

Towards nonlinear thermohydrodynamic simulations via the Onsager-regularized lattice-Boltzmann method

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This work presents a generalized, assumption-free, and stencil-independent theoretical analyses of the recently proposed Onsager-regularized (OReg) lattice Boltzmann (LB) method [Jonnalagadda *et al.*, *Phys. Rev. E* **104**, 015313 (2021)] and demonstrates its ability to mitigate spurious errors associated with the insufficient isotropy of standard first-neighbor lattices without the inclusion of any external correction terms. The hydrodynamic limit recovered by the OReg scheme is derived for two equilibrium distribution functions, namely the so-called thermal guided equilibrium and the popular second order polynomial equilibrium, to show that the OReg scheme yields macroscopic dynamics that are $\mathcal{O}(u)$ times more accurate than that of the bare BGK collision model. Specifically, we show that, with the guided equilibrium on the D2Q9 standard lattice, the OReg scheme inherently compensates for the insufficient lattice isotropy of the standard D2Q9 lattice by automatically adjusting the lattice viscosity, yielding $\mathcal{O}(u^4)$ and $\mathcal{O}(u^2)$ accurate kinetic models when operated at the reference and arbitrary temperatures, respectively. Further, we also show that the OReg scheme presents an $\mathcal{O}(u^3)$ accurate kinetic model for the D2Q9 lattice when used with the second order polynomial equilibrium formulation. Thereafter, the accuracy of the OReg-guided-equilibrium kinetic model is numerically demonstrated for quasi-one-dimensional simulations of the rotated decaying shear wave and isothermal shocktube problems. The present work lays the theoretical foundation of a generic framework which can enable fully local, correction-free, nonlinear thermohydrodynamic LB simulations on standard lattices, thereby facilitating scalable simulations of physically challenging fluid flows.

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I. INTRODUCTION

The evolution of a lattice Boltzmann (LB) system [1–7] emulates the Boltzmann transport equation in D dimensions through microscopic operations on discrete populations, f_i , in a lattice-discretized velocity space having N velocities $c_{i\alpha}$, $i \in \{1, \dots, N\}$. In the single relaxation framework, the lattice-BGK update is defined as

$$\begin{aligned} f_i(x_\alpha + c_{i\alpha} \Delta t, t + \Delta t) - f_i(x_\alpha, t) &= -\frac{1}{\tau} f_i^{(neq)}(x_\alpha, t) \\ &= -\frac{1}{\tau} (f_i(x_\alpha, t) - f_i^{(eq)}(x_\alpha, t)), \end{aligned} \quad (1)$$

where τ is the relaxation time, and $f_i^{(eq)}, f_i^{(neq)} = (f_i - f_i^{(eq)})$ are the equilibrium and nonequilibrium contributions of f_i , respectively. In such a discrete framework, exactly recovering

Navier-Stokes-Fourier (NSF) macrodynamics places explicit constraints on both the equilibrium and nonequilibrium contributions of f_i .

Specifically, the discrete equilibrium is required to recover the following Maxwell-Boltzmann (MB) moments:

$$\langle f_i^{(eq)}, \{1, c_{i\alpha}, c_i^2/2\} \rangle = \{\rho, \rho u_\alpha, E\}, \quad (2a)$$

$$\Pi_{\alpha\beta}^{(eq)} = \Pi_{\alpha\beta}^{MB} = p \delta_{\alpha\beta} + \rho u_\alpha u_\beta, \quad (2b)$$

$$q_\alpha^{(eq)} = q_\alpha^{MB} = u_\alpha (E + p), \quad (2c)$$

where $\langle \varphi_i, \psi_i \rangle = \sum_i \varphi_i \psi_i$, the quantities ρ , ρu_α and $E =$

$\Pi_{\alpha\alpha}^{(eq)}/2 = (Dp + \rho u^2)/2$ are the mass, momentum, and energy density, respectively, with $p = \rho \theta$ being the thermodynamic pressure given through the ideal gas law, where $\theta = RT$ is the reduced temperature, and $\Pi_{\alpha\beta}^{(eq)} = \langle f_i^{(eq)}, c_{i\alpha} c_{i\beta} \rangle$ and $q_\alpha^{(eq)} = \langle f_i^{(eq)}, \frac{1}{2} c_i^2 c_{i\alpha} \rangle$ are the equilibrium contributions of the pressure tensor and heat flux vector. Note that Eq. (2) corresponds to 8 and 13 linearly independent constraints on $f_i^{(eq)}$ in two and three dimensions. Thus, one can completely describe the equilibrium state even on standard lattices (Fig. 1) lying within the first Brillouin zone. In contrast, on standard lattices, the description of the nonequilibrium populations, $f_i^{(neq)}$, and

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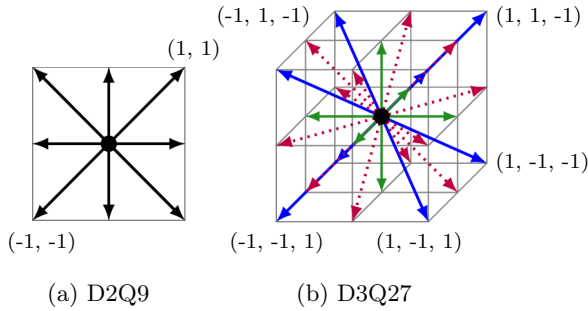


FIG. 1. Velocity space representations in two and three dimensions using the standard D2Q9 and D3Q27 lattices, respectively.

consequently the resulting out-of-equilibrium macrodynamics, requires more care.

