Development of a 3D Spectral Boltzmann Solver for Plasma Modeling

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Abstract: A numerical framework for studying plasma flows in electric propulsion systems is developed. The *novelty* of this kinetic-theory-based method is the spectral treatment of the Boltzmann collision operator using Fourier-Galerkin scheme coupled with the computational efficiency of the streaming of the lattice Boltzmann method. This spectral treatment (i) avoids the low Mach number restriction of the lattice Boltzmann method or gas-kinetic method and (ii) makes the present scheme valid over a wider range of Knudsen numbers. The sum of two three-dimensional Maxwell distributions were used for verification of the method. Spectral order accurate computations of plasma flows in electric propulsion systems are achievable with this approach.

Nomenclature

$\boldsymbol{A}$	= magnetic potential
$\boldsymbol{a}$	= particle acceleration
$\boldsymbol{B}$	= magnetic induction
B	= kernel in collision integral
$\boldsymbol{D}$	= electric displacement field
$\boldsymbol{E}$	= electric field
f	= particle velocity distribution function
$\hat{f}$	= Fourier coefficients
f_N	= truncated Fourier series approximating f
ϕ	= electric potential
$\boldsymbol{g}$	= relative particle velocity
$\boldsymbol{H}$	= magnetic field
$\boldsymbol{J}$	= net current density
L	= loss term in collision operator
m	= mass
N	= number of spectral modes
Q	= collision operator
q	= charge
ρ_e	= net charge density
$\boldsymbol{v}$	= particle velocity

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I. Introduction

Kinetic-theory-based methods are becoming increasingly popular for computing many types of rarefied/plasma-type flows.[1–12] However, many of these approaches use the linearized Botzmann.[9,13] The linearized-Boltzmann-based methods are not useful for flows where the density varies greatly such that the Knudsen number varies by orders of magnitudes, e.g., in electric propulsion (EP) systems,[14–16] an important application where erosion of ion thruster components is an issue. The spectral decomposition of the Boltzmann collision operator used in this study offers a way of analyzing all the flow regimes where the density can vary by orders of magnitudes as is done using the Direct Simulation Monte Carlo (DSMC).[17–20] A motivation for this work is the relation of Boltzmann's equation to DSMC.[21–24] The spectral treatment allows for spectral order accurate computations of important phenomena in thrust production using plasmas in different EP systems, erosion of critical EP components and onset of different types of plasma instabilities. The spectral decomposition of Boltzmann's collision integral has the potential to be fast and less oscillatory than other algorithms besides being spectral-order accurate as in many comparative studies.[25–31]

A numerical framework for studying plasma flows in electric propulsion systems is developed based on kinetic-theory. The framework uses the spectral decomposition of the Boltzmann collision operator coupling a Fourier-Galerkin scheme with the computational efficiency of the streaming of the lattice Boltzmann method (LBM). In contrast, previous kinetic-theory-based methods used the linearized Bhatnagar-Gross-Krook (BGK) collision operator. This spectral treatment (i) avoids the low Mach number restriction of LBM[9,32] or gas-kinetic method (GKM)[13] and (ii) makes the present scheme valid over a wider range of Knudsen numbers.[33] The approach uses the computational infrastructure of LBM (mostly streaming) because LBM is established, verified and validated[9,10,34–37] for non-rarefied flows but the fact that this approach uses a spectral decomposition of the *full* Boltzmann collision integral makes it *not* LBM. There exists here the potential to use different types of spectral decompositions and even to use the spectral decompositions on different types of collision operators[38,39] or computational or experimental data.[40] This spectral algorithm is also straightforward for later incorporation of multi-species effects.[41]

