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Title: assistée par ordinateur des fluides à plusieurs phases immiscibles

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UNIVERSITÉ DE MONTRÉAL

ÉTUDE D'UN MODÈLE DE BOLTZMANN SUR RÉSEAU POUR LA SIMULATION
ASSISTÉE PAR ORDINATEUR DES FLUIDES À PLUSIEURS PHASES IMMISCIBLES

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Cette thèse intitulée :

ÉTUDE D'UN MODÈLE DE BOLTZMANN SUR RÉSEAU POUR LA SIMULATION
ASSISTÉE PAR ORDINATEUR DES FLUIDES À PLUSIEURS PHASES IMMISCIBLES

présentée par : LECLAIRE Sébastien

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*À mon père,
pour la passion et la curiosité
que tu as su me transmettre
envers les sciences et les ordinateurs...*

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RÉSUMÉ

Depuis quelques décennies, la simulation assistée par ordinateur de la dynamique des fluides est un sujet de recherche qui s'est démarqué en permettant la résolution d'une multitude de problèmes scientifiques, tant au niveau académique qu'industriel. Dans ce domaine, la simulation des fluides à plusieurs phases immiscibles demeure un défi en raison de la complexité de l'interaction des différentes interfaces entre les phases. Différentes méthodes numériques sont disponibles pour étudier ces phénomènes et, ces dernières années, la méthode de Boltzmann sur réseau s'est montrée bien adaptée pour résoudre ce type d'écoulement complexe.

Dans cette thèse, un modèle de Boltzmann sur réseau pour la simulation des fluides à deux phases immiscibles est étudié. Le principal objectif de cette thèse est de développer davantage cette méthode prometteuse afin d'étendre son champ de validité. Pour ce faire, cette recherche est subdivisée en cinq thèmes distincts. Les deux premiers se concentrent à corriger certaines lacunes du modèle original. Le troisième généralise le modèle afin de supporter la simulation des fluides à N phases immiscibles. Le quatrième thème vise à modifier le modèle afin de permettre la simulation des fluides immiscibles avec variation de densité entre les phases. Avec la classe de modèle de Boltzmann sur réseau étudiée dans cette thèse, la variation de densité entre les phases était modélisée inadéquatement et cette problématique était non résolue depuis une vingtaine d'années. Le cinquième thème, complémentaire à cette thèse, est un sujet connexe à la méthode de Boltzmann sur réseau. Ce dernier généralise la théorie des gradients isotropes 2D et 3D pour un ordre de précision spatial élevé.

Chacun de ces thèmes a résulté en un article scientifique mis en annexe de cette thèse. En relation avec les objectifs de cette recherche, ce document se résume à une synthèse qui explique les liens entre les différents articles ainsi que les contributions scientifiques. Dans l'ensemble, plusieurs cas tests qualitatifs et quantitatifs issus de la théorie des écoulements à plusieurs phases ont permis de mettre en évidence des problématiques concernant le modèle de simulation. Il s'en est suivi différentes modifications qui ont eu pour effet de réduire ou d'éliminer certains artefacts numériques dont souffrait la méthode. Ces cas tests ont aussi permis de valider les extensions qui ont été appliquées au modèle original.

ABSTRACT

The computer assisted simulation of the dynamics of fluid flow has been a highly rewarding topic of research for several decades now, in terms of the number of scientific problems that have been solved as a result, both in the academic world and in industry. In the fluid dynamics field, simulating multiphase immiscible fluid flow remains a challenge, because of the complexity of the interactions at the flow phase interfaces. Various numerical methods are available to study these phenomena, and, the lattice Boltzmann method has been shown in recent years to be well adapted to solving this type of complex flow.

In this thesis, a lattice Boltzmann model for the simulation of two-phase immiscible flows is studied. The main objective of the thesis is to develop this promising method further, with a view to enhancing its validity. To achieve this objective, the research is divided into five distinct themes. The first two focus on correcting some of the deficiencies of the original model. The third generalizes the model to support the simulation of N-phase immiscible fluid flows. The fourth is aimed at modifying the model itself, to enable the simulation of immiscible fluid flows in which the density of the phases varies. With the lattice Boltzmann class of models studied here, this density variation has been inadequately modeled, and, after 20 years, the issue still has not been resolved. The fifth, which complements this thesis, is connected with the lattice Boltzmann method, in that it generalizes the theory of 2D and 3D isotropic gradients for a high order of spatial precision.

These themes have each been the subject of a scientific article, as listed in the appendix to this thesis, and together they constitute a synthesis that explains the links between the articles, as well as their scientific contributions, and satisfy the main objective of this research. Globally, a number of qualitative and quantitative test cases based on the theory of multiphase fluid flows have highlighted issues plaguing the simulation model. These test cases have resulted in various modifications to the model, which have reduced or eliminated some numerical artifacts that were problematic. They also allowed us to validate the extensions that were applied to the original model.

TABLE DES MATIÈRES

DÉDICACE	iii
REMERCIEMENTS	iv
RÉSUMÉ	vi
ABSTRACT	vii
TABLE DES MATIÈRES	viii
LISTE DES FIGURES	x
LISTE DES ANNEXES	xi
LISTE DES SIGLES ET ABRÉVIATIONS	xii
CHAPITRE 1 INTRODUCTION	1
1.1 Mise en contexte	1
1.2 Hypothèses de modélisation	3
1.2.1 Hypothèses de modélisation pour un système à une phase	3
1.2.2 Hypothèses de modélisation pour un système à plusieurs phases immiscibles	5
1.3 Cadre théorique de cette recherche doctorale	8
1.3.1 Description de l'équation de Boltzmann	8
1.3.2 Discrétisation de l'équation de Boltzmann	11
1.3.3 Modèle de Boltzmann sur réseau de base à une phase	14
1.3.4 Modèle de Boltzmann sur réseau plus général	16
1.3.5 Modèle de Boltzmann sur réseau à deux phases de Reis et Phillips	17
1.4 Problématique	22
1.5 Objectifs	24
CHAPITRE 2 REVUE CRITIQUE DE LA LITTÉRATURE	26
2.1 Les modèles de type SC, FE, MF et FM	27
2.2 Les modèles de type RK	29
2.2.1 Thème 1 : Opérateur de recoloriage	30

2.2.2	Thème 2 : La discrétisation du gradient de couleur	31
2.2.3	Thème 3 : Les modèles de type RK à plusieurs phases	32
2.2.4	Thème 4 : Le problème de discontinuité des modèles RK	33
2.3	Thème 5 complémentaire : Les différences finies isotropes	34
CHAPITRE 3 SYNTHÈSE DE L'ENSEMBLE DU TRAVAIL		36
3.1	Thème 1 : Opérateur de recoloriage	36
3.1.1	Contribution théorique	37
3.1.2	Contribution appliquée	38
3.2	Thème 2 : La discrétisation du gradient de couleur	42
3.2.1	Contribution théorique	42
3.2.2	Contribution appliquée	43
3.3	Thème 3 : Modèle RK à plusieurs phases	45
3.3.1	Contribution théorique	45
3.3.2	Contribution appliquée	48
3.4	Thème 4 : Le problème de discontinuité	52
3.4.1	Contribution théorique	52
3.4.2	Contribution appliquée	54
3.5	Thème 5 complémentaire : Les gradients isotropes d'ordre spatial élevé	55
3.5.1	Contribution théorique	55
3.5.2	Contribution appliquée	55
CHAPITRE 4 DISCUSSION GÉNÉRALE		57
4.1	Discussion des problématiques résolues et améliorées	57
4.2	Discussion des problématiques non résolues	61
CHAPITRE 5 CONCLUSION ET RECOMMANDATIONS		63
5.1	Recommandations	64
LISTE DES RÉFÉRENCES		66
ANNEXES		75

LISTE DES FIGURES

Figure 1.1	Réseau D2Q9.	14
Figure A.1	Avis de réception par les éditeurs de l'article : « Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model ».	75
Figure B.1	Avis de réception par les éditeurs de l'article : « Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model ».	90
Figure C.1	Avis de réception par les éditeurs de l'article : « Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios ».	107
Figure D.1	Avis de réception par les éditeurs de l'article : « Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models ».	127
Figure E.1	Avis de réception par les éditeurs de l'article : « High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs ».	139

LISTE DES ANNEXES

Annexe A	Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model	75
Annexe B	Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model	90
Annexe C	Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios	107
Annexe D	Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models	127
Annexe E	High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs	139

LISTE DES SIGLES ET ABRÉVIATIONS

BGK	Bhatnagar, Gross et Krook
CFD	Computational Fluid Dynamics
DmQn	Réseau à m dimensions et à n vitesses microscopiques discrètes
DNAPL	Dense, Non-Aqueous Phase Liquid
FE	Free Energy
FM	Field Mediator
Kn	Knudsen
LBM	Lattice Boltzmann Method (à lire, méthode de Boltzmann sur réseau)
LUMINOS	Laboratoire Universitaire de Modélisation Ingénierie Numérique et Optimisation des Systèmes
Ma	Mach
MF	Mean Field
MRT	Multi-Relaxation Time
Opérateur I	Opérateur de recoloriage original
Opérateur II	Opérateur de recoloriage modifié
$O(\cdot)$	De l'Ordre de $(\cdot)$
Re	Reynold
RK	Rothman-Keller
SC	Shan-Chen
TRT	Two-Relaxation Time
(I)	Ordre Isotrope
(S)	Ordre Spatial

CHAPITRE 1

INTRODUCTION

1.1 Mise en contexte

Au sens large, cette recherche fait partie de celles qui étudient l'équation de Boltzmann. Cette équation développée par Ludwig Boltzmann est célèbre et a donné lieu à des dizaines de milliers de recherches. Issue de la théorie cinétique des gaz, l'équation de Boltzmann est généralement présentée comme une équation décrivant le comportement spatio-temporel d'un gaz dilué qui n'est pas dans un équilibre thermodynamique. Un survol rapide de cette équation dans le cadre de cette recherche doctorale est présenté dans cette introduction.

De manière plus spécifique, un modèle de Boltzmann sur réseau pour la simulation assistée par ordinateur des fluides à plusieurs phases immiscibles a été étudié, développé et amélioré durant cette recherche. Tout d'abord, il convient de définir ce qui est sous-entendu par l'expression « fluides à plusieurs phases immiscibles ».

Un système à une phase est défini comme un système homogène à un ou plusieurs composants chimiques. Par exemple, l'air est un système à une phase homogène, mais composé principalement d'azote, d'oxygène et de dioxyde de carbone. Similairement, tel qu'indiqué par Zemansky [1], un système à plusieurs phases se définit comme un système composé d'un ou de plusieurs composants chimiques homogènes et séparé par une frontière bien définie. Un exemple de système à deux phases et avec un seul composé chimique serait un système avec de l'eau liquide et de la vapeur d'eau. L'eau et l'huile forment un système à deux phases avec deux composants chimiques. Dans cette optique, l'air et l'eau peuvent être vus comme un système à deux phases composé principalement de quatre composants chimiques. L'ajout du terme immiscible implique que les différentes phases ne se mélangent pas. Autrement dit, l'état de la matière ne se modifie pas en passant d'une phase à une autre ou pour former une nouvelle phase comme c'est le cas lors de la dissolution de l'encre dans de l'eau. Par exemple, dans le cas où les phases sont de l'eau liquide avec de la vapeur d'eau, l'immiscibilité implique qu'il n'y a pas de passage de la phase liquide vers la phase gazeuse et vice-versa.

La définition d'un système à plusieurs phases immiscibles ou non, proposée dans le paragraphe précédent, mène à beaucoup de systèmes possibles. Une liste est illustrée sous forme de diagramme dans le livre de Kolev [2]. Ce diagramme expose 28 différents schémas d'écoulements allant de gaz, de liquide, de solide, de solide-liquide, etc. Les combinaisons sont nombreuses dans l'étude de ce type d'écoulement et, comme précisé par Brennen [3], il n'existe

pas de formulation unique et bien établie permettant de décrire toutes les possibilités. Par bien établie, Brennen [3] sous-entend que les modèles utilisés pour représenter les écoulements à phases multiples sont encore sujets à des débats scientifiques.

La simulation des fluides à plusieurs phases est un domaine de recherche en pleine évolution et connaît aussi plusieurs applications pratiques. L'industrie pétrolière en est un bon exemple, les simulations faites par Ingrain [4] sont utilisées pour mieux prédire l'extraction du pétrole ou des gaz naturels des sols. D'autre part, l'industrie pharmaceutique s'intéresse au domaine de la microfluidique [5], où l'on essaie de prédire le comportement du dépôt de gouttes sur des substrats à une échelle microscopique. De plus, l'industrie nucléaire est aussi concernée par le transfert de chaleur au niveau des écoulements à bulles [5] ainsi que par les vibrations générées par ces écoulements qui se produisent dans les systèmes de conduites [6, 7]. La thèse de doctorat de Chiappini [8] énumère plusieurs autres champs d'applications pratiques de la simulation des fluides à plusieurs phases.

La communauté scientifique s'intéresse aussi à la modélisation du transport des contaminants dans les sols [9]. Pour mettre en contexte, il existe une classe de contaminants très dangereux pour la santé soit les DNAPL (Dense, Non-Aqueous Phase Liquid). Les DNAPL sont des liquides plus denses que l'eau et généralement immiscibles avec l'eau. Étant plus denses que l'eau, ces contaminants ont tendance à descendre par gravité dans les sols profonds et contaminent ainsi les eaux souterraines.

La méthode de Boltzmann sur réseau tente de se démarquer en ce qui concerne le calcul du coefficient de perméabilité pour les écoulements à une phase [10] et des coefficients de perméabilité relatifs pour les écoulements à phases multiples [11]. En milieu poreux, la loi de Darcy prédit que la vitesse moyenne de l'écoulement dans la direction d'une force, par exemple un gradient de pression, est proportionnelle au coefficient de perméabilité [12]. Ce dernier est seulement en fonction de la géométrie intrinsèque du matériau. Par contre, pour les écoulements à plusieurs phases, il est possible que la phase mouillante qui adhère plus facilement à la paroi solide, couvre la surface solide et se déplace le long de celle-ci. La phase non mouillante, quant à elle, circule dans l'espace restant tout en étant enrobée de la phase mouillante. Par conséquent, il y a un fort couplage visqueux à l'interface entre le fluide mouillant et le non mouillant. Pour tenir compte de ce couplage visqueux, il faut introduire les coefficients de perméabilité relatifs dans la loi de Darcy généralisée pour calculer la perméabilité effective des écoulements à plusieurs phases [13]. Basés sur des données expérimentales, ces coefficients peuvent être obtenus à l'aide de modèles simplifiés. Par contre, ce processus est très dispendieux et difficile à déterminer en raison de l'anisotropie des milieux poreux. Conceptuellement, l'idée est d'utiliser les méthodes de Boltzmann sur réseau pour calculer ces coefficients à un niveau microscopique et d'ensuite les utiliser comme référence dans des

modèles macroscopiques hydrogéologiques de transport de contaminants. Les méthodes de Boltzmann sur réseau pourraient réduire les coûts associés à des expériences en laboratoire faites par des équipes spécialisées, et ce, en utilisant la distribution géométrique des matériaux pour en déduire par simulation la valeur de ces coefficients. Il y a présentement un effort fait par la communauté scientifique de Boltzmann sur réseau pour développer un modèle capable de calculer ces coefficients correctement, avec fiabilité et robustesse [13, 14].

Bien qu'il soit approprié d'avoir mentionné divers champs d'applications de la méthode développée dans cette recherche, les développements et les contributions effectués dans **cette thèse se concentrent sur l'amélioration de l'aspect théorique et numérique d'un modèle de simulation** et non pas sur l'application de celui-ci à des situations complexes comme pour le calcul des coefficients de perméabilité. Comme toutes les autres méthodes, celle de Boltzmann sur réseau s'améliore de jour en jour, mais elle est encore en phase de développement en ce qui concerne la simulation des écoulements à plusieurs phases. La vision à long terme de cette thèse est qu'il est possible de développer un modèle de Boltzmann sur réseau permettant d'appuyer concrètement et de manière systématique les recherches ou les études qui s'intéressent à la dispersion des contaminants dans les sols.

1.2 Hypothèses de modélisation

Il est important de mentionner les hypothèses de modélisation sous lesquelles les modèles de simulation étudiés dans cette thèse sont valides. Au prochain chapitre, la revue de littérature présente certains aspects ou hypothèses, par rapport à ceux présentés ci-dessous, qui peuvent être différents dépendamment du type de modèle de Boltzmann sur réseau considéré. D'abord, les hypothèses de modélisation pour un système à une seule phase sont évoquées et pour ce cas simplifié, ce sont celles couramment utilisées pour les modèles de Boltzmann sur réseau de base. Par la suite, certaines hypothèses supplémentaires sont ajoutées pour obtenir un modèle d'un système à plusieurs phases.

1.2.1 Hypothèses de modélisation pour un système à une phase

D'un point de vue macroscopique, il est d'abord considéré que :

H1a) Le régime d'évolution du système est isotherme, c'est-à-dire à température constante. Cette hypothèse permet de ne pas avoir à considérer l'énergie interne du fluide comme une inconnue du système. Les régimes de simulation thermodynamique ne peuvent donc pas être simulés. Les régimes possibles de simulation sont limités à l'hydrodynamique ce qui implique alors que :

H2a) Les inconnues d'un système à régime hydrodynamique sont :

- la masse volumique ρ_k ;
- la quantité de mouvement $\rho_k \vec{u}_k$;
- et la pression p_k dans le fluide.

Bien que seulement les systèmes à une phase soient traités dans cette sous-section, l'indice k fait référence à un fluide « de couleur k ». Cela permet de faire une différence avec la notation définie dans la prochaine section qui traite des systèmes avec plusieurs phases. Avec c_s^k la vitesse du son dans le fluide, seulement les systèmes à très faible nombre de Mach sont considérés :

H3a) $\text{Ma}_k = \frac{\|\vec{u}_k\|}{c_s^k} \ll 1$

Il est à noter que c_s^k est la vitesse du son isotherme ou Newtonnienne, c'est-à-dire $(c_s^k)^2 = \frac{\partial p_k}{\partial \rho_k}$ à température constante et non pas à entropie constante comme c'est usuellement le cas [15].

H4a) La viscosité cinématique ν_k du fluide est considérée constante.

Comme la viscosité cinématique dépend généralement de la température, cette dernière hypothèse est raisonnable étant donné que le système est supposé isotherme.

H5a) Le fluide est newtonien.

La viscosité dynamique est notée $\mu_k = \rho_k \nu_k$. Le tenseur des contraintes déviatoriques est alors donné par $\mathbf{T}_k = \mu_k [\vec{\nabla} \vec{u}_k + (\vec{\nabla} \vec{u}_k)^T] - 2/3 (\vec{\nabla} \cdot \vec{u}_k) \mathbf{I}$. Dans la limite d'un faible nombre de Mach, la divergence du champ de vitesses $\vec{\nabla} \cdot \vec{u}_k$ est pratiquement nulle ainsi que la variation de la densité ρ_k . Par conséquent, le tenseur des contraintes de cisaillement $\mathbf{S}_k = \vec{\nabla} \cdot \mathbf{T}_k$ se simplifie à sa forme incompressible $\mathbf{S}_k = \mu_k \vec{\nabla}^2 \vec{u}_k$.

Un système, qui respecte les hypothèses précédentes, peut être modélisé par deux équations au niveau macroscopique. La conservation de la masse mène à l'équation de continuité et la conservation de la quantité de mouvement mène aux équations de la quantité de mouvement :

$$\vec{\nabla} \cdot \vec{u}_k = 0 \quad (1.1)$$

$$\rho_k \left(\frac{\partial \vec{u}_k}{\partial t} + \vec{u}_k \cdot \vec{\nabla} \vec{u}_k \right) = -\vec{\nabla} p_k + \mu_k \vec{\nabla}^2 \vec{u}_k \quad (1.2)$$

Une méthode de Boltzmann sur réseau de base est équivalente à ce système d'équations seulement dans la limite d'un faible nombre de Mach et de Knudsen. La méthode est dite quasi-incompressible, car il y a toujours une faible variation de la densité dans un modèle de Boltzmann sur réseau de base. Dans ce cas, l'utilisation de l'équation d'état isotherme permet de ne plus avoir à considérer la pression comme une inconnue :

H6a) L'équation d'état isotherme est $p_k = \rho_k (c_s^k)^2$.

La pression p_k ne varie alors que légèrement en raison de l'hypothèse d'un faible nombre de Mach. L'ensemble de ces hypothèses sous-entend que la méthode de Boltzmann sur réseau de base est seulement une solution approchée des équations de Navier-Stokes incompressibles.

1.2.2 Hypothèses de modélisation pour un système à plusieurs phases immiscibles

Dans un modèle à plusieurs phases immiscibles, différentes hypothèses de modélisations sont possibles. Un choix doit être fait quant à la nature de l'interface entre chacun des fluides. Les premières hypothèses sont que :

H1b) L'interface est diffuse.

H2b) La tension de surface entre chacune des paires d'interfaces est prise en compte, mais l'interaction par tension de surface entre deux fluides à une interface ne dépend pas de la présence des autres fluides.

Tel que proposé par Lafaurie et al. [16], lorsque l'interface est diffuse et que seulement deux phases sont présentes, le tenseur des contraintes capillaires responsable de l'introduction de la tension de surface entre deux fluides k et l a la forme suivante : $\mathbf{C}_{kl} = \sigma_{kl} (\mathbf{I} - \vec{n}_{kl} \otimes \vec{n}_{kl}) \delta_{kl}$. L'expression σ_{kl} est associée à l'intensité de la tension de surface, le vecteur $\vec{n}_{kl}$ est un vecteur normal à l'interface et l'expression δ_{kl} est une fonction delta concentrée à l'interface. Le symbole $\otimes$ indique le produit tensoriel. Il est intéressant de noter que Lafaurie et al. [16] ont démontré que la divergence de ce tenseur est proportionnelle à la courbure de l'interface. L'approche proposée par Reis et Phillips [17] suggère d'écrire :

$$\mathbf{H3b)} \quad \mathbf{C}_{kl} = \sigma_{kl} \left(\left| \vec{F}_{kl} \right|^2 \mathbf{I} - \vec{F}_{kl} \otimes \vec{F}_{kl} \right)$$

où $\vec{F}_{kl}$ est le gradient d'un paramètre d'ordre mesurant la composition du fluide. Le vecteur $\vec{F}_{kl}$ est en fait une mesure de la fonction delta δ_{kl} et orienté dans la direction $\vec{n}_{kl}$ normale à l'interface. Avec cette approche, plusieurs choix sont possibles pour $\vec{F}_{kl}$ et selon le choix, il faut déterminer une expression pour σ_{kl} qui fera en sorte que la tension de surface du système dans la simulation soit la même que celle prédite par la théorie. Intuitivement, plus l'expression pour σ_{kl} est grande, plus la tension de surface entre les fluides est grande. Selon la forme de l'expression σ_{kl} , il est alors possible de contrôler la tension de surface entre deux fluides k et l .

Pour modéliser un système à plusieurs phases, l'approche la plus générale est de considérer chacune des phases séparément et de les représenter par plusieurs équations individuelles couplées. L'approche adoptée ici consiste plutôt à définir un fluide « sans couleur » représentant le plus simplement et le plus fidèlement possible la dynamique globale de l'ensemble des fluides individuels k .

H4b) Le fluide sans couleur est la somme des propriétés individuelles de chacun des fluides k .

- Densité du fluide sans couleur : $\rho = \sum_k \rho_k$
- Quantité de mouvement du fluide sans couleur : $\rho \vec{u} = \sum_k \rho_k \vec{u}_k$
- Viscosité dynamique du fluide sans couleur : $\mu = \sum_k \mu_k$
- Pression du fluide sans couleur : $p = \sum_k p_k$

Cette dernière hypothèse peut sembler injustifiée, mais elle fait en sorte de donner un poids plus important aux fluides qui sont prépondérants à une position donnée. À cause de l'hypothèse d'incompressibilité, il semble logique de donner, à une certaine position, plus d'importance aux particules de fluides présentes en plus grande quantité. L'effet local d'un fluide de couleur k à un endroit donné est donc proportionnel à la quantité de celui-ci présent à cette position. Cet argument justifie la définition de la densité du fluide sans couleur et de sa quantité de mouvement. Pour la viscosité, cette hypothèse correspond en fait à une interpolation de la viscosité cinématique pondérée par la densité. Cela est une approximation standard dans les méthodes numériques pour la simulation de plusieurs phases immiscibles [16]. D'autres types d'interpolations sont possibles [18]. Pour la pression du fluide sans couleur, son effet se traduit dans les équations par une force par unité de volume, $\vec{\nabla} p$, il est donc normal que la somme des pressions soit choisie pour représenter la pression du fluide sans couleur.

Il est aussi supposé que les contraintes capillaires dans le fluide sans couleur sont égales à la somme des contraintes capillaires générées individuellement par chacune des paires d'interfaces :

H5b) Tenseur des contraintes capillaires du fluide sans couleur : $\mathbf{C} = \sum_{kl} \mathbf{C}_{kl}$

Similairement à la pression, les contraintes capillaires se traduisent par des forces par unité de volume, $\vec{\nabla} \cdot \mathbf{C}$, dans les équations. Il est donc normal de faire une sommation des contraintes pour représenter le tenseur des contraintes capillaires du fluide sans couleur.

Pour simplifier la dynamique du système, une hypothèse supplémentaire est ajoutée :

H6b) Chacun des fluides k se déplace avec la même vitesse que le fluide sans couleur.

Cette dernière hypothèse fait en sorte qu'il y a seulement le champ de vitesse $\vec{u}$ du fluide sans couleur qui est inconnu. Par conséquent, une partie de l'information concernant la dynamique complète d'un système réel à plusieurs phases est perdue. Par contre, cela permet de simplifier considérablement la procédure de résolution numérique du modèle. En procédant ainsi, un système à plusieurs phases distinctes est en fait modélisé par une seule phase, le fluide sans

couleur, dont les propriétés, ρ et μ , ou les forces par unité de volume, $-\vec{\nabla}p$ et $\vec{\nabla} \cdot \mathbf{C}$, agissant sur celui-ci varient spatialement et temporellement en fonction du détail et de l'évolution des champs de densité ρ_k de chacun des fluides k . En fait, puisque chacun des fluides k est immiscible l'un avec l'autre, c'est seulement à l'interface entre les fluides où l'information est perdue concernant les vitesses individuelles de chacun des fluides. Cette hypothèse de simplification est donc probablement acceptable pour plusieurs situations pratiques.

Les équations considérées issues de la conservation de la masse et de la conservation de la quantité de mouvement du fluide sans couleur sont :

$$\vec{\nabla} \cdot \vec{u} = 0 \quad (1.3)$$

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{u} \right) = -\vec{\nabla}p + \mu \vec{\nabla}^2 \vec{u} + \vec{\nabla} \cdot \mathbf{C} \quad (1.4)$$

Au niveau macroscopique, ce modèle est incomplet puisque rien ne garantit l'immiscibilité des fluides, ou encore l'immiscibilité des champs de densité ρ_k . À ce stade, il n'est pas du tout évident de garantir l'immiscibilité des fluides. Pour garantir cette propriété des fluides à l'interface, l'approche utilisée dans cette thèse exige de modifier l'état des champs de couleur au niveau microscopique. Ainsi, un « opérateur de recoloriage » est appliqué dans les équations discrètes de l'équation de Boltzmann sur réseau. Le terme « opérateur de recoloriage » peut sembler non physique de par son nom, mais il est choisi judicieusement pour conserver, au minimum, la masse et la quantité de mouvement du fluide sans couleur ainsi que la masse de chacun des fluides individuels k . Seulement alors, le régime hydrodynamique du fluide sans couleur peut être conservé. La quantité de mouvement des fluides individuels k n'a pas besoin d'être conservée puisque de toute manière cette dynamique est effacée du système par l'hypothèse que chacun des fluides k se déplace avec la vitesse du fluide sans couleur. Un tel opérateur peut être construit avec les méthodes de Boltzmann sur réseau puisque certains degrés de liberté sont libres au niveau de l'équation de Boltzmann sur réseau et peuvent être ainsi ajustés sans perturber le régime hydrodynamique du fluide sans couleur. Dans la prochaine section, les bases de la méthode de Boltzmann sur réseau sont établies et d'autres détails concernant cet opérateur sont donnés.

Maintenant que le modèle a été présenté d'un point de vue macroscopique, la prochaine section aborde quelques aspects théoriques des méthodes de Boltzmann sur réseau étudiées dans cette thèse.

1.3 Cadre théorique de cette recherche doctorale

Cette section discute de l'équation de transport de Boltzmann ainsi que sa discrétisation pour obtenir un modèle de Boltzmann sur réseau. L'objectif de cette section est d'établir le plus brièvement et succinctement possible les bases nécessaires à la compréhension des contributions scientifiques de cette thèse. Le but n'est pas de faire une description détaillée de la théorie de Boltzmann sur réseau qui ne ferait qu'alourdir le chemin vers la compréhension des contributions scientifiques. Par contre, lorsque des détails ne sont pas discutés, des citations vers des références appropriées sont indiquées. La description sommaire de l'équation de Boltzmann effectuée dans cette thèse est commune et a souvent fait l'objet de discussions similaires dans des mémoires, des thèses, des livres ainsi que des articles scientifiques [19–24].

Cette section se termine par la présentation du modèle de Boltzmann sur réseau à deux phases de Reis et Phillips [17]. Ce modèle est en fait le point de départ de cette recherche scientifique. Dans la prochaine section, la problématique concernant ce modèle est abordée.

Notez que l'indice k pour la notation d'un fluide de couleur k est généralement omis dans cette section pour éviter d'alourdir le texte et, à moins d'indication contraire, il est sous-entendu qu'on ne discute pas du fluide sans couleur, mais plutôt d'un système simplifié à une phase.

1.3.1 Description de l'équation de Boltzmann

L'équation de Boltzmann décrit au niveau microscopique le comportement d'un ensemble ou d'un groupe de particules à l'aide d'une fonction f de densité de probabilité [19]. Cette fonction f est communément appelée la fonction de distribution et est définie dans l'espace des phases $\{(\vec{x}, \vec{\xi}) \in \mathbb{R}^3 \times \mathbb{R}^3\}$ où $\vec{\xi}$ est la vitesse microscopique caractéristique d'un groupe de particules à la position $\vec{x}$. D'un point de vue mathématique, la fonction f est une variable aléatoire continue décrivant la probabilité relative que cette variable prenne une certaine valeur. L'expression $f(\vec{x}, \vec{\xi}) d\vec{x} d\vec{\xi}$ représente alors le nombre de particules probable dans le cube $\vec{x} \pm d\vec{x}/2$ avec une vitesse microscopique située dans le cube $\vec{\xi} \pm d\vec{\xi}/2$.

Au niveau macroscopique, l'équation de Boltzmann décrivant la dynamique d'un système de particules identiques est donnée par :

$$\frac{\partial f}{\partial t} + \vec{\xi} \cdot \vec{\nabla}_{\vec{x}} f + \vec{F}_e \cdot \vec{\nabla}_{\vec{\xi}} f = C(f) \quad (1.5)$$

L'opérateur $\vec{\nabla}_{\vec{x}} = [\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]$ est le gradient par rapport à la position $\vec{x}$. L'opérateur $\vec{\nabla}_{\vec{\xi}} = [\frac{\partial}{\partial \xi_x}, \frac{\partial}{\partial \xi_y}, \frac{\partial}{\partial \xi_z}]$ est le gradient par rapport aux vitesses microscopiques $\vec{\xi}$ où, par exemple, ξ_x est la composante dans la direction x de la vitesse microscopique $\vec{\xi}$.

L'expression $\vec{F}_e$ est une force externe par unité de masse agissant sur les particules. Pour modéliser les forces externes dans les modèles de Boltzmann sur réseau, différentes approches ont été proposées par plusieurs auteurs [17, 25–27]. Tel que mentionné par He et al. [26], cela est dû au fait que l'intégration de l'expression $\vec{\nabla}_{\vec{\epsilon}} f$ mène à un terme qui ne peut pas être calculée aisément. Bien que certaines approches procurent des avantages par rapport à d'autres, les avantages sont la plupart du temps reliés à l'ajout d'une complexité supplémentaire, comme par exemple : des méthodes numériques temporellement implicites [25]. Le traitement numérique des termes sources est sans doute l'un des plus grands défis auquel les méthodes de Boltzmann sur réseau ont été, et sont encore, confrontées ces dernières années. Le sujet des termes sources dans le cadre des méthodes de Boltzmann sur réseau est encore relié à des réflexions scientifiques et ceux-ci ne sont pas le sujet de cette thèse. Ils ne sont alors plus discutés dans cette section.

Les conditions aux frontières pour l'équation de Boltzmann représentent aussi tout un défi. En effet, il n'est pas évident à priori de transposer les variables macroscopiques que l'on désire imposer aux frontières, telles que la pression ou la vitesse, avec les fonctions de distributions au niveau microscopique. Le problème se complique aussi lorsque la géométrie des frontières est courbe. Différentes stratégies existent dans la littérature scientifique, par exemple, les méthodes de Guo et al. [28] et de Bouzidi et al. [29], pour ne nommer que celles-ci. Récemment, il y a une approche intéressante et très générale pour obtenir les variables microscopiques à partir des variables macroscopiques qui a été développée par Vanderhoydonc et Vanroose [30]. Pour le présent ouvrage, l'interaction avec les frontières a été minimisée afin d'étudier et d'analyser le coeur même du comportement de la méthode de Boltzmann sur réseau.

Le membre de droite $C(f)$ de l'Éq. (1.5) est la collision modélisant uniquement les collisions binaires entre les particules. Cette dernière hypothèse, à propos des collisions binaires, suggère que l'équation de Boltzmann est valide que pour un gaz dilué. En effet, c'est sous cette dernière hypothèse que Boltzmann a initialement développé son équation. Dans un gaz dilué, il y a moins de chance que des collisions à plusieurs particules surviennent. En réalité, tel que réalisé plus tard par Knudsen [31], ce n'est pas vraiment la densité du gaz qui compte, mais plutôt le nombre de Knudsen, Kn , qui exprime le nombre moyen de collisions que subit une particule d'un certain rayon par unité de temps. Suivant la relation de von Kármán, le nombre de Knudsen peut s'exprimer par :

$$Kn = \alpha \frac{Ma}{Re} = \frac{\lambda}{L} \quad (1.6)$$

où α est une constante de proportionnalité. Les expressions Ma et Re sont respectivement le nombre de Mach et de Reynolds. Le nombre de Knudsen est aussi égal au ratio entre

la distance moyenne λ parcourue par une particule entre les collisions et la longueur L de référence caractéristique de l'écoulement à l'étude. Lorsque le nombre de Knudsen est faible, la formulation de l'équation de Boltzmann tel que présentée dans cette thèse est valide. Des explications supplémentaires concernant la physique derrière les collisions binaires sont données dans les références qui suivent [19, 20].

Bhatnagar et al. [32] ont simplifié considérablement cet opérateur et ont été en mesure d'obtenir un modèle de la collision $C(f)$ mathématiquement simple et capable de modéliser suffisamment bien la physique de base. En effet, le modèle de collision de Bhatnagar, Gross et Krook (BGK) a été utilisé dans le cadre de plusieurs centaines de recherches utilisant les méthodes de Boltzmann sur réseau et les résultats de recherche semblent cohérents avec la physique modélisée dans ces recherches. La collision BGK s'exprime par l'expression :

$$C(f) = -\frac{(f - f^{(e)})}{\tau} \quad (1.7)$$

Cette collision est donc une relaxation de la fonction de distribution f vers un état d'équilibre représenté par une fonction de distribution d'équilibre $f^{(e)}$ où τ est le temps de relaxation relatif entre les collisions de particules. La fonction d'équilibre $f^{(e)}$ est la fonction de distribution de Maxwell-Boltzmann :

$$f^{(e)} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left(-\frac{|\vec{\xi} - \vec{u}|^2}{2RT}\right) \quad (1.8)$$

Les quantités ρ , $\vec{u}$ et T représentent respectivement, au niveau macroscopique, la masse par unité de volume, la vitesse et la température en Kelvin du fluide. Les constantes R et D sont respectivement la constante universelle des gaz parfaits et la dimension spatiale. Il est important de noter que la constante des gaz parfaits $R = N_A k_B$ est en relation avec le nombre d'Avogadro N_A et la constante de Boltzmann k_B . La relation entre les propriétés macroscopiques du fluide et microscopiques des particules est donnée par les moments successifs de la fonction de distribution f ou $f^{(e)}$ par rapport aux vitesses microscopiques $\vec{\xi}$:

$$\rho = \int f d\vec{\xi} = \int f^{(e)} d\vec{\xi} \quad (1.9)$$

$$\rho \vec{u} = \int f \vec{\xi} d\vec{\xi} = \int f^{(e)} \vec{\xi} d\vec{\xi} \quad (1.10)$$

$$\rho DRT = \int f |\vec{\xi} - \vec{u}|^2 d\vec{\xi} = \int f^{(e)} |\vec{\xi} - \vec{u}|^2 d\vec{\xi} \quad (1.11)$$

1.3.2 Discrétisation de l'équation de Boltzmann

Pour être en mesure de faire des simulations assistées par ordinateur avec l'équation de Boltzmann, il faut discrétiser temporellement et spatialement les équations sur un réseau et aussi discrétiser l'espace des phases.

Discrétisation spatio-temporelle de l'équation de Boltzmann

La méthode suggérée par Dellar [15] illustre comment discrétiser temporellement l'Éq. (1.5) en suivant les directions caractéristiques $\vec{\xi}$. D'abord, la dérivée totale $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{\xi} \cdot \vec{\nabla}$ est introduite :

$$\frac{Df}{Dt} = -\frac{(f - f^{(e)})}{\tau} \quad (1.12)$$

En intégrant l'équation précédente sur un intervalle de temps Δt , l'équation se transforme en :

$$f(\vec{x} + \vec{\xi}\Delta t, t + \Delta t) - f(\vec{x}, t) = -\frac{1}{\tau} \int_0^{\Delta t} \left[f(\vec{x} + s\vec{\xi}, t + s) - f^{(e)}(\vec{x} + s\vec{\xi}, t + s) \right] ds \quad (1.13)$$

L'intégrale est approximée avec une méthode trapézoïdale :

$$\begin{aligned} f(\vec{x} + \vec{\xi}\Delta t, t + \Delta t) - f(\vec{x}, t) = \\ -\frac{\Delta t}{2\tau} \left[f(\vec{x} + \Delta t\vec{\xi}, t + \Delta t) - f^{(e)}(\vec{x} + \Delta t\vec{\xi}, t + \Delta t) + f(\vec{x}, t) - f^{(e)}(\vec{x}, t) \right] \end{aligned} \quad (1.14)$$

Présentée ainsi, la discrétisation spatio-temporelle suivant les caractéristiques $\vec{\xi}$ est d'ordre 2 et implicite, mais le stratagème initialement proposé par He et al. [26] permet de récupérer une formulation explicite en effectuant les changements de variables suivants [15] :

$$g^{(e)} = f^{(e)} \quad (1.15)$$

$$g = f + \frac{\Delta t}{2\tau} (f - f^{(e)}) \quad (1.16)$$

$$\omega = \frac{\Delta t}{\tau + \Delta t/2} \quad (1.17)$$

Une approximation de l'Éq. (1.5) suivant les caractéristiques $\vec{\xi}$ est alors donnée par :

$$g(\vec{x} + \vec{\xi}\Delta t, t + \Delta t) - g(\vec{x}, t) = -\omega (g(\vec{x}, t) - g^{(e)}(\vec{x}, t)) \quad (1.18)$$

Bien que la discrétisation soit d'ordre 2 en temps, il a été démontré par Lätt [33] que la méthode de Boltzmann sur réseau pour la simulation des écoulements incompressibles se comporte en fait comme un schéma d'ordre 1 en temps à cause des erreurs reliées aux effets de compressibilité.

D'autre part, il est possible de remarquer qu'avec le changement de variable (1.15) et (1.16), les fonctions de distribution g et $g^{(e)}$ respectent aussi les équations (1.9) à (1.11).

Discrétisation de l'espace des vitesses microscopiques

Physiquement, les particules sont libres de se déplacer dans n'importe quelle direction. Par contre, dans le cadre des méthodes de Boltzmann sur réseau, la discrétisation de l'espace sur un réseau discret nécessite de considérer uniquement un sous-ensemble de vitesses microscopiques discrètes $\vec{c}_i$ pour représenter l'ensemble des vitesses microscopiques $\vec{\xi}$. Ici, la notation pour les vitesses microscopiques est différente selon que l'espace considéré soit continu, avec $\vec{\xi}$, ou discret, avec $\vec{c}_i$. Le choix des vitesses microscopiques discrètes $\vec{c}_i$ n'est pas fait au hasard. Tel que mentionné par Lätt [33], les vitesses $\vec{c}_i$ doivent respecter une certaine symétrie pour que l'équation de Boltzmann sur réseau soit en mesure de reproduire des équations aux dérivées partielles au niveau macroscopique. Pour la simulation hydrodynamique incompressible de Navier-Stokes, il est suffisant de considérer des réseaux où les vitesses microscopiques $\vec{c}_i$ respectent les équations suivantes :

$$\begin{aligned}
& - \sum_i W_i = 1 \\
& - \sum_i W_i c_{i\alpha} c_{i\beta} = \lambda^{(2)} \delta_{\alpha\beta} \\
& - \sum_i W_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \lambda^{(4)} (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \\
& - \sum_i W_i c_{i\alpha} = 0 \\
& - \sum_i W_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0 \\
& - \sum_i W_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} c_{i\epsilon} = 0
\end{aligned}$$

où W_i est une liste de poids à déterminer étant donné le choix du sous-ensemble de vitesses microscopiques $\vec{c}_i$ et, $\lambda^{(2)}$ et $\lambda^{(4)}$, sont aussi des coefficients à déterminer qui dépendent du réseau [24]. Dans les expressions ci-dessus, δ est le symbole de Kronecker. Il est assez évident que ce n'est pas n'importe quel sous-ensemble de vitesses microscopiques $\vec{c}_i$ qui permet de satisfaire un tel système d'équations. La thèse de Lätt [33] et l'article de Nourgaliev et al. [24] présentent quelques exemples de réseaux en 2 et 3 dimensions.

He et al. [23] ont proposé de discrétiser les intégrales (1.9) à (1.11) en utilisant une quadrature Gaussienne d'un ordre approprié :

$$\int p(\vec{\xi})g(\vec{x}, \vec{\xi}, t)d\vec{\xi} = \sum_i w_i p(\vec{c}_i)g(\vec{x}, \vec{c}_i, t) \equiv \sum_i p(\vec{c}_i)N_i(\vec{x}, t) \quad (1.19)$$

où $p(\cdot)$ est un polynôme en $\vec{\xi}$ ou $\vec{c}_i$ qui dépend de l'intégrale à discrétiser. Il doit être noté que les vitesses $\vec{c}_i$ agissent comme point de quadrature et que les w_i sont les poids correspondants de la quadrature. Le nombre de points et de poids pour la quadrature dépend du degré maximum du polynôme $p(\cdot)$ et de la dimension (2D ou 3D généralement) de l'espace des vitesses $\vec{\xi}$ [15]. La fonction de distribution continue est notée g tandis que les fonctions de distribution discrètes sont notées N_i et sont définies par $N_i \equiv N_i(\vec{x}, t) \equiv w_i g(\vec{x}, \vec{c}_i, t)$. La fonction de distribution d'équilibre $g^{(e)}$ doit aussi respecter l'Éq. (1.19) pour chacune des intégrales (1.9) à (1.11). En suivant cette procédure, les intégrales (1.9) et (1.10) sont approximées de sorte que :

$$\rho = \sum_i N_i = \sum_i N_i^{(e)} \quad (1.20)$$

$$\rho \vec{u} = \sum_i N_i \vec{c}_i = \sum_i N_i^{(e)} \vec{c}_i \quad (1.21)$$

Comme seulement les écoulements isothermes sont considérés, l'Éq. (1.11) relative à l'énergie n'est pas tenue en compte.

En procédant à un développement en série de Taylor autour de 0 de la fonction d'équilibre par rapport à la vitesse macroscopique $\vec{u}$, l'Éq. (1.8) devient :

$$g^{(e)} = f^{(e)} = \left[\frac{\rho}{(2\pi RT)^{D/2}} \exp\left(\frac{-(\vec{\xi} \cdot \vec{\xi})}{2RT}\right) \right] \left(1 + \frac{\vec{\xi} \cdot \vec{u}}{RT} + \frac{(\vec{\xi} \cdot \vec{u})^2}{2(RT)^2} - \frac{\vec{u}^2}{2RT} \right) + O(\vec{u}^3) \quad (1.22)$$

Cette dernière expression est valide pour les écoulements dans la limite d'un faible nombre de Mach. Il est possible de considérer plus de termes dans le développement pour récupérer le moment (1.11) concernant l'énergie [34]. Si le carré de la vitesse du son isothermale du système est donné par $c_s^2 = RT$, la fonction d'équilibre dans l'espace discret s'écrit :

$$N_i^{(e)} = \rho W_i \left(1 + \frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + \frac{(\vec{c}_i \cdot \vec{u})^2}{2c_s^4} - \frac{\vec{u}^2}{2c_s^2} \right) \quad (1.23)$$

Cette dernière équation pour la fonction d'équilibre est la plus courante dans la littérature scientifique des méthodes de Boltzmann sur réseau. Le lien entre les poids de la quadrature w_i

et les poids du réseau W_i est donné par la relation :

$$w_i = (2\pi RT)^{D/2} \exp\left(\frac{\vec{c}_i \cdot \vec{c}_i}{2RT}\right) W_i \quad (1.24)$$

En utilisant la formulation (1.18) de l'équation de Boltzmann discrète dans le temps suivant les caractéristiques $\vec{\xi}$, l'équation de Boltzmann discrète dans le temps et dans l'espace des phases se résume à la formulation suivante :

$$N_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) - N_i(\vec{x}, t) = -\omega \left(N_i(\vec{x}, t) - N_i^{(e)}(\vec{x}, t) \right) \quad (1.25)$$

avec $i = 1..n$ et n est le nombre de vitesses microscopiques discrètes $\vec{c}_i$ considérées dans la discrétisation de l'espace des phases.

1.3.3 Modèle de Boltzmann sur réseau de base à une phase

Pour décrire un modèle de Boltzmann sur réseau, il faut d'abord choisir un réseau. En deux dimensions, le réseau le plus commun est D2Q9 illustré à la figure (1.1). Le pas de temps Δt et le pas géométrique Δx sont reliés par l'expression $c = \Delta x / \Delta t$. Dans les méthodes de Boltzmann sur réseau, c'est une procédure commune d'adimensionnaliser le réseau en fixant $c = \Delta x = \Delta t = 1$ et ensuite, d'adimensionnaliser les paramètres restant de la simulation suivant ce réseau adimensionnel. À partir de ce point, cette convention est utilisée dans cette thèse ainsi que dans les articles scientifiques, soumis et publiés, en annexe.

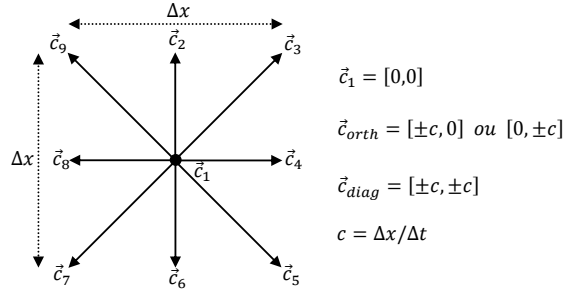


Figure 1.1 Réseau D2Q9.

Pour le réseau D2Q9, les valeurs les plus communes sont :

$$W_1 = 4/9 \quad (1.26)$$

$$W_{\text{orth}} = 1/9 \quad (1.27)$$

$$W_{\text{diag}} = 1/36 \quad (1.28)$$

$$\vec{c}_1 = [0, 0] \quad (1.29)$$

$$\vec{c}_{\text{orth}} = [\pm 1, 0] \text{ et } [0, \pm 1] \quad (1.30)$$

$$\vec{c}_{\text{diag}} = [\pm 1, \pm 1] \quad (1.31)$$

$$\lambda^{(2)} = c_s^2 = 1/3 \quad (1.32)$$

$$\lambda^{(4)} = c_s^4 = 1/9 \quad (1.33)$$

Tel que démontré par Nourgaliev et al. [24], pour être en mesure de récupérer au niveau macroscopique les Éqs. (1.1) et (1.2) de Navier-Stokes incompressibles dans la limite d'un faible nombre de Mach, la fonction d'équilibre de l'Éq. (1.23) doit respecter certaines relations constitutives :

$$\sum_i N_i^{(e)} = \rho \quad (1.34)$$

$$\sum_i N_i^{(e)} c_{i\alpha} = \rho u_\alpha \quad (1.35)$$

$$\sum_i N_i^{(e)} c_{i\alpha} c_{i\beta} = P_{\alpha\beta} + \rho u_\alpha u_\beta \quad (1.36)$$

$$\sum_i N_i^{(e)} c_{i\alpha} c_{i\beta} c_{i\gamma} = M(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) \quad (1.37)$$

où $P_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta}$ est le tenseur de pression et $M = \rho \frac{\lambda^{(4)}}{\lambda^{(2)}} = \rho/3$ est un coefficient relié à la viscosité du fluide.

En utilisant la formulation (1.25), l'équation de Boltzmann sur réseau prend la forme adimensionnelle suivante dans le cas simplifié du réseau D2Q9 :

$$N_i(\vec{x} + \vec{c}_i, t + 1) - N_i(\vec{x}, t) = -\omega \left(N_i(\vec{x}, t) - N_i^{(e)}(\vec{x}, t) \right) \quad (1.38)$$

avec :

$$\rho = \sum_i N_i = \sum_i N_i^{(e)} \quad (1.39)$$

$$\rho \vec{u} = \sum_i N_i \vec{c}_i = \sum_i N_i^{(e)} \vec{c}_i \quad (1.40)$$

$$p = \rho c_s^2 = \rho/3 \quad (1.41)$$

$$N_i^{(e)} = \rho W_i \left(1 + 3(\vec{c}_i \cdot \vec{u}) + \frac{9}{2}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}\vec{u}^2 \right) \quad (1.42)$$

$$\nu = \frac{1}{3} \left(\frac{1}{\omega} - \frac{1}{2} \right) \quad (1.43)$$

En utilisant précisément les Éqs. (1.38) à (1.43) , les auteurs Hou et al. [35] ont démontré avec détails que dans la limite d'un faible nombre de Mach, cette formulation de Boltzmann sur réseau est équivalente aux équations de Navier-Stokes incompressibles. Cette démonstration, à elle seule, occupe une douzaine de pages dans leur article.

1.3.4 Modèle de Boltzmann sur réseau plus général

Une analyse plus approfondie faite par Nourgaliev et al. [24] révèle en fait un degré de liberté supplémentaire dans l'équation de Boltzmann sur réseau permettant d'obtenir une fonction d'équilibre plus générale. En théorie, cette généralisation au niveau des équations de Boltzmann sur réseau ne change pas le comportement asymptotique des équations macroscopiques.

Pour un réseau D2Q9 plus général, le poids $W_1 \in]0, 1[$ et :

$$W_{\text{orth}} = 4W_{\text{diag}} \quad (1.44)$$

$$W_{\text{diag}} = \frac{1 - W_1}{20} \quad (1.45)$$

$$\lambda^{(2)} = \frac{3(1 - W_1)}{5} = c_s^2 \quad (1.46)$$

$$\lambda^{(4)} = \frac{(1 - W_1)}{5} \quad (1.47)$$

$$N_{i=1}^{(e)} = \rho \left[1 - \frac{1 - W_1}{\lambda^{(2)}} c_s^2 - \frac{\vec{u}^2}{2} \left(\frac{\lambda^{(2)}}{\lambda^{(4)}} - \frac{1 - W_1}{\lambda^{(2)}} \right) \right] \quad (1.48)$$

$$N_{i \neq 1}^{(e)} = \rho W_i \left[\frac{c_s^2}{\lambda^{(2)}} + \frac{\vec{c}_i \cdot \vec{u}}{\lambda^{(2)}} + \frac{(\vec{c}_i \cdot \vec{u})^2}{2\lambda^{(4)}} - \frac{\vec{u}^2}{2\lambda^{(2)}} \right] \quad (1.49)$$

La fonction d'équilibre donnée par l'Éq. (1.42) est en fait un cas particulier lorsque $W_1 = 4/9$.

1.3.5 Modèle de Boltzmann sur réseau à deux phases de Reis et Phillips

Le point de départ de cette thèse est le modèle de Boltzmann sur réseau à deux phases de Reis et Phillips [17]. Leur modèle est donc énoncé dans cette section. La description de leur modèle est issue de la Ref. [36], qui est la première contribution scientifique de cette recherche doctorale. Tel qu'il sera décrit plus loin dans la revue de littérature, ce modèle de Boltzmann sur réseau possède divers avantages par rapport à d'autres modèles de Boltzmann sur réseau. Il fait aussi partie d'une catégorie de modèles issue et du même type que le premier modèle de Boltzmann sur réseau pour la simulation des fluides à plusieurs phases immiscibles [37]. La littérature scientifique concernant ce type de modèle est donc assez variée par rapport à d'autres types de modèles disponibles. Comme le modèle de Reis et Phillips est aussi très bien expliqué dans leur article, la compréhension pour les non-initiés des modèles à plusieurs phases de Boltzmann sur réseau a donc été facilitée. Leur modèle a ainsi été sélectionné pour être étudié et analysé davantage. Cette thèse est donc, d'une certaine manière une extension du travail de Reis et Phillips. Après avoir présenté le modèle en détail, il s'en suivra une discussion sur les problématiques qu'engendre l'utilisation de ce modèle pour la simulation des fluides à deux phases.

Dans ce modèle à deux dimensions, il y a deux ensembles de fonctions de distribution, une pour chaque fluide, se déplaçant sur un réseau D2Q9 avec les vitesses microscopiques $\vec{c}_i$. Avec $\theta_i = \frac{\pi}{4}(4 - i)$ les vitesses microscopiques sont définies par :

$$\vec{c}_i = \begin{cases} (0, 0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)], & i = 2, 4, 6, 8 \\ [\sin(\theta_i), \cos(\theta_i)] \sqrt{2}, & i = 3, 5, 7, 9 \end{cases} \quad (1.50)$$

Les fonctions de distribution pour un fluide de couleur k (avec $k = r$ pour rouge et $k = b$ pour bleu) sont notées $N_i^k(\vec{x}, t)$, alors que $N_i(\vec{x}, t)$ est utilisé pour la somme $N_i^r(\vec{x}, t) + N_i^b(\vec{x}, t)$. La fonction de distribution $N_i(\vec{x}, t)$ représente celle du fluide sans couleur. L'algorithme suit alors l'équation d'évolution suivante :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t) + \Omega_i^k(N_i^k(\vec{x}, t)) \quad (1.51)$$

où l'opérateur de collision Ω_i^k est le résultat de la combinaison de trois sous-opérateurs (similairement à la Réf. [38]) :

$$\Omega_i^k = (\Omega_i^k)^{(3)} [(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)}] \quad (1.52)$$

Dans l'algorithme, l'équation d'évolution est résolue en quatre étapes par séparation des

opérateurs de la façon suivante :

1. Opérateur de collision à une phase :

$$N_i^k(\vec{x}, t_*) = (\Omega_i^k)^{(1)}(N_i^k(\vec{x}, t))$$

2. Opérateur de collision à deux phases (perturbation) :

$$N_i^k(\vec{x}, t_{**}) = (\Omega_i^k)^{(2)}(N_i^k(\vec{x}, t_*))$$

3. Opérateur de collision à deux phases (recoloriage) :

$$N_i^k(\vec{x}, t_{***}) = (\Omega_i^k)^{(3)}(N_i^k(\vec{x}, t_{**}))$$

4. Opérateur de propagation :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t_{***})$$

Opérateur de collision à une phase

Le premier sous-opérateur $(\Omega_i^k)^{(1)}$ est l'opérateur BGK standard de la méthode de Boltzmann sur réseau à une phase, où les fonctions de distribution relaxent vers un équilibre local avec ω_k désignant le facteur de relaxation :

$$(\Omega_i^k)^{(1)}(N_i^k) = N_i^k - \omega_k \left(N_i^k - N_i^{k(e)} \right) \quad (1.53)$$

Voici quelques détails concernant cet opérateur : la densité du fluide k est donnée par le premier moment des fonctions de distribution :

$$\rho_k = \sum_i N_i^k = \sum_i N_i^{k(e)} \quad (1.54)$$

où l'exposant (e) dénote l'équilibre. La densité totale du fluide (sans couleur) est donnée par $\rho = \rho_r + \rho_b$, tandis que la quantité de mouvement du fluide (sans couleur) est définie comme le second moment des fonctions de distribution :

$$\rho \vec{u} = \sum_i \sum_k N_i^k \vec{c}_i = \sum_i \sum_k N_i^{k(e)} \vec{c}_i \quad (1.55)$$

où $\vec{u}$ est la vitesse macroscopique du fluide (sans couleur). Les fonctions de distribution d'équilibre sont définies par :

$$N_i^{k(e)} = \rho_k \left(\phi_i^k + W_i \left[3\vec{c}_i \cdot \vec{u} + \frac{9}{2}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}(\vec{u})^2 \right] \right) \quad (1.56)$$

Les poids W_i sont ceux du réseau D2Q9 standard :

$$W_i = \begin{cases} 4/9, & i = 1 \\ 1/9, & i = 2, 4, 6, 8 \\ 1/36, & i = 3, 5, 7, 9 \end{cases} \quad (1.57)$$

Avec,

$$\phi_i^k = \begin{cases} \alpha_k, & i = 1 \\ (1 - \alpha_k)/5, & i = 2, 4, 6, 8 \\ (1 - \alpha_k)/20, & i = 3, 5, 7, 9 \end{cases} \quad (1.58)$$

Avec quelques manipulations, il est possible de remarquer que l'expression (1.56) est la même que la fonction d'équilibre plus générale définie par les Éqs. (1.48) et (1.49). Ces deux expressions pour la fonction d'équilibre ont un degré de liberté.

Tel qu'introduit par Grunau et al. [39], pour obtenir un interface stable, le ratio de densité γ entre les fluides à besoin d'être pris tel que :

$$\gamma = \frac{\rho_r^0}{\rho_b^0} = \frac{1 - \alpha_b}{1 - \alpha_r} \quad (1.59)$$

où l'indice supérieur « 0 » au-dessus de ρ_k^0 indique la valeur initiale de ρ_k au début de la simulation.

Sans perdre de généralité, il est supposé que $\rho_r^0 \geq \rho_b^0$. La pression dans le fluide de couleur k est :

$$p_k = \frac{3\rho_k(1 - \alpha_k)}{5} = \rho_k(c_s^k)^2 \quad (1.60)$$

où, dans l'expression précédente, soit α_r ou α_b est un paramètre libre, et c_s^k est la vitesse du son dans le fluide de couleur k [17, 40]. Théoriquement, la contrainte $\alpha_k \leq 1$ doit être respectée pour éviter des pressions négatives. Il est aussi possible de démontrer que $0 \leq \alpha_b \leq \alpha_r \leq 1$ est toujours vrai lorsque $\rho_r \geq \rho_b$ et $0 \leq \alpha_b \leq 1$. En pratique, la valeur de α_b est choisie entre 0 et 1. Ainsi, la valeur de α_r est calculée à partir du ratio de densité γ et de α_b .

Le paramètre de relaxation ω_k est choisi de manière à ce que l'équation d'évolution (1.51) respecte les équations macroscopiques des écoulements à une phase dans les régions où une seule phase est présente [17]. Ce paramètre est une fonction de la viscosité cinématique du fluide ν_k , donné par $\omega_k = 1/(3\nu_k + \frac{1}{2})$. Aussi introduit par Grunau et al. [39], lorsque les viscosités des fluides sont différentes, une interpolation est appliquée pour définir le paramètre

ω_k à l'interface. Pour ce faire, la fonction « champ de couleur » est introduite :

$$\psi = \frac{\rho_r - \rho_b}{\rho_r + \rho_b} \quad (1.61)$$

Le champ de couleur ψ est une fonction avec son image entre -1 et 1 . Cette fonction prend la valeur 1 ou -1 , selon qu'elle est évaluée à une position qui contient seulement du fluide rouge ou seulement du fluide bleu. À l'interface, le champ de couleur est évidemment entre -1 et 1 . Le facteur de relaxation ω_k dans l'Éq. (1.53) est remplacé par le facteur de relaxation effectif ω_{eff} :

$$\omega_{\text{eff}} = \begin{cases} \omega_r, & \psi > \delta \\ f_r(\psi), & \delta \geq \psi > 0 \\ f_b(\psi), & 0 \geq \psi \geq -\delta \\ \omega_b, & \psi < -\delta \end{cases} \quad (1.62)$$

où δ est un paramètre libre et

$$\begin{aligned} f_r(\psi) &= \chi + \eta\psi + \kappa\psi^2 \\ f_b(\psi) &= \chi + \lambda\psi + v\psi^2 \end{aligned} \quad (1.63)$$

avec

$$\begin{aligned} \chi &= 2\omega_r\omega_b/(\omega_r + \omega_b) \\ \eta &= 2(\omega_r - \chi)/\delta \\ \kappa &= -\eta/(2\delta) \\ \lambda &= 2(\chi - \omega_b)/\delta \\ v &= \lambda/(2\delta) \end{aligned} \quad (1.64)$$

Le paramètre libre δ est requis pour calculer ω_{eff} , il est généralement choisi égal à 0.1 [17]. C'est un paramètre qui influence l'épaisseur de l'interface lorsque la viscosité des fluides est différente. Le plus grand est δ , le plus large est l'interface entre les fluides. Si la viscosité des fluides est la même, le paramètre δ n'a pas d'impact sur la solution parce que, dans ce cas, $\omega_{\text{eff}} = \omega_r = \omega_b$.

Opérateur de perturbation

Dans ce type de modèle de Boltzmann sur réseau, la tension de surface est modélisée à l'aide de l'opérateur de perturbation [17, 41, 42]. Premièrement, le gradient de couleur en

terme de la différence de couleur est défini par :

$$\vec{F}(\vec{x}) = \sum_i \vec{c}_i (\rho_r(\vec{x} + \vec{c}_i) - \rho_b(\vec{x} + \vec{c}_i)) \quad (1.65)$$

Le gradient de couleur est une approximation de la perpendiculaire à l'interface entre les fluides. Cet opérateur est défini par l'expression suivante :

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \frac{A_k}{2} |\vec{F}| \left[W_i \frac{(\vec{F} \cdot \vec{c}_i)^2}{|\vec{F}|^2} - B_i \right] \quad (1.66)$$

où

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (1.67)$$

Sous les hypothèses de conservation de la masse et de la conservation de la quantité de mouvement, Reis et Phillips [17] ont démontré que cet opérateur concorde au niveau macroscopique avec la forme du tenseur des contraintes capillaires, c'est-à-dire que l'Éq. (1.66) au niveau macroscopique est proportionnelle à l'expression $\sigma(|\vec{F}|^2 \mathbf{I} - \vec{F} \otimes \vec{F})$. Cet opérateur gère le couplage entre les deux fluides avec le paramètre libre A_k choisi pour modéliser la tension de surface. La valeur de la tension de surface théorique σ_{th} en fonction des paramètres du modèle est donnée par l'expression :

$$\sigma_{th} = \frac{4}{3} \frac{\rho_r^0 + \rho_b^0}{\omega_{eff}} (A_r + A_b) \quad (1.68)$$

Bien que cet opérateur génère la tension de surface, il ne garantit pas l'immiscibilité des fluides. Pour minimiser le mélange des fluides, l'opérateur de recoloriage $(\Omega_i^k)^{(3)}$ doit être introduit.

Opérateur de recoloriage

Ce dernier opérateur a l'objectif de maximiser la quantité de fluide rouge envoyée dans la région du fluide rouge et la quantité de fluide bleu envoyée dans la région du fluide bleu, tout en respectant la conservation de la masse et de la quantité de mouvement totale. Au niveau microscopique, la conservation de la masse et la quantité de mouvement totale sont

équivalentes à :

$$\begin{aligned} N_i^r + N_i^b &= N_i \\ \sum_i N_i^r &= \rho_r \end{aligned} \quad (1.69)$$

La procédure algorithmique est heuristique et dans le modèle de Reis et Phillips [17], elle est réalisée comme suit. Premièrement, les vecteurs $\vec{c}_i$ sont réordonnés en ordre croissant relativement à leur angle avec le gradient de couleur $\vec{F}$. Le vecteur $\vec{c}_1 = [0, 0]$ est placé au centre des neuf directions. Il est à noter que le gradient de couleur $\vec{F}$ pointe dans la direction du fluide rouge. La deuxième étape consiste à envoyer un maximum de fluide rouge dans la direction la plus proche de $\vec{F}$, toujours sous les contraintes (1.69). En utilisant la quantité de fluide rouge restant, une quantité maximum de fluide rouge est envoyée dans la deuxième direction la plus près de $\vec{F}$, toujours en respectant les contraintes (1.69). Ce processus est répété jusqu'à ce que tout le fluide rouge ait été redistribué. À la fin de la redistribution du fluide rouge, le fluide bleu occupe l'espace restant.