We recall from kinetic theory that $f_i^{(neq)}$ must satisfy the so-called compatibility conditions Eq. (3a) and should recover the NSF constitutive relations for the viscous stress tensor Eq. (3b) and heat flux vector Eq. (3c);

$$\langle f_i^{(neq)}, \{1, c_{i\alpha}, c_{i\alpha}^2/2\} \rangle = 0, \quad (3a)$$

$$\Pi_{\alpha\beta}^{(neq)} = \Pi_{\alpha\beta}^{\text{NSF}} = -\mu \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D} \partial_\chi u_\chi \delta_{\alpha\beta} \right), \quad (3b)$$

$$q_\alpha^{(neq)} = q_\alpha^{\text{NSF}} = -\kappa \partial_\alpha \theta. \quad (3c)$$

The quantities μ and κ are the dynamic viscosity and thermal conductivity, respectively.

In order to evaluate Eq. (3), closed form expressions of $f_i^{(neq)}$ are needed; while newer regularization schemes prescribe analytical expressions [8], historically, $f_i^{(neq)}$ is simply computed as $f_i^{(neq)} = (f_i - f_i^{(eq)})$. However, since f_i is a computationally evaluated quantity, such a representation is not amenable for a theoretical evaluation of Eq. (3). Consequently, the following approach is adopted for enabling theoretical analyses: First, the compatibility conditions given by Eq. (3a) are *assumed* to hold. However, kinetic theory requires these conditions to be imposed on nonequilibrium descriptions of the distribution function [9] and, as evidenced by theoretical works on higher-order continuum transport equations [10–13], such an assumption may not be valid even in the continuous phase space. Second, Eqs. (3b) and (3c) are evaluated by coupling $\Pi_{\alpha\beta}^{(neq)} = \langle f_i^{(neq)}, c_{i\alpha} c_{i\beta} \rangle$ and $q_\alpha^{(neq)} = \langle f_i^{(neq)}, \frac{1}{2} c_{i\alpha}^2 c_{i\alpha} \rangle$ to $f_i^{(eq)}$ via higher-order equilibrium moments $Q_{\alpha\beta\gamma}^{(eq)} = \langle f_i^{(eq)}, c_{i\alpha} c_{i\beta} c_{i\gamma} \rangle$ and $R_{\alpha\beta\gamma\mu}^{(eq)} = \langle f_i^{(eq)}, c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\mu} \rangle$. However, this coupling to higher order equilibrium moments has severe repercussions in that spurious numerical errors are introduced on standard lattices due to insufficient lattice isotropy. In order to retain the computational advantage provided by LB on standard lattices, significant efforts have been made over the past three decades to eliminate these spurious errors [14–26]. The current state-of-the-art incorporates nonlocal correction terms into the lattice update to exactly recover the desired thermohydrodynamics [21,22,25]. However, it is noteworthy that this strategy is not only hard to generalize to different collision kernels and equilibrium representations, but is also detrimental

to the parallel efficiency offered by LB on standard lattices. Furthermore, this performance sacrifice is exacerbated in numerical implementations that incorporate advanced meshing paradigms such as, e.g., grid refinement, needed for addressing complex problems involving fluid flow.

In this work, we demonstrate that the recently proposed Onsager-regularized (OReg) LB method [8,27,28] facilitates simulations of nonlinear NSF hydrothermal transport phenomenon by alleviating the adverse standard lattice anisotropy effects without resorting to nonlocal corrections. Specifically, we first present a generalized, assumption-free, and stencil-independent theoretical analysis of the OReg scheme via the Chapman-Enskog (CE) procedure [5,6] that is valid for any equilibrium representation. We then employ the so-called $\mathcal{O}(u^4)$ guided equilibrium [22–24] and the $\mathcal{O}(u^2)$ polynomial equilibrium representation to obtain OReg kinetic models for the NSF equations on standard lattices. Thereafter, we present numerical results for canonical quasi-one-dimensional problems demonstrating the improved accuracy obtained with the OReg model with the guided equilibrium, and, finally, present our conclusions.

II. ONSAGER-REGULARIZED LBM

The OReg scheme uses the principles of linear irreversible thermodynamics and prescribes the nonequilibrium contribution of the distribution function at the NSF level in terms of viscous and thermal irreversible processes [29,30] that comply with Onsager's symmetry principle. Here, for the sake of brevity, we restrict the discussion to isothermal flows of monatomic gases and direct the interested reader to Ref. [28] and the references therein for a more detailed exposition. In such a setting, the nonequilibrium thermodynamics representation of the NSF contribution of the distribution function is given as

$$f^{(1)} = f^{\text{OReg}} = -\tau f^{\text{MB}} \left(C_\alpha C_\beta - \frac{C^2}{D} \delta_{\alpha\beta} \right) \left(\frac{\partial_\beta u_\alpha + \partial_\alpha u_\beta}{2\theta} \right). \quad (4)$$

Here, f^{MB} is the continuous Maxwell-Boltzmann equilibrium distribution function and $C_\alpha = (c_\alpha - u_\alpha)$ is the peculiar velocity. Note that Eq. (4) can be recast into the same form [28] that is obtained from a CE expansion of the continuous, force-free, integro-differential Boltzmann equation and thus recovers the isothermal Navier-Stokes (NS) equations exactly in the nondiscrete setting. Here we remark that, much like the entropic LB which connects the discrete equilibrium and path length to kinetic theory via the discrete H Theorem [31], the OReg formulation explicitly connects the description of the nonequilibrium lattice populations to kinetic theory via nonequilibrium thermodynamic descriptions. This is done by simply projecting Eq. (4) onto lattice stencils by representing f^{MB} and C_α as $f_i^{(eq)}$ and $C_{i\alpha} = (c_{i\alpha} - u_\alpha)$, respectively, to obtain

$$f_i^{\text{OReg}} = -\tau f_i^{(eq)} \left(C_{i\alpha} C_{i\beta} - \frac{C_i^2}{D} \delta_{\alpha\beta} \right) \left(\frac{\partial_\beta u_\alpha + \partial_\alpha u_\beta}{2\theta} \right). \quad (5)$$

