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Auteur: Mohamed Amine Bouguezzoul
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**Conditional Quadrature Method of Moments for Populations of Non-Spherical
Particles**

MOHAMED AMINE BOUGUEZZOUL

Département de génie mécanique

Mémoire présenté en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*
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Particles**

présenté par **Mohamed Amine BOUGUEZZOUL**

en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

a été dûment accepté par le jury d'examen constitué de :

Roberto PAOLI, président

Fabian DENNER, membre et directeur de recherche

Bruno BLAIS, membre et codirecteur de recherche

Bianca VIGGIANO, membre et codirectrice de recherche

Yann-Meing LAW, membre

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RÉSUMÉ

Ce mémoire étudie la dynamique complexe des écoulements multiphasiques dispersés et dilués contenant des particules non sphériques, plus particulièrement des ellipsoïdes oblates. Le suivi de l'évolution de telles populations nécessite la résolution d'une équation de bilan de population (PBE) définie sur un espace des phases à haute dimension et fortement couplé. Plus précisément, cette étude considère un espace des états en cinq dimensions (5D) comprenant le diamètre équivalent en volume, le rapport d'aspect et les trois composantes de la vitesse de translation de la particule. Étant donné que la discrétisation classique sur grille souffre d'une augmentation exponentielle du coût de calcul, ce travail implémente et évalue des solveurs macroscopiques eulériens basés sur la méthode des moments en quadrature conditionnelle (CQMOM).

En suivant dynamiquement les moments statistiques de la fonction de densité en nombre (NDF) et en exploitant un suivi hiérarchique des variétés, le cadre proposé permet de simuler efficacement l'advection aérodynamique dépendante de la forme, l'attrition de surface continue et la fragmentation binaire discrète. Afin d'évaluer rigoureusement la stabilité du solveur dans des régimes fortement hors équilibre, le modèle est soumis à un environnement d'écoulement d'air tourbillonnaire entièrement couplé. Au sein de cet espace des phases hautement chaotique, les particules subissent simultanément une ablation de surface dictée par l'énergie cinétique (attrition en v^2), une dissipation continue de la variance (traînée aérodynamique) et une injection discontinue de la variance (recul stochastique lors de la fragmentation). Une analyse comparative est menée entre une approche explicite de transport direct des moments (MT), entièrement couplée, et une approche de transport hybride (HT) à opérateurs scindés de Strang de manière symétrique, en utilisant des simulations lagrangiennes de Monte Carlo (MC) comme référence.

Les résultats mettent en évidence la fragilité mathématique fondamentale des fermetures aux moments lorsqu'elles sont entièrement couplées. Lorsqu'elle est contrainte de traiter simultanément des termes sources continus et discontinus violemment opposés, la méthode explicite MT souffre d'un mauvais conditionnement sévère de la matrice. Cela déclenche des mécanismes de repli de quadrature localisés qui corrompent à la fois la conservation géométrique de la masse et la variance cinématique, entraînant finalement des effondrements catastrophiques de la réalisabilité et des fuites d'énergie non physiques. À l'inverse, la méthode HT, s'appuyant sur une scission de Strang, réussit à découpler ces opérateurs, préservant ainsi la stricte définition positive de la matrice de covariance. Bien que les gradients ciné-

matiques extrêmes de cet environnement explicitement couplé exposent une erreur inhérente de fermeture de quadrature dans l'ensemble des moments — se manifestant par une dissipation graduelle de la variance dans la température granulaire —, l'architecture HT contourne entièrement la singularité matricielle. En maintenant la stabilité structurelle sans dégradation numérique catastrophique, la méthode HT atteint la fidélité macroscopique d'un solveur stochastique à une fraction du coût de calcul.

ABSTRACT

This work investigates the complex dynamics of dilute dispersed multiphase flows containing non-spherical, oblate ellipsoidal particles. Tracking the evolution of such populations requires solving a Population Balance Equation (PBE) defined over a highly coupled, high-dimensional phase space. Specifically, this study considers a 5D state space comprising particle volume-equivalent diameter, aspect ratio, and three translational velocity components. Because conventional grid-based discretization suffers from exponential computational scaling, this work implements and evaluates macroscopic Eulerian solvers based on the Conditional Quadrature Method of Moments (CQMOM).

By dynamically tracking the statistical moments of the Number Density Function (NDF) and utilizing hierarchical manifold tracking, the proposed framework allows for the efficient simulation of shape-dependent aerodynamic advection, continuous surface attrition, and discrete binary breakage. To rigorously evaluate solver stability in highly non-equilibrium regimes, the framework is subjected to a fully coupled swirling airflow environment. Within this highly chaotic phase space, particles experience simultaneous kinetic-energy-driven surface ablation (v^2 -attrition), continuous variance dissipation (aerodynamic drag), and discontinuous variance injection (stochastic breakage recoil). A comparative analysis is conducted between an explicit fully coupled Moment Transport (MT) approach and a symmetric Strang-splitting Hybrid Transport (HT) approach against Lagrangian Monte Carlo (MC) benchmarks.

The results expose the fundamental mathematical fragility of fully coupled moment closures. When forced to simultaneously process competing continuous and discontinuous source terms, the explicit MT method suffers from severe matrix ill-conditioning. This triggers localized quadrature fallbacks that corrupt both geometric mass conservation and kinematic variance, ultimately resulting in detrimental realizability collapses and unphysical energy leaks. In contrast, the Strang-split HT method successfully decouples these operators, preserving the strict positive-definiteness of the Hankel matrices. While the extreme kinematic gradients of this explicitly cross-coupled environment expose an inherent quadrature closure error in the moment set—manifesting as a gradual variance dissipation in the granular temperature—the HT architecture entirely circumvents matrix singularity. By maintaining structural stability without numerical degradation, the HT method achieves the macroscopic fidelity of a stochastic solver at a fraction of the computational cost.

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LIST OF SYMBOLS AND ACRONYMS

CFD	computational fluid dynamics
CHyQMOM	conditional hyperbolic quadrature method of moments
CQMOM	conditional quadrature method of moments
FVM	finite volume method
GQMOM	generalized quadrature method of moments
HT	hybrid transport
HyQMOM	hyperbolic quadrature method of moments
MC	Monte Carlo
MT	moment transport
MTE	moment transport equation
NDF	number density function
ODE	ordinary differential equation
PBE	population balance equation
PDE	partial differential equation
QBMM	quadrature-based moment methods
QMOM	quadrature method of moments
QSO	quasi-steady orientation
RK	Runge–Kutta
SSP-RK	strong stability preserving Runge–Kutta
SSP-RK3	strong stability preserving third-order Runge–Kutta
TP	tensor-product

CHAPTER 1 INTRODUCTION

Non-spherical, specifically ellipsoidal, particles are widely encountered in natural and industrial multiphase flows, ranging from atmospheric aerosols and ice crystals to biomass processing and pharmaceutical manufacturing [2, 3]. Accurately modeling their coupled geometry and kinematics under physical forces is crucial for predicting macroscopic system dynamics. However, tracking the evolution of such populations requires solving a population balance equation (PBE) defined over a high-dimensional phase space. Because conventional Eulerian bin-based methods suffer from an exponential scaling of computational cost with each added dimension, resolving this highly coupled state space remains computationally prohibitive [4, 5]. To overcome this fundamental bottleneck, this work focuses on developing, validating, and applying macroscopic numerical solvers based on the conditional quadrature method of moments (CQMOM) [4]. By tracking a small set of statistical moments rather than the full distribution, we aim to formulate a computationally feasible framework that accurately accounts for particle advection, continuous kinetic-energy-driven surface attrition, shape evolution, orientation-dependent drag forces, and discrete fragmentation events within a 5-dimensional (5D) phase space.

The PBE is a fundamental mathematical framework for describing the evolution of a dispersed multiphase flow—such as solid particles, bubbles, or droplets—within a continuous carrier medium [3]. It governs the time evolution of the number density function (NDF), denoted as $n(t; \mathbf{x}, \mathbf{u}, \boldsymbol{\xi})$, which characterizes the probable number of particles at a given time t , physical spatial location $\mathbf{x}$, velocity $\mathbf{u}$, and internal phase space variables $\boldsymbol{\xi}$ (e.g., volume-equivalent diameter, aspect ratio). The general form of the PBE is given by:

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{x}} \cdot (n\mathbf{u}) + \nabla_{\boldsymbol{\xi}} \cdot (n\dot{\boldsymbol{\xi}}) = \mathcal{S}, \quad (1.1)$$

where $\dot{\boldsymbol{\xi}}$ represents the continuous advection rate within the internal phase space, and $\mathcal{S}$ denotes the discontinuous source and sink terms representing discrete macroscopic phenomena such as coalescence, continuous growth, or fragmentation [1, 3].

In this work, the primary focus is exclusively on the complex, high-dimensional internal phase space dynamics (size, shape, and velocity). Consequently, we operate under the assumption of spatial homogeneity for the control volume being analyzed, allowing us to explicitly neglect the physical space advection term $\nabla_{\mathbf{x}} \cdot (n\mathbf{u})$. In comprehensive 3D computational fluid dynamics (CFD) frameworks, resolving this spatial advection is a separate numerical challenge,

typically addressed using robust Eulerian techniques such as the finite volume method (FVM) [6] or Discontinuous Galerkin methods [7]. By decoupling the spatial transport, we can rigorously isolate and validate the numerical treatment of the internal coordinates $\boldsymbol{\xi}$.

To provide a tractable solution to Equation (1.1), moment methods close the PBE by tracking only a finite, lower-dimensional set of statistical moments rather than the full NDF itself [3]. The statistical moment of order $\mathbf{k}$ of the distribution is defined by integrating the NDF over the internal phase space Ω :

$$M_{\mathbf{k}} = \int_{\Omega} \boldsymbol{\xi}^{\mathbf{k}} n(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad \text{with } \mathbf{k} \in \mathbb{N}^d. \quad (1.2)$$

When the moment operator $\int_{\Omega} \boldsymbol{\xi}^{\mathbf{k}}(\cdot) d\boldsymbol{\xi}$ is applied to the homogeneous PBE, it yields the moment transport equation (MTE):

$$\frac{\partial M_{\mathbf{k}}}{\partial t} = - \int_{\Omega} \boldsymbol{\xi}^{\mathbf{k}} \nabla_{\boldsymbol{\xi}} \cdot (\dot{\boldsymbol{\xi}} n) d\boldsymbol{\xi} + \int_{\Omega} \boldsymbol{\xi}^{\mathbf{k}} \mathcal{S} d\boldsymbol{\xi} \quad (1.3)$$

The right-hand side of the MTE, denoted as the $\mathbf{k}$ -th order flux, might contain unclosed integral source terms [3]. To achieve mathematical closure, quadrature method of moments (QMOM) approximates the continuous NDF as a finite summation of weighted Dirac delta functions [3]:

$$n(\boldsymbol{\xi}) \approx \sum_{i=1}^N w_i \delta(\boldsymbol{\xi} - \boldsymbol{\xi}_i), \quad (1.4)$$

where w_i are the discrete probability weights and $\boldsymbol{\xi}_i$ are the abscissas (quadrature nodes) reconstructed directly from the transported moments via an inversion algorithm. This Dirac delta representation is mathematically equivalent to a Gaussian quadrature, allowing the unclosed integral source terms in the MTE to be evaluated efficiently and accurately at the discrete node locations, thus closing the Eulerian transport system [3, 8].

While the theoretical foundation of the PBE is well established, accurately simulating the dynamics of non-spherical particles in highly inertial, non-equilibrium flows introduces severe mathematical and computational challenges [8]. The core of this problematic is three-fold: the curse of dimensionality, the geometric rigidity of standard quadrature grids, and the severe mathematical stiffness induced by explicitly cross-coupled phase-space fluxes.

First, solving the continuous PBE directly using conventional discretization techniques, such as sectional methods [5], is unfeasible for multivariate distributions due to the exponential scaling of computational cost [3, 4]. To fully capture the physics of size-dependent drag, shape relaxation, and aerodynamic surface attrition for oblate spheroids, the NDF must be tracked within a highly coupled 5D phase space, specifically comprising the volume-equivalent

diameter (d), the aspect ratio (χ), and the three components of the translational velocity vector (u, v, w). Attempting to discretize this 5D domain using standard bin-based methods requires millions of transported scalars per spatial control volume, rendering the approach completely intractable for industrial CFD applications [3, 4].

Second, while standard moment closures (QMOM) resolve the dimensionality issue for 1D phase spaces, extending them naively to 5D domains utilizing Tensor-Product grids results in severe inefficiencies [4, 9]. Multidimensional NDFs in multiphase flows are highly correlated; for instance, a particle’s terminal settling velocity and its susceptibility to surface attrition are tightly coupled to its diameter and shape. Tensor-Product grids force quadrature nodes into a rigid Cartesian structure, placing the vast majority of computational nodes in completely empty, unphysical regions of the phase space. This not only wastes computational resources but actively induces ill-conditioning in the moment inversion algorithms [3, 9].

Third, and most critically, resolving explicitly cross-coupled flows featuring simultaneous continuous advection and discrete fragmentation exposes fundamental mathematical fragilities in standard Eulerian moment closures. In realistic multiphase systems, aerodynamic drag acts as a continuous focusing operator that dissipates velocity variance, driving the local distribution toward a singularity [8, 10]. Simultaneously, kinetic-energy-driven surface attrition [11, 12] (v^2 -attrition) couples this kinematic variance directly to the geometric phase space, accelerating mass loss at high slip velocities. Conversely, violent fragmentation events—accompanied by stochastic recoil—act as discontinuous diffusion operators that isotropically inject variance back into the system. Attempting to balance these violently opposed, highly coupled source terms simultaneously within a single continuous Ordinary Differential Equation (ODE) integration step induces extreme numerical stiffness [3]. This conflict forces standard solvers to overshoot the realizable moment space, destroying the positive-definiteness of the underlying Hankel matrices and triggering detrimental algorithmic failures [3, 10]. Consequently, a novel mathematical architecture is strictly required to process these competing fluxes without artificial numerical degradation.

The primary objective of this research is to develop, validate, and optimize a computationally tractable and mathematically realizable macroscopic Eulerian solver capable of tracking the fully coupled 5D phase-space evolution of non-spherical particle populations.

To achieve this primary goal, the specific sub-objectives are defined as follows:

- **Implement and verify the CQMOM:** Develop a robust multivariate moment inversion framework utilizing adaptive Wheeler algorithms to track highly correlated phase-space manifolds without relying on rigid tensor grids.

- **Derive a dimensionally reduced physical model:** Conduct a rigorous time-scale analysis of the rotational and translational relaxation times of oblate spheroids to mathematically justify the quasi-steady orientation (QSO) assumption, safely reducing the phase space to 5 tractable dimensions.
- **Develop a mathematically stable transport architecture:** Formulate a split-operator Hybrid Transport (HT) method to completely decouple continuous variance dissipation and geometric attrition from discontinuous breakage variance injection, preventing matrix ill-conditioning.
- **Validate against high-fidelity stochastic benchmarks:** Rigorously assess the macroscopic kinematic and geometric accuracy of the proposed Eulerian solvers against exact Lagrangian Monte Carlo (MC) simulations under explicitly cross-coupled flow conditions.

This thesis is structured to systematically build and validate the 5D multiphase framework. Following the literature review in Chapter 2, Chapter 3 introduces the fundamental mathematics of the 1D QMOM, detailing the adaptive Wheeler inversion algorithm and verifying its accuracy on a continuous non-linear growth problem. Chapter 4 extends this mathematical foundation to multivariate distributions, detailing the hierarchical conditional inversion of CQMOM and verifying its capability to track highly correlated rotating manifolds.

Chapter 5 shifts to the physical modeling, defining the orientation-dependent aerodynamic forces acting upon oblate spheroids and conducting the rigorous time-scale analysis required to justify the 5D QSO phase-space reduction. Chapter 6 begins coupling the mathematics and the physics, applying the framework to a monomodal particle population undergoing simultaneous advection and binary breakage. This chapter introduces the split-operator Hybrid Transport (HT) architecture and contrasts its numerical stability against standard Moment Transport (MT). Chapter 7 evaluates the framework against highly non-equilibrium initial conditions, utilizing multimodal crossing jets to test solver survivability under discrete variance injection. Finally, Chapter 8 pushes the framework to its absolute limit, subjecting the particle population to a fully coupled swirling airflow environment featuring simultaneous v^2 -driven surface attrition, aerodynamic advection, and stochastic fragmentation. Chapter 9 synthesizes the findings, discusses the inherent numerical limitations of the current moment closures, and outlines pathways for future algorithmic research.

To ensure the complete transparency, verification, and reproducibility of the numerical methodologies developed throughout this Master’s research, the entire codebase has been publicly released as open-source software under the terms of the MIT License. The computational

frameworks are organized into two dedicated libraries, hosted actively on GitHub for ongoing version control and permanently archived on Zenodo:

- **QMOM-Intro:** An introductory and foundational Python framework that implements the standard univariate QMOM to solve generic PBEs, validating the moment closure against discrete Monte Carlo simulations.

GitHub: <https://github.com/polycfd/QMOM-Intro>

Zenodo Archive: DOI: 10.5281/zenodo.20090578

- **5D CQMOM Particle Simulation Framework:** The primary research suite of this thesis, providing a macroscopic 5-dimensional Eulerian solver that tracks highly polydisperse populations of non-spherical oblate spheroids via CQMOM coupled with an isolated Strang-splitting Hybrid Transport architecture.

GitHub: <https://github.com/polycfd/CQMOM-Ellipsoidal-Particles>

Zenodo Archive: DOI: 10.5281/zenodo.20044545

CHAPTER 2 LITERATURE REVIEW

The foundational work by Fox, Marchisio, and colleagues [3, 8, 13] established quadrature-based moment methods as a robust and flexible Eulerian approach for simulating multiphase systems involving aggregation, fragmentation, and turbulent flows. By tracking a finite set of integer moments rather than the full probability density, these methodologies bypass the severe computational bottlenecks associated with grid-based discretization. To address specific physical constraints and numerical limitations inherent to the classical QMOM, a variety of mathematical extensions have since been developed within the literature.

For instance, rather than tracking the moments themselves, the Direct QMOM (DQMOM) tracks the transport equations for the quadrature weights and abscissas directly, a formulation that can significantly simplify the coupling of the dispersed phase with Eulerian CFD solvers [1, 3, 14]. In physical scenarios where the reconstruction of a continuous NDF is strictly necessary—such as modeling continuous evaporation or condensation—the Extended QMOM (EQMOM) was introduced to replace the discrete Dirac delta functions with continuous kernel density functions, such as Gaussian or log-normal distributions [1, 3, 15].

However, standard moment closures frequently suffer from artificial numerical artifacts, particularly the formation of delta-shocks when simulating highly inertial, multi-modal crossing trajectories. For multivariate distributions governed by purely hyperbolic transport equations (e.g., the scalar advection equation, $\partial_t n + u \partial_x n = 0$), the mathematical inability of standard polynomial closures to capture converging variance without losing realizability led to the development of the Hybrid QMOM (HyQMOM) and Conditional HyQMOM (CHyQMOM) [1, 8, 16–18]. These advanced formulations overcome the shortcomings of EQMOM and DQMOM by explicitly transporting the velocity variance as a strictly conserved variable, preventing artificial shock formation. Furthermore, the Generalized QMOM (GQMOM) provides a more accurate and stable moment closure than the standard Wheeler algorithm by extending the quadrature representation to an over-determined system ($N > n$ terms). By incorporating prior knowledge of the distribution’s shape, GQMOM preserves known moments while situating higher-order moments strictly within the interior of the realizable moment space, achieving superior stability at a comparable computational cost [19].

For higher-dimensional phase spaces, the extension of moment methods historically relied on rigid Tensor-Product grids, which suffer from severe empty-node inefficiencies and matrix ill-conditioning [9]. To resolve this, Yuan and Fox [4] formulated the CQMOM, utilizing adaptive hierarchical conditioning to strictly place quadrature nodes on the non-zero probability

manifolds, successfully avoiding the exponential scaling of standard grids. Recent efforts in the field have heavily focused on extending these hierarchical moment methods to 3D and 4D phase spaces for complex fluid dynamics [4, 13, 18, 20]. Simultaneously, there is a growing necessity to incorporate geometric shape factors and orientation as internal phase-space variables to accurately model the complex aerodynamic dynamics of non-spherical particles, biomass, and atmospheric aerosols [2]. The present work aims to directly contribute to these ongoing efforts by developing, stabilizing, and validating a fully coupled CQMOM framework specifically tailored for the highly correlated 5D phase-space evolution of non-spherical oblate ellipsoids.

CHAPTER 3 THE QUADRATURE METHOD OF MOMENTS

3.1 The Challenge of the Population Balance Equation

The description of polydispersed multiphase flows is fundamentally governed by the PBE, a continuity equation defined over a high-dimensional phase space. As formulated in Equation (1.1), the evolution of the NDF, $n(t; \mathbf{x}, \boldsymbol{\xi})$, depends not only on physical space $\mathbf{x}$ and time t , but also on a set of internal coordinates $\boldsymbol{\xi}$.

Solving this equation directly using conventional grid-based Eulerian discretization techniques, such as the discrete sectional method, is severely hindered by the exponential scaling of computational cost [3, 4]. As each internal coordinate adds an independent dimension to the computational domain, the required degrees of freedom become prohibitively numerous.

To quantify the prohibitive nature of this cost, consider a phase space Ω defined by five internal coordinates. In a conventional bin approach, each dimension is discretized into N intervals. To adequately resolve the shape of the NDF and prevent excessive numerical diffusion across bins, especially for problems with collisions and coagulation, sectional methods typically require 20 to 100 bins per internal dimension [21]. Let us assume a coarse discretization grid to establish a theoretical lower bound for the cost—using only 20 bins per dimension. The total number of degrees of freedom (scalars) required to be transported at every single spatial mesh point becomes:

$$N_{DoF} = 20^5 \approx 3,200,000 \text{ scalars per cell.} \quad (3.1)$$

For a typical engineering CFD simulation utilizing a spatial mesh of 10^6 (1 million) cells, the memory requirement for the dispersed phase alone would be:

$$\text{Memory} \approx 10^6 \text{ cells} \times 3.2 \times 10^6 \text{ doubles/cell} \times 8 \text{ bytes/double} \approx 25.6 \text{ Terabytes.} \quad (3.2)$$

This memory requirement far exceeds the capacity of standard high-performance computing nodes. Furthermore, the computational cost of advecting 3,200,000 transport equations per time step is fundamentally intractable.

In stark contrast, quadrature-based moment methods bypass this exponential scaling by projecting the distribution onto a lower-dimensional subspace. Instead of tracking the full NDF, QMOM approximates it using N discrete quadrature nodes. Mathematically, to uniquely determine the N discrete weights and the N spatial abscissas, exactly $2N$ independent degrees

of freedom are required [22]. Consequently, the quadrature rule must be constructed using exactly $2N$ consecutive integer moments. This specific mathematical requirement guarantees the exact integration of any polynomial up to degree $2N - 1$ over the phase space [3].

For a standard 5-dimensional implementation, choosing $N = 2$ quadrature nodes per dimension is widely considered sufficient for engineering applications [4, 13, 23, 24]. This low-order approximation accurately captures the total number, mean, variance, and skewness of the distribution (up to the 3rd-order moment). Using CQMOM, the number of transported scalars for an $N = 2$ tracking strategy scales cumulatively as:

$$2N_1 + 2N_1N_2 + 2N_1N_2N_3 + 2N_1N_2N_3N_4 + 2N_1N_2N_3N_4N_5 = 124 \text{ moments.} \quad (3.3)$$

Consequently, the memory requirement is drastically reduced to:

$$\text{Memory} \approx 10^6 \text{ cells} \times 124 \text{ doubles/cell} \times 8 \text{ bytes/double} \approx 992 \text{ Megabytes.} \quad (3.4)$$

This represents a data compression ratio of order $\mathcal{O}(10^4)$, rendering the 5-dimensional simulation computationally feasible on standard hardware.

3.2 The Moment Closure Problem

The moment reduction strategy mitigates the exponential scaling of the computational cost with dimensionality by projecting the continuous distribution onto a finite subspace. Integrating the NDF over the internal phase space Ω yields the statistical moments. The k -th moment is defined as:

$$M_k = \int_{\Omega} \xi^k n(\xi) d\xi, \quad (3.5)$$

where ξ represents an internal coordinate. In this work, internal coordinates include the volume-equivalent diameter, the aspect ratio and the velocities. The aspect ratio is specifically tracked to characterize the geometry of ellipsoidal particles, as it directly dictates the orientation-dependent drag, lift, and torque coefficients required for accurate kinematic modeling [25], as further discussed in Chapter 5.

Applying the moment operator to the PBE (1.1) in 1D generates the MTE $\frac{\partial M_k}{\partial t} = \Phi_k$, where the flux Φ_k is defined as

$$\Phi_k \stackrel{def}{=} -\nabla_{\mathbf{x}} \cdot \int_{\Omega} \xi^k \mathbf{u}(\xi) n d\xi - \int_{\Omega} \xi^k \frac{\partial}{\partial \xi} (\xi n) d\xi + \int_{\Omega} \xi^k \mathcal{S} d\xi. \quad (3.6)$$

However, this might introduce a fundamental mathematical difficulty known as the clo-

sure problem. Even if the internal phase space advection and discrete event source terms are closed, spatial transport introduces a distinct closure challenge [3]. When the spatial velocity of a particle depends non-linearly on its internal coordinates (such as size- and shape-dependent settling velocity), the macroscopic spatial flux of the k -th moment, $\nabla_{\mathbf{x}} \cdot \int_{\Omega} \mathbf{u}(\xi) \xi^k n(\xi) d\xi$, cannot be expressed as a simple function of $M_0, M_1, \dots, M_k$. This non-linear dependence strictly requires information about the next higher moments, rendering the spatial advection unclosed [3]. Similarly, integral source terms representing fragmentation or aggregation often depend on fractional or higher-order moments that are not explicitly transported. In what follows, we focus exclusively on the dynamics in phase space, assuming a homogeneous control volume in the physical space.

