Adaptive Finite Volume numerical method

L Bilbao

INFIP-CONICET, and Physics Department (FCEN-UBA),
Ciudad Universitaria, Pab. I, 1428 Buenos Aires, Argentina

E-mail: bilbao@df.uba.ar

Abstract. This work describes a Finite Volume computational method for the parametric study of phenomena in plasmas, i.e. in situations where numerous runs of three-dimensional simulations are required (in many cases, thousands or tens of thousands). Such problems require simple codes, robust, modular (to add or remove physical processes) and do not require high precision. The code is based on a complex multi-component species program with transport and radiation terms. The integration domain is represented with a structured irregular mesh, with fixed connectivity. A new algorithm for the hydrodynamics was implemented in order to improve the computational efficiency plus the improved capability of adapting the mesh to the solution. The improved hydrodynamics method worked well in an ample range of Mach number from subsonic ($10^{-3}$) to supersonic. After each calculation cycle, mesh vertices are moved arbitrary over the fluid. This is done in order to dynamically adapt the mesh to the solution. The adaptive method consists of shifting mesh vertices over the fluid in order to keep a reasonable mesh structure and increase the spatial resolution where the physical solution demands. As an example, we show the results of the development of the Kelvin-Helmholtz instability in local plane slab models of the magnetopause, showing the development and saturation of the instability in an initially unperturbed structure, i.e., the temporal response approach; and the response of a background equilibrium to the excitation by finite amplitude perturbations generated upstream, i.e., the spatial response of the system.

1. Introduction

The scope for developing the present numerical method was to perform parametric studies for optimization of several problems in plasma physics. Nowadays there exist several efficient numerical codes in the subject. However the construction of own computational codes brings the following important advantages: (a) to get a deeper knowledge of the physical processes involved and the numerical methods used to simulate them; and, (b) more flexibility to adapt the code to particular situations in a more efficient way than a closed general code would.

On those premises a new Arbitrary Lagrangian-Eulerian (ALE) Finite Volume algorithm was developed based on a previously reported code [1]. As in the previous version, Three-Dimensional (3D), time depend, multi-component, two-temperature code was used.

The code includes ion viscosity, thermal conduction (electrons and ions), magnetic diffusion, thermonuclear or chemical reaction, Bremsstrahlung radiation, EOS (from the ideal gas to the degenerate electron gas). In the next paragraph the main improvements will be highlighted.
2. Numerical resolution

We have used an ALE Finite Volume method with hexahedral cells that move at arbitrary velocity. The notation and definition of the geometry is described elsewhere [1]. The main advantage of this method is that the geometry is imposed to the cells and not to the operators.

This method consists of integrating conserved quantities over a cell. For a general fluid property $\Psi$, the following identity holds

$$\frac{d}{dt} \int_{V(t)} \Psi \, dV = \frac{\partial}{\partial t} \int_{V(t)} \Psi \, dV + \int_{S(t)} \Psi \cdot \mathbf{w} \cdot dS$$

where integration is performed over a cell of arbitrary volume $V(t)$ with boundary $S(t)$ moving at an arbitrary speed $\mathbf{w}$. By choosing $\mathbf{w} = 0$, that is both $V$ and $S$ remain fixed, a full Eulerian formulation is retrieved. On the other hand, setting $\mathbf{w} = \mathbf{v}(x,t)$ -fluid velocity- leads to the standard Lagrangian formulation. The adaptive method consists of choosing an appropriated $\mathbf{w}(x,t)$ over the fluid in order to keep a reasonable mesh structure and increase the spatial resolution where the physical solution demands.

For the ideal MHD, the equations for mass ($M$), momentum ($P$), internal energy ($E$), and, magnetic flux ($\Phi$), are

$$\frac{dM}{dt} = \frac{d}{dt} \int_{V(t)} \rho \, dV = - \int_{S(t)} \rho (\mathbf{v} - \mathbf{w}) \cdot dS$$

$$M \frac{dY_k}{dt} = - \int_{S(t)} \rho (\mathbf{v} - \mathbf{w}) \cdot dS - \int_{S(t)} dS \cdot q_k^D + \int_{V(t)} dV \omega_k$$

$$\frac{dP}{dt} = \frac{d}{dt} \int_{V(t)} \mathbf{v} \rho dV = - \int_{S(t)} \rho \mathbf{v} (\mathbf{v} - \mathbf{w}) \cdot dS - \int_{S(t)} p dS + \int \mathbf{j} \times \mathbf{B} \, dV$$

