On recovering the second-order convergence of the lattice Boltzmann method with reaction-type source terms

Grzegorz Gruszczyński\textsuperscript{a,b,*}, Michał Dzikowski\textsuperscript{b}, Łukasz Łaniewski-Wollk\textsuperscript{c}

\textsuperscript{a}Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology, Warszawa, Poland
\textsuperscript{b}Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Warszawa, Poland
\textsuperscript{c}School of Mechanical and Mining Engineering, The University of Queensland, St Lucia, Australia

Abstract
This study analyses an approach to consistently recover the second-order convergence of the lattice Boltzmann method (LBM), which is frequently degraded by an improper discretisation of the required source terms. Current work focuses on advection-diffusion models, in which the source terms are dependent on the intensity of transported fields. Such terms can be observed in reaction-type equations used in heat and mass transfer problems or multiphase flows. The investigated scheme is applicable to a wide range of formulations within the LBM framework. All considered source terms are interpreted as contributions to the zeroth-moment of the distribution function. These account for sources in a scalar field, such as density, concentration, temperature or a phase field. Further application of this work can be find in the method of manufactured solutions or in the immersed boundary method.

This paper is dedicated to three aspects regarding proper inclusion of the source term in LBM schemes. Firstly, it identifies the differences observed between the ways in which source terms are included in the LBM schemes present in the literature. The algebraic manipulations are explicitly presented in this paper to clarify the observed differences, and to identify their origin. Secondly, it analyses in full detail, the implicit relation between the value of the transported macroscopic field, and the sum of the LBM densities. This relation is valid for any source term discretization scheme. It is a crucial ingredient for preserving the second-order convergence in the case of complex source terms. Moreover, three equivalent forms of the second-order accurate collision operator are presented. Finally, closed form solutions of this implicit relation are shown for a variety of common models, including general linear and second order terms; population growth models, such as the Logistic or Gompertz model and the Allen-Cahn equation.

The second-order convergence of the proposed LBM schemes is verified on both linear and non-linear source terms. The pitfalls of the commonly used acoustic and diffusive scalings are identified and discussed. Furthermore, for a simplified case, the competing errors are shown visually with isolines of error in the space of spatial and temporal resolutions.

\textbf{Keywords:} lattice Boltzmann method, reaction equation, source term, second-order convergence

1. Introduction

The lattice Boltzmann method (LBM) is a widely used numerical scheme for solving both the Navier Stokes equations and advection-diffusion-reaction equation (ADRE). Its popularity has significantly risen in the recent three decades due to its ability to handle complex boundary shapes and its relative ease of implementation and parallelisation. In general, the second-order convergence of the LBM is known the literature [1, 2]. However, it is often degraded through inconsistent discretisation of the source terms. This inconsistency may be a significant limitation when applying the LBM. It can lead to excessive computational requirements to achieve accuracies observed in other formulations.

*Corresponding author.
Email addresses: ggruszczynski@gmail.com (Grzegorz Gruszczyński), mjdzikowski@gmail.com (Michał Dzikowski)

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The concepts presented in this paper are applicable to a wide range of problems. To simplify derivations, the scope is narrowed to an advection-diffusion-reaction equation,

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (u\phi) = \nabla \cdot (M \nabla \phi) + Q(\phi, x, t),
\]

(1)

where \( \phi \) denotes the scalar field, \( u \) refers to an advection velocity, \( M \) is a diffusion coefficient, and \( Q \) is the source term.

In this work, a consistent discretisation for source terms is discussed in order to recover the second-order convergence of the underlying scheme. We highlight the often neglected details of the derivation of the LBM in the case where \( Q \) is a function of the scalar field \( \phi \). Most importantly, it is shown that to recover the second-order convergence one has to solve an implicit, potentially non-linear, relation between the macroscopic scalar field \( \phi \), and the zeroth-moment of the LBM densities, \( \tilde{\phi} = \sum_i \tilde{h}_i \) (see Section 2.1 for details):

\[
\phi - \frac{1}{2} Q(\phi, x, t) = \tilde{\phi}.
\]

(2)

Furthermore, special care has to be taken during initialization of the LBM densities.

### 1.1. Discussion on the state of the art

From an application point-of-view, there is a wide range of physical phenomena which can be described by a form of the advection-diffusion-reaction equation. Models based on the LBM were developed for processes such as multicomponent reaction [3], combustion [4], solid and fluid dissolution related to underground CO\(_2\) storage [5, 6], crystallization and melting [7, 8], Joule heating in electro-osmotic flows [9] and heat transfer [1, 10–19]. Last but not least, the numerical solvers can be verified by the method of manufactured solutions [20–22] in which the source term modelling is extensively used. Selected studies involving the use of LBM are listed below to present both the scope of modelling approaches, and applicability of the concepts discussed in this work.

One of the earliest studies in which the LBM framework was applied to simulate reaction-diffusion equations has been conducted by Dawson et al. [23] in 1993. The group investigated the classical Selkov model (originating from biological studies of glycolysis). They used a hexagonal lattice with a BGK relaxation model and an explicit first-order integration of source term. The proposed technique was used to simulate pure diffusion, homogenous reaction and the formation of Turing patterns. Later, the model was re-formulated on a square lattice by Blaak and Sloot [24]. The first order approximation of the source term was present in both works.

Arguably, the most widely explored application of the advection-diffusion LBM is found in coupled flow-heat transfer problems [1, 10–19]. To model the underlying physics, a two-population approach is frequently used. One of the populations simulates motion of the fluid, while the second one uses some form of the energy balance equation to resolve the heat transfer. The primary benefit of using the same numerical framework for fluid flow and heat transfer is that it greatly simplifies the computational implementation.

The LBM framework has also been extended to capture the conjugate heat transfer and or phase change between solid and liquid phases. Huang et al. [7, 8] incorporated the term responsible for the latent heat of fusion into the equilibrium distribution function. As a result, moments of equilibrium have been adjusted to recover the desired partial differential equation. A similar effect has been obtained by Hosseini et al. [25], who presented a set of weight coefficients to tune the second-order moments of a source-like term, which was added to the equilibrium distribution function. Karani and Huber [26], and later Chen et al. [27], studied the macroscopic energy equation suitable to model conjugate heat transfer in comparison with the standard advection-diffusion equation. The difference was expressed as a corrective source term, and was added to the standard LBM routine for the ADRE to obtain the correct energy balance. While the aforementioned works [25–27] introduce a source term specific for conjugate heat transfer problems, they do not discuss its proper treatment which potentially leads to the use of explicit first-order schemes. Interested readers are referred to a comprehensive review of methods related to phase-change, heat transfer and multiphase flows by Li et al. [28].

The source term technique can be also used to implement a boundary condition on a moving or curved wall. The intensity of the heat source is adjusted in each iteration to match the Dirichlet, Neumann, or Robin boundary condition. Models that use this technique are commonly referred to as immersed boundary method. Seta [29] performed a
comprehensive work on its thermal variant, including an analysis of the error terms present. Many authors have recognised the importance of consistently treating the source term with an appropriate scheme [29–35], however, it is not always taken into account [36–38]. Alternative approach to couple the fluid-solid interaction is through the partially saturated method [39], where a lattice node is categorised as a pure fluid, pure solid or mixed node. Recent applications can be found in the studies of heat transfer in particle suspensions [40, 41].

To simulate advection-diffusion-reaction in a compressible medium, Aursjø et al. [42] have defined the concentration of the scalar quantity relatively to density of fluid. Later, the same research group proposed a scheme for including a mass source term in the Navier Stokes equations and showed its application for imposing a pressure boundary condition [43].

While problems relating to heat transfer represent the majority of work conducted with the advection-diffusion equation resolved in the LBM framework, other physical phenomena are also studied. When multiple components are present in the same volume, a reaction between them may occur [4, 23, 44, 45]. Kang et al. [44] managed to reduce the number of equations required to solve the problem of dividing species by separating their interaction into reaction rate-, and diffusion-dominated. Again, the convergence was not discussed in [4, 23, 44].

Shi and Guo [46] and Chai et al. [47] provided general studies on the non-linear and anisotropic variants of the advection-diffusion equations in the LBM framework, respectively. The influence of source term treatment is highlighted, but the numerical examples are focused on other aspects of the ADRE and do not include an example of solving non-linear source term preserving both temporal and spatial derivatives. The asymptotic analysis of the LBM schemes for the advection-diffusion equation have been discussed in detail by Yoshida and Nagaoka [48] and Chai and Shi [49]. The authors gave a detailed expansion analysis for both single relaxation time and multiple relaxation time collision operators for the advection-diffusion-reaction system. For the diffusive scaling, second-order accuracy was reported. However, the test cases presented did not include source terms, which were integrated with a first-order scheme.

From a theoretical point-of-view, detailed studies of LBM schemes for the 1D advection-diffusion equation have been conducted by Dellacherie [50]. The systematic analysis presented by Dellacherie provided a framework to quantify the behaviour of D1Q2 LBM schemes in \( L^\infty \) norm, allowing one to check both consistency and convergence. It is worth noting, that the author indicated a need to integrate the collision operator with a higher-order integration scheme. Additionally, a link was shown between the periodic 1D LBM schemes and the finite-difference schemes, namely, leap-frog for the temporal discretisation, centred-difference for convective terms and Du Fort-Frankel for the diffusive term. The interested reader is referred to the discussion on stability analysis and convergence of a 1D LBM in the work of Junk and Yang [51].

Although less common in the literature, the final family of discretisation schemes for the diffusion and advection-diffusion within the LBM framework were derived based on the finite-volume concept. The scheme was proposed by Onishi et al. [52]. It adapts the particle distribution function used to resolve the NSE to calculate the scalar flux similar to the finite-volume approach. The method was later extended by Osmanlic and Körner [53] to include an upwind-type switch in flux calculation. The interested read is directed to the review by Küng et al. [54] for more information on this formulation and the details relating to it.

Having outlined the range of applications, the mathematical methodology is now presented. Readers interested in a detailed discussion on analysis methods are refereed to the work of Chai and Shi [49]. In general, the derivations of the conventional LBM numerical schemes present in the literature, can be broadly divided into two groups. First one refer to as bottom-up and second one to top-down approach.