To resolve these unclosed spatial and internal fluxes, QMOM approximates the underlying NDF as a summation of N weighted Dirac delta functions: As established by McGraw [22],

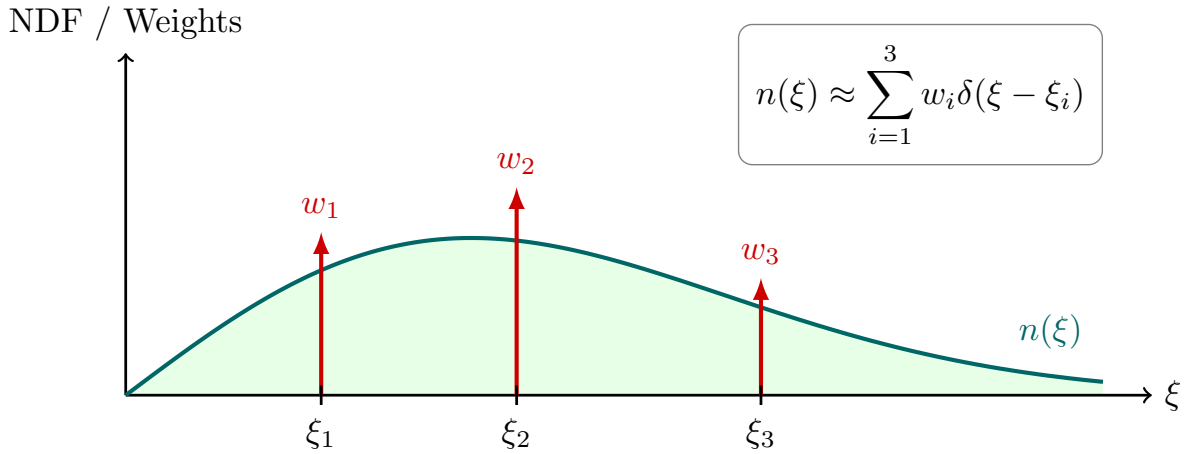


Figure 3.1 Conceptual representation of QMOM with $N = 3$

uniquely determining these N weights and N abscissas requires exactly $2N$ degrees of freedom. Consequently, the quadrature rule must be constructed using the first $2N$ consecutive integer moments, $\mathcal{M}_{2N} = \{M_0, M_1, \dots, M_{2N-1}\}$. This specific requirement guarantees the exact integration of any polynomial up to order $2N - 1$ over Ω . More importantly, this discrete representation allows the solver to extrapolate unclosed higher-order or fractional moments directly from the finite set of known integer moments, thereby numerically closing the MTEs [3].

3.3 Moment Inversion Mathematics

3.3.1 Realizability of a moment set

Before attempting to invert a finite set of moments into a discrete quadrature rule, one must verify that the moment set is physically and mathematically valid. A set of moments $\mathcal{M}_{2N} = \{M_0, M_1, \dots, M_{2N-1}\}$ is defined as strictly realizable if, and only if, there exists a non-negative measure function $n(\xi) \geq 0$ defined over the domain Ω that can produce those exact moments [3].

In the context of multiphase flows, realizability ensures that the statistical moments correspond to a physically possible particle population. For example, the total number density (M_0) must be positive, and the variance of the distribution ($M_0M_2 - M_1^2$) must be non-negative. If numerical errors—such as diffusion or dispersion introduced by spatial advection schemes—corrupt the transported moment vector, the sequence may exit the realizable moment space. Attempting to apply a quadrature inversion to an unrealizable moment set will invariably lead to algorithm failure, producing complex or negative quadrature weights that fatally crash the simulation.

The classical mathematical criteria for moment realizability are strictly governed by the properties of Hankel determinants. For a given moment sequence to be realizable over the real line $\mathbb{R}$, certain Hankel matrices constructed from the moments must be positive definite [3, 19]. The Hankel matrix of order n , denoted as $\mathbf{H}_n$, is the symmetric matrix defined for $n = 0, 1, \dots, N$ as:

$$\mathbf{H}_n = \begin{bmatrix} M_0 & M_1 & M_2 & \dots & M_n \\ M_1 & M_2 & M_3 & \dots & M_{n+1} \\ M_2 & M_3 & M_4 & \dots & M_{n+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ M_n & M_{n+1} & M_{n+2} & \dots & M_{2n} \end{bmatrix}. \quad (3.7)$$

The necessary and sufficient condition for strict realizability is that the determinants of all such Hankel matrices, $\det(\mathbf{H}_n)$, remain strictly greater than zero for all $n \leq N$ [3].

Early moment inversion algorithms, such as the Product-Difference (PD) algorithm proposed by Gordon [26], relied explicitly on calculating these Hankel determinants to build the quadrature. However, as a continuous particle distribution approaches a monodisperse state (a single Dirac delta function), the higher-order moments become increasingly linearly dependent. Consequently, the Hankel matrices become severely ill-conditioned, and their determinants rapidly approach the machine precision limit, often evaluating to zero or negative values due to floating-point truncation [3]. Another significant issue arises from the fact that

when dealing with distributions that have a zero mean ($M_1 = 0$), the algorithm becomes unstable and fails [3].

This inherent numerical instabilities motivate the absolute necessity for alternative inversion techniques in CFD applications. This work utilizes the Wheeler algorithm specifically because it bypasses the direct computation of Hankel determinants, reconstructing the necessary orthogonal polynomial coefficients through a significantly more stable modified Chebyshev procedure and can handle problems with $M_1 = 0$ [3, 27].

3.3.2 Wheeler Algorithm

The core numerical task in QMOM is the moment inversion problem. Given the known moment set $\mathcal{M}_{2N}$, the objective is to determine the unique set of weights w_i and abscissas ξ_i satisfying:

$$M_k = \sum_{i=1}^N w_i \xi_i^k \quad \text{for } k = 0, \dots, 2N - 1. \quad (3.8)$$

This relationship is expressed compactly as a non-linear matrix equation:

$$\mathbf{V} \mathbf{R} \mathbf{1}_N = \mathbf{M}, \quad (3.9)$$

where $\mathbf{R} \in \mathbb{R}^{N \times N}$ is the diagonal matrix containing the weights w_i along its main diagonal. The matrix $\mathbf{V} \in \mathbb{R}^{2N \times N}$ represents the Vandermonde matrix constructed from the abscissas:

$$\mathbf{V} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \xi_1 & \xi_2 & \cdots & \xi_N \\ \xi_1^2 & \xi_2^2 & \cdots & \xi_N^2 \\ \vdots & \vdots & \ddots & \vdots \\ \xi_1^{2N-1} & \xi_2^{2N-1} & \cdots & \xi_N^{2N-1} \end{bmatrix}. \quad (3.10)$$

The term $\mathbf{1}_N \in \mathbb{R}^N$ denotes a column vector of ones, and $\mathbf{M} \in \mathbb{R}^{2N}$ is the column vector of the moments M_k .

This non-linear mapping from moment space to quadrature space relies on the theory of orthogonal polynomials [27]. For any realizable measure $n(\xi)$, there exists a sequence of polynomials $\{P_k(\xi)\}_{k=0}^\infty$ that are orthogonal with respect to the inner product $\langle P, Q \rangle = \int_\Omega n(\xi) P(\xi) Q(\xi) d\xi$. These polynomials satisfy a unique three-term recurrence relation:

$$P_{k+1}(\xi) = (\xi - a_k)P_k(\xi) - b_k P_{k-1}(\xi), \quad (3.11)$$

with initial conditions $P_{-1}(\xi) = 0$ and $P_0(\xi) = 1$. The quadrature nodes ξ_i correspond precisely to the roots of the N -th order orthogonal polynomial $P_N(\xi)$ [3, 27].

To compute the recurrence coefficients a_k and b_k directly from the moments, this work implements the Wheeler algorithm [27]. The procedure initializes a 2D array $\sigma_{k,l}$, referred to as the sigma table, strictly from the transported moments:

$$\sigma_{-1,l} = 0 \quad \text{for } l = 1, \dots, 2N - 2, \quad (3.12)$$

$$\sigma_{0,l} = M_l \quad \text{for } l = 0, \dots, 2N - 1, \quad (3.13)$$

with the initial recurrence coefficients defined as $a_0 = M_1/M_0$ and $b_0 = 0$. The Wheeler algorithm then iteratively updates the table using the algebraic relation:

$$\sigma_{k,l} = \sigma_{k-1,l+1} - a_{k-1}\sigma_{k-1,l} - b_{k-1}\sigma_{k-2,l}. \quad (3.14)$$

Following the table update, the subsequent recurrence coefficients are systematically extracted from the diagonal and sub-diagonal elements for $k = 1, \dots, N - 1$ and $l = k + 1, \dots, 2N - k - 1$:

$$a_k = \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \quad b_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \quad (3.15)$$

This construction remains numerically stable provided the input moments correspond to a strictly non-degenerate distribution.

Once the coefficients a_k and b_k are derived, they are assembled to form the symmetric tridiagonal Jacobi matrix J_N :

$$J_N = \begin{bmatrix} a_0 & \sqrt{b_1} & 0 & \dots \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & \dots \\ 0 & \sqrt{b_2} & a_2 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{bmatrix}. \quad (3.16)$$

The Golub-Welsch algorithm [3, 28] is then utilized to solve the associated eigenvalue problem, $J_N \mathbf{v}_i = \lambda_i \mathbf{v}_i$. The resulting eigenvalues λ_i correspond exactly to the quadrature nodes ξ_i . The corresponding weights are determined from the first component of the normalized eigenvectors, $v_{i,0}$, scaled by the zeroth moment:

$$w_i = M_0 \cdot (v_{i,0})^2. \quad (3.17)$$

This spectral decomposition mathematically ensures that the computed weights are strictly positive and the nodes are distinct, satisfying the fundamental realizability conditions of the

moment set [3].

3.3.3 Adaptive Implementation and Stability Preservation

A significant numerical challenge in solving the MTEs is the potential for matrix ill-conditioning. When the particle distribution becomes nearly monodisperse, higher-order moments become linearly dependent. This dependency leads to a singular sigma table and potential failure of the Wheeler algorithm [3]. To ensure robustness, this framework utilizes the adaptive Wheeler algorithm found in the work of Marchisio *et al.* (2013) [3] relying on three critical stability checks executed dynamically during runtime.

First, a basic realizability check is enforced prior to inversion by verifying that the zeroth moment remains strictly positive ($M_0 > 0$). If the moment set represents an unphysical state, the algorithm returns an error flag to prevent solver divergence. Second, a rank deficiency check is performed during the construction of the sigma table. The diagonal elements $\sigma_{k,k}$ are closely monitored; if an element falls below a predefined machine-precision cutoff (ϵ_{cutoff}), the matrix is deemed singular. This indicates that the distribution can be adequately represented by fewer than N nodes, prompting the algorithm to truncate the quadrature order to $N' < N$. Finally, post-solution conditioning ensures the physical validity of the extracted nodes. After computing the quadrature set, the quality of the solution is verified against user-defined tolerances for the weight ratio (r_{min}) and absolute node separation distance (e_{abs}). If these conditions are violated, indicating clustered nodes or vanishing weights, the algorithm iteratively reduces the number of nodes and re-solves the system.

Another critical requirement when updating the MTEs is the strict preservation of moment space realizability [3]. Standard Runge-Kutta schemes treat the transport of each moment independently. Because the moment space is bounded by strict, non-linear inequalities (e.g., $M_0 M_2 - M_1^2 \geq 0$), independent integration might introduce numerical dispersion (oscillations) that pushes the moment set outside the realizable space, causing the inversion algorithms to crash [29]. To mitigate this risk, the strong stability preserving third-order Runge-Kutta (SSP-RK3) time integration scheme is employed [3, 30, 31]. This time-stepping strategy, combined with the adaptive fallback mechanisms of the Wheeler algorithm, ensures a robust integration and $\mathcal{O}(\Delta t^3)$ accuracy of the coupled moment system [29].

The numerical implementation proceeds systematically through a closed-loop algorithmic workflow evaluated at each computational cell. This workflow operates via the sequence illustrated in Figure 3.2.

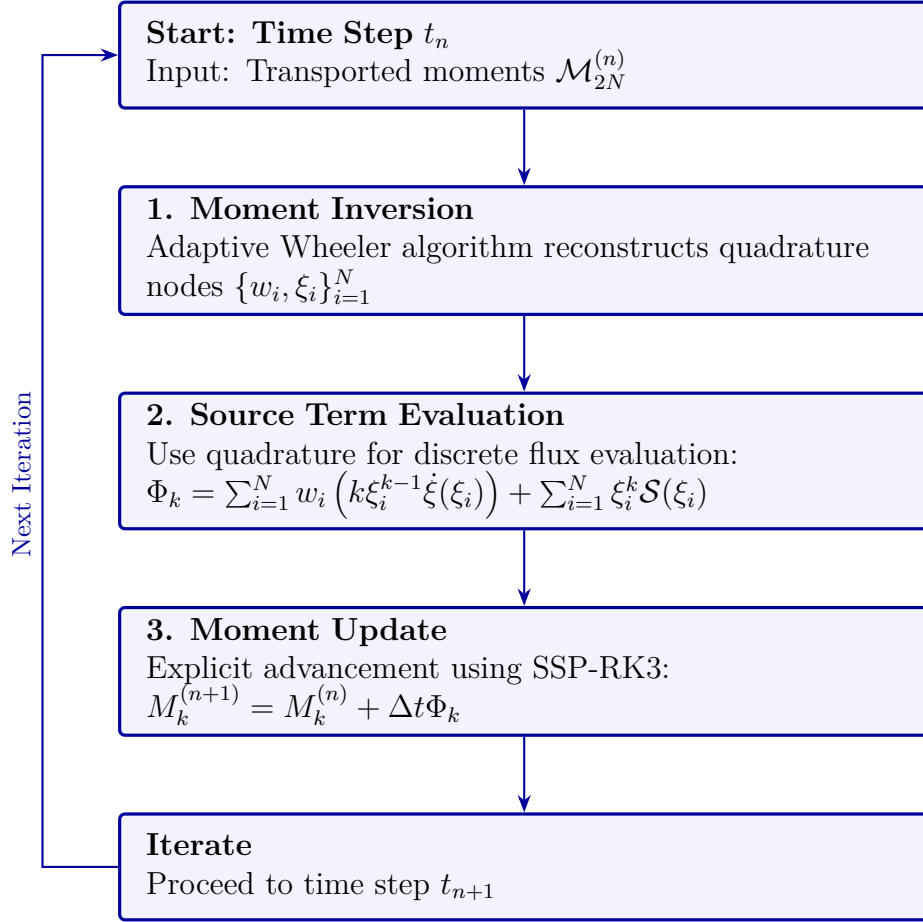


Figure 3.2 Algorithmic flow for the 1D QMOM

3.4 1D Verification Case: Non-Linear Growth

3.4.1 Problem Formulation and the Closure Requirement

To robustly verify the implementation of the 1D QMOM and the adaptive Wheeler inversion algorithm, a canonical test case involving the non-linear continuous growth of a particle population is simulated. This case isolates the internal phase-space advection from spatial complexities, allowing for a direct assessment of the quadrature closure accuracy across different quadrature orders ($N = 1, 2$, and 3).

The physical system is defined by a single internal coordinate ξ evolving according to the non-linear rate equation:

$$\frac{d\xi}{dt} = \xi - \frac{\xi^3}{9}. \quad (3.18)$$

To initialize the simulation, the initial Number Density Function (NDF) at $t = 0$ for a

population of 10,000 particles is prescribed as a Gaussian distribution centered at $\mu = 3.0$ with a covariance of $\sigma^2 = 0.7$. From this analytical distribution, the exact initial integer moments are calculated directly to initialize the moment vector.

Applying the moment operator to the governing PBE (3.18) yields the following MTE:

$$\frac{dM_k}{dt} = kM_k - \frac{k}{9}M_{k+2}. \quad (3.19)$$

This formulation explicitly reveals the closure problem discussed in Section 3.2: calculating the evolution of the k -th moment strictly requires the unclosed higher-order moment M_{k+2} . To close the system, the QMOM framework approximates the right-hand side utilizing the dynamically calculated quadrature nodes:

$$\frac{dM_k}{dt} \approx \sum_{i=1}^N w_i \left(k\xi_i^k - \frac{k}{9}\xi_i^{k+2} \right). \quad (3.20)$$

The simulations are integrated temporally using the SSP-RK3 scheme (see Section 3.3.3) over a duration of 3.0 seconds, and the results are compared against a high-fidelity benchmark generated via a MC method.

3.4.2 Geometric Adaptation of Quadrature Nodes

The ability of the QMOM framework to dynamically adapt to the underlying distribution is visually confirmed in Figure 3.3. The figure presents the temporal evolution of the continuous normalized MC distribution (gray histogram) alongside the discrete quadrature representations using $N = 1, 2, 3$ nodes at three distinct simulation times ($t = 0.0, 0.75$, and 1.5 s).

Initially at $t = 0.0$ s, the distribution follows the prescribed Gaussian shape. The single-node approximation ($N = 1$, purple marker) effectively captures only the mean of the distribution ($\xi \approx 3$). Expanding to $N = 2$ (teal markers) allows the quadrature to capture the variance, placing two symmetrical nodes on either side of the peak. The $N = 3$ approximation (yellow markers) achieves the highest geometric fidelity, allocating a central node with a dominant weight to capture the peak, and two lower-weight satellite nodes to approximate the curvature and tails. As the simulation progresses to $t = 1.5$ s, the non-linear growth dynamics cause the continuous distribution to narrow and become sharper. In response, the adaptive Wheeler algorithm dynamically shifts the quadrature nodes inward. The nodes cluster more tightly around the central peak, automatically concentrating the transported degrees of freedom directly into the regions of highest probability mass.

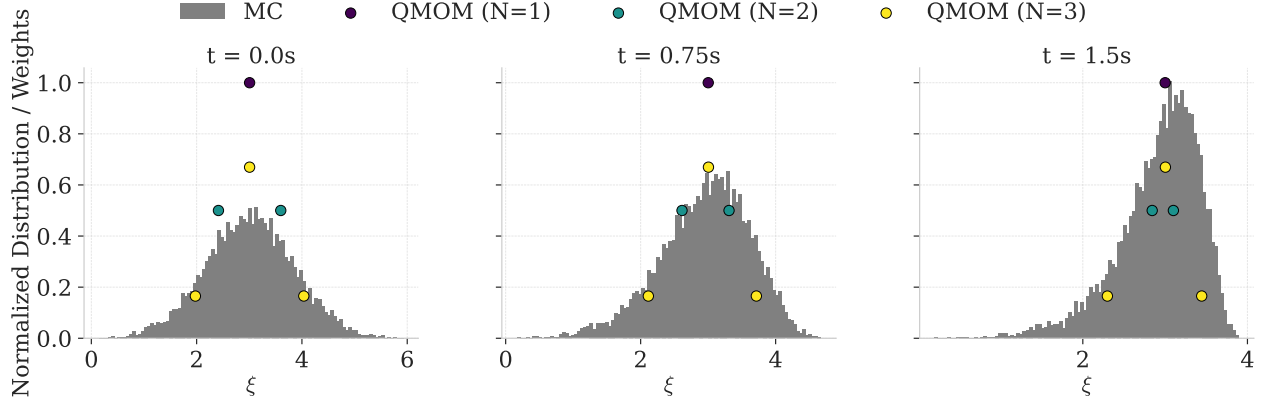


Figure 3.3 Evolution of the NDF and optimal node placement at $t = 0.0, 0.75$, and 1.5 s. The gray histogram represents the MC benchmark. The discrete markers represent the QMOM approximations for $N = 1$ (purple), $N = 2$ (teal), and $N = 3$ (yellow), illustrating how quadrature nodes follow the NDF

3.4.3 Moment Evolution and Closure Accuracy

The mathematical superiority of higher-order quadrature closures is quantified by examining the transient evolution of the statistical moments, presented in Figure 3.4. The figure compares the time history of the low-order moments (M_0, M_1, M_2) and the highly non-linear high-order moments (M_6, M_7, M_8) against the MC benchmark.

For all tested quadrature orders, the zeroth moment M_0 remains strictly constant at 1.0, confirming that the numerical scheme perfectly conserves the total probability mass. The low-order moments (M_1 and M_2) undergo a slight transient drop around $t \approx 0.5$ s before recovering toward their steady-state values. Both the $N = 2$ and $N = 3$ implementations track this behavior closely, whereas the $N = 1$ approximation deviates noticeably.

The critical impact of the closure problem becomes undeniable when observing the higher-order moments (M_6, M_7, M_8). These moments exhibit magnitudes of order $\mathcal{O}(10^3)$ to $\mathcal{O}(10^4)$ and experience a severe transient drop before exhibiting a slow recovery. The mono-disperse assumption ($N = 1$) completely fails to resolve these extreme non-linear dynamics, yielding flat predictions that fundamentally misrepresent the physical state. Incorporating the variance via $N = 2$ significantly improves the response, but it is the $N = 3$ approximation that demonstrates exceptional fidelity, nearly perfectly tracking the deep transient curve of the MC benchmark. This demonstrates that sufficient quadrature resolution is necessary to accurately extrapolate the unclosed source terms driven by higher-order phase space dependencies.

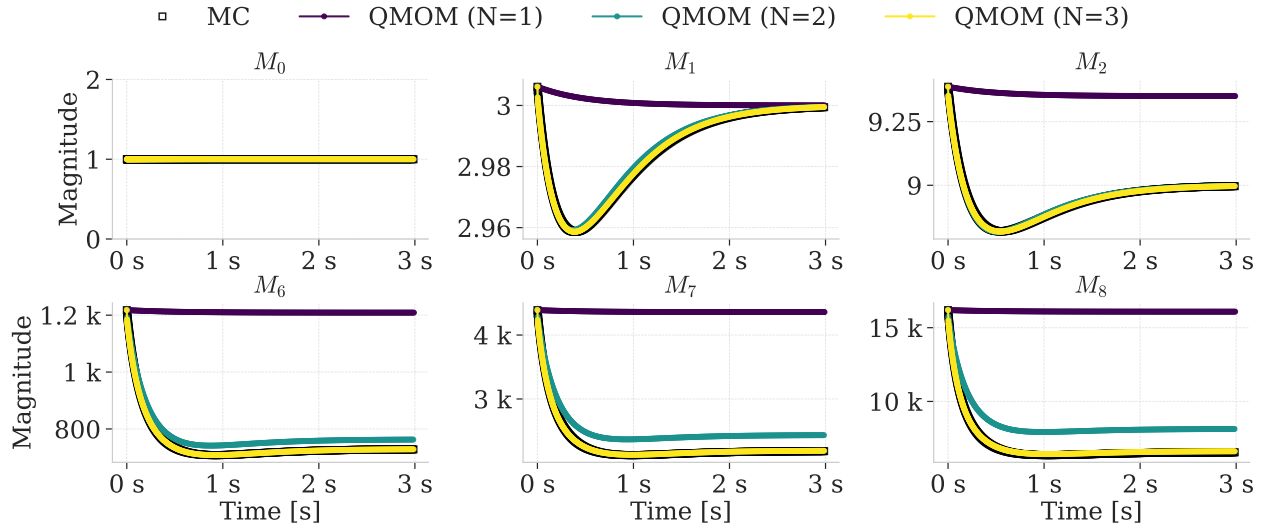


Figure 3.4 Temporal evolution of the statistical moments. The solid black squares denote the MC benchmark. The colored lines correspond to QMOM predictions of varying order. With $N = 1$ the Wheeler algorithm can only track the first moment M_1 with a maximum relative error of 1.3%. While $N = 2$ fails to capture the transient dynamics of the higher-order moments (M_6 - M_8), $N = 3$ demonstrates excellent agreement with the exact solution

CHAPTER 4 THE CONDITIONAL QUADRATURE METHOD OF MOMENTS

4.1 Introduction: The need for a multivariate approach

While the standard QMOM efficiently resolves the closure problem for one-dimensional phase spaces, extending it to multivariate distributions presents significant geometric and computational challenges. The most straightforward approach to discretizing a multidimensional NDF, $n(t; \mathbf{x}, \boldsymbol{\xi})$, is to apply the Wheeler algorithm independently along each coordinate axis to construct a tensor-product (TP) grid [3, 9]. For a 2D phase space (d, u) representing particle diameter and velocity, utilizing N nodes per dimension results in a rigid, rectilinear grid defined by the Cartesian product of the independent abscissas $(\xi_{d,i}, \xi_{u,j})$.

However, in dispersed multiphase flows, internal coordinates are almost never statistically independent; they are tightly coupled by macroscopic physical laws resulting in a joint NDF that is coupled (e.g. $n(t; d, u)$). For example, the Stokesian terminal settling velocity of a particle depends strictly on its squared diameter ($u_t \propto d^2$). Consequently, the actual probability density of the physical population does not fill the entire phase space. Instead, it effectively collapses onto a lower-dimensional manifold, forming a narrow, curved trajectory in the $d - u$ domain [3].

A TP quadrature forces nodes to populate the entire rectilinear grid. To adequately resolve a strongly correlated diagonal manifold, the TP method requires a highly dense grid [3, 9]. This forces the algorithm to place the vast majority of its quadrature nodes in completely empty regions of the phase space—such as the coordinates representing very large particles with near-zero velocities. This geometric mismatch leads many nodes to carry negligible or zero probability weight ($w_{i,j} \approx 0$). Transporting these zero-weight nodes wastes computational resources on empty phase space regions and rapidly induces catastrophic ill-conditioning in the moment inversion algorithm [3].

To overcome the inefficiency and instability of the TP grid, a multivariate quadrature scheme must adaptively track the geometric support of the NDF rather than imposing a rigid Cartesian structure upon it. A physically faithful representation requires that the velocity quadrature nodes be free to migrate off the Cartesian axes and align themselves directly with the non-linear correlation curves dictated by the physics.

Instead of solving for a global, independent set of velocity nodes that applies equally to all particle sizes, the problem requires a hierarchical, leader-follower arrangement between

the coordinates. In this arrangement, the primary variable (e.g., size) is discretized first, and the secondary variable (e.g., velocity) is discretized locally, with its placement explicitly dependent on the specific value of the primary node. By making the velocity abscissa a mathematical function of the diameter (i.e. considering the marginal NDF $n(t; u|d)$), the computational nodes naturally populate only the lower-dimensional manifold where the actual physical states exist. This eliminates unnecessary static weightless nodes entirely. Every transported node represents a realizable physical state, ensuring that computational resources are strictly dedicated to regions of non-zero probability. This intuitive physical requirement for hierarchical coordinate dependence forms the fundamental motivation for the mathematical formulation of conditional probability utilized in the CQMOM.

4.2 Mathematical Formulation of Conditional Quadrature Method of Moments

To mathematically realize the adaptive manifold tracking described above, CQMOM abandons the assumption of statistical independence. Instead, it exploits the exact factorization of the multivariate NDF into a product of a marginal distribution and a sequence of conditional distributions [3, 4].

For a bivariate phase space characterized by variables ξ_1 and ξ_2 , the joint number density function $n(t; \xi_1, \xi_2)$ can be expressed as:

$$n(\xi_1, \xi_2) = n(\xi_1) n(\xi_2|\xi_1). \quad (4.1)$$

In this formulation, $n(\xi_1)$ represents the marginal distribution of the first internal coordinate, integrated over all possible states of the second coordinate. The term $n(\xi_2|\xi_1)$ represents the conditional distribution of the second coordinate, given that the first coordinate is exactly fixed at a specific value ξ_1 .

