Coupling of the MPI-AMRVAC MHD code with the iPIC3D kinetic code

K. Makwana, R. Keppens, G. Lapenta

Center for mathematical Plasma Astrophysics, KU Leuven, Leuven, Belgium

Magnetic reconnection is a ubiquitous plasma phenomenon in which magnetic field lines break and reconnect in a local region, changing the global topology. This change in magnetic topology drives global flows and energy conversion. Often kinetic physics is required to explain the observed rate of reconnection. In order to simulate this kinetic particle-in-cell (PIC) codes are utilized, which tend to be more computationally intensive than magnetohydrodynamic (MHD) codes because they simulate hundreds of quasi-particles in each computational cell. However, kinetic effects are often localized to the small diffusion region where field lines break and reconnect. Therefore, such a problem can be suitably modeled by treating only the localized diffusive region kinetically and the outer region by MHD. We can expect an ideal scale-up in the computation speed by the inverse fraction of PIC domain volume to MHD domain volume, compared to a fully kinetic simulation. Such an approach will require a coupling between the larger MHD domain and the smaller, embedded PIC domain.

We describe such a coupling between the versatile MHD code MPI-AMRVAC and the implicit particle-in-cell (PIC) code iPIC3D. MPI-AMRVAC is a block-adaptive-mesh advection code suitable for MHD computations [1], [2]. Each grid-block can be refined/coarsened by a factor of two at user-specified time intervals, giving rise to hierarchically nested grids, which is useful for making grids compatible with PIC requirements. It can also solve Hall-MHD which can be useful in coupling with kinetic simulations. It has been widely used for a variety of heliospheric and astrophysical problems. iPIC3D uses an implicit-moment method to solve the field equations which are linearized by using a Taylor expansion [3], [4]. Thereby, the field equations do not need particle information at the next time step. The particles are advanced implicitly. This method allows the time-step to be $5X - 10X$ longer and grid spacing to be $10X - 50X$ bigger compared to explicit PIC codes. This has allowed iPIC3D to simulate magnetic reconnection with realistic mass ratios in physically large systems. iPIC3D has also been coupled with the BATS-R-US MHD code for studying planetary magnetospheres [5].

One-way coupling from MPI-AMRVAC to iPIC3D has been implemented for steady-state configurations. At regular intervals in MPI-AMRVAC, the grid blocks to be converted into PIC blocks are identified. The MHD values of density(ρ), velocity($\mathbf{v}$), magnetic field($\mathbf{B}$), pressure(p), and current density($\mathbf{J}$) at the cell-corners of these grid blocks are output to binary files. The iPIC3D has been made into a C++ library which can be called as an object from within MPI-

AMRVAC. iPIC3D initializes its grid and physical state from the files written by AMRVAC. A linear interpolation function is used to get physical values at any position within a cell. A separate MPI-communicator is utilized for iPIC3D so that it can run on the same processors as AMRVAC, making the computing as efficient as possible. The electromagnetic fields are taken directly from the MHD values. The particle distribution function is assumed to be a Maxwellian, whose temperature is taken from AMRVAC, with mean velocities given by

$$\mathbf{v}_{e,i} = \frac{n_{i,e}q_{i,e}(\rho_i + \rho_e)\mathbf{u} - \rho_{i,e}\mathbf{j}}{n_{i,e}q_{i,e}\rho_{e,i} - \rho_{i,e}n_{e,i}q_{e,i}} \tag{1}$$

with the usual meaning for symbols. Quasi-neutrality is assumed, so $n_i = n_e$. The ρ_i and ρ_e is determined by the user-defined mass ratio of ion to electrons. The next step is to take alternate time steps of MHD and PIC with each code giving updated boundary conditions for the other code at every time step.

