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One-stage simplified lattice Boltzmann method for two- and three-dimensional magnetohydrodynamic flows

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In this paper, we propose a new simplified lattice Boltzmann method (SLBM) for magnetohydrodynamic flows that outperforms the classical one in terms of accuracy, while preserving its advantages. A very recent paper [A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021)] demonstrated that the SLBM enforces the divergence-free condition of the magnetic field in an excellent manner and involves the lowest amount of virtual memory. However, the SLBM is characterised by the poorest accuracy. Here, the two-stages algorithm that is typical of the SLBM is replaced by a one-stage procedure following the approach devised for non-conductive fluids in a very recent effort [A. Delgado-Gutierrez, P. Marzocca, D. Cardenas, and O. Probst, “A single-step and simplified graphics processing unit lattice Boltzmann method for high turbulent flows”, International Journal for Numerical Methods in Fluids (2021)]. The Chapman-Enskog expansion formally demonstrates the consistency of the present scheme. The resultant algorithm is very compact and easy to be implemented. Given all these features, we believe that the proposed approach is an excellent candidate to perform numerical simulations of two- and three-dimensional magnetohydrodynamic flows.

Keywords: Lattice Boltzmann method, Magnetohydrodynamics

NOMENCLATURE

Abbreviations
BGK Bhatnagar-Gross-Krook
LBE lattice Boltzmann equation
LBM lattice Boltzmann method
MRT multiple-relaxation time
SLBM two-stages simplified lattice Boltzmann method
SSLBM one-stage simplified lattice Boltzmann method

Dimensionless numbers
Ma Mach number
Prm Magnetic Prandtl number
Re Reynolds number

Superscripts
† Quantity computed at the predictor stage

Subscripts
i index spanning the lattice directions

Symbols
ζ vorticity vector
B magnetic field vector
\( g_i^{eq} \) equilibrium distributions for the magnetic field
\( j \) density of the electric current vector
\( m \) fluid momentum vector
\( u \) velocity vector
\( \nabla \) spatial derivative operator
\( \Delta \) Laplacian operator
\( \epsilon \) dissipation rate
\( c_i \) lattice directions
\( \nu \) kinematic viscosity
\( \rho \) density
\( \tau_{\nu}, \tau_{\eta} \) relaxation times
\( c_s \) lattice sound speed
\( E \) total energy
\( E_k \) kinetic energy
\( E_m \) magnetic energy
\( f_i^{eq} \) equilibrium distributions for the velocity field
\( t \) time
\( w_i \) weighting factors

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I. INTRODUCTION

The investigation of the behaviour of electrically conducting fluids, also known as magnetohydrodynamics (MHD), is nowadays an important topic in contemporary computational fluid dynamics. Indeed, its area of employment is impressively wide. The design of electromagnetic pumps and cooling systems for nuclear reactors, the predictions of solar flares, the measurement of flow velocities in hot and aggressive liquids, and drop-on-demand printability are just few compelling examples of the most challenging applications of MHD.

From a mathematical viewpoint, the flow of an electrically conductive fluid is governed by the magnetic induction equation:

\[ \partial_t B = \nabla \times (u \times B) + \eta \Delta B, \]

where \( t \) is the time, \( \eta \) is the magnetic diffusivity, \( u \) and \( B \) are the velocity and magnetic field vectors, respectively, accompanied by the divergence-free condition

\[ \nabla \cdot B = 0, \]

together with the incompressible Navier-Stokes equations for MHD, i.e.

\[ \partial_t u + (u \cdot \nabla) u = -\frac{\nabla \rho}{\rho} + \nu \Delta u + \frac{j \times B}{\rho}, \]

\[ \nabla \cdot u = 0, \]

where \( \rho \) is the mass density, \( p \) is the pressure, \( \nu \) is the fluid kinematic viscosity, \( j = \nabla \times B \) is the density of electric current vector.

A closed-form solution of this set of equations is available only in few cases, where the flow and the geometry undergo significant simplifications. The most popular example is the simple (laminar) Hartmann flow, where an electrically conductive fluid flows between two parallel plates with an external magnetic field being perpendicular to the channel walls. Unfortunately, the aforementioned practical applications involve complex (turbulent) flows and geometries. Therefore, the usage of numerical methods is essential. Spectral and pseudo-spectral methods represent a very well-consolidated approach to MHD problems. However, the capability to accurately simulate flows in complex geometries with possibly moving parts is one of the key current issues in computational MHD.

An alternative to classical macroscopic-based approaches can be found in the mesoscopic-based lattice Boltzmann method (LBM). In the LBM, the flow is idealised by collections (also known as populations or distributions) of fictitious particles, colliding and streaming along the links of a Cartesian lattice that is kept fixed through the whole analysis. Before going any further, let us highlight that fluid dynamics stems from the computation of the evolution of populations. Despite the algorithmic simplicity of the resultant algorithm, it should be noted that it might lead to a very large memory usage, especially when running three-dimensional simulations, due to the storage of the particle distribution functions at each lattice node. Interestingly, the simplified lattice Boltzmann method (SLBM) avoids the computation of the space-time evolution of the particle distribution functions, as it involves only macroscopic variables. Hence, the SLBM demands to compute and store only these quantities at each lattice site, while the computation and storage of populations are completely neglected. As a consequence, the amount of involved virtual memory is drastically reduced.

The earliest attempts to demonstrate the suitability of the LBM to simulate MHD flows were carried out by Succi et al., Chen et al. and Martínez et al. Later, Dellar proposed a seminal contribution, where the physics of an electrically conductive fluid is governed by two sets of populations: a scalar one retaining the fluid flow, and a vector-valued one recovering the solution of the magnetic induction equation. Despite the very accurate predictions performed by this approach, De Rosis et al. demonstrated that it is unsuitable when the magnetohydrodynamic flows are turbulent. This behaviour must be addressed to the disadvantages of the Bhatnagar-Gross-Krook (BGK) collision operator, that is the one adopted by Dellar. Indeed the intrinsic unavoidable presence of non-hydrodynamic ghost modes, which undermine the stability of the algorithm through spurious couplings with hydrodynamic ones, accompanies the common practice to relax populations to an incomplete local equilibrium, promotes a sudden blow-up of the BGK-based simulations when the fluid kinematic viscosity reduces.