Following this continuous factorization, CQMOM applies a discrete quadrature approximation to each probability distribution sequentially. For a bivariate system comprising internal coordinates ξ_1 and ξ_2 , the marginal distribution of the primary variable is first approximated utilizing N_1 nodes:

$$n(\xi_1) \approx \sum_{i=1}^{N_1} w_i \delta(\xi_1 - \xi_{1,i}). \quad (4.2)$$

Subsequently, for each discrete realization of the primary variable $(\xi_{1,i})$, the conditional

distribution of the secondary variable is approximated utilizing N_2 nodes:

$$n(\xi_2|\xi_{1,i}) \approx \sum_{j=1}^{N_2} w_{i,j} \delta(\xi_2 - \xi_{2,i,j}). \quad (4.3)$$

Multiplying these two discrete expressions yields the full bivariate CQMOM approximation of the joint NDF:

$$n(\xi_1, \xi_2) \approx \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} w_i w_{i,j} \delta(\xi_1 - \xi_{1,i}) \delta(\xi_2 - \xi_{2,i,j}). \quad (4.4)$$

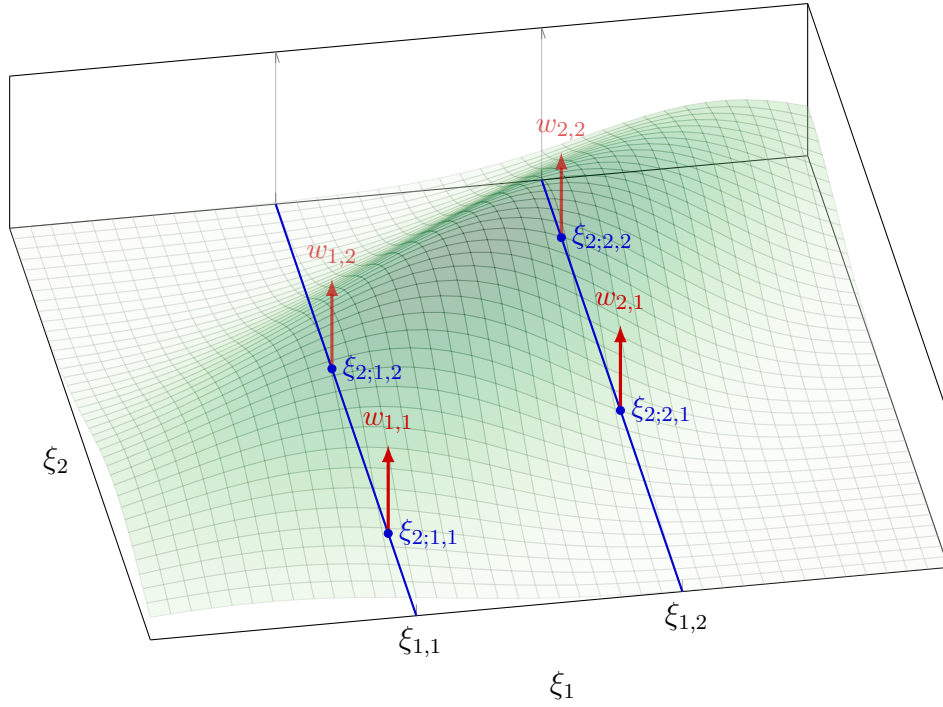


Figure 4.1 Conceptual 3D representation of the bivariate CQMOM ($N_1 = 2$, $N_2 = 2$). The translucent surface represents a highly correlated continuous NDF. Instead of forming a square grid, the secondary nodes ($\xi_{2,i,j}$) slide along the primary nodes ($\xi_{1,i}$) to perfectly align with the underlying probability manifold

This mathematical structure explicitly enforces the geometric dependence required to track strongly correlated physical manifolds. The secondary abscissas, $\xi_{2,i,j}$, and their corresponding conditional weights, $w_{i,j}$, carry an index i , strictly dictating that their values are uniquely determined for, and dependent upon, each specific primary node $\xi_{1,i}$ as illustrated in Figure 4.1.

To determine these hierarchical weights and abscissas, the algorithm requires a predefined set of mixed integer moments. The mixed moment of order k with respect to ξ_1 and order l

with respect to ξ_2 is defined as:

$$M_{k,l} = \int_{\Omega} \xi_1^k \xi_2^l n(\xi_1, \xi_2) d\xi_1 d\xi_2. \quad (4.5)$$

Substituting the discrete approximation (Equation 4.4) into this exact integral definition yields the fundamental non-linear CQMOM moment constraint:

$$M_{k,l} = \sum_{i=1}^{N_1} w_i \xi_{1,i}^k \left(\sum_{j=1}^{N_2} w_{i,j} \xi_{2;i,j}^l \right). \quad (4.6)$$

The numerical inversion process required to solve this coupled system proceeds in three sequential stages. To illustrate, the complete algorithmic workflow for the bivariate CQMOM inversion is visually summarized in Figure 4.2. First, the marginal moments of the primary variable are extracted by setting $l = 0$, yielding $M_{k,0}$. Because these moments depend exclusively on the primary variable ξ_1 , this subset of $2N_1$ moments is passed directly to the standard Wheeler algorithm (see Section 3.3.2) to compute the primary weights w_i and primary abscissas $\xi_{1,i}$ [3, 4].

Second, to isolate the parameters for the secondary variable, the inner summation of Equation(4.6) is mathematically isolated. This inner term physically represents the conditional moments of the secondary variable at each fixed primary node i , defined as:

$$M_{i,l}^{(2)} = \sum_{j=1}^{N_2} w_{i,j} \xi_{2;i,j}^l. \quad (4.7)$$

Substituting this definition back into the main constraint forms a linear system of equations linking the known mixed moments to the unknown conditional moments:

$$M_{k,l} = \sum_{i=1}^{N_1} \left(w_i \xi_{1,i}^k \right) M_{i,l}^{(2)}. \quad (4.8)$$

For a fixed secondary moment order l , this system is cast as a matrix equation where the coefficient matrix is a Vandermonde matrix constructed from the previously computed primary abscissas $\xi_{1,i}$, scaled row-by-row by their respective primary weights w_i . Because the primary abscissas are strictly distinct—a fundamental property of the orthogonal polynomials established previously—this Vandermonde matrix is non-singular [3, 4]. Consequently, it can be inverted numerically to solve for the unknown conditional moments $M_{i,l}^{(2)}$ for all primary nodes i [3, 4].

Finally, once the set of $2N_2$ conditional moments is obtained for a given primary node i , they

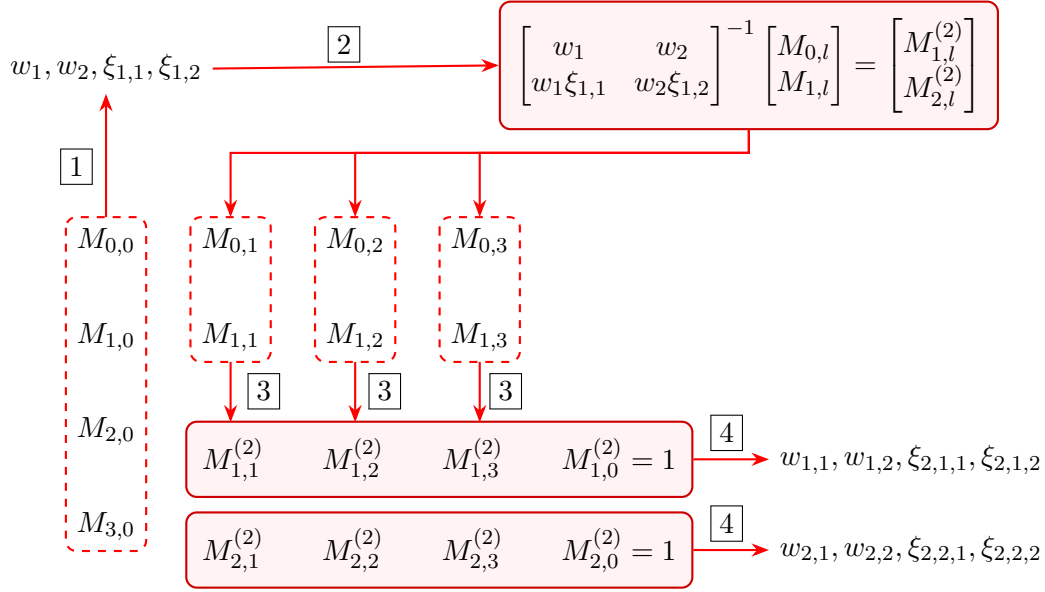


Figure 4.2 Algorithmic workflow of the bivariate CQMOM inversion ($N_1 = 2, N_2 = 2$). [1] The marginal moments of the primary variable ($M_{k,0}$) are inverted via the Wheeler algorithm. [2] The modified Vandermonde matrix is constructed from the primary nodes and weights. [3] The linear systems are solved column-by-column to yield the sets of conditional moments $M_{i,l}^{(2)}$. [4] These conditional moments are inverted via independent Wheeler algorithms to yield the secondary nodes and weights. The diagram is inspired by Li *et al.* [1]

are passed as an independent moment vector into the Wheeler algorithm. This terminal step computes the secondary conditional weights $w_{i,j}$ and abscissas $\xi_{2,i,j}$. This 1D inversion is repeated for every primary node $i = 1, \dots, N_1$, completely defining the bivariate quadrature using $2N_1 + 2N_1N_2$ moments without requiring multi-dimensional optimization solvers [3].

This bivariate framework naturally extends to higher dimensions through the recursive conditioning of later coordinates on prior ones [3]. For an arbitrary D -dimensional phase space, the joint continuous distribution is mathematically factorized as a chain of conditional probabilities: $n(\xi_1, \dots, \xi_D) = n(\xi_1)n(\xi_2|\xi_1) \dots n(\xi_D|\xi_1, \dots, \xi_{D-1})$.

The numerical inversion mirrors this continuous chain rule by recursively constructing linear Vandermonde systems at each hierarchical level. Once the conditional nodes and weights for the m -th variable are computed via the Wheeler algorithm, they immediately populate the coefficient matrix required to isolate the conditional moments of the $(m+1)$ -th variable. The complete sequence of these algorithmic steps, from the primary marginal inversion through the discrete source term evaluation, is visualized in Figure 4.3. For a general quadrature formulation assigning an order N_m to the m -th internal coordinate, this hierarchical chain perfectly closes the system using exactly $\sum_{k=1}^D \left(2 \prod_{m=1}^k N_m \right)$ transported mixed moments [3].

In the context of this work, the full 5-dimensional phase space is inverted by strictly following the physical hierarchy of the dispersed phase: particle size (d), aspect ratio (χ), and the three spatial velocity components (u_p, v_p, w_p). The ordering of these variables is not arbitrary, but physically motivated. The fundamental geometric properties (d and χ) dictate the aerodynamic response times and drag coefficients, which in turn directly govern the conditional velocity distributions [20]. By recursively chaining these Vandermonde inversions, the complete 5D CQMOM rule is systematically constructed. For a uniform quadrature order of $N = 2$ across all dimensions, this hierarchical chain perfectly closes the system using the 124 transported mixed moments, entirely circumventing the exponential scaling of computational cost with dimensionality while strictly preserving the underlying physical correlations.

4.3 2D Verification Case: Harmonic Oscillator

4.3.1 Problem Formulation and Correlated Dynamics

To verify the multivariate CQMOM implementation and its ability to track highly correlated distributions, a 2D phase-space harmonic oscillator benchmark is simulated. This canonical test case isolates the advection of the internal coordinates, providing a stringent evaluation of the conditional quadrature’s geometric adaptability and moment-preservation capabilities. The physical system is defined over a bivariate phase space (ξ_1, ξ_2) , evolving according to the coupled, linear differential equations:

$$\frac{d\xi_1}{dt} = \xi_2, \quad \frac{d\xi_2}{dt} = -\xi_1. \quad (4.9)$$

To evaluate the handling of coupled variables, the initial NDF is prescribed as a bivariate Gaussian distribution centered at $\boldsymbol{\mu}(\xi_1, \xi_2)_{t=0} = [0, 1]^\top$ with $\mathbf{cov}(\xi_1, \xi_2)_{t=0} = 0.01 \mathbf{I}$. In this configuration, the harmonic oscillator ODE induces a rigid-body rotation of the NDF around the phase space origin. Analytically, the initial covariance matrix is strictly diagonal and isotropic, meaning the continuous distribution forms a perfectly symmetric circle with a constant conditional variance. However, within the discrete numerical simulation, statistical sampling artifacts introduce microscopic artificial cross-correlations. As the discrete moment set evolves, the inherently ill-conditioned Vandermonde matrices within the higher-order ($N = 3$) CQMOM inversion amplify this numerical noise, causing the computed conditional variance to artificially fluctuate and compress. This intentionally provides a stringent stress test for the algorithm’s adaptive realizability safeguards.

4.3.2 Adaptive Order Reduction and Realizability

A fundamental numerical challenge in multi-dimensional moment methods is the preservation of realizability when the conditional variance of the distribution becomes negligible. If the conditional distribution becomes excessively narrow, attempting to invert a high-order quadrature rule leads to an ill-conditioned Vandermonde matrix, generating spurious nodes with near-zero weights and eventually causing numerical instability.

To counteract this, the adaptive Wheeler algorithm present at each stage of the CQMOM procedure (see Section 4.2) implements a dynamic order-reduction mechanism governed by a strict tolerance ($r_{\min} \leq \min_{i,j \in \{1, \dots, N\}} (w_i/w_j)$) that we set equal to 10^{-3} in this simulation. During the sequential inversion process, if the extracted conditional variance drops below $r_{\min}$, the algorithm automatically truncates the local quadrature order to prevent singularity.

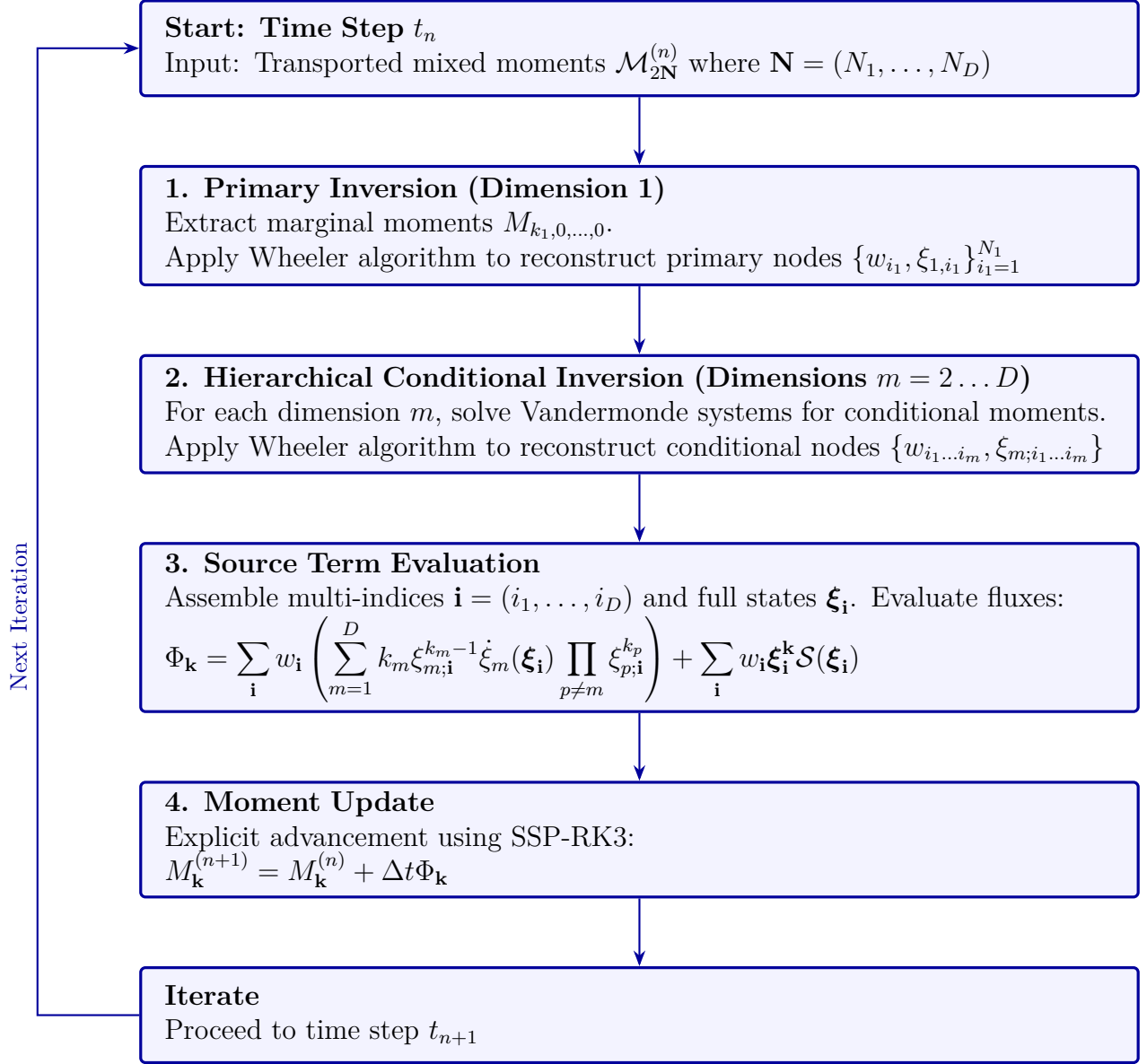
The success of this adaptive scheme is visually confirmed in Figure 4.4. Initially, the $N = 3$ formulation perfectly allocates $3 \times 3 = 9$ nodes to capture the skewed geometry of the initial NDF. As the distribution rotates and the conditional spread along the primary axis narrows, the algorithm intelligently sheds redundant degrees of freedom, gracefully reducing the active node count from 9 to 6. This confirms that the hierarchical tracking mechanism dedicates computational resources exclusively to regions of non-zero probability mass.

4.3.3 High-Order Moment Evolution

The mathematical fidelity of the dynamic closure is quantified by comparing the temporal evolution of the mixed moments against a high-fidelity MC benchmark. The simulations evaluate the performance of the mono-disperse assumption ($N = 1$) against higher-order conditional closures ($N = 2$ and $N = 3$).

As illustrated in Figure 4.5, all quadrature orders successfully conserve the total mass ($M_{0,0}$) and accurately track the mixed moments ($M_{1,1}$ and $M_{2,2}$). However, the necessity of the higher-order multivariate closure becomes explicitly clear when observing higher order moments. Because the $N = 1$ approximation essentially assumes a mono-disperse state, it completely fails to capture the shifting cross-correlations as the distribution rotates through phase space, heavily damping the magnitude of the higher-order moments.

Most notably, the robust tracking of extreme high-order moments, such as $M_{8,8}$ and $M_{9,9}$, underscores the stability of the $r_{\min}$ regularizer. Despite the massive magnitudes and rapid oscillatory gradients of these moments, the adaptive $N = 3$ CQMOM framework seamlessly reproduces the MC benchmark without inducing numerical instability, effectively validating the solver for coupling with complex aerodynamic source terms.

Figure 4.3 Algorithmic flow for the D -Dimensional CQMOM

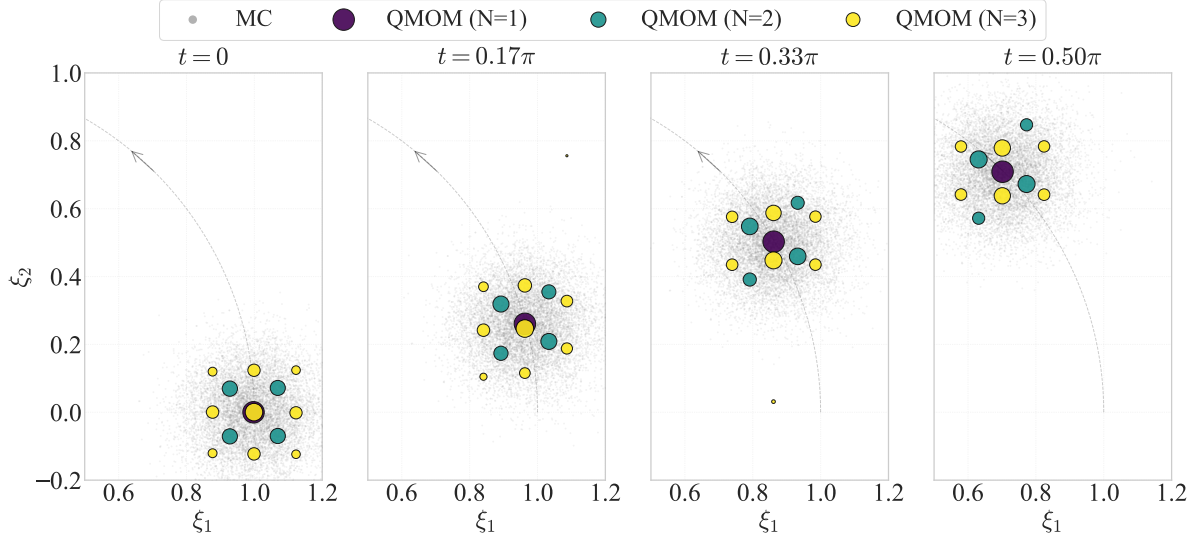


Figure 4.4 Phase space trajectory of the dispersed nodes tracking the rotating multi-variate Gaussian distribution. The adaptive CQMOM algorithm dynamically reduces the active number of nodes (from 9 down to 6) when the conditional variance drops below the $r_{\min}$ threshold, preserving numerical stability

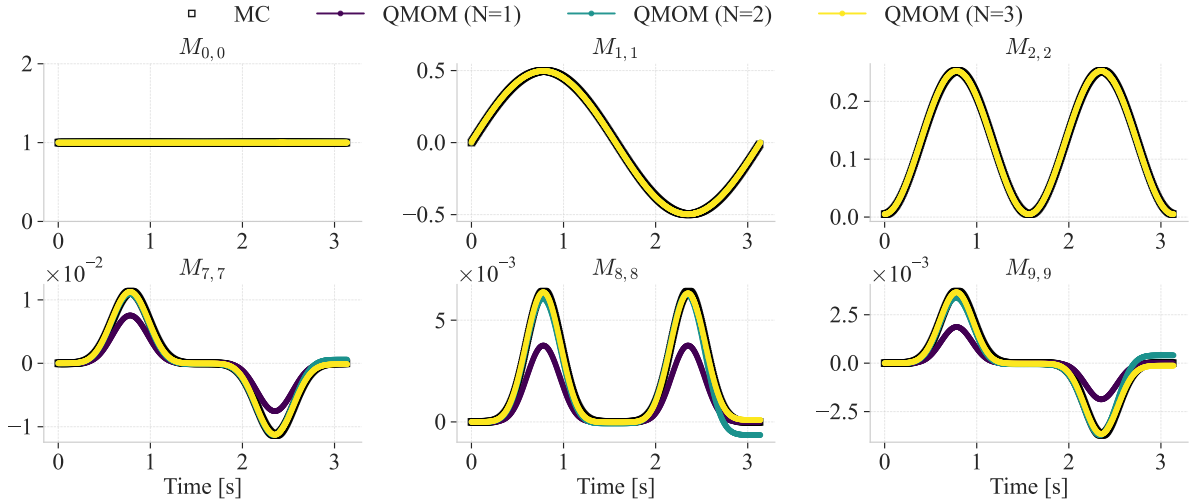


Figure 4.5 Temporal evolution of selected mixed moments ($M_{0,0}$ through $M_{9,9}$) over a half-period ($t \leq \pi$). The adaptive $N = 3$ CQMOM closure (yellow markers) perfectly tracks the oscillatory dynamics of the extreme high-order moments, whereas the lower-order closures suffer from severe truncation errors

CHAPTER 5 MATHEMATICAL MODELING AND TIME-SCALE ANALYSIS OF OBLATE SPHEROID POPULATIONS

5.1 Introduction

In the preceding chapters, the CQMOM was established as a mathematically robust, realizable framework for tracking the evolution of multidimensional NDFs. However, the accuracy of any Eulerian moment method [3, 32]—where the particle population is represented as a continuous distribution field rather than tracked individually— is fundamentally dictated by the physical fidelity of the underlying phase-space source terms. While the classical assumption of spherical particles greatly simplifies these source terms by reducing the internal phase space to a single size parameter, it introduces severe physical discrepancies in many industrial and environmental multiphase flows.

In reality, dispersed populations—such as liquid droplets undergoing aerodynamic deformation or engineered industrial powders—frequently have non-spherical geometries. Among these, oblate spheroids represent a canonical geometry of critical importance. The departure from sphericity alters the aerodynamic coupling between the dispersed and continuous phases. The drag coefficient (C_D) becomes strictly dependent on both the particle’s orientation and its aspect ratio (χ), while asymmetric pressure distributions generate hydrodynamic torques that induce complex rotational dynamics.

To accurately close the macroscopic MTE (1.3), these microscopic forces must be rigorously defined. This chapter details the mathematical modeling of the physical forces acting upon a population of oblate spheroids. Furthermore, a time-scale analysis is conducted to compare the characteristic relaxation times of translational acceleration and rotational response. By quantifying the disparity between these hydrodynamic timescales, we demonstrate that the rotational degrees of freedom relax faster than the translational ones. This physical separation of scales justifies a dimension reduction of the phase space: rather than tracking the full orientational state, the particle’s alignment can be treated as a quasi-steady function of the local velocity. Consequently, the system is reduced to a 5-dimensional manifold (d, χ, u_p, v_p, w_p) , which serves as the sufficient state space for the subsequent CQMOM implementation.

5.2 Kinematics and the Quasi-Steady Orientation Hypothesis

To accurately model the dispersed phase, we consider a dilute suspension of solid, oblate spheroidal particles immersed in a continuous Newtonian fluid characterized by a uniform density ρ_f , dynamic viscosity μ_f , and a macroscopic velocity field $\mathbf{u}_f$. The assumption of a macroscopic dilute regime is a fundamental prerequisite for the hydrodynamic modeling in this work. In a dilute suspension, the mean inter-particle distance is sufficiently large that complex multi-body hydrodynamic interactions—such as wake-drafting, lubrication forces, and localized shear-layer modifications—can be safely neglected [33]. Consequently, each dispersed spheroid is treated as hydrodynamically isolated. This physical isolation is strictly required to mathematically justify the use of single-particle empirical closures, specifically the aerodynamic drag correlations of Ouchene [25] and the rotational friction model of Perrin [34], which are derived exclusively for solitary particles in an undisturbed free-stream flow.

Instead of treating the particles as point masses, their shape is represented as oblate spheroids. Each particle is defined by an equatorial semi-axis a and a polar semi-axis b , where $a > b$ as illustrated in Figure 5.1. The flattening is quantified by the aspect ratio $\chi = b/a \leq 1$. To interface these geometric parameters with standard aerodynamic correlations, the particle size is expressed via its volume-equivalent diameter $d = \sqrt[3]{8a^2b}$.

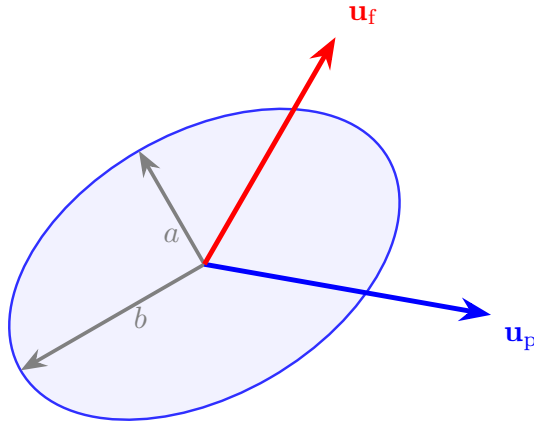


Figure 5.1 Geometric representation of an oblate spheroid

The kinematic state of the particle is defined by its translational velocity vector $\mathbf{u}_p$ and its angular velocity $\boldsymbol{\omega}$. Consequently, the relative slip velocity between the particle and the

continuous phase is given by $\mathbf{u}_{\text{rel}} = \mathbf{u}_f - \mathbf{u}_p$, yielding a particle Reynolds number of:

$$\text{Re} = \frac{\rho_f \|\mathbf{u}_{\text{rel}}\| d}{\mu_f}. \quad (5.1)$$

A full description of an ellipsoid's rotational kinematics in a 3D flow field requires tracking three Euler angles (θ, φ, ψ) and three angular velocity components $(\dot{\theta}, \dot{\varphi}, \dot{\psi})$ [3]. However, for microscopic particles advecting in moderate flows or creeping flows, we hypothesize that the rotational relaxation time—driven by viscous fluid damping—is significantly smaller than the macroscopic transport time scales. This proposed mechanism, which we denote the quasi-steady orientation (QSO) assumption, implies that the particle rapidly aligns its broadside area perpendicular to the relative slip velocity vector $\mathbf{u}_{\text{rel}}$ [25].