The bottom-up procedure starts from an a priori postulated discrete evolution scheme. It proceeds with an expansion procedure (such as Chapman-Enskog) to recover the macroscopic equations and to analyse its order of accuracy. Knowing the difference between the target and recovered equation, one can apply corrections to account for the missing terms. Regarding the advection-diffusion-reaction equation, the missing terms are recognised as spatio-temporal derivatives of the source term. To regain second-order accuracy of the numerical scheme, two approaches can be distinguished. Shi et al. [46, 55] evaluated the derivatives using standard finite-difference stencils. On the other hand, Seta [29] and Chai et al. [47] realised that a redefinition of variables allowed the problem to be resolved, while preserving the locality of the underlying scheme. Readers interested in the analysis of a forcing term in the Navier Stokes equations are referred to the work of Guo et al. [56].

In the top-down approach, the discrete Boltzmann equation (DBE) is first constructed. It is then integrated along its characteristics to derive the fully discrete scheme [57–59]. In most cases, the resulting time integration scheme...
will be implicit. Again, redefinition of variables can be used to transform it into explicit equations [1]. Finally, it is interesting to notice, that some alternative LBM schemes are also being developed [60–62].

1.2. Structure

With the state of the art, and the common methodologies for deriving an LBM scheme introduced, the remainder of this paper is structured as follows. In Section 2.1, a general framework based on a top-down approach is discussed in detail. From this, a general method which preserve the second-order nature of the underlying LBM with source terms is analysed. A simplified relaxation procedure using a moment-based collision operator is then presented in Section 2.4.1. Section 3 outlines the non-dimensionalisation procedure for a PDE and the required scaling of parameters on LBM grids. Subsequently, Section 4.1 describes how leading components of error affect the accuracy of a solution in terms of both spatial and temporal resolution. To illustrate the methodology, the proposed approach for solving a formally implicit source term is applied to the Allen-Cahn equation in Section 4.2. With the use of symbolic algebra, a solution with an explicit algorithm, which preserves second-order accuracy is proposed. Finally, the methodology is validated numerically by comparison with a finite-element method solution in Section 4.2.2 and a convergence study is provided in Sections 4.2.1 and 4.2.3. The summary of the findings and major outcomes of this work are presented in Section 5.

| Nomenclature |
|---------------|
| **Abbreviations** | | **Symbols** |
| ADE | advection-diffusion equation | $eq$ | Equilibrium |
| ADRE | advection-diffusion-reaction equation | $\Delta t$ | Temporal resolution (1/T) |
| DBE | discrete Boltzmann equation | $\Delta x$ | Spatial resolution (1/L) |
| FD | finite difference | $h_i$ | $i$-th distribution function for the $\phi$ field |
| FEM | finite element method | $M$ | Transformation matrix |
| LBM | lattice Boltzmann method | $S$ | Relaxation matrix |
| MRT | multiple relaxation time | $e$ | Characteristic lattice velocity |
| ODE | ordinary differential equation | $u$ | Macroscopic velocity vector |
| PDE | partial differential equation | $x$ | Position vector |
| SRT | single relaxation time | $\omega_i$ | $i$-th relaxation frequency |
| TRT | two relaxation time | $\phi$ | Density of the scalar field |
| Da | Damköhler number | $\tau$ | Relaxation time |
| Fo | Fourier number | $i$ | Imaginary number |
| Pe | Péclet number | $Y_i$ | $i$-th raw moment of the distribution function |
| **Dimensionless Variables** | | $c_s$ | Lattice speed of sound |
| $L$ | Number of lattice elements per length | $M$ | Macroscopic diffusion coefficient |
| $Q$ | Macroscopic source term | $T$ | Number of time iterations (time steps) |
| **Superscripts** | | $\sim$ | redefined (shifted) distribution function or its moment |
| $\star$ | Post-collision variable | $\wedge$ | Variables from the future (t+1) |
2. Model description

2.1. Discrete Boltzmann equation (DBE)

Here, the iterative scheme is derived using the top-down approach, i.e. by direct integration of the DBE. For a set of densities \( h_i(x, t) \), and velocity vectors \( \mathbf{e}_i \), the DBE is known as ([2, Chapter 3.4 and 8.3]),

\[
\frac{\partial}{\partial t} h_i + e_i^j \frac{\partial}{\partial x_j} h_i = \frac{1}{\tau} (h_i^{eq}(\phi, \mathbf{u}) - h_i) + q_i(\phi, x, t),
\]

(3)

where \( h_i^{eq} \) is the equilibrium distribution, \( q \) is the source term, \( \phi = \sum_i h_i \) is the scalar field, and \( \mathbf{u} \) is the advection velocity. It is important to reiterate here that the source term depends on the investigated scalar field. To the best of the authors’ knowledge, such a form has not been discussed in the literature. With an appropriate choice of equilibrium distribution [63], this equation can be shown to represent the advection-diffusion-reaction equation with, \( \phi = \sum_i h_i \), and \( Q = \sum q_i \). The equations for the equilibrium distribution are presented in Section 2.4. An important property of the equilibrium that will be used, is,

\[
\sum_i h_i^{eq}(\phi, \mathbf{u}) = \phi.
\]

(4)

Contrary to classical numerical methods, such as finite-volume or finite-element method, the space and time integration can not be treated independently in the construction of a conventional LBM scheme. For a fixed \( i, s \) and \( t \), the characteristic of DBE is given by

\[
\int_{I_1}^1 \left( \frac{\partial}{\partial t} h_i + e_i^j \frac{\partial}{\partial x_j} h_i \right) ds = \int_{I_2}^1 \left( \frac{1}{\tau} (h_i^{eq} - h_i) + q_i \right) ds.
\]

(5)

Two integrals, \( I_1 \) and \( I_2 \), can be identified in the integration process of the DBE. To denote the future variables, the hat superscript is used in this work. Namely, \( \hat{x} = x + s \mathbf{e}_i, \hat{t} = t + 1, \hat{\phi} = \phi(\hat{x}, \hat{t}) \) and \( \hat{\mathbf{u}} = \mathbf{u}(\hat{x}, \hat{t}) \). The first integral can be evaluated directly, as it is a material derivative of \( h_i \),

\[
I_1 = \int_0^1 \left( \frac{\partial}{\partial t} h_i + e_i^j \frac{\partial}{\partial x_j} h_i \right) ds = h_i(\hat{x}, \hat{t}) - h_i(x, t).
\]

(6)

The second integral can be approximated by the trapezoidal rule,

\[
I_2 = \int_0^1 \left( \frac{1}{\tau} (h_i^{eq} - h_i) + q_i \right) ds \approx \frac{1}{2} \left[ \frac{1}{\tau} (h_i^{eq}(\hat{\phi}, \hat{\mathbf{u}}) - h_i(x, \hat{t})) + q_i(\hat{\phi}, \hat{x}, \hat{t}) + \frac{1}{\tau} (h_i^{eq}(\phi, \mathbf{u}) - h_i(x, t)) + q_i(\phi, x, t) \right].
\]

(7)

Integrating Equation (7) over the characteristics, and collecting the future variables (which depend on \( \hat{x} \) and \( \hat{t} \)) on the left hand side gives,

\[
1 + \frac{1}{2\tau} h_i(\hat{x}, \hat{t}) - \frac{1}{2\tau} h_i^{eq}(\hat{\phi}, \hat{\mathbf{u}}) - \frac{1}{2} q_i(\hat{\phi}, \hat{x}, \hat{t}) = \left[ 1 - \frac{1}{2\tau} \right] h_i(x, t) + \frac{1}{2\tau} h_i^{eq}(\phi, \mathbf{u}) + \frac{1}{2} q_i(\phi, x, t).
\]

(8)

Next, a shifted distribution, \( \hat{h}_i \), is introduced to remove the implicit relation from Equation (8). It shall be underlined, that the one solved in the numerical scheme. To illustrate the idea, a simple example of variable shift in a ordinary differential equation is presented in Appendix A. General description of this procedure in the contexts of LBM can be found in a textbook Krüger et al. [2, Chapter 3.5]).
The new (shifted) distribution, denoted with a tilde, is defined as,

$$\tilde{h}_i(\bullet) = \left[ 1 + \frac{1}{2\tau} \right] h_i(\bullet) - \frac{1}{2\tau} \tilde{h}_i^{eq}(\bullet) - \frac{1}{2} q_i(\bullet)$$ (9)

$$\implies h_i(\bullet) = \frac{1}{1 + \frac{1}{\tau} t\tau} \left( \tilde{h}_i(\bullet) + \frac{1}{2\tau} \tilde{h}_i^{eq}(\bullet) + \frac{1}{2} q_i(\bullet) \right).$$ (10)

where $\bullet$ is a placeholder for variables in either $t$ or $\tilde{t}$. Substituting Equation (9) into the left-hand side of Equation (8) and Equation (10) into the right-hand side of Equation (8) leads to a fully explicit evolution scheme (see Appendix B for details),

$$\tilde{h}_i(x + e_i, t + 1) = \tilde{h}_i^*(x, t) = (1 - \omega)\tilde{h}_i(x, t) + \omega \tilde{h}_i^{eq}(\phi, u) + \left( 1 - \frac{\omega}{2} \right) q_i(\phi, x, t),$$ (11)

where a relaxation frequency, $\omega = \frac{1}{\tau + 1/2}$, has been introduced to simplify the expression. The post-collision densities are denoted as $h^*$. It is important to reiterate, that $\tilde{h}$ is the variable solved in the implementation of a LBM scheme, and is denoted with a tilde in this paper to distinguish it from the non-shifted population, $h$. The differences in the discretisation schemes available in the literature are discussed in Appendix C.

