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KINETIC MODELS AND ALGORITHMS FOR SOLUTION OF THE MAGNETOGASDYNAMIC PROBLEMS ON THE MODERN SUPERCOMPUTING SYSTEMS

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Abstract. *The impressive progress of the kinetic schemes in the solution of gas dynamics problems and the development of effective parallel algorithms for modern high performance parallel computing systems led to the development of advanced methods for the solution of the magnetohydrodynamics problem in the important area of plasma physics. The novel feature of the method is the formulation of the complex Boltzmann-like distribution function of kinetic method with the implementation of electromagnetic interaction terms. The numerical method is based on the explicit schemes. Due to logical simplicity and its efficiency, the algorithm is easily adapted to modern high performance parallel computer systems including hybrid computing systems with graphic processors.*

1 INTRODUCTION

The tremendous progress in the development of high performance computing systems, especially expecting drastically new exascale computing systems, including the challenges in architecture, scale, power and reliability, gives new opportunities for the mathematical modelling of important physical phenomena in the present and future. Nevertheless the complexity of the challenges in science and engineering continues to outpace our ability to adequately address them through impressively growing computational power.

A feature of the present is that the development of technologies and computer systems architecture are well ahead of software development. The software problems are primarily associated with the complexity of the algorithms adaptation for the differential equations of mathematical physics to high performance computing systems architecture. In particular they refer to one of the important requirements as the accuracy in combination with the correctness of the initial mathematical models. Another requirement for the methods is their logical simplicity and high efficiency at the same time. The numerical algorithms should be simple and transparent from a logical point of view.

One of the important directions to overcome these problems is the development of a nontraditional approach to initial mathematical models and computational algorithms. In the present study for the solution of the multidimensional gas dynamics and magnetohydrodynamics problems kinetic difference scheme is proposed. It is convenient from the physics point of view to define the gas dynamics and magnetohydrodynamics quantities from close relations between the kinetic and gas dynamics description of physics processes [1, 2, 3, 4, 5, 6].

Another aspect is the study of the explicit finite difference schemes, which seem to be preferable for future high performance parallel computing, especially in terms of their simplicity and well adaptability to parallel program realization, including hybrid high performance parallel computing systems. The weakness of explicit schemes is a strictly limited time step that ensures computational stability. This restriction becomes critical with the growing number of nodes and the reduction in the step of a spatial mesh. The advanced explicit kinetic finite difference schemes have a soft stability condition giving the opportunity to enhance the stability and to use very fine meshes [7].

The mentioned aspects are used for the development of the framework for the study of the dynamics of the conducting gas media in strong magnetic fields at high performance parallel computing systems.

2 THEORETICAL ISSUES

2.1 Gas Dynamics Processes

The kinetic theory describes the gas dynamics by the Boltzmann differential equation through the evolution of the distribution function $f\left(\mathbf{x},\boldsymbol{\xi},t\right)$ [8]:

$$\frac{\partial f\left(\mathbf{x},\boldsymbol{\xi},t\right)}{\partial t}+\boldsymbol{\xi}\cdot\nabla f\left(\mathbf{x},\boldsymbol{\xi},t\right)=C\left(f\right) \tag{1}$$

where $C\left(f\right)$ is a nonlinear integral operator which describes the collisions between gas molecules.

This evolution equation follows naturally from the relations between the kinetic and the gas dynamics description of continuous media. The macroscopic observables such as density, momentum, energy flux as a function of $\mathbf{x}$ and t are obtained from the moments of the distribution function with respect to the macroscopic velocity. The evolution equations for these gas dynamics quantities are obtained by integrating Eq. (1) over molecular velocities $\boldsymbol{\xi}$ with summational invariants m,$m\boldsymbol{\xi}$,$\frac{1}{2}m\boldsymbol{\xi}^2$. The computational interest in kinetic formulations of the gas dynamics is high due to the linearity of the differential operator on the left side of Eq. (1). Nonlinearity is confined by the collision term, which is generally local in $\mathbf{x}$ and t.

An important feature is that the collision integral vanishes in the equilibrium state when the local Boltzmann distribution function f is a Maxwellian:

$$f(\mathbf{x},\boldsymbol{\xi},t) = \frac{\rho(\mathbf{x},t)m^{1/2}}{\left(2\pi kT\left(\mathbf{x},t\right)\right)^{3/2}} exp\left\{-\frac{m}{2kT(t,\mathbf{x})}(\boldsymbol{\xi}-\mathbf{u}(t,\mathbf{x}))^2\right\} \tag{2}$$

This leads to the use of this model for numerical methods and possible generalisations in order provide a natural kinetic description of the system of conservation laws. This approximation is sufficient for the gas dynamics processes and is called the kinetic approach [8].

2.2 Magneto Gas Dynamic Processes

In [9] it was shown that electromagnetic fields do not destroy the validity of the Boltzmann equation and this opened the way for the implementation of the electromagnetic term in the Boltzmann-like distribution function. From the vector nature of the electromagnetic interaction, the distribution function should taking into account the vector behaviour and provide correct formulation for the evolution of the magnetic field, i. e. the magnetic field should be generally defined as the momentum of the Boltzmann-like distribution function.