Thereafter, the derivative terms appearing in Eq. (5) are locally evaluated by using the definition of the second-order

trace-free stress tensor [8,27,28] to generically represent the OReg populations as

$$f_i^{\text{OReg}} = \frac{f_i^{(eq)}}{2\rho\theta^2} \left(C_{i\alpha} C_{i\beta} - \frac{C_i^2}{D} \delta_{\alpha\beta} \right) \times \sum_{k=1}^N \left(c_{k\alpha} c_{k\beta} - \frac{c_k^2}{D} \delta_{\alpha\beta} \right) f_k^{(neq)}. \quad (6)$$

Note that Eq. (6) is agnostic to the lattice stencil as well as the spatial discretization and therefore yields a fully local formulation. It is also noteworthy that, as opposed to earlier works [8,27,28], the OReg scheme as presented in Eq. (6) is generalized to include temperature dependence and is a significantly simpler representation of the scheme valid for monatomic gases. We highlight that the presence of $f_i^{(neq)}$ in Eq. (6) allows the OReg scheme to be interpreted as a one-step predictor-corrector method where the prediction $f_i^{(1)} \approx f_i^{(neq)}$ is corrected to $f_i^{(1)} = f_i^{\text{OReg}}$ evaluated using Eq. (6). The predictor $f_i^{(neq)}$ can be evaluated through any existing regularization scheme [8]; however, for the sake of simplicity, we use $f_i^{(neq)} = (f_i - f_i^{(eq)})$. Finally, in line with regularized LBM schemes, the OReg lattice update is realized by reworking Eq. (1) as

$$f_i(x_\alpha + c_{i\alpha} \Delta t, t + \Delta t) = f_i^{(eq)}(x_\alpha, t) + \left(1 - \frac{1}{\tau} \right) f_i^{\text{OReg}}(x_\alpha, t). \quad (7)$$

Before proceeding, we remark that Eq. (6) is strikingly similar to those obtained with the projected regularized

scheme [32] and is visually almost identical to the Galilean Invariant Filtered (GIFR) collision model [33]; this is an expected outcome since these schemes aim to recover the same macroscopic equations. However, it is important to note that the projected regularized scheme, along with systematic improvements such as the recursively regularized [34,35], hybrid-recursively regularized [36], and GIFR schemes, are *functional approximations* of the lattice-discretized nonequilibrium distribution function expressed in a Hermitian basis [8]. In contrast, the OReg scheme, represented by Eq. (6), is simply a fully local lattice-discretized representation of the nonequilibrium distribution function [8]. It is, therefore, reasonable to expect that the OReg scheme would yield improved stability characteristics as compared to other regularization strategies; indeed, previous work [28] has demonstrated such a behavior for flows with large Reynolds (Re) and Mach (Ma) numbers on standard lattices.

III. HYDRODYNAMIC LIMIT USING THE CHAPMAN-ENSKOG MULTISCALE EXPANSION

A. General outcomes

We now briefly describe the procedure to obtain the hydrodynamic limit of single relaxation time LB schemes through the Chapman-Enskog (CE) multiscale expansion [5,6]. The quantities appearing in Eq. (1) are expressed in terms of a perturbation series as $f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \mathcal{O}(\epsilon^3)$, $\partial_t = \partial_t^{(0)} + \epsilon \partial_t^{(1)} + \mathcal{O}(\epsilon^2)$, and $\partial_\alpha = \epsilon \partial_\alpha^{(1)}$, where the perturbation parameter, ϵ , corresponds to the Knudsen number (Kn). Subsequently, after a series of algebraic manipulations, during which it is revealed that $f_i^{(0)} = f_i^{(eq)}$, the following $\mathcal{O}(\epsilon^3)$ equations are recovered:

$$\partial_t \varphi_i^{(eq)} + \partial_\alpha \varphi_{i\alpha}^{(eq)} = -\frac{\epsilon}{\tau} \varphi_i^{(1)} - \frac{\epsilon^2}{\tau} \varphi_i^{(2)} - \epsilon^2 \left\{ \partial_t^{(1)} \left[\left(1 - \frac{\Delta t}{2\tau} \right) \varphi_i^{(1)} \right] + \partial_\alpha^{(1)} \left[\left(1 - \frac{\Delta t}{2\tau} \right) \varphi_{i\alpha}^{(1)} \right] \right\}, \quad (8a)$$

$$\partial_\alpha \varphi_{i\alpha}^{(eq)} + \partial_\alpha \underbrace{\langle f_i^{(eq)}, c_{i\alpha} c_{i\beta} \rangle}_{\Pi_{\alpha\beta}^{(eq)}} + \partial_\alpha \left[\epsilon \left(1 - \frac{\Delta t}{2\tau} \right) \underbrace{\langle f_i^{(1)}, c_{i\alpha} c_{i\beta} \rangle}_{\Pi_{\alpha\beta}^{(1)}} \right] = -\frac{\epsilon}{\tau} \varphi_{i\alpha}^{(1)} - \frac{\epsilon^2}{\tau} \varphi_{i\alpha}^{(2)} - \epsilon^2 \partial_t^{(1)} \left[\left(1 - \frac{\Delta t}{2\tau} \right) \varphi_{i\alpha}^{(1)} \right], \quad (8b)$$

where $\{\varphi_i^{(eq)}, \varphi_i^{(1)}, \varphi_i^{(2)}\} = \langle \{f_i^{(eq)}, f_i^{(1)}, f_i^{(2)}\}, 1 \rangle$ and $\{\varphi_{i\alpha}^{(eq)}, \varphi_{i\alpha}^{(1)}, \varphi_{i\alpha}^{(2)}\} = \langle \{f_i^{(eq)}, f_i^{(1)}, f_i^{(2)}\}, c_{i\alpha} \rangle$. Note that, with $f_i^{(0)} = f_i^{(eq)}$, the resultant nonequilibrium populations become $f_i^{(neq)} = \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \mathcal{O}(\epsilon^3)$, and upon introducing the constraints of Eq. (2) and Eq. (3), Eq. (8a) directly yields the equation of mass conservation, while Eq. (8b), pending closure of $\Pi_{\alpha\beta}^{(1)}$, approximates the NS momentum conservation equations; as alluded to earlier, this closure is typically performed via $\mathcal{Q}_{\alpha\beta\gamma}^{(eq)}$.

