Particle-Gas Hybrid Schemes in the PLUTO Code

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Abstract. Hybrid codes treating composite systems made up of fluid and particle components are becoming increasing more popular in order to address multiple scale in complex astrophysical environments. Here we review some recent additions to the PLUTO code consisting of three flexible particle physics implementations targeting i) cosmic ray particles, ii) sub-grid electron acceleration and emission from high-energy astrophysical environments and iii) dust grains in protoplanetary disks. While the fluid equations are generally solved using standard finite-volume techniques, integration of particles as well as their feedback onto the gas is treated using standard techniques borrowed from Particle-In-Cell (PIC) frameworks. Some novel numerical benchmarks, not discussed in the original method papers, are also presented.

1. Introduction

Magnetohydrodynamics (MHD) simulations constitute the standard simulation paradigm to address large-scale, low-frequency phenomena in plasma astrophysics. For this reason, the last two decades have seen a significant proliferation of publicly available MHD codes such as FLASH\textsuperscript{1}, PLUTO\textsuperscript{2}, Athena\textsuperscript{3}, Nirvana\textsuperscript{4}, MPI-AMRVAC\textsuperscript{5}, PENCIL\textsuperscript{6}, to cite just a few. The availability of increasingly more sophisticated tools together with the growing computational resources has fostered MHD modeling of a large variety of astrophysical environments. The PLUTO code, for instance, is no exception and it has been employed to study stellar jet evolution\textsuperscript{7}, relativistic jet propagation\textsuperscript{8}, shearing-box simulations of the magneto-rotational instability\textsuperscript{9}, mass accretion to young stars\textsuperscript{10}, pressure-driven 3D instabilities in accretion mounds on neutron stars\textsuperscript{11}, models of the circumstellar medium of evolving massive runaway stars\textsuperscript{12} among others. Because of its nature, however, the basic MHD approach is applicable on scales much larger than the Larmor radius, and it completely neglects important kinetic effects relevant to the microscales which are, on the other hand, consistently described using Particle-In-Cell (PIC) codes. This severely compromises the possibility of extending the range of applicability of MHD to smaller spatial and temporal scales thus preventing any attempt to bridge the formidable gap between large and kinetic scales.

An attempt to overcome this limitation leans on the construction of hybrid numerical frameworks, where both fluid and particle approaches coexist. This approach is certainly not new and it is commonly adopted in space physics and laboratory plasma codes (see, e.g.,\textsuperscript{13, 14})
where ions are treated as particles moving in a neutralizing electron fluid. The BATS’R’US code is also an example (see [15] and the contribution by Moschou et al. in this conference proceeding).

Here we review the gas-particle hybrid numerical methodology recently implemented in the PLUTO code which, at present, incorporate three different kinds of particles. The Cosmic-Ray implementation (see [16]) is appropriate to capture the dynamical evolution of a plasma consisting of a thermal fluid and a non-thermal component represented by relativistic charged particles, or cosmic rays (CR). The second implementation addresses sub-grid electron physics by introducing Lagrangian, tracer-like particles and it has been designed to specifically address the problem of non-thermal emission from highly energetic particles (typically electrons) embedded in a large-scale classical or relativistic MHD flow, [17]. Finally, the dust module (see [18]) describes the physics of dust grains coupled to the gas via drag forces and it is mainly intended for the numerical modeling of protoplanetary disks in which solid and gas interact via aerodynamic drag. In §2 we illustrate the relevant equations and formalism, while the three module are described in §3, §4 and §5.