2.2. Calculation of the scalar field

Equation (11) would be an explicit iterative scheme for $\tilde{h}$, if not for the implicit dependence on the scalar field, $\phi$. One can calculate $\phi$ from $\tilde{h}$ by summation of Equation (9) noting that both $\sum_i h_i$ and $\sum_i \tilde{h}_i^{eq}$ are equal to $\phi$,

$$\tilde{\phi} = \sum_i \tilde{h}_i = \left( 1 + \frac{1}{2\tau} \right) \sum_i h_i(x, t) - \frac{1}{2\tau} \sum_i h_i^{eq}(\phi, u) - \frac{1}{2} \sum_i q_i(\phi, x, t)$$

$$= \left[ 1 + \frac{1}{2\tau} \right] \phi - \frac{1}{2\tau} \phi - \frac{1}{2} Q(\phi, x, t)$$

$$= \phi - \frac{1}{2} Q(\phi, x, t).$$ (12)

Since the source term depends on the scalar field, $Q = Q(\phi, x, t)$, one must solve the implicit equation for $\phi$ to retain the second-order convergence of the underlying scheme. This can be done with a sub-iteration routine, such as bisection or Newton’s method, and in certain cases it can be solved analytically. In Table 1, a set of common source terms is presented with corresponding equations for the scalar field, $\phi$. In some cases multiple solutions to the implicit equation can exist, and physical limitations must be applied to select the appropriate value. For these cases, the relevant conditions are listed in the notes. If $Q$ is dependent only on the spatial, $x$, and temporal, $t$, location, the equation reduces to, $\phi = \bar{\phi} + \frac{1}{2} Q(x, t)$, which is commonly encountered in the literature.

Observe, that the equation for the macroscopic quantity, $\phi$, is independent of the LBM scheme being used. Namely, for any collision operator, for example single relaxation time, multiple relaxation time or cascaded LBM, and any discretisation of the source term, $q_i$, the equation will stay the same.

2.3. Initialization

As the densities simulated in the LBM are different than the DBE densities, the difference must to be taken into account in the initialization procedure. Namely, if one assumes the DBE to be initialized by the equilibrium distribution function, the LBM densities need to be initialized as,

$$\tilde{h}_i(x, 0) = h_i^{eq}(\phi_0, u_0) - \frac{1}{2} q_i(\phi_0, x, 0)$$

$$= h_i^{eq}(\phi_0, u_0),$$ (13)
The discrete, raw moments in 2D are defined as,

\[ \phi = \tilde{\phi} + \frac{1}{2} Q(x, t) \]

which can be easily extended to 3D with three indices. For moments of LBM densities, \( \tilde{h} \), post-collision densities, \( \tilde{h}' \), equilibrium distribution, \( h^{eq} \) and source term, \( q \), we will use \( \tilde{\Upsilon} \), \( \tilde{\Upsilon}' \), \( \tilde{\Upsilon}^{eq} \) and \( R \) respectively.

As the set of densities is finite, and the velocities \( \mathbf{e} \) are distinct, one can select a finite set of linearly independent moments to fully represent any set of densities. For the D2Q9 lattice, the following set of moments are chosen,

\[ \Upsilon = \begin{bmatrix} \Upsilon_{00} & \Upsilon_{10} & \Upsilon_{01} & \Upsilon_{20} & \Upsilon_{02} & \Upsilon_{11} & \Upsilon_{21} & \Upsilon_{12} & \Upsilon_{22} \end{bmatrix}^\top. \]

### Table 1: Calculation of the value of the macroscopic scalar field \( \phi \) from the sum of LBM densities \( \tilde{\phi} = \sum_{i} \tilde{h}_i \). In cases of higher order terms, only one branch of the implicit function is selected, based on physical considerations.

| Class | Source term | Equation for \( \phi \) | Notes |
|-------|-------------|--------------------------|-------|
| No source term | \( Q = 0 \) | \( \phi = \tilde{\phi} \) | |
| \( \phi \) independent term | \( Q = Q(x, t) \) | \( \phi = \tilde{\phi} + \frac{1}{2} Q(x, t) \) | |
| General 1st order term | \( Q = -\lambda(\phi - \gamma) \) | \( \phi = \tilde{\phi} + \frac{1}{2\gamma\lambda}(\gamma - \tilde{\phi}) \) | |
| Linear decay | \( Q = -\lambda \phi \) | \( \phi = \frac{1}{\lambda} \phi \) | |
| General 2nd order term | \( Q = -\lambda(\phi^2 - B\phi + C) \) | \( \phi = \alpha + \sqrt{\frac{\lambda}{\gamma} \phi + \alpha^2 - C} \) for \( \phi > \alpha \), where \( \alpha = \frac{B}{2\gamma} \) | |
| Logistic model | \( Q = \lambda \phi(1 - \frac{\phi}{\gamma}) \) | \( \phi = \alpha + \sqrt{\frac{\lambda}{\gamma} \phi + \alpha^2} \) for \( \phi > \alpha \), where \( \alpha = \gamma \left( \frac{1}{2} \right) \) | |
| Gompertz model | \( Q = -\lambda \phi \ln \frac{\phi}{\gamma} \) | \( \phi = \alpha e^{\lambda(\frac{\phi}{\gamma})} \) for \( \phi > \alpha \), where \( \alpha = \gamma e^{-\frac{
}{\gamma}} \), and \( \lambda \) is the Lambert W function | |
| Allen-Cahn equation | \( Q = \lambda \phi \left( 1 - \phi^2 \right) \) | \( \phi = \frac{A}{2} - C \) for \( \lambda < 2 \), where \( A = \frac{2 - B}{C} \), \( B = \frac{C}{2} \), and \( C = \sqrt{\frac{B^2 + A^2 - B}{2}} \) | |
| General term | \( Q = Q(\phi, x, t) \) | \( \phi - \frac{1}{2} Q(\phi, x, t) = \tilde{\phi} \) implicit equation, which can be solved with sub-iterations | |

where \( \tilde{\phi}_0 \) and \( u_0 \) are the initial values of the macroscopic field, \( \phi \), and advection velocity respectively. Taking advantage of Equation (12), the initialization procedure can be simplified by calculating \( \tilde{\phi}_0 \). Omission of this crucial adjustment of the initialization procedure will result in a solution inconsistent with the desired initial condition, and will reduce the order of convergence. Note, that Equation (13) gives the value of the initial distribution functions after streaming and before collision.

### 2.4. Moments of the distribution

In order to formally discuss different LBM schemes, the concept of moments of the distribution is introduced in this section. Here, the D2Q9 lattice will be adopted for illustrational purposes, but without the loss of generality. The D2Q9 is the most popular lattice discretisation used for 2D problems, and it defines the discrete velocity vectors \( \mathbf{e}_i \) as,

\[
\begin{align*}
\mathbf{e}_1 &= [0, 0] \\
\mathbf{e}_2 &= [1, 0] \\
\mathbf{e}_3 &= [0, 1] \\
\mathbf{e}_4 &= [-1, 0] \\
\mathbf{e}_5 &= [0, -1] \\
\mathbf{e}_6 &= [1, 1] \\
\mathbf{e}_7 &= [-1, 1] \\
\mathbf{e}_8 &= [-1, -1] \\
\mathbf{e}_9 &= [1, -1]
\end{align*}
\]

The discrete, raw moments in 2D are defined as,

\[ \Upsilon_{mn} = \sum_i (e_i^m)^q (e_i^n)^q \tilde{h}_i, \]  \hspace{1cm} (14)

which can be easily extended to 3D with three indices. For moments of LBM densities, \( \tilde{h} \), post-collision densities, \( \tilde{h}' \), equilibrium distribution, \( h^{eq} \) and source term, \( q \), we will use \( \tilde{\Upsilon}, \tilde{\Upsilon}', \tilde{\Upsilon}^{eq} \) and \( R \) respectively.

As the set of densities is finite, and the velocities \( e \) are distinct, one can select a finite set of linearly independent moments to fully represent any set of densities. For the D2Q9 lattice, the following set of moments are chosen,

\[ \Upsilon = \begin{bmatrix} \Upsilon_{00} & \Upsilon_{10} & \Upsilon_{01} & \Upsilon_{20} & \Upsilon_{02} & \Upsilon_{11} & \Upsilon_{21} & \Upsilon_{12} & \Upsilon_{22} \end{bmatrix}^\top. \]  \hspace{1cm} (15)
The transformation from the densities, $h$, to the vector of moments can be expressed through matrix multiplication as $\mathbf{Y} = \mathbf{M} \mathbf{h}$. In the case of D2Q9, this matrix reads,

$$
\mathbf{M} = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 & 0 \\
0 & 1 & 0 & -1 & 1 & 1 & -1 & 1 & 0 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & 0 \\
1 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & 0 \\
0 & 1 & 0 & 1 & 0 & 1 & 1 & -1 & 0 \\
0 & 0 & 1 & 0 & 1 & 1 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0
\end{bmatrix}.
$$

(16)

It is convenient to express LBM schemes in terms of moments, and not densities themselves. This is because they represent specific mechanics, and or have physical interpretations, which the densities themselves do not possess. The LBM collision operator defined in equation Equation (11), can be expressed using moments as,

$$
\tilde{\mathbf{Y}}(t, x) = (1 - \omega)\mathbf{Y}(t, x) + \omega \mathbf{Y}^\text{eq}(\phi, u) + (1 - \frac{\omega}{2})\mathbf{R}(\phi, u, x, t).
$$

(17)

The moments of the discrete equilibrium, $\mathbf{Y}^\text{eq}$, are defined to be equal to moments of the continuous Maxwell-Boltzmann distribution function, $\mathbf{Y}^\text{eq}(\phi, u) = \phi \mathbf{\Gamma}(u)$, where,

$$
\mathbf{\Gamma}(u) = \begin{bmatrix}
1 & u_x & u_y & c_s^2 + u_x^2 & c_s^2 + u_y^2 & u_x u_y & u_x (c_s^2 + u_y^2) & u_x (c_s^2 + u_x^2) & c_s^2 + c_s^2 (u_x^2 + u_y^2) + u_x^2 u_y^2
\end{bmatrix}^\top.
$$

(18)

One can clearly see that these moments fulfill the conditions required for representation of the advection-diffusion-reaction equation by the DBE. A common choice of the speed of sound $c_s$ is $1 / \sqrt{3}$, which reduces the error in higher moments. The moments of the equilibrium distribution are truncated by some authors on the second order terms [1, 7, 10, 11, 13, 41, 64–67], by not including the terms $u_x^2 u_y$, $u_x u_y^2$ and $u_y^2 u_x^2$. Furthermore, it can be truncated at first-order terms [25–27, 48, 68] giving,

$$
\mathbf{\Gamma}^\text{1st order}(u) = \begin{bmatrix}
1 & u_x & u_y & c_s^2 & c_s^2 & 0 & u_x c_s^2 & u_y c_s^2 & c_s^2
\end{bmatrix}^\top.
$$

(19)

Formulas analogous to Equation (18) can be used for the D2Q5 lattice [16]. Similarly, the moments of the source term can be expressed as $\mathbf{R} = \mathbf{Q}(\phi, x, t) \mathbf{\Gamma}(u)$. Again, some authors simplify the source term by truncating the velocity [48, 69]. Investigation of an error related to the order of velocity expansion of the equilibrium distribution function has been conducted by Chopard et al. [70]. It has been shown that the full order velocity expansion enhances both the Galilean invariance [15, 71–74] and stability of the LBM schemes [71, 74].