La prochaine section traite des problématiques rencontrées avec cette méthode de Boltzmann sur réseau lorsqu'elle est utilisée pour la simulation des fluides à plusieurs phases immiscibles.

1.4 Problématique

Dans les lignes qui suivent, une liste des problématiques rencontrées avec ce modèle est dressée. Bien que la liste peut sembler longue, elle n'est peut-être pas exhaustive. Elle ne comprend que les éléments aperçus durant le cadre de cette recherche doctorale. Il est à noter que certains éléments ont été identifiés dès le début de la recherche tandis que d'autres ont été identifiés beaucoup plus tard. Certains problèmes ne sont donc pas abordés et analysés dans cette thèse, mais il est quand même important de les mentionner.

1. Par rapport à l'algorithme dans son ensemble, l'opérateur de recoloriage $(\Omega_i^k)^{(3)}$, de l'Éq. (1.52), est difficile à programmer.
2. L'interface souffre du « lattice pinning ». Ce problème peut se produire à l'interface de deux fluides lorsque la convection dans l'écoulement est faible. Dans la pratique, cela signifie que l'interface peut ne pas bouger et devient « épinglée » au réseau, et ce, aussi longtemps que la convection n'est pas assez importante.
3. Le modèle est affecté par des « courants parasites » artificiels aux interfaces entre les fluides. Ces courants parasites devraient être théoriquement nuls, mais ils perturbent le champ de vitesse $\vec{u}$ de manière non physique. Les courants parasites sont généralement

faibles, mais diminuent néanmoins la stabilité et la précision du schéma numérique.

4. L'interface est très mince et l'épaisseur de l'interface n'est pas ajustable. Le fait que l'interface soit très mince, deux à trois unités de réseau, engendre certaines difficultés étant donné que la théorie concernant le tenseur des contraintes capillaires est développée en supposant une interface diffuse. Étant donné les quasi-discontinuités dans les champs de densités des fluides aux interfaces, le calcul du vecteur normal $\vec{F}$ à l'interface à l'aide de méthode numérique est donc peu précis.
5. Dans le cas d'écoulements théoriquement stationnaires, la convergence de la solution numérique de l'algorithme vers un état stationnaire numérique n'est généralement pas atteinte. Il y a donc un « bruit » dans l'algorithme dont la cause exacte est difficilement identifiable.
6. Le modèle n'est pas en mesure de simuler des ratios de densité élevés, et ce, même pour des cas tests théoriquement stationnaires.
7. Dans ce modèle, des bulles initialement circulaires ont tendance à se déformer et à adopter une forme anisotrope à l'état stationnaire.
8. Le modèle est imprécis lorsque la tension de surface est faible.
9. Le comportement du modèle dans le cas mixte de variation de densité et de viscosité est pratiquement inconnu.
10. Le modèle est limité à la simulation d'écoulements à deux phases. La généralisation du modèle pour simuler trois phases immiscibles et plus n'est pas directe.
11. Lorsqu'il y a un ratio de densité non unitaire entre les fluides, le modèle n'est pas en mesure de simuler correctement l'écoulement de Couette à plusieurs phases. Il y a une discontinuité dans le champ de la quantité de mouvement théorique qui n'est pas capturée par le schéma numérique.

À partir de ce point, les problématiques suivantes ne sont pas traitées dans cette thèse.

12. Le modèle n'est pas en mesure de simuler des ratios de viscosité très élevés, c'est-à-dire $> O(100)$, même pour des cas tests théoriquement stationnaires.
13. Le modèle a été initialement formulé pour deux dimensions spatiales. La généralisation à trois dimensions n'est pas directe.
14. La condition d'écoulement à faible nombre de Mach est de plus en plus difficile à respecter lorsque le ratio de densité entre les fluides augmente. Effectivement, selon la condition (1.59) concernant les écoulements avec ratio de densité non unitaire, la vitesse du son dans le fluide dense peut être très petite limitant ainsi la vitesse maximale que peut atteindre le fluide pour respecter un faible nombre de Mach.

Avec l'ensemble des problèmes précédemment mentionnés, il est normal de se demander pourquoi développer et examiner ce modèle davantage. En fait, ce modèle possède aussi des points positifs très appréciables. Il est facilement parallélisable. À l'exception de l'opérateur de recoloriage, il est aussi très simple à programmer. De plus, cette méthode est très bien adaptée pour simuler des écoulements dans des géométries complexes, tels que les milieux poreux. Le modèle est en mesure de simuler le changement de la topologie des interfaces, comme la coalescence ou la séparation des bulles, de manière très naturelle et sans difficulté.

1.5 Objectifs

Cette dernière section de l'introduction décrit les objectifs de la thèse. L'objectif de la recherche a été de faire à la fois des progrès touchant la modélisation théorique et numérique du modèle de Reis et Phillips [17]. Voici les **objectifs principaux** :

- 1^{er} objectif** Modifier l'opérateur de recoloriage $(\Omega_i^k)^{(3)}$, de l'Éq. (1.52), afin de réduire l'impact sur le modèle des problématiques 1, 2, 3, 4, 5, 6 et 8 données à la page 22.
- 2^e objectif** Employer une discrétisation isotrope pour calculer le gradient de couleur $\vec{F}$, de l'Éq. (1.65), afin réduire l'impact sur le modèle des problématiques 3, 4, 6, 7 et 8 données à la page 22.
- 3^e objectif** Généraliser le modèle afin de simuler des écoulements avec plus de deux phases. Le but est d'améliorer le modèle concernant les problématiques 6, 9 et 10 données à la page 23.
- 4^e objectif** Capturer la discontinuité du champ de la quantité de mouvement présent dans l'écoulement de Couette à plusieurs phases avec ratio de densité non unitaire. Le but est d'améliorer le modèle concernant les problématiques 6, 9 et 11 données à la page 23.

Le chapitre concernant la synthèse des contributions montre en quoi chacun des changements énumérés ci-dessus contribuent à améliorer un ou plusieurs éléments de la problématique ayant trait avec le modèle de Reis et Phillips [17]. Un **objectif complémentaire** de cette thèse est de :

- 5^e objectif** Généraliser la théorie des gradients pour des ordres spatiaux et isotropes élevés.

Avant de faire la synthèse des contributions, une revue de la littérature scientifique se

rapportant aux méthodes de Boltzmann sur réseau pour la modélisation des fluides à plusieurs phases est présentée.

CHAPITRE 2

REVUE CRITIQUE DE LA LITTÉRATURE

Depuis maintenant deux décennies, une nouvelle méthode numérique pour la simulation des écoulements des fluides a été développée et utilisée. Cette approche, connue sous le nom de la LBM (à lire comme « méthode de Boltzmann sur réseau » de l'anglais « Lattice Boltzmann Method »), utilise des fonctions de distribution [43] et a été initialement construite comme une extension des automates cellulaires [44]. Ce n'est que plus tard, qu'il a été découvert, que la méthode peut également être considérée comme une troncature systématique de l'équation de Boltzmann dans l'espace des phases [23].

Un des avantages de la LBM réside dans la façon dont elle est en mesure de traiter les problèmes de calcul dans les géométries complexes. Même dans ces situations, la LBM est bien adaptée pour le calcul sur des architectures parallèles [45–47]. De plus, étant donné la linéarité de l'opérateur de propagation, cette méthode est simple d'application. L'une des caractéristiques de la LBM est sa grande souplesse dans le traitement additionnel de physiques complexes, parfois moins évident pour les méthodes CFD traditionnelles basées sur les équations de Navier-Stokes.

Les écoulements à phases multiples sont un exemple typique de physiques complexes où la LBM s'est révélée être bien adaptée [17, 39, 41, 42, 48–50]. Cela inclut, par exemple, la formation et la coalescence des gouttes [51, 52], le déplacement de bulles [53–55], les écoulements de fluides en milieu poreux [38, 56–58], les écoulements sanguins [59], la dissolution de gouttelettes de liquide dans un autre liquide [40], et la transition solide/liquide des phases [60, 61]. Dans ces travaux, des comparaisons avec la physique expérimentale ont également été effectuées [38, 51, 53].

Les modèles de la LBM pour la simulation des fluides à phases multiples peuvent généralement être classifiés en cinq catégories. Ces dernières, nommées en ordre chronologique, sont les méthodes de : Rothman-Keller (RK) [17, 38, 39, 41, 42, 48, 49, 51, 59, 62–64], Shan-Chen (SC) [40, 50, 65–68], « free energy » (FE) [53, 55, 56, 58, 69–72], « mean-field » (MF) [26, 73, 74] et « field mediator » (FM) [75]. Il est à noter que cette classification n'est pas universelle et qu'il y a d'autres méthodes non abordées dans ce travail.

Note

Cette revue de littérature est en fait une unification des différentes revues de littérature contenues dans les articles en annexe de la thèse. Elle est réorganisée de la manière suivante. Tout d’abord, une brève présentation des différents modèles de Boltzmann sur réseau de type SC, FE, MF, FM est donnée. Puisque le modèle de simulation développé dans cette thèse est de type RK, une discussion plus détaillée traitant de ces modèles est abordée. Dans la section concernant les modèles RK, la revue de littérature discute aussi de quatre thèmes se rapportant aux quatre premiers objectifs de la thèse. La dernière section discute de la thématique complémentaire concernant le cinquième et dernier objectif de la thèse. À la fin de chacune des différentes thématiques, chacun des objectifs de la thèse est rappelé.

2.1 Les modèles de type SC, FE, MF et FM

Le modèle développé par Shan et Chen [50] utilise une force d’interaction entre les fonctions de distribution pour simuler les interactions microscopiques et ainsi séparer automatiquement la phase concentrée de la phase diluée. Cette ségrégation spontanée des phases est une fonctionnalité qui a attiré les praticiens de la LBM et a contribué à la popularité du modèle SC. La catégorie SC permet l’utilisation des équations d’états non idéaux en abandonnant la conservation de la quantité de mouvement locale pour ne respecter que la conservation de la quantité de mouvement dans un sens global [76]. Les modèles SC ont également l’avantage d’être facile à mettre en oeuvre et sont capables de simuler des fluides avec un ratio de densité élevé, mais les différents paramètres du modèle ne peuvent pas être choisis indépendamment [63]. Il y a quelques années, Hou et al. [77] ont comparé les modèles RK et SC. L’une des conclusions de leur étude préliminaire était que le modèle SC fournit de meilleurs résultats, car cette méthode produisait des courants parasites moins intenses à l’interface.

La méthode FE de Swift et al. [69] décrit une approche qui, à l’équilibre, conduit à un état pouvant être associé à une fonctionnelle concernant une énergie libre. La méthode utilise des règles de collision qui assurent l’évolution du système vers le minimum de la fonctionnelle d’énergie libre. Cette fonctionnelle possède à la fois une composante d’énergie associée au fluide pur et une autre à l’interface. La première composante veut décrire le comportement de

l'équilibre des phases pures, tandis que la tension de surface concerne la seconde composante. Comme le modèle SC, cette formulation est également capable de réaliser automatiquement la séparation des phases. Les méthodes de type FE font face à d'autres types de problèmes. Par exemple, ils ne respectent pas l'invariance galiléenne [63]. Néanmoins, les méthodes FE ont deux avantages : elles peuvent produire des interfaces aussi minces que deux unités de réseau et elles permettent l'utilisation de l'équation d'état de Van der Waals [58] à la place de l'équation d'état isothermale [70].

Les trois approches RK, SC, et FE sont théoriquement capables de simuler un nombre arbitraire de phases immiscibles [50, 59, 72].

Les méthodes MF simulent l'attraction entre les fonctions de distribution de la même façon que l'interaction de Coulomb est traitée dans l'équation de Vlasov [26]. Ces modèles, contrairement aux modèles SC, peuvent simuler les systèmes liquide-vapeur de manière thermodynamiquement conforme.

La méthode FM utilise des fonctions de distribution de masse nulle, dont l'unique rôle est d'inverser la quantité de mouvement des fonctions de distribution du réseau dans la couche de transition pour ainsi séparer les différents fluides [75]. Elle présente l'avantage d'être apte à intégrer la diffusivité binaire et, par conséquent, elle est également adaptée pour simuler les fluides miscibles.

Un autre défi, auquel est confrontée la LBM appliquée aux écoulements à plusieurs phases, est la simulation des ratios de densité élevés entre les phases. Des ratios de $O(160)$ ont été simulés par Kuzmin et Mohamad [67] à l'aide d'un modèle à interaction étendue et MRT (multi-relaxation time). Cependant, cette méthode SC améliorée est toujours incapable de simuler un rapport de densité air-eau $O(1000)$. Les travaux récents de Bao and Schaefer [68] ont permis la simulation d'écoulements à plusieurs phases avec de hauts ratios de densité en utilisant l'approche SC. Une méthode de projection basée sur un schéma FE mis au point par Inamuro et al. [54, 78] a permis de simuler des ratios de densité allant jusqu'à $O(1000)$. Malheureusement, cette méthode requiert, à chaque pas de temps, la résolution d'une équation de Poisson qui est coûteuse d'un point de vue de l'effort de calcul. Sur la base des méthodes MF et d'une discrétisation stable de l'équation de Boltzmann sur réseau, un modèle récent de Lee et al. [74] a été introduit et a montré des résultats prometteurs. Bien que cette discrétisation semble assez complexe, elle fonctionne bien, selon les auteurs. Ces derniers ont été capables de simuler des systèmes liquide-vapeur non idéaux avec une stabilité numérique accrue, et ce, pour un grand ratio de densité $O(1000)$. Une autre approche prometteuse a été développée par Zheng et al. [79], qui peut également atteindre des ratios de densité $O(1000)$ et ne nécessite pas la solution d'une équation de Poisson ou la mise en oeuvre de traitements complexes de dérivées numériques. Une méthode ne pouvant pas être classifiée dans l'une des

cinq catégories est celle de Becker et al. [80]. Ils ont réussi à simuler des ratios de densité aussi élevés que $O(1000)$ en utilisant la LBM ainsi que la méthode « level set ». Cependant, le couplage de la LBM avec la méthode « level set » n'est pas simple, car cela nécessite la connaissance de deux domaines de recherche différents. Une revue de la littérature récente et plus complète est présentée par Gokaltun et McDaniel [81] concernant la LBM conçue pour simuler les écoulements avec, simultanément, des ratios de densité et de viscosité élevés.

D'autre part, les discrétisations isotropes ont été initialement introduites dans les méthodes SC par Shan lui-même [82], et ce, pour le gradient de la fonction effective de masse représentant les interactions entre les fonctions de distribution. Il est démontré que plus il y a d'isotropie dans la discrétisation du gradient, plus l'intensité des courants parasites diminue. Une description détaillée des gradients isotropes, comme les points et les poids nécessaires à la discrétisation, est donnée dans le travail de Sbragaglia et al. [83] pour les espaces 2D et 3D.

2.2 Les modèles de type RK

Ces modèles de Boltzmann sur réseau pour la simulation des fluides à plusieurs phases sont issus du modèle d'automate cellulaire de Rothman et Keller [84]. Quelques années plus tard, Gunstensen et al. [41] ont développé une version « Boltzmann sur réseau » du modèle RK. Il doit être noté que toutes les références à propos des modèles RK sont en effet basées sur la thèse de doctorat de Gunstensen [48].

Le modèle RK d'origine considère deux types de fluides, rouge et bleu, chacun d'entre eux avec des fonctions de distribution suivant sa propre équation de Boltzmann sur réseau. Parce qu'il y a deux fluides impliqués, l'étape de collision, intrinsèque à toute formulation de Boltzmann sur réseau, prend en compte les interactions entre les fonctions de distribution de la même couleur ainsi que les interactions croisées entre les fonctions de distribution de couleurs différentes. Cette dernière interaction est liée à la tension de surface entre les deux phases, ce qui nécessite le gradient de la fonction de couleur. La séparation des phases est obtenue par une étape supplémentaire en utilisant un opérateur de recoloriage. L'avantage de cette approche est dans la souplesse avec laquelle les paramètres du modèle peuvent être choisis. Les modèles RK permettent le contrôle indépendant de la tension de surface, le ratio de densité et le ratio de viscosité des différents fluides de part et d'autre de l'interface ainsi que le contrôle de l'angle de contact concernant le comportement du mouillage aux phases solides [41].

Un problème majeur commun aux modèles de la LBM pour la simulation des écoulements à plusieurs phases est qu'ils semblent tous souffrir de la présence de courants parasites à l'interface entre les fluides. Ces courants parasites perturbent le champ de vitesse des fluides.

Ils affectent également la stabilité numérique, limitent les ratios de densité maximaux et réduisent la précision du modèle.

Les courants parasites à l'interface dans la méthode RK ont été étudiés par Ginzbourg et Adler [62]. Ils ont noté qu'un choix approprié des valeurs propres de la matrice de collision conduit à l'élimination de ces courants dans certaines circonstances. Malheureusement, les auteurs concluent que ces courants non physiques ne peuvent pas être éliminés ou réduits uniquement avec le choix des valeurs propres. Le phénomène des courants parasites à proximité d'une interface a également été mentionné par Halliday et al. [42], où il a été constaté que ces courants sont plus forts au centre de l'interface entre les fluides. Pour les réduire, Dupin et al. [59] ont proposé d'ajuster la tension de surface entre les fluides en perturbant les fonctions de distribution en conformité avec les orientations du réseau. Cette idée semblait prometteuse, mais n'a pas été plus explorée.

La capacité à simuler des écoulements avec un ratio de densité variable a été introduite par Grunau et al. [39], qui ont présenté des simulations instationnaires avec des ratios de densité allant jusqu'à $O(10)$. Depuis lors, la capacité de la famille RK pour simuler les écoulements avec un ratio de densité variable a été peu étudiée. Tölke et al. [38] rapportent un ratio de densité $O(30)$ pour une simulation d'un écoulement permanent et un rapport de densité de $O(4)$ pour une simulation d'écoulement instationnaire. Récemment, Reis et Phillips [17] ont apporté une contribution importante au modèle RK, qui a été d'adapter le modèle de Grunau et al. [39] pour le populaire réseau D2Q9. Plus important encore, ils ont réussi à construire un opérateur de perturbation qui introduit la tension de surface d'une manière qui est compatible, dans la limite macroscopique, avec la forme du tenseur des contraintes capillaires. Pour certains cas tests et avec la formulation de Reis et Phillips [17], des ratios de densité plus élevés que ceux des autres modèles RK peuvent être abordés. Un ratio de densité allant jusqu'à $O(18)$ a été rapporté pour une simulation instationnaire. D'autre part, Liu et al. [85, 86] ont développé une version 3D de l'opérateur de perturbation de Reis et Phillips pour le réseau D3Q19.

2.2.1 Thème 1 : Opérateur de recoloriage

Une amélioration majeure a été la redéfinition de l'opérateur recoloriage qui est intégré dans le modèle pour conserver l'immiscibilité des fluides.

Tölke et al. [38] ont constaté que l'étape de recoloriage du modèle d'origine rendait les simulations instables dans certaines situations. Une de leurs conclusions est que le principal problème réside dans le fait que le modèle d'origine génère une interface trop mince entre les fluides. Avec le nouvel opérateur de recoloriage de Tölke et al. [38], l'épaisseur de l'interface est un peu plus large que dans le modèle d'origine. Cependant, le contrôle précis de l'épaisseur

de l'interface n'est pas disponible. Tölke et al. sont parvenus tout de même à obtenir des simulations préliminaires qui sont en accord avec certaines données expérimentales [38].

D'Ortona et al. [87] ont rapporté que les courants parasites ont été significativement réduits avec leur nouvel opérateur de recoloriage destiné pour un modèle d'automate cellulaire à deux phases. Plus tard, Latva-Kokko et Rothman [49] ont modifié l'opérateur de recoloriage de D'Ortona et al. [87] pour éviter des fonctions de distribution négative dans le contexte de la LBM. Pour les modèles RK d'origines, l'étape de recoloriage est également considérée comme difficile à programmer. Toutefois, les idées de Latva-Kokko et Rothman [49] ont permis de construire un opérateur de recoloriage qui est très simple à mettre en oeuvre avec la possibilité supplémentaire de contrôler l'épaisseur de l'interface.

Leur nouvel opérateur de recoloriage réduit aussi considérablement le problème de « lattice pinning » du modèle d'origine [49]. Ce problème peut se produire à l'interface de deux fluides lorsque la convection est faible. Dans la pratique, cela signifie que l'interface ne peut pas bouger et devient « épinglée » au réseau, aussi longtemps que la convection n'est pas assez forte. Le problème du « lattice pinning » a été reconnu par plusieurs auteurs : Reis et Dellar [88], Latva-Kokko et Rothman [49], Dupin et al. [89], et Halliday et al. [90, 91]. Il est inconnu si ce problème est également présent dans les autres types de modèle de Boltzmann sur réseau. Il est important de noter que le modèle de Reis et Phillips n'utilise pas ces nouveaux opérateurs de recoloriage et que ces auteurs ont indiqué que leur modèle pourrait aussi souffrir du « lattice pinning ».

Le premier objectif de cette thèse est d'adapter l'opérateur de recoloriage de Latva-Kokko et Rothman [49] pour fonctionner avec le modèle de Reis et Phillips ainsi que pour des ratios de densité non unitaire. Cette modification permettra d'améliorer la stabilité et la précision du modèle. Plus de détails sont donnés dans le prochain chapitre concernant la synthèse des contributions.

2.2.2 Thème 2 : La discrétisation du gradient de couleur

Une caractéristique, qui distingue les modèles RK des autres modèles, est la présence d'un gradient de couleur. Pour les écoulements à deux phases de Boltzmann sur réseau, le gradient de couleur a été introduit par Rothman et Keller [84] avec leur modèle basé sur les automates cellulaires. C'est en utilisant le gradient de couleur que l'interface entre les fluides est maintenue. L'évaluation du gradient de couleur est une étape clé dans la discrétisation des différents éléments du modèle.

Lors de l'application de la méthode RK, des gradients de type non isotropes sont principalement utilisés [38, 39, 42, 49, 51, 59, 62, 77]. En fait, les gradients isotropes, c'est-à-dire avec une erreur de discrétisation qui est invariante par rapport à la rotation [92], sont rarement utilisés

et ont seulement été trouvés dans [63,93]. Malheureusement, dans ces études, ni l'avantage d'utiliser une telle discrétisation pour le gradient, ni la raison de le faire ne sont expliqués. À notre connaissance, il n'existe aucune étude systématique montrant que la mise en oeuvre d'un gradient isotrope dans les modèles RK offre une réduction significative des courants parasites, élargit la gamme d'applications de la tension superficielle ou augmente considérablement le ratio de densité maximal traité entre les deux phases.

Plus précisément, le deuxième objectif de cette thèse est de montrer que l'utilisation d'une discrétisation isotrope du gradient de couleur dans la formulation de Reis et Phillips devrait augmenter la robustesse de la méthode. Ceci est d'une importance primordiale, car cela minimise l'accumulation des erreurs de discrétisations directionnelles. Une conséquence bénéfique est la réduction des courants parasites. Cela signifie qu'il sera possible de résoudre des problèmes avec un ratio de densité plus élevé et/ou avec une gamme de tension superficielle plus large que précédemment obtenue avec d'autres modèles de type RK. Plus de détails sont donnés dans le prochain chapitre concernant la synthèse des contributions.

2.2.3 Thème 3 : Les modèles de type RK à plusieurs phases

Beaucoup moins d'attention a été accordée à la simulation des écoulements avec trois phases ou plus. La première étude sur ce sujet a été présentée dans la thèse de doctorat de Gunstensen [37].

Son modèle a toutefois ses limites, car la méthode pour prolonger le modèle à deux phases vers son homologue à trois phases ne peut pas être généralisée à un modèle à N -phases ou, du moins, il n'est pas évident de savoir comment faire. L'approche fonctionne bien pour trois phases, mais seulement parce qu'il y a exactement trois interfaces fluide-fluide ce qui correspond au nombre de phases. Parce que ce modèle a été introduit il y a 20 ans, il ne contient aussi aucune des améliorations subséquentes apportées au modèle RK.

Un autre modèle RK pour la simulation d'écoulements à plusieurs phases est celui de Dupin et al. [59]. Par la définition d'un gradient de couleur pour chacune des interfaces fluide-fluide, ils ont évité le problème de la généralisation du modèle à plus de trois phases de Gunstensen [37]. Une approche similaire est offerte par Halliday et al. [94], dans lequel une généralisation possible de l'opérateur de recoloriage est présentée pour N phases. Une version plus récente, similaire au modèle de Halliday et al. [94], est décrite par Spencer et al. [95]. Malheureusement, aucun de ces modèles à plusieurs phases a été construit pour simuler des ratios de densité variables. Il est avantageux d'envisager un modèle à N phases qui le permet tout en consolidant l'applicabilité et les avantages des modèles RK précédents. Il s'agit du troisième objectif de cette thèse.

Afin d'améliorer la capacité du modèle à simuler des ratios de densité élevés, nous avons

intégré les discrétisations isotropes d'ordre élevé pour le gradient de couleur qui doivent être calculées à chaque pas de temps. Comme indiqué précédemment par Leclaire et al. [96], ce type de discrétisation augmente la précision du modèle. En raison du coût en temps de calculs associés à l'évaluation du gradient, l'un des objectifs est de réduire le nombre d'approximations de gradients différents à calculer. Halliday et al. [94] ont affirmé que l'évaluation des gradients est une source importante de calcul supplémentaire. Ces auteurs ont d'ailleurs décidé d'examiner la possibilité d'approximer le gradient avec une méthode locale lorsque la courbure de l'interface est faible. Lors de la généralisation du modèle à N phases, une attention particulière doit être apportée pour minimiser le nombre d'approximations différentes de gradient. Plus de détails sont donnés dans le prochain chapitre concernant la synthèse des contributions.

2.2.4 Thème 4 : Le problème de discontinuité des modèles RK

Tel que dans d'autres études [97–99], l'auteur du présent document a réalisé que les modèles RK ne sont pas en mesure de simuler l'écoulement de Poiseuille ou de Couette à plusieurs phases avec une variation de densité. En effet, la quantité de mouvement théorique de cet écoulement n'est pas bien résolue.

Après une étude approfondie de la littérature scientifique, nous avons trouvé quelques travaux dans lesquels les auteurs ont démontré que leur modèle est en mesure de simuler correctement l'écoulement de Couette ou de Poiseuille à plusieurs phases. L'écoulement de Couette est plus simple à résoudre que celui de Poiseuille puisqu'aucun terme source simulant un gradient de pression n'est requis.

Lishchuk et al. [100] ont développé un modèle à plusieurs phases pour les fluides avec variation de densité. Ils ont démontré que l'écoulement de Couette est bien résolu avec leur modèle. Cependant, il n'est pas clair comment leurs idées pourraient être utilisées pour appliquer une correction simple aux modèles RK précédents qui ne fonctionnent pas bien [17, 18, 36, 38, 39, 85, 96, 97]. Dans l'article de Knutson et Noble [101], l'écoulement de Couette est aussi simulé avec succès. Néanmoins, les auteurs indiquent clairement que leur méthode, telle que présentée, ne convient pas pour des configurations d'écoulements plus complexes. Beaucoup d'efforts sont encore nécessaires pour généraliser leur méthode afin de résoudre des écoulements généraux plus complexes. En outre, pour utiliser cette méthode, il sera peut être nécessaire de la combiner avec un résolveur de type « level set » [101], ce qui signifierait que l'élégance de la LBM serait perdue. Yiotis et al. [58] ont montré que leur modèle est capable de simuler correctement l'écoulement de Poiseuille à plusieurs phases avec variation de densité. Il faudrait beaucoup d'efforts pour adapter leurs idées à la formulation RK actuelle puisque leur modèle utilise une nouvelle formulation de fonctions de distribution

pour la pression.

Holdych et al. [102] ont modifié le tenseur des contraintes d'équilibre du modèle FE de Swift et al. [69] afin de récupérer la solution analytique de l'écoulement de Couette à plusieurs phases avec des ratios de densité variable. Le quatrième objectif de cette thèse est de montrer que leur approche peut être adaptée au modèle RK afin de récupérer correctement les équations de Navier-Stokes dans les régions à phases pures, et ce, dans la limite d'un petit nombre de Knudsen et d'un faible gradient de pression. Plus de détails sont donnés dans le prochain chapitre concernant la synthèse des contributions.

2.3 Thème 5 complémentaire : Les différences finies isotropes

Les méthodes de différences finies pour calculer les gradients de fonctions sont largement utilisées dans la communauté scientifique. Lors du calcul du gradient d'une fonction de plusieurs variables, une différence finie 1D est généralement utilisée pour chacune des directions. Cependant, ces dernières années, il a été démontré que cette procédure peut introduire un certain degré d'anisotropie dans les résultats numériques [92].

Pour surmonter ce problème, Kumar a introduit le concept de la différence finie isotrope qui garantit que le terme d'erreur principal de la discrétisation par différences finies est isotrope et donc invariant par rapport à la rotation [92]. Cela assure que le schéma n'ajoute pas sa propre anisotropie à la simulation numérique [92]. Dans les travaux de Kumar, la simulation de la solidification symétrique dendritique est plus précise si des différences finies isotropes sont utilisées plutôt que des différences finies classiques. Dans la première approche, originalement proposée par Kumar, seulement des approximations 2D et 3D à l'aide des différences finies d'un ordre spatial et isotrope peu élevé ont été présentées.

Peu de temps après, Xiao et al. [103] ont utilisé des différences finies 3D isotropes pour discrétiser un cas particulier de l'équation de Maxwell et ont amélioré les résultats numériques. Des discrétisations isotropes ont également amélioré les résultats de Shen et al. [104], qui simulent la propagation d'une onde électromagnétique transitoire en 2D.

Suite à l'idée de Shan [82], pour la simulation numérique des écoulements à plusieurs phases en utilisant la méthode de Boltzmann sur réseau, Sbragaglia et al. [83] ont généralisé les gradients 2D et 3D isotropes à des ordres supérieurs. Bien que n'étant pas explicitement mentionné dans leur travail [83], l'approche qu'ils ont développée conduit à une approximation du gradient qui est précise au second ordre en espace. Pour leur modèle, l'utilisation de discrétisation isotrope pour le calcul des gradients a permis de réduire les courants parasites de leur modèle. Leur technique de gradient isotrope a également été utilisée par Leclaire et al. [96] et a permis la simulation de ratios de densité jusqu'à $O(10000)$ pour une bulle circulaire

et stationnaire. La discrétisation isotrope réduit l'anisotropie dans le schéma numérique et évite la déformation non physique de la bulle en plus de réduire les courants parasites.

Pour permettre la discrétisation 3D de gradients pseudo-isotropes sur maillage irrégulier, Grogger [105] a utilisé un processus d'optimisation qui minimise l'erreur associée à l'anisotropie, tout en assurant une approximation non dissipative, qui est une propriété importante dans la solution des équations aux dérivées partielles hyperboliques. Dans l'investigation faite par Grogger [105], il est à noter que pour un ordre donné de la discrétisation spatiale, l'erreur d'isotropie mène probablement à un ordre isotrope approximativement égal à l'ordre spatial. Le but étant d'augmenter la limite de stabilité de son schéma numérique, cela signifie que la méthode de Grogger est un compromis entre l'isotropie et la limite de la stabilité. Selon l'application prévue, la limite de stabilité n'est pas un paramètre requis et une meilleure isotropie peut être souhaitable.

Dans le cadre de la détection de contours sur les images numériques, Sayed et al. [106] ont développé un filtre omnidirectionnel ou isotrope. Les auteurs soutiennent que leur technique pourrait conduire à des filtres séparables qui permettent la détection très rapide des bords dans une image. Toutefois, étant donné que leur approche a émis l'hypothèse de la continuité du filtre et que le filtre réel est en fait discret, il y a une perte de précision due à un processus d'interpolation. Dans le contexte spécifique de la détection des contours, cette perte de précision n'est peut-être pas importante, mais dans d'autres applications scientifiques, où le filtre peut être appliqué fréquemment, cette perte de précision pourrait être importante, puisque la propriété d'isotropie décroît en qualité à cause du processus d'interpolation. En outre, la précision spatiale de leur méthode de discrétisation n'est pas connue.

D'autres opérateurs différentiels discrets isotropes peuvent être développés. Par exemple, Thampi et al. [107] ont montré que l'opérateur de Laplace peut être obtenu à partir des poids de la fonction d'équilibre discrète de Maxwell-Boltzmann, qui est largement utilisée dans la communauté de Boltzmann sur réseau. Patra et al. [108] ont également développé des poids isotropes pour le Laplacien, le bi-Laplacien (ou bi-harmonique) et le gradient du Laplacien.

Dans toutes les recherches précédentes, la conclusion est la même : les discrétisations isotropes des opérateurs différentiels sont plus précises que les différences finies classiques. Partant de ce constat, les chercheurs devraient tester les discrétisations isotropes.

Le cinquième et dernier objectif de cette thèse est de généraliser les différences finies isotropes pour l'approximation des gradients d'ordre élevé spatialement, tout en assurant en même temps que l'ordre d'isotropie est strictement plus grand que l'ordre spatial. Il s'agit d'une extension et d'une généralisation du travail de Sbragaglia et al. [83] pour les gradients d'un ordre spatial supérieur. Plus de détails sont donnés dans le prochain chapitre concernant la synthèse des contributions.

CHAPITRE 3

SYNTHÈSE DE L'ENSEMBLE DU TRAVAIL

Ce chapitre fait la synthèse des contributions de cette thèse. Il est organisé en cinq thèmes correspondants à ceux présentés dans la revue de la littérature. Pour les quatre premiers thèmes, les objectifs associés sont rappelés et dans chaque cas, deux types de contributions sont discutées :

- Contribution d'un apport théorique concernant le modèle de simulation.
- Contribution d'un apport appliqué concernant l'amélioration des résultats numériques.

Le cinquième thème, étant complémentaire, présente aussi des contributions d'un apport théorique et appliqué, mais il ne concerne pas le modèle de simulation de Boltzmann sur réseau développé dans cette thèse. Les détails précis concernant la méthodologie à suivre pour produire les résultats numériques ne sont pas donnés dans ce chapitre. Pour plus de détails, le lecteur est invité à consulter les articles en annexe de la thèse. Afin de mieux illustrer les contributions, les sections des articles correspondants sont indiquées en gras et entre parenthèses.

3.1 Thème 1 : Opérateur de recoloriage

1^{er} objectif Modifier l'opérateur de recoloriage $(\Omega_i^k)^{(3)}$, de l'Éq. (1.52), afin de réduire l'impact sur le modèle des problématiques 1, 2, 3, 4, 5, 6 et 8 données à la page 22.

L'article suivant répond à ce premier objectif :

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, "Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model", *Applied Mathematical Modelling*, vol. 36, n. 5, pp. 2237–2252, 2012.

Une version de cet article soumise au journal *Applied Mathematical Modelling* est donnée à la page 76 de cette thèse.

3.1.1 Contribution théorique

Tout d'abord, l'opérateur de recoloriage d'origine des modèles RK est rappelé pour mieux saisir les changements entre le modèle de Reis et Phillips d'origine et le modèle obtenu après les modifications.

Opérateur de recoloriage d'origine des modèles RK

Cet opérateur a l'objectif de maximiser la quantité de fluide rouge envoyée dans la région du fluide rouge et la quantité de fluide bleu envoyée dans la région du fluide bleu, tout en respectant la conservation de la masse et de la quantité de mouvement totale. Au niveau microscopique, la conservation de la masse et de la quantité de mouvement totale sont équivalentes à :

$$\begin{aligned} N_i^r + N_i^b &= N_i \\ \sum_i N_i^r &= \rho_r \end{aligned} \quad (3.1)$$

La procédure algorithmique est heuristique et est réalisée comme suit. Premièrement, les vecteurs $\vec{c}_i$ sont réordonnés en ordre croissant relativement à leur angle avec le gradient de couleur $\vec{F}$. Le vecteur $\vec{c}_1 = [0, 0]$ est placé au centre des neuf directions. Il est à noter que le gradient de couleur $\vec{F}$ pointe dans la direction du fluide rouge. La deuxième étape consiste à envoyer un maximum de fluide rouge dans la direction la plus proche de $\vec{F}$, toujours sous les contraintes (3.1). En utilisant la quantité de fluide rouge restante, une quantité maximale de fluide rouge est envoyée dans la deuxième direction la plus près de $\vec{F}$, toujours en respectant les contraintes (3.1). Ce processus est répété jusqu'à ce que tout le fluide rouge ait été redistribué. À la fin de la redistribution du fluide rouge, le fluide bleu occupe l'espace restant. De manière générale et d'un point de vue informatique, cet algorithme n'est pas simple à comprendre et à mettre en oeuvre.

Opérateur de Latva-Kokko et Rothman ainsi que l'opérateur modifié

Issu du modèle de D'Ortona et al. [87], le modèle de Latva-Kokko et Rothman [49] propose

de définir l'opérateur de recoloriage comme suit :

$$(\Omega_i^r)^{(3)}(N_i^r) = \frac{\rho_r}{\rho} N_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) N_i^{(e)}(\rho, 0) \quad (3.2)$$

$$(\Omega_i^b)^{(3)}(N_i^b) = \frac{\rho_b}{\rho} N_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) N_i^{(e)}(\rho, 0) \quad (3.3)$$

où les fonctions de distribution du fluide sans couleur sont $N_i^{(e)}$. D'origine, cet opérateur de Latva-Kokko et Rothman est défini pour une valeur constante de α_r et α_b . Alors, pour combiner cet algorithme avec celui de Reis et Phillips, il est important de tenir compte que la vitesse du son isotherme est un paramètre libre dans le modèle de Reis et Phillips. À cet égard, une contribution théorique de cette thèse est l'adaptation de l'opérateur de recoloriage de Latva-Kokko pour une vitesse du son variable. Le nouvel opérateur de recoloriage prend alors la forme suivante :

$$(\Omega_i^r)^{(3)}(N_i^r) = \frac{\rho_r}{\rho} N_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \quad (3.4)$$

$$(\Omega_i^b)^{(3)}(N_i^b) = \frac{\rho_b}{\rho} N_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \quad (3.5)$$

où β est un paramètre libre et $\cos(\varphi_i)$ est le cosinus de l'angle entre le gradient de couleur $\vec{F}$ et la vitesse $\vec{c}_i$. Les fonctions de distribution d'équilibre $N_i^{(e)}$ dans les Éqs. (3.2) et (3.3) sont remplacées par la somme des fonctions d'équilibre de chacun des fluides $N_i^{k(e)}$ et sont évaluées en utilisant une vitesse nulle et la valeur respective de α_k . La valeur de $\cos(\varphi_1)$ doit être nulle pour conserver la masse dans le système. De plus, le paramètre β doit être choisi entre 0 et 1 pour assurer une valeur positive des fonctions de distribution [49]. Le paramètre β influence l'épaisseur de l'interface : le plus petit est cette valeur, le plus large est l'interface.

3.1.2 Contribution appliquée

Pour facilement différencier l'opérateur de recoloriage original de l'opérateur de recoloriage modifié, ils sont respectivement notés opérateur de recoloriage *I* et *II*. En passant de l'opérateur *I* à *II*, les résultats numériques du modèle de Reis et Phillips sont grandement améliorés, et ce, pour plusieurs cas tests. En résumé :

- L'interface planaire (**p. 79, section 3.1**)

L'interface planaire correspond à la simulation de deux fluides de différentes couleurs de part et d'autre d'une interface immobile. Comme l'interface et les fluides sont immobiles,

cet écoulement est en théorie stationnaire. Mathématiquement, la convergence vers un état stationnaire du système discrétisé est atteinte lorsque l'expression suivante est nulle :

$$\max_{\text{Toutes les fonctions de distribution}} \{|(N_i^k)^{(n)} - (N_i^k)^{(n-1)}|\} \quad (3.6)$$

où n dénote le nombre de pas de temps. Plusieurs résultats numériques indiquent que l'opérateur de recoloriage I empêche le précédent critère de converger vers 0, tandis qu'avec l'opérateur de recoloriage II , cette problématique est résolue. Un graphique décrivant cette expression en fonction du temps démontre la meilleure convergence obtenue avec l'opérateur de recoloriage II , et ce, pour plusieurs paramètres différents lors de la simulation d'une interface planaire (**p. 86, Fig. 1**).

D'autre part, le but principal de cette expérience numérique est d'attester la capacité du modèle à créer une tension de surface entre les fluides conforme avec la définition mécanique [17, 41, 42, 62]. Idéalement, il faut que le modèle soit en mesure d'obtenir la tension de surface désirée seulement en ajustant les paramètres libres A_k du modèle. Plusieurs simulations corroborent que la tension de surface prédite par le modèle est la même que celle prédite par la tension de surface mécanique lorsque le ratio de densité est unitaire, et ce, pour les deux opérateurs de recoloriage. Par contre, lorsque le ratio de densité n'est pas unitaire, l'opérateur de recoloriage I introduit une erreur numérique significative par rapport à la tension de surface prédite. En revanche, l'opérateur de recoloriage II génère de meilleurs résultats en terme d'exactitude (**p. 80, Tab. 2**).

- Bulle stable circulaire (**p. 80, section 3.2**)

Cette expérience numérique implique une bulle rouge d'un certain rayon immergée dans un fluide bleu. En trois dimensions, cela correspond plutôt à un cylindre immergé. Le but consiste à vérifier si oui ou non la tension de surface du modèle est conforme avec la tension de surface prédite par l'équation de Laplace [17, 41]. Les expériences numériques démontrent que les deux opérateurs de recoloriage produisent des résultats d'une précision comparable lorsque la densité des deux fluides est égale. Par contre, une erreur importante est obtenue par l'opérateur de recoloriage I lorsque le ratio de densité est non unitaire et que la tension de surface est faible. L'opérateur de recoloriage II donne des résultats valables pour les mêmes paramètres et cela indique que le modèle modifié est valide pour un éventail plus large de paramètres (**p. 86, Tab. 3**).

De plus, l'effet des deux opérateurs de recoloriage sur les courants parasites, phénomène dont l'origine est méconnue, a également été comparé. Ces courants, se trouvant à l'interface entre les fluides, devraient être absents. Dans la littérature des modèles d'automates cellulaires [87], il a été mentionné qu'un opérateur de recoloriage similaire à l'opérateur II peut réduire les courants parasites. Ces résultats sont confirmés pour ce modèle de Boltzmann sur réseau. En effet, l'opérateur II réduit jusqu'à 2 ordres de grandeur ces courants parasites lorsque le ratio de densité est non unitaire et lorsque la tension de surface est faible (**p. 86, Tab. 3**).

D'autre part, tout comme pour l'interface planaire, l'opérateur de recoloriage I ne permet pas la convergence de la solution vers un état stationnaire numérique, tandis que pour l'opérateur II , la convergence est graduelle en fonction du temps.

- Écoulement de Poiseuille à deux phases (**p. 80, section 3.3**)

Cet écoulement se compose de deux couches de fluide, avec des viscosités dynamiques différentes, entre deux plaques immobiles. Les fluides subissent aussi un gradient de pression dans la même direction que la tangente des plaques. Le but de cette expérience numérique est de comparer les profils de la quantité de mouvement analytiques à ceux numériques. Dans les faits, le changement de l'opérateur de recoloriage de I vers II ne contribue pas à améliorer les résultats numériques. Les erreurs sont du même ordre de grandeur pour les deux opérateurs. L'écoulement de Poiseuille à deux phases est tout de même un cas test important à effectuer puisque celui-ci permet de démontrer que ce modèle de Boltzmann sur réseau n'est pas en mesure d'obtenir la solution analytique pour le cas avec variation de densité entre les fluides. La cause de ce phénomène non physique est abordé au quatrième thème de ce chapitre.

- Coalescence des bulles (**p. 81, section 3.4**)

Cette expérience numérique simule la coalescence de deux bulles de densité égale ou différente. En trois dimensions, cela équivaut à une collision de deux cylindres très rapprochés et de longueur infinie. Ce test est utilisé pour évaluer la capacité des opérateurs de recoloriage à effectuer une simulation d'un écoulement instationnaire où une solution finale stationnaire existe sur laquelle il est possible de mesurer et de prédire la tension de surface finale. L'algorithme est suffisamment stable pour que l'opérateur de recoloriage I

puisse simuler un ratio de densité pouvant aller jusqu'à $O(45)$. Par contre, pour les mêmes conditions, l'opérateur de recoloriage II procure une simulation stable jusqu'à un ratio $O(85)$. En ce qui a trait à l'exactitude entre la tension de surface du modèle et celle prédite théoriquement, l'opérateur II est plus précis puisqu'il peut atteindre des niveaux d'exactitude jusqu'à un ordre de grandeur plus élevé (**p. 82, Tab. 5**).

Encore une fois, un autre avantage de l'opérateur de recoloriage II est l'économie qu'il génère en terme de temps de calcul qui est lié au nombre de pas de temps nécessaire pour arriver à un état stationnaire numérique.

- « Lattice pinning » (**p. 82, section 3.5**)

Cette section de l'article propose une nouvelle configuration originale permettant de mesurer la présence et l'intensité du « lattice pinning ». Cette expérience consiste à accélérer horizontalement une particule très petite de fluide rouge initialement immobile et immergée dans le fluide bleu. L'accélération est constante pendant un certain temps, puis devient nulle par la suite. Aucune tension de surface, ratio de densité ou de viscosité cinématique n'est considéré. Cette particule doit alors suivre le comportement du fluide environnant. Dans ce cas, il existe une solution analytique qui exprime la vitesse moyenne et la position de la particule en fonction du temps. Pour les deux opérateurs de recoloriage, les résultats numériques indiquent que les vitesses moyennes horizontales des particules de fluides rouges sont en accord avec la vitesse d'écoulement du fluide local. Par contre, la position des particules n'est pas en accord avec la théorie. Avec ces simulations, il est possible de conclure que l'opérateur de recoloriage I révèle un phénomène physique inexistant puisque la particule ne se déplace pas malgré une vitesse non nulle, tandis que l'opérateur de recoloriage II se comporte beaucoup mieux dans un tel cas (**p. 89, Fig. 4**). À cet égard, avec l'opérateur II , une réduction du paramètre β peut réduire le « lattice pinning » davantage, mais l'interface devient plus large.

L'ensemble de ces contributions théoriques et appliquées répond au premier objectif de la thèse et montre une amélioration du modèle de Reis et Phillips concernant les problématiques 1, 2, 3, 4, 5, 6 et 8 données à la page 22 de cette thèse.

3.2 Thème 2 : La discrétisation du gradient de couleur

2^e objectif Employer une discrétisation isotrope pour calculer le gradient de couleur $\vec{F}$, de l'Éq. (1.65), afin réduire l'impact sur le modèle des problèmes 3, 4, 6, 7 et 8 données à la page 22.

L'article suivant répond à ce deuxième objectif :

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, “Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model”, *Computers & Fluids*, vol. 48, n. 1, pp. 98–112, 2011.

Une version de cet article soumise au journal *Computers & Fluids* est donnée à la page 91 de cette thèse.

3.2.1 Contribution théorique

Le gradient de couleur $\vec{F}$ est un élément important des modèles RK. Il définit la direction normale à l'interface et permet aussi de contrôler la tension de surface entre deux fluides. L'évaluation de $\vec{F}$ correspond à calculer le gradient de la fonction représentant la différence de densité $\Delta \equiv \rho_r - \rho_b$ entre les fluides. Dans le modèle original, une discrétisation non isotrope est utilisée pour évaluer ce gradient numériquement.

Les gradients isotropes ont l'avantage de permettre, dans certaines situations, le calcul très précis de la direction normale à l'interface et ainsi d'améliorer le comportement des interfaces entre les phases. Les sections suivantes décrivent en détail la différence mathématique entre une discrétisation non isotrope et une discrétisation isotrope du gradient (**p. 94, section 2.2.1 et 2.2.2**).

Bref, pour mettre en application les discrétisations isotropes, il suffit de modifier la discrétisation du gradient de couleur original :

$$\vec{F}(\vec{x}) = \sum_i \vec{c}_i \Delta(\vec{x} + \vec{c}_i) \quad (3.7)$$

$$(3.8)$$

par :

$$\vec{F}(\vec{x}) = \sum_i \xi_i \vec{d}_i \Delta(\vec{x} + \vec{d}_i) \quad (3.9)$$

Ces deux dernières expressions correspondent à une sommation pondérée des valeurs discrètes de la fonction à différents points du réseau. Selon l'ordre d'isotropie de la discrétisation, différents choix sont possibles pour les poids ξ_i et les points $\vec{d}_i$ (**p. 95 et 96, Tab. 1 et 2**).

En changeant la discrétisation du gradient de couleur pour une discrétisation isotrope, la tension de surface dans le modèle est ajustée différemment. Au lieu d'utiliser l'Éq. (1.68), l'expression suivante doit être utilisée :

$$\sigma_{th} = \frac{1}{9}(\rho_r^0 + \rho_b^0) \frac{(A_r + A_b)}{\omega_{eff}} \quad (3.10)$$

3.2.2 Contribution appliquée

Pour évaluer l'isotropie du schéma numérique, le meilleur cas test en deux dimensions est celui d'une bulle rouge cylindrique circulaire immergée dans un fluide bleu. Plusieurs centaines de simulations ont été sélectionnées pour étudier l'influence des différents paramètres du modèle sur l'exactitude des résultats. C'est seulement lorsque les résultats sont regardés en moyenne qu'une tendance globale se présente concernant certaines caractéristiques du modèle. En particulier, le choix de la discrétisation du gradient de couleur influence la précision de la loi de Laplace, la forme des bulles, les courants parasites ainsi que le ratio de densité maximal que peut simuler le modèle.

- Bulle stable circulaire : Loi de Laplace (**p. 97, section 3.1**)

Comme pour le premier thème, le but de ce cas test est de vérifier si oui ou non la tension de surface prédite par le modèle est conforme avec la loi de Laplace. Cette loi célèbre prédit le saut de pression à travers une interface en fonction de la courbure de l'interface et de la tension de surface entre les fluides. Dans les faits, selon les résultats obtenus, il y a une tendance très claire démontrant que la loi de Laplace est beaucoup plus précise avec un gradient de couleur isotrope qu'avec un gradient de couleur non isotrope. Par rapport aux différents paramètres des simulations, la tendance peut être résumée comme suit. Lorsque la tension de surface décroît, l'erreur avec la loi de Laplace diminue seulement lorsque l'épaisseur de l'interface augmente ou lorsque l'ordre d'isotropie du gradient de couleur augmente. Ce comportement devient de plus en plus évident lorsque le ratio de densité entre les fluides augmente. L'épaisseur de l'interface

et l'isotropie du gradient de couleur sont deux facteurs clés nécessaires pour simuler avec précision des ratios de densité importants, et ce, pour une large gamme de tensions de surface (**p. 98-101, Fig. 3 à 6**).

- Bulle stable circulaire : Déformation (**p. 99, section 3.2**)

Pour ce cas test, quatre simulations ont été effectuées avec un ratio de densité moyen et une faible tension de surface. La forme des bulles à l'état stationnaire numérique est observée et, selon le choix de la discrétisation pour le gradient, la forme initiale circulaire de la bulle n'est pas nécessairement conservée. Il est évident que plus l'ordre d'isotropie du gradient est élevé, plus la forme circulaire de la bulle est conservée (**p. 106, Fig. 7**).

- Bulle stable circulaire : Courants parasites (**p. 100, section 3.3**)

Les courants parasites peuvent être représentés par la vitesse maximale $\vec{u}$ de l'ensemble du domaine de calcul du fluide sans couleur. Théoriquement, la quantité $\vec{u}$ devrait être nulle sur l'ensemble du domaine de calcul pour ces simulations. Encore une fois, la tendance est très marquée : plus l'isotropie du gradient augmente, plus ces courants parasites sont diminués (**p. 103-105, Fig. 9 à 11**).

D'autre part, les courants parasites peuvent être réduits, de deux ordres de grandeur en choisissant $\beta = 0.7$ au lieu de $\beta = 0.99$, et réduits davantage lorsque l'épaisseur de l'interface augmente (**p. 106, Fig. 12**). Deux avenues sont proposées pour réduire les courants parasites : augmenter l'isotropie de la discrétisation du gradient de couleur ou augmenter l'épaisseur de l'interface, ce qui a pour effet de réduire les erreurs de discrétisation reliées au calcul du gradient et ainsi réduire les courants parasites.

- Bulle stable circulaire : Ratio de densité très élevé (**p. 102, section 3.4**)

Ce dernier cas test a pour but d'explorer la limite du modèle. En fait, tout en conservant une interface de 5 à 6 unités de réseau d'épaisseur, il a été possible pour certains paramètres de simuler un ratio de densité à $O(10000)$ avec une précision de 0.5 % concernant la loi de Laplace (**p. 102, Tab. 7**). Cet exemple ne fonctionne pas sans une discrétisation isotrope du gradient et il illustre bien que l'isotropie du gradient peut augmenter significativement la précision et la stabilité des simulations de la loi Laplace

combinée à un très grand ratio de densité entre les phases.

L'ensemble de ces contributions théoriques et appliquées répond au deuxième objectif de la thèse et montre une nette amélioration du modèle de Reis et Phillips concernant les problématiques 3, 4, 6, 7 et 8 données à la page 22 de cette thèse.

3.3 Thème 3 : Modèle RK à plusieurs phases

3^e objectif Généraliser le modèle afin de simuler des écoulements avec plus de deux phases. Le but est d'améliorer le modèle concernant les problématiques 6, 9 et 10 données à la page 23.

L'article suivant répond à ce troisième objectif :

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, "Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios", *Journal of Computational Physics*, vol. 246, n. 1, pp. 318-342, 2013.

Une version de cet article soumise au *Journal of Computational Physics* est donnée à la page 108 de cette thèse.

3.3.1 Contribution théorique

Plusieurs modifications doivent être apportées au modèle afin de pouvoir simuler plusieurs phases immiscibles. Les composantes des opérateurs doivent être redéfinies pour tenir compte de chacun des fluides et de chacune des paires d'interfaces. Le détail complet des modifications est donné à la section 2 de la page 109. Par contre, ces modifications sont résumées dans les lignes qui suivent.

Tout d'abord, la méthode d'interpolation à deux fluides pour le facteur de relaxation ω_{eff} , de l'Éq. (1.62), est complexe et il est difficile de l'adapter pour la simulation de trois phases ou plus. Effectivement, il convient d'opter pour une approche plus simple telle que des moyennes pondérées par les densités ρ_k de chacun des fluides. Pour ce faire, la fonctionnelle barre est introduite et elle est définie par la moyenne- q pondérée par la densité. Par exemple, pour une variable X_k définie pour chacun des fluides k , la moyenne- q pondérée par la densité de cette

variable est définie par :

$$\overline{X}|_q = \begin{cases} \left(\sum_k \frac{\rho_k (X_k)^q}{\rho} \right)^{\frac{1}{q}}, & q \neq 0 \\ \left(\prod_k (X_k)^{\rho_k} \right)^{\frac{1}{\rho}}, & q = 0 \end{cases} \quad (3.11)$$

Si ν_k est la viscosité cinématique du fluide k , alors, selon la moyenne- q , un choix possible pour le facteur de relaxation effectif est :

$$\omega_{\text{eff}} = \frac{1}{3 \left(\overline{\nu}|_q \right) + \frac{1}{2}} \quad (3.12)$$

Le choix de définir ω_{eff} de cette manière n'est pas la seule option et différentes possibilités sont examinées, soit les moyennes- q avec $q = -1, 0, 1$ et 2 .

Plusieurs phases de différentes densités peuvent se présenter simultanément. Il faut donc définir les différents ratios de densité de la façon suivante pour obtenir des interfaces stables entre les différentes phases :

$$\gamma_{kl} = \frac{\rho_k^0}{\rho_l^0} = \frac{1 - \alpha_l}{1 - \alpha_k} \quad (3.13)$$

Dans ces expressions, un seul des α_k est un paramètre libre. On note par κ l'indice du fluide le moins dense. Généralement, au début d'une simulation, la valeur de α_κ est imposée, il est alors garanti que la relation $0 < \alpha_\kappa \leq \alpha_k < 1$ est vraie pour chacun des fluides k . Cette dernière relation doit obligatoirement être respectée pour éviter des pressions négatives.

Un autre détail important concerne l'évaluation du gradient de couleur. Dans le modèle original de Reis et Phillips, ce dernier est défini comme le gradient de la différence de densité des deux fluides, c'est-à-dire $\vec{F} = \vec{\nabla}(\rho_r - \rho_b)$. Malheureusement, cette approche ne fonctionne pas bien en pratique lorsque plus de deux phases sont en contact. Pour la présente généralisation du modèle à plusieurs phases, le gradient de couleur est alors défini par l'expression suivante :

$$\vec{F}_{kl} = \frac{\rho_l}{\rho} \vec{\nabla} \left(\frac{\rho_k}{\rho} \right) - \frac{\rho_k}{\rho} \vec{\nabla} \left(\frac{\rho_l}{\rho} \right) \quad (3.14)$$

Ce type de vecteur définissant la normale d'une interface est issue d'un modèle de simulation des interfaces et des jonctions de fluides à plusieurs phases [109]. Il est intéressant de noter que l'ordre de complexité par rapport au nombre d'approximation de gradient différent est $O(N)$ où N est le nombre de phases. En d'autres mots, lors de l'évaluation des gradients,

l'information contenue aux sites voisins est utilisée seulement avec une complexité à $O(N)$. Il s'agit d'une nette amélioration par rapport à d'autres modèles [94, 95] où l'ordre de complexité est à $O(N^2)$.

L'opérateur de perturbation doit être modifié pour prendre en compte la tension de surface entre chacune des combinaisons possibles deux à deux d'interfaces :

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \sum_{\substack{l \\ l \neq k}} \frac{A_{kl}C_{kl}}{2} |\vec{F}_{kl}| \left[W_i \frac{(\vec{F}_{kl} \cdot \vec{c}_i)^2}{|\vec{F}_{kl}|^2} - B_i \right] \quad (3.15)$$

où

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (3.16)$$

et

$$C_{kl} = \min \left\{ \eta_1 \frac{\rho_k \rho_l}{\rho_k^0 \rho_l^0}, 1 \right\} \quad (3.17)$$

avec η_1 , un paramètre libre. Des tests avec $\eta_1 = 10^6$ donnent de bons résultats. La fonction C_{kl} est un facteur de concentration qui limite l'activation de la tension de surface à une interface k - l seulement lorsque les deux fluides k et l sont présents.

Afin d'ajuster la tension de surface entre deux fluides k et l , l'Éq. (3.10) est modifiée. Cette nouvelle relation est la suivante :

$$\sigma_{kl} = \frac{1}{9} \frac{(A_{kl} + A_{lk})}{\omega_{\text{eff}}} \quad (3.18)$$

Dans cette dernière relation, la différence principale entre ce modèle et le modèle à deux phases provient de la normalisation du gradient de couleur par la densité totale ρ du fluide sans couleur.

L'opérateur de recoloriage doit aussi être modifié pour assurer l'immiscibilité des différents fluides à travers chacune des paires possibles d'interfaces, et ce, tout en conservant la masse de chacun des fluides k et la quantité de mouvement totale du fluide sans couleur. Adapté pour permettre la variation de densité entre les phases, cet opérateur est une combinaison des idées essentielles de Latva-Kokko et Rothman [49] et Halliday et al. [94] :

$$(\Omega_i^k)^{(3)}(N_i^k) = \frac{\rho_k}{\rho} N_i^k + \sum_{\substack{l \\ l \neq k}} \beta_{kl} \frac{\rho_k \rho_l}{\rho^2} \cos(\varphi_i^{kl}) N_i^{(e)}(\rho, 0, \bar{\alpha}|_{q=1}) \quad (3.19)$$

où β_{kl} est un paramètre libre contrôlant l'épaisseur des interfaces $k-l$. La variable φ_i^{kl} correspond à l'angle entre le gradient de couleur $\vec{F}_{kl}$ et la direction du réseau $\vec{c}_i$. La fonction d'équilibre du fluide sans couleur $N_i^{(e)}$ est évaluée avec une vitesse nulle et la moyenne $\bar{\alpha}|_{q=1}$. Il est important de prendre la moyenne avec $q = 1$, sinon le modèle n'est pas stable. De plus, il faut noter que $\beta_{kl} = \beta_{lk}$ pour conserver la masse et la quantité de mouvement totale.

La prochaine et dernière modification est optionnelle et valide seulement pour trois phases. Elle améliore le comportement du modèle au point triple de contact des fluides. En effet, il existe un possible équilibre statique des angles de contacts θ_{kl} entre les fluides lorsque les tensions de surface forment un triangle de Neumann (**p. 112, Fig. 1**). En suivant les idées de Spencer et al. [95], ces angles de contact statiques sont seulement respectés lorsqu'une relation spéciale pour β_{kl} est utilisée. Elle est donnée par :

$$\beta_{kl} = \begin{cases} \beta^0, & kl \text{ avec } \theta_{\max} \\ \beta^0 (1 + c_{triple} (\sin(\pi - \theta_{\max} - \theta_{kl}) - 1)), & \text{autrement} \end{cases} \quad (3.20)$$

où β^0 est une constante entre 0 et 1 contrôlant l'épaisseur globale des trois interfaces et

$$c_{triple} = \min \left\{ \eta_2 \frac{\rho_r \rho_g \rho_b}{\rho^3}, 1 \right\} \quad (3.21)$$

est une fonction qui varie aussi entre 0 et 1. Le paramètre η_2 est un paramètre libre. Des tests avec $\eta_2 = 35$ donnent de bons résultats.

3.3.2 Contribution appliquée

Différents cas tests ont été étudiés et développés pour évaluer à la fois certaines propriétés qualitatives et quantitatives de ce modèle de simulation à plusieurs phases.

- Décomposition spinodale à plusieurs phases (**p. 112, section 3.1**)

La décomposition spinodale peut être vue comme le processus physique de la séparation des phases d'une émulsion. Ce cas test étudie le comportement d'une mixture de plusieurs phases initialement placées de manière aléatoire dans un domaine de calcul. C'est une expérience numérique servant à analyser la stabilité du présent modèle de Boltzmann sur réseau. Tous les modèles construits pour la simulation de plusieurs phases immiscibles doivent être en mesure de réussir la décomposition spinodale. Bien que les résultats sont qualitatifs, ils permettent de tester la robustesse du code numérique et de voir l'aggrégation des différents fluides. Dans les faits, les résultats montrent que

l'algorithme est stable et que la décomposition spinodale a effectivement lieu, et ce, même pour des ratios de densité et de viscosité cinématique élevées à $O(1000)$ et $O(100)$ respectivement (**p. 113, Fig. 2 à 5**).

- Interfaces planaires à plusieurs phases (**p. 113, section 3.2**)

Le but de ce cas test est de vérifier si le modèle est en mesure de simuler avec précision la tension de surface entre plusieurs fluides de différentes propriétés situés de part et d'autre d'interfaces planaires. En théorie, la tension de surface est indépendante de la viscosité du fluide. Toutefois, dans ce modèle, pour définir une tension de surface spécifique entre deux fluides au moyen de l'Éq. (3.18), la viscosité cinématique du fluide doit être pris en compte parce que le facteur de relaxation ω_{eff} dépend de ce paramètre.

Dans les études antérieures [17, 36, 96], l'exactitude de la tension de surface du modèle a été vérifiée uniquement pour des ratios de viscosité cinématique unitaire et n'a pas été vérifiée pour des ratios de viscosité cinématique variables entre les phases. Cette question est adressée et il est montré que le modèle simule avec précision la tension de surface, c'est-à-dire que l'Éq. (3.18) fonctionne correctement quand il y a simultanément des ratios de densité et de viscosité cinématique entre des interfaces planaires. Des ratios de densité jusqu'à $O(900)$ et des ratios de viscosité cinématique jusqu'à $O(50)$ ont été simulés. Dans ces simulations, le paramètre $\beta_{kl} = 1$. Cependant, il peut être abaissé afin d'obtenir une interface plus large, ce qui conduit à une meilleure stabilité et augmente encore plus les ratios de densité et de viscosité cinématique possibles. Les différentes moyennes- q pour les méthodes d'interpolations ont été testées et il a été conclu que c'est en utilisant $q = 1$ et $q = 2$ que les meilleurs résultats sont obtenus (**p. 125, Tab. 3 et 4**).