2. Equations and General Formalism

We begin by writing the MHD equations in a form which is more suited for incorporating particle effects. The equations describe the temporal evolution of density $\rho$, momentum $\rho v$, energy $E$ and magnetic fields $B$ and are best written in conservative fashion as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0,$$  \hspace{1cm} (1)

$$\frac{\partial (\rho v)}{\partial t} + \nabla \cdot \left( \frac{1}{2} \rho v^2 + \rho e + p \right) v = \rho a_g + f_p,$$  \hspace{1cm} (2)

$$\frac{\partial E}{\partial t} + \nabla \cdot \left( \frac{1}{2} \rho v^2 + \rho e + p \right) v = \rho v \cdot a_g + W_p,$$  \hspace{1cm} (3)

$$\frac{\partial B}{\partial t} + \nabla \times (cE) = 0,$$  \hspace{1cm} (4)

where $p_t = p_g + B^2/8\pi$ is the total (gas + magnetic) pressure, $I$ is the identity matrix and the total energy density accounts for kinetic, thermal and magnetic contributions, $E_g = \rho v_g^2/2 + \rho e + B^2/8\pi$. Here $\rho e = p/(\Gamma - 1)$ is the typical closure adopted for the internal energy with $\Gamma$ being the specific heat ratio. The electric field $E$ is specified by Ohm’s law, whose form depend on the particular model at hand. In Eq. (1)-(3) we have introduced $f_p$ and $W_p$ which are coupling terms introduced to express, respectively, the force and work (per unit volume) done by the particles onto the gas. Here the “p” subscript refer to a particle-related quantity. The precise form of $f_p$, $W_p$ and $E$ depends on the physic module at hand, described in the following.

On the other side, particles are described in terms of their position and velocity coordinates $(x_p, v_p)$ and are evolved by solving the six differential ordinary differential equations

$$\begin{align*}
\frac{dx_p}{dt} &= v_p \\
\frac{dv_p}{dt} &= a_p(x_p, v_p, U). 
\end{align*}$$  \hspace{1cm} (5)

Note that the particle acceleration vector $a_p$ can depend on the particle coordinates as well as on fluid quantities, denoted with $U$.

At the discrete level, Eq. (1)–(4) are solved on a computational grid using finite-volume numerical schemes for MHD, properly modified to account for the particle back-reaction
terms. The basic algorithms for the MHD-PIC, Lagrangian macroparticles and and dust-grain modules have been described in detail in [16, 17, 18], respectively. The divergence-free condition is enforced using either constrained transport or divergence cleaning approaches. By contrast, particles are treated kinetically using conventional Particle-In-Cell (PIC) time-reversible integrators (for dust and CR) or simple Runge-Kutta schemes in the case of the Lagrangian module.

A 2nd-order predictor-corrector method is used to advance both the fluid and particle components which, in compact form, can be written as

\[
U_i^{n+\frac{1}{2}} = U_i^n + \frac{\Delta t}{2} L_i^{n} + \frac{\Delta t}{2} S_{p,i}^n, \tag{6}
\]

\[
(x_p, v_p)^n \rightarrow (x_p, v_p)^{n+1}, \tag{7}
\]

\[
U_i^{n+1} = U_i^n + \Delta t L_i^{n+\frac{1}{2}} + \Delta t S_{p,i}^{n+\frac{1}{2}}, \tag{8}
\]

where \(i = (i, j, k)\) identify the computational zone, \(L\) and \(S\) are the two-point flux difference operator and source terms, respectively given by

\[
L_i^{n+\frac{1}{2}} = \sum_d \frac{\mathcal{F}_i^{n+\frac{1}{2}} - \mathcal{F}_i^{n+\frac{1}{2}}}{\Delta x_d} + S_{g,i}^{n+\frac{1}{2}}, \quad S_{p,i}^{n+\frac{1}{2}} = \sum_p W(x_i - x_p^{n+\frac{1}{2}}) \left( \frac{\Delta m_p}{\Delta E_{k,p}} \right). \tag{9}
\]

In the previous expressions \(\mathcal{F}_{i\pm e_d/2}\) are the numerical fluxes obtained at cell interfaces (here \(e_d\) is the unit vector in the direction \(d = x, y, z\)) by solving a Riemann problem between suitably reconstructed left and right states. Note that the previous relations also hold in the case of a Strong-Stability-Preserving (SSP) RK method by replacing \(U^{n+\frac{1}{2}} = (U^n + U^*)/2\), \(L^{n+\frac{1}{2}} = (L^n + L^*)/2\) where \(U^* = U^n + \Delta t(L^n + S^n)\) is the full-step predictor.