In a very recent paper, De Rosis et al. have performed a comprehensive comparison of four different LBMs for MHD: (i) the BGK LBM, the multiple-relaxation-time (MRT) LBMs based on (ii) raw and (iii) central moments, and (iv) the simplified lattice Boltzmann method. From the reported extensive analysis, two main results have been found. First, the adoption of the D2Q9 discretization for the populations addressing the evolution of \( B \) instead of the D2Q5 one (as suggested by Dellar) is instrumental to achieve more accurate computations. Secondly, the divergence-free condition of the magnetic field (which should be ensured by any scheme for MHD flows) is enforced in an excellent manner only by the SLBM, which shows results very close to the round-off error. However, the SLBM shows the lowest accuracy, and this is particularly emphasised when coarse grid resolutions are adopted. This should be addressed to its level of numerical dissipation that is generally higher than the one obtained by the BGK or MRT LBMs.

In this work, we present a new simplified scheme for magnetohydrodynamic flows. Instead of using the classical two-stages predictor-corrector technique, we develop a one-stage lattice Boltzmann method (SSLBM). While keeping the same excellent properties on the satisfaction of the divergence-free condition, our proposed strategy
exhibits a superior accuracy, that is particularly evident in three-dimensional scenarios. The resultant procedure is very compact and easy to be implemented.

The rest of the paper is organized as follows. In Sec. II, the numerical methodology is devised. Results from two- and three-dimensional analyses are discussed in Sec. III. Eventually, some conclusions are drawn in Sec. IV.

II. LATTICE BOLTZMANN METHOD

In this section, first the simplified LBM by De Rosis et al. is recalled. Secondly, our one-stage simplified LBM for two-dimensional magnetohydrodynamic flows is devised. Eventually, we demonstrate that its extension to three dimensions is straightforward and its algorithm is outlined.

A. Two-dimensional two-stages simplified LBM by De Rosis et al.

Let us consider a two-dimensional Cartesian space \( x = [x,y] \) and the D2Q9 velocity discretization, where lattice directions are \( c_i = [c_{ix}, c_{iy}] \) with
\[
c_{ix} = [0, 1, 0, -1, 0, 1, -1, 1],
\]
\[
c_{iy} = [0, 0, 1, 0, -1, 1, 1, -1].
\]

In two dimensions, the velocity and magnetic field vectors have two components, i.e. \( \mathbf{u} = [u_x, u_y], \mathbf{B} = [B_x, B_y] \). Conversely, the density of electric current and the vorticity possess only one component, i.e. \( j = [j] \) and \( \zeta = [\zeta] \). Let us also introduce the vector of the fluid momentum \( \mathbf{m} = \rho \mathbf{u} = [m_x, m_y] \).

Given the solution at the time \( t \), the classical simplified LBM involves a two-stages fractional step technique, i.e.

**Predictor step:**
\[
\rho^\dagger (x, t + \Delta t) = \sum_i f_i^eq (x - c_i \Delta t, t),
\]
\[
m^\dagger (x, t + \Delta t) = \sum_i c_i f_i^eq (x - c_i \Delta t, t),
\]
\[
B^\dagger (x, t + \Delta t) = \sum_i g_i^eq (x - c_i \Delta t, t),
\]

where the superscript \( \dagger \) denotes predicted (intermediate) quantities, and

**Corrector step:**
\[
\rho (x, t + \Delta t) = \rho^\dagger (x, t + \Delta t),
\]
\[
m (x, t + \Delta t) = m^\dagger (x, t + \Delta t) + (\tau_v - 1) \sum_i c_i f_i^{eq,\dagger} (x + c_i \Delta t, t + \Delta t) -
\]
\[
(\tau_v - 1) m (x, t),
\]
\[
B (x, t + \Delta t) = B^\dagger (x, t + \Delta t) + (\tau_\eta - 1) \sum_i g_i^{eq,\dagger} (x + c_i \Delta t, t + \Delta t) -
\]
\[
(\tau_\eta - 1) B (x, t).
\]

The two relaxation times, \( \tau_v \) and \( \tau_\eta \), are linked to the fluid kinematic viscosity and magnetic diffusivity as
\[
\nu = \left( \tau_v - \frac{1}{2} \right) c_s^2,
\]
\[
\eta = \left( \tau_\eta - \frac{1}{2} \right) c_s^2,
\]

respectively. Within the framework of the one-stage and two-stages simplified LBM, equilibrium populations are usually written by a second-order truncated expression. Here, \( f_i^{eq} \) is computed by expanding onto the full basis of Hermite polynomials (up to the fourth order) according to De Rosis et al., that is
\[
f_i^{eq} = w_i \rho \left[ 1 + \frac{\mathcal{H}_i^{(1)} \cdot \mathbf{u}}{2 c_s^2} + \frac{1}{2 c_s^4} \mathcal{H}_i^{(2)} : \mathbf{uu} + \frac{1}{2 c_s^6} \mathcal{H}_i^{(3)} \cdot \mathbf{uu} \cdot \mathbf{uu} + \frac{1}{4 c_s^8} \mathcal{H}_i^{(4)} \cdot \mathbf{uu} \cdot \mathbf{uu} \cdot \mathbf{uu} + \frac{1}{2 c_s^{10}} \left| \mathbf{B} \right|^2 \right],
\]

\[
g_i^{eq} = w_i \left[ B_z + \frac{c_m}{c_s} (u_y B_x - u_x B_y) \right],
\]

\[
g_i^{eq} = w_i \left[ B_y + \frac{c_m}{c_s} (u_x B_y - u_y B_x) \right],
\]