A few useful attempts to formulate the vector Boltzmann-like distribution function can be found in [10, 11, 12], but physical meaning was not clearly defined.

We propose an evaluation of the electromagnetic processes in the context of the distribution function, taking into account the axial nature of the magnetic field. The electromagnetic interaction processes contributions are considered as a complex velocities vector, described by kinetic motion of charged particles in magnetic field [13]. Using the above definitions we define the local complex Maxwellian distribution function of magnetohydrodynamics with drift velocity $\mathbf{u}$ in magnetic field $\mathbf{B}$ at the equilibrium:

$$f_M = \frac{\rho m^{1/2}}{\left(2\pi kT\right)^{3/2}} \exp\left\{-\frac{m}{2kT}\left|(\boldsymbol{\xi}-\mathbf{u}) - i\frac{\mathbf{B}}{\sqrt{\mu_m \rho}}\right|^2\right\}, \tag{3}$$

The first term on the right-hand side of (3) includes the kinetic energy and the second term is contribution from electromagnetic interactions. The hydrodynamics observables are real scalars and vectors. The complex components include the dynamics of the macroscopic observables introduced by the evolution of the magnetic field, keeping their specific pseudo-vectorial nature.

The hydrodynamic and electromagnetic observables are obtained respectively as the real and imaginary part of the integral of the distribution function (3) with the summational invariants $\left(m, m\boldsymbol{\xi}, \frac{1}{2}m\boldsymbol{\xi}^2, m\boldsymbol{\xi}^*\right)$ along the line L parallel to the real axis and shifted by $i\mathbf{B}/\sqrt{\mu\rho}$ in the imaginary axis direction.

$$\rho = \int_L m f_M d^3\boldsymbol{\xi} \tag{4}$$

$$\mathbf{u} = \frac{1}{\rho}\int_L m\boldsymbol{\xi} f_M d^3\boldsymbol{\xi} \tag{5}$$

$$E = \int_L \frac{1}{2} m\boldsymbol{\xi}^2 f_M d^3\boldsymbol{\xi} \tag{6}$$

$$\mathbf{B} = -\sqrt{\frac{\mu_m}{\rho}}\int_L m\boldsymbol{\xi}^* f_M d^3\boldsymbol{\xi} \tag{7}$$

For the compressible media, we use the linear approximation of the magnetic permeability:

$$\mu_m = \mu_\rho \rho \tag{8}$$

where μ_ρ is a constant representing the magnetic permeability per unit density.

The proposed complex Boltzmann Maxwell like distribution function contains the hydrodynamics terms and the electromagnetic terms. Thus by using this distribution function to calculate the mass, momentum, energy and magnetic field fluxes, most of the electromagnetic contributions are calculated directly, i.e. one does not have to solve the hydrodynamics and magnetic force components separately or differently, as will be shown below.

3 THE IDEAL MAGNETO GAS DYNAMICS EQUATIONS

To provide the first step of the formulation of the MHD conservation laws equation, the equilibrium state is considered with the proposed distribution function. The MHD system of equations is obtained by the integration of (1) with vanishing collision integral with the summational invariants following the definition in (7):

$$\int_L m\frac{\partial f}{\partial t} + \int_L m\boldsymbol{\xi}\cdot\nabla f d^3\boldsymbol{\xi} = 0 \tag{9}$$

$$\int_L m\boldsymbol{\xi}\frac{\partial f}{\partial t} + \int_L m\boldsymbol{\xi}\boldsymbol{\xi}\cdot\nabla f d^3\boldsymbol{\xi} = 0 \tag{10}$$

$$\int_L \frac{1}{2}m\boldsymbol{\xi}^2\frac{\partial f}{\partial t} + \int_L \frac{1}{2}m\boldsymbol{\xi}^2\boldsymbol{\xi}\cdot\nabla f d^3\boldsymbol{\xi} = 0 \tag{11}$$

$$\int_L m\boldsymbol{\xi}^*\frac{\partial f}{\partial t} + \int_L m\boldsymbol{\xi}^*\boldsymbol{\xi}\cdot\nabla f d^3\boldsymbol{\xi} = 0 \tag{12}$$

The result obtained, set of Eq. (12), is the ideal magnetohydrodynamics system of equations:

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x_i}\rho u_i = 0 \tag{13}$$

$$\frac{\partial}{\partial t}\rho u_i + \frac{\partial}{\partial x_k}\left[\left(p + \frac{B^2}{2\mu_M}\right)\delta_{ik} + \rho u_i u_k - \frac{B_i B_k}{\mu_M}\right] = 0 \tag{14}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i}\left[u_i\left(E + p + \frac{B^2}{2\mu_M}\right) - \frac{B_i u_k B_k}{\mu_M}\right] = 0 \tag{15}$$

$$\frac{\partial B_i}{\partial t} + \frac{\partial}{\partial x_k}\left[u_k B_i - u_i B_k\right] = 0 \tag{16}$$