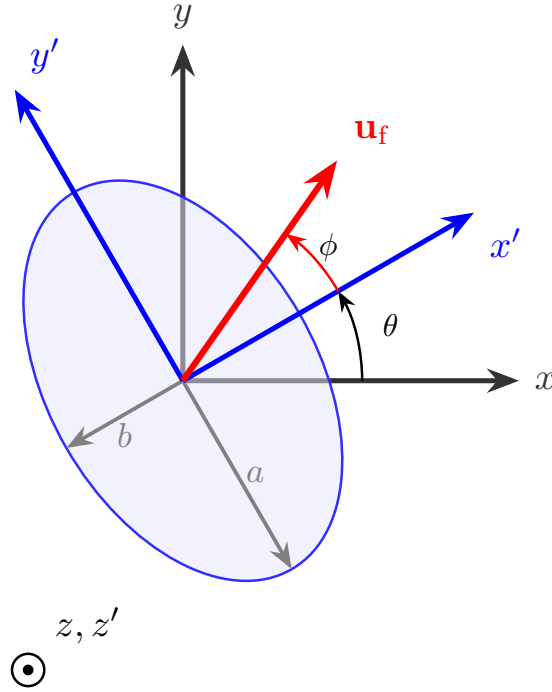


Figure 5.2 Fluid velocity in the reference frame (x, y, z) and the particle frame (x', y', z') . The angle of incidence ϕ is the angle between the fluid velocity vector $\mathbf{u}_f$ and the equatorial plane. θ is the absolute angle between the equatorial plane and the horizontal plane

To mathematically frame and ultimately verify this hypothesis, we restrict the rotational analysis to a two-dimensional planar projection, where the particle orientation is defined by a single in-plane angle θ , and its angular velocity reduces to a scalar $\omega = \dot{\theta}$. The instantaneous angle of incidence ϕ is subsequently defined as the angle between the relative velocity vector

and the particle's equatorial plane, as illustrated in Figure 5.2.

5.3 General Hydrodynamic Drag and Torque Models

Before the QSO dimensionality reduction can be applied, the fully coupled translational and rotational dynamics must be explicitly defined. The translational motion of a dispersed particle is governed by Newton's second law, balancing the particle's inertia with the aerodynamic forces and gravity:

$$\rho_p V_p \frac{d\mathbf{u}_p}{dt} = \mathbf{F}_D + \mathbf{F}_L + \mathbf{F}_g, \quad (5.2)$$

where $V_p = \frac{\pi}{6}d^3$ is the particle volume, $\mathbf{F}_g = \rho_p V_p \mathbf{g}$ is the gravitational force, $\mathbf{F}_D$ is the hydrodynamic drag, and $\mathbf{F}_L$ is the orientation-induced lift force.

Using the semi-empirical correlations developed by Ouchene [25], these forces depend explicitly on the angle of incidence ϕ and are modeled as:

$$\mathbf{F}_D = \frac{1}{2} \rho_f A_p C_D(\phi, \text{Re}, \chi) \|\mathbf{u}_{\text{rel}}\| \mathbf{u}_{\text{rel}}, \quad (5.3)$$

$$\mathbf{F}_L = \frac{1}{2} \rho_f A_p C_L(\phi, \text{Re}, \chi) \|\mathbf{u}_{\text{rel}}\| (\mathbf{u}_{\text{rel}} \times \mathbf{e}_z), \quad (5.4)$$

where $A_p = \pi d^2/4$ is the reference area of the particle and $\mathbf{e}_z$ is unit vector defining the axis of rotation (pointing toward the viewer in Figure 5.2). The drag coefficient interpolates smoothly between its two limiting values, $C_{D,0}$ and $C_{D,90}$, corresponding respectively to flow aligned with and perpendicular to the particle symmetry axis [25]:

$$C_D(\phi, \text{Re}, \chi) = C_{D,0} + (C_{D,90} - C_{D,0}) \sin^2 \phi, \quad (5.5)$$

$$C_L(\phi, \text{Re}, \chi) = \left(C_{D,0} - C_{D,90} + 2 \frac{(1/\chi - 1)^{0.542}}{(1 + \chi)^{7.85}} \text{Re}^{0.1516} \right) \sin \phi \cos \phi. \quad (5.6)$$

The empirically-fitted limits are given by [25]:

$$C_{D,0}(\text{Re}, \chi) = \frac{24}{\text{Re}} \left(K_0 + 0.15 \chi^{95.91} \text{Re}^{0.687} + 0.2927(1 - \chi)^{0.4374} \text{Re}^{0.7512} \right), \quad (5.7)$$

$$C_{D,90}(\text{Re}, \chi) = \frac{24}{\text{Re}} \left(K_{90} + 0.15 \chi^{100.7} \text{Re}^{0.687} + 0.1411(1 - \chi)^{24.75} \text{Re}^{0.7143} \right), \quad (5.8)$$

where K_0 and K_{90} are purely geometric shape factors dependent on the aspect ratio [25]:

$$K_0 = \frac{8}{3}\chi^{-\frac{1}{3}} \left[\frac{2\chi}{1-\chi^2} + \frac{2(1-2\chi^2)}{(1-\chi^2)^{\frac{3}{2}}} \tan^{-1} \left(\frac{\sqrt{1-\chi^2}}{\chi} \right) \right]^{-1}, \quad (5.9)$$

$$K_{90} = \frac{8}{3}\chi^{-\frac{1}{3}} \left[\frac{-\chi}{1-\chi^2} - \frac{2\chi^2-3}{(1-\chi^2)^{\frac{3}{2}}} \sin^{-1}(\sqrt{1-\chi^2}) \right]^{-1}. \quad (5.10)$$

Simultaneously, the hydrodynamic torque governing the rotational acceleration of the spheroid is modeled as the sum of a flow-induced restoring torque and a viscous frictional damping term [25]:

$$I \frac{d\omega}{dt} = \tau(\phi, \text{Re}, \chi) = -C_T(\phi, \text{Re}, \chi) \rho_f \|\mathbf{u}_{\text{rel}}\|^2 \frac{\pi d^3}{8} - C_R \omega, \quad (5.11)$$

where $I = \frac{1}{20} \rho_p V_p d^2 (\chi^{-2/3} + \chi^{4/3})$ is the moment of inertia. The empirical torque coefficient C_T drives the particle toward its stable broadside alignment and is given by:

$$C_T(\phi, \text{Re}, \chi) = 1.85 \left(\frac{1}{\chi} - 1 \right)^{0.832} \text{Re}^{-0.146} \sin \phi \cos \phi. \quad (5.12)$$

The second term in Equation 5.11 represents the rotational friction. Because robust empirical algebraic closures for oblate spheroids at high rotational Reynolds numbers do not exist, the rotational friction coefficient C_R is evaluated using the exact analytical framework established by Perrin [34, 35]. It is imperative to note that Perrin's formulation is strictly derived for the creeping flow (Stokes) regime ($\text{Re} \ll 1$) and is given by [34, 35]:

$$C_R = \pi \mu_f d^3 F_{\text{eq}}(\chi), \quad (5.13)$$

where $F_{\text{eq}}(\chi)$ is the shape correction factor for rotation about the equatorial axis [34, 35]:

$$F_{\text{eq}}(\chi) = \frac{4}{3} \frac{\frac{1}{\chi^2} - \chi^2}{2 - S(\chi) \left(2 - \frac{1}{\chi^2} \right)}, \quad (5.14)$$

with the auxiliary function $S(\chi)$ defined as [34, 35]:

$$S(\chi) = \begin{cases} 2, & \chi \approx 1, \\ 2^{\frac{\arctan(\xi)}{\xi}}, & \text{otherwise,} \end{cases} \quad \xi = \frac{\sqrt{1-\chi^2}}{\chi}. \quad (5.15)$$

5.4 Time-Scale Analysis and Numerical Verification

To numerically justify the QSO assumption—and thus allow the removal of the rotational degrees of freedom from the macroscopic CFD solver—it is necessary to quantify and compare the translational (τ_t) and rotational (τ_r) relaxation times across the parameter space. We define τ_t as the time required for the particle to reach 99% of the background fluid velocity. To ensure physical consistency, an equivalent 1% relative tolerance is applied to τ_r , measured against the maximum theoretical angular displacement a particle can undergo before reaching a stable broadside equilibrium ($\Delta\theta_{max} = \pi/2$).

Using Equation(5.6) and assuming a quiescent vertical flow field with no gravity to isolate aerodynamic relaxation, the equations of motion are given by:

$$\frac{d}{dt} \begin{pmatrix} \omega \\ \theta \\ u_p \\ v_p \end{pmatrix} = \begin{pmatrix} \tau(\phi, \text{Re}, \chi)/I \\ \omega \\ (F_{D,x} + F_{L,x})/m \\ (F_{D,y} + F_{L,y})/m \end{pmatrix}, \quad (5.16)$$

where $m = \rho_p V_p$ is the particle mass. The simulated particle has a volume-equivalent diameter $d = 150 \mu\text{m}$, density $\rho_p = 2000 \text{ kg/m}^3$, and an aspect ratio varied between 0 and 1. The fluid properties are $\rho_f = 1.225 \text{ kg/m}^3$ and $\mu_f = 1.48 \times 10^{-5} \text{ Pa}\cdot\text{s}$. The horizontal background fluid velocity is evaluated at $u_f \in \{0.01, 0.1\} \text{ m/s}$, corresponding to translational Reynolds numbers of $\text{Re} = 0.12$ and $\text{Re} = 1.24$.

Figures 5.3 and 5.4 illustrate the resulting phase space of relaxation times for 18,000 distinct simulation cases, varying both χ and θ_0 . The data reveals that the entire phase-space manifold is strictly confined below the line of equality ($\tau_t = \tau_r$). For every geometry and initial condition tested, the rotational relaxation time is consistently shorter than the translational relaxation time. Highly oblate particles ($\chi \rightarrow 0$) generate severe asymmetric drag and immense restoring torques, snapping to broadside alignment rapidly. As the particle approaches a spherical geometry ($\chi \rightarrow 1$), the restoring torque diminishes, stretching the relaxation times.

As stated previously, the Perrin rotational friction coefficient (C_R) is analytically derived for strict creeping flow [34, 35]. As the translational Reynolds number enters the transitional regime ($\text{Re} \approx 1.24$), convective inertia alters the boundary layer, technically invalidating the strict assumption of decoupled linear Stokes drag. However, this approximation acts as a mathematically conservative bound for our hypothesis. The onset of translational inertia

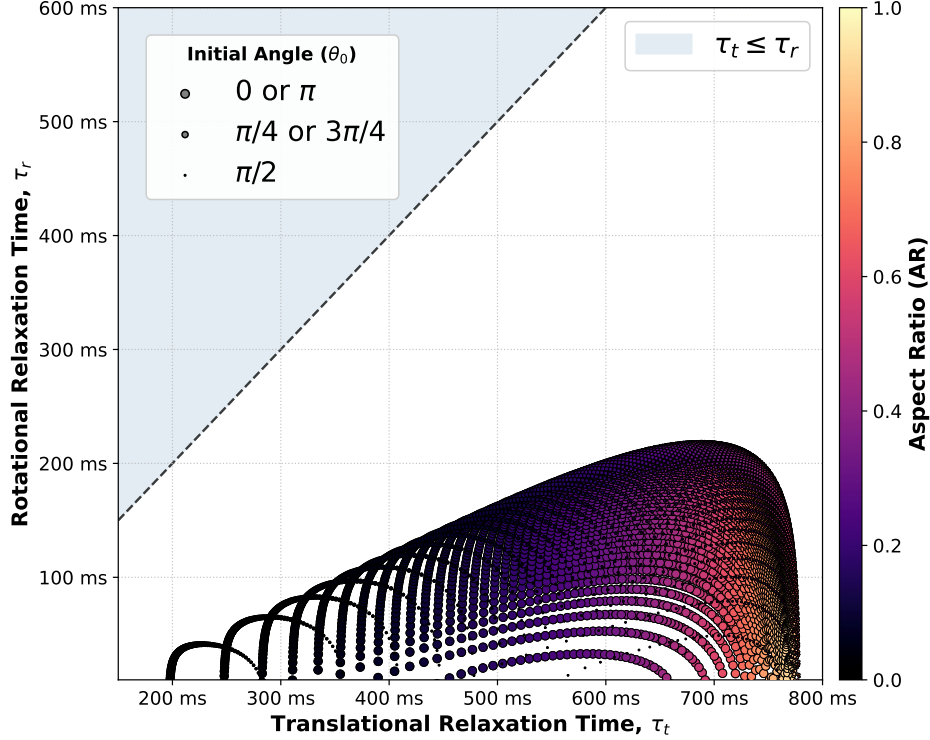


Figure 5.3 Comparison of translational (τ_t) and rotational (τ_r) relaxation times for oblate spheroids with $Re = 0.12$. The shaded region denotes the regime where rotation is relaxed slower than translation. All simulated data points lie strictly below the line of equality, confirming $\tau_t > \tau_r$.

and wake formation inevitably *increases* the true rotational damping experienced by the particle compared to the linear Stokes prediction. Since increased rotational friction would only serve to arrest the particle's rotation more rapidly, the true rotational relaxation time will be strictly less than the theoretical values computed here. Therefore, demonstrating that $\tau_r \leq \tau_t$ holds under the under-damped Perrin assumption mathematically guarantees that the QSO assumption remains robust in the physical inertial regime.

5.5 Phase Space Reduction and the 5D PBE

Due to the QSO assumption, the orientation-dependent physical forces can be radically simplified. Because the particle is treated as instantaneously and permanently aligned broadside to the flow, the angle of incidence becomes a fixed algebraic constant ($\phi \approx \pi/2$). Consequently, the orientation-induced lift force vanishes ($C_L \approx 0$), and the effective drag coefficient reduces strictly to its perpendicular limit ($C_D \approx C_{D,90}$) [25].

In the context of the macroscopic CQMOM solver, removing the periodic orientation angles

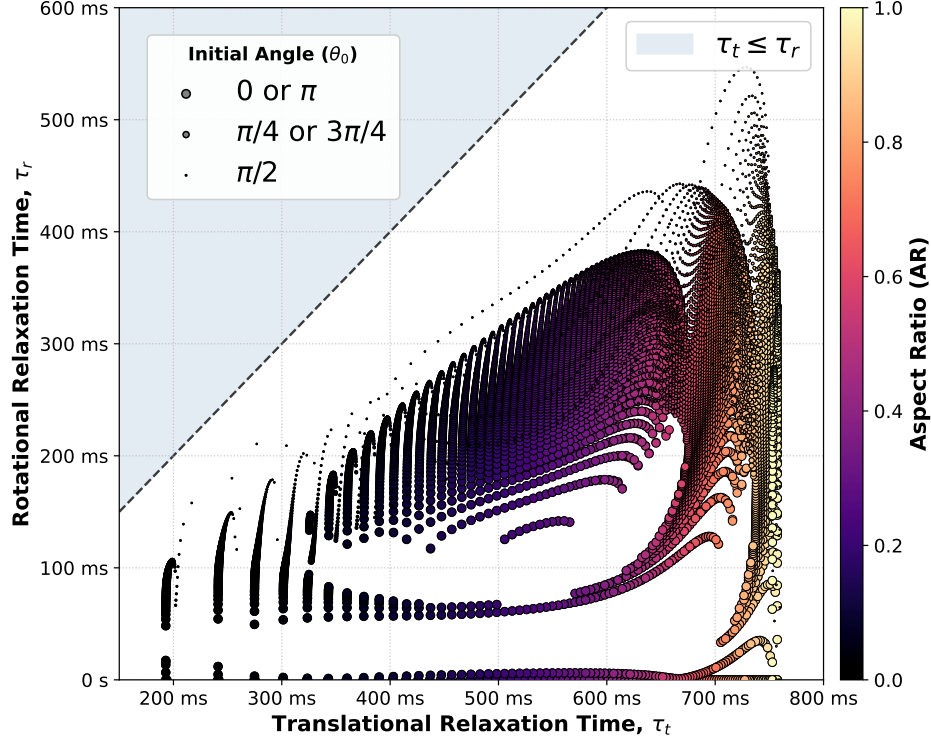


Figure 5.4 Comparison of translational (τ_t) and rotational (τ_r) relaxation times for oblate spheroids with $\text{Re} = 1.24$, confirming $\tau_t > \tau_r$ at the upper limits of the Stokes regime

(θ, ϕ, ψ) and their derivatives $(\dot{\theta}, \dot{\phi}, \dot{\psi})$ entirely avoids the severe mathematical complexities associated with enforcing periodic boundary conditions within the moment inversion framework [3]. Assuming the geometry is invariant ($\dot{d} = 0, \dot{\chi} = 0$), dividing Newton's second law by the particle mass $\rho_p V_p$, and assuming a steady, uniform macroscopic fluid velocity field ($\dot{\mathbf{u}}_f = 0$), the final explicit system of ordinary differential equations governing the reduced 5D state vector $\boldsymbol{\xi} = [d, \chi, u_p, v_p, w_p]^\top$ arises naturally as:

$$\frac{d}{dt} \begin{bmatrix} d \\ \chi \\ u_p \\ v_p \\ w_p \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{F_{D,x}}{\rho_p V_p} + g_x \\ \frac{F_{D,y}}{\rho_p V_p} + g_y \\ \frac{F_{D,z}}{\rho_p V_p} + g_z \end{bmatrix}. \quad (5.17)$$

This system explicitly demonstrates that the particle acceleration is driven solely by the shape-dependent broadside drag and gravity, firmly grounding the macroscopic model in the

derived physical forces without introducing arbitrary unclosed terms.

By applying the QSO assumption, we are able to reduce the phase space from 11 dimensions, $n(t; d, \chi, u_p, v_p, w_p, \theta, \varphi, \psi, \dot{\theta}, \dot{\varphi}, \dot{\psi})$, to just 5 dimensions, $n(t; d, \chi, u_p, v_p, w_p)$. This considerable dimensional reduction markedly simplifies the mathematical description of the system. The spatial and temporal evolution of this 5-dimensional dispersed phase is ultimately governed by the PBE :

$$\frac{\partial n}{\partial t} + \nabla_{\xi} \cdot (\dot{\xi} n) = \mathcal{S}(\xi). \quad (5.18)$$

Physically, this equation acts as a continuity equation for the particles in phase space; it tracks how the probability of finding a particle with a specific size, shape, and velocity shifts over time as the aerodynamic forces accelerate them. Expanding the internal phase-space divergence using the explicit ODEs derived in Equation(5.17) yields the final macroscopic governing equation:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial u_p}(u_p n) + \frac{\partial}{\partial v_p}(v_p n) + \frac{\partial}{\partial w_p}(w_p n) = \mathcal{S}(\xi). \quad (5.19)$$

The right-hand source term $\mathcal{S}(\xi)$ accounts for discontinuous processes such as fragmentation and collisions, which fall outside the scope of the continuous aerodynamic advection modeled in this work.

5.6 Summary and Outlook

In this chapter, the orientation-dependent aerodynamic forces acting upon oblate spheroids were mathematically formulated. Furthermore, a numerical time-scale analysis of the translational and rotational relaxation times was conducted, justifying the quasi-steady orientation (QSO) assumption. This critical physical insight allowed for the safe dimensional reduction of the phase space to five tractable dimensions (d, χ, u_p, v_p, w_p) , completely circumventing the computational burden of resolving high-frequency angular kinematics.

With the multivariate moment inversion algorithm established in Chapter 4 and the physical aerodynamic source terms derived herein, the theoretical and physical foundations of this thesis are now complete. The following chapters will systematically implement, stress-test, and validate this 5D Eulerian framework across increasingly complex multiphase environments.

Specifically, Chapter 6 will serve as the foundational integration of the mathematics and physics. It will introduce the split-operator Hybrid Transport (HT) architecture, applying it to a particle population undergoing simultaneous continuous aerodynamic advection and discontinuous binary breakage. By contrasting the HT method directly against the stan-

dard, fully coupled Moment Transport (MT) approach, this chapter will expose the severe numerical stiffness induced by competing phase-space fluxes. It will formally establish how Strang splitting preserves the positive-definiteness of the Hankel matrices and prevents the catastrophic realizability collapses that plague traditional solvers.

Building upon this mathematically stabilized architecture, Chapter 8 will then push the framework to its absolute limits. The dispersed phase will be subjected to a fully coupled swirling airflow featuring kinetic-energy-driven (v^2) surface attrition. Through rigorous comparative analysis against Lagrangian Monte Carlo (MC) benchmarks, the final chapter will definitively establish the operational superiority, macroscopic fidelity, and inherent mathematical boundaries of the proposed Eulerian solver in extreme non-equilibrium regimes.

CHAPTER 6 MONOMODAL NON-SPHERICAL PARTICLE POPULATION UNDER AERODYNAMIC TRANSPORT AND BREAKAGE

6.1 Physical Modeling and Phase-Space Definition

The primary objective of this chapter is to evaluate the numerical performance and stability of the CQMOM framework by solving the fully coupled, 5-dimensional PBE. To achieve this, we consider a dilute, polydispersed population of oblate spheroids undergoing simultaneous aerodynamic advection, gravity-driven free fall and discrete binary breakage. The state of each particle is completely defined by the internal coordinate vector $\boldsymbol{\xi} = [d, \chi, u_p, v_p, w_p]^\top$, where d is the volume-equivalent diameter, χ is the aspect ratio, and $\mathbf{u}_p = (u_p, v_p, w_p)$ is the particle velocity. The dispersed particles possess a material density of $\rho_p = 2000 \text{ kg/m}^3$ and are immersed in a carrier fluid representing air at standard conditions ($\rho_f = 1.225 \text{ kg/m}^3$, $\mu_f = 1.48 \times 10^{-5} \text{ Pa} \cdot \text{s}$). The evolution of the NDF, $n(t; \boldsymbol{\xi})$, is governed by the continuous advection in phase-space ($\dot{\boldsymbol{\xi}}$) and the discontinuous breakage source terms ($\mathcal{S}$), expressed as:

$$\frac{\partial n}{\partial t} + \nabla_{\boldsymbol{\xi}} \cdot (\dot{\boldsymbol{\xi}} n) = \mathcal{S}(\boldsymbol{\xi}, t). \quad (6.1)$$

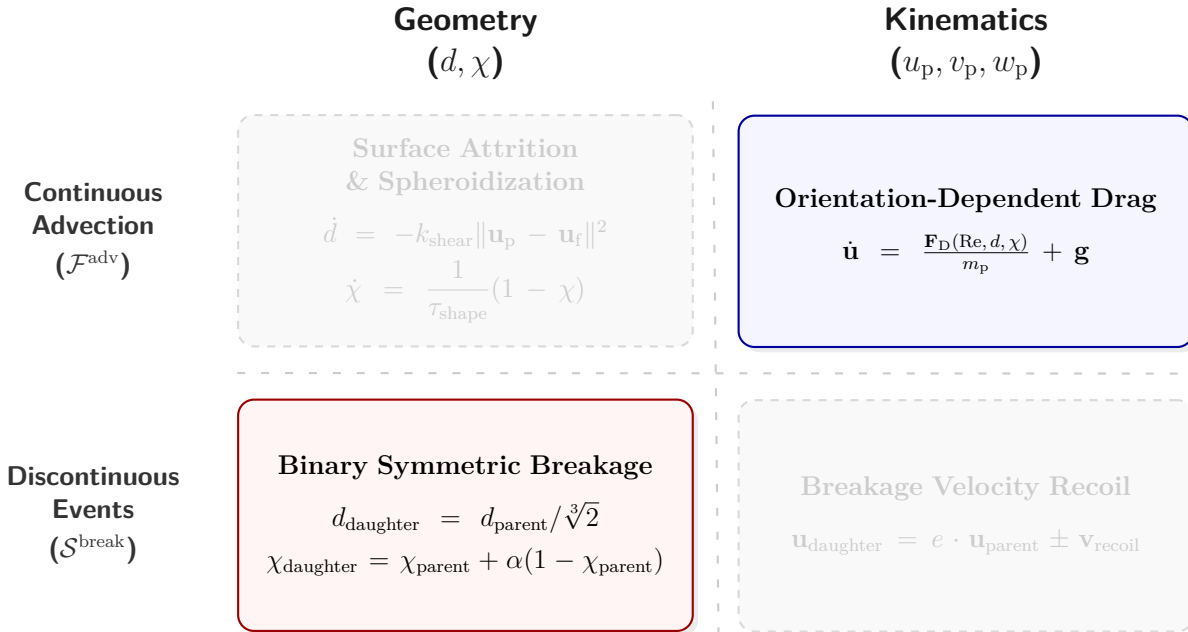


Figure 6.1 Physical Roadmap of the Monomodal Settling with Breakage

Before exposing the fully coupled 5D CQMOM framework to the non-linearities of industrial

flows, it is imperative to validate its foundational numerical stability. This chapter establishes that baseline. As illustrated in the physical roadmap (Figure 6.1), the mathematical complexity is initially restricted to isolate the core advection and fragmentation mechanics.

Between discontinuous breakage events, the particles evolve continuously according to Newton's second law. The geometry is assumed not to be advected in phase-space during flight ($\dot{d} = 0, \dot{\chi} = 0$), while the translational acceleration is driven by gravity and aerodynamic drag ($\dot{\mathbf{u}}_p = \mathbf{F}_D/m_p + \mathbf{g}$). The drag force $\mathbf{F}_D$ is modeled utilizing the oblate spheroid drag correlations under the QSO assumption, as established in Chapter 5. This aerodynamic formulation introduces a strong, non-linear coupling between the first dimensions (d, χ) and the velocity dimensions (u, v, w), because smaller particles decelerate significantly faster than larger ones due to their lower inertia. To test the solver's ability to track these shifting correlations, the macroscopic fluid velocity field $\mathbf{u}_f$ imposes a time-varying rotating background flow defined as $\mathbf{u}_f(t) = [A \cos(\omega t), A \sin(\omega t), 0]^\top$, utilizing an amplitude $A = 2.0$ m/s and a frequency $\omega = 2\pi$ rad/s to induce complex aerodynamic mixing. An illustration is shown in Figure 6.2.