II. Computational Approach

A. Spectral Decomposition of the Boltzmann Collision Integral

The numerical approach uses a spectral decomposition of the homogeneous Boltzmann equation as developed by Pareschi and Giovanni.[33] In this formulation, the collision operator is split into gain and loss parts $Q(f,f) = Q^+(f,f) - fL(f)$. Then the homogeneous Boltzmann equation is rewritten as

$$\frac{\partial f}{\partial t} + fL(f) = Q^+(f,f) \tag{1}$$

where $f = f(\boldsymbol{x}, \boldsymbol{v}, t)$ and

$$Q^+(f,f) = \int_{\mathbb{R}^d}\int_{S^{d-1}} B(|\boldsymbol{g}|, \boldsymbol{\theta}) f(\boldsymbol{v}') f(\boldsymbol{v}_1') d\boldsymbol{\omega} d\boldsymbol{g} \tag{2}$$

$$L(f) = \int_{\mathbb{R}^d}\int_{S^{d-1}} B(|\boldsymbol{g}|, \boldsymbol{\theta}) f(\boldsymbol{v} - \boldsymbol{g}) d\boldsymbol{\omega} d\boldsymbol{g}, \tag{3}$$

where B depends on the type of collision, $\boldsymbol{g} = \boldsymbol{v} - \boldsymbol{v}_1$, $\boldsymbol{\omega}$ is the direction of $\boldsymbol{g}$, $\boldsymbol{\theta}$ is the deflection angle and

$$\boldsymbol{v}' = \boldsymbol{v} - \frac{1}{2}(\boldsymbol{g} - |\boldsymbol{g}|\boldsymbol{\omega}), \quad \boldsymbol{v}_1' = \boldsymbol{v} - \frac{1}{2}(\boldsymbol{g} + |\boldsymbol{g}|\boldsymbol{\omega}). \tag{4}$$

In order to create the spectral approximation, consider the distribution function $f(\mathbf{v})$ restricted on the cube $[-T,T]^3$ with $T \geq (2+\sqrt{2})R$, and assume that $f(\boldsymbol{v}) = 0$ on $[-T,T]^3/\mathcal{B}(0,R)$ and extend it as a periodic function on $[-T,T]^3$. Then $R = \lambda T$ where $\lambda = 2/(3+\sqrt{2})$. A truncated Fourier series approximates the function f_N as

$$f_N(\boldsymbol{v}) = \sum_{\boldsymbol{k}=-\boldsymbol{N}}^{\boldsymbol{N}} \hat{f}_{\boldsymbol{k}} e^{i\frac{\pi}{T}\boldsymbol{k}\cdot\boldsymbol{v}}, \tag{5}$$

$$\hat{f}_{\boldsymbol{k}} = \frac{1}{(2T)^d}\int_{[-T,T]^d} f(\boldsymbol{v}) e^{-i\frac{\pi}{T}\boldsymbol{k}\cdot\boldsymbol{v}} d\boldsymbol{v}. \tag{6}$$

Here $\boldsymbol{k} = (k_1, k_2, k_3)$ with $(k_1, k_2, k_3) = -\boldsymbol{N}, ..., \boldsymbol{N}$. A Fourier-Galerkin method is used to find the unknown coefficients $\hat{f}_{\boldsymbol{k}}$. For $\boldsymbol{k} = -\boldsymbol{N}, ..., \boldsymbol{N}$

$$\int_{[-T,T]^d} \left(\frac{\partial f_N}{\partial t} + f_N L(f_N) - Q^+(f_N, f_N) \right) e^{-i\frac{\pi}{T}\boldsymbol{k}\cdot\boldsymbol{v}} d\boldsymbol{v} = 0. \tag{7}$$

By requiring that the residual of (7) be orthogonal to all trigonometric polynomials of degree $\leq N$, a set of ordinary differential equations for the $\hat{f}_{\boldsymbol{k}}$ coefficients results:

$$\frac{d\hat{f}_{\boldsymbol{k}}}{dt} + \sum_{\boldsymbol{m}=-N}^{N} \hat{f}_{\boldsymbol{k}-\boldsymbol{m}} \hat{f}_{\boldsymbol{m}} \hat{B}(\boldsymbol{m}, \boldsymbol{m}) = \sum_{\boldsymbol{m}=-N}^{N} \hat{f}_{\boldsymbol{k}-\boldsymbol{m}} \hat{f}_{\boldsymbol{m}} \hat{B}(\boldsymbol{k}-\boldsymbol{m}, \boldsymbol{m}), \tag{8}$$

