Titre: Title:	Wave-DNA: a software tool for simulating nonlinear acoustic waves emitted by moving boundaries
Auteurs: Authors:	Sören Schenke, Fabian Sewerin, Berend van Wachem, & Fabian Denner
Date:	2025
Type:	Article de revue / Article
Référence: Citation:	Schenke, S., Sewerin, F., van Wachem, B., & Denner, F. (2025). Wave-DNA: a software tool for simulating nonlinear acoustic waves emitted by moving boundaries. SoftwareX, 30, 102101 (6 pages). https://doi.org/10.1016/j.softx.2025.102101

SoftwareX 30 (2025) 102101

Contents lists available at ScienceDirect

SoftwareX

journal homepage: www.elsevier.com/locate/softx

Original software publication

Wave-DNA: A software tool for simulating nonlinear acoustic waves emitted by moving boundaries

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ARTICLE INFO

Keywords:
Nonlinear acoustics
Kuznetsov equation
FDTD method
Doppler effect

ABSTRACT

The investigation of nonlinear acoustics requires sophisticated and tailored methods to advance the state of the art. Here we present the software tool Wave-DNA for the simulation of nonlinear acoustic waves emitted by stationary or moving boundaries in quiescent or moving fluids, assuming a one-dimensional or spherically-symmetric geometry. At its core, Wave-DNA is based on the convective Kuznetsov equation, a second-order nonlinear acoustic wave equation that accounts for the background flow and may be reduced to alternative wave equations by applying simplifying assumptions. A tailored finite-difference time-domain method with time-dependent coordinate transformation enables the accurate simulation of acoustic waves emitted by moving boundaries.

Code metadata

Current code version	v1.3
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-24-00360
Legal Code License	MIT License
Code versioning system used	Git
Software code languages, tools, and services used	C
Compilation requirements, operating environments & dependencies	GCC (or a similar C compiler)
Link to developer documentation/manual	https://github.com/polycfd/Wave-DNA/blob/main/documentation/WaveDNA-Documentation.pdf
Support email for questions	Please use the GitHub issue tracker

1. Motivation and significance

Acoustic waves are ubiquitous in nature and technology and play a pivotal role across a broad spectrum of disciplines, ranging from seismology and medical imaging to the remote sensing of ocean currents and industrial non-destructive testing. Even though acoustics and, in particular, sound have been studied for centuries, the complicated nonlinear interactions between acoustic waves, moving boundaries and moving fluids is an active field of research [1–7]. Acoustic waves are affected by the properties of the fluid they propagate in, the motion of their source and the prevailing flow conditions [8,9], which makes isolating and distinguishing the physical mechanisms that are responsible for their modulation essential for harnessing the information they carry in technical applications. For instance, the realistic modeling and detailed understanding of acoustic wave propagation and scattering can improve imaging techniques and the interpretation of their results in medical ultrasound applications [10,11], as well as the study of marine environments [12]. More generally, any acoustic monitoring and remote sensing application stands to benefit from new insights into the modulation of acoustic waves emitted by moving boundaries and propagating in moving fluids [13].

However, in classical acoustics, the acoustic wave is commonly assumed to be plane, the emitter to be rigid, and the carrier flow to be quiescent [14,15]. Although these simplifications are justified for many applications, they often stand in direct contradiction to reality, since conventional acoustic emitters, such as an ultrasound transducer or a simple loudspeaker, feature a moving wave-emitting boundary

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https://doi.org/10.1016/j.softx.2025.102101
Received 2 July 2024; Received in revised form 7 February 2025; Accepted 14 February 2025
Available online 26 February 2025

that displaces the adjacent fluid, introducing Doppler shifts [1,4] and amplitude modulations [7]. Moreover, while the acoustic impedance of a plane wave is a real-valued function of the fluid density and speed of sound, the acoustic impedance experienced by an acoustic wave with a curved wavefront is complex [15], an effect that becomes dominant for emitters that are smaller than the wavelength of the acoustic waves they emit. At the moment, the understanding of these effects and their interrelation is incomplete, particularly in the realm of nonlinear acoustics. Developed with the objective of closing this gap in our understanding, Wave-DNA offers a state-of-the-art software tool for the study of acoustic waves emitted by moving boundaries, featuring a tailored finite-difference time-domain method [16] and supporting different acoustic wave equations.