D'autre part, une nouvelle méthode pour initialiser les écoulements à plusieurs phases utilisant un modèle de type RK a été proposée. En effet, la condition initiale usuelle est la fonction d'équilibre qui, pour ce type de problème, peut entraîner une instabilité, car les champs de la fonction de distribution du fluide sans couleur N_1 et/ou les densités des fluides ρ_k sont initialement discontinus. Il est alors préférable d'initialiser ces champs avec des fonctions plus continues. Une possibilité est décrite par Mei et al. [110]. Cette approche est adaptée pour le contexte des écoulements à plusieurs phases. Elle consiste donc à résoudre les équations du modèle pour un certain nombre de pas de temps avec $A_{kl} = 0$ tout en imposant $\vec{u} = 0$ dans les fonctions de distribution d'équilibre.

- Loi de Laplace à plusieurs phases (**p. 115, section 3.3**)

Cette expérience numérique implique l'évolution d'un écoulement à trois phases où la solution à l'état d'équilibre correspond à une configuration analogue à celle de la loi de Laplace à deux phases. Ce cas test a été spécialement développé pour vérifier le respect de la loi de Laplace lors de la généralisation du modèle de deux à trois phases. En effet, cette expérience est utilisée pour évaluer la capacité du modèle à réaliser une simulation instationnaire, où le comportement qualitatif de l'évolution de l'écoulement peut être prédit. Un état stable et final existe pour cet écoulement sur lequel il est possible de mesurer et de prédire la tension de surface (**p. 115, Fig. 7**). Pour le modèle développé ici, les erreurs relatives avec la loi de Laplace à trois phases sont faibles, même pour un ratio de densité $O(1000)$ et un ratio de viscosité cinématique $O(100)$ (**p. 116, Tab. 6**).

De plus, il a été démontré que le choix du gradient de couleur lors du passage d'un modèle à deux phases à un modèle à plusieurs phases est très important. Effectivement, si un gradient de couleur de la même forme que le modèle original est utilisé, c'est-à-dire $\vec{F}_{kl} = \vec{\nabla}(\rho_k - \rho_l)$, il y a des écoulements non physiques de fluides dans les directions tangentielles aux interfaces. Ce phénomène est évidemment faux et indésirable, et, en fonction du type simulation, peut facilement compromettre les résultats (**p. 116, Fig. 8**). Avec le gradient de couleur $\vec{F}_{kl}$ tel que défini dans l'Éq. (3.14), ce comportement non physique est évité.

- Loi de Laplace-Young (**p. 116, section 3.4**)

Le but de ce cas test est de vérifier l'aptitude du modèle à simuler correctement les angles de contact statiques à la jonction triple des fluides en fonction des tensions de surface pour un écoulement à trois phases. Ce test numérique est le seul qui vérifie de manière quantitative le comportement du modèle pour un écoulement à trois phases. Un objectif complémentaire est de définir un indice de qualité simple et robuste pour mesurer la précision par rapport aux angles de contact statiques d'un modèle de simulation à plusieurs phases. À partir des résultats, il est possible de déduire que ce modèle de Boltzmann sur réseau est compatible avec la solution analytique de la loi de Laplace-Young parce que l'ordre de convergence de l'indice de qualité est d'environ 1, même pour des ratios de densité et de viscosité cinématique allant jusqu'à $O(1000)$ et $O(100)$ respectivement (**p. 125, Tab. 7 à 9**). Il a été conclu que la loi de Laplace-Young est

correctement intégrée dans ce modèle, autrement dit, l’ajustement des tensions de surface du modèle suffit à atteindre les angles de contact théoriques entre les fluides à l’état stationnaire.

Il est important de souligner que les modèles de Boltzmann sur réseau sont généralement considérés comme précis au second ordre [33], mais cela n’est vrai que pour un écoulement à une phase et ne l’est pas nécessairement pour les écoulements à plusieurs phases. De plus, il convient de noter que la méthode de Boltzmann sur réseau de base se comporte comme une méthode de premier ordre en temps à cause des erreurs de compressibilité [33]. Il n’est pas surprenant que le schéma soit du premier ordre en terme de l’indice de qualité puisque cet indice n’est pas une variable primitive du résolveur.

- Écoulement de Couette à plusieurs phases (**p. 118, section 3.5**)

Le but de ce test numérique est d’étudier la capacité du modèle à simuler un écoulement avec des viscosités dynamiques variables. L’écoulement de Couette à plusieurs phases consiste en plusieurs couches de fluide entre deux plaques infinies et mobiles. Une contribution a été d’obtenir une solution analytique pour cet écoulement à N phases. Aussi, il a été démontré que le choix de la moyenne- q pour la méthode d’interpolation des viscosités cinématiques des fluides peut avoir un impact positif sur l’exactitude de la solution numérique. Clairement, les résultats indiquent que la moyenne- q avec $q = -1$ procure de meilleurs résultats que les autres moyennes. Par la suite, l’exactitude diminue à mesure que q augmente (**p. 126, Tab. 10**). Cela est intrigant puisque les simulations avec les interfaces planaires donnent de meilleurs résultats avec $q = 2$. Il existe encore de nombreux facteurs qui ne sont pas pris en compte et la précision du schéma en fonction de la méthode d’interpolation pour la viscosité cinématique semble dépendre beaucoup du type d’écoulement. Ainsi, il est possible de conclure que d’autres choix pour la méthode d’interpolation pourraient être mieux adaptés pour d’autres situations données.

Il a été démontré précédemment que les modèles RK ne sont pas en mesure de capturer la discontinuité dans le profil de la quantité de mouvement (ou le profil de vitesse) de l’écoulement de Poiseuille à plusieurs phases avec variation de densité [97]. Puisque l’écoulement de Poiseuille est généralement simulé en utilisant des termes sources pour simuler un gradient de pression, cela complique l’analyse des résultats par rapport à un écoulement de Couette conventionnel. Le modèle proposé dans cet article n’est pas plus en mesure de capturer la discontinuité dans le profil de la quantité de

mouvement de l'écoulement de Couette à plusieurs phases (**p. 122, Fig. 16**). Capturer cette discontinuité avec ce schéma numérique constitue le prochain objectif de cette thèse.

- Réduction du nombre de fonctions de distribution (**p. 122, section 4**)

Ce modèle de Boltzmann sur réseau à plusieurs phases tel que présenté suggère d'utiliser un ensemble de fonctions de distribution pour chacun des fluides. Par contre, il n'est pas nécessaire de procéder ainsi. En effet, il est possible de réduire le nombre d'ensembles de fonctions de distribution nécessaire. Conceptuellement, seulement la fonction de distribution du fluide sans couleur ainsi que les champs de densité de chacun des fluides k sont nécessaires. Cela permet de réduire considérablement la quantité de mémoire requise pour simuler un système à plusieurs phases.

L'ensemble de ces contributions théoriques et appliquées répond au troisième objectif de la thèse et constitue une généralisation ou une amélioration du modèle de Reis et Phillips concernant les problématiques 6, 9 et 10 données à la page 23 de cette thèse.

3.4 Thème 4 : Le problème de discontinuité

- | | |
|-------------------------------|--|
| 4^e objectif | Capturer la discontinuité du champ de la quantité de mouvement présent dans l'écoulement de Couette à plusieurs phases avec ratio de densité non unitaire. Le but est d'améliorer le modèle concernant les problématiques 6, 9 et 11 données à la page 23. |
|-------------------------------|--|

L'article suivant, à la page 128 de cette thèse, répond à ce quatrième objectif :

Sébastien Leclaire, Nicolas Pellerin, Marcelo Reggio and Jean-Yves Trépanier, "Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models", manuscript submitted to *International Journal of Multiphase Flow* in February 2013.

3.4.1 Contribution théorique

Il y a été démontré précédemment que les modèles RK ne sont pas en mesure de capturer la discontinuité dans le profil de la quantité de mouvement présent dans l'écoulement de

Couette à plusieurs phases. Idéalement, une simple modification devrait être mise au point pour permettre aux modèles RK de capturer cette discontinuité. Pour atteindre cet objectif, il est proposé de modifier la fonction d'équilibre du modèle original de la manière suivante :

$$N_i^{k(e)}(\rho_k, \vec{u}, \alpha_k) = \rho_k \left(\phi_i^k + W_i \left[\frac{3}{c^2} \vec{c}_i \cdot \vec{u} + \frac{9}{2c^4} (\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2c^2} (\vec{u})^2 \right] \right) + \Phi_i^k \quad (3.22)$$

où l'expression Φ_i^k est ajoutée à la fonction d'équilibre originale. Elle est définie comme suit :

$$\Phi_i^k = \begin{cases} -3 \bar{\nu}|_q (\vec{u} \cdot \vec{\nabla} \rho_k) / c^2, & i = 1 \\ +4 \bar{\nu}|_q (\mathbf{G}^k : \vec{c}_i \otimes \vec{c}_i) / c^4, & i = 2, 4, 6, 8 \\ +1 \bar{\nu}|_q (\mathbf{G}^k : \vec{c}_i \otimes \vec{c}_i) / c^4, & i = 3, 5, 7, 9 \end{cases} \quad (3.23)$$

où $\otimes$ est le produit tensoriel et le symbole « : » représente la contraction tensorielle. Le tenseur $\mathbf{G}^k$ est défini par :

$$\mathbf{G}^k = 1/8 \left[(\vec{u} \otimes \vec{\nabla} \rho_k) + (\vec{u} \otimes \vec{\nabla} \rho_k)^T \right] \quad (3.24)$$

Cette procédure est issue du modèle « Free Energy » de Holdych et al. [102]. Elle est adaptée ici pour ce modèle RK. En effet, Holdych et al. ont remarqué qu'en changeant les fonctions de distribution d'équilibre de leur modèle, l'équation de Boltzmann sur réseau devient alors compatible avec les équations Navier-Stokes sous l'hypothèse d'un faible gradient de pression et dans la limite des petits nombres de Mach et de Knudsen, et ce, même avec un large gradient de densité. Ils ont aussi démontré que sans le terme additif Φ_i^k , un gradient de densité non nul fait en sorte de diverger, dans la limite macroscopique, les équations de Boltzmann sur réseau des équations de Navier-Stokes. Les fonctions d'équilibre n'ont pas été données explicitement dans l'article de Holdych et al. [102]. D'autres auteurs [111] ont explicitement présenté les fonctions d'équilibres à utiliser dans le cas d'un fluide à un seul composant avec variation de densité et avec une équation d'état « non idéale ».

En bref, pour adapter ces idées au modèle RK, les expressions Φ_i^k sont définies de manière à ce que la fonction d'équilibre du fluide sans couleur soit la même, dans les régions de phase pure, que celle dans le modèle de Holdych et al. [102]. La seule différence concerne le tenseur de pression, où dans ce modèle RK, une équation d'état isothermale différente est utilisée dans chacune des régions de phase pure. Ces modifications visent à corriger le problème de discontinuité dans l'écoulement de Couette et cette approche n'a jamais été testée auparavant pour les modèles RK.

3.4.2 Contribution appliquée

- Écoulement de Couette à deux phases (**p. 132, section 3**)

Les profils de la quantité de mouvement analytique et numérique sont comparés en utilisant le modèle original ($\Phi_i^k = 0$) et le modèle modifié ($\Phi_i^k \neq 0$). Les résultats indiquent sans équivoque que le modèle modifié est en mesure de capturer la discontinuité tandis que le modèle original ne capture pas cette discontinuité lorsqu'il y a une variation de densité entre les phases (**p. 135-137, Tab. 3 à 5**). Les tests montrent aussi que le schéma est stable et précis, même avec un ratio simultané de densité et de viscosité cinématique de $O(1000)$ et de $O(100)$ respectivement.

De plus, pour tous les tests, l'erreur en norme L^2 se rapportant à la quantité de mouvement diminue en fonction du nombre de sites dans le réseau. La précision du schéma en espace concernant la quantité de mouvement est d'ordre 2 sans variation de densité et d'ordre 1 lorsqu'il y a une discontinuité avec variation de densité entre les phases. Il est clair que le modèle proposé est compatible avec la solution analytique de l'écoulement de Couette à plusieurs phases en présence de ratios de densité.

Dans l'ensemble, l'approche présentée élargit la validité de ce modèle RK. De plus, il y a tout lieu de s'attendre à ce que cette technique fonctionne également pour les autres modèles RK [17, 36, 38, 39, 85, 96, 97], qui souffrent également du problème de discontinuité.

L'ensemble de ces contributions théoriques et appliquées répond au quatrième objectif de la thèse et procure une amélioration du modèle de Reis et Phillips concernant les problématiques 6, 9 et 11 données à la page 23 de cette thèse.

3.5 Thème 5 complémentaire : Les gradients isotropes d'ordre spatial élevé

5^e objectif Généraliser la théorie des gradients pour des ordres spatiaux et isotropes élevés.

L'article suivant, à la page 140 de cette thèse, répond à ce cinquième objectif :

Sébastien Leclaire, Maud El-Hachem, Marcelo Reggio and Jean-Yves Trépanier, “High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs”, manuscript submitted to *Journal of Scientific Computing* in September 2012.

3.5.1 Contribution théorique

Basé sur le concept des différences finies centrées et isotropes, ce travail généralise à un ordre spatial supérieur, en 2D et en 3D, l'opérateur gradient isotrope. Une méthode est utilisée pour obtenir un ensemble d'équations à partir duquel il est possible de déduire les poids et les points nécessaires afin d'obtenir une approximation numérique du gradient d'un ordre spatial et isotrope élevé (**p. 141, section 2**).

L'ordre spatial (S) contrôle l'ordre de précision spatial de la **norme** et de la **direction** du gradient, tandis que l'ordre d'isotropie (I) contrôle l'ordre de précision spatial de la **direction** du gradient. Une liste utile des poids et des points nécessaires à la construction de différents gradients d'un ordre spatial et isotrope élevé est donnée (**p. 144 et 145, Tab. 1 et 2**).

D'autre part, différents algorithmes de convolution sont utilisés pour calculer efficacement des gradients de fonctions ou d'images. Aussi, différentes plates-formes sur CPU et GPU sont étudiées, tel que : MATLAB de base, le plug-in Jacket [112] pour MATLAB et CUDA. Il est important de noter que cette partie de l'article, concernant les algorithmes de convolution, n'est pas discutée dans cette thèse puisqu'il s'agit d'une contribution issue majoritairement d'un travail de collaboration et non pas d'une contribution développée à majorité significative par l'auteur de cette thèse.

3.5.2 Contribution appliquée

- Ordre de précision (**p. 148, section 3.1**)

Trois tests numériques sont développés afin de démontrer que les discrétisations des gradients proposées permettent d'obtenir l'ordre spatial et isotrope prédit par la théorie.

Le premier test évalue l'ordre de précision spatial (S) des gradients lors de l'évaluation du gradient d'un polynôme de haut degré et à plusieurs variables ; le second test implique l'évaluation d'une fonction sinusoïdale à plusieurs variables pour mesurer l'ordre de précision spatial (S) et le troisième test valide simultanément l'ordre spatial (S) et isotrope (I) des gradients à l'aide d'une fonction unidimensionnelle qui a subi une rotation.

C'est ce dernier cas test qui est le plus intéressant. Effectivement, il permet de démontrer qu'à mesure que l'espacement entre les points de la discrétisation diminue, l'erreur associée à la norme du gradient peut seulement être réduite à un taux plus élevé si l'ordre spatial (S) du gradient est augmenté. Par contre, l'erreur par rapport à la direction du gradient peut être réduite à un taux plus élevé si l'ordre spatial (S) est augmenté, ou bien, si l'ordre isotrope (I) est augmenté.

Tous les tests numériques démontrent que l'ordre de précision spatial et isotrope des gradients numériques sont les mêmes que ceux prédits par la théorie (**p. 149-151, Tab. 6 à 11**). Cela confirme que les poids et les points des différentes discrétisations sont adéquatement définis.

L'ensemble de ces contributions théoriques et appliquées répond au cinquième et dernier objectif de la thèse.

CHAPITRE 4

DISCUSSION GÉNÉRALE

Ce chapitre remet en perspective les contributions des quatres premiers thèmes apportées au modèle de Reis et Phillips. Les problématiques sont rappelées et les solutions apportées y sont expliquées au sens de comment elles améliorent le présent modèle. De plus, les problématiques non résolues sont aussi détaillées. L'ordre de présentation est le même que celui utilisé dans les chapitres précédents. Pour le cinquième thème, il s'agit d'une contribution complémentaire et il ne concerne pas les méthodes de Boltzmann sur réseau. Il n'est donc pas discuté dans ce chapitre.

4.1 Discussion des problématiques résolues et améliorées

1. Par rapport à l'algorithme dans son ensemble, l'opérateur de recoloriage $(\Omega_i^k)^{(3)}$, de l'Éq. (1.52), est difficile à programmer.

Cette problématique est étudiée au thème 1. Effectivement, la procédure algorithmique originale de l'opérateur de recoloriage exige tout d'abord la programmation d'un algorithme de tri. Ensuite, la redistribution des fluides est effectuée selon les contraintes de conservation de la masse et de la quantité de mouvement. Ces caractéristiques contribuent à la complexité de l'algorithme dans son ensemble. En adaptant l'opérateur de Latva-Kokko et Rothman [49] pour le modèle de Reis et Phillips, cette problématique est résolue puisque la programmation des Éqs. (3.4) et (3.5) est simplifiée et les contraintes de conservation de la masse et de la quantité de mouvement sont automatiquement respectées.

2. L'interface souffre du « lattice pinning ». Ce problème peut se produire à l'interface de deux fluides lorsque la convection dans l'écoulement est faible. Dans la pratique, cela signifie que l'interface peut ne pas bouger et devient « épinglée » au réseau, et ce, aussi longtemps que la convection n'est pas assez importante.

Cette problématique est étudiée au thème 1. Tel que conjecturé par les auteurs Reis et Phillips [17], il a été démontré que ce modèle souffre de ce problème lorsque l'interface est simulée avec l'opérateur de recoloriage original. L'adaptation de l'opérateur de

Latva-Kokko et Rothman a considérablement réduit le « lattice pinning » et peut être réduit davantage en augmentant l'épaisseur de l'interface entre les fluides. Cela ajoute une nouvelle caractéristique du modèle puisqu'il n'est pas possible d'ajuster l'épaisseur de l'interface avec l'opérateur de recoloriage original.

3. Le modèle est affecté par des « courants parasites » artificiels aux interfaces entre les fluides. Ces courants parasites devraient être théoriquement nuls, mais ils perturbent le champ de vitesse $\vec{u}$ de manière non physique. Les courants parasites sont généralement faibles, mais diminuent néanmoins la stabilité et la précision du schéma numérique.

Cette problématique est étudiée aux thèmes 1 et 2. Dans le cas d'une bulle circulaire avec tension de surface non nulle, l'adaptation de l'opérateur de Latva-Kokko et Rothman pour le modèle de Reis et Phillips a permis de réduire ces courants parasites. En fait, l'intensité de ces courants peut être contrôlée en ajustant l'épaisseur de l'interface entre les fluides. Plus l'épaisseur de l'interface augmente, plus les courants parasites diminuent. De plus, il a été montré que l'augmentation de l'isotropie de la discrétisation du gradient de couleur réduit également ces courants parasites.

4. L'interface est très mince et l'épaisseur de l'interface n'est pas ajustable. Le fait que l'interface soit très mince, deux à trois unités de réseau, engendre certaines difficultés étant donné que la théorie concernant le tenseur des contraintes capillaires est développée en supposant une interface diffuse. Étant donné les quasi-discontinuités dans les champs de densités des fluides aux interfaces, le calcul du vecteur normal $\vec{F}$ à l'interface à l'aide de méthode numérique est donc peu précis.

Cette problématique est étudiée aux thèmes 1 et 2. La possibilité d'ajuster l'épaisseur de l'interface avec l'opérateur de recoloriage modifié réconcilie ce schéma de Boltzmann sur réseau avec la théorie. En effet, le développement du tenseur des contraintes capillaires émet l'hypothèse d'une interface diffuse. Cette dernière est mieux respectée avec le nouvel opérateur de recoloriage. D'autre part, le calcul de la direction normale à l'interface est plus précis avec les discrétisations isotropes du gradient.

5. Dans le cas d'écoulements théoriquement stationnaires, la convergence de la solution numérique de l'algorithme vers un état stationnaire numérique n'est généralement pas atteinte. Il y a donc un « bruit » dans l'algorithme dont la cause exacte est difficilement identifiable.

Cette problématique est étudiée au thème 1. L'opérateur de recoloriage modifié pour le modèle de Reis et Phillips réduit ou élimine certains bruits numériques du modèle original. Effectivement, lorsqu'une solution théorique stationnaire existe, comme pour les interfaces planaires ou les bulles immobiles, l'algorithme modifié converge généralement vers un état stationnaire numérique à la précision machine, et ce, pour un éventail beaucoup plus large de paramètres.

6. Le modèle n'est pas en mesure de simuler des ratios de densité élevés, et ce, même pour des cas tests théoriquement stationnaires.

Cette problématique est étudiée aux thèmes 1, 2, 3 et 4. Le changement de l'opérateur de recoloriage a permis d'augmenter la stabilité du modèle puisque des ratios de densité plus élevés peuvent être simulés avec le cas test de la loi de Laplace. Aussi, les gradients isotropes permettent de réduire les courants parasites et cela augmente alors la stabilité du modèle et permet la simulation de ratios de densité plus élevés pour la loi de Laplace. Pour le modèle à trois phases et certains paramètres, le schéma numérique est compatible avec la loi de Laplace-Young même pour des ratios de densité élevés. Avec la fonction d'équilibre modifiée, l'écoulement de Couette à plusieurs phases peut être simulé même avec des ratios de densité élevés. Ces cas tests peuvent être simulés pour des ratios de densité jusqu'à $O(1000)$.

7. Dans ce modèle, des bulles initialement circulaires ont tendance à se déformer et à adopter une forme anisotrope à l'état stationnaire.

Cette problématique est étudiée dans le thème 2. En effet, pour réduire ou corriger ce comportement non physique du modèle, l'utilisation d'une discrétisation isotrope pour le gradient de couleur est nécessaire. Ce type de discrétisation permet un calcul beaucoup plus précis de la direction normale à l'interface et cela permet d'éliminer le problème de déformation des bulles.

8. Le modèle est imprécis lorsque la tension de surface est faible.

Cette problématique est étudiée aux thèmes 1 et 2. Deux hypothèses sont avancées pour expliquer ce phénomène. Sans l'opérateur de recoloriage modifié, l'interface est très mince entre les fluides et il devient alors difficile de calculer précisément la norme du

gradient de couleur. Lorsque la tension de surface est faible, la perturbation résultante à l'interface est également faible tandis que les erreurs de calcul reliées au gradient de couleur sont constantes. À une certaine limite, les erreurs de calcul deviennent prédominantes. Avec l'opérateur de recoloriage modifié l'interface est plus large, ce qui permet ainsi de diminuer les erreurs de calcul relié au gradient de couleur. Similairement, avec la discrétisation isotrope, c'est le calcul de la direction du gradient qui est plus précis et cela évite la déformation des bulles. Par conséquent, la loi de Laplace est plus exacte avec une bulle circulaire qu'avec une bulle déformée.

9. Le comportement du modèle dans le cas mixte de variation de densité et de viscosité est pratiquement inconnu.

Cette problématique est étudiée aux thèmes 3 et 4. Les cas tests suivants ont démontré qualitativement et quantitativement que le modèle est adapté pour simuler plusieurs phases avec variation mixte de densité et viscosité : la décomposition spinodale, les interfaces planaires, la loi de Laplace, la loi de Laplace-Young et l'écoulement de Couette à plusieurs phases.

10. Le modèle est limité à la simulation d'écoulements à deux phases. La généralisation du modèle pour simuler trois phases immiscibles et plus n'est pas directe.

Cette problématique est étudiée au thème 3. Effectivement, pour généraliser le modèle à plusieurs phases, il faut changer la méthode d'interpolation de la viscosité, les opérateurs de perturbation et de recoloriage ainsi que la définition du gradient de couleur. Ce dernier changement exige une nouvelle expression pour la tension de surface du modèle. De plus, afin d'intégrer la loi de Laplace-Young à trois phases, il faut ajuster l'épaisseur des interfaces avec une relation spéciale.

11. Lorsqu'il y a un ratio de densité non unitaire entre les fluides, le modèle n'est pas en mesure de simuler correctement l'écoulement de Couette à plusieurs phases. Il y a une discontinuité dans le champ de la quantité de mouvement théorique qui n'est pas capturée par le schéma numérique.

Cette problématique est étudiée au thème 4. Avec la modification de la fonction d'équilibre, il est possible de rendre compatible ce schéma de Boltzmann sur réseau avec la solution analytique de l'écoulement de Couette en dépit d'une variation de densité

entre les phases.

4.2 Discussion des problématiques non résolues

12. Le modèle n'est pas en mesure de simuler des ratios de viscosité très élevés, c'est-à-dire $> O(100)$, même pour des cas tests théoriquement stationnaires.

Avec toutes les modifications, les aptitudes de ce modèle de Boltzmann sur réseau concernant la simulation de ratios de viscosité élevés sont similaires au modèle de Reis et Phillips original. Il est difficile d'obtenir des ratios de viscosité très élevés entre les phases. À l'exception de l'écoulement de Poiseuille ou de Couette, tous les autres cas tests effectués dans cette recherche sont limités à des ratios de viscosité inférieurs à $O(100)$.

13. Le modèle a été initialement formulé pour deux dimensions spatiales. La généralisation à trois dimensions n'est pas directe.

En effet, la généralisation à trois dimensions de ce modèle n'est pas complète. Liu et al. [85] suggèrent une approche pour obtenir l'opérateur de perturbation sur le réseau D3Q19. Ce n'est pas explicitement mentionné dans leur article, mais ce modèle souffre du problème de discontinuité. Il faut donc trouver une généralisation pour les réseaux 3D de la fonction d'équilibre corrigée développée au thème 4 de cette thèse.

14. La condition d'écoulement à faible nombre de Mach est de plus en plus difficile à respecter lorsque le ratio de densité entre les fluides augmente. Effectivement, selon l'Éq. (1.59) concernant les écoulements avec ratio de densité non unitaire, la vitesse du son dans le fluide dense peut être très petite limitant ainsi la vitesse maximale que peut atteindre le fluide pour respecter un faible nombre de Mach.

Cette problématique est sans doute la plus limitante pour ce modèle. Ce dernier exploite la possibilité d'utiliser différentes vitesses du son isothermale pour chaque phase. Dans la LBM, il est connu que la valeur $\sqrt{1/3}$ pour la vitesse du son isothermale est seulement une possibilité et que c'est la valeur la plus commune [33]. La vitesse du son isothermale est ajustée avec le poids α_k du réseau qui est celui associé à la vitesse microscopique nulle [24]. Différentes vitesses du son isothermale signifient que les

équations de Navier-Stokes sont récupérées dans chacune des phases avec leur propre vitesse du son isothermale. En fait, ces vitesses du son isothermale ne servent que de paramètres « pseudo-compressible » pour relaxer la solution du système de la LBM vers la solution incompressible et visqueuse de Navier-Stokes [24]. Examinons la condition d'incompressibilité de la LBM dans le contexte de ce modèle. Puisque la vitesse du son isothermale dans la phase dense (fluide rouge) est plus petite que celle dans la phase légère (fluide bleu), le nombre de Mach à chaque position du domaine de calcul de l'écoulement est plus petit ou approximativement égal à :

$$\text{Ma} \approx \frac{|\vec{u}|}{c_s^r} \quad (4.1)$$

Pour vérifier la limite incompressible, il faut alors conserver un faible nombre de Mach dans l'écoulement, par exemple plus petit que $\text{Ma} = 0.1$. Cette condition mène à la contrainte suivante :

$$|\vec{u}| \leq (0.1)c_s^r = (0.1)\sqrt{3/5(1 - \alpha_r)} = (0.1)\frac{\sqrt{3/5(1 - \alpha_b)}}{\sqrt{\gamma}} \quad (4.2)$$

Il est possible de remarquer que dans le système d'unité de la LBM, la vitesse maximale que le fluide peut atteindre est inversement proportionnelle à la racine carrée du ratio de densité. Il est important de toujours respecter cette dernière contrainte pour obtenir une simulation stable respectant aussi la limite d'incompressibilité de la LBM.

CHAPITRE 5

CONCLUSION ET RECOMMANDATIONS

Les schémas numériques ont pour but de résoudre les équations théoriques de modèles simplifiés censés représenter la réalité. Chaque modèle ou schéma numérique a des avantages et des inconvénients par rapport aux autres. Le choix d'un modèle plutôt qu'un autre dépend généralement du problème à résoudre. Tout au long de cette recherche doctorale, le modèle de Reis et Phillips [17] a été étudié à l'aide de plusieurs cas tests qualitatifs et surtout analytiques et quantitatifs. En résumé, les contributions théoriques et appliquées des quatre thèmes principaux de cette thèse ont permis d'étendre la validité de ce modèle de Boltzmann sur réseau.

Le premier thème a démontré que l'adaptation de l'opérateur de recoloriage de Latva-Kokko et Rothman permet de converger les solutions numériques vers l'état stationnaire théorique lorsqu'elles existent, d'améliorer la stabilité numérique et la précision des solutions pour un éventail de paramètres plus large, de réduire de façon significative l'intensité des courants parasites et de diminuer le problème du « lattice pinning ». Le deuxième thème a introduit la discrétisation isotrope du gradient de couleur permettant la réduction des courants parasites, la conservation de la forme circulaire des bulles et, pour la loi de Laplace, d'élargir la fenêtre d'application de la tension de surface et des ratios de densité. Les avantages de l'opérateur de recoloriage modifié, et des gradients isotropes, peuvent être étendus à tous les modèles de Boltzmann sur réseau de type RK.

Le troisième thème a généralisé le modèle pour simuler N phases immiscibles tout en étant en mesure de reproduire la physique essentielle. En effet, cette généralisation réussit la simulation de plusieurs cas tests tels que : la décomposition spinodale ; les interfaces planaires ; la loi de Laplace et la loi de Laplace-Young. Les cas tests ont démontré certains accords avec des points qualitatifs et quantitatifs de la théorie des écoulements à plusieurs phases immiscibles. L'étude approfondie de ces trois premiers thèmes a permis de révéler que le modèle original n'est pas en mesure de capturer la discontinuité de la quantité de mouvement dans l'écoulement de Couette à plusieurs phases en présence de variation de densité. Le quatrième thème de cette thèse a apporté une modification à la fonction d'équilibre du modèle de Boltzmann sur réseau permettant à l'écoulement de Couette d'être correctement simulé même dans le cas simultané de grands ratios de densité $O(1000)$ et de viscosité $O(100)$. En fait, en présence d'un faible gradient de pression et dans la limite d'un faible nombre de Mach et de Knudsen, le nouveau modèle est équivalent à une formulation de Navier-Stokes au niveau

macroscopique. De plus, cette solution simple peut également s'appliquer directement aux modèles RK suivants : [17, 18, 36, 38, 39, 85, 96, 97] et peut être également appliquée à d'autres types de modèle de Boltzmann sur réseau avec des problématiques similaires [97].

Il est important de reconnaître que la plupart des cas tests examinés dans les thèmes antérieurs sont toujours valables avec cette nouvelle fonction d'équilibre corrigée. Ceci s'explique par le fait que le modèle original et le nouveau modèle coïncident dans la limite d'un gradient de densité nul ou d'une quantité de mouvement nulle. Pour la majorité des cas tests précédemment effectués, l'une de ces deux conditions est satisfaite.

D'autre part, le cinquième thème, complémentaire à cette thèse, a présenté une généralisation de la discrétisation des gradients d'un ordre spatial et isotrope élevé. Sur la base des dérivations théoriques, il est maintenant possible de calculer les poids et les points nécessaires pour ajuster librement l'ordre spatial et/ou isotrope de l'opérateur gradient discret 2D et 3D. La méthode présentée dans cette thèse peut être généralisée à d'autres types d'opérateurs différentiels, tels que l'opérateur de Laplace ou d'autres opérateurs avec des dérivées mixtes d'ordres supérieurs.

5.1 Recommandations

Ce travail se termine avec quelques recommandations ou idées qui pourraient être utiles pour résoudre ou améliorer les problématiques non résolues du modèle développé.

Tout d'abord, la simulation de ratios de viscosité élevés avec ce modèle reste un défi. Pour éviter une très grande surrelaxation du paramètre effectif de relaxation, une des viscosités du fluide doit être très petite, ce qui cause des instabilités. L'opérateur BGK original est connu pour être instable lorsque la viscosité est faible. D'autres opérateurs de collision tels que le « two-relaxation time (TRT) operator » [113] ou le « multi-relaxation time (MRT) operator » [114] se comportent mieux avec de faibles viscosités et pourraient résoudre ce problème. L'introduction de la condition de stabilité de Brownlee et al. [115] pourrait aussi aider ce modèle. Une des conséquences de l'utilisation de la condition de stabilité Brownlee et al. est l'introduction de dissipation artificielle jusqu'à un ordre donné et cela permet de stabiliser les méthodes de Boltzmann sur réseau. Les modèles de Boltzmann sur réseau entropiques pourraient aussi être envisagés comme autre alternative [116].

En ce qui concerne la généralisation du modèle en trois dimensions, les poids B_i présents dans l'opérateur de perturbation ne sont connus que pour le réseau D2Q9 et D3Q19. Il serait intéressant de trouver les poids pour les réseaux D3Q15 et D3Q27 qui sont aussi des réseaux populaires pour la simulation en trois dimensions avec LBM. Par contre, il est important de noter que la fonction d'équilibre corrigée pour les réseaux 3D est inconnue. En effet, le

développement de ces poids requiert énormément de manipulations algébriques. L'utilisation de logiciels symboliques tels que Maple [117] ou Mathematica [118] pourrait rendre cette tâche beaucoup plus facile et permettre la généralisation de ce modèle pour trois dimensions spatiales.

La principale raison pour laquelle la limite incompressible du modèle est difficile à respecter avec des ratios de densité élevés provient du fait que la vitesse du son isothermale du modèle est variable. D'autre part, c'est en exploitant une vitesse du son variable que le modèle est en mesure de simuler des interfaces planaires immobiles en présence de variation de densité entre les phases. Pour éviter alors cette problématique, il faudrait éviter une vitesse du son isothermale variable, mais cela requiert de changer le tenseur de pression de manière à ce qu'une interface plane à vitesse nulle reste immobile, malgré une variation de densité entre les phases et une pression égale de chaque côté de l'interface. Une analyse approfondie des différents tenseurs de pression utilisés par les différents modèles de Boltzmann sur réseau pour la simulation des fluides à plusieurs phases permettrait une meilleure compréhension de la situation et éventuellement de démystifier cette problématique.

Pour l'instant, un point important à régler est la généralisation en trois dimensions. Par la suite, l'état du modèle serait assez avancé pour résoudre des problèmes beaucoup plus pratiques que les cas tests étudiés dans cette thèse. En effet, l'application d'ingénierie éventuelle, qui est ciblée par le travail effectué dans cette thèse, est le calcul des coefficients de perméabilité relatifs des écoulements à plusieurs phases immiscibles en milieux poreux. Cette application nécessite un modèle en trois dimensions et des ressources informatiques de grande envergure. Éventuellement, il est envisagé que ces coefficients pourraient être précalculés par des ordinateurs pour ensuite être utilisés dans des logiciels modélisant le transport macroscopique des contaminants. C'est dans cette optique que s'est inscrite la vision à plus long terme de ce projet doctoral.

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ANNEXE A

Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model

Il est important de noter que cet article a peut être été sujet à des changements avant la publication finale de celui-ci.

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, “Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model”, manuscript submitted to *Applied Mathematical Modelling* in August 2011.

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Numerical evaluation of two recoloring operators for an immiscible two-phase flow lattice Boltzmann model

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Abstract

The lattice Boltzmann method is applied to the study of immiscible two-phase flows using a Rothman-Keller-type (RK) model. The focus is on the algorithm proposed by Latva-Kokko and Rothman, which has been modified and integrated into the Reis and Phillips model, which belongs to the RK family. A key element of the RK model is the recoloring step applied at the interface of two fluids, at which the fluids are separated and sent to their own region. When convection is weak, the interface in the Reis and Phillips model suffers from “lattice pinning”, which is a problem that may prevent the interface from moving. While the recoloring algorithm proposed by Latva-Kokko and Rothman diminishes this problem, it was not used in the work of Reis and Phillips. This is the framework in which the present study has been conducted. Its scope is twofold : first, to integrate and adapt the Latva-Kokko and Rothman recoloring algorithms for reducing the lattice pinning problem found in the Reis and Phillips model ; and second, to conduct a set of numerical tests to show that the combination of the two algorithms leads to an improvement in the quality of the results, along with a better convergence. The context of the work is two-dimensional, with the D2Q9 lattice used as the basic computational element.

1 Introduction

The recently devised lattice Boltzmann method (LBM), historically derived from cellular automata [6, 32], has been shown to be well suited to simulating complex flows, including immiscible multiphase flows [12, 13, 14, 17, 26, 31, 34]. These include the formation and coalescence of drops [39, 40], rising bubbles [9, 25, 35], flows of immiscible fluids in porous media [19, 36, 41, 42], blood flow [7], and the dissolution of liquid droplets in another liquid [4], among others. Comparisons with experiments have also been performed [9, 36, 39].

Models for lattice Boltzmann immiscible multiphase flows can generally be classified in five categories : the Rothman-Keller (RK) [7, 10, 13, 14, 12, 17, 26, 31, 37, 36, 39, 43], Shan-Chen (SC) [4, 5, 24, 34], free energy (FE) [9, 18, 19, 35], mean-field (MF) [22, 20], and field mediator (FM) methods [33]. In this study, the Reis and Phillips model [31], which belongs to the RK family and is based on color gradients to maintain sharp interfaces, has been adopted. The advantage of this approach is the flexibility with which the model’s parameters can be chosen. It allows independent control of the surface tension, density ratio, and viscosity ratio of the various fluids on either side of an interface, as well as control of the contact angle and the wetting behavior of the solid phases [14]. With the representation of Reis and Phillips [31], higher density ratios can be tackled than with other RK models.

Some years ago, Hou et al. [23] compared the RK and SC models. One of the conclusions of their study was that the SC model provides better results, as it produces less intense spurious currents at the interface. In our current work, we will show that, when Latva-Kokko’s recoloring operator is adapted to the Reis and Phillips RK model, a significant reduction in the spurious currents is achieved. Ginzbourg and Adler [10] also showed that, with an RK model, these currents can be removed completely with a particular choice of eigenvalues in the collision operator. However, these authors only demonstrate that the improvement is valid for a simple test case. The above-referenced RK-based models follow Gunstensen’s [13] Ph.D. thesis, which mentions that the lattice Boltzmann representation recovers Galilean invariance with a proper assignment of the rest equilibrium particles. The ability to simulate flow with a variable density ratio was introduced by Grunau et al. [12], who presented unsteady flow simulations with density ratios up to 10. Since then, the ability of the RK family to simulate flows with a variable density ratio has been investigated very little. In one study [36], Tölke et al. reported a density ratio of 30 for a steady flow simulation, and a density ratio of 4 for an unsteady flow simulation. With the Reis and Phillips representation [31], higher density ratios can be tackled than with other RK models, i.e. a density ratio of up to 18.5 has been reported for an unsteady simulation. In addition, their approach has been shown to be compatible with the macroscopic equations for two-phase flows.

The models in the SC family also have the advantage of being easy to implement and capable of readily simulating fluids with a high-density ratio, but the various parameters of the model cannot be chosen independently [37]. The SC family allows the use of non-ideal equations of state by abandoning the conservation of local momentum and respecting only the conservation of momentum in a global sense [2]. Methods such as the FE type face other kinds of problems ; for example, they do not respect Galilean invariance [37]. Nevertheless, the FE methods have two advantages : they can produce interfaces as thin as two lattice units [42], and they allow the use of a van der Waals equation of state for gas flows, instead of the ideal gas law [28]. The three families, RK, SC, and FE, are theoretically able to simulate an arbitrary number of fluid components [7, 34, 44]. The MF methods simulate interparticle attraction in the same way as the Coulomb interaction is treated in the Vlasov equation [22]. These models can simulate thermodynamically consistent liquid-vapour systems, where the SC models fail [21]. Based on the MF methods and stable discretization of the lattice Boltzmann equation, a recent model from Lee et al. [27] was introduced and shows promising results. They were able to simulate non-ideal gaseous systems with increased numerical stability for a large density ratio $O(1000)$. The FM methods use null-mass particles, the only role of which is to invert the momentum of lattice particles in the transition layer to segregate fluids of different

colors [33]. They have the advantage of being able to incorporate binary diffusivity, and this method can also, therefore, be adapted to simulate miscible fluids.

In our study here, numerical experiments were conducted, closely following the work of Reis and Phillips, to validate the integration of the recoloring algorithm of Ref. [26] into the model of Ref. [31]. These include the surface tension predicted for a planar interface, the Laplace equation for surface tension, and the Poiseuille equation for a layered immiscible fluid with different viscosities. All three test cases are compared with theoretical results. As a fourth test case, the coalescence of two circular bubbles of the same density immersed in a fluid of a higher/lower density is discussed. Finally, a numerical experiment to test the problem of lattice pinning is proposed and investigated. We should mention that another recoloring algorithm has been presented in Ref. [36], but is not studied in this work.

2 Lattice Boltzmann immiscible two-phase model

For the Reis and Phillips model [31] in two dimensions, there are two sets of distribution functions, one for each fluid, moving on a D2Q9 grid with the velocity vectors $\vec{c}_i$. With $\theta_i = \frac{\pi}{4}(4-i)$, the velocity vectors are defined as :

$$\vec{c}_i = \begin{cases} (0, 0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)], & i = 2, 4, 6, 8 \\ [\sin(\theta_i), \cos(\theta_i)] \sqrt{2}, & i = 3, 5, 7, 9 \end{cases} \quad (1)$$

The distribution functions for a fluid of color k (with $k = r$ for red and $k = b$ for blue) are noted $N_i^k(\vec{x}, t)$, while $N_i(\vec{x}, t)$ is used for the sum $N_i^r(\vec{x}, t) + N_i^b(\vec{x}, t)$. If the time step is $\Delta t = 1$, the algorithm from [31] uses the following evolution equation :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t) + \Omega_i^k(N_i^k(\vec{x}, t)) \quad (2)$$

where the collision operator Ω_i^k is the result of the combination of three sub-operators (similar to Ref. [36]) :

$$\Omega_i^k = (\Omega_i^k)^{(3)} \left[(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)} \right] \quad (3)$$

In the algorithm, the evolution equation is solved in four steps with operator splitting, as follows :

1. Single-phase collision operator :

$$N_i^k(\vec{x}, t_*) = (\Omega_i^k)^{(1)}(N_i^k(\vec{x}, t))$$

2. Two-phase collision operator (perturbation) :

$$N_i^k(\vec{x}, t_{**}) = (\Omega_i^k)^{(2)}(N_i^k(\vec{x}, t_*))$$

3. Two-phase collision operator (recoloring) :

$$N_i^k(\vec{x}, t_{***}) = (\Omega_i^k)^{(3)}(N_i^k(\vec{x}, t_{**}))$$

4. Streaming operator :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t_{***})$$

2.1 Single-phase collision operator

The first sub-operator $(\Omega_i^k)^{(1)}$ is the standard BGK operator of the single-phase LBM, where the distribution functions are relaxed towards a local equilibrium in which ω_k denotes the relaxation factor :

$$(\Omega_i^k)^{(1)}(N_i^k) = N_i^k - \omega_k (N_i^k - N_i^{k(e)}) \quad (4)$$

A few details concerning this operator are the following : The density of the fluid k is given by the first moment of the distribution functions :

$$\rho_k = \sum_i N_i^k = \sum_i N_i^{k(e)} \quad (5)$$

where the superscript (e) denotes equilibrium. The total fluid density is given by $\rho = \rho_r + \rho_b$, while the total momentum is defined as the second moment of the distribution functions :

$$\rho \vec{u} = \sum_i \sum_k N_i^k \vec{c}_i = \sum_i \sum_k N_i^{k(e)} \vec{c}_i \quad (6)$$

in which $\vec{u}$ is the total and local velocity of the fluid. The equilibrium functions are defined by [31] :

$$N_i^{k(e)} = \rho_k \left(\phi_i^k + W_i \left[3\vec{c}_i \cdot \vec{u} + \frac{9}{2}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}(\vec{u})^2 \right] \right) \quad (7)$$

These equilibrium distribution functions, $N_i^{k(e)}$, are chosen to respect the conservation of mass and momentum [31]. The weights W_i are those of a standard D2Q9 lattice :

$$W_i = \begin{cases} 4/9, & i = 1 \\ 1/9, & i = 2, 4, 6, 8 \\ 1/36, & i = 3, 5, 7, 9 \end{cases} \quad (8)$$

Moreover,

$$\phi_i^k = \begin{cases} \alpha_k, & i = 1 \\ (1 - \alpha_k)/5, & i = 2, 4, 6, 8 \\ (1 - \alpha_k)/20, & i = 3, 5, 7, 9 \end{cases} \quad (9)$$

As introduced in [12], to obtain a stable interface, the density ratio γ needs to be taken as follows :

$$\gamma = \frac{\rho_r}{\rho_b} = \frac{1 - \alpha_b}{1 - \alpha_r} \quad (10)$$

Without loss of generality, in this paper $\rho_r \geq \rho_b$. The pressure of the fluid of color k is :

$$p^k = \frac{3\rho_k(1 - \alpha_k)}{5} = \rho_k(c_s^k)^2 \quad (11)$$

where, in the above expressions, either α_r or α_b represents a free parameter, and c_s^k is the sound speed in the fluid of color k [4, 31]. These parameters are important when the density ratio γ is large [31]. Theoretically, the constraint $\alpha_b \leq 1$ must be respected in order to avoid negative pressures. It is also possible to show that $0 \leq \alpha_b \leq \alpha_r \leq 1$ is always true when $\rho_r \geq \rho_b$ and $0 \leq \alpha_b \leq 1$.

The relaxation parameters ω_k are chosen so that the evolution equation (2) respects the macroscopic equations for single-phase flow in the single-phase regions [31]. This parameter is a function of the fluid kinematic viscosity ν_k , given by $\omega_k = 1/(3\nu_k + \frac{1}{2})$. As introduced in [12], when the viscosities of the fluids are different, an interpolation is applied to define the parameter ω_k at the interface. To do this, it is necessary to introduce the color field :

$$\psi = \frac{\rho_r - \rho_b}{\rho_r + \rho_b} \quad (12)$$

The color field ψ is a function with its image between -1 and 1 . It takes the value 1 or -1 , depending on whether it is evaluated at a position that contains only red fluid or only blue fluid. In an interface, the color field is obviously between -1 and 1 . The relaxation factor ω_k in Eq. 4 is replaced by ω :

$$\omega = \begin{cases} \omega_r, & \psi > \delta \\ f_r(\psi), & \delta \geq \psi > 0 \\ f_b(\psi), & 0 \geq \psi \geq -\delta \\ \omega_b, & \psi < -\delta \end{cases} \quad (13)$$

in which δ is a free parameter and

$$\begin{aligned} f_r(\psi) &= \chi + \eta\psi + \kappa\psi^2 \\ f_b(\psi) &= \chi + \lambda\psi + v\psi^2 \end{aligned} \quad (14)$$

with

$$\begin{aligned} \chi &= 2\omega_r\omega_b/(\omega_r + \omega_b) \\ \eta &= 2(\omega_r - \chi)/\delta \\ \kappa &= -\eta/(2\delta) \\ \lambda &= 2(\chi - \omega_b)/\delta \\ v &= \lambda/(2\delta) \end{aligned} \quad (15)$$

The free parameter δ is required to calculate ω , and is chosen to be 0.1 for all the simulations in this paper. It is a parameter that influences the thickness of the interface when the fluid viscosities are different [31]. The larger δ , the thicker the fluid interface. If the fluid viscosities are the same, the parameter δ does not have an impact on the solution, because, in this case, $\omega = \omega_r = \omega_b$.

2.2 Perturbation operator

In the RK model, surface tension is modeled by means of the perturbation operator [14, 17, 31]. First, the color gradient in terms of the color difference is defined by :

$$\vec{F}(\vec{x}) = \sum_i \vec{c}_i (\rho_r(\vec{x} + \vec{c}_i) - \rho_b(\vec{x} + \vec{c}_i)) \quad (16)$$

The color gradient direction is an approximation of the perpendicular to the interface between the fluids. This perturbation operator is defined by :

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \frac{A_k}{2} |\vec{F}| \left[W_i \frac{(\vec{F} \cdot \vec{c}_i)^2}{|\vec{F}|^2} - B_i \right] \quad (17)$$

where

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (18)$$

Reis and Phillips [31] have shown that this operator complies with the macroscopic equations for two-phase flows. It handles the coupling between the two fluids, with the free parameters A_k chosen to model the surface tension. Although this operator generates the surface tension, it does not guarantee the fluid's immiscibility. To minimize the mixing of the two fluids, the recoloring operator $(\Omega_i^k)^{(3)}$ must be introduced.

2.3 Recoloring operator

2.3.1 Original Reis recoloring algorithm

This last operator is used to maximize the amount of red fluid at the interface sent to the red fluid region, and the amount of blue

fluid sent to the blue fluid region, while respecting the conservation of mass and total momentum. Reis' model uses a recoloring method that produces a very thin interface, but, as recognized by the authors, it has the problem of lattice pinning [31]. By defining the color flux :

$$\vec{K}(\vec{x}) = \sum_i (N_i^r - N_i^b) \vec{c}_i, \quad (19)$$

the recoloring operator is used to maximize the work W performed by the color gradient against the color flux [14, 31, 32] :

$$W = \vec{K} \cdot \vec{F} \quad (20)$$

subject to the following equivalent constraints of mass and total momentum conservation :

$$\begin{aligned} N_i^r + N_i^b &= N_i \\ \sum_i N_i^r &= \rho_r \end{aligned} \quad (21)$$

The standard optimization techniques, such as Lagrange multipliers, cannot be used to solve this problem [31]. Instead, the usual RK model method is used, which consists of maximizing the number of red particles sent in the direction of the color gradient $\vec{F}$, while respecting the constraints given in Eq. 21. This is achieved as follows.

First, the $\vec{c}_i$ directions are reordered, with the first one pointing in the direction closest to $\vec{F}$, then the second closest is placed, and so on. The vector $\vec{c}_1$ is located at the center of the nine directions. Then, a maximum mass of red fluid is sent in the direction closest to $\vec{F}$, always within the constraints imposed by Eq. 21. Using the amount of red fluid remaining, the maximum quantity of red fluid is sent in the second direction closest to $\vec{F}$, still respecting the constraints required by Eq. 21. This process is repeated until all the red fluid has been redistributed. In this paper, this operator is called *recoloring operator I*.

2.3.2 Original Latva-Kokko and modified recoloring algorithm

In the model proposed by Latva-Kokko and Rothman [26], the recoloring operator is defined as follows :

$$(\Omega_i^r)^{(3)}(N_i^r) = \frac{\rho_r}{\rho} N_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) N_i^{(e)}(\rho, 0) \quad (22)$$

$$(\Omega_i^b)^{(3)}(N_i^b) = \frac{\rho_b}{\rho} N_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) N_i^{(e)}(\rho, 0) \quad (23)$$

where the color-blind equilibrium function is $N_i^{(e)}$, and therefore the recoloring operator is defined for a constant value of α_r and α_b . Thus, when combining the Latva-Kokko and Rothman [26] recoloring operator with the Reis and Phillips model [31], it is important to take into account that the sound speed is a free parameter in the Reis and Phillips model. In this respect, a contribution of this paper is the adaptation of the Latva-Kokko recoloring operator for a variable speed of sound. The new recoloring operator takes the following form :

$$(\Omega_i^r)^{(3)}(N_i^r) = \frac{\rho_r}{\rho} N_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \quad (24)$$

$$(\Omega_i^b)^{(3)}(N_i^b) = \frac{\rho_b}{\rho} N_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \quad (25)$$

where β is a free parameter and $\cos(\varphi_i)$ is the cosine of the angle between the color gradient $\vec{F}$ and the direction $\vec{c}_i$. The color-blind equilibrium distributions $N_i^{(e)}$ in Eqs. 22 and 23 are replaced with

the sum of the equilibrium distributions of each fluid $N_i^{k(e)}$ in Eqs. 24 and 25, and are evaluated using the respective value of α_k and a zero velocity. The value of $\cos(\varphi_1)$ must equal 0 in order to conserve mass. Also, the parameter β must be between 0 and 1 to ensure that the distribution functions remain positive [26]. It is important to mention that other factors in a simulation could lead to negative distribution functions. Parameter β influences the thickness of the interface : the smaller its value, the thicker the interface. The value of β used in this paper is 0.99, unless otherwise stated. The recoloring operator defined by Eqs. 24 and 25 is called *recoloring operator II* in this paper.

3 Numerical Results

The simulations were performed with a single-threaded MATLAB program running on a desktop equipped with an Intel core i7 970 CPU. In our setting, this processor can compute, on average, approximately 70 and 90 time steps per second for recoloring operators I and II respectively, for a lattice with 100x100 sites and periodic boundary conditions. It should be noted that the code was not intended to be particularly efficient. With it, we can nevertheless show that one advantage of the current recoloring operator (II) over the former operator (I) is the smaller computational cost per time step.

3.1 Planar interface

In a similar way to that shown in Ref. [31], we consider a planar interface parallel to the standard y-axis with a stationary fluid of a different color on each side of the interface. In such a case, and for the current model, it was shown by [31] that the surface tension is given by the following equation when measured from any line of integration perpendicular to the interface :

$$\sigma_{model} = \frac{(A_r + A_b)}{9\omega} \sum_{\vec{x}} |\vec{F}| \quad (26)$$

Equation 26 relates the surface tension in the model as a function of the color gradient and other parameters [31].

The mechanical definition of surface tension is [10, 14, 17, 31] :

$$\sigma_{mec} = \int_{-\infty}^{+\infty} (P_N(z) - P_T(z)) dz \quad (27)$$

where P_N and P_T are the normal and tangential components of the pressure tensor. The z-axis is a line of integration perpendicular to the interface. By setting θ_z to be the angle of the z-axis with respect to the standard x-axis, and θ_i to be the relative angle between the x-axis and the vector $\vec{c}_i$, the components P_N and P_T are given by [31] :

$$\begin{aligned} P_N &= \sum_i N_i (|\vec{c}_i| \cos(\theta_i - \theta_z))^2 \\ P_T &= \sum_i N_i (|\vec{c}_i| \sin(\theta_i - \theta_z))^2 \end{aligned} \quad (28)$$

To perform numerical simulations on the planar interface, a computational domain of 64×64 sites is defined. Initially, all sites on the left-hand side of the computational domain are initialized with a red fluid using zero velocity equilibrium functions. The remaining sites are initialized in a same way, but with blue fluid. Periodic boundary conditions are used at each end of the computational domain. The viscosity of both fluids is $\nu_r = \nu_b = 1/6$. A value of $\alpha_b = 0.2$ is used. By directly applying Eqs. 26 and 27 on a horizontal line of integration, the surface tension measured is twice the desired value,

as the line of integration passes through an interface twice. This is a consequence of the finite computational domain and the periodic boundary conditions.

The goal of this numerical experiment is to attest to the model's ability to create a surface tension between the fluids that is consistent with the mechanical definition. An additional goal is to show that it is possible to arrive at a desired surface tension by setting only the free parameters A_k of the model.

A total of 54 numerical simulations were conducted to study how the various parameters in the current model influence the surface tension. The total number of all possible combinations of input parameters is 54 ($2 \times 3 \times 3 \times 3$), as summarized in Table 1.

Recoloring Operator	$A_r = A_b$	ρ_r	γ
I	0.01	1	1
II	0.002	4	4
	0.0004	6	6

TABLE 1: Combination of parameters for the planar interface case.

The stopping criterion applied to all planar interface simulations is :

$$\max_{\text{all distribution functions}} \left\{ |(N_i^k)^{(n)} - (N_i^k)^{(n-1)}| \right\} \leq \epsilon \quad (29)$$

with $\epsilon = 10^{-10}$ and n denoting the iteration number. If the criterion was not met within a maximum of 20000 iterations, the simulations were stopped. The results after all 54 simulations showed that recoloring operator I failed to converge under the imposed convergence criterion. In contrast, operator II converges without difficulty. In fact, the maximum number of iterations required for all 54 simulations with operator II was 6000. Therefore, the limit of 20000 iterations to allow convergence was appropriate for the planar interface problem. To demonstrate the better convergence of recoloring operator II over recoloring operator I, a plot showing the left-hand side of Eq. 29 versus the time step is presented in Fig. 1.

It was already known that the surface tension can be set in an RK model using only the free parameters. Work has been done by [31] and their predecessors to obtain the surface tension as a function of ρ , ω , A_r , and A_b . The expression obtained varies from one model to another, but they are always very similar. For the current model, by analyzing the simulation results of the previous setting, the value for the surface tension as a function of the various model parameters is generalized for the case of the variable density ratio (as in Ref. [36]) :

$$\sigma_{predict} = \frac{4}{3} \frac{\rho_r + \rho_b}{\omega} (A_r + A_b) = \frac{4}{3} \left(1 + \frac{1}{\gamma}\right) \frac{\rho_r}{\omega} (A_r + A_b) \quad (30)$$

Equation 30 can therefore be used to approximately set the surface tension between the fluids.

Let us define the error corresponding to the i^{th} simulation as follows :

$$\begin{aligned} E_i^m &= \frac{\left| \frac{\sigma_{mec}^i}{2} - \frac{\sigma_{model}^i}{2} \right|}{\frac{\sigma_{mec}^i}{2}} \\ E_i^p &= \frac{\left| \frac{\sigma_{mec}^i}{2} - \sigma_{predict}^i \right|}{\frac{\sigma_{mec}^i}{2}} \end{aligned} \quad (31)$$

and compare the accuracy of recoloring operators I and II. Table 2 reports some relative errors for various simulation groups and norms. The first line compares the maximum surface tension errors obtained for all simulations when the density ratio γ between the two fluids

is unity. The next three lines are similar, except that the simulations with $\gamma \neq 1$ are considered to calculate the norms. Note that the integral in Eq. 27 is numerically evaluated with a simple midpoint method, with the lattice sites taken as the integration node. The symbol $\langle \cdot \rangle$ stands for the average.

	Recoloring I		Recoloring II	
	E^m (%)	E^p (%)	E^m (%)	E^p (%)
$\max \{E_i \gamma = 1\}$	0	0	0	0
$\max \{E_i \gamma \neq 1\}$	93.456	93.467	0	0.0095
$\min \{E_i \gamma \neq 1\}$	7.5198	7.5524	0	0.0053
$\langle \{E_i \gamma \neq 1\} \rangle$	51.222	51.261	0	0.0074

TABLE 2: Error comparison based on different norms for the planar interface problem.

Regarding Table 2, it is important to note that, when $\gamma = 1$, the surface tension predicted by Eqs. 26 and 30 is the same as the mechanical surface tension, regardless of the recoloring operator. It has already been mentioned that it is the perturbation operator that introduces the surface tension in the numerical model. This means that, for the 18 simulations with $\gamma = 1$, neither recoloring operator introduces numerical errors into the surface tension generated by the perturbation operator. With $\gamma \neq 1$, recoloring operator I introduces a significant error in the surface tension produced by the perturbation operator. In contrast, with $\gamma \neq 1$, recoloring operator II performs better, in terms of both accuracy and the number of iterations required to reach convergence.

3.2 Steady bubble

The next numerical experiment involves a steady red bubble of radius R immersed in a blue fluid. The aim of this second numerical experiment is to verify whether or not the surface tension predicted by Eq. 30 is consistent with the Laplace equation [14, 31] :

$$\sigma_{laplace} = R\Delta p \quad (32)$$

where $\Delta p = p_{in} - p_{out}$ is the pressure jump between the inside and outside of the bubble. For these simulations, the computational domain is discretized with a lattice size of 128×128 . Initially, the red fluid is placed at a distance of at most R from the center of the computational domain. The fluid is initialized with the zero velocity equilibrium distribution functions. The field is initialized in the same way for the blue fluid. Periodic boundary conditions are used at the four ends of the computational domain. A value of $\alpha_b = 0.6$ is used for all the steady bubble simulations. The pressures inside and outside the bubble are measured according to :

$$\begin{aligned} p_{in} &= \frac{3}{\pi^2} \rho_{in} (1 - \alpha_r) \\ p_{out} &= \frac{3}{\pi^2} \rho_{out} (1 - \alpha_b) \end{aligned} \quad (33)$$

where

$$\begin{aligned} \rho_{in} &= \langle \{\rho_r | \psi \geq \xi\} \rangle \\ \rho_{out} &= \langle \{\rho_b | \psi \leq -\xi\} \rangle \end{aligned} \quad (34)$$

For example, ρ_{in} is the average of the density ρ_r for all sites, such that the color field ψ is greater than or equal to ξ . The variable ξ is

the nearest value to 1 in the following set : $\{1 - 0.1^n | n \leq 10\}$, such that there exists at least one site with $\psi \geq \xi$.

Let us denote by E_I the relative error between the surface tension $\sigma_{laplace}$ and $\sigma_{predict}$, with $\sigma_{predict}$ as a reference when a simulation was performed with recoloring operator I and by E_{II} if a simulation was performed with recoloring operator II. Table 3 illustrates the parameters and the errors resulting from the various simulations of the steady bubble.

Simulations not shown here revealed that, for $\gamma = 6$ and low surface tension, the Laplace equation leads to a negative surface tension when using recoloring operator I and $\alpha_b = 0.2$. It is important to note that recoloring operator II gives accurate results for $\alpha_b = 0.2$ and $\alpha_b = 0.6$.

Table 3 shows that the two recoloring operators produce results of similar accuracy when the density of the two fluids is equal. This result indicates the same behavior as in the simulation of the planar interface. In contrast, a large error is obtained by recoloring operator I when the density ratio is high and the surface tension is small. This indicates that recoloring operator II gives valid results for a wider range of parameters.

For the steady bubble experiment, we also looked at the effect of recoloring operators I and II on the spurious currents. These currents, found at the interface between two fluids, should be absent, and their origin is poorly understood. In the cellular automata literature [6], it has been mentioned that a recoloring operator of the form of recoloring operator II can reduce spurious currents. These results are confirmed for the current lattice Boltzmann model. Table 3 shows that recoloring operator II greatly reduces these spurious currents ($\max \|\vec{u}\|$), by up to 2 orders of magnitude when the density ratio is high and the surface tension is small. This could explain why there is a large error in the measured surface tension obtained with recoloring operator I.

To obtain convergence with recoloring operator II, the average number of iterations under the stopping criterion with $\epsilon = 10^{-10}$ in Eq. 29 is 73875. Note that all simulations with recoloring operator I were stopped after 200000 iterations.

3.3 Layered Poiseuille flow

In the same manner as in Ref. [31], a simulation of a Poiseuille flow between two infinite plates is performed to study the model's ability to simulate two fluids of different viscosity. The simulation is conducted on a lattice containing 1×32 sites (the analytical solution is 1D). The flow is centered at $y = 0$ and is initialized with the red fluid using the zero velocity equilibrium distribution functions for the 16 sites with $y < 0$, and similarly with the blue fluid for $y > 0$. Periodic boundary conditions are used in the x-direction. The first and last sites are used to implement the standard "bounce back" boundary condition. With this condition, the walls are located at $y = -15$ and $y = 15$, which correspond to a channel half height of $h = 15$. When implementing the wall boundary condition for the current model, the "density" of the wall must be known in order to calculate the color gradient. For the current simulation, the top wall is set to be red wet, so $\rho_r = 1$ and $\rho_b = 0$ on the last site. Similarly, the bottom wall is set to be blue wet, with $\rho_r = 0$ and $\rho_b = 1$. The parameters of the simulation are : $\rho_r = 1$, $\gamma = 1$, $A_r = A_b = 0$, $\alpha_b = 0.2$, $\nu_r = 1/6$, and viscosity ratio $\nu = \frac{\nu_r}{\nu_b}$. For this case, only recoloring operator II converges the solution to steady state, with $\epsilon = 10^{-11}$. The convergence of recoloring operator I is unsatisfactory, because it is similar to the planar interface simulations. For this particular flow, with the "shear viscosities" μ_r and μ_b , and when the compressibility

effects are neglected, an analytical solution exists :

$$\begin{aligned} u^r &= \frac{Gh^2}{2\mu_r} \left[-\left(\frac{y}{h}\right)^2 + \frac{y}{h} \left(\frac{\mu_r - \mu_b}{\mu_r + \mu_b} \right) + \frac{2\mu_r}{\mu_r + \mu_b} \right], -h \leq y \leq 0 \\ u^b &= \frac{Gh^2}{2\mu_b} \left[-\left(\frac{y}{h}\right)^2 + \frac{y}{h} \left(\frac{\mu_r - \mu_b}{\mu_r + \mu_b} \right) + \frac{2\mu_b}{\mu_r + \mu_b} \right], 0 \leq y \leq h \end{aligned} \quad (35)$$

where G is the pressure gradient between the two ends of the channel. That pressure gradient is simulated using an equivalent body force, which is implemented by adding G/ω to the horizontal component of the total velocity when computing the equilibrium distribution function $N_i^{k(e)}$ in the operator $(\Omega_i^k)^{(1)}$. Note that the pressure gradient G is chosen to achieve a speed at the center of the channel of $u_c = 0.000045$:

$$G = \frac{u_c (\mu_r + \mu_b)}{h^2} \quad (36)$$

As with the stationary bubble, E_I and E_{II} denote the relative error between the theoretical total velocity and the numerical total velocity when a simulation is performed with recoloring operators I and II respectively. For the numerical simulations considered here, it should be noted that the errors obtained are practically the same with both recoloring operators, i.e. $E_I \approx E_{II}$. Errors at four different positions in the channel are listed in Table 4 for different viscosity ratios.

