J Stat Phys (2010) 139: 1090–1143
DOI 10.1007/s10955-010-9969-9

Optimal Stability of Advection-Diffusion Lattice Boltzmann Models with Two Relaxation Times for Positive/Negative Equilibrium

Irina Ginzburg · Dominique d'Humières · Alexander Kuzmin

Received: 15 June 2009 / Accepted: 7 April 2010 / Published online: 27 April 2010

Abstract Despite the growing popularity of Lattice Boltzmann schemes for describing multi-dimensional flow and transport governed by non-linear (anisotropic) advection-diffusion equations, there are very few analytical results on their stability, even for the isotropic linear equation. In this paper, the *optimal two-relaxation-time* (OTRT) model is defined, along with necessary and sufficient (easy to use) von Neumann stability conditions for a very general anisotropic advection-diffusion equilibrium, in one to three dimensions, with or without numerical diffusion. Quite remarkably, the OTRT stability bounds are the same for any Peclet number and they are defined by the adjustable equilibrium parameters. Such *optimal stability* is reached owing to the free ("kinetic") relaxation parameter. Furthermore, the sufficient stability bounds tolerate negative equilibrium functions (the distribution divided by the local mass), often labeled as "unphysical". We prove that the non-negativity condition is (i) a sufficient stability condition of the TRT model with any eigenvalues for the *pure diffusion equation*, (ii) a sufficient stability condition of its OTRT and BGK/SRT subclasses, for *any linear anisotropic advection-diffusion equation*, and (iii) unnecessarily more restrictive for any Peclet number than the optimal sufficient conditions. Adequate choices of the two relaxation rates and the free-tunable equilibrium parameters make the OTRT subclass more efficient than the BGK one, at least in the advection-dominant regime, and allow larger time steps than known criteria of the forward time central finite-difference schemes (FTCS/MFTCS) for both, advection and diffusion dominant regimes.

I. Ginzburg (✉)
Cemagref, Antony Regional Centre, HBAN, Parc de Tourvoie BP 44, 92163 Antony Cedex, France
e-mail: irina.ginzburg@cemagref.fr

D. d'Humières
Laboratoire de Physique Statistique, École Normale Supérieure, Associated to CNRS, Pierre and Marie Curie and D. Diderot Universities, 24 Rue Lhomond, 75231 Paris Cedex 05, France
e-mail: dominiq@lps.ens.fr

A. Kuzmin
Mechanical and Manufacturing Engineering, Schulich School of Engineering, University of Calgary, Calgary, T2N 1N4 AB, Canada
e-mail: shurik.kuzmin@gmail.com

Keywords Lattice Boltzmann equation · Advection-diffusion equation · Necessary and sufficient stability conditions · Von Neumann stability analysis · Two-relaxation-time model · Forward time finite-difference schemes · BGK

1 Introduction

Developed for solving the Navier-Stokes equation, [3, 15, 16], then rapidly adapted for the diffusion equation [7, 35], the Lattice-Boltzmann schemes (LBE) become more and more popular for solving different problems governed by linear or non-linear, isotropic or anisotropic advection-diffusion equations (AADE), e.g., [9, 20, 30, 32, 38]. In contrast to the explicit finite-difference schemes which discretize the AADE in terms of the primary (conserved) variables, the primary variables of the LBE are *populations*, and the corresponding velocity sets implicitly define the discretization stencil. The populations are linearly relaxed towards prescribed equilibrium distribution, constructed such that the mass (sum) of populations is conserved and its evolution obeys, with second-order accuracy, the prescribed advection-diffusion equation. It is very convenient to examine the LBE schemes with a central-symmetry argument where all the populations are split into their symmetric and anti-symmetric components, their values being respectively equal or opposite for any pair of populations leaving the node in two opposite directions. The two-relaxation-times collision operator (TRT) [8] is the minimal one which enables individual relaxation rates for the symmetric and anti-symmetric components. It includes the BGK [25] (or (single-relaxation-time) SRT model) when the two relaxation rates are the same. All the diffusion coefficients of the TRT AADE equations are related to the relaxation rate of the anti-symmetric components and to (anisotropic) equilibrium mass weights [8, 13, 30]. This is to be contrasted with the link-wise operators [8, 13, 37] for which anisotropic tensors can be obtained with isotropic weights and different anti-symmetric relaxation rates. The relaxation parameter of the symmetric components is free and restricted only by linear stability arguments. While any user knows that the effective stability of LBE schemes depends on the selected values of free parameters, the exact dependency is however unknown so far.

The von Neumann stability analysis is suitable for linear LBE schemes, but analytically tedious in a parameter space spanned by Q populations and d physical (velocity) dimensions. Recent results [29, 31] of *numerical* von Neumann stability analysis for one and two-dimensional BGK models suggest that the highest stable Courant number (or lattice velocity $U = u\frac{\Delta t}{\Delta x}$), decreases in the advection limit (when the diffusion coefficient vanishes) but the BGK model remains stable provided that all equilibrium functions (divided by mass quantity) are kept non-negative. Similar stability analysis of the TRT operator [28] draws a much more complicated scenario, due to the presence of the free relaxation parameter. A possible impact of the “kinetic” modes on stability/accuracy was also revealed in reference [34] for the minimal diffusion model and numerical studies [5, 24] for multiple-relaxation-times models.

The analytical results of Rheinländer [27] for the simplest advection-diffusion one-dimensional BGK scheme with two populations (d1Q2) show that this scheme is stable up to the Courant number $U = 1$, for any relaxation parameter τ. However, the d1Q2 scheme is unable to (locally) cancel its numerical diffusion, equal to $-U^2$, [8, 28]. Suga [31] develops analytical study on the spectrum of the BGK evolution equation for several multi-dimensional velocity sets, including the d2Q9 schemes for one particular equilibrium, but restricting the BGK model to $\tau = 1$. In fact, this particular scheme (*optimal* OBGK hereafter) is equivalent to forward time central finite-difference advection diffusion schemes (FTCS) on suitable spatial stencils, e.g., [33]. We will show that the time/space steps stability criteria of FTCS and (modified) MFTCS (those schemes reduce the numerical diffusion, [17]) can be directly re-interpreted for the OBGK model, in terms of the equilibrium weights and the advection velocity U.

In contrast to the dispersion [19], perturbation [26] and structural [2] (and references herein) approaches for hydrodynamic LBE models, we mainly develop the analytical von Neumann stability analysis for the TRT AADE schemes. We first show that there exists the *optimal* sub-class of the TRT operator which retains the *equilibrium* stability bounds of the OBGK for *any value* of diffusion (anti-symmetric) relaxation parameter, hence, for any value of grid Peclet number. The OTRT sub-class reaches such an *optimal stability* when the product of the two relaxation functions, the so-called "magic" parameter Λ, keeps the value one fourth, and includes both the OBGK model and the FTCS/MFTCS when both relaxation rates are equal. The effect of Λ on the accuracy of boundary [4, 14, 23], interface [10] and overall truncation errors [8, 28] has already been reported. It is also known that all the coefficients of the infinite Chapman-Enskog *steady state expansion* are explicitly set [4, 11] as functions of Λ, for the TRT schemes with any eigenvalues and any equilibrium. In this paper, we prove, for any velocity set, any equilibrium, and any individual values of the two relaxation times, that $\Lambda = \frac{1}{4}$ reduces the Qth-order characteristic equation of mass-conserving models to a quadratic one. Then we establish necessary and sufficient bounds for the Courant number U, for the largest available number of equilibrium degrees of freedom.

There is a common belief, coming certainly from the kinetic interpretation of the LBE, e.g., [1] that the equilibrium functions must be non-negative. We first derive the generic sufficient OTRT stability conditions, suitable for any AADE equilibrium. We proof that the non-negativity condition is stronger, hence it is also sufficient for stability of the OTRT sub-class. We then show that stable equilibrium parameters partially lie in the domain where the equilibrium functions of *moving populations* are negative. Assuming the non-negativity as necessary condition for the BGK models in the advection limit, the OTRT sub-class overcomes it in stability, operating (i) with more efficient equilibrium parameters, along with (ii) more stable eigenvalue functions. Moreover, the d2Q9 velocity set tolerates negative equilibrium function even for its *immobile weight*. Altogether, assuming the non-negativity of equilibrium as a necessary condition puts severe limits on the numerical efficiency of the LBE, at least for the OTRT AADE schemes.

The paper is organized as follows. Section 2 presents the methodology for the TRT AADE and (anisotropic) equilibrium distributions for "minimal", d1Q3, d2Q5, d3Q7, and "full", d2Q9 and d3Q15 models. Necessary stability conditions for isotropic tensors in the advection limit are first derived from the positive semi-definiteness of the diffusion tensor. We show that, similarly to finite-difference schemes and in agreement with numerical studies [29], the stability of the TRT schemes drastically differs, first, when the diagonal elements of the second-order tensor are removed (all the schemes with immobile population reach this), second, when the cross-diagonal numerical diffusion is cancelled ("full" models only).

Section 3 develops analytical von Neumann stability analysis. More specifically, we (1) derive characteristic equation of the OTRT sub-class; (2) build the OTRT sufficient stability conditions; (3) show that the non-negativity condition satisfies them; (4) prove that the non-negativity condition is sufficient for stability of the TRT *pure diffusion equation* with no advection, for any relaxation times; (5) prove that the non-negativity condition is sufficient for stability of the BGK model for any τ; (6) derive necessary stability conditions for the TRT model in diffusion limit: they constrain specific (model dependent) linear combinations of symmetric equilibrium components to interval [0, 1].

Section 4 works out necessary (all the TRT schemes) and sufficient (only the OTRT subclass) conditions for the minimal models. We show that time steps larger than those of the FTCS/MFTCS can be used for a suitable choice of the equilibrium parameters and eigenvalue functions. Section 5 delineates necessary stability conditions for the d2Q9 and d3Q15 TRT models and prescribes sufficient conditions for several OTRT schemes with interesting equilibrium weights. They are mostly elaborated for isotropic diffusion tensor, but in the presence of the full anisotropic tensor of numerical diffusion. Section 6 summarizes the main results of this work and concludes the paper. Some known mathematical results are given and extended in Appendix A. Appendix B gives the non-negativity conditions for the equilibrium of the d2Q9 and d3Q15 models with free weights. Appendix C applies the developed methodology for the derivation of sufficient, then necessary and sufficient, stability conditions of "full" OTRT schemes.

1.1 Linear Anisotropic Advection-Diffusion Equation

We consider the TRT modeling of the linear anisotropic-advection diffusion equation (AADE) in d-dimensional space, with the constant advection velocity $\mathbf{u}$ and a symmetric diffusion tensor $\mathbf{K} = \{K_{\alpha\beta}\}$:

$$\partial_t s + \mathbf{u} \cdot \nabla s = \sum_{\alpha,\beta} K_{\alpha\beta} \partial^2_{\alpha\beta} s, \quad \{\alpha, \beta\} = 1, \ldots, d. \tag{1}$$

The problem is well-posed if the diagonal components $\{K_{\alpha\alpha}\}$ are non-negative and the diffusion tensor is positive semi-definite (e.g., [13, 17] and references herein). The space transformation, from the rectangular physical grid on the cuboid computational grid is defined via selection of space steps $\{\Delta_\alpha\}$. The physical value of one iteration of population update is set equal to Δ_t. Then the "computational" diffusion tensor $\mathbf{K}' = \{K'_{\alpha\beta}\}$ and advective velocity $\mathbf{U} = \{U_\alpha\}$ are prescribed as:

$$K'_{\alpha\beta} = K_{\alpha\beta} \frac{\Delta_t}{\Delta_\alpha \Delta_\beta}, \qquad U_\alpha = \frac{u_\alpha \Delta_t}{\Delta_\alpha}, \quad \{\alpha, \beta\} = 1, \ldots, d. \tag{2}$$

We will distinguish "minimal" velocity sets: {d1Q3, d2Q5, d3Q7}, abbreviated dDQ(2D+1) and "full" sets with two non-zero velocity amplitudes, such as the d2Q9 and d3Q15 schemes. The immobile (zero velocity) population has index 0. A minimal model has $2 \times d$ non-zero velocities: $\mathbf{c}_q = \{\pm \mathbf{1}_\alpha, \alpha = 1, \ldots, d\}$, all parallel to the coordinate axes. The d2Q9 velocity set has four "coordinate" velocities $\mathbf{c}_q = \{(\pm 1, 0), (0, \pm 1)\}$ and four "diagonal" velocities $\mathbf{c}_q = \{(\pm 1, \pm 1)\}$. The d3Q15 velocity set has six "coordinate" velocities $\mathbf{c}_q = \{(\pm 1, 0, 0),\ (0, \pm 1, 0),\ (0, 0, \pm 1)\}$, and eight "diagonal" velocities $\mathbf{c}_q = \{(\pm 1, \pm 1, \pm 1)\}$.

Each nonzero velocity $\mathbf{c}_q$ has an opposite one $\mathbf{c}_{\bar{q}} = -\mathbf{c}_q$, $q = 1, \ldots, Q_m$, $Q_m = Q - 1$. Hereafter we call "*links*" such pairs of anti-parallel velocities $(\mathbf{c}_q, \mathbf{c}_{\bar{q}})$. We assume (without loss of generality) that the first $Q_m/2$ velocities are anti-parallel to the last ones. When the symmetric and anti-symmetric equilibrium components: e_q^+ and e_q^-, are prescribed, the TRT update rule is performed with two relaxation parameters, λ^+ and λ^-, one for the symmetric and one for the anti-symmetric non-equilibrium components, n_q^+ and n_q^-, respectively:

$$f_q(\mathbf{r} + \mathbf{c}_q, t + 1) = f_q + \lambda^+ n_q^+ + \lambda^- n_q^-, \tag{3}$$

where

$$n_q^\pm = (f_q^\pm - e_q^\pm), \quad \text{and} \quad f_q^\pm = \frac{1}{2}(f_q \pm f_{\bar{q}}). \tag{4}$$

The two populations of any link have the same symmetric components whereas their anti-symmetric components have opposite signs. The immobile population coincides with its symmetric part. In what follows, we operate with two positive eigenvalue functions Λ^- and Λ^+, and their product Λ:

$$\text{TRT:}\quad \Lambda = \Lambda^-\Lambda^+,\quad \Lambda^\pm = -\left(\frac{1}{2}+\frac{1}{\lambda^\pm}\right),\quad -2<\lambda^\pm<0. \tag{5}$$

The eigenvalues are restricted by linear stability analysis [15, 16] for any (e.g., zero) equilibrium function. The BGK model [25] operates with one relaxation parameter, commonly called τ:

$$\text{BGK:}\quad \tau = -\frac{1}{\lambda^+} = -\frac{1}{\lambda^-},\quad \text{then}\quad \Lambda = \Lambda^{+2} = \Lambda^{-2} = \frac{(2\tau-1)^2}{4}. \tag{6}$$

The diffusion coefficients of the derived equations are all proportional to Λ^- (see below). Then Λ^+ is a free parameter for all the TRT AADE models, including the BGK operator when $\Lambda^+ = \Lambda^-$. The infinite number of combinations $\{\Lambda^+, \Lambda^-\}$ defines the *optimal OTRT sub-class* if their product is equal to $\frac{1}{4}$:

$$\text{OTRT:}\quad \Lambda = \frac{1}{4},\quad \text{or equivalently:}$$

$$\lambda^+ + \lambda^- = -2\quad \text{or}\quad \lambda^\star = \frac{\lambda^+ + \lambda^-}{2} = -1,\quad \text{when} -2<\lambda^\pm<0. \tag{7}$$

The BGK sub-class intersects the OTRT sub-class only for $\tau = 1$:

$$\text{OBGK:}\quad \Lambda^- = \Lambda^+ = \frac{1}{2},\quad \text{i.e.,}\ \lambda^+ = \lambda^- = -1\quad \text{or}\quad \tau = 1. \tag{8}$$

Remark 1.1 We will prove that for any choice of the eigenvalues λ^+ and λ^-, the OTRT sub-class has the same stability bounds, which only depend on the equilibrium parameters, hence they are the same as for the OBGK model. This enables the optimal sub-class to model advection-diffusion equation with the same equilibrium parameters for any Peclet number.

1.2 Equilibrium Function

1.2.1 General Form

The general form of equilibrium distribution $\{e_q^\pm\}$ is considered as:

$$\begin{cases} e_q^+ = sE_q^+, \quad s = \sum_{q=0}^{Q_m} f_q, \quad E_q^+ = E_q^{(m)} + g^{(u)}E_q^{(u)}(\mathbf{U}), \quad g^{(u)} \in \{0,1\}, \\ e_0^+ = e_0 = sE_0, \quad E_0 = 1 - \sum_{q=1}^{Q_m} E_q^+, \quad e_0^- = 0, \\ e_q^- = sE_q^-, \quad E_q^- = t_q^{(a)}(\mathbf{U}\cdot\mathbf{c}_q), \quad q = 1,\dots,Q_m. \end{cases} \tag{9}$$

The models without rest population are included with $E_0 \equiv 0$ and $f_0 \equiv 0$. In what follows we refer to $\{E_q^+\}$ as *the symmetric weights*, assuming $q \in \{1,\dots,Q_m\}$, and E_0 as *the "immobile" weight*. We also call $E_q = \{E_q^+ + E_q^-, E_0\}$ *the equilibrium weights*. A vector in

Q-dimensional population space is said *isotropic* when its components have the same value per velocity class. Isotropic weights $t_q = t_q^{(a)}$ are restricted to obey two conditions:

$$(1)\ t_q \geq 0 \quad \text{and} \quad (2) \sum_{q=1}^{Q_m} t_q c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta}, \quad \forall\{\alpha,\beta\} \in \{1,\dots,d\}. \tag{10}$$

Hereafter, $\delta_{\alpha\beta}$ is the Kronecker symbol.

Definition 1.2.1 Let $\mathcal{D} = \{\mathcal{D}_{\alpha\beta}\}$ be the symmetric tensor obtained from $\{K'_{\alpha\beta}\}$, and c_e be *the arithmetic mean of its diagonal elements*:

$$\mathcal{D}_{\alpha\beta} = \frac{K'_{\alpha\beta}}{\Lambda^-} = \frac{K_{\alpha\beta}\Delta_t}{\Lambda^-\Delta_\alpha\Delta_\beta}, \quad \text{and} \quad c_e = \frac{\sum_{\alpha=1}^d \mathcal{D}_{\alpha\alpha}}{d} = \frac{\sum_{\alpha=1}^d K'_{\alpha\alpha}}{d\Lambda^-}. \tag{11}$$

When $\mathbf{K}'$ is isotropic then

$$\mathcal{D}_{\alpha\beta} = c_e \delta_{\alpha\beta}, \quad c_e \geq 0, \quad \forall\{\alpha,\beta\} \in \{1,\dots,d\}. \tag{12}$$

The set $\{E_q^{(m)}\}$ solves the following linear system of equations, [8, 13] :

$$\mathcal{D}_{\alpha\beta} = \sum_{q=1}^{Q_m} E_q^{(m)} c_{q\alpha} c_{q\beta}. \tag{13}$$

The TRT operator needs an anisotropic set $\{E_q^{(m)}\}$ for any anisotropy of the diffusion tensor. The set $\{E_q^{(m)}\}$ is specified below for the minimal, d2Q9 and d3Q15 velocity sets (relations (16), (21) and (24), respectively). In the presence of advection ($\mathbf{U} \neq 0$), the full (second-order accurate) tensor $\mathcal{D}^{(num)}$ of numerical diffusion is:

$$\mathcal{D}_{\alpha\beta}^{(num)} = -U_\alpha U_\beta, \quad \forall\{\alpha,\beta\} \in \{1,\dots,d\}. \tag{14}$$

Then the effective diffusion tensor $\mathcal{D}^{(eff)}$ is:

$$\begin{aligned} \mathcal{D}_{\alpha\beta}^{(eff)} &= \mathcal{D}_{\alpha\beta}^{+} + \mathcal{D}_{\alpha\beta}^{(num)}, \\ \mathcal{D}_{\alpha\beta}^{+} &= \sum_{q=1}^{Q_m} E_q^{+} c_{q\alpha} c_{q\beta} = \mathcal{D}_{\alpha\beta} + g^{(u)} \sum_{q=1}^{Q_m} E_q^{(u)} c_{q\alpha} c_{q\beta}. \end{aligned} \tag{15}$$

The equilibrium term $E_q^{(u)}$ removes $\mathcal{D}^{(num)}$, partially or completely, when $g^{(u)} = 1$.

For convenience, we separate the non-negativity and stability conditions into four specific groups, using notation $U^2 = \sum_{\alpha=1}^d U_\alpha^2$ hereafter.

Definition 1.2.1.A We refer to function $U_d^2(c_e)$, $c_e \in [0, c_e^{(0)}]$, such that $E_0(c_e, U_d^2) = 0$ and $U_d^2(c_e = c_e^{(0)}) = 0$ as the *E_0-non-negativity line* or *E_0-n-line*. Then $E_0 \geq 0$ if $U^2 \leq U_d^2(c_e)$ and $c_e \in [0, c_e^{(0)}]$.

Definition 1.2.1.B We refer to (minimal value) function $U_n^2(c_e)$ where at least one of the moving weights E_q is equal to zero as the *non-negativity line* or *n-line*. Then $\{E_q > 0\}$, $q = 1,\dots,Q_m$, if $U^2 \leq U_n^2(c_e)$.

Definition 1.2.1.C We refer to (minimal value) function $U_a^2(c_e)$ obtained as a necessary stability limit when the effective diffusion coefficients vanish as the *advection line* or *a-line*.

Definition 1.2.1.D We refer to (minimal value) functions $\{U_{d,1}^2(c_e), U_{d,2}^2(c_e), \dots\}$ obtained as necessary stability bounds in the diffusion-dominant limit (where the impact of $\{E_q^-\}$ vanishes) as the *diffusion lines* or *d-lines*. We denote as $c_e^{(\max)}$ the (minimal value) $c_e > 0$ where at least one of *d-lines* is equal to zero.

1.2.2 Minimal Models: d1Q3, d2Q5 and d3Q7

Their equilibrium parameters (9) are:

$$\begin{cases} E_q^{(m)} = \frac{1}{2}\mathcal{D}_{\alpha\alpha}, \quad t_q^{(a)} = \frac{1}{2}, \quad E_q^{(u)} = \frac{U_\alpha^2}{2} \quad \text{if } c_{q\alpha} \neq 0,\ q = 1, \dots, Q_m, \\ E_0 = 1 - dc_e - g^{(u)} U^2. \end{cases} \tag{16}$$

As an example, the effective diffusion tensor (15) of the d2Q5 takes the form:

$$\mathcal{D}^{(eff)} = \begin{pmatrix} \mathcal{D}_{xx} + (g^{(u)} - 1)U_x^2 & -U_x U_y \\ -U_x U_y & \mathcal{D}_{yy} + (g^{(u)} - 1)U_y^2 \end{pmatrix}. \tag{17}$$

This model describes anisotropic diagonal elements $\mathcal{D}_{xx} \neq \mathcal{D}_{yy}$ with $E_q = \frac{1}{2}\mathcal{D}_{xx}$ and $E_q = \frac{1}{2}\mathcal{D}_{yy}$ for the links along the x- and y-axes, respectively. However, neither the d2Q5 nor the d3Q7 model with *local equilibrium* is able to set nonzero off-diagonal elements: $\mathcal{D}_{xy}$ or $\{\mathcal{D}_{xy}, \mathcal{D}_{xz}, \mathcal{D}_{yz}\}$. Hence, they cannot locally remove the off-diagonal elements of the numerical diffusion: $-U_\alpha U_\beta$, $\alpha \neq \beta$. The set $\{E_q^+ = E_q^{(m)} + g^{(u)} E_q^{(u)}\}$ becomes for isotropic tensor (12):

$$E_q^+ = \frac{1}{2}\left(c_e + g^{(u)} \sum_{\alpha=1}^{d} U_\alpha^2 c_{q\alpha}^2\right), \quad q = 1, \dots, Q_m. \tag{18}$$

Remark 1.2.2.A The TRT AADE minimal models are specified with two *independent* groups of parameters: (1) a triplet $\{c_e, \Lambda^-, \mathbf{U}\}$, with $c_e \geq 0$ and $\Lambda^- \geq 0$ (when strictly positive, they are related to the grid Peclet number by $Pe_{\Delta x} = \frac{|\mathbf{U}|}{c_e \Lambda^-}$), and (2): a free eigenvalue function $\Lambda^+ \geq 0$.

Immobile Weight Immobile weight E_0 is given by relation (16), either for isotropic or anisotropic diffusion tensor. The non-negativity conditions for E_0 are:

$$\begin{aligned} &\mathbf{U} \equiv 0 \quad \text{or} \quad g^{(u)} = 0: \quad E_0 \geq 0 \quad \text{if} \quad 0 \leq c_e \leq c_e^{(0)} = \frac{1}{d}. \\ &g^{(u)} = 1: \quad E_0 \geq 0 \quad \text{if} \quad 0 \leq U^2 \leq U_d^2 = 1 - dc_e,\ 0 \leq c_e \leq c_e^{(0)}. \end{aligned} \tag{19}$$

Remark 1.2.2.B We will prove that these conditions are necessary diffusion-dominant stability conditions of the minimal models.

1.2.3 "Full" Velocity Sets: d2Q9 and d3Q15

They describe full anisotropic symmetric tensors with the help of their diagonal links [8, 13] and completely remove $\mathcal{D}^{(num)}$ if:

$$\sum_{q=1}^{Q_m} E_q^+ c_{q\alpha} c_{q\beta} = \mathcal{D}_{\alpha\beta} - \mathcal{D}_{\alpha\beta}^{(num)} \quad \text{when } g^{(u)} g_{\alpha\beta}^{(u)} = 1. \tag{20}$$

Definition 1.2.3.A Let us distinguish three situations:

(1) *The numerical diffusion is not cancelled*. We will refer to as $g^{(u)} = 0$.
(2) *Only the diagonal elements of numerical diffusion are cancelled*. We will refer to as $g^{(u)} = 1$, or $g^{(u)} = 1$ and $g_{\alpha\beta}^{(u)} = 0$, assuming all possible $\alpha \neq \beta$.
(3) *The whole tensor $\mathcal{D}^{(num)}$ is cancelled*. We will refer to as $g_{\alpha\beta}^{(u)} g^{(u)} = 1$, or $g^{(u)} = 1$ and $g_{\alpha\beta}^{(u)} = 1$, assuming all possible $\alpha \neq \beta$.