B. Onsager-regularized macrodynamics for a generic equilibrium distribution function

Now that the generalized outcome of the CE expansion at the NS level is available in Eq. (8), we move on to obtain the macroscopic limit of the OReg scheme for a generic equilib-

rium representation. Note that such a generic representation need not satisfy Eq. (2) in its entirety for recovering athermal/isothermal hydrodynamics. Indeed, on standard lattices, only the so-called consistent equilibrium [37], when operated at the standard lattice reference temperature $\theta_0 = 1/3$, satisfies Eq. (2) completely. Therefore, we introduce $\Phi'_i = \Phi_i^{(eq)} - \Phi_i^{\text{MB}}$ as the generic deviation of an equilibrium moment $\Phi_i^{(eq)}$ from its MB counterpart Φ_i^{MB} and $\Pi'_{\alpha\beta}$, q'_α , $Q'_{\alpha\beta\gamma}$, and $R'_{\alpha\beta\gamma\mu}$ as the respective deviations of the equilibrium pressure tensor, heat flux vector, and the third- and fourth-order moments, respectively. Note that the conserved quantities are expected to not have any deviations, i.e., $\rho' = (\rho u_\alpha)' = 0$. Thereafter, since we are interested in NS level thermohydrodynamics, we assume that the compatibility conditions hold for the Burnett and higher order contributions; thus, $\varphi_i^{(2)}$ and $\varphi_{i\alpha}^{(2)}$ are always taken to be zero while $\varphi_i^{(1)}$, $\varphi_{i\alpha}^{(1)}$ are evaluated explicitly

using $f_i^{(1)} = f_i^{\text{OReg}}$ given in Eq. (5). Note that this is the first deviation from the standard procedure followed in the LB

literature which assumes that Eq. (3a) holds for all levels of approximation in ϵ . Explicitly, we obtain

$$\varphi_i^{(1)|\text{OReg}} = \langle f_i^{\text{OReg}}, 1 \rangle = -\frac{\tau}{2\theta} (\partial_\beta^{(1)} u_\alpha + \partial_\alpha^{(1)} u_\beta) \left(\Pi'_{\alpha\beta} - \frac{\delta_{\alpha\beta}}{2D} \Pi'_{\chi\chi} \right), \quad (9a)$$

$$\varphi_{i_\gamma}^{(1)|\text{OReg}} = \langle f_i^{\text{OReg}}, c_{i_\gamma} \rangle = -\frac{\tau}{2\theta} (\partial_\beta^{(1)} u_\alpha + \partial_\alpha^{(1)} u_\beta) \left[\mathcal{Q}'_{\alpha\beta\gamma} - u_\alpha \Pi'_{\beta\gamma} - u_\beta \Pi'_{\gamma\alpha} - \frac{\delta_{\alpha\beta}}{D} \left(q'_\gamma - \frac{u_\gamma}{2} \Pi'_{\chi\chi} \right) \right], \quad (9b)$$

where the derivative terms have the superscript (1) since f_i^{OReg} is of $\mathcal{O}(\epsilon)$. The next deviation from the standard procedure is in closing Eq. (8b) which is achieved through directly evaluating $\Pi_{\alpha\beta}^{(1)}$ using f_i^{OReg} . This direct evaluation yields

$$\begin{aligned} \Pi_{\alpha\beta}^{(1)|\text{OReg}} = & \underbrace{\langle f_i^{\text{OReg}}, c_{i_\alpha} c_{i_\beta} \rangle}_{\Pi_{\alpha\beta}^{\text{NSF}}} = -\tau \rho \theta \left(\partial_\alpha^{(1)} u_\beta + \partial_\beta^{(1)} u_\alpha - \frac{2}{D} \partial_\chi^{(1)} u_\chi \delta_{\alpha\beta} \right) \\ & - \underbrace{\frac{\tau}{2\theta} (\partial_\mu^{(1)} u_\gamma + \partial_\gamma^{(1)} u_\mu) [R'_{\alpha\beta\gamma\mu} - u_\gamma \mathcal{Q}'_{\alpha\beta\mu} - u_\mu \mathcal{Q}'_{\alpha\beta\gamma} + u_\gamma u_\mu \Pi'_{\alpha\beta} - \frac{\delta_{\gamma\mu}}{D} (R'_{\alpha\beta\chi\chi} - 2u_\chi \mathcal{Q}'_{\alpha\beta\chi} + u_\chi^2 \Pi'_{\alpha\beta})]}_{(\Pi_{\alpha\beta}^{(neq)})'}, \end{aligned} \quad (10)$$

where $(\Pi_{\alpha\beta}^{(neq)})'$ is the error contribution to the NSF stress tensor. Here, we highlight that, while Eqs. (9) and (10) can be simplified depending on the constraints on $f_i^{(eq)}$, spurious contributions from $\mathcal{Q}'_{\alpha\beta\gamma}$ and $R'_{\alpha\beta\gamma\mu}$ are still retained on standard lattices. Nevertheless, it is important to note that Eq. (10) recovers the NSF stress tensor, albeit with the erroneous $(\Pi_{\alpha\beta}^{(neq)})'$ contribution, irrespective of the employed equilibrium $f_i^{(eq)}$. It is worth noting that the derivative terms premultiplying the error terms increase the magnitude of $(\Pi_{\alpha\beta}^{(neq)})'$ by $\mathcal{O}(u)$. Thus, the overall equilibrium-dependent spurious contributions brought in by $\mathcal{Q}'_{\alpha\beta\gamma}$ and $R'_{\alpha\beta\gamma\mu}$ are

diluted by at least one order of magnitude and, consequently, may be small enough to be ignored. In contrast, when the closure of Eq. (8b) is performed via $\mathcal{Q}_{\alpha\beta\gamma}^{(eq)}$, only the consistent equilibrium of Ref. [37] yields a trace-free NSF stress tensor.