ν	$y = -7.5$	$y = -0.5$	$y = 0.5$	$y = 7.5$
10	0.0439	0.0343	0.5776	0.3635
100	0.0485	0.0418	2.2146	0.4848
1000	0.0521	0.0464	3.3110	0.5133
10000	0.0502	0.0442	3.4807	0.5094

TABLE 4: Relative errors (%) in the velocity profile at different positions in the channel for the layered Poiseuille flow and different viscosity ratio, ν .

Figure 2 shows the numerical solution and the analytical solution when using recoloring operator II and for different viscosity ratios. The solution with recoloring operator I (not shown) is almost the same as the solution with recoloring operator II.

For the chosen parameters, the current model can accurately simulate a high viscosity ratio for the layered Poiseuille flow without any velocity discontinuity at the interface. As in Ref. [29], velocity discontinuity does arise in the current model if the kinematic viscosity of one of the fluids is too high. To solve such a discontinuity in the velocity profile, a two-relaxation-time (TRT) collision operator can be used instead of a simpler BGK operator [11, 29].

Based on the results obtained, it can be concluded, for this numerical experiment, that the two recoloring operators behave similarly and lead to a satisfactory solution. The similarity of the results for both recoloring operators is not surprising, since, for the planar interface and steady bubble, the results are also similar when the density ratio is unitary.

3.3.1 Layered Poiseuille flow with density ratios larger than unity

An analytical solution for a layered Poiseuille flow with larger density ratios can be found in the section above, or in Refs. [38, 31, 29]. In a similar manner as for a unit density ratio, we tried to simulate the flow by adding a body force $\frac{G}{\rho\omega}$ to the equilibrium velocity. The simulation results in a large discrepancy between the numerical and analytical solutions when the density ratio is larger than unity, i.e.

a discontinuity arises in the velocity profile at the interface between the fluids. This behavior has also been found in Ref. [29].

The artifact of adding a body force to mimic a pressure gradient may be one cause of the inaccuracy. As pointed out by Buick and Greated [3], adding $\frac{G}{\rho\omega}$ to the equilibrium velocity is less valid in the presence of a density gradient. It is not yet clear to us how to implement a consistent body force with a variable density ratio. Another possible cause of the inaccuracy, mentioned by Rannou [29], may be the inability of the LB model to guarantee a simultaneous continuity of the shear stress and velocity when the density ratio is larger than one. This problem clearly deserves more attention and further research.

In fact, the ability of the current LB model to simulate flow with a density ratio larger than unity is questionable. As shown by Rannou [29], this comment can be made for at least four types of LB model (RK, SC, FE, and MF), for which a discontinuity arises in the velocity profile. We note that this problem has only recently been identified, and, as stated by Aidun and Clausen, it is known as the "discontinuity problem" [1].

Nevertheless, it appears that recoloring operator II corrects the inaccuracy found with recoloring operator I when density ratio is not unity, at least for the planar interface and steady bubble case. In this respect, the multiphase LB community should attempt to successfully simulate layered Poiseuille flow with density ratios larger than unity.

3.4 Bubble coalescence

The next numerical experiment involves the coalescence of two bubbles of equal density in a fluid with an equal, lower, or higher density, which is equivalent to a 3D collision of two cylinders of infinite length. This test is used to assess the ability of recoloring operator II to perform an unsteady simulation where a final steady solution exists on which we can measure and predict the final surface tension.

A lattice of 100×100 sites is used, with periodic boundary conditions at the four ends. The computational domain then measures 99 lattice units in both height and width. The corner at the bottom left of the domain is located at the origin (0,0). Using zero velocity equilibrium distribution functions, two red/blue fluid bubbles of radius $R = 18$, with density $\rho_r = 1$ or $\rho_b = \frac{1}{\gamma}$, are initialized at the following respective positions :

$$(x - 49.5)^2 + (y - 49.5 \pm 18)^2 \leq 18^2 \quad (37)$$

The remaining sites are similarly initialized with the blue/red fluid, and respecting a certain density ratio γ . The simulation parameters are set with $\alpha_b = 0.6$, $A_r = A_b$, $\sigma_{predict} = 6 \cdot 10^{-3}$, and $\nu_r = \nu_b = 1/6$. "Snapshots" of the color field ψ showing the collision of two dense red bubbles for density ratio $\gamma = 35$ and with recoloring operator II are presented in Fig. 3 for different times. The results shown in Fig. 3 are very similar to those obtained by Reis and Phillips [31]. The reason why they differ qualitatively is that the surface tension in our simulation is about half that in the simulation presented by Reis and Phillips [31].

The fluids are immiscible and a surface tension exists between them. Because of this, at steady state, the surface contact "area" between the two fluids is minimal, and only one big red bubble remains. It is stated in [31] that the final radius of the red fluid bubble should be equal to $R_f = \sqrt{2}R$. Therefore, at steady state, when using this predicted radius, R_f , in the Laplace equation (32), the Laplace surface tension obtained, $\sigma_{Laplace}$, should be equal to the predicted surface tension $\sigma_{predict}$ that was set with Eq. 30 at the beginning of the simulation. Simulation of bubble coalescence was performed for different density ratios and with both recoloring operators. Some re-

sults are shown in Tab. 5, with the errors and the pressure calculated as in the steady bubble simulation.

γ	Red dense bubbles		Blue light bubbles	
	E_I (%)	E_{II} (%)	E_I (%)	E_{II} (%)
1	3.352	0.469	3.352	0.469
35	17.55	3.951	36.06	0.643
40	34.86	4.592	N/A	0.733
45	113.7	5.269	N/A	0.825
50	N/A	5.940	N/A	0.920
80	N/A	11.49	N/A	1.487
85	N/A	12.13	N/A	1.585
90	N/A	N/A	N/A	N/A

TABLE 5: Error after the coalescence of the two dense/light bubbles between the predicted and calculated surface tensions $\sigma_{predict}$ and $\sigma_{Laplace}$.

The algorithm was stable enough that both recoloring operators were able to simulate a high-density ratio of up to 45. Note that recoloring operator I is unstable for $\gamma = 85$, while recoloring operator II provides a numerically stable solution. As shown in Tab. 5, recoloring operator II is certainly more accurate and stable than recoloring operator I, as it can achieve error levels smaller than one order of magnitude. Another advantage of recoloring operator II is the economy it generates in terms of computational cost, which is related to the number of time steps needed to arrive at the steady state. The convergence criterion is $\epsilon = 10^{-8}$. To reach the steady-state solution, the mean number of iterations for recoloring operator II is about 46000, while the simulations carried out with recoloring operator I did not reach convergence at the maximum number of iterations allowed, that is, 200000.

3.5 Lattice pinning

For the RK model, the pinning problem in multiphase flows has been recognized by several authors : Reis and Dellar [30], Latva-Kokko and Rothman [26], Dupin et al. [8], and Halliday et al. [15, 16]. This problem can arise at the interface of two fluids when there is weak convection. In practice, this means that the interface cannot move and becomes “pinned” to the lattice, as long as the convection flow is not strong enough.

To our knowledge, it is unknown whether or not this problem is also present in other type of LB model. In this section, a numerical experiment is proposed to test the presence of lattice pinning. This test, which we could call a tool, may also be applied to other LB schemes to test the presence of pinning.

Although the model of Reis and Phillips is an improvement over others in the same group, the authors indicate that it could suffer from lattice pinning. Latva-Kokko and Rothman have proposed a recoloring algorithm to prevent lattice pinning, or at least diminish it. The next numerical experiment illustrates that combining the two algorithms leads to an improvement in the results.

3.5.1 Numerical experiment 1

The ability of recoloring operator II to reduce the lattice pinning effect is illustrated with the next simulation. A computational domain of 257×33 sites and geometrically located over $[0, -16] \times [256, 16]$ is used with periodic boundary conditions in all directions. All sites are initialized with blue fluid using zero velocity equilibrium functions, except that the sites located at $x = 10$ and $y = \pm 8$ are initialized

with red fluid. The simulation parameters are $\beta = 0.8$, $\nu_r = \nu_b = 1/6$, $A_r = A_b = 0$, $\rho_r = 1$, and $\gamma = 1$. All simulations are iterated to 10000 time steps. A body force is added to the fluid, so that it undergoes an acceleration of 0.000005 lattice units per time step squared up to time $t = 6000$. Recoloring operator I is used for all sites, such that $y \geq 0$, and operator II is used elsewhere. This configuration allows simultaneous testing of recoloring operators I and II for the lattice pinning problem. The red fluid particle with $y \geq 0$ is called red fluid particle I (the same name as the recoloring operator used in this area), and, similarly, the red fluid particle with $y < 0$ is called red fluid particle II. Because there is no surface tension ($A_r = A_b = 0$) and no density or viscosity difference between the two fluids, the horizontal velocity and position of the red fluid particle are the known theoretical ones, given by :

$$\begin{aligned} u_{x,th}(t) &= \begin{cases} \frac{5}{1000000}t, & t < 6000 \\ \frac{3}{100}, & t \geq 6000 \end{cases} \\ x_{th}(t) &= \begin{cases} 10 + \frac{25}{1000000}t^2, & t < 6000 \\ 100 + \frac{3}{100}(t - 6000), & t \geq 6000 \end{cases} \end{aligned} \quad (38)$$

To compare the numerical results with the analytical results, the average horizontal component of the total fluid velocity of red fluid particles I and II, $u_{x,I}$ and $u_{x,II}$, and the average horizontal positions of red fluid particles I and II, x_I and x_{II} , are calculated using the color field :

$$\begin{aligned} u_{x,I} &= \langle \{u_x | \psi \geq -0.9 \text{ and } y \geq 0\} \rangle \\ u_{x,II} &= \langle \{u_x | \psi \geq -0.9 \text{ and } y < 0\} \rangle \\ x_I &= \langle \{x | \psi \geq -0.9 \text{ and } y \geq 0\} \rangle \\ x_{II} &= \langle \{x | \psi \geq -0.9 \text{ and } y < 0\} \rangle \end{aligned} \quad (39)$$

In Figure 4 and for $\alpha_b = 0.2$, the average horizontal velocity and position of red fluid particles I and II versus time are presented, together with the analytical solution. In Figure 4a, it is apparent that the average horizontal velocities of the two red fluid particles are in agreement with the local fluid flow velocity.

But, Figure 4b clearly shows that recoloring operator I was not able to move the red fluid particle, the position of which did not change over time. When looking at recoloring operator II, the behavior of the particle is much better, because it moves from left to right. Note, however, that lattice pinning has not been avoided completely, because particle II does not move during the first 2000 iterations. In the limit $t \rightarrow \infty$, the relative error for the position of the particle diverges to ∞ when recoloring operator I is used, compared to 0% with recoloring operator II. A reduction of parameter β could reduce lattice pinning further, but the interface would become very thick. With this simulation, we can conclude that recoloring operator I reveals a nonexistent physical phenomenon, and that recoloring operator II behaves much better in such a case.

3.5.2 Numerical experiment 2

To further analyze recoloring operator II, the behavior of red fluid particle II is studied as a function of α_b . In theory and without lattice pinning, the integral of the average total fluid velocity of the particle should be equal to the distance traveled, but, when there is lattice pinning, the integrated speed will be greater than the distance traveled. This is because lattice pinning prevents the particle from moving, even if there is a convection current that “tells” it to move.

To approximate the intensity of lattice pinning as a function of α_b , the integral of the total average speed versus time of particle II is compared with the distance traveled. Table 6 indicates the error between the integral of the average speed and the final position of particle II for different values of α_b . The numerical integration is performed with a basic midpoint method using 200 points uniformly distributed between $t = 0$ and $t = 10000$. Although an error is introduced with the numerical integration, it is in the order of the round-off error, because the midpoint method is of second order and the velocity profile is linear in the worst case. The behavior of the error suggests that lattice pinning is reduced with an increasing value of α_b .

For the value of α_b used in Table 6, we can point out that pinning is not prevented at all for recoloring operator I. Because α_b is related to the speed of sound, the results suggest that the slower the speed of sound, the less lattice pinning is taking place.

α_b	$t = 10000$		$\int_0^{10000} (u_{x,II})dt$	Error (%)
	$x_{th} - 10$	$x_{II} - 10$		
0.1	210	150.0	210	28.6
0.2	210	156.0	210	25.7
0.4	210	166.5	210	20.7
0.5	210	171.0	210	18.6
0.6	210	175.0	210	16.7
0.8	210	178.0	210	15.2
0.9	210	182.0	210	13.3

TABLE 6: Measure of lattice pinning intensity.

3.5.3 Numerical experiment 3

Numerical experiment 1 showed that lattice pinning can occur when there is not enough convection and a small red fluid particle is immersed in a blue fluid. This case is extreme, because, initially, the red fluid particle consisted of only a single lattice site, which means that there is a lack of spatial resolution. The next numerical experiment will show that, when the red bubbles cover more lattice sites (better spatial resolution), then the lattice pinning effect disappears and the analytical solution is recovered. The setup is as in numerical experiment 1, but with $\beta = 0.99$ and the red fluid zone initially consisting of larger bubbles, with the following equation respected :

$$(x - 10)^2 + (y \pm 8)^2 \leq 6^2 \quad (40)$$

Figure 5 presents the numerical and analytical horizontal velocity and position in such a case. As in numerical experiment 1, and, as expected, in Figure 5a, the average horizontal velocities of the two red particles are in agreement with the theoretical solution. For the results obtained in Figure 5b, the small error between the numerical solution and the analytical one may come from the way the positions of the red fluid particles are measured, and also, again, from a lack of spatial resolution (even though the results are a great deal better in this numerical experiment). Lattice pinning is a problem that occurs in very particular cases (degenerate), and better spatial resolution appears to fix it for both recoloring operators. It can be concluded that lattice pinning should not be a problem in the majority of the immiscible two-phase flow applications, because, in general, a high enough spatial resolution is chosen to resolve the scale of interest.

However, this is not always possible. For example, in porous media with intricate geometry, a passage could reach the lattice size and the fluid could easily remain (artificially) stuck, impeding the flow. Obviously, this would produce a fake solution. Therefore, it is important

to use recoloring operator II instead of operator I for simulating flows for these kinds of media.

4 Conclusion

The Latva-Kokko and Rothman algorithm [26] has been adapted and incorporated into the two-phase lattice Boltzmann model of Reis and Phillips [31]. Numerical simulations were conducted to determine the benefits of such a modification. Simulations of a planar interface, a steady bubble, layered Poiseuille flow, and bubble coalescence showed that the proposed recoloring operator leads to a stationary solution in many fewer iterations than the original recoloring operator use by Reis and Phillips. Regarding accuracy, the two recoloring operators provide similar results for the selected test cases when the density ratio of the two fluids is unity. For the planar interface, and when the density ratio is not unity, the recoloring operator in [31] introduces a significant error in the surface tension, while the current recoloring operator is very accurate. For the steady bubble simulation, a problem showed up when the density ratio was not unity and the surface tension was low. In that case, the recoloring operator in the Reis and Phillips model introduced a large error in the surface tension, while the present recoloring operator provided satisfactory results. Moreover, the intensity of spurious currents was much lower with the Latva-Kokko recoloring operator than with the recoloring operator in the Reis and Phillips model. For a layered Poiseuille flow problem, the introduction in the model of the recoloring operator of Latva-Kokko and Rothman did not show an improvement over the standard recoloring operator in terms of the accuracy of the results; however, the Latva-Kokko recoloring operator showed an improvement in the number of iterations required to achieve a steady-state solution. A viscosity ratio as high as 10000 was accurately simulated for the layered Poiseuille flow. We mentioned the discontinuity problem, which is an open problem with the LB model when the density ratio is not unity in the layered Poiseuille flow. This problem definitely needs more attention. In the bubble coalescence simulation, the current recoloring operator showed better numerical stability and accuracy, as the maximum density ratio simulated was 85, which is an improvement over the results in Reis and Phillips's original paper. A simulation conducted to illustrate the problem of lattice pinning revealed that Reis and Phillips's recoloring operator is much more sensitive to this problem than the proposed recoloring operator. For the new model, the numerical results suggest that a low speed of sound can diminish the problem. The last numerical experiment showed that lattice pinning seems to come mainly from a lack of spatial resolution, because, when enough lattice sites are used to define a bubble, the phenomenon disappears. Because, in general, a high enough spatial resolution is chosen to resolve the scale of interest, we can conclude that lattice pinning should not be a problem in the majority of immiscible two-phase flow applications. In conclusion, when the results are compared with those of the Reis and Phillips model [31], the adaptation of the Latva-Kokko and Rothman recoloring operator for this model greatly increases the rate of convergence, improves the numerical stability and accuracy of the solutions over a wide range of model parameters, and significantly reduces the intensity of the spurious currents and lessens the lattice pinning problem.

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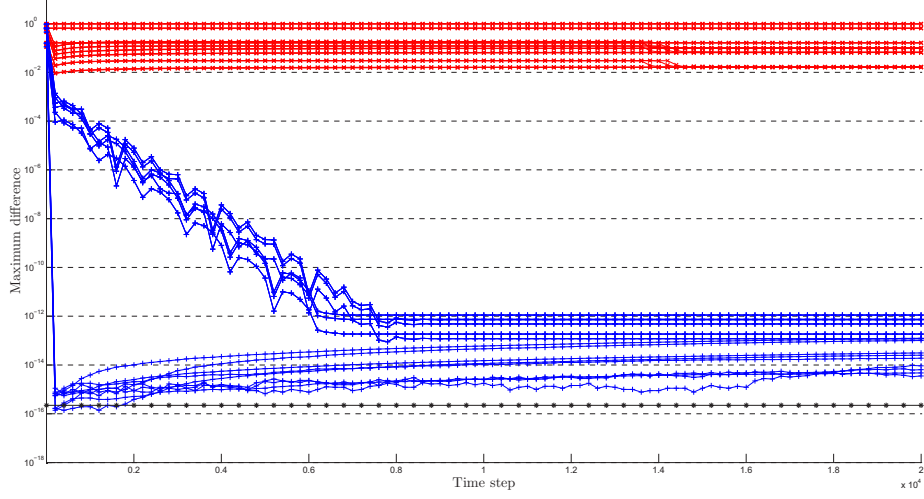


FIGURE 1: Convergence of all planar interface simulations for recoloring operator I (red cross) and operator II (blue plus sign). Reference : machine epsilon (black star), y-axis is in log-scale.

γ	A	ρ_r	R	$\sigma_{predict}$	Recoloring I		Recoloring II	
					$\max \ \vec{u}\ $	$E_I(\%)$	$\max \ \vec{u}\ $	$E_{II}(\%)$
1	4e-04	1	20	1.066e-03	1.969e-04	3.36	3.308e-04	1.83
1	4e-04	1	40	1.066e-03	2.242e-04	2.55	2.639e-04	2.65
1	4e-04	6	20	6.400e-03	1.894e-04	3.33	3.308e-04	1.83
1	4e-04	6	40	6.400e-03	2.242e-04	2.54	2.639e-04	2.65
1	1e-02	1	20	2.666e-02	5.360e-03	3.17	1.296e-03	0.58
1	1e-02	1	40	2.666e-02	6.349e-03	2.76	1.299e-03	0.40
1	1e-02	6	20	1.600e-01	5.526e-03	3.30	1.296e-03	0.58
1	1e-02	6	40	1.600e-01	6.349e-03	2.76	1.299e-03	0.40
6	4e-04	1	20	6.222e-04	2.092e-02	84.8	4.493e-04	0.36
6	4e-04	1	40	6.222e-04	1.452e-02	74.3	2.133e-04	1.37
6	4e-04	6	20	3.733e-03	2.017e-02	60.3	4.493e-04	0.36
6	4e-04	6	40	3.733e-03	1.446e-02	88.0	2.133e-04	1.37
6	1e-02	1	20	1.555e-02	2.066e-02	1.51	2.726e-03	2.46
6	1e-02	1	40	1.555e-02	2.543e-02	3.56	2.884e-03	0.80
6	1e-02	6	20	9.333e-02	2.069e-02	1.50	2.726e-03	2.46
6	1e-02	6	40	9.333e-02	2.543e-02	3.47	2.884e-03	0.80

TABLE 3: Parameters, maximum spurious currents, and errors for the steady bubble test case.

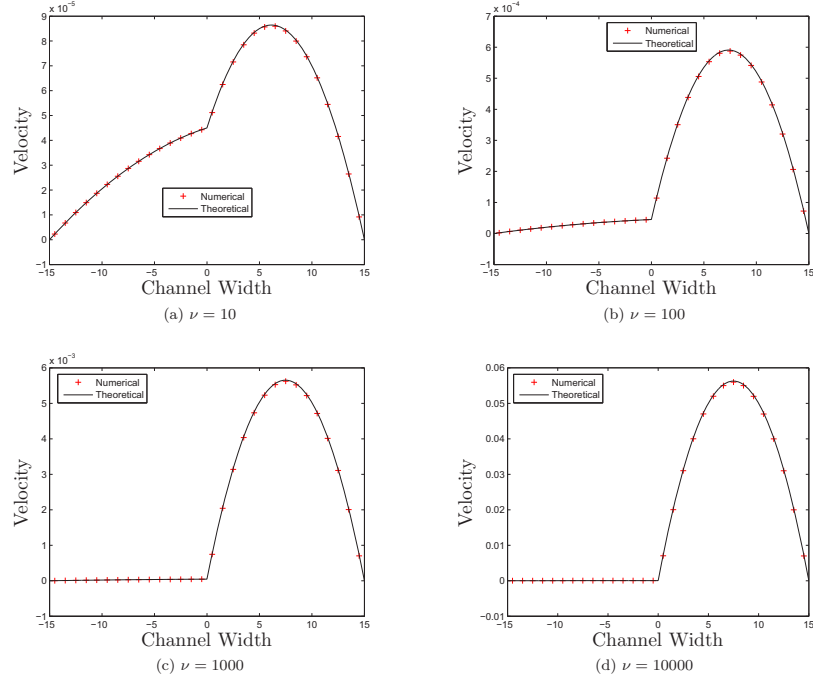


FIGURE 2: Numerical and theoretical velocity profile for the layered Poiseuille flow obtained with recoloring operator II and a different viscosity ratio, ν .

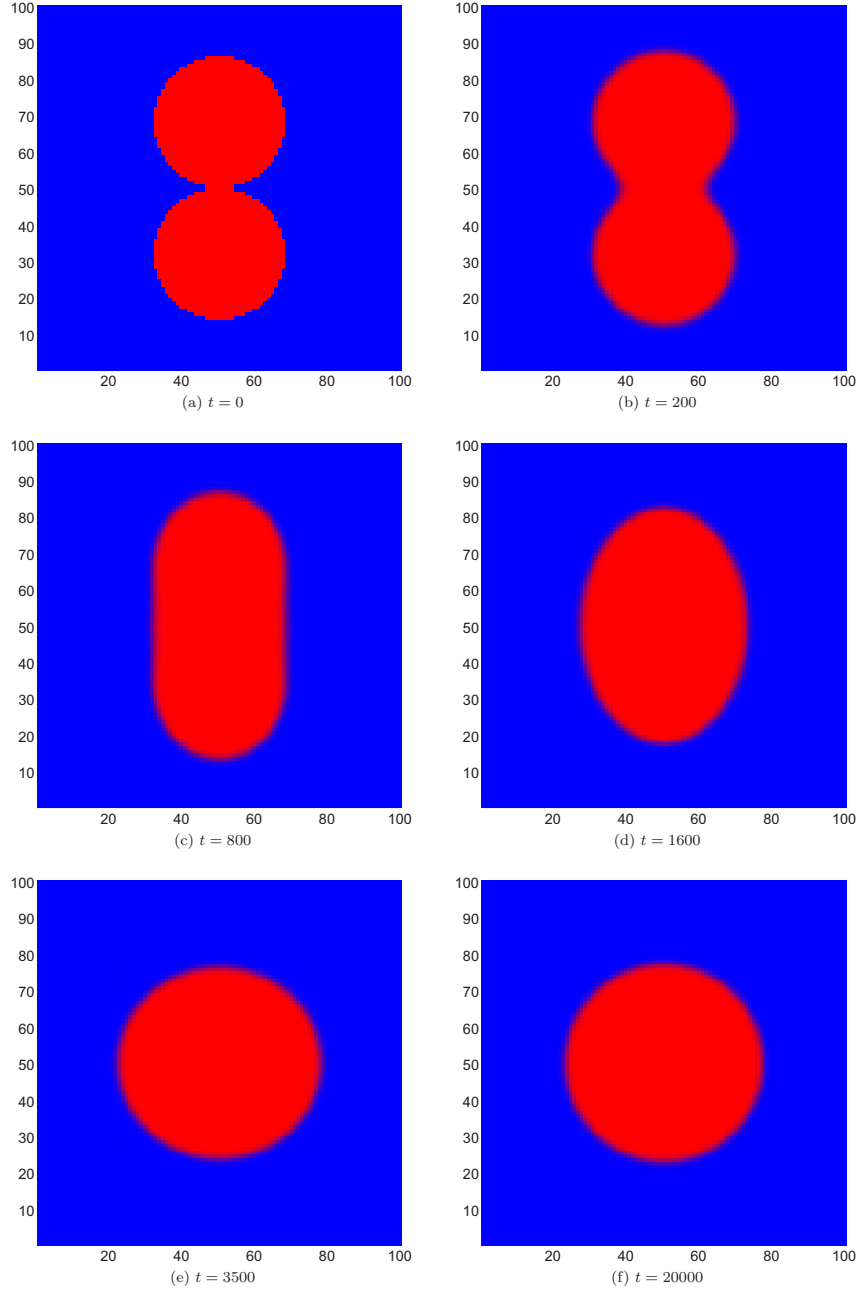


FIGURE 3: Collision of two dense red bubbles in a less dense fluid at different times ($\gamma = 35$).

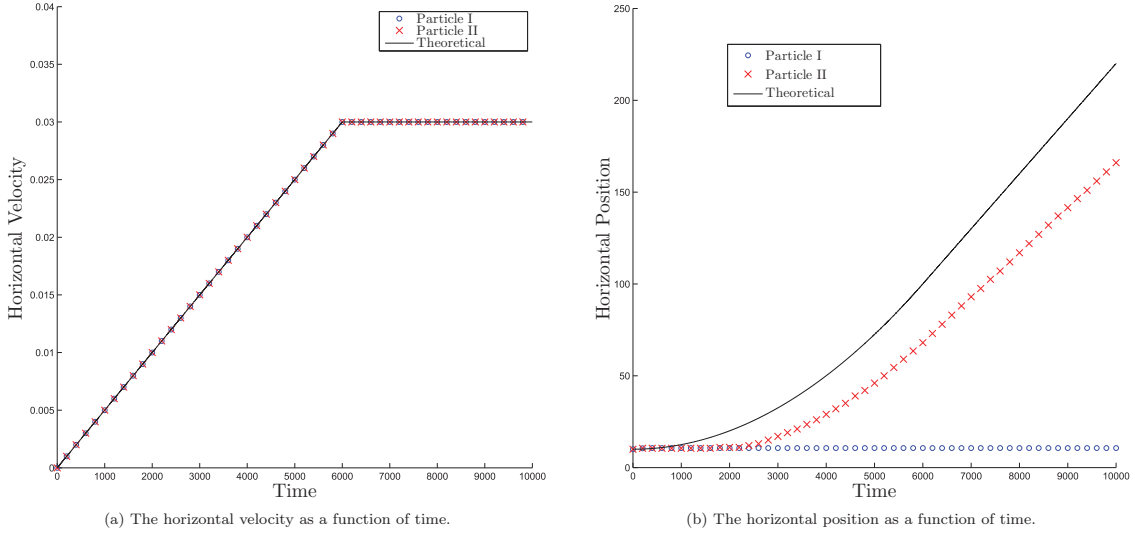


FIGURE 4: Study of the lattice pinning problem.

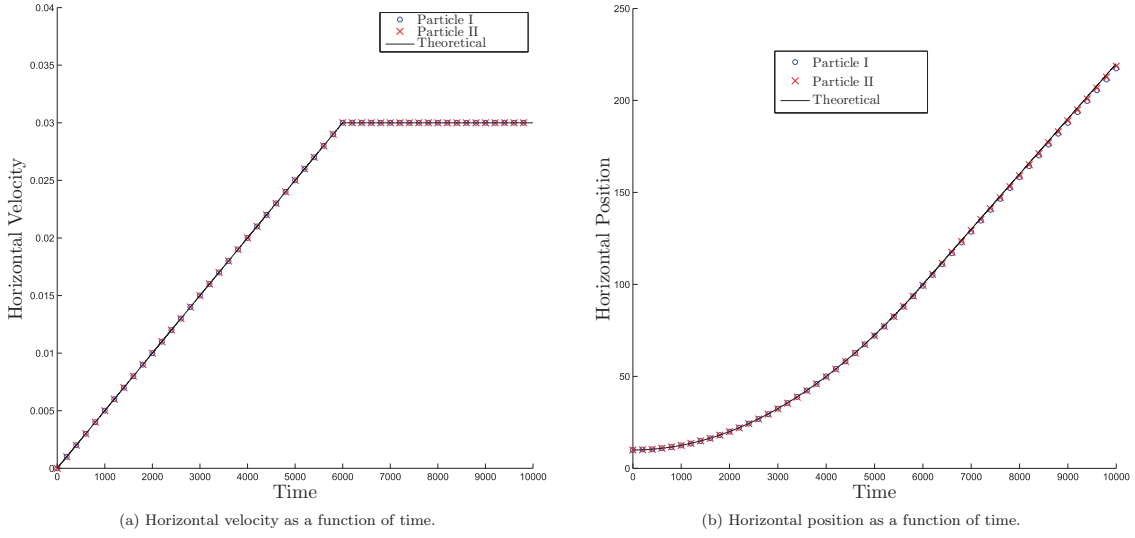


FIGURE 5: Recovery of the analytical solution with a better spatial resolution.

ANNEXE B

Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model

Il est important de noter que cet article a peut être été sujet à des changements avant la publication finale de celui-ci.

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, “Isotropic color gradient for simulating very high-density ratios with a two-phase flow lattice Boltzmann model”, manuscript submitted to *Computers & Fluids* in October 2010.

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Isotropic color gradient for simulating very high density ratios with a two-phase flow lattice Boltzmann model

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Abstract

This study presents the integration of isotropic color gradient discretization into a lattice Boltzmann Rothman-Keller (RK) model designed for two-phase flow simulation. The proposed model removes one limitation of the RK model, which concerns the handling of $O(1000)$ large density ratios between the fluids for a wide range of parameters. Taylor's series expansions are used to characterize the difference between an isotropic gradient discretization and the commonly used anisotropic gradient. The proposed color gradient discretization can reduce, by one order of magnitude, the spurious current problem that affects the interface between the phases. A set of numerical tests is conducted to show that a rotationally invariant discretization enables widening of the parameter range for the surface tension. Surface tensions from $O(10^{-2})$ to $O(10^{-8})$, depending on the density ratio, are accurately simulated. An extreme density ratio of $O(10000)$ is successfully tested for a steady bubble with an error of 0.5% for Laplace's law across a sharp interface, with a thickness of about 5-6 lattice units.

1 Introduction

For two decades now, a new method for examining fluids in the molecular state, rather than at the classical macroscopic level, has been developed and used as a tool for numerical flow simulation. This alternative, known as the lattice Boltzmann method (LBM), uses continuous distribution functions [27], and was originally built as an extension of the lattice gas automata [5]. Later, it was discovered that the method can also be regarded as a systematic truncation of the Boltzmann equation in the velocity space [12]. The advantages of the LBM are the way in which it addresses computational issues in complex geometries, and that it is simple to apply, because the streaming operator is linear.

One of the features of the LBM is its great flexibility in dealing with additional complex physics, which is difficult for the traditional CFD methods, based on the Navier-Stokes equations, to handle. Multiphase flow is a typical example of such complex physics. In this case, even some existing LBMs still face problems because of their limited parameter window with respect to surface tension and density ratio, which hampers its application in practical engineering problems. Before setting out the specific goal of this study, we briefly recall the techniques commonly used to predict multiphase flows within the lattice Boltzmann framework.

The lattice Boltzmann (LB) models for immiscible two-phase flows can generally be classified in five groups : Rothman-Keller (RK) [24, 10, 6, 23, 8, 7, 4, 38, 39, 40], Shan-Chen (SC) [35], Free Energy (FE) [36, 11], mean-field (MF) [15, 13], and field mediator (FM) [32].

The original RK model considers two types of fluids, red and blue, each of them with particle distributions following its own LB equation. Because there are two fluids involved, the collision step, intrinsic to any LB formulation, takes into account interactions among particles of the same color, as well as cross interactions between particles of different colors. These latter are related to the surface tension between the two phases, which requires the gradient of the color function. The phase separation is achieved with an additional recoloring step. For the original RK models, this step is seen as cumbersome to program. Recently, however, the ideas of Latva-Kokko and Rothman [23] have made it very easy and straightforward to implement, along with the additional capability of interface thickness adjustment. Work to introduce thermodynamics into the RK model has also been carried out, by Kono et al. [20].

The model developed by Shan and Chen [35] uses an interaction force between the particles to mimic microscopic interactions and automatically separate the concentrated and diluted phases. This spontaneous phase segregation is a feature that has attracted LB practitioners and contributed to the popularity of the SC model.

The free energy method of Swift et al. [36] describes an approach which, in equilibrium, leads to a steady state that can be associated with a free energy. The method uses collision rules, which ensure that the system evolves towards the minimum of an input free energy functional. This functional includes both the pure fluid part and the interface part. The first accounts for the equilibrium between two phases, while the second concerns surface tension. Like the SC model, this formulation is also capable of achieving automatic phase separation.

The MF methods simulate interparticle attraction in the same way as the Coulomb interaction is treated in the Vlasov equation [15]. These models can simulate thermodynamically consistent liquid-vapor systems, where the SC models fail [14].

The FM methods use null-mass particles, the only role of which is to invert the momentum of lattice particles in the transition layer to segregate fluids of different colors [32]. They have the advantage of being able to incorporate binary diffusivity, and this method can therefore be adapted to simulate miscible fluids.

A major problem common to these five methods is that they all appear to suffer from the presence of spurious currents at the interface between the fluids. These currents affect numerical stability, limit the density ratio, and reduce accuracy.

Spurious currents at a two-fluid interface in the RK method have been studied by Ginzbourg and Adler [6], who noted that an appropriate choice of the eigenvalues of the collision matrix leads to the elimination of these currents under certain circumstances. Unfortunately, the authors conclude that these unrealistic currents cannot be eliminated or reduced solely with the choice of eigenvalues. The spu-

rious current phenomenon near an interface has also been mentioned by Halliday et al. in [10], where it was found that these currents are strongest at the interface between two fluids. To reduce them, Dupin et al. [4] proposed adjusting the surface tension between the fluids by disturbing the distribution functions in accordance with the directions of the lattice. This idea seemed promising, but has not been further explored.

In this paper, an improvement to the RK-type model, described in Refs. [24, 30], is proposed which reduces spurious currents. It should be noted that the methodology presented here can be applied to any RK-type LB model.

A characteristic that distinguishes the RK model from other models is the presence of a color gradient. For two-phase LB flows, the color gradient was introduced by Rothman and Keller [31] with their model based on cellular automata. It is by using the color gradient that the interface between the fluids is maintained, and evaluating the color gradient is the key point that we address in this study. Specifically, the goal of this work is to show that an isotropic discretization of the color gradient, that is, with a leading discretization error that is rotationally invariant [21], increases the robustness of the method. This is of primary importance, because it ensures less accumulation of directionally biased discretization errors, and one consequence of using it is a reduction in spurious currents. This ultimately means that it will be possible to solve problems with a higher density ratio and/or with lower surface tension than previously achieved with other RK-type models.

Another challenge facing LBMs designed to simulate two-phase flows is handling the high-density ratio between the phases. Ratios of $O(160)$ were simulated by Kuzmin and Mohamad [22] using a multi-range, multi-relaxation time LB scheme. However, this improved SC method is still unable to simulate a $O(1000)$ air-to-water density ratio. With the projection method, an FE scheme devised by Inamuro et al. [17, 18] succeeded in simulating density ratios of up to $O(1000)$. Unfortunately, this method requires the solution of a costly Poisson equation at every time step. Other methods, such as the one proposed by Lee and Lin [25], can treat high-density ratios, like $O(1000)$, using a special discretization of the LB equation. Although it seems quite complex, this discretization works well, according to the authors. Another promising approach has been developed by Zheng et al. [41], which can also achieve $O(1000)$ density ratios and does not require the solution of a Poisson equation or the implementation of a complex treatment of derivatives. More recently, Becker et al. [1] succeeded in simulating density ratios as high as $O(1000)$ using the LBM and the level set method. However, coupling the LBM and the level set method is not straightforward, because doing so requires knowledge from two different research fields.

The RK model has been shown to be capable of simulating complex two-phase flow problems, but with density ratios reaching only $O(80)$ [24]. Our study will show that this limit can be substantially increased. The method is based on a modified recoloring operator presented by Leclaire et al. [24], which, when combined with the improvement presented in this work, can handle high-density ratios, up to $O(10000)$, with great accuracy for Laplace's law. Specifically, the model is based on that of Reis and Phillips [30], with a variant of the recoloring operator from Latva-Kokko et al. [23]. This improvement is expected to allow high-density ratios to be addressed for all RK models.

When applying the RK method, anisotropic color gradients are mostly used [10, 38, 4, 7, 23, 6, 16, 40]. In fact, an isotropic color gradient is seldom used, and can only be found in [39, 19]. Unfortunately, in these studies, neither the advantage of using such a gradient discretization, nor the reason for doing so, is explained.

In contrast, for the three LBMs for multiphase flows, FE, MF, and

SC, isotropic gradients have been used. For the FE methods, Tiribocchi et al. [37] show that there is a reduction in the spurious current by one order of magnitude when the gradient in the source term of their model is defined using a rotationally invariant discretization. Spurious currents were also reduced in the work of Pooley and Furtado [29] when an isotropic gradient is used, along with the addition of a special forcing term.

More recently, Chiappini et al. [3] proposed an MF model which completely eliminates spurious currents, but, unfortunately, the model does not respect the principle of mass conservation.

Similarly, isotropic discretizations have been introduced for the SC methods [34] for the gradient of the “effective mass function”, represented by the interparticle interactions. Again, it is shown that the more isotropy there is in the gradient, the lower the spurious currents. A detailed description of isotropic gradient stencils and weights can be found in the work of Sbragaglia et al. [33] for 2D and 3D spaces.

In this paper, we present the development of a second order color gradient discretization, while for higher order gradients, the stencils and weights developed by Sbragaglia et al. [33] will be used. This choice will make it possible to improve the accuracy of the RK model presented in [24]. To our knowledge, there is no study showing that the implementation of an isotropic color gradient in RK models provides a significant reduction in spurious currents, widens the range of application of the surface tension, or greatly increases the maximum density ratio handled between the two phases.

This paper is organized in two major sections. In the first, the LB model is given, along with theoretical details to illustrate the difference between isotropic and anisotropic gradients. In the second, a large number (hundreds) of numerical simulations are performed for a steady bubble, combining the various parameters of the model. These tests allow us to analyze the influence of gradient discretization on the solution and to demonstrate the need for an isotropic gradient, and its superiority, versus the standard anisotropic approximation. The primary goal of our paper is to demonstrate the usefulness of an isotropic gradient discretization for the RK model.

2 Lattice Boltzmann immiscible two-phase model

The current LB approach follows the model of Reis and Phillips [30], along with the improvement presented by Leclaire et al. [24] for the recoloring operator. For the sake of clarity, we recall the model described in Refs. [24, 30]. For this two-dimensional LB model, there are two sets of distribution functions, one for each fluid, moving on a D2Q9 grid with the velocity vectors $\vec{c}_i$. With $\theta_i = \frac{\pi}{4}(4 - i)$, the velocity vectors are defined as ($\Delta x = \Delta y = 1$) :

$$\vec{c}_i = \begin{cases} (0, 0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)], & i = 2, 4, 6, 8 \\ [\sin(\theta_i), \cos(\theta_i)] \sqrt{2}, & i = 3, 5, 7, 9 \end{cases} \quad (1)$$

The distribution functions for a fluid of color k (with $k = r$ for red or $k = b$ for blue) are noted $N_i^k(\vec{x}, t)$, while $N_i(\vec{x}, t)$ is used for the sum $N_i^r(\vec{x}, t) + N_i^b(\vec{x}, t)$. If the time step is $\Delta t = 1$, the algorithm uses the following evolution equation :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t) + \Omega_i^k(N_i^k(\vec{x}, t)) \quad (2)$$

where the collision operator Ω_i^k is the result of the combination of three sub operators (similar to Ref. [38]) :

$$\Omega_i^k = (\Omega_i^k)^{(3)} \left[(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)} \right] \quad (3)$$

In the algorithm, the evolution equation is solved in four steps with operator splitting, as follows :

1. Single-phase collision operator :

$$N_i^k(\vec{x}, t_*) = (\Omega_i^k)^{(1)}(N_i^k(\vec{x}, t))$$

2. Two-phase collision operator (perturbation) :

$$N_i^k(\vec{x}, t_{**}) = (\Omega_i^k)^{(2)}(N_i^k(\vec{x}, t_*))$$

3. Two-phase collision operator (recoloring) :

$$N_i^k(\vec{x}, t_{***}) = (\Omega_i^k)^{(3)}(N_i^k(\vec{x}, t_{**}))$$

4. Streaming operator :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t_{***})$$

2.1 Single-phase collision operator

The first sub operator, $(\Omega_i^k)^{(1)}$, is the standard BGK operator of the single-phase LBM, where the distribution functions are relaxed towards a local equilibrium in which ω_k denotes the relaxation factor :

$$(\Omega_i^k)^{(1)}(N_i^k) = N_i^k - \omega_k (N_i^k - N_i^{k(e)}) \quad (4)$$

Here, some details concerning this operator are given. The density of the fluid k is given by the first moment of the distribution functions :

$$\rho_k = \sum_i N_i^k = \sum_i N_i^{k(e)} \quad (5)$$

where the superscript (e) denotes equilibrium. The total fluid density is given by $\rho = \rho_r + \rho_b$, while the total momentum is defined as the second moment of the distribution functions :

$$\rho \vec{u} = \sum_i \sum_k N_i^k \vec{c}_i = \sum_i \sum_k N_i^{k(e)} \vec{c}_i \quad (6)$$

in which $\vec{u}$ is the density weighted average velocity of the fluid. The equilibrium functions are defined by [30] :

$$N_i^{k(e)} = \rho_k \left(\phi_i^k + W_i \left[3\vec{c}_i \cdot \vec{u} + \frac{9}{2}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}(\vec{u})^2 \right] \right) \quad (7)$$

These equilibrium distribution functions $N_i^{k(e)}$ are chosen to respect the principles of mass and momentum conservation. The weights W_i are those of a standard D2Q9 lattice :

$$W_i = \begin{cases} 4/9, & i = 1 \\ 1/9, & i = 2, 4, 6, 8 \\ 1/36, & i = 3, 5, 7, 9 \end{cases} \quad (8)$$

Besides,

$$\phi_i^k = \begin{cases} \alpha_k, & i = 1 \\ (1 - \alpha_k)/5, & i = 2, 4, 6, 8 \\ (1 - \alpha_k)/20, & i = 3, 5, 7, 9 \end{cases} \quad (9)$$

As introduced in [7], in order to obtain a stable interface, the density ratio γ is defined by :

$$\gamma = \frac{\rho_r}{\rho_b} = \frac{1 - \alpha_b}{1 - \alpha_r} \quad (10)$$

Without loss of generality, $\rho_r \geq \rho_b$ in this paper. The pressure of the fluid of color k is :

$$p^k = \frac{3\rho_k(1 - \alpha_k)}{5} = \rho_k(c_s^k)^2 \quad (11)$$

where, in the above expressions, either α_r or α_b represents a free parameter, and c_s^k is the sound speed in the fluid of color k [30, 2].

The relaxation parameters ω_k are chosen so that the evolution equation (2) respects the macroscopic equations for single-phase flow in the single-phase regions [30]. This parameter is a function of the fluid viscosity ν_k , given by $\omega_k = 1/(3\nu_k + \frac{1}{2})$. As introduced in [7], when the viscosities of the fluids are different, an interpolation is applied to define the parameter ω_k at the interface. To do this, it is necessary to introduce the color field :

$$\psi = \frac{\rho_r - \rho_b}{\rho_r + \rho_b} \quad (12)$$

The color field ψ is a function with its image between -1 and 1 . It takes the value 1 or -1 , depending on whether it is evaluated at a position that contains only the red fluid or only the blue fluid. At an interface, the color field is obviously between -1 and 1 . The relaxation factor ω_k in Eq. 4 is replaced by ω :

$$\omega = \begin{cases} \omega_r, & \psi > \delta \\ f_r(\psi), & \delta \geq \psi > 0 \\ f_b(\psi), & 0 \geq \psi \geq -\delta \\ \omega_b, & \psi < -\delta \end{cases} \quad (13)$$

in which δ is a free parameter and

$$\begin{aligned} f_r(\psi) &= \chi + \eta\psi + \kappa\psi^2 \\ f_b(\psi) &= \chi + \lambda\psi + \nu\psi^2 \end{aligned} \quad (14)$$

with

$$\begin{aligned} \chi &= 2\omega_r\omega_b/(\omega_r + \omega_b) \\ \eta &= 2(\omega_r - \chi)/\delta \\ \kappa &= -\eta/(2\delta) \\ \lambda &= 2(\chi - \omega_b)/\delta \\ \nu &= \lambda/(2\delta) \end{aligned} \quad (15)$$

The free parameter δ is required to calculate ω , and influences the thickness of the interface when the fluid viscosities are different [30]. The larger δ , the thicker the fluid interface. If the fluid viscosities are the same, the parameter δ does not have an impact on the solution, because, in this case, $\omega = \omega_r = \omega_b$.

2.2 Perturbation operator

In the RK model, surface tension is modeled by means of the perturbation operator [10, 30, 9]. In this model, with $\vec{F}$, the color gradient in terms of the color difference, the perturbation operator, is defined by :

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \frac{A_k}{2}|\vec{F}| \left[W_i \frac{(\vec{F} \cdot \vec{c}_i)^2}{|\vec{F}|^2} - B_i \right] \quad (16)$$

where

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (17)$$

Reis and Phillips [30] have shown that this operator complies with the macroscopic equations for two-phase flows. It handles the coupling between the two fluids, with the free parameters A_k chosen to model

the surface tension. Although this operator generates the surface tension, it does not guarantee the fluid's immiscibility. To minimize the mixing and segregate the two fluids, the recoloring operator (Ω_i^k)⁽³⁾ needs to be properly selected. This process is introduced in the next subsection. But first, some insight concerning the discretization of the color gradient is needed.

2.2.1 Standard anisotropic color gradient

The color gradient direction is an approximation of the perpendicular to the interface between the fluids. Usually, the color gradient in the RK model is defined by :

$$\vec{F}(\vec{x}) = \sum_i \vec{c}_i (\rho_r(\vec{x} + \vec{c}_i) - \rho_b(\vec{x} + \vec{c}_i)) = \sum_i \vec{c}_i \Delta(\vec{x} + \vec{c}_i) \quad (18)$$

with $\Delta = \rho_r - \rho_b$ introduced to simplify the following derivation. Without loss of generality, the function Δ is expressed using a two-dimensional Taylor series expansion around the zero vector :

$$\begin{aligned} \Delta(x, y) = & \Delta(0, 0) + x \frac{\partial \Delta}{\partial x} \Big|_{(0,0)} + y \frac{\partial \Delta}{\partial y} \Big|_{(0,0)} + \frac{1}{2} x^2 \frac{\partial^2 \Delta}{\partial x^2} \Big|_{(0,0)} \\ & + xy \frac{\partial^2 \Delta}{\partial x \partial y} \Big|_{(0,0)} + \frac{1}{2} y^2 \frac{\partial^2 \Delta}{\partial y^2} \Big|_{(0,0)} + \frac{1}{6} x^3 \frac{\partial^3 \Delta}{\partial x^3} \Big|_{(0,0)} \\ & + \frac{1}{2} x^2 y \frac{\partial^3 \Delta}{\partial x^2 \partial y} \Big|_{(0,0)} + \frac{1}{2} x y^2 \frac{\partial^3 \Delta}{\partial x \partial y^2} \Big|_{(0,0)} \\ & + \frac{1}{6} y^3 \frac{\partial^3 \Delta}{\partial y^3} \Big|_{(0,0)} + O(x^n y^m) \end{aligned}$$

with $n + m > 3$. To approximate the gradient in the x direction, the following stencil values, marked with a "red cross" in Fig. 1, can be taken : $\Delta(h, h)$, $\Delta(h, 0)$, $\Delta(h, -h)$, $\Delta(-h, -h)$, $\Delta(-h, 0)$, and $\Delta(-h, h)$.

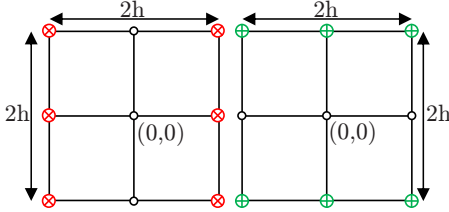


FIGURE 1: Stencil points.

When these stencil values are combined, as in the case of the standard anisotropic color gradient (Eq. 18), an approximation of the gradient in the x direction at $(0, 0)$ is obtained :

$$\begin{aligned} \frac{\partial \Delta}{\partial x} \Big|_{(0,0)} = & \frac{1}{6h} \left[\Delta(h, h) + \Delta(h, 0) + \Delta(h, -h) \right. \\ & \left. - \Delta(-h, -h) - \Delta(-h, 0) - \Delta(-h, h) \right] \\ & - \frac{h^2}{6} \frac{\partial^3 \Delta}{\partial x^3} \Big|_{(0,0)} - \frac{h^2}{3} \frac{\partial^3 \Delta}{\partial x^2 \partial y} \Big|_{(0,0)} + O(h^3) \end{aligned} \quad (19)$$

Using the stencil values marked with a "green plus sign" in Fig. 1, a

similar expression is found for the y direction :

$$\begin{aligned} \frac{\partial \Delta}{\partial y} \Big|_{(0,0)} = & \frac{1}{6h} \left[\Delta(-h, h) + \Delta(0, h) + \Delta(h, h) \right. \\ & \left. - \Delta(h, -h) - \Delta(0, -h) - \Delta(-h, -h) \right] \\ & - \frac{h^2}{6} \frac{\partial^3 \Delta}{\partial y^3} \Big|_{(0,0)} - \frac{h^2}{3} \frac{\partial^3 \Delta}{\partial x \partial y^2} \Big|_{(0,0)} + O(h^3) \end{aligned} \quad (20)$$

In the approximate gradients of Eq. 19 and 20, the leading differential operator of the second order error term ($O(h^2)$) can be written in vector form :

$$\vec{E}^{(2)} = -\frac{h^2}{6} \left[\frac{\partial^3}{\partial x^3} + 2 \frac{\partial^3}{\partial x^2 \partial y}, \frac{\partial^3}{\partial y^3} + 2 \frac{\partial^3}{\partial x \partial y^2} \right] \quad (21)$$

Using the following partial derivative operator transformation :

$$\frac{\partial}{\partial x} = \cos(\theta) \frac{\partial}{\partial r} - \frac{1}{r} \sin(\theta) \frac{\partial}{\partial \theta} \quad (22)$$

$$\frac{\partial}{\partial y} = \sin(\theta) \frac{\partial}{\partial r} + \frac{1}{r} \cos(\theta) \frac{\partial}{\partial \theta} \quad (23)$$

and by supposing that $\Delta = \Delta(r)$, it is possible to show (after a lengthy algebraic manipulation) that, when the differential operator $\vec{E}^{(2)}$ is applied to $\Delta(r)$, the resulting vector will have a Euclidean norm that is a function of θ and r , except if $\Delta(r)$ is a constant. This result, that is, the norm $\|\vec{E}^{(2)} \Delta(r)\| \equiv f(r, \theta)$, is an equation that takes up almost a page and so is not presented here. This result can easily be obtained with symbolic mathematics software. For a vector function to be rotationally invariant, it must have a Euclidean norm that is a function of the radius only. Therefore, this color gradient approximation is not isotropic to the second order in space, but anisotropic. It is worth noting that, even if the function Δ is isotropic (i.e. $\Delta = \Delta(r)$) around $(0, 0)$, the calculated derivatives have an error leading term that is not isotropic. This means that, when the color gradient is approximated with this finite difference stencil, the color gradient calculated will not conserve the isotropic property of the differentiated function.

2.2.2 Isotropic color gradient

Taking into consideration the anisotropy problem of the standard color gradient, it is possible to change the weights of the grid points when computing the gradient to make them isotropic up to the second order in space by defining the gradients in the x and y directions, as follows :

$$\begin{aligned} \frac{\partial \Delta}{\partial x} \Big|_{(0,0)} = & \frac{1}{12h} \left[\Delta(h, h) + 4\Delta(h, 0) + \Delta(h, -h) - \Delta(-h, -h) \right. \\ & \left. - 4\Delta(-h, 0) - \Delta(-h, h) \right] - \frac{h^2}{6} \frac{\partial}{\partial x} \left(\frac{\partial^2 \Delta}{\partial x^2} + \frac{\partial^2 \Delta}{\partial y^2} \right) \Big|_{(0,0)} \\ & - \frac{h^4}{72} \frac{\partial}{\partial x} \left(\frac{\partial^4 \Delta}{\partial x^4} + 2 \frac{\partial^4 \Delta}{\partial x^2 \partial y^2} + \frac{\partial^4 \Delta}{\partial y^4} \right) \Big|_{(0,0)} \\ & - \frac{h^4}{180} \frac{\partial^5 \Delta}{\partial x^5} \Big|_{(0,0)} + O(h^5) \end{aligned} \quad (24)$$

$$\begin{aligned}
\left. \frac{\partial \Delta}{\partial y} \right|_{(0,0)} &= \frac{1}{12h} \left[\Delta(-h, h) + 4\Delta(0, h) + \Delta(h, h) - \Delta(h, -h) \right. \\
&\quad \left. - 4\Delta(0, -h) - \Delta(-h, -h) \right] - \frac{h^2}{6} \frac{\partial}{\partial y} \left(\frac{\partial^2 \Delta}{\partial x^2} + \frac{\partial^2 \Delta}{\partial y^2} \right) \Big|_{(0,0)} \\
&\quad - \frac{h^4}{72} \frac{\partial}{\partial y} \left(\frac{\partial^4 \Delta}{\partial y^4} + 2 \frac{\partial^4 \Delta}{\partial x^2 \partial y^2} + \frac{\partial^4 \Delta}{\partial x^4} \right) \Big|_{(0,0)} \\
&\quad - \frac{h^4}{180} \frac{\partial^5 \Delta}{\partial y^5} \Big|_{(0,0)} + O(h^5)
\end{aligned} \tag{25}$$

With this new discretization, the dominant differential operator of the second order error term takes the form :

$$\bar{E}^{(2)} = [E_x^{(2)}, E_y^{(2)}] = -\frac{h^2}{6} \left[\frac{\partial}{\partial x} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right), \frac{\partial}{\partial y} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] \tag{26}$$

If a gradient has a small dependence on direction, this would imply that the dominant error term has only an axial dependence when the function being derived also only depends on the radius. That is, the operator in Eq. 26 applied on $\Delta(r)$ would lead to a function that depends only on the radius :

$$\bar{E}^{(2)} \Delta(r) \equiv \vec{e}_r f(r) \tag{27}$$

with $\vec{e}_r = [\cos(\theta), \sin(\theta)]$ being the unit radial vector. Using the partial derivative operator transformation of Eqs. 22 and 23, and supposing that $\Delta = \Delta(r)$ around (0,0), the components $E_x^{(2)} \Delta(r)$ and $E_y^{(2)} \Delta(r)$ are :

$$E_x^{(2)} \Delta(r) = \frac{h^2 \cos(\theta)}{6r^2} \left(-\frac{\partial \Delta(r)}{\partial r} + r \frac{\partial^2 \Delta(r)}{\partial r^2} + r^2 \frac{\partial^3 \Delta(r)}{\partial r^3} \right) \tag{28}$$

$$E_y^{(2)} \Delta(r) = \frac{h^2 \sin(\theta)}{6r^2} \left(-\frac{\partial \Delta(r)}{\partial r} + r \frac{\partial^2 \Delta(r)}{\partial r^2} + r^2 \frac{\partial^3 \Delta(r)}{\partial r^3} \right) \tag{29}$$

which can be rewritten in the same form as Eq. 27. Similarly, the first differential operator of the fourth order error term in Eqs. 24 and 25 takes the form :

$$\begin{aligned}
\bar{E}_{iso}^{(4)} = [E_{x,iso}^{(4)}, E_{y,iso}^{(4)}] &= -\frac{h^4}{72} \left[\frac{\partial}{\partial x} \left(\frac{\partial^4}{\partial x^4} + 2 \frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial y^4} \right), \right. \\
&\quad \left. \frac{\partial}{\partial y} \left(\frac{\partial^4}{\partial y^4} + 2 \frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial x^4} \right) \right]
\end{aligned} \tag{30}$$

and the associated components in polar coordinates, when applied to a rotationally invariant function $\Delta(r)$ around (0,0), are given by :

$$\begin{aligned}
E_{x,iso}^{(4)} \Delta(r) &= \frac{h^4 \cos(\theta)}{72} \left(3 \frac{\partial \Delta(r)}{\partial r} - 3r \frac{\partial^2 \Delta(r)}{\partial r^2} + 3r^2 \frac{\partial^3 \Delta(r)}{\partial r^3} \right. \\
&\quad \left. - 2r^3 \frac{\partial^4 \Delta(r)}{\partial r^4} - r^4 \frac{\partial^5 \Delta(r)}{\partial r^5} \right)
\end{aligned} \tag{31}$$

$$\begin{aligned}
E_{y,iso}^{(4)} \Delta(r) &= \frac{h^4 \sin(\theta)}{72} \left(3 \frac{\partial \Delta(r)}{\partial r} - 3r \frac{\partial^2 \Delta(r)}{\partial r^2} + 3r^2 \frac{\partial^3 \Delta(r)}{\partial r^3} \right. \\
&\quad \left. - 2r^3 \frac{\partial^4 \Delta(r)}{\partial r^4} - r^4 \frac{\partial^5 \Delta(r)}{\partial r^5} \right)
\end{aligned} \tag{32}$$

which again meet the rotational invariance requirement and can be rewritten in the same form as given in Eq. 27. The last differential error operator of the fourth order error term in Eqs. 24 and 25 is :

$$\bar{E}_{ani}^{(4)} = -\frac{h^4}{180} \left[\frac{\partial^5}{\partial x^5}, \frac{\partial^5}{\partial y^5} \right] \tag{33}$$

and can be shown to be anisotropic (i.e. f in Eq. 27 would also be a function of θ). Therefore, the error associated with the anisotropy is lower by two orders when compared to the main second order leading term. It is important to point out that both gradient approximations presented so far are second order approximations in space, but only the latter is a second order approximation in space for the isotropy.

In order to link the gradient approximation to the current LB formulation, $h = 1$ needs to be taken for the lattice spacing. In a more general way, the stencil points with the corresponding weights needed to obtain 2D and 3D isotropic gradients can be found in Ref. [33].

In this paper, the focus is on the four color gradient approximations presented in Table 1 : the standard second order anisotropic color gradient $\bar{F}_I$ (Eq. 18), the second order isotropic color gradient $\bar{F}_{II}$ (Eqs. 24 and 25), a fourth order isotropic color gradient $\bar{F}_{III}$, and a sixth order isotropic color gradient $\bar{F}_{IV}$. The weights for calculating $\bar{F}_{III}$ and $\bar{F}_{IV}$ were taken from [33]. The vectors $\vec{d}$ and the weights ξ of Table 1 could be represented, for example, by the vectors and weights of a pseudo D2Q25 lattice numbered as in Table 2.

24	25	10	11	12
23	9	2	3	13
22	8	1	4	14
21	7	6	5	15
20	19	18	17	16

TABLE 2: Analogy with a D2Q25 lattice for numbering the vector $\vec{d}$ and the weight ξ needed to compute the color gradient approximation.

2.3 Recoloring operator

This last operator is used to maximize the amount of red fluid at the interface sent to the red fluid region, and the amount of blue fluid sent to the blue fluid region, while respecting the principles of conservation of mass and total momentum. The recoloring operator presented in [24] is used, which was derived from [23] :

$$(\Omega_i^r)^{(3)}(N_i^r) = \frac{\rho_r}{\rho} N_i + \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \tag{34}$$

$$(\Omega_i^b)^{(3)}(N_i^b) = \frac{\rho_b}{\rho} N_i - \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\varphi_i) \sum_k N_i^{k(e)}(\rho_k, 0, \alpha_k) \tag{35}$$

where β is a free parameter and $\cos(\varphi_i)$ is the cosine of the angle between the color gradient $\vec{F}$ and the direction $\vec{c}_i$. The equilibrium distributions of each fluid $N_i^{k(e)}$ in Eqs. 34 and 35 are evaluated using the respective value of α_k and a zero velocity. The value of $\cos(\varphi_1)$ must equal 0 in order to conserve mass. Also, the parameter β must be between 0 and 1 to ensure that the distribution functions remain positive [23]. The parameter β influences the thickness of the interface : the smaller its value, the thicker the interface.

In the work [24], the recoloring operator used by Reis and Phillips is compared with that of Latva-Kokko, which has been adapted for the Reis and Phillips model [30]. Detailed comparisons were performed on : the planar interface, the steady bubble, unsteady bubble collision, the variable viscosity layered Poiseuille flow, and lattice pinning. We conclude that the Latva-Kokko recoloring operator adapted to the current model greatly increases the accuracy of the Reis and Phillips model for a wide range of parameters. But, as is shown in this paper, the Reis and Phillips model with the Latva-Kokko recoloring algorithm alone (and with the second order anisotropic color gradient) is not sufficient to tackle high density on a steady bubble

$\vec{F}(\vec{x}) = \sum_{i=1}^{i=25} \xi_i \vec{d}_i \Delta(\vec{x} + \vec{d}_i)$	
$\vec{F}_I$	$\vec{\xi} = [0, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$
$\vec{F}_{II}$	$\vec{\xi} = [0, 4, 1, 4, 1, 4, 1, 4, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]/12$
$\vec{F}_{III}$	$\vec{\xi} = [0, 32, 12, 32, 12, 32, 12, 32, 12, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0]/120$
$\vec{F}_{IV}$	$\vec{\xi} = [0, 960, 448, 960, 448, 960, 448, 960, 448, 84, 32, 1, 32, 84, 32, 1, 32, 84, 32, 1, 32, 84, 32, 1, 32, 84, 32, 1, 32]/5040$

TABLE 1: Different color gradient stencils and weights.

with accuracy. Therefore, in the numerical results section, the accuracy of the isotropic discretization for the color gradient is compared to the standard second order anisotropic color gradient. The use of the isotropic discretization for the color gradient led to a significant increase in the accuracy of the model.