3. The MHD-PIC Model

The MHD-PIC model [19, 16] describes the dynamical interaction between a thermal plasma and a non-thermal population of collisionless cosmic rays (CR henceforth). While the thermal component, that comprises ions and massless electrons, is described through a fluid approach making use of shock-capturing MHD methods, CR particles (typically representing energetic ions) are treated kinetically using a conventional PIC techniques. In this formalism only the Larmor (gyration) scale must be properly resolved thereby extending the range of applicability of the MHD-PIC model to much larger spatial (and temporal) scales when compared to the standard PIC approach, inasmuch the particle gyroradius largely exceeds the plasma skin depth \(c/\omega_{pi} \approx 2.27 \times 10^7/\sqrt{n_i} \text{ cm.}\)

The relevant equations (see also §2 in [16]) are given by (1)–(4) with

\[
f_p = -F_{CR} = -q_{CR}E - \frac{1}{c} J_{CR} \times B, \tag{10}
\]

\[
W_p = -v_g \cdot F_{CR},
\]

where \(q_{CR}\) and \(J_{CR} = q_{CR}v_{CR}\) are the CR charge and current densities, respectively, whereas the electric field follows directly from the thermal massless electrons equation of motion (after neglecting the Hall and electron pressure terms):

\[
\mathbf{e}E = -\mathbf{v}_g \times \mathbf{B} - R(\mathbf{v}_{CR} - \mathbf{v}_g) \times \mathbf{B}, \tag{11}
\]
where $R$ represents the ratio of the CR charge density to the total charge density:

$$ R = \frac{q_{CR}}{q_i + q_{CR}} = \frac{\alpha_{CR} \varrho_{CR}}{\alpha_g \varrho_g + \alpha_{CR} \varrho_{CR}}. $$

(12)

In the expression above we have introduced the charge to mass ratios $\alpha_{CR} = (e/mc)_{CR}$ and $\alpha_g = (e/mc)_g$, where $e$ is the elementary charge.

CR particles are subject to the standard Lorentz force,

$$ \frac{d(\gamma v_p)}{dt} = \alpha_{CR} (cE + v_p \times B), $$

(13)

where $\gamma = 1/\sqrt{1 - v^2_p/C^2}$ is the Lorentz factor. Note that while the speed of light never appears in the MHD fluid equations, it has been denoted here with $C$ to specify an artificial value, which, for consistency, must be greater than any characteristic MHD velocity. Eq. (13) is solved by means of a standard $2^{nd}$ order Boris pusher with spatial and velocity coordinates defined at the same time level, in order to allow computations to be carried out with varying time steps (see §3.2 in [16]). We point out that the MHD-PIC formalism cannot describe kinetic effects arising from the thermal component (e.g. Weibel-like filamentation) and that the CR-particle injection cannot be consistently modeled, unless specifically prescribed.

3.1. Linear Growth of the Bell Instability with non-negligible CR Hall term

The Bell instability is driven by the relative streaming between gas and CR particles along magnetic field lines, and it takes place when the CR drift velocity exceeds the local Alfvén speed [20, 21, 19, 16]. Local magnetic field perturbations are amplified by the return current of the thermal plasma in the attempt to restore charge neutrality. The instability is non-resonant and it excites nearly purely growing modes with

$$ k_m = J_{CR} \frac{1}{2B_0c} f, \quad \text{Im}(\omega) = v_A \frac{J_{CR}}{2B_0c} \frac{1}{\sqrt{f}}, $$

(14)

being the most unstable wavenumber and corresponding growth rate, as shown by the linear analysis of [19]. In the expressions above $B_0$ is the background magnetic field, $v_A$ is the Alfvén speed, while

$$ J_{CR} = (ne)_{CR} \frac{v_A}{\epsilon}, \quad f = 1 + (\Lambda/2)^2, \quad \Lambda = R \frac{|v_{CR} - v_g|}{v_A} \approx \frac{R}{\epsilon}, $$

(15)

where $\epsilon = v_A/v_{CR} < 1$ is the ratio between the CR velocity and the local Alfvén speed.

