An innovative, particle-supported Lagrangian method for MHD plasma simulations

F. Bacchini, V. Olshevsky, G. Lapenta

Centre for mathematical Plasma Astrophysics, Department of Mathematics, KU Leuven,
Celestijnenlaan 200B, B-3001 Leuven, Belgium

Particle-in-Cell (PiC) methods are well-established techniques for plasma simulations. The basic idea behind the method consists of the exchange of information between a computational grid, in which fields are advanced in time, and a large number of particles which act as sources for the fields.

The basic computational cycle of PiC methods is composed of four steps:

- Projection from particles to the grid: information from the particles is gathered at the grid points in order to compute the fields.
- Field advancing: the grid quantities are evolved in time according to the preferred discretisation scheme.
- Projection from grid to particles: the advanced field quantities are used to compute forces acting on particles.
- Particle advancing: the particles are moved in the domain according to the governing equations of motion.

Depending on the considered physical model, the fields and the equations of motion differ in simulations. The four basic steps, however, remain the same.

“Classical” PiC methods are usually employed in kinetic simulations of multi-species plasmas. Here, particles represent portions of the six-dimensional phase space where the distribution function governs the statistics of kinetic phenomena. The electric and magnetic fields are computed at the grid points by using the charge density and current, interpolated from the particles, as sources. After the field advancing phase, the particles are pushed by the Lorentz force and the cycle can start over. Although this approach is more fundamental, it is very expensive due to the limited size of the grid cells imposed by the need to resolve kinetic scales.

For very large domains, commonly studied in astrophysical contexts, magnetohydrodynamics (MHD) gives an acceptable approximation as the particles are treated like a single magnetised fluid, subjected to the effects of electromagnetic fields, in a continuum description. Particle-based MHD follows the same principle described above for the kinetic approach, but in this case the employed particles are not subjected to actual single-particle dynamics. In “fluid” PiC, particles are, in facts, a less coarse representation of the fluid description than the computational grid [1]. As a consequence, they also carry macroscopic properties. In pure hydrodynamics, the projection of the conserved quantities from particles to grid allows one to compute the advection of mass, momentum and energy throughout the domain in a Lagrangian description of the system, without the need to move the grid. Exchange of information from particles to grid is carried on according to

$$C_g = \sum_p c_p W_{pg}, \tag{1}$$

where C_g and c_p represent the same conserved quantity in the grid and particle frames, respectively. The interpolation function W_{pg} is chosen in order to guarantee that the gathering of information on a grid element involve a sufficiently high number of particles (usually, b-splines of some order are employed). An approximate inverse of the above relation is used when projecting grid quantities on the particles. In the grid advancing phase, any preferred formulation of the fluid equations can be solved on the fixed grid. This avoids a number of computational issues which are common in classical Lagrangian MHD solvers.

A full MHD particle-supported simulation has to deal with several issues affecting particle methods. Two fundamental aspects to be addressed are the so-called ringing instability, which occurs in explicit PiC simulations, and the preservation of the solenoidality condition by suitably linking particles to the magnetic field.

The ringing instability is due to aliasing occurring when information is exchanged between particles and grid. The effect in fluid PiC simulations is to increase the interpolation error to what it would be if there were one particle per cell. The results obtained in this case are obviously not reliable and counter-measures are necessary. An effective but expensive solution consists of implicitly differencing the dynamical equations. It is desirable, however, to avoid such level of complication in order to obtain a fast, portable code that can run on small machines while retaining the advantage of particle methods.

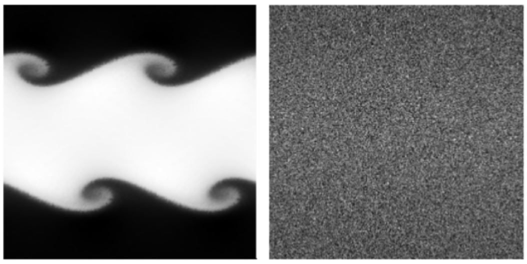

Figure 1: *2D Kelvin-Helmholtz instability at t=2.5 with (left) and without (right) the volume evolution procedure switched on.*

In our work, we introduce a particle volume evolution procedure in order to increase the overall accuracy of the method. The cell volume is interpolated from the particles along with the other quantities. Particle volume V_p is updated during the computation in a similar fashion to the Material Point Method (MPM) for solid mechanics [2]. The evolution depends on gradients of the velocity $\mathbf{u}$ as $V_p^{n+1} = V_p^n |J_p^{n+1}|$, where

$$J_p^{n+1} = (\mathbf{I} + \Delta t \nabla \mathbf{u}_p^{n+1}) J_p^n, \tag{2}$$

and $\nabla \mathbf{u}_p^{n+1} = \sum_g \nabla W_{pg} \mathbf{u}_g^{n+1}$.

The above procedure improves the method's performance and brings in the additional advantage of suppressing the ringing instability. The normalisation introduced in the density appears to be enough to avoid spreading the aliasing effects on the other macroscopic variables in explicit simulations. Figure 1 shows the comparison between two simulations with and without the volume evolution procedure switched on.