2.4 Setting the surface tension

Following a theoretical development from Ref. [30] and his predecessors [10], it is possible to predict the surface tension between the two fluids using only the basic parameters of the model. Knowing the form of the expression describing the surface tension and performing simulations on planar interfaces, as in Refs. [24, 30], a function of ρ_r , γ , ω , A_r , and A_b can be determined to approximately describe the surface tension. In this work, different color gradient approximations are used and, depending on which is selected, the surface tension is set in a slightly different way. When the second order anisotropic color gradient is used, $\vec{F}_I$, the surface tension is adjusted by combining the model parameters, as follows [24] :

$$\sigma_{ani} = \frac{4}{3} \frac{(1 + \frac{1}{\gamma}) \frac{\rho_r}{2}}{\omega} (A_r + A_b) \quad (36)$$

A similar expression is used for the second $\vec{F}_{II}$, fourth $\vec{F}_{III}$, and sixth order $\vec{F}_{IV}$ isotropic color gradient. The surface tension is also adjusted in a same way, but with a different multiplicative constant :

$$\sigma_{iso} = \frac{2}{9} \frac{(1 + \frac{1}{\gamma}) \frac{\rho_r}{2}}{\omega} (A_r + A_b) \quad (37)$$

2.5 Incompressible limit of the model

The current model exploits the possibility of using different speeds of sound in each phase. It is known that the value of $\sqrt{1/3}$ for the speed of sound in the LBM is only one possibility, and that it is only the most common one [26]. The speed of sound in the LBM is set by the value of the rest lattice weight α_k [28]. Different speeds of sound mean that the Navier-Stokes equations are recovered in each phase with their own speed of sound. Moreover, and most importantly, at the interface, Reis and Phillips have shown that the equations for two-phase flows are also recovered [30]. It is by exploiting the fact that different speeds of sound can be taken in each phase that the RK model can simulate the density ratios between the phases [7].

Now let us look at the incompressible condition of the LBM in the context of this model. Because the speed of sound in the high-density phase (red fluid in our model) is lower than in the low-density phase, the maximum possible Mach number, $M_{\max}$, in the flow at each position in the computational domain is approximately equal to :

$$M_{\max} \approx \frac{|\vec{u}|}{c_s^r} \quad (38)$$

To verify the incompressible limit, we want to keep a small Mach number, let's say smaller than 0.1. This leads to the following constraint :

$$|\vec{u}| \leq (0.1) c_s^r \quad (39)$$

Eq. 11 then gives :

$$|\vec{u}| \leq (0.1) \sqrt{3/5(1 - \alpha_r)} \quad (40)$$

Finally, Eq. 10 gives :

$$|\vec{u}| \leq (0.1) \frac{\sqrt{3/5(1 - \alpha_b)}}{\sqrt{\gamma}} \quad (41)$$

For the light phase, as low a value of α_b as possible, is always chosen to help the incompressible limit constraint of the red phase. In this paper, we chose $\alpha_b = 0.2$. It is then found that, in the LB unit system, maximum velocity is inversely proportional to the square root of the density ratio. Because of the square root, the constraint is not as limiting as might be expected, and further research may one day remove it altogether. When the density ratio is high, it is important to respect the constraint in Eq. 41. In this paper, when the results are accurate, the incompressible limit of the LBM is respected.

3 Numerical Results

The focus of the numerical simulations is on the circular steady bubble, because it is the best test case for evaluating the isotropy of the numerical scheme. In this section, we concentrate on a steady (red) bubble of radius R immersed in a different (blue) fluid.

Only calculations aimed at stationary solutions are performed here, so it is convenient to introduce the stopping criterion common to all simulations :

$$\max_{\text{all distribution functions}} \left\{ |(N_i^k)^{(n)} - (N_i^k)^{(n-1)}| \right\} \leq \epsilon \quad (42)$$

with $\epsilon = 10^{-9}$ and n denoting the time step number. This condition is only checked every 2000 time steps, in order to reduce the computational cost. Under this criterion, all the numerically stable simulations performed in this paper converge in a finite number of time steps. Even though this criterion is rigorous, it does not necessarily guarantee that all solutions will be fully steady. However, all the numerically stable simulations converge to results that represent the steady state solutions well. The number of time steps required to converge the solution to such a small value of ϵ could be high, and, because many numerical simulations were undertaken, the computational cost limited the choice for ϵ .

Some input parameters are the same for all numerical simulations, and these are listed in Table 3. We can see that, depending on γ , the

α_b	δ	ν_r	ν_b
0.2	0.1	1/6	1/6

TABLE 3: Constant input parameters for all simulations.

value of α_r is found from Eq. 10. The value for α_k should normally be chosen to obtain the standard weight (4/9) when the density ratio is unity. However, in our particular case, to compare the overall trend for many density ratios, it is better to choose the same α_b for all simulations. Therefore, we chose a value of $\alpha_b = 0.2$ that is not too high, to help reduce the incompressible LBM constraint in the red, higher density phase (Eq. 41).

The free parameter δ does not influence the solution, because only the unit viscosity ratio is simulated. The decision to choose fluid viscosities that will yield a unit relaxation time was made for simplicity. Note that $\omega = 1$ is not necessarily the most accurate.

3.1 Steady bubble : Laplace's law

The aim of this subsection is to verify whether or not the surface tensions of the model predicted by Eqs. 36 and 37 are consistent with Laplace's law [9, 30] :

$$\sigma_{Laplace} = R\Delta p \quad (43)$$

where $\Delta p = p_{in} - p_{out}$ is the pressure jump across the inside and outside of the bubble. The pressures of the bubble, inside p_{in} and outside p_{out} , are measured as follows :

$$\begin{aligned} p_{in} &= p_{in}^r + p_{in}^b = \frac{3}{5}\rho_{r,in}(1 - \alpha_r) + \frac{3}{5}\rho_{b,in}(1 - \alpha_b) \\ p_{out} &= p_{out}^r + p_{out}^b = \frac{3}{5}\rho_{r,out}(1 - \alpha_r) + \frac{3}{5}\rho_{b,out}(1 - \alpha_b) \end{aligned} \quad (44)$$

with

$$\begin{aligned} \rho_{r,in} &= \langle \{\rho_r | \psi \geq 0.999999\} \rangle \\ \rho_{b,in} &= \langle \{\rho_b | \psi \geq 0.999999\} \rangle \\ \rho_{r,out} &= \langle \{\rho_r | \psi \leq -0.999999\} \rangle \\ \rho_{b,out} &= \langle \{\rho_b | \psi \leq -0.999999\} \rangle \end{aligned} \quad (45)$$

where the symbol $\langle \cdot \rangle$ stands for the average.

In a previous work [24], the internal and external pressures were computed for each fluid separately in the single fluid regions considered. That is to say, the internal and external pressure calculations were performed using only the red and blue fluids respectively. According to the numerical model, the more consistent, easier, and more robust method is to compute the pressure by including the pressure contributions of both fluids, even if these are small on regions where one of them is fully predominant.

For these simulations, the computational domain is discretized with a lattice of 128×128 sites geometrically located over the computational domain $[1, 128] \times [1, 128]$. Initially, the red fluid is placed at a distance of at most R from the center of the computational domain $((x - 64.5)^2 + (y - 64.5)^2 \leq R^2)$. The fluid is initialized with zero velocity equilibrium distribution functions. For the blue fluid, the field is initialized in the same way. Periodic boundary conditions are used at the four ends of the computational domain. Depending on the color gradient, the parameters $A_r = A_b$ are obtained from Eqs. 36 or 37 and by using the surface tension σ_{ani} or σ_{iso} , and the other three parameters ρ_r , γ , and ω .

A total of 674 simulations were selected to study how the various parameters in the current model influence the accuracy of the results. This is the number of all the possible combinations of input parameters, i.e. $674 = 4 \times 7 \times 2 \times 3 \times 3 \times 1 + 4 \times 7 \times 2 \times 3 \times 1 \times 1$. Tables 4 and 5 summarize these combinations.

Color gradient	$\sigma_{ani} = \sigma_{iso}$	R	ρ_r	γ	β
$\vec{F}_I$	10^{-2}	20	0.2	1	0.99
$\vec{F}_{II}$	10^{-3}	30	1	100	
$\vec{F}_{III}$	10^{-4}		5	1000	
$\vec{F}_{IV}$	10^{-5}				
	10^{-6}				
	10^{-7}				
	10^{-8}				

TABLE 4: Some combinations of parameters for the steady bubble simulations.

Color gradient	$\sigma_{ani} = \sigma_{iso}$	R	ρ_r	γ	β
$\vec{F}_I$	10^{-2}	20	0.2	1000	0.7
$\vec{F}_{II}$	10^{-3}	30	1		
$\vec{F}_{III}$	10^{-4}		5		
$\vec{F}_{IV}$	10^{-5}				
	10^{-6}				
	10^{-7}				
	10^{-8}				

TABLE 5: Some combinations of parameters for the steady bubble simulations.

Below, the superscript i indicates a quantity obtained at the end of the i^{th} simulation. Let us denote by :

$$E_I^i = 100 \frac{|\sigma_{Laplace}^i - \sigma_{ani}^i|}{\sigma_{ani}^i} \quad (46)$$

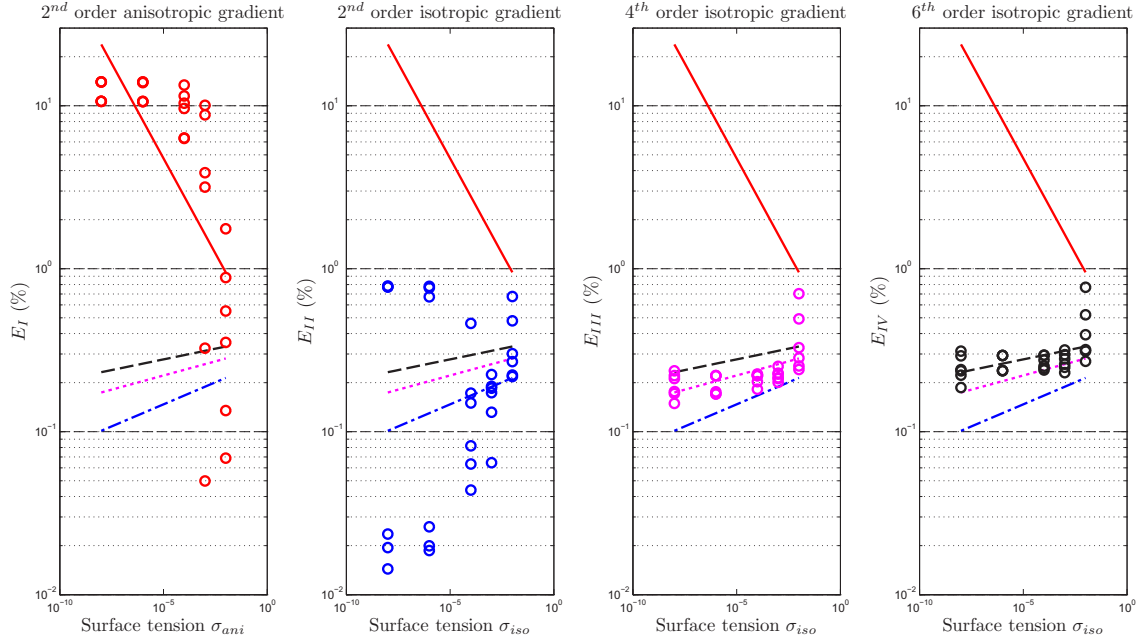
the relative error, as a percentage, between the surface tension σ_{ani} and $\sigma_{Laplace}^i$, with σ_{ani} as a reference when the simulation is performed with the anisotropic color gradient $\vec{F}_I$. Similarly, when the simulation is performed with the isotropic color gradients $\vec{F}_{II}$, $\vec{F}_{III}$, or $\vec{F}_{IV}$, the relative error is denoted E_{II}^i , E_{III}^i , or E_{IV}^i , but with σ_{iso} used as reference.

For a density ratio $\gamma = 1$, Fig. 3 shows the relative error as a function of the surface tension resulting from the various simulations listed in Table 4. In the same way, Figs. 4 and 5 show the relative errors for $\gamma = 100$ and $\gamma = 1000$ respectively. For a clear reading of the results presented in these figures, the plot convention must be explained : The axes are on a log-log scale. From left to right, they show the results obtained from the second order anisotropic gradient, second order isotropic gradient, fourth order isotropic gradient, and sixth order isotropic gradient. On each of these plots, there are four lines, each of them corresponding to a "linear best fit" obtained from the simulation results of a particular color gradient. This allows a better appreciation and comparison of the general behavior of the error as a function of surface tension for each of the four color gradients. The figures can be more easily understood when they are represented in color (available online), because the "best fit lines" are the same color as the points they fit. The line style specifiers used to associate the best fit lines with the color gradient are shown in Fig. 2.

The results displayed in Fig. 3 merit a few comments. First, for $\gamma = 1$, the gradient $\vec{F}_I$ leads to accurate and valid results only for a high surface tension. When low surface tensions are simulated, the gradient approximation $\vec{F}_I$ yields inaccuracy, represented by a non circular bubble at steady state. Further details of this behavior are given in the next subsection. In general, all isotropic gradient discretizations lead to more accurate results than the anisotropic gradient over all the surface tensions in the spectrum that were simulated, i.e. $O(10^{-2})$



FIGURE 2: Line style specifiers associated with the color gradient.

FIGURE 3: (Color online) Steady bubble : relative error with the Laplace surface tension as a function of surface tension ($\gamma = 1$ and $\beta = 0.99$).

to $O(10^{-8})$. Surprisingly, with the second order isotropic gradient, the results are more accurate, on average, than with the fourth and sixth order isotropic gradients. This strange behavior is found in the error for the surface tension plot only (Fig. 3), and not in the spurious currents plot (Fig. 9). It is important to keep in mind the way the inside pressure and outside pressure of the bubble are measured. The way to do this is heuristic (Eq. 44), which may have something to do with the observed behavior. We can only have full confidence in the surface tension errors when we look at the results on average, i.e. by looking at the overall trend of all 674 simulations. The tendency clearly shows improvement for the surface tension with an isotropic color gradient versus the original anisotropic discretization. Also note that the results for the spurious currents are more reliable, because their measurement is not heuristic, and this confirms the same trend in behavior. Nevertheless, we would have expected that the higher order gradients would always perform better than the lower order gradients. However, gradient-order effects are expected to be much more significant as the grid is refined, and better results could be expected on a fine grid with a higher order gradient. At least it can be said that the lower the surface tension, the better the precision (less scatter) with the higher order gradients. Results for the fourth and sixth order isotropic gradients are practically the same, with an error that is always less than 1%.

For $\gamma = 100$ in Fig. 4, the second order anisotropic gradient still leads to the worst results on average. An important fact to note is that, when increasing the density ratio to $O(100)$, the two second order gradient discretizations, both the isotropic and anisotropic, be-

have in the same way when the surface tension is low, i.e. the results are less accurate, or are inaccurate. This again can be explained by the deformation of the bubble shape. For the fourth order and sixth order isotropic gradients, the results are still similar, but the sixth order gradient starts to produce more accurate results in the low surface tension regime. This difference increases when the density ratio climbs to $O(1000)$. We need to point out that 10 of the simulations with $\gamma = 100$ were unstable in the $O(10^{-2})$ surface tension regime, and that this instability affects all four color gradients. To avoid distorting the pattern of the best fit lines, all simulations with $\sigma = 10^{-2}$ have been removed from Fig. 4.

For $\gamma = 1000$ in Fig. 5 and for the $O(10^{-2})$ and $O(10^{-3})$ surface tension regimes, 29 simulations among the four color gradients were unstable. As a result, all the simulations with $\sigma = 10^{-2}$ and $\sigma = 10^{-3}$ have been removed from Fig. 5. Overall, these simulations were unstable because the incompressible limit of the LBM was not respected. The spurious currents were too high and pulled in a high, non physical Mach number, which renders the simulation unstable. The results obtained for the two second order gradients were shown to be very similar to those of the previous case with $\gamma = 100$. These two gradients lacked sufficient isotropy to accurately simulate a low surface tension with a large density ratio. Looking at Fig. 5 for $\sigma = 10^{-4}$, it can be seen that the results are practically the same for all the isotropic gradients, and, as surface tension decreases, the higher order isotropic gradient always performs better than the second order isotropic gradient. With these model parameters, it also appears that the isotropy of the fourth and sixth order isotropic gradients is not sufficient

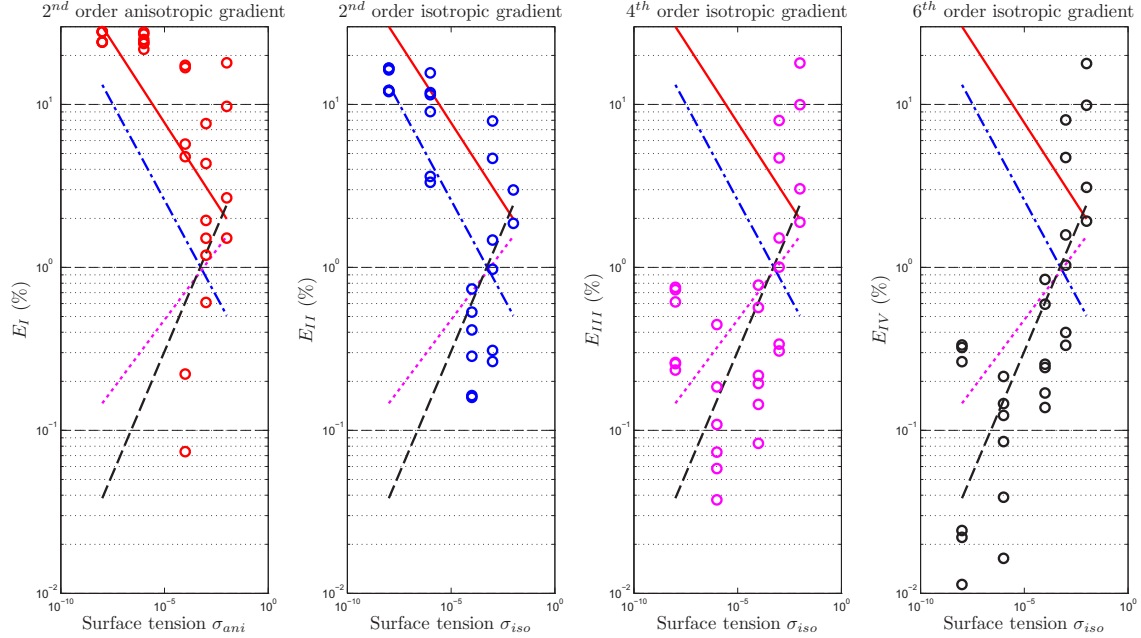


FIGURE 4: (Color online) Steady bubble : relative error with the Laplace surface tension as a function of surface tension ($\gamma = 100$ and $\beta = 0.99$).

to simulate the steady bubble accurately when the surface tension is very low, $O(10^{-7})$ or $O(10^{-8})$, as, at this limit, the error was found to be high for some simulations. Nevertheless, we can note that the sixth order isotropic gradient performs better than the fourth order one for a low surface tension.

To be able to accurately simulate very low surface tension with a large density ratio such as $O(1000)$, we can adjust the thickness of the interface to reduce the errors of the gradient discretization. By changing the parameter β from 0.99 to 0.7, the thickness of the interface increases slightly and the results become much more accurate. We can see from the simulation results of Table 5 shown in Fig. 6 that, for a density ratio of $O(1000)$ and for surface tensions from $O(10^{-8})$ to $O(10^{-4})$, the error with the Laplace surface tension is almost always less than 1% when the fourth or sixth order isotropic gradients are used. It might be possible, if the problem is well posed and not subject to numerical round-off error accumulation, to accurately simulate even lower surface tension, but this has not been tested. Also, it might be possible to use a higher value than 0.7 for β to achieve similar accuracy; however, this has not been tested either. Moreover, we note that the outcome of the two second order gradients, both isotropic and anisotropic, is unsatisfactory.

Overall, the above results can be summarized as follows. As the surface tension decreases, the error becomes smaller with an increase in the interface thickness and in the isotropy of the color gradient. This behavior becomes increasingly strong as the ratio of the density of the two fluids increases. In short, the interface thickness and the isotropy of the color gradient are two key factors required to accurately simulate large density ratios for a wide range of surface tensions. We must be careful to select an interface thickness that is not too large, because the numerical position of the interface may differ greatly from

the true physical one.

3.2 Steady bubble : Bubble deformation

In this subsection, four numerical simulations illustrate the reason why large errors are found when the second order isotropic or anisotropic color gradients are used with a low surface tension. In these simulations, the surface tension is set to 10^{-6} , also $\rho_r = 1$, $R = 30$, $\beta = 0.99$, and $\gamma = 10$. For each of the four color gradients, a snapshot of the color field ψ at steady state is shown in Fig. 7. The error with the Laplace surface tension obtained at steady state and the number of time steps needed to reach steady state are also listed in Table 6.

	$\vec{F}_I$	$\vec{F}_{II}$	$\vec{F}_{III}$	$\vec{F}_{IV}$
E_X (%)	24.31	1.639	0.207	0.239
t_{end}	190000	1808000	1096000	1028000

TABLE 6: Surface tension errors and time step number at steady state.

Looking at Fig. 7, it seems clear that the errors from Table 6 are mainly due to bubble deformation. The results obtained with the second order isotropic gradient are better than the diamond shaped bubble obtained with the second order anisotropic gradient. Note that the accuracy and the bubble shape obtained at steady state are much better with the higher order isotropic color gradient for this case. Since the bubble is deformed significantly with $\vec{F}_{II}$ and γ is relatively small, one conclusion is that the isotropy of this gradient

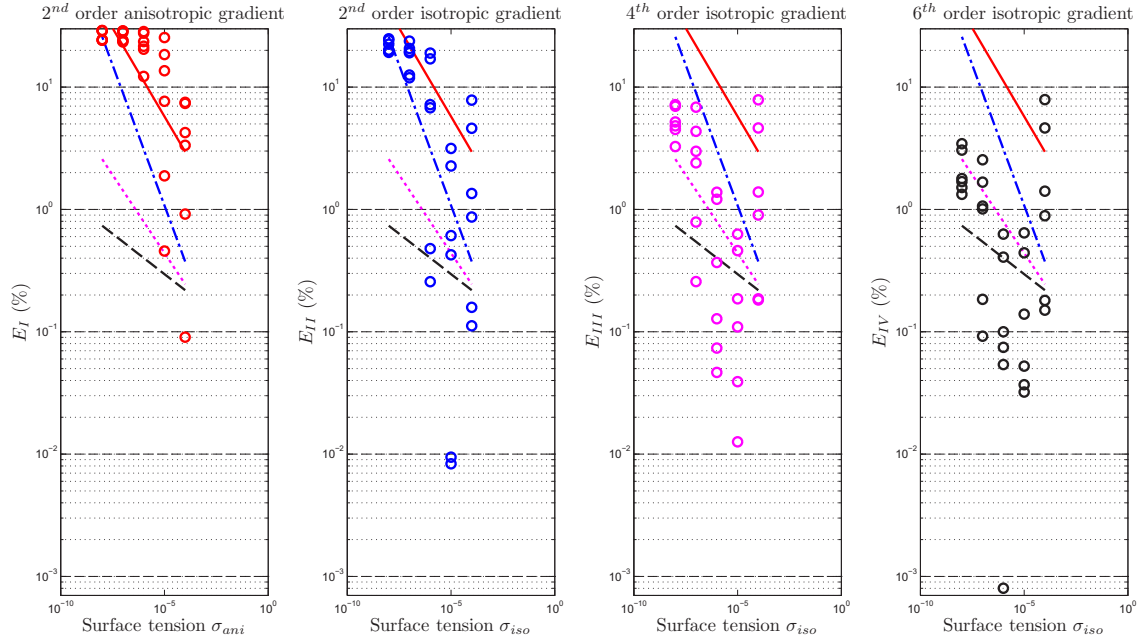


FIGURE 5: (Color online) Steady bubble : relative error with the Laplace surface tension as a function of surface tension ($\gamma = 1000$ and $\beta = 0.99$).

is not sufficient to produce accurate results for a low surface tension and a high density ratio.

When the surface tension is low, the effect of the gradient discretization errors may be of the same order as the effect of the cohesive force between the molecules, which is introduced by the perturbation operator to minimize the contact area between the two fluids. Note that more mass is added in the direction normal to the interface when perturbation is high. When the discretization errors generated by the gradient anisotropy are too large, the cohesive forces may not be able to maintain a minimal contact area. In other words, when using high order isotropic discretization, the effects of the errors arising from anisotropic discretization are probably less than the effects of the forces of cohesion, or at least not high enough to significantly deform the bubble. Similarly, when perturbation is low, the mass added in the direction normal to the interface cannot counter the effect of the accumulation of directionally biased discretization errors. This reasoning may explain, at least in part, the bubble deformation at low surface tension, along with the poor accuracy.

Spurious currents constitute another factor that needs to be taken into account, as they may also deform the bubble, although the anisotropic discretization error is probably the main cause of inaccuracy. The interface deformation may not be occurring primarily because of the effect of the velocity $\vec{u}$ in the equilibrium distribution of the single phase collision operator, but rather because of the anisotropic forces, caused by anisotropic discretization, that are present in the perturbation and recoloring operator. It is thought that this is the main problem, because, with a higher order isotropic color gradient, the approximation of the color gradient is better and the bubble deformation disappears. Spurious currents could also come from an anisotropic discretization of the Boltzmann equation. Therefore, spu-

rious currents seem to be a problem caused by anisotropy. Naturally, spurious currents are extremely important to numerical stability, as higher ones directly increase the Mach number in a non physical way. From this perspective, we can understand why high order isotropic color gradients are better at simulating fluids with a low surface tension.

Generally, the fourth order isotropic color gradient will be a better choice, for two reasons. The first is obvious : the bubble shape and accuracy at steady state are usually better. The second is less so : the bubble deformation with $\vec{F}_{II}$ happens very slowly, and therefore causes the simulation to reach steady state with many more time steps than with the fourth order isotropic gradient $\vec{F}_{III}$ (Table 6). Even though $\vec{F}_{III}$ costs more to calculate than $\vec{F}_{II}$, because some neighbors of neighbors are involved in calculating $\vec{F}_{III}$, the total simulation time is usually less with $\vec{F}_{III}$, owing to the smaller number of time steps needed to reach steady state (almost half, in this case).

3.3 Steady bubble : Spurious currents

First, we illustrate the problem of spurious currents with four numerical simulations. The surface tension, σ , is set to 10^{-2} , also $\rho_r = 1$, $R = 30$, $\beta = 0.99$, and $\gamma = 10$. For each of the four color gradients, a snapshot of the velocity magnitude field at steady state is shown in Fig. 8. (Color is available online, and is needed to fully appreciate these snapshots.) For each of the four plots, the velocity magnitude is scaled using the maximum velocity over the computational domain that was obtained at steady state from the simulation performed with the sixth order isotropic gradient. This makes it easier to compare the color gradients in terms of the magnitude of the spurious currents. The color bar is therefore scaled with two color "spectra". In order to

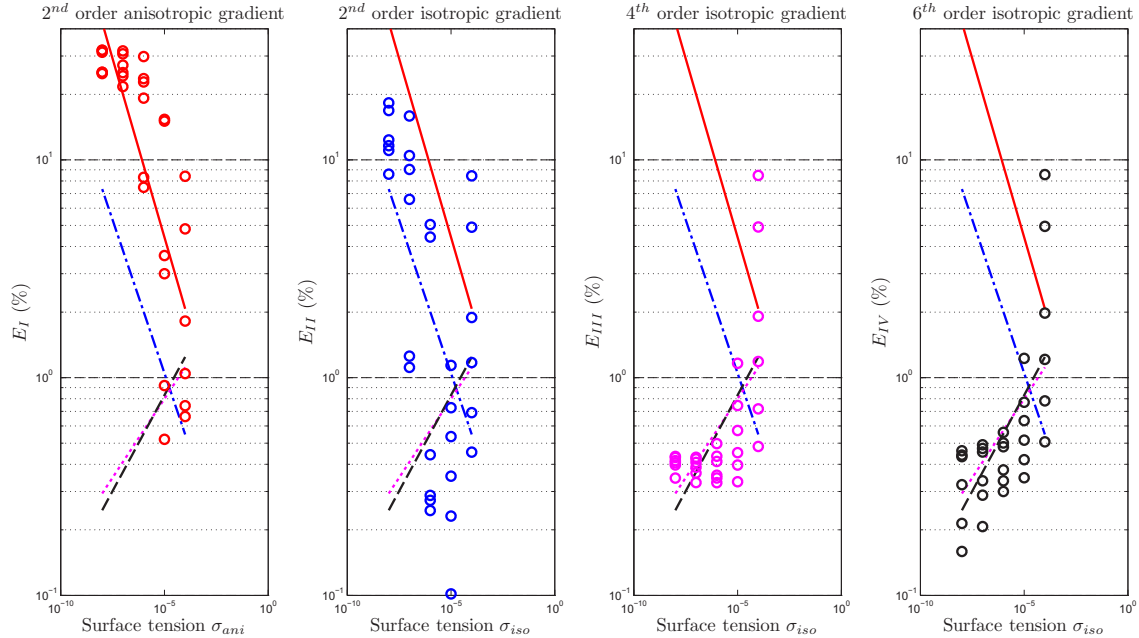


FIGURE 6: (Color online) Steady bubble : relative error with the Laplace surface tension as a function of surface tension ($\gamma = 1000$ and $\beta = 0.7$).

illustrate a velocity less than the maximum obtained with the sixth order isotropic gradient, the first color of the spectrum goes from white to green to represent a velocity ratio from 0 to 1. If the velocity ratio is greater than 1, then a second color spectrum is used that goes from white, to yellow, to red, to black, where black represents the magnitude of the maximum velocity of the current simulation. The bubble shape is also plotted over the velocity magnitude field. An important feature of the bubble shape, because surface tension is high, is that it is circular at steady state for all gradient discretizations.

Looking at the color bar in Figs. 8a and 8b, we can see that the spurious currents are reduced by one order of magnitude ($\approx 18/1.8$) when the second order isotropic gradient is used instead of the second order anisotropic gradient. This result is very similar to the findings of [37, 34] with the FE and SC methods. As did Halliday et al. in [10], we found that the spurious currents are strongest at the interface.

It is also important to note that a significant, but not very large, reduction in the spurious currents is achieved using the fourth order isotropic gradient instead of the second order isotropic gradient. Between the fourth and sixth order gradient, there is almost no reduction in spurious currents. It seems, therefore, that the fourth order isotropic gradient is worth the cost for these cases versus the second order isotropic gradient. Here, the sixth order isotropic gradient has not been shown to be worth applying when its results are compared with those obtained with the fourth order isotropic gradient.

Figs. 9, 10, and 11 show the maximum velocity magnitude at steady state as a function of the surface tension in the same way as the relative error is shown as a function of the surface tension in Figs. 3, 4, and 5. Again, these plots are drawn using the simulation results obtained with the various input parameters in Table 4, which provides a much better overview of the spurious currents as a function of the

model parameters.

From Fig. 9, we can note that, for $\gamma = 1$, the intensity of the spurious currents is linearly proportional to the surface tension. This suggests that the perturbation operator (Eq. 16) introduces anisotropic forces, since the importance of this operator is also linearly dependent on the surface tension. Perhaps a perturbation operator that would distribute the tension forces in a more isotropic way would greatly reduce the spurious currents. In other words, perhaps the whole perturbation operator is not highly isotropic, despite the fact that the discretization of the color gradient is highly isotropic. This is reminiscent of the idea of Dupin et al. [4], who adjusted the surface tension differently, depending on the direction of the lattice, in order to reduce the spurious currents. These currents are probably linked to the anisotropy problem at different steps of the numerical scheme. However, it is encouraging to see that, as the gradient approximation becomes more isotropic, the spurious currents are reduced. This is in agreement with the work of Ref. [33].

The results of $\gamma = 100$ in Fig. 10 reveal that the spurious currents are stronger than with $\gamma = 1$. We conclude from this that an important factor influencing these currents is the density ratio. Their intensity is also roughly a linear function of the surface tension. We note that, on average and when the surface tension is low, the second order isotropic gradient does not seem capable of reducing the spurious currents. It is important to remember that the error associated with the Laplace surface tension was also high in this regime, and so was the deformation of the bubbles. This may affect the spurious currents. The fourth and sixth order isotropic gradients have almost the same behavior and produce smaller spurious currents than the second order gradients, which make them more accurate with respect to spurious currents than the other gradients.

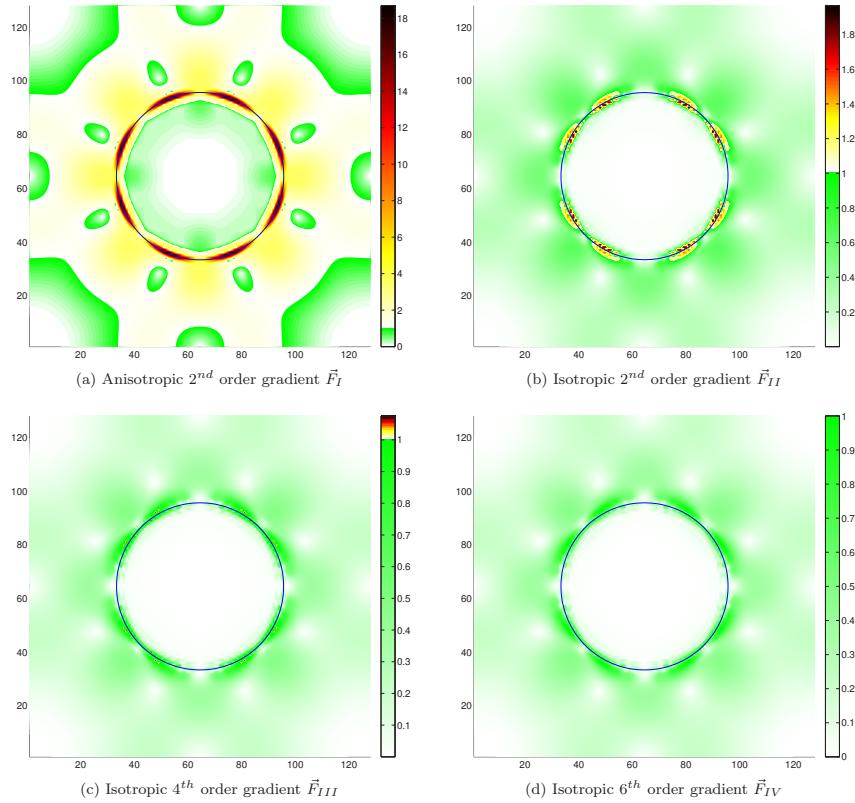


FIGURE 8: (Color online) Spurious currents at steady state obtained from different color gradient ($\gamma = 10$).

For $\gamma = 1000$, the figures are very similar to the case with $\gamma = 100$. By increasing the density ratio, the spurious currents increase, but, this time, the sixth order isotropic gradient reduces them significantly compared to the fourth order isotropic gradient. As for the figures that show the errors with the Laplace surface tension, the spurious currents indicate that the isotropy of the color gradient is an important factor influencing accuracy.

The simulation results in Table 5 show that the effect of the interface thickness does influence the spurious currents in a significant way. Those for $\gamma = 1000$ and $\beta = 0.7$ are shown in Fig. 12. The spurious currents can be reduced by as much as two orders of magnitude by choosing $\beta = 0.7$ instead of $\beta = 0.99$, and even more when the interface thickness is further decreased. Two alternatives are proposed for reducing the spurious currents : increase the isotropy of the color gradient discretization, or increase the interface thickness to reduce the gradient discretization errors.

3.4 Steady bubble : Very high density ratio

To test the stability limit and accuracy of the model, a final simulation with a very high density ratio between the fluids was performed ($\gamma = 10000$) using the fourth order isotropic color gradient. For this simulation, the input parameters and the results are summarized in Table 7. The accuracy of the result is very good with a 0.507% er-

Color gradient	γ	ρ_r	R	β	σ_{iso}	E_{III} (%)
$\vec{F}_{III}$	10000	1	30	0.99	10^{-5}	0.507

TABLE 7: Input parameters and the error obtained with the Laplace surface tension for a very high density ratio steady bubble ($\gamma = 10000$).

ror at steady state between the Laplace surface tension (Eq. 43) and the surface tension set using the model parameters (Eq. 37). To fully appreciate the numerical steady state solution, there is a plot of the density profile at $x = 64$ for each fluid in Figs. 13a and 13b. These density profiles show that the interface is fairly clean and sharp, with a thickness of about 5-6 lattice units. The results obtained are excellent for such an extreme case. Moreover, the bubble shape at steady state is circular, as illustrated in Fig. 13c. With this model and for the steady bubble case, we can conclude that the fourth order isotropic color gradient can lead to accurate simulation of a very high density ratio.

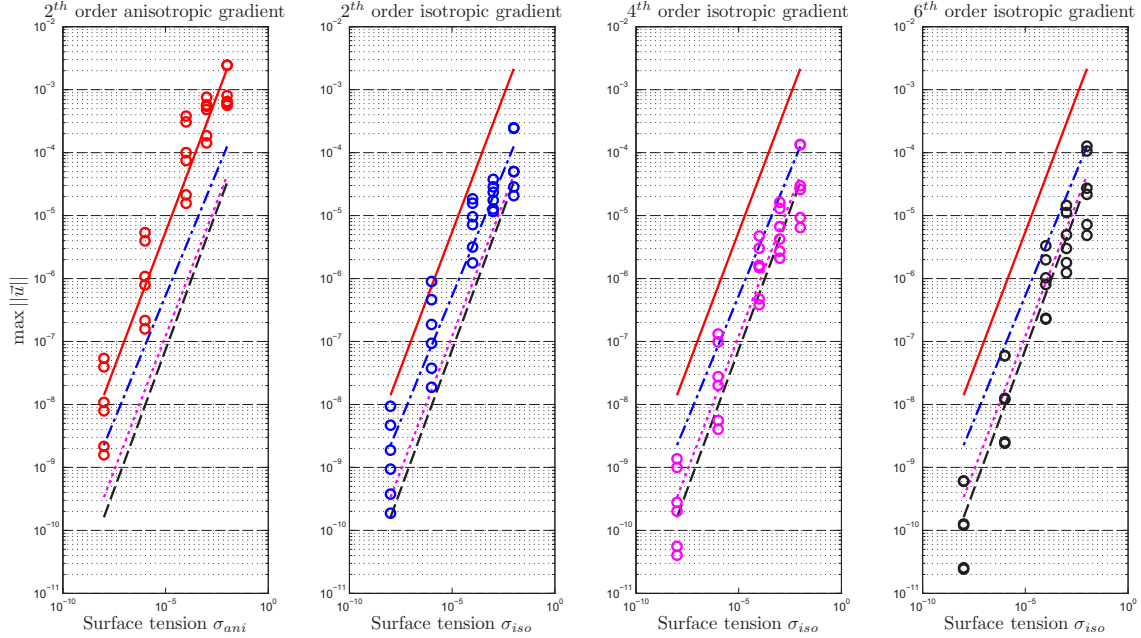


FIGURE 9: (Color online) Maximum velocity magnitude as a function of the surface tension resulting from the various simulations of the steady bubble ($\gamma = 1$ and $\beta = 0.99$).

4 Conclusion

In this study, we showed that the isotropy of the color gradient is crucial to RK-type lattice Boltzmann schemes for the solution of two-phase flow problems. The simulations revealed that, when the isotropy of the color gradient is poor, the surface tension result is not reliable. For a steady bubble problem, we showed that isotropic color gradients up to second order in space are not sufficient to treat low surface tension (bubble deformation), with an average density variation of $O(10)$. However, the isotropic color gradients of the fourth and sixth order make it possible to accurately simulate density ratios as high as $O(1000)$, depending on the surface tension. To be able to accurately simulate very low surface tension with a $O(1000)$ density ratio, the interface thickness must also be carefully selected, and our investigation here indicates that it is possible to simulate two-phase air-to-water density ratio with the LB color gradient method. In such a case, an isotropic gradient of higher order (fourth or sixth) capable of handling a high density ratio is worth its cost. For this model, our study also suggests that the spurious currents are mainly caused by anisotropic forces introduced at the various stages of the numerical scheme. Overall, the isotropic color gradient reduces the spurious currents, widens the range of applicability of the surface tension, and allows the accurate simulation of high density ratios for Laplace's law. In practice, this also can be appreciated by keeping the circular shape of a two-dimensional bubble at steady state. Finally, we believe that the advantages of isotropic color gradients can be extended to all RK-type schemes.

Acknowledgement

The authors thank the anonymous reviewers for their insightful and constructive comments. This work was supported by a grant from FQRNT "Le Fonds Québécois de la Recherche sur la Nature et les Technologies".

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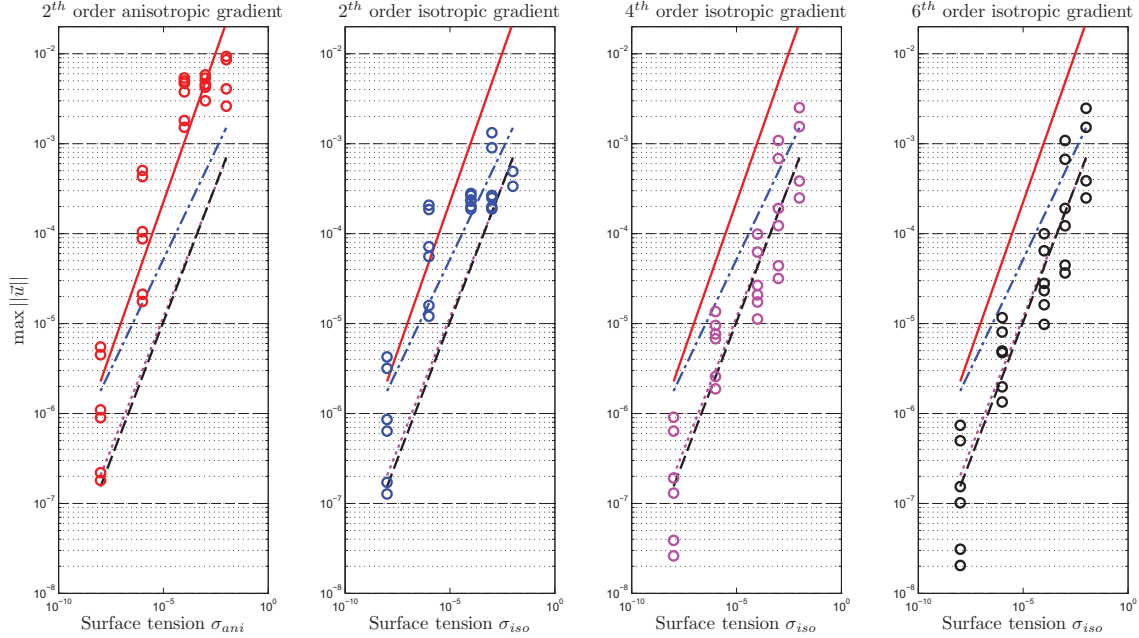


FIGURE 10: (Color online) Maximum velocity magnitude as a function of the surface tension resulting from the various simulations of the steady bubble ($\gamma = 100$ and $\beta = 0.99$).

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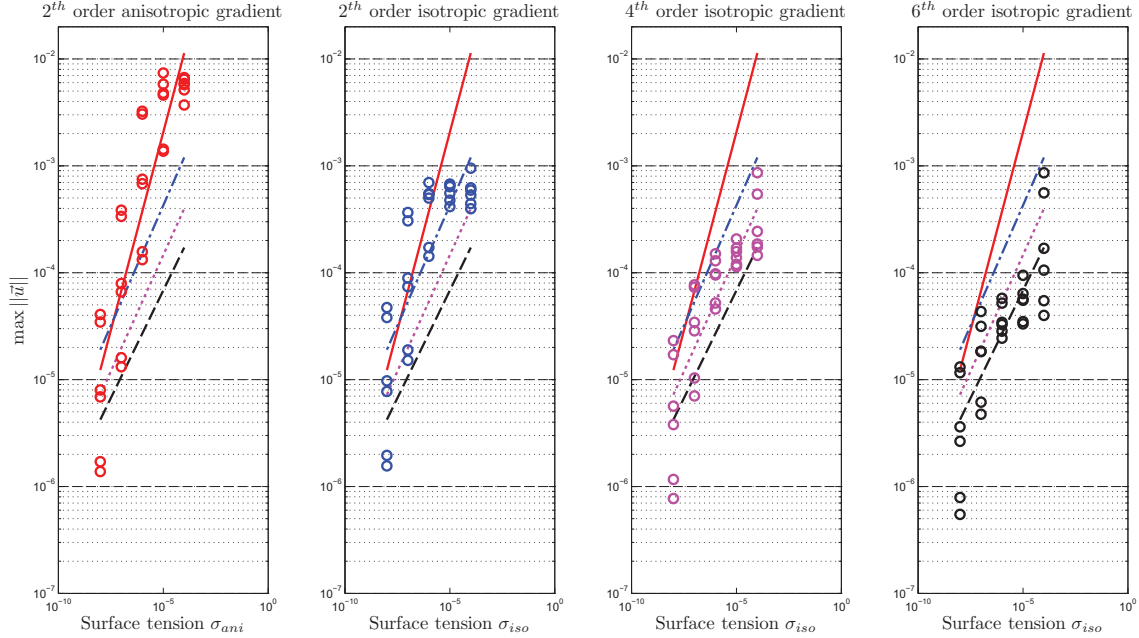


FIGURE 11: (Color online) Maximum velocity magnitude as a function of the surface tension resulting from the various simulations of the steady bubble ($\gamma = 1000$ and $\beta = 0.99$).

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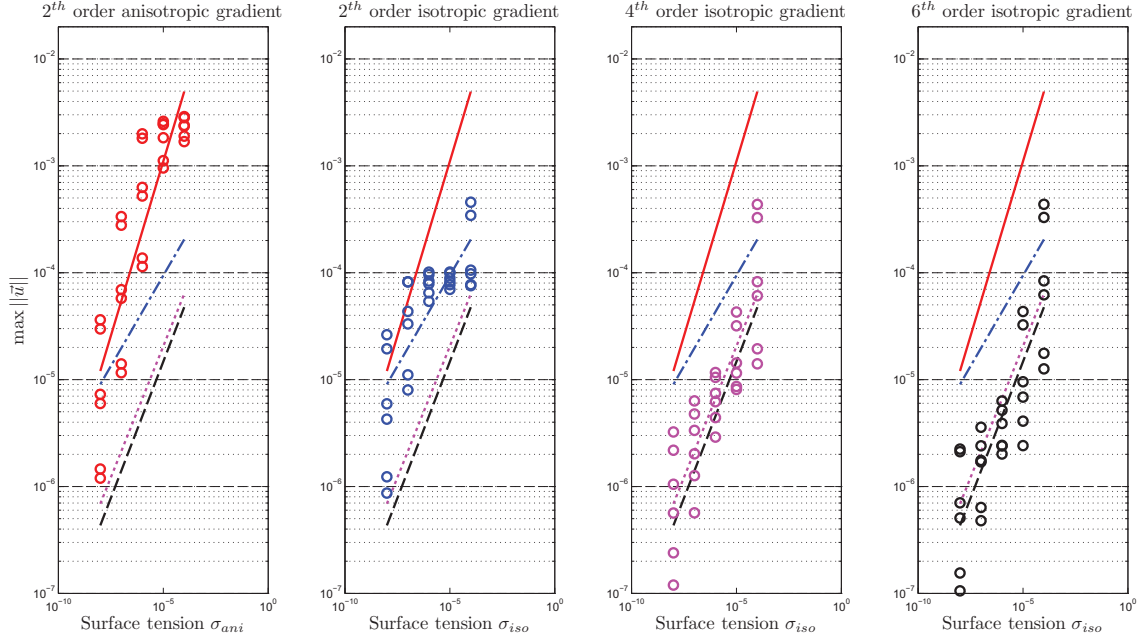


FIGURE 12: (Color online) Maximum velocity magnitude as a function of the surface tension resulting from the various simulations of the steady bubble ($\gamma = 1000$ and $\beta = 0.7$).

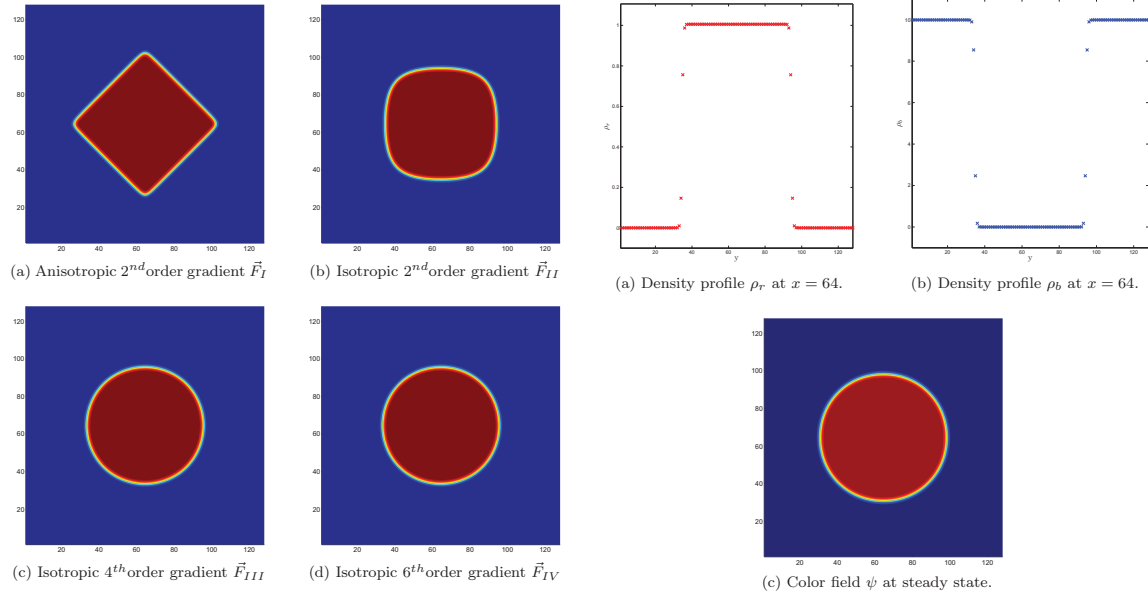


FIGURE 7: Bubble shape at steady state for different color gradients ($\gamma = 10$).

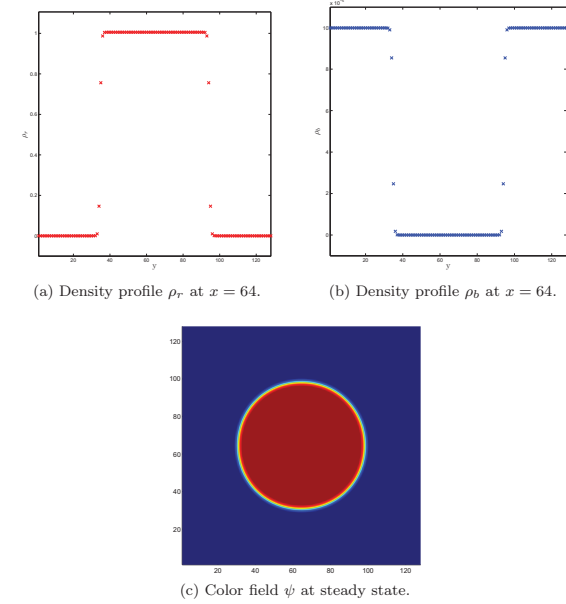


FIGURE 13: Steady state results for the very high density ratio steady bubble simulation ($\gamma = 10000$).

ANNEXE C

Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios

Il est important de noter que cet article a peut être été sujet à des changements avant la publication finale de celui-ci.

Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier, “Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios”, manuscript submitted to *Journal of Computational Physics* in July 2012.

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Progress and investigation on lattice Boltzmann modeling of multiple immiscible fluids or components with variable density and viscosity ratios

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July 17, 2012

Abstract

Lattice Boltzmann models for simulating multiphase flows are relatively new, and much work remains to be done to demonstrate their ability to solve fundamental test cases before they are considered for engineering problems. From this perspective, a hydrodynamic lattice Boltzmann model for simulating immiscible multiphase flows with high density and high viscosity ratios, up to $O(1000)$ and $O(100)$ respectively, is presented and validated against analytical solutions. The method is based on a two phase flow model with operators extended to handle N immiscible fluids. The current approach is $O(N)$ in computational complexity for the number of different gradient approximations. This is a major improvement, considering the $O(N^2)$ complexity found in most works. A sequence of systematic and essential tests have been conducted to establish milestones that need to be met by the proposed approach (as well as by other methods). First, the method is validated qualitatively by demonstrating its ability to address the spinodal decomposition of immiscible fluids. Second, the model is quantitatively verified for the case of multilayered planar interfaces. Third, the multiphase Laplace law is studied for the case of three fluids. Fourth, a quality index is developed for the three-phase Laplace-Young's law, which concerns the position of the interfaces between the fluids resulting from the different surface tensions. The current model is compatible with the analytical solution, and is shown to be first order accurate in terms of this quality index. Finally, the multilayered Couette's flow is studied. In this study, numerical results can recover the analytical solutions for all the selected test cases, as long as unit density ratios are considered. For high density and high viscosity ratios, the analytical solution is recovered for all tests, except that of the multilayered Couette's flow. Numerical results and a discussion are presented for this unsuccessful test case. It is believed that other LB models may have the same problem in addressing the simulation of multiphase flows with variable density ratios.

1 Introduction

Two decades ago, the lattice Boltzmann (LB) model for simulating immiscible fluids was derived from the cellular automata model [36]. Shortly after that, Gunstensen and Rothman [17] adapted the idea of Rothman and Keller (RK) [36], and created an LB model for immiscible two phase flows. This type of model (RK) uses color gradients to separate and model the interaction at the interface of the fluids. Another idea for simulating immiscible fluids was developed by Shan and Chen [39] (SC), which consisted of introducing an effective mass function to simulate the interaction between the fluids. A third method was presented by Swift et al. [41], where collision rules are chosen to ensure that the system evolves towards the minimum of an input

free energy (FE) functional. A fourth method, the mean-field (MF) method, simulate interparticle attraction in the same way as the Coulomb interaction is treated in the Vlasov equation [21]. Finally, the field mediator (FM) methods use null mass particles, the only role of which is to invert the momentum of lattice particles in the transition layer to segregate fluids of different colors [37]. Each of these five models, RK [17,36], SC [39], FE [41], MF [21], and FM [37], belongs to one class of LB model for simulating immiscible two phase flows. It is worth noting that this classification is not universal, and that there are other methods, not discussed in this work, which may not be classified among those mentioned above. Recent work by Bao and Schaefer [3] allowed multiphase and multicomponent flow with high density ratios using the SC approach. A recent and more complete literature review is presented by Gokaltun and McDaniel [14] on LB modeling designed to simulate flow with both high density and high viscosity ratios.

In this work, an RK type LB model based on the Reis and Phillips [35] approach is studied. Grunau et al. [15] have removed some of the limitations of the original RK model of Gunstensen and Rothman [17] by introducing variable density and viscosity ratios. However, the Grunau et al. model can only simulate very low density or viscosity ratios. A major improvement was the redefinition of the recoloring operator, which is incorporated into the model to segregate the fluids. D'Ortona et al. [9] reported that spurious currents were significantly reduced with the new recoloring operator. Later, Latva-Kokko and Rothman [26] modified D'Ortona et al.'s recoloring operator to avoid a negative probability distribution. The new recoloring operator also substantially reduced the "lattice pinning" problem [26]. Recently, Reis and Phillips [35] made an important contribution to the RK model, which was to adapt the model of Grunau et al. [15] for the popular D2Q9 lattice. Most importantly, they managed to construct a perturbation operator which introduces the surface tension in a way that is compatible, within the macroscopic limit, with the form of the capillary stress tensor. For some test cases, their model is able to simulate higher density ratios than previous RK models, even when neither the recoloring operator of D'Ortona et al. [9] nor that of Latva-Kokko and Rothman [26] is used. More recently, Leclaire et al. [29] have adapted the recoloring operator of Latva-Kokko and Rothman to the Reis and Phillips [35] model. Doing so has substantially increased the density ratio between the fluids for several test cases, and the noise in the model has been reduced in such a way that numerical steady state solutions have become possible. In addition, Leclaire et al. [28] showed that, by using an isotropic gradient discretization for the color gradient, it is possible to accurately simulate Laplace's law with density ratios as high as 10000. Moreover, the spurious currents are significantly reduced and accurate simulations with a very low surface tension are possible. With these latter results, the accuracy

and range of the model parameters have been greatly improved in the RK model.

Still, in the lattice Boltzmann RK model, much less attention has been paid to the simulation of multiphase flows with three or more fluids. The first study on this topic was presented in the Ph.D. thesis of Gunstensen [16]. His model has limitations, however, because the method for extending the two-phase model to its three-phase counterpart cannot be generalized, nor is it obvious how it could be generalized to N -phase flows. The approach works well for three phases, but only because there are only three fluid-fluid interfaces, which is equal to the number of fluids. Because this model was introduced almost 20 years ago, it does not contain any of the improvements subsequently made to the RK model. Another RK-based model for simulating multicomponent flows is that of Dupin et al. [10]. By defining a color gradient for each of the fluid-fluid interfaces, they avoided the problem that someone may encounter when attempting to generalize to N -phase the Gunstensen model [16]. A similar alternative was offered by Halliday et al. [18], in which a possible generalization of the recoloring operator is presented for N phases. A more recent version, similar to the Halliday et al. model, is described by Spencer et al. [40]. Unfortunately, none of these multiphase models was built to simulate variable density ratios. In this paper, we introduce a model that does so, by consolidating the applicability and advantages of two-phase flows into an N -phase flow model.

In order to improve the model's ability to simulate high density ratios, we incorporated high-order isotropic gradient discretization for the color gradient computed at each time step. As previously shown [28], this kind of discretization increases the accuracy of the model [28]. Because of the cost associated with gradient computing, this model is designed to reduce, as much as possible, the number of different gradient approximations to be calculated. As stated by Halliday et al. [18], gradient calculation is a source of a significant computational overhead, to the point where these authors decided to consider local gradient approximation when the interface curvature is small. The basis of this approach allows us to consider generalization to N -phase flows, with the number of different gradient approximations $O(N)$ in computational complexity, i.e. neighbor information is needed only with $O(N)$ complexity. This is a clear improvement over most models, which are $O(N^2)$ in complexity [18, 40].

In a previous RK model [10], the computational complexity was shown to be reduced from $O(N^2)$ to $O(\approx 5)$ by neglecting the effect of some fluids. This procedure could also be applied here to obtain similar results. However, if all the fluid interactions must be taken into account, then $O(N)$ complexity is preferable to $O(N^2)$.

This paper is organized in two major sections. First, the LB model for N immiscible fluids is presented. Novel numerical details of the model requirements are given and discussed throughout this work. Then, various numerical simulations for multiphase flows are introduced, performed, and analyzed. When possible, the results are compared with the available analytical solutions for multiphase flows. This new multiphase RK model is able to simulate large density and viscosity ratios, up to $O(1000)$ and $O(100)$ respectively, for all but one of the selected test cases. The unsuccessful test case for variable density ratios is the multilayered Couette's flow. Numerical results and an investigation are presented for this test case in section (3.5).

2 Lattice Boltzmann immiscible multiphase model

The current LB approach follows the two-phase model of Reis and Phillips [35], along with the improvements presented by Leclaire et al. [28, 29] for the recoloring operator and the color gradient. For this

2D LB model, conceptually, there are N sets of distribution functions, one for each fluid, moving on a D2Q9 lattice with the velocity vectors $\vec{c}_i$. We say conceptually, because, in reality, only the color-blind set of distribution functions is needed (see section (4) for technical details). With $\Delta x = \Delta y = 1$ and $\theta_i = \frac{\pi}{4}(4-i)$, the velocity vectors are defined as :

$$\vec{c}_i = \begin{cases} (0, 0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)], & i = 2, 4, 6, 8 \\ [\sin(\theta_i), \cos(\theta_i)] \sqrt{2}, & i = 3, 5, 7, 9 \end{cases} \quad (1)$$

The distribution functions for a fluid of color k (e.g. $k = r$ for red, $k = g$ for green, and $k = b$ for blue) are noted $N_i^k(\vec{x}, t)$, while $N_i(\vec{x}, t) = \sum_k N_i^k(\vec{x}, t)$ is used for the color-blind distribution function. If the time step is $\Delta t = 1$, the algorithm uses the following evolution equation :

$$N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t) + \Omega_i^k(N_i^k(\vec{x}, t)) \quad (2)$$

where the collision operator Ω_i^k is the result of the combination of three sub operators (similar to Ref. [42]) :

$$\Omega_i^k = (\Omega_i^k)^{(3)} \left[(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)} \right] \quad (3)$$

The evolution equation is solved in four steps, as follows :

1. Single phase collision operator (BGK) :
 $N_i^k(\vec{x}, t_*) = (\Omega_i^k)^{(1)}(N_i^k(\vec{x}, t))$
2. Multiphase collision operator (perturbation) :
 $N_i^k(\vec{x}, t_{**}) = (\Omega_i^k)^{(2)}(N_i^k(\vec{x}, t_*))$
3. Multiphase collision operator (recoloring) :
 $N_i^k(\vec{x}, t_{***}) = (\Omega_i^k)^{(3)}(N_i^k(\vec{x}, t_{**}))$
4. Streaming operator :
 $N_i^k(\vec{x} + \vec{c}_i, t + 1) = N_i^k(\vec{x}, t_{***})$

2.1 Single phase collision operator

The first sub operator, $(\Omega_i^k)^{(1)}$, is the standard BGK operator of the single phase LB model, where the distribution functions are relaxed towards a local equilibrium, in which ω_{eff} denotes the effective relaxation factor :

$$(\Omega_i^k)^{(1)}(N_i^k) = N_i^k - \omega_{\text{eff}} \left(N_i^k - N_i^{k(e)} \right) \quad (4)$$

The details of this operator are the following. The density of the fluid k is given by the first moment of the distribution functions :

$$\rho_k = \sum_i N_i^k = \sum_i N_i^{k(e)} \quad (5)$$

where the superscript (e) denotes equilibrium. The total fluid density is given by $\rho = \sum_k \rho_k$, while the total momentum is defined as the

second moment of the distribution functions :

$$\rho \vec{u} = \sum_i \sum_k N_i^k \vec{c}_i = \sum_i \sum_k N_i^{k(e)} \vec{c}_i \quad (6)$$

in which $\vec{u}$ is the density weighted arithmetic average velocity of the fluid. The equilibrium functions are defined by [35] :

$$N_i^{k(e)}(\rho_k, \vec{u}, \alpha_k) = \rho_k \left(\phi_i^k + W_i \left[3\vec{c}_i \cdot \vec{u} + \frac{9}{2}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}(\vec{u})^2 \right] \right) \quad (7)$$

These equilibrium distribution functions $N_i^{k(e)}$ are chosen to satisfy the principles of conservation of mass and momentum. The weights W_i are those of a standard D2Q9 lattice :

$$W_i = \begin{cases} 4/9, & i = 1 \\ 1/9, & i = 2, 4, 6, 8 \\ 1/36, & i = 3, 5, 7, 9 \end{cases} \quad (8)$$

Besides,

$$\phi_i^k = \begin{cases} \alpha_k, & i = 1 \\ (1 - \alpha_k)/5, & i = 2, 4, 6, 8 \\ (1 - \alpha_k)/20, & i = 3, 5, 7, 9 \end{cases} \quad (9)$$

As introduced in Ref. [15] for two-phase flows, the different density ratios between k and l fluids are γ_{kl} , and must be taken as follows to obtain a stable interface :

$$\gamma_{kl} = \frac{\rho_k^0}{\rho_l^0} = \frac{1 - \alpha_l}{1 - \alpha_k} \quad (10)$$

where the superscript "0" over ρ_k^0 indicates the initial value of ρ_k at the beginning of the simulation.

The pressure of the fluid of color k is :

$$p^k = \frac{3\rho_k(1 - \alpha_k)}{5} = \rho_k(c_s^k)^2 \quad (11)$$

In the above expressions, one of the α_k represents a free parameter. We let κ be the index of the least dense fluid. Generally, we set the value of $\alpha_\kappa > 0$, then the relation $0 < \alpha_\kappa \leq \alpha_k < 1$ is guaranteed to hold for each fluid k . These parameters set the sound speed c_s^k in each fluid of color k [35].

The effective relaxation parameter ω_{eff} is chosen so that the evolution equation, Eq. (2), respects the macroscopic equations for a single-phase flow in the single-phase regions. When the viscosities of the fluids are different, an interpolation is applied to define the parameter ω_{eff} at the interface. For flows with more than two phases, it is easier to consider only a simple interpolation, which is different from the quadratic-type interpolation from the basic two phase flow model [15, 35]. It is very important to note that ω_{eff} must be the same for each fluid, since, without it, the amount of computer memory required for this model is much larger. If ω_{eff} is not the same for each fluid color, the distribution functions of each fluid color will need to be kept in the computer memory, instead of only the color blind distribution functions as it is explained in section (4).

In this paper, we define the bar functional as the density weighted q -average. For example, for a variable X_k defined for each fluid k , the density weighted q -average of this variable is defined as :

$$\bar{X}|_q = \begin{cases} \left(\sum_k \frac{\rho_k (X_k)^q}{\rho} \right)^{\frac{1}{q}}, & q \neq 0 \\ \left(\prod_k (\rho_k)^{X_k} \right)^{\frac{1}{p}}, & q = 0 \end{cases} \quad (12)$$

If ν_k is the kinematic viscosity of the fluid k , then, depending on the q -average, one possible choice for the effective relaxation parameter is :

$$\omega_{\text{eff}} = \frac{1}{3 \left(\bar{\nu}|_q + \frac{1}{2} \right)} \quad (13)$$

The choice to define ω_{eff} in this way is not the only option, and, since the accuracy of the model seems to greatly depend on that

choice, different choices for ω_{eff} are investigated in this study, namely the q -average with $q = -1, 0, 1$ and 2 .