In addition an equation for $\nabla \cdot \mathbf{B}$ is obtained as the imaginary part of the integral of the summational invariant (m) respect to the velocities $\boldsymbol{\xi}$:

$$\int_L m\frac{\partial f}{\partial t} + \int_L m\boldsymbol{\xi} \cdot \nabla f d^3\boldsymbol{\xi} = 0 \tag{17}$$

$$\frac{\partial B_i}{\partial x_i} = 0 \tag{18}$$

4 THE QUASI MAGNETO GAS DYNAMIC SYSTEM OF EQUATIONS

The quasi MHD system of equations for the real gases is obtained using the integration technique outlined in section 2 and the balance relation based on the Taylor expansion of the variation of the local distribution function in spatial variables up to third order infinitesimal [2]:

$$\frac{f^{j+1} - f^j}{\Delta t} + \xi_i \frac{\partial f^j}{\partial x_i} = \xi_i \xi_k \frac{\partial}{\partial x_i} \frac{\tau}{2} \frac{\partial f^j}{\partial x_k} \tag{19}$$

The evaluation equation for the magneto gas dynamic variables (quasi magneto gas dynamic equations) obtained as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\rho u_i = \frac{\partial}{\partial x_i}\left(\frac{\tau}{2}\frac{\partial}{\partial x_k}\Pi_{ik}\right) \tag{20}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_k}\Pi_{ik} = \frac{\partial}{\partial x_k}\Pi^D_{ik} + \frac{\partial}{\partial x_k}\left[\left(\frac{\tau}{2}\frac{\partial}{\partial x_k}\Pi_{ik}\right)u_k\right] \tag{21}$$

$$\frac{\partial E}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial Q_i}{\partial x_i} + \frac{\partial}{\partial x_i}\Pi^D_{ik}u_k + \frac{\partial}{\partial x_i}\left[\left(\frac{E+p}{\rho} + \frac{1}{\mu_m}\frac{B^2}{2\rho}\right)\frac{\tau}{2}\frac{\partial}{\partial x_k}\Pi_{ik}\right] \tag{22}$$

$$\frac{\partial B_i}{\partial t} + \frac{\partial}{\partial x_k}M^B_{ik} = \frac{\partial}{\partial x_k}\Pi^{DB}_{ik} \tag{23}$$

The right-hand of the kinetic magneto gas dynamic Eq. (20-23) contains dissipative terms. In comparison with other methods, the dissipative terms are obtained not by phenomenology with some assumptions about magneto gas dynamics processes but in consistency with the difference scheme of the Boltzmann equation.

Π_{ik} is the momentum flux density tensor for a perfect gas in magnetic field:

$$\Pi_{ik} = \left(p + \frac{B^2}{2\mu_m}\right)\delta_{ik} + \rho u_i u_k - \frac{1}{\mu_m}B_i B_k \tag{24}$$

F_i is the heat transfer flux of a perfect gas in magnetic field:

$$F_i = \left[\left(E + p + \frac{B^2}{2\mu_m}\right)u_i - \frac{1}{\mu_m}B_i u_k B_k\right] \tag{25}$$

M^B_{ik} is the asymmetric product between velocity $\mathbf{u}$ and magnetic field flux $\mathbf{B}$:

$$M^B_{ik} = u_k B_i - u_i B_k \tag{26}$$

The dissipative terms:

$$
\begin{aligned}
\Pi_{ik}^{D} =&\frac{\tau}{2}\left(p\frac{\partial u_i}{\partial x_k}+p\frac{\partial u_k}{\partial x_i}-\frac{2}{3}p\frac{\partial u_l}{\partial x_l}\delta_{ik}\right)\\
&+\frac{\tau}{2}\left[\left(\frac{1}{\mu_m}\frac{B^2}{2}\delta_{lk}-\frac{1}{\mu_m}B_lB_k\right)\frac{\partial u_i}{\partial x_l}+\left(\frac{1}{\mu_m}\frac{B^2}{2}\delta_{il}-\frac{1}{\mu_m}B_iB_l\right)\frac{\partial u_k}{\partial x_l}\right.\\
&\left.-\left(\frac{1}{\mu_m}\frac{B^2}{2}\delta_{ik}-\frac{1}{\mu_m}B_iB_k\right)\frac{\partial u_l}{\partial x_l}\right]\\
&+\frac{\tau}{2}\left[\frac{1}{\mu_m}B_l\left(-B_k\frac{\partial u_i}{\partial x_l}-B_i\frac{\partial u_k}{\partial x_l}+B_n\frac{\partial u_n}{\partial x_l}\delta_{ik}\right)\right]\\
&+\frac{\tau}{2}\left[\rho u_iu_l\frac{\partial u_k}{\partial x_l}+u_i\frac{\partial p}{\partial x_k}+u_i\frac{\partial}{\partial x_k}\frac{1}{\mu_m}\frac{B^2}{2}-u_i\frac{\partial}{\partial x_l}\frac{1}{\mu_m}B_lB_k\right]\\
&+\frac{\tau}{2}\left[u_l\frac{\partial p}{\partial x_l}+\gamma p\frac{\partial u_l}{\partial x_l}\right]\delta_{ik}+\frac{\tau}{2}\left[\frac{1}{\mu_m}B_n^2\frac{\partial u_l}{\partial x_l}-\frac{B_nB_l}{\mu_m}\frac{\partial u_n}{\partial x_l}\right.\\
&\left.+\frac{1}{\mu_m}B_nu_l\frac{\partial B_n}{\partial x_l}\right]\delta_{ik}+\frac{\tau}{2}\left[-\frac{B_iB_k}{\mu_m}\frac{\partial u_l}{\partial x_l}+\frac{B_iB_l}{\mu_m}\frac{\partial u_k}{\partial x_l}-\frac{B_i}{\mu_m}u_l\frac{\partial B_k}{\partial x_l}\right]\\
&+\frac{\tau}{2}\left[-\frac{B_kB_i}{\mu_m}\frac{\partial u_l}{\partial x_l}+\frac{B_kB_l}{\mu_m}\frac{\partial u_i}{\partial x_l}-\frac{B_k}{\mu_m}u_l\frac{\partial B_i}{\partial x_l}\right]
\end{aligned}
\tag{27}
$$