$$\frac{dE}{dt} = \frac{d}{dt} \int_{V(t)} \varepsilon \rho dV = - \int_{S(t)} \rho \varepsilon (\mathbf{v} - \mathbf{w}) \cdot dS + \int_{S(t)} \left( \frac{c_p k T}{e} \right) \cdot dS - \int_{V(t)} \rho \nabla \cdot \mathbf{v} \, dV$$

$$\frac{d\Phi}{dt} = \frac{d}{dt} \int_{\Sigma(t)} \mathbf{B} \cdot dS = - \int_{C(t)} \mathbf{dI} \cdot \mathbf{E}' + \int \left[ (\mathbf{v} - \mathbf{w}) \times \mathbf{B} \right] \cdot d\mathbf{l}$$

where $\mathbf{j}$ is the electrical current density, $\varepsilon = \rho / (\rho\gamma - 1)$ the internal energy density ($c_p$ is the specific heat at constant pressure) and $e$ the charge of the electron. In the last equation $\Sigma$ is an arbitrary open surface bounded by a closed path $C$, which moves according to $\mathbf{w}(x,t)$.

The integration domain is represented with a structured irregular mesh, with fixed connectivity made of hexahedral cells. Each cell is surrounded by 6 faces and 8 vertices. Fluid variables are assigned to staggered locations in the mesh. Pressure, internal energy, density, species concentration, cell volume and mass are all assigned to cell centres. Coordinates $(x,y,z)$ and velocities $(u_x,u_y,u_z)$ are assigned to cell vertices.

For example, using $\mathbf{w} = 0$ the evolution of the cell mass $M \approx \langle \rho \rangle V$, $\langle \rho \rangle$ being a mean value of the density over de cell, and $V$ the volume, is written as
\[
\frac{dM}{dt} = -\sum_{i} \rho_i v_i \cdot S_i
\]  

(6)

where \( S_i, v_i, \rho_i \) are the surface, velocity and mass density of the \( i \)-th face of the cell. Analogously, the momentum of a cell, \( P \approx \langle \rho \rangle \langle v \rangle V \), evolves according to

\[
\frac{dP}{dt} = -\sum_{i} \rho_i v_i (S_i \cdot v_i) - \sum_{i} \rho_i S_i + \frac{1}{4\pi} (\sum_{i} S_i \cdot B_i) \times \langle B \rangle
\]  

(7)

where \( \langle B \rangle \) is the mean value of the magnetic field on a cell.

Using the same ideas all integral equations are discretized. In order to set the values on the faces, appropriate mean values over adjacent cells are used.

Global conservation of the above magnitudes is checked during calculation. Also, condition \( d\tau(B) = 0 \) is controlled over the whole integration domain.

The same method may be applied for more complex modelling of plasmas that includes ion viscosity, thermal conduction (electrons and ions), magnetic diffusion, chemical or thermonuclear reactions, Bremsstrahlung radiation, and realistic equation of state (EOS) from the ideal gas to the degenerate electron gas. The integration in time is sequential. This means that each process is integrated with a different uncoupled method during a time step. The overall truncation error is \( O(\Delta x, \Delta y, \Delta z, \Delta t) \). Solution does not dependent on the integration order of the terms.

Calculation proceeds as follows:

- Hydrodynamics is integrated using an improved Predictor-Corrector method [2].
- Diffusion processes (of species concentration and energy) are integrated with ADI methods (Alternating Direction Implicit) for the 2D/3D case, and with full implicit methods for the 1D case.
- Source terms from chemical or nuclear reactions are explicitly integrated in time.
- Mesh vertices are moved arbitrary over the fluid as described below.

Lagrangian cell methods are not adequate for describing flows undergoing large distortions, because cells may undergo severe deformations.

Nuclear burning, combustion structures, or instabilities may present steep gradient of temperature, species concentration, and heat release. The adaptive method consists of shifting mesh vertices over the fluid in order to keep a reasonable mesh structure and increase the spatial resolution where the physical solution demands.

The rezone velocity \( U \) with which vertices are moved over the fluid is calculated in order to increase spatial resolution where steep temperature gradients and high chemical/nuclear heat release are produced. The new coordinates for each vertex are calculated in such a way that the Lagrangian distance remains uniformly distributed. A possibility is to define \( U \) in order to restore an Eulerian grid. This calculation is performed following one computational direction. The procedure is repeated over several paths where corrections are needed.

Vertex \( i \) moves from \( i \) to \( i' \) according to

\[
x_{i}' = x_i + U \Delta t
\]  

(8)

where \( U \) is the rezone velocity. During this process there is an exchange of mass, species, energy and momentum among neighbourhood cells.