While a numerical study of the linear phases in the regime $\Lambda \sim 0$ has already been presented in our previous work [16] we establish here some complementary results not shown in that paper. In particular, we codify the setup in a somewhat different way which is more suitable to explore the regimes for arbitrary $\Lambda$ (without violating the condition $R \ll 1$). From the linear analysis of [19], we write the wavenumber relative to the fastest growing mode as

$$ \left\{ \begin{array}{c} k_m = k_{max} \frac{\epsilon R}{\epsilon^2 + R^2/4} \\ \omega_m = k_{max} v_A \frac{R}{\sqrt{\epsilon^2 + R^2/4}} \end{array} \right. $$

where $k_{max} = \frac{(ne)_{CR} v_A}{2cB_0 R}$.

(16)
The expression above indicates that $k_m$ is maximum when $\epsilon = R/2$ where $k_m = k_{\text{max}}$. Since $1/R \approx (ne)/ne_{\text{cr}} = (\alpha \rho)/\epsilon \rho_{\text{cr}}$, we also conclude that the wavelength of the fastest growing mode never falls below the ion skin depth of the fluid:

$$\lambda_{\text{min}} = \frac{2\pi}{k_{\text{max}}} \approx \frac{4\pi B_0}{(\alpha \rho) g v_A} = \frac{16\pi^2 c}{\omega_{p,g} R},$$

(17)

where $\omega_{p,g}$ is the (ion) plasma frequency of the gas.

In our configuration, therefore, we fix the value of $R$ while leave $\epsilon$ as a free parameter controlling the CR current through Eq. (15). Our analysis also suggests to set the reference length equal to the minimum value (Eq. 17), and change the computational domain size to fit one most unstable wavelength accordingly. In code units, therefore, $k_{\text{max}} = 2\pi = \alpha g/2$ while the domain size is determined by $\epsilon$ and $R$ through the relation $L_0 = k_{\text{max}}/k_m$.

The background medium consists of a constant uniform density $\rho_0 = 1$ and pressure $p_0 = 1$ threaded by constant a magnetic field $B_0 = B_0 \hat{e}_x$ with $B_0 = \sqrt{4\pi} \left(v_A = 1\right)$. Particles travel along the initial field direction creating a current density (from Eq. 15) $J_{\text{cr}}/(\epsilon) \approx (\alpha \rho) v_A / \epsilon$, where $\alpha_{\text{cr}}$ and $\rho_{\text{cr}}$ are the charge to mass ratio and density of the CR particles. In order to have $J_{\text{cr}}$ approximately constant in time, $\alpha_{\text{cr}} = (\epsilon/mc)_{\text{cr}}$ is chosen to be a small number (large inertia) and the CR density is recovered from the definition of $R$ (Eq. 12) yielding

$$\rho_{\text{cr}} = \rho_0 \frac{\alpha_g R}{\alpha_{\text{cr}} (1 - R)}.$$  

(18)

The speed of light used in the definition of the CR Lorentz factor (Eq. 13) has been set to $C = 10^6$.

The background state is perturbed with the exact eigenvectors (see [19]) yielding, at $t = 0$, the following condition on velocity and transverse magnetic field:

$$\delta v_g = v_A \frac{b_\perp}{B_0} \left[ \left( \frac{\Lambda}{2} \cos \phi + \sqrt{f} \sin \phi \right) \hat{e}_y + \left( \frac{\Lambda}{2} \sin \phi - \sqrt{f} \cos \phi \right) \hat{e}_z \right],$$

$$\delta B = \frac{b_\perp}{B_0} \left( \cos \phi \hat{e}_y + \sin \phi \hat{e}_z \right),$$

(19)

where $\phi = k_m x$ and $b_\perp = 10^{-5}$ is the initial perturbation amplitude. We investigate the linear phase in 1, 2 and 3D dimensions. In 1D we employ 64 cells while in 2D and 3D we rotate the configuration as in [16] and use $L_x = 2L_y = \sqrt{5}L_0$ with 64 $\times$ 32 zones (in 2D) and $L_x = 2L_y = 2L_z = 3L_0$ with 96 $\times$ 48 $\times$ 48 zones (in 3D).