The minimal models can only reach the two first configurations. The d2Q9 model achieves all of them prescribing the equilibrium (9) for $q = 1, \ldots, Q_m$ as:

$$\begin{cases} \text{d2Q9:} \quad E_q^+ = E_q^{(m)} + g^{(u)} E_q^{(u)}(\mathbf{U}), \quad E_q^{(m)} = t_q^{(m)} c_e + E_q^{(a)}, \quad \text{where} \\ E_q^{(u)}(\mathbf{U}) = t_q^{(u)} \frac{U^2}{2} + \frac{U_x^2 - U_y^2}{4} p_q^{(xx)} + g_{xy}^{(u)} \frac{U_x U_y}{4} p_q^{(xy)}, \\ E_q^{(a)} = \frac{\mathcal{D}_{xx} - \mathcal{D}_{yy}}{4} p_q^{(xx)} + \frac{\mathcal{D}_{xy}}{4} p_q^{(xy)}, \\ \quad \text{with } \mathbf{p}^{(xx)} = \{p_q^{(xx)} = c_{qx}^2 - c_{qy}^2\}, \ \mathbf{p}^{(xy)} = \{p_q^{(xy)} = c_{qx} c_{qy}\}. \end{cases} \tag{21}$$

We restrict the three families of weights: $\{t_q^{(m)}\}$, $\{t_q^{(a)}\}$, and $\{t_q^{(u)}\}$ be non-negative, isotropic, and satisfy relation (10). Hence, there exists a single degree of freedom per family of weights, e.g., if the "coordinate" weight t_c is selected, then the diagonal weight t_d is:

$$\text{d2Q9:} \quad t_d = \frac{1 - 2t_c}{4}, \quad 0 \leq t_c \leq \frac{1}{2}, \quad t_q = \{t_q^{(m)}, t_q^{(a)}, t_q^{(u)}\}. \tag{22}$$

The effective tensor of the d2Q9 schemes is:

$$\mathcal{D}^{(eff)} = \begin{pmatrix} \mathcal{D}_{xx} + (g^{(u)} - 1)U_x^2 & \mathcal{D}_{xy} + (g_{xy}^{(u)} g^{(u)} - 1)U_x U_y \\ \mathcal{D}_{xy} + (g_{xy}^{(u)} g^{(u)} - 1)U_x U_y & \mathcal{D}_{yy} + (g^{(u)} - 1)U_y^2 \end{pmatrix}. \tag{23}$$

Similarly, we specify equilibrium function (16) for moving populations of the d3Q15 model as:

$$\begin{cases} \text{d3Q15:} \quad E_q^+ = E_q^{(m)} + g^{(u)} E_q^{(u)}(\mathbf{U}), \quad E_q^{(m)} = t_q^{(m)} c_e + E_q^{(a)}, \quad q = 1, \ldots, Q_m, \\ E_q^{(u)}(\mathbf{U}) = t_q^{(u)} \frac{U^2}{3} + \frac{2U_x^2 - (U_y^2 + U_z^2)}{12} p_q^{(xx)} + \frac{U_y^2 - U_z^2}{4} p_q^{(ww)} \\ \qquad + \sum_{(\alpha\neq\beta)} g_{\alpha\beta}^{(u)} \frac{U_\alpha U_\beta}{8} p_q^{(\alpha\beta)}, \\ E_q^{(a)} = \frac{2\mathcal{D}_{xx} - (\mathcal{D}_{yy} + \mathcal{D}_{zz})}{12} p_q^{(xx)} + \frac{\mathcal{D}_{yy} - \mathcal{D}_{zz}}{4} p_q^{(ww)} + \sum_{(\alpha\neq\beta)} \frac{\mathcal{D}_{\alpha\beta}}{8} p_q^{(\alpha\beta)}, \\ p_q^{(xx)} = 2c_{qx}^2 - (c_{qy}^2 + c_{qz}^2), \quad p_q^{(ww)} = c_{qy}^2 - c_{qz}^2, \quad p_q^{(\alpha\beta)} = c_{q\alpha} c_{q\beta}, \quad \alpha \neq \beta. \end{cases} \tag{24}$$

Here, $\sum_{(\alpha\neq\beta)}$ includes each component only once, e.g., $\{\alpha\beta\} = \{(xy), (yz), (xz)\}$. Again, the non-negative and isotropic weights $\{t_q^{(m)}\}$, $\{t_q^{(a)}\}$ and $\{t_q^{(u)}\}$ satisfy relation (10) such that:

$$\text{d3Q15:}\quad t_d = \frac{1-2t_c}{8}, \quad 0 \le t_c \le \frac{1}{2}, \quad t = \{t^{(m)}, t^{(a)}, t^{(u)}\}. \tag{25}$$

We parametrize the non-negative weights $\{t^{(u)}\}$ with the free parameter γ_u:

$$\begin{aligned} &\text{d2Q9:}\quad t_c^{(u)} = \frac{1+2\gamma_u}{6}, \quad t_d^{(u)} = \frac{1-\gamma_u}{6}, \quad -\frac{1}{2} \le \gamma_u \le 1, \\ &\text{d3Q15:}\quad t_c^{(u)} = \frac{\gamma_u}{2}, \quad t_d^{(u)} = \frac{1-\gamma_u}{8}, \quad 0 \le \gamma_u \le 1. \end{aligned} \tag{26}$$

When $\gamma_u = 1$ (or, $\gamma_u = -\frac{1}{2}$ (d2Q9) and $\gamma_u = 0$ (d3Q15)) then the isotropic U^2-component of $E_q^{(u)}$ is completely "absorbed" by the coordinate, or, respectively, diagonal links.

Remark 1.2.3.A The d2Q9 and d3Q15 schemes reduce to the d2Q5 and d3Q7 schemes, respectively, when

$$t_c^{(m)} = t_c^{(a)} = t_c^{(u)} = \frac{1}{2} \quad \text{and} \quad \mathcal{D}_{\alpha\beta} = 0, \quad g_{\alpha\beta}^{(u)} \equiv 0, \ \forall\{\alpha \neq \beta\}. \tag{27}$$

Remark 1.2.3.B On top of the parameters of the minimal models: $\{\Lambda^-, c_e, U^2\}$ and Λ^+, the "full" models have three additional degrees of freedoms which are related to the distribution of weights between the two velocity classes. Any suitable choice of weights is equivalent for the second order equations. However, as we show below, different weight combinations may give very different stability bounds.

Remark 1.2.3.C The equilibrium commonly used for isotropic diffusion tensors, hereafter called "standard" form, is prescribed (a): with both $\{t_q^{(m)}\}$ and $\{t_q^{(a)}\}$ equal to the "hydrodynamic" isotropic weights $\{t_q^\star\}$ (they obey additional constraint (28)) and (b): with $\{E_q^{(u)}\} = \{E_q^\star\}$, for $q = 1, \dots, Q_m$:

$$E_q^\star = \frac{t_q^\star}{2}(3(\mathbf{U}\cdot\mathbf{c}_q)^2 - U^2), \quad 3\sum_{q=1}^{Q_m} t_q^\star c_{q\alpha}^2 c_{q\beta}^2 = 1, \quad \forall \alpha \neq \beta, \tag{28}$$

then

$$\text{d2Q9:}\quad t_c^\star = \frac{1}{3}, \quad t_d^\star = \frac{1}{12}, \quad \text{and} \quad \text{d3Q15:}\quad t_c^\star = \frac{1}{3}, \quad t_d^\star = \frac{1}{24}. \tag{29}$$

Definition 1.2.3.B The "standard" form (28)–(29) is defined with:

$$\text{d2Q9}^{(stan)}, \text{d3Q15}^{(stan)}:\quad t_c^{(m)} = t_c^{(a)} = \frac{1}{3}, \quad \gamma_u = 0. \tag{30}$$

Immobile Weight The weight E_0 is independent of the anisotropy and takes the form:

$$\text{d2Q9:}\quad E_0 = 1 - c_e(1 + 2t_c^{(m)}) - g^{(u)}(2+\gamma_u)\frac{U^2}{3}, \tag{31}$$

$$\text{d3Q15:} \quad E_0 = 1 - c_e(1 + 4t_c^{(m)}) - g^{(u)}(1 + 2\gamma_u)\frac{U^2}{3}. \tag{32}$$

Then $E_0 \ge 0$ when $U^2 \le U_d^2(c_e)$ and the E_0-*n-line* functions $U_d^2(c_e)$ are defined as:

$$\text{d2Q9:} \quad U_d^2 = \frac{3}{2+\gamma_u}\left(1 - \frac{c_e}{c_e^{(0)}}\right), \quad 0 \le c_e \le c_e^{(0)} = \frac{1}{1+2t_c^{(m)}}, \tag{33}$$

$$\text{d3Q15:} \quad U_d^2 = \frac{3}{1+2\gamma_u}\left(1 - \frac{c_e}{c_e^{(0)}}\right), \quad 0 \le c_e \le c_e^{(0)} = \frac{1}{1+4t_c^{(m)}}. \tag{34}$$

Remark 1.2.3.D Sufficient conditions for the mass weights have been proposed by Banda et al. [2] in the frame of the BGK Navier-Stokes equation and $\mathbf{U} = 0$. One can re-interpret them for the d2Q9 and d3Q15 schemes such that $E_0 \ge 0$ when $t_c^{(m)} = \frac{1}{3}$ ("standard" choice).

Remark 1.2.3.E The condition $E_0 \ge 0$ is given by relations (19), (33) and (34) for the minimal models, d2Q9 and d3Q15 schemes, respectively. When $\mathbf{U} = 0$ or $g^{(u)} = 0$, this condition restricts c_e to the interval $[0, c_e^{(0)}]$, where, respectively, $c_e^{(0)} = \{\frac{1}{d}, \frac{1}{1+2t_c^{(m)}}, \frac{1}{1+4t_c^{(m)}}\}$. The "full" models yield the largest interval $[0, c_e^{(0)}]$ for $t_c^{(m)} = 0$, then $c_e^{(0)} = 1$, and the smallest one for $t_c^{(m)} = \frac{1}{2}$, then $c_e^{(0)} = \frac{1}{d}$, $d = 2$ and $d = 3$. Then $E_0 \ge 0$ in the interval $[0, \frac{1}{d}]$ for all the models. The analysis of the diffusion-dominant conditions will prescribe $E_0 \ge 0$ as *a necessary condition* for the minimal and d3Q15 models, but not for the d2Q9 schemes. Moreover, the *sufficient stability conditions* obtained for the d2Q9 OTRT schemes will not respect the non-negativity of the immobile weight, in general.

1.3 Advection-Dominant Stability Constraints

Necessary stability conditions in the advection limit ($\mathcal{D}_{\alpha\beta} \to 0$) can be directly derived from the condition that the *effective* diffusion tensor $\mathcal{D}^{(eff)}$ is positive semi-definite. As a basic example, let us compute $\det[\mathcal{D}^{(eff)}]$ in the isotropic case (12):

$$\begin{cases} g^{(u)} = 0, d \in \{1,2,3\} : & \det[\mathcal{D}^{(eff)}] = c_e^{d-1}(c_e - U^2), \\ g^{(u)} = 1, d = 2 \quad : & \det[\mathcal{D}^{(eff)}] = c_e^2 - U_x^2 U_y^2, \\ g^{(u)} = 1, d = 3 \quad : & \det[\mathcal{D}^{(eff)}] = c_e^3 - 2U_x^2U_y^2U_z^2 \\ & \qquad - c_e(U_y^2U_z^2 + U_x^2U_y^2 + U_x^2U_z^2). \end{cases} \tag{35}$$

The following conditions guarantee the non-negativity of $\det[\mathcal{D}^{(eff)}]$ for any direction of velocity vector $\mathbf{U}$:

$$\begin{cases} g^{(u)} = 0,\ d \in \{1,2,3\} : & U^2 \le U_{a,0}^2 = c_e, \\ g^{(u)} = 1,\ d = 2 \quad : & U^2 \le U_{a,1}^2 = 2c_e, \\ g^{(u)} = 1,\ d = 3 \quad : & U^2 \le U_{a,2}^2 = \frac{3}{2}c_e. \end{cases} \tag{36}$$

When $\mathcal{D}^{(num)}$ is completely cancelled, e.g., for the d1Q3, d2Q9 or d3Q15 velocity sets, then the effective diffusion tensor is equal, at the second order, to the modeled tensor:

$$g_{\alpha\beta}^{(u)} g^{(u)} = 1 : \mathcal{D}^{(eff)} = \mathcal{D}. \tag{37}$$

Hence $\mathcal{D}^{(eff)}$ is positive semi-definite and the necessary advection-dominant conditions are prescribed by the effective high-order velocity corrections to $\mathcal{D}^{(eff)}$.

Remark 1.3 Conditions (36) are necessary for all models, they define the *a-lines* (see Definition 1.2.1.C). When the numerical diffusion is removed, the velocity components are not restricted by the *second-order analysis* in the advection limit which only prescribes $c_e \geq 0$ as the stability boundary for isotropic tensors (cf. relation (37)). Moreover, the advection limit is only a subset of all the *necessary stability conditions*. The linear von Neumann stability analysis gives *necessary and sufficient* stability bounds for periodic solutions of the evolution equation. They are also necessary for any other boundary conditions.

2 Von Neumann Stability Analysis

In this section, we first present two different but equivalent forms for the TRT characteristic equation assuming the generic AADE equilibrium form (9). We then develop several general results which are valid for any velocity set. They concern: (1) distinguished stability properties of the OTRT sub-class, (2) its sufficient stability conditions for any equilibrium, (3) the sufficiency of positivity of the whole equilibrium set $\{E_q = e_q/s = E_q^+ + E_q^-\}$ for stability of the OTRT sub-class, (4) the sufficiency of positivity of the whole set $\{E_q = E_q^+\}$ for the stability of *the pure diffusion equation* (when $\mathbf{U} = 0$, hence $E_q^- \equiv 0$), for any values of the two relaxation rates, (5) the sufficiency of positivity of the whole equilibrium set $\{E_q\}$ for the stability of the BGK AADE model *at any* τ, (6) the derivation of *necessary* stability conditions in the diffusion-dominant regime. These results are illustrated with simple examples, then worked out for all the models considered in Sects. 3 and 4 along with Appendices B and C.

2.1 Characteristic Equation

Von Neumann stability analysis is based on the Fourier transform of the evolution equation (3). Plugging there Fourier modes, $f_q(\mathbf{r}, t) = \Omega^t \mathcal{F}_q \exp(i\mathbf{r} \cdot \mathbf{k})$, $\mathbf{k} = \{k_x, k_y, k_z\}$, $-\pi < k_\alpha < \pi$, the amplification factor Ω satisfies Qth-order characteristic equation of the evolution matrix L:

$$\begin{cases} \det|\mathsf{L} - \Omega \mathsf{I}| = 0, \quad \mathsf{L} = \mathsf{K}^{(-1)} \cdot [\mathsf{I} + \mathsf{C}], \quad \text{with} \\ C_{0j} = \lambda^+(\delta_{0j} - E_0), \quad \forall j = 0, \ldots, Q_m, \\ C_{qj} = \lambda^+(\frac{\delta_{qj}+\delta_{\bar{q}j}}{2} - E_q^+) + \lambda^-(\frac{\delta_{qj}-\delta_{\bar{q}j}}{2} - E_q^-), \\ \mathsf{K}^{(-1)}_{q,j} = \exp\{-ik_q\}\delta_{qj}, \quad k_q = (\mathbf{k} \cdot \mathbf{c}_q), \quad \{q, j\} = 0, \ldots, Q_m. \end{cases} \tag{38}$$

The model is stable in von Neumann sense, e.g. [22], if for all the roots $\Omega \in \{\Omega_q\}$:

$$|\Omega| \leq 1, \quad \forall \mathbf{k}, \quad \forall \Omega \in \{\Omega_q\}, \quad q = 0, \ldots, Q_m. \tag{39}$$

Let us now divide the populations by the local mass quantity s, assuming $s \neq 0$, then we define: $F_q^\pm(\mathbf{r}, t) = \mathcal{F}_q^\pm / s$. This set solves the (reduced by s) TRT evolution equation:

$$\Omega(F_q^+ + F_q^-)e^{ik_q} = (1+\lambda^+)F_q^+ + (1+\lambda^-)F_q^- - \lambda^+ E_q^+ - \lambda^- E_q^-, \\ q = 0, \ldots, Q_m. \tag{40}$$

Taking into account that F_q^+ and E_q^+ are equal for two anti-parallel velocities, and F_q^- and E_q^- have opposite signs, with $F_0^- = E_0^- = 0$, the solution of (40) takes the form (with

$q = 1, \ldots, Q_m$):

$$\begin{cases} F_0^+ = \frac{E_0\lambda^+}{1+\lambda^+-\Omega}, \\ F_q^+ = [(1-\Omega\cos[k_q]+\lambda^-)\lambda^+ E_q^+ + i\Omega\sin[k_q]\lambda^- E_q^-]z_q, \\ F_q^- = [(1-\Omega\cos[k_q]+\lambda^+)\lambda^- E_q^- + i\Omega\sin[k_q]\lambda^+ E_q^+]z_q, \\ z_q = [\Omega^2 - \Omega\cos[k_q](2+\lambda^+ + \lambda^-) + (1+\lambda^-)(1+\lambda^+)]^{-1}. \end{cases} \tag{41}$$

Definition 2.1.1 We define the Qth-order TRT characteristic equation:

$$\sum_{q=0}^{Q_m} F_q^+ = F_0^+ + 2\sum_{q=1}^{Q_m/2} F_q^+ = 1, \tag{42}$$

where F_q^+ are defined by relations (41).

Remark 2.1.A An interesting property of the TRT characteristic equation is that the product of its Q roots, $\Pi_{q=0}^{Q_m}\Omega_q$, given by the constant term of the characteristic equation, is:

$$\Pi_{q=0}^{Q_m}|\Omega_q| = |\Pi_{q=0}^{Q_m}\Omega_q| = |1+\lambda^+|^{\frac{Q_m}{2}}|1+\lambda^-|^{\frac{Q_m}{2}}, \quad \forall E_q^+, \quad \forall E_q^-, \tag{43}$$

Therefore, the product of roots is independent of the equilibrium parameters.

2.2 Optimal Sub-Class (OTRT)

The coefficients of the characteristic equation, then the stability bounds of the TRT operator, *generally* depend on:

1. $\{E_q^+\}$, then on $\{\mathcal{D}_{\alpha\beta}\}$ and $U_\alpha U_\beta$ (when $g^{(u)} = 1$);
2. $\{E_q^-\}$, then on $\mathbf{U}$;
3. λ^-, then on Λ^-;
4. λ^+, then on Λ^+.

We prove below that the OTRT sub-class sets stability condition (39) with relations (45)–(46), then they only depend on the parameters of $\{E_q^+\}$ and $\{E_q^-\}$.

2.2.1 The Characteristic Equation on the OTRT Sub-class

Lemma 2.2.1 *Let $\lambda^+ + \lambda^- = -2$, then any root Ω of (42) satisfies equation $P^{(2)}(\Omega) = 0$, where*

$$P^{(2)}(\Omega) = \Omega^2 - \Omega((1+p)\mathcal{A} - i(1-p)\mathcal{B}) + p, \quad p = 1+\lambda^-, \tag{44}$$

and $\mathcal{A}(\mathbf{k})$ and $\mathcal{B}(\mathbf{k})$ are defined as:

$$\mathcal{A} = E_0 + \sum_{q=1}^{Q_m}\cos[k_q]E_q^+, \quad \textit{and} \quad \mathcal{B} = \sum_{q=1}^{Q_m}\sin[k_q]E_q^-. \tag{45}$$

Proof of Lemma 2.2.1 When $\lambda^+ + \lambda^- = -2$ then all the z_q in relation (41) are equal and the characteristic equation (42) becomes: $P^{(2)}(\Omega) = 0$. □

Theorem 2.2.1 *Let* $\lambda^+ + \lambda^- = -2$, $-2 < \lambda^\pm < 0$, *and* Ω *be any root of* (42). *Then conditions*: $|\Omega| \le 1$, $\forall \mathbf{k}$, $\Omega \in \{\Omega_q, q = 0, \dots, Q_m\}$, *is equivalent to*

$$\mathcal{A}^2 + \mathcal{B}^2 \le 1, \quad \forall \mathbf{k}, \tag{46}$$

where $\mathcal{A}$ *and* $\mathcal{B}$ *are defined by relations* (45).

Proof of Theorem 2.2.1 From Lemma 2.2.1, the stability bounds are set by the roots of $P^{(2)}(\Omega)$. For $\lambda^\pm \in]-2, 0[$ this polynomial satisfies the conditions of the Miller's Theorem 6.1 [21]: $|P^{(2)}(0)| = |p| = |1 + \lambda^-| < 1 = |\tilde{P}^{(2)}(0)|$ (see relations (113)). The reduced polynomial (113) is $P^{(1)}(\Omega) = (\Omega - (A - iB))(1 - p^2)$. Since $P^{(1)}(\Omega)$ has equivalent stability properties then the condition $|\Omega|^2 \le 1$ is set by relation (46), which is equivalent to the case $p = 0$ of the original equation $P^{(2)}(\Omega) = 0$. □

Remark 2.2.1.A Theorem 2.2.1 tells us that the stability bounds of the OTRT sub-class are set by the magnitude of the roots:

$$\Omega = \mathcal{A} \pm i\mathcal{B}, \tag{47}$$

where $\mathcal{A}$ and $\mathcal{B}$ only depend on the equilibrium parameters via relations (45). Using $\pm i$ does not change $|\Omega|^2$ but corresponds to the two equivalent solutions of the evolution equation: $f_q(\mathbf{r}, t) = \Omega^t \mathcal{F}_q \exp(i\mathbf{r} \cdot (\pm\mathbf{k}))$.

Remark 2.2.1.B The remarkable property of the OTRT sub-class is that its (equilibrium) stability bounds are the same for any value of the grid Peclet number $Pe_{\Delta x}$. When c_e and $U(c_e)$ are chosen, then any $Pe_{\Delta x}$ can be adjusted with a suitable choice of the eigenvalue function Λ^-. All the elements of the optimal sub-class have then the same stability bounds as the OBGK model ($p = 0$). The characteristic equation of the OBGK model is equivalent to forward time central finite difference schemes with equivalent spatial stencils. We compare the relative efficiency of these schemes and OTRT sub-class in Sect. 3.3.

Examples 2.2.1 In the limit $\mathbf{k} \to 0$, the series for $|\Omega|^2 = \mathcal{A}^2 + \mathcal{B}^2$ takes the following form when the diffusion tensor (12) is isotropic:

$$\begin{cases} g^{(u)} = 0 & : \ |\Omega|^2 = 1 - c_e \sum_{\alpha=1}^{d} k_\alpha^2 + (\sum_{\alpha=1}^{d} U_\alpha k_\alpha)^2 + O(k^4), \\ g^{(u)} = 1 & : \ |\Omega|^2 = 1 - c_e \sum_{\alpha=1}^{d} k_\alpha^2 + \sum_{\alpha \ne \beta} U_\alpha U_\beta k_\alpha k_\beta + O(k^4), \\ g_{\alpha\beta}^{(u)} g^{(u)} = 1 : & \ |\Omega|^2 = 1 - c_e \sum_{\alpha=1}^{d} k_\alpha^2 + O(k^4). \end{cases} \tag{48}$$

The necessary conditions (36) follow from these relations. When $g^{(u)} = 0$, then, necessarily, $U^2 \le c_e$, $\forall$ $\mathbf{U}$ when $\mathbf{k}$ is parallel to $\mathbf{U}$. When $g^{(u)} = 1$, and $\mathbf{U}$ and $\mathbf{k}$ are along the diagonal, $U_\alpha^2 = \frac{U^2}{d}$ and $k_\alpha^2 = \frac{k^2}{d}$, then $|\Omega|^2 = 1 - c_e k^2 + k^2 U^2 (d-1)/d + O(k^4)$, and, necessarily, $U^2 \le \frac{d}{d-1} c_e$, $d > 1$. Hence, the limits are the same for the d2Q5 and d2Q9 models: $U^2 \le 2c_e$, and for the d3Q7 and d3Q15 models: $U^2 \le \frac{3}{2} c_e$, unless the d2Q9 and d3Q15 models cancel the numerical cross-diffusion. Then, when $g_{\alpha\beta}^{(u)} g^{(u)} = 1$, the only k^2-restriction is $c_e \ge 0$.

2.3 Sufficient Stability Conditions on the OTRT Sub-class

We derive the OTRT sufficient stability conditions valid for modeling of the mass-conservation equation with equilibrium (9).

2.3.1 Sufficient Equilibrium Condition

Theorem 2.3.1 *Let $\Omega = A \pm iB$ where A and B are related to equilibrium components $\{E_q^-\}$ and $\{E_q^+\}$ via relations (45). Then $|\Omega|^2 \le 1$, $\forall$ $\mathbf{k}$, if $\{E_q^-\}$ and $\{E_q^+\}$ satisfy conditions (49-1) and (49-2):*

$$\begin{cases} (1)\ E_0 \ge 0 \quad and \quad E_q^+ > 0, \quad q = 1, \dots, Q_m, \\ (2)\ 0 \le \sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} \le 1. \end{cases} \tag{49}$$

The proof of this theorem is inspired by techniques [17].

Proof of Theorem 2.3.1

$$|\Omega|^2 = \mathcal{A}^2 + \mathcal{B}^2 = \left(\sum_{q=0}^{Q_m} \cos[k_q] E_q^+\right)^2 + \left(\sum_{q=1}^{Q_m} \sin[k_q] E_q^-\right)^2. \tag{50}$$

When conditions (49-1) and (49-2) are satisfied, using Corollaries A.1.B and A.1.C with $a_q = E_q^-$ it comes

$$|\Omega|^2 \le 1 - \left(1 - \sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+}\right)\left(\sum_{q=1}^{Q_m} E_q^+ \sin^2[k_q]\right) \le 1,$$

using $\sum_{q=1}^{Q_m} E_q^+ \sin^2[k_q] \le \sum_{q=1}^{Q_m} E_q^+ \le 1$ when (49-1) is satisfied. □

Remark 2.3.1.A The theorem formally rules out $E_q^+ = 0$. However, when $E_q^- = 0$ and $E_q^+ \ge 0$, the theorem is still valid (see Remark A.1.B). This includes the pure diffusion, $E_q^- \equiv 0$, $\forall q$, then $\mathcal{B}^2 \equiv 0$ and the non-negativity of symmetric weights gives the sufficient OTRT condition. Theorem 2.4 extends this result for the TRT modeling of pure diffusion equation.

Remark 2.3.1.B The theorem enables the derivation of stability bounds from prescribed equilibrium distributions. This avoids the analysis of Ω for all possible $\mathbf{k}$. Based upon Theorem 2.3.1, the sufficient conditions are worked out for all models considered in Sects. 3 and 4.

Examples 2.3.1 Let us consider the isotropic diffusion tensors (12) when the numerical diffusion is not cancelled ($g^{(u)} = 0$) and $t_q^{(m)} = t_q^{(a)}$. Then $E_q^+ = t_q^{(a)} c_e$ and $E_q^- = t_q^{(a)} \sum_{\alpha=1}^{d} U_\alpha c_{q\alpha}$, with $t_q^{(a)} = \frac{1}{2}$ for dDQ(2D+1). We rule out the links with $t_q^{(a)} = 0$ and take into account relation (10). Then

$$\sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} = \frac{1}{c_e} \sum_{q=1}^{Q_m} t_q^{(a)} \left(\sum_{\alpha=1}^{d} U_\alpha c_{q\alpha}\right)^2 = \frac{1}{c_e} \sum_{\alpha=1}^{d} U_\alpha^2 \sum_{q=1}^{Q_m} t_q^{(a)} c_{q\alpha}^2 = \frac{U^2}{c_e}. \tag{51}$$

The conditions of Theorem 2.3.1 are satisfied when $E_0 = (1 - \sum_{q=1}^{Q_m} t_q^{(m)} c_e) \ge 0$. The sufficient conditions of the OTRT sub-class become for all the models:

$$g^{(u)} = 0\colon \quad U^2 \le U_{a,0}^2 = c_e \quad \text{and} \quad 0 \le c_e \le c_e^{(0)} = \frac{1}{\sum_{q=1}^{Q_m} t_q^{(m)}}. \tag{52}$$

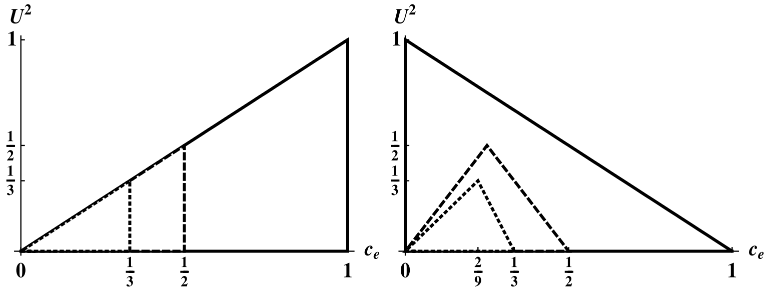

Fig. 1 The stable triangles are shown for the minimal OTRT models: d1Q3 (*large*), d2Q5 (*middle*) and d3Q7 (*small*). *Left*: with numerical diffusion, $g^{(u)} = 0$, the *a-line* is $U^2 = c_e$ and the E_0-*n-line* is $c_e = \frac{1}{d}$, the available interval is $c_e \in [0, c_e^{(0)} = \frac{1}{d}]$. *Right*: the diagonal numerical diffusion is removed, $g^{(u)} = 1$. The *a-line* and *d-line* become, respectively, $U^2 = \frac{dc_e}{d-1}$, $d \geq 2$ and $U^2 = 1 - dc_e$. These stability bounds are specified by relations (52) and (71) for $g^{(u)} = 0$ and relations (73) for $g^{(u)} = 1$. The "best" stability domains are the two large triangles for the d1Q3 model (cf. relations (74))

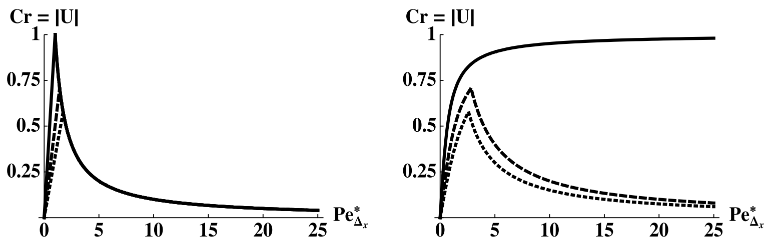

Fig. 2 The sufficient stability bounds (76) are plotted for the minimal OTRT models as $Cr = |\mathbf{U}|$ function of $Pe^*_{\Delta x} = \frac{|\mathbf{U}|}{c_e}$. The numerical diffusion is not removed on the *left* picture ($g^{(u)} = 0$), and its diagonal elements are removed on the *right* one ($g^{(u)} = 1$). The stable domain is below the curve, d1Q3: *solid*, d2Q5: *dashed*, d3Q7: *dotted*. The small $Pe^*_{\Delta x}$ values are bounded by the (increasing) E_0-*n-line*; the large $Pe^*_{\Delta x}$ values are bounded by the (decreasing) *a-line*. The *a-line* has the same form when $g^{(u)} = 0$ (*solid*) and it vanishes for the d1Q3 when $g^{(u)} = 1$. Using the OTRT sub-class, these bounds are valid $\forall \Lambda^- > 0$ (hence, for all grid Peclet numbers $Pe_{\Delta x} = Pe^*_{\Delta x}/\Lambda^-$)

Two stability conditions [31] for the $d2Q4$ and d2Q9 schemes are matched when $c_e = \frac{1}{2}$ and $c_e = \frac{1}{3}$, respectively.