where \( g_i^{eq} = [g_i^{eq, x}, g_i^{eq, y}] \), the weights are \( w_0 = 4/9, w_1, ..., w_5 = 1/9, w_6, ..., w_8 = 1/36 \), the lattice sound speed is \( c_s = 1/\sqrt{3} \) and Hermite polynomials are
\[
\mathcal{H}^{(1)}_{ix} = c_{ix},
\]
\[
\mathcal{H}^{(1)}_{iy} = c_{iy},
\]
\[
\mathcal{H}^{(2)}_{ixx} = c_{ix}^2 - c_s^2,
\]
\[
\mathcal{H}^{(2)}_{ixy} = c_{iy}^2 - c_s^2,
\]
\[
\mathcal{H}^{(2)}_{iyy} = c_{iy}^2 c_{ix},
\]
\[
\mathcal{H}^{(3)}_{ixxx} = (c_{ix}^2 - c_s^2)^2 c_{iy},
\]
\[
\mathcal{H}^{(3)}_{ixxy} = (c_{ix}^2 - c_s^2) (c_{iy}^2 - c_s^2) c_{ix},
\]
\[
\mathcal{H}^{(4)}_{ixxxy} = (c_{ix}^2 - c_s^2)^2 (c_{iy}^2 - c_s^2).
\]

Notice that the equilibrium states \( f_i^{eq,\dagger} \) and \( g_i^{eq,\dagger} \) are computed by adopting the predicted values, i.e. \( f_i^{eq,\dagger} = f_i^{eq} (\rho^\dagger, \mathbf{u}^\dagger, \mathbf{B}^\dagger) \) and \( g_i^{eq,\dagger} = g_i^{eq} (\mathbf{u}^\dagger, \mathbf{B}^\dagger) \).

B. Two-dimensional one-stage simplified LBM

More recently, Delgado-Gutierrez et al. proposed a one-stage simplified lattice Boltzmann method, where
the two-stages predictor-corrector strategy is replaced by an algorithm spanning the lattice point just once per time step. We now derive an SSLBM for MHD flows.

For simplicity, let us just consider one of the particle distribution functions, $g_{ix}$. The lattice Boltzmann equation (LBE) can be written as

$$ g_{ix}(x + c_i \Delta t, t + \Delta t) - g_{ix}(x, t) = \frac{g_{eq}(x, t) - g_{ix}(x, t)}{\tau_\eta}. $$

(15)

By applying a Taylor series expansion at the left-hand side of Eq. (15) followed by a Chapman-Enskog analysis, it is possible to write the following equations:

$$ \frac{g_{ix}^{(0)} - g_{eq}}{\tau_\eta \Delta t} = 0, $$

(16)

$$ \Delta g_{ix}^{(0)} + \frac{g_{ix}^{(1)}}{\tau_\eta \Delta t} = 0, $$

(17)

$$ \frac{\partial g_{ix}^{(0)}}{\partial t_1} + \left(1 - \frac{1}{2\tau_\eta}\right) \Delta g_{ix}^{(1)} = 0. $$

(18)

From Eqs. (16,17), we obtain

$$ g_{ix}^{(0)} = g_{eq}, $$

(19)

$$ g_{ix}^{(1)} = g_{eq} - \tau_\eta \Delta t g_{eq}. $$

(20)

Following the SLBM, it is possible to get

$$ g_{eq}^{(0)}(x, t) = -\tau_\eta [g_{eq}^{eq}(x, t) - g_{eq}^{eq}(x - c_i \Delta t, t - \Delta t)]. $$

(21)

We can further write

$$ \frac{\partial g_{ix}^{(0)}}{\partial t_0} = -c_i \cdot \nabla g_{ix}^{(0)}, $$

(22)

$$ \frac{\partial g_{ix}^{(1)}}{\partial t_0} = - \left(1 - \frac{1}{2\tau_\eta}\right) \Delta g_{ix}^{(1)}. $$

(23)

By combining these two equations, we have

$$ \frac{\partial g_{ix}^{(0)}}{\partial t} = -c_i \cdot \nabla g_{ix}^{(0)} - \left(1 - \frac{1}{2\tau_\eta}\right) \Delta g_{ix}^{(1)}. $$

(24)

Let us sum the above equation over the lattice directions, i.e.

$$ \sum_i \left[ \frac{\partial g_{ix}^{(0)}}{\partial t} + c_i \cdot \nabla g_{ix}^{(0)} + \left(1 - \frac{1}{2\tau_\eta}\right) \Delta g_{ix}^{(1)} \right] = 0. $$

(25)

Interestingly, it is possible to write

$$ \frac{\partial g_{ix}^{(0)}}{\partial t} = g_{ix}^{(0)}(x, t + \Delta t) - g_{ix}^{(0)}(x, t), $$

(26)

$$ c_i \cdot \nabla g_{ix}^{(0)} = \frac{g_{ix}^{(0)}(x + c_i \Delta t, t) - g_{ix}^{(0)}(x - c_i \Delta t, t)}{2}, $$

(27)

$$ \Delta g_{ix}^{(1)} = \frac{\partial}{\partial t_0} g_{ix}^{(1)} + c_i \cdot \nabla g_{ix}^{(1)} = \frac{\partial g_{ix}^{(1)}}{\partial c_i} = g_{ix}^{(1)}(x + c_i \Delta t, t) - g_{ix}^{(1)}(x, t) $$

$$ -\tau_\eta \left[ g_{ix}^{(0)}(x + c_i \Delta t, t) - 2g_{ix}^{(0)}(x, t) + g_{ix}^{(0)}(x - c_i \Delta t, t) \right]. $$

(28)

Then, we get

$$ \sum_i \left[ g_{ix}^{(0)}(x, t + \Delta t) + 2 (\tau_\eta - 1) g_{ix}^{(0)}(x, t) - \tau_\eta g_{ix}^{(0)}(x + c_i \Delta t, t) - \tau_\eta g_{ix}^{(0)}(x - c_i \Delta t, t) \right] = 0. $$

(29)