2. Software description

Wave-DNA, which is short for *Wave Doppler effects in Nonlinear Acoustics*, is a simulation tool for one-dimensional and spherically-symmetric nonlinear acoustic waves in transient and spatially variable background flow fields. The propagation of acoustic waves in a quiescent or moving background fluid is modeled by a convective form of the lossless Kuznetsov wave equation [6]. The background flow field in which the acoustic waves propagate is treated as an input to the wave solver; it may be obtained from analytical considerations, numerical simulations, or experimental measurements. The moving boundary represents a moving wave emitter or scatterer, which may move relative to the fluid or displace the fluid. The motion of the domain boundary is conveniently taken into account by a generic coordinate transformation of the governing wave equation that relates the moving physical domain to a fixed computational domain. This technique facilitates accurate numerical solutions of the wave propagation problem without the necessity to interpolate data between moving grid points in the physical domain. The numerical technique is based on an explicit finite-difference time-domain (FDTD) method that is equipped with a predictor–corrector method to counteract the onset and growth of dispersive numerical noise due to broad frequency bands or shock waves [16].

2.1. Software architecture

Wave-DNA is written in C and, aside from the C standard library, has no external dependencies. Scripts to compile Wave-DNA in debug or release mode using CMake are available. The user communicates all desired options for a simulation to Wave-DNA via a human-readable text file, which is read at the beginning of each simulation. Wave-DNA can output the results for the acoustic pressure, velocity and other variables of interest in the form of space-dependent results at predefined time instants, in the form of time-dependent results at predefined spatial locations, or as space–time plots. The repository of Wave-DNA contains Python scripts to visualize the simulation results of the provided examples, which may be adapted by the user to visualize their own simulation results.

Structures are used in Wave-DNA to group variables and functions, and to provide a modular layout of the code. There are four main structures, the instances of which are created in `main.c`:

- `struct DNA_RunOptions` contains variables and function pointers associated with the run options.
- `struct DNA_FluidProperties` contains the fluid properties, such as the background density and speed of sound.
- `struct DNA_Fields` contains all scalar fields for the computational grid, the background flow field and the acoustic perturbation field.
- `struct DNA_MovingBoundary` contains the variables associated with the moving boundary of the physical domain.

Table 1
First- and second-order wave equations currently available in Wave-DNA.

Wave equation	Order	u_0	β	$\mathcal{L}$
Convective Kuznetsov equation [6]	2	$\neq 0$	$\neq 0$	$\neq 0$
Standard Kuznetsov equation [17,18]	2	$= 0$	$\neq 0$	$\neq 0$
Convective Westervelt equation	<2	$\neq 0$	$\neq 0$	$= 0$
Standard Westervelt equation [19]	<2	$= 0$	$\neq 0$	$= 0$
Convective linear wave equation [20,21]	1	$\neq 0$	$= 0$	$= 0$
Standard linear wave equation	1	$= 0$	$= 0$	$= 0$

The declarations of all constants, macros, structures and functions, as well as the required headers of the C standard library, are contained in three header files:

- `DNA.h` declares all structures used throughout the program.
- `DNA-functions.h` declares the function prototypes.
- `DNA-constants.h` contains macros of constants and mathematical operators. To enable a straightforward change in floating-point precision, such as an extension to quad precision, regularly used mathematical functions of the C standard library and the data type `double` are renamed (for instance, `DNA_SQRT(a)` replaces `sqrt(a)` and `DNA_FLOAT` replaces `double`) and consistently used throughout the code.

A description of all options, functions and structures used in Wave-DNA can be found in the Wave-DNA documentation.

2.2. Software functionalities

Wave-DNA models the formation and propagation of nonlinear acoustic waves in a quiescent or moving fluid along the spatial coordinate r by a first- or second-order wave equation, which may account for the influence of a background flow. To this end, the velocity $u = u_0 + u_1$, the pressure $p = p_0 + p_1$ and the density $\rho = \rho_0 + \rho_1$ are formally decomposed into background flow contributions, denoted by the subscript 0, and acoustic perturbations, denoted by the subscript 1. The acoustic perturbations, which are described by the acoustic velocity potential ϕ_1, defined as $u_1 = \partial\phi_1/\partial r$, are assumed to capture all compressibility effects of the barotropic fluid, with $\mathrm{d}p/\mathrm{d}\rho = c_0^2 \approx p_1/\rho_1$. The background flow is assumed to be inviscid, with a constant density ρ_0 and speed of sound c_0, and may be spatially non-uniform and time dependent. Under these assumptions, the acoustic waves are modeled by the lossless convective Kuznetsov equation for the acoustic wave potential ϕ_1 [6],