Remark 2.3.1.C It follows that the *necessary condition* (36) is also *sufficient* for the OTRT sub-class when c_e is restricted to the interval $[0, c_e^{(0)}]$, $g^{(u)} = 0$ and the equilibrium mass/velocity weights are equal: $t_q^{(m)} = t_q^{(a)}$, at least. The sufficient conditions for $U^2(c_e)$ are illustrated in Fig. 1. They are replotted for $Cr(Pe^*_{\Delta x})$ in Fig. 2 (the notations of [29] have been adapted for convenience, the Courant number Cr is equal to $|\mathbf{U}|$ and $Pe^*_{\Delta x} = Pe_{\Delta x}\Lambda^-$).

2.3.2 Non-negativity of the Equilibrium Set $\{E_q = E_q^+ + E_q^-\}$: Sufficient Stability Condition for the OTRT Sub-class

It is easy now to show that the positivity of the whole equilibrium set $\{E_q\}$, along with $E_0 \geq 0$, necessarily implies Theorem 2.3.1.

Lemma 2.3.2 *Let $E_0 \geq 0$ and $\{E_q = E_q^+ + E_q^- > 0\}$ for $\forall q = 1, \dots, Q_m$ then conditions (49) are satisfied.*

Proof of Lemma 2.3.2 Let us consider the pairs of opposite velocities, with $E_q = E_q^+ \pm E_q^-$. It follows that, if $E_q > 0$, then $E_q^+ > 0 \; \forall \; q$, hence condition (49-1) is satisfied. Also $E_q \geq 0$ implies $(E_q^-)^2 \leq (E_q^+)^2$, then

$$0 \leq \sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} \leq \sum_{q=1}^{Q_m} E_q^+ = (1 - E_0) \leq 1. \tag{53}$$

The last inequality follows from the assumption $E_0 \geq 0$. □

Remark 2.3.2.A Lemma 2.3.2 can be extended to $E_q \geq 0$ when $E_q^- = 0$ and $E_q^+ \geq 0$, then the corresponding link does not contribute to $\sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+}$.

Remark 2.3.2.B Lemma 2.3.2 proves that the non-negativity of equilibrium presents *stronger* sufficient stability conditions for the OTRT sub-class than sufficient conditions from Theorem 2.3.1.

Examples 2.3.2 Let us consider again an example of isotropic diffusion tensor when $g^{(u)} = 0$ and $t_q^{(m)} = t_q^{(a)}$, both weights differ from $\{0, \frac{1}{2}\}$ for "full" models. Then the non-negativity is guaranteed for all "moving" weights and E_0 if:

$$g^{(u)} = 0, \text{minimal models:} \quad U^2 \leq U_n^2 = c_e^2, \quad 0 \leq c_e \leq c_e^{(0)} = \frac{1}{d}.$$

$$g^{(u)} = 0, \text{d2Q9\&d3Q15:} \quad U^2 \leq U_n^2 = \frac{c_e^2}{d}, \quad 0 \leq c_e \leq c_e^{(0)}. \tag{54}$$

The first (minimal) condition is reached when $\mathbf{U}$ is parallel to one of the coordinate axes. The "full" models reach the minimal velocity on the diagonal links when $\mathbf{U}$ is parallel to a diagonal lattice direction. Obviously, relations (54) are stronger than relations (52), this confirms Lemma 2.3.2. The non-negativity conditions are illustrated in Fig. 3 for minimal models and re-plotted in Fig. 4 for $Cr(Pe^*_{\Delta x})$. Further details can be found in Sect. 3.2.

2.4 Non-negativity of Equilibrium Set $\{E_q^+\}$: Sufficient Stability Condition of the TRT Model for Pure Diffusion Equation

We refer to AADE as *pure diffusion equation* when $\mathbf{u} \equiv 0$. Our goal is to prove that the non-negativity of all symmetric weights $\{E_q^+\}$, together with $E_0 \geq 0$, is a sufficient stability condition for any TRT diffusion scheme when the eigenvalues are found in their stability interval.

Theorem 2.4 *Let Ω be any root of (42) when $E_q^- \equiv 0$ for all q and $-2 \leq \lambda^\pm \leq 0$. Then condition $|\Omega| \leq 1$ is satisfied provided that $E_0 \geq 0$ and $E_q^+ > 0$, $q = 1, \dots, Q_m$.*

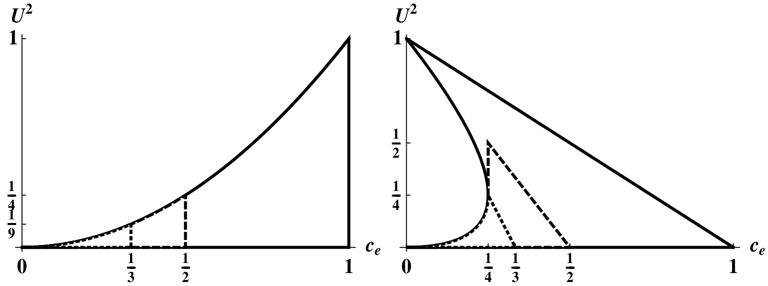

Fig. 3 The non-negativity domains where $\{E_q \geq 0, q = 1, \ldots, Q_m\}$ and $E_0 > 0$ are shown for the minimal models when $g^{(u)} = 0$ (*left*) and $g^{(u)} = 1$ (*right*), d1Q3: large (*solid boundary*), d2Q5: middle-size, (*dashed boundary*), and d3Q7: smallest (*dotted boundary*). The non-negativity lines, *n-line* and E_0-*n-line*, are predicted by relations (54) and (78) (with $\mathcal{D}^{min} = c_e$ for isotropic tensors)

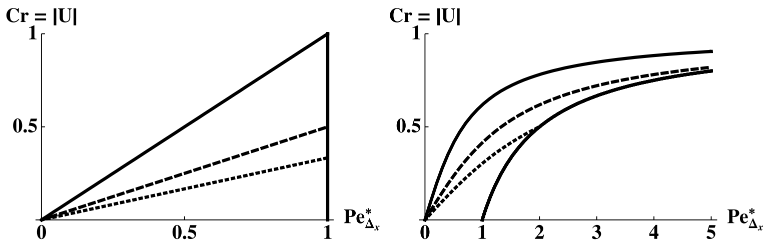

Fig. 4 The non-negativity conditions (79) of the minimal models are plotted in the $\{Cr, Pe^*_{\Delta x}\}$ plane for $g^{(u)} = 0$ (*left*) and $g^{(u)} = 1$ (*right*), $Pe^*_{\Delta x} = \frac{|\mathbf{U}|}{c_e}$. The non-negativity domain for $g^{(u)} = 0$ is below the E_0-*n-line* $Cr = \frac{Pe^*_{\Delta x}}{d}$ whereas the *n-line* is vertical, $Pe^*_{\Delta x} = 1$. The non-negativity domain for $g^{(u)} = 1$ is between the *n-line* (the common *solid* (*lower*) *line*) and the E_0-*n-line*, d1Q3: *solid*, d2Q5: dashed, and d3Q7: *dotted*

Proof of Theorem 2.4 We substitute $E_q^- \equiv 0$ and multiply each equation (40) by its complex conjugate. Dividing then the obtained relations by E_q^+, their sum yields:

$$|\Omega|^2\left(\sum_{q=0}^{Q_m}\frac{|F_q^+|^2}{E_q^+} + \sum_{q=1}^{Q_m}\frac{|F_q^-|^2}{E_q^+}\right)$$
$$= -\lambda^+(2+\lambda^+) + (1+\lambda^+)^2\sum_{q=0}^{Q_m}\frac{|F_q^+|^2}{E_q^+} + (1+\lambda^-)^2\sum_{q=1}^{Q_m}\frac{|F_q^-|^2}{E_q^+}. \quad (55)$$

We have taken into account that

(a) opposite populations have equal E_q^+ and F_q^+ components,
(b) opposite populations have opposite F_q^- components,
(c) $E_q^+ \in \Re$, $F_q^+ + F_q^{+\star} = 2\Re(F_q^+)$ if $F_q^{+\star}$ is the complex conjugate of F_q^+,
(d) and $\sum_{q=0}^{Q_m}\Re(F_q^+) = \sum_{q=0}^{Q_m} E_q^+ = 1$.

Since $E_0^+ \equiv 0$ implies $F_0^+ \equiv 0$, these terms do not appear in the sums and the models without rest population are included in relation (55). This relation can be rewritten as

$$(1-|\Omega|^2)\left(\sum_{q=0}^{Q_m}\frac{|F_q^+|^2}{E_q^+}+\sum_{q=1}^{Q_m}\frac{|F_q^-|^2}{E_q^+}\right)$$
$$=-\lambda^+(2+\lambda^+)\left(\sum_{q=0}^{Q_m}\frac{|F_q^+|^2}{E_q^+}-1\right)-\lambda^-(2+\lambda^-)\sum_{q=1}^{Q_m}\frac{|F_q^-|^2}{E_q^+}. \quad (56)$$

Using Corollary A.1.A with $a_q=|F_q^+|^2$ and $E_q=E_q^+$, the right-hand side of relation (56) is non-negative, the term multiplying $(1-|\Omega|^2)$ is also non-negative, hence $|\Omega|^2\le 1$, □

Remark 2.4.A Theorem 2.4 extends for models without rest population where $E_0\equiv 0$. Also, if $E_q^+=E_q^-\equiv 0$ then $F_q^+=F_q^-\equiv 0$ in relation (41), and those links are ruled out from the above consideration.

Remark 2.4.B In fact, the "unconditional stability" of the LBE diffusion schemes, e.g., [34], means that any diffusion coefficient can be modeled for any value of the time step Δ_t, owing to the freedom in the selection of Λ^-, provided that all the symmetric weights, $\{E_q^+\}$ and E_0, are positive.

2.5 Non-negativity of the Equilibrium Set $\{E_q=E_q^++E_q^-\}$: Sufficient Stability Condition for the BGK Model

We aim to prove that the non-negativity of all equilibrium distributions $\{E_q\}$ (since their sum is equal to 1, at least one is strictly positive) is a sufficient stability condition for any BGK model with a mass-conservation equation.

Theorem 2.5 *Let Ω be any root of system (40) when $\lambda^+=\lambda^-$. Then condition $|\Omega|\le 1$ is satisfied provided that $E_q\ge 0$, for all $q=0,\dots,Q_m$.*

Proof Taking both eigenvalues equal to λ^-, equation (40) becomes:

$$\Omega F_q e^{ik_q}=(1+\lambda^-)F_q-\lambda^-E_q,\quad \text{with } \sum_{q=0}^{Q_m}\Re(F_q)=\sum_{q=0}^{Q_m}E_q=1. \quad (57)$$

If $E_q=0$ for some q, then from (57) either $\Omega=(1+\lambda^-)e^{-ik_q}$, then $|\Omega|\le 1$, or $\Omega\ne(1+\lambda^-)e^{-ik_q}$, then $F_q=0$ and the summations in (57) can be restricted to the q such that $E_q>0$. Multiplying all (57) with $E_q>0$ by their complex conjugate, then dividing by E_q and taking their sum, we obtain:

$$|\Omega|^2\mathcal{X}=-\lambda^-(2+\lambda^-)+(1+\lambda^-)^2\mathcal{X},$$

where

$$\mathcal{X}=\sum_{q:E_q>0}\frac{|F_q|^2}{E_q}>0\quad\text{and}\quad -\lambda^-(2+\lambda^-)\ge 0. \quad (58)$$

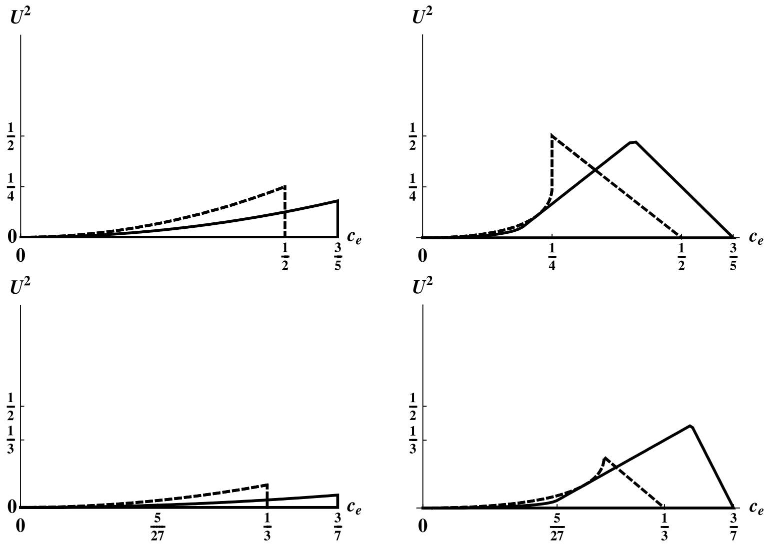

Fig. 5 The non-negativity areas are shown for the d2Q5/d2Q9$^{(stan)}$ (*top row*) and the d3Q7/d3Q15$^{(stan)}$ (*bottom row*) when $g^{(u)} = 0$ (*left*) and $g^{(u)} = 1$ (*right*). The dashed line bounds the non-negativity domain of the minimal models (cf. Fig. 3); the "*solid*" line is for "full" schemes: their non-negativity boundaries (*n-lines*) are specified, respectively, by relations (54) when $g^{(u)} = 0$ and by relations (118) and (122) when $g^{(u)} g^{(u)}_{\alpha\beta} = 1$

Using Corollary A.1.A and Remark A.1.B with $a_q = F_q$, then $\mathcal{X} \geq 1$, then

$$|\Omega|^2 = \frac{-\lambda^-(2+\lambda^-)}{\mathcal{X}} + (1+\lambda^-)^2 \leq -\lambda^-(2+\lambda^-) + (1+\lambda^-)^2 = 1. \tag{59}$$

This gives the assertion: $|\Omega| \leq 1$, □

Remark 2.5.A It follows from relation (58) that for all q, $|\Omega_q| \geq |1 + \lambda^-|$ for the BGK model. Hence, restricting condition (43) to the BGK model: $|\Pi_{q=0}^{Q_m} \Omega_q| = |1 + \lambda^-|^{Q-1}$ then $|\Omega_q| \leq 1$ for all q. This presents an alternative proof of relation (59). Then, for the BGK model with positive equilibrium, all the roots are such that

$$|1 + \lambda^-| \leq |\Omega_q| \leq 1. \tag{60}$$

Remark 2.5.B The non-negativity condition can be used as a sufficient estimate of the stability bounds for the OTRT sub-class (Lemma 2.3.2) and the BGK model (Theorem 2.5). It is noted that $\{E_q \geq 0\}$ implies $\{E_q^+ \geq 0\}$, hence, the non-negativity conditions cannot relax the constraints of Theorem 2.3.1. The non-negativity conditions are derived in Sects. B.1 and B.2 for the d2Q9 and d3Q15 schemes, respectively, with isotropic diffusion tensor but retaining all degrees of freedom for the weights, with and without the anisotropic tensor of numerical diffusion. They are compared in Fig. 5 for the pairs of models: d2Q5/d2Q9$^{(stan)}$ and d3Q7/d3Q15$^{(stan)}$. Altogether the non-negativity conditions strongly depend on the equilibrium weights and the amount of numerical diffusion (see examples below for "full" models).

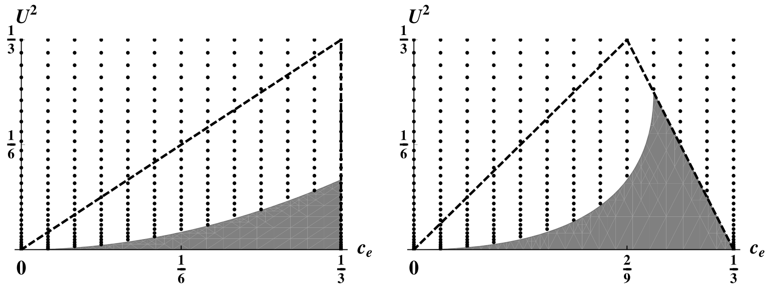

Fig. 6 The unstable points (obtained with the numerical stability analysis) for the d3Q7 BGK model with $\tau = 0.51$ are shown for $g^{(u)} = 0$ (*left*) and $g^{(u)} = 1$ (*right*). The non-negativity areas (77) and (78) (with $\mathcal{D}^{min} = c_e$) are "filled". For comparison, the OTRT stability boundary is plotted by a *dashed line*. The vertical ($g^{(u)} = 0$) or decreasing ($g^{(u)} = 1$) boundary is the E_0-*n-line*. The set of "moving" equilibrium weights $\{E_q\}$ contains the negative elements when U^2 lies between the *a-line* and the *n-line*

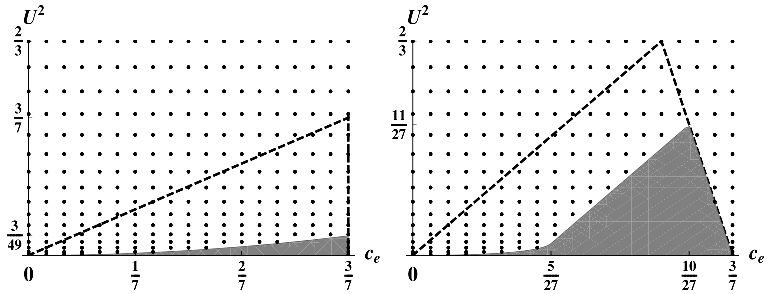

Fig. 7 The unstable points for the d3Q15$^{(stan)}$ BGK model with $\tau = 0.51$ are shown for $g^{(u)} = 0$ (*left*) and $g^{(u)}_{\alpha\beta} g^{(u)} = 1$ (*right*). The non-negativity areas (121) are "*filled*". They can be compared to the non-negativity domains of the d3Q15$^{(unif)}$ scheme in Fig. 15. The stable area of the OTRT sub-class is limited by dashed line

Remark 2.5.C We emphasize that the non-negativity line is especially restrictive in the advection-dominant (but relatively large) zone $c_e \to 0$ when the numerical diffusion is removed. The necessity of the non-negativity conditions for the BGK model in the advection limit is confirmed for all minimal models and the selected "full" models, as illustrated in Figs. 6 and 7. The proof is out of the scope of this work. Assuming the non-negativity condition as the necessary advection condition, it becomes imperative for the BGK model to avoid small c_e values when $\Lambda^- \to 0$ ($\tau \to \frac{1}{2}$). The velocity weights should be equal: $t_q^{(a)} = t_q^{(m)}$, for the two limit cases, $t_c^{(m)} = 0$ and $t_c^{(m)} = \frac{1}{2}$, otherwise their non-negativity domain reduces to $U^2 = 0$, with or without the numerical diffusion. The "standard" equilibrium weights give relatively large non-negativity domains. Selecting properly the equilibrium weights and c_e (especially), one may improve the stability of the BGK schemes in the advection limit.

2.6 Necessary Stability Conditions of the TRT Model in the Diffusion-Dominant Limit

We consider three principal orientations of the wave vector $\mathbf{k}$: (1) when $\mathbf{k}$ is parallel to one of the coordinate axis, say α: $\mathbf{k} = k\mathbf{1}_\alpha$, (2) when $\mathbf{k}$ is along the diagonal lattice direction:

$\mathbf{k} = k\mathbf{1}_d$, $\mathbf{1}_d \in \{1, (1, 1), (1, 1, 1)\}$, (3) when $\mathbf{k}$ is along the diagonal on two-dimensional sub-lattice: $\mathbf{k} = k\mathbf{1}_d^{(\gamma)}$, $\mathbf{1}_d^{(\gamma)} \in \{(0, 1, 1), (1, 1, 0), (1, 0, 1)\}$. When $\mathbf{k} = \pi\mathbf{1}_d$, then $\cos(\pi\mathbf{c}_q \cdot \mathbf{1}_d) \equiv -1$ for all links of the minimal models and d3Q15.

Definition 2.6.1 *The diffusion-dominant limit* corresponds to $k = \pi$ for any $\mathbf{k}$ mentioned above, when the set $\{E_q^-\}$ vanishes in the characteristic equation (42) with relations (41), since $\sin[k_q] = 0$. This also includes the pure diffusion equation $\mathbf{U} \equiv 0$ (then $E_q^- \equiv 0$). The characteristic equation (42) takes the form:

$$\begin{aligned}
&(1 + \lambda^- + \Omega)(\Omega^2 + \Omega\lambda^+(1 - 2s^+) - (1 + \lambda^+)) = 0, \quad \text{for} \\
&\qquad \mathbf{k} = \pi\mathbf{1}_\alpha, \quad s^+ = \mathcal{S}_\alpha^+: \quad \text{all models}, \\
&\qquad \mathbf{k} = \pi\mathbf{1}_d, \quad s^+ = \mathcal{S}^+: \quad \text{dDQ(2D+1)},\ \text{d3Q15}, \\
&\qquad \mathbf{k} = \pi\mathbf{1}_d, \quad s^+ = \mathcal{S}_c^+: \quad \text{d2Q9}, \\
&\qquad \mathbf{k} = \pi\mathbf{1}_d^{(\gamma)}, \quad s^+ = \mathcal{S}_c^{+,\gamma}: \quad \text{d3Q15},
\end{aligned} \tag{61}$$

with

$$\begin{cases}
\mathcal{S}^+ = \sum_{q=1}^{Q_m} E_q^+ = 1 - E_0, \\
\mathcal{S}_\alpha^+ = \sum_{q:c_{q\alpha}\neq 0} E_q^+ = \sum_{q=1}^{Q_m} E_q^+ c_{q\alpha}^2 = \mathcal{D}_{\alpha\alpha}^+ = \mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2, \\
\mathcal{S}_c^+ = \sum_{q:c_{q\alpha}c_{q\beta}=0,\alpha\neq\beta} E_q^+, \\
\mathcal{S}_c^{+,\gamma} = \sum_{q:c_{q\alpha}c_{q\beta}=0,c_{q\gamma}=0} E_q^+, \quad \gamma \neq \alpha \neq \beta.
\end{cases} \tag{62}$$

Here, $\mathcal{S}^+$, $\mathcal{S}_\alpha^+$, $\mathcal{S}_c^+$ and $\mathcal{S}_c^{+,\gamma}$ denote, respectively, the sum of all moving weights E_q^+, their sum for all populations with non-zero α-component of $\mathbf{c}_q$, the sum of E_q^+ for all coordinate links and finally, the sum of E_q^+ for two of three coordinate links, those with zero γ-component of their velocity $\mathbf{c}_q$. The second order polynomial (61) satisfies the conditions of the Miller's theorem (see relation (113)) when $\lambda^+ \in]-2, 0[$, such that its stability bounds are set by the case $\lambda^+ = -1$:

$$\Omega = 1 - 2s^+, \quad \text{then } |\Omega| \leq 1 \text{ if only } 0 \leq s^+ \leq 1. \tag{63}$$

Using relations (62) for s^+ in inequality (63), we derive four principal necessary diffusion-dominant stability conditions:

1. The first condition is:

$$\mathbf{k} = \pi\mathbf{1}_\alpha, \quad \text{all models:} \quad 0 \leq \mathcal{S}_\alpha^+ \leq 1. \tag{64}$$

2. The second condition is:

$$\mathbf{k} = \pi\mathbf{1}_d, \quad \text{dDQ(2D+1)} \quad \text{and} \quad \text{d3Q15:} \quad 0 \leq \mathcal{S}^+ \leq 1, \quad 0 \leq E_0 \leq 1. \tag{65}$$

3. The third condition is:

$$\mathbf{k} = \pi\mathbf{1}_d, \quad \text{d2Q9:} \quad 0 \leq \mathcal{S}_c^+ \leq 1, \quad 0 \leq E_0 + \sum_{q:c_{qx}c_{qy}\neq 0} E_q^+ \leq 1. \tag{66}$$

4. The fourth condition is:

$$\mathbf{k} = \pi \mathbf{1}_d^{(\gamma)}, \quad \text{d3Q15:} \quad 0 < \mathcal{S}_c^{+,\gamma} \leq 1, \quad \forall \gamma = 1, \ldots, d. \tag{67}$$

Remark 2.6.A We stress that the obtained diffusion conditions are necessary for the TRT model with any eigenvalues. They are straightforward for the OTRT sub-class using solution (47) where $\mathcal{B}$ vanishes. One can replace any $\sum_q E_q^+$ in relations above with $\sum_q E_q$ owing to the symmetry.

Remark 2.6.B The first condition (64) restricts the sub-set $\{E_q^+\}$ with a common nonzero velocity coordinate to [0, 1]. Hence, $E_q^+ \in [0, \frac{1}{2}]$ for the minimal models. Since $0 \leq \mathcal{D}_{\alpha\alpha}^+ \leq 1$ and $\mathcal{D}_{\alpha\alpha}^+ = \mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2 \geq \mathcal{D}_{\alpha\alpha}$ then, for all the models, $c_e = \frac{\sum_{\alpha=1}^d \mathcal{D}_{\alpha\alpha}}{d}$ is confined to [0, 1] and U^2 is limited by $1 - c_e$ when $g^{(u)} = 1$:

$$\begin{aligned} g^{(u)} = 1: \quad & U_\alpha^2 \leq 1 - \mathcal{D}_{\alpha\alpha}, \quad 0 \leq \mathcal{D}_{\alpha\alpha} \leq 1, \quad \forall \alpha = 1, \ldots, d, \\ \text{then:} \quad & U^2 \leq 1 - \max_\alpha \{\mathcal{D}_{\alpha\alpha}\} \leq 1 - c_e, \quad 0 \leq c_e \leq 1. \end{aligned} \tag{68}$$

Remark 2.6.C The second condition (65) constraints E_0 and, equivalently, $\sum_{q=1}^{Q_m} E_q^+$ to the interval [0, 1] but only for the minimal models and d3Q15. Indeed, the third condition (66) for the d2Q9 scheme does not restrict E_0 alone to [0, 1], but only together with $\sum_q E_q^+$ for the diagonal links. This sum alone is not restricted to [0, 1], unless it vanishes when the d2Q9 model reduces to the d2Q5 model (then $E_0 \geq 0$). Therefore, the necessary condition (66) is *weaker* than the condition $E_0 > 0$. The sufficient stability conditions in Sect. 4 respect, mostly, neither $E_0 > 0$ nor $\{E_q^+ > 0\}$. This is illustrated in Fig. 13.

Remark 2.6.D Finally, the d3Q15 scheme restricts to [0, 1]: (i) E_0 (hence $\sum_{q=1}^{Q_m} E_q^+$), (ii) $\sum_q E_q^+$ for any two of three coordinate links, and (iii) $\sum_q E_q^+$ for any coordinate link with all the diagonal links.

