Simulating the interaction between supra-thermal particles and the magnetic field in astrophysical shocks

A. J. van Marle¹, F. Casse¹ & A. Marcowith²
¹Laboratoire AstroParticle & Cosmologie (APC), Université Paris Diderot, CNRS/IN2P3, CEA/Irfu, Observatoire de Paris, Sorbonne Paris Cité, 10, rue Alice Domon et Leonie Duquet, F-75205 Paris Cedex 13, France.
²Laboratoire Univers et Particules de Montpellier (LUPM) Université Montpellier, CNRS/IN2P3, CC72, place Eugène Bataillon, 34095, Montpellier Cedex 5, France.
E-mail: vanmarle@apc.univ-paris7.fr

Abstract. In order to model the magnetic field amplification and particle acceleration that takes place in astrophysical shocks, we need a code that can efficiently model the large-scale structure of the shock, while still taking the kinetic aspect of supra-thermal particles into account. Starting from the proven MPI-AMRVAC magnetohydrodynamics code we have created a code that combines the kinetic treatment of the Particle-in-Cell (PIC) method for supra-thermal particles with the large-scale efficiency of grid-based hydrodynamics (MHD) to model the thermal plasma, including the use of adaptive mesh refinement. Using this code we simulate astrophysical shocks, varying both the Mach-number and the angle between the magnetic field and the shock to test our code against existing results and study both the evolution of the shock and the behaviour of supra-thermal particles. We find that the combined PIC-MHD method can accurately recover the results that were previously obtained with pure PIC codes. Furthermore, the efficiency of the code allows us to explore the available parameter space to a larger degree than has been done in previous work. Our results suggest that efficient particle acceleration can take place in near-oblique shocks were the magnetic field makes a large angle with the direction of the flow.

1. Introduction
Astrophysical shocks accelerate particles to high velocities in a process known as Fermi-acceleration, which involves repeated crossings of the shock. We observe these particles as cosmic rays (CRs). This process also influence the evolution of the shock, causing turbulence and triggering instabilities in the magnetic field in both the pre-shock and post-shock areas (see [1] for a review.) Simulating this process numerically is difficult because of the different length scales involved. Astrophysical shocks are best modelled using grid-based magnetohydrodynamics (MHD), which is a computationally efficient method that allows for the modelling of large scale structures by treating the gas as a fluid that can be represented by average values. Unfortunately, MHD does not include particle physics and can therefore not be used to simulate the behaviour of particles that behave in a supra-thermal fashion. The movement of individual particles in a gas can be modelled using the Particle-in-Cell (PIC) approach, which treats the gas a
collection of individual particles. However, although the PIC method can accurately model the acceleration of individual particles, it is computationally expensive and difficult to apply to large scale structures.

In order to be able to model both the shock and the particle acceleration, we combine these two methods in a a single code, using the prescription by [2]. This model is based on the assumption that an astrophysical plasma can be described as being primarily thermal, with a relatively small supra-thermal component. The thermal part of the plasma can be modelled using grid-based MHD. The supra-thermal part can be modelled using the PIC method. The effect of the thermal plasma on the particles can be expressed using the electromagnetic field generated by the thermal plasma. For the influence of the supra-thermal particles on the thermal component, [2] used a modified version of Ohm’s law. We now present a computer code that uses a similar approach. The main advantage of this approach over the more traditional PIC and PIC-hybrid codes lies in its computational efficiency. Because the thermal gas can be modelled as a fluid, rather than as individual particles, the total number of particles in the simulation can be greatly reduced, which in turn allows us to focus on those particles that behave in a supra-thermal fashion.

We have used this code to repeat simulations of a high-Mach shock travelling into a weakly magnetized gas done by [2] who used the same approach. Simulations of this situation were done previously by [3,4] using a spherical harmonic expansion of the Vlasov-Fokker-Planck equation and by [5–7] using the PIC-hybrid approach.

2. Particles in MHD cells II: physics
The underlying assumption for the Particles in MHD Cells method is that the plasma can be described as a thermal plasma with a (relatively) small correction term caused by the presence of supra-thermal particles. The thermal plasma can be described by a series of conservation equations for mass, momentum and energy and the magnetic induction equation, as is the case in classical MHD. However, the equations contain additional terms to incorporate the effect that the presence of the supra-thermal articles have on the thermal plasma.