The extension of the fluid PiC to MHD has been tackled in several ways. The first step is the definition of a link between particles and the magnetic field, which differs from the other macroscopic quantities as it is not a conserved variable. If the particles are assigned a certain fraction of magnetization, several divergence cleaning approaches are allowed, which however do not always guarantee that $\nabla \cdot \mathbf{B} = 0$ be maintained to machine precision. A projection method, suitably formulated, can satisfy such condition at the cost of solving a Poisson equation at each time step [3]. This is again an undesirable aspect, especially in explicit codes, as it greatly raises the computational cost.

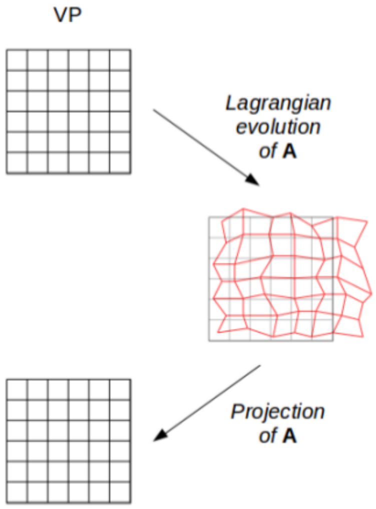

Figure 2: *Schematisation of the VP strategy. The vector potential evolves on a separate grid and its values at the fixed grid points are retrieved via interpolation.*

A vector potential (VP) strategy ensures that the discrete divergence-free condition be respected at each time step [4]. In this case, however, the link between particles and magnetic field quantities cannot imply conserved variables. A natural solution, however, is to relegate $\mathbf{B}$ (and, as a consequence, the vector potential $\mathbf{A}$) to the role of pure grid quantity. In this case, a moving grid can be employed to advect the vector potential through the domain. In 2D, this can be done according to the particularly advantageous equation $dA_z/dt = 0$, as the z-component of $\mathbf{A}$ is the only one needed to compute $B_x = \partial_y A_z$ and $B_y = -\partial_x A_z$. The grid points of the moving grid can therefore be assigned a value of A_z which will not change during the simulation. Simple interpolation between the two grids allows one to retrieve the necessary value of the vector potential at the fixed grid nodes and obtain a solenoidal magnetic field to be used in the momentum equation. The procedure is sketched in Figure 2.

The use of a moving grid, although only for magnetic field-related effects, brings back the usual downsides which are avoided by the presence of particles. While the ultimate goal remains to link the particles to the vector potential in a direct way, the formulation is very efficient in two dimensions as it only requires a one-way interpolation per time step, thus minimising the dissipation and computational cost. No higher-order procedure, such as solving a Poisson equation, is necessary.

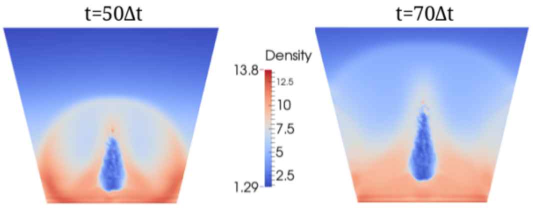

Figure 3: *Simulation of a CME propagating through the solar atmosphere at two consecutive moments in time.*

The particle method expresses all its potential in multiple applications. Where the system dynamics would cause large deformations in the grid structure, the particles can instead supply the necessary level of accuracy without degeneracy of the grid. This peculiarity has remarkable efficiency in, e.g., solid mechanics simulations [5]. In astrophysical contexts, large interstellar moving structures such as Coronal Mass Ejections (CME) can be followed throughout their propagation in the background medium thanks to the Lagrangian formulation of the system. This feature permits to avoid simulating a very large domain when the dynamics of interest is involving only a small part of it. Figure 3 shows an example of application to CME dynamics through a portion of the solar atmosphere [6].

The method is fully functional for 2D ideal MHD simulations. Extension to full 3D, non-ideal MHD is currently being pursued with the final aim of applying the particle method to solar-related phenomena. CMEs, solar flares, solar wind dynamics are possible candidates for testing the potential of the strategy.

References

[1] J.U. Brackbill and H.M. Ruppel, Journal of Computational Physics **65**, 314 (1986)

[2] A. Sadeghirad, R.M. Brannon and J. Burghardt, International Journal for Numerical Methods in Engineering **86**, 1435 (2011)

[3] J.U. Brackbill, Journal of Computational Physics **96**, 163 (1991)

[4] D.J. Price, Monthly Notices of the Royal Astronomical Society **401**, 3 (2009)

[5] S.G. Bardenhagen, J.U. Brackbill and D. Sulsky, Computer Methods in Applied Mechanics and Engineering **187**, 529 (2000)

[6] F. Bacchini, R. Susino, A. Bemporad and G. Lapenta, The Astrophysical Journal **809**, 58 (2015)