PIC simulation of the thermal pressure-driven expansion of a blast shell into a magnetized ambient medium

> Mark Eric Dieckmann, Department of Science and Technology (ITN), Linköping University, Campus Norrköping, Sweden.

Overview

• The kinetic equations.

- Numerics of the particle-in-cell method.
- Laser-plasma experiments.
- Reproducing the experimental findings.
- A 'textbook' MHD shock in 1D.
- Expansion of a radial blast shell into a magnetized plasma.
- Summary.

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Maxwell's equations
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The evolution of the electromagnetic fields is described by : Faraday's law, Ampere's law and Gauss' law.

 $\partial/\partial t B = \nabla \times E$ $\mu \partial \varepsilon \partial \partial t E = \nabla \times B - \mu \partial J$

 $\nabla \cdot E = \rho / \varepsilon 0$ $\nabla \cdot B = 0$

Gauss' law of electrostatics is related to Ampere's law:

Continuity equation: $\epsilon_0 \partial/\partial t \nabla \cdot E = \partial/\partial t \rho = -\nabla \cdot J \Rightarrow \nabla \cdot (\partial/\partial t \epsilon \partial E + J) = 0$

Electric field update: solve Ampere's law and make sure Gauss' law is fulfilled. **Magnetic field update:** solve Faraday's law and make sure $\nabla \cdot B = 0$ is fulfilled.

Charge and current densities

- The plasma enters through the charge density ρ and the current density J.
- Both are functions of space and time in a magneto-fluid: $\rho(x,t)$ and J(x,t).
- If collisions are absent in the plasma, then the particles change their velocity only via electromagnetic fields: velocity becomes an independent variable.
- Species *i* is described by a phase space density distribution $f_i(x, v, t)$.
- We obtain from it the charge- and current densities as:
- $\rho_i(x,t)=q_i \int f_i(x,v,t) d^3v$ and $J_i(x,t)=q_i \int v f_i(x,v,t) d^3v$ (q_i is the particle charge).
- The total charge is $\rho = \sum_{i} \rho_{i}$ and the total current is $J = \sum_{i} J_{i}$.

Effects of electromagnetic field on plasma

- The charge- and current density of the plasma drives electromagnetic fields.
- The electromagnetic fields act back on the plasma.
- The phase space density is preserved in a Lagrangian frame if there is no ionization and recombination of charges: $(d/dt) f_i(x(t), v(t), t) = 0$.
- We obtain the evolution equation for the phase space density of species *i* in a Eulerian frame

 $\partial/\partial t fi(x,v,t) + dx/dt \nabla fi(x,v,t) + qi/mi(E+v \times B) \cdot \nabla v fi(x,v,t) = 0.$

We need to find suitable numerical schemes for updating the phase space density distribution and the fields.

Numerical scheme: *E*, *B* and *J*.

We solve the field equations in the Eulerian frame: $\mu 0 \varepsilon 0 \partial / \partial t E = \nabla \times B - \mu 0 J$ $\partial / \partial t B = \nabla \times E$

We place *E*, *B* and *J* on a numerical grid.

- Most PIC simulations employ uniform spacing for Δx , Δy , Δz and for Δt .
- Maxwell's equations can be solved explicitly with a finite difference time domain (FDTD) scheme.
- E is defined at integer time steps.
- B and J at half-integer time steps.



Yee lattice for a PIC code

Numerical scheme: $f_i(x, v, t)$

Vlasov equation: $\partial/\partial t fm(x,v,t) + dx/dt \nabla fm(x,v,t) + qm/mm(E+v \times B) \cdot \nabla v fm(x,v,t) = 0.$

pproximate fm(x, v, t) by N_m computational ම 0.5 articles (CPs). -2⁻ he CP with index α is characterized by a position -1.5-0.5 -1 0 0.5 1 $_{\alpha} = (X_{\alpha x}, X_{\alpha y}, X_{\alpha z})$ and velocity V_{α} . () 。 0.5 (ξ) is a B-spline of order *j* and $\xi = x - X_{\alpha y}$ ample the shape function on the grid as: $S_{ijk\alpha} = (x_i - X_{\alpha x}, y_j - X_{\alpha y}, z_k - X_{\alpha z})$, where x_i , y_j and z_k -1.5-0.50.5 (E) 0.5 prrespond to cell coordinates. formalization of splines $\Rightarrow \sum_{\alpha} q_{\alpha} S_{ijk\alpha} \approx \rho_m(x, t)$ 0--2 -0.5 0.5 -1.50

s initialized with a random number generator with the probability density function $f_m(x,v,t)$.

1.5

1.5

1.5

2

Coupling fields and computational particles

- Faraday's and Ampere's law evolve the electric field and the magnetic field on a grid with the help of the total current density *J* of the plasma.
- The electric field *E* is known at integer time steps $n\Delta_t$.
- The magnetic field B and the current density J are known at times $(n+1/2)\Delta_t$.
- It makes sense to update particle positions and velocities at different times.
- The current density J is obtained by summing up the current contributions of all CPs \Rightarrow we define particle velocities at times $(n+1/2)\Delta_t$.
- We define particle positions at integer time steps $n\Delta_t$.