3 Optimal Minimal Models and Finite-Difference Schemes

3.1 Minimal OTRT Models

We consider the minimal TRT models: dDQ(2D+1) = $\{d1Q3, d2Q5, d3Q7\}$. Their optimal stability bounds are set by relations (46) with (45), where the equilibrium components $E_q^\pm$ are prescribed by relations (9) with (16), then:

$$\Omega = 1 + \sum_{\alpha=1}^{d} \mathcal{D}_{\alpha\alpha}^+ (\cos[k_\alpha] - 1) - i \sum_{\alpha=1}^{d} U_\alpha \sin[k_\alpha], \quad \mathcal{D}_{\alpha\alpha}^+ = \mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2. \tag{69}$$

We prescribe the *necessary and sufficient* conditions for all minimal models:

$$\begin{cases} (1)\ 0 \leq E_0 \leq 1, \quad \text{or, equivalently,} \quad 0 \leq \sum_{\alpha=1}^d (\mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2) \leq 1, \\ (2)\ \sum_\alpha \frac{U_\alpha^2}{\mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2} \leq 1, \quad g^{(u)} = \{0, 1\}. \end{cases} \tag{70}$$

Their sufficiency immediately follows from relations (49). The necessity of the first (diffusion-dominant) condition is stated by relation (65). Then the *d-line* boundary reduces to the E_0-*n-line* for the minimal models. The necessity of the second, advection condition can be derived from relation (69) in the limit $\mathbf{k} \to 0$, similarly as it was demonstrated above for isotropic tensors (see relations (36) and (48)). More rigorous proof can be obtained using techniques [17] (see also Sect. 3.3). When the diffusion tensor (12) is isotropic and $\{E_q^+\}$ is prescribed with relation (18), conditions (70) become:

$$g^{(u)} = 0: \quad U^2 \le U_{a,0}^2 = c_e, \quad 0 \le c_e \le c_e^{(\max)} = c_e^{(0)} = \frac{1}{d}. \tag{71}$$

Here, the optimal advection line, *a-line*, is $U^2 = U_{a,0}^2$ and the non-negativity line, E_0-*n-line*, reduces to $c_e = \frac{1}{d}$ (see Definitions 1.2.1.C and D). The stability bounds are illustrated by the left diagram in Fig. 1. Then the highest velocity amplitude, $U^2 = \frac{1}{d}$, is reached on the E_0-*n-line*, the highest possible Courant number is $Cr = \frac{1}{\sqrt{d}}$. When $c_e = 1$, the d1Q3 model reduces to d1Q2 where the $Cr = 1$. The work by Rheinländer [27] shows that the d1Q2 BGK model has this condition for any τ. However, without immobile population, the d1Q2 cannot remove the numerical diffusion with *local* equilibrium distribution.

When $g^{(u)} = 1$, replacing c_e with $c_e + U_\alpha^2$ in relation (71), and summing over α, the stability conditions become:

$$g^{(u)} = 1: \quad U^2(c_e) \le \min\left\{1 - dc_e, \forall d, \frac{d}{d-1}c_e, d \ge 2\right\}, \quad 0 \le c_e \le \frac{1}{d}. \tag{72}$$

This can also be obtained noting that the functions (70) with isotropic diffusion components have their maximum for diagonal velocity direction. The stability bounds are illustrated by the right diagram in Fig. 1. They are all limited by the (decreasing) E_0-*n-line* function $U_d^2 = 1 - dc_e$ and the (increasing) *a-line* function $U^2(c_e) \le \frac{d}{d-1}c_e$, except the d1Q3 model where the *a-line* reduces to the boundary segment $0 \le U^2(c_e = 0) \le 1$. The intersection of the *a-line* and the E_0-*n-line* when $c_e = c_e^{opt}$ gives the highest stable velocity: $U_{opt}^2 = U^2(c_e^{opt})$:

$$\begin{aligned}
&g^{(u)} = 1: \\
&\text{d1Q3:} \quad 0 \le c_e \le 1, U^2 \le U_d^2 = 1 - c_e, \\
&\qquad\qquad \text{then} \quad c_e^{opt} = 0, U_{opt}^2 = 1. \\
&\text{d2Q5:} \quad 0 \le c_e \le \frac{1}{2}, \quad U^2 \le U_d^2 = 1 - 2c_e \quad \text{and} \quad U^2 \le U_{a,1}^2 = 2c_e, \\
&\qquad\qquad \text{then} \quad c_e^{opt} = \frac{1}{4}, U_{opt}^2 = \frac{1}{2}. \\
&\text{d3Q7:} \quad 0 \le c_e < \frac{1}{3}, U^2 \le U_d^2 = 1 - 3c_e \quad \text{and} \quad U^2 \le U_{a,2}^2 = \frac{3}{2}c_e, \\
&\qquad\qquad \text{then} \quad c_e^{opt} = \frac{2}{9}, U_{opt}^2 = \frac{1}{3}.
\end{aligned} \tag{73}$$

Remark 3.1.A The stability bounds of the d1Q3 model are:

$$\begin{aligned}
&\text{d1Q3}, g^{(u)} = 0: \quad U^2 \le U_{a,0}^2 = c_e, \quad 0 \le c_e \le 1, \\
&\text{d1Q3}, g^{(u)} = 1: \quad U^2 \le U_d^2 = 1 - c_e, \quad 0 \le c_e \le 1.
\end{aligned} \tag{74}$$

These conditions are necessary for all velocity sets (see relations (36) and (68)) and we refer to them as "best" (possible) stability.

Remark 3.1.B Let $\mathcal{D}^{min}$ be the smallest diagonal diffusion coefficient $\{\mathcal{D}_{\alpha\alpha}\}$ ($\mathcal{D}^{min} \leq c_e$). The sufficient advection condition (70-2) for anisotropic tensors can be simplified using the stronger condition:

$$\sum_{\alpha=1}^{d} \frac{U_\alpha^2}{\mathcal{D}^{min} + g^{(u)} U_\alpha^2} \leq 1. \tag{75}$$

Then the conditions (71)–(72) can be adapted by replacing c_e with $\mathcal{D}^{min}$, but uniquely for the advection lines: $\{U_{a,0}^2, U_{a,1}^2, U_{a,2}^2\}$.

The stability bounds for $Cr = |\mathbf{U}| = \sqrt{U^2}$ versus $Pe_{\Delta x}^* = \Lambda^- Pe_{\Delta x} = \frac{|\mathbf{U}|}{c_e}$ are shown in Fig. 2. They are obtained by replacing c_e with $\frac{|U|}{Pe_{\Delta x}^*}$ in relations (71) and (73):

$$\begin{aligned}
&g^{(u)} = 0: \\
&\quad 0 \leq Cr \leq Cr_0 = \frac{Pe_{\Delta x}^*}{d}, \quad \text{if } 0 \leq Pe_{\Delta x}^* \leq Pe_0^* = \sqrt{d}, \quad \text{else } 0 \leq Cr \leq \frac{1}{Pe_{\Delta x}^*}. \\
&g^{(u)} = 1: \quad 0 \leq Cr \leq Cr_0, \quad Cr_0 = \frac{-d + \sqrt{d^2 + 4(Pe_{\Delta x}^*)^2}}{2Pe_{\Delta x}^*}, \\
&\quad \text{if } 0 \leq Pe_{\Delta x}^* \leq Pe_0^* = \frac{d\sqrt{d}}{d-1}, \quad \text{else } 0 \leq Cr \leq \frac{d}{(d-1)Pe_{\Delta x}^*}, d \neq 1.
\end{aligned} \tag{76}$$

The E_0-*n-line* $Cr = Cr_0$ dominates when $Pe_{\Delta x}^*$ is small, while the *a-line* bounds the domain for $Pe_{\Delta x}^* > Pe_0^*$. The use of $Pe_{\Delta x}^*$ enables us to cover all grid Peclet numbers $Pe_{\Delta x}$ on the same diagram. When the diagonal elements of the numerical diffusion are removed, all the models reach higher Courant values Cr for equal $Pe_{\Delta x}^*$ values in the advection-dominant regime. The d1Q3 model is then "unconditionally" stable until $Cr = 1$ when $Pe_{\Delta x}^* \to \infty$. The necessary and sufficient stability conditions (76) are valid for any Λ^- using the OTRT sub-class, with $\Lambda^- = \frac{1}{2}$ for the OBGK model.

Examples 3.1 The spectrum of the characteristic equation (38) is computed with the help of numerical eigenmode routines (the CLAPACK library) when both $\mathbf{U}$ and $\mathbf{k}$ vary in a d-dimensional space. Typically, we use 8 points per every variation of $\mathbf{U}$: $\mathbf{U} = U\{\cos\psi \sin\alpha, \sin\psi \sin\alpha, \cos\alpha\})$ and 8 points per every variation of $\mathbf{k}$ with respect to $\mathbf{U}$, with 72 points for $|k| \in [0, \pi\sqrt{d}]$, once U is set. We first confirm that $\Lambda = \frac{1}{4}$ gives the same stable areas as the OBGK model, for very different values of Λ^-. The numerical analysis validates the predicted stability bounds, as illustrated in Fig. 8. In fact, for isotropic minimal models in two and three dimensions, it turns out that the necessary and sufficient stability conditions are set by the diagonal directions. We emphasize that the stability bounds $U^2(c_e)$ (Figs. 1, 2, and 8) are valid $\forall \Lambda^+ > 0$ and $\forall \Lambda^- > 0$ such that $\Lambda = \Lambda^+\Lambda^- = \frac{1}{4}$.

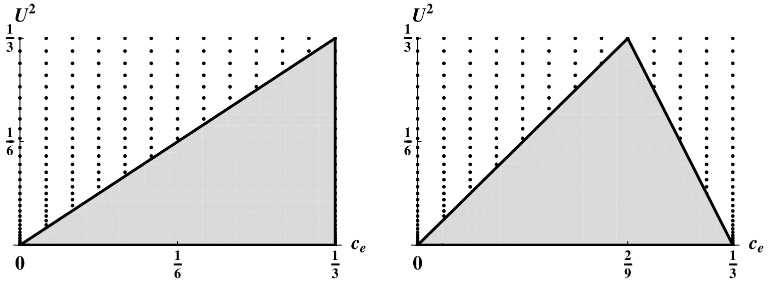

Fig. 8 The unstable points $(c_e, |\mathbf{U}|^2)$ are shown for the d3Q7 OBGK model (where $|\Omega| \geq 1+\epsilon$, $\epsilon = 10^{-14}$, with the numerical stability analysis). They perfectly fit the predicted necessary and sufficient bounds (52) and (71) for $g^{(u)} = 0$ (*left*) and (73) for $g^{(u)} = 1$ (*right*). These stability domains are valid for the whole OTRT sub-class

3.2 Optimal and Non-negativity Conditions

Let $\mathcal{D}^{min} \leq c_e \leq \frac{1}{d}$ be the smallest diagonal coefficient. The non-negativity equilibrium conditions for minimal models are:

$$g^{(u)} = 0, d = \{1, 2, 3\}: \quad U^2 \leq U_n^2 = \mathcal{D}^{min2}, 0 \leq c_e \leq \frac{1}{d} \tag{77}$$

and

$$\begin{cases} g^{(u)} = 1, d = \{1, 2, 3\}: & U^2 \leq U_n^2 = 1 - dc_e, \\ \text{and} & \\ g^{(u)} = 1, d = 1 \quad : & (U^2 \leq U_n^{2(-)}) || (U^2 \geq U_n^{2(+)}), \\ g^{(u)} = 1, d = \{2, 3\} \quad : & U^2 \leq U_n^{2(-)}, \quad U_n^{2(\pm)} = \frac{(1 \pm \sqrt{1-4\mathcal{D}^{min}})^2}{4}. \end{cases} \tag{78}$$

These relations apply for isotropic tensors with $\mathcal{D}^{min} = c_e$, as illustrated in Fig. 3. First condition (78) ($E_0 \geq 0$) is common for both, non-negativity and optimal stability conditions. The non-negativity line (*n-line*) envelopes conditions $\{E_q \geq 0\}$ for the moving populations. This condition rules out the whole area between the optimal boundary *a-line* and the *n-line*. Figure 6 confirms that the stability boundary of the BGK model approaches solution (78) when $\Lambda^- \to 0$.

Lemma 2.3.2 states that the non-negativity conditions are stronger than the sufficient conditions (70). For isotropic tensors and $g^{(u)} = 0$, the optimal condition: $U^2 \leq c_e$ is obviously weaker than the non-negativity condition: $U^2 \leq c_e^2$. Let us illustrate this property for anisotropic tensors. In fact, when the non-negativity condition is verified, each velocity component $U_\alpha > 0$ is such that $\mathcal{D}_{\alpha\alpha} - U_\alpha + g^{(u)} U_\alpha^2 \geq 0$, then

$$\sum_{\alpha=1}^{d} \frac{U_\alpha^2}{\mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2} \leq \sum_{\alpha=1}^{d} \frac{(\mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2)^2}{\mathcal{D}_{\alpha\alpha} + g^{(u)} U_\alpha^2} \leq 1 - E_0 \leq 1.$$

For isotropic diffusion tensor, the non-negativity domain in the plane $(Cr, Pe^*_{\Delta x})$ is given by

$$\begin{cases} g^{(u)} = 0: & 0 \leq Cr \leq Cr_0, \quad 0 \leq Pe^*_{\Delta x} \leq 1. \\ g^{(u)} = 1: & \max\{0, \frac{Pe^*_{\Delta x} - 1}{Pe^*_{\Delta x}}\} \leq Cr \leq Cr_0, \quad \forall Pe^*_{\Delta x}. \end{cases} \tag{79}$$

The E_0-*n-line* $Cr = Cr_0$ is given by relations (76). Conditions (79) agree with the non-negativity solution [29] (see their Sects. (A.1)–(B.1) for the d1Q3 model with $g^{(u)} = \{0, 1\}$ and d2Q5 with $g^{(u)} = 0$, respectively). The non-negativity conditions are illustrated in Fig. 4. In the presence of numerical diffusion, the non-negativity condition $U^2 \le c_e^2$ restricts $Pe^*_{\Delta x}$ to $[0, 1]$. When the numerical diffusion is removed, then higher $Pe^*_{\Delta x}$ values can be reached inside the non-negativity domain in multi-dimensions. In one dimension, any $Pe^*_{\Delta x}$ value is available but the non-negativity condition rules out the stable area for $0 \le Cr(Pe^*_{\Delta x}) \le \frac{Pe^*_{\Delta x}-1}{Pe^*_{\Delta x}}$ when $Pe^*_{\Delta x} > 1$.

Remark 3.2 Altogether, the OTRT sub-class is stable for any grid Peclet number $Pe_{\Delta x}$ when the necessary and sufficient conditions (70) are verified, even when some of the "moving" equilibrium distributions are negative.

3.3 The OTRT Sub-class Against the Forward-Time Central-Differences Schemes

We mainly follow the work by Hindmarsch, Grescho & Griffiths [17]. The minimal diffusion stencils contain 3, 5 and 7 points in one, two and three dimensions, respectively. The neighbors are the same as for dDQ(2D+1) models. The minimal forward-time central-differences scheme (FTCS) for the advection-diffusion equation reads:

$$\frac{s(\mathbf{r}, t+\Delta_t) - s(\mathbf{r}, t)}{\Delta_t} + \sum_{\alpha=1}^{d} U_\alpha \bar{\Delta}_\alpha s(\mathbf{r}, t) = \sum_{\alpha=1}^{d} K_{\alpha\alpha} \Delta_\alpha^2 s(\mathbf{r}, t), \tag{80}$$

where $\bar{\Delta}_\alpha$ and $\Delta_\alpha^2 s(\mathbf{r}, t)$ are respectively the central-difference and Laplace operators along the α-axis. Let us define the dimensionless parameters:

$$\mathcal{D}_{\alpha\alpha}^{f.d.} = 2\frac{K_{\alpha\alpha}\Delta_t}{\Delta_\alpha^2}, \quad U_\alpha = \frac{u_\alpha \Delta_t}{\Delta_\alpha}, \quad \text{and} \quad Pe^*_{\Delta\alpha} = \frac{u_\alpha \Delta_\alpha}{2K_{\alpha\alpha}} = \frac{U_\alpha}{\mathcal{D}_{\alpha\alpha}^{f.d.}}. \tag{81}$$

Substituting the Fourier mode, $s(\mathbf{r}, t) = \Omega^t \exp(i\mathbf{r} \cdot \mathbf{k})$, the solution of the FTCS for the amplification factor Ω is:

$$\Omega = 1 + \sum_{\alpha=1}^{d} \mathcal{D}_{\alpha\alpha}^{f.d.} (\cos[k_\alpha] - 1) - i \sum_{\alpha=1}^{d} U_\alpha \sin[k_\alpha]. \tag{82}$$

Hindmarsch et al. [17] prove that this scheme is stable in the von Neumann sense, if and only if the following conditions take place:

$$\begin{cases} (1)\ 0 \le \sum_{\alpha=1}^{d} \mathcal{D}_{\alpha\alpha}^{f.d.} \le 1, \quad \text{or, equivalently,} \quad c_e^{(f.d.)} = \frac{\sum_{\alpha=1}^{d} \mathcal{D}_{\alpha\alpha}^{f.d.}}{d} \le \frac{1}{d}, \\ (2)\ \sum_{\alpha=1}^{d} \frac{U_\alpha^2}{\mathcal{D}_{\alpha\alpha}^{f.d.}} \le 1, \quad \text{or, equivalently,} \quad \sum_{\alpha=1}^{d} U_\alpha Pe^*_{\Delta\alpha} \le 1. \end{cases} \tag{83}$$

The (modified) MFTCS scheme, also known as Lax-Wendroff scheme in one dimension, removes the diagonal elements of the numerical diffusion, taking $K_{\alpha\alpha} = K_{\alpha\alpha} + \frac{u_\alpha^2}{2}$. Its stability conditions can be obtained replacing in both relations (83):

$$\text{MFTCS:} \quad \mathcal{D}_{\alpha\alpha}^{f.d.} \to \mathcal{D}_{\alpha\alpha}^{f.d.} + U_\alpha^2. \tag{84}$$

The characteristic equation (82) is equivalent to (44) for the OBGK scheme ($\Lambda^- = \frac{1}{2}$, $p = 0$, $\Omega = \mathcal{A} - i\mathcal{B}$), with $g^{(u)} = 0$ for the FTCS and $g^{(u)} = 1$ for the MFTCS. It follows that the proofs [17] of the necessity and sufficiency are also suitable for the OTRT conditions (70), replacing $\mathcal{D}_{\alpha\alpha}^{f.d.} = 2\frac{K_{\alpha\alpha}\Delta_t}{\Delta_\alpha^2}$ with $\mathcal{D}_{\alpha\alpha} = \frac{K_{\alpha\alpha}\Delta_t}{\Lambda^-\Delta_\alpha^2}$.

Let us now compare the OTRT sub-class and FTCS in efficiency on the same grid, with respect to their available time-steps Δ_t and $\Delta_t^{f.d.}$. Keeping in mind that $Pe_{\Delta x}^* = \frac{U}{c_e} = \Lambda^- Pe_{\Delta x}$, ${Pe_{\Delta x}^*}^{f.d.} = \frac{U}{c_e^{(f.d.)}} = \frac{1}{2} Pe_{\Delta x}$, then $Pe_{\Delta x}^* = 2\Lambda^- {Pe_{\Delta x}^*}^{f.d.}$ and the two principal stability criteria of both schemes give when $g^{(u)} = 0$:

$$\begin{cases} \text{diffusion-dominant:} \quad 0 \le Cr \le \text{Const}\, Pe_{\Delta x}^*, \quad \text{then } \Delta_t > \Delta_t^{f.d.} \quad \text{if } \Lambda^- > \frac{1}{2}. \\ \text{advection-dominant:} \quad 0 \le Cr \le \frac{\text{Const}}{Pe_{\Delta x}^*}, \quad \text{then } \Delta_t > \Delta_t^{f.d.} \quad \text{if } \Lambda^- < \frac{1}{2}. \end{cases}$$

Selecting $\Lambda^- > \frac{1}{2}$ the time-step condition of the OTRT sub-class is more efficient than the one of the FTCS in the diffusion-dominant regime. This is conversely in the advection-dominant regime where $\Lambda^- < \frac{1}{2}$ allows larger time steps. When $\Lambda^- = \frac{1}{2}$ then the OTRT and BGK schemes coincide with the FTCS. In summary, owing to Λ^-, both the BGK and OTRT sub-classes allow larger time steps than the explicit finite-difference schemes in the diffusion-dominant regime, where predominates the non-negativity of the immobile weight. Owing to the free relaxation parameter, the OTRT sub-class also allows larger time steps in the advection-dominant regime, provided that c_e and Λ^- are properly selected.

4 The d2Q9 and d3Q15 Models

The objectives of this section are: (a) to specify the set of necessary (any eigenvalues) stability conditions based on the above results for the advection-dominant and the diffusion-dominant limits, (b) to derive sufficient specific OTRT stability conditions with the help of Theorem 2.3.1 (for this we first need to derive the non-negativity conditions for symmetric weights $\{E_q^+\}$), and (c), to build *necessary and sufficient* OTRT stability conditions for the most interesting cases. The restriction $\{E_q^{(a)} = 0\}$ is applied to all results of this section. For comparison, the non-negativity conditions $\{E_q = E_q^+ + E_q^- \ge 0\}$ are plotted along with the OTRT sufficient conditions for all figures.

4.1 Non-negativity of the Symmetric Weights $\{E_q^+\}$: d2Q9 and d3Q15 Models

The equilibrium parameter c_e is found in the interval $[0, 1]$ (cf. relation (68)). The non-negativity of the immobile weight, E_0-*n-line* function $U_d^2(c_e)$, is prescribed by relations (33) and (34), respectively, for the d2Q9 and d3Q15 schemes. We first derive the non-negativity conditions per class, for *the coordinate weights*: $U^2 \le U_{p,c}^2(c_e)$ and for *the diagonal weights*: $U^2 \le U_{p,d}^2(c_e)$. Interestingly, both functions are the same for the d2Q9 and d3Q15 schemes.

Coordinate Links The whole set $\{E_q^+\}$ is non-negative for the coordinate links when $E_q^{(a)} = 0$ and $g^{(u)} = 0$. However, when $g^{(u)} = 1$ the minimum $\min_q E_q^+(c_e, \mathbf{U})$ is equal to $c_e t_c^{(m)} + \frac{(\gamma_u - 1)}{6} U^2$, and it is reached on the link perpendicular to the coordinate axis parallel to $\mathbf{U}$. Then $\{E_q^+ \ge 0\}$ for all the coordinate links provided that $U^2 \le U_{p,c}^2(c_e)$ where:

$$g^{(u)} = 1, \quad g_{\alpha\beta}^{(u)} = \{0, 1\}: \quad U_{p,c}^2 = k_c c_e, \quad k_c = \frac{6 t_c^{(m)}}{1 - \gamma_u}, \quad \gamma_u \ne 1. \tag{85}$$

Hence $E_q^+ \geq 0$ for all the coordinate links and $\forall \mathbf{U}$ when $\gamma_u = 1$ ($t_c^{(u)} = \frac{1}{2}$), i.e., when only the coordinate links obtain the U^2-term, as the minimal models. When $t_c^{(m)} \equiv 0$ then $U^2_{p,c}(c_e) = 0$, except $\gamma_u = 1$. It follows that Theorem 2.3.1 can be applied for $t_c^{(m)} = 0$ only with $t_c^{(a)} = 0$ and $\gamma_u = 1$.

Diagonal Links When $E_q^{(a)} = 0$ and $g^{(u)}_{\alpha\beta} g^{(u)} = 0$ then $E_q^+ \geq 0$ for all the diagonal links. However, when $g^{(u)}_{\alpha\beta} g^{(u)} = 1$, the minimal diagonal weight E_q^+ is proportional to $6c_e(1 - 2t_c^{(m)}) - U^2(1 + 2\gamma_u)$. Then $\{E_q^+ \geq 0\}$ for all diagonal links if only $U^2 \leq U^2_{p,d}$:

$$g^{(u)}_{\alpha\beta} g^{(u)} = 1: \quad U^2_{p,d} = k_d c_e, \quad k_d = \frac{6(1 - 2t_c^{(m)})}{1 + 2\gamma_u}, \quad \gamma_u \neq -\frac{1}{2}. \tag{86}$$

This condition may vanish only when $\gamma_u = -\frac{1}{2}$. We recall that $\gamma_u \in [-\frac{1}{2}, 1]$ for the d2Q9 scheme but γ_u is limited to $[0, 1]$ for the d3Q15 scheme (then $\{t_q^{(u)} > 0\}$, see relation (26)). The condition (86) is the most restrictive when $\gamma_u = 1$ once $t_c^{(m)}$ is set.

Coordinate and Diagonal Links The highest common slope value for $U^2(c_e)$, when *both conditions* (85) *and* (86) are respected, is $k_c = k_d = 2$. This can be achieved only when γ_u is linked to $t_c^{(m)}$ via specific rule, hereafter referred to as $\gamma_u = \gamma_u^{(m)}$:

$$g^{(u)}_{\alpha\beta} g^{(u)} = 1: \quad k_c = k_d = 2 \quad \text{if only } \gamma_u = \gamma_u^{(m)} = 1 - 3t_c^{(m)}. \tag{87}$$

It is noted that the family (87) rules out the minimal models (27) but includes the "standard" schemes (30). In fact, $\gamma_u = \gamma_u^{(m)}$ separates two sub-intervals where either $k_c \geq 2$ (when $\gamma_u^{(m)} \leq \gamma_u \leq 1$) or $k_d \geq 2$ ($\gamma_u \leq \gamma_u^{(m)}$). When $\gamma_u = \gamma_u^{(m)}$, the E_0-*n-lines* and weights $\{t_q^{(u)}\}$ become

$$\begin{aligned}
\text{d2Q9:} \quad & U_d^2(c_e) = \frac{1 - c_e(1 + 2t_c^{(m)})}{1 - t_c^{(m)}}, \quad t_c^{(u)} = \frac{1 - 2t_c^{(m)}}{2}, \quad t_d^{(u)} = \frac{t_c^{(m)}}{2}. \\
\text{d3Q15:} \quad & U_d^2(c_e) = \frac{1 - c_e(1 + 4t_c^{(m)})}{1 - 2t_c^{(m)}}, \quad t_c^{(u)} = \frac{1 - 3t_c^{(m)}}{2}, \quad t_d^{(u)} = \frac{3t_c^{(m)}}{8}.
\end{aligned} \tag{88}$$

Interestingly, all the E_0-*n-lines* (88) intersect the non-negativity line (87) $U^2(c_e) = 2c_e$ for $c_e = \frac{1}{3}$, $\forall t_c^{(m)} \in [0, \frac{1}{2}]$. Then, all the symmetric weights $\{E_q^+\}$ and E_0 are non-negative provided that U^2 is confined into the following triangle:

$$U^2 \leq 2c_e \quad \text{if} \quad 0 \leq c_e \leq \frac{1}{3}, \quad \text{and} \quad U^2 \leq U_d^2(c_e) \quad \text{if} \quad \frac{1}{3} \leq c_e \leq c_e^{(0)}. \tag{89}$$

Figure 9 illustrates these conditions for the d2Q9 and d3Q15 schemes when $t_c^{(m)}$ varies. The highest possible velocity is $U^2 = \frac{2}{3}$:

$$g^{(u)}_{\alpha\beta} g^{(u)} = 1: \quad \text{if } E_0 \geq 0 \quad \text{and} \quad \{E_q^+ \geq 0\} \quad \text{then } U^2 \leq \frac{2}{3}. \tag{90}$$

Finally, we emphasize that relation (49-2) of Theorem 2.3.1 predicts the sufficient stability conditions for the OTRT models with the weight family (87) provided that $U^2 \leq 2c_e$ and $E_0 \geq 0$.