By noticing that

$$ \sum_i g_{ix}^{(0)}(x, t + \Delta t) = B_x(x, t + \Delta t), $$

(30)

we end up with

$$ B_x(x, t + \Delta t) = B_x(x, t) + (\tau_\eta - 1) (B_{xf} - 2B_{xc} + B_{xb}). $$

(32)

Having achieved this result, we are now in the position to deploy the one-stage simplified lattice Boltzmann method as follows:

$$ \rho(x, t + \Delta t) = \frac{1}{2} \rho_f - \rho_c + \frac{3}{2} \rho_b, $$

$$ m(x, t + \Delta t) = m_b + (\tau_\eta - 1) (m_f - 2m_c + m_b), $$

$$ B(x, t + \Delta t) = B_b + (\tau_\eta - 1) (B_{f} - 2B_{c} + B_{b}). $$

(33)

where

$$ \rho_f = \sum_i f_i^{eq}(x + c_i \Delta t, t), $$

$$ \rho_b = \sum_i f_i^{eq}(x - c_i \Delta t, t), $$

$$ \rho_c = \rho(x, t), $$

$$ m_f = \sum_i f_i^{eq}(x + c_i \Delta t, t) c_i, $$

$$ m_b = \sum_i f_i^{eq}(x - c_i \Delta t, t) c_i, $$

$$ m_c = \rho(x, t) u(x, t). $$
\[ B_f = \sum_i g^q_i(x + c_i \Delta t, t), \]
\[ B_b = \sum_i g^q_i(x - c_i \Delta t, t), \]
\[ B_c = B(x, t). \]  
(34)

Eventually, the fluid velocity can then be simply computed as
\[ u(x, t + \Delta t) = \frac{m(x, t + \Delta t)}{\rho(x, t + \Delta t)}. \]  
(35)

Eqs. (33, 34, 35), accompanied by the expressions of the equilibrium populations in Eqs. (11, 12, 13), represent the core of the algorithm of the proposed SSLBM.

Let us underline that the present (one-stage) SSLBM retains the salient advantages of the (two-stages) SLBM. First, the computation of the evolution of the particle distribution functions is completely avoided. Overall, it demands to store an amount of information that is 5.4 times lower than the virtual memory requested by the LBMs with evolution of populations (BGK and MRT). This is even more emphasised in three dimensions, where the D3Q19 and D3Q27 discretizations could be used. In these cases, the amounts of information to be saved are 9.8 and 15.6 times lower, respectively. Secondly, boundary conditions just consist of assigning the desired values of the macroscopic variables, without involving any particular (populations-based) treatment and additional implementation.

C. Extension to three dimensions of the one-stage simplified LB

In three dimensions, let us consider a two-dimensional Cartesian space \( x = [x, y, z] \) and the D3Q19 velocity discretization, where lattice directions are \( c_i = [c_{ix}, c_{iy}, c_{iz}] \) with
\[
\begin{align*}
 c_{ix} &= [0, 1, -1, 0, 0, 0, 1, -1, 1, \\
          & -1, 1, -1, 1, -1, 0, 0, 0, 0], \\
 c_{iy} &= [0, 0, 0, 0, 0, -1, 0, 0, -1, 1], \\
 c_{iz} &= [0, 0, 0, 0, 0, 1, -1, 0, 0, 0, 1, -1, 1, -1, 1, -1, 1].
\end{align*}
\]  
(36)

In this case, the velocity, magnetic field and density of electric current and vorticity vectors have three components, i.e. \( u = [u_x, u_y, u_z], B = [B_x, B_y, B_z], J = [J_x, J_y, J_z] \) and \( \zeta = [\zeta_x, \zeta_y, \zeta_z] \). The fluid momentum is \( m = [m_x, m_y, m_z] \).

Coreixas et al.\(^{37}\) proposed a derivation of the equilibrium that is compliant with all collision models, and the corresponding expressions are
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{18}[1 - (u_x^2 + u_y^2 + u_z^2) + 3(u_x^2u_y^2 + u_x^2u_z^2 + u_y^2u_z^2)],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{18}[1 + 3\sigma u_x + 3(u_x^2 - u_y^2 - u_z^2) - 9\sigma(u_x^2u_y^2 + u_x^2u_z^2) - 9(u_x^2u_y^2 + u_x^2u_z^2)],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{18}[1 + 3\lambda u_y + 3(-u_x^2 + u_y^2 - u_z^2) - 9\lambda(u_x^2u_y^2 + u_y^2u_z^2) - 9(u_x^2u_y^2 + u_y^2u_z^2)],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{18}[1 + 3\chi u_z + 3(-u_x^2 - u_y^2 + u_z^2) - 9\chi(u_x^2u_y^2 + u_y^2u_z^2) - 9(u_x^2u_y^2 + u_y^2u_z^2)],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{36}[1 + 3(\sigma u_x + \lambda u_y) + 3(u_x^2 + u_y^2) + 9\sigma\lambda u_xu_y + 9(\lambda u_x^2u_y + \sigma u_xu_y^2) + 9u_x^2u_y^2],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{36}[1 + 3(\sigma u_x + \chi u_z) + 3(u_x^2 + u_z^2) + 9\sigma\chi u_xu_z + 9(\chi u_x^2u_z + \sigma u_xu_z^2) + 9u_x^2u_z^2],
\]
\[
f_{(0,0,0)}^{eq} = \frac{\rho}{36}[1 + 3(\lambda u_y + \chi u_z) + 3(u_y^2 + u_z^2) + 9\lambda\chi u_yu_z + 9(\chi u_y^2u_z + \lambda u_yu_z^2) + 9u_y^2u_z^2],
\]  
(37)

where, for the sake of compactness, the tensor product notation has been adopted\(^{38}\) with \((\sigma, \gamma, \chi) \in \{-1\}^3\) are three indices assuming the same value of the components of the lattice directions vectors. These expressions are then corrected by adding the term
\[
\frac{u_l}{2c_s^3} \left[ \frac{1}{3} |c_l|^2 |\mathbf{B}|^2 - (c_l \cdot \mathbf{B})^2 \right],
\]  
(38)