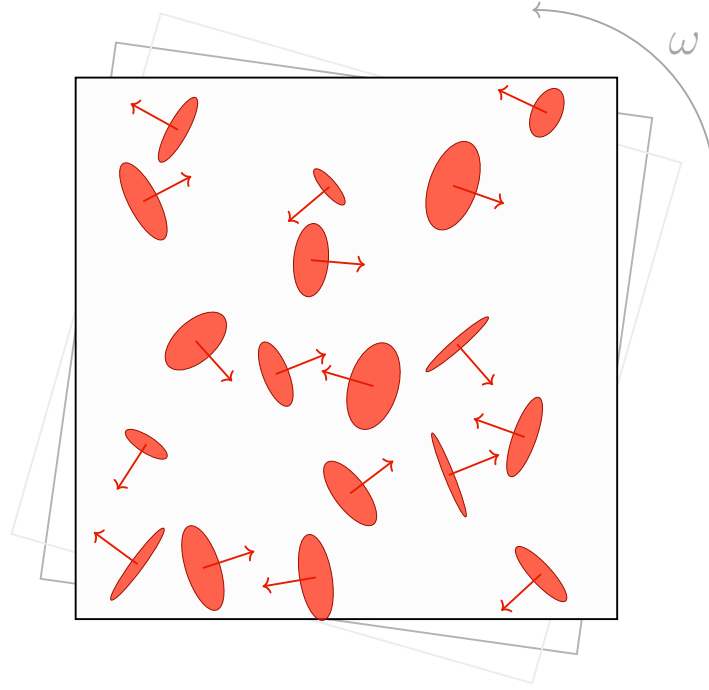


Figure 6.2 Illustration of the monomodal test case in the xy plane. The square describes the rotating background flow. The QSO assumption implies that the particles are broadsided with their relative velocity vector

Simultaneously, the population undergoes discrete binary breakage. In the PBE, the net rate of change for the number density at state ξ is dictated by a classical birth-death integral

source term [3]:

$$S_{\text{break}}(\boldsymbol{\xi}) = \int_{\Omega} \beta(\boldsymbol{\xi}|\boldsymbol{\xi}') R_{\text{break}}(\boldsymbol{\xi}') n(\boldsymbol{\xi}') d\boldsymbol{\xi}' - R_{\text{break}}(\boldsymbol{\xi}) n(\boldsymbol{\xi}) \quad (6.2)$$

where $R_{\text{break}}(\boldsymbol{\xi})$ is the breakage frequency of a particle at state $\boldsymbol{\xi}$, and $\beta(\boldsymbol{\xi}|\boldsymbol{\xi}')$ is the daughter distribution function representing the probability density of forming a daughter state $\boldsymbol{\xi}$ from a parent state $\boldsymbol{\xi}'$, scaled by the stoichiometric generation factor.

The frequency of these discrete breakage events is modeled using a size-dependent power-law kernel [3]:

$$R_{\text{break}}(d) = k \cdot d^{\gamma} \quad (6.3)$$

In this formulation, the exponent is strictly set to $\gamma = 2$, mathematically dictating that the breakage rate is directly proportional to the available surface area of the particle. The pre-exponential rate constant $k = 10^8$ is calibrated to ensure multiple breakage generations occur within the simulation timeframe. The quadratic scaling is selected because it preserves analytical simplicity while maintaining a physically consistent dependence on particle surface area.

The breakage kernel assumes deterministic binary breakage. To strictly obey physical conservation laws, the daughters inherit mass and velocity from the parent. The daughter distribution function is therefore expressed via a Dirac delta formulation [3]:

$$\beta(\boldsymbol{\xi}|\boldsymbol{\xi}') = 2 \delta(\boldsymbol{\xi} - \boldsymbol{\xi}_{\text{daughter}}) \quad (6.4)$$

Upon fracture, a parent particle splits into two identical daughter particles. Volume conservation dictates that $d_{\text{daughter}} = d_{\text{parent}}/\sqrt[3]{2}$, while perfect momentum conservation in the inertial reference frame ensures that the daughters strictly inherit the absolute particle velocity ($\mathbf{u}_{\text{daughter}} = \mathbf{u}_{\text{parent}}$). However, the violent nature of the fracture induces a geometric shape relaxation, modeled as $\chi_{\text{daughter}} = \chi_{\text{parent}} + \alpha(1 - \chi_{\text{parent}})$. The relaxation parameter $\alpha \in [0, 1]$ models the tendency of fragments to become more equant after splitting. We set the value of $\alpha = 0.5$ that serves as a sensible physical heuristic, approximating a geometric split along the major axis while ensuring asymptotic convergence to a perfectly spherical shape ($\chi \rightarrow 1$) for highly fragmented populations.

6.2 Numerical Methodology

The simulation tracks the evolution of the dispersed particle population across the five-dimensional phase-space $\Omega \subset \mathbb{R}^5$. To solve the governing PBE accounting for size-dependent

drag, gravity, and binary breakage, we implement and evaluate three distinct numerical strategies: the moment transport (MT) approach, the split-operator hybrid transport (HT) approach, and a stochastic Monte Carlo (MC) benchmark.

6.2.1 Method 1: Direct Moment Transport (MT)

The MT method resolves the phase-space directly by solving the MTE. This equation is derived by multiplying the PBE by a continuous monomial test function $\xi^{\mathbf{k}}$ and integrating over the entire phase-space. The transport of the $\mathbf{k}$ -th moment $M_{\mathbf{k}}$ is thereby governed by the sum of its source terms:

$$\frac{dM_{\mathbf{k}}}{dt} = \mathcal{F}_{\mathbf{k}}^{\text{adv}} + \mathcal{S}_{\mathbf{k}}^{\text{break}} \quad (6.5)$$

The discrete breakage source term $\mathcal{S}_{\mathbf{k}}^{\text{break}}$ is formulated from the birth-death integrals. By substituting the Dirac delta daughter distribution and representing the moments of the daughter distribution as $\bar{b}_{\mathbf{k}}(\xi') = \int_{\Omega} \xi^{\mathbf{k}} \beta(\xi|\xi') d\xi$, the term is analytically factored and closed via quadrature:

$$\begin{aligned} \mathcal{S}_{\mathbf{k}}^{\text{break}} &= \int_{\Omega} \xi^{\mathbf{k}} S_{\text{break}}(\xi) d\xi \\ &= \int_{\Omega} R_{\text{break}}(\xi') n(\xi') \left[\int_{\Omega} \xi^{\mathbf{k}} \beta(\xi|\xi') d\xi \right] d\xi' - \int_{\Omega} R_{\text{break}}(\xi) n(\xi) \xi^{\mathbf{k}} d\xi \\ &= \int_{\Omega} R_{\text{break}}(\xi') n(\xi') \left[\bar{b}_{\mathbf{k}}(\xi') - (\xi')^{\mathbf{k}} \right] d\xi' \\ &\approx \sum_{i=1}^{N_q} w_i R_{\text{break}}(d_i) \left[\bar{b}_{\mathbf{k}}(\xi_i) - (\xi_i)^{\mathbf{k}} \right] \end{aligned} \quad (6.6)$$

Similarly, the advection flux $\mathcal{F}_{\mathbf{k}}^{\text{adv}}$ is derived using integration by parts. Assuming the distribution vanishes at the phase-space boundaries, the spatial derivative is transferred from the number density to the test function. The closed source term is subsequently evaluated via quadrature over the N_q nodes:

$$\begin{aligned} \mathcal{F}_{\mathbf{k}}^{\text{adv}} &= - \int_{\Omega} \xi^{\mathbf{k}} \nabla_{\xi} \cdot (n(\xi) \dot{\xi}) d\xi \\ &= \int_{\Omega} n(\xi) \dot{\xi} \cdot \nabla_{\xi} (\xi^{\mathbf{k}}) d\xi \\ &= \int_{\Omega} n(\xi) \sum_{j=1}^5 \dot{\xi}_j \left(k_j \xi_j^{k_j-1} \prod_{l \neq j} \xi_l^{k_l} \right) d\xi \\ &\approx \sum_{i=1}^{N_q} w_i \left[\sum_{j=1}^5 k_j \xi_{i,j}^{k_j-1} \dot{\xi}_{i,j} \prod_{l \neq j} \xi_{i,l}^{k_l} \right] \end{aligned} \quad (6.7)$$

This fully coupled formulation mathematically guarantees the exact conservation of moments during continuous transport. The closure is achieved via the CQMOM inversion algorithm, where the phase-space nodes ξ_i and weights w_i must be dynamically reconstructed from the transported moments at every intermediate stage of the SSP-RK3 time integrator.

6.2.2 Method 2: Hybrid Transport (HT)

To mitigate the computational cost of frequent matrix inversions while maintaining higher-order temporal accuracy, the HT method employs an advanced split-operator architecture [6, 36]. While the conceptual strategy of decoupling advection and source terms via operator splitting is inspired by the first-order approach of *Heylmun et al.* [20], the present work significantly elevates this technique by implementing a symmetric, second-order Strang splitting sequence [36]. This upgraded architecture mathematically decouples the continuous aerodynamic transport from the discrete breakage events within a macroscopic time step Δt using a symmetric operator-splitting sequence. Let $M_{\mathbf{k}}^{(n)}$ represent the $\mathbf{k}^{\text{th}}$ -order moment at time t_n . The evolution to t_{n+1} proceeds in three distinct steps.

In the first step, the HT method reconstructs the quadrature nodes $\xi_i^{(n)}$ and advects them strictly along their physical phase-space trajectories for a half time-step ($\Delta t/2$). This integration is performed using an adaptive Bogacki–Shampine Runge–Kutta 2(3) (RK23) scheme. Since transporting the nodes involves solving a localized system of ODEs, the total variation diminishing properties of a Strong Stability Preserving (SSP) method are unnecessary, allowing for a more computationally efficient integration. During this phase, the nodal velocities are evolved by directly integrating the physical ODEs (5.17) to find the intermediate state:

$$\xi_i^{(n+1/2)} = \xi_i^{(n)} + \int_{t_n}^{t_n + \Delta t/2} \dot{\xi}(\tau) d\tau \quad (6.8)$$

Intermediate moments $M_{\mathbf{k}}^{(n+1/2)}$ are then analytically reconstructed from these advected nodes via direct summation, such that $M_{\mathbf{k}}^{(n+1/2)} = \sum_{i=1}^{N_q} w_i (\xi_i^{(n+1/2)})^{\mathbf{k}}$.

Subsequently, in the second step, these intermediate moments are evolved for a full time-step (Δt) strictly under the isolated influence of the breakage source term. Using the state from the first step as the input, the moments are updated via explicit integration using the SSP-RK3 with embedded 2nd-order Runge–Kutta scheme (RK2) for adaptive time stepping, yielding the modified intermediate state $\widetilde{M}_{\mathbf{k}}^{(n+1/2)}$:

$$\widetilde{M}_{\mathbf{k}}^{(n+1/2)} = M_{\mathbf{k}}^{(n+1/2)} + \Delta t \cdot \sum_{i=1}^{N_q} w_i R_{\text{break}}(d_i^{(n+1/2)}) \left[\bar{b}_{\mathbf{k}}(\xi_i^{(n+1/2)}) - (\xi_i^{(n+1/2)})^{\mathbf{k}} \right] \quad (6.9)$$

Finally, in the third step, a new set of nodes $\tilde{\xi}_j^{(n+1/2)}$ is reconstructed from the fragmented moments $\tilde{M}_{\mathbf{k}}^{(n+1/2)}$ via a CQMOM inversion. These freshly inverted nodes are then advected for the remaining half time-step ($\Delta t/2$) to complete the integration cycle:

$$\xi_j^{(n+1)} = \tilde{\xi}_j^{(n+1/2)} + \int_{t_n+\Delta t/2}^{t_{n+1}} \dot{\xi}(\tau) d\tau \quad (6.10)$$

The final moments $M_{\mathbf{k}}^{n+1}$ at t_{n+1} are calculated directly from these final nodal positions. This symmetric operator sequence ($\mathcal{L}_{\Delta t/2}^{\text{adv}} \circ \mathcal{L}_{\Delta t}^{\text{break}} \circ \mathcal{L}_{\Delta t/2}^{\text{adv}}$) ensures second-order accuracy $\mathcal{O}(\Delta t^2)$ for the local splitting error [6, 36], significantly improving the mathematical coupling between the particle trajectory and breakage history compared to the standard first-order architecture of *Heylmun et al.* [20].

The complete algorithmic execution of this symmetric splitting sequence is visually summarized in Figure 6.3. By mapping the fractional-step workflow, the computational advantage of the decoupled architecture becomes readily apparent. The computationally expensive CQMOM matrix inversion is strictly isolated to a single evaluation per macroscopic time step (Step 3). This architectural isolation shields the sensitive inversion algorithm from the stiff, intermediate evaluations of the continuous advection ODEs, providing a stark contrast to MT where the fully coupled SSP-RK3 demands moment inversions at every stage.

6.2.3 Method 3: Monte Carlo (MC)

To establish a definitive, high-fidelity ground truth for validating the macroscopic moment closures, a stochastic MC method is utilized as the third numerical strategy. The MC solver tracks a statistical ensemble of N_p discrete computational parcels throughout the simulation domain. Each individual parcel p evolves continuously according to the exact Newtonian equations of motion, defined as $d\xi_p/dt = \dot{\xi}(\xi_p)$, see Equation (5.17), without any reliance on finite mathematical closures or numerical inversions.

Simultaneously, the discrete breakage mechanism is treated strictly as a random Poisson process. The probability of a particle breaking within a given time step Δt is evaluated as $P_{\text{break}} = 1 - e^{-R_{\text{break}}(d)\Delta t}$. Upon fracture, the mass and momentum of the parent particle are perfectly conserved and distributed to the generated daughter parcels according to the established physical rules. Finally, the global macroscopic moments of the population are recovered at any given time via statistical ensemble averaging, expressed as $M_{\mathbf{k}}(t) \approx \sum_{p=1}^{N_p} w_p \xi_p(t)^{\mathbf{k}}$. Because the MC method accurately resolves the full five-dimensional probability manifold by tracking discrete physical realizations, it serves as the baseline reference for evaluating the kinematic and geometric accuracy of the MT and HT solvers.

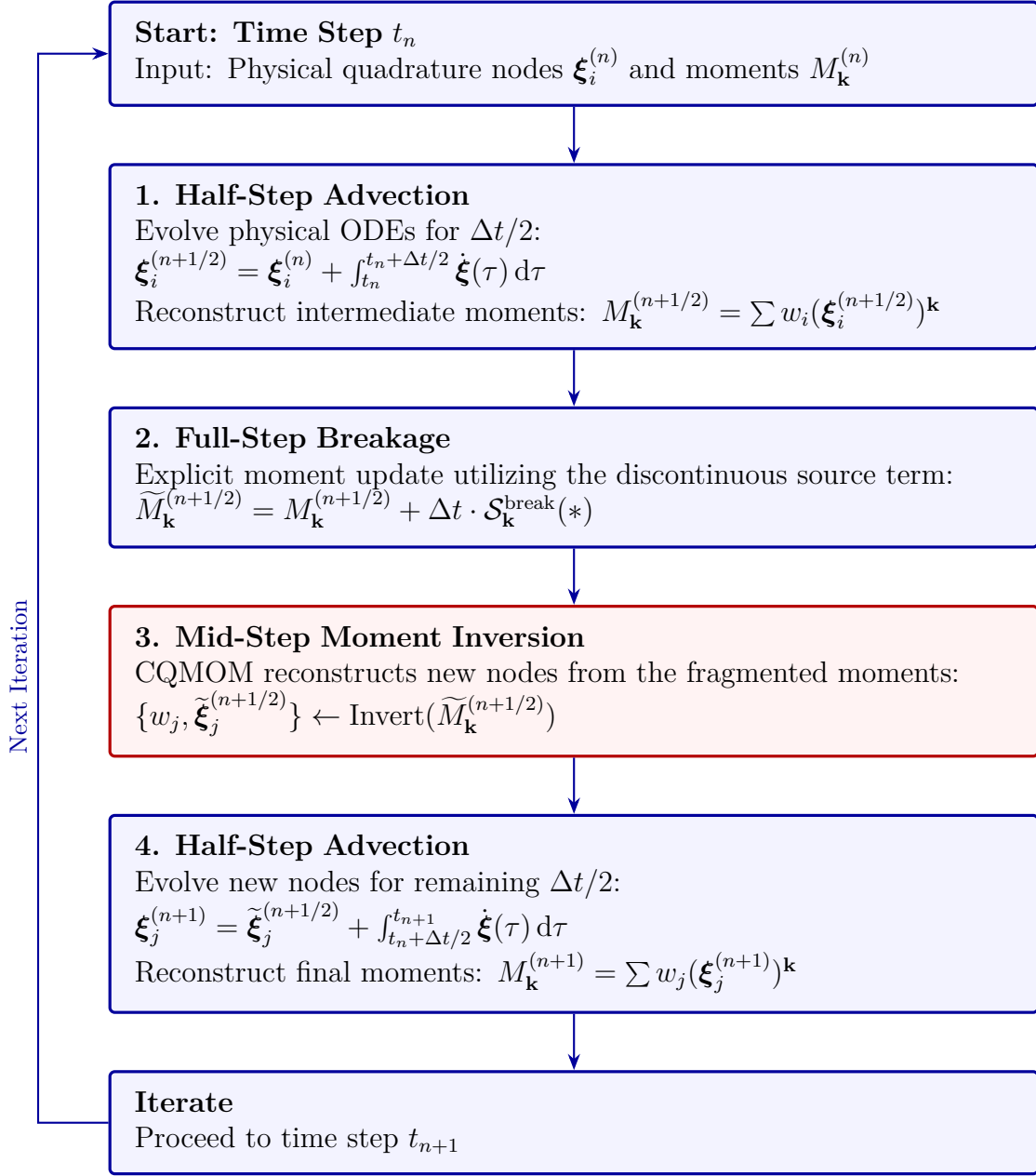


Figure 6.3 Algorithmic flow for the split-operator HT method, illustrating the symmetric Strang splitting sequence $(\mathcal{L}_{\Delta t/2}^{\text{adv}} \circ \mathcal{L}_{\Delta t}^{\text{break}} \circ \mathcal{L}_{\Delta t/2}^{\text{adv}})$. The computationally expensive CQMOM inversion (highlighted) is strictly isolated from the continuous ODE integration

6.3 Key Validation Metrics

To evaluate the numerical fidelity of the MT and HT solvers against the MC benchmark, we track a specific set of moments that correspond directly to macroscopic physical conservation laws and coupling phenomena, as defined in Table 6.1.

Table 6.1 Key Moments and Derived Metrics for Solver Validation

Physical Quantity	Moment	Validation Goal
Total Volume (V)	$M_{3,0,0,0,0}$	Conservation Check. Must remain strictly constant throughout the whole simulation.
Total Number (N)	$M_{0,0,0,0,0}$	Breakage Rate. Validates the numerical integration of the birth-death kernel.
Mean Surface Area	$M_{2,0,0,0,0}$	Drag Coupling. Governs the momentum exchange rate since $F_D \propto d^2$.
Mean Aspect Ratio	$M_{0,1,0,0,0}$	Shape Relaxation. Tracks the dynamic spheroidization toward $\chi = 1$.
Mean Velocity ($\langle u_{p,i} \rangle$)	$M_{0,0,\delta_x^i,\delta_y^i,\delta_z^i}$	Drift Response. Verifies the macroscopic response to the continuous fluid field.
Velocity Covariance	$M_{0,0,1,1,0}$	Shear Detection. Checks for unphysical correlations or node alignment artifacts.

Beyond these standard moments, the kinetic energy metrics require strict physical differentiation. The Directional Kinetic Energy ($E_{k,i} \propto M_{3,0,2\delta_x^i,2\delta_y^i,2\delta_z^i}$) represents the total energy of the system and is heavily mass weighted (d^3), making it an excellent indicator of whether the solver correctly captures the inertial lag of the largest, unfragmented parent particles. However, to evaluate the kinematic dispersion of the population, we must extract the true Granular Temperature Θ , where $\Theta_i = \langle u_{p,i}^2 \rangle - \langle u_{p,i} \rangle^2$. This variance metric isolates the velocity spread induced by polydispersity; in a pure settling flow, Θ_i should initially rise as particles of different sizes differentiate their terminal velocities, providing a stringent test for the multivariate closure capabilities of the CQMOM framework.

6.4 Results and Analysis

6.4.1 Initial Conditions and Phase-Space Configuration

To evaluate the numerical stability of the CQMOM framework, an initial monomodal test case is constructed. The dispersed phase of $N_p = 10\,000$ particles is initialized utilizing a narrow log-normal size distribution with a mean diameter of $\mu_d = 150\,\mu\text{m}$ and an initial aspect ratio beta distribution centered at highly oblate geometries ($\mu_\chi = 0.3$) and the particles are injected into the continuous fluid phase according to a centered Gaussian profile for velocities. The full statistics are shown in Figure 6.4. To ensure that multiple breakage generations occur and interact with the aerodynamic drag within the 1.0 s physical simulation window, the

breakage rate constant is calibrated to $k = 10^8$.

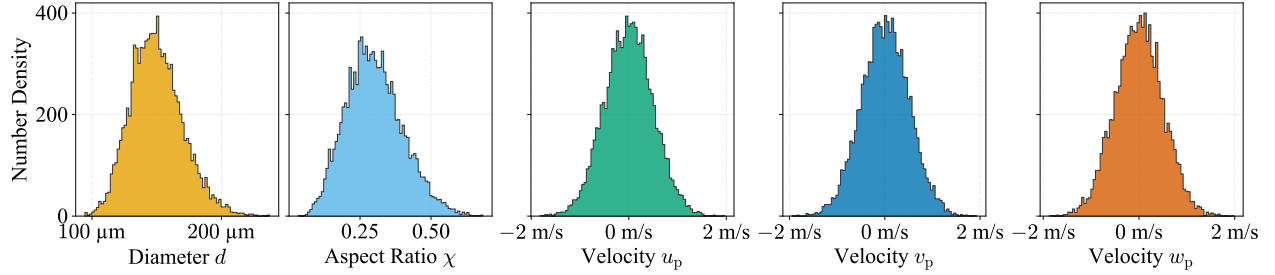


Figure 6.4 Initial distribution for the monomodal test case

6.4.2 Solver Stability and Failure Modes Under Strict Conditioning

In quadrature-based algorithms, a critical parameter governing solver stability is the reciprocal condition number threshold (**rcond**). This parameter establishes the singular value cutoff during the iterative Wheeler inversion of the conditional moment matrices. If a matrix's condition number falls below this threshold, the algorithm assumes the moments are linearly dependent and actively discards quadrature nodes to artificially force mathematical stability via a low-order fallback. To test the extreme sensitivity of the solvers to this parameter, a significantly strict, arbitrary uniform threshold of **rcond** = 0.5 is applied to a quadrature setup of $N_q = [2, 1, 2, 2, 2]$ nodes. This specific tensor configuration is strategically calibrated to resolve the critical macroscopic physics while minimizing computational cost. Resolving the diameter and the three translational velocity components with two discrete nodes each ($N_d = 2$, $N_u = N_v = N_w = 2$) is the strict mathematical minimum required to capture both the internal size variance driving the non-linear fragmentation and the granular temperature necessary to prevent artificial trajectory merging. Conversely, because the fragments relax toward a spherical shape, a single node ($N_\chi = 1$) is sufficient to track the mean aspect ratio, keeping the total phase-space realizations computationally tractable at 16 nodes.

As illustrated in Figure 6.5, imposing this arbitrarily strict threshold reveals distinct behavioral differences between the two macroscopic solvers. Both the HT and MT methods perfectly conserve the total volume throughout the simulation. However, a subtle discrepancy emerges between the HT formulation and the MC ground truth when evaluating the mean diameter and surface area. Notably, the HT geometric drift begins well before any mathematical inversion failures occur ($t < 500$ ms). This early drift is a direct consequence of numerical truncation; the strict **rcond** = 0.5 threshold prematurely truncates the singular values during the standard CQMOM inversion, artificially destroying the physical variance of the size distribution. Because the HT method isolates the breakage step, evaluating the

non-linear breakage rate ($R_{\text{break}} \propto d^2$) on this artificially narrowed size distribution creates a compounding mass error. Conversely, the fully coupled MT method integrates all terms simultaneously, maintaining sufficient moment consistency to track the MC geometric reference accurately despite the strict threshold.

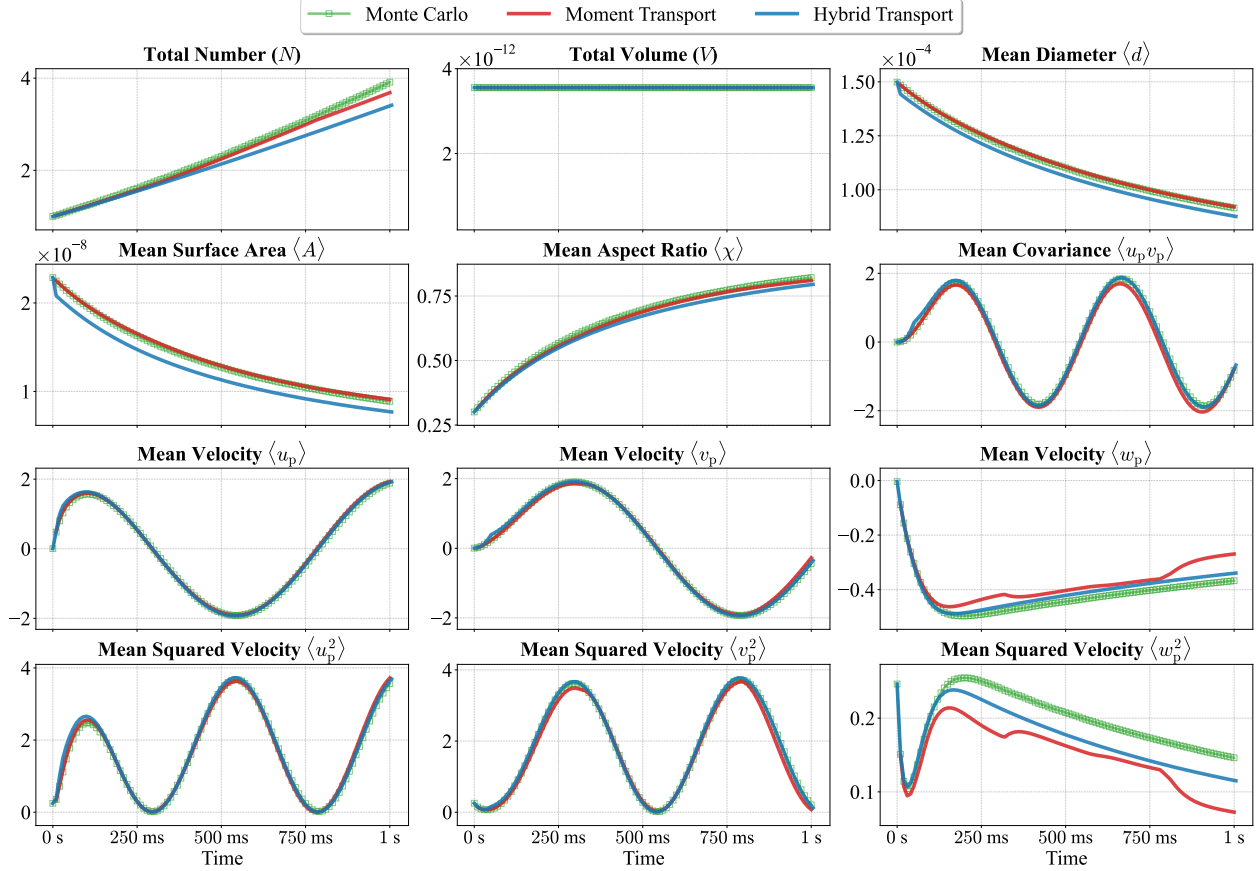


Figure 6.5 Geometric and mass moment evolution utilizing an arbitrarily strict conditioning threshold ($\text{rcond} = 0.5$). While volume is conserved, the HT method underpredicts the mean diameter and surface area and introduce spurious bumps for horizontal velocities moments before $t = 125$ ms, whereas the MT method tracks geometry accurately but introduces spurious perturbations in the velocity fields

While the MT solver excels geometrically, an analysis of the mean and higher-order kinematics reveals severe corruption. As seen in the mean vertical velocity ($\langle w_p \rangle$), the MT solution suffers from continuous spurious perturbations. The strict rcond threshold effectively strangles the CQMOM algorithm, causing it to treat valid phase-space variance as numerical noise. For the MT solver, this triggers a continuous chain of unrecoverable low-order fallbacks starting as early as $t \approx 300$ ms, which persist continuously until $t \approx 780$ ms. Because the SSP-RK3 integrator couples all source terms simultaneously, a single threshold failure

corrupts the continuous temporal integration, trapping the solver in an ill-conditioned state. As demonstrated in Figure 6.6, this continuous reliance on the fallback representation physically manifests as a massive, unphysical overshoot in the vertical kinetic energy ($E_{k,z}$), where the solver completely detaches from the MC benchmark.