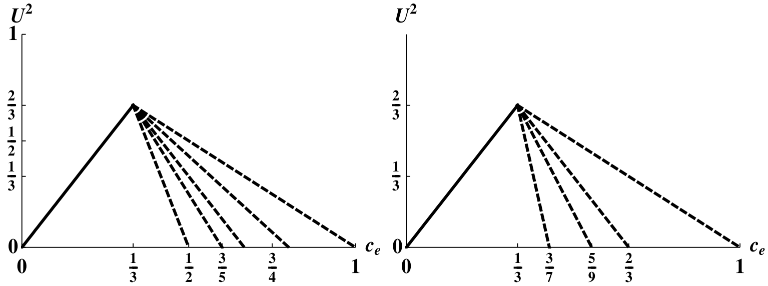

Fig. 9 The best possible domains (89) for non-negative *symmetric weights* ($E_q^+ \geq 0\ \forall q$ and $E_0 \geq 0$), are shown for the d2Q9 schemes (*left*) and d3Q15 schemes (*right*), when $t_c^{(m)}$ varies and $0 \leq \gamma_u = 1 - 3t_c^{(m)} \leq 1$ (relation (87)). The boundary segment $U^2 = 2c_e$ (*solid line*) guarantees $\{E_q^+ > 0\}$ for these weights. The E_0-*n-line* is the decreasing (*dashed*) edge, from right to left: $t_c^{(m)} = \{0, \frac{1}{8}, \frac{1}{4}, \frac{1}{3}, \frac{1}{2}\}$ for the d2Q9 scheme, and: $t_c^{(m)} = \{0, \frac{1}{8}, \frac{1}{5}, \frac{1}{3}\}$ for the d3Q15 scheme. The d2Q9$^{(stan)}$ and d3Q15$^{(stan)}$ models have $t_c^{(m)} = \frac{1}{3}$; the d2Q9$^{(unif)}$ and d3Q15$^{(unif)}$ models have $t_c^{(m)} = \frac{1}{4}$ and $t_c^{(m)} = \frac{1}{5}$, respectively. The peak is for $c_e = \frac{1}{3}$ for any $t_c^{(m)}$

4.2 The d2Q9 Model

4.2.1 The d2Q9 Model: Necessary Stability Conditions for Any Eigenvalues

With Numerical Diffusion $g^{(u)} = 0$ The necessary diffusion-dominant conditions (64) and (66) become:

$$\begin{cases} (1)\ \mathbf{k} = \pi\{1, 0\}: & 0 \leq c_e \leq 1, \\ (2)\ \mathbf{k}^{\pi} = \pi\{1, 1\}: & 0 \leq c_e \leq \frac{1}{4t_c^{(m)}}. \end{cases} \tag{91}$$

Together, these two conditions give:

$$0 \leq c_e \leq c_e^{(\max)}, \quad c_e^{(\max)} = \min\left\{1, \frac{1}{4t_c^{(m)}}\right\}, \quad 0 \leq t_c^{(m)} \leq \frac{1}{2}. \tag{92}$$

Hence, c_e is available in the whole interval $[0, 1]$ when $t_c^{(m)} \in [0, \frac{1}{4}]$. Combining condition (92) with the necessary advection-dominant condition (36), *the necessary conditions in the presence of numerical diffusion* become:

$$g^{(u)} = 0: \quad U^2 \leq U_{a,0}^2 = c_e, \quad 0 \leq c_e \leq c_e^{(\max)}, \quad c_e^{(\max)} = \min\left\{1, \frac{1}{4t_c^{(m)}}\right\}. \tag{93}$$

Without Diagonal Numerical Diffusion $g^{(u)} = 1,\ g_{xy}^{(u)} = 0$ When $g^{(u)} = 1$, the necessary diffusion-dominant conditions (64) and (66) become:

$$U^2 \leq \min\{U_{d,1}^2, U_{d,2}^2\} \quad \text{where}$$
$$\begin{cases} (1)\ \mathbf{k} = \pi\{1, 0\}: \ U_{d,1}^2 = 1 - c_e, 0 \leq c_e \leq 1, \\ (2)\ \mathbf{k}^{\pi} = \pi\{1, 1\}: U_{d,2}^2 = \frac{3}{(1+2\gamma_u)}(1 - \frac{c_e}{c_e^{(\max)}}), 0 \leq c_e \leq c_e^{(\max)}. \end{cases} \tag{94}$$

Combining necessary conditions (36) and (94), *the necessary conditions in the presence of cross-diagonal elements* $\{\mathcal{D}_{\alpha\beta}^{(num)}, \alpha \neq \beta\}$ become:

$$g^{(u)} = 1, g_{xy}^{(u)} = 0: \quad U^2 \leq \min\{U_{a,1}^2 = 2c_e, U_{d,1}^2, U_{d,2}^2\}. \tag{95}$$

Remark 4.2.1.B We emphasize that the diffusion-dominant conditions do not require $E_0 \geq 0$ unless $\min\{U_{d,1}^2, U_{d,2}^2\} = U_d^2$ (the E_0-*n-line* function $U_d^2(c_e)$ is given by relation (33)). When $t_c^{(m)} \in [0, \frac{1}{4}]$ or $\gamma_u = -\frac{1}{2}$ ($t_c^{(u)} = 0$) then $\min\{U_{d,1}^2, U_{d,2}^2\} = U_{d,1}^2$ and $U_{d,1}^2 = U_d^2$ if $t_c^{(m)} \equiv 0$. When $t_c^{(m)} \in]\frac{1}{4}, \frac{1}{2}]$ and $\gamma_u = 1$ ($t_c^{(u)} = \frac{1}{2}$) then $\min\{U_{d,1}^2, U_{d,2}^2\} = U_{d,2}^2 > U_d^2$ since $c_e^{(\max)} > c_e^{(0)}$. Finally, when $t_c^{(m)} \in]\frac{1}{4}, \frac{1}{2}]$ and $-\frac{1}{2} < \gamma_u < 1$, the diffusion boundary *d-line* consists from two segments, the first one is $U_{d,1}^2$ and the second one is $U_{d,2}^2$. Examples can be found in Figs. 10 to 14.

Without Numerical Diffusion, $g_{xy}^{(u)} g^{(u)} = 1$ When the numerical diffusion is cancelled, the condition $U^2 \leq \min\{U_{d,1}^2, U_{d,2}^2\}$ is still necessary but the advection-dominant condition $U^2 \leq U_{a,1}^2 = 2c_e$ is not retained. For example, the necessary conditions for all the schemes with $t_c^{(m)} \in [0, \frac{1}{4}]$ are:

$$\begin{cases} g^{(u)} = 0 & : \quad U^2 \leq U_{a,0}^2 = c_e, \quad 0 \leq c_e \leq 1. \\ g^{(u)} = 1 & : \quad U^2 \leq U_{a,1}^2 = 2c_e, \quad 0 \leq c_e \leq \frac{1}{3}, \\ & \quad\;\; U^2 \leq U_{d,1}^2 = 1 - c_e, \quad \frac{1}{3} \leq c_e \leq 1. \\ g_{xy}^{(u)} g^{(u)} = 1 & : \quad U^2 \leq U_{d,1}^2 = 1 - c_e, \quad 0 \leq c_e \leq 1. \end{cases} \tag{96}$$

However, in contrast with the d1Q3 model, condition $U^2 \leq 1 - c_e$ is not sufficient for all the weights $\{t_q^{(a)}\}$ and $\{t_q^{(u)}\}$ when the numerical diffusion is removed. Let us consider several examples.

4.2.2 The d2Q9 OTRT Schemes: Examples

Examples 4.2.2.A The "uniform" scheme d2Q9$^{(unif)}$ and "optimal" family d2Q9$^{(opt)}$. Let us first introduce

$$\text{d2Q9}^{(unif)}: \quad t_c^{(a)} = t_c^{(m)} = t_c^{(u)} = \frac{1}{4}, \quad \text{then } \gamma_u = \frac{1}{4}. \tag{97}$$

Theorem 2.3.1 predicts for this scheme the best possible advection boundary, $U^2 = c_e$ when $g^{(u)} = 0$ and $U^2 = 2c_e$ when $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$ (see relations (96) and (126)), and this is the only d2Q9 scheme with equal mass/advection weights satisfying at the same time condition (87) and the necessary advection conditions from Theorem 2.3.1. However, Theorem 2.3.1 restricts the domain of validity of the advection conditions to the E_0-*n-line* given by $U_d^2 = \frac{4}{3} - 2c_e$ for the d2Q9$^{(unif)}$ scheme. Moreover, this theorem cannot predict larger stable area than $U^2 \leq 2c_e$, even without numerical diffusion, because of its non-negativity precondition $\{E_q^+ > 0\}$. Based on the exact analysis of $|\Omega|^2$ (Ω is specified by relations (128)), Proposition C.1.2.1 first proves the extension of the stability interval $[0, c_e^{(0)}]$ to the larger interval $[0, c_e^{(\max)}]$ when $\mathbf{U} = 0$, for any d2Q9 OTRT scheme. Then Proposition C.1.2.2 proves that $U^2 \leq c_e$ (advection line) is a sufficient condition when $g^{(u)} = 0$ and $c_e \in [0, c_e^{(\max)}]$, for any d2Q9 OTRT scheme provided that their mass and velocity weights are equal. Finally, Proposition C.1.2.4 confirms that necessary conditions (93) and (95) are sufficient provided

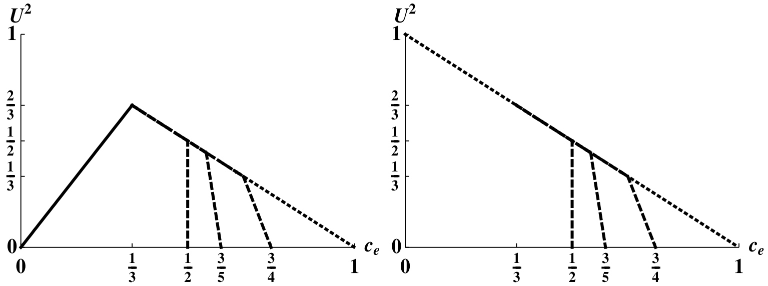

Fig. 10 The stability boundaries for the d2Q9 OTRT schemes with the "optimal" advection weight $t_c^{(a)} = \frac{1}{4}$ are shown when $t_c^{(m)}$ varies and $\gamma_u = 1 - 3t_c^{(m)}$ (relation (87)). *Left*: $g_{xy}^{(u)} = 0$, the stable domain is bounded by the necessary conditions (95), $U_{a,1}^2 = 2c_e$ and the diffusion line, $U^2 \le \min\{U_{d,1}^2, U_{d,2}^2\}$. *Right*: $g_{xy}^{(u)} = 1$, the only boundary is the diffusion line. When $t_c^{(m)} \in [0, \frac{1}{4}]$, then $\min\{U_{d,1}^2, U_{d,2}^2\} = U_{d,1}^2 = 1 - c_e$ (*dotted line*). Otherwise, the diffusion line is composed of two linear segments, $U_{d,1}^2$ and $U_{d,2}^2$, as shown for $t_c^{(m)} = \{\frac{1}{3}, \frac{5}{12}, \frac{1}{2}\}$, from the right to the left decreasing boundary

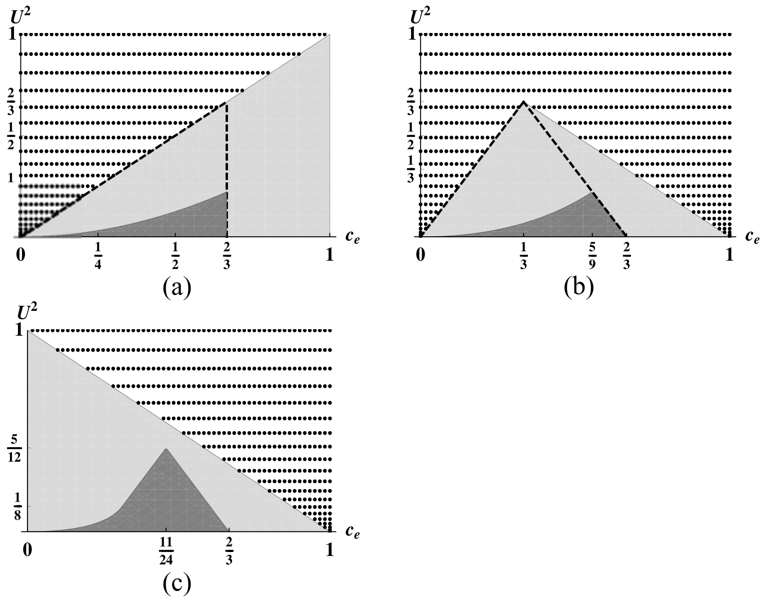

Fig. 11 The "uniform" d2Q9$^{(unif)}$ OTRT scheme (97). The unstable points are shown for: (**a**) $g^{(u)} = 0$, (**b**) $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$, and (**c**) $g_{xy}^{(u)} g^{(u)} = 1$. The stable area obtained from Theorem 2.3.1 is bounded by the *dashed lines* (see the two first pictures). The effective ("filled") stable sub-domains are bounded by the necessary stability conditions (96). The d1Q3 stability (74) is reached when $g^{(u)} = 0$ (a) and when $g_{xy}^{(u)} g^{(u)} = 1$ (c). For comparison the non-negativity areas (*dark grey*) are plotted. This scheme is also illustrated in Fig. 13

that $t_c^{(a)} = \frac{1}{4}$, for any choice of the other weights, and that the stable domain is uniquely bounded by the decreasing diffusion line when the numerical diffusion is removed, as illustrated in Fig. 10. Hereafter, we call the equilibrium weights as "optimal" if they allow to

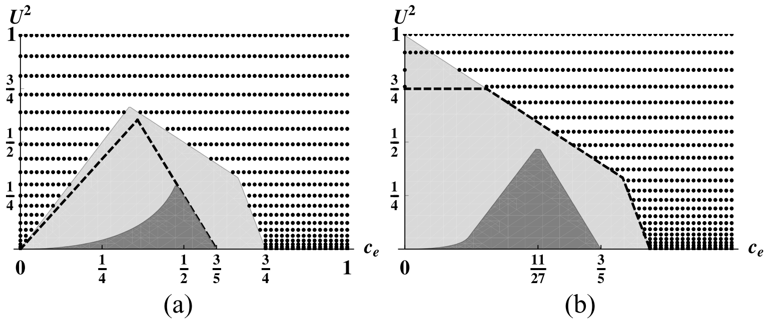

Fig. 12 The "standard" OTRT model d2Q9$^{(stan)}$ (30). The unstable points are shown for: (**a**) $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$ (*left*) and (**b**) $g_{xy}^{(u)} g^{(u)} = 1$ (*right*). The sufficient boundaries given by Theorem 2.3.1 (*left*) and Proposition C.1.2.5 (*right*) are plotted with *dashed lines*. The "filled" areas (light grey) are limited by necessary boundary (99). The non-negativity sub-domains (118) are plotted (*dark grey*) for comparison

reach the d1Q3 stability on the OTRT sub-class:

$$\text{d2Q9}^{(opt)}: \quad t_c^{(a)} = \frac{1}{4}, \quad t_d^{(a)} = \frac{1}{8}, \quad t_c^{(m)} \in \left[0, \frac{1}{4}\right], \quad \forall \gamma_u. \tag{98}$$

Hence, the d2Q9$^{(unif)}$ scheme is the "extreme" element of the d2Q9$^{(opt)}$ family. Figure 11 confirms the sufficiency of the stability bounds (96) with the help of eigenmode analysis of the characteristic equation (38). Similar results are obtained for $t_c^{(m)} \neq \frac{1}{4}$, e.g., $t_c^{(m)} = 0$ taking $\gamma_u = \gamma_u^{(m)}$ ($t_c^{(u)} = \frac{1}{2}$). The non-negativity conditions: $\{E_q \geq 0\}$ and $\{E_q^+ \geq 0\}$, then necessary and sufficient conditions, are illustrated for the "uniform" scheme in Fig. 13 (right diagram).

Examples 4.2.2.B The "standard" scheme d2Q9$^{(stan)}$. The necessary conditions (93) and (95), along with the exact analysis of $|\Omega(c_e = 0)|$ when the numerical diffusion is removed, give for the d2Q9$^{(stan)}$:

$$\begin{cases} g^{(u)} = 0 & : \quad U^2 \leq c_e, 0 \leq c_e \leq c_e^{(\max)} = \frac{3}{4}. \\ g^{(u)} = 1, g_{xy}^{(u)} = 0 & : \quad U^2 \leq 2c_e, 0 \leq c_e \leq \frac{1}{3}. \\ g^{(u)} = 1, g_{xy}^{(u)} = 1 & : \quad U^2(c_e = 0) \leq \frac{3}{4}. \\ g^{(u)} = 1, g_{xy}^{(u)} = \{0, 1\} : & \quad U^2 \leq 1 - c_e, \frac{1}{3} \leq c_e \leq \frac{2}{3}, \\ g^{(u)} = 1, g_{xy}^{(u)} = \{0, 1\} : & \quad U^2 \leq 3 - 4c_e, \frac{2}{3} \leq c_e \leq c_e^{(\max)} = \frac{3}{4}. \end{cases} \tag{99}$$

The standard scheme has equal mass/velocity weights, then extension of the stability interval up to $c_e^{(\max)}$ is predicted by Proposition C.1.2.2 when $g^{(u)} = 0$. The results of the eigenmode analysis are illustrated in Fig. 12 when $g^{(u)} = 1$. They suggest that the necessary conditions (95) are also sufficient when $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$ (left diagram). At the same time, the sufficient conditions derived with the help of Theorem 2.3.1 (see relation (126)) give a smaller stable area, $U^2 \leq \frac{1+\sqrt{33}}{4} c_e$, further limited by the E_0-*n-line* $U_d^2 = \frac{3-5c_e}{2}$. Next, the Proposition C.1.2.5 and Proposition C.1.2.6 confirm the sufficiency of conditions (95), e.g., when $\gamma_u = \{-\frac{1}{2}, 0, 1\}$. This suggests that they may be sufficient $\forall \gamma_u \in [-\frac{1}{2}, 1]$. When $g_{xy}^{(u)} g^{(u)} = 1$, the selected γ_u value affects not only the segment $U^2 = U_{d,2}^2(c_e)$ of the diffusion boundary, *d-line*, but also the advection limit. Proposition C.1.2.5 predicts for $\gamma_u = 0$ that the line $U^2(c_e) = \frac{3}{4}$ is a sufficient condition up to its intersection with $U_{d,1}^2$ at $c_e = \frac{1}{4}$. Next we observe that $U^2(c_e = 0)$ drops to 0 for $\gamma_u = -\frac{1}{2}$, in contrast to both cases $\gamma_u = \{0, 1\}$. Hence,

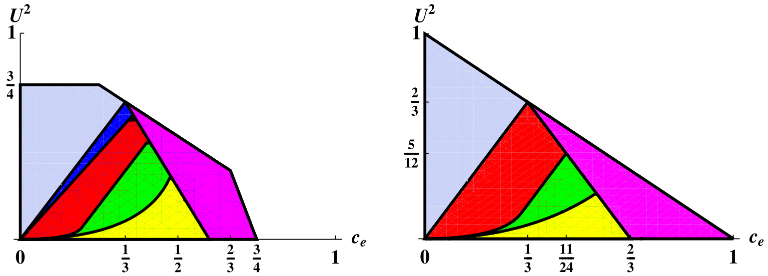

Fig. 13 (Color online) The non-negativity areas and stable sub-domains of the OTRT schemes are plotted for the d2Q9$^{(stan)}$ (30) (*left*) and the d2Q9$^{(unif)}$ (97) (*right*) when the numerical diffusion is removed, partially or completely. Two non-negativity areas (117) have curvilinear boundaries: they are smaller when $g_{xy}^{(u)} = 0$ (*yellow*) than when $g_{xy}^{(u)} = 1$ (*green+yellow*). The stable sub-domains predicted by Theorem 2.3.1 for $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$ are small (*red+green+yellow*) *triangles*: their left boundary is $U^2 = \frac{1+\sqrt{33}}{4} c_e$ for the d2Q9$^{(stan)}$ and $U^2 = 2c_e$ (the *a-line*) for the d2Q9$^{(unif)}$, and the right edge is the E_0-*n-line*. The *effective stable* domains include the area above the E_0-*n-line* where $E_0 < 0$ (*magenta*), and it also extends to the *a-line* for the d2Q9$^{(stan)}$ (narrow triangle (*dark-blue*)). The (*blue*) domain above $U^2 = 2c_e$ is stable only for $g_{xy}^{(u)} = 1$ and the symmetric weights E_q^+ may become negative there. The total triangle $0 \le U^2 \le 1 - c_e$ (the d2Q9$^{(unif)}$ only) is the best stability area (74)

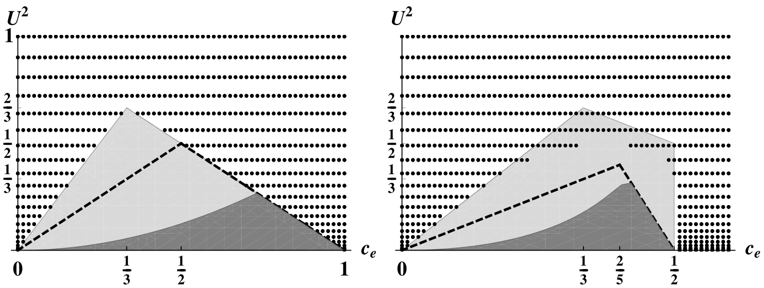

Fig. 14 Two "limit" equilibrium schemes (100): the d2Q9$^{(diag)}$ (*left*) and the d2Q9$^{(coor)}$ (*right*) are shown for $g^{(u)} = 1$, $g_{xy}^{(u)} = 0$. The "filled" sub-domains are bounded by necessary conditions (96) in the available intervals. The sufficient conditions obtained from Theorem 2.3.1 are plotted by *dashed lines*. Proposition C.1.2.7 extends them up to the necessary conditions for the d2Q9$^{(diag)}$. The (principal) necessary conditions *are not sufficient* for the d2Q9$^{(coor)}$. The non-negativity areas (117) are plotted (*dark grey*) for comparison (they are set by the coordinate links for the d2Q9$^{(coor)}$)

the results suggest that the choice $\gamma_u = -\frac{1}{2}$ ($t_c^{(u)} = 0$, when the U^2-term is completely absorbed by the diagonal links) is unfavorable in the advection-dominant limit.

The non-negativity, necessary and sufficient conditions can be compared for the "standard" and "uniform" weights in Fig. 13. The d2Q9$^{(unif)}$ has larger stability domains on the OTRT sub-class but smaller velocity peaks of its non-negativity conditions: $U_n^2(c_e = \frac{11}{27}) = \frac{13}{27}$ for the d2Q9$^{(stan)}$ against $U_n^2(c_e = \frac{11}{24}) = \frac{5}{12}$ for the d2Q9$^{(unif)}$ when the numerical diffusion is removed.

Examples 4.2.2.C The d2Q9$^{(diag)}$ "diagonal" and d2Q9$^{(coor)}$ "coordinate" schemes. The two previous examples may give the impression that a (minimal) combination of the necessary advection-dominant and diffusion-dominant conditions is always sufficient. This is however not always so. Let us consider two "extreme" elements of family (87), called d2Q9$^{(diag)}$ and d2Q9$^{(coor)}$, with $(t_c^{(m)}, \gamma_u)$ equal to $(0, 1)$ and $(\frac{1}{2}, -\frac{1}{2})$, respectively:

$$\begin{aligned} &\text{d2Q9}^{(diag)}: \quad t_c^{(m)} = t_c^{(a)} = t_d^{(u)} = 0, \quad t_d^{(m)} = t_d^{(a)} = \frac{t_c^{(u)}}{2} = \frac{1}{4}. \\ &\text{d2Q9}^{(coor)}: \quad t_c^{(m)} = t_c^{(a)} = 2t_d^{(u)} = \frac{1}{2}, \quad t_d^{(m)} = t_d^{(a)} = t_c^{(u)} = 0. \end{aligned} \tag{100}$$

Unlike the five populations based schemes, such as the d2Q5 or the "rotated" d2Q5, both d2Q9$^{(diag)}$ and d2Q9$^{(coor)}$ schemes use two different sub-classes for their equilibrium mass term and the isotropic U^2-term. Moreover, they use both velocity classes for the anisotropic component of $E_q^{(u)}$. When $g^{(u)} = 0$ or $g^{(u)} = 1$ and $g_{xy}^{(u)} = 0$, the necessary conditions of both schemes are the same as for the d2Q9$^{(unif)}$ (cf. relations (96)) but the d2Q9$^{(coor)}$ is defined only when $c_e \in [0, \frac{1}{2}]$. Theorem 2.3.1 predicts the same stability boundary $U^2 \le c_e$ for both schemes and for both cases: either with numerical diffusion (where this condition is necessary) or without it. However, Proposition C.1.2.7 expands this result and predicts that the necessary conditions (96) are sufficient for the d2Q9$^{(diag)}$, as well, except when $g_{xy}^{(u)} g^{(u)} = 1$. The exact analysis of $|\Omega|^2$ tells us that the necessary conditions *are not sufficient* for d2Q9$^{(coor)}$ when $g^{(u)} = 1$. The results of the eigenmode stability analysis in Fig. 14 confirm all these predictions. Again, the choice $\gamma_u = -\frac{1}{2}$ $(t_c^{(u)} = 0)$ is unfavorable. In brief, the d2Q9$^{(diag)}$ has the larger non-negativity domain and much better stability properties than the d2Q9$^{(coor)}$.

4.3 The d3Q15 Model

4.3.1 The d3Q15 Model: Necessary Stability Conditions for Any Eigenvalues

In the advection-dominant limit, they are set by relation (36):

$$\begin{aligned} g^{(u)} = 0: &\quad U^2 \le U_{a,0}^2 = c_e. \\ g^{(u)} = 1: &\quad U^2 \le U_{a,2}^2 = \frac{3}{2} c_e. \end{aligned} \tag{101}$$

The first condition has the same form for all models, and the second condition is the same as for the d3Q7 model. In the diffusion limit $\mathbf{U} = 0$, the necessary conditions are set by relations (64), (65) and (67):

$$\begin{cases} (1)\ \mathbf{k} = \pi \mathbf{1}_\alpha \ : \quad 0 \le c_e \le 1, \\ (2)\ \mathbf{k} = \pi \mathbf{1}_d \ : \quad 0 \le c_e \le \frac{1}{1+4t_c^{(m)}}, \\ (3)\ \mathbf{k} = \pi \mathbf{1}_d^{(\gamma)}: \quad 0 \le c_e \le \frac{1}{4t_c^{(m)}}. \end{cases} \tag{102}$$

Then the minimal relation is:

$$0 \le c_e \le c_e^{(0)} = c_e^{(\max)} = \frac{1}{1 + 4t_c^{(m)}}, \quad \text{when} \quad 0 \le t_c^{(m)} \le \frac{1}{2}. \tag{103}$$

This condition guarantees the non-negativity of the immobile weight, hence it is sufficient for pure diffusion *isotropic* equation (Theorem 2.4). When $g^{(u)}=1$ and $0\le c_e\le c_e^{(\max)}$, the necessary diffusion-dominant conditions (64), (65), and (67) become:

$$\begin{cases} (1)\ \mathbf{k}=\pi\mathbf{1}_\alpha\ : & U^2\le U_{d,1}^2=1-c_e,\\ (2)\ \mathbf{k}=\pi\mathbf{1}_d\ : & U^2\le U_d^2=\frac{3(1-c_e(1+4t_c^{(m)}))}{1+2\gamma_u},\\ (3)\ \mathbf{k}=\pi\mathbf{1}_d^{(\gamma)}: & 0\le\frac{12c_et_c^{(m)}+U^2(1+2\gamma_u)-3U_\gamma^2}{3}\le 1.\end{cases} \tag{104}$$

Again, the second condition requires $E_0(c_e,U^2)\ge 0$. When $\mathbf{k}=\pi\mathbf{1}_d^{(\gamma)}$ ($\mathbf{1}_d^{(\gamma)}$ is parallel to diagonal axis in $2d$ plane perpendicular to the γ-axis) then two conditions are imposed. The minimal case of the (left) inequality (104-3) imposes $U^2\le U_{p,c}^2$, the function $U_{p,c}^2(c_e)$ is given by relation (85). We recall that condition $U^2\le U_{p,c}^2$ ensures the non-negativity of the symmetric weights for all coordinate links. At the same time, condition (104-2) is stronger than the right inequality (104-3) (≤ 1). Then the necessary stability conditions of the d3Q15 model become:

$$\begin{cases} g^{(u)}=0 & : \quad U^2\le c_e,\ 0\le c_e\le c_e^{(0)}=c_e^{(\max)}=\frac{1}{1+4t_c^{(m)}},\\ g^{(u)}=1,\ g_{\alpha\beta}^{(u)}=0: & U^2\le\min\{\frac{3}{2}c_e,U_{d,2}^2,U_d^2\},\quad 0\le c_e\le c_e^{(0)},\\ g^{(u)}=1,\ g_{\alpha\beta}^{(u)}=1: & U^2\le\min\{U_d^2,U_{d,2}^2\},\quad 0\le c_e\le c_e^{(0)}\\ & U_d^2=\frac{3(1-c_e(1+4t_c^{(m)}))}{1+2\gamma_u},\quad U_{d,2}^2=U_{p,c}^2=\frac{6t_c^{(m)}}{1-\gamma_u}c_e.\end{cases} \tag{105}$$

When $\gamma_u=\gamma_u^{(m)}$ then $U_{d,2}^2=2c_e$, whereas when $\gamma_u^{(m)}<\gamma_u<1$ the restriction $U^2\le U_{d,2}^2$ is weaker than $U^2\le 2c_e$ and it vanishes when $\gamma_u=1$ ($t_c^{(u)}=\frac{1}{2}$). Hence, the particularity of the d3Q15 model is that the *diffusion-dominant* condition $U^2\le U_{d,2}^2$ restricts the *advection-dominant* zone, except for $\gamma_u=1$ ($t_c^{(u)}=\frac{1}{2}$).