The equilibrium and source term distribution functions can be easily calculated from their moments as $\mathbf{h}^\text{eq} = \mathbf{M}^{-1} \mathbf{Y}^\text{eq}$ and $\mathbf{q} = \mathbf{M}^{-1} \mathbf{R}$.

2.4.1. The collision operator

If the moments of the source term are chosen to be $\mathbf{R} = \mathbf{Q}(\phi, x, t) \mathbf{\Gamma}(u)$, and $\mathbf{Y}^\text{eq}(\phi, u) = \phi \mathbf{\Gamma}(u)$, one can use Equations (12) and (18) to express the collision operator in three equivalent forms,

$$
\tilde{\mathbf{Y}} = (1 - \omega)\mathbf{Y} + \omega \mathbf{Y}^\text{eq}(\phi, u) + \left(1 - \frac{\omega}{2}\right)\mathbf{R}
$$

(20)

$$
\tilde{\mathbf{Y}} = (1 - \omega)\mathbf{Y} + \omega \mathbf{Y}^\text{eq}(\phi, u) + \mathbf{R}
$$

(21)

$$
\tilde{\mathbf{Y}} = (1 - \omega)\left(\mathbf{Y} - \mathbf{Y}^\text{eq}(\phi, u)\right) + \mathbf{Y}^\text{eq}(\phi + \mathbf{Q}, u).
$$

(22)

The form provided in Equation (21) can be viewed as a simplification of a relaxation procedure expressed in central moments space by Fei and Luo [16]. On the other hand, the form in Equation (22) can be interpreted as a natural extension of the exact difference method [75] for reaction-type source terms. Even though Equations (21) and (22)
use $\Upsilon^\text{eq}(\tilde{\phi}, \mathbf{u})$ instead of $\Upsilon^\text{eq}(\phi, \mathbf{u})$, the implicit Equation (12) must still be resolved as the source term $Q$ is dependent on $\phi$.

For a comparison of forcing schemes, the reader is referred to the studies [56, 76, 77]. Further discussion concerning discretisation and the order of the velocity expansion of the forcing scheme in the central moment space can be found in [78–80] and references therein.

2.4.2. two relaxation time

The two relaxation time (TRT) collision operator was shown to have superior accuracy and stability [81–86] when compared to the single relaxation time collision presented in the previous section. The TRT approach consists of decomposing the distribution function into symmetric and anti-symmetric components [81],

$$
\begin{align*}
  h_{j}^{\text{even}} &= \frac{h_{j} + h_{k}}{2}, \\
  h_{j}^{\text{odd}} &= \frac{h_{j} - h_{k}}{2},
\end{align*}
$$

for $k$ chosen such that $e_{j} = -e_{k}$. For the two components, two different relaxation times, $\tau$, are used resulting in two different relaxation coefficients, $\omega$.

The symmetric component, $h_{j}^{\text{even}}$, has only even order moments, and the anti-symmetric component has only odd order moments that are non-zero. This means that a TRT collision can be constructed from Equation (21) as,

$$
\tilde{\Upsilon}^{\text{stellar}} = (1 - S)\tilde{\Upsilon} + S\Upsilon^\text{eq}(\tilde{\phi}, \mathbf{u}) + R,
$$

where $S$ is the diagonal relaxation matrix, which has $\omega_{\text{odd}}$ in rows corresponding to moments of odd order, and $\omega_{\text{even}}$ otherwise. For D2Q9 the matrix is as follows,

$$
S = \text{diag}([\omega_{\text{even}}, \omega_{\text{odd}}, \omega_{\text{odd}}, \omega_{\text{even}}, \omega_{\text{even}}, \omega_{\text{odd}}, \omega_{\text{odd}}, \omega_{\text{even}}]).
$$

This means that the non-orthogonal matrix of raw moments, $M$, provided in Equation (16), diagonalises the TRT collision operator [87]. For additional information on the TRT method, the interested reader is directed to the work of Ginzburg [81], although this particular property has not been explicitly stated there. In case of the advection-diffusion equation, the relaxation rate for odd moments, $\omega_{\text{odd}}$, has to correspond to the macroscopic diffusion coefficient,

$$
\omega_{\text{odd}} = \frac{1}{c_{s}^{2}} + 1/2.
$$

On the other hand, the (tunable) relaxation rate for even moments, $\omega_{\text{even}}$, can be defined based on the so-called magic parameter,

$$
\Lambda = \left(\frac{1}{\omega_{\text{odd}}} - \frac{1}{2}\right)\left(\frac{1}{\omega_{\text{even}}} - \frac{1}{2}\right).
$$

Fixing the magic parameter at different constant values, results in a minimisation of specific types of discretisation errors, and can improve stability and or accuracy of commonly used boundary conditions [81, 86].

2.4.3. Streaming

As usual, the collision step, given by Equation (24), is followed by the streaming step,

$$
\tilde{h}_i(x + e_i, t + 1) = \tilde{h}_i^*(x, t) = M^{-1}\tilde{\Upsilon}^{\text{stellar}}(x, t).
$$

Concluding, the order of operations in the LBM scheme can be presented as in Figure 1.
3. Scaling of LBM

To represent the same physical problem, the non-dimensional form of the investigated differential equation must be preserved on a set of LBM grids. Let us consider a source term \( Q = \lambda P(\phi) \), where \( P \) has the same unit as \( \phi \), and \( \lambda \) is a scaling coefficient (see Table 1). Using \( L, T \) and \( U \) as reference length, time and velocity, respectively, one can define non-dimensional coordinates \( x = x' L, t = t' T, u = u' U \). For a constant \( M \) one can express the Equation (1) in non-dimensional form \[88]\[
\frac{\partial}{\partial t'} \phi + Pe Fo \nabla \cdot (u' \phi) = Fo \Delta' \phi + Da Fo \phi, \tag{29}
\]
where \( Fo, Da \) and \( Pe \) are dimensionless numbers:

- Fourier number \( Fo = \frac{MT}{L^2} \) — the ratio of the diffusive term to the temporal term;
- (second) Damköhler number \( Da = \frac{LU}{M} \) — the ratio of the reaction term to diffusive term;
- Péclet number \( Pe = \frac{UL}{M} \) — the ratio of the convective term to the diffusive term.

Observe, that the Fourier number incorporates the temporal scale of the simulation and as such can be considered as a non-dimensional time. An alternative approach would be to fix \( Fo = 1 \), and quote the time of simulation for each case.

The LBM grids are described by their characteristic length and time \( (L, T) \) expressed in number of elements and time-steps. The element size, and time-step can be expressed as their inverse, \( \Delta x = \frac{1}{L} \) and \( \Delta t = \frac{1}{T} \). For each grid, there are corresponding values of \( M, \lambda, \) and \( U \) that preserve the dimensionless numbers: \( M = Fo \frac{L^2}{T}, \lambda = Da Fo \frac{1}{T} \) and \( U = Pe Fo \frac{1}{T} \).

For the so-called acoustic scaling, one uses a series of lattices with \( L_k = \varepsilon_k^{-1} L_0 \) and \( T_k = \varepsilon_k^{-2} T_0 \), for some scaling factor \( \varepsilon_k \to 0 \). Using the previously mentioned equations for the simulation parameters one obtains, \( M_k = \varepsilon_k^{-1} M_0, U_k = U_0, \) and \( \lambda_k = \varepsilon_k \lambda_0 \). This scaling is called acoustic, as it preserves the velocity scale, making the speed of sound constant across the series of LBM grids. On the other hand, for diffusive scaling, one has \( L_k = \varepsilon_k^{-1} L_0 \) and \( T_k = \varepsilon_k^{-2} T_0 \). This in turn gives, \( M_k = M_0, \lambda_k = \varepsilon_k^{-1} \lambda_0 \). This scaling is called diffusive, as the diffusion coefficient \( M \) is constant across the series of LBM grids.

4. Model Verification and Validation

To test the numerical properties of the described LBM scheme, two equations were investigated, an advection diffusion equation, with a linear source term, and the Allen-Cahn equation. As analytical solutions are easy to obtain for the first example, a detail analysis of error is performed in that case. Also, for the first equation, the results are compared with the situation in which one would naively assume \( \phi = \phi' \). In the case of the Allen-Cahn equation, which has a bi-stable, highly non-linear source term, convergence is checked for both uniform, and non-trivial initial conditions.
If not stated differently, error between numerical solution $\phi(x_i)$ defined on lattice points $x_i$ and reference solution $\phi_{\text{ref}}$ is quantified using $L_2$ norm, defined as:

$$L_2 \text{ norm of error} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\phi(x_i) - \phi_{\text{ref}}(x_i))^2},$$

where $N$ is the number of points in the lattice.

4.1. Linear advection-diffusion-reaction model

Here, a simple equation with a linear source term is considered,

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (u \phi) = \nabla \cdot (M \nabla \phi) + \lambda (\eta(x) - \phi),$$

where $\gamma$ is a known constant function. On a periodic domain with constant velocity, $u$, the problem is a first order linear differential equation, which acts independently on all wavelengths. That means that for any selected wavevector $k$, we can solve analytically the equation for initial condition $\phi|_{t=0} = Pe^{ikx}$ and $\eta = Ge^{ikx}$, where upright i denotes the imaginary unit. The analytical solution will be a transition between the initial condition and the steady state,

$$\phi_{\text{analytical}}(x, t) = \left(e^{-\omega t} P + (1 - e^{-\omega t})A^{-1}AG\right)e^{ikx},$$

where $a = \lambda + i(u \cdot k) + M(k \cdot k)$. As the equation is linear, one can take the imaginary or real part of the above analytical solution to obtain a real valued solution. If not specifically mentioned, the real part is used in tests. By varying $P$ and $G$ one can study the influence of the initial condition and the steady-state solution respectively.