$$\left(1 + \frac{2\beta}{c_0^2}\frac{\mathrm{D}\phi_1}{\mathrm{D}t}\right)\frac{\mathrm{D}^2\phi_1}{\mathrm{D}t^2} + \frac{2}{\rho_0}\frac{\mathrm{D}\mathcal{L}}{\mathrm{D}t} + \frac{\partial u_0}{\partial r}\left(\frac{\partial\phi_1}{\partial r}\right)^2 = c_0^2\nabla_{\mathrm{A}}^2\phi_1, \tag{1}$$

where β is the nonlinearity coefficient, $\nabla_{\mathrm{A}}^2 = \partial^2/\partial r^2 + (1/A)(\partial A/\partial r)\,\partial/\partial r$ is the Laplace operator accounting for a potentially spatially variable cross-sectional area A, and $\mathrm{D}/\mathrm{D}t = \partial/\partial t + u_0\partial/\partial r$ denotes the material derivative. The Lagrangian density $\mathcal{L}$, which represents the difference between the acoustic kinetic and potential energy densities, is defined as

$$\mathcal{L} = \frac{\rho_0}{2}\left(\frac{\partial\phi_1}{\partial r}\right)^2 - \frac{\rho_0}{2c_0^2}\left(\frac{\mathrm{D}\phi_1}{\mathrm{D}t}\right)^2. \tag{2}$$

In Eq. (1), the first term contains the cumulative nonlinearity, the second term contains the local nonlinearity, and the third term contains the convective nonlinearity arising from the interaction of the flow field and the acoustic wave. A detailed derivation of the convective Kuznetsov equation from first principles based on perturbations of the continuity and momentum equations can be found in the supplementary material of Ref. [6].

Depending on the modeling assumptions and background flow field, different wave equations can be obtained on the basis of Eq. (1), summarized in Table 1. Westervelt-type equations are obtained by assuming that the acoustic velocity and pressure are in phase ($\mathcal{L} = 0$) and linear wave equations are obtained by neglecting both cumulative and local nonlinearities ($\beta, \mathcal{L} = 0$).

To account for a moving wave-emitting boundary, the governing wave equation, Eq. (1), is transformed from the physical domain with a moving wave-emitting boundary $R(t)$ and a stationary boundary R_{stat}, to a stationary computational domain with fixed left and right boundaries $\mathcal{X}_R$ and $\mathcal{X}_\infty$, by a time-dependent linear coordinate transformation,

$$\xi(r,t) = \mathcal{X}_\infty + \left(r - R_{\text{stat}}\right) \frac{\mathcal{X}_\infty - \mathcal{X}_R}{R_{\text{stat}} - R(t)}. \tag{3}$$

In this stationary computational domain, the wave equation is discretized and solved on a spatially uniform grid using an explicit FDTD method [16]. This FDTD method is based on central differences in space and a predictor–corrector method [22,23] to suppress any dispersive numerical noise. A wave-scattering or wave-absorbing [24] boundary condition may be applied at the non-emitting boundary of the domain.

2.3. Software limitations

The implementation of Wave-DNA is subject to a number of limitations in its current form, in addition to the inherent limitations of the considered wave equation (see Table 1). The considered wave-flow system is limited to one spatial dimension and is one-way coupled, since the convective wave equation couples the behavior of the acoustic waves to the background flow, but not vice versa. Consequently, any modulation of the fluid flow by the acoustic waves is neglected. Moreover, thermoviscous dissipation is currently not taken into account by Wave-DNA, but may be added in the form of a source term that is based on the time derivative of the Laplacian of the acoustic potential [25,26]. Nevertheless, the numerical dissipation of the employed FDTD method is sufficient to predict the attenuation of shock waves, as demonstrated in Section 3.1. Lastly, Wave-DNA currently supports boundary conditions at which acoustic waves reflect perfectly (i.e., the wave-scattering boundary condition) or through which acoustic waves leave the computational domain (i.e., the wave-absorbing boundary condition), but does not include a partially reflecting boundary condition.