$$
\begin{aligned}
Q_i^D =&\frac{\tau}{2}\left(\frac{5}{2}p\frac{\partial}{\partial x_i}\frac{p}{\rho}\right)\\
&+\frac{\tau}{2}\left[\frac{5}{2}\left(\frac{B^2}{2\mu_m}\delta_{ik}-\frac{B_iB_k}{\mu_m}\right)\frac{\partial}{\partial x_k}\frac{p}{\rho}\right]\\
&+\frac{\tau}{2}\left[\frac{3}{2}\left(p\delta_{ik}+\frac{B^2}{2\mu_m}\delta_{ik}-\frac{B_iB_k}{\mu_m}\right)\frac{\partial}{\partial x_k}\frac{B^2}{2\mu_m\rho}-\left(p+\frac{B^2}{2\mu_m}\right)\frac{\partial}{\partial x_k}\frac{B_iB_k}{\mu_m\rho}\right.\\
&\left.-\frac{B_iB_k}{\mu_m\rho}\frac{\partial}{\partial x_k}\frac{B^2}{2\mu_m}\right]+\frac{\tau}{2}\left[\rho u_iu_k\frac{\partial}{\partial x_k}\frac{3}{2}\frac{p}{\rho}\right]\\
&+\frac{\tau}{2}\left[\rho u_iu_k\left(p+\frac{B^2}{\mu_m}\right)\frac{\partial}{\partial x_k}\frac{1}{\rho}-u_i\frac{B^2}{\mu_m}\frac{\partial u_k}{\partial x_k}\right]\\
&+\frac{\tau}{2}\left[u_i\frac{B_l}{\mu_m}\left(B_l\frac{\partial u_k}{\partial x_k}-B_k\frac{\partial u_l}{\partial x_k}+u_k\frac{\partial B_l}{\partial x_k}\right)\right]\\
&+\frac{\tau}{2}\left[\frac{1}{2}\rho u_iu_k\left(\frac{B^2}{2\mu_m}\frac{\partial}{\partial x_k}\frac{1}{\rho}-\frac{1}{\rho}\frac{\partial}{\partial x_k}\frac{B^2}{2\mu_m}\right)\right]\\
&+\frac{\tau}{2}\left[B_iB_l\left(-u_k\frac{\partial u_l}{\partial x_k}-\frac{1}{\rho}\frac{\partial p}{\partial x_l}-\frac{1}{\rho}\frac{\partial}{\partial x_l}\frac{B^2}{2\mu_m}+\frac{1}{\rho}\frac{\partial}{\partial x_k}\frac{B_lB_k}{\mu_m}\right)\right]
\end{aligned}
\tag{28}
$$

$$
\begin{aligned}
\Pi_{ik}^{DB} =& \frac{\tau_l}{2}\left[\frac{1}{\rho}\left(p+\frac{B^2}{2\mu_m}\right)\left(\frac{\partial B_i}{\partial x_k}-\frac{\partial B_k}{\partial x_i}\right)\right] \\
&+ \frac{\tau}{2}\left[\left(p+\frac{B^2}{2\mu_m}\right)\left(B_i\frac{\partial}{\partial x_k}\frac{1}{\rho}-B_k\frac{\partial}{\partial x_i}\frac{1}{\rho}\right)\right] \\
&+ \frac{\tau}{2}\left[u_kB_l\frac{\partial u_i}{\partial x_l}-u_iB_l\frac{\partial u_k}{\partial x_l}\right]+\frac{\tau}{2}\left[\frac{1}{\rho}\frac{B_iB_l}{\mu_m}\frac{\partial B_k}{\partial x_l}-\frac{1}{\rho}\frac{B_kB_l}{\mu_m}\frac{\partial B_i}{\partial x_l}\right] \\
&+ \frac{\tau}{2}\left[u_kB_i\frac{\partial u_l}{\partial x_l}-u_kB_l\frac{\partial u_i}{\partial x_l}+u_ku_l\frac{\partial B_i}{\partial x_l}\right] \\
&+ \frac{\tau}{2}\left[B_iu_l\frac{\partial u_k}{\partial x_l}+\frac{B_i}{\rho}\frac{\partial p}{\partial x_k}+\frac{B_i}{\rho}\frac{\partial}{\partial x_k}\frac{B^2}{2\mu_m}-\frac{B_i}{\rho}\frac{\partial}{\partial x_l}\frac{B_kB_l}{\mu_m}\right] \\
&+ \frac{\tau}{2}\left[-u_iB_k\frac{\partial u_l}{\partial x_l}+u_iB_l\frac{\partial u_k}{\partial x_l}-u_iu_l\frac{\partial B_k}{\partial x_l}\right] \\
&+ \frac{\tau}{2}\left[-B_ku_l\frac{\partial u_i}{\partial x_l}-\frac{B_k}{\rho}\frac{\partial p}{\partial x_i}-\frac{B_k}{\rho}\frac{\partial}{\partial x_i}\frac{B^2}{2\mu_m}+\frac{B_k}{\rho}\frac{\partial}{\partial x_l}\frac{B_iB_l}{\mu_m}\right]
\end{aligned} \tag{29}
$$