The three panels in Fig. 1 show the growth of transverse magnetic field in time (normalized to the inverse growth rate $\omega$) on top of the exact growth rates (solid lines). Our results well recover the linear stages of the instability in which the magnetic field is amplified well beyond the initial background state. The instability eventually saturates once the magnetic tension term $\nabla \times B$ becomes large enough to oppose the stretching and bending of magnetic field line induced by CR current $J_{\text{cr}}$ (see [21] for a more detailed description). It is worth pointing out that, while in absence of the CR Hall term ($\Lambda \sim R/\epsilon \sim 0$) the growth rate of the most unstable mode increases indefinitely as $\epsilon \to 0$, the presence of a non-negligible $\Lambda$ has the effect of reducing the growth rate eventually saturating at $\omega \sim k_{\text{max}} v_A^2/\sqrt{R}$ as $\epsilon \to 0$.

### 3.2. Test Particle Acceleration in Relativistic Current Sheets

As a proof of concept, we illustrate an application of the MHD-PIC module to a composite system made of a relativistic thermal plasma and test particles (i.e. no feedback on the fluid).
Figure 1. Growth of the transverse magnetic field as a function of time for different values of the $\epsilon$ parameter, $\epsilon = 10^{-1}$ (black), $\epsilon = 10^{-2}$ (purple), $\epsilon = 10^{-3}$ (red) and $\epsilon = 10^{-4}$ (blue). The solid lines indicate the corresponding analytical growth rates. The three panels show, from left to right, the results obtained in 1D, 2D and 3D.

Figure 2. Left: density snapshots at $t_1 \approx 6.34 \times 10^4 \omega_p^{-1}$ and $t_2 = 7.56 \times 10^4 \omega_p^{-1}$ for the relativistic current sheet problem using $\sigma = 10$. Right: particle energy as a function of time. The inset shows the density maps at $t_3 = 8.28 \times 10^4 \omega_p^{-1}$. The positions of the particle are shown with blue dots in the different panels while the corresponding acceleration phases $t_1, t_2$ and $t_3$ are marked in the energy plot.

We consider a 2D Cartesian grid of size $2L \times L$ ($L = 10^4 c/\omega_p$) hosting, at $t = 0$, a Harris current sheet defined by

$$B = B_0 \tanh \left( \frac{2\pi y}{w} \right) \hat{e}_x, \quad p_y = \frac{B_0^2}{8\pi} (\beta + 1) - \frac{B^2}{8\pi},$$

(20)

where $w$ denotes the width of the current sheet chosen to be $20\Delta y$, $B_0$ is the magnetic field strength, $\beta = 10^{-2}$ while the second equation ensures pressure equilibrium. The field strength is controlled by the $\sigma$ parameter, defined as $\sigma = B_0^2/(4\pi \rho)$. A random perturbation in the vertical velocity localized around $y = 0$ is applied to trigger the onset of the tearing instability. We fix our unit density to $\rho = 1$ and solve the ideal relativistic MHD equations as described in [22]. Periodic boundaries hold in the $x$-direction while reflective conditions are applied at $y = \pm L/2$. We place one particle per cell and initialize their velocity using a Maxwellian distribution with temperature equal to the gas temperature. Here $\mathcal{C} = 1$ for obvious reasons while the numerical resolution is set to $1536 \times 768$. Numerical simulations are performed with $\sigma = 1, 10, 30$.

The reconnecting layer becomes tearing-unstable breaking into a chain of magnetic islands separated by ‘X’ points. Islands gradually merge leading to the formation of larger structures, as shown in the left panels of Fig. 2. Particles initially drift and convey towards the reconnecting layer where, in the presence of an ‘X’-point, they experience abrupt acceleration in a way similar
Figure 3. Particle energy spectra at different times (given by the colors) for the three simulation cases: $\sigma = 1$ (left), $\sigma = 10$ (middle) and $\sigma = 30$ (right).

to [23]. This is illustrated in the right panel of Fig. 2 for one of the most energetic particles. Particles are accelerated in the $z$-direction by the convective electric field (note that, in this simple model, the amount of resistivity is set only by numerical diffusion). As particles become trapped inside magnetic islands, the acceleration process continues either through the formation of secondary ‘X’ points (at island merging) or by Fermi-like mechanism whereby particles are repeatedly reflected by the contracting walls of the island.