The new conservation equations for the thermal gas can be written as follows:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \]  
\[ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \otimes \mathbf{v} - \frac{\mathbf{B} \otimes \mathbf{B}}{4\pi} + P_{\text{tot}} \mathbf{I} \right) = - \mathbf{F}_{\text{part}}, \]

with \( \mathbf{B} \) the magnetic field and \( P_{\text{tot}} = P + B^2/8\pi \) the total pressure. The energy equations is

\[ \frac{\partial e}{\partial t} + \nabla \cdot \left( (e + P_{\text{tot}}) \mathbf{v} + (\mathbf{E} - \mathbf{E}_0) \times \frac{\mathbf{B}}{4\pi} \right) = - \mathbf{u}_{\text{part}} \cdot \mathbf{F}_{\text{part}} \]

where \( e \) is the total energy density of the thermal plasma, \( \mathbf{E}_0 = -\mathbf{v}/c \times \mathbf{B} \) is the electric field generated by the motion of the thermal plasma, and \( \mathbf{E} \) is the electric field generated by the thermal plasma and the supra-thermal particles combined. \( \mathbf{E} \) is obtained through a modified version of Ohm’s law:

\[ c \mathbf{E} = -((1-R) \mathbf{v} + R \mathbf{u}_{\text{part}}) \times \mathbf{B}, \]
density applied by the electromagnetic field upon the supra-thermal particles $F_{\text{part}}$, which is defined as

$$F_{\text{part}} = (1 - R) \left( n_{\text{part}}q E_0 + \frac{J_{\text{part}}}{c} \times B \right),$$

with $n_{\text{part}}q$ the particle charge density and $J_{\text{part}}$ the current generated by the supra-thermal particles. We close this set of equations with the induction equation:

$$\frac{\partial B}{\partial t} = c \nabla \times E,$$

and an equation of state, for which we assume an ideal gas.

Defined this way, equations 1-3 and 6 can be solved together in a self-consistent way. The only outside information required, are the charge and current density generated by the supra-thermal particles.

The motion of the supra-thermal particles can be calculated through the momentum equation of a charged particle in an electromagnetic field:

$$\frac{\partial p_{\alpha,j}}{\partial t} = q_j \left( E + \frac{u_{\alpha,j}}{c} \times B \right),$$

with $p_{\alpha,j}$, $q_j$ and $u_{\alpha,j}$ the momentum, charge, and velocity of a particle with index $j$ and type $\alpha$. (In practice we will treat all particles as protons in this paper, but the code allows for multiple particle species.) Note that there is no direct interaction between the particles because we assume that they behave in a non-collisional fashion.

3. Particles in MHD cells II: numerics

In order to combine the PIC and MHD methods into a single code we start with an existing grid-based finite volume MHD code: MPI-AMRVAC [8]. This is a well-tested code that uses the OCTREE system of adaptive mesh refinement [9] and can run in parallel on distributed memory platforms. We retain the existing MHD module but add the extra terms described in the previous section to the conservation equations. In addition we have written a new module to handle the particle motion. This module uses the existing MHD grid, including the adaptive mesh refinement and adds particles. At the beginning of each time step, the MHD quantities of the thermal gas are updated according to the conservation equations. Simultaneously, the particles are moved according to the momentum equation (Eq. 7) by means of a relativistic Boris-pusher [10], which uses the electromagnetic field as it was at the beginning of the time-step. Once the particles have been moved, their effective charge and current is interpolated onto the cell-centres of the MHD grid, where they will contribute to the integration of the conservation equations for the next time step.

In order to maintain numerical stability we limit the time-step using the CFL condition:

$$\Delta t \leq C \min \left( \frac{\Delta x}{v_{\text{max}}} \right),$$

with $\Delta t$ the time step, $C$ a constant (usually less than one), $\Delta x$ the size of a gridcell and $v_{\text{max}}$ the maximum speed at which any kind of signal travels through the gas. The latter is calculated as the maximum value of the sum of the bulk motion of the thermal fluid various wave velocities, such as sound speed and Alfvén speed. This is then compared to the maximum particle velocity. In addition we limit the time-step to a predetermined fraction of the gyro-time to ensure that we capture the motion of individual particles.

A problem that occurs when combining PIC and MHD is that the local magnetic field deviates from being divergence free as a result of local charge concentrations. We have implemented a Constrained Transport algorithm based on [11] to ensure that the magnetic field remains divergence free.
4. Simulations

We test our code by performing two simulations of moving shocks in a weak magnetic field. For the first simulation we duplicate the input parameters used by [2]: The shock moves parallel to the magnetic field with a shock velocity equal to 30 times the Alfvén speed. Unlike [2] we simulate in the frame of reference of the shock in order to reduce the size of the simulation. At the start of the simulation we fill the gas with a thermal plasma conform the Rankine-Hugoniot conditions for a standing shock with an upstream velocity of \( V_{sh} = 3.10^{-3}c \) along the \( x \)-axis, flowing from the right \( x \)-boundary toward the left \( x \)-boundary. Furthermore the gas contains a magnetic field corresponding to an Alfvén speed of \( V_{A0} = 10^{-4}c \) and the upstream medium is considered to follow equipartition. For a pure MHD simulation this is a stable situation, which should only display minor deviation at the shock due to the size of individual gridcells.