4.1.1. Second-order convergence

To test the convergence, the Equation (31) was solved on a periodic domain of size $L \times L$ elements for a time $t$ with $Fo = 0.001$ and $Da = 1000$. In all computations of this case, the single relaxation time collision operator was used. The number of time steps was increased by a factor of 2 from $T = 2^9$ to $T = 2^{15}$, while maintaining the number of elements per length, $L$, proportional such that $16L = T$ (acoustic scaling). The velocity was varied between $Pe = 0$ and $Pe = 1000$ and the wave number $k$ was $0 \frac{\pi}{L}, 1 \frac{2\pi}{L}$ or $2 \frac{2\pi}{L}$. For each setup, two cases were executed. One with $P = 1$ and $G = 0$, and the other with $P = 0$ and $G = 1$. LBM solutions were compared with the analytical solution of Equation (31), and the $L_2$ norm of the difference was computed. The proposed scheme consistently recovered second-order convergence for all the cases, with the slope varying from 1.99 to 2.2 as calculated with a least square fit. Figure 2 provides an indication of the convergence for $k = 1 \frac{2\pi}{L}$, $P = 1$ and $G = 0$. The convergence observed was compared to results obtained when ignoring the implicit Equation (12) and assuming $\phi = \phi$ in the calculation of $Q$.

4.1.2. Convergence of DBE to ADRE

The LBM can be treated as a discretisation of the DBE, which in turn converges to the ADRE that one originally wanted to solve. This means that two types of error need to be considered, namely, the error of discretisation, and the error (difference) between the DBE and ADRE. Readers interested in a more detailed study regarding equivalent partial differential equations for the lattice Boltzmann schemes are referred to the recent work of Fučík and Straka [89] and references therein.

In the case of the linear source term, $q = Q(\phi)\gamma(u)$, $h^{eq} = \phi\gamma(u)$ and $\gamma(u) = M^{-1}\Gamma(u)$, the DBE given in Equation (3) can be solved analytically and its solution can be conveniently expressed using matrix exponents,

$$h^{\text{DBE}}_{\text{analytical}}(x, t) = \left(e^{-At}\phi\gamma(u)P + (I - e^{-At})A^{-1}\gamma(u)AG\right)e^{ikx},$$

where $A_{\phi} = i\delta_{\phi}(e_j \cdot k) - \frac{1}{2}\left(\gamma_j(u) - \delta_{\phi}\right) + \lambda\gamma_j(u)$. Substitution of all variables indicates that the analytical solution of the ADRE is independent of $L$ and $T$, as one would expect, however, the analytical solution of the DBE is only dependent on ratio of $L$ to $T$ (the velocity scale).
Figure 2: Convergence of the solution of Equation (31) compared with analytical solution given by Equation (32), for $k = \frac{1}{2\pi}, P = 1$ and $G = 0$.

Figure 3 provides the $L_2$ norm of the difference between the complex solutions of DBE and ADRE. The two components of the error can be observed, namely, the fourth-order, velocity dependent error, and second-order, velocity independent error.

Figure 3: $L_2$ norm of the difference between the analytical solutions of the discrete Boltzmann Equation (3) and the advection-diffusion-reaction Equation (1). Evaluated for $k = \frac{1}{2\pi}, M = 0.001 \frac{1}{T}, G = 0$, and $P = 1$.

4.1.3. Error landscape

Better understanding of the behaviour of the LBM method for advection-diffusion-reaction equation, and LBM in general, can be gained by looking at the dependence of the error on both spatial and temporal resolution. In this work, this is termed the error landscape. For most of physical problems it is prohibitively expensive to calculate the full error landscape, even if an analytical solutions is available. Nevertheless, the landscape for this case is discussed here, as the general trends and slopes of this landscape will be similar in any LBM application.

A set of 23 and 31 distinct values of $L$ and $T$ were selected, generating a solution set that is close to a linear distribution in log space. For each pair, two simulations were performed, one with the method presented in this paper, and one in which $Q$ is calculated from $\tilde{\phi}$, not $\phi$. In total, 1426 simulations were performed to populate the error landscape. The results were compared to both the analytical solutions of the ADRE and DBE. Figure 4 presents
the isolines of the error. One can observe, that the convergence to the DBE is only driven by competing temporal

\textbf{vs. ADRE} \hspace{1cm} \textbf{vs. DBE}

![Figure 4: The isolines of error of the LBM solution are compared to Equation (32) or Equation (33) in the T-L space. Error is defined as } \|L\|^2 - \text{norm of the difference between LBM solution and analytical solution. All combinations of 23 and 31 distinct values of } L \text{ and } T \text{ respectively, were simulated. Evaluated for } k = \frac{2\pi}{L}, M = 0.001 \frac{2\pi}{L}, G = 0, P = 1, \text{ and } u = 0.\]

and spatial discretisation errors. On the other hand, the \(T/L\) dependent error between DBE and ADRE dominates the temporal error in convergence to ADRE. In either case, if the source term is inappropriately integrated, its first-order error reduces the accuracy greatly in almost the entire landscape (marked with dashed lines).

In order to provide a clear view of the trends present in the error landscape, approximations of all the separate errors were established to create a smoothed landscape presented in Figure 5.

To quantify the impact of the source term discretisation, the computational cost was compared to achieve the same level of error using either a first- or second-order scheme. Both for the present method, and for the inconsistent integration, an optimal selection of number of time-steps, \(T\), and number of elements, \(L\), was made, to achieve error of no more than \(10^{-5}\). In this specific example, the use of the inconsistent integration scheme for the source term leads to a 500 times increase computational cost \((L^2 T)\) to achieve an equivalent error level.

The landscapes presented in Figures 4 and 5 indicate the pitfalls of analysing the convergence of LBM. It has to be reiterated that the Boltzmann equation is integrated along the characteristics, thus the space and time integration can not be treated independently in the construction of a conventional LBM scheme. As a consequence, a properly implemented LBM scheme has second-order convergence. The isolines of error, presented in Figure 5, are commonly traversed along the directions marked by the so-called acoustic and diffusive scaling. Given a specific scaling, i.e. ratio of temporal to spatial resolution between subsequent refinements, a researcher may get a biased view of the error and the order of convergence. For instance, under the diffusive scaling, a second order convergence in space will be observed for both the trapezoidal and Euler’s implementation of the reaction term integrator. An example of first order implementation leading to aforementioned misinterpretation can be found in [90]. Next, the second order convergence in time is clearly visible in the acoustic scaling, while the diffusive scaling can give a misleading impression of being only first order in time (see Figure 10). Moreover, in the lower right corner of the landscape, the error caused by Euler’s implementation is relatively small, thus it may not affect the order of convergence. Concluding, the same gain in accuracy can be completed along different pathways. Looking solely at one of the axes (either the temporal or spatial as in Figure 10) of the refinement does not make the method to change its order of convergence.
Figure 5: The schematic isolines of error in the T–L space. See Figure 4 for the plot of actual error, measured in simulation. First three of the top four plots show the trends of: error between discrete Boltzmann equation solution and advection-diffusion-reaction equation ($\sim (T/L)^{-2}$), error of the spatial discretisation ($\sim L^{-2}$), 1st order temporal error introduced by improper integration of the source term ($\sim T^{-1}$). The last of the top four plots presents the trend of the cost of the simulation for 2D lattice ($\sim L^2T$). The large black circles mark optimal (CPU cheapest) selections of $L$ and $T$ to achieve the error of no more then $10^{-5}$. The ratio of the computational cost for the optimal setup in the naive approach ($\phi = \tilde{\phi}$) compared to the present study is approximately 500 times. The vectors indicate the direction of spatio-temporal refinement using either acoustic or diffusive scaling. Assuming that the length of a vector corresponds to a single refinement step, a misleading impression of second order convergence can be deduced (as two isolines of errors are crossed) when looking solely at the diffusive scaling and setting $\phi = \tilde{\phi}$. 

---

\[ \text{DBE vs ADRE error} \]
\[ \text{spatial error} \]
\[ \text{1st ord. temp. error} \]
\[ \text{cost} \]

$\text{Time steps (T)}$
$\text{Elements per length (L)}$

100 101 102 103 104 105 106

$10^−9$
$10^−8$
$10^−7$
$10^−6$
$10^−5$
$10^−4$
$10^−3$

Figure 4: The plot of actual error, measured in simulation. First three of the top four plots show the trends of: error between discrete Boltzmann equation solution and advection-diffusion-reaction equation ($\sim (T/L)^{-2}$), error of the spatial discretisation ($\sim L^{-2}$), 1st order temporal error introduced by improper integration of the source term ($\sim T^{-1}$). The last of the top four plots presents the trend of the cost of the simulation for 2D lattice ($\sim L^2T$). The large black circles mark optimal (CPU cheapest) selections of $L$ and $T$ to achieve the error of no more then $10^{-5}$. The ratio of the computational cost for the optimal setup in the naive approach ($\phi = \tilde{\phi}$) compared to the present study is approximately 500 times. The vectors indicate the direction of spatio-temporal refinement using either acoustic or diffusive scaling. Assuming that the length of a vector corresponds to a single refinement step, a misleading impression of second order convergence can be deduced (as two isolines of errors are crossed) when looking solely at the diffusive scaling and setting $\phi = \tilde{\phi}$. 

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\[ \text{Isolines of constant cost in 2D} \]
\[ \bullet \text{Optimal configuration with error} < 10^{-5} \]
4.2. The Allen-Cahn equation — illustrative advection-diffusion-reaction problem.

In this section a solidification problem was selected in order to illustrate the impact of the non-linear dependence of the source term on the transported field. The problem solved is the Allen-Cahn equation in the form,

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (u \phi) = \nabla \cdot (M \nabla \phi) + \lambda \phi (1 - \phi^2).
\]

(34)

The details for this equation can be found in the dedicated literature, for example Cahn and Hilliard [91], Jacqmin [92]. To formulate the implicit relation between \(\phi\) and \(\tilde{\phi}\), the source term, \(Q(\phi)\), it was substituted into Equation (12),

\[
\tilde{\phi} = \sum_i \tilde{h}_i = \phi - \frac{1}{2}Q(\phi) = \phi - \frac{1}{2} \lambda \phi (1 - \phi^2) = \phi \left(1 - \frac{\lambda}{2} (1 - \phi^2)\right).
\]

(35)

As previously discussed, this equation has to be solved to express \(\phi\) as a function of \(\tilde{\phi} = \sum_i h_i\) to resolve the implicit relation introduced by \(Q = Q(\phi)\). The exact solution can be readily derived for this third order polynomial. For \(\lambda < 2\), there is only one real-valued solution,

\[
\phi(\tilde{\phi}) = \frac{A}{C} - C, \text{ where } A = \frac{2 - \lambda}{3\lambda}, B = \frac{\tilde{\phi}}{A}, \text{ and } C = \sqrt{B^2 + A^3} - B.
\]

(36)

In the next sections, this analytical expression is used in the LBM collision operator to calculate \(\phi\), and \(Q(\phi)\). To illustrate the dependence of \(\phi\) and \(Q(\phi)\) is plotted as a function of \(\tilde{\phi}\) in Figure 6. Two stable fixed points correspond to the roots of \(Q\), present at \(\phi = \tilde{\phi} = 1\) and \(-1\), and one unstable at 0.