The particles energy spectra, for the three simulation cases, are shown in Fig. 3 at different times and they typically feature: a low-energy Maxwellian residue, a power-law portion and high-energy cut-off. The power-law becomes harder as the magnetization is increased, progressively shifting the maximum Lorentz factors to larger values ($\gamma_{\text{max}} \sim 6 \times 10^3$ when $\sigma = 30$). The index $p$ of the power-law, $dN/d\gamma \propto \gamma^p$, decreases in absolute value as the magnetization grows yielding, for increasing $\sigma$, $p = -2.11$, $p = -1.72$ and $p = -1.68$. Our simple toy-model yields results which are roughly consistent with those obtained by PIC codes, [23]. Future work will address this problem in a more scrupulous way by including physical resistivity.

4. Sub-grid Electron Physics through Lagrangian Particles

This module employs a particle approach for solving the transport equation for cosmic rays propagation and energization in a scattering medium. A large number of Lagrangian (i.e. passive) macro-particles is used to sample the distribution function in physical space. A macro-particle represents an ensemble of actual particles (leptons or hadrons) that are very close in physical space but with a finite distribution in energy (or momentum) space (see [17]). Introducing the number density ratio $\chi_p = N_p/n$ representing the number of electrons normalized to the fluid number density, it is straightforward to show that $\chi_p$ obeys to the following equation:

$$\frac{d\chi_p}{dt} + \frac{\partial}{\partial E} \left[ \left( -\frac{E}{3} \nabla u^\mu + \dot{E}_l \right) \chi_p \right] = 0 .$$  \hspace{1cm} (21)

The solution of Eq. (21) is carried out separately into a transport step (during which we update the spatial coordinates of the particles) followed by a spectral evolution step (corresponding to the evolution of the particle energy distribution), see §2.3.1 and 2.3.2 in [17]. Note that macroparticles are advected at the fluid speed and that energy distributions associated with particles are assumed to be isotropic.

In addition, our model also incorporates diffusive shock acceleration (DSA) as a sub-grid model that recomputes the energy spectrum of a macro-particle encountering a shocked region. This is achieved by first computing the shock orientation and strength and then by resetting
the particle spectrum to a power-law within the energy bounds and normalisation obtained through Eqs. (29)-(32) in [17]. An alternative form of spectral update, that partially preserves the spectral history of the particle (not presented in the original paper), is also possible. The approach, similar to [24], involves convolving the upstream spectrum of the particle with the power-law spectrum predicted by the theory of diffusive shock acceleration (DSA) [17] to obtain the downstream energy spectrum. The details of this approach can be in [25]. In addition, the method ensures that the cosmic ray energy and number densities are equal to or below the equipartition threshold, whose value is set as a parameter. This can be particularly important when the particle experiences multiple shock crossing thus avoiding spurious energy losses while adhering to the basic assumptions of energy equipartition at shock sites. We point out that this approach is valid at very large scales (typically parsec or more) where the typical time step size largely exceeds the DSA relaxation time scale.