Once the simulation starts we introduce individual particles directly behind the shock at such a rate that they contain 0.2 percent of the total mass that flows through the shock, conform [2], which in turn derived this percentage from [5–7]. These particles are introduced at 3 times the shock velocity and move in a random direction relative to the speed of the post-shock gas.

For the second simulation, we repeat the model described previously, but with the magnetic field at a 70 degree angle with the direction of the flow in the pre-shock medium. Note that this means that the post-shock magnetic field is stronger than the pre-shock field as a result of compression of perpendicular component of the field in the shock. This configuration has not yet been explored using the combined PIC-MHD method, but similar simulations have been performed using the PIC-hybrid method by [5–7].

4.1. Results: 1 parallel model

The results of our first simulation are shown in Fig. 1, which shows the magnetic field strength, thermal gas density, and relative supra-thermal particle density to thermal gas density at three stages of the parallel shock simulation.
Figure 2. Time evolution of the energy spectrum of supra-thermal particles injected at energy $E_{\text{inj}}/m_i c^2 = 4 \times 10^{-5}$, for the simulation shown in Fig. 1. In the late stages of the simulation a supra-thermal tail is forms, which tends to a power-law spectrum in agreement with a diffusive shock acceleration process.

As a result of the disturbance in the magnetic field, particles start to move back and forth across the shock, being accelerated in the process. This is shown in Fig. 2, which shows the particle spectra at various moments in time. As time progresses, the number of high velocity particles increases and they form the kind of spectral energy distribution that is expected from Fermi-acceleration.

4.2. Results: 2 near-perpendicular model

The results of the second simulation show a different behaviour compared to the first simulation, as shown in Fig. 3. Initially, a long wavelength pattern appears in the upstream medium. This pattern is the result of small-scale corrugation of the shock, which causes particles to move upstream, not as a smooth flow, but in the form of localized streams. As this pattern interacts with the shock, the shock corrugation increases in strength and downstream turbulence appears. Eventually, she shock itself is disturbed to the point where we have to stop the simulation.
Figure 3. Similar to Fig. 1, this figure demonstrates the evolution of the gas for the near-perpendicular shock (70 degree angle between flow and magnetic field.) From an early stage, the upstream medium shows a long-wavelength pattern caused by particle streams moving upstream from the shock. Over time this phenomenon causes both increased shock corrugation as well as downstream turbulence.

The particle acceleration for this model follows a different pattern as well as shown in Fig. 4. Initially, only a limited acceleration occurs. This is the result of particles circling the streamlines near the shock and crossing the shock repeatedly as they move [13]. Only when the upstream and downstream magnetic disturbance increases does the pattern of Fermi-acceleration emerge.

5. Discussion
Our parallel simulation recovers the results obtained by [2] as well as the PIC-hybrid simulations by [5–7], proving the validity of our code. However, our results for the near-perpendicular case differ radically from those obtained by [6] for a similar situation. Upon closer investigation we can identify two reasons for this: Firstly, the PIC-hybrid models have trouble generating a sufficient number of high velocity particles. Although the absolute number of particles in these simulations is much higher than in our own, which typically contains no more than 10 million particle at any given time, a PIC-hybrid code uses most of its particles to simulate the thermal plasma, leaving only a small fraction to behave in a supra-thermal fashion. By contrast, all our particles behave supra-thermally, because the thermal gas is represented by the MHD part of the code. This leaves us with a larger effective particle population. Without such a population, it is impossible to generate an upstream disturbance of the magnetic field. The second reason lies in the size of the simulation box. The progression of events in the near-perpendicular model relies on the formation of the long-wavelength pattern in the upstream medium. The PIC-hybrid models did not have sufficient space in the perpendicular (y) direction to resolve this wave, being smaller than the wavelength. This demonstrates the advantage of the combined PIC-MHD approach, which allows for larger simulations without becoming prohibitively computationally expensive.

6. Conclusions
We have shown the initial results obtained with our new combined PIC-MHD code. For a parallel shock we have recovered the results obtained with several models ranging from combined PIC-MHD, through PIC-hybrid, to Vlasov-Fokker-Planck. In the case of the near-perpendicular shock model, the computational efficiency of the combined PIC-MHD method has allowed us to increase the scale of the simulations, which has led to a new result, showing that particle
Figure 4. Similar to Fig. 2 but for the simulation shown in Fig. 3. Initially, the particles show only limited acceleration as they circle back and forth across the shock. In the later stages a plateau corresponding to Fermi-acceleration appears.

acceleration can occur even in near-oblique shocks. A full description of our code and results will soon be published and has appeared in pre-print [14].

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