where the weights are \(w_0 = 1/3, w_{1,...,6} = 1/18\) and \(w_{7,...,18} = 1/36\). The equilibrium populations of the magnetic field are \(g_i^{eq} = [g_{ix}^{eq}, g_{iy}^{eq}, g_{iz}^{eq}],\) which assume the following form:
\[
g_{ix}^{eq} = w_i \left[ B_x + \frac{c_{ix}}{c_s} (u_yB_x - u_xB_y) + \frac{c_{iz}}{c_s} (u_zB_x - u_xB_z) \right],
\]  
(39)
\[
g_{iy}^{eq} = w_i \left[ B_y + \frac{c_{iy}}{c_s} (u_xB_y - u_yB_x) + \frac{c_{iz}}{c_s} (u_zB_y - u_yB_z) \right],
\]  
(40)
\[
g_{iz}^{eq} = w_i \left[ B_z + \frac{c_{iz}}{c_s} (u_xB_z - u_zB_x) + \frac{c_{iy}}{c_s} (u_yB_z - u_zB_y) \right].
\]  
(41)

By simply changing the equilibrium populations and the lattice directions, we are immediately in the position to solve Eqs. (33, 34, 35) to run a three-dimensional simulation without any additional change.

For the sake of completeness, let us just mention that this three-dimensional model can be adapted straightforwardly to the D3Q27 lattice discretization by simply changing the lattice directions as
\[
c_{ix} = [0, 1, -1, 0, 0, 0, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1].
\]
and by expanding the equilibrium distribution onto the complete basis composed of 27 Hermite polynomials

\[ f_i^{eq} = w_i \rho \left( 1 + \frac{c_{\tau} \cdot u}{c_s^2} + \frac{1}{2c_s^2} \left[ \mathcal{H}_{i}^{(2)}u_x^2 + \mathcal{H}_{i}^{(2)}u_y^2 + \mathcal{H}_{i}^{(2)}u_z^2 + \right. \right. \]

\[ + 2 \left( \mathcal{H}_{i}^{(2)}u_x u_y + \mathcal{H}_{i}^{(2)}u_x u_z + \mathcal{H}_{i}^{(2)}u_y u_z \right) \left. \right] + \]

\[ \frac{1}{2c_s^2} \left[ \mathcal{H}_{i}^{(3)}u_x^2 u_y + \mathcal{H}_{i}^{(3)}u_x^2 u_z + \mathcal{H}_{i}^{(3)}u_y^2 u_z + \right. \]

\[ + \mathcal{H}_{i}^{(3)}u_x u_y u_z \right) + \]

\[ \frac{1}{4c_s^2} \left[ \mathcal{H}_{i}^{(4)}u_{xy}^2 u_y + \mathcal{H}_{i}^{(4)}u_{xz}^2 u_y + \mathcal{H}_{i}^{(4)}u_{yz}^2 u_y + \right. \]

\[ + \left. \mathcal{H}_{i}^{(4)}u_x u_y u_z \right] + \]

\[ \frac{1}{4c_s^4} \left[ \mathcal{H}_{i}^{(5)}u_x^2 u_y^2 + \mathcal{H}_{i}^{(5)}u_x^2 u_z^2 + \right. \]

\[ + \left. \mathcal{H}_{i}^{(5)}u_y^2 u_z^2 \right] + \]

\[ \frac{1}{8c_s^4} \mathcal{H}_{i}^{(6)}u_{xyz}^2 \right) + \]

\[ \frac{w_i}{2c_s^2} \left[ \frac{1}{3} |c_i|^2 |B|^2 - (c_i \cdot B)^2 \right], \] (43)

where the weights are \( w_0 = 8/27, w_{1...6} = 2/27, w_{7...18} = 1/54 \) and \( w_{19...26} = 1/216 \). \( \mathcal{H}_{n}^{(m)} \) denotes the \( n \)-th order Hermite polynomial tensor. Coefficients before these tensors are \( (n_x!n_y!n_z!c_s^2)^{-1} \), where \( n_x, n_y, \) and \( n_z \) are the number of occurrences of \( x, y \) and \( z \) respectively.\(^{44}\)

### III. RESULTS AND DISCUSSION

In this section, we report the results of simulations in two and three dimensions.

#### A. Two-dimensional simulations

Here, the accuracy of the above-outlined one-stage simplified lattice Boltzmann method is tested against the numerical predictions of the two-dimensional the Orszag-Tang vortex problem\(^{11}\) by De Rosis et al.\(^{45}\) obtained by four different LBMs: (i) the one-relaxation-time LBM (BGK), the multiple-relaxation-time LBM based on the relaxation of (ii) raw (MRT) and (iii) central moments (CMS), and (iv) the two-stages simplified LBM.

Let us consider a doubly-periodic domain of size \( A = 2\pi \times 2\pi \). The velocity and magnetic fields are initialised as

\[ u(x, t = 0) = u_0 [-\sin y, \sin x], \quad B(x, t = 0) = b_0 [-\sin y, \sin 2x]. \] (44)

where \( u_0 = b_0 = 2 \). The density is initially set equal to 1 everywhere. The kinetic and magnetic energies averaged by the domain size are

\[ E_k = \frac{1}{2A} \sum_x \rho(x) |u(x)|^2, \quad E_m = \frac{1}{2A} \sum_x |B(x)|^2, \] (45)

respectively. The total energy is \( E = E_k + E_m \). The kinetic and magnetic enstrophies averaged by the domain size are

\[ \Omega_k = \frac{1}{2A} \sum_x \zeta(x)^2, \quad \Omega_m = \frac{1}{2A} \sum_x j(x)^2, \] (46)

where

\[ \zeta(x) = \nabla \times u(x) = \partial_x u_y(x) - \partial_y u_x(x), \] (47)

\[ j(x) = \nabla \times B(x) = \partial_y B_z(x) - \partial_z B_y(x) \] (48)

are the vorticity and the density of electric current, respectively. The dissipation rate is

\[ \epsilon = \nu \Omega_k + \eta \Omega_m. \] (49)