4.1. Planar Shock and Particle Acceleration

To understand the evolution of electron spectra with time, we have introduced 2048 uniformly spaced Lagrangian macro-particles in a 2D X-Y plane of size $400 \times 200$ pc with a resolution of $512 \times 256$ cells. Initially, the electron spectra is prescribed as a steep power-law i.e., $\chi_p \propto E^{-\alpha}$ with $\alpha = 9$ within an energy range of 62.5 MeV to 62.5 TeV. The proportionality constant is related to the total number density of micro-particle (electron in this case) within a single macro-particle. A MHD shock with non-relativistic speed of $0.063c$ is injected from left to right. The downstream ambient medium has mean density of unity along with added random perturbation and gas pressure $p_g = 10^{-4}$ in units of $\rho_0 c^2$, where $\rho_0$ is $10^{-2}$ cm$^{-3}$ and $c$ being speed of light. The magnetic field has magnitude prescribed by the plasma $\beta = 100$ and makes an angle of 30° with respect to the x-axis. The macro-particle under consideration is shown as red dot in the 2D density map at time $\tau = 4.4$ kyr in the top panel of Fig 4. This macro-particle undergoes a shock acceleration resulting in a flatter spectra consistent with the input compression ratio of 3.55. A comparison of the spectral evolution of a particular macro-particle for $\approx 15$ kyr for two different spectral update strategies is shown in the bottom panels Fig 4.

The maximum energy is estimated by equating the acceleration time scale with the radiative cooling time. In both the cases, negligible changes in the high energy part of the spectrum are observed. However, the lower energy part shows changes due to the manner in which the upstream spectra is modified through convolution.

5. Dust Grains

The physics of dust grains plays also an important role in forging the dynamical evolution of protoplanetary disks. Dynamic coupling between dust and fluid takes place through aerodynamic drag forces causing the two components to exchange momentum through mutual feedback terms. In the Epstein regime, the drag force is proportional to the relative velocity between the two species,

$$a_p = \tilde{a}_p - \frac{v_p - v_g}{\tau_{s,p}}$$

(22)

where $\tilde{a}_p$ accounts for external forces (e.g., gravity, Coriolis and so forth) while the second term is the actual viscous drag. The particle stopping time is denoted by $\tau_{s,p}$.

The particle feedback on the gas is described by

$$f_p = -\left(\varrho_D \frac{v_g - v_D}{\tau_s}\right),$$

(23)

representing the average cumulative drag force accounting for feedback from dust particles to the gas and it is obtained by first computing the drag acceleration at the particle position and
Figure 4. Top: 2D density map for the planar shock test at time $\tau = 4.4$ kyr, with the selected macro-particle (shown as a red dot) being just out of the shock. Bottom: panels compare the evolution of the normalized spectra of the same macro-particle using the approach of [17] (left) and the convolution method of [24] (right). Different times (in kyr) are colored as shown in the legend.

then distributing it back on the grid (see §3.1 in [18]). Magnetic fields are neglected on the gas (dust grains are neutral) and an isothermal equation of state is used so that the energy equation is not necessary.

Despite its simplicity (feedback is modeled as a linear term in the relative velocity), the drag acceleration can become stiff for tightly coupled grains ($\tau_{s,p} \ll \Delta t$), thus forcing an explicit scheme to abnormally small time stepping. While implicit methods can be used to overcome this limitation [26], we rely instead on the employment of a new 2nd-order, time-reversible exponential integrator which has shown to possess better convergence properties in that i) it provides energy errors that are always bounded and ii) it remains stable in the limit of arbitrarily small particle stopping times, yielding the correct asymptotic solution. The proposed exponential midpoint method [18] advances the particle coordinates by a time step $\Delta t$ in the following way

$$x_{p}^{n+\frac{1}{2}} = x_{p}^{n} + \frac{\Delta t}{2} v_{p}^{n},$$

$$v_{p}^{n+1} = e^{-\Delta t/\tau_{s,p}} v_{p}^{n} + h_{1} G \left( x_{p}^{n+\frac{1}{2}}, v_{p}^{n+\frac{1}{2}}, v_{g}^{n+\frac{1}{2}} \right),$$

$$x_{p}^{n+1} = x_{p}^{n+\frac{1}{2}} + \frac{\Delta t}{2} v_{p}^{n+1},$$

(24)

where $v^{n+\frac{1}{2}} = (v^{n} + v^{n+1})/2$, $G = \tilde{a}_{p} + v_{g}/\tau_{s,p}$ while $h_{1} = \tau_{s,p}(1 - e^{-\Delta t/\tau_{s,p}})$ is the exponential propagator.
5.1. Convergence & Turbulence Properties in the Streaming Instability

The streaming instability [27] is driven by the relative motion between solid (dust) particle and gas which are coupled through dissipative drag forces. The instability draws its energy from the radial gas pressure gradient and it plays a fundamental role in the dynamical evolution of protoplanetary disks [28]. The growth of the instability results in particle-density enhancements which can potentially trigger planetesimal formation.