Esirkepov's charge-conserving scheme

ne scheme proposed by *T. Zh. Esirkepov,* Computer Physics Communications 135, 144 2001) fulfills the continuity equation.

ne charge is defined in the center of the cell.

ne currents and fields are specified around it milarly to the distribution in the Yee lattice.

uses gradient operators with forward and ackward schemes.

$$\mathbf{E}^{n} = \left(E_{i,j+1/2,k+1/2}^{1}, E_{i+1/2,j,k+1/2}^{2}, E_{i+1/2,j+1/2}^{3}, E_{i+1/2,j+1/2}^{3}\right)$$
$$\mathbf{B}^{n+1/2} = \left(B_{i+1/2,j,k}^{1}, B_{i,j+1/2,k}^{2}, B_{i,j,k+1/2}^{3}\right)^{n+1/2}$$

$$\rho^{n} = \rho^{n}_{i+1/2, j+1/2, k+1/2},$$

$$\mathcal{J}^{n+1/2} = \left(\mathcal{J}^{1}_{i, j+1/2, k+1/2}, \mathcal{J}^{2}_{i+1/2, j, k+1/2}, \mathcal{J}^{3}_{i+1/2, j+1/2}, \mathcal{J}^{3$$

$$\nabla^{+} f_{i,j,k} = \left(\frac{f_{i+1,j,k} - f_{i,j,k}}{dx}, \frac{f_{i,j+1,k} - f_{i,j,k}}{dy}, \frac{f_{i,j,k+1} - f_{i,j,k}}{dz}\right),$$
$$\nabla^{-} f_{i,j,k} = \left(\frac{f_{i,j,k} - f_{i-1,j,k}}{dx}, \frac{f_{i,j,k} - f_{i,j-1,k}}{dy}, \frac{f_{i,j,k} - f_{i,j,k-1}}{dz}\right).$$

Esirkepov's charge-conserving scheme

- Equations are given in normalized units (see paper).
- The electric field, the charge and particle positions are known at integer time steps.
- The magnetic field, the current and particle velocities are known at half-integer time steps.
- The scheme works if the computational particles' shape function is a B-spline.

$$\frac{\mathbf{E}^{n+1} - \mathbf{E}^n}{dt} = \nabla^+ \times \mathbf{B}^{n+1/2} - \mathcal{J}^{n+1/2},$$
$$\frac{\mathbf{B}^{n+1/2} - \mathbf{B}^{n-1/2}}{dt} = -\nabla^- \times \mathbf{E}^n,$$
$$\nabla^+ \cdot \mathbf{E}^n = \rho^n,$$
$$\nabla^- \cdot \mathbf{B}^{n+1/2} = 0,$$

$$\frac{\mathbf{u}_{\alpha}^{n+1/2} - \mathbf{u}_{\alpha}^{n-1/2}}{dt} = 2\pi \frac{q_{\alpha}}{m_{\alpha}} \frac{m_{e}}{e} \left(\mathbf{E}^{n} \left(\mathbf{x}_{\alpha}^{n}, t \right) + \frac{\mathbf{u}_{\alpha}^{n}}{\gamma_{\alpha}} \times \mathbf{B}^{n} \left(\mathbf{x}_{\alpha}^{n+1} - \mathbf{x}_{\alpha}^{n}\right) \right) + \frac{\mathbf{u}_{\alpha}^{n}}{\gamma_{\alpha}} \times \mathbf{B}^{n} \left(\mathbf{x}_{\alpha}^{n+1} - \mathbf{x}_{\alpha}^{n}\right) + \frac{\mathbf{u}_{\alpha}^{n}}{\gamma_{\alpha}} \times \mathbf{B}^{n} \left(\mathbf{x}_{\alpha}^{n}, t \right) + \frac{\mathbf{u}_{\alpha}^{n}}{\gamma_{\alpha}} \times \mathbf{B}^{n} \left(\mathbf{x}_{\alpha}^{$$

Experimental setup

- The interaction beam ablates a target, thereby generating a dense blast shell of plasma.
- Radiation from this plasma ionizes residual gas in the vessel.
- Shocks form where the blast shell collides with the ambient plasma.
- The CPA beam generates fast protons, which cross the plasma and hit the RCF stack.
- The probing protons are deflected by electromagnetic fields, which yields a spatially varying irradiation of the RCF films.
- The electromagnetic field distribution can be reconstructed from the irradiation pattern.



Sketch from G. Sarri et al, New J. Phys. 12, 045006, 20

Experimental result

- The blast shell was launched at the bottom and moved up.
- The magnetic field lines point horizontally.
- The plasma *8≈1/3.5*.
- The ambient plasma frequency $\omega_p \approx 10^{12}$
- The electron gyro-frequency $\omega_{ce} \approx 10^{11}$.
- We observe a turbulent wave field and a flat front at $t\omega_p \approx 10^3$ or $t\omega_{ce} \approx 10^2$.
- The oscillations have a wave length of the order of the electron thermal gyro-radius.

Image provided by D. Doria, G. Sarri, H. Ahmed and M. Borghesi (CPP, Queens University Belfast, UK)



PIC Simulations:

1D simulation along horizontal direction.2D simulation of radially expanding blast shell.

Initial conditions for 1D simulation

- D simulation box with length 0.75 m.
- eflecting boundary conditions.
- lectron density *n₀* = 2.75 ·10¹⁴cm⁻³
- lectron temperature $T_0 = 2 \text{ keV}$
- patial density / temperature profiles are nown to the right.
- spatially uniform magnetic field $B_{z0} = 0.85 T$ Ils the simulation box.
- lectron thermal gyro-radius $r_{qe} = 1.25 \cdot 10^{-4} m$
- ons : fully ionized nitrogen with temperature /12.5 and density that yields charge eutrality.



Early time

We track the blast shell expansion for 1.1 ns.

The 10-logarithmic ion phase space density distributions are compared for (a) $B_{z0} = 0$ and (b) $B_{z0} = 0.85 T$.

Both