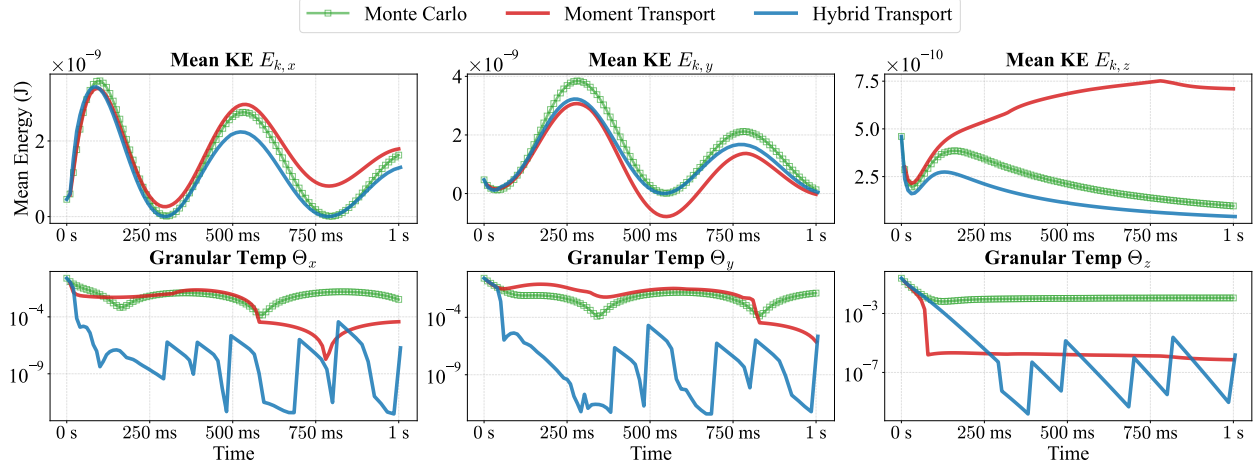


Figure 6.6 Evolution of directional Kinetic Energy and Granular Temperature (Θ) utilizing an arbitrarily strict conditioning threshold ($\text{rcond} = 0.5$). The MT method becomes trapped in a continuous fallback state, causing a massive energy overshoot. The HT method exhibits "tooth-shaped" artifacts, representing a cycle of physically dissipating variance via drag and artificially injecting variance via forced mathematical regularization

The HT method avoids this continuous trapping due to the natural smoothing effect of its operator splitting, running cleanly until halfway through the simulation. However, when it finally breaches the strict threshold, it fails in distinct, intermittent bursts. This behavior is accurately captured in the "tooth-shaped" profiles of the granular temperature (Θ), particularly in the vertical variance (Θ_z). This jagged profile represents a continuous cycle of kinetic variance dissipation and sudden artificial variance injection. The downward diagonal slope occurs as aerodynamic drag continuously forces the distinct particle velocities to converge, consequently draining the kinematic dispersion from the system. As this variance shrinks, the moment matrix becomes highly ill-conditioned. Once the arbitrary $\text{rcond} = 0.5$ limit is breached, the Wheeler algorithm fails. To preserve the realizability of the moment set during integration, the solver triggers a robust fallback mechanism that abandons the fully coupled conditional inversion. Instead, it artificially constructs a decoupled two-node quadrature based strictly on independent marginal means and variances ($\mu \pm \sigma$). While this forces mathematical realizability, it implicitly zeroes out the cross-covariances between geometry and kinematics, severely degrading the physical accuracy of the multiphase system. This mathematical intervention abruptly injects unphysical variance back into the system before

the drag immediately begins dissipating it away again.

Notably, the frequency of these cyclic fallbacks is directly governed by the operator splitting architecture. To illustrate this, the simulation is rerun utilizing a classical first-order splitting sequence (the original Heylmun approach [20]), which applies a full time-step of advection prior to breakage ($\mathcal{L}_{\Delta t}^{\text{adv}} \circ \mathcal{L}_{\Delta t}^{\text{break}}$). As shown in Figure 6.7, removing the Strang splitting results in a significantly higher density of fallback spikes for the HT solver. Because the uninterrupted advection step acts over a full Δt , the aerodynamic drag has more time to significantly compress the velocity nodes, repeatedly driving the matrix into singularity. In contrast, the symmetric Strang splitting applied in the baseline formulation ($\Delta t/2$) interrupts this compressive drag phase twice as often. By updating the discrete size distribution via breakage midway through the time step, Strang splitting allows differential drag to immediately act on the new daughter particles. This physical mechanism actively pulls the velocity nodes apart earlier in the integration cycle, effectively buffering the moment matrix against ill-conditioning and minimizing the frequency of mathematical collapses.

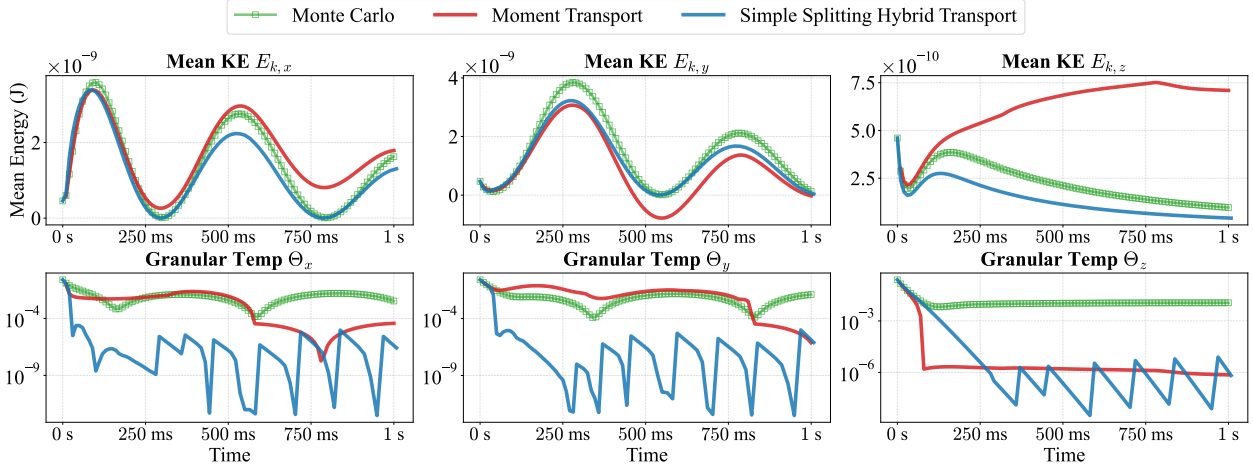


Figure 6.7 Logarithmic Granular Temperature (Θ) evolution utilizing a first-order splitting sequence (full advection step prior to breakage) with an arbitrarily strict conditioning threshold ($\text{rcond} = 0.5$). The HT method (blue) exhibits a significantly higher density of fallback "teeth" compared to the Strang splitting baseline, as the uninterrupted drag phase repeatedly drives the moment matrix into singularity. Other moments aren't displayed here because there's no visible difference between Strang and simple splitting approaches

Ultimately, the stark contrast in these failure modes demonstrates that imposing a bad, arbitrary conditioning threshold causes severe numerical malfunctions and physical inaccuracies. Rather than a mere numerical technicality, rcond emerges as a parameter of critical importance to the CQMOM framework. Its improper specification either traps the fully coupled formulation in a continuous state of kinematic corruption, or triggers cyclical, unphysical

variance injections in the split formulation. On the other hand, imposing a highly relaxed threshold ($\mathbf{rcond}_{\text{HT}} = 10^{-5}$) accurately restores the statistical and geometric fidelity of the HT solver—rendering it effectively indistinguishable from the MC benchmark. Remarkably, the HT formulation demonstrates exceptional algorithmic robustness under these relaxed conditions; lowering the threshold even further to near-zero limits ($\mathbf{rcond}_{\text{HT}} = 10^{-50}$) yields the exact same stable, high-fidelity results. This demonstrates that the split-operator architecture can safely process highly stiff, ill-conditioned moment matrices without relying on artificial mathematical truncation. In direct contrast, applying these same relaxed thresholds causes the highly sensitive, fully coupled MT solver to fatally explode and crash early in the integration ($t \approx 100$ ms), as its SSP-RK3 integrator fails to process the un-truncated stiff source terms. Consequently, effectively resolving the strongly coupled 5D phase-space requires a split-operator HT architecture together with a highly relaxed conditioning strategy.

6.4.3 Macroscopic Fidelity Under Optimized Conditioning

To evaluate the true mathematical capabilities of the moment closures without the interference of arbitrary numerical truncation, the solvers are subjected to an optimized conditioning strategy. Through iterative parameter sweeping to delay the first fallback while minimizing total fallbacks events, optimal thresholds are identified as $\mathbf{rcond}_{\text{HT}} = 10^{-5}$ for the HT method and $\mathbf{rcond}_{\text{MT}} = 0.05$ for the MT method.

As illustrated in Figure 6.8, applying these optimally relaxed thresholds fundamentally cures the geometric drift previously observed in the split-operator formulation. The terminal execution logs confirm that the HT solver achieves 100% integration completion with zero fallback occurrences. By lowering the threshold to 10^{-5} , the algorithm avoids the silent truncation of singular values during the routine CQMOM inversion. The solver is permitted to retain size nodes that are closely spaced, thereby accurately preserving the statistical variance and the wide tails of the size distribution. Because this full mathematical spread is maintained, the non-linear breakage rate ($R_{\text{break}} \propto d^2$) is integrated flawlessly, keeping the mean diameter and surface area in perfect agreement with the MC ground truth throughout the entire simulation.

In contrast, the optimized MT solution explicitly demonstrates the inherent architectural fragility of evaluating highly coupled, stiffening moment matrices. Even when tuned to its optimal threshold of 0.05, the MT solver only survives cleanly until $t \approx 340$ ms. At this critical juncture, aerodynamic drag sufficiently compresses the phase-space velocities to breach the threshold, plunging the SSP-RK3 integrator into a continuous, unbroken chain of low-order fallbacks that persists until $t \approx 790$ ms. As shown in Figure 6.9, this continuous

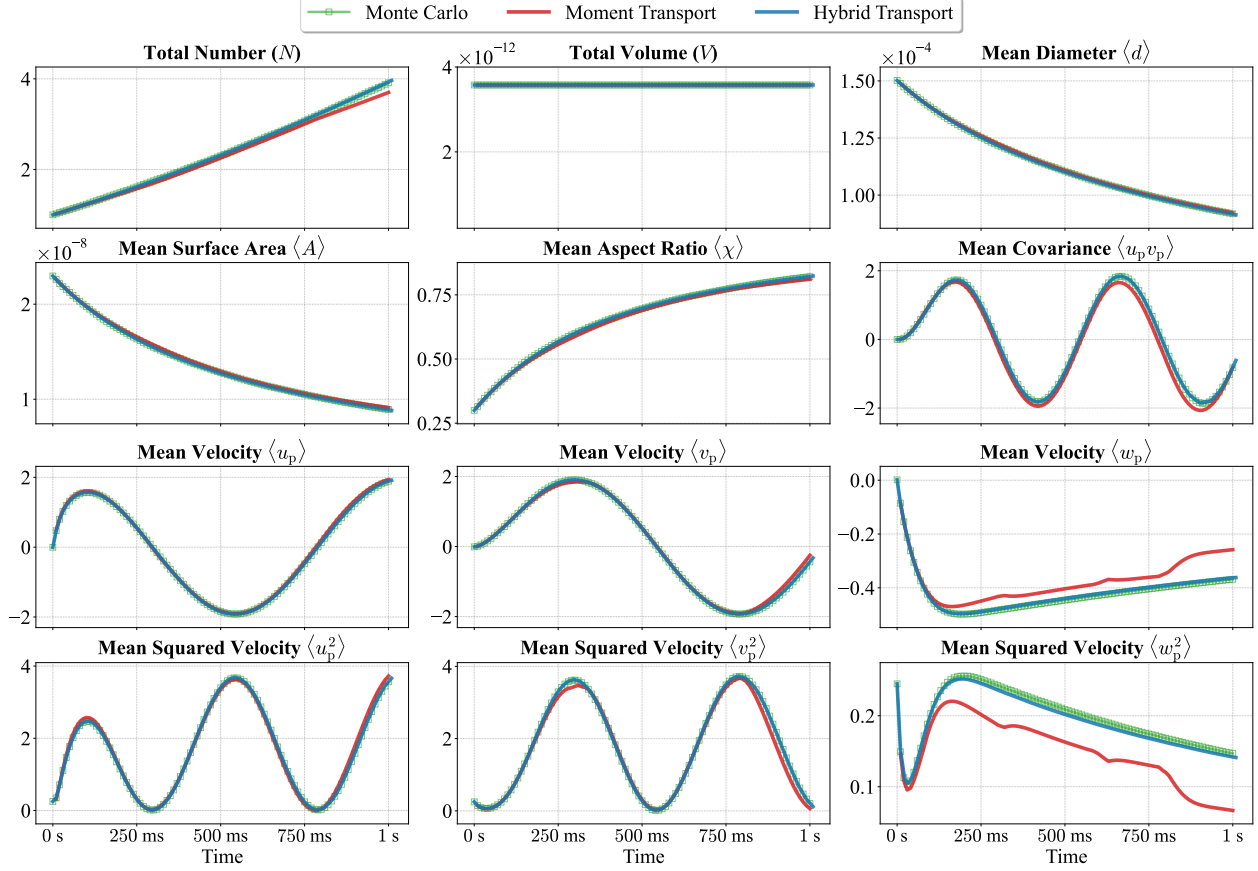


Figure 6.8 Evolution of the global mean moments utilizing optimized conditioning parameters ($\mathbf{rcond}_{\text{HT}} = 10^{-5}$, $\mathbf{rcond}_{\text{MT}} = 0.05$). The HT method perfectly resolves the geometric moments by avoiding silent truncation, while the MT method exhibits a late-stage deviation in the mean vertical velocity ($\langle w_p \rangle$)

trapping explicitly corrupts the macroscopic integration; the mean vertical velocity ($\langle w_p \rangle$) permanently deviates from the true trajectory, and the vertical kinetic energy ($E_{k,z}$) suffers a massive numerical overshoot. The MT solver only escapes this fallback trap after 790 ms because continuous breakage eventually generates a sufficient population of tiny daughter particles, radically increasing the velocity spread and spontaneously restoring the matrix conditioning at the expense of accuracy for moments of order 2 or higher.

The most profound difference between the two formulations, however, is revealed in their treatment of the second-order kinematics. As demonstrated by the granular temperature (Θ) in Figure 6.9, the HT method accurately tracks the MC ground truth across all three spatial dimensions. The advection step processes the tightening velocity nodes without artificially destroying their dispersion, allowing the HT solver to flawlessly capture the physical variance dynamically generated by differential drag.

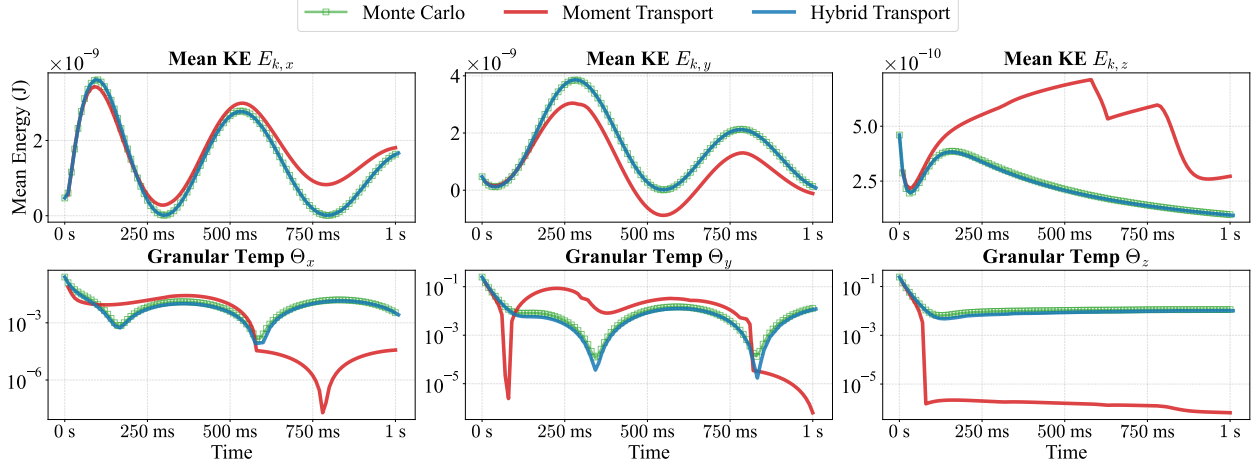


Figure 6.9 Evolution of directional Kinetic Energy and Granular Temperature (Θ) utilizing optimized conditioning. The HT method accurately tracks the MC benchmark. In contrast, the MT method suffers severe variance collapse and a clear energy overshoot

Conversely, the MT formulation fails to preserve this second-order phase-space. In the vertical settling direction (Θ_z), the MT solver suffers a severe collapse exceptionally early in the simulation ($t \approx 100$ ms), dropping straight to the numerical floor. Furthermore, in the transverse directions (Θ_x and Θ_y), the variance severely plunges multiple orders of magnitude below the correct trajectory. Because the MT formulation evaluates all coupled source terms simultaneously inside the sensitive SSP-RK3 loop, the highly ill-conditioned velocity nodes lose their linear independence far more rapidly than those evolving under the HT method. Consequently, the MT algorithm truncates the internal variance of the particle population long before the explicit fallback chain begins, rendering the solver unable to resolve the actual kinematic dispersion of the multiphase flow.

6.4.4 Computational Efficiency and Runtime Analysis

Beyond mathematical robustness and physical accuracy, the choice of closure architecture profoundly impacts computational efficiency. While stochastic MC methods provide a high-fidelity ground truth, their application in three-dimensional industrial CFD requires tracking billions of computational parcels, often rendering them computationally intractable. CQMOM is specifically employed to bypass this bottleneck. To quantify the relative efficiency of the proposed macroscopic architectures, the total execution time for this idealized 0D monomodal scenario is recorded. The MC benchmark, utilizing an ensemble of $N_p = 10\,000$ particles, required 27 seconds to complete the simulation. The MT solver required 70 seconds; while this still represents a macroscopic continuum solution, this extended

runtime highlights the severe computational penalty of the fully coupled formulation. The SSP-RK3 integrator struggles to process the highly stiff moment matrices, requiring computationally expensive Wheeler inversions at every intermediate sub-step just to maintain stability.

Conversely, the HT method completed the identical simulation in just 2.5 seconds. By decoupling the physics through operator splitting and utilizing a node-advection step, the HT formulation entirely bypasses the expensive, continuous matrix inversions required by the MT loop. Ultimately, the HT solver not only flawlessly replicates the high-fidelity 5D phase-space resolution of the MC benchmark, but achieves this at a $28\times$ reduction in computational cost compared to the coupled MT approach, strongly suggesting that the HT architecture provides a more robust framework for this class of multiphase flows.

CHAPTER 7 MULTIMODAL PARTICLE JET DYNAMICS WITH STOCHASTIC BREAKAGE RECOIL

7.1 Physical Model Formulation and Initial Conditions

Having established the baseline stability of the HT solver in Chapter 6, the framework is now subjected to severe kinematic stress. In highly inertial multiphase flows, aerodynamic drag dissipates velocity variance, while fragmentation isotropically injects variance. As highlighted in the updated roadmap (Figure 7.1), we activate in this chapter a discontinuous velocity recoil mechanism. Forcing the phase space to simultaneously process these competing phenomena directly exposes the mathematical fragilities of standard explicit moment methods and demonstrates the necessity of the split-operator HT architecture.

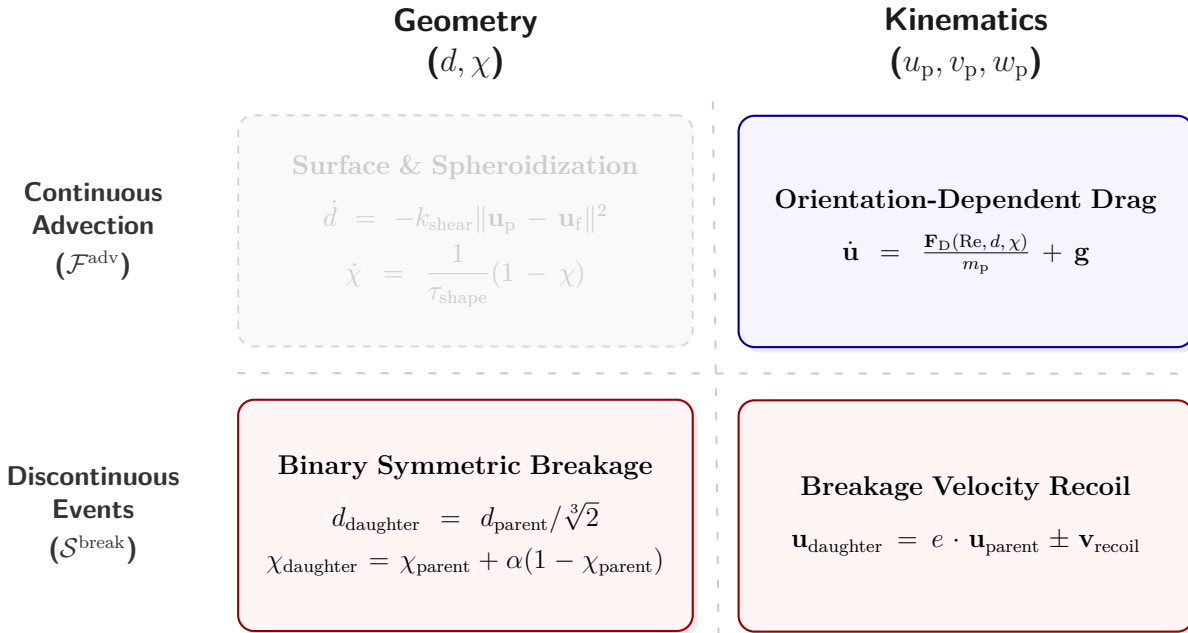


Figure 7.1 Physical Roadmap of the Multimodal Crossing Jets

Physically, this extends the breakage kinematics to account for the liberation of internal strain energy. Rather than daughters perfectly inheriting their parent's velocity, the continuous momentum transfer is replaced by a dissipative recoil model. The center of mass of the newly formed fragments retains a fraction ($e = 0.5$) of the parent's momentum, representing non-elastic damping. Concurrently, an isotropic, stochastic recoil vector $\mathbf{v}_{\text{recoil}}$ is superimposed to simulate kinetic ejection. To strictly conserve momentum across the fracture event, the

two identical daughters receive equal and opposite recoils (Figure 7.2):

$$\mathbf{u}_{\text{daughter},1} = e \cdot \mathbf{u}_{\text{parent}} + \mathbf{v}_{\text{recoil}} \quad (7.1)$$

$$\mathbf{u}_{\text{daughter},2} = e \cdot \mathbf{u}_{\text{parent}} - \mathbf{v}_{\text{recoil}} \quad (7.2)$$

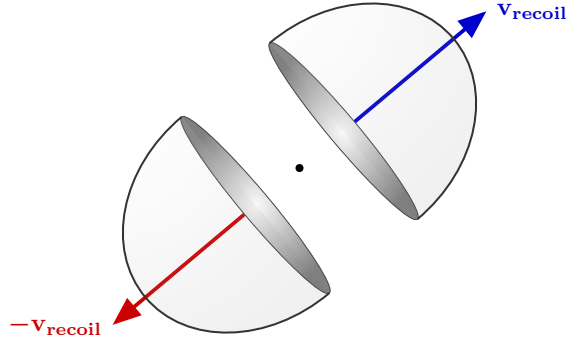


Figure 7.2 Illustration of the stochastic recoil mechanism

The components of this random recoil vector are sampled from a normal distribution, $\mathbf{v}_{\text{recoil}} \sim \mathcal{N}(\mathbf{0}, \sigma_{\text{recoil}}^2 \mathbf{I})$, with a variance of $\sigma_{\text{recoil}} = 0.5 \text{ m/s}$. This intentionally high magnitude stress-tests the solver's realizability under severe variance injection. By continuously injecting microscopic granular temperature, this mechanism establishes a sustained thermal floor that counteracts the aerodynamic focusing effect.

Implementing this stochastic recoil requires distinct strategies based on the numerical framework. In the MC benchmark, the velocity damping and opposite recoils are applied directly to the discrete daughter parcels upon fracture.

Conversely, within the CQMOM framework (MT and HT methods), this stochastic energy injection must be embedded analytically into the macroscopic moment equations to avoid random sampling. The breakage flux for an arbitrary moment $M_{\mathbf{k}}$ evaluates the net change utilizing the mathematical expectation of the daughter states, $\langle \mathbf{u}_{\text{daughter}}^{\mathbf{k}} \rangle$. Assuming each velocity component follows an independent Gaussian distribution, the expectation is analytically closed using the exact expansion for raw normal moments. For an arbitrary velocity component (e.g., u_p), this yields:

$$\langle u_{p,\text{daughter}}^k \rangle = \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{2j} (2j-1)!! \sigma_{\text{recoil}}^{2j} (e \cdot u_{p,\text{parent}})^{k-2j} \quad (7.3)$$

By embedding this analytical formulation, the CQMOM solvers exactly capture the granular

temperature injection directly within the macroscopic Eulerian fluxes.