The divergence of the magnetic field is

\[ \nabla \cdot B(x) = \partial_x B_z(x) + \partial_y B_y(x). \] (50)

The spatial derivatives of any field variable, namely \( \chi \), are computed as

\[ \nabla \chi(x) = \frac{1}{c_s^2} \sum_i w_i \chi(x + c_i) c_i. \] (51)

The problem is governed by two dimensionless parameters: the Reynolds numbers, \( \text{Re} = \frac{2\pi u_0}{\nu} \), and the magnetic Prandtl number, \( \text{Pr}_m = \frac{\nu}{\eta} \). Consistently with De Rosis et al.\(^{49}\), a low Mach number equal to \( \text{Ma} = \frac{u_0}{S_v c_s} \approx 0.028 \) is adopted in all the simulations, where \( S_v \) is a scaling factor allowing us to transform the velocity \( u_0 \) into LB units.\(^{40}\)

Our numerical campaign begins by simulating a scenario where \( \nu = \eta = 0.02 \), corresponding to a Reynolds number of \( \text{Re} \approx 628 \). TABLES I, II and III report the peak values of (i) the vorticity, \( \zeta_{\text{max}} = \max_x |\zeta(x)| \), (ii) the density of electric current, \( j_{\text{max}} = \max_x |j(x)| \), and (iii) the divergence of the magnetic field, \( \max_x |\nabla \cdot B(x)| \)
normalised by $b_0$. Two salient time instants are considered: $t = 0.5$ and 1. The grid resolution varies as $L = 128, 256$ and 512. Results indicate that the SSLBM increases the accuracy of the computations of both the velocity and magnetic fields with respect to the SLBM. This is particularly evident for the coarsest lattice, where the advantage is particularly prominent. We address this behaviour to the lower numerical dissipation introduced by the present method with respect to the classical simplified strategy. Interestingly, the proposed scheme is also able to keep very low peak values of the divergence of the magnetic field, i.e. $10^{-16} - 10^{-15}$, that can be considered an excellent numerical approximation of the divergence-free condition. The aggregate view

<table>
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<td>14.18</td>
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Table I. Two-dimensional MHD vortex flow at $\nu = \eta = 0.02$: peak values of the vorticity at salient time instants and different grid resolutions by the present approach and other LBMs from De Rosis et al., together with findings from Dellar (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing. Reproduced with permission from J. Comput. Phys. 179, 1 (2002). Copyright 2002 Elsevier.).

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Table II. Two-dimensional MHD vortex flow at $\nu = \eta = 0.02$: peak values of the density of electric current at salient time instants and different grid resolutions by the present approach and other LBMs from De Rosis et al., together with findings from Dellar (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing. Reproduced with permission from J. Comput. Phys. 179, 1 (2002). Copyright 2002 Elsevier.).

in FIG. 1 clearly highlights the large discrepancy of the density of electric current and vorticity at representative time instants. In agreement with Refs. 31, 49, thin layers with large currents and vorticities arise in the domain as the time advances.

Let us investigate further scenarios characterised by different Reynolds numbers Prandtl number equal to 1. This is achieved by varying the fluid kinematic viscosity.
Table III. Two-dimensional MHD vortex flow at $\nu = \eta = 0.02$: peak values of the divergence of the magnetic field normalised by $b_0$ at salient time instants and different grid resolutions by the present approach and other LBMs from by De Rosis et al.\textsuperscript{49}, together with findings from Dellar\textsuperscript{31} (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing. Reproduced with permission from J. Comput. Phys. 179, 1 (2002). Copyright 2002 Elsevier.).

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<td>$2.28 \times 10^{-15}$</td>
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Figure 2. Two-dimensional MHD vortex flow at $\nu = \eta = 0.02$: contour lines of the density of electric current at (a) $t = 0.2$, (b) 0.6, (c) 0.85 and vorticity at (d) $t = 0.2$, (e) 0.6, (f) 0.85.

as $\nu = \eta = 0.08, 0.04, 0.01$ and 0.05. All the runs are carried out by assuming $L = 1024$. Maxima of the dissipation rate, max$_{t} |\epsilon(t)|$, are reported in TABLE IV for all the considered approaches. While the LBMs with evolution of populations show identical results, the SLBM differs from these, especially when more turbulent scenarios are involved. Interestingly, findings obtained by the SSLBM are closer to those provided by the BGK, MRT.
and CMS LBMs. Again, this behaviour should be addressed to the lower dissipation and subsequent superior accuracy properties of the proposed approach. Interestingly, the SSLMB demonstrates that the maximum value of \( \epsilon \left( \max_j \left[ \epsilon(t) \right] \right) \) decreases of \( \approx 20\% \) when the viscosity reduces by a half, as observed in the seminal work by Orszag & Tang\(^{11} \) and more recently in De Rosis et al.\(^{19} \). For the sake of completeness, these findings are also plotted in FIG. 3. FIG. 4 sketches the contour map of the density of electric current at salient time instants.

Moreover, it tends to dissipate earlier in time for larger values of the viscosity. A vis-à-vis comparison with the results reported in FIG. 8 of the work by De Rosis et al.\(^{19} \) clearly highlights an optimal consistency of the proposed SSLBM with the schemes based on the evolution of populations.