A numerical investigation of the linear phase of the instability was already presented in the reference paper [18]. Here we describe the nonlinear evolution and address the problem of numerical convergence with respect to resolution. The setup is identical to §4.3 in [18] and it consists of a background equilibrium state,

\[
\begin{align*}
\mathbf{v}_g &= \left[ \frac{2c_s^2}{\Delta} \hat{e}_x - \frac{1 + \epsilon \tau_s^2}{1 + \epsilon} \hat{e}_y \right] \eta v_K, \\
\mathbf{v}_p &= -\left[ \frac{2c_s^2}{\Delta} \hat{e}_x + \left( 1 - \frac{\tau_s^2}{\Delta} \right) \frac{1}{1 + \epsilon} \hat{e}_y \right] \eta v_K,
\end{align*}
\]

(25)

where \( \epsilon \) denotes the density ratio of particles to gas, \( \Delta = (1 + \epsilon)^2 + \tau_s^2 \), \( \tau_s = \Omega \tau_s \) is the Stokes number and \( \eta v_K \) measures the amount by which the gas azimuthal velocity is reduced from the Keplerian value by the global radial pressure gradient. Note that in our original paper [18], the particle x-velocity contains an incorrect extra factor \( \epsilon \). We solve the 2D, axisymmetric shearingbox equations in the \( x - z \) plane with \( \Omega = 1, q = 3/2 \) and adopt an isothermal equation of state \( p = c_s^2 \rho \) with \( c_s = 0.1 v_K \) (\( v_K = 1 \)).

The orbital advection scheme of [29] is used to subtract the linear shear contribution from the total velocity. We employ 9 particles per cell with dust to gas density ratio \( \epsilon = 1 \) and stopping time \( \tau_{s,p} = 0.1 \), corresponding to run 'AB' in [26]. The initial equilibrium state is perturbed by randomly displacing particles inside each cell.

We carry out a resolution study using \( 256^2, 512^2, 1024^2 \) and \( 2048^2 \) grid zones.

Particle clumping takes place on smaller scales as the resolution is increased, as shown in the left panels of Fig. 5, where we show the colored maps of the dust density at \( t = 30 \Omega^{-1} \) for...
the four different runs. A quantitative measure of dust concentration is obtained by calculating the cumulative distribution function (CDF), i.e., the number of cells (normalized to the total) in which the dust density exceeds the average value. We follow [26] and use a long averaging period over the time window $80 \leq t \Omega^{-1} \leq 160$. The CDF is plotted in the top right panel for the four different grid resolutions showing excellent convergence properties in agreement with the results of [26]. In the bottom right panel, we show the maximum dust density as a function of time: the initial linear phase is strongly dependent on the grid resolution but, during the nonlinear phases, the maximum density saturates around $60 \lesssim \max(\varrho_D) \lesssim 80$ for $N_x \gtrsim 512$.

6. Summary

A review of the new hybrid gas-particle implementations in the PLUTO code has been presented. The new algorithmic framework combines Particle-in-Cell (PIC) techniques with a Godunov-type finite volume schemes offering three different physics modules extending the range of validity of conventional MHD in the attempt of restoring some small scale physics or kinetic effects. These include: i) the MHD-PIC module suitable to study cosmic-ray propagation and acceleration at the ion Gyration scale; ii) a Lagrangian particle module modeling sub-scale electron acceleration applicable to large scales and high-energy astrophysical phenomena; iii) a gas-particle hybrid numerical model to simulate the mutual interaction between gas and dust grains, coupled via an aerodynamic drag force that is linear in the relative velocity. The proposed framework is suitable in the context of dust dynamics in protoplanetary accretion discs. The three modules have been described in detail by [16], [17] and [18] while some unpublished results have been presented in this work.

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