![Figure 6: Plot presents the real solution of Equation (36), namely \(\phi = \phi(\tilde{\phi})\) and \(Q = Q(\tilde{\phi})\) for \(\lambda = 1\).](image)

The following subsections are ordered by a growing complexity. First, only the reaction term is benchmarked. Then, a non-uniform initial condition is applied to observe the diffusive effects. Finally, an external velocity field is imposed to obtain the full advection-diffusion-reaction problem.

4.2.1. Uniform reaction benchmark — comparison with an analytical solution

This section analyses the evolution of a uniform initial distribution of the scalar field, \(\phi\), in the absence of an external velocity field. The spatial derivatives in Equation (34) reduce to zero and the problem simplifies to ordinary differential equation,

\[
\frac{d\phi}{dt} = \lambda \phi (1 - \phi^2).
\]

(37)
The analytical solution of this equation is,

$$\phi(t) = \pm \left( C_1 e^{-2\lambda t} + 1 \right)^{-\frac{1}{2}},$$

where $C_1 = (\phi(0))^{-2} - 1$. (38)

The results obtained from LBM using the Equation (36), were compared with the analytical solution of the ODE. In Figure 7, both local and global (accumulated) truncation errors are presented. The local time-step error was calculated as the difference between the numerical and analytical solution after a single time step. For this case, the third-order convergence up to the level of computational accuracy was recovered. As there is no diffusion, the Fourier number is undefined. The global convergence rate was determined by comparison of the numerical and analytical solution after a fixed time $t \in 1, 10, 100$. The coefficient responsible for the intensity of reaction was set to $\lambda = 0.01$.

As observed in Figure 7b, the scheme recovered the expected second-order convergence. From this result it can be concluded that the presented implementation recovers the trapezoidal integration scheme for the special case in which the Allen-Cahn partial differential equation reduces to an ODE.

Figure 7: Convergence study of the reaction component of the Allen-Cahn Equation (34), on a $D2Q9$ lattice with uniform initial condition and on periodic domain with $\lambda = 0.01$. In such a case, the problem simplifies to ODE given by Equation (37). The operator $|\cdot|$ denotes a scalar absolute value. It is used to evaluate the error against analytical solution. In general, a method which converges with $O(n + 1)$ local truncation error, has a global error of order $O(n)$. In this example, convergence is limited by truncation error at $\approx 10^{-16}$ in local error.

It is reminded that to obtain accurate solution, a precise initialisation procedure which took into account the shift in calculated values (see Equation (13)) must be applied.

4.2.2. Reaction-diffusion benchmark (2D, periodic) — comparison with a finite-element solution

To ensure that the proposed collision kernel properly recovers the diffusion process, the LBM solver has been qualitatively compared against finite-element method (FEM). A spatially varying, periodic initial condition was applied on a square, unit domain using the exponential function,

$$\phi |_{t=0}(x, y) = \frac{1}{2e - e^{-1}} \left(e^{\sin(2\pi x L)} - 2e^{\sin(4\pi y L)}\right).$$

(39)

Figure 8a shows the result of the initialisation.

The FEM results were obtained using the FEniCS [93, 94] solver. We used fourth-order Lagrange interpolation for spatial discretisation. Fourth-order Runge-Kutta (ESDIRK43a) with adaptive time-stepping was used for time integration, as implemented in Gryphon package [95]. The FEM was solved on a regular, triangular mesh in the 2D square domain of unit length. There were 25 divisions along each side of the domain resulting in $\sim 26^2$ elements in total. The time step ranged from approximately $10^{-4}$ to $10^{-5}$. Diffusivity in FEM solver was set to one, while the reaction rate was defined by setting $Da = 500$. The LBM domain was discretised with $256 \times 256$ lattice nodes and the
diffusivity was set to 1/6 in lattice units, and magic number was set to 1/12. To match the solutions obtained by two different solvers, the results were reported for a specific non-dimensional time. There was no external velocity field, thus $Pe = 0$.

Figure 8b provides a qualitative comparison between the FEM and LBM solutions at a time defined by $Fo = 7.26 \cdot 10^{-3}$. Here, the colour contours from the FEM solution are aligned with the dashed iso-lines of the LBM solution. Figure 8c quantitatively compares the time evolution of the scalar field, $\phi$, computed by both solvers, through the cross section denoted by the vertical dashed line in Figure 8a and Figure 8b. The initial condition, and three subsequent times are provided in the same figure. It can be clearly seen that the LBM and FEM solutions agree.

![Figure 8a](image-url) ![Figure 8b](image-url) ![Figure 8c](image-url)

(a) The initial condition, given by Equation (39), used to initialize the intensity of the phase field, $\phi$, for both the FEM and LBM solvers.
(b) The intensity of the phase field, $\phi$, at the final time, $Fo = 7.26 \cdot 10^{-3}$. Both FEM (colors) and LBM (lines) solutions are presented.
(c) The time evolution of the phase field, $\phi$, is captured for four different Fourier numbers at a cross-section defined at $x/L = 0.2$. The FEM and LBM solutions are marked with crosses and lines respectively.

Figure 8: Comparison of the FEM and LBM solutions for reaction-diffusion problem specified in section 4.2.2. The LBM lattice consists of 256x256 nodes. Domain is periodic. The Pécle and Damköhler numbers are $Pe = 0, Da = 500$.

4.2.3. Advection-diffusion-reaction benchmark (2D, periodic) — impact of the Damköhler number on self-convergence

This section investigates the convergence of the advection-diffusion-reaction equation Equation (34). The exponential initial condition was used again, as per Equation (39). For this study, a TRT collision was used with the magic
coefficient, $A$, set to 1/12 in order to cancel out the third-order spatial error and provide optimal results for advection dominated problems [96]. The scalar field was advected with a uniform external velocity, $U_s$, corresponding to $Pe = 500$. The time of the simulation was determined by setting $Fo = 1 \times 10^{-3}$. The convergence of the scheme was assessed using both acoustic and diffusive scaling techniques. The parameters used during these studies are provided in Table 2 and Table 3, respectively. Here, number of elements per the domain length, $L$, is provided, as is the number of iterations, $T$.

Table 2: Simulation parameters in lattice units, acoustic scaling, for $Pe = 500$ and $Fo = 0.001$.

| $L$ | $T$ | $U_s$ | $M$ | $\lambda_{Da=0.001}$ | $\lambda_{Da=1000}$ |
|-----|-----|-------|-----|-----------------------|---------------------|
| 32  | 4096| $3.91 \times 10^{-3}$ | $2.50 \times 10^{-4}$ | $2.44 \times 10^{-10}$ | $2.44 \times 10^{-4}$ |
| 64  | 8192| $3.91 \times 10^{-3}$ | $5.00 \times 10^{-4}$ | $1.22 \times 10^{-10}$ | $1.22 \times 10^{-4}$ |
| 128 | 16384| $3.91 \times 10^{-3}$ | $1.00 \times 10^{-3}$ | $6.10 \times 10^{-11}$ | $6.10 \times 10^{-5}$ |
| 256 | 32768| $3.91 \times 10^{-3}$ | $2.00 \times 10^{-3}$ | $3.05 \times 10^{-11}$ | $3.05 \times 10^{-5}$ |
| 512 | 65536| $3.91 \times 10^{-3}$ | $4.00 \times 10^{-3}$ | $1.53 \times 10^{-11}$ | $1.53 \times 10^{-5}$ |

Table 3: Simulation parameters in lattice units, diffusive scaling, for $Pe = 500$ and $Fo = 0.001$.

| $L$ | $T$ | $U_s$ | $M$ | $\lambda_{Da=0.001}$ | $\lambda_{Da=1000}$ |
|-----|-----|-------|-----|-----------------------|---------------------|
| 32  | 256 | $6.25 \times 10^{-2}$ | $4.00 \times 10^{-3}$ | $3.91 \times 10^{-9}$ | $3.91 \times 10^{-3}$ |
| 64  | 1024| $3.12 \times 10^{-2}$ | $4.00 \times 10^{-3}$ | $9.77 \times 10^{-10}$ | $9.77 \times 10^{-4}$ |
| 128 | 4096| $1.56 \times 10^{-2}$ | $4.00 \times 10^{-3}$ | $2.44 \times 10^{-10}$ | $2.44 \times 10^{-4}$ |
| 256 | 16384| $7.81 \times 10^{-3}$ | $4.00 \times 10^{-3}$ | $6.10 \times 10^{-11}$ | $6.10 \times 10^{-5}$ |
| 512 | 65536| $3.91 \times 10^{-3}$ | $4.00 \times 10^{-3}$ | $1.53 \times 10^{-11}$ | $1.53 \times 10^{-5}$ |

Figure 9 provides the result of the finest resolution simulated for the scalar variable, $\phi$, and the implicit source term, $Q(\phi)$. Starting from the initial condition, it can be observed that $\phi$ was advected half of the domain in the specified dimensionless time. As there does not exist an analytical solution to the complete advection-diffusion-reaction equation, this finest mesh solution is used to provide a reference point of convergence tests.