C. Onsager-regularized macrodynamics using the guided equilibrium

As an explicit illustration of the above arguments, we first consider the OReg scheme coupled with the guided equilibrium distribution representation [22–24]:

$$f_i^{(eq)|G} = \rho \prod_{\alpha=x,y} \frac{(1 - 2c_{i_\alpha}^2)}{2c_{i_\alpha}^2} [c_{i_\alpha}^2 - 1 + c_{i_\alpha} u_\alpha + u_\alpha^2 + \theta]. \quad (11)$$

Note that Eq. (11), defined for the D2Q9 lattice obeys six out of the eight constraints imposed on $f_i^{(eq)}$ with Eq. (2c) not being obeyed. Using Eq. (11) in Eq. (5), we explicitly obtain the OReg nonequilibrium populations which we denote using $f_i^{\text{OReg}|G}$. Thereafter, substituting $f_i^{\text{OReg}|G}$ into Eq. (10) gives us the OReg NS pressure tensor using the guided equilibrium as

$$\Pi_{\alpha\beta}^{(1)|\text{OReg}|G} = -\mu_{\alpha\beta}^{\text{OReg}|G} (\partial_\alpha u_\beta + \partial_\beta u_\alpha - \partial_\chi u_\chi \delta_{\alpha\beta}) + (\Pi_{\alpha\beta}^{(neq)|G})', \quad (12a)$$

$$\text{where, } \mu_{\alpha\beta}^{\text{OReg}|G} = \tau \rho \theta \begin{cases} \frac{1}{2\theta^2} (\theta - u_\alpha^2) (1 - \theta - u_\alpha^2) & \text{if } \alpha = \beta \\ 1 & \text{otherwise,} \end{cases} \quad (12b)$$

$$(\Pi_{\alpha\beta}^{(neq)|G})' = \begin{cases} 0 & \text{if } \alpha = \beta \\ \rho \frac{\tau}{2\theta} u_x u_y (u_x^2 - u_y^2) (\partial_x u_x - \partial_y u_y) \sim \mathcal{O}(u^6) & \text{otherwise.} \end{cases} \quad (12c)$$

It is remarkable to note from Eq. (12c) that the diagonal components of the nonequilibrium pressure tensor are naturally error free while the off-diagonal components have an $\mathcal{O}(u^6)$ error (recall that $\tau \propto u$). Thus, the contribution of $(\Pi_{\alpha\beta}^{(neq)|G})'$ to $\Pi_{\alpha\beta}^{\text{OReg}|G}$ is indeed negligible and can be safely ignored. Now, with a vanishing $(\Pi_{\alpha\beta}^{(neq)|G})'$, Eq. (12a) explicitly yields

a traceless second-order pressure tensor having a velocity and temperature dependant dynamic viscosity of $\mu_{\alpha\beta}^{\text{OReg}|G}$ as shown in Eq. (12b). It is through $\mu_{\alpha\beta}^{\text{OReg}|G}$ that the OReg scheme compensates for the insufficient lattice isotropy of the D2Q9 lattice by intrinsically modifying the lattice viscosity of the diagonal components of $\Pi_{\alpha\beta}^{\text{OReg}|G}$.

Next, we evaluate Eqs. (9a) and (9b) using the guided equilibrium to obtain

$$\varphi_i^{(1)|\text{OReg|G}} = \langle f_i^{\text{OReg|G}}, 1 \rangle = 0, \quad (13a)$$

$$\varphi_{i_\alpha}^{(1)|\text{OReg|G}} = \langle f_i^{\text{OReg|G}}, c_{i_\alpha} \rangle = \frac{\tau \rho u_\alpha}{\theta} (u_\alpha^2 + 3\theta - 1) \left(\partial_\alpha u_\alpha - \frac{1}{2} \partial_\chi u_\chi \right) = \begin{cases} \mathcal{O}(u^5) & \text{if } \theta = 1/3 \\ \mathcal{O}(u^3) & \text{otherwise} \end{cases}. \quad (13b)$$

From Eq. (13a), it can be seen that Eq. (9a) vanishes with the OReg scheme and the guided equilibrium as required by the compatibility conditions; in contrast, $\varphi_{i_\alpha}^{(1)|\text{OReg|G}}$ is nonzero with errors having magnitudes as shown in Eq. (13b). Consequently, due to the $(1/2\tau)$ factor in Eq. (8), the corresponding mass and momentum conservation equations contain $\mathcal{O}(u^4)/\mathcal{O}(u^2)$ errors depending on the value of the isothermal temperature. Thus, with the OReg scheme and the guided equilibrium, one can conduct correction-free isothermal NS simulations with $\mathcal{O}(u^3)/\mathcal{O}(u)$ accuracy at the lattice reference temperature and arbitrary lattice temperatures, respectively.

In order to isolate the accuracy gained by using OReg scheme from those brought about by using the guided equilibrium, we consider the momentum equation obtained from the CE expansion of the Lattice-BGK scheme with the guided equilibrium from Ref. [22]:

$$\partial_t(\rho u_\alpha) + \partial_\beta \Pi_{\alpha\beta}^{\text{MB}} + \partial_\beta \left[-\tau \rho \theta \left(1 - \frac{\Delta t}{2\tau} \right) (\partial_\alpha u_\beta + \partial_\beta u_\alpha - \partial_\chi u_\chi \delta_{\alpha\beta}) \right] = -\partial_\gamma \left[\left(1 - \frac{\Delta t}{2\tau} \right) (\Pi_{\alpha\gamma}^{(neq)})' \right], \quad (14a)$$