with initial condition

$$\hat{f}_{\boldsymbol{k}}(0) = \frac{1}{(2T)^d} \int_{[-T,T]^d} f_0(\boldsymbol{v}) e^{-i\boldsymbol{k}\cdot\boldsymbol{v}} d\boldsymbol{v}. \tag{9}$$

where the Fourier coefficients $\hat{f} = 0$ for $|k_j| > N$, $j = 1, 2, 3$. This means that the value of $\hat{f}_{\boldsymbol{k}-\boldsymbol{m}} = 0$ if the index $\boldsymbol{k} - \boldsymbol{m}$ falls outside the range of $-\boldsymbol{N}, ..., \boldsymbol{N}$.

Given any initial particle velocity distribution, one can compute the evolution of the distribution with time in the frequency domain of the velocity space. After an inverse Fourier transform, one can then compute macroscopic physical properties from moments of the resulting distribution function.

B. Coupling The Spectral Boltzmann Solver with Maxwell's Equations

The modeling of plasmas using the spectral Boltzmann solver requires including the forcing term in the Boltzmann equation and to include all the species (ions and electrons) that wold be present in the plasma. This is Boltzmann's equation written in a general form for a N-component mixture:[42]

$$\begin{aligned} \frac{\partial f^i}{\partial t} + \boldsymbol{v}^i \cdot \boldsymbol{\nabla} f^i + \boldsymbol{a}^i \cdot \boldsymbol{\nabla}_{\boldsymbol{v}} f^i &= \sum_{j=1}^{N} \int \left[f'^i f'^j (1 + \vartheta_i f^i)(1 + \vartheta_j f^j) - f^i f^j (1 + \vartheta_i f'^i)(1 + \vartheta_j f'^j) \right] d\varphi d\boldsymbol{v}^j \\ &= \sum_{j=1}^{N} Q(f^i,\, f^j), \end{aligned} \tag{10}$$

where $\vartheta_i = -1$ 0, +1, for Fermi-Dirac, Maxwell-Boltzmann, and Einstein-Bose statistics; $d\varphi = 2\pi\sigma \sin\chi d\chi$, the quantities σ and χ are the differential scattering cross-section and the angle of deflection, respectively; $f^i = f(\boldsymbol{x},\, \boldsymbol{v}^i,\, t)$ and $f'^i = f'(\boldsymbol{x},\, \boldsymbol{v}'^i,\, t)$ are the distributions before and after collision for the i-th species, and $\boldsymbol{a}^i$ is the acceleration due to external force fields or a mean-field interaction written as

$$\boldsymbol{a}^i = \left(\frac{q}{m} \right)^i (\boldsymbol{E} + \boldsymbol{v}^i \times \boldsymbol{B}) \tag{11}$$

The electric and magnetic fields are found from Maxwell's equations:

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = \rho_e \tag{12}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0 \tag{13}$$

$$\boldsymbol{\nabla} \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \tag{14}$$

$$\boldsymbol{\nabla} \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \tag{15}$$

where

$$\rho_e = \sum_{i=1}^{N} \left(\frac{q}{m} \right)^i \int f^i d\boldsymbol{v}^i$$

$$\boldsymbol{J} = \sum_{i=1}^{N} \left(\frac{q}{m} \right)^i \int f^i \boldsymbol{v}^i d\boldsymbol{v}^i$$

$\boldsymbol{D} = \epsilon \boldsymbol{E}, \boldsymbol{H} = \mu \boldsymbol{B}, \epsilon$ is the electric permittivity of matter and μ is the magnetic permeability of matter. However, we simplify the set of equations in this first implementation by looking at only a single conducting species and simplify the set of Maxwell's equations, to be coupled with the single-species Boltzmann, as