It was shown in [2] that the dissipative terms of the gas dynamics system of equations are small in comparison with the convective terms. The corresponding dissipative terms are associated with the real physics processes and an important remark is that in this case the gas dynamics parameters such as viscosity and heat conductivity are obtained from the kinetic theory.

The Navier-Stokes viscosity is identified as the first term of Eq. (27):

$$
\Pi_{ik}^{NS} = \frac{\tau}{2}\left(p\frac{\partial u_i}{\partial x_k}+p\frac{\partial u_k}{\partial x_i}-\frac{2}{3}p\frac{\partial u_l}{\partial x_l}\delta_{ik}\right) = \mu\left(\frac{\partial u_i}{\partial x_k}+\frac{\partial u_k}{\partial x_i}-\frac{2}{3}\frac{\partial u_l}{\partial x_l}\delta_{ik}\right) \tag{30}
$$

where the bulk viscosity component is neglected and the shear viscosity μ is related to the gas pressure p and the characteristic time τ as $\mu = \frac{\tau}{2}p$.

The Navier-Stokes thermal flux vector is identified as the first term of Eq. (28):

$$
Q_i^{NS} = \frac{\tau}{2}\left(\frac{5}{2}p\frac{\partial}{\partial x_i}\frac{p}{\rho}\right) = k\frac{\partial T}{\partial x_i} \tag{31}
$$

with T gas temperature and k thermal coefficient expressed as $k = \frac{1}{Pr}\frac{5}{2}R\frac{\tau}{2}p$, with Pr Prandtl number.

A similar analysis of the dissipative terms of the electromagnetic processes gives the estimation of their smallness. The correct magnetic viscosity is represented as part of dissepative term. The gas resistivity is identified as the first term of Eq. (29) and also appears as a result of the kinetic formulation:

$$
\Pi_{ik}^{B} = \frac{\tau_m}{2}\left[\left(p+\frac{B^2}{2}\right)\left(\frac{\partial B_i}{\partial x_k}-\frac{\partial B_k}{\partial x_i}\right)\right] = \eta\left(\frac{\partial B_i}{\partial x_k}-\frac{\partial B_k}{\partial x_i}\right) \tag{32}
$$

Where the $\eta = \frac{\tau_m}{2}\left(p+\frac{B^2}{2}\right)$ represents the resistivity.

5 THE COMPUTATIONAL ALGORITHM

The computational task consists of the solution of the kinetic consistent MHD system of equations (20 - 23).

The computational algorithm used in this paper is build upon the Finite Volume method applied to the gas dynamic equations and on the Constrained Transport method applied to the magnetic induction equation [14, 15].

In the finite volume method the conserved gas dynamics variables, density, gas momentum and energy, are averaged above the volume of the computational cell. The contrained transport method treatment is based on the area-averaging of the magnetic field through the surfaces of the grid cells.

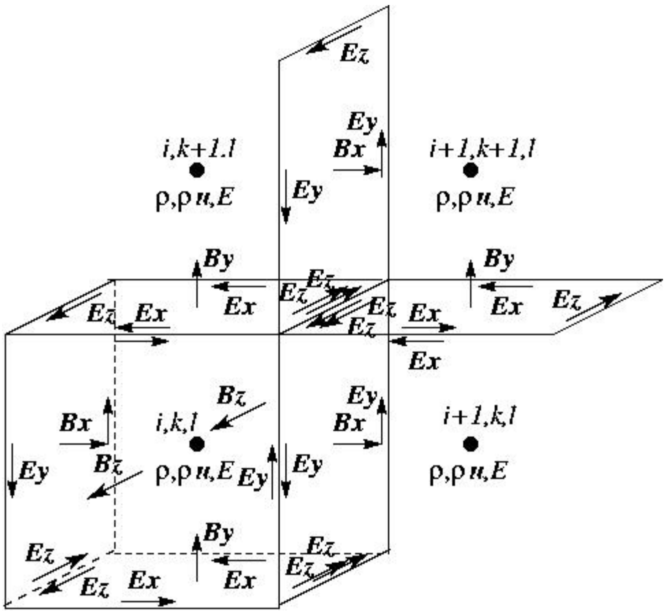

Figure 1: 3D Computational Domain

Fig. 1 shows the four neighbour to the cell (i, k, l) used in evaluations of the hydrodynamics and electromagnetic variables.