Then the following steps must be applied

- Calculate the new coordinates using (8), then calculate the volume exchange among neighbourhood cells
- Associated with the volume exchange there will also be a mass, species concentration and total energy exchange. The mass, concentration or energy per unit mass assigned to this volume are computed using a donor cell flux. Finally, fluid conserved properties are updated.
- Once updated the conserved cell and vertex properties, cell volume, density and species concentration are calculated from the new vertex coordinates.

3. Development of the KH instability
A physical problem studied by means of the numerical code is related to the turbulent mixing layers of plasma at the near equatorial flanks of the terrestrial magnetopause. The numerical 3D code was used to simulate the large amplitude perturbations and waves at the dusk side low latitude boundary layer of the magnetopause generated by an interplanetary tangential discontinuity.

We focused on the motion and structure of the magnetopause/boundary layer observed in response to a joint tangential discontinuity/vortex sheet (TD/VS) observed by the ACE spacecraft on December 7, 2000. Sharp polarity reversals in the east-west components of the field and flow occurred at the discontinuity. These rotations were followed by a period of strongly northward IMF. These two factors elicited a two-stage response at the magnetopause, as observed by Cluster spacecraft situated in the boundary layer at the dusk side terminator.

These studies were aimed to clarify some particular physical properties of the instability of velocity shear flows and mixing layers, such as the 3D vorticity amplification mechanism and non conservation of vorticity flux.

The most common of these is the Kelvin-Helmholtz instability feeding on the flow shears which exist across the magnetosheath/magnetosphere interface (see figure 1). Ever since Dungey [3] pointed out the possibility of the magnetopause going Kelvin-Helmholtz unstable, many studies have been devoted to this instability, the surface waves it causes, their coupling to the geomagnetic field giving rise to field line resonances, and how this instability might mediate the entry of magnetosheath plasma into the magnetosphere [4-13].

Attention has been drawn to two other interplanetary parameters whose changes may occasion considerable deformation and motion of the magnetopause. One is a variable orientation of the interplanetary magnetic field (IMF). Fairfield et al. [14] showed that, even when the dynamic pressure is constant, the magnetopause and inner-magnetosphere boundaries may be in motion. They attributed these motions to pressure changes generated in the foreshock region by the IMF changes. These pressure changes subsequently convect through the bow shock and impinge on the magnetopause. The authors thus concluded that even in the presence of a solar wind that is absolutely steady in velocity and density but which carries an embedded interplanetary magnetic field of variable orientation; there will be a variation of pressure exerted on the magnetopause.

**Figure 1.** Sketch of vortex formation due to the Kelvin Helmholtz instability in the magnetopause

For the observations at the magnetopause we focused on Cluster 3 data. The Cluster spacecrafts were on an outbound trajectory just tail ward of the dusk terminator and at northern latitudes. (At this
early stage of the mission, the spacecraft separation was of order a few hundred km and all spacecraft see the same features.). For some hours prior to our observations, the spacecraft stayed in the vicinity of the magnetopause because the magnetopause boundary was expanding slowly outward due to a slow decrease in dynamic pressure. From 14:00 to 14:30 UT the spacecraft stays within a distance of 0.4 RE from the magnetopause. We may reasonably assume that Cluster 3 is inside the boundary layer according to the model, in agreement with instrument readings.

We carried out a stability analysis of a limited segment of the magnetopause, where the boundary layer may be considered to lie in a local tangent plane. The boundary layer is then modelled as a planar plasma slab with stratified density, flow velocity, and magnetic field. The physical quantities on either side of the magnetosheath-magnetosphere transition are obtained from the Cluster 3 readings at the extremes of the large oscillations recorded after 13:58 UT. Specifically, we selected the second oscillation, where the lowest speed was recorded at maximum $T$. That is, we assume that at the extremes of the oscillation, Cluster 3 samples alternately the high density-low temperature magnetosheath plasma, and the low density-high temperature magnetosphere plasma. In this way the local instability is examined by parameters measured locally and in temporal proximity.

The full description of the problem and main results are presented in [15]. Anyhow, some sample outputs showing the 3D, complex character of the problem are presented. Figure 2 shows streamlines complexity and formation of a swirling flow in the large eddy at $t = 84$ s. Figure 3 shows the development of kinetic helicity, $t = 132$ s, contours of kinetic helicity density are displayed. Figure 2 illustrates the progression from the simple, parallel shear flow, where the kinetic helicity density is initially zero, to a complex stage with a large vortex core and deformations of large magnitude of the vorticity layer. Kinetic helicities of both sign arise from the initial velocity field perturbation. Note that the KH waves appear already after a few theoretical e-folding times, due to the great oscillations generated by the tangential discontinuity stress that has reduced the amplification time. In order to get an appropriated resolution, up to 1,000,000 cells were used.