4.3.2 The d3Q15 OTRT Schemes: Examples

Examples 4.3.2.A "Uniform" scheme d3Q15$^{(unif)}$ is introduced with:

$$\text{d3Q15}^{(unif)}:\quad t_c^{(a)}=t_c^{(m)}=t_c^{(u)}=\frac{1}{5},\quad \text{then}\quad \gamma_u=\frac{2}{5}. \tag{106}$$

On the one hand, as the d2Q9$^{(unif)}$, this scheme satisfies condition (87), and, on the other hand, Theorem 2.3.1 gives to this scheme the best possible, necessary and sufficient, advection boundaries, $U^2=c_e$ when $g^{(u)}=0$ and $U^2=\frac{3}{2}c_e$ when $g^{(u)}=1$, $g_{\alpha\beta}^{(u)}=0$ (see relations (135)). However, since the d3Q15$^{(unif)}$ has $\gamma_u\ne 1$, this scheme cannot have better left boundary than $U^2=2c_e$, even when the numerical diffusion is removed. The sufficiency of this condition when $g_{\alpha\beta}^{(u)}g^{(u)}=1$ is addressed by Proposition C.2.2.1 (Ω is given by relation (136) for the d3Q15 model). The independent eigenmode analysis of the spectrum of (38) confirms the predicted sufficient conditions as shown in Fig. 15.

Examples 4.3.2.B The "standard" scheme d3Q15$^{(stan)}$. The equilibrium distribution (30) of this scheme is built with the "hydrodynamic" weights and it satisfies relation (87). Hence,

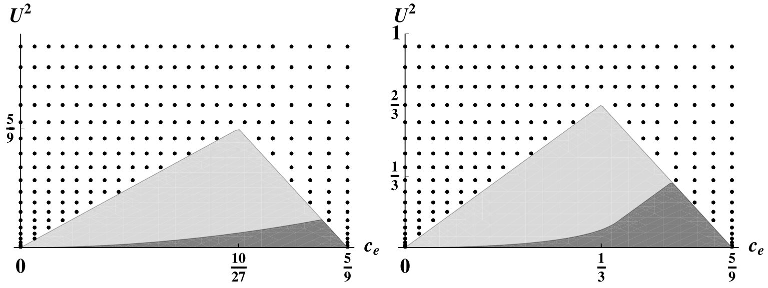

Fig. 15 The unstable points and stable ("filled") area are shown for the d3Q15$^{(unif)}$ OTRT model (106). The stable domain is limited by the necessary and sufficient stability boundaries: $U^2 = \frac{3}{2}c_e$ (*left*, $g^{(u)} = 1$, $g^{(u)}_{\alpha\beta} = 0$) and $U^2 = 2c_e$ (*right*, $g^{(u)}_{\alpha\beta} g^{(u)} = 1$), up to their intersection with the E_0-*n-line*. The non-negativity domain (121) is plotted (*dark grey*) for comparison

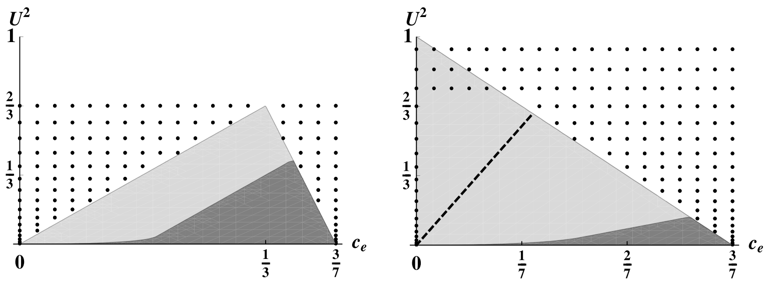

Fig. 16 The unstable points for the d3Q15$^{(stan)}$ OTRT model are shown for two values of the equilibrium parameter γ_u: *left*, $\gamma_u = 0$ (standard choice), and *right*, $\gamma_u = 1$, when $g^{(u)}_{\alpha\beta} g^{(u)} = 1$. The "filled" areas are limited by necessary conditions: (*left*) $U^2 \le \min\{U^2_{d,2} = 2c_e, U^2_d\}$ where $U^2_d(c_e)$ is the E_0-*n-line* $U^2_d = 3 - 7c_e$; (*right*) $U^2 \le U^2_d(c_e)$, given by relations (105). When $\gamma_u = 1$, right, the velocity increases in the advection zone, at least up to $U^2 = 4c_e$ (*dashed line*), but the necessary conditions are not sufficient. The non-negativity domain (*dark grey*) is much smaller for $\gamma_u = 1$

like the d3Q15$^{(unif)}$ model, the d3Q15$^{(stan)}$ model respects the necessary lines (105): $U^2 = \frac{3}{2}c_e$ or $U^2 = 2c_e$, when $g^{(u)} = 1$ and $g^{(u)}_{\alpha\beta} = 0$ or $g^{(u)}_{\alpha\beta} = 1$, respectively. However, in contrast to the d3Q15$^{(unif)}$ model, the sufficient advection line predicted by Theorem 2.3.1 is weaker, $U^2 = \sqrt{\frac{3}{2}c_e}$. The results of the numerical eigenmode stability analysis in Fig. 16 and an extensive analysis of $|\Omega|^2$ on the assumed boundary (Proposition C.2.2.1) both suggest that the necessary conditions (105) are sufficient. Hence, the d3Q15$^{(unif)}$ and d3Q15$^{(stan)}$ have very similar effective stable areas, with a larger available interval for the d3Q15$^{(unif)}$, $c_e \in [0, \frac{5}{9}]$ compared to $[0, \frac{3}{7}]$ for the d3Q15$^{(stan)}$. When the numerical diffusion is removed, the peak is for $c_e^{opt} = \frac{1}{3}$, then $U^2_{opt} = \frac{2}{3}$, for both schemes. When $\gamma_u = 1$ the stability line $U^2 = 2c_e$ improves at least as $U^2 = 4c_e$ for the "standard" scheme. At the same time, the E_0-*n-line* is more restrictive and the non-negativity area is much smaller for $\gamma_u = 1$ than for "standard choice" $\gamma_u = 0$ (see Fig. 16).

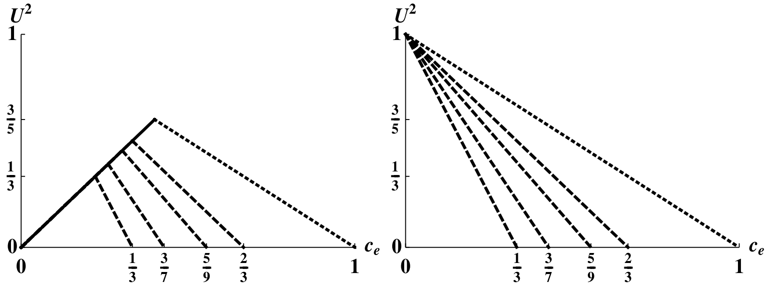

Fig. 17 The stable triangles predicted by Proposition C.2.2.1 for the d3Q15 OTRT schemes with the coordinate weights $\{t_c^{(a)}, t_c^{(u)}\} = \{\frac{1}{4}, \frac{1}{2}\}$ are shown for $g^{(u)} = 1$, $g_{\alpha\beta}^{(u)} = 0$ (*left*) and $g_{\alpha\beta}^{(u)} g^{(u)} = 1$ (*right*), $t_c^{(m)}$ varies between 0 and $\frac{1}{2}$ (from right to *left*: $t_c^{(m)} = \{0, \frac{1}{8}, \frac{1}{5}, \frac{1}{3}, \frac{1}{2}\}$). The advection line *a-line* $U^2 = \frac{3}{2}c_e$ is sufficient when the cross-diffusion is not cancelled (*left*). The right edge of all triangles is the E_0-*n-line*: $U_d^2(\gamma_u = 1) = 1 - c_e(1 + 4t_c^{(m)})$. It bounds the stable area when $g_{\alpha\beta}^{(u)} g^{(u)} = 1$ (*right*)

Examples 4.3.2.C "Optimal" family d3Q15$^{(opt)}$. Neither the d3Q15$^{(unif)}$ nor the d3Q15$^{(stan)}$ achieve the stability of the d1Q3 OTRT model. As a last example, we introduce the "optimal" family, again based on $t_c^{(a)} = \frac{1}{4}$:

$$\text{d3Q15}^{(opt)}: \quad t_c^{(a)} = \frac{1}{4}, \quad t_c^{(u)} = \frac{1}{2}, \quad 0 \le t_c^{(m)} \le \frac{1}{2},$$
$$\text{then:} \quad t_d^{(a)} = \frac{1}{16}, \quad t_d^{(u)} = 0. \tag{107}$$

For the choice $t_c^{(u)} = \frac{1}{2}$ ($\gamma_u = 1$), the necessary condition $U^2 \le U_{d,2}^2$ disappears. Combining the predictions of the fourth-order analysis in k for the advection limit and the eigenmode analysis for $|\Omega|^2$, Proposition C.2.2.1 predicts that the "optimal" schemes match the d1Q3 stability (96) in the available interval $c_e \in [0, c_e^{(0)}]$, when either $g^{(u)} = 0$ or $g_{\alpha\beta}^{(u)} g^{(u)} = 1$, their stability bounds are illustrated in Fig. 17. These findings are also confirmed by an independent analysis of the whole spectrum. However, in contrast to the "optimal" d2Q9$^{(opt)}$ family, the whole interval $c_e \in [0, 1]$ is available only for the "limit" weights: zero coordinate mass weight $t_c^{(m)} = 0$. Further extension of this work [18] suggests to avoid such "extreme" weight configurations (which are the limits of some necessary and/or non-negativity conditions) when $\Lambda \ne \frac{1}{4}$. The d3Q15$^{(unif)}$ model or the d3Q15$^{(opt)}$ with $t_c^{(m)} = t_c^{(a)} = \frac{1}{4}$ and $t_c^{(u)} = \{\frac{1}{4}, \frac{1}{2}\}$ are predicted as good stability candidates also beyond the OTRT.

5 Summary

This paper develops a von Neumann analytical analysis of the TRT operator for the linear advection-diffusion equation. The key point is the splitting of the linear equilibrium function $\{e_q = sE_q\}$ into symmetric and anti-symmetric components: $\{E_q = E_q^+ + E_q^-\}$, which have equal and opposite values, respectively, for two anti-parallel velocities called *a link*. Let us subdivide the findings of this paper into three groups. The first group addresses general statements, valid for any velocity set and equilibrium weights $\{E_q^\pm\}$ constrained to the mass-conservation, $\sum_{q=0}^{Q_m} E_q^+ = 1$. The BGK model is included as a particular sub-class of the TRT model. The second group addresses specific results for the TRT modeling of the advection-diffusion equation, namely their necessary conditions for any values of the two relaxation rates. The results in the third group are derived for the OTRT sub-class. Its exceptional feature is the independence of the stability bounds from the individual values of the two relaxation times, provided that their specific combination Λ is kept equal to $\frac{1}{4}$.

I. The four following statements have been proved:

– *A particular OTRT sub-class of the TRT operator* (3)*, defined for any positive eigenvalue functions Λ^+ and Λ^- such that $\Lambda = \Lambda^+\Lambda^- = \frac{1}{4}$, is stable in the von Neumann sense provided that, $\forall \mathbf{k}$, $|\Omega|^2 = \mathcal{A}^2 + \mathcal{B}^2 \leq 1$, with*

$$\mathcal{A} = 1 + \sum_{q=1}^{Q_m} (\cos[k_q] - 1) E_q^+, \qquad \mathcal{B} = \sum_{q=1}^{Q_m} \sin[k_q] E_q^-, \quad k_q = \mathbf{k} \cdot \mathbf{c}_q.$$

This result is stated as Theorem 2.2.1. Exact, necessary and sufficient *equilibrium* stability conditions are set when $\max_{\mathbf{k}} |\Omega(\mathbf{k})|^2 = 1$. The solution for amplification factor Ω is specified by relations (69) for the minimal models, then by relations (128) and (136) for the d2Q9 and d3Q15 velocity sets with the equilibrium functions (21)–(22) and (24)–(25), respectively.

– *The OTRT sub-class is stable if $\sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} \leq 1$, provided that $E_0 \geq 0$ and $\{E_q^+ > 0\}$ for all $q = 1, \ldots, Q_m$.* This result is stated as Theorem 2.3.1. This still applies when $E_q^- \equiv 0$ and $E_q^+ \geq 0$. Using this result, one avoids a tedious eigenmode analysis. However, the derived sufficient conditions may appear as more restrictive than necessarily.

– *If the equilibrium weights are non-negative, $E_0 \geq 0$ and $\{E_q > 0\}$ for all $q = 1, \ldots, Q_m$, then $\sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} \leq 1$ and the OTRT sub-class is stable.* This result is stated as Lemma 2.3.2. This still applies when $E_q \geq 0$ and $E_q^+ > 0$, or when $E_q^- \equiv 0$ and $E_q^+ \geq 0$. The non-negativity of all equilibrium functions gives *stronger* sufficient stability condition than the conditions obtained from Theorem 2.3.1.

– *If $E_0 \geq 0$ and $\{E_q \geq 0\}$ for all $q = 1, \ldots, Q_m$ (at least one is strictly positive), then the BGK model is stable.* This result is stated as Theorem 2.5. Hence, the non-negativity of all equilibrium functions is also sufficient for the stability of the BGK model.

– *If $E_0 \geq 0$, $E_q^- \equiv 0$ and $\{E_q^+ \geq 0\}$ for all $q = 1, \ldots, Q_m$ (at least one is strictly positive), then the TRT model is stable.* The result is stated as Theorem 2.4. It tells us that the non-negativity of the symmetric equilibrium weights is sufficient for stability of the diffusion equation with no advection, for any eigenvalues. When the mass weights $\{t_q^{(m)}\}$ are non-negative, the non-negativity of E_0 is then sufficient for *isotropic* diffusion equation. In other words, owing to Λ^-, any value of the diffusion coefficient can be obtained with the same equilibrium parameters, hence with the same physical time steps.

II. The TRT modeling of the advection-diffusion equations (AADE) is examined in the following framework: (a) $\{E_q^- = t_q^{(a)}(\mathbf{U} \cdot \mathbf{c}_q)\}$; (b) the mean diffusion coefficient is equal to $\Lambda^- c_e$, where $c_e \in [0, c_e^{(\max)}]$ is a free parameter of $\{E_q^+\}$; (c) if $g^{(u)} = 0$ then $\{E_q^+ = t_q^{(m)} c_e\}$ and this results in a full tensor of numerical diffusion $\mathcal{D}_{\alpha\beta}^{(num)} = \{-U_\alpha U_\beta\}$; (d) the numerical diffusion is partially ($g^{(u)} = 1$, $g_{\alpha\beta}^{(u)} = 0$) or completely ($g_{\alpha\beta}^{(u)} g^{(u)} = 1$) cancelled via the anisotropic equilibrium term $\{E_q^{(u)}\}$, governed by the weights $\{t_q^{(u)}\}$;

(e) the minimal models only cancel the diagonal elements $\{\mathcal{D}^{(num)}_{\alpha\alpha}\}$; the "full" models may also remove the cross-diffusion elements $\{\mathcal{D}^{(num)}_{\alpha\beta}, \alpha \neq \beta\}$; (f) all equilibrium weights $\{t^{(m)}_q, t^{(a)}_q, t^{(u)}_q\}$ are non-negative, isotropic, found in the interval $[0, \frac{1}{2}]$ and satisfy relation (10). We stress that their non-negativity is not *a-priori* a necessary stability condition but a deliberate choice. The equilibrium term $\{E^{(a)}_q\}$ which introduces the anisotropy of the diagonal elements $\{\mathcal{D}_{\alpha\alpha}\}$ for all the models, plus the anisotropy of the cross-diagonal elements for the d2Q9 and d3Q15 schemes, is set equal to zero for modeling of *isotropic* diffusion tensor.

II.1 *The non-negativity of the symmetric weights* $\{E^+_q\}$ *and the immobile weight* E_0.
The non-negativity condition $E_0 \geq 0$ is prescribed by relations (19), (33) and (34), for the minimal models, d2Q9 and d3Q15 schemes, respectively, and independently of the anisotropy of the modeled tensor. In the presence of the $\{E^{(u)}_q\}$ term, the symmetric weights $\{E^+_q\}$ of the "full" models may become negative. Their non-negativity conditions are the same for the d2Q9 and d3Q15 schemes, at least when the modeled tensor is isotropic. They are prescribed by relations (85) and (86), separately for the coordinate and diagonal links. When the numerical diffusion is completely removed ($g^{(u)}g^{(u)}_{\alpha\beta} = 1$), the non-negativity of all the weights $\{E^+_q\}$ necessarily restricts U^2 to be smaller than $2c_e$, and the whole interval $U^2 \in [0, 2c_e]$ is only available when $2t^{(u)}_c = 1 - dt^{(m)}_c$, as given by relation (88). The intersection of the boundary $U^2 = 2c_e$ with the E_0-*n-lines* then occurs for $c_e = \frac{1}{3}$, hence the highest possible velocity value is $U^2(c_e = \frac{1}{3}) = \frac{2}{3}$ (see relation (89)), for any mass weights $\{t^{(m)}_q\}$. Note that the non-negativity of two equilibrium weights per link, $E_q = E^+_q \pm E^-_q$, necessarily implies the non-negativity of their symmetric components E^+_q.

II.2 *The non-negativity of the whole set* $\{E_q\}$.
When the diffusion tensor is isotropic and the numerical diffusion is not corrected, then the non-negativity condition is $U^2 \leq U^2_n = c^2_e$ for all the minimal models. The d2Q9 and d3Q15 schemes have the best non-negativity limits when their mass/velocity weights are equal ($t^{(m)}_q = t^{(a)}_q \neq 0$) but their highest available velocity is only $U^2_n = \frac{c^2_e}{d}$ when $g^{(u)} = 0$ (see relations (115)). These situations are illustrated by the left diagrams in Fig. 5.

This situation changes when $g^{(u)} = 1$ (see the right diagrams in Fig. 5). The non-negativity area is $U^2 \leq U^2_n = \min\{U^2_{n,c}, U^2_{n,d}\}$ where $U_{n,c}$ and $U_{n,d}$ are the (minimal) velocity values in relations (116) and (120) for the d2Q9 and d3Q15 schemes, respectively. These relations take the form (117) and (121) for the family $\gamma_u = \gamma^{(m)}_u$ and equal mass/velocity weights, $\{t^{(a)}_q = t^{(m)}_q\}$. Since $E_q > 0$ implies $E^+_q \geq 0$ for all the links, all non-negativity areas (117) and (121) are confined to the triangle (89) (see Fig. 9). The diagonal links prescribe two different non-negativity domains when $g^{(u)}_{\alpha\beta} = 0$ and $g^{(u)}_{\alpha\beta} = 1$, the domain is larger when the numerical cross-diffusion is removed ($g^{(u)}_{\alpha\beta}g^{(u)} = 1$) (see Fig. 13 for the d2Q9 schemes and Figs. 16 and 17 for the d3Q15 schemes). The coordinate links give the same non-negativity conditions for $g^{(u)}_{\alpha\beta} = 0$ or $g^{(u)}_{\alpha\beta} = 1$ but this condition dominates only when $t^{(u)}_c \to 0$, as in Fig. 14. In all the considered cases, the highest velocity inside the non-negativity domain is reached when $c_e > \frac{1}{3}$ (note that $c_e = \frac{1}{3}$ is the commonly used value). The non-negativity domain is especially narrow in the advection zone $c_e \to 0$. When considering the non-negativity as a necessary condition in the limit $\Lambda^- \to 0$ for the BGK model (a proof for the minimal models is reported in [18]), one should pay a special attention on the selection of all the equilibrium weights and equilibrium parameter c_e.

II.3 *Necessary stability conditions* (*any eigenvalues*) are:

- *the advection-dominant stability conditions* (35) for isotropic tensors. They restrict $U^2(c_e)$ to $[0, c_e]$ in the presence of numerical diffusion, $g^{(u)} = 0$. When the diagonal elements $\{-U_\alpha^2\}$ of the numerical diffusion tensor $\{\mathcal{D}_{\alpha\beta}^{(num)}\}$ are cancelled, then U^2 may lie in the intervals $[0, 2c_e]$ and $[0, \frac{3}{2}c_e]$, respectively, in two and three dimensions. When $\{\mathcal{D}_{\alpha\beta}^{(num)}\}$ is completely cancelled (the d1Q3, d2Q9 and d3Q15 schemes), then the only *second-order* restriction is $c_e \geq 0$. However, this does not mean the "unconditional" stability: $U^2(c_e = 0) \in [0, 1]$, except for several schemes such as the d1Q3, d2Q9$^{(opt)}$ and d3Q15$^{(opt)}$.

- *the diffusion-dominant stability conditions* (64)–(67) constrain the specific linear combinations of symmetric equilibrium weights $\{E_q^+\}$ (whatever they are) as:
  1. $\sum_{q=1}^{Q_m} E_q^+ c_{q\alpha}^2$ to $[0, 1]$, $\forall \alpha = 1, \ldots, d$, then c_e to $[0, 1]$, for all models. It follows that the selected value Λ^- should be higher than the mean diagonal element of the rescaled diffusion tensor: $\Lambda^- > \frac{\sum_{\alpha=1}^{d} K'_{\alpha\alpha}}{d}$ (cf. relations (11) and (12)).
  2. $\sum_q E_q^+$ to the interval $[0, 1]$: for any two parallel velocities (one link) of the minimal model; for all four coordinate velocities (two links) of the d2Q9, and any two coordinate links for the d3Q15 schemes.
  3. E_0, or equivalently $\sum_{q=1}^{Q_m} E_q^+$, to the interval $[0, 1]$, but only for the minimal and d3Q15 models. This condition dominates all previous ones when all moving weights $\{E_q^+\}$ are non-negative.

These conditions are then elaborated for all the considered schemes with isotropic diffusion tensors. The *sufficient* stability conditions (70) of the minimal models on the OTRT sub-class, further precised by relations (72) and (73) for the isotropic minimal models, are *necessary* for all eigenvalues. It follows that no choice of the eigenvalues may have better stability criteria. Moreover, the necessary conditions of the d1Q3 model are also necessary for all the others. It follows that no one velocity set may have better stability than the d1Q3 OTRT scheme. The *necessary* conditions are specified, respectively, by relations (93) and (95) and (104)–(105) for isotropic d2Q9 and d3Q15 schemes, with any eigenvalues. The d2Q9 and d3Q15 models differ on two principal points. First, the non-negativity of the immobile weight is necessary for the d3Q15 model, as for the minimal ones. Second, the non-negativity of the coordinate values E_q^+ is one of the additional necessary conditions (cf. (85) and (105)), unless the U^2-term is covered by the coordinate links ($t_c^{(u)} = \frac{1}{2}$, or $\gamma_u = 1$).

These necessary advection and diffusion dominant conditions should be further explored for full anisotropic diffusion tensors, to estimate the impact of the anisotropy on the stability and to derive its effective available range. In fact, prescribing the positivity for all the symmetric weights $\{E_q^+\}$, the cross-diagonal elements $\{\mathcal{D}_{\alpha\beta}\}$ of the modeled diffusion tensor are restricted to the condition: $|\mathcal{D}_{\alpha\beta}| \leq \min_\alpha \mathcal{D}_{\alpha\alpha}$, at least, for the d2Q9 and d3Q15 models, [13].

III. *Necessary and sufficient stability conditions on the OTRT sub-class.*
As it has been mentioned above, the sufficient conditions predicted by Theorem 2.3.1 for the minimal models are also necessary. Actually, one can predict the sufficient conditions for the d2Q9 and d3Q15 models with any weights using relations (124) when $g^{(u)} = 0$, then relations (126) (for the d2Q9) and (134) (for the d3Q15) when $g^{(u)} = 1$,

further restricted by the non-negativity conditions (85) and (86) (both models), and $E_0 \geq 0$. In some cases, e.g., when $g^{(u)} = 0$ and mass/velocity weights are equal, the sufficient conditions predicted by Theorem 2.3.1 are also necessary: $U^2 \leq c_e$. In general, the sufficient conditions (enforcing the non-negativity of the immobile weight, $E_0 \geq 0$) are more restrictive than necessarily for the diffusion (decreasing) boundary of the d2Q9 schemes. Similarly, when the numerical diffusion is completely removed, the derived advection line (enforcing all the symmetric weights to be non-negative, $\{E_q^+ \geq 0\}$) is often stronger than necessarily. The exact analysis of $|\Omega(\mathbf{k})|$ may offer higher stable velocity amplitudes, along with larger available c_e intervals, but this (dependent on $\mathbf{k}$) analysis is more tedious than the equilibrium control offered by Theorem 2.3.1.

Altogether, the selected nine and fifteen velocity OTRT schemes, such as d2Q9$^{(opt)}$ and d3Q15$^{(unif)}$, d3Q15$^{(stan)}$ and d3Q15$^{(opt)}$ are provided with the *necessary and sufficient* conditions. Their stability conditions cannot be improved for any other eigenvalue choice. Moreover, the d2Q9$^{(opt)}$ and d3Q15$^{(opt)}$ OTRT schemes reach the d1Q3 stability. Curiously, the "optimal" advection weights of the d2Q9$^{(opt)}$ family are equivalent to the central-difference nine-point advection stencil with the weights $\{\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\}$. When the numerical diffusion is cancelled, this choice is delineated (without proof) for retaining "unconditional" stability of Lax-Wendroff scheme in multi-dimensions [17]. We believe that further extensions of this work for $d3Q19$ and $d3Q27$ velocity sets and anisotropic tensors are straightforward and that our findings are interesting for explicit finite-difference schemes on "full" stencils.

6 Concluding Remarks

From a practical point of view, the OTRT sub-class makes possible an efficient optimization of the equilibrium and relaxation parameters for a given interval of Peclet numbers, solving the physical problem. The OTRT model is "unconditionally" stable in the sense that any Peclet number can be modeled with equal values of the physical time steps. At the same time, the OTRT model is only conditionally stable in the sense that the available Courant numbers are limited and controlled by the equilibrium parameters. In brief, selecting the equilibrium parameter c_e and eigenvalue function Λ^-, one can take an advantage of $U^2(c_e)$ and the (equivalent) $Cr(Pe^*_{\Delta x})$ stability diagrams (with $Pe^*_{\Delta x} = \Lambda^- Pe_{\Delta x} = \frac{|\mathbf{U}|}{c_e}$). The highest velocity is reached at the intersection of the advection (increasing) and diffusion (decreasing) lines. The established "hierarchy" of the equilibrium weights is, *a-priori*, valid only on the OTRT sub-class. Beyond it, the most stable schemes may lose their robustness. Further analysis [18] indicates that the advection-diffusion schemes with the same weight families for all the terms are most capable for retaining of the OTRT stability when $\Lambda \in]\frac{1}{8}, \frac{1}{4}]$.

When the selected OTRT schemes possess the necessary (best possible) stability among all the TRT schemes, there is no reason to select $\Lambda \neq \frac{1}{4}$, however, the smaller values of Λ may become more efficient to reduce higher-order truncation errors, [8, 28, 30]. A good compromise between accuracy and efficiency plays a decisive role in the choice of the numerical parameters. Two comparative elements are still lacking: the accuracy properties of the OTRT sub-class and the stability properties of the TRT schemes when $\Lambda \neq \frac{1}{4}$.

Exact time-dependent *recurrence equations* [12] re-interpret the OTRT sub-class as a three-time-level central link-wise finite-difference schemes which share the properties of the Du Fort-Frankel diffusion scheme [6], distinctive in what it is both explicit and unconditionally stable for pure diffusion equation. The particularity of OTRT temporal and spatial discretization is not limited to the advection-diffusion equation. We believe that our results are valuable for the hydrodynamic LBE models where, most likely, all advection-diffusion stability constraints are also necessary (replacing c_e with "sound" velocity c_s^2), and perhaps for deriving stability conditions for other kinetic schemes.