$$\text{where, } \partial_\gamma (\Pi_{\alpha\gamma}^{(neq)})' = \mp \frac{\tau}{2} \partial_\alpha \{ \rho u_x (1 - 3\theta) - \rho^2 u_x^3 \} - \partial_\gamma [\rho u_y (1 - 3\theta) - \rho^2 u_y^3] \sim \begin{cases} \mathcal{O}(u^4) & \text{if } \theta = 1/3 \\ \mathcal{O}(u^2) & \text{otherwise} \end{cases}, \quad (14b)$$

where Eq. (14b) takes the negative value if $\alpha = x$ and vice versa if $\alpha = y$, respectively. It can be seen that, with the $1/2\tau$ factor from Eq. (14a), Eq. (14b) culminates into an $\mathcal{O}(u^3)$ and $\mathcal{O}(u)$ representation of the momentum equation when $\theta = 1/3$ and $\theta \neq 1/3$, respectively, for the Lattice-BGK scheme used with the guided equilibrium. However, we highlight that, since Eq. (14a) is derived under the assumption that Eq. (3a) holds, there may be additional unaccounted errors that remain. In contrast, under the same assumptions, the OReg scheme with the guided equilibrium yields a negligible error irrespective of the lattice temperature with $(\Pi_{\alpha\beta}^{(neq)|G})' \sim \mathcal{O}(u^6)$. Thus, if the compatibility conditions are assumed to hold, the OReg scheme used with the guided equilibrium exactly models the NSF momentum equations with $\mu_{\alpha\beta}^{\text{OReg|G}}$ compensating for the lattice anisotropy. We highlight that it

is *only* due to the explicit evaluation of the compatibility condition $\langle f_i^{\text{OReg|G}}, c_{i_\alpha} \rangle$ that the OReg scheme yields $\mathcal{O}(u^4)$ and $\mathcal{O}(u^2)$ accurate momentum representations when $\theta = 1/3$ and $\theta \neq 1/3$, respectively. Note that this is still an order of magnitude better than the BGK/guided equilibrium formulation.

D. Onsager-regularized macrodynamics using the second order polynomial equilibrium

As a further illustration, we consider the OReg scheme when used with the popular $\mathcal{O}(u^2)$ polynomial form of the equilibrium distribution commonly used at the lattice reference temperature $\theta_0 = 1/3$:

$$f_i^{(eq)|\mathcal{O}(u^2)} = \rho W_i \left[1 + \frac{u_\alpha c_\alpha}{\theta_0} + \frac{(u_\alpha c_\alpha)^2}{2\theta_0^2} \right], \quad (15)$$

where the weights W_i for the D2Q9 lattice are obtained as tensor products of $W_{\pm 1} = \theta_0/2$ and $W_0 = (1 - \theta_0)$. Evaluating Eqs. (9) and (10) with $f_i^{\text{OReg}|\mathcal{O}(u^2)}$ yields

$$\varphi_i^{(1)|\text{OReg}|\mathcal{O}(u^2)} = \langle f_i^{\text{OReg}|\mathcal{O}(u^2)}, 1 \rangle = 0, \quad (16a)$$

$$\varphi_{i_\alpha}^{(1)|\text{OReg}|\mathcal{O}(u^2)} = \langle f_i^{\text{OReg}|\mathcal{O}(u^2)}, c_{i_\alpha} \rangle = \frac{\tau \rho}{2\theta_0} u_\alpha [(u_x^2 - u_y^2)(\partial_x u_x - \partial_y u_y) + 2u_x u_y (\partial_y u_x - \partial_x u_y)], \quad (16b)$$

$$\text{and, } (\Pi_{\alpha\beta}^{(neq)|\mathcal{O}(u^2)})' = -\underbrace{u_\beta \varphi_{i_\alpha}^{(1)|\text{OReg}|\mathcal{O}(u^2)}}_{\mathcal{O}(u^6)} - \underbrace{\frac{\tau \rho}{2\theta_0} u_\alpha u_\beta (\partial_x u_x - \partial_y u_y)}_{\mathcal{O}(u^4)} \times \begin{cases} \pm 1 & \text{if } \alpha = \beta = x/y \\ 0 & \text{if } \alpha \neq \beta \end{cases}. \quad (17)$$

Equation (16b) shows that the error in the first order compatibility condition obtained using $f_i^{\text{OReg}|\mathcal{O}(u^2)}$ has a magnitude of

$\mathcal{O}(u^5)$ and can be safely ignored, while from Eq. (17) the error $(\Pi_{\alpha\beta}^{(neq)|\mathcal{O}(u^2)})' \sim \mathcal{O}(u^4)$. Correspondingly, the momentum

equations from the OReg scheme using $f_i^{\text{OReg}|\mathcal{O}(u^2)}$ are $\mathcal{O}(u^3)$ accurate. Again, the OReg scheme yields an improvement in accuracy of an order of magnitude as compared to the bare BGK scheme.

IV. NUMERICAL BENCHMARKS

We now proceed to numerically benchmark the OReg scheme used with the guided equilibrium for two canonical quasi-one-dimensional problems. First, the classical linear benchmark case of a decaying shear wave [21,24,26] is considered. In the absence of any spurious numerical errors, observed statistics for waves described by a wave vector $\mathbf{k} = m\hat{e}_\parallel + n\hat{e}_\perp$, where $\hat{e}_\parallel$ and $\hat{e}_\perp$ are unit vectors parallel and perpendicular to the wave, theoretically display an exponential time decay. Here we take the amplitude of the x -velocity component, $u_x^{\text{max}}(t)$, as the statistic of interest and compute the numerical kinematic viscosity, $\tilde{\nu}$, through the following curve fitting expression: $u_x^{\text{max}}(t) \propto \exp(-|\mathbf{k}|^2 \tilde{\nu} t)$. We consider two situations, namely an axis-aligned and a $\pi/4$ -rotated wave, respectively. Both cases are initialized with a unit density. The initial velocity field for the axis-aligned case is given as

$$u_x = A_0 \sin\left(\frac{2\pi y}{L_y}\right), \quad u_y = \text{Ma}\sqrt{\theta}, \quad (18a)$$

and that for the rotated wave case is given as

$$u_x = A_0 \sin\left(\frac{2\pi}{L_y\sqrt{2}}(-x + y)\right),$$

$$u_y = \text{Ma}\sqrt{\theta} + A_0 \sin\left(\frac{2\pi}{L_y\sqrt{2}}(-x + y)\right). \quad (18b)$$