As will be discussed further in sections (3.2) and (3.5) concerning the multilayered planar interface and the multilayered Couette's flow, none of the effective relaxation parameters ω_{eff} studied here seems to be the perfect candidate in all circumstances. Nevertheless, from these two test cases, we suggest that $q = -1$ is the best choice when simulating unit density ratios, while $q = 1$ appears to be a better choice when non unit density ratios are treated. We note that depending on what is important, e.g. surface tension or velocity, other alternatives for q could lead to better results. In the work of Refs. [10, 42, 43], when three or more phases are simulated, $q = 1$ is used.

2.2 Perturbation operator

In the RK model, surface tension is modeled by means of the perturbation operator [17, 19, 35]. First, to introduce the surface tension into this model, a "color" gradient $\vec{F}$ that approximates the interface normal needs to be defined for each of the fluid-fluid interfaces.

The first possibility that may be considered is the natural extension for N phases of the color gradient present in the basic two phase model [28] :

$$\vec{F}_{kl}^{\text{natural}} = \vec{\nabla}(\rho_k - \rho_l) \quad (14)$$

According to this form, the number of different gradient approximations is $O(N^2)$ in complexity, because one gradient approximation for each interface needs to be computed at each lattice site. This follows from the number of possible interfaces in a N -phase flow, which is equal to $N(N-1)/2$. Instead of applying the gradient operator to the density difference, it is also possible to distribute the gradient operator to each fluid density, in order to obtain :

$$\vec{F}_{kl}^{\text{natural}} = \vec{\nabla}\rho_k - \vec{\nabla}\rho_l \quad (15)$$

Clearly, the number of different gradient approximations is now $O(N)$ in complexity. Only one gradient approximation for each phase needs to be computed at each lattice site. Note that, in this particular case, the two color gradients in Eqs. (14) and (15) are analytically/numerically equivalent.

Unfortunately, the color gradient in Eq. (15) leads to non physical results when three or more phases are simulated. In fact, in section (3.3.1), it is shown that this natural extension leads to a non physical mass flow along the direction tangential to the interfaces.

Another possible color gradient or phase field gradient is the one presented in the model of Spencer et al. [40] :

$$\vec{F}_{kl}^{\text{phase}} = \vec{\nabla} \left(\frac{\rho_k - \rho_l}{\rho_k + \rho_l} \right) \quad (16)$$

Once more, this color gradient is $O(N^2)$ in complexity for the number of different gradient approximations. It is again possible to distribute the gradient operator to obtain a color gradient that is $O(N)$ in complexity :

$$\vec{F}_{kl}^{\text{phase}} = 2 \frac{\rho_l \vec{\nabla}\rho_k - \rho_k \vec{\nabla}\rho_l}{(\rho_k + \rho_l)^2} \quad (17)$$

It is important to note that this time the two gradients in Eqs. (16) and (17) are not numerically equal, because the discrete gradient operator is a linear combination of stencil values, while the color gradient $\vec{F}_{kl}^{\text{phase}}$ in Eq. (17) is not a linear combination of the density gradients. Therefore, the results that would be obtained in a simulation using Eq. (16) will not be the same as with Eq. (17). It should be noted that the color gradient $\vec{F}_{kl}^{\text{phase}}$ is undefined when both fluids ρ_k and

ρ_l are absent. This situation arises when three or more phases occur. This phase field gradient is clearly suited to two-phase flows, but will be prone to numerical instability and inaccuracy when three or more phases occur.

For this model, we found only one color gradient $O(N)$ in complexity that leads to physical results and not prone to numerical instability. Based on the Allen-Cahn system [11], the color gradient in this model is defined as :

$$\vec{F}_{kl} = \frac{\rho_l}{\rho} \vec{\nabla} \left(\frac{\rho_k}{\rho} \right) - \frac{\rho_k}{\rho} \vec{\nabla} \left(\frac{\rho_l}{\rho} \right) \quad (18)$$

It is interesting to note that the color gradient in Eq. (18) from the Allen-Cahn system is very similar to the phase field gradient in Eq. (17). In fact, it can be shown that for two-phase flows these two gradients are exactly the same, except that the color gradient $\vec{F}_{kl}^{phase}$ is twice the length of $\vec{F}_{kl}$. Therefore, we can conclude that the gradient $\vec{F}_{kl}$ is a more rigorous generalization for N -phase flows than $\vec{F}_{kl}^{phase}$, because $\vec{F}_{kl}$ is a vector function that is always defined.

In order not to neglect any fluid interaction, $O(N)$ complexity is preferable when the number of phases is growing. Therefore, the way the algorithm is implemented is very important. Specifically, if N different gradient approximations need to be computed with the same stencils for every lattice site, this can be achieved very quickly using convolution products and storing them in computer memory for future use [27]. This is an important point we are making in this paper, and one that becomes increasingly important as the order of the gradient discretization grows. Also, high-order gradient discretization is preferred in some cases, in order to accurately simulate high density ratios with this type of model [28]. In this work, an eighth order isotropic discrete gradient operator is used for the gradient of the density fraction ρ_k/ρ of each fluid. More details about this isotropic discrete gradient operator are given in section (2.4).

The perturbation operator, for the fluid k , is therefore defined by :

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \sum_{l \neq k} \frac{A_{kl} C_{kl}}{2} |\vec{F}_{kl}| \left[W_i \frac{(\vec{F}_{kl} \cdot \vec{c}_i)^2}{|\vec{F}_{kl}|^2} - B_i \right] \quad (19)$$

where

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (20)$$

and

$$C_{kl} = \min \left\{ \eta_1 \frac{\rho_k \rho_l}{\rho_k^0 \rho_l^0}, 1 \right\} \quad (21)$$

where $\eta_1 = 10^6$ is a threshold and the function C_{kl} is a concentration factor that limits the activation of the surface tension at the k - l interface only where both the k and l fluids are present. The accuracy of the model depends on the choice of η_1 , but its effect appears to be very small for a very wide range of values. To our knowledge, this is the first time that the concentration factor in Eq. (21) has been used. There are other concentration factors in the literature, in the work of Dupin et al. [10], for example :

$$C_{kl} = 1 - \left| \frac{\rho_k - \rho_l}{\rho_k + \rho_l} \right| \quad (22)$$

Again, it can be noted that, for three or more phases, this concentration factor can be undefined over some regions of the computational domain.

Reis and Phillips [35] have shown that the perturbation operator complies, within the macroscopic limit, with the capillary stress tensor present in the macroscopic equations for two-phase flows. It handles the coupling between the two fluids, with the space- and time-dependent parameters A_{kl} chosen to model the surface tension between the k - l fluid interface. Although this operator generates the surface tension, it does not guarantee the fluid's immiscibility. To minimize the mixing and segregate the fluids, the recoloring operator $(\Omega_i^k)^{(3)}$ needs to be properly selected.

2.3 Recoloring operator

This last operator is used to maximize the amount of fluid of color k at the interface that is sent to the k fluid region, while respecting the conservation of mass and total momentum. The recoloring operator presented here is a combination of the essential ideas from Latva-Kokko and Rothman [26] and Halliday et al. [18] :

$$(\Omega_i^k)^{(3)}(N_i^k) = \frac{\rho_k}{\rho} N_i^k + \sum_{l \neq k} \beta_{kl} \frac{\rho_k \rho_l}{\rho^2} \cos(\varphi_i^{kl}) N_i^{(e)}(\rho, 0, \vec{\alpha}|_{q=1}) \quad (23)$$

where β_{kl} is a parameter controlling the thickness of the k - l interface [26]. The variable φ_i^{kl} corresponds to the angle between the color gradient $\vec{F}_{kl}$ and the lattice direction vector $\vec{c}_i$. The equilibrium distributions of the color-blind fluid $N_i^{(e)}$ in Eq. (23) are evaluated using Eq. (7), a zero velocity, and the respective value of $\vec{\alpha}|_{q=1}$. It should be noted that, for $i = 1$, there is a division by 0. In such a case, the numerator is also 0, and we release the indeterminacy by setting the whole term equal to 0 to respect mass conservation. Also, the parameter β_{kl} must be between 0 and 1 to ensure, at least for a two-fluid interface, that the distribution functions remain positive [26]. When three or more fluids are present at an interface, it is not clear whether or not the distribution functions will remain positive, but the current numerical results seem to indicate that the numerical evolution of the solution is stable with $0 \leq \beta_{kl} \leq 1$. Moreover, it should also be noted that $\beta_{kl} = \beta_{lk}$, in order to guarantee mass and momentum conservation.

2.4 Isotropic discrete gradient operator

In this work, an eighth order isotropic discrete gradient operator is used. This kind of gradient operator was generalized by Sbragaglia et al. for 2D and 3D higher order isotropic operators [38]. In Ref. [28], it is shown that this type of discretization enhances the accuracy of the RK model significantly. The eighth order isotropic gradient operator takes the following form :

$$\vec{\nabla} f(x, y) = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] f(x, y) \approx \sum_{i=1}^{25} \xi_i [d_i^x, d_i^y] f(x + d_i^x, y + d_i^y) \quad (24)$$

with

$$\begin{aligned} \vec{\xi} &= [0, 960, 448, 960, 448, 960, 448, 960, 448, 84, \\ &\quad 32, 1, 32, 84, 32, 1, 32, 84, 32, 1, 32, 84, 32, 1, 32] / 5040 \\ \vec{d}^x &= [0, 0, 1, 1, 1, 0, -1, -1, -1, 0, 1, 2, 2, 2, 2, 1, \\ &\quad 0, -1, -2, -2, -2, -2, -2, -2, -1] \\ \vec{d}^y &= [0, 1, 1, 0, -1, -1, -1, 0, 1, 2, 2, 2, 1, 0, -1, -2, \\ &\quad -2, -2, -2, -2, -1, 0, 1, 2, 2] \end{aligned} \quad (25)$$

Note that the previous operator assumes a unit lattice spacing in the " x " and " y " directions.

2.5 Setting the surface tension

Following a theoretical development by Reis and Phillips [35] and his predecessors [19], it is possible to predict the surface tension between the two fluids using only the basic parameters of the model. As in Refs. [29, 35], knowing the form of the expression describing the surface tension and performing simulations on planar interfaces, a function of the model parameters can be determined to approximately describe the surface tension across an interface. It is very important to realize that the appropriate setting of the surface tension depends on the form of the color gradient and the discretization of the gradient operator.

For the isotropic color gradient discretization defined in Ref. [29] and in Eq. (14), the surface tension is set as follows [28] :

$$\sigma_{kl} = \frac{2}{9} \frac{\rho_k^0 + \rho_l^0}{\omega} (A_{kl} + A_{lk}) = \frac{2}{9} \left(1 + \frac{1}{\gamma_{kl}}\right) \frac{\rho_k^0}{\omega} (A_{kl} + A_{lk}) \quad (26)$$

In previous studies [28, 29, 35], the different values for σ_{kl} were set at the beginning of a simulation. Then, the parameters $A_{kl} = A_{lk}$ were simulation constants calculated from the initial values of ρ_k , σ_{kl} and ω . Note that when the surface tension was not zero in these studies, the parameter ω was a constant.

For isotropic color gradients defined as in Eq. (18), the surface tension is set as follows :

$$\sigma_{kl} = \frac{1}{9} \frac{(A_{kl} + A_{lk})}{\omega_{\text{eff}}} \quad (27)$$

The main difference between Eqs. (26) and (27) is that the color gradient in Eq. (18) is normalized by the total density. The different values for σ_{kl} are also set at the beginning of a simulation. However, the values for $A_{kl} = A_{lk}$ are space- and time-dependent, because, in this study, ω_{eff} may depend on space and time. So, the value for q in Eq. (13) is a new input parameter that needs to be properly selected when variable viscosity ratios are simulated.

2.6 Adjustment of the interface width for static contact angles

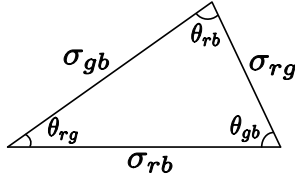


FIGURE 1: Neumann's Triangle.

For three-phase flows and when the surface tension yields a Neumann triangle, as shown in Fig. (1), there is a possible equilibrium state where static contact angles θ_{kl} will be formed between the fluids. Here, we follow the idea of Spencer et al. [40], who have found and demonstrated theoretically that a particular relation for β_{kl} at the triple fluid junction must be used, otherwise the angle θ_{kl} will not be satisfied at steady state. This is more noticeable when one of the angles, θ_{kl} , shown in Fig. (1), is small. The value of the angle θ_{kl} can be found from the surface tension σ_{kl} using the law of cosines. By setting θ_{max} as the largest θ_{kl} in Fig. (1), the special relation for β_{kl}

is :

$$\beta_{kl} = \begin{cases} \beta^0, & kl \text{ with } \theta_{\text{max}} \\ \beta^0 (1 + c_{\text{triple}} (\sin(\pi - \theta_{\text{max}} - \theta_{kl}) - 1)), & \text{otherwise} \end{cases} \quad (28)$$

where β^0 is a constant between 0 and 1 controlling the overall thickness of all three interfaces and

$$c_{\text{triple}} = \min \left\{ \eta_2 \frac{\rho_r \rho_g \rho_b}{\rho^3}, 1 \right\} \quad (29)$$

is a function that also varies between 0 and 1. It should be noted that the function c_{triple} is very similar to the one provided by Spencer et al. [40]. However, in [40], the threshold $\eta_2 = 27$ and the "min" function are absent. In the setting of Spencer et al., c_{triple} does not really reach unit value, and is usually less than 0.95. This cause some inaccuracy when one of the θ_{kl} angles is small, i.e. the interface thickness ratio at the interface is not respected. In order to obtain the correct interface thickness ratio, $c_{\text{triple}} = 1$ must be ensured for a certain number of sites at the triple fluid function. This is why we used the free threshold parameter $\eta_2 = 35$, along with the "min" function. Therefore, the special form of the function c_{triple} makes it possible to fully activate the special relation for β_{kl} only at the triple fluid junction and for a reasonable number of lattice sites.

It is important to mention that, when there is no Neumann triangle, no relation for β_{kl} is known regarding the dynamic contact angles. The behavior of these contact angles is an active research topic in the LB community [7, 23]. So, in this study, when there is no Neumann triangle, we merely set each of the β_{kl} to the same constant.

It can also be noted that, when the θ_{kl} angles are close to 60 degrees, i.e. an equilateral Neumann triangle, the setting of all β_{kl} to the same value does not really affect the solution, because $\sin(60) \approx 0.866$, which is close to 1 [40].

Moreover, generalizing these relations is not straightforward when more than four fluids are in contact. One possibility, which is not easy to implement, would be to use only the three fluids most in evidence at each lattice site, and compute c_{triple} for these three fluids if there is a Neumann triangle. Then, we could use the relation in Eq. (28) for these three interfaces and set $\beta_{kl} = \beta^0$ for the other interfaces. This would be equivalent to neglecting the effect of some fluids, and may not always work well, but would yield a reasonable approximation for some applications.

3 Numerical Simulation

In this work, the figures showing multiphase flow are RGB images of size $N_x \times N_y \times 3$ given by :

$$RGB = \frac{\begin{bmatrix} \rho_r \\ \rho_g \\ \rho_b \end{bmatrix}}{\sum_k \frac{\rho_k}{\rho_k^0}} \quad (30)$$

where N_x and N_y denote the number of lattice sites in the horizontal and vertical direction.

3.1 Multiphase spinodal decomposition

Spinodal decomposition can be viewed as the physical process of phase separation of an emulsion. Here, we study the spinodal decomposition of an initial and random multiphase mixture. This is a very good numerical experiment in which to test the stability of the current LB model, and, in any case, any immiscible multicomponent

model must pass the spinodal decomposition test. Although the results in this section are qualitative, they make it possible to test the robustness of the numerical code and see how the various fluids aggregate. A quantitative study of spinodal decomposition involving an RK model can be found in the work of Alexander et al. [2].

The setup is as follows. The computational domain is discretized with a lattice of $N_x = 64$ by $N_y = 64$ sites. Initially, for each site and with three fluid colors available (red, green, and blue), a uniform probability distribution is used to select a fluid color. Then, the site is filled with that fluid color using zero velocity equilibrium distribution functions. For the other fluids, the site is filled with zero density and velocity equilibrium distribution functions. The initial mixture is depicted in Fig. (2). Periodic boundary conditions are used at the four ends of the computational domain.

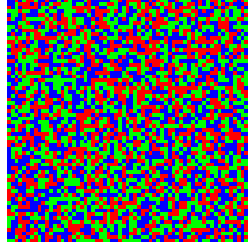


FIGURE 2: (*Color available online*) Initial mixture for the spinodal decomposition simulation ($t = 0$).

Three simulations were performed : Case I with a unit density and viscosity ratio, Case II with a high density and unit viscosity ratio, and Case III with a high density ratio and a high viscosity ratio. The simulation results are shown in Figures (3), (4), and (5) respectively. The results show that the algorithm is stable, and that spinodal decomposition is effectively taking place. Note that the unsteady behavior of the flow varies greatly, depending on the density and/or viscosity ratios. Also, with $\alpha_\kappa = 4/9$ (κ is the index of the least dense fluid) and $\beta_{kl} = 0.5$, the properties of the other fluids used are shown in Table (1). From the discussion in section (2.6) on the adjustment

Parameters	Case I	Case II	Case III
ρ_r	1	100	100
ρ_g	1	10	10
ρ_b	1	1	1
ν_r	1/6	1/6	1
ν_g	1/6	1/6	1/10
ν_b	1/6	1/6	1/100
σ_{kl}	10^{-1}	10^{-1}	10^{-1}
q	N/A	N/A	1

TABLE 1: Input parameters for the multiphase spinodal decomposition tests.

of the interface width for static contact angles, since β_{kl} is the same for every interface, the contact angles at $t = 1000000$ in Figures (3), (4), and (5) are about 60 degrees. This is a quantitative behavior that is theoretically expected. It is no surprise that the 60 degree angle is more accurate in the case of unit density ratios than in the other cases. In the section on the Laplace-Young law (3.4), the static contact angles are studied quantitatively in greater detail.

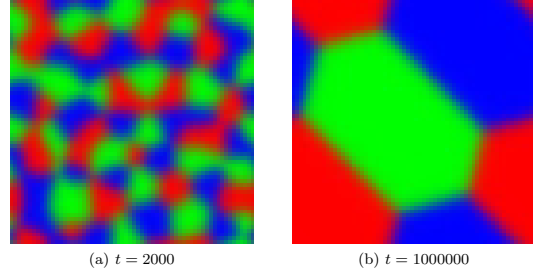


FIGURE 3: (*Color available online*) Spinodal decomposition with *unit* density and *unit* viscosity ratios.

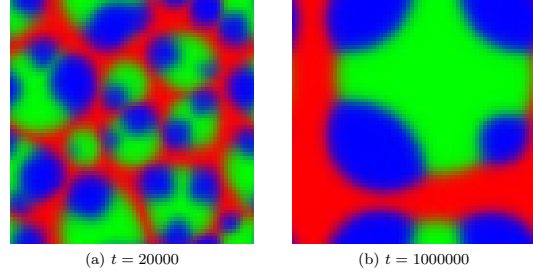


FIGURE 4: (*Color available online*) Spinodal decomposition with *high* density and *unit* viscosity ratios.

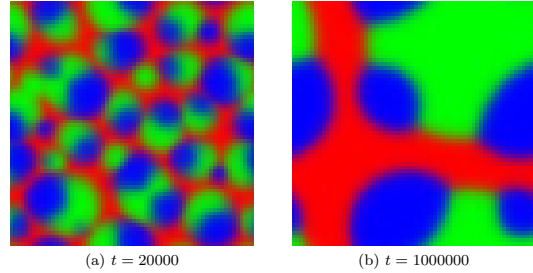


FIGURE 5: (*Color available online*) Spinodal decomposition with *high* density and *high* viscosity ratios.

3.2 Multilayered planar interfaces

The goal in this section is to test the model's ability to accurately simulate surface tension across different fluid interfaces. In theory, surface tension is independent of fluid viscosity. However, in this model, to set a specific surface tension between two fluids by means of Eq. (27), the fluid viscosity has to be taken into account, because the relaxation factor ω_{eff} depends on it. In previous investigations [28, 29, 35], the correctness of the surface tension across a planar interface was only conducted for unit viscosity ratios and not verified for variable viscosity ratios between the interfaces. We will now address this issue, to show that the model accurately simulates surface tension, i.e. Eq. (27) is working properly, when there are both density and viscosity ratios across a planar interface.

The easiest way to test the multilayered planar interfaces is with the following flow configuration, as shown in Fig. (6). The variable

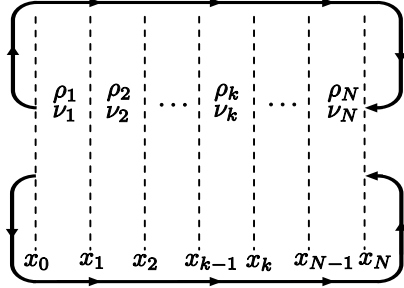


FIGURE 6: Multilayered planar interface flow configuration.

x_k is used to note the different interface position between the fluids. The flow must be considered to be periodic in the x-axis, i.e. x_0 and x_N are physically in the same fluid line.

The mechanical surface tension σ_{mec} is defined or studied, or both, in Refs. [12, 17, 19, 35] for different flow configurations. Here, in the context of the previous specific flow setting, σ_{mec} takes the following form :

$$\sigma_{\text{mec}} = \int_{x_0}^{x_N} (P_n(x) - P_t(x)) dx \quad (31)$$

where P_n and P_t are the normal and tangential components of the pressure tensor. The x-axis is a line of integration perpendicular to the interface. By setting φ_i^x as the relative angle between the x-axis and the vector $\vec{c}_i$, the components P_n and P_t are given by [35] :

$$\begin{aligned} P_n &= \sum_i N_i (|\vec{c}_i| \cos(\varphi_i^x))^2 \\ P_t &= \sum_i N_i (|\vec{c}_i| \sin(\varphi_i^x))^2 \end{aligned} \quad (32)$$

The setting of this test is described in the context of an LB simulation. First, only three layers of fluids, $N = 3$, are considered. The red fluid is on the left-hand side, the green fluid is in the middle, and the blue fluid is on the right-hand side. Since the mechanical surface tension is integrated along the x-axis and must take into account the surface tension of each fluid-fluid interfaces, we can conclude that the following relation must hold :

$$\sigma_{\text{mec}} = \sigma_{rg} + \sigma_{gb} + \sigma_{br} \quad (33)$$

The analytical flow solution for the surface tension is 1D, therefore a lattice containing 90×1 sites is used and is geometrically located over the interval $[x_0, x_N] = [0, 89]$. Each fluid section is initialized with the zero velocity equilibrium distribution functions and is 30 sites wide. All fluid layers are 30 lattice units wide. The interfaces x_k are located between the fluid lattice sites. Periodic boundary conditions are applied in all four directions. The values $\alpha_\kappa = 4/9$ (κ is the index of the least dense fluid) and $\beta_{kl} = 1$ are used. For all multilayered planar interface simulations, the stopping criterion is the same, and is :

$$\frac{\sigma_{\text{mec}}^n - \sigma_{\text{mec}}^{n-2000}}{\sigma_{\text{mec}}^n} < 10^{-6} \quad (34)$$

with n the time step number. This check is only performed at every 2000 time steps.

A total of 192 numerical simulations were conducted to study how the various parameters in the current model influence the surface

$\bar{\nu}_q$	σ	ν_r	ν_g	ν_b	ρ_r	ρ_g	ρ_b
$q = -1$	10^{-5}	1/2	1/6	1/6	30	1	1
$q = 0$	10^{-3}	1/6		1/100	1		1/30
$q = 1$	10^{-1}						
$q = 2$							

TABLE 2: Some combinations of parameters for the multilayered planar interface simulations.

tension. The total number of all possible combinations of input parameters is 192 ($4 \times 3 \times 2 \times 1 \times 2 \times 2 \times 1 \times 2$), as summarized in Table (2). The values for the surface tension must be of the same order, e.g. $\sigma_{rg} = \sigma_{gb} = \sigma_{br} = \sigma$, otherwise the computed value for $\sigma_{rg} + \sigma_{gb} + \sigma_{br}$ will not represent each surface tension individually.

The initial condition for this problem can lead to instability, because the color-blind density distribution, N_1 , and/or the fluid densities ρ_k , are initially discontinuous. It is then preferable to initialize the flow with a more continuous function. One way of doing this is described by Mei et al. [31], and is applied here in the context of multiphase flow. It consists in solving the model equation for a certain number of time steps with $A_{kl} = 0$, while imposing $\vec{u} = 0$ in the equilibrium density distribution in Eq. (7). So, for the simulations presented here, the first 2000 time steps only serve to stabilize the density distribution to a more continuous function.

Let us define the superscript index j corresponding to the j^{th} simulation. The error for the j^{th} simulation is defined as follows :

$$E_j = \frac{|\sigma_{rg}^j + \sigma_{gb}^j + \sigma_{br}^j - \sigma_{\text{mec}}^j|}{\sigma_{\text{mec}}^j} \quad (35)$$

Tables (3) and (4) show the percentage error based on various norms applied over different simulation groups. More precisely, Table (3) displays the error as a function of the surface tension, while Table (4) shows the error when the following are considered : i) only unit density and unit viscosity ratios; ii) only non unit density and unit viscosity ratios; iii) only unit density and non unit viscosity; and iv) only non unit density and non unit viscosity ratios. The symbol $\langle \cdot \rangle$ stands for the average.

From Table (3), it can be concluded for this simple test case that, whatever the viscosity q -average interpolation, the higher the surface tension, the greater is the relative accuracy of the model.

From Table (4), all the viscosity q -average interpolations seem to lead to similar accuracy, except for one case. Indeed, when simulating non unit density and viscosity ratios and small surface tension, the harmonic average, i.e. with $q = -1$, for interpolating viscosity leads to large inaccuracies.

For this test case, even if the accuracy is similar, we can still see from Table (3) and (4) that $q = 2$ provides better results, then the accuracy decreases as q decreases.

To conclude, a careful analysis of the results will reveal that, based on our input parameters in Table (1), the multilayered planar interface is accurately simulated with errors under 2% for density ratios up to $O(900)$ and viscosity ratios up to $O(50)$ when using $q = 1$ or 2. Note that we used the parameter $\beta_{kl} = 1$ here. Now, β_{kl} can be lowered to obtain a larger interface, which would lead to a reduction in computational error and/or spurious current, and so improve stability. In the next two sections, we simultaneously obtain stable and accurate simulations with high density and viscosity ratios of up to $O(1000)$ and $O(100)$ respectively by lowering β_{kl} to 0.5.

3.3 Multiphase Laplace law

The next numerical experiment involves the evolution of a three-phase flow, where the steady state solution corresponds to a similar setup of a Laplace law numerical experiment [28]. This test is used to assess the ability of the model to perform an unsteady simulation, where the qualitative behavior of the flow evolution can be predicted. Moreover, a final steady state solution exists on which we can measure and predict the final surface tension. Note that this section is presented primarily to show that the generalization of the model from two phases to N phases does not break Laplace's law.

The setup is as follows. A lattice of 128×128 sites is used with periodic boundary conditions at the four ends. The computational domain then measures 127 lattice units in both height and width. The corner at the bottom left of the domain is located at the origin $(0,0)$. The fluids are initialized using the zero velocity equilibrium distribution functions. The red fluid is initialized at the following position :

$$(x - 63.5)^2 + (y - 73.5)^2 \leq 30^2 \text{ and } y > 73.5 \quad (36)$$

$$(x - 63.5)^2 + (y - 53.5)^2 \leq 30^2 \text{ and } y < 53.5 \quad (37)$$

The green fluid is initialized at the following position :

$$33.5 < x < 93.5 \text{ and } 53.5 < y < 73.5 \quad (38)$$

The remaining lattice sites are filled with blue fluid. Figure (7a) shows the initial condition of this setup. A numerical simulation is performed for each of the three cases, I, II, and III. The input parameters for these simulations are presented in Table (5).

Parameters	Case I	Case II	Case III
β_{kl}	0.7	0.7	0.5
α_b	4/9	4/9	4/9
ρ_r	1	1000	1000
ρ_g	1	$\sqrt{1000}$	$\sqrt{1000}$
ρ_b	1	1	1
ν_r	1/6	1/6	1
ν_g	1/6	1/6	1/10
ν_b	1/6	1/6	1/100
σ_{rg}	8e-02	8e-02	8e-02
σ_{rb}	8e-02	8e-02	8e-02
σ_{gb}	4e-01	4e-01	4e-01
q	N/A	N/A	1

TABLE 5: Input parameters for the three phase flow Laplace law tests.

As described in section (3.2), the initial condition of this problem can lead to instability. Therefore, the first 2000 time steps are used to stabilize that condition.

By adding the surface tension forces at the initial triple junction point of the fluids, we can see that, because the flow is initially at rest and σ_{gb} is significantly larger than the sum of the other two surface tension forces, the red fluid will start to encircle the green fluid. In fact, it will completely surround the green fluid, and the green-blue interface will disappear. Because σ_{rg} and σ_{rb} are non zero, in the long run, the steady state solution is a green circular bubble inside a red circular annulus, the outside of which is surrounded by blue fluid. The numerical solution at steady state and at intermediate times is presented in Figure (7) for case III with a high density and a high viscosity ratio. It should be noted that case I with unit density ratio is similar. Moreover, the qualitative behavior of the flow agrees well with the previously expected scenario.

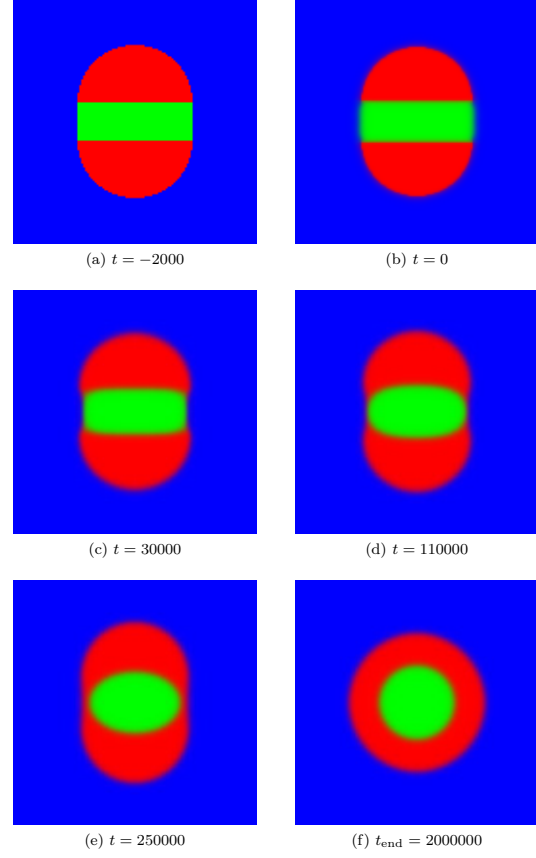


FIGURE 7: (Color available online) Unsteady flow converging to a steady state three phase flow configuration.

At steady state, if the Laplace law for two-phase flow is applied iteratively across the two interfaces $r-g$ and $r-b$, we should obtain the following result :

$$\sigma_{rg} + \sigma_{rb} = \Delta P_{gr} R_g + \Delta P_{rb} R_r \quad (39)$$

where $\Delta P_{gr} = P_g - P_r$ and $\Delta P_{rb} = P_r - P_b$ indicate the pressure jumps across the various fluid interfaces. Also, R_g is the radius of the green circular bubble and R_r is the outer radius of the red fluid annulus.

Here, the average pressure inside the fluid section of color j is measured as the sum of the local average pressure of each fluid k , as follows :

$$P_j = \sum_k \frac{3 \langle \rho_{k,j} \rangle (1 - \alpha_k)}{5} \quad (40)$$

with $\langle \rho_{k,j} \rangle = \langle \{ \rho_k \mid \rho_j^0 \rho_j \geq 0.99 \} \rangle$. The symbol $\langle \cdot \rangle$ stands for the average. There are 2828 red and 1200 green sites initially, and, because of the incompressible limit of the LB model, the radii R_g and R_r can be estimated to be equal to $\sqrt{1200/\pi}$ and $\sqrt{(1200 + 2828)/\pi}$ respectively.

For each parameter case, I, II, and III, Table (6) shows the relative percentage errors with Eq. (39) obtained at steady state for different concentration factors, i.e. Eqs. (21) or (22). The left-hand side of Eq. (39) is used as the reference to calculate the relative errors. The model greatly underestimates the surface tension when using Eq. (22) instead of Eq. (21).

C_{kl}	Case I	Case II	Case III
Eq. (21)	0.073%	2.891%	4.076%
Eq. (22)	54.17%	52.24%	53.29%

TABLE 6: Relative errors for the three phase flow Laplace law tests.

Note that the numerical steady state in Case I and Case II is regarded as achieved when :

$$\max_{\text{all sites}} \left\{ \left| \left(\sum_k N_t^k \right)^{(n)} - \left(\sum_k N_t^k \right)^{(n-1)} \right| \right\} \leq \epsilon \quad (41)$$

with $\epsilon = 10^{-7}$, while n denotes the time step number. To reduce the computational cost, this condition is only checked every 2000 time steps. Note that in Case III, with both high density and high viscosity ratios, numerical noise is present and prevents the simulation from converging with such a restrictive numerical steady state condition. This might be related to the fact that the numerical scheme is at the limit of numerical stability. So, for Case III, the simulations were stopped after 2000000 time steps.

Fortunately, with the current model and for this test case, the relative errors for the three phase Laplace law are acceptable, even with high density and high viscosity ratios up to $O(1000)$ and $O(100)$ respectively. The large discrepancies obtained with the concentration factor in Eq. (22) show that it is very important for the numerical method to be carefully designed so that the generalization to N -phase flow does not break Laplace's law. Here, we do not repeat further results concerning Laplace's law, as this has been extensively studied in [28].

It is important to note that we do not think that the concentration factor in Eq. (22) is incorrect, but, by choosing that concentration factor, another multiplicative constant ($\neq 1/9$) would need to be chosen in Eq. (27) for the definition of the surface tension. It appears to us much more difficult to find a multiplicative constant that works well for a wide range of parameters. With the concentration factor in Eq. (22), this multiplicative constant could be determined using a planar interface simulation prior to any more complex simulations, but it would be a heuristic determination and would not work in the case of a simulation with variable surface tension.

In order to correctly simulate the unsteady multiphase flow converging to the Laplace law setup, two choices were carefully made. First, an appropriate definition of the concentration factor, i.e. Eq. (21), and second, a suitable definition of the color gradient, i.e. Eq. (18).

3.3.1 Appropriate choice of the color gradient

In this section, we show numerically why the choice of color gradient is important when generalizing the model from two to N phases. With the same setting as with Case II in section (3.3), except that $\sigma_{rg} = \sigma_{rb} = 8\text{e-}05$ and $\sigma_{gb} = 4\text{e-}04$, Figure (8) shows the results obtained for ρ_r , ρ_g , and ρ_b , depending on the choice of color gradient, i.e. Eq. (15) or Eq. (18). The online version of Fig. (8) may provides a better understanding. Paying careful attention to the images, it becomes clear that there is a non physical mass flow leak in the direction

tangential to the interfaces when the color gradient $\vec{F}_{kl}^{natural}$ is use. This false phenomenon is obviously undesired, and, depending on the setting of a simulation, may easily spoil the results. We have not yet investigated why this is so. Fortunately, when using $\vec{F}_{kl}$ in Eq. (18), this non physical behavior does not occur.

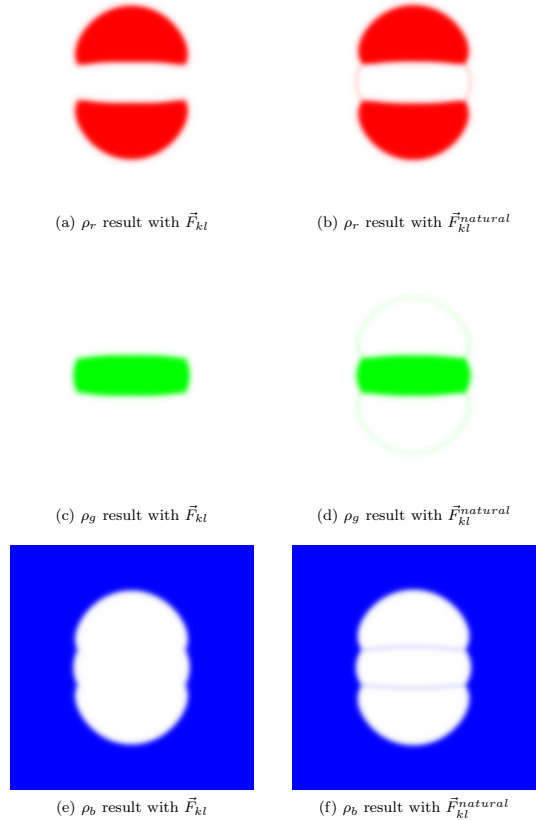


FIGURE 8: (Better quality and color available online) Mass flow leakage in the direction tangential to the interface at $t = 8000$.

3.4 Laplace-Young's law

The goal in this section is to verify whether or not the model can correctly simulate the static contact angles at a triple fluid junction as a function of the surface tension. In the current study, this numerical test is the only one that really checks the quantitative behavior of the model for a flow with three phases. It will then be numerically investigated and described in detail. A complementary goal is to define a simple and robust quality index to measure the accuracy of any LB model with respect to the static contact angles. Before going into the details of this test, we wish to point out that Refs. [40, 43] have addressed the subject of contact angles with three phases within the LB framework. This study has also been conducted in Refs. [6, 24] using other numerical methods.

We now discuss the flow configuration in the context of an LB

setting. A lattice of $N_x \times N_y$ sites is used with periodic boundary conditions at the four ends. The corner at the bottom left of the domain is located at the origin $(0, 0)$. The fluids are initialized using the zero velocity equilibrium distribution functions. The green fluid is initialized at the following position :

$$\left(x - \left(\frac{N_x - 1}{2}\right)\right)^2 + \left(y - \left(\frac{N_y - 1}{2}\right)\right)^2 \leq \left(\frac{N_x}{2}\right)^2 \quad (42)$$

The red fluid is initialized at the remaining sites available in the section $y < \frac{N_y - 1}{2}$. The other lattice sites are filled with blue fluid. Fig. (9) shows the initial conditions of this setup for $N_x = 1024$ and $N_y = 1024$. The green bubble may appear small when compared to the computational domain, but its size has been chosen to accommodate the simulations with very small contact angles. Also, the green bubble is small, in order to avoid the perturbation coming from the periodic boundary conditions. As described in section (3.2), the initial condition of this problem can lead to instability. Therefore, the first 2000 time steps are used to stabilize the initial condition.

The stopping criterion for all simulations is a dynamic procedure which combines two criteria. Let us denote n the time step number and Q_{old} , updated every 2000 time steps, the last quality index of the simulation that is kept in the computer memory. First, $|Q^n - Q_{old}| < 10^{-5}$ must be true for 50000 time steps in a row. If the previous condition is true, then $|\frac{Q^n - Q_{old}}{Q^n}| < 10^{-5}$ is checked. If it is true, the simulation stops, if not, the counter, which is then at 50000, is reset to 0 and the simulation continues. As in section (3.3), with both high density and high viscosity ratios, numerical noise is present and may prevents the simulation from converging with such a restrictive numerical steady state condition. So, in Table (9), the simulations (a) with lattice size 128×128 and 256×256 were stopped after 5000000 time steps. All the others simulations have converged correctly.

In all the simulations, the following parameters are constant : $\sigma_{rb} = 10^{-2}$, and $\alpha_\kappa = 4/9$. Three sets of simulations are considered :

1. One with unit density and viscosity ratios, i.e. with $\rho_k = 1$, $\nu_k = 1/6$, and $\beta_0 = 0.7$.
2. One with high density ratios, but unit viscosity ratios, i.e. with $\rho_r = 1$, $\rho_g = 1000$, $\rho_b = 1$, $\nu_k = 1/6$, and $\beta_0 = 0.7$.
3. One with both high density and high viscosity ratios, i.e. with $\rho_r = 1$, $\rho_g = 1000$, $\rho_b = 1$, $\nu_r = 1/100$, $\nu_g = 1$, $\nu_b = 1/100$, and $\beta_0 = 0.5$.

For each simulation set, the surface tensions σ_{rg} and σ_{gb} are varied, in order to generate different contact angles, θ_{rg} and θ_{gb} . Tables (7), (8), and (9) show the missing parameters and the results of these simulations.

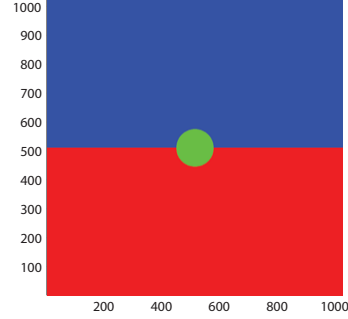


FIGURE 9: (Color available online) Typical initial condition for a Laplace-Young law simulation.

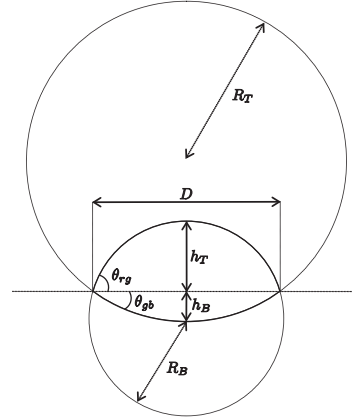


FIGURE 10: Expected steady state configuration for the green fluid deduced from the Laplace-Young law.

At steady state, the expected flow configuration is shown in Fig. (10) when a Neumann triangle exists. This is deduced from Laplace-Young's law. Based on geometric considerations, we can define the following variables :

$$D = 2 \sqrt{\frac{A_g}{\sum_{kl=r,g,b} \frac{1}{\sin(\theta_{kl})} \left(\frac{\theta_{kl}}{\sin(\theta_{kl})} - \cos(\theta_{kl}) \right)}} \quad (43)$$

$$h_T = \frac{D}{2} \left(\frac{1 - \cos(\theta_{rg})}{\sin(\theta_{rg})} \right) \quad (44)$$

$$h_B = \frac{D}{2} \left(\frac{1 - \cos(\theta_{gb})}{\sin(\theta_{gb})} \right) \quad (45)$$

$$L_i = \sqrt{h_i^2 + (D/2)^2}, \quad i = T, B \quad (46)$$

$$R_i = \frac{\left(\frac{L_i}{2}\right)^2}{\sqrt{1 - \left(\frac{D/2}{L_i}\right)^2}}, \quad i = T, B \quad (47)$$

$$\theta_i = 2 \arccos \left(\frac{R_i - h_i}{R_i} \right), \quad i = T, B \quad (48)$$

where A_g is the initial area of the green fluid. In our case, A_g equals the initial number of green sites. Following this, a *quasi-analytical solution*, i.e. two arc circles, for the position of the top and bottom interface can be found :

$$R_T e^{\theta_i} + x_c + i(y_c - (R_T - h_T)), +\pi - \theta_T \leq 2\theta \leq +\pi + \theta_T \quad (49)$$

$$R_B e^{\theta_i} + x_c + i(y_c + (R_B - h_B)), -\pi - \theta_B \leq 2\theta \leq -\pi + \theta_B \quad (50)$$

Note that $i = \sqrt{-1}$ in the previous two arc circle equations, and that $x_c = (N_x - 1)/2$. We describe the above equations as a quasi-analytical solution, because the position of y_c is not known a priori when the simulation is started. This is because of the periodic boundary and initial conditions. For example, with variable density ratios and depending on the surface tension, a large amount of momentum is transferred between the various fluid colors and the position of y_c changes. Moreover, the final value of y_c is not known, which is why we describe it now. First, a set of y values is defined :

$$\{y_1, y_2, \dots, y_n, \dots, y_{16}\} = \{y \mid 16 \text{ sites with } \frac{\rho_r \rho_b \rho_g}{\rho^3} \text{ maximum}\} \quad (51)$$

Then, the value used for y_c is defined as :

$$y_c = \frac{\sum_{n=1}^{16} y_n \left(\frac{\rho_r \rho_b \rho_g}{\rho^3} \right)_n}{\sum_{n=1}^{16} \left(\frac{\rho_r \rho_b \rho_g}{\rho^3} \right)_n} \quad (52)$$

$$(53)$$

3.4.1 Laplace-Young's law : Quality index

From the quasi-analytical position of the interfaces, we can define the following quality index :

$$Q = \sqrt{\left(\frac{\rho_k^{tot} - \rho_k^{out}}{\rho_k^{tot}} \right)^2 + \left(\frac{\rho_b^{tot} - \rho_b^{out}}{\rho_b^{tot}} \right)^2 + \left(\frac{\rho_g^{tot} - \rho_g^{in}}{\rho_g^{tot}} \right)^2} \quad (54)$$

where ρ_k^{tot} is the total amount of k fluid in the computational domain. Also, ρ_k^{out} is the amount of k fluid that is outside the two quasi-analytical arc circles, while ρ_k^{in} is the amount of k fluid inside them. Note that $Q = 0$ indicates *indirectly* that the interfaces between the fluids are located exactly where predicted by the analytical solution. Also, this quality index is easier to use, and is more robust and reliable than any heuristic method of calculating the contact angles numerically.

3.4.2 Laplace-Young's law : Results

Table (7) shows, for unit density ratios, the quality index Q obtained at steady state for different lattice sizes, ranging from 128×128 to 1024×1024 . Tables (8) and (9) show the same test, but for high density ratios and unit or high viscosity ratios.

The order of convergence of the quality index in terms of lattice size is also computed, and presented in Tables (7), (8), and (9). The order of convergence is computed as the absolute value of the slope of the best fit line in a log-log scale of the quality index Q versus the lattice size N_x .

From these results, we can deduce that this LB model is compatible with the analytical solution of Laplace-Young's law, because the order of convergence of the quality index Q is about 1. Note that, where

the order of convergence is much lower than 1, e.g. case (a) with a convergence order equal to 0.76 in Table (7), the value for Q_{512}/Q_{1024} equals 1.921 and is about 2, which confirms first order accuracy and indicates that the lattice would need to contain, for this case, more sites, in order to see the first order accuracy appear. For the high density ratios and the high viscosity ratio simulations, since $\beta_0 = 0.5$ and so the interface fluids are thicker, the quality index Q for these simulations is higher, but the order of convergence is still about 1.

It is important to emphasize that LB models are usually thought to be second order accurate, but that is true for a single-phase flow and not necessarily for multiphase flows. From our knowledge, only the basic LB streaming combined with the BGK collision was shown to be second order accurate in time and space [30] for the conserved variables ρ and $\rho \vec{u}$, and not with the multiphase collision operator. So it is no surprise that the scheme is first order in terms of the quality index. It is believed that LB models for simulating multiphase flow may only be first order accurate in space and time *at the interface* for the conserved variables ρ and $\rho \vec{u}$. Second order accuracy is only achieved in regions of a pure phase. Obtaining second order accuracy at the interface is difficult, because the combination of all the operators would need to be constructed in such a way as to satisfy, at the macroscopic level, the Navier-Stokes equations to second order. This appears to be difficult to achieve, but may be possible.

Even though the contact angles are small, the model still captures the correct contact angles. We recall that this is not possible, at least for this model, without the special relations in Eq. (28) for β_{kl} . Without these special formulas, the scheme simply becomes incompatible with the analytical solution. In other words, the order of convergence would rapidly decrease to zero as the lattice size increases. For example, when case (a), with unit density ratios from Table (7), was simulated by setting the coefficients to $\beta_{kl} = \beta^0$ instead of using the special relations in Eq. (28), we found that the order of convergence for the quality index Q dropped to 0.635. Moreover, $Q_{512}/Q_{1024} = 1.564$ for that case, so there was no sign of compatibility with the analytical solution using $\beta_{kl} = \beta^0$.

Figure (11) shows the numerical solution of the simulations at steady state with the unit density ratios presented in Table (7). Figures (12) and (13) show the same solutions, but with the simulations presented in Tables (8) and (9) with high density ratios and with unit/high viscosity ratios. The quasi analytical arc circles and the contours of the functions $\rho_g/\rho_g^0 = 0.5$ and $\rho_g/\rho_g^0 = 0.01$ are also plotted, in order to visualize the theoretical versus the numerical position of the interface. The two contour values give an idea of the interface width. These figures are provided to make it possible to visualize that the density and viscosity ratios have very little effect on the numerical steady state contact angles. Note that the axes were rescaled in order to emphasize the plot on the green bubble.

In concluding this section, we can infer that Laplace-Young's law is correctly embedded in this model, i.e. the surface tension alone is enough to achieve the theoretical steady state contact angles between the fluids.

3.5 Multilayered Couette's flow

The purpose of this numerical test is to investigate the model's ability to simulate flow with variable dynamic viscosity. The multilayered Couette's flow consists of multiple layers of fluids between two infinite moving plates, as shown in Fig. (14).

The variable x_k is used to denote the interface position between the fluids with properties (ρ_k, μ_k) and (ρ_{k+1}, μ_{k+1}) , where $\mu_k = \rho_k \nu_k$ is the dynamic viscosity. The walls located at positions x_0 and x_N are moving vertically at a velocity of v_0^y and v_N^y respectively.

At steady state and applying the incompressibility hypothesis, an

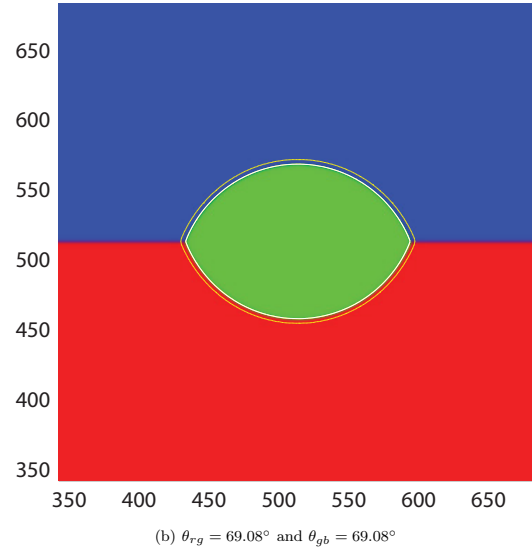
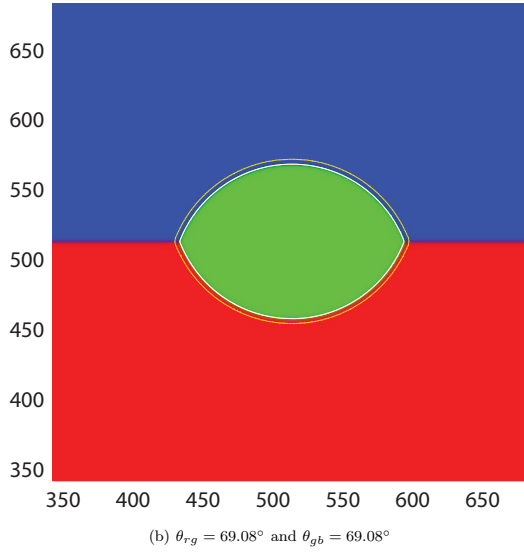
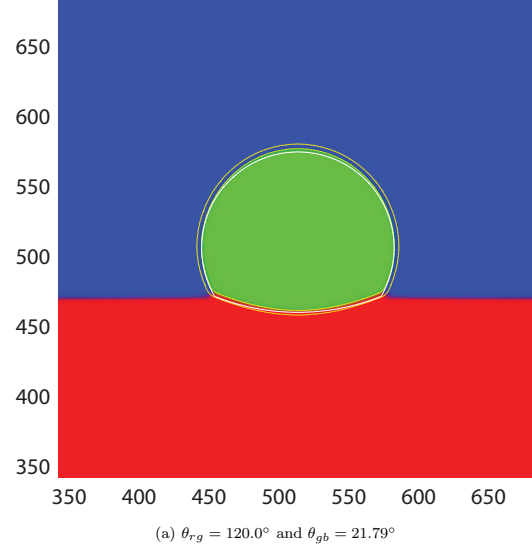
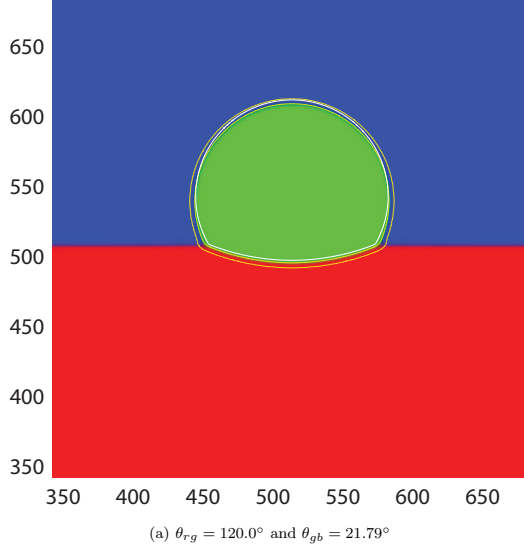


FIGURE 11: (*Better quality and color available online*) Steady state solution at *unit* density and *unit* viscosity ratios for different contact angles.

FIGURE 12: (*Better quality and color available online*) Steady state solution at *high* density and *unit* viscosity ratios for different contact angles.

analytical solution exists for the previous flow setting (see Ref. [22] for the three-layer case). Here, we derive a generalized solution for the N phase Couette's flow. From the Navier-Stokes equations, each fluid layer k should respect :

$$\frac{\partial^2}{\partial x^2} v_k^y = 0 \quad (55)$$

This leads to multiple linear velocity profiles within each interval

$x_{k-1} \leq x \leq x_k$, of the form :

$$v_k^y = a_k x + b_k \quad (56)$$

Both boundary conditions and interface conditions must be provided to solve the partial differential equation problem. Physical considerations imply that the velocity in Eqs. (59) and the shear stress in Eqs. (60) must be continuous at each of the interfaces [4]. Therefore,

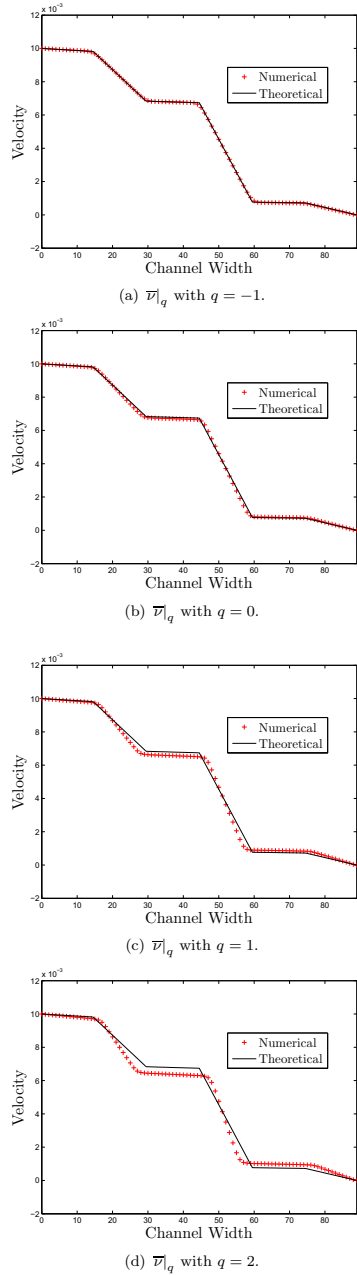


FIGURE 15: Numerical and theoretical velocity profile for the multilayered Couette's flow with *unit* density ratios.

fluid layers. It is also important to show that the choice of viscosity interpolation $\overline{\nu}|_q$ can have a positive impact, because the accuracy

of the model depends on this choice. The densities and viscosities used in this simulation are $\rho_k = 1$, $\nu_1 = 1/6$, $\nu_2 = 1/96$, $\nu_3 = 1/3$, $\nu_4 = 1/192$, $\nu_5 = 2/3$, and $\nu_6 = 1/24$ respectively.

The numerical velocity profile that was obtained at steady state is compared in Fig. (15) to the theoretical profile for each of the possible viscosity interpolations considered in this study. Let us denote as $E(x_j)$ the difference between the numerical and theoretical velocity of the fluid at site $x = x_j$. Table (10) shows the error with the theoretical profile using different norms. A norm is calculated with all the lattice sites. Clearly, from Fig. (15) and Table (10), the q -average with $q = -1$ used to compute $\overline{\nu}|_q$ provides better results than the other alternatives. Afterwards, the accuracy decreases as q increases. The numerical profile in Fig. (15a) agrees better with the theoretical profile than that in Figs. (15b-15d). Moreover, for some norms, errors can be lowered by one order of magnitude compared to other choices for $\overline{\nu}|_q$, and for the same lattice size.

From section (3.2), the q -average with $q = 2$ was the best choice. This leads to a kind of contradiction, however. The planar interface simulations tell us to take $q = 2$, while the Couette's flow tells us to take $q = -1$. We think that $q = -1$ is a better choice when simulating unit density ratio, and $q = 1$ appears to be the better choice when dealing with a non unit density ratio. Nevertheless, there are still many factors that are not taken into account, and the accuracy resulting from the viscosity interpolation may depend more on the type of flow than we may think. Thus, depending on what is most important, e.g. surface tension or velocity, other choices might be better suited to a given situation.

3.5.2 Multilayered Couette's flow with *variable* density ratios

In this section, the current model is tested against the multilayered Couette's flow with variable density ratios between the fluid interfaces. The density and viscosity of the different fluids are $\rho_k = 7 - k$ and $\nu_k = 1/6$.

It turns out that the model fails this numerical test. In [34], it was shown that an RK model fails the multilayered Poiseuille's flow with variable density ratios. Poiseuille's flow is more complicated than Couette's flow, because of the source term involved in the model that mimics a pressure gradient. In an earlier work [29], failure of the Poiseuille's flow test was blamed on a possible inaccuracy of the source term in the presence of variable density ratios. It is possible that this hypothesis may not be correct, because, even though no source term is needed to simulate Couette's flow, the model is still unsuccessful. Note that Poiseuille's flow, which is a similar problem, can be simulated with very high viscosity ratios, $O(10000)$, as long as the unit density ratio is considered [29].

The numerical solution for the density, velocity, and momentum is presented with the analytical solution in Fig. (16). At steady state, the numerical density profile matches the theoretical profile, but the numerical velocity and the momentum profile are incorrect.

From Fig. (16b), we can realize that momentum decreases smoothly and linearly from the left to the right boundary, without being affected *at all* by the change in the fluid density across the interface. This shows the model's inability to simulate flow with variable density ratios in the presence of non zero momentum or a non zero momentum gradient. In all the preceding test cases, the analytical solution at steady state was calculated with zero momentum. This may well explain why these test cases provide good results at steady state, but not for the Couette's flow with variable density ratios. Note that the validity of the unsteady process at high density ratios in the earlier test cases is also open to discussion.

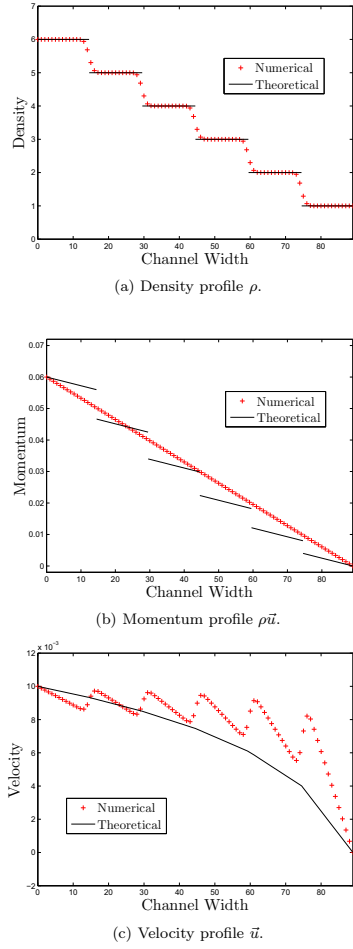


FIGURE 16: Numerical and theoretical solution profile for the multi-layered Couette's flow with *variable* density ratios.

It should be pointed out, however, that the numerical density profile in Fig. (16a) is correct, and that it agrees well with the fact that previous tests only investigated the model's behavior in terms of density. First, in section (3.3), the pressure jump is linearly related to density with the equation of state in Eq. (11). Second, in order to introduce surface tension, the role of the perturbation operator is to deplete mass (density behavior) perpendicular to the color gradient and add mass in the direction of the color gradient *while conserving momentum*. Third, the special interface thickness adjustment set by Eq. (28) only adjusts to the different color density profile. All the previous tunings seem to work well with variable density ratios with a momentum that is theoretically zero. However, when a variable density ratio is simulated along with non zero momentum or a non zero momentum gradient, this RK model fails.

In the [34] study, an RK [34], an SC [34], an FE [32, 44], and an MF [20] model were tested against a three-layer Poiseuille's flow

with variable density ratios. None of these models passed the test. Moreover, it is thought that they would also fail the simpler Couette's flow test with variable density ratios. In this respect, we have not been able to find a study in the reviewed literature which discusses a successful simulation obtained with a pure LB model. There is one exception, however, which we found in the Knutson and Noble [25] paper, where this basic flow was successfully simulated. Nevertheless, the authors clearly state that their method, as presented, is not suitable for more complicated flow configurations. A great deal of effort is still needed to generalize their method to solve general complex flows. Moreover, this method may need to be combined with a level set solver, which would mean that the elegance of a pure LB model would be lost.

From the above results, we conclude that there remains a missing link for pure multiphase LB schemes with variable density ratios, and that, unfortunately, these schemes may not be ready for engineering applications. However, for applications where density ratios can be neglected, i.e. unit density ratios, this numerical scheme works very well.

4 Technical details

This section is included to explain how this numerical algorithm can be constructed in such a way that the computer memory required is significantly reduced. This is an important factor to take into account when simulating N -phase flow when N is large. The pseudo-algorithm for the LB model in this paper is the following :

1. Initialization of the density field ρ_k for each fluid k .
2. Initialization of the color-blind distribution functions N_i . Usually, N_i is initialized with the equilibrium :

$$N_i|_{t=0} = \sum_k N_i^{k(e)} \quad (64)$$

It is important to note the following property of the color-blind equilibrium :

$$N_i^{(e)} = \sum_k N_i^{k(e)}(\rho_k, \vec{u}, \alpha_k) = N_i^{(e)}(\rho, \vec{u}, \vec{\alpha}|_{q=1}) \quad (65)$$

3. Main loop :
 - BGK collision on the color-blind distribution functions N_i using the effective relaxation factor ω_{eff} . Note that :

$$\begin{aligned} (\Omega_i)^{(1)}(N_i) &= \sum_k (\Omega_i^k)^{(1)}(N_i^k) = \\ &= \sum_k N_i^k - \sum_k \omega_{\text{eff}}(N_i^k - N_i^{k(e)}) = \\ &= N_i - \omega_{\text{eff}}(N_i - N_i^{(e)}) \end{aligned} \quad (66)$$

It is from the previous equation that we realize how important it is to choose the same ω_{eff} for each fluid color. Without this, the previous equation does not hold and the BGK collision cannot be performed only on the color-blind distribution functions.

- Compute and store the gradient of the color density fraction $\vec{\nabla} \left(\frac{\rho_k}{\rho} \right)$ for each fluid k .
- Apply the perturbation to the color-blind distribution functions N_i . Note that :

$$\begin{aligned} (\Omega_i)^{(2)}(N_i) &= \sum_k (\Omega_i^k)^{(2)}(N_i^k) = \\ N_i &+ \sum_k \sum_{l \neq k} \frac{A_{kl} C_{kl}}{2} |\vec{F}_{kl}| \left[W_i \frac{(\vec{F}_{kl} \cdot \vec{c}_i)^2}{|\vec{F}_{kl}|^2} - B_i \right] \end{aligned} \quad (67)$$

- Set $N_i^{\text{temp}} = 0$ and $\rho_k^{\text{temp}} = \rho_k$.
- Loop over each fluid k :
 - Recolor fluid k in order to obtain N_i^k using the recoloring operator $(\Omega_i^k)^{(3)}$, the fluid density of each fluid ρ_k^{temp} , and the color-blind distribution functions N_i .
 - Stream the distribution functions N_i^k using the streaming operator $(\Omega_i^k)^{(4)}$.
 - Store the new values for the density and color-blind distribution functions :

$$N_i^{\text{temp}} = N_i^{\text{temp}} + N_i^k \quad (68)$$

$$\rho_k = \sum_k N_i^k \quad (69)$$

So, the idea of the previous loop is to recolor and stream one fluid color at a time.