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = \frac{1}{\epsilon_0} \sum_{i=1}^{N} \left(\frac{q}{m}\right)^i \int f^i d\boldsymbol{v}^i \tag{16}$$

$$\boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J} \tag{17}$$

where ϵ_0 is the electric permittivity of free space and μ is the magnetic permeability of free space. The left-hand side of Boltzmann's equation can be integrated along a characteristic (without the acceleration term) as is done in the lattice-Boltzmann method. This approach is used here to compare the results with the established formulation of LBM and to ease implementation by building on the LBM infrastructure while benefiting on the computational efficiency of the streaming achieved through integrating along a characteristic with LBM. For the spectral implementation of Maxwell's equations, they can be rearranged as:[43]

$$\boldsymbol{\nabla}^2 \boldsymbol{E} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \frac{\boldsymbol{\nabla} \rho_e}{\epsilon_0} \tag{18}$$

and

$$\boldsymbol{\nabla}^2 \boldsymbol{B} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{B}}{\partial t^2} = -\mu_0 \boldsymbol{\nabla} \times \boldsymbol{J} \tag{19}$$

where $c = \sqrt{\epsilon_0 \mu_0}$ is the speed of light. A spectral discretization of these wave equations for the electric and magnetic fields is implemented, without the second time derivative as none of the plasma processes of interest will be anywhere near the speed of light. This spectral discretization is also Fourier based to allow for use of the same implementation of the Fast Fourier Transform (FFT) used by the spectral Boltzmann solver in the same code, if desired. The spectral discretization of Maxwell's equations follows already published implementations.[44,45] A finite difference solution of Maxwell's equations are incorporated as another option in the modeling schemes in the code using central differences for testing and verification purposes. As an alternative, and to not require derivatives of the charge current density, the electric and magnetic potentials are also incorporated in the code as an option. The electric potential, ϕ, such that $\boldsymbol{E} = -\boldsymbol{\nabla}\phi$ and the magnetic potential, $\boldsymbol{A}$, such that, $\boldsymbol{A} = \boldsymbol{\nabla} \times \boldsymbol{B}$ allow the wave equations to be written as

$$\boldsymbol{\nabla}^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho_e}{\epsilon_0} \tag{20}$$

and

$$\boldsymbol{\nabla}^2 \boldsymbol{A} - \frac{1}{c^2} \frac{\partial^2 \boldsymbol{A}}{\partial t^2} = -\mu_0 \boldsymbol{J} \tag{21}$$

Once the electromagnetic fields are obtained, rather than modifying the integral along the characteristic used from LBM, we add these fields effects to a modified equilibrium distribution as done by Dellar[34] and elsewhere[37] for magnetohydrodynamic (MHD) simulations to allow recovering the Maxwell stress tensor in the macroscopic continuum fluid equations. This reassures that the formulation can also recover these macroscopic continuum fluid equations if needed and allows comparison with MHD simulations. This is done as this modified equilibrium distribution is simply an additive term in the implementations (here and Dellar's). Another reason for implementing the single-species model is to compare with established models such as used in the MHD simulations.[34,37,46]

III. Results

A. Verification Test: Two distinct 3D Maxwellians

The test case simulated initially has two three-dimensional Maxwellians. This case serves to check the evolution of the distribution function and the relaxation to equilibrium as in previous computations.[33,47] This case can represent two similar fluids initially separated by a wall which is then suddenly removed at the start of the simulation. The initial distribution is shown in Fig. 1.After 3000 time steps (0.0001 non-dimensional time step size), the two three-dimensional distributions evolve into one (See Fig. 2) as the two fluids merge and relax to a new state of equilibrium as one fluid.