3. Illustrative examples

We demonstrate the capabilities of Wave-DNA using three representative examples. These examples are, alongside other examples, included in the Wave-DNA repository, to demonstrate the capabilities and verify the correct functionality of Wave-DNA.

3.1. Formation and attenuation of a shock wave

The formation and attenuation of a shock wave is a classical example of nonlinear acoustics. In the absence of sufficient thermoviscous dissipation, the wave progressively steepens and eventually forms a shock wave as a result of the constitutive nonlinearity of the fluid. We consider here an initially sinusoidal acoustic wave, emitted by a planar emitter into a quiescent and inviscid fluid. The wave is emitted at the left boundary and travels to the right. The excitation frequency f_a, the excitation amplitude Δp_a, and the nonlinearity coefficient β are set such that the shock-formation distance is [27]

$$x_\text{sh} = \frac{\rho_0 c_0^3}{2\pi \beta f_\text{a} \Delta p_\text{a}} = 10. \tag{4}$$

The progressively steepening wave first starts to develop a discontinuity at the shock-formation distance x_sh and, subsequently, the wave profile approaches asymptotically the analytical solution for the peak pressure $\hat{p}_1 = \pi \Delta p_\text{a}/(1 + x/x_\text{sh})$ of Fay [28], as the wave evolves into a fully developed sawtooth shape. Fig. 1 shows that Wave-DNA predicts the development and decay of the shock wave accurately, approaching the Fay envelope after the shock wave has started to form. It is noted that the predictor–corrector method drives the attenuation associated with the dissipation across the shock front [16].

3.2. Pulsating spherical emitter

Following the recent work of Denner [7], we consider a spherical emitter that pulsates with angular frequency $\omega_\text{b} = 2\pi f_\text{b}$. The time-dependent radius of this emitter is defined as $R(t) = R_0 + \Delta \dot{R}_\text{b} \sin(\omega_\text{b} t)/\omega_\text{b}$, where $\Delta \dot{R}_\text{b} = c_0/4$ is the velocity amplitude of the pulsation. The emitter emits small-amplitude acoustic waves with frequency $f_\text{a} = 10 f_\text{b}$ and has an initial radius of $R_0 = \lambda_\text{a}/2$, where $\lambda_\text{a} = c_0/f_\text{a}$ is the acoustic wavelength. Fig. 2 shows the wave characteristics in the space–time plane for three different cases: (a) the emitter has a constant radius ($\Delta \dot{R}_\text{b} = 0$, $u_0 = 0$); (b) the emitter oscillates but does not induce a flow ($\Delta \dot{R}_\text{b} = c/4$, $u_0 = 0$); (c) the emitter oscillates and induces a corresponding flow ($\Delta \dot{R}_\text{b} = c/4$, $u_0 \neq 0$). In addition, Fig. 3 shows the spatial profile of the acoustic pressure at $f_\text{a} t = 10$. The pressure of the acoustic waves emanating from the emitter with constant radius show the decay expected for a diverging spherical wave, with $p_1 \propto 1/r$. Setting the boundary of the emitter in motion, but neglecting the induced flow, different parts of the acoustic wave are emitted at different emitter radii, giving the spatial pressure profile a more complicated shape. Taking, in addition to the pulsation of the emitter, also the flow induced by this pulsation into account, the emitted acoustic wave propagates through a non-uniform flow field. As a consequence, the spatial pressure profile exhibits a phase shift and an amplitude modulation, resulting from a nonlinear interaction between the acoustic wave and the background flow [6,7].

3.3. Acoustic black hole analogue

This example shows how Wave-DNA can be used to simulate the propagation of acoustic waves in a spherical acoustic black hole analogue [21], which we employed to study the modulation of acoustic waves in accelerating flows [6]. This acoustic black hole analogue and its counterpart, the acoustic white hole analogue, provide convenient model systems for the analysis of acoustic waves in accelerating flows, since they allow to trap a wave characteristic at the point of sonic transition (i.e., the sonic horizon), where it is subject to a non-zero background flow acceleration. Due to this non-zero acceleration, neighboring wave characteristics diverge away from the sonic horizon. Fig. 4 shows (a) the space–time diagram and (b) the instantaneous acoustic pressure profiles for such a spherical acoustic black hole analogue. The entire physical domain in Fig. 4 is initially located outside the acoustic black hole. Subsequently, the moving wave-emitting boundary collapses and eventually passes the sonic horizon while emitting outgoing acoustic waves.