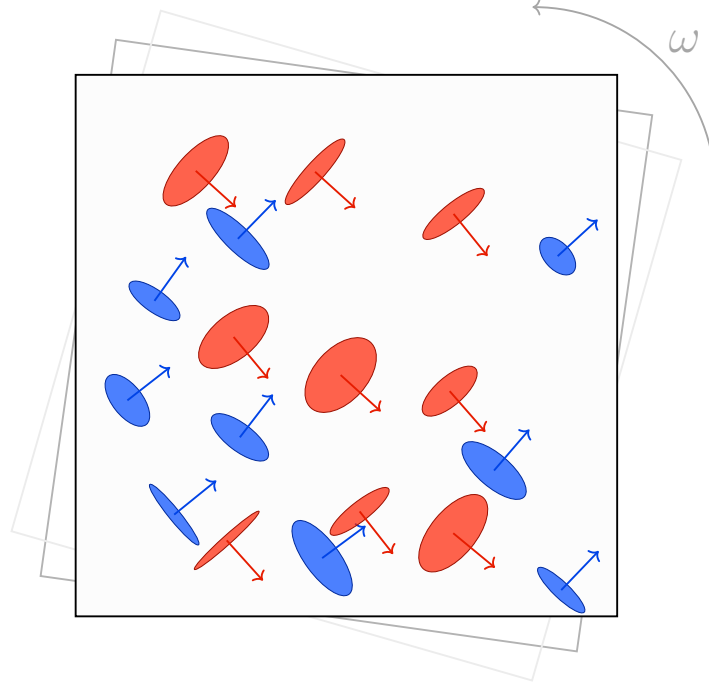


Figure 7.3 Illustration of counter flowing jets in the xy plane with two distinct colors along with the rotating background flow

To test the solver's ability to preserve distinct phase-space modes without suffering from artificial numerical homogenization, the system is initialized with a challenging bimodal distribution of $N_p = 10000$ particles, representing two counter-flowing jets along the y -axis. The initial condition represents two equal-weight modes, with a 50% mixture weight assigned to each jet as illustrated in Figure 7.3. Both populations share identical geometric distributions, with a mean volume-equivalent diameter of $\mu_d = 150 \mu\text{m}$ ($\sigma_d = 20 \mu\text{m}$) and an oblate mean aspect ratio of $\mu_\chi = 0.3$ ($\sigma_\chi = 0.1$). Kinematically, both jets translate uniformly in the streamwise direction with a mean velocity of $\langle u_p \rangle = 1.0 \text{ m/s}$. However, they oppose each other in the transverse direction, with Jet 1 traveling at $\langle v_p \rangle = 1.0 \text{ m/s}$ and Jet 2 traveling at $\langle v_p \rangle = -1.0 \text{ m/s}$. The vertical velocity is initialized at absolute rest ($\langle w_p \rangle = 0.0 \text{ m/s}$). A uniform isotropic velocity standard deviation of 0.5 m/s is applied across all three spatial dimensions for both modes as shown in Figure 7.4. For the numerical QMOM inversion stability during this highly discontinuous scenario, the relaxed regularizer threshold is set to $\text{rcond}_{\text{HT}} = 10^{-6}$ for the HT method, while a severely strict, empirically tuned threshold of $\text{rcond}_{\text{MT}} = 0.9$ is required for the fully coupled MT method to maintain realizability.

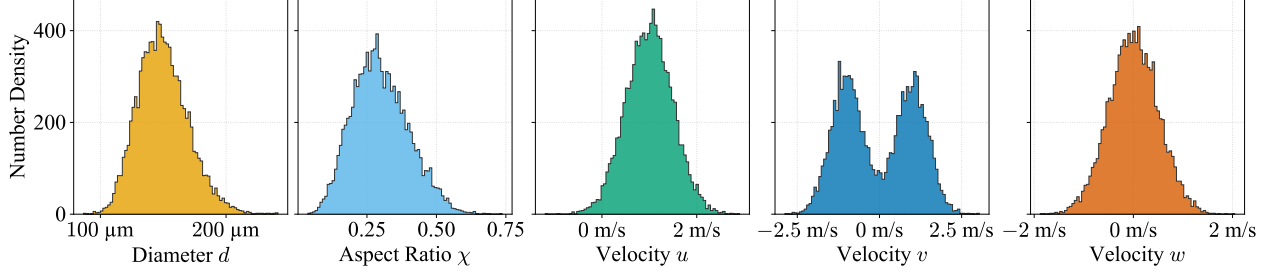


Figure 7.4 Initial distribution of the multimodal particle jets. The symmetric bimodal nature of the counter-flowing system ($\langle v \rangle = \pm 1.0$ m/s) is distinctly resolved prior to the onset of continuous aerodynamic advection and discrete breakage events

7.2 Results and Analysis

7.2.1 Solver Stability and Execution Performance

The numerical integration of multimodal particle jets undergoing stochastic recoil exposes the underlying mathematical limitations of fully coupled CQMOM closures. Evaluated over a physical simulation time of 1.0 s, the operator-splitting architecture of the HT method demonstrates clear numerical superiority. By mathematically decoupling the continuous aerodynamic advection ($\mathcal{L}_{\text{adv}}$) from the discontinuous, energy-injecting breakage events ($\mathcal{L}_{\text{break}}$), the HT solver strictly maintains the realizability of the moment set. This isolation allows the CQMOM inversion to operate seamlessly at a strict regularization threshold of $\text{rcond}_{\text{HT}} = 10^{-6}$, completing the simulation in 5.7 s with zero quadrature failures.

Conversely, the MT method attempts to evaluate the continuous variance dissipation (due to drag) and the discontinuous variance injection (due to the recoils) simultaneously within the same SSP-RK3 integration stage. This fundamental competition induces extreme mathematical stiffness in the moment transport equations, driving the zeroth conditional moment of the 4th and 5th-stage conditional systems into unphysical negative states. Consequently, the adaptive Wheeler algorithm is forced to abort and trigger low-order fallback mechanisms at the onset of the simulation and again at $t \approx 760$ ms. These algorithmic collapses drastically inflate the execution time to over 4 minutes and significantly degrade the physical predictions.

7.2.2 Macroscopic Geometric Fidelity

The macroscopic fidelity of the solvers is first assessed through the lower-order conservation and geometric moments presented in Figure 7.5. All three methodologies successfully enforce

strict mass conservation, as evidenced by a perfectly stable total volume (V). The HT method serves as an excellent Eulerian surrogate for the MC ground truth, precisely capturing the phase and amplitude of the crossing trajectories ($\langle u_p \rangle, \langle v_p \rangle$) and accurately reproducing the continuous generation of particles up to the final normalized population of $N = 4.0$.

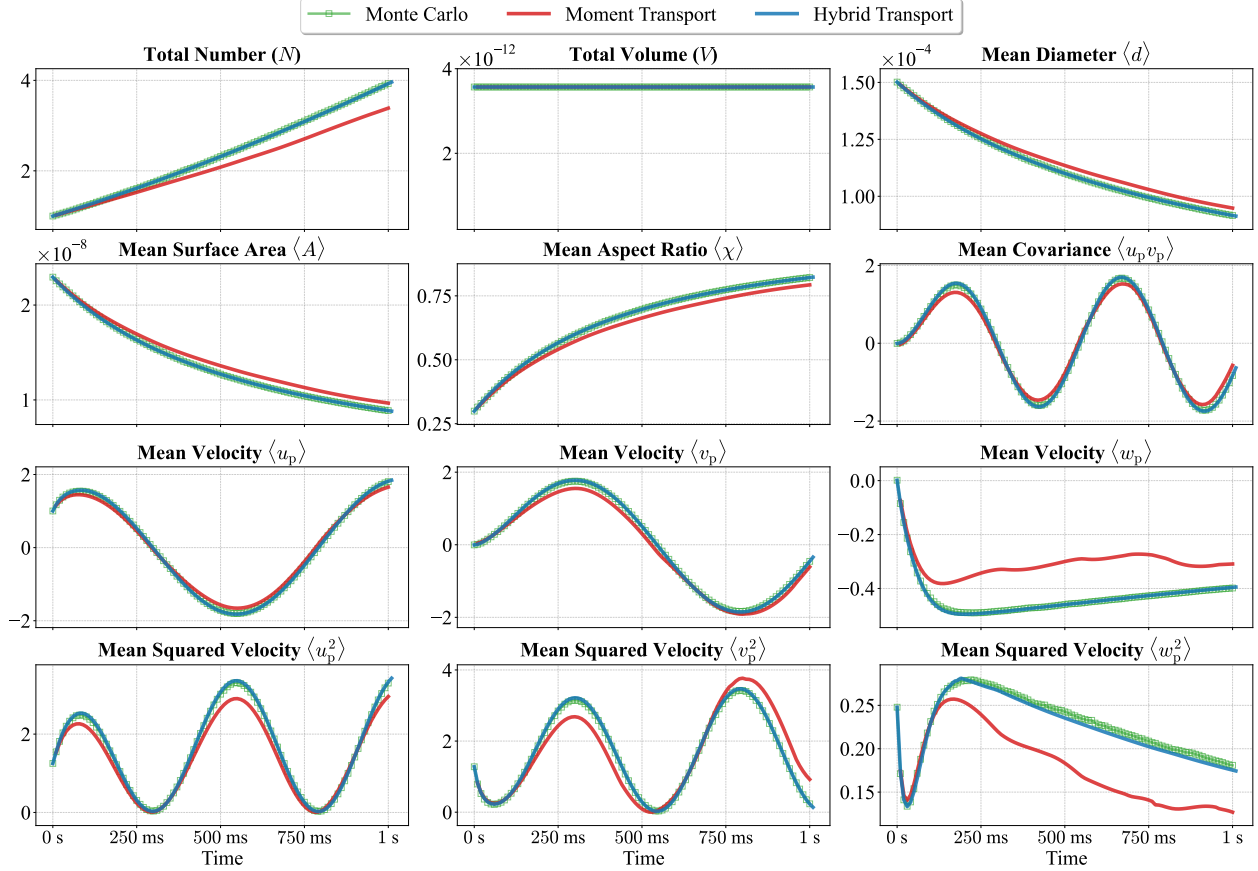


Figure 7.5 Comparative evolution of the global lower-order moments. The HT serves as an excellent surrogate for the MC benchmark across all geometric and kinematic variables, while the MT artificially overshoots the tracked moments due to repeated quadrature fallbacks

However, the consequences of the MT method's quadrature failures manifest distinctly in the geometric evolution. Because the MT solver frequently reverts to a lower-order moment subset, it artificially truncates the phase-space resolution required to accurately integrate the size-dependent breakage kernel and the shape relaxation rate. Consequently, the MT method underpredicts the particle generation rate and exhibits an artificial lag in both the decay of the mean diameter ($\langle d \rangle$) and the rounding of the mean aspect ratio ($\langle \chi \rangle$). The HT method integrates these deterministic geometric fluxes with negligible error relative to the MC reference while maintaining its full quadrature tensor throughout the simulation.

7.2.3 Kinematic Variance and Thermal Floor Tracking

The defining theoretical contribution of this multimodal scenario is the evaluation of the granular temperature (Θ) as shown in Figure 7.6. In standard Eulerian models, aerodynamic drag drives the phase-space velocities to converge, ultimately triggering a numerical delta-shock (where $\Theta \rightarrow 0$) [37]. The stochastic recoil mechanism counteracts this by continuously injecting kinetic energy. The MC benchmark establishes the physical reality of this balance: the vertical granular temperature (Θ_x, Θ_y) decay initially but oscillate stably around a sustained thermal floor of approximately $10^{-1.5}$ instead of 10^{-3} in Chapter 6, preventing the mono-kinetic collapse.

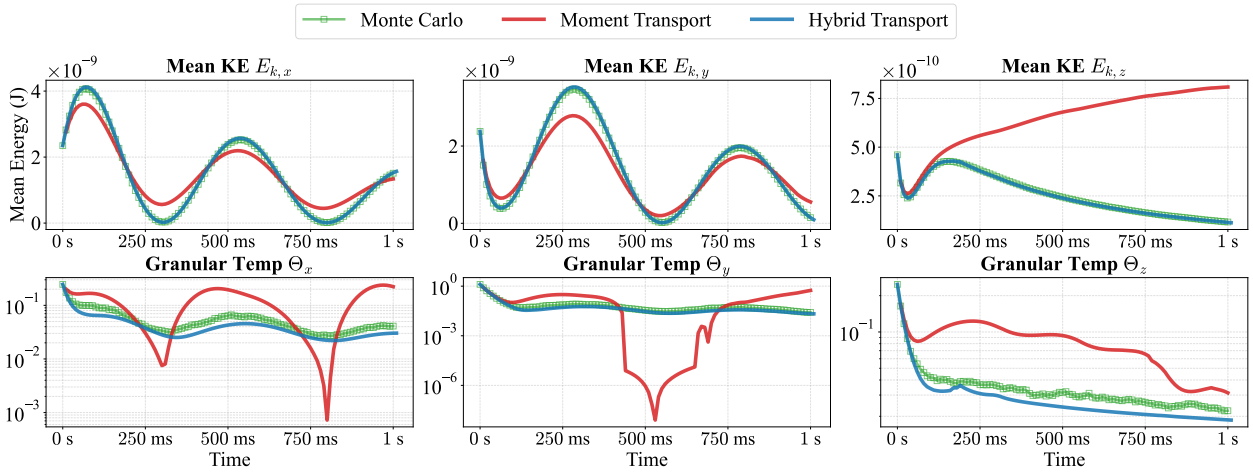


Figure 7.6 Evolution of directional kinetic energy and granular temperature (Θ) plotted on a logarithmic scale. The HT method successfully captures the stabilized thermal floor generated by the stochastic recoil, effectively preventing a delta-shock. The MT method exhibits severe numerical singularities and unphysical spurious heating in the unforced z -axis

The HT method flawlessly reproduces this variance regularization. By explicitly evaluating the analytical Gaussian expectation of the daughter states, the split-operator framework accurately injects the required thermal energy, tracing the logarithmic decay and the stabilized plateau of the MC benchmark across all spatial dimensions.

In stark contrast, the MT method fails to resolve the energy dynamics due to the severe numerical stiffness induced by coupling the competing source terms. In the MTE framework, aerodynamic drag continuously dissipates velocity variance, driving the moment set toward the boundary of the realizable space where the higher-order Hankel determinants approach zero [3]. Simultaneously, the stochastic recoil flux attempts to inject variance and broaden the distribution. When the SSP-RK3 integrator attempts to balance these strongly competing fluxes within a single continuous step, the resulting numerical stiffness causes the solver to

overshoot the realizable phase space. This violates the positive-definiteness of the Hankel matrices, causing the CQMOM inversion to fail and triggering the low-order fallbacks.

This algorithmic collapse forces numerical singularities within the moment set, evident in Figure 7.6 via the unphysical, v-shaped collapses of Θ_x down to 10^{-3} , and a total severe drop in Θ_y to 10^{-8} at approximately $t = 550$ ms.

7.2.4 Unphysical Energy Leaks in the Transverse Plane

This fundamental failure is further exacerbated in the vertical axis (z). Because the macroscopic carrier fluid flow is zero in the vertical direction ($\langle w_p \rangle = 0$), the z -axis dynamics are governed strictly by gravitational settling and the isotropic distribution of the breakage recoil. As shown in Figure 7.6, the HT method correctly models the dissipation of the initial vertical kinetic energy ($E_{k,z}$), peaking at 4.5×10^{-10} J before decaying. However, as continuous aerodynamic drag forces the velocity variance in the x and y planes toward zero, the moments become highly linearly dependent. This severe ill-conditioning corrupts the CQMOM root-finding algorithm, causing the reconstructed velocity nodes to skew unphysically and lose their expected geometric symmetry. To balance the global moment equations under this severe ill-conditioning, the solver artificially leaks unresolved turbulent energy into the unforced z -axis. This causes the MT prediction for $E_{k,z}$ to diverge upward to 8.0×10^{-10} J, accompanied by a granular temperature (Θ_z) that remains nearly an order of magnitude higher than the physical truth.

Ultimately, this analysis confirms that the HT method successfully captures non-equilibrium variance injection. By mathematically decoupling the competing operators, the HT framework systematically avoids the severe matrix ill-conditioning and realizability boundary violations inherent to fully coupled explicit integration. This approach preserves the strict positive-definiteness of the moment set, providing the accuracy of a Lagrangian solver at a fraction of the computational cost, and demonstrating that operator splitting is essential for stabilizing CQMOM closures in discontinuous, high-variance fragmentation regimes.

CHAPTER 8 FULLY COUPLED PARTICLE DYNAMICS IN A SWIRLING AIRFLOW

8.1 Physical Model Formulation and Initial Conditions

The preceding chapters have systematically evaluated the CQMOM framework against isolated kinematic and geometric complexities, establishing the stability of the Strang splitting numerical architecture. This final results chapter presents a comprehensive evaluation of the framework under a fully coupled environment, modeling the processing of oblate particles in a high-speed rotating airflow. As shown in the updated physical roadmap (Figure 8.1), all macroscopic operators within the 5D phase space are simultaneously active.

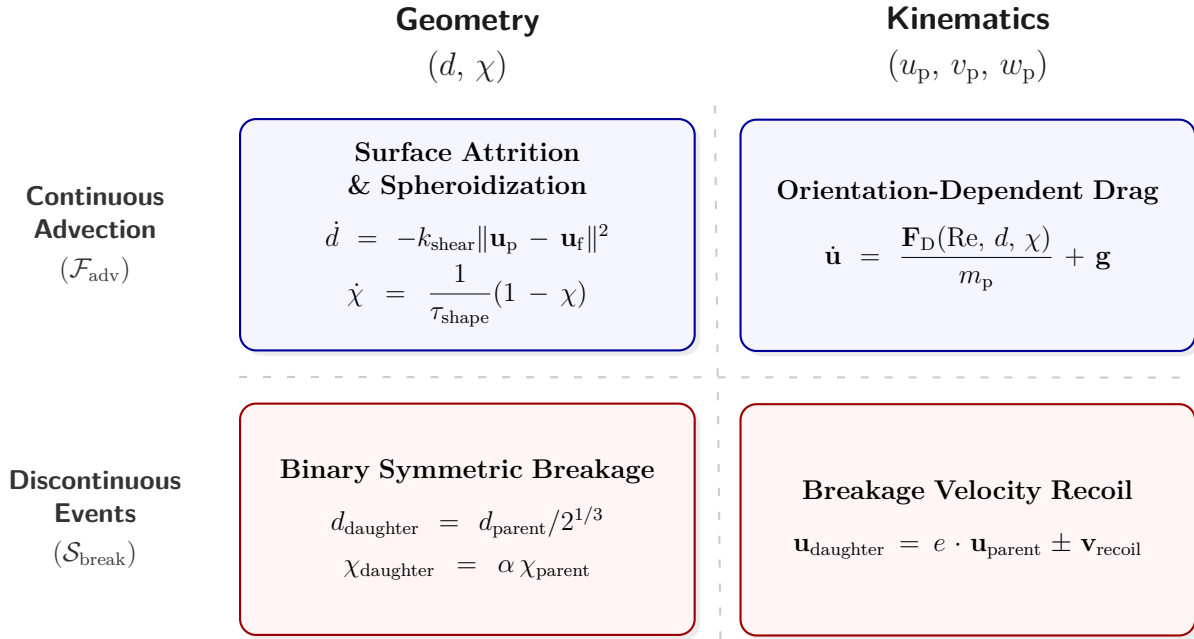


Figure 8.1 Physical roadmap of the fully coupled 5D CQMOM framework. The phase-space configuration incorporates simultaneous kinetic-energy-driven surface attrition and swirling aerodynamic advection, coupled with discontinuous volume-conserving fragmentation and stochastic velocity recoil

The dispersed phase is initialized with $N_p = 10\,000$ particles following the statistical distribution detailed in Chapter 7, and subjected to an environment characterized by highly coupled multidimensional mechanisms.

First, the particles experience continuous surface attrition modeled as a drift in the geometric phase space. In industrial cyclones, macroscopic empirical correlations, such as those estab-

lished by Reppenhagen and Werther (2000)[12] as well as Ghadiri and Zhang (2002)[11], demonstrate that the total abrasive mass loss scales with the square of the characteristic gas velocity. To embed this kinetic-energy-driven attrition into the CQMOM phase space, the macroscopic correlation is localized. Assuming the microscopic mass attrition rate ($\dot{m}_p$) scales with the particle cross-sectional area (d^2) and the local specific kinetic energy of the slip velocity ($\|\mathbf{u}_p - \mathbf{u}_f\|^2$), it follows that $\dot{m}_p \propto -d^2\|\mathbf{u}_p - \mathbf{u}_f\|^2$. Relating this to the geometric rate of mass change ($\dot{m}_p = \rho_p \frac{\pi}{2} d^2 \dot{d}$) cancels the geometric d^2 dependencies, reducing the particle shrinking rate to a direct function of the squared relative velocity:

$$\dot{d} = -k_{\text{shear}}\|\mathbf{u}_p - \mathbf{u}_f\|^2 \quad (8.1)$$

Simultaneously, this abrasive action wears down the sharp edges of the oblate fragments, driving a continuous geometric relaxation toward a spherical shape:

$$\dot{\chi} = \frac{1}{\tau_{\text{shape}}}(1 - \chi) \quad (8.2)$$

Second, the particles undergo discrete structural fragmentation. To strictly enforce mass conservation during binary symmetric breakage, the daughter particle diameter (d_{daughter}) is dictated by the parent's volume, yielding:

$$d_{\text{daughter}} = \frac{d_{\text{parent}}}{\sqrt[3]{2}} \quad (8.3)$$

To establish a direct physical competition within the geometric phase space, the discrete fragmentation kernel is designed to drive the aspect ratio toward an infinitely oblate limit ($\chi \rightarrow 0$). This discrete flattening mechanism actively opposes the continuous aerodynamic spheroidization ($\chi \rightarrow 1$) governed by Equation 8.2. Specifically, daughter particles assume a reduced aspect ratio proportional to the parent via a flattening coefficient $\alpha = 0.5$, such that:

$$\chi_{\text{daughter}} = \alpha \chi_{\text{parent}} \quad (8.4)$$

Concurrently, fragmentation introduces variance into the kinematic space via the isotropic velocity recoil $\mathbf{v}_{\text{recoil}}$. Mathematically, this explicitly cross-coupled formulation, illustrated conceptually in Figure 8.2, requires the CQMOM solver to balance continuous kinetic-energy-driven geometric reduction, continuous aerodynamic variance dissipation, and discontinuous variance injection simultaneously across all five phase-space dimensions.

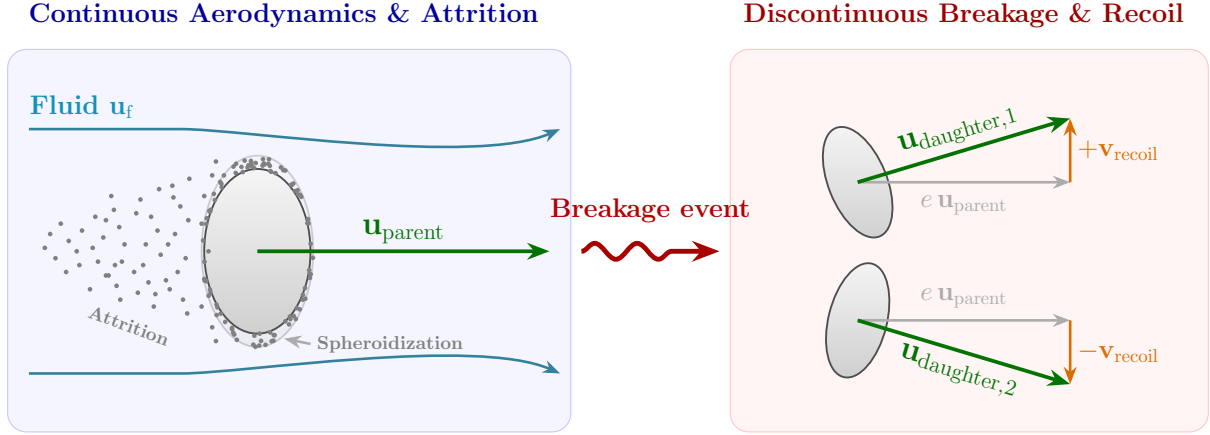


Figure 8.2 Illustration of the fully coupled dynamics test case featuring simultaneous v^2 -attrition, fragmentation and aerodynamic advection

8.2 Results and Analysis

8.2.1 Algorithmic Stability and Computational Efficiency

The numerical integration of this explicitly cross-coupled system exposes the underlying mathematical limitations of fully coupled CQMOM closures. Evaluated over the physical simulation time, the operator-splitting architecture of the HT method demonstrates clear numerical stability. By isolating the continuous advection from the discontinuous fragmentation into sequential integration steps via Strang splitting, the decoupling mitigates numerical stiffness and allows the Hankel matrices to remain strictly positive-definite. The HT solver successfully navigates the phase space utilizing a highly relaxed regularization threshold ($\text{rcond}_{\text{HT}} = 10^{-10}$), requiring no emergency fallbacks and maintaining full quadrature resolution throughout the simulation.

Conversely, the integration of the fully coupled MTE via the MT method induced substantial mathematical stiffness. Attempting to balance continuous v^2 -driven mass loss, continuous aerodynamic drag, and discontinuous recoil simultaneously within the explicit integrator forced the MT solver into severe matrix ill-conditioning. The solver systematically failed to maintain realizability, repeatedly triggering Wheeler inversion errors. To prevent simulation termination, the MT algorithm relied heavily on localized fallback inversions, frequently reducing the optimal 16-node quadrature down to 8, 4, and occasionally 2 nodes.

This operational stability directly impacts computational efficiency. The Lagrangian MC benchmark required 21 s to process the population. Due to the repeated matrix conditioning

iterations and quadrature collapses, the MT solver required 156 s (2 minutes and 36 seconds). The HT solver executed the entire 5D phase-space evolution in 3 s—a 52-fold reduction in computational time compared to the explicit MT approach.

8.2.2 Macroscopic and Geometric Evolution

As presented in Figure 8.3, the total particle count (N) exhibits exponential growth consistent with a continuous binary breakage cascade. The geometric coupling is verified by the evolution of the total volume (V), mean diameter ($\langle d \rangle$), and mean surface area ($\langle A \rangle$). Because the attrition is driven by the slip kinetic energy, these macroscopic parameters do not decay as smooth exponentials; rather, they exhibit a wave-like trajectory. The mass loss accelerates when the oscillating fluid vortex creates a high slip velocity and flattens out when the particle velocity aligns with the fluid streamlines. The HT method successfully captures this complex aerodynamic-geometric coupling, closely matching the MC benchmark.