The gas dynamics observables - mass density, momentum and energy density are defined at the cell centre. The components of the magnetic field are defined at the face centers of the cells. A duality is established between the electric field and the fluxes. This duality is utilised to obtain the electric field at the edges of the computational cell through a reconstruction process that is applied directly to the properly up-winded fluxes. The electric field is then utilised to make an update of the magnetic fields that preserves the solenoidal nature of the magnetic field and ensures that the magnetic field in a magnetohydrodynamics model remains strictly solenoidal up to discretisation errors.

The explicit finite volume computational algorithm for the magneto gas gas dynamics are used. This method has the convenient stability conditions and very important for adaptation on the massive parallel computing systems.

6 RESULTS OF NUMERICAL MODELLING

The parallel implementation of the numerical algorithm is obtained through the domain decomposition in distributed memory approach. The communication between processors is performed via MPI protocol. The computational method needs only one layer of ghost cells at the boundary and along the edges of each subdomain which is exchanged between the domains with MPI calls. The algorithm is well suited to distributed memory clusters as it is time explicit and requires only one MPI call per time step, reducing significantly the processor communication time contribution to the total computational time.

The demonstration of the method is performed on the basis of the solution of the spherical expansion problem of ionised gas and the solution of the expansion of an ionised gas in strong magnetic field. The initial conditions are the same as proposed in [16] and are expressed in normalised units in order to provide a direct comparison. They consist of a sphere with radius 0.1 placed in the centre of the physical region with pressure of 100 in comparison to the overall represented area with pressure 1. The density is uniform and equal to 1 in the full computational domain. For the study of ionised gas in a strong magnetic field the uniform magnetic field $B_z = 5/\sqrt{\pi}$ aligned with the z coordinate is added to the initial conditions. The adiabatic coefficient of the gas is chosen as $\gamma = 5/3$. Reflective border conditions are used throughout the simulation.

The simulations are performed for a Cartesian rectangular mesh $100 \times 100 \times 100$ in the physics domain [0,1].

Fig. 2 present the state of the 3D simulation of the processes for relative time 0.03. On the 3D pictures the arrows represent the velocities of the ionised gas and the colour represents the density of gas. 3D figures clearly show the confinement of the ionized gas in the cylindrical area along z due to the magnetic field.

Fig. 3,4 represent the $2D$ projections of the density, pressure and kinetic energy of the gas expansion without magnetic field and the $1D$ density profile for these condition at time $t = 0.03$.

Fig. 5,6 represents the $2D$ projections of the density, pressure, magnetic pressure and kinetic energy for the gas expansion problem of the ionized gas with initial magnetic field and Fig. 7 shows the $1D$ profile of the density for these conditions at time $t = 0.03$.

This test demonstrates the ability of the computational algorithm in preserving perfect symmetry. The comparison of the results in [16] shows a reasonable agreement and will be analysed further.

Another significant numerical test is the implosion. It consists of a 3-dimensional generalisation of the Sod shock tube problem [17]. The initial condition corresponds to hydrogen gas presenting a discontinuity perpendicular to the diagonal of the computational domain. The left state has initial density $\rho_l = 0.719$ Kg/m^3 and pressure $P_r = 722680$ Pa. The right state has initial density $\rho_r = 0.125 \times \rho_l$ and pressure $P_r = 0.14 \times P_l$. The initial magnetic field of 0.1 T is aligned with the y-axis. Reflective boundary conditions are used.

The simulations are performed for a Cartesian rectangular mesh $2000 \times 2000 \times 2000$ in the physics domain [0,10] μm.

Fig. 8 represents the $2D$ projections of the density at time t = 1.76×10^{-8} for the two cases with and without magnetic field.

The reflection of the shock generated by the initial contact discontinuity drives consequent vortices and instabilities. The result is characterised by complex shock reflections and rarefactions. In absence of magnetic field the symmetry along the diagonal is preserved. The presence of the magnetic field changes dramatically the picture. The deflection of the charged media flow in the direction of the magnetic field is clearly visible. Another observed effect is the strong smoothing of the instabilities of the gas dynamics, which corresponds to a physical experimental evidence. The possibility of such observation is the basis of the importance of the very detailed space discretisation, which is available with the proposed method.