The wave vectors for the two cases are $\frac{2\pi}{L_y}\hat{j}$ and $\frac{\pi}{L_y}(-\hat{i} + \hat{j})$, respectively. The values of the wave amplitude (A_0) and spatial discretization ($L_x \times L_y$) are taken to be 0.001 and 1×200 , respectively. Simulations are conducted using the lattice-BGK, OReg, and projected regularized (PR) schemes at the reference temperature $\theta = 1/3$ with an imposed kinematic viscosity $\nu = 0.01$ for different Mach numbers.

In the axis-aligned case, the spurious errors due to lattice anisotropy are dormant [24], and consequently the lattice-BGK and PR schemes recover the correct dissipation rate as shown in Fig. 2(a); it can be seen that the OReg scheme also recovers the correct dissipation rate. For the rotated wave case, the spurious contributions are activated and, as shown in Fig. 2(b), the uncorrected lattice-BGK and PR models fail to recover the dissipation accurately; the PR scheme yields significantly larger deviations from the expected value as shown on the right vertical axis of Fig. 2(b). In contrast, the OReg scheme yields the accurate dissipation rate without having to incorporate any correction terms.

The second benchmark we consider is that of a shocktube operating at appreciably small viscosities and lattice temperatures of $\theta \neq 1/3$. It has been previously shown that the OReg scheme, used with an $\mathcal{O}(u^4)$ polynomial equilibrium representation, exactly recovers the analytical solution in an athermal setting where $\theta = 1/3$ for a lattice viscosity $\nu = 10^{-7}$ [28]. Here, we examine the behavior of the OReg scheme with the guided equilibrium when employed at elevated operating tem-

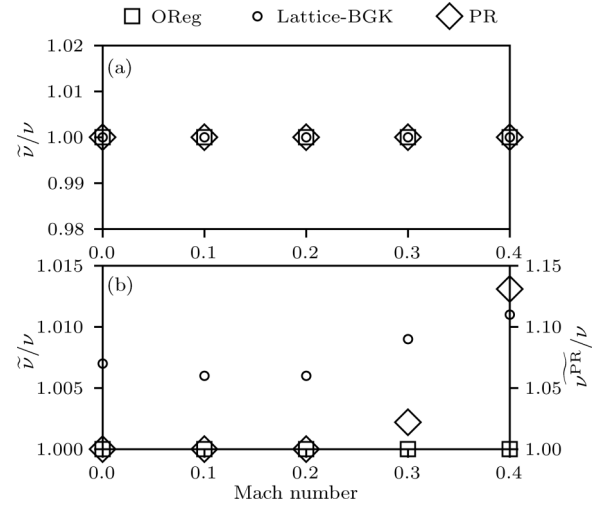


FIG. 2. Comparison of the numerically computed and physically imposed fluid viscosities, $\tilde{\nu}$ and ν , for a decaying shear wave at different Mach numbers obtained with the OReg, Lattice-BGK, and projected regularized (PR) LB schemes using the guided equilibrium on the D2Q9 lattice. For the axis-aligned shear wave [panel (a)], all schemes correctly model the viscous dissipation as demonstrated by $\tilde{\nu}/\nu = 1$ while for the $\pi/4$ rotated wave [panel (b)] only the OReg scheme recovers the imposed viscous dissipation rate.

peratures and lattice viscosities of $\theta = 0.35$, $\nu = 10^{-5}$ and $\theta = 0.4$, $\nu = 10^{-9}$, respectively.

In Figs. 3 and 4, we present the numerical results obtained from the lattice-BGK, the state-of-the-art first-order essentially entropic (EE) [38], the projected regularized (PR) and the OReg LB schemes, along with comparisons against analytical solutions. The simulation is run on a 800×1 grid for 500 time steps and employs the fullway bounce-back treatment for the walls. It can be seen that while the lattice-BGK yields the largest oscillations and the EE and PR schemes significantly reduces those oscillations, the OReg scheme completely eliminates them. The results for the EE and PR schemes display an interesting trend, namely, for smaller values of θ and Re (larger ν), the EE scheme performs relatively better, while at higher values of θ and Re (smaller ν), the PR scheme performs relatively better. Note that the OReg scheme yields a slightly incorrect slope in the high-density region due to the first-order nature of the resulting hydrodynamics at temperatures of $\theta \neq 1/3$. However, a computation of the L_2 errors reveals that the OReg scheme captures the density with an accuracy of approximately 98.88% and 98.20%, respectively, for the two cases investigated herein. The simulations conducted on halved and doubled grids also yield similar accuracy hinting at a reasonable level of grid independence of the solution. Lastly, it is noteworthy that while the accuracy of the EE and PR schemes improves with increasing grid size, it still retains spurious oscillations; in contrast even on halved grids, the OReg scheme demonstrates no spurious oscillations.