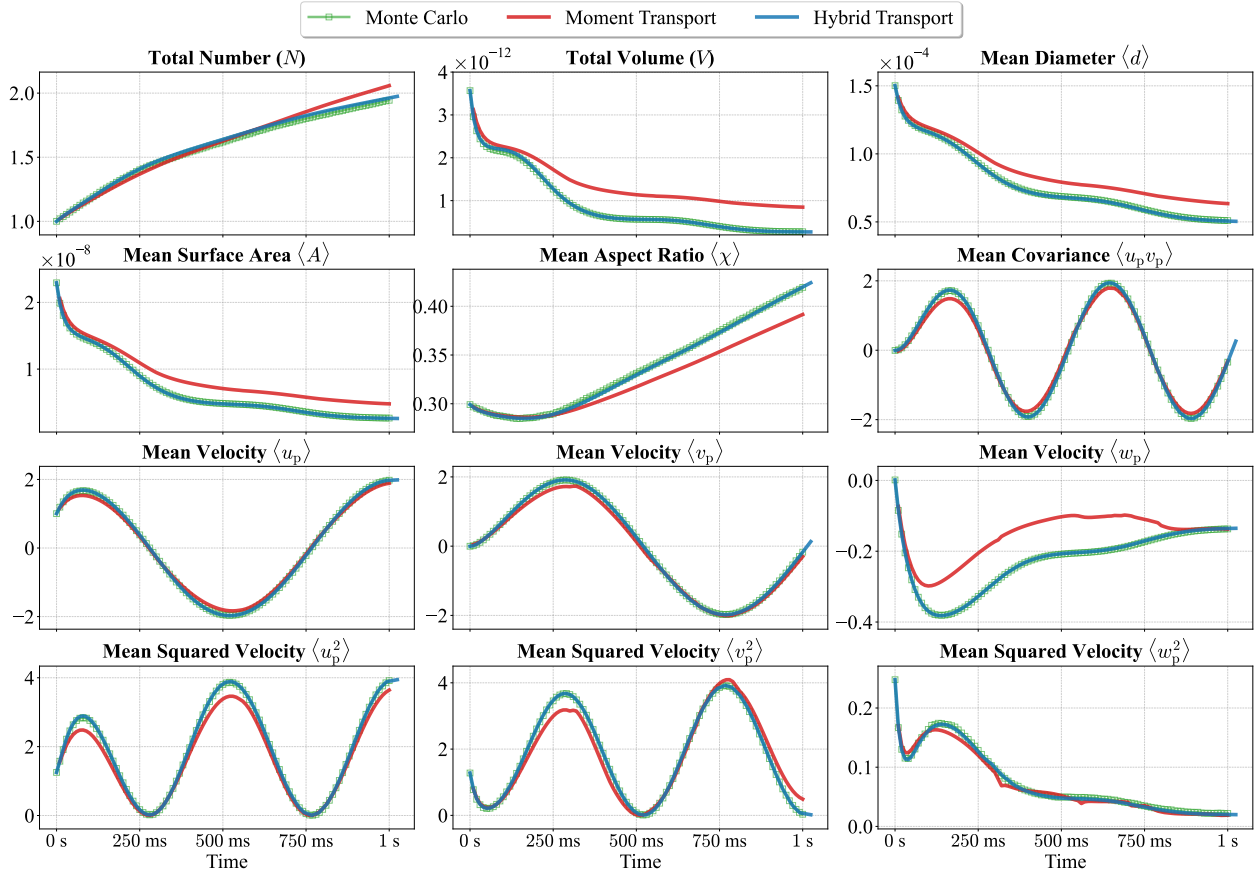


Figure 8.3 Temporal evolution of the primary geometric and kinematic moments for the fully coupled particle dynamics test case. Comparing the explicit MT and HT methods against MC benchmark

The consequences of the MT method's quadrature failures manifest distinctly in the geometric phase space. Because MT frequently reverts to a lower-order moment subset, it fails to resolve the velocity variance accurately. This artificially underestimates the local slip kinetic energy, causing the MT solver to systematically under-predict the physical abrasion. Consequently, the MT method erroneously overpredicts the retained volume (V) and mean diameter ($\langle d \rangle$), highlighting that numerical stiffness in the kinematic space fundamentally corrupts physical mass conservation in the geometric space.

Furthermore, while the mean planar kinematic drift ($\langle u_p \rangle$, $\langle v_p \rangle$) is accurately captured by both solvers, the MT method fails to correctly model the vertical settling velocity ($\langle w_p \rangle$). The MT trajectory exhibits a massive artificial plateau, whereas the HT method tracks the MC reference stably.

8.2.3 Kinematic Variance and Thermal Energy Conservation

The limitations of the explicit MT approach become apparent upon analysis of the granular temperature profiles (Θ_x , Θ_y , Θ_z) detailed in Figure 8.4. Accurately predicting the macroscopic granular temperature and kinetic energy moments requires maintaining the integrity of the phase-space cross-covariances under simultaneous variance dissipation and injection.

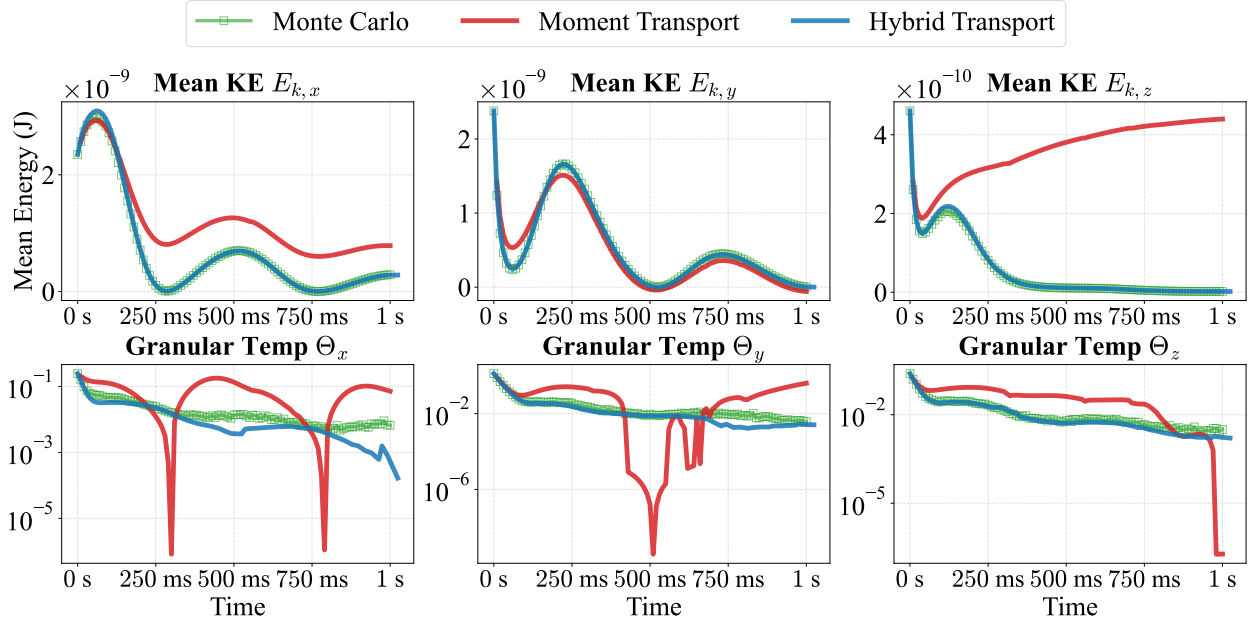


Figure 8.4 Temporal evolution of the mean kinetic energy and granular temperature (Θ). The HT method tracks the MC benchmark closely, whereas the explicit MT method exhibits severe numerical deviations and unphysical energy leaks associated with quadrature fallback mechanisms induced by Hankel-matrix ill-conditioning

The explicit MT solver exhibits severe collapses, dropping the granular temperature to unphysical values correlated with the solver triggering low-order fallback inversions. Collapsing the quadrature to a minimal node representation drops the velocity variance near zero.

This numerical failure is further exacerbated by an unphysical energy leak in the unforced z -axis. The MC and HT methods correctly model the dissipation of the initial vertical kinetic energy ($E_{k,z}$), decaying smoothly as aerodynamic drag acts on the settling particles. However, because the CQMOM algorithm relies on sequential conditional inversion, the severe matrix ill-conditioning generated in the highly coupled x and y planes propagates directly into the vertical dimension. As the solver triggers localized quadrature fallbacks and applies heavy algebraic regularization ($\mathbf{rcond}_{\text{MT}} = 0.9$) to prevent a total singularity, the conditional nodes for the z -axis are artificially distorted. This loss of matrix rank forces a spurious widening of the vertical velocity abscissas to satisfy the global moment constraints, causing the MT prediction for $E_{k,z}$ to erroneously diverge upward to 4×10^{-10} J.

The HT formulation systematically avoids the severe numerical instability inherent to the explicit MT approach. By employing Strang splitting, the decoupling preserves the strict positive-definiteness of the Hankel matrices, allowing the CQMOM inversion to maintain full multidimensional node resolution at standard time steps. Consequently, the HT method successfully captures the initial stochastic thermal floor established by the breakage recoil, avoiding the zero-variance singularity and the severe unphysical energy leaks observed in the MT solver.

However, an examination of the granular temperature profiles (Θ_x, Θ_y) reveals that the HT prediction does not accurately track the MC benchmark throughout the entirety of the simulation. After $t = 400$ ms, the HT trajectory exhibits a slow downward drift, underpredicting the steady-state variance. This deviation highlights a fundamental limitation of applying CQMOM closures to highly discontinuous, non-equilibrium regimes. The simultaneous application of v^2 -driven attrition, aerodynamic drag, and stochastic recoil generates a severely non-smooth underlying distribution.

Ultimately, while the exact mathematical mechanism driving this variance leakage remains an open question for future investigation, the data indicates an absolute resolution limit of the globally integrated moment set when processing competing, extreme-gradient phase spaces. Nevertheless, despite this inherent limitation, the HT method entirely circumvents the explicit matrix singularity failures of fully coupled integration, achieving significantly improved macroscopic fidelity and algorithmic stability over traditional solvers.

CHAPTER 9 CONCLUSION AND PERSPECTIVES

9.1 Summary of Works

This thesis establishes a comprehensive 5D macroscopic moment framework for resolving the complex multidimensional phase-space dynamics of non-spherical particle populations. The foundational effort focused on overcoming the severe dimensional curse associated with the PBE. By implementing the CQMOM, the framework replaces the exponential computational scaling of traditional TP grids with an adaptive, hierarchical inversion strategy.

Initial verification cases utilizing one-dimensional continuous growth and two-dimensional harmonic oscillators confirmed that the dynamically adapting Wheeler algorithm accurately tracks strongly correlated physical manifolds. It intelligently sheds redundant degrees of freedom when conditional variances collapse, while strictly preserving the mass and higher-order mixed moments of the NDF.

To elevate the solver to physically realistic industrial flows, the mathematical modeling was extended to accommodate the orientation-dependent aerodynamic forces acting upon oblate spheroids. A rigorous timescale analysis quantified the disparity between the rotational and translational relaxation times, validating the QSO assumption for the Stokes and intermediate inertial regimes. This critical physical insight permitted a safe dimensional reduction, yielding a highly tractable 5D state space (d, χ, u_p, v_p, w_p) where particle acceleration is explicitly governed by shape-dependent broadside drag and gravity, entirely circumventing the need to track the high-frequency angular kinematics.

The crowning achievement of this work is the successful coupling of this 5D continuous aerodynamic advection with kinetic-energy-driven surface attrition and discrete, non-equilibrium stochastic breakage events. The comparative analysis between the explicit MT method and the split-operator HT method exposed the severe mathematical fragilities of fully coupled CQMOM closures.

Attempting to simultaneously balance continuous v^2 -driven mass loss against discontinuous variance injection forced the MT solver into extreme matrix ill-conditioning, ultimately triggering unphysical energy leaks (e.g., in the $E_{k,z}$ trajectories) and detrimental losses of realizability.

Conversely, the HT architecture demonstrated profound operational superiority. By mathematically isolating the continuous operators from the discontinuous events utilizing Strang splitting, the HT method preserved the strict positive-definiteness of the Hankel matrices.

This approach provided the macroscopic fidelity of a Lagrangian Monte Carlo benchmark at a fraction of the computational cost, establishing it as an essential methodology for explicitly cross-coupled, high-variance fragmentation regimes.

9.2 Limitations

While the proposed HT framework coupled with CQMOM demonstrates exceptional numerical stability and computational efficiency, its underlying physical and mathematical assumptions introduce specific limitations that must be acknowledged.

First, the aerodynamic formulation heavily relies on the QSO assumption. While this dimensional reduction is rigorously justified for microscopic particles settling in moderate or creeping flows, its validity diminishes in highly turbulent macroscopic regimes or for particles with massive rotational inertia ($St \gg 1$). In such environments, the tumbling timescale may become comparable to the translational advection, rendering the instantaneous broadside drag assumption physically inaccurate.

Second, the framework is strictly constrained to the dilute multiphase regime. The governing PBE and the utilized empirical oblate drag closures explicitly assume hydrodynamically isolated particles. Consequently, the current solver cannot accurately model dense granular flows where four-way coupling [38], lubrication forces, and continuous particle-particle collisions dictate the macroscopic momentum transfer [39].

Finally, a fundamental numerical limitation of the globally integrated moment set was identified during the fully coupled 5D simulations. In extreme non-equilibrium environments—where continuous v^2 -attrition and drag actively compete against discontinuous stochastic recoil—the underlying population develops a severely non-smooth, non-Gaussian distribution.

While the HT effectively captures the bulk macroscopic trajectories, the extreme tails of this chaotic phase space expose the inherent limits of finite-node moment reconstruction. In such highly non-equilibrium regimes, the solver yields a gradual artificial variance dissipation of the granular temperature (Θ)—a drift driven by fundamental quadrature closure error rather than temporal truncation, meaning it cannot be mitigated by simply reducing the integration time step.

Framework Limitations: Topological Bifurcations

While the HT operator-splitting architecture successfully stabilizes Eulerian moment closures in high-variance, discontinuous fragmentation regimes, the framework exhibits funda-

mental mathematical limitations when subjected to severe topological bifurcations. Because Eulerian moment methods rely on globally integrated, low-order polynomial bases, they inherently struggle to resolve populations that undergo drastic, non-linear phase-space deformations—such as splitting across a separatrix, clustering into disconnected attractors, or converging onto a limit cycle.

To isolate and evaluate the solver’s structural response to these fundamental topological challenges, the framework is tested against a canonical non-linear oscillator. Rather than simulating a specific physical flow, this idealized mathematical surrogate serves as a strict, generalized test case for bifurcation dynamics. Specifically, it forces an initial continuous population to diverge from an unstable equilibrium and converge onto a stable limit cycle, ultimately stretching into a hollow annular distribution.

The dynamics of this topological test case are governed by a continuous 2D phase-space advection field (ξ_1, ξ_2) , defined by the following coupled non-linear ordinary differential equations:

$$\dot{\xi}_1 = \mu\xi_1 - \xi_2 - (\xi_1^2 + \xi_2^2)\xi_1 \quad (9.1)$$

$$\dot{\xi}_2 = \xi_1 + \mu\xi_2 - (\xi_1^2 + \xi_2^2)\xi_2 \quad (9.2)$$

where the bifurcation parameter is strictly set to $\mu = 1$, dictating a supercritical Hopf bifurcation that establishes a stable limit cycle at a radius of $r = 1$. A phase portrait is shown in Figure 9.1.

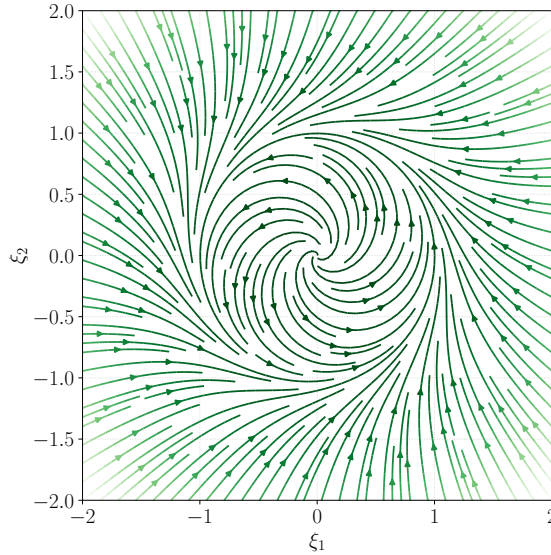


Figure 9.1 Phase portrait of the continuous advection field

The dispersed phase is initialized as an isotropic Gaussian distribution centered directly on the unstable origin, defined by the initial mean vector and covariance matrix:

$$\boldsymbol{\mu}_{t=0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{\Sigma}_{t=0} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (9.3)$$

Resolving this rotational topology presents a distinct mathematical challenge for globally integrated Eulerian moment methods, as a continuous 1D ring must be dynamically represented by a finite set of discrete quadrature nodes.

For the split-operator HT method, the spatial decoupling successfully allows the discrete quadrature nodes to continuously advect along the circular trajectory while maintaining geometric symmetry. However, because a continuous annular distribution is being approximated by a sparse set of rotating Dirac delta functions, the globally integrated macroscopic moments naturally oscillate around the true MC baseline. This behavior is a direct, fundamental artifact of the discrete quadrature representation. As the node count is systematically increased, the solver does not alter the geometric footprint of the ring; rather, it populates the exact same annular trajectory with a higher density of discrete points. This improved angular resolution smoothly distributes the mass along the orbit, heavily dampening the numerical oscillations and allowing the HT moment predictions to stably converge toward the ground truth as illustrated in Figure 9.2. Conversely, the explicit MT formulation with 2×2 nodes fails to resolve this rotational advection.

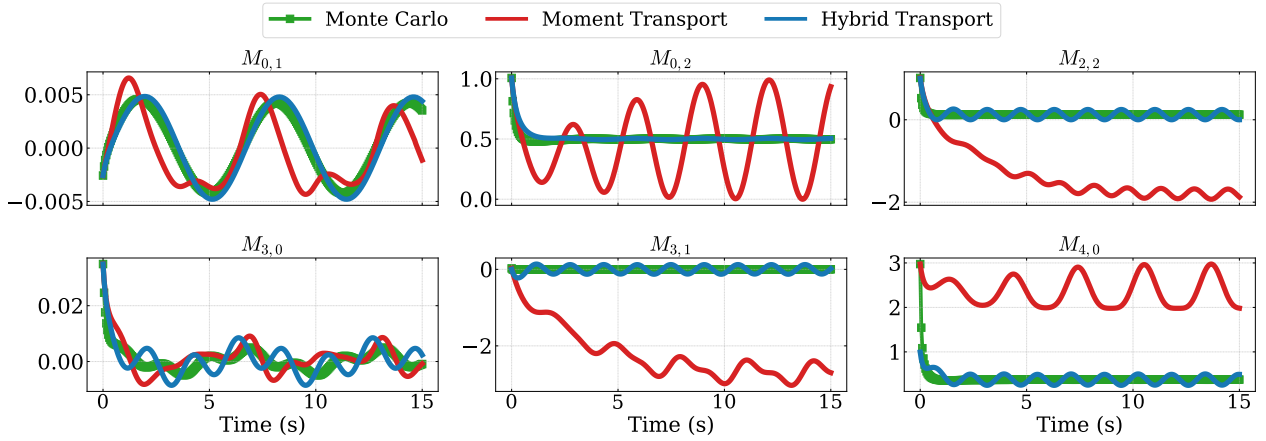


Figure 9.2 Temporal evolution of the macroscopic moments for HT and MT solvers for a simulation time of 15 s and a time step $\Delta t = 50$ ms

Rather than smoothly translating along the limit cycle, the MT quadrature nodes exhibit spurious, unphysical oscillations (Figure 9.3). This inability to properly advect the discrete

weights shatters the physical symmetry of the distribution, causing the predicted global moments to continuously diverge from the real trajectory.

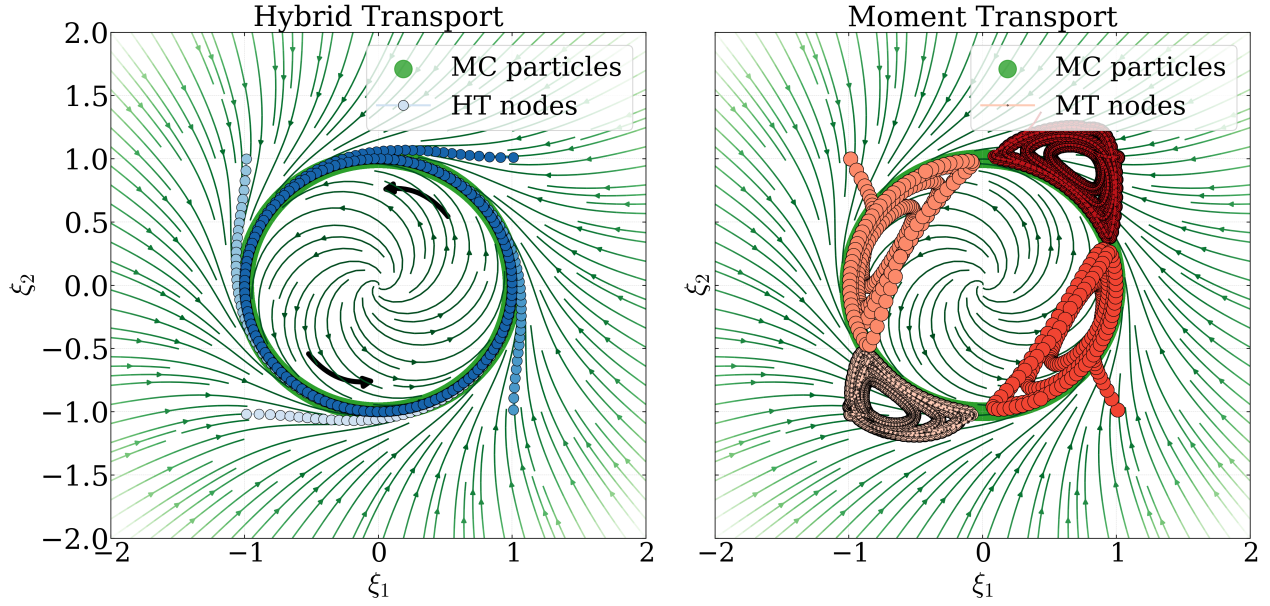


Figure 9.3 Comparative topological response of the HT and MT solvers with 2×2 nodes to a stable limit cycle. While the HT quadrature nodes (left) correctly translate along the continuous rotational streamlines, the explicit MT nodes (right) become artificially anchored, oscillating spuriously and failing to resolve the hollow annular phase space. Marker areas represent instantaneous discrete quadrature weights

Furthermore, the MT formulation demonstrates a fatal inability to scale. While the HT method stably improves with higher-order quadratures, attempting to resolve this complex annular topology in the MT solver by increasing the node count induces immediate matrix ill-conditioning. The fully coupled SSP-RK3 integrator cannot mathematically balance the highly non-linear, stiff rotational fluxes within a high-order polynomial basis, causing the adaptive Wheeler inversion to catastrophically fail and terminate the simulation. This severe numerical breakdown is captured globally in the comparative error heatmaps (Figure 9.4).

Ultimately, this analysis establishes an absolute operational boundary for macroscopic moment closures. While the HT formulation provides exceptional mathematical stability—successfully processing complex rotating limit cycles at the cost of expected, node-dependent moment oscillations—traditional explicit integration (MT) fundamentally breaks down in severely rotational phase spaces, underscoring the absolute necessity of operator splitting for multi-dimensional CFD applications.

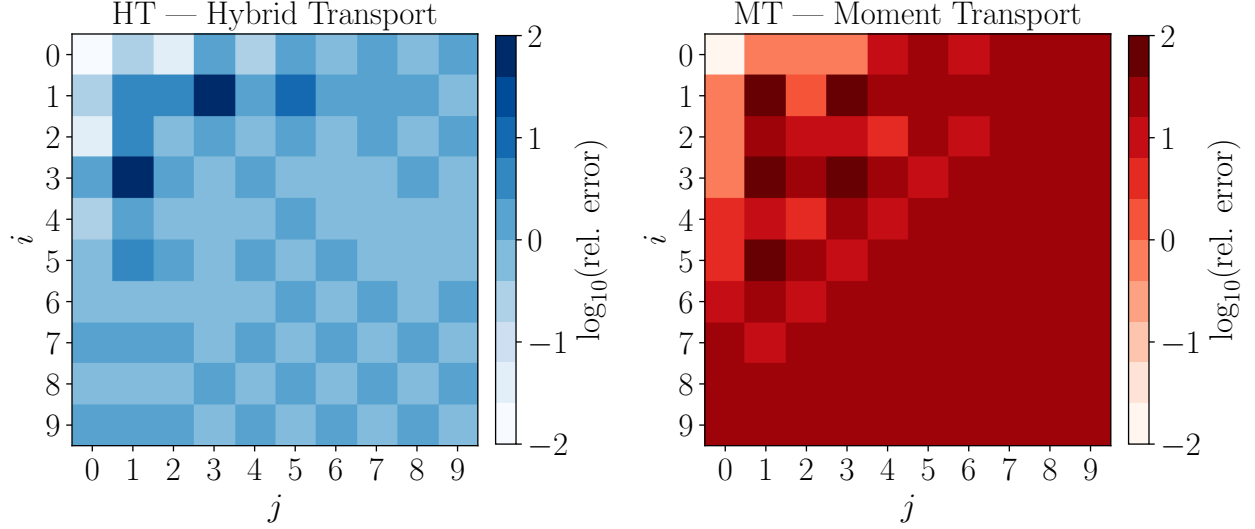


Figure 9.4 Comparative heatmap of the relative error across the moment set $M_{i,j}$ compared to MC benchmark. The direct MT formulation rapidly accumulates massive error due to matrix ill-conditioning, whereas the split-operator HT architecture maintains stable moment transport

9.3 Perspectives for Future Research

To directly address the current limitations and further expand the robust applicability of the moment-based solver, three primary algorithmic avenues for future research are proposed.

Extension to the generalized quadrature method of moments (GQMOM):

The current CQMOM implementation, utilizing the Wheeler algorithm, is mathematically constrained by the strict requirement of using exactly $2N$ moments to reconstruct N quadrature nodes. To surpass the quadrature closure error observed in the fully coupled phase space, the framework can be extended to integrate the GQMOM inversion algorithm.

Rather than being restricted by an exact moment-to-node ratio, GQMOM provides the mathematical flexibility to expand the quadrature representation to an arbitrary number of nodes by incorporating prior physical information regarding the underlying “shape” of the NDF. By formulating an over-determined system that perfectly preserves the transported moments while utilizing this shape constraint, GQMOM can provide a more physically faithful representation of the extreme phase-space tails without requiring highly sensitive, higher-order mixed moments.

Extension to the conditional hyperbolic quadrature method of moments:

While the HT method successfully prevents matrix collapses during discontinuous break-

age, standard CQMOM closures still inherently struggle with variance preservation when differential drag and attrition forces severely distort the physical manifold.

Because the split-operator architecture successfully decouples the phase-space transport, it naturally facilitates a direct upgrade to a conditionally hyperbolic closure. By explicitly formulating the velocity variance (granular temperature) as a strictly transported, conserved macroscopic variable rather than a derived quadrature property, conditional hyperbolic quadrature method of moments (CHyQMOM) is a good candidate to prevent the artificial variance dissipation observed in the HT solver, ensuring the perfect preservation of kinetic energy in highly inertial, multimodal particulate flows.

Extension to Multidimensional Physical Space Advection:

While the current framework has been validated in a zero-dimensional spatial context to isolate and resolve the severe mathematical stiffness of the internal phase-space operators, the ultimate objective for industrial computational fluid dynamics remains the simulation of spatially varying, multidimensional flows.

The necessary progression of this research is to embed the 5D HT-CQMOM architecture into a fully coupled spatial Eulerian solver. This requires extending the macroscopic moment equations to include physical spatial fluxes, $\nabla_{\mathbf{x}} \cdot (\mathbf{u}_p M_{\mathbf{k}})$. Because the split-operator HT scheme successfully stabilizes the internal source terms and breakage mechanics, future efforts can concentrate directly on the distinct numerical challenges of spatial advection. Specifically, this involves the implementation of high-resolution, realizability-preserving finite volume schemes to prevent the corruption of the moment set as the highly inertial, non-spherical particle populations are transported across complex computational grids.

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