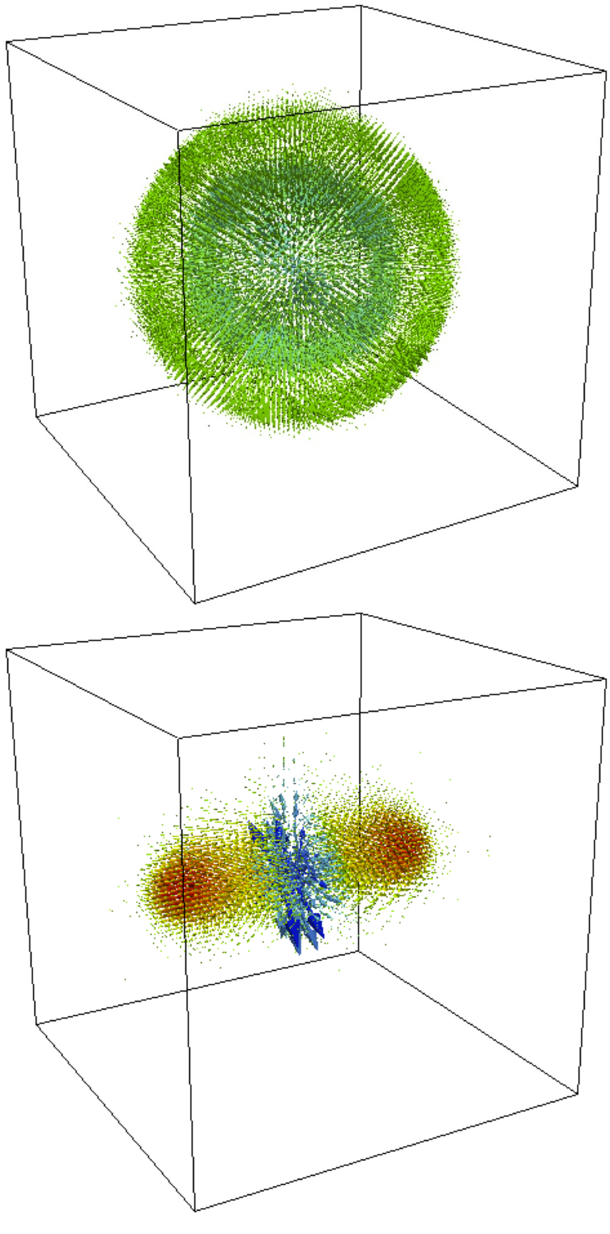

Figure 2: $3D$ view of the conductive gas expansion in strong magnetic field

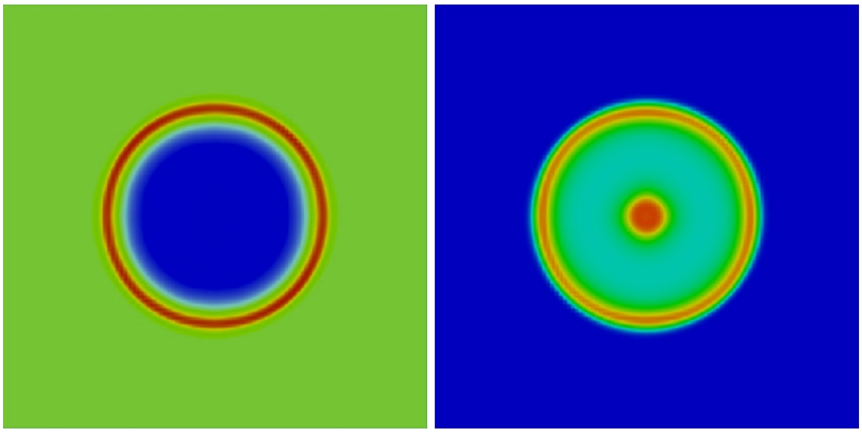

Figure 3: $2D$ gas density and 2D gas pressure projections

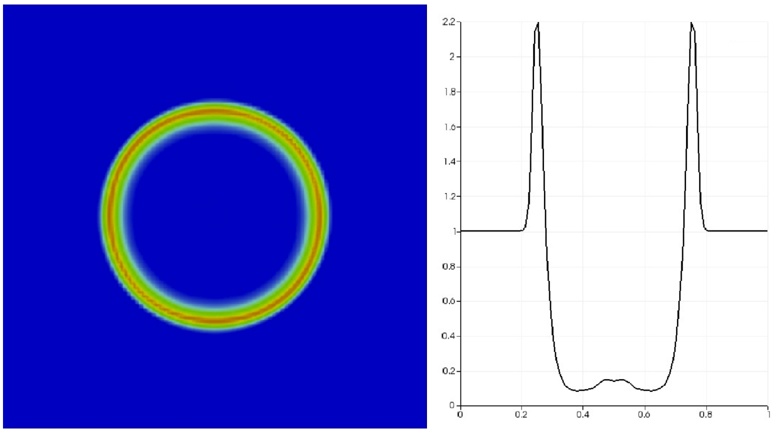

Figure 4: $2D$ kinetic energy and 1D density profile

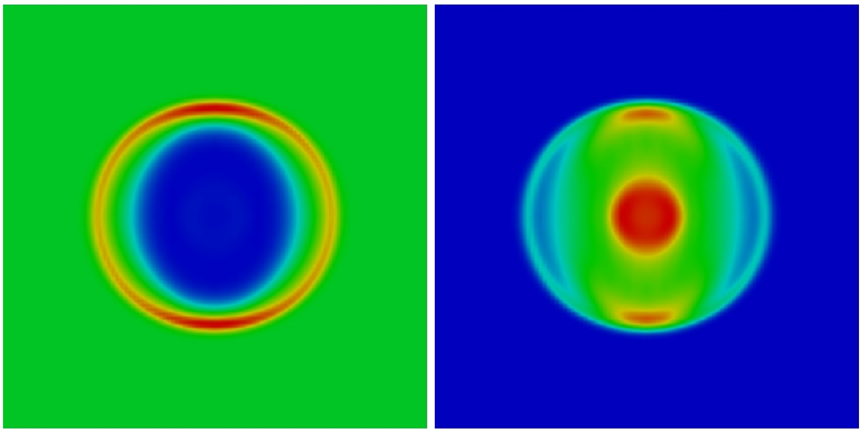

Figure 5: $2D$ gas density and $2D$ gas pressure projections in the magnetic field $5/\sqrt{\pi}$