The two scaling approaches (acoustic and diffusive) are evaluated in Figure 10 for both low and high $Da$. The spatial and temporal resolution are calculated as $\Delta x = 1/L$ and $\Delta t = 1/T$, respectively. In the first case, with $Da = 0.001$, a scenario in which diffusion dominates the reaction in investigated. The latter case, with $Fo = 1000$, provides the opposite situation in which the diffusion terms dominate the reaction behaviour. In both scenarios, the proposed scheme provided second-order convergence with respect to the grid spacing. However, when diffusive scaling is applied, the spatial discretisation error dominates (see Fig. 5) which manifests as first-order dependence of error on time step. To understand the impact these convergence rates have in practice, the $L_2$ error norm is shown as a function of the computational cost, defined as $CPU_{cost} = TL^2$, in Figure 10. Assuming that the simulation parameters will be maintained within the stability regime of the LBM (namely, $U_{max} \ll 0.1, \nu < 2$), one may conclude that for a given set of dimensionless numbers, it is more computationally effective to use acoustic scaling for mesh refinement, and diffusive scaling for mesh rarefaction. It is noted here, however, that a domain-specific simulation may affect the scaling approach. For example, one may prefer to use diffusive scaling in the simulation of flow through a porous medium as the effective boundary location is known to be affected by the choice of relaxation frequency [97, 98].

In addition to the above, the convergence rates reported in this test case highlight the importance of the error landscape previously introduced. The rates observed in Figure 10, indicate that the set of simulations were conducted below the diagonal of Figure 5. Based on this, one could select the spatio-temporal parameters of the simulation to progress along the iso-error line in order to obtain the desired result with a lower computational cost. For the particular scenario investigated here, the spatial error dominates indicating that one could increase the time-step. Furthermore, this apparent diagonal line sets the limit on the accuracy that could be obtained by means of a single acoustically scaled set of grids, and should be noted by practitioners looking to study the convergence of their LBM scheme.
5. Conclusions

Since its initial formulation, the lattice Boltzmann method (LBM) has been developed and adapted to solve a variety of equations, addressing different physical scenarios. This paper is focused on the details of the usage of LBM for advection-diffusion-reaction equation (ADRE) in which the source term directly depends on the advected field. Such source terms arise in the study of heat and mass transfer, phase-transition or evolution of species populations. Moreover, most implementations of Immerse Boundary Method for heat flows, use source terms to account for desired thermal boundary conditions. In this paper, the state-of-the-art applications of the LBM for ADRE were presented, and the main differences in discretisation were shown. A clear framework for derivation of the LBM numerical scheme from discrete Boltzmann equation (DBE) was discussed, and the algebraic manipulations needed for it, were explicitly shown. Next, a simplification of the collision operator in the moments’ space has been proposed.

The article shows that an implicit relation, Equation (12), between the value of the macroscopic field, and the zeroth-moment (sum) of the LBM densities is a the key component for recovering the second-order convergence of the resulting LBM numerical scheme. Furthermore, closed form solutions of this relation were presented for a variety of common source terms, ranging from simple linear terms to Gompertz model and the Allen-Cahn equation. Using this implicit relation, the paper presented a local and explicit single- or two relaxation time (TRT) LBM for ADRE with source terms dependent of the transported field.

The convergence of error of the proposed scheme was tested on two distinct equations, involving a linear source term, and a third-order source term (Allen-Cahn equation). In the case of the linear source term, analytical solutions for both ADRE and DBE were derived, allowing for study of the dependence of the error of the LBM on both spatial and time resolution. This dependence was visualized as isolines, forming an error landscape. Different competing sources of error were discussed, as was the dependence of the convergence graph on choice of scaling and initial parameters. Moreover, by investigating the isolines of error one can find point which minimizes the computational effort for a given accuracy.

To demonstrate the order of convergence of the proposed approach, the Allen-Cahn equation was selected for the second benchmark. The analytical solution of the non-linear, implicit macroscopic field relation, was embedded into the explicit, local evaluation of the LBM collision operator. The resulting numerical scheme was evaluated on three different test problems. Firstly, the domain was initialised with a uniform initial distribution to verify the accuracy of
Figure 10: Convergence study of an advection-diffusion-reaction, Equation (34), on a $D_2Q_9$ lattice for $Pe = 500$ and $Fo = 0.001$. Notice, that the second-order LBM scheme gives impression of being a first-order only with respect to time if the refinement is done along the diffusive pathway (see Section 4.1.3).
the time integration of the source term independently. The uniform initial distribution removed the spatial derivatives from the governing equation and allowed an analytical solution to be derived. In this scenario, the proposed scheme recovered the expected second-order global, and third-order local-in-time convergence. Next, the diffusion term was included in the assessment along with a periodic initial condition based on the exponential function. The result of a two-dimensional LBM simulation was compared to a fourth-order finite element method (FEM) solution, as an analytical solution for such case is no longer obtainable. Finally, an external velocity field was added to drive the phase field to introduce advective effects. Mesh-convergence was investigated for different scales of the source term described by the Damköhler number \( Da \). For both low and high \( Da \), the expected, second-order of convergence was recovered indicating a consistent derivation and implementation of the proposed method. The TRT collision operator was required to eliminate the influence of numerical artefacts in the results.

All examples confirmed the consistency of the proposed approach and have shown second-order convergence. The same implicit relation of the macroscopic field to zeroth moment of the LBM densities, can be applied in the case of a system of ADRE, simply by replacing \( \phi \) in Equation (12) by a vector of fields of interest. However, detailed analysis of the behaviour of the resulting LBM schemes is beyond the scope of this paper.

6. 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.

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Appendix A. Example: Direct derivation of the 0D scheme from ODE

As an illustrative exercise, a direct derivation of numerical scheme for an ordinary differential equation (ODE), analogous to the proposed LBM scheme, is presented. Given an ODE,

\[
\frac{d}{dt} \phi = Q(\phi, t),
\]

an implicit scheme can be obtained by integration of:

\[
\int_t^{t+\delta t} \frac{d}{dt} \phi \, dt = \int_t^{t+\delta t} Q \, dt,
\]

with the trapezoidal rule. This leads to the update formula,

\[
\phi(t + \delta t) = \phi(t) + \frac{\delta t}{2} \left( Q(\phi(t), t) + Q(\phi(t + \delta t), t + \delta t) \right),
\]

which is also called a trapezoidal rule, and is an example of a wider class of implicit Adams–Moulton methods. Introduction of a \( \frac{\delta t}{2} \) shift, similarly to the LBM derivation presented in Section 2.1,

\[
\tilde{\phi} = \phi - \frac{\delta t}{2} Q \longrightarrow \phi = \tilde{\phi} + \frac{\delta t}{2} Q,
\]
allows to transform this update formula into an explicit one,

$$\tilde{\phi}(t + \delta t) + \frac{\delta t}{2} \frac{Q(\phi(t + \delta t), t + \delta t)}{2} = \tilde{\phi}(t) + \frac{\delta t}{2} Q(\phi(t), t) + \frac{\delta t}{2} \left( Q(t) + \frac{Q(\phi(t + \delta t), t + \delta t)}{2} \right).$$

as long as the transformation between $\phi$ and $\tilde{\phi}$ is bijective. This lead to a numerical scheme, identical to one obtained in LBM methodology,

$$\tilde{\phi}(t + \delta t) = \tilde{\phi}(t) + \delta t Q(\phi(t), t) \quad \text{where} \quad \phi(t) = \tilde{\phi}(t) + \frac{\delta t}{2} Q(\phi(t), t).$$

### Appendix B. Notes on integration of the discrete Boltzmann equation

To ease the reading of the main text, some of the algebraic transformations are listed here. The substitutions can prove a useful reference for the reader, especially for newcomers, although similar derivations can be also found LBM textbooks [2, 63].

Substituting Equation (9) into the left-hand side of Equation (8) and Equation (10) into the right-hand side of Equation (8) gives,

$$\tilde{h}_i(\tilde{x}, \tilde{t}) = \left[ 1 - \frac{1}{2r_1} \right] \frac{\tilde{h}_i(\tilde{x}, t) + \frac{1}{2} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)}{1 + \frac{1}{2r_1}} + \frac{1}{2r_1} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)$$

$$= \left[ 1 - \frac{1}{2r_1} \right] \frac{\tilde{h}_i(\tilde{x}, t) + \frac{1}{2} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)}{1 + \frac{1}{2r_1}} + \frac{1}{2r_1} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)$$

$$= \left[ 1 + \frac{2r - 1}{2r_1} \right] \frac{\tilde{h}_i(\tilde{x}, t) + \frac{1}{2} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)}{1 + \frac{2r - 1}{2r_1}} + \frac{1}{2} \left[ 1 + \frac{2r - 1}{2r_1} \right] q_i(x, t)$$

$$= \left[ 1 + \frac{2r - 1}{2r_1} \right] \frac{\tilde{h}_i(\tilde{x}, t) + \frac{1}{2} h_i^{eq}(\phi, u) + \frac{1}{2} q_i(x, t)}{1 + \frac{2r - 1}{2r_1}} + \frac{1}{2} \left[ 1 + \frac{2r - 1}{2r_1} \right] q_i(x, t). \quad \text{(B.1)}$$

Next, introducing the relaxation frequency, $\omega = \frac{1}{\frac{1}{2} + \frac{1}{2}}$, simplifies the expressions further,

$$F_1 = \frac{2r - 1}{2r + 1} = \frac{2r + 1}{2r + 1} - \frac{2}{2r + 1} = 1 - \frac{1}{\frac{1}{2} + \frac{1}{2}} = 1 - \omega. \quad \text{(B.2)}$$

$$F_2 = \frac{1}{2} \left[ 1 + \frac{2r - 1}{2r + 1} \right] = \frac{1}{2} \left[ \frac{2r + 1}{2r + 1} - \frac{2}{2r + 1} \right] = \omega. \quad \text{(B.3)}$$

$$F_3 = \frac{1}{2} \left[ 1 + \frac{2r - 1}{2r + 1} \right] = \frac{2r + 1}{2r + 1} - \frac{2}{2r + 1} = 1 - \frac{1}{2} \omega. \quad \text{(B.4)}$$

Substituting Equations (B.2-B.4) into Equation (B.1), the desired Equation (11) emerges,

$$\tilde{h}_i(x + e_i, t + 1) = \tilde{h}_i(x, t) = (1 - \omega)\tilde{h}_i(x, t) + \omega h_i^{eq}(\phi, u) + \left( 1 - \frac{\omega}{2} \right) q_i(x, t). \quad \text{(B.5)}$$
Appendix C. Comparison of approaches to the source term integration

The appropriate integration of the DBE with the trapezoidal rule and redefinition of variables allows one to derive a second-order accurate, local, and explicit evolution scheme as presented in Equation (11). To broaden the discussion of approaches available in the literature, this appendix briefly analyses the spatio-temporal derivatives of the source term that appears in the works of Shi et al. [46, 55] and Chai et al. [47, 49]. If the source term is not included in the shift of variables, then the evolution equation reads,

\[ \vec{h}_i(x + e_i, t + 1) = \vec{h}^*_i(x, t) = (1 - \omega)\vec{h}_i(x, t) + \omega h^3_i(\phi, u) + q_i(\phi, x, t) + \frac{1}{2} \left( \frac{\partial}{\partial t} + e_i \cdot \nabla \right) q_i(\phi, x, t), \tag{C.1} \]

where contrary to the presented scheme, \( \phi = \vec{\phi} = \sum \vec{h}_i \) and \( \vec{h} \) is a shifted variable, analogous to \( \vec{h}_i \), but without the contribution of \( q_i \).