- Set $N_i = N_i^{\text{temp}}$.

The previous pseudo-procedure implies that, for each fluid color k , the density ρ_k , the gradient of the density fraction $\vec{\nabla} \left(\frac{\rho_k}{\rho} \right)$, and the color-blind distribution functions N_i for each lattice site needs to be always kept in memory. Depending on the software implementation, a temporary copy of these variables may also need to be kept in memory. What is important to note is that there is no need to always store the distribution functions N_i^k of each fluid k , but only their density ρ_k .

In addition, the use of sparse arrays could be used for each fluid ρ_k and the gradient of the density fraction $\vec{\nabla} \left(\frac{\rho_k}{\rho} \right)$, in order to reduce the total computer memory required. Of course, this would be at the expense of losing mass conservation, but this may be controlled. Moreover, if the norm of the color gradient is near zero for a certain k - l fluid interface, the value β_{kl} could be set to zero to decrease the computational complexity of the recoloring operators. The same strategy can be applied for the perturbation operator by setting $A_{kl} = 0$, if the color gradient is negligible. All these numerical techniques will be studied in a future work and have not been applied here.

5 Conclusion

In this paper, a lattice Boltzmann model for the simulation of multiple immiscible fluids was developed and numerically investigated. Our results show that, as long as the momentum is theoretically zero at steady state, the model can effectively simulate high density and high viscosity ratios, up to $O(1000)$ and $O(100)$ respectively, with stability and accuracy. In spite of this success, the multilayered Couette's flow with variable density ratios is a test case that the current model fails to simulate. However, for unit density ratios, this model appears to be very accurate. The generalization from two phases to N phases is not straightforward, because all the collision operators need to be generalized for N phases and still capture some of the essential physics. Particular attention has been paid to the definition of the color gradient, in order to avoid numerical instability and non physical mass flow tangential to the interfaces. Fortunately, there was a definition of that vector in the Allen-Cahn system that works properly. Moreover, this definition has the advantage of generalizing the model to N -phase flows while only using neighbor information with $O(N)$ in computational complexity. Also, the concentration factor in our model, which is used to limit the activation of the surface tension to the desired interface, and which is absent in the two-phase flow simulation, is carefully selected. The choice of the effective relaxation factor seems to be an important factor affecting the accuracy of the model as well. For three-phase flow, the interface width at the triple

fluid junction must be considered in a special way, in order to capture the correct static contact angles. All the previous details were needed, even for unit density ratios, to correctly embed Laplace's law and Laplace-Young's law in this N phase LB model. This LB model can be constructed in such a way that there is no need to keep all the various color distribution functions in memory, as only the color-blind distribution functions are needed. We believe that this model may be able to achieve both high density and high viscosity ratios up to $O(1000)$ simultaneously for several test cases. When simulating high viscosity ratios, to avoid a large over-relaxation of the effective relaxation parameters, one of the fluid viscosities must be very low, which might cause instability. The BGK collision operator, as used in this work, is known to result in unstable simulation for low viscosity. Other collision operators like the two-relaxation time (TRT) operator [13] or the multi-relaxation time (MRT) operator [33], which behave better in such situations, might solve this problem. The introduction of the Brownlee et al. stability condition into this model could also help [8]. Another alternative might be the entropic lattice Boltzmann methods [5]. It would be interesting to investigate these options in future work. Also, further research needs to be conducted to find a cure for the discontinuity problem of the multiphase LB model [1] and allow high density ratios to be accurately simulated in the multilayered Couette's flow. For now, this model can only be used with confidence when the various density ratios can be neglected and set to unity.

Acknowledgments

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Simulations sets				
	$\{E_j \mid \sigma_{kl} = 10^{-5}\}$	$\{E_j \mid \sigma_{kl} = 10^{-3}\}$	$\{E_j \mid \sigma_{kl} = 10^{-1}\}$	$\bar{\nu} _q$
$\max\{\cdot\}$	3.961e+01	2.063e+00	1.501e+00	$q = -1$
	4.469e+00	1.712e+00	1.693e+00	$q = 0$
	1.122e+00	8.442e-01	8.442e-01	$q = 1$
	1.427e+00	1.670e-01	1.672e-01	$q = 2$
$\langle\{\cdot\}\rangle$	3.706e+00	7.712e-01	7.297e-01	$q = -1$
	9.807e-01	6.937e-01	6.906e-01	$q = 0$
	4.111e-01	3.350e-01	3.351e-01	$q = 1$
	2.411e-01	5.422e-02	5.263e-02	$q = 2$

TABLE 3: Errors in percentage (%) based on various norms, simulations sets, and effective relaxation factors for the multilayered planar interfaces.

Simulations sets $\{E_j \mid [\cdot]\}$					
	$[\rho_k = 1, \nu_k = 1/6]$	$[\nu_k = 1/6, \exists k : \rho_k \neq 1]$	$[\rho_k = 1/6, \exists k : \nu_k \neq 1]$	$[\exists k : \nu_k \neq 1/6, \exists k : \rho_k \neq 1]$	$\bar{\nu} _q$
$\max\{\cdot\}$	1.430e-03	1.587e-01	1.501e+00	3.961e+01	$q = -1$
	1.430e-03	1.587e-01	1.693e+00	4.469e+00	$q = 0$
	1.430e-03	1.587e-01	8.442e-01	1.122e+00	$q = 1$
	1.430e-03	1.587e-01	4.549e-02	1.427e+00	$q = 2$
$\langle\{\cdot\}\rangle$	1.430e-03	6.001e-02	9.918e-01	2.735e+00	$q = -1$
	1.430e-03	6.001e-02	9.488e-01	1.065e+00	$q = 0$
	1.430e-03	6.001e-02	4.745e-01	4.624e-01	$q = 1$
	1.430e-03	6.001e-02	3.187e-02	1.754e-01	$q = 2$

TABLE 4: Errors in percentage (%) based on various norms, simulations sets, and effective relaxation factors for multilayered planar interfaces.

Unit density ratios					Quality index : Q				Order	Q_{512}/Q_{1024}
	$\sigma_{rg} \cdot 10^2$	$\sigma_{gb} \cdot 10^2$	θ_{rg}	θ_{gb}	128x128	256x256	512x512	1024x1024		
(a)	1.40	0.60	120.0	21.79	1.44e-01	9.20e-02	5.62e-02	2.93e-02	0.760	1.921
(b)	1.40	1.40	69.08	69.08	1.40e-01	6.80e-02	3.47e-02	1.79e-02	0.986	1.937

TABLE 7: Quality index and order of convergence for different static contact angles with *unit* density ratios.

High density ratios					Quality index : Q				Order	Q_{512}/Q_{1024}
	$\sigma_{rg} \cdot 10^2$	$\sigma_{gb} \cdot 10^2$	θ_{rg}	θ_{gb}	128x128	256x256	512x512	1024x1024		
(a)	1.40	0.60	120.0	21.79	2.60e-01	1.17e-01	5.57e-02	2.61e-02	1.101	2.130
(b)	1.40	1.40	69.08	69.08	1.24e-01	6.35e-02	3.20e-02	1.55e-02	0.998	2.066

TABLE 8: Quality index and order of convergence for different static contact angles with *high* density ratios.

High density and viscosity ratios					Quality index : Q				Order	Q_{512}/Q_{1024}
	$\sigma_{rg} \cdot 10^2$	$\sigma_{gb} \cdot 10^2$	θ_{rg}	θ_{gb}	128x128	256x256	512x512	1024x1024		
(a)	1.40	0.60	120.0	21.79	3.29e-01	1.56e-01	6.03e-02	2.56e-02	1.243	2.357
(b)	1.40	1.40	69.08	69.08	1.86e-01	9.26e-02	4.55e-02	2.34e-02	0.999	1.948

TABLE 9: Quality index and order of convergence for different static contact angles with *high* density and *high* viscosity ratios.

	ω_{eff} calculated with $\overline{v} _q$			
	$q = -1$	$q = 0$	$q = 1$	$q = 2$
$\max E(x_i) $	9.445e-05	2.923e-04	6.332e-04	9.104e-04
$\frac{1}{x_N - x_0} \sqrt{\sum_i (E(x_i))^2}$	2.434e-06	9.598e-06	2.261e-05	3.684e-05
$\frac{1}{N_x} \sum_i E(x_i) $	1.455e-05	6.419e-05	1.605e-04	2.733e-04

TABLE 10: Error comparison based on different norms for the multilayered Couette's flow with *unit* density ratios.

ANNEXE D

**Enhanced equilibrium distribution functions for simulating immiscible
multiphase flows with variable density ratios in a class of lattice Boltzmann
models**

Il est important de noter que cet article pourrait être sujet à des changements d'ici la publication finale de celui-ci dans une revue scientifique.

Sébastien Leclaire, Nicolas Pellerin, Marcelo Reggio and Jean-Yves Trépanier, "Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models", manuscript submitted to *International Journal of Multiphase Flow* in February 2013.

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Enhanced equilibrium distribution functions for simulating immiscible multiphase flows with variable density ratios in a class of lattice Boltzmann models

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Abstract

This research examines the behavior of a class of lattice Boltzmann (LB) models designed to simulate immiscible multiphase flows. There is some debate in the scientific literature as to whether or not the "color gradient" models, also known as the Rothman-Keller (RK) models, are able to simulate flow with density variation. In this paper, we show that it is possible, by modifying the original equilibrium distribution functions, to capture the discontinuity present in the analytical momentum profile of the two-layered Couette flow with variable density ratios. Investigations carried out earlier were not able to simulate such a flow correctly. Now, with the proposed approach, the new scheme is compatible with the analytical solution, and it is also possible to simulate the two-layered Couette flow with simultaneous density ratios of $O(1000)$ and viscosity ratios of $O(100)$. The authors believe that this improvement can be made to other RK models as well, which will allow the range of validity of these models to be extended. This is, in fact, what we found for the method proposed in this article.

1 Introduction

Lattice Boltzmann models of multiphase flow can be classified in various categories. One possible classification could be the following :

- the RK from Rothman and Keller [1988];
- the SC from Shan and Chen [1993];
- the Free-Energy (FE) from Swift et al. [1996];
- the Mean-Field (MF) from He et al. [1998] and
- the Field-Mediator (FM) from Santos et al. [2003].

It is worth noting that this classification is not universally adopted, and there are other models, not discussed in this work, that may be classified differently. Our goal here is to improve the RK category, and we begin by providing a short literature review of the RK lattice Boltzmann models.

The RK lattice Boltzmann model for simulating multiphase flow is derived from the lattice gas model of Rothman and Keller [1988]. A couple of years later, Gunstensen et al. [1991] developed a lattice Boltzmann version of the RK model. Grunau et al. [1993] then modified the Gunstensen et al. model to accommodate variable density and viscosity ratios between the fluids in several test cases.

Tölke [2002] and Latva-Kokko and Rothman [2005] realized that the original recoloring step performed at the interface of the fluids in the above model was making the scheme unstable in some situations, or resulting in non physical behavior such as lattice pinning. New recoloring schemes were developed in both studies and the authors of both agreed that the main problem with the original model was a very thin interface between the fluids. Tölke [2002] managed to

achieve preliminary simulations that agreed well with experimental data.

Reis and Phillips [2007] changed the forcing scheme of the perturbation operator to induce the appropriate surface tension term in the macroscopic equations. Even without the newest recoloring operators, Reis and Phillips showed that their model could be used to simulate flow with large density ratios in some test cases. Leclaire et al. [2012c] adapted the recoloring operator of Latva-Kokko and Rothman for the Reis and Phillips model in the case of variable density ratios. This modification led researchers to conclude that numerical "noise" in the model could be substantially reduced. Also, higher density ratios were tackled for the same Reis and Phillips test cases. However, as was the case in other studies (Rannou [2008]; Aidun and Clausen [2010]; Yang and Boek [2013]), the current RK model was not able to simulate flow with density variation for the multilayered Poiseuille or Couette flow test cases.

While some sought a cure for this problem, Leclaire et al. [2011a] aimed to develop the RK model in order to increase precision in terms of simulating Laplace's law with isotropic discretization for the color gradient. Also, Liu et al. [2012] developed a 3D version of the Reis and Phillips perturbation operator for the D3Q19 lattice. Satisfactory agreement with some experimental results was obtained in the Liu et al. research. Other efforts were also made by Leclaire et al. [2011b] to develop an N-phase model. This latter study showed that the RK model was not able to capture the theoretical momentum discontinuity in the simple multilayered Couette flow. Our objective in the current research is to find a solution to this serious problem, which affects RK models in general.

Fortunately, a review of the scientific literature has revealed that models have been developed with demonstrable ability to simulate the multilayered Couette or Poiseuille flow. Lishchuk et al. [2008], for example, developed a multicomponent LB method for fluids with density contrast, which was shown to recover the multilayered Couette flow with a density ratio different from 1. It is not clear, however, how their idea could be used to apply a simple fix to the RK models that were previously not working (Grunau et al. [1993]; Tölke [2002]; Reis and Phillips [2007]; Rannou [2008]; Leclaire et al. [2012c, 2011a]; Liu et al. [2012]). Although this basic flow was successfully simulated in the work of Knutson and Noble [2009], the authors clearly state that their method, as presented, is not suitable for more complicated flow configurations, and a great deal of effort is still needed to generalize their method to solving general complex flows. Moreover, this method may need to be combined with a level set solver, in which case the elegance of a pure LB model would be lost. Yiotis et al. [2007] show that their model can simulate the multilayered Poiseuille flow with density ratios; nevertheless, considerable effort would be required to adapt their ideas to the current RK formulation, as their model use

a new pressure distribution function.

Holdych et al. [1998] modified the equilibrium stress tensor of the free energy model of Swift et al. [1996], in order to recover the analytical solution of the multilayered Couette flow with variable density ratios. In fact, we show here that their approach can be readily and easily adapted to the RK model to correctly recover the Navier-Stokes equations in the single phase region with a weak pressure gradient and within the limits of small Mach and Knudsen numbers. Moreover, our method does allow the current RK model to correctly simulate the multilayered Couette flow, even in the case of simultaneous high density $O(1000)$ and high viscosity $O(100)$ ratios. This simple fix can also be applied in a straightforward manner to the following RK model (Grunau et al. [1993]; Tölke [2002]; Reis and Phillips [2007]; Rannou [2008]; Leclaire et al. [2012c, 2011a]; Liu et al. [2012]), and perhaps to other LB models with similar issues (Rannou [2008]).

2 Lattice Boltzmann immiscible multi-phase model

The current LB approach follows the two-phase model of Reis and Phillips [2007], along with the improvements presented by Leclaire et al. [2012c, 2011a,b] for the recoloring operator, the isotropic color gradient, and the model generalization to N-phase flows. For this 2D LB model, there are N sets of distribution functions, one for each fluid, moving on a D2Q9 lattice with the velocity vectors $\vec{c}_i$. With $\theta_i = \frac{\pi}{4}(4 - i)$, these velocity vectors are defined as :

$$\vec{c}_i = \begin{cases} (0, 0), & i = 1 \\ [\sin(\theta_i), \cos(\theta_i)] c, & i = 2, 4, 6, 8 \\ [\sin(\theta_i), \cos(\theta_i)] \sqrt{2}c, & i = 3, 5, 7, 9 \end{cases} \quad (1)$$

where $c = \Delta x / \Delta t$, $\Delta y = \Delta x$, Δx is the lattice spacing, and Δt is the time step.

The distribution functions for a fluid of color k (e.g. $k = r$ for red, $k = g$ for green, and $k = b$ for blue) are noted $N_i^k(\vec{x}, t)$, while $N_i(\vec{x}, t) = \sum_k N_i^k(\vec{x}, t)$ is used for the color-blind distribution function. The algorithm uses the following evolution equation :

$$N_i^k(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = N_i^k(\vec{x}, t) + \Omega_i^k(N_i^k(\vec{x}, t)) \quad (2)$$

where the collision operator Ω_i^k is the result of the combination of three sub operators (similar to Tölke [2002]) :

$$\Omega_i^k = (\Omega_i^k)^{(3)} \left[(\Omega_i^k)^{(1)} + (\Omega_i^k)^{(2)} \right] \quad (3)$$

These original operators are rewritten in such a way that the evolution equation is solved in four steps with operator splitting, as follows :

1. Single phase collision operator :
 $N_i^k(\vec{x}, t_*) = (\Omega_i^k)^{(1)}(N_i^k(\vec{x}, t))$
2. Multiphase collision operator (perturbation) :
 $N_i^k(\vec{x}, t_{**}) = (\Omega_i^k)^{(2)}(N_i^k(\vec{x}, t_*))$
3. Multiphase collision operator (recoloring) :
 $N_i^k(\vec{x}, t_{***}) = (\Omega_i^k)^{(3)}(N_i^k(\vec{x}, t_{**}))$
4. Streaming operator :
 $N_i^k(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = N_i^k(\vec{x}, t_{***})$

The model presented with the evolution equation (2) suggests the use of one set of distribution functions for each fluid. Leclaire et al.

[2011b] explains how the number of distribution functions necessary for the simulation of N-phase flows can be reduced. Conceptually, only the distribution functions of the color-blind fluid and each density field are required to implement the model, although it is much easier to describe the theoretical model using one set of distribution functions for each fluid.

2.1 Original single phase collision operator

The first sub operator, $(\Omega_i^k)^{(1)}$, is the standard BGK operator of the single phase LB model, where the distribution functions are relaxed towards a local equilibrium, in which ω_{eff} denotes the effective relaxation factor :

$$(\Omega_i^k)^{(1)}(N_i^k) = N_i^k - \omega_{\text{eff}} (N_i^k - N_i^{k(e)}) \quad (4)$$

Below are the details of this operator. The density of the fluid k is given by the first moment of the distribution functions :

$$\rho_k = \sum_i N_i^k = \sum_i N_i^{k(e)} \quad (5)$$

where the superscript (e) denotes equilibrium. The total fluid density is given by $\rho = \sum_k \rho_k$, while the total momentum is defined as the second moment of the distribution functions :

$$\rho \vec{u} = \sum_i \sum_k N_i^k \vec{c}_i = \sum_i \sum_k N_i^{k(e)} \vec{c}_i \quad (6)$$

in which $\vec{u}$ is the velocity of the color-blind distribution functions. The equilibrium functions are defined by :

$$N_i^{k(e)}(\rho_k, \vec{u}, \alpha_k) = \rho_k \left(\phi_i^k + W_i \left[\frac{3}{c^2} \vec{c}_i \cdot \vec{u} + \frac{9}{2c^4} (\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2c^2} (\vec{u})^2 \right] \right) + \Phi_i^k \quad (7)$$

It should be noted that $\Phi_i^k \equiv 0$ for the original single phase collision operator. The weights W_i are those of a standard D2Q9 lattice :

$$W_i = \begin{cases} 4/9, & i = 1 \\ 1/9, & i = 2, 4, 6, 8 \\ 1/36, & i = 3, 5, 7, 9 \end{cases} \quad (8)$$

Besides,

$$\phi_i^k = \begin{cases} \alpha_k, & i = 1 \\ (1 - \alpha_k)/5, & i = 2, 4, 6, 8 \\ (1 - \alpha_k)/20, & i = 3, 5, 7, 9 \end{cases} \quad (9)$$

As established by Grunau et al. [1993], the various density ratios between fluids k and l are γ_{kl} for two-phase flows, and must be taken as follows to obtain a stable interface :

$$\gamma_{kl} = \frac{\rho_k^0}{\rho_l^0} = \frac{1 - \alpha_l}{1 - \alpha_k} \quad (10)$$

where the superscript "0" over ρ_k^0 indicates the initial value of ρ_k at the beginning of the simulation.

The pressure of the fluid of color k is :

$$p_k = \rho_k \frac{3(1 - \alpha_k)}{5} c^2 = \rho_k (c_s^k)^2 \quad (11)$$

In the above expressions, one of the α_k is a free parameter. We let κ be the index of the least dense fluid. Generally, we set the value of $\alpha_\kappa > 0$, so that the relation $0 < \alpha_\kappa \leq \alpha_k < 1$ is guaranteed to hold

for each fluid k . These parameters set the isothermal sound speed c_s^k in each fluid of color k .

Using the index notation (m, n, o, p) and δ for the Kronecker function, [Nourgaliev et al. \[2003\]](#) note that the equilibrium distribution functions $N_i^{k(e)}$ satisfy the following principles of conservation of mass and momentum, momentum flux tensor, and constitutive physics :

$$\sum_i N_i^{k(e)} = \rho_k \quad (12)$$

$$\sum_i N_i^{k(e)} c_{i,m} = \rho_k u_m \quad (13)$$

$$\sum_i N_i^{k(e)} c_{i,m} c_{i,n} = P_{mn}^k + \rho_k u_m u_n \quad (14)$$

$$\sum_i N_i^{k(e)} c_{i,m} c_{i,n} c_{i,o} = \frac{\rho_k c^2}{3} (u_m \delta_{no} + u_n \delta_{mo} + u_o \delta_{mn}) \quad (15)$$

with the pressure tensor $P_{mn}^k = \rho_k (c_s^k)^2 \delta_{mn}$.

The effective relaxation parameter ω_{eff} is chosen so that the evolution equation, Eq. (2), respects the macroscopic equations for a single phase flow in the single phase regions. When the viscosities of the fluids are different, an interpolation is applied to define the parameter ω_{eff} at the interface.

Like [Leclaire et al. \[2011b\]](#), we define the bar functional as the density weighted q -average. For example, for a variable X_k defined for each fluid k , the density weighted q -average of this variable is defined as :

$$\bar{X}|_q = \begin{cases} \left(\sum_k \frac{\rho_k (X_k)^q}{\rho} \right)^{\frac{1}{q}}, & q \neq 0 \\ \left(\prod_k (\rho_k)^{X_k} \right)^{\frac{1}{\rho}}, & q = 0 \end{cases} \quad (16)$$

If ν_k is the kinematic viscosity of the fluid k , then, depending on the q -average, one possible choice for the effective relaxation parameter is :

$$\omega_{\text{eff}} = \frac{2c^2 \Delta t}{6 \left(\bar{\nu}|_q \right) + c^2 \Delta t} \quad (17)$$

In this study, we use $q = -1$ to interpolate the viscosity $\bar{\nu}|_q$ of the fluid. This interpolation corresponds to the density weighted harmonic average. For the simulation of multiphase flows of different viscosities, the interpolation of the viscosity at the interface is a widely used approximation.

In the numerical results section, we show that, with this current form, our model as it stands is not able to correctly simulate flows with variable density ratios in the two-layered Couette flow. In order to be able to do this, correction terms can be added to the equilibrium distribution functions.

2.2 Single phase collision operator with corrected equilibrium

In their free energy LB model, [Holdych et al. \[1998\]](#) noticed that they were able, by changing the equilibrium distribution functions, to obtain error terms in the macroscopic formulation of the lattice Boltzmann equation compatible with the Navier-Stokes equations under the hypothesis of a weak pressure gradient and within the limits of small Mach and Knudsen numbers. The corrected equilibrium distribution functions were not given in the original scientific paper of [Holdych et al. \[1998\]](#). However, [Che Sidik and Takahiko \[2007\]](#) explicitly describe the changes that need to be made to the equilibrium

distribution functions in the case of a one-component fluid with a variable density ratio and a "non ideal" equation of state. Their idea is adapted here for our immiscible multiphase RK model, which is aimed at correcting the discontinuity problem in the Couette flow. This approach has not been tested before, and is introduced specifically for the model in this paper. We define Φ_i^k in Eq. (7) such that :

$$\Phi_i^k = \begin{cases} -3 \bar{\nu}|_q \left(\vec{u} \cdot \vec{\nabla} \rho_k \right) / c^2, & i = 1 \\ +4 \bar{\nu}|_q \left(\mathbf{G}^k : \vec{c}_i \otimes \vec{c}_i \right) / c^4, & i = 2, 4, 6, 8 \\ +1 \bar{\nu}|_q \left(\mathbf{G}^k : \vec{c}_i \otimes \vec{c}_i \right) / c^4, & i = 3, 5, 7, 9 \end{cases} \quad (18)$$

where $\otimes$ is the tensor product and the symbol ":" stand for the tensor contraction. The tensor $\mathbf{G}^k$ is defined by :

$$\mathbf{G}^k = 1/8 \left[\left(\vec{u} \otimes \vec{\nabla} \rho_k \right) + \left(\vec{u} \otimes \vec{\nabla} \rho_k \right)^T \right] \quad (19)$$

After summing the equilibrium distribution functions of each fluid k , the color-blind distribution functions $N_i^{(e)}$ are the same as $N_i^{k(e)}$, except that ρ_k is replaced by ρ , and α_k is replaced by $\bar{\alpha}|_{q=1}$. This means that

$$N_i^{(e)} \equiv N_i^{(e)}(\rho, \vec{u}, \bar{\alpha}|_{q=1}) = \sum_k N_i^{k(e)}(\rho_k, \vec{u}, \alpha_k) \quad (20)$$

With the modifications from Eq. (18), the color-blind distribution functions respect the following constraints of mass and momentum conservation, momentum flux tensor, and constitutive physics :

$$\sum_i N_i^{(e)} = \rho \quad (21)$$

$$\sum_i N_i^{(e)} c_{i,m} = \rho u_m \quad (22)$$

$$\begin{aligned} \sum_i N_i^{(e)} c_{i,m} c_{i,n} &= P_{mn} + \rho u_m u_n \\ &+ \bar{\nu}|_q [u_m \partial_n(\rho) + u_n \partial_m(\rho) + u_o \partial_o(\rho) \delta_{mn}] \end{aligned} \quad (23)$$

$$\sum_i N_i^{(e)} c_{i,m} c_{i,n} c_{i,o} = \frac{\rho c^2}{3} (u_m \delta_{no} + u_n \delta_{mo} + u_o \delta_{mn}) \quad (24)$$

With regard to the color-blind distribution functions, the only difference between the original model ($\Phi_i^k = 0$) and the new model ($\Phi_i^k \neq 0$) is in the definition of the momentum flux tensor, where the terms on the second line of Eq. (23) with a density gradient are added to take into account the density variation in multiphase flow. This is the main idea of [Holdych et al. \[1998\]](#), and is applied here to solve the discontinuity problem of the RK model.

When $\alpha_k = 4/9$, we can see that the color-blind distribution functions of Eq. (20) are the same as those in the free energy model of [Che Sidik and Takahiko \[2007\]](#) in the single phase region. This is because Eqs. (21) to (24) are the same in the single phase region as in the work of [Che Sidik and Takahiko \[2007\]](#). The only difference is in the pressure tensor P_{mn} , of which we only consider the "ideal" part in our study, so that a different isothermal equation of state is used in each phase :

$$P_{mn} = \rho \frac{3}{5} \left(1 - \bar{\alpha}|_{q=1} \right) c^2 \delta_{mn} = \rho \left. \overline{c_s^2} \right|_{q=1} \delta_{mn}. \quad (25)$$

Without source terms and in the single phase region only, it is therefore correct to conclude that the color-blind distribution functions of this new model will lead to the same macroscopic equations as

defined by [Holdych et al. \[1998\]](#) and [Che Sidik and Takahiko \[2007\]](#) : with

$$\partial_t \rho_k + \partial_m (\rho_k u_m) = O(Kn^2) \quad (26)$$

$$\partial_t (\rho_k u_m) + \partial_n (\rho_k u_m u_n) = \quad (27)$$

$$- \partial_n P_{mn}^k + \nu_k [\partial_n \rho_k (\partial_n (u_m) + \partial_m (u_n) + \partial_o (u_o) \delta_{mn})] \quad (28)$$

$$- 3\nu_k \partial_n [u_m \partial_o P_{no}^k + u_n \partial_o P_{mo}^k + \partial_o (\rho_k u_m u_n u_o)] / c^2 \quad (29)$$

$$- 3\nu_k \partial_n [(\partial_n P_{mn}^k)(\partial_o \rho_k u_o)] / c^2 \quad (30)$$

$$- 3\nu_k \partial_n [u_m \partial_o (u_n \partial_o \rho_k + u_o \partial_n \rho_k + \delta_{on} u_p \partial_p \rho_k)] / c^2 \quad (31)$$

$$- 3\nu_k \partial_n [u_n \partial_o (u_m \partial_o \rho_k + u_o \partial_m \rho_k + \delta_{mo} u_p \partial_p \rho_k)] / c^2 \quad (32)$$

$$+ 3\nu_k \partial_n [\partial_t (u_m \partial_n \rho_k + u_n \partial_m \rho_k + \delta_{mn} u_p \partial_p \rho_k)] / c^2 + O(Kn^2) \quad (33)$$

where the first three lines are the compressible continuity and Navier-Stokes momentum equations, and the subsequent lines are the error terms, all negligible with weak pressure gradients and within the small Mach and Knudsen Kn number limit ([Holdych et al. \[1998\]](#)).

Again, the single phase collision operator is chosen to respect the macroscopic equations of a single phase flow in the single phase region only. Most multiphase LB models do not consider the viscosity variation in the theoretical development of the model ([Grunau et al. \[1993\]](#); [Dupin et al. \[2003\]](#); [Kang et al. \[2004\]](#); [Halliday et al. \[2009\]](#)). As in this model, the development is achieved by first supposing a constant viscosity, and then applying an interpolation to describe the viscosity at the interface. It is important to note that the interpolation of the viscosity at the interface is a method commonly used in other multiphase flow models ([Lafaurie et al. \[1994\]](#); [Akhlaghi Amiri and Hamouda \[2013\]](#)). The viscosity interpolation is already used in the definition of the relaxation factor ω_{eff} , and here we only apply the viscosity interpolation $\bar{\nu}|_q$ once more to construct the correction terms Φ_i^k . In fact, it is not clear what happens at the interface because of this interpolation. However, based on the numerical results, it seems that our method effectively corrects the discontinuity problem of the RK model in the two-layered Couette flow.

2.3 Perturbation operator

Although we do not use it in this work, surface tension in the RK model is modeled by means of the perturbation operator ([Halliday et al. \[1998\]](#); [Reis and Phillips \[2007\]](#); [Gunstensen et al. \[1991\]](#)). To introduce surface tension into this model, a "color" gradient $\vec{F}_{kl}$ would need to be defined first, which approximates the normal interfaces for each of the k - l fluid interfaces. With multiple interfaces, a simplification is made such that the surface tension between each pair of fluids is taken into account, but the interaction related to surface tension between two fluids in an interface does not depend on the presence of the other fluids. In others words, as in [Dupin et al. \[2003\]](#), the two-phase flow theory is applied individually to each k - l fluid interface.

The color gradient in this model is defined as :

$$\vec{F}_{kl} = \frac{\rho_l}{\rho} \vec{\nabla} \left(\frac{\rho_k}{\rho} \right) - \frac{\rho_k}{\rho} \vec{\nabla} \left(\frac{\rho_l}{\rho} \right) \quad (34)$$

For flow with three phases or more, this formulation for the color gradient has been shown to be superior to the usual RK color gradient ([Leclaire et al. \[2011b\]](#)).

The perturbation operator for the fluid k is therefore defined by

$$(\Omega_i^k)^{(2)}(N_i^k) = N_i^k + \sum_{l \neq k} \frac{A_{kl} C_{kl}}{2} |\vec{F}_{kl}| \left[W_i \frac{(\vec{F}_{kl} \cdot \vec{c}_i)^2}{|\vec{F}_{kl}|^2 c^2} - B_i \right] \quad (35)$$

$$B_i = \begin{cases} -4/27, & i = 1 \\ 2/27, & i = 2, 4, 6, 8 \\ 5/108, & i = 3, 5, 7, 9 \end{cases} \quad (36)$$

and

$$C_{kl} = \min \left\{ \eta_1 \frac{\rho_k \rho_l}{\rho_k^0 \rho_l^0}, 1 \right\} \quad (37)$$

where $\eta_1 = 10^6$ is a threshold and the function C_{kl} is a concentration factor that limits surface tension activation at the k - l interface only where both the k and l fluids are present.

[Reis and Phillips \[2007\]](#) has shown that the perturbation operator complies, within the macroscopic limit, with the capillary stress tensor present in the macroscopic equations for two-phase flows. It handles the coupling between the two fluids, with the space- and time-dependent parameters A_{kl} chosen to model the surface tension at the k - l fluid interface.

The surface tension σ_{kl} is set as follows :

$$\sigma_{kl} = \frac{1}{9} \frac{(A_{kl} + A_{lk})}{\omega_{\text{eff}}} c^2 \Delta t \quad (38)$$

The values for σ_{kl} are set at the beginning of a simulation. However, the values for $A_{kl} = A_{lk}$ are space- and time-dependent, because ω_{eff} may depend on space and time.

Although this operator generates the surface tension, it does not guarantee the fluid's immiscibility. To minimize the mixing and segregate the fluids, the recoloring operator $(\Omega_i^k)^{(3)}$ needs to be properly selected.

2.4 Recoloring operator

This latter operator is used to maximize the amount of fluid of color k at the interface that is sent to the k fluid region, while respecting the conservation of mass and total momentum. The recoloring operator presented here is a combination of the essential ideas in [Latva-Kokko and Rothman \[2005\]](#) and [Halliday et al. \[2007\]](#), and is as follows :

$$(\Omega_i^k)^{(3)}(N_i^k) = \frac{\rho_k}{\rho} N_i + \sum_{l \neq k} \beta_{kl} \frac{\rho_k \rho_l}{\rho^2} \cos(\varphi_i^{kl}) N_i^{(e)}(\rho, 0, \bar{\alpha}|_{q=1}) \quad (39)$$

where β_{kl} is a parameter controlling the thickness of the k - l interface. The variable φ_i^{kl} corresponds to the angle between the color gradient $\vec{F}_{kl}$ and the lattice direction vector $\vec{c}_i$. The equilibrium distributions of the color-blind fluid $N_i^{(e)}$ in Eq. (39) are evaluated using Eq. (7), a zero velocity, and the respective value of $\bar{\alpha}|_{q=1}$. This operator keeps the fluids immiscible while conserving the mass and momentum of the color-blind fluid and the mass of each individual fluid k . The momentum dynamics of each fluid k is not conserved, or, more accurately, does not exist, in this model. However, it should be noted that, in each single-phase region, the color-blind fluid coincides with each fluid of color k . So, it is only at the interface that some information concerning the individual momentum dynamics of each fluid k is lost.

2.5 Isotropic discrete gradient operator

In this work, a fourth order isotropic discrete gradient operator is used for the discretization of the gradient in Eqs. (18) and (34). This kind of isotropic gradient operator was presented by [Sbragaglia et al. \[2007\]](#) for 2D and 3D, and further generalized by [Leclaire et al. \[2012b\]](#) for higher order spatial and isotropic operators. [Leclaire et al.](#)

[2011a] show that this type of discretization enhances the accuracy of the RK model significantly. The fourth order isotropic gradient operator takes the following form :

$$\bar{\nabla} f(x, y) = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] f(x, y) \approx \sum_{i=1}^9 \frac{\xi_i [d_i^x, d_i^y] f(x + d_i^x, y + d_i^y)}{(\Delta x)^2} \quad (40)$$

with

$$\begin{aligned} \vec{\xi} &= [0, 4, 1, 4, 1, 4, 1, 4, 1]/12 \\ \vec{d}^x &= [0, 0, 1, 1, 1, 0, -1, -1, -1]\Delta x \\ \vec{d}^y &= [0, 1, 1, 0, -1, -1, -1, 0, 1]\Delta x \end{aligned} \quad (41)$$

Note that this operator supposes that $\Delta y = \Delta x$. To compute this type of gradient efficiently, convolution products may be used, as explained by [Leclaire et al. \[2012a,b\]](#).

2.6 Adjustment of the interface width for static contact angles

For three-phase flows, and when the surface tension yields a Neumann triangle, there is a possible equilibrium state where static contact angles θ_{kl} will be formed between the fluids. [Spencer et al. \[2010\]](#) found, and demonstrated theoretically, that a particular relation for β_{kl} at the triple fluid junction must be used, otherwise the angle θ_{kl} will not be satisfied at steady state. The value of the angle θ_{kl} can be found from the surface tension σ_{kl} using the law of cosines. By setting $\theta_{\max}$ as the largest θ_{kl} , the special relations for β_{kl} are as follows :

$$\beta_{kl} = \begin{cases} \beta^0, & kl \text{ with } \theta_{\max} \\ \beta^0 (1 + c_{triple} (\sin(\pi - \theta_{\max} - \theta_{kl}) - 1)), & \text{otherwise} \end{cases} \quad (42)$$

where β^0 is a constant between 0 and 1 controlling the overall thickness of all three interfaces, and

$$c_{triple} = \min \left\{ \eta_2 \frac{\rho_r \rho_g \rho_b}{\rho^3}, 1 \right\} \quad (43)$$

is a function that also varies between 0 and 1. The free threshold $\eta_2 = 35$. This value for η_2 has been shown to provide good results ([Leclaire et al. \[2011b\]](#)). However, in this study, these special relations are not used, and each β_{kl} is set to the same constant.

3 Numerical Simulation

3.1 Two-layered Couette flow

The purpose of this numerical test is to investigate the model's ability to simulate flow with variable dynamic viscosity. The two-layered Couette flow consists of two layers of fluid between two infinite moving plates.

The variable x_I is used to denote the interface position between the fluids with properties (ρ_r, μ_r) on the left-hand side and (ρ_b, μ_b) on the right-hand side, where $\mu_k = \rho_k \nu_k$ is the dynamic viscosity. The walls located at positions x_0 and x_N move vertically at a velocity of u_0^y and u_N^y respectively.

At steady state and applying the incompressibility hypothesis, an analytical solution exists for the previous flow setting ([Leclaire et al. \[2011b\]](#)). This leads to two theoretical momentum profiles within each interval $x_0 \leq x < x_I$ and $x_I < x \leq x_N$ of the form :

$$(\rho u^y)(x)|_{\text{th}} = \begin{cases} \rho_r^0 (a_r x + b_r), & x_0 \leq x < x_I \\ \rho_b^0 (a_b x + b_b), & x_I < x \leq x_N \end{cases} \quad (44)$$

with the constants a_r , b_r , and a_b , and b_b solutions of the following system :

$$\begin{pmatrix} x_0 & 1 & 0 & 0 \\ \mu_r & 0 & -\mu_b & 0 \\ x_I & 1 & -x_I & -1 \\ 0 & 0 & x_N & 1 \end{pmatrix} \cdot \begin{pmatrix} a_r \\ b_r \\ a_b \\ b_b \end{pmatrix} = \begin{pmatrix} u_0^y \\ 0 \\ 0 \\ u_N^y \end{pmatrix} \quad (45)$$

Now that the analytical solution for the two-layered Couette flow has been presented, the setting for this test is described in the context of an LB simulation. It is common in lattice Boltzmann methods to set the lattice spacing $\Delta x = 1$ and the time step Δt so that $c = 1$. We do this here. Since the analytical solution is 1D, a lattice containing $N_x = 160$ by $N_y = 1$ sites is used, unless stated otherwise, and is located over the interval $[x_0, x_N]$. The interface $x_I = (x_0 + x_N)/2$ is located halfway along the channel, and each fluid section is initialized with the zero velocity equilibrium distribution functions. The wall located at x_0 and x_N passes over the lattice sites, while the interfaces x_I pass between the fluid lattice sites. Because the model is 2D, periodic boundary conditions are applied in the y-direction. The first and last sites are located where the velocity boundary conditions are implemented. The standard [Zou and He \[1997\]](#) velocity boundary condition is applied. The wall velocities are set to $u_0^y = 0.0001$ and $u_N^y = -0.01$. The values $\alpha_\kappa = 4/9$ (κ index of the least dense fluid) and $\beta_{kl} = 0.8$ are used. The density $\rho_b = 1$, and the viscosity $\nu_r = 1/2$.

A special nomenclature, shown in Table (1), is introduced to describe the various simulations. Depending on the simulation case, with its different density and viscosity ratios, additional information is provided in Table (2).

Nomenclature	
U	Unit
L	Low
M	Medium
H	High
D	Density ratio
V	Viscosity ratio

TABLE 1: Nomenclature used for the various simulation cases.

Case	ρ_r/ρ_b	ν_r/ν_b	# Table
UD-LV	1	2	(3)
UD-MV	1	20	(3)
UD-HV	1	100	(3)
LD-UV	2	1	(4)
MD-UV	20	1	(4)
HD-UV	1000	1	(4)
LD-LV	2	2	(5)
MD-MV	20	20	(5)
HD-HV	1000	100	(5)

TABLE 2: Additional simulation parameters for the two-layered Couette flow.

As previously explained by [Leclaire et al. \[2011b\]](#), the initial condition for this problem can lead to instability, because the color-blind density distribution N_1 and the fluid densities ρ_k are initially discontinuous. In this case, it is preferable to initialize the flow with a more continuous function. To do so, the model equations are solved for a certain number of time steps with $A_{kl} = 0$, while $\vec{u} = 0$ is imposed in

the equilibrium density distribution in Eq. (7). So, for the simulations presented here, the first 2000 time steps only serve to stabilize the initial density distribution and fluid densities to a more continuous function.

Note that the numerical steady state is regarded as achieved when :

$$\max_{\text{all sites}} \left\{ \left| \frac{(N_i)^{(n)} - (N_i)^{(n-1)}}{(N_i)^{(n)}} \right| \right\} \leq \epsilon \quad (46)$$

with $\epsilon = 10^{-10}$, while n denotes the time step number. To reduce the computational cost, this condition is only checked every 2000 time steps.

3.1.1 Discussion of the numerical results

To compare the original model ($\Phi_i^k = 0$) and the new model ($\Phi_i^k \neq 0$) in terms of the numerical and theoretical momentum profiles, three sets of simulations were undertaken. The first set, shown in Table (3), contains simulations that illustrate the behavior of the two models with unit density but variable viscosity ratios. The second set, given in Table (4), illustrates the case with variable density ratios, but a unit viscosity ratio. The last set, shown in Table (5), presents the case with both variable density and variable viscosity ratios. All the tables, (3) to (5), display cases with unit and/or low, medium, and high density and/or viscosity ratios. The numerical density profiles are not shown, because both models are able to capture the theoretical density profile correctly in all cases.

The results in Table (3) indicate that the behavior of the momentum in the original model is identical to that in the new model, with unit density and variable viscosity ratios. This is because $\Phi_i^k = 0$ when the density gradient is zero. In fact, without density variation, the two models become theoretically the same. The work of [Leclaire et al. \[2012c\]](#) shows that the model is able to simulate the multilayered Poiseuille flow with a very high viscosity ratio $O(10000)$, but with unit density ratio only. Therefore, it is not surprising that this model is also able to simulate the two-layered Couette flow with unit density ratio and large viscosity ratios.

With variable density and unit viscosity ratios, the results in Table (4) reveal that the behavior of the momentum in the original and in the new model are different. In fact, in our case here, the original model yields a momentum profile which is not affected at all by the change in density across the interface. This clearly indicates the inability of the original model to simulate flows with variable density ratios. In contrast, the new model shows the expected theoretical behavior, i.e. the discontinuity in the momentum profile is well captured by the numerical scheme.

With both variable density and variable viscosity ratios, the results displayed in Table (5) indicate that the behavior of the momentum in the original and in the new model are again different. Only the new model works as expected. Even when using viscosity interpolation, the new model is still able to capture the two-layered Couette flow correctly. Our tests indicate that the scheme is stable, with a simultaneous density ratio of $O(1000)$ and a viscosity ratio of $O(100)$. Any further increase in viscosity ratio leads to instability.

For each of the nine tests, Table (6) shows the L2 errors that occur with the new model as the lattice size increases. It is clear that the proposed model is compatible with the analytical solution, as the order of accuracy is > 1 . It is important to point out that the model is only second order accurate in space with unit density ratios for this test case. With variable density ratios, a discontinuity arises in the momentum profile and the order of accuracy drops to 1. We can see that the MD-MV case yielded an order of accuracy of 1.478, but this is

only because the jump discontinuity is small for this situation, and the momentum profile decreases monotonically.

Overall, the approach presented in this paper enhances the range of validity of this RK model. Moreover, there is every reason to expect that this technique will also work for the other RK models ([Grunau et al. \[1993\]](#); [Tölke \[2002\]](#); [Reis and Phillips \[2007\]](#); [Rannou \[2008\]](#); [Leclaire et al. \[2012c, 2011a\]](#); [Liu et al. \[2012\]](#)), which also suffer from the discontinuity problem. The current approach should correct the behavior of these models with respect to momentum for the test case involving the multilayered Couette flows with variable density ratios.

4 Conclusion

In this research, the equilibrium distribution functions of the current RK lattice Boltzmann model have been modified to correctly recover the Navier-Stokes equations with weak pressure gradients and within the limits of a small Mach and Knudsen number. Because of the way in which the original model was used by various researchers, it was not able to capture the momentum discontinuity in the two-layered Couette flow with density ratios other than 1. The new model is able to do so, even with a large density ratio $O(1000)$ and a viscosity ratio $O(100)$. However, the discontinuity problem of the RK models mentioned by [Aidun and Clausen \[2010\]](#) is only partially resolved, since the model is valid only when the pressure gradients are weak, which is usually the case when the current isothermal equation of state is used. We also believe that other LB models in the RK class, and perhaps even other classes, could also use the current corrected equilibrium distribution functions to improve their range of validity. We end this article on this final note : It is important to acknowledge that most of the test cases examined in our previous works ([Leclaire et al. \[2011a, 2012c, 2011b\]](#)) are still valid with the current corrected equilibrium. This is because the original model and the new model coincide within the limit of 0 momentum or of 0 density gradient. Often in these works, one of the two conditions is, for practical purposes, met.

Acknowledgments

We applied the SDC (sequence-determines-credit) approach in listing the authors of this article ([Tscharntke et al. \[2007\]](#)). The work was supported by a grant from the NSERC (Natural Sciences and Engineering Research Council of Canada).

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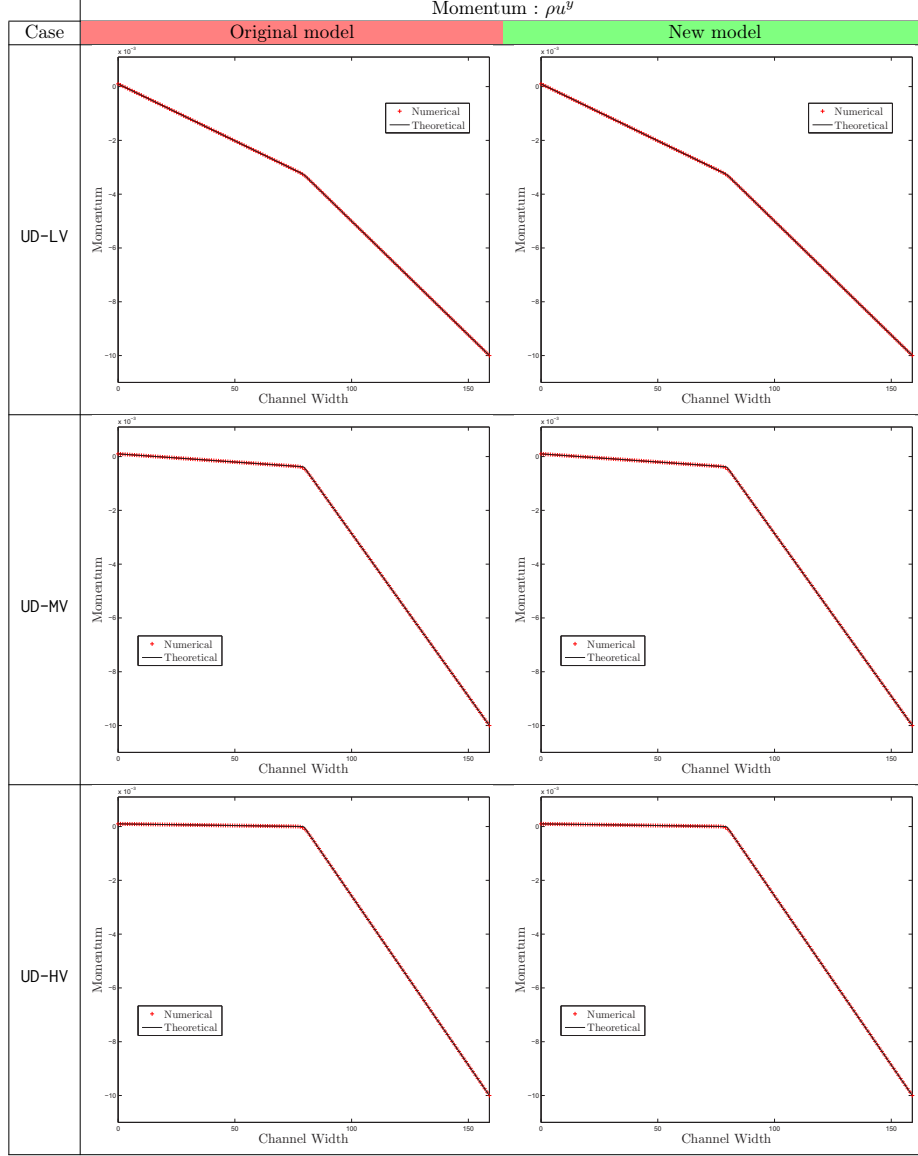
TABLE 3: Two-layered Couette flow with *unit* density and *variable* viscosity ratios.

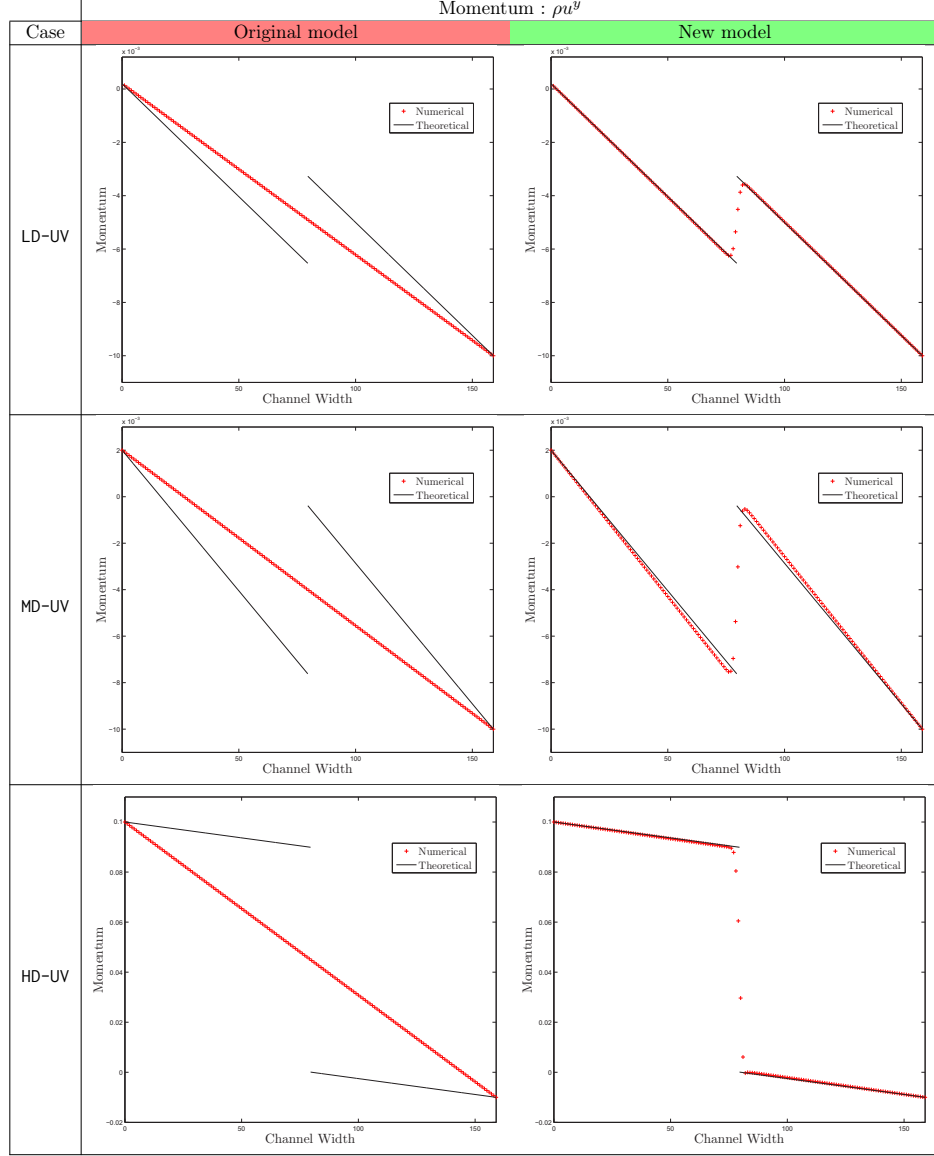
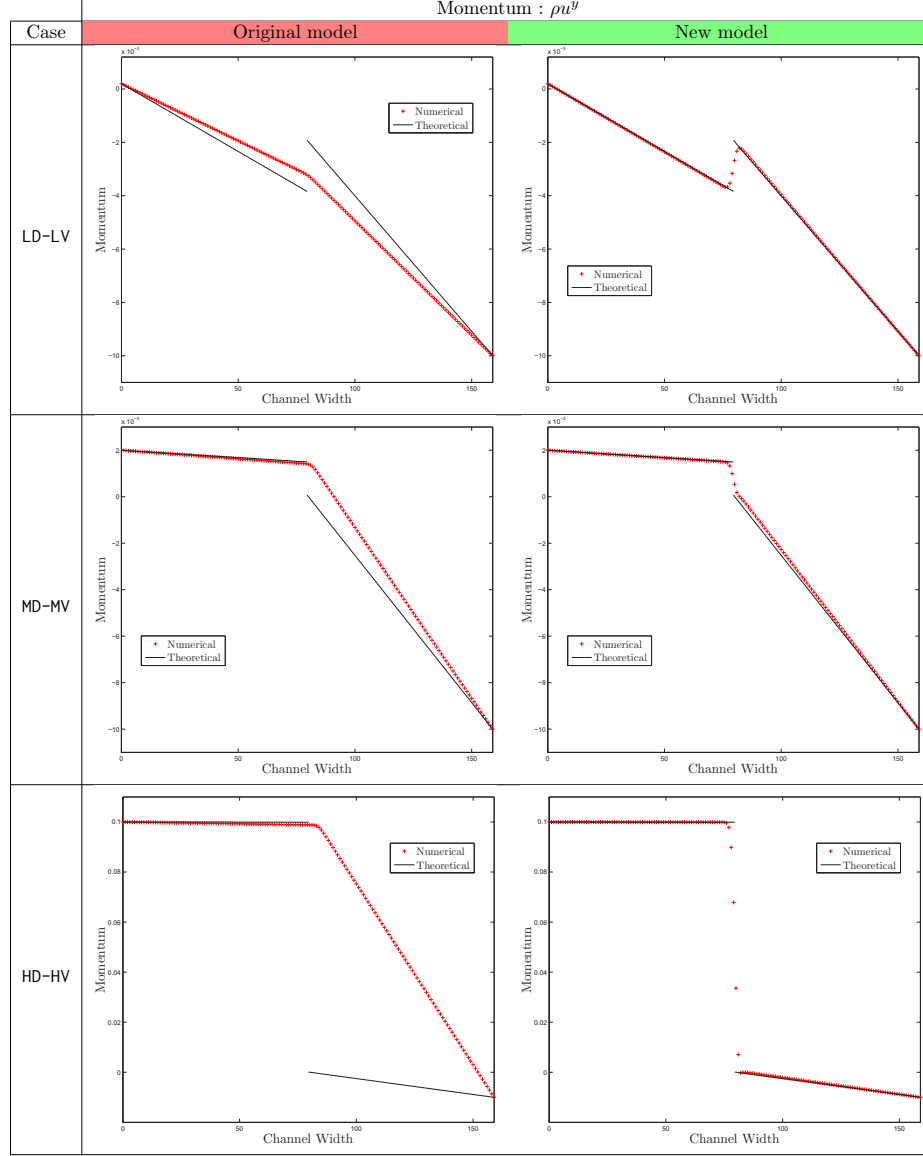
TABLE 4: Two-layered Couette flow with *variable* density and *unit* viscosity ratios.

TABLE 5: Two-layered Couette flow with *variable* density and *variable* viscosity ratios.

$\sqrt{\frac{\sum_j ((\rho u^y)(x_j) _{\text{th}} - (\rho u^y)(x_j) _{\text{num}})^2}{N_x - 1}}$				
Case	$N_x = 40$	$N_x = 80$	$N_x = 160$	Order
UD-LV	1.970e-06	4.789e-07	1.169e-07	2.038
UD-MV	5.347e-06	1.302e-06	3.220e-07	2.027
UD-HV	5.791e-06	1.411e-06	3.864e-07	1.953
LD-UV	4.557e-05	2.255e-05	1.124e-05	1.010
MD-UV	1.282e-04	5.771e-05	2.745e-05	1.112
HD-UV	1.165e-03	5.589e-04	2.741e-04	1.044
LD-LV	2.772e-05	1.358e-05	6.717e-06	1.023
MD-MV	8.958e-05	3.223e-05	1.154e-05	1.478
HD-HV	1.257e-03	6.128e-04	3.028e-04	1.027

TABLE 6: Errors between theoretical and numerical momentum for the two-layered Couette flow and the new model.

ANNEXE E

High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs

Il est important de noter que cet article pourrait être sujet à des changements d'ici la publication finale de celui-ci dans une revue scientifique.

Sébastien Leclaire, Maud El-Hachem, Marcelo Reggio and Jean-Yves Trépanier, "High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs", manuscript submitted to *Journal of Scientific Computing* in September 2012.

Journal of Scientific Computing <rajeswari.sundaram@springer.com>
To: Sébastien Leclaire <sebastien.leclaire@polymtl.ca>

Wed, Sep 5, 2012 at 10:04 PM

Dear Mr. Sébastien Leclaire:

Thank you for submitting your manuscript entitled "High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs" for possible publication in the Journal of Scientific Computing.

The paper will be assigned to a member of the editorial board who will handle the review process. Every effort will be made to ensure a timely review. We will let you know as soon as the review process is finished.

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Sincerely,

Professor Chi-Wang Shu and Professor Christine Bernardi
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Figure E.1 Avis de réception par les éditeurs de l'article : « High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs ».

High order spatial generalization of 2D and 3D isotropic discrete gradient operators with fast evaluation on GPUs

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September 5, 2012

Abstract

Based on the concept of isotropic centered finite differences, this work generalizes to higher order the spatial order of accuracy of the 2D and 3D isotropic discrete gradient operators. A suitable methodology is used to obtain a set of equations from which it is possible to deduce stencil weights to achieve numerical approximations of both high order spatial and high order isotropic gradients. We consider that the suggested discretization will be useful for enhancing the quality of the results in various scientific fields. The spatial order (S) controls the spatial order of accuracy of the gradient **norm** and **direction**, while the isotropic order (I) controls the spatial order of accuracy of the gradient **direction**. A useful list of the stencil weights needed to construct different high order spatial and isotropic gradients is given. Numerical tests show that the numerical spatial and isotropic orders of accuracy of the gradient approximation are the same as those predicted by theory. A series of benchmarks comparing various efficient convolution algorithms used to compute function or image gradients is presented. Different platforms implemented on CPU and GPU are studied, namely : plain MATLAB; the Jacket plugin for MATLAB; and CUDA. The results show situations in which substantial computational speedup can be obtained, e.g. by more than 250x with CUDA and the Jacket plugin for MATLAB versus MATLAB on CPU.

1 Introduction

The numerical finite difference method for calculating gradient functions is widely used in the scientific community. When calculating the gradient of a function with several variables, a 1D finite difference is usually used for each direction. In recent years, however, it has been shown that this procedure may cause some degree of anisotropy in the results [11].

To overcome this problem, Kumar introduced the concept of the isotropic finite difference [11], which ensures that the error term of the finite difference discretization is isotropic. This guarantees that the scheme does not add its own anisotropy to the numerical simulation [11]. In Kumar's work, the simulation of a 6-fold symmetric dendritic solidification is more accurate if isotropic finite differences, rather than conventional finite differences, are used. For the gradient operator, in the first approach that Kumar [11] proposed, only 2D and 3D approximation using finite differences of low spatial and isotropic order were presented (i.e. $I = S + 2 = 4$ - see section (2.1) for the detailed definition of S and I).

Shortly thereafter, Xiao et al. [24] used 3D isotropic finite differences to discretize a special case of Maxwell's equation and improve the numerical results. Isotropic discretizations have also improved an application of Shen et al. [21], which is a 2D numerical simulation of 2D transient electromagnetic wave propagation.

Following the idea of Shan [20] for the numerical simulation of multiphase flow using the lattice Boltzmann method, Sbragaglia et al. [19] generalized the 2D and 3D gradients of higher isotropic order (i.e. $I \geq S + 2 = 4$). Although not explicitly stated in their work [19], the approach presented here can show that the weights they developed lead to a gradient approximation that is second order accurate in space (i.e. $S = 2$). For their model, the use of isotropic discretization for the calculation of gradients allowed the simulation of high-density ratios between different fluids. Their isotropic gradient technique has also been used by Leclaire et al. [13], and allowed the simulation of density ratios up to $O(10000)$ for a stationary isotropic bubble. Isotropic discretization reduces the anisotropy in the numerical scheme to prevent non physical bubble deformation and to reduce spurious currents, which constitute a numerical artifact at the fluid interface.

To allow the discretization of a 3D pseudo-isotropic gradient on irregular mesh, Grogger [8] used an optimization process that minimized the error associated with isotropy, while ensuring non dissipative approximation, which is an important property in the solution of hyperbolic partial differential equations. It is worth noting that, in Grogger's [8] investigation, for a given spatial order of discretization, the isotropy error minimized by the optimization process may lead to an isotropic order approximately equal to the same spatial order (i.e. $I \approx S$). He did this in order to increase the stability limit of his numerical scheme. This means that Grogger's method is a compromise between the stability limit and the isotropy. Depending on the intended application, the stability limit is not a required parameter, and better isotropy is often desirable.

Other isotropic discrete differential operators can be developed. For example, Thampi et al. [22] have shown that isotropic Laplacian operators can be obtained from the weights of the discrete Maxwell-Boltzmann equilibrium, which is widely used in the lattice Boltzmann community. Patra et al. [16] have also developed isotropic stencil weights for the Laplacian, the Bilaplacian and the gradient of the Laplacian operators.

In all previous investigations, the conclusion has been the same : the isotropic discretizations of differential operators are more accurate than conventional finite differences. Based on this fact, researchers should test the isotropic discretization.

In this work, which was developed based on regular meshes, we generalize isotropic finite differences for highly spatially accurate gradient approximations, while at the same time ensuring that the order of isotropy is greater than the spatial order (i.e. $I \geq S + 2 \geq 4$). This is an extension and generalization of the work of Sbragaglia et al. [19] for high order spatial gradient discretizations. We can add that, depending on the order of accuracy, our method is built to use the minimum number of closest neighbors required to achieve the target accuracy. As in Ref. [8], because of the symmetry of the weights and the stencils, the non dissipative approximation is also respected by our various discretizations. We believe that the weights and stencils developed in this work may be useful for scientific applications other than those related to the lattice Boltzmann method. In this paper, we first show how the necessary equations are obtained to determine the various weights of the discretization, and then we show, numerically, that the spatial and isotropic orders of the gradients are actually the same as those predicted theoretically. Finally, various platforms and algorithms are used to compare the evaluation performance of the gradient discretizations, using MATLAB, the JACKET plugin for MATLAB, and CUDA. These benchmarking tests led us to conclude that the computation of high order spatial 2D and 3D isotropic gradients is a great deal faster with a GPU than with plain MATLAB.

2 Methodology

In this section, a methodology for obtaining high order spatial and isotropic finite differences for the gradient operator is described, and an efficient method on the CUDA architecture is presented, using convolution products for computing the function gradients. Previous works [11–13] may be useful for clarifying the mathematical differences between isotropic and anisotropic discretizations.

2.1 High order accurate gradient in space and isotropy

In this section, we describe how to construct a high order spatial and isotropic centered finite difference on a square lattice for the first derivative. Without loss of generality, the finite difference method is derived by supposing that the gradient of the function F is evaluated at the origin $(0, 0)$ of a 2D Cartesian space. Evaluating F at other positions in space is a straightforward application of this simplified case.

First, we define a stencil, or a set of discrete positions $c^{(i,j)} = [c_x^{(i)}, c_y^{(j)}]$, around zero :

$$c_x^{(i)} = ih, \quad i = -R, -R + 1, \dots, 0, \dots, R - 1, R \quad (1)$$

$$c_y^{(j)} = jh, \quad j = -R, -R + 1, \dots, 0, \dots, R - 1, R \quad (2)$$

where h is the spacing between the various discrete positions, and the integer R is the radius of the stencil for a specific set of discrete positions.