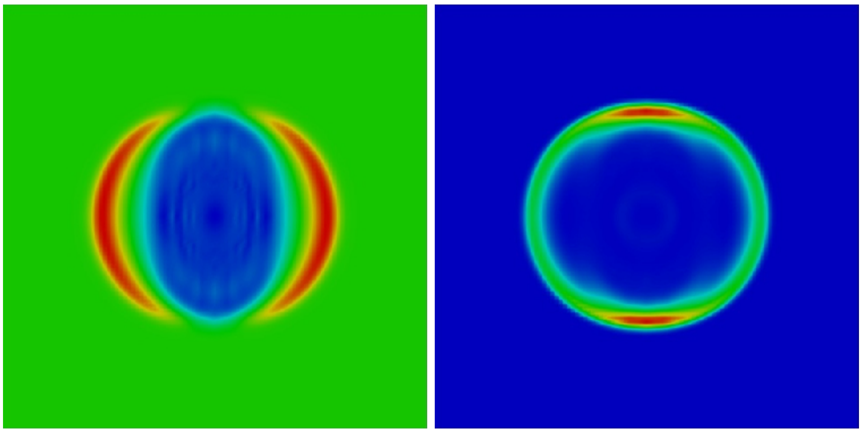

Figure 6: $2D$ magnetic pressure and $2D$ kinetic energy in the magnetic field $5/\sqrt{\pi}$

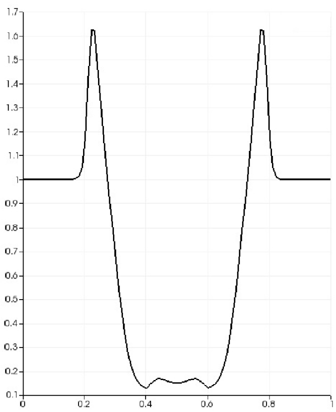

Figure 7: $1D$ density profile in the magnetic field $5/\sqrt{\pi}$

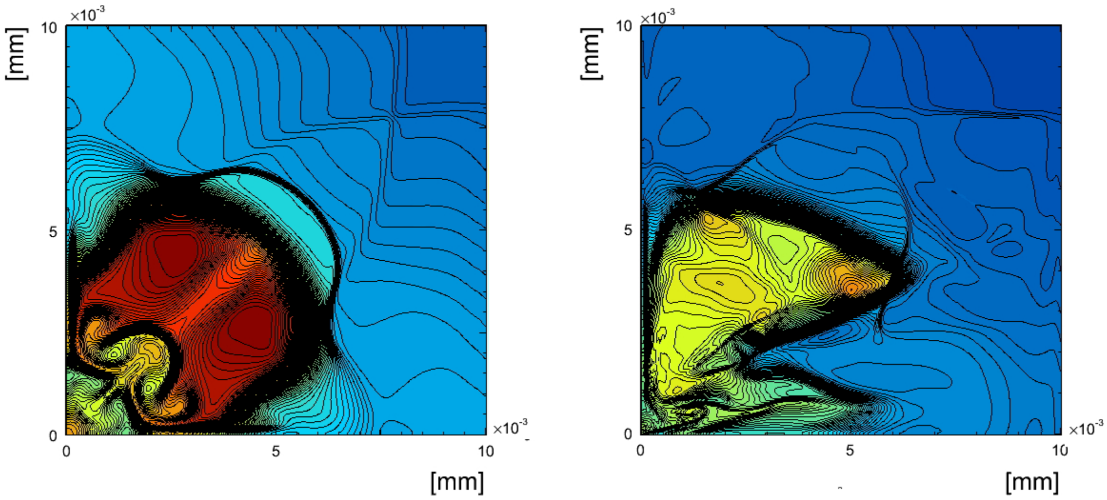

Figure 8: Sod shocktube problem: 2D gas density projections at time 1.76×10^{-8} s without (a) and with (b) magnetic field.

7 CONCLUSIONS

A new 3D kinetic algorithm has been developed for the solution of the magnetohydrodynamics problems. The novel feature of the method is that the local complex Boltzmann-like distribution function incorporated most of the electromagnetic processes terms. The fluxes of mass, momentum and energy across the cell interface as well as the magnetic field are calculated by integrating a local complex Boltzmann-like distribution function over the velocity space. Thus by using this distribution function to calculate the mass, momentum and energy fluxes, most of the electromagnetic contributions are calculated directly, i.e. one does not have to solve the hydrodynamics and magnetic force components separately or differently.

A staggered, divergence free mesh configuration is used for the evaluation of the electromagnetic behaviour.

Numerical examples demonstrate that the proposed method can achieve high numerical accuracy and resolve strong shock waves of the magnetohydrodynamics problems.

The explicit method is chosen with respect to optimal adaptation on the large scale parallel computing systems. The improvement of the stability conditions which is one of the limiting factor for the explicit method will be studied by the implementation of the hyperbolic type of the magneto gas dynamic equations.

8 ACNOWLEDGEMENT

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