To understand the relation between Equation (C.1), and the one described in the present study (given by Equation (11)), consider the right hand side of Equation (5). The \( I_2 \) integral consist of two parts, first related to collision and second to the source term. In fact, any number of different numerical techniques can be applied to each of them. For example, instead of applying the trapezoidal rule, one can use a first order approximation of the source term,

\[
q_i(x + se_i, t + s) = q_i(x, t) + s \frac{\partial}{\partial s} q_i(x + se_i, t + s) + O(s^2)
\]

where \( O(s^2) \) stands for terms of order \( s^2 \) or higher.

This approximation can be integrated giving,

\[
\int_0^1 q_i(x + se_i, t + s) ds = \left[ q_i(x + se_i, t + s) + \frac{s^2}{2} \left( \frac{\partial}{\partial t} + e_i \cdot \nabla \right) q_i(x + se_i, y, t) + O(s^2) \right]_0^1
\]

In the case of the bottom-up approach, the last term in Equation (C.3) is usually recognised as an artefact \[29\]. As pointed out by Seta \[29\], it can be removed by redefinition of variables or by addition of a correction with regard to the derivative of the source term. The derivative can be computed using a forward or backward finite difference (FD) expression. As one would expect, if a forward FD is used, than the result is equivalent to that obtained through the trapezoidal rule,

\[
q_i(\phi, x, t) + \frac{1}{2} \left( \frac{\partial}{\partial t} + e_i \cdot \nabla \right) q_i(\phi, x, t) = q_i(\phi, x, t) + \frac{1}{2} \left( q_i(\phi, x, t) - q_i(\phi, x, t) \right) = \frac{1}{2} \left( q_i(\phi, x, t) + q_i(\phi, x, t) \right).
\]

The influence of the spatial component of the derivative, \( e_i \cdot \nabla \), and various FD stencils has been analysed in \[55\]. As long as the source term does not depend on \( \phi \), both forward and backwards FD are computationally trivial. However, if there is a dependence, the backwards FD would require additional transfer of data, while the forward FD, without the appropriate shift of variables, results in a globally implicit scheme.

References

[1] X. He, S. Chen, G. D. Doolen, A Novel Thermal Model for the Lattice Boltzmann Method in Incompressible Limit, Journal of Computational Physics 146 (1998) 282–300.
[2] T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shadr, G. Silva, E. M. Viggen, The Lattice Boltzmann Method, 2017.
Boltzmann method, International Journal of Heat and Fluid Flow 60 (2016) 31–46.

[37] S. Karimnejad, A. Amiri Deloew, M. Nazari, M. M. Shahnardan, M. M. Rashidi, S. Wongwises, Immerged boundary—thermal lattice Boltzmann method for the moving simulation of non-isothermal elliptical particles, Journal of Thermal Analysis and Calorimetry 138 (2019) 4003–4017.

[38] K. Suzuki, T. Kawasaki, N. Furumachi, Y. Tai, M. Yoshino, A thermal immersed boundary–lattice Boltzmann method for moving-boundary flows with Dirichlet and Neumann conditions, International Journal of Heat and Mass Transfer 121 (2018) 1099–1117.

[39] D. Noble, J. Torczyński, A lattice-boltzmann method for partially saturated computational cells, International Journal of Modern Physics C 9 (1998) 1189–1201.

[40] J. McCullough, S. Aminossadati, B. Jones, C. Leonardi, J. Williams, Lattice Boltzmann methods for the simulation of heat transfer in particle suspensions, International Journal of Heat and Fluid Flow 62 (2016) 150–165.

[41] J. W. McCullough, C. R. Leonardi, B. D. Jones, S. M. Aminossadati, J. R. Williams, Investigation of local and non-local lattice Boltzmann models for transient heat transfer between non-stationary, disparate media, Computers and Mathematics with Applications (2018) 1–21.

[42] O. Aursjö, E. Jettestuen, J. L. Vinningland, A. Hioth. An improved lattice Boltzmann method for simulating advective diffusive processes in fluids, Journal of Computational Physics 332 (2017) 363–375.

[43] O. Aursjö, E. Jettestuen, J. L. Vinningland, A. Hioth, On the inclusion of mass source terms in a single-relaxation-time lattice Boltzmann method, Physics of Fluids 30 (2018).

[44] Q. Kang, P. C. Lichtner, D. Zhang, Lattice Boltzmann pore-scale model for multicomponent reactive transport in porous media, Journal of Geophysical Research: Solid Earth 111 (2006).

[45] S. A. Hosseini, A. Eshghnejadafard, N. Darabia, D. Thévenin, Weakly compressible Lattice Boltzmann simulations of reacting flows with detailed thermo-chemical models, Computers and Mathematics with Applications 79 (2020) 141–158.

[46] B. Shi, Z. Guo, Lattice Boltzmann model for nonlinear convection-diffusion equations, Physical Review E - Statistical, Nonlinear, and Soft Matter Physics 79 (2009).

[47] Z. Chai, B. Shi, Z. Guo, A Multiple-Relaxation-Time Lattice Boltzmann Model for General Nonlinear Anisotropic Convection-Diffusion Equations, Journal of Scientific Computing 69 (2016) 355–390.

[48] H. Yoshida, M. Nagaoka, Multiple-relaxation-time lattice Boltzmann model for the convection and anisotropic diffusion equation, Journal of Computational Physics 229 (2010) 7774–7795.

[49] Z. Chai, B. Shi, Multiple-relaxation-time lattice Boltzmann method for the Navier-Stokes and nonlinear convection-diffusion equations: Modeling, analysis, and elements, Physical Review E 102 (2020) 24–26.

[50] S. Delligacherie, Construction and Analysis of Lattice Boltzmann Methods Applied to a 1D Convection-Diffusion Equation, Acta Applicandae Mathematicae 131 (2013) 69–140.

[51] M. Junk, Z. Yang, L2 convergence of the lattice boltzmann method for one dimensional convection-diffusion-reaction equations, Communications in Computational Physics 17 (2015) 1225–1245.

[52] J. Onishi, Y. Chen, H. Ohashi, A Lattice Boltzmann model for polymeric liquids, Progress in Computational Fluid Dynamics, An International Journal 5 (2005) 75.

[53] F. Osmanlic, C. Körner, Lattice Boltzmann method for Oldroyd-B fluids, Computers & Fluids 124 (2016) 190–196.

[54] V. E. Küng, F. Osmanlic, M. Markl, C. Körner, Comparison of passive scalar transport models coupled with the Lattice Boltzmann method, Computers & Mathematics with Applications (2018).

[55] B. Shi, B. Deng, R. Du, X. Chen, A new scheme for source term in LBGK model for convection-diffusion equation, Computers and Mathematics with Applications 55 (2008) 1568–1575.

[56] Z. Guo, C. Zheng, B. Shi, Discrete lattice effects on the forcing term in the lattice Boltzmann method, Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics 65 (2002) 6.

[57] X. He, X. Shan, G. D. Doolen, Discrete Boltzmann equation model for nonideal gases, Physical Review E 57 (1998) R13–R16.

[58] T. Lee, C.-L. Lin, A stable discretization of the lattice Boltzmann equation for simulation of incompressible two-phase flows at high density ratio, Journal of Computational Physics 206 (2005) 16–47.

[59] X. Guo, B. Shi, Z. Chai, General propagation lattice Boltzmann model for nonlinear advection-diffusion equations, Physical Review E 97 (2018) 043310.

[60] A. Krämer, D. Wilde, K. Kullmer, D. Reith, H. Fossy, W. Jopich, Lattice boltzmann simulations on irregular grids: Introduction of the ntrum library, Computers and Mathematics with Applications 79 (2020) 34–54.

[61] D. Wilde, A. Krämer, K. Kullmer, H. Fossy, D. Reith, Multistep lattice boltzmann methods: Theory and applications, International Journal for Numerical Methods in Fluids 90 (2019) 156–169.

[62] D. Strzeleckiak, M. Matyka, How nodes layout, refinement and velocity discretization influence convergence of the meshless lattice boltzmann method, SSRN Electronic Journal (2022).

[63] S. Succi, The Lattice Boltzmann Equation For Complex States of Flowing Matter, Oxford University Press, 2019.

[64] L. Fei, K. H. Luo, Cascaded Lattice Boltzmann method for thermal flows on standard lattices, International Journal of Thermal Sciences 132 (2018) 368–377.

[65] J. H. Lu, H. Y. Lei, C. S. Dai, A lattice Boltzmann algorithm for simulating conjugate heat transfer through virtual heat capacity correction, International Journal of Thermal Sciences 116 (2017) 22–31.

[66] J. H. Lu, H. Y. Lei, C. S. Dai, A unified thermal lattice Boltzmann equation for conjugate heat transfer problem, International Journal of Heat and Mass Transfer (2018).

[67] J. H. Lu, H. Y. Lei, C. S. Dai, An optimal two-relaxation-time lattice Boltzmann equation for solid-liquid phase change: The elimination of unphysical numerical diffusion, International Journal of Thermal Sciences 135 (2019) 17–29.

[68] H. Yoshida, T. Kobayashi, H. Hayashi, T. Kinjo, H. Washizu, K. Fukuzawa, Boundary condition at a two-phase interface in the lattice Boltzmann method for the convection-diffusion equation, Physical Review E - Statistical, Nonlinear, and Soft Matter Physics 90 (2014) 13303.

[69] J. Wang, M. Wang, Z. Li, A lattice boltzmann algorithm for fluid-solid conjugate heat transfer, International Journal of Thermal Sciences