Furthermore, let us consider the following four configurations with variable Re and Pr\(_m\): (a) \( \nu = \eta = 0.02 \); (b) \( \nu = 0.04 \) and \( \eta = 0.02 \); (c) \( \nu = 0.02 \) and \( \eta = 0.04 \); (d) \( \nu = \eta = 0.04 \). TABLE V reports the peak values of the density of electric current at salient time instants obtained the MRT LBM, \( j_{\text{max,MRT}} \), together with the absolute discrepancies of the other LBMs with respect to it. These discrepancies are computed as

\[
\begin{align*}
    d_{\text{BGK}} &= |j_{\text{max,MRT}} - j_{\text{max,BGK}}|, \\
    d_{\text{CMS}} &= |j_{\text{max,MRT}} - j_{\text{max,CMS}}|, \\
    d_{\text{SLBM}} &= |j_{\text{max,MRT}} - j_{\text{max,SLBM}}|, \\
    d_{\text{SSLBM}} &= |j_{\text{max,MRT}} - j_{\text{max,SSLBM}}|, \\
\end{align*}
\]

where \( j_{\text{max,BGK}} \), \( j_{\text{max,SLBM}} \), \( j_{\text{max,SSLBM}} \) are the peak values of the density of electric current computed by BGK, SLBM and SSLBM, respectively, and \( d_{\text{max,BGK}} \), \( d_{\text{max,SLBM}} \), \( d_{\text{max,SSLBM}} \) are the corresponding absolute deviations from the values provided by the MRT LBM. From this table, one can immediately appreciate that results provided by the CMS are identical to those form the MRT. The BGK LBM exhibits very small deviations. The SLBM shows the highest discrepancies, which are considerably alleviated by the SSLBM. Independently from the configuration, one can appreciate that the SSLBM generates results which are in closer agreement to those obtained by LBMs with evolution of distribution functions (BGK, MRT and CMS) than is obtained by SLBM.

In the following, configuration (a) is adopted to compare the run time of all the adopted schemes. Specifically, FIG. 5 depicts the CPU time taken to simulate the range \( t \in [0:1] \) with different grid resolutions. MRT, CMS and BGK LBMs are observed to take the least CPU time, with little variation between them. SSLBM is observed to be the slowest. Its overhead in time is due additional arithmetic operations per lattice point as described in Section II. Nevertheless, the accuracy improvements over the SLBM are self-evident, and will be further demonstrated in the following section in the application to three dimensional scenarios. Furthermore, it is relevant to note that this cost is expected to be more than offset by computational efficiencies brought by a reduced numerical stencil size when employed on memory-bound computer hardware such as GPU processing (see Mawson & Revel\(^{59} \)).

### B. Three-dimensional simulations

Let us test the ability of the proposed scheme to simulate a three-dimensional scenario by considering the

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TABLE IV. Two-dimensional MHD vortex flow at Pr\(_m\) = 1 and variable Re: maxima of the dissipation rate \( \epsilon \left( \times 10 \right) \) obtained by the present approach and other LBMs in De Rosis et al.\(^{19} \). (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing.)

![Figure 3. Two-dimensional MHD vortex flow at Pr\(_m\) = 1 and variable Re: plot of the maxima of the dissipation rate (max\(_j\) [\( \epsilon(t) \] \times 10) reported in Table IV. Findings are obtained from BGK LBM (circles), two-stages simplified LBM (diamonds), and present one-stage simplified LBM (crosses) (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing.)](image-url)
Figure 4. Two-dimensional MHD vortex flow at Pr$_{m}$ = 1 and variable Re: map of the density of electric current at salient time instants for different values of $v$. $v = 0.08$ at (a) $t = 0.5$, (b) 1, (c) 1.5, (d) 2. $v = 0.005$ at (e) $t = 0.5$, (f) 1, (g) 1.5, (h) 2. Colour map ranges from 0 (black) to 20 (dark red).

Table V. Two-dimensional MHD vortex flow at variable Re and Pr$_{m}$: peak value of the density of electric current $j_{\text{max},\text{MRT}}$ at salient time instants by the MRT together with the absolute discrepancies of the other LBMs in De Rosis et al.\textsuperscript{10} with respect to it under different configurations. (Reproduced from A. De Rosis, J. Al-Adham, H. Al-Ali and R. Meng, “Double-D2Q9 lattice Boltzmann models with extended equilibrium for two-dimensional magnetohydrodynamic flows”, Phys. Fluids 33, 035143 (2021), with the permission of AIP Publishing.)

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Figure 5. CPU time (normalized by the minimum value corresponding to the fastest run) against grid resolution $2\pi/L$ involved by different schemes: BGK (black solid line with squares), raw-moments-based (MRT, red dashed line with circles), central-moments-based (CMS, green dotted line with triangles), two-stages simplified LBM (SLBM, blue dash-dotted line with inverted triangles), and single-stage simplified LBM (SSLBM, magenta dash-dot-dotted line with diamonds).

MHD vortex flow developing in a cubic periodic box of volume $2\pi \times 2\pi \times 2\pi$ with the initial conditions defined
We can compute the peak value of the density of the electric current as:

\[ j_{\text{max}} = \max_{x} |j(x)|, \]

where \( j \) is the electric current density. Notice that the divergence of the magnetic field is computed as \( \nabla \cdot B = \partial_x B_x + \partial_y B_y + \partial_z B_z \) in three dimensions.

Let us consider a scenario where \( \nu = \eta = 0.057 \). The box is represented by 128³ lattice points and the Mach number of the simulations is \( \text{Ma} = \frac{u_0}{\sqrt{c_s^2 + c_	ext{e}^2}} \approx 0.00407 \).

The D3Q19 lattice discretization is adopted. In FIG. 6, the time evolution of \( j_{\text{max}} \) is depicted. Findings obtained by the present SSLBM are plotted together with the results obtained by a high-resolution pseudo-spectral analysis and those coming from SLBM and BGK runs. The latter is characterised by large-amplitude oscillations in the earliest stage \( (t < 0.1) \) of the simulations, which vanish rapidly and do not deteriorate the solution in the later stage. Interestingly, one can immediately observe that the SSLBM generates results which are considerably closer to the reference pseudo-spectral solution than those achieved by the SLBM. When \( t > 0.45 \), the SLBM produces a solution that largely underestimates \( j_{\text{max}} \). This is particularly evident with respect to the maximum value. Conversely, the SSLBM is able to capture well the knee at \( t \sim 0.95 \) and the subsequent bell-shaped behaviour. This is further quantified in TABLE VI, where the discrepancy of the BGK, SLBM and SLBM with respect to the pseudo-spectral values is computed as:

\[ \varepsilon_{\text{BGK}} = \frac{|\max_t \{j_{\text{max,PS}}(t)\} - \max_t \{j_{\text{max,BGK}}(t)\}|}{\max_t \{j_{\text{max,PS}}(t)\}} \times 100, \]
\[ \varepsilon_{\text{S}} = \frac{|\max_t \{j_{\text{max,PS}}(t)\} - \max_t \{j_{\text{max,S}}(t)\}|}{\max_t \{j_{\text{max,PS}}(t)\}} \times 100, \]
\[ \varepsilon_{\text{SS}} = \frac{|\max_t \{j_{\text{max,PS}}(t)\} - \max_t \{j_{\text{max,SS}}(t)\}|}{\max_t \{j_{\text{max,PS}}(t)\}} \times 100, \]

where \( \max_t \) denotes the maximum value of the desired quantity over the considered time range, \( j_{\text{max,PS}} \), \( j_{\text{max,BGK}} \), \( j_{\text{max,S}} \) and \( j_{\text{max,SS}} \) are the time-dependent peak values of the density of the electric current obtained by the pseudo-spectral analysis, the BGK LBM, the simplified lattice Boltzmann method and the present scheme, respectively. From this table, it is possible to appreciate that the error obtained by the present method is about seven times lower than the one made by the classical two-steps simplified approach. Moreover, it is just 1.7 times larger than the one achieved by the BGK run. Present errors are computed by discretising each side of the domain by 128 points, as mentioned. Such an apparently coarse grid resolution has been chosen as a trade-off between accuracy and computational cost. Nevertheless, the usage of finer grids will certainly reduces the mismatch with respect to the pseudo-spectral reference values.

In FIG. 7, the contour plot of the magnitude of the density of electric current is depicted at representative time instants. Thin sheets characterised by strong currents arise in the range \( t \in [1 : 1.5] \), that is consistent with the high values of \( |j| \) reported in FIG. 6. Interestingly, regions with high currents correspond to vanishing values of the magnetic field (see FIG. 8). These findings corroborate the results shown in Refs.\cite{15,32}, in two and three dimensions, respectively, as well as the observations in the work by De Rosi et al.\cite{62}, where a central-moments-based collision operator was adopted. Notably, the transition to turbulence of the Orszag-Tang vortex has been recently investigated by direct numerical simulations in a recent work by Jadhav & Chandy\cite{63}.
Table VI. Three-dimensional MHD vortex flow: maximum of the peak values of the density of the electric current by a high-resolution pseudo-spectral analysis, the BGK LBM, the two-stage SLBM and the present one-stage method and relative discrepancies.

<table>
<thead>
<tr>
<th></th>
<th>PS</th>
<th>BGK</th>
<th>SLBM</th>
<th>SSLBM</th>
<th>$\varepsilon_{\text{BGK}}$ [%]</th>
<th>$\varepsilon_{\text{S}}$ [%]</th>
<th>$\varepsilon_{\text{SS}}$ [%]</th>
</tr>
</thead>
</table>

Eventually, it is worth to underline that both the adopted LBMs satisfy very well the condition $\nabla \cdot \mathbf{B} = 0$. In fact, our computations are characterised by values of this quantity of order $10^{-16}$, which is an excellent numerical approximation.

With respect to other efforts, here we elucidate the role of the magnetic Prandtl number in the three-dimensional vortex flow. Specifically, we re-run the same simulation by varying $\text{Pr}_m$ as $\text{Pr}_m = 0.5, 1, 2$. In FIG. 9, the time evolution of the peak value of the density of electric current is reported for these scenarios. One can immediately observe that $j_{\text{max}}$ tends to grow with $\text{Pr}_m$. We address this behaviour to the fact that scenarios characterised by higher value of $\text{Pr}_m$ correspond to lower values of $\eta$ (i.e., $\nu$ is kept fixed). Therefore, the diffusion coefficient of the magnetic field reduces and more magnetically turbulent scenarios are achieved. These findings are confirmed in FIG. 10, where the time evolution of the magnetic, kinetic and total energies are depicted. While $E_k$ and $E$ tend to monotonically decrease, $E_m$ under-
goes larger variations due to an exchange of energy which corroborates the observations in two-dimensional simulations\cite{11,32,49}.

**IV. CONCLUSIONS**

In a very recent effort\cite{49}, the simplified LBM has been shown able to enforce the divergence-free condition $\nabla \cdot \mathbf{B} = 0$ in an excellent manner. However, it has demonstrated poorer accuracy if compared to the adoption of the BGK and MRT collision operators. In this paper, we presented, tested and validated a simplified lattice Boltzmann method for two- and three-dimensional magnetohydrodynamic flows with improved accuracy. Differently from its classical formulation, here the two-stages procedure is replaced by a one-stage one. While keeping the same excellent performance of the SLBM in the satisfaction of the divergence-free condition of the magnetic field, we demonstrated that the SSLBM is characterised by a superior accuracy. This is particularly evident when three-dimensional scenarios are considered, where the dissipation properties of the SLBM dominate excessively the flow physics.

In summary, we believe that the SSLBM is an excellent candidate to perform numerical simulations of magnetohydrodynamic flows for the following reasons:

- $\nabla \cdot \mathbf{B} = 0$ excellently satisfied, with values which are several orders of magnitude lower than those achieved by LBMs with evolution of populations;
- low amount of required virtual memory, allowing us to use one tenth of the one required by LBMs with evolution of populations;
- superior accuracy with respect to findings obtained by the SLBM.
In a future work, we aim at performing systematic comparisons of the statistical properties of MHD turbulence.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

SUPPLEMENTARY MATERIAL

In order to help the reader to reproduce our results, we add in the supplementary material a C++ programs, SSLBM.cpp, which implement the present one-stage models. It allows the interested reader to simulate the two-dimensional MHD flows discussed in SEC. III. The code used in this work is included in the supplementary material, along with a README file containing details and compilation instructions needed to run. In this way the interested reader is able to reproduce the results in this paper.

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REFERENCES


12W. J. T. Bos for the help in understanding the physics of magnetohydrodynamic turbulence.