4. Impact

Wave-DNA fills a gap in the open-source software domain by providing a simulation tool that features a tailored FDTD method and supports different first- and second-order wave equations for the study of acoustic waves emitted by moving boundaries in one spatial dimension. This enables the user to study nonlinear Doppler effects associated with moving wave emitters/scatterers and/or non-uniform background flow fields.

Wave-DNA has already been instrumental in the formulation of an acoustic black hole analogy for the study of nonlinear acoustics [21] and the subsequent identification and quantification of an acoustic pressure modulation driven by accelerating flows [6,7]. Three distinct features of Wave-DNA have enabled these new discoveries and promise to facilitate further research in nonlinear acoustics:

1. The employed wave equation, Eq. (1), accounts for the background flow ($u_0 \neq 0$), which may vary in time and space.
2. The user is free to define a flow field analytically, or use a flow field obtained from experimental measurements or other numerical simulations, because the employed wave equation, Eq. (1), does not assume a particular flow field.

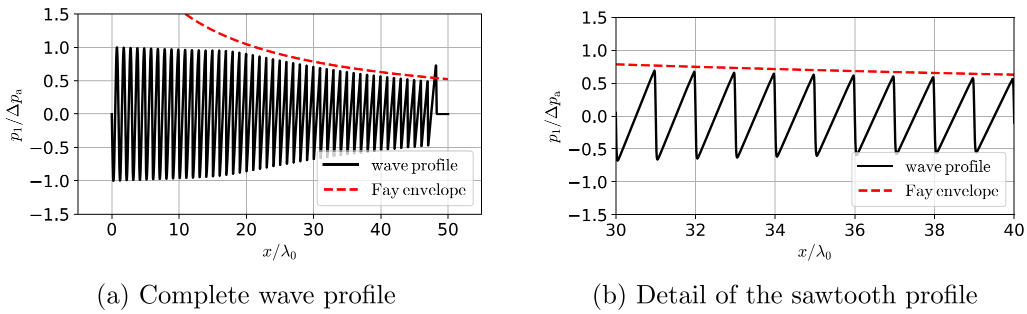

Fig. 1. An initially sinusoidal wave that evolves to form a shock wave. The analytical solution of the pressure amplitude of Fay [28] is shown for reference.

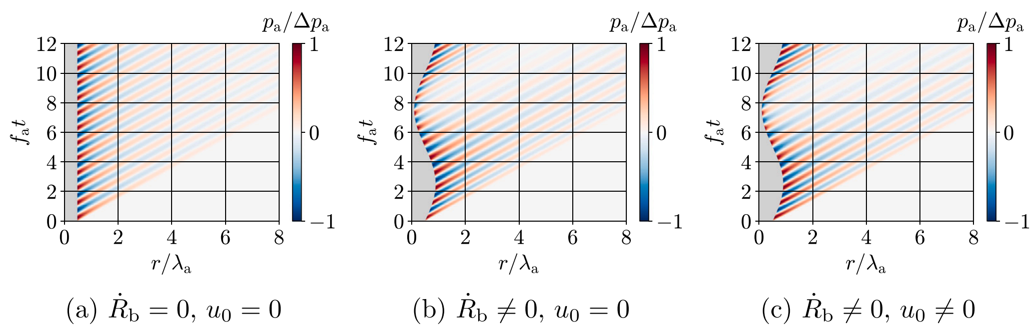

Fig. 2. Characteristics of the acoustic waves emitted by a spherical emitter in the space–time plane for three different cases: (a) The emitter has a constant radius and does not induce a flow, (b) the emitter oscillates but does not induce a flow, and (c) the emitter oscillates and induces a corresponding flow.

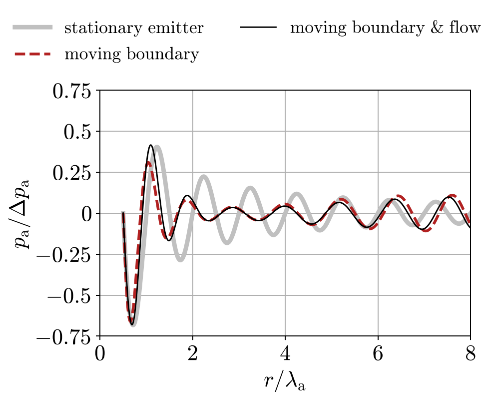

Fig. 3. Pressure profile of the acoustic wave emitted by a spherical emitter as a function of space at $f_a t = 10$ for the three scenarios shown in Fig. 2.