The next step is to use the Taylor series expansion of the function F around the origin :

$$\begin{aligned} F(x, y) = & F(0, 0) + x \frac{\partial F}{\partial x} \Big|_{(0,0)} + y \frac{\partial F}{\partial y} \Big|_{(0,0)} + \frac{1}{2} x^2 \frac{\partial^2 F}{\partial x^2} \Big|_{(0,0)} + xy \frac{\partial^2 F}{\partial x \partial y} \Big|_{(0,0)} \\ & + \frac{1}{2} y^2 \frac{\partial^2 F}{\partial y^2} \Big|_{(0,0)} + \frac{1}{6} x^3 \frac{\partial^3 F}{\partial x^3} \Big|_{(0,0)} + \frac{1}{2} x^2 y \frac{\partial^3 F}{\partial x^2 \partial y} \Big|_{(0,0)} + \frac{1}{2} xy^2 \frac{\partial^3 F}{\partial x \partial y^2} \Big|_{(0,0)} \\ & + \frac{1}{6} y^3 \frac{\partial^3 F}{\partial y^3} \Big|_{(0,0)} + \dots + O(x^n y^m) \end{aligned}$$

where n and m are integers that define the order of the Taylor series expansion $T = n + m - 1$.

Given a certain order T of the Taylor series expansion and neglecting $O(h^{T+1})$ terms, the truncated series can be evaluated at the various positions $c^{(i,j)}$ of the stencil :

$$\begin{aligned} F(c_x^{(i)}, c_y^{(j)}) = & F(0, 0) + ih \frac{\partial F}{\partial x} \Big|_{(0,0)} + jh \frac{\partial F}{\partial y} \Big|_{(0,0)} + \frac{1}{2} (ih)^2 \frac{\partial^2 F}{\partial x^2} \Big|_{(0,0)} \\ & + (ih)(jh) \frac{\partial^2 F}{\partial x \partial y} \Big|_{(0,0)} + \frac{1}{2} (jh)^2 \frac{\partial^2 F}{\partial y^2} \Big|_{(0,0)} + \frac{1}{6} (ih)^3 \frac{\partial^3 F}{\partial x^3} \Big|_{(0,0)} \\ & + \frac{1}{2} (ih)^2 (jh) \frac{\partial^3 F}{\partial x^2 \partial y} \Big|_{(0,0)} + \frac{1}{2} (ih)(jh)^2 \frac{\partial^3 F}{\partial x \partial y^2} \Big|_{(0,0)} \\ & + \frac{1}{6} (jh)^3 \frac{\partial^3 F}{\partial y^3} \Big|_{(0,0)} + \dots + O(h^{T+1}) \end{aligned}$$

As in Ref. [7], the gradient of the function F at $(0, 0)$ can be approximated using a linear weighted combination of the values $F(c_x^{(i)}, c_y^{(j)})$,

such as :

$$\left. \frac{\partial F}{\partial x} \right|_{(0,0)} \approx \frac{1}{h^2} \sum_{\substack{i,j \\ i^2+j^2 \leq D}} F(c_x^{(i)}, c_y^{(j)}) w^{(i,j)} c_x^{(i)} \quad (3)$$

$$\left. \frac{\partial F}{\partial y} \right|_{(0,0)} \approx \frac{1}{h^2} \sum_{\substack{i,j \\ i^2+j^2 \leq D}} F(c_x^{(i)}, c_y^{(j)}) w^{(i,j)} c_y^{(j)} \quad (4)$$

where $w^{(i,j)}$ are weights that need to be carefully selected to ensure that the result of the linear combination does indeed correspond to a gradient approximation. The integer D , associated with the distance relative to the origin, is a parameter that can further reduce the number of discrete positions considered in the stencil. This parameter will be set later on, in order to uniquely define the different weights $w^{(i,j)}$. For symmetry considerations, the weights $w^{(i,j)}$ are chosen to be radially symmetric, i.e. $w^{(i,j)} = w^{(j,i)}$, and $w^{(i,j)} = w^{(|i|,|j|)}$.

As in Refs. [12, 13, 19], to study the isotropy of the discretization, we suppose that the function F to be derived is isotropic, i.e. $F \equiv F(r)$. Then, to be isotropic, the gradient also needs to be a vector function that depends only on the radius, i.e. $\vec{\nabla} F \equiv f(r)\vec{e}_r$, where $\vec{e}_r = [\cos(\theta), \sin(\theta)]$ is the unit radial vector, and $f(r)$ is another isotropic function. However, in the discrete space, this is impossible to achieve with a finite set of discrete positions $\vec{c}^{(i,j)}$, since, in this case, the best we can do is choose the weights $w^{(i,j)}$ such that the error term is isotropic up to a certain order [19]. Therefore, to study the isotropy of the discretization, it is easier to change the spatial coordinates from Cartesian to polar using the following partial derivative operator :

$$\frac{\partial}{\partial x} = \cos(\theta) \frac{\partial}{\partial r} - \frac{1}{r} \sin(\theta) \frac{\partial}{\partial \theta} \quad (5)$$

$$\frac{\partial}{\partial y} = \sin(\theta) \frac{\partial}{\partial r} + \frac{1}{r} \cos(\theta) \frac{\partial}{\partial \theta} \quad (6)$$

After these transformations have been made and by only considering an error term up to order T , the gradient approximation with the error term in polar coordinates can always be rewritten as follows :

$$\left. \frac{\partial F}{\partial x} \right|_{(0,0)} \approx \frac{1}{h^2} \sum_{\substack{i,j \\ i^2+j^2 \leq D}} F(c_x^{(i)}, c_y^{(j)}) w^{(i,j)} c_x^{(i)} + \underbrace{\cos(\theta) \sum_{t=2}^{T-2} h^t E_{x,polar}^{(t)}}_{\text{Error term}} \quad (7)$$

$$\left. \frac{\partial F}{\partial y} \right|_{(0,0)} \approx \frac{1}{h^2} \sum_{\substack{i,j \\ i^2+j^2 \leq D}} F(c_x^{(i)}, c_y^{(j)}) w^{(i,j)} c_y^{(j)} + \underbrace{\sin(\theta) \sum_{t=2}^{T-2} h^t E_{y,polar}^{(t)}}_{\text{Error term}} \quad (8)$$

where $E_{x,polar}^{(t)}$ and $E_{y,polar}^{(t)}$ are expressions that are a function of the variables r and θ , and the weights $w^{(i,j)}$. Note that these expressions are not a function of the spacing h , because that spacing already appears outside these expressions.

For purposes of clarity, we are dropping the subindex "polar" for the rest of this work :

$$E_x^{(t)} \equiv E_{x,polar}^{(t)} \quad (9)$$

$$E_y^{(t)} \equiv E_{y,polar}^{(t)} \quad (10)$$

Note that, because of the symmetry of the weights $w^{(i,j)}$, the expressions $E_x^{(t)}$ and $E_y^{(t)}$ are zero for t odd.

Knowing the form of the expression $E_x^{(t)}$ allowed us to construct a set of equations having, by solution, the weights $w^{(i,j)}$, in such a way that :

1. The gradient approximation is space accurate up to the spatial order S . Mathematically, this means that $E_x^{(t)}$ and $E_y^{(t)}$ are zero up to h^{S-2} . The spatial order thus controls the rate at which the error of the gradient **norm** and **direction** decrease with the spacing h .
2. The gradient is isotropic accurate up to the isotropic order I . Mathematically, this means that the whole error term in Eqs. (7) and (8) written in vector form is equivalent to a radially symmetric vector (i.e. $f(r)\vec{e}_r$) up to h^{I-2} . The isotropic order thus controls the rate at which the error of the gradient **direction** decreases with the spacing h .

Note that discretizations with spatial order S are automatically of isotropic order I , because, when $E_x^{(t)}$ and $E_y^{(t)}$ are zero, they are also radially symmetric.

Next, we describe the way to construct the set of equations to find the weights $w^{(i,j)}$ under the specific spatial order and isotropic order S and I respectively. Obviously, this is very tedious to do by hand, and we so used the symbolic computation software Maple [2] to obtain the full set of equations. The method for obtaining the equations is explained below.

Note that, because of the symmetry of the weights $w^{(i,j)}$, we only need to search for specific conditions in the error term of the x-derivative when building the set of equations to find the weights $w^{(i,j)}$, because searching for conditions in the error term of the y-derivative would lead to exactly the same set of equations.

First, Eq. (7) can be rewritten as :

$$\frac{1}{h^2} \underbrace{\sum_i \sum_j}_{i^2+j^2 \leq D} F(c_x^{(i)}, c_y^{(j)}) w^{(i,j)} c_x^{(i)} \approx A \left. \frac{\partial F}{\partial x} \right|_{(0,0)} + \underbrace{B}_{\text{Error term}} \quad (11)$$

where A is a function of the weights $w^{(i,j)}$, and B is an expression involving the error term. Following the previous definition, the next equation defines the scaling of the gradient, and it is required that :

$$A = 1 \quad (12)$$

Next, given the spatial order S of the gradient discretization, we impose the spatial order of the gradient discretization by adding the following condition :

$$\cos(\theta) h^t E_x^{(t)} \equiv 0 \quad \forall \theta, \quad t = 2, 4, \dots, S-2 \quad (13)$$

The Maple symbolic computation software can solve the problem in Eq. (13) and provide a set of equations that are a function of $w^{(i,j)}$ and which respect these identities.

The last set of equations that is needed will establish the isotropic order I of the gradient discretization. In obtaining this set of equations, we should note that error term $E_x^{(t)}$ in Eq. (7) has the following form :

$$E_x^{(t)}(r, \theta, w^{(i,j)}) = g^{(t,0)}(r, w^{(i,j)}) + \sum_{k=2}^{2(I-2)} g^{(t,k)}(r, w^{(i,j)}) [\cos(\theta)]^k \quad (14)$$

with $g^{(t,k)}$ being functions of the variable r and the weights $w^{(i,j)}$. So, to impose isotropy up to order I , i.e. $E_x^{(t)}(r, \theta, w^{(i,j)}) \equiv E_x^{(t)}(r, w^{(i,j)})$ for $S \leq t \leq I-2$, the next conditions that we need are the following :

$$g^{(t,k)}(r, w^{(i,j)}) [\cos(\theta)]^k \equiv 0 \quad \forall \theta, \quad \begin{cases} k = 2, 4, \dots, 2(I-2) \\ t = S, S+2, \dots, I-2 \end{cases} \quad (15)$$

Again, the Maple software can solve the problem in Eq. (15) and provide a set of equations that are a function of $w^{(i,j)}$ and which respect these identities.

2.2 Weights and stencils

For example, if we consider the spatial order and isotropy of order $I = S + 2 = 4$, then, to build the set of equations, we choose $T = 4$, $R = 1$, and $D = 2$. Therefore, Eq. (12) will be :

$$4w^{(1,1)} + 2w^{(1,0)} = 1 \quad (16)$$

In this case, the set of equations that would come from the identities in Eq. (13) will be empty. Finally, the set of equations that set isotropy are deduced from Eq. (15), as follows :

$$\begin{aligned} w^{(1,0)} &= 4w^{(1,1)} \\ w^{(1,1)} &= w^{(1,1)} \end{aligned} \quad (17)$$

with solutions $w^{(0,1)} = 1/3$ and $w^{(1,1)} = 1/12$. These weights are already known and correspond to those given in Refs. [11, 19].

Let us consider a second example. If the spatial order and isotropic order are of order $I = S + 2 = 6$, then, with $R = 2$ and $D = 5$, Eq. (12) becomes :

$$20w^{(2,1)} + 8w^{(2,0)} + 4w^{(1,1)} + 2w^{(1,0)} = 1 \quad (18)$$

The equations that set the spatial order now exist, and are deduced from Eq. (13) :

$$\begin{aligned} w^{(1,0)} &= -16w^{(2,0)} - 18w^{(2,1)} \\ w^{(2,0)} &= w^{(2,0)} \\ w^{(1,1)} &= -8w^{(2,1)} \\ w^{(2,1)} &= w^{(2,1)} \end{aligned} \quad (19)$$

The group of equations that sets the isotropy are deduced from Eq. (15), as follows :

$$\begin{aligned} w^{(1,0)} &= 70w^{(2,1)} + 8w^{(1,1)} - 64w^{(2,0)} \\ w^{(2,0)} &= w^{(2,0)} \\ w^{(1,1)} &= w^{(1,1)} \\ w^{(2,1)} &= w^{(2,1)} \end{aligned} \quad (20)$$

TABLE 1: Stencil weights needed to construct 2D high order spatial and isotropic gradient discretization.

	Spatial and isotropic order (S, I)							Weights
	(2, 4)	(4, 6)	(6, 8)	(8, 10)	(10, 12)	(12, 14)	(14, 16)	
	1/3	13/30	31/70	27/70	16/63	215/12012	-9769/25740	$w^{(1,0)}$
	1/12	2/15	27/140	88/315	1145/2772	626/1001	49861/51480	$w^{(1,1)}$
$w^{(7,0)}$	-1/420420	-1/120	0	1/30	575/5544	11177/48048	2947/6435	$w^{(2,0)}$
$w^{(6,6)}$	0	-1/60	-3/70	-53/630	-5/33	-2115/8008	-11711/25740	$w^{(2,1)}$
$w^{(6,5)}$	0	0	3/560	2/105	65/1386	100/1001	371/1872	$w^{(2,2)}$
$w^{(6,4)}$	0	0	-1/630	-1/105	-125/4158	-1985/27027	-12187/77220	$w^{(3,0)}$
$w^{(6,3)}$	0	0	1/280	4/315	25/792	205/3003	91/660	$w^{(3,1)}$
$w^{(6,2)}$	-1/41184	0	0	-1/630	-5/693	-515/24024	-7/132	$w^{(3,2)}$
$w^{(6,1)}$	1/25740	0	0	0	5/8316	10/3003	119/10296	$w^{(3,3)}$
$w^{(6,0)}$	-1/38610	5/432432	0	1/1440	85/22176	1219/96096	287/8580	$w^{(4,0)}$
$w^{(5,5)}$	0	0	0	-1/1260	-5/1386	-87/8008	-707/25740	$w^{(4,1)}$
$w^{(5,4)}$	0	0	0	0	5/11088	5/2002	56/6435	$w^{(4,2)}$
$w^{(5,3)}$	-1/12870	0	0	0	0	-5/24024	-7/5148	$w^{(4,3)}$
$w^{(5,2)}$	1/1716	1/12012	0	0	0	0	7/82368	$w^{(4,4)}$
$w^{(5,1)}$	-2/2145	-1/12012	0	0	-1/4950	-123/100100	-581/128700	$w^{(5,0)}$
$w^{(5,0)}$	149/128700	1/50050	-1/17325	0	1/5544	1/1001	7/1980	$w^{(5,1)}$
$w^{(4,4)}$	-1/9152	0	0	0	0	-1/8008	-7/8580	$w^{(5,2)}$
$w^{(4,3)}$	7/5148	5/24024	0	0	0	0	7/102960	$w^{(5,3)}$
$w^{(4,2)}$	-5/858	-5/3432	-1/3696	0	0	0	0	$w^{(5,4)}$
$w^{(4,1)}$	7/780	5/3432	0	0	0	0	0	$w^{(5,5)}$
$w^{(4,0)}$	-29/2340	-205/96096	5/22176	1/3360	0	23/432432	7/19305	$w^{(6,0)}$
$w^{(3,3)}$	-4/429	-5/2002	-1/2079	0	0	-1/24024	-7/25740	$w^{(6,1)}$
$w^{(3,2)}$	155/5148	115/12012	2/693	1/1260	0	0	7/205920	$w^{(6,2)}$
$w^{(3,1)}$	-56/1287	-95/12012	1/693	1/630	0	0	0	$w^{(6,3)}$
$w^{(3,0)}$	5171/77220	2005/108108	5/2079	-1/630	-1/630	0	0	$w^{(6,4)}$
$w^{(2,2)}$	-17/208	-25/1001	-1/154	-1/420	-1/560	0	0	$w^{(6,5)}$
$w^{(2,1)}$	61/572	5/1001	-2/77	-11/420	-1/70	0	0	$w^{(6,6)}$
$w^{(2,0)}$	-327/1430	-4313/48048	-185/5544	-1/90	0	1/120	-17/1261260	$w^{(7,0)}$
$w^{(1,1)}$	-79/715	15/182	5/33	17/105	1/7	1/10	1/102960	$w^{(7,1)}$
$w^{(1,0)}$	7967/8580	7957/12012	370/693	289/630	27/70	4/15		
Weights	(12, 16)	(10, 14)	(8, 12)	(6, 10)	(4, 8)	(2, 6)		
Spatial and isotropic order (S, I)								

It is important to mention that some of the above equations, given by the Maple software, are sometimes equivalent, in the sense that they may define the same linear space. So, we can see that the previous set of equations in Eq. (20) is obtained twice by this software, but that multiple equivalent linear spaces do not cause a problem to the software when a linear system is solved symbolically.

The solution for the weights is $w^{(0,1)} = 13/30$, $w^{(2,0)} = -1/120$, $w^{(1,1)} = 2/15$, and $w^{(2,1)} = -1/60$. We believe that this is the first time that these weights have been found.

If the spatial order and isotropy become larger, the set of equations turns out to be very large indeed. So, up to $I = S + 2 = 16$, only the solution of the system of equations with different weights $w^{(i,j)}$ is given in Table (1). For convenience, Table (1) also provides the weights up to $S = 12$ for the case where $I = S + 4$. The sparsity pattern of the various filters can be determined when the weights $w^{(i,j)}$ that are zero are known.

Up to now, we have only presented a methodology to obtain high order spatial and isotropic gradient discretization in 2D. The methodology in 3D is very similar, except that, to achieve isotropy, we need to consider a spherical coordinate system instead of polar coordinates. Although this results in additional complexity, it is still possible to build a set of equations in a similar fashion with the weights $w^{(i,j,k)}$ unknown. These equations, once solved, will lead to 3D high order spatial and isotropic gradient discretizations. Up to order $I = S + 2 = 10$, Table (2) shows the weights $w^{(i,j,k)}$ needed to achieve these discretizations. Table (2) provides the weights for the 3D case, with $I = S + 4$ up to $S = 6$.

We may add that, if $I = S + 2 = T = 2R + 2$, the set of equations obtained from Eqs. (12), (13), and (15) has no solution for the weights $w^{(i,j)}$ (or $w^{(i,j,k)}$) if $D < R^2 + 1$. It has a unique solution if $D = R^2 + 1$, and an infinite number of solutions if $D > R^2 + 1$. For $I = S + 4 = T = 2R + 2$, the set of equations has no solution for the weights if $D < R^2$. It has a unique solution if $D = R^2$, and an infinite number of solutions if $D > R^2$. Note that, in both cases where there is a unique solution, the resulting weights will form, by the construction

TABLE 2: Stencil weights needed to construct 3D high order spatial and isotropic gradient discretization.

Spatial and isotropic order (S, I)					
	(2, 4)	(4, 6)	(6, 8)	(8, 10)	Weights
	1/6	1/15	-41/140	-347/315	$w^{(1,0,0)}$
	1/12	1/5	3/7	32/35	$w^{(1,1,0)}$
$w^{(4,0,0)}$	1/3360	-1/30	-9/70	-13/35	$w^{(1,1,1)}$
$w^{(3,3,3)}$	0	1/40	33/280	5/14	$w^{(2,0,0)}$
$w^{(3,3,2)}$	0	-1/60	-9/140	-17/90	$w^{(2,1,0)}$
$w^{(3,3,1)}$	0	0	3/280	2/35	$w^{(2,1,1)}$
$w^{(3,3,0)}$	0	0	3/560	1/35	$w^{(2,2,0)}$
$w^{(3,2,2)}$	0	0	0	-1/210	$w^{(2,2,1)}$
$w^{(3,2,1)}$	0	0	0	0	$w^{(2,2,2)}$
$w^{(3,2,0)}$	1/1260	0	-11/1260	-2/45	$w^{(3,0,0)}$
$w^{(3,1,1)}$	1/420	0	1/280	2/105	$w^{(3,1,0)}$
$w^{(3,1,0)}$	-1/315	0	0	-1/315	$w^{(3,1,1)}$
$w^{(3,0,0)}$	1/315	-1/630	0	-1/630	$w^{(3,2,0)}$
$w^{(2,2,2)}$	0	0	0	0	$w^{(3,2,1)}$
$w^{(2,2,1)}$	1/210	0	0	0	$w^{(3,2,2)}$
$w^{(2,2,0)}$	-1/84	-1/560	0	0	$w^{(3,3,0)}$
$w^{(2,1,1)}$	4/105	-1/140	0	0	$w^{(3,3,1)}$
$w^{(2,1,0)}$	17/420	0	0	0	$w^{(3,3,2)}$
$w^{(2,0,0)}$	-22/315	1/280	1/120	0	$w^{(3,3,3)}$
$w^{(1,1,1)}$	23/140	3/70	1/60	23/10080	$w^{(4,0,0)}$
$w^{(1,1,0)}$	-2/21	1/14	1/15	-1/1260	$w^{(4,1,0)}$
$w^{(1,0,0)}$	181/315	17/70	2/15		
Weights	(6, 10)	(4, 8)	(2, 6)		
Spatial and isotropic order (S, I)					

itself, the smallest possible set of weights with non zero values near the origin. So, given the orders S and I , the high order spatial and isotropic gradient discretization developed in this work uses the closest set of neighbors.

The methodology presented in section (2.1) is general enough to calculate the weights $w^{(i,j)}$ that are needed for gradient discretization with an isotropic order much higher than the spatial order, i.e. the case where $I > S + 4$. To compare our results with the work described in Ref. [19], the weights for the most local isotropic discretization are given in 2D with $S = 2$ and $I = 4, \dots, 16$, and in 3D with $S = 2$ and $I = 4, \dots, 10$. Based on our findings, the method presented in this work generalizes the method presented in Ref. [19] to a higher spatial order.

2.3 Gradient evaluation by convolution

The computational method derived from Eq. (3) to obtain an approximation of the gradient is to add the function values in all the discrete positions $\vec{c}^{(i,j)}$ and to weight these values using stencil values. The generalization of this method leads to convolution, which is a generic procedure used to compute gradients [3]. In this section, we explain the convolution computation by splitting the process into two methods : the first implemented in the spatial domain and the second in the frequency domain. Below is a review of the theoretical background of this alternative. As was done in Ref. [12], we present examples that occur in 2D, but the formalism can easily be extended to 3D.

The convolution product of two continuous 2D functions $g(x, y)$ and $h(x, y)$, defined by Eq. (21), calculates an average function by sliding the filter h all over the image g . Simply put, we say that the function h acts as a filter of the function g .

$$(g * h)(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x, y) h(x - s, y - t) ds dt \quad (21)$$

The present case requires discrete functions and, for simplicity, periodic boundary conditions. The circular convolution of the discrete functions $G(x, y)$ and $H(x, y)$ is presented in Eq. (22). In practice, the procedure consists of flipping the filter H , in each dimension, aligning G and H into 1D vectors, and then sliding H from one boundary of G to the opposite side, where G starts again, at the first boundary. At each position, within a window of the filter dimensions, the weighted scalar product of G is computed, with the weights given by H .

$$(G \circledast H)(x, y) = \sum_i \sum_j G(i, j) H[(x - i) \bmod N, (y - j) \bmod N] \quad (22)$$

As stated by the convolution theorem in Eq. (23) and concisely described in Ref. [5, chap. 4], the convolution of two functions in the space domain is also equivalent to the pointwise product of these functions in the frequency domain, where $\mathcal{F}\{g\}$ and $\mathcal{F}\{h\}$ are the Fourier transform of g and h , and the symbol $\mathcal{F}^{-1}$ represents the inverse Fourier transform. In mathematics, the Fourier transform of a function generates its frequency spectrum, where high frequencies correspond to information varying rapidly in the original function and low frequencies correspond to slow variations. The inverse transform rebuilds a function from its frequency spectrum. The second way of convoluting the discrete functions G and H would be to use the sequence set out in Eq. (24), as follow, where DFT stands for Discrete Fourier Transform as described in Ref. [4, chap. 6] : compute image and filter discrete Fourier transforms, multiply the resulting Fourier coefficients, and apply Fourier inverse transform on the product of the coefficients.

$$g * h = \mathcal{F}^{-1}\{\mathcal{F}\{g\} \cdot \mathcal{F}\{h\}\} \quad (23)$$

$$G * H = \text{DFT}^{-1}\{\text{DFT}\{G\} \cdot \text{DFT}\{H\}\} \quad (24)$$

We decide whether to use the discrete Fourier transform pipeline or spatial circular convolution based first and foremost on a comparison of complexity functions. In the spatial domain, the convolution of an $N \times N$ image with a $K \times K$ filter requires $N^2 K^2$ multiplications and nearly $N^2 K^2$ additions. In the frequency domain, the discrete Fourier transform and its inverse are computed via the divide-and-conquer algorithm of the Fast Fourier Transform (FFT), the fundamental notions of which can be found in Ref. [4, chap. 8]. In 2D and 3D DFT implementation, the separability property reduces the 2D DFT complexity from $O(N^2 \log_2(N))$ to $O(N \log_2(N))$, since it is decomposed into two operational sequences, where 1D DFT is applied successively in each dimension. To the Fourier transform computational complexity is added the cost of the product of two complex numbers (4 multiplications and 2 additions) when Fourier coefficients are multiplied. The resulting complexity of convoluting an $N \times N$ image by a $K \times K$ filter would then give $2N \log_2(N) + K \log_2(K) + 6N^2$ operations.

In conclusion, convoluting in the spatial domain will yield better performance than using Fourier transforms for small filters only, because $O(N^2 K^2) > O(N \log_2(N) + K \log_2(K) + N^2)$ for fixed N and large K . This observation is enhanced in 3D, where spatial convolution complexity is $O(N^3 K^3)$ while passing by FFT and IFFT complexity is in $O(N \log_2(N) + K \log_2(K) + N^3)$.

2.4 Gradient computation with CUDA

In this work, CUDA (Compute Unified Device Architecture) and C language are used to implement the filter sliding in the spatial domain and the filter application in the frequency domain. The GPU manufacturer's Nvidia offers CUDA as a platform to implement general purpose computing on GPUs that are suited for vector calculus, as is required for graphics rendering. For highly arithmetic kernels executed on a large set of data, the performance gained by GPUs vs. CPUs is achieved because GPUs devote more transistors to data processing and fewer to data caching and flow control. As introduced in Ref. [14, chap. 2], the data nodes are partitioned into 2D or 3D blocks of 2D or 3D threads, which execute independently. From within the launched kernel, threads and blocks are accessible through their indices, providing an intuitive way to invoke the kernel across the 2D or 3D dataset elements. Device linear memory can be allocated in one, two, or three dimensions, but its size should be a multiple of 16 in order to be aligned with the half warp size. All threads have access to a global linear memory, while shared memory is a local memory that is only accessible from threads within a block.

2.4.1 Padding

Real data dimensions are not usually multiples of 16, and so we must pad them. In addition to aligning data size, padding should regulate boundary conditions to make borders repeat from one side to the other. As suggested in Ref. [17], we implemented a padding kernel to be called before the convolution is launched. This increases data size by at least the radius R on each border, where $K = 2R + 1$, and fills out the data dimensions to the required size with periodic borders. The kernel fetches the values to copy from a texture memory object binded to the global linear memory. Using texture memory in this way offers performance advantages, as listed in Ref. [6], because texture mapping hardware is optimized for interpolation techniques. One texture unit, or texel, comprises four 8-bit channels, one for each color (red, green, and blue), plus one for transparency. Since the maximum built-in precision is 32 bits, we store each double precision value in two texels. We present in Table (3) an invented example, where the original 14×14 image with a 3×3 stencil gives a 16×16 padded image. Besides adding the stencil halos, padding should increase the size of the data until it reaches the nearest multiple of 16, filling the space after the halos with no particular required values. As explained in the section (2.4.2), for the FFT and IFFT cases, the size should equal a power of 2.

2.4.2 CUDA with FFT convolution

We took advantage of the CUFFT (CUDA Fast Fourier Transform) library to implement the convolution via a discrete Fourier transform. CUDA provides a mechanism, called a "plan", which calculates the optimal execution configuration "in terms of minimum floating-point operations (FLOPs) for a particular FFT size and data type" [15]. Before calculating its transform, the stencil should be expanded to the size of the padded data, as demonstrated in Ref. [17] : we place the central element of the stencil, given in Table (4) for example, at $(0, 0)$ of the padded stencil, as shown in Table (5), and periodically shift the excess to the remaining corners of the extended image, so that the stencil

TABLE 3: Image with original 14 by 14 size, after padding for a 3 by 3 stencil.

196	183	184	185	...	196	183
14	1	2	3	...	14	1
28	15	16	17	...	28	15
42	29	30	31	...	42	29
...	...	...	...	...	...	...
196	183	184	185	...	196	183
14	1	2	3	...	14	1

wraps each data element it passes during circular convolution. We must remember that the divide-and-conquer DFT algorithm requires a power of 2 data size, because it factorizes each FFT step into two subdivisions to recombine them at end of the recursion. Passing the configured plan handle as a parameter, we use the *cufftExecZ2Z* function to perform the forward real-to-complex transform and the inverse complex-to-real transform, where Fourier coefficients are complex numbers made up of two double precision numbers, and request twice the padded size from global memory.

TABLE 4: Original stencil.

1	2	3
4	5	6
7	8	9

TABLE 5: Cyclically shifted and padded stencil.

5	6	0	0	...	4
8	9	0	0	...	7
0	0	0	0	...	0
...	...	...	...	...	...
2	3	0	0	...	1

As expressed in Eq. (24), the Fourier transform image is modulated by a Fourier transform kernel and an inverse transform is applied on the result. The following routine shows the main execution steps :

1. Create an execution plan for the forward and inverse transforms ;
2. Pad the image and the stencil ;
3. Call the forward FFT function on the padded image and stencil ;
4. Generate a pointwise product of the coefficients ;
5. Call the inverse FFT function on the result ;
6. Unpad the output.

2.4.3 CUDA with spatial convolution

In this section, the convolution does not require padding the stencil. We simply reverse the stencil and slide it onto the padded image and calculate the scalar product of the current window, weighted by the stencil. The convolution of the image and stencil in Table (3) and Table (4) requires 9 multiplications of the input value and 8 additions to output value at the final position (0,0) : $1 \times 16 + 2 \times 15 + 3 \times 28 + 4 \times 2 + 5 \times 1 + 6 \times 14 + 7 \times 184 + 8 \times 185 + 9 \times 196$. Furthermore, the global data input will require 9 memory read accesses. One position will be read 9 times after we have processed the convolution for the whole image. As recommended in Ref. [18], the global memory bandwidth is reduced by loading into shared memory the neighborhood related to all the indices within a block of threads. Most positions, except the thread block borders within a radius of R , would then be loaded once. The remaining positions will have to be loaded at most $3R + 1$ times in 2D and $4R + 1$ times in 3D to ensure that the data padding is stored in shared memory. In order to optimize coalescence in shared memory, the scalar product operations (multiplication and addition) must be unrolled, since they can be performed in any order. Finally, the stencil is loaded into the constant memory, to reduce bandwidth usage, since constant memory is cached and can be broadcast to other threads.

Fined-grained parallelism depends on the size of the shared memory, which means that the size of the 2D thread block, which could be as much as 32×32 in Nvidia version 2.0 cards, has to be reduced to a 16×16 tile, so that the padded tile will fit into a 48 kB shared memory. In 3D, the block size used is $16 \times 4 \times 4$.

We implemented convolution for any stencil form in 2D and 3D. Isotropic centered finite differences with the stencil weights presented in Tables (1) and (2) reveal a distribution pattern of weights among positions with many zero values. These could eventually be discarded when computing the scalar product. It would be interesting to take these patterns into account, but the resulting CUDA code would not be suitable for all types of stencils.

3 Numerical Results

In this section, we first demonstrate that the numerical spatial order and isotropic order of the various gradient discretizations shown in Tables (1) and (2) are compatible with the theoretical spatial order and isotropic order developed in the methodology section (2.1).

After providing a numerical proof of the spatial and isotropic order accuracy, the next step is to create a performance benchmark for the various gradient discretizations over different computing platforms. As we mentioned in section (2.3), the convolution product is an efficient way of evaluating the gradient of a function or image. Consequently, we use this evaluation method to compare the performance of the gradient discretizations on the following platforms : MATLAB, the Jacket plugin for MATLAB, and CUDA.

3.1 Order of accuracy

Here, we present three numerical tests demonstrating that the gradient discretization provided in section (2.2) achieves the theoretical predicted spatial and isotropic order of accuracy. The first test case evaluates the spatial order of accuracy of the gradient discretization when evaluating the gradient of a high order multivariable polynomial; the second test case involves a multivariable periodic sinusoidal function; and the third test case validates the spatial and isotropic order of accuracy using a rotated 1D sinusoidal function. In summary, the spatial order is validated for the case where $I = S + 2$ and $I = S + 4$, while the more interesting isotropic order is only validated in the case where $I = S + 4$. We do this for reasons of clarity, as the validation with $I = S + 2$ is scientifically equivalent.

3.1.1 High order multivariable polynomial (spatial order)

The aim of this numerical test is to verify whether or not different gradient discretizations of order $S \geq n$ obtained from the weights in Tables (1) and (2) can be used to accurately evaluate the gradient of a multivariable polynomial of order n . The only case validated for this test is where $I = S + 2$. This is a standard numerical experiment performed to verify the spatial accuracy of a gradient discretization, because gradient discretization of spatial order $S \geq n$ must accurately evaluate the gradient of a multivariable polynomial of order n [9]. The multivariable polynomial chosen for this test is the following :

$$p(x, y) = (x + y + 1)^n \quad (25)$$

and

$$p(x, y, z) = (x + y + z + 1)^n \quad (26)$$

in 2D and in 3D respectively. Without loss of generality, the methodology is presented here only for the 2D case and for the derivative in the x-direction. The case with 3D and/or for other derivative directions can be expressed and obtained in a straightforward manner.

The error between the numerical and theoretical results is computed as follows :

$$\text{Error}(S, n) = \left| \frac{\partial p}{\partial x} \Big|_{(0,0)}^{(\text{num}, S)} - \frac{\partial p}{\partial x} \Big|_{(0,0)}^{(\text{th})} \right| = \left| \frac{\partial p}{\partial x} \Big|_{(0,0)}^{(\text{num}, S)} - n \right| \quad (27)$$

given a spatial order value of S . The numerical derivative in the x-direction is computed using Eq. (3), along with the associated weights $w^{(i,j)}$ from Table (1). Note that in our case, $h = 1/16$, any value of h leads to the same main conclusion.

The errors obtained from Eq. (27) are shown in Tables (6) and (7) for the 2D and 3D cases respectively. It is clear that, as predicted theoretically, the gradient discretization of spatial order $S \geq n$ does precisely evaluate the gradient of the multivariable polynomial up to order n , because the error is of the order of the machine accuracy. This is a clear numerical indication that the stencils weights $w^{(i,j)}$ are correct.

3.1.2 Multivariable sinusoidal function (spatial order)

The evaluation of a multivariable polynomial derivative is an important test, but rather a simple one. We present a more complex case now, which involves computing the gradient of a periodic multivariable sinusoidal function, and evaluating the discretization error over the entire periodic domain of the function. Achieving the target numerical spatial accuracy is therefore more difficult. The only case validated for this test is with $I = S + 2$.

The periodic multivariable sinusoidal functions chosen for this test are the following :

$$F(x, y) = \sin(2\pi x) + \sin(2\pi y) \quad (28)$$

and

$$F(x, y, z) = \sin(2\pi x) + \sin(2\pi y) + \sin(2\pi z) \quad (29)$$

in 2D and 3D respectively. Again, without loss of generality, the methodology is presented only for the 2D case and for the derivative in the x-direction. The case with 3D and/or of other derivative directions can also be developed in a straightforward manner.

The function $F(x, y)$ is periodic over the domain $(x, y) \in [-1/2, 1/2] \times [-1/2, 1/2]$, and therefore the error is evaluated as follows :

$$\text{Error}(S, h) = \left[\int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left(\frac{\partial F}{\partial x} \Big|^{(\text{num}, S)} - \frac{\partial F}{\partial x} \Big|^{(\text{th})} \right)^2 dx dy \right]^{1/2} \quad (30)$$

TABLE 6: Errors with the x-derivative of a multivariable polynomial for different gradient discretizations in 2D.

Polynomial order	Spatial and isotropic order (S, I)						
	(2, 4)	(4, 6)	(6, 8)	(8, 10)	(10, 12)	(12, 14)	(14, 16)
$n = 1$	0	0	0	0	0	0	0
$n = 2$	2.22e-16	0	8.88e-16	4.44e-16	4.44e-16	8.88e-16	2.66e-15
$n = 3$	7.81e-03	8.88e-16	4.44e-16	0	4.44e-16	8.88e-16	6.66e-15
$n = 4$	3.13e-02	8.88e-16	2.66e-15	8.88e-16	8.88e-16	3.55e-15	4.00e-15
$n = 5$	7.82e-02	2.44e-04	8.88e-16	1.78e-15	0	9.77e-15	1.78e-15
$n = 6$	1.57e-01	1.46e-03	1.78e-15	8.88e-16	8.88e-16	2.66e-15	8.88e-16
$n = 7$	2.75e-01	5.14e-03	1.72e-05	8.88e-16	1.78e-15	1.15e-14	3.55e-15
$n = 8$	4.43e-01	1.38e-02	1.37e-04	1.78e-15	3.55e-15	5.33e-15	2.66e-15
$n = 9$	6.68e-01	3.12e-02	6.20e-04	2.15e-06	7.11e-15	1.60e-14	8.88e-15
$n = 10$	9.61e-01	6.29e-02	2.08e-03	2.15e-05	0	5.33e-15	5.33e-15
$n = 11$	1.33e+00	1.17e-01	5.77e-03	1.18e-04	4.19e-07	1.78e-15	1.07e-14
$n = 12$	1.79e+00	2.02e-01	1.40e-02	4.77e-04	5.03e-06	2.84e-14	8.88e-15
$n = 13$	2.35e+00	3.34e-01	3.08e-02	1.57e-03	3.28e-05	1.18e-07	8.88e-15
$n = 14$	3.03e+00	5.28e-01	6.27e-02	4.46e-03	1.55e-04	1.65e-06	2.66e-14
$n = 15$	3.84e+00	8.07e-01	1.20e-01	1.14e-02	5.88e-04	1.24e-05	4.51e-08
$n = 16$	4.79e+00	1.20e+00	2.19e-01	2.65e-02	1.91e-03	6.70e-05	7.22e-07

TABLE 7: Errors with the x-derivative of a multivariable polynomial for different gradient discretization in 3D.

Polynomial order	Spatial and isotropic order (S, I)			
	(2, 4)	(4, 6)	(6, 8)	(8, 10)
$n = 1$	0	0	0	0
$n = 2$	2.22e-16	6.66e-16	2.22e-15	3.11e-15
$n = 3$	1.17e-02	0	3.55e-15	4.89e-15
$n = 4$	4.69e-02	0	8.88e-16	1.78e-15
$n = 5$	1.17e-01	5.49e-04	1.78e-15	2.66e-15
$n = 6$	2.35e-01	3.30e-03	6.22e-15	9.77e-15
$n = 7$	4.14e-01	1.16e-02	5.79e-05	1.15e-14
$n = 8$	6.66e-01	3.10e-02	4.63e-04	1.24e-14
$n = 9$	1.01e+00	7.02e-02	2.09e-03	1.09e-05
$n = 10$	1.45e+00	1.42e-01	7.02e-03	1.09e-04

with a given spatial order value of S . The numerical derivative in the x-direction is computed using Eq. (3), along with the associated weights $w^{(i,j)}$ from Table (1). This time, the error is computed as a function of the spacing h . The error in Eq. (30) is the L^2 norm of the difference between the numerical and theoretical derivatives as a function of the spatial order S and the spacing h .

Again, the errors obtained from Eq. (30) are shown in Tables (8) and (9) for the 2D and 3D cases. As expected, the error decreases at the predicted rate as the spacing h decreases. In Tables (8) and (9), the numerical spatial order is computed following the definition of spatial order accuracy [10]. In our case, this can be simplified to the absolute slope of the linear best fit line obtained from the logarithm of the error as a function of the logarithm of the spacing h . Some of the errors in Tables (8) and (9) are noted as $O(\epsilon)$. These are not used in the computation of the numerical spatial order, because, at that level of accuracy, the machine accuracy is achieved, or almost achieved, and the errors do not decrease at the same rate as theoretically predicted.

It is clear that, as predicted by the theory, the gradient discretization of spatial order S evaluates the gradient of the periodic multivariable sinusoidal function at the spatial accuracy S in the L^2 norm. This is another clear numerical indication that the stencil's weights $w^{(i,j)}$ are correct.

3.1.3 Rotated 1D sinusoidal function (isotropic order)

The goal of the last test case is to corroborate the fact that the isotropic order of accuracy is the same as that predicted theoretically. At the same time, it can be demonstrated that the spatial order of accuracy is also correctly predicted. This test case consists of calculating the gradient of a rotated 1D sinusoidal function, and of checking the error between the theoretical and numerical gradients. As the spacing h is reduced, the error associated with the norm of the gradient can only be reduced at a greater rate if the spatial order of accuracy is

TABLE 8: Errors with the x-derivative of a periodic multivariable sinusoidal function for different gradient discretizations in 2D.

	Theoretical spatial and isotropic order (S, I)						
	(2, 4)	(4, 6)	(6, 8)	(8, 10)	(10, 12)	(12, 14)	(14, 16)
$h = 1/8$	4.43e-01	5.24e-02	6.61e-03	8.62e-04	1.15e-04	1.55e-05	2.13e-06
$h = 1/16$	1.13e-01	3.46e-03	1.13e-04	3.82e-06	1.32e-07	4.65e-09	1.65e-10
$h = 1/32$	2.85e-02	2.19e-04	1.81e-06	1.54e-08	1.35e-10	1.19e-12	$O(\epsilon)$
$h = 1/64$	7.13e-03	1.37e-05	2.84e-08	6.07e-11	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$
$h = 1/128$	1.78e-03	8.60e-07	4.44e-10	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$
$h = 1/256$	4.46e-04	5.37e-08	6.94e-12	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$
Numerical spatial order S	1.99	3.98	5.97	7.92	9.85	11.8	13.7

TABLE 9: Errors with the x-derivative of a periodic multivariable sinusoidal function for different gradient discretizations in 3D.

	Theoretical spatial and isotropic order (S, I)			
	(2, 4)	(4, 6)	(6, 8)	(8, 10)
$h = 1/8$	4.43e-01	5.24e-02	6.61e-03	8.63e-04
$h = 1/16$	1.13e-01	3.46e-03	1.13e-04	3.82e-06
$h = 1/32$	2.85e-02	2.19e-04	1.80e-06	1.54e-08
$h = 1/64$	7.13e-03	1.37e-05	2.84e-08	6.07e-11
$h = 1/128$	1.78e-03	8.60e-07	4.44e-10	$O(\epsilon)$
$h = 1/256$	4.46e-04	5.37e-08	6.93e-12	$O(\epsilon)$
Numerical spatial order S	1.99	3.98	5.97	7.92

higher. However, the error with respect to the gradient direction can be reduced at a greater rate if either the spatial or the isotropic order of accuracy is increased.

Without loss of generality, for a given 2D or 3D rotation for a 1D sinusoidal function, only the error with respect to the x-derivative has to be validated. The errors associated with the y- and z-derivatives are of the same order. Therefore, the order of the error concerning the norm of the gradient is proportional to the error of the x-derivative. In 2D, only one angle is needed to represent the gradient direction, so its error has to be validated. In 3D, when the spherical coordinates are used, only two angles are needed to represent the direction of the gradient. By rotational symmetry, the error of only one of the angles needs to be validated. We have chosen to validate the error of the angle between the gradient and the x-axis in 2D, and with the error between the gradient and the z-axis in 3D.

The rotated 1D sinusoidal function used for this test is the following :

$$F(x, y, z) = \sin(4\pi x') \quad (31)$$

with

$$\begin{aligned} x' = & \cos(\theta) \cos(\psi)x + \\ & [\cos(\phi) \sin(\psi) + \sin(\phi) \sin(\theta) \cos(\psi)]y + \\ & [\sin(\phi) \sin(\psi) - \cos(\phi) \sin(\theta) \cos(\psi)]z \end{aligned} \quad (32)$$

The angles ϕ , θ , and ψ are associated with a rotation around the x-axis, y-axis, and z-axis respectively. To check the order of accuracy, we first randomly choose a rotation. In 2D : $\phi = 0$, $\theta = 0$, and $\psi = 7/8\pi$; and in 3D : $\phi = 3/8\pi$, $\theta = 5/8\pi$, and $\psi = 7/8\pi$. It should be noted that the conclusion is the same, whatever the rotation, except if the 1D sinusoidal function is aligned with the stencil, in which case the isotropy error is zero.

For all cases, the error between the theoretical gradient and the numerical gradient is only computed at the origin of the system of coordinates for different gradient discretizations ($I = S + 4$) and spacing h . In 2D, Table (10) shows the errors with the x-derivative and the errors with the gradient direction, and Table (11) shows the errors for the 3D case. In both Tables, the numerical spatial and isotropic orders of accuracy are also computed.

Clearly, we can conclude that the numerical spatial and isotropic orders of accuracy of the gradient discretizations are the same as those predicted theoretically. This confirms that the stencil weights are correct.

The important point here is that the error with respect to the gradient direction decreases at a greater rate than the error with respect to the norm of the gradient, even if the function to be derived is not isotropic. This can only happen because the stencil weights are chosen specifically to lead to an isotropic error term.

TABLE 10: Errors with different gradient discretizations for a 1D rotated sinusoidal function in 2D.

	Theoretical spatial and isotropic order (S, I)						
	(2, 6)	(4, 8)	(6, 10)	(8, 12)	(10, 14)	(12, 16)	
$h = 1/17$	1.21e+00	1.36e-01	1.57e-02	1.87e-03	2.25e-04	2.74e-05	Errors with the x-derivative.
$h = 1/33$	3.33e-01	1.02e-02	3.25e-04	1.06e-05	3.50e-07	1.17e-08	
$h = 1/65$	8.65e-02	6.91e-04	5.72e-06	4.84e-08	4.16e-10	3.66e-12	
$h = 1/129$	2.20e-02	4.47e-05	9.43e-08	2.03e-10	4.12e-13	$O(\epsilon)$	
$h = 1/257$	5.55e-03	2.84e-06	1.51e-09	8.90e-13	$O(\epsilon)$	$O(\epsilon)$	
Numerical spatial order S	1.99	3.97	5.96	7.92	9.93	11.8	Errors with the angle between the gradient and the x-axis.
Numerical isotropic order I	6.02	7.97	9.92	11.8	13.8	15.7	
$h = 1/17$	1.21e-05	1.24e-06	1.40e-07	1.97e-08	3.29e-09	5.79e-10	
$h = 1/33$	2.15e-07	6.45e-09	2.00e-10	7.69e-12	3.50e-13	1.69e-14	
$h = 1/65$	3.64e-09	2.89e-11	2.33e-13	2.66e-15	$O(\epsilon)$	$O(\epsilon)$	
$h = 1/129$	5.94e-11	1.20e-13	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	
$h = 1/257$	9.49e-13	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	$O(\epsilon)$	

TABLE 11: Errors with different gradient discretizations for a 1D rotated sinusoidal function in 3D.

	Theoretical spatial and isotropic order (S, I)			
	(2, 6)	(4, 8)	(6, 10)	
$h = 1/17$	4.64e-01	5.19e-02	6.01e-03	Errors with the x-derivative.
$h = 1/33$	1.27e-01	3.91e-03	1.24e-04	
$h = 1/65$	3.31e-02	2.64e-04	2.19e-06	
Numerical spatial order S	1.97	3.94	5.90	Errors with the angle between the gradient and the z-axis
Numerical isotropic order I	6.04	7.96	9.94	
$h = 1/17$	1.54e-06	2.90e-07	1.53e-07	
$h = 1/33$	2.74e-08	1.50e-09	2.15e-10	
$h = 1/65$	4.64e-10	6.72e-12	2.48e-13	

3.2 Performance benchmark of MATLAB, Jacket, and CUDA

The main objective in this section is to benchmark various algorithms for computing high order spatial and isotropic gradients. Doing so will enable us to understand that the choice of algorithm or computational platform, or both, can actually reduce the computational time. The benchmark presented here is very similar to the one in Ref. [12], the main difference being that the filters and algorithms used here may be different. In a similar fashion and for convenience, we reuse structural ideas from our previous work and repeat some of the comments that we have made there [12]. We also refer the reader to this work for details on how to perform efficient isotropic gradient computation with a convolution product using MATLAB.

First, all performance testing consists of evaluating gradients of random 2D and 3D double precision images. Note that we suppose a periodic padding for these images. When using MATLAB for computing the image gradient, the `-singleCompThread` startup option is used. This is done for benchmarking purposes, because the reference case should be computed using a sequential algorithm, that is, with a single core only. The CPU used in this work is an Intel Core i7-970 processor, while the GPU is an Nvidia GeForce GTX 580 card. The computations on the GPU are performed either in MATLAB via the Jacket plugin developed by AccelerEyes or by using a precompiled CUDA code. The version of MATLAB is R2010b, the Jacket version is 2.1 (build e2c1fa6), and the CUDA version is 4.1.

To test performance, five different algorithms/platforms are considered for computing the gradient :

1. MATLAB CPU singlethread [REFERENCE CASE]
2. MATLAB GPU Jacket
3. MATLAB GPU Jacket with GFOR
4. CUDA with FFT convolution
5. CUDA with spatial convolution

MATLAB GPU with the Jacket plugin, Case (2), is the GPU equivalent of Case (1), the reference case, MATLAB CPU singlethread. MATLAB GPU Jacket with GFOR, Case (3), is a special case that is not available on the CPU. To explain this, let us suppose that the user wishes to evaluate the gradient of n different images simultaneously. This cannot be done using MATLAB without `parfor`, which is only available with the Parallel Computing Toolbox. Also note that `parfor` is usually used for coarse-grained parallelism, while `gfor` can be

used for fine-grained parallelism. Without `parfor`, or if fine-grained parallelism is required, a `for` loop is needed to evaluate the gradients of the images sequentially, and to store the results in a large matrix by subassignment. With Jacket, it is possible to perform these n gradient evaluations in parallel on the GPU using a `gfor` loop. Usually, this significantly reduces computational time, compared to the sequential `for` loop. More details on the functionality and limitations of the `gfor` loop can be found in [1]. In order to be able to compare the `gfor` loop case (3) with the other cases (1, 2, 4, and 5), all the performance tests were conducted with $n = 3$, unless otherwise stated, i.e. we suppose that the user needs to evaluate three image gradients simultaneously. A summary of the algorithms used for cases 1, 2, and 3 can be found in Ref. [12], and those for cases 4 and 5 are presented in section (2.4). Note that the algorithms in cases 4 and 5 use the CUDA platform to compute the gradients. Moreover, the convolution algorithms differ, depending on the case selected. Case (4) computes the convolution in the frequency domain using FFT, while case (5) computes the convolution in the spatial domain.

The timing method on the CPU is the usual MATLAB `tic`; `m-code`; `toc`; procedure. However, this method is not suitable for timing m-code on the GPU with Jacket. A method that is capable of doing this has been proposed by AccelerEyes [1]. In CUDA, we record two events and measure the time lapse between them, at the beginning and at the end of the simulation, with a synchronization that completes all events before the last one is recorded. Note that in Figures (1-4), the time taken for one simulation "dot", or result "dot", is the average of one hundred simulations. All results differ with respect to machine accuracy in double precision, and the padding of the images is computed on the fly to save computer memory. This is because padding is very cheap in terms of computing cost, relative to the cost of evaluating the gradient. For each case, the computational time only includes the time to pad the image and the actual gradient evaluation. The time to transfer the data from the CPU memory to the GPU memory is not taken into account.

The figures show performance behavior on a log scale. CUDA with spatial convolution performance decreases dramatically with a larger stencil size, due to smaller threads block and therefore smaller shared memory. In order to gain performance, the number of padding positions in shared memory should not exceed the current block number of threads, because those padding positions request a higher memory bandwidth, as we saw in section (2.4.1). These situations were simply disregarded in the results figures and tables.

Figures (1a) and (1b) show the performance speedup for 2D gradients with orders $(S, I) = (2, 4)$ and $(S, I) = (14, 16)$ as a function of image size. When the CUFFT library is used, e.g. Fig. (1b), the overall performance speedup increases with the image size, however abrupt speedup drops can be seen near sizes 256 and 512. The FFT algorithm requests a power of 2 input size : 16, 32, 64, 128, 256, 512, 1024. When data size is greater than the closest power of 2, then it should be extended to the next greater power of 2, even if only half the requested input memory will contribute to the final results. The spatial convolution is not affected by this limitation and speedup performance steadily grows as the image size increases. Note that for the 3x3 stencil in Fig. (1a), the spatial convolution algorithms for small images is much faster with CUDA. As the image size increases, Jacket speedup performance is better and can be compared with that of CUDA. This could be attributed to the fact that there might be some computational overhead with the Jacket plugin for MATLAB. However, as the image size grows and the computational complexity increases, this becomes less noticeable.

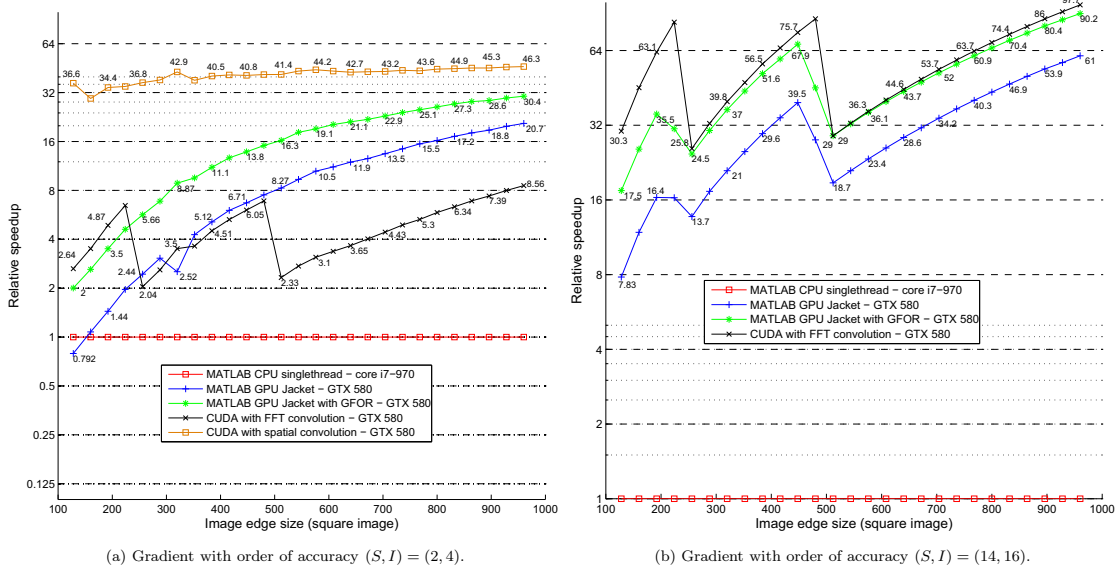
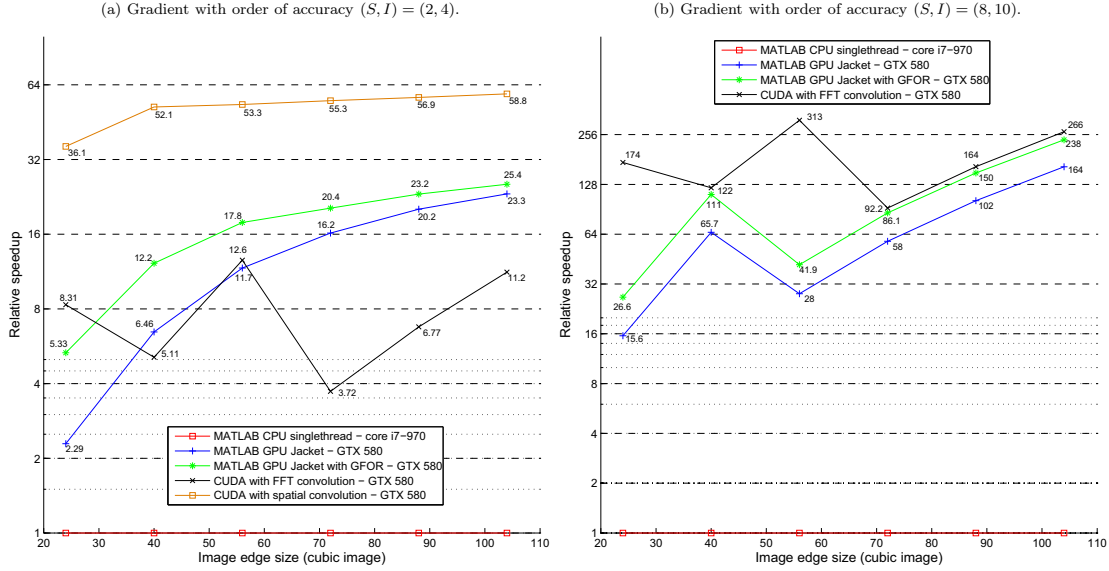


FIGURE 1: Speedup as a function of image size (2D gradient).

Figures (2a) and (2b) show the same situation, but for 3D gradients of orders $(S, I) = (2, 4)$ and $(S, I) = (8, 10)$. The same comments that were made for the 2D case can be made for the 3D case. The main difference is that, for a 3D image, the performance speedup that can be achieved compared to MATLAB CPU singlethread is much higher, up to 313x in the best conditions.

FIGURE 2: Speedup as a function of image size (3D gradient).



Figures (3a) and (3b) show the speedup with the 2D and 3D gradients as a function of the spatial and isotropic order at a fixed image size. In 2D, the image sizes are 960x960, and in 3D, they are 104x104x104. For both the 2D and 3D cases, as the spatial/isotropic order or the number of images to evaluate simultaneously increases, the speedup that can be achieved using the GPU also increases. This was to be expected, since the computational complexity increases with the stencil radius R . Looking at the CUDA algorithm in Figures (3a) and (3b), it is possible to identify the performance speedup crossing between the FFT and spatial convolution. Note that Jacket version 2.1 automatically uses spatial convolution instead of FFT convolution for stencil sizes up to 9x9 in 2D, and 3x3x3 in 3D.

Figure (4) shows the speedup for the 3D gradients of order $(S, I) = (8, 10)$ as a function of n , the number of images to be evaluated simultaneously at a fixed image size of 104x104x104. As more images need to be evaluated in parallel, the performance speedup grows significantly for MATLAB GPU Jacket with GFOR, and for CUDA with FFT convolution. This is because the same filter is used for evaluating each of the image gradients. When using FFT convolution, we need to compute the FFT of the filter. In doing so, it is possible to exploit the fact that the FFT of the filter can only be calculated once for the first image, and is reused for evaluating the other image gradients. This is what we have done in CUDA, and we suspect that Jacket automatically detects that the filter is the same for each loop iterator, and so accelerates the computation with GFOR using this technique. However, this might not be the case, as we do not have access to the Jacket library.

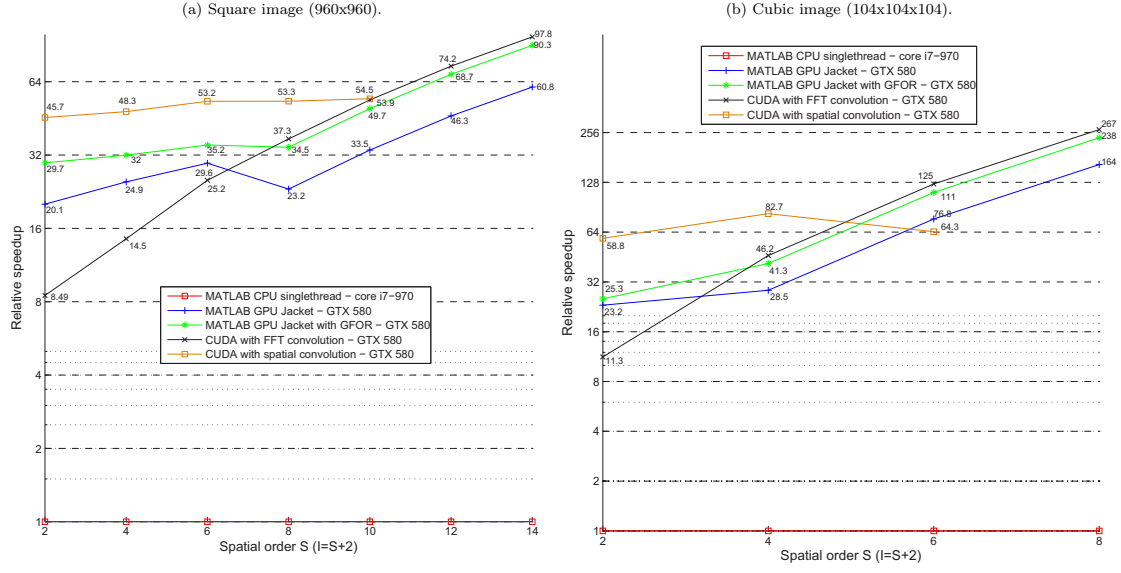
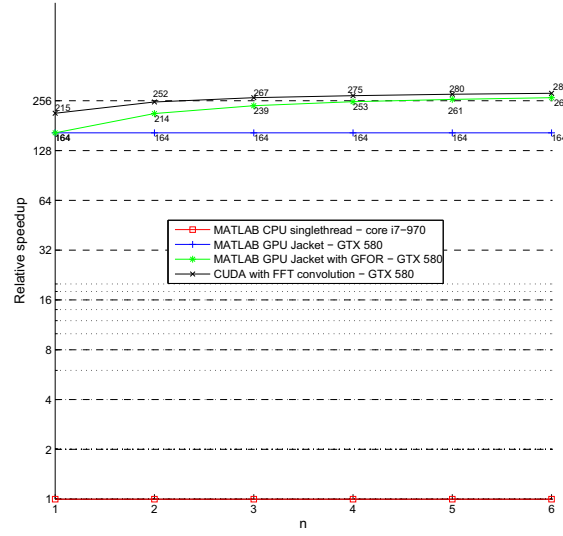
For the larger image size, Table (12) contains a summary of the results presented in Figs. (1-4). If both CUDA algorithms are considered, i.e. FFT and spatial convolution, CUDA is always faster than Jacket. However, the performance gap is not a large one, especially with the FFT convolution. Depending on the target application, it might not be necessary to use the more complicated CUDA programming platform. Instead, we could simply use Jacket for MATLAB to accelerate the application, as it is much simpler to program in MATLAB language than CUDA.

Based on the results presented in this section, we can conclude that, in our case, high order spatial and isotropic gradient computation can be accelerated using the GPU with CUDA or the Jacket plugin for MATLAB, instead of plain MATLAB. As long as the filters are the same size, the performance benchmark presented here, and our conclusion, are valid for any other convolution filter.

4 Conclusion

In this work, a detailed description of high order spatial and isotropic gradient discretizations has been presented. Based on our theoretical derivation, it is now possible to calculate the stencil weights needed to freely adjust the spatial and/or isotropic order of the 2D and 3D discrete gradient operator. Although the various discrete differential operators presented here usually use non compact stencils, and are therefore computationally expensive, we have addressed this issue by combining the convolution product and GPU hardware. We have shown that when computing image or function gradients, either CUDA or the Jacket plugin for MATLAB can outperform, by more than 250x in some situations, the widely used plain MATLAB programming environment. In addition, researchers will be able to benefit from isotropic discretizations, since they make it possible to reduce the anisotropy of numerical methods considerably. We believe that the method presented in this work can be generalized to other types of differential operators, such as the Laplacian or other operators containing higher

FIGURE 3: Speedup as a function of the spatial and isotropic order of the gradient.

FIGURE 4: Speedup as a function of the number of cubic images (104x104x104) to be evaluated simultaneously using the 3D gradient with order of accuracy $(S, I) = (8, 10)$.

order or mixed derivatives. Future development of stencil weights for other differential operators that would lead to high order spatial and isotropic accuracy could provide significant benefits for some scientific applications. Note, too, that with larger stencils, there may be opportunities to incorporate other properties into the finite difference discretization.

TABLE 12: Speedup summary for large image size.

n	2D							3D					
	3							3				1	
Spatial order S ($I = S + 2$)	2	4	6	8	10	12	14	2	4	6	8	1	8
MATLAB CPU singlethread	1	1	1	1	1	1	1	1	1	1	1	1	1
MATLAB GPU Jacket	20	25	30	23	34	46	61	23	29	77	164	164	164
MATLAB GPU Jacket with GFOR	30	32	35	35	50	69	91	25	41	111	238	164	267
CUDA with FFT convolution	8	14	25	37	54	74	98	11	46	125	267	215	284
CUDA with spatial convolution	46	48	53	53	54	N/A	N/A	59	82	64	N/A	N/A	N/A

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