We have setup a force-free current sheet to check the coupling between MPI-AMRVAC and iPIC3D. The sheet has $B_x = 0.1 * tanh(0.5y - 8)$ and $B_z = 0.1 * sech(0.5y - 8)$. The resolution in MHD is 200×200 cells and 110×160 cells in PIC. Same cell sizes are used in AMRVAC and iPIC3D, although the code is capable of handling different resolution in the PIC part. There are 343 particles per PIC cell. The magnetic field in the z direction of the current sheet is shown in Fig. 1. The smaller red box shows the B_z field from the PIC simulation superimposed on the MHD simulation. The color scale is made same for both the regions. The PIC simulation is run for 50 gyro periods and the MHD simulation runs for 2 Alfven times. The boundary conditions in the PIC domain are implemented in the Maxwell solver of the electric fields by specifying the electric field on the outermost cell-centers as the MHD values. The magnetic field is calculated from the Faraday's law, with the magnetic field in the three outermost cell-centers of the PIC domain set from the MHD values. The current sheet remains stable throughout the

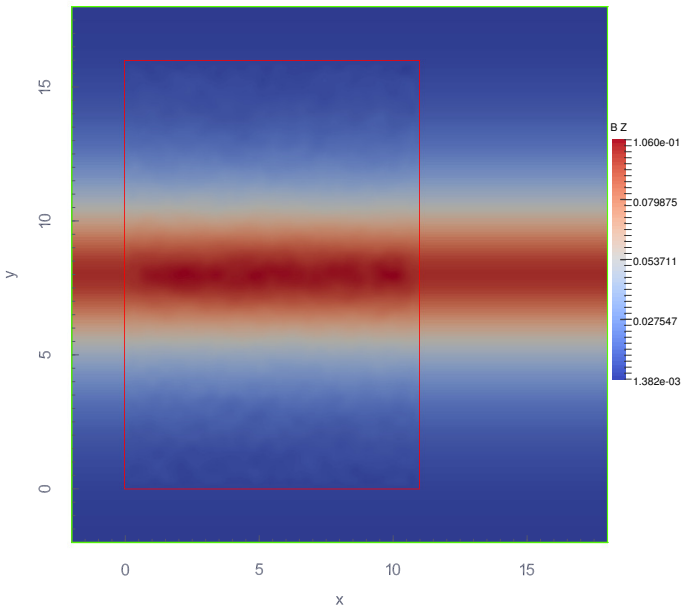

Figure 1: *B_z magnetic field of a current sheet after 100 cycles of iPIC3D run, outlined by the red box, superimposed on the B_z field from MHD simulation.*

simulation and the interface between MHD and PIC regions does not develop any errors, showing good coupling of the electromagnetic fields. There are small fluctuations due to the PIC particle noise, these can be reduced by increasing the number of particles.

In the above simulation we also look at the energy conservation. The energy conservation is perfect in the MPI-AMRVAC part of the simulation. The energy evolution in PIC region is shown in Fig. 2. The magnetic energy is conserved very well and the energy in electric fields is negligible for this setup. The kinetic energy is the energy in thermal motion of particles, there is no mean flow kinetic energy. The kinetic energy also seems very well-conserved. Typically explicit PIC codes show particle heating due to the finite grid instability. However, implicit PIC codes show particle cooling. For example, a full iPIC3D simulation of a uniform plasma with similar box-size, resolution, particles-per-cell, and time length shows a decrease in total energy by 0.1%. In Fig. 2 for the current sheet case the total energy increases by 0.05%. This is very good energy conservation, well within the error range. The increase in energy maybe due to the particle injection implemented at the boundaries in order to couple with MHD. In order to implement the particle boundary conditions, at every time step the particles in the three outermost PIC cells are deleted and repopulated with thermal plus mean velocities supplied by the MHD as given in Eq. 1.

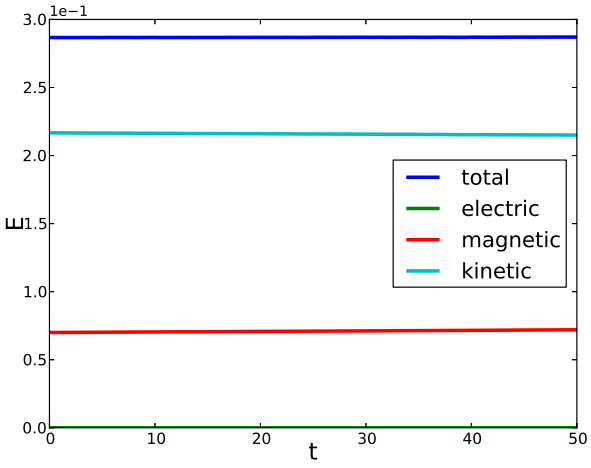

Figure 2: *Time evolution of different energy components in iPIC3D simulation of stable current sheet.*