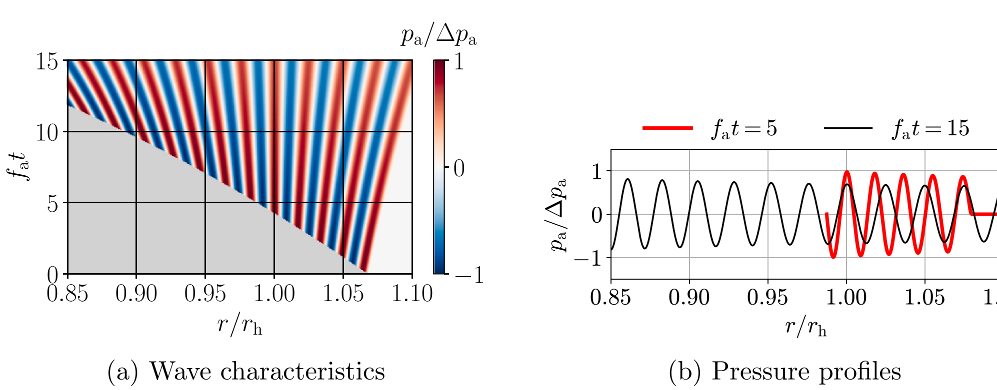

Fig. 4. Characteristics of the acoustic waves emitted by a spherical acoustic black hole analogue in the space–time plane and the corresponding instantaneous pressure profiles at two time instants.

3. The employed wave equation, Eq. (1), accounts for the complex impedance of curved waves and the resulting non-zero Lagrangian density ($\mathcal{L} \neq 0$).

This unique set of features allows in-depth quantitative analyses of, for instance, the Doppler-related generation of frequency sidebands [4], Doppler shifts driven by a moving wave-emitting boundary [1], and the influence of accelerating flows on the amplitude and shape of finite-amplitude acoustic waves [7]. Moreover, Wave-DNA allows to study the influence of the emitter size relative to the length of the emitted acoustic waves as a result of a complex acoustic impedance. These phenomena are difficult to measure and quantify experimentally and, as a consequence, not yet fully understood. Nevertheless, they are of direct relevance for a broad spectrum of applications, such as the highly nonlinear acoustic emissions of collapsing cavitation bubbles in medical high-intensity focused ultrasound applications [29,30] or the acoustic remote sensing of fast-moving objects [31]. Wave-DNA offers a tailored numerical framework to study these phenomena and to provide high-fidelity data, for example, for the training of machine learning algorithms.

Because Wave-DNA is easy to install and use, it is also attractive as a virtual laboratory for nonlinear acoustics in higher education. The canonical examples available in the Wave-DNA repository may be used to introduce students to, for example, Doppler effects or the formation and attenuation of shock waves.

5. Conclusions

The field of nonlinear acoustics still holds many open questions for physicists and engineers. To help address these questions, we have developed Wave-DNA, a software tool that features a state-of-the-art numerical framework designed for the simulation of spatially one-dimensional nonlinear acoustic waves emitted by stationary or moving boundaries in quiescent or moving fluids. Wave-DNA's unique capabilities offer a powerful platform for exploring intricate nonlinear and interrelated wave phenomena, as demonstrated in recent studies [6,7,21]. The origins of these phenomena may be elucidated through a successive simplification of the governing wave equation, and their influence on realistic applications can be studied by introducing different user-defined flow fields. To our awareness, there is currently no other open-source software tool offering similar features and capabilities as Wave-DNA.

CRediT authorship contribution statement

Sören Schenke: Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Conceptualization. **Fabian Sewerin:** Writing – review & editing, Methodology, Conceptualization. **Berend van Wachem:** Writing – review & editing, Supervision, Resources, Methodology, Funding acquisition, Conceptualization. **Fabian Denner:** Writing – review & editing, Writing – original draft, Validation, Supervision, Software, Resources, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), grant number 441063377, and by the Natural Sciences and Engineering Research Council of Canada (NSERC), funding reference number RGPIN-2024-04805.

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