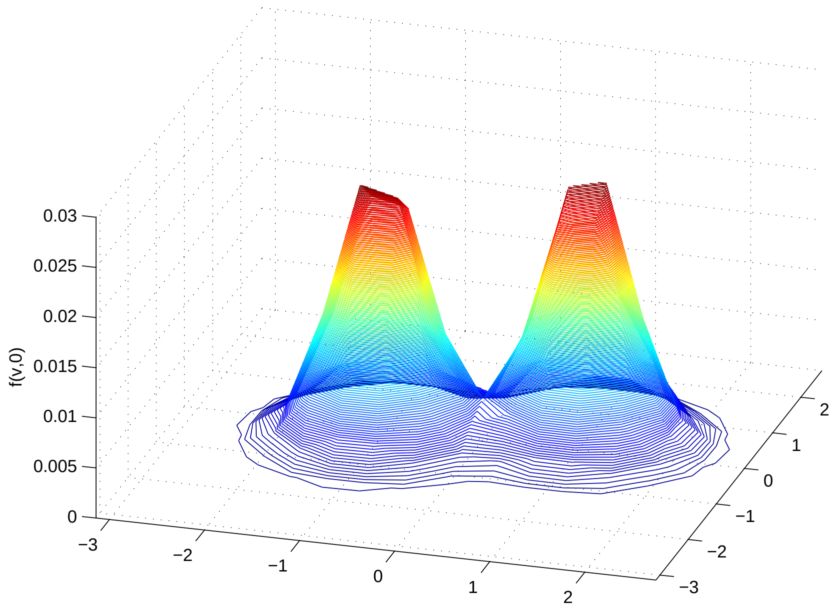

Figure 1. Initial distribution of two Maxwellians.

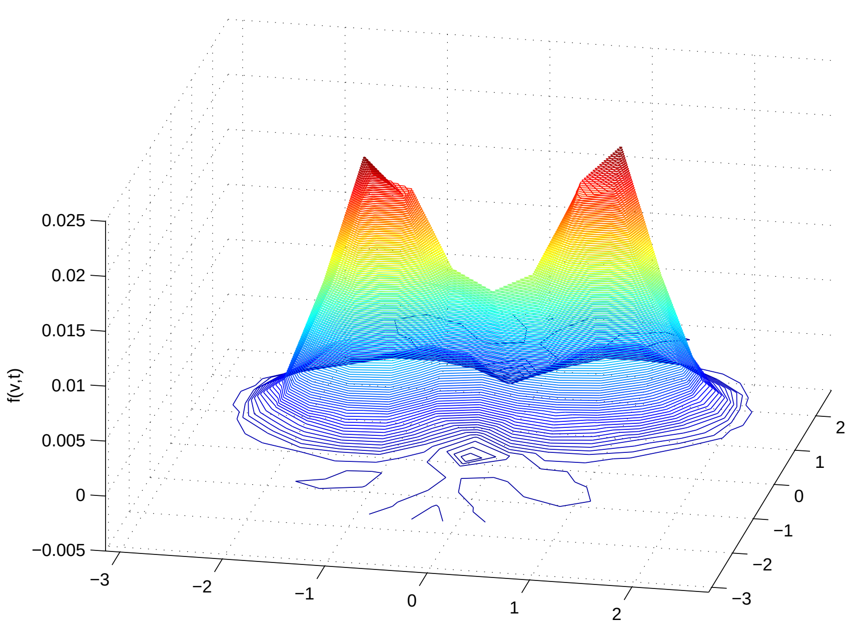

Figure 2. Distribution function after 3000 time steps.

The method successfully and accurately captured the evolution of two Maxwellian distributions. Spectral-order accurate computations of typical plasma flows in electric propulsion systems will be presented in the full paper.