Acknowledgements A. Kuzmin wants to thank Alberta Ingenuity Fund for their financial support. I. Ginzburg is thankful to Professor A. A. Mohamad for the hospitality in Calgary University.

Appendix A: Theory

A.1 Corollaries of the Cauchy-Schwartz Inequality

In several places we need the following variants of the Cauchy-Schwartz inequality for sets of (real or) complex quantities $\{a_1, \dots, a_n\}$ and $\{b_1, \dots, b_n\}$:

$$\left|\sum_{q=1}^{n} a_q b_q\right|^2 \le \sum_{q=1}^{n} |a_q|^2 \sum_{q=1}^{n} |b_q|^2. \tag{108}$$

Lemma A.1 *Any sets of $Q = Q_m + 1$ complex numbers a_q and b_q obey the following inequality for any set of Q positive numbers E_q*:

$$\left|\sum_{q=0}^{Q_m} a_q b_q\right|^2 \le \left(\sum_{q=0}^{Q_m} \frac{|a_q|^2}{E_q}\right)\left(\sum_{q=0}^{Q_m} E_q |b_q|^2\right), \quad E_q > 0,\ \forall q \in \{0, \dots, Q_m\}. \tag{109}$$

This is the Cauchy-Schwartz inequality written for $a_q/\sqrt{E_q}$ and $b_q\sqrt{E_q}$.

Corollary A.1.A *If the complex numbers a_q and the positive numbers E_q are such that $\sum_{q=0}^{Q_m} a_q = \sum_{q=0}^{Q_m} E_q = 1$, then*

$$\left(\sum_{q=0}^{Q_m} \frac{|a_q|^2}{E_q}\right) \ge 1, \quad E_q > 0,\ \forall q \in \{0, \dots, Q_m\}. \tag{110}$$

This is obtained from Lemma A.1 with $b_q = 1,\ \forall q \in \{0, \dots, Q_m\}$.

Corollary A.1.B *If the positive numbers E_q are such that $\sum_{q=0}^{Q_m} E_q = 1$ with $a_q = E_q$ and $b_q = \cos(k_q)$ (k_q real), then Lemma A.1 gives*

$$\left(\sum_{q=0}^{Q_m} E_q \cos(k_q)\right)^2 \le 1 - \sum_{q=0}^{Q_m} E_q \sin^2(k_q), \quad E_q > 0,\ \forall q \in \{0, \dots, Q_m\}. \tag{111}$$

Corollary A.1.C *If the E_q are positive numbers and $b_q = \sin(k_q)$ (k_q real), then Lemma A.1 gives*

$$\left|\sum_{q=0}^{Q_m} a_q \sin(k_q)\right|^2 \le \left(\sum_{q=0}^{Q_m} \frac{|a_q|^2}{E_q}\right)\left(\sum_{q=0}^{Q_m} E_q \sin^2(k_q)\right),$$
$$E_q > 0, \quad \forall q \in \{0, \dots, Q_m\}. \tag{112}$$

Remark A.1.B The positivity condition for the E_q can be replaced by a non-negativity condition ($E_q \ge 0$) in Corollary A.1.B, since the terms corresponding to $E_q = 0$ do not contribute to the sums. This can also be extended to Corollaries A.1.A and A.1.C, iff the terms $|a_q|^2/E_q$ go to zero when the corresponding E_q goes to zero.

A.2 Miller's Theorem

Miller's Theorem 6.1, [21], p. 403 Starting from a nth-order polynomial $P(z) = \sum_{j=0}^{n} a_j^* z^j$, let us built the reduced $(n-1)$th-order polynomial $P_1(z)$ (where a^* denotes complex conjugate of a):

$$P_1(z) = \frac{\tilde{P}(0)P(z) - \tilde{P}(z)P(0)}{z}, \qquad \tilde{P}(z) = \sum_{j=0}^{n} a_{n-j}^* z^j. \tag{113}$$

The Miller's theorem 6.1 states that if, $|\tilde{P}(0)| > |P(0)|$, then $P(z)$ is a von Neumann polynomial when $P_1(z)$ is a von Neumann polynomial (Neumann polynomials are polynomials with all their zeros either in the open unit disk or on the unit circle).

Appendix B: Non-negativity Equilibrium Conditions

B.1 Non-negativity Conditions of the d2Q9 Model

The non-negativity of the immobile weight $E_0 \ge 0$ is guaranteed by conditions (33). The interval $c_e \in [0, c_e^{(0)} = \frac{1}{1+2t_c^{(m)}}]$ is assumed for all conditions below. The non-negativity condition of moving populations, the *n-line* $U^2 = U_n^2(c_e)$ will bound the non-negativity area up to its intersection with the E_0-*n-line* (33). Relations (114) define the minimal equilibrium functions: E_c^{min} and E_d^{min} which give $\min_\psi\{E_q\}$ taking $\mathbf{U} = U(\cos\psi, \sin\psi)$, for the coordinate and the diagonal links, respectively. Without loss of generality, each relation below is valid when it is non-negative for $U \ge 0$:

$$\begin{cases}
\text{coordinate and diagonal links for } g^{(u)} = 0: \\
E_c^{min} = -Ut_c^{(a)} + c_e t_c^{(m)}, \quad E_d^{min} = \frac{c_e(1-2t_c^{(m)}) + \sqrt{2}(-1+2t_c^{(a)})U}{4} \\
\\
\text{coordinate links for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = \{0, 1\}: \\
E_c^{min,1} = \frac{U^2(2+\gamma_u) + 6(c_e t_c^{(m)} - t_c^{(a)} U)}{6}, \quad E_c^{min,2} = \frac{U^2(-1+\gamma_u) - 3({t_c^{(a)}}^2 - 2c_e t_c^{(m)})}{6}, \\
\\
\text{diagonal links for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = 0: \\
E_d^{min} = \frac{c_e(3-6t_c^{(m)}) + U(3\sqrt{2}(-1+2t_c^{(a)}) + U(1-\gamma_u))}{12}, \\
\\
\text{or for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = 1: \\
E_d^{min,1} = \frac{(5-2\gamma_u)U^2 + 6c_e(1-2t_c^{(m)}) - 6U\sqrt{2}(1-2t_c^{(a)})}{24}, \quad \text{and} \\
E_d^{min,2} = \frac{-(1+2\gamma_u)U^2 - 3((1-2t_c^{(a)})^2 - 2c_e(1-2t_c^{(m)}))}{24}.
\end{cases} \tag{114}$$

The equilibrium distributions of coordinate/diagonal links are non-negative provided that $U \in [0, \min\{U_{n,c}\}]$ or $U \in [0, \min\{U_{n,d}\}]$, respectively, where $\{U_{n,c}\}$ and $\{U_{n,d}\}$ are all suitable roots of equations $\{E_c^{min}(U)=0\}$ and $\{E_d^{min}(U)=0\}$, respectively. When the numerical diffusion is present, the non-negativity domain is $U^2 \le U_n^2 = \min\{U_{n,c}^2, U_{n,d}^2\}$, with:

$$g^{(u)}=0:$$
$$\begin{cases} U_n = U_{n,c} = \frac{c_e t_c^{(m)}}{t_c^{(a)}} \quad \text{if } t_c^{(a)} \ge \frac{\sqrt{d} t_c^{(m)}}{1+2(\sqrt{d}-1)t_c^{(m)}}, \quad \text{else } U_n = U_{n,d} = \frac{\sqrt{d} c_e (2t_c^{(m)}-1)}{d(2t_c^{(a)}-1)} \\ \text{then:} \quad U_n^2 = \frac{c_e^2}{d} \quad \text{if } t_c^{(a)} = t_c^{(m)} \neq \frac{1}{2} \quad \text{and} \quad U_n^2 = c_e^2 \quad \text{if } t_c^{(a)} = t_c^{(m)} = \frac{1}{2}, d=\{2,3\}. \end{cases} \tag{115}$$

These relations are valid for the d2Q9 model ($d=2$) and the d3Q15 model ($d=3$) (see next section). When $\{t_q^{(a)} = t_q^{(m)}\}$, the *n-line* $U_n^2 = \frac{c_e^2}{d}$ is set by the diagonal links, except for the d2Q5 and d3Q7 with $t_c^{(a)} = t_c^{(m)} = \frac{1}{2}$. Note that these minimal models has better non-negativity condition than all others when $c_e \in [0, \frac{1}{d}]$. In the two limit cases: $t_c^{(m)} = 0$ and $t_c^{(m)} = \frac{1}{2}$, the velocity is restricted to zero unless mass and velocity weights are equal, $\{t_q^{(a)} = t_q^{(m)}\}$.

When the numerical diffusion is removed, then the diagonal links prescribe different non-negativity conditions when $g_{xy}^{(u)} = 0$ and $g_{xy}^{(u)} = 1$. Again, $U^2 \le U_n^2 = \min\{U_{n,c}^2, U_{n,d}^2\}$, with:

$$\begin{cases} \text{coordinate links for } g^{(u)}=1,\ g_{xy}^{(u)}=\{0,1\}: \\ U_{n,c} = \frac{3t_c^{(a)} - \sqrt{9 t_c^{(a)2} - 6c_e(2+\gamma_u)t_c^{(m)}}}{2+\gamma_u}, \quad 0 \le c_e \le c_e^{bis},\ c_e^{bis} = \frac{(4-\gamma_u)t_c^{(a)2}}{6t_c^{(m)}}. \\ U_{n,c}^2 = \frac{3(t_c^{(a)2} - 2c_e t_c^{(m)})}{-1+\gamma_u}, \quad \gamma_u \neq 1,\ c_e^{bis} \le c_e \le c_e^{(0)}, \\ \\ \text{diagonal links for } g^{(u)}=1 \quad \text{and} \quad g_{xy}^{(u)}=0: \\ U_{n,d} = \frac{-3(1-2t_c^{(a)}) + \sqrt{9(2t_c^{(a)}-1)^2 - 6c_e(-1+\gamma_u)(2t_c^{(m)}-1)}}{\sqrt{2}(-1+\gamma_u)}, \quad \gamma_u \neq 1,\ 0 \le c_e \le c_e^{(0)}, \\ U_{n,d} = \frac{\sqrt{2} c_e (2t_c^{(m)}-1)}{2(2t_c^{(a)}-1)}, \quad \gamma_u = 1,\ t_c^{(a)} \neq \frac{1}{2},\ 0 \le c_e \le c_e^{(0)}, \\ \\ \text{or for } g^{(u)}=1 \quad \text{and} \quad g_{xy}^{(u)}=1: \\ U_{n,d} = \frac{\sqrt{2}(-3+\sqrt{-3c_e(2\gamma_u-5)(2t_c^{(m)}-1)+9(2t_c^{(a)}-1)^2} + 6t_c^{(a)})}{2\gamma_u-5}, \quad 0 \le c_e \le c_e^{bis}, \\ U_{n,d}^2 = -\frac{3(-2c_e(2t_c^{(m)}-1)+(2t_c^{(a)}-1)^2)}{1+2\gamma_u}, \quad \gamma_u \neq -\frac{1}{2},\ c_e^{bis} \le c_e \le c_e^{(0)}, \\ \quad c_e^{bis} = -\frac{(7+2\gamma_u)(2t_c^{(a)}-1)^2}{12(2t_c^{(m)}-1)},\ t_c^{(m)} \neq \frac{1}{2}. \end{cases} \tag{116}$$

The relations above are defined when $\gamma_u \in [-\frac{1}{2}, 1]$ and $\{t_c^{(a)}, t_c^{(m)}\} \in [0, \frac{1}{2}]$, except for some limit cases which should be considered separately. The non-negativity condition of coordinate links consists of two segments where the first one (for $U_{n,c}$) is set when $\mathbf{U}$ is parallel to the coordinate axis. The non-negativity condition of diagonal links is prescribed by the diagonal velocity when $g_{xy}^{(u)} = 0$. When $g_{xy}^{(u)} = 1$, the non-negativity condition of the diagonal links also consists from two segments where the first one (for $U_{n,d}$) is set when $\mathbf{U}$ is parallel to the diagonal axis.

Let us now specify the non-negativity conditions when $\{t_q^{(a)} = t_q^{(m)}\}$, $\gamma_u = 1 - 3t_c^{(m)}$ (relation (87)) and the E_0-*n-lines* are prescribed by relation (88). The case $g^{(u)} = 0$ and $\{t_q^{(a)} = t_q^{(m)}\}$ is addressed by relations (115). When $g^{(u)} = 1$, relations (116) become:

$$\begin{cases} \text{coordinate links for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = \{0, 1\}: \\ U_{n,c} = \frac{-t_c^{(m)} + \sqrt{t_c^{(m)}(2c_e(-1+t_c^{(m)}) + t_c^{(m)})}}{-1+t_c^{(m)}}, \quad 0 \le c_e \le \frac{t_c^{(m)}}{2}(1 + t_c^{(m)}), \\ \text{else } U_{n,c}^2 = 2c_e - t_c^{(m)}, \\ \\ \text{diagonal links for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = 0: \\ U_{n,d} = -\frac{\sqrt{(-1+2t_c^{(m)})(-1+2(1+c_e)t_c^{(m)})} - 1 + 2t_c^{(m)}}{\sqrt{2}t_c^{(m)}}, \\ \\ \text{or for } g^{(u)} = 1 \quad \text{and} \quad g_{xy}^{(u)} = 1: \\ U_{n,d} = -\frac{\sqrt{2}(\sqrt{(-1+2t_c^{(m)})(-1+c_e+2(1+c_e)t_c^{(m)})} - 1 + 2t_c^{(m)})}{1+2t_c^{(m)}}, \\ \quad \text{if } 0 \le c_e \le \frac{3}{4} + (-2 + t_c^{(m)})t_c^{(m)}, \quad \text{else } U_{n,d}^2 = 2c_e + 2t_c^{(m)} - 1. \end{cases} \tag{117}$$

All the non-negativity areas (117) lie inside the triangle prescribed by relations (89)–(90). In the limit case $t_c^{(m)} = \frac{1}{2}$ (here $t_c^{(u)} = 0$), the equilibrium weights $\{E_q\}$ are all non-negative for the diagonal links and the non-negativity condition is set by the coordinate links. The non-negativity conditions (117) become for the d2Q9$^{(stan)}$ (30):

$$\begin{cases} g^{(u)} = 0 \qquad\qquad : \quad U_n^2 = \frac{c_e^2}{2}, \quad 0 < c_e \le \frac{3}{5}. \\ g^{(u)} = 1, g_{xy}^{(u)} = 0 : \quad U_n^2 = \frac{1}{2}(-1 + \sqrt{1 - 2c_e})^2, \quad 0 \le c_e \le c_e^{bis}, \\ \qquad\qquad\qquad\qquad U_n^2 = \frac{3-5c_e}{2}, \quad c_e^{bis} < c_e \le \frac{3}{5}, \; c_e^{bis} = \frac{-1+2\sqrt{7}}{9}. \\ g^{(u)} = g_{xy}^{(u)} = 1 \quad : \quad U_n^2 = \frac{2}{25}(1 - \sqrt{1 - 5c_e})^2, \quad 0 \le c_e \le \frac{7}{36}, \\ \qquad\qquad\qquad\qquad U_n^2 = 2c_e - \frac{1}{3}, \quad \frac{7}{36} \le c_e \le \frac{11}{27}, \quad U_n^2 = \frac{3-5c_e}{2}, \quad \frac{11}{27} < c_e \le \frac{3}{5}. \end{cases} \tag{118}$$

This solution agrees with [28] (see their formulas (A.27) for $g^{(u)} = 0$ and (40) for $g_{xy}^{(u)} g^{(u)} = 1$). It is plotted in Figs. 12 and 13.

B.2 Non-negativity Conditions of the d3Q15 Model

The non-negativity of the immobile weight is prescribed by relation (34). As for the nine-velocity schemes, we first determine the set of minimal conditions $\{E_{c,d}^{min} = \min_{m,n}\{E_q\}\}$, separately for each sub-class, taking $\mathbf{U} = U\{\cos\psi \sin\alpha, \sin\psi \sin\alpha, \cos\alpha\}$ and using $\{m, n\} = \{\tan[\frac{\alpha}{2}], \tan[\frac{\psi}{2}]\}$ for trigonometric operations. The domain of validity of each relation (119) is $E_{c,d}^{min} \geq 0$ when $U \geq 0$:

$$\begin{cases} \text{coordinate links and diagonal links for } g^{(u)} = 0: \\ E_c^{min} = -U t_c^{(m)} + c_e t_c^{(m)}, \quad E_d^{min} = \frac{c_e(1-2t_c^{(m)})+\sqrt{3}(-1+2t_c^{(a)})U}{8}, \\ \\ \text{coordinate links for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = \{0, 1\}: \\ E_c^{min,1} = \frac{(\gamma_u+2)U^2-6(Ut_c^{(a)}-c_e t_c^{(m)})}{6}, \quad E_c^{min,2} = \frac{(\gamma_u-1)U^2+3(2c_e t_c^{(m)}-{t_c^{(a)}}^2)}{6}, \\ \\ \text{diagonal links for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = 0: \\ E_d^{min} = \frac{U(3\sqrt{3}(2t_c^{(a)}-1)-U(\gamma_u-1))-3c_e(2t_c^{(m)}-1)}{24}, \\ \\ \text{or for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = 1: \\ E_d^{min,1} = \frac{U(3\sqrt{3}(2t_c^{(a)}-1)+(4-\gamma_u)U)-3c_e(1-2t_c^{(m)})}{24}, \\ E_d^{min,2} = \frac{-(1+2\gamma_u)U^2+3(2c_e(1-2t_c^{(m)})-(1-2t_c^{(a)})^2)}{48}. \end{cases} \tag{119}$$

The equilibrium weights $\{E_q\}$ of "moving" populations are all non-negative provided that $U \in [0, U_n]$, $U_n = \min\{U_{n,c}, U_{n,d}\}$, where $\{U_{n,c} > 0, U_{n,d} > 0\}$ are all suitable roots of equations $\{E_{c,d}^{min}(U) = 0\}$. When $g^{(u)} = 0$, the relations (115) are valid for the d3Q15 ($d = 3$). When the numerical diffusion is removed, the solution becomes:

$$\begin{cases} \text{coordinate links for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = \{0, 1\}: \\ \\ U_{n,c} = \frac{3t_c^{(a)}-\sqrt{9{t_c^{(a)}}^2-6c_e t_c^{(m)}(2+\gamma_u)}}{\gamma_u+2}, \quad 0 \leq c_e \leq c_e^{bis}, \\ U_{n,c}^2 = \frac{3({t_c^{(a)}}^2-2c_e t_c^{(m)})}{-1+\gamma_u}, \quad c_e^{bis} < c_e < c_e^{(\max)}, c_e^{bis} = \frac{{t_c^{(a)}}^2(4-\gamma_u)}{6t_c^{(m)}}, \gamma_u \neq 1. \\ \\ \text{with diagonal links for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = 0: \\ U_{n,d} = \frac{\sqrt{3}}{2} \frac{3(1-2t_c^{(a)})-\sqrt{9(1-2t_c^{(a)})^2-4c_e(1-2t_c^{(m)})(1-\gamma_u)}}{1-\gamma_u}, \quad 0 \leq c_e \leq c_e^{(\max)}, \\ \\ \text{or for } g^{(u)} = 1 \quad \text{and} \quad g_{\alpha\beta}^{(u)} = 1: \\ U_{n,d} = \frac{\sqrt{3}}{2} \frac{3(1-2t_c^{(a)})-\sqrt{9(1-2t_c^{(a)})^2-4c_e(1-2t_c^{(m)})(4-\gamma_u)}}{(4-\gamma_u)}, \quad 0 \leq c_e \leq c_e^{bis}, \\ U_{n,d}^2 = -\frac{3((1-2t_c^{(a)})^2+2c_e(-1+2t_c^{(m)}))}{1+2\gamma_u}, \quad c_e^{bis} \leq c_e \leq c_e^{(\max)}, c_e^{bis} = \frac{(-1+2t_c^{(a)})^2(5+\gamma_u)}{9(1-2t_c^{(m)})}. \end{cases} \tag{120}$$

Further analysis is similar as for the d2Q9 model. We specify the non-negativity conditions when $\gamma_u = 1 - 3t_c^{(m)}$ and $\{t_q^{(a)} = t_q^{(m)}\}$, $\frac{1}{3} \leq t_c^{(a)} \leq \frac{1}{2}$, then:

$$\begin{cases} g^{(u)}=0: \quad U^2 \le \frac{c_e^2}{d}, d=3: \\ \text{coordinate links, } g^{(u)}=1,\, g^{(u)}_{\alpha\beta}=\{0,1\}: \\ U_{n,c}=\frac{-t_c^{(m)}+\sqrt{t_c^{(m)}(2c_e(-1+t_c^{(m)})+t_c^{(m)})}}{-1+t_c^{(m)}}, \quad 0\le c_e \le \frac{t_c^{(m)}}{2}(1+t_c^{(m)}), \\ \qquad\qquad \text{else } U^2_{n,c}=2c_e-t_c^{(m)}. \\ \\ \text{with diagonal links for } g^{(u)}=1,\, g^{(u)}_{\alpha\beta}=0: \\ U_{n,d}=\frac{\sqrt{3}(1-2t_c^{(m)})-\sqrt{(-1+2t_c^{(m)})(-3+(6+4c_e)t_c^{(m)})}}{2t_c^{(m)}} \\ \\ \text{or for } g^{(u)}=1,\, g^{(u)}_{\alpha\beta}=1: \\ U_{n,d}=\frac{\sqrt{3}(1-2t_c^{(m)})-\sqrt{(-1+2t_c^{(m)})(-3+6t_c^{(m)}+4c_e(1+t_c^{(m)}))}}{2(1+t_c^{(m)})}, \\ \qquad\qquad \text{if } 0\le c_e\le \frac{(-2+t_c^{(m)})(-1+2t_c^{(m)})}{3}, \quad \text{else } U^2_{n,d}=2c_e+2t_c^{(m)}-1. \end{cases} \tag{121}$$

These relations are illustrated in Fig. 15. All non-negativity areas (121), together with condition $E_0 \ge 0$, are confined inside the triangle (89), as for the d2Q9 schemes (Fig. 9). Again, the non-negativity domain is larger when the cross-diffusion is removed. The solution for U_n^2 takes the following form for d3Q15$^{(stan)}$ (30):

$$\begin{cases} g^{(u)}=0 & : \quad U_n^2=\frac{c_e^2}{3}, \quad 0\le c_e\le \frac{3}{7}. \\ \\ g^{(u)}=1,\, g^{(u)}_{\alpha\beta}=0: & \quad U_n^2=\frac{(\sqrt{3}-\sqrt{3-4c_e})^2}{4}, \quad 0\le c_e\le\frac{5}{12}, \\ & \quad U_n^2=3-7c_e, \quad \frac{5}{12}\le c_e\le\frac{3}{7}. \\ \\ g^{(u)}=g^{(u)}_{\alpha\beta}=1 & : \quad U_n^2=\frac{(\sqrt{3}-\sqrt{3-16c_e})^2}{64}, \quad 0\le c_e\le\frac{5}{27}, \\ & \quad U_n^2=2c_e-\frac{1}{3}, \quad \frac{5}{27}\le c_e\le\frac{10}{27}, \quad U_n^2=3-7c_e, \quad \frac{10}{27}\le c_e\le\frac{3}{7}. \end{cases} \tag{122}$$

This solution is plotted in Figs. 7 and 16.

Appendix C: Spectrum of the d2Q9 and d3Q15 OTRT Schemes

The Sects. C.1.1 and C.2.1 apply Theorem 2.3.1 to derive sufficient stability conditions, with a focus on the equilibrium weights where these conditions are also necessary. Sections C.1.2 and C.2.2 derive *necessary and sufficient* stability conditions with the help of direct analysis of the condition $|\Omega(\mathbf{k})|=1$ for the OTRT sub-class. All these results are restricted to isotropic symmetric weights $\{E_q^{(m)}\}$, when $\{E_q^{(a)}=0\}$.

C.1 The d2Q9 OTRT Schemes: Necessary and Sufficient Stability Conditions

C.1.1 The d2Q9 OTRT Model: Sufficient Stability Conditions

We apply condition (49-2) from Theorem 2.3.1 to build sufficient stability conditions for the d2Q9 scheme with $E_q^{(a)}=0$:

$$\begin{cases} S_s = \sum_{q=1}^{Q_m} \frac{(E_q^-)^2}{E_q^+} \le 1, \quad \text{where } S_s = 12 t_c^{(a)2} S_c - \frac{3(1-2t_c^{(a)})^2}{2} S_d, \\ \text{with} \\ S_c = \frac{U_x^2}{6c_e t_c^{(m)} + g^{(u)}((2+\gamma_u)U_x^2 + (-1+\gamma_u)U_y^2)} + \frac{U_y^2}{6c_e t_c^{(m)} + g^{(u)}((2+\gamma_u)U_y^2 + (-1+\gamma_u)U_x^2)} \\ S_d = \frac{(U_x+U_y)^2}{3c_e(-1+2t_c^{(m)}) + g^{(u)}((-1+\gamma_u)(U_x^2+U_y^2) - 3g_{xy}^{(u)} U_x U_y)} \\ \quad + \frac{(U_x-U_y)^2}{3c_e(-1+2t_c^{(m)}) + g^{(u)}((-1+\gamma_u)(U_x^2+U_y^2) + 3g_{xy}^{(u)} U_x U_y)}. \end{cases} \tag{123}$$

Here, S_c and S_d are the total respective contributions from the coordinate and diagonal links. Next step consists in seeking for maximum: $S_s^{(max)} = \max_n S_s(\mathbf{U}(n))$ (we replace: $\cos\psi \to \frac{1-n^2}{1+n^2}$, $\sin\psi \to \frac{2n}{1+n^2}$, with $n = \tan\frac{\psi}{2}$ for $\mathbf{U} = U(\cos\psi, \sin\psi)$). The stability boundary $U^2(c_e)$ satisfies equation $S_s^{(max)} = 1$ provided that $\{E_q^+ > 0\}$ (relations (85) and (86)) and $E_0 \ge 0$ (relation (33)).

With Numerical Diffusion $g^{(u)} = 0$ In such a case, all $\{E_q^+ > 0\}$ when $t_c^{(m)} \ne \{0, \frac{1}{2}\}$ and $E_0 \ge 0$ when $c_e \in [0, c_e^{(0)}]$. Then condition (123) prescribes the following stable area:

$$g^{(u)} = 0: \quad U^2 \le k_s c_e, \quad k_s = \frac{1 - 2t_c^{(m)}}{1 - 2t_c^{(a)}(2 - \frac{t_c^{(a)}}{t_c^{(m)}})}, t_c^{(m)} \notin \left\{0, \frac{1}{2}\right\}. \tag{124}$$

This sufficient condition is weaker than the non-negativity conditions (115), in agreement with the predictions of Lemma 2.3.2. When the mass and advection weights take the limit values, $t_c^{(a)} = t_c^{(m)} \in \{0, \frac{1}{2}\}$, the theorem still applies excluding either S_c or S_d, respectively, from S_s. These models are five populations schemes (a "rotated" d2Q5 and the d2Q5, respectively) and in both cases, $U^2 \le c_e$ is the sufficient condition. The theorem cannot be applied when $t_c^{(m)} \in \{0, \frac{1}{2}\}$ but $\{t_q^{(a)} \ne t_q^{(m)}\}$. Finally, the necessary (93) and sufficient (124) conditions coincide only if the mass and velocity weights are equal:

$$g^{(u)} = 0, \quad 0 \le t_c^{(m)} = t_c^{(a)} \le \frac{1}{2}: \quad U^2 \le c_e, \quad 0 \le c_e \le c_e^{(0)}. \tag{125}$$

Remark C.1.1.A Theorem 2.3.1 predicts the necessary and sufficient conditions for equal mass and velocity weights when $g^{(u)} = 0$ but does not rule out $k_s = 1$ for other combinations of weights.