We vary the size of the PIC domain in the current sheet simulation to see how the total MHD+PIC computing time changes. This is shown in the adjoining table. As the PIC part takes the majority of the time, the scaling of computing time with fraction of PIC domain size is close to ideal. Of course, this will change depending on the problem and will also change with time evolving setups. In real applications, the size of the PIC domain will be decided on the basis of physical considerations. Therefore this code will work best when the PIC region is

PIC size	PIC fraction	Time
17600 cells	0.44	480 secs
8800 cells	0.22	262 secs
4800 cells	0.12	164 secs

a small fraction of the MHD region.

We also simulate a steady flow in the simulation box as shown in Fig. 3. The velocities are $v_x = v_y = 0.01c$, $v_z = 0$. It is simulated with periodic boundary conditions in AMRVAC, and with the MHD-coupling boundary conditions in iPIC3D. The flow tests the particle boundary conditions in both X and Y boundaries. The streamlines of the flow are shown in Fig. 3. The streamlines in MHD and PIC regions are perfectly aligned, with the magnitude of the velocities also perfectly matched, showing good coupling of the particles. MPI-AMRVAC has no fluctuations whereas iPIC3D develops some fluctuations with r.m.s. values less than 10% of the mean velocity. The total energy increases by less than 0.001%, showing very good energy conservation in this case also.

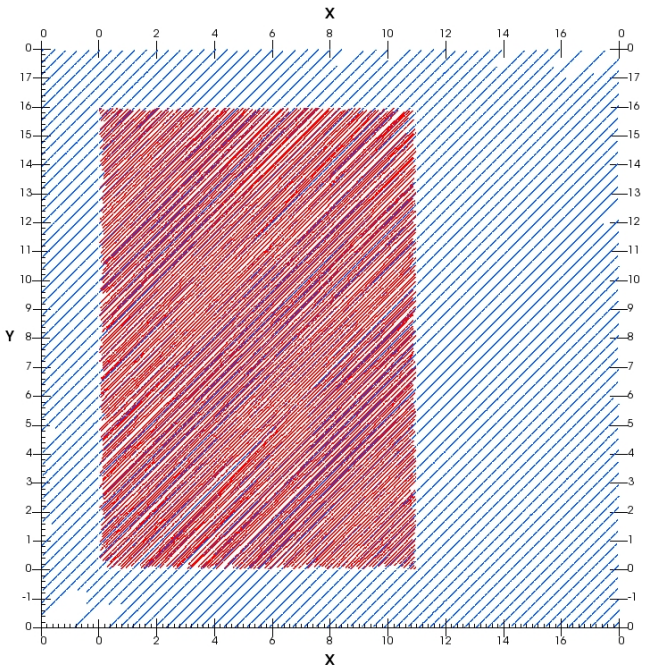

Figure 3: *Blue lines are the streamlines from MHD simulation, superimposed by the streamlines from PIC simulation shown in red. PIC region shows fluctuations in velocity, but the average value is 0.014c, which matches very well with the AMRVAC value. The PIC snapshot is again taken after 50 gyro periods.*

There are several steps to be taken in the future to utilize the full power of this coupling. The time stepping has to be implemented such that evolving systems are seamlessly simulated. The back-coupling of the code will be implemented where PIC data is used to update the MHD simulation. Currently the PIC region is selected arbitrarily, but using physical conditions for selecting PIC regions will make this tool very powerful.

References

[1] O. Porth, C. Xia, T. Hendrix, S. P. Moschou and R. Keppens, The Astrophysical Journal Supplement **214**, 4 (2014).

[2] R. Keppens, Z. Meliani, A. J. van Marle, P. Delmont, A. Vlasis, and B. van der Holst, Journal of computational Physics **231**, 718 (2012).

[3] G. Lapenta, Journal of Computational Physics **231**, 795 (2012).

[4] S. Markidis, G. Lapenta, and Rizwan-uddin, Mathematics and Computers in Simulation **80**, 1509 (2010).

[5] L. K. S. Daldorff, G. Toth, T. I. Gombosi, G. Lapenta, J. Amaya, S. Markidis, and J. U. Brackbill, Journal of Computational Physics **268**, 236 (2014).