B. Plasma Jet Simulations

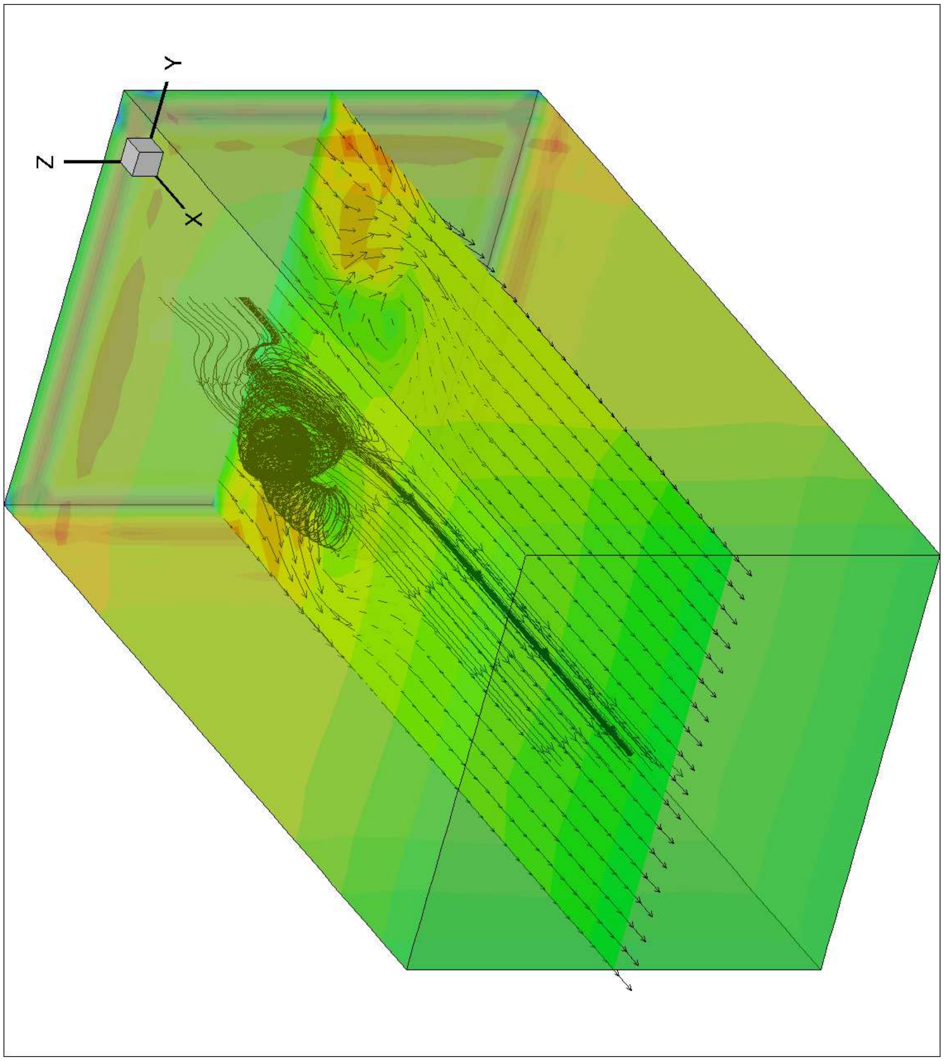

Figure 3. Plasma jet simulation using LBM.

As an illustration of an EP type simulation, the spectral Boltzmann-Maxwell solver is applied to the flow a jet of plasma through one or more circular current loops, imposing an external magnetic field on the jet, to simulate flow similar to that through a magnetic nozzle.[48,49] Different numbers of modes are used with different size grids in the simulations. These are from 2 to 16 modes, 2^3 to 16^3 uniform grids in velocity space with uniform grids for physical space ranging from 16^3 to $132 \times 32 \times 32$. Grid convergence studies were conducted and finer grids were deemed unnecessary for some simulations as L_2 error norms met tolerances less than 10^{-5} for finer grids computed. The comparison was made between the spectral Boltzmann-Maxwell solver and LBM using the same code but with different solver options. Since the same streaming was used, data was distributed over the larger number points in going from a 19-velocity LBM to large numbers of spectral modes and points were skipped according to the ratio of the spectral to LBM in going the other direction. Other interpolation schemes were available as options but these generally better recovered the distribution, which could be like one of the distributions in Fig. 1, in each cell or equivalent lattice where