Some interesting features of the phenomenon are obtained from the numerical results. For example, high temperature rises in a compact vortex core correlated with local density depletion while gas, and magnetic pressure (roughly constant across the structure) are near to surrounding values. Also detected a high density patch in a vorticity structure correlated with a local increase of gas pressure, whereas temperature stays near to surrounding values.

Figure 2. Mixing layer, $t = 84$ s, vorticity contours and streamlines. Comparing streamlines views: left, fixed (Earth) frame, and right, moving frame with average velocity ($U$= 78.5 km/s). In the moving frame magnetosheath and magnetopause plasmas are seen counter streaming.
Figure 3. Development of kinetic helicity, $t = 132$ s. The plot shows contours of kinetic helicity density (left). Details of vorticity evolution at $t = 180$ s with a view of the distortions of shape of the BL flow and some streamlines of swirling flows.

Concomitant with 3-D vortex stretching, kinetic helicity density rises at the vorticity cores. Finally, non conservation of vorticity becomes manifest at about (or even before) one rollover time, where in addition to vortices with positive rotation (the same sign of the original vorticity sheet) other coherent structures with strong negative vorticity also arise.

The rise of these coherent structures has important consequences for the properties of the mixing layer. There is a broadening of the boundary layer's width, and a substantial lengthening of the transit time of plasma, compared with that of a stable laminar boundary layer.

4. Conclusions
The numerical simulation was a powerful tool for the parametric analysis of the development of Kelvin-Helmholtz instability. The sequential implementation resulted of practical use, because each physical process was treated with a different numerical method. The improved hydrodynamics method worked well in an ample range of Mach number from subsonic ($10^{-3}$) to supersonic.

We reported here a study of the MHD development of vortices in compressible, non-homogeneous, mixing layers due to the velocity gradient instability. The non-linear evolution was computed with a new 3D+t FV code of temporal mixing layers tailored to represent distinctive conditions of the terrestrial magnetopause. The boundary layer is characterized by the growth of large-scale vortices, and becomes a site of mass mixing favouring enhanced plasma diffusion. The rise of counter-rotating vortices from the evolution of the original vortex sheet is one of the noteworthy processes revealed by the simulation. The adaptive grid process was able to keep a reasonable mesh structure and resolution inside the vortices.

5. Acknowledgments
Work partially supported by grant UBA 20020100100866, University of Buenos Aires.

6. References
[1] Bilbao L 1990 *J Comp Physics* 91 361.
[2] Bilbao L 2009 “Computational Plasmadynamics applied to parametric studies” *Journal of*
Physics: Conference Series 166, 012020.

[3] Dungey J W 1955 “Electrodynamics of the outer atmospheres” Report 69, Ions Res Lab. Pa State Univ, University Park.

[4] Southwood D J 1979 Proceedings of Magnetospheric Boundary Layers Conference ESA SP-148 Eur Space Agency Paris 359

[5] Miura A 1984 J Geophys Res 89 801

[6] Chen S H, Kivelson M G, Gosling J T, Walker R J, Lazarus A J 1993 J Geophys Res 98 5727.

[7] Kivelson M G, Chen S H 1995 in Physics of the Magnetopause (edited by P Song, B U O Sonnerup and M F Thomsen) Geophys Monogr Ser 90 AGU Washington DC 257.

[8] Seon J L, Frank A, Lazarus A J, Lepping R P 1995 J Geophys Res 100 (11) 907.

[9] Fairfield D H, Otto A, Mukai T, Kokubun S, Lepping R P, Steinberg J T, Lazarus A J, Yamamoto T 2000 J Geophys Res 105 (22),159.

[10] Otto A, Fairfield D H 2000 J Geophys Res 105 (A9) 21175-21190.

[11] Farrugia C J, Gratton F T, Contin J, Cochechi J C C, Arnoldy R L, Ogilvie K W, Lepping R P, Zastenker G N, Nozdrachev M N, Fedorov A, Sauvaud J A, Steinberg J T, Rostoker G 2000 J Geophys Res 105 (A4) 7639-7667.

[12] Gratton F T, Bender L, Farrugia C J, Gnvi G 2004 J Geophys Res 109 (A04211) 1-13.

[13] Farrugia C J, Gratton F T, Torbert R 2001 Space Sci Rev 95 (1/2) 443-456

[14] Fairfield D H, Baumjohann W, Paschmann G, Luehr H, Sibeck D G 1990 J Geophys Res 95 3773-3786.

[15] Gratton F T, Bilbao L, Farrugia C J, Gnvi G 2009 “Large eddy simulations in MHD: the rise of counter-rotating vortices at the magnetopause” Journal of Physics: JPCS 166, 012023.