Remark C.1.1.B When $\mathbf{U} \equiv 0$, the non-negativity of the immobile weight, $c_e \in [0, c_e^{(0)}]$, is sufficient from both Theorems 2.3.1 and 2.4. Proposition C.1.2.1 extends the stable interval $[0, c_e^{(0)} = \frac{1}{1+2t_c^{(m)}}]$ to the larger one, $c_e \in [0, c_e^{(\max)}]$, where $c_e^{(\max)} = \min\{1, \frac{1}{4t_c^{(m)}}\}$, as predicted by the necessary diffusion conditions (93). Then $E_0(c_e) \le 0$ when $c_e \in [c_e^{(0)}, c_e^{(\max)}]$.

Remark C.1.1.C In the presence of the advection, and when $\{t_q^{(a)} = t_q^{(m)}\}$, Proposition C.1.2.2 extends the necessary and sufficient condition (125) to the larger interval $c_e \in [0, c_e^{(\max)}]$. Then $E_0(c_e, U^2)$ is negative *inside the stable area* $U^2 \le c_e$ when $c_e \in [c_e^{(0)}, c_e^{(\max)}]$.

Remark C.1.1.D Proposition C.1.2.3 extends Proposition C.1.2.2 for different weights $\{t_q^{(m)} \le t_q^{(a)}\}$ when they lie in the interval $[0, \frac{1}{4}]$.

Without Diagonal Numerical Diffusion, $g^{(u)}=1$ *and* $g^{(u)}_{xy}=0$ Assuming $E_0 \geq 0$, then either the necessary advection-dominant condition (95) (when $g^{(u)}_{xy}=0$) or the non-negativity condition $\{E^+_q > 0\}$ (when $g^{(u)}_{xy}=1$) reduces the stable area to the triangle (89). When $g^{(u)}_{xy}=0$, relation (123) reaches its maximum for the diagonal velocity $U_x=U_y=U\frac{\sqrt{2}}{2}$, then the stability boundary $U^2(c_e)$ satisfies the inequality:

$$\frac{3(1-2t_c^{(a)})^2U^2}{3c_e(1-2t_c^{(m)})+(1-\gamma_u)U^2}+\frac{24{t_c^{(a)}}^2U^2}{12c_et_c^{(m)}+(1+2\gamma_u)U^2}\leq 1. \qquad (126)$$

The above inequality gives the stability boundary $U^2=k_sc_e$ where k_s depends on all three weights. The best value $k_s=2$ is reached when $t_c^{(a)}$ is related to the two other weights by:

$$t_c^{(a)}=\frac{1+2(\gamma_u+3t_c^{(m)})}{12} \quad \text{or, equivalently,} \quad t_c^{(u)}=2t_c^{(a)}-t_c^{(m)}. \qquad (127)$$

The condition $U^2\leq 2c_e$ is sufficient for the non-negativity of all $\{E^+_q\}$ when $\gamma_u=\gamma_u^{(m)}$ (cf. relation (87)). This choice reduces relation (127) to $t_c^{(a)}=\frac{1}{4}$. Then the advection line $U^2=2c_e$ is sufficient when $t_c^{(a)}=\frac{1}{4}$ and $g^{(u)}=1$, up to its intersection with the E_0-*n-line*. In this case, the predicted sufficient area coincides with the non-negativity triangle $\{E^+_q\geq 0\}$, given by conditions (89) and illustrated in Fig. 9.

Remark C.1.1.E The non-negativity domain (89) is also sufficient for case $g^{(u)}_{xy}g^{(u)}=1$ when $t_c^{(a)}=\frac{1}{4}$. However, in this and many other cases, the conditions derived with the assumptions $\{E^+_q>0\}$ and $E_0\geq 0$ are unnecessarily restrictive. We then proceed with the exact study of $|\Omega|$.

C.1.2 The d2Q9 OTRT Schemes: Necessary and Sufficient Stability Conditions

The characteristic equation of the OTRT sub-class is given by relation (44) with (45). Its stability properties are defined taking there $p=0$, then

$$\begin{cases} \Omega &= \Omega_r - i\Omega_i, \\ \text{where} & \\ \Omega_r &= 1-c_e\Omega_0+g^{(u)}(U_x^2\Omega_x+U_y^2\Omega_y-g^{(u)}_{xy}U_xU_y\sin k_x\sin k_y), \\ \Omega_0 &= (1-\cos k_x\cos k_y)+2t_c^{(m)}(1-\cos k_x)(1-\cos k_y), \\ \Omega_x &= \frac{1}{3}(-(2+\gamma_u)(1-\cos k_x)+(\gamma_u-1)(1-\cos k_x)\cos k_y), \\ \Omega_y &= \frac{1}{3}(-(2+\gamma_u)(1-\cos k_y)+(\gamma_u-1)(1-\cos k_y)\cos k_x), \\ \Omega_i &= (2t_c^{(a)}+(1-2t_c^{(a)})\cos k_y)U_x\sin k_x+(2t_c^{(a)}+(1-2t_c^{(a)})\cos k_x)U_y\sin k_y. \end{cases} \qquad (128)$$

The stability conditions which are both necessary and sufficient need, first, to maximize $|\Omega(U,c_e)|^2$ over three variables: $\{m_x,\ m_y\}$ and n (we use substitutions $\cos[k_\alpha]\rightarrow\frac{1-m_\alpha^2}{1+m_\alpha^2}$, $\sin[k_\alpha]\rightarrow\frac{2m_\alpha}{1+m_\alpha^2}$ and $\cos\psi\rightarrow\frac{1-n^2}{1+n^2}$, $\sin\psi\rightarrow\frac{2n}{1+n^2}$ for $\mathbf{U}=U(\cos\psi,\sin\psi)$, with $m_\alpha=\tan\frac{k_\alpha}{2}$ and $n=\tan\frac{\psi}{2}$), then to derive the solution $U^2(c_e)$ from stability boundary $|\Omega|^2=1$.

Proposition C.1.2.1 *When* $\mathbf{U}=0$, *then* $|\Omega|^2=(1-c_e\Omega_0)^2\leq 1$ *provided that* $c_e\leq c_e^{(\max)}=\min\{1,\frac{1}{4t_c^{(m)}}\}$, $0\leq t_c^{(m)}\leq\frac{1}{2}$.

Proof When $\mathbf{U}=0$, $\Omega=1-c_e\Omega_0$ and $1-|\Omega|^2=c_e\Omega_0(2-c_e\Omega_0)$. Then $|\Omega|^2\le 1$ iff $c_e\ge 0$, $\Omega_0\ge 0$, and $(2-c_e\Omega_0)\ge 0$ for all m_x and m_y. In fact, using

$$\Omega_0=\frac{2(m_x^2+m_y^2+4t_c^{(m)}m_x^2m_y^2)}{(1+m_x^2)(1+m_y^2)}, \tag{129}$$

$$2-c_e\Omega_0=\frac{2(1+(1-c_e)(m_x^2+m_y^2)+(1-4c_et_c^{(m)})m_x^2m_y^2)}{(1+m_x^2)(1+m_y^2)}, \tag{130}$$

these conditions are fulfilled iff $c_e\le c_e^{(\max)}=\min\{1,\frac{1}{4t_c^{(m)}}\}$ and $0\le t_c^{(m)}\le\frac{1}{2}$, □

Proposition C.1.2.2 *When* $g^{(u)}=0$ *and* $\{t_q^{(m)}=t_q^{(a)}\}$, *then* $|\Omega|^2\le 1$ *provided that* $0\le U^2\le c_e$ *and* $0\le c_e\le c_e^{(\max)}=\min\{1,\frac{1}{4t_c^{(m)}}\}$.

Proof When $g^{(u)}=0$ then $|\Omega|^2=(1-c_e\Omega_0)^2+\Omega_i^2$. Then, with the help of the Cauchy-Schwartz inequality:

$$\Omega_i^2\le(U_x^2+U_y^2)w_i^2,\quad \text{where } w_i^2=(2t_c^{(a)}(1-\cos k_y)+\cos k_y)^2\sin^2 k_x + (2t_c^{(a)}(1-\cos k_x)+\cos k_x)^2\sin^2 k_y. \tag{131}$$

We substitute the assumed stability boundary: $(U_x^2+U_y^2)\le c_e$, then:

$$|\Omega|^2\le W^2(c_e,t_c^{(m)},t_c^{(a)},m_x^2,m_y^2),\ W^2=(1-c_e\Omega_0)^2+c_ew_i^2,$$

where

$$w_i^2=\frac{4(m_x^2(1-(1-4t_c^{(a)})m_y^2)^2+m_y^2(1-(1-4t_c^{(a)})m_x^2)^2)}{(1+m_x^2)^2(1+m_y^2)^2}. \tag{132}$$

We then confirm that $W^2\le 1$ when $0\le t_c^{(a)}=t_c^{(m)}\le\frac{1}{2}$ and $c_e\in[0,c_e^{(\max)}]$. □

Proposition C.1.2.3 *When* $g^{(u)}=0$ *and* $0\le t_q^{(m)}\le t_q^{(a)}\le\frac{1}{4}$, *then* $|\Omega|^2=((1-c_e\Omega_0)^2+\Omega_i^2)\le 1$ *provided that* $0\le U^2\le c_e$ *and* $0\le c_e\le c_e^{(\max)}=1$.

Proof We again use the Cauchy-Schwartz estimate W^2 (relation (132)) and confirm that $\max_{m_x,m_y}W^2=1$ when all pre-conditions are set. □

Proposition C.1.2.4 *When* $t_c^{(a)}=\frac{1}{4}$ $(t_d^{(a)}=\frac{1}{8})$ *and* $0\le c_e\le c_e^{(\max)}=\min\{1,\frac{1}{4t_c^{(m)}}\}$ *then the necessary and sufficient conditions are given by relations* (133), *for any* $t_c^{(m)}\in[0,\frac{1}{2}]$ *and any* $\gamma_u\in[-\frac{1}{2},1]$:

$$\begin{cases} g^{(u)}=0 & : \quad U^2\le U_{a,0}^2=c_e. \\ g^{(u)}=1,\ g_{xy}^{(u)}=0: & \quad U^2\le\min\{U_{a,1}^2=2c_e,U_{d,1}^2,U_{d,2}^2\}. \\ g^{(u)}=1,\ g_{xy}^{(u)}=1: & \quad U^2\le\min\{U_{d,1}^2,U_{d,2}^2\}. \end{cases} \tag{133}$$

Here, $U_{d,1}^2$ *and* $U_{d,2}^2$ *are the diffusion-dominant conditions* (94).

Proof (a) When $g^{(u)}=0$, we confirm that $W^2\le 1$ for any $t_c^{(m)}\in[0,\frac{1}{2}]$ when $c_e\in[0,c_e^{(\max)}]$ provided that $t_c^{(a)}=\frac{1}{4}$. (b) When $g^{(u)}=1$, we consider exact solution (128) on the assumed stability boundaries and confirm, with the help of exact maximization routines [36] that $|\Omega|^2\le 1$ for the limit cases and several intermediate cases, e.g., $t_c^{(m)}=\{0,\frac{1}{4},\frac{1}{2}\}$, $\gamma_u=-\{\frac{1}{2},0,1\}$. We either keep c_e as a variable, or use the (dense) grid of c_e values in the available interval $c_e\in[0,c_e^{(\max)}]$ (this accelerates the maximization procedure).

This proposition first extends Proposition C.1.2.3 for the second part of the available interval, $t_c^{(m)}\in[\frac{1}{4},\frac{1}{2}]$, but uniquely for $t_c^{(a)}=\frac{1}{4}$. Second, the proposition extends the sufficient conditions predicted by Theorem 2.3.1 for "uniform" weights $t_c^{(a)}=t_c^{(m)}=\frac{1}{4}$ when $g^{(u)}=1$ and $g_{\alpha\beta}^{(u)}=0$ to the whole interval $t_c^{(m)}\in[0,\frac{1}{2}]$, again, provided that $t_c^{(a)}=\frac{1}{4}$. Third, the stability condition for $g_{xy}^{(u)}g^{(u)}=1$ predicts the "unconditional" stability: $0\le U^2(c_e=0)\le 1$ for $t_c^{(a)}=\frac{1}{4}$. The principal necessary conditions (93) and (95) are then sufficient. Hence, the d1Q3 model and d2Q9 schemes with $t_c^{(a)}=\frac{1}{4}$ (for any $t_c^{(m)}\in[0,\frac{1}{4}]$ and any γ_u) have the same stability conditions. This proposition is illustrated in Fig. 10 when $\gamma_u=\gamma_u^{(m)}$, $t_c^{(m)}$ varies and in Figs. 11 and 13 (right diagram) for the "uniform" weights. □

Proposition C.1.2.5 *When $g^{(u)}=0$, or $g^{(u)}=1$ with $g_{xy}^{(u)}=0$, and the equilibrium weights are related by conditions* (30) *(d2Q9$^{(stan)}$), then the necessary stability conditions* (99) *are also sufficient. When $g_{xy}^{(u)}g^{(u)}=1$, the sufficient condition is $U^2\le\frac{3}{4}$ when $c_e\in[0,\frac{1}{4}]$, and $U^2\le\min\{U_{d,1}^2,U_{d,2}^2\}$ when $c_e\in[\frac{1}{4},c_e^{(\max)}]$, $c_e^{(\max)}=\frac{3}{4}$.*

Indeed, the case $g^{(u)}=0$ is already addressed by Proposition C.1.2.2. When $g^{(u)}=1$, the proposition is verified along the same lines as Proposition C.1.2.4. This proposition expands the sufficient conditions predicted by Theorem 2.3.1 towards the necessary conditions and gives the (sufficient) stability boundary for $g_{xy}^{(u)}g^{(u)}=1$. In this last case, $U^2\le\frac{3}{4}$ is necessary only for $c_e=0$. The stability boundaries of the d2Q9$^{(stan)}$ scheme are confirmed by independent eigenmode analysis in Fig. 12 and illustrated in Fig. 13 (left diagram).

Proposition C.1.2.6 *For "standard" weights $t_c^{(a)}=t_c^{(m)}=\frac{1}{3}$, (a) the necessary stability conditions* (95) *are sufficient for any γ_u when $g^{(u)}=1$, $g_{xy}^{(u)}=0$, (b) when $g_{xy}^{(u)}g^{(u)}=1$ then $U^2=4c_e$, $0\le c_e\le\frac{1}{5}$, and $U^2=1-c_e$, $\frac{1}{5}\le c_e\le\frac{3}{4}$, is sufficient for $\gamma_u=-\frac{1}{2}$, (c) when $g_{xy}^{(u)}g^{(u)}=1$, then $U^2=\frac{11}{12}(1-3c_e)+\frac{5}{3}c_e$, $0\le c_e\le\frac{1}{3}$, and $U^2=1-\frac{4}{3}c_e$, $\frac{1}{3}\le c_e\le\frac{3}{4}$, is sufficient for $\gamma_u=1$.*

This proposition extends the previous one (where $\gamma_u=0$) for all γ_u when $g^{(u)}=1$, and proposes the sufficient boundaries for two limit cases, $\gamma_u=-\frac{1}{2}$ and $\gamma_u=1$. The proposition is verified similarly as Proposition C.1.2.4.

Proposition C.1.2.7 *For the d2Q9$^{(diag)}$ model* (100)*: $t_c^{(a)}=t_c^{(m)}=0$ with $\gamma_u=\gamma_u^{(m)}=1$, then (a) the necessary stability conditions* (95)*: $U^2\le 2c_e$ when $c_e\in[0,\frac{1}{3}]$ and $U^2\le 1-c_e$ when $c_e\in[\frac{1}{3},1]$, are sufficient when $g^{(u)}=1$, $g_{xy}^{(u)}=0$. (b) $U^2\le\frac{4}{5}$ when $c_e\in[0,\frac{1}{5}]$ and $U^2\le 1-c_e$ when $c_e\in[\frac{1}{5},1]$ is sufficient when $g_{xy}^{(u)}g^{(u)}=1$. The proposition is verified similarly as Proposition C.1.2.4 and confirmed in Fig. 14.*

C.2 The d3Q15 OTRT Schemes: Necessary and Sufficient Stability Conditions

C.2.1 The d3Q15 OTRT Model: Sufficient Stability Conditions

With Numerical Diffusion, $g^{(u)}=0$ We consider the sufficient conditions (49). When $g^{(u)}=0$, they result in relation (124), the same as for the d2Q9 schemes, where $c_e^{(\max)}$ obeys (103). This condition is stronger than the necessary condition (101) except for equal mass/velocity weights, $\{t_q^{(m)}=t_q^{(a)}\}$, where they coincide.

Without Numerical Diffusion, $g^{(u)}=1$ The non-negativity condition (49-1): $\{E_q^+\geq 0\}$ is set by relations (85) and (86), as for the d2Q9 model. Then we examine condition (49-2): $S_s=\sum_{q=1}^{Q_m}\frac{(E_q^-)^2}{E_q^+}\leq 1$ for equilibrium (24). The diagonal velocity $\mathbf{U}=\{U_\alpha=\frac{U}{\sqrt{3}}\}$ gives:

$$\frac{(1-2t_c^{(a)})^2U^2}{3c_e(1-2t_c^{(m)})+(1-\gamma_u)U^2}+\frac{4{t_c^{(a)}}^2U^2}{(6c_et_c^{(m)}+\gamma_uU^2)}\leq\frac{1}{9}. \tag{134}$$

The best possible advection boundary: $U^2=U_{a,2}^2=k_sc_e$ with $k_s=\frac{3}{2}$ is obtained only if $t_c^{(a)}$ is related to $t_c^{(m)}$ and γ_u by:

$$t_c^{(a)}=\frac{4t_c^{(m)}+\gamma_u}{6}\quad\text{or, equivalently, } t_c^{(u)}=3t_c^{(a)}-2t_c^{(m)}. \tag{135}$$

When $\gamma_u=\gamma_u^{(m)}$ (relation (87)) then $k_s=\frac{3}{2}$ for $t_c^{(a)}=\frac{1+t_c^{(m)}}{6}$ and the diagonal velocity gives the maximum for S_s. The sufficient (stable) triangle is then bounded by the advection line $U^2=k_sc_e$ and the E_0-*n-line*. Equal mass/velocity weights $\{t_q^{(a)}=t_q^{(m)}\}$ then result in the "uniform" weights (106).

C.2.2 The d3Q15 OTRT Schemes: Necessary and Sufficient Stability Conditions

We consider the root Ω of the OTRT characteristic equation (44) for $p=0$:

$$\begin{cases}\Omega=\Omega_r-i\Omega_i,\quad \text{where } \Omega_r=1-c_e\Omega_0+g^{(u)}(\frac{1}{3}\sum_{\alpha=\{x,y,z\}}U_\alpha^2\Omega_\alpha-\Omega_{xyz}),\\ \Omega_0=2t_c^{(m)}(3-\cos k_x-\cos k_y-\cos k_z)+(1-2t_c^{(m)})(1-\cos k_x\cos k_y\cos k_z),\\ \Omega_\alpha=(3\cos[k_\alpha]-1-2\gamma_u)\\ \qquad +(\gamma_u-1)(\cos[k_\alpha]+\cos[k_\beta]+\cos[k_\gamma]-\cos[k_\alpha]\cos[k_\beta]\cos[k_\gamma]),\quad \alpha\neq\beta\neq\gamma.\\ \Omega_{xyz}=\sum_{\alpha\neq\beta\neq\gamma}g_{\alpha\beta}^{(u)}\sin k_\alpha\sin k_\beta\cos k_\gamma U_\alpha U_\beta,\\ \Omega_i=\sum_{\alpha\neq\beta\neq\gamma}\sin k_\alpha U_\alpha(\sin k_\beta\cos k_\gamma(1-2t_c^{(a)})+2t_c^{(a)}).\end{cases} \tag{136}$$

Proposition C.2.2.1 *When* $t_c^{(a)}=\frac{1}{4}$ *then* (*a*) *the necessary conditions* (105) *are sufficient*; (*b*) *when* $g_{\alpha\beta}^{(u)}g^{(u)}=1$ *and* $\gamma_u=1$, *then the necessary and sufficient condition is* $U^2\leq U_d^2$ *when* $c_e\in[0,c_e^{(0)}]$.

This proposition predicts $U(c_e=0)\in[0,1]$ when $t^{(a)}=\frac{1}{4}$ but only for $\gamma_u=1$ ($t_c^{(u)}=\frac{1}{2}$), when the necessary diffusion-dominant condition $U^2\leq U_{d,2}^2=U_{p,c}^2$ (relation (105)) vanishes. This proposition is illustrated in Fig. 17. It is also confirmed by the eigenmode analysis, in particular for $t_c^{(m)}=0$.

Proposition C.2.2.2 *For $d3Q15^{(stan)}$ (30) and $d3Q15^{(unif)}$ (106), the necessary conditions (105) are also sufficient. Replacing $\gamma_u = 0$ with $\gamma_u = 1$ for $d3Q15^{(stan)}$, its stability boundary $U^2 \leq 2c_e$ improves at least as $U^2 \leq 4c_e$ when $g^{(u)}_{\alpha\beta} g^{(u)} = 1$. This proposition is confirmed by the eigenmode analysis in Figs. 15 and 16.*

The two propositions are confirmed computing $|\Omega|^2$ on the assumed stability boundary $U^2(c_e)$ with a dense variation of $\mathbf{U}$ and $\mathbf{k}$ in three dimensions (60^5 points) and confirmed by independent numerical analysis of the spectrum of the evolution equation (38).

References

1. Asinari, P., Karlin, I.V.: Generalized Maxwell state and H-theorem for computing fluid flows using the lattice Boltzmann method. Phys. Rev. E **79**(3), 036703(5) (2009)
2. Banda, M.K., Yong, W.A., Klar, A.: A stability notion for Lattice Boltzmann equations. SIAM J. Sci. Comput. **27**(6), 2098–2111 (2006)
3. d'Humières, D.: Generalized Lattice-Boltzmann equations. AIAA rarefied gas dynamics: theory and simulations. Prog. Astronaut. Aeronaut. **59**, 450–548 (1992)
4. d'Humières, D., Ginzburg, I.: Viscosity independent numerical errors for Lattice Boltzmann models: from recurrence equations to "magic" collision numbers. Comput. Math. Appl. **58**(5), 823–840 (2009)
5. d'Humières, D., Ginzburg, I., Krafczyk, M., Lallemand, P., Luo, L.-S.: Multiple-relaxation-time lattice Boltzmann models in three dimensions. Phil. Trans. R. Soc. Lond. A **360**, 437–451 (2002)
6. Du Fort, E.C., Frankel, S.P.: Stability conditions in the numerical treatment of parabolic differential equations. Math. Tab. Aids Comput. **7**, 135 (1953)
7. Flekköy, E.G.: Lattice Bathnagar-Gross-Krook models for miscible fluids. Phys. Rev. E **47**(6), 4247–4257 (1993)
8. Ginzburg, I.: Equilibrium-type and Link-type Lattice Boltzmann models for generic advection and anisotropic-dispersion equation. Adv. Water Resour. **28**, 1171–1195 (2005)
9. Ginzburg, I.: Variably saturated flow described with the anisotropic Lattice Boltzmann methods. J. Comput. Fluids **25**, 831–848 (2006)
10. Ginzburg, I.: Lattice Boltzmann modeling with discontinuous collision components. Hydrodynamic and advection-diffusion equations. J. Stat. Phys. **126**, 157–203 (2007)
11. Ginzburg, I.: Consistent Lattice Boltzmann schemes for the Brinkman model of porous flow and infinite Chapman-Enskog expansion. Phys. Rev. E **77**, 0666704:1-12 (2008)
12. Ginzburg, I.: Magic recipes for Lattice Boltzmann modeling of micro and macro flow. Habilitation Thesis, University Paris VI (2009). http://cemadoc.cemagref.fr/cemoa/PUB00025772
13. Ginzburg, I., d'Humières, D.: Lattice Boltzmann and analytical modeling of flow processes in anisotropic and heterogeneous stratified aquifers. Adv. Water Resour. **30**, 2202–2234 (2007)
14. Ginzburg, I., Verhaeghe, F., d'Humières, D.: Two-relaxation-time Lattice Boltzmann scheme: about parametrization, velocity, pressure and mixed boundary conditions. Commun. Comput. Phys. **3**, 427–478 (2008)
15. Higuera, F.J., Jiménez, J.: Boltzmann approach to lattice gas simulations. Europhys. Lett. **9**, 663–668 (1989)
16. Higuera, F.J., Succi, S., Benzi, R.: Lattice gas dynamics with enhanced collisions. Europhys. Lett. **9**, 345–349 (1989)
17. Hindmarsch, A.C., Grescho, P.M., Griffiths, D.F.: The stability of explicit time-integration for certain finite difference approximation of the multi-dimensional advection-diffusion equation. Int. J. Num. Methods Fluids **84**(4), 853–897 (1984)
18. Kuzmin, A., Ginzburg, I., Mohamad, A.A.: A role of the kinetic parameter on the stability of two-relaxation-times advection-diffusion Lattice Boltzmann scheme. *Comput. Math. Appl.* (2010, revised)
19. Lallemand, P., Luo, L.-S.: Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability. Phys. Rev. E **61**, 6546–6562 (2000)
20. Li, Y., Huang, P.: A coupled lattice Boltzmann model for advection and anisotropic dispersion problem in shallow water. Adv. Water Resour. **31**(12), 1719–1730 (2008)
21. Miller, J.J.H.: On the location of zeros of certaines classes of polynomials with application to numerical analysis. J. Inst. Math. Appl. **8**, 397–406 (1971)
22. Mitchell, A.R., Griffiths, D.F.: The Finite Difference Method in Partial Differential Equations. Wiley, Chichester (1980)

23. Pan, C., Luo, L.-S., Miller, C.T.: An evaluation of lattice Boltzmann schemes for porous media simulation. J. Comput. Fluids **35**(4), 898–909 (2006)
24. Premnach, K.N., Abraham, J.: Three-dimensional multi-relaxation time (MRT) lattice-Boltzmann models for multiphase flow. J. Comput. Phys. **224**, 539–559 (2007)
25. Qian, Y., d'Humières, D., Lallemand, P.: Lattice BGK models for Navier-Stokes equation. Europhys. Lett. **17**, 479–484 (1992)
26. Reis, T., Phillips, T.N.: Alternative approach to the solution of the dispersion relation for a generalized lattice Boltzmann equation. Phys. Rev. E. **77**, 026702-8 (2008)
27. Rheinländer, M.: Stability and multiscale analysis of an advective lattice Boltzmann scheme. Prog. Comput. Fluid Dyn. **8**(1–4), 56–68 (2008)
28. Servan-Camas, B., Tsai, F.T.C.: Lattice Boltzmann method for two relaxation times for advection-diffusion equation: third order analysis and stability analysis. Adv. Water Resour. **31**, 1113–1126 (2008)
29. Servan-Camas, B., Tsai, F.T.C.: Non-negativity and stability analysis of Lattice Boltzmann method for advection-diffusion equation. J. Comput. Phys. **228**, 236–256 (2009)
30. Servan-Camas, B., Tsai, F.T.C.: Saltwater intrusion modeling in heterogeneous confined aquifers using two-relaxation -time Lattice Boltzmann method. Adv. Water. Resour. **32**(4), 620–631 (2009)
31. Suga, S.: Numerical schemes obtained from Lattice Boltzmann equations for advection diffusion equations. Int. J. Modern Phys. C **17**(11), 1653–1677 (2006)
32. Sukop, M.C., Thorne, Jr. D.T.: Lattice Boltzmann Modeling. An Introduction for Geoscientists and Engineers. Springer, Berlin, Heidelberg (2006)
33. van der Sman, R.G.M.: Finite Boltzmann schemes. Comput. Fluids **35**, 849–854 (2006)
34. van der Sman, R.G.M., Ernst, M.H.: Diffusion lattice Boltzmann scheme on an orthorhombic lattice. J. Stat. Phys. **94**(1/2), 203–217 (1999)
35. Wolf-Gladrow, D.: Lattice gas cellular automata and lattice Boltzmann models: an introduction. In: Lecture Notes in Mathematics, vol. 1725. Springer, Berlin (2000). ISBN 3-540-66973-6
36. Wolfram, S.: Software package "Mathematica 6" (2010)
37. Zhang, X., Bengough, A.G., Deeks, L.K., Crawford, J.W., Young, I.M.: A lattice BGK model for advection and anisotropic dispersion equation. Adv. Water Resour. **25**, 1–8 (2002)
38. Zhang, X., Bengough, A.G., Deeks, L.K., Crawford, J.W., Young, I.M.: A novel three-dimensional lattice Boltzmann model for solute transport in variably saturated porous media. Water Resour. Res. **38**, 1167–1177 (2002)