V. CONCLUSION

In conclusion, we have shown that the OReg scheme yields stable and accurate results on computationally efficient first-neighbor lattices, coping with the long-standing limitations

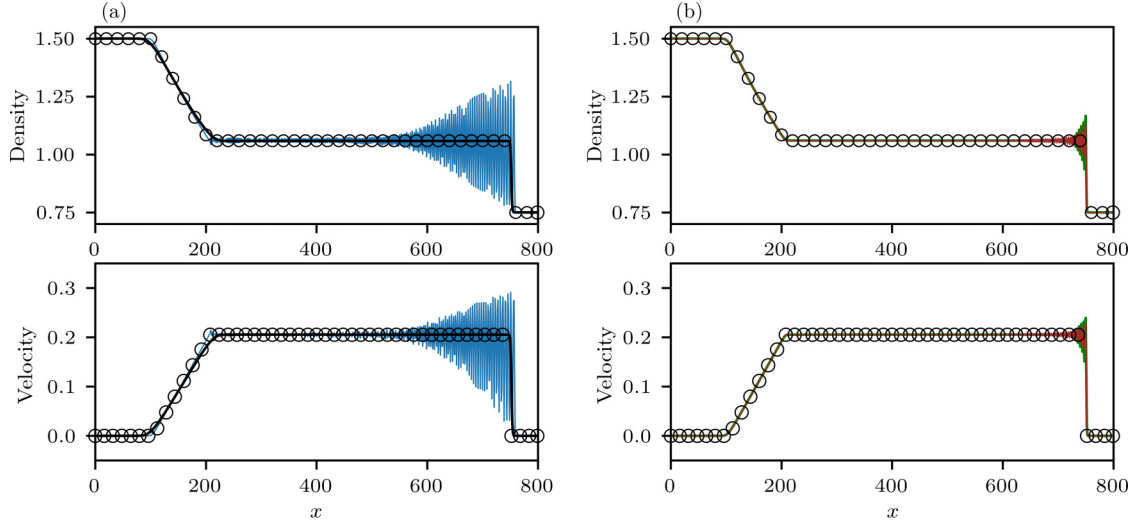


FIG. 3. Isothermal shocktube results obtained using the guided equilibrium on the D2Q9 lattice using different LB schemes at $\theta = 0.35$ and $\nu = 10^{-5}$. Panel (a) shows the OReg (black) and the Lattice-BGK (blue) schemes, while panel (b) shows the first order essentially entropic LB (brown) and the projected regularized (green) schemes. The round black symbols correspond to the analytical solution.

induced by the anisotropy error, which have plagued LB simulations so far. Specifically, with the guided equilibrium defined on the D2Q9 lattice, the OReg scheme is shown to recover isothermal hydrodynamics with third-order accuracy for simulations conducted at the lattice reference temperature and with first-order accuracy at arbitrary lattice temperatures. Recall that the guided equilibrium is not fully constrained as Eq. (11) does not recover the equilibrium heat flux vector Eq. (2c); indeed, the deviations in $Q'_{\alpha\beta\gamma}$ and $R'_{\alpha\beta\gamma\mu}$ for a fully constrained equilibrium representation, may yield a more accurate model for isothermal temperatures of $\theta \neq 1/3$. Nevertheless, even in the current form, the OReg scheme can be coupled to a second population to conduct fully local thermal and compressible flow simulations on standard lattices. Additionally, in comparison to the bare BGK collision

model, the OReg scheme is shown to recover macroscopic dynamics with an accuracy improved by a factor of $\mathcal{O}(u)$ for two equilibrium formulations, further demonstrating the practical usability of the scheme. Indeed, it can be appreciated that the OReg scheme shifts the focus from modeling accuracy to numerical stability obtained from using different equilibrium formulations. We also highlight that the OReg scheme presented in Eq. (6) is generic and can be seamlessly generalized to any lattice stencil. Indeed, the OReg scheme can be directly integrated into high-performance codes such as, e.g., waLBerla [39] and highly optimized GPU implementations [40,41]. Further, the OReg scheme also offers a promising alternative to locally defining the so-called Grad boundary conditions [42,43] and coupling to thermal boundary conditions such as those presented in [44]. Thus, the

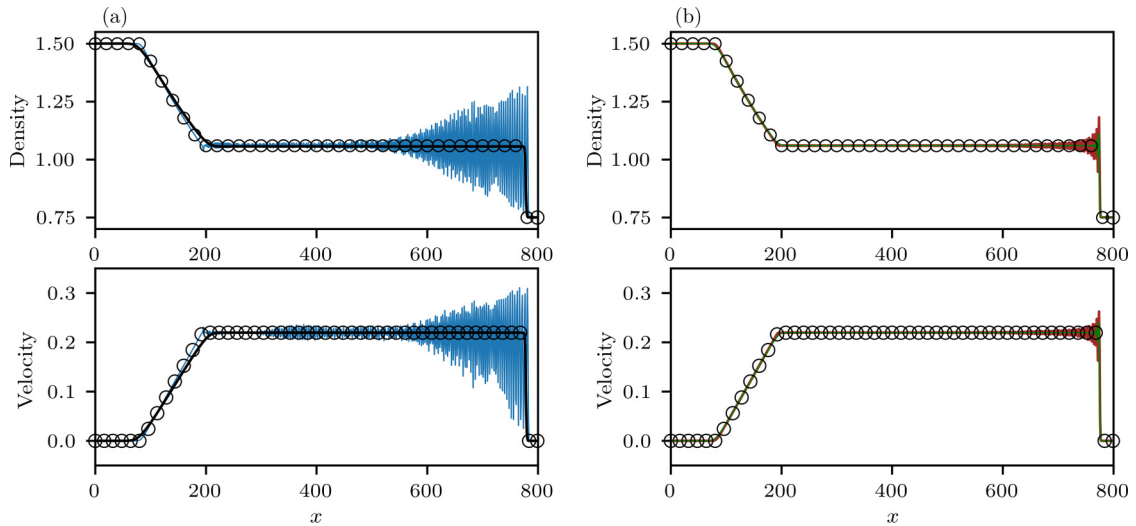


FIG. 4. Isothermal shocktube results obtained using the guided equilibrium on the D2Q9 lattice using different LB schemes at $\theta = 2/5$ and $\nu = 10^{-9}$. The curves have the same meaning as in Fig. 3.

OReg scheme presents a significant advance for conducting scalable simulations of physically relevant nonlinear dissipative transport problems (see, e.g., [45]) characterized by multi-scale phenomena, in complex geometries. Explorations into these avenues will be the subject of future work.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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