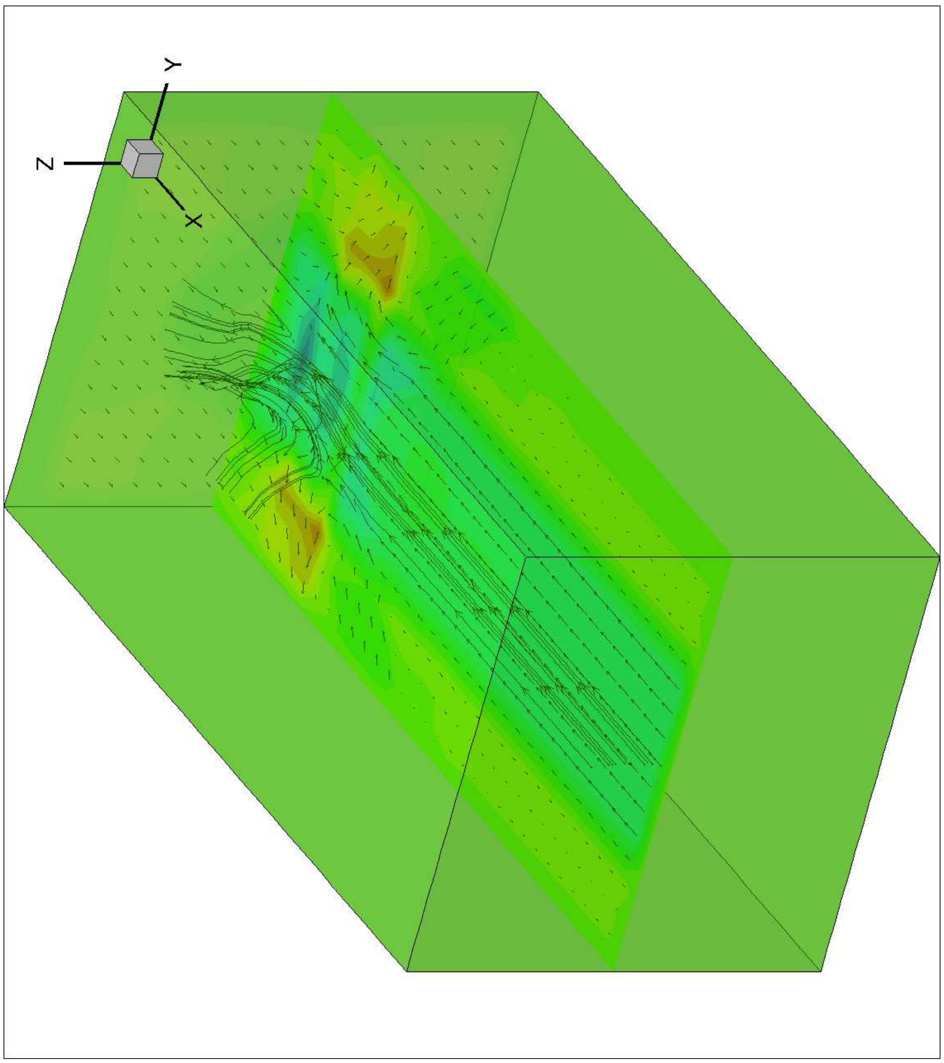

Figure 4. Plasma jet simulation using the spectral Boltzmann-Maxwell solver.

the spectral modes were being computed.

In the incompressible MHD simulation of the plasma jet, Dellar's MHD is coupled with the multiple-relaxation time (MRT) formulation of LBM, shown to be better at higher Reynolds numbers.[37] The plasma accelerates as expected but the flow around the current loops show more of the flow being slowed after some initial acceleration (Fig. 3). This is primarily due to the incompressible simulation. The same flow pattern may be seen with the spectral solver (Fig. 4). A compressible simulation has not yet been conducted.

IV. Conclusion

Generally, more accurate simulations could be performed with the spectral Boltzmann-Maxwell solver than with LBM but at great computational expense as the latter was 20-30 times faster. Others have established the spectral Boltzmann solver as faster than other techniques for rarefied flows. The accuracy was the driving motivation for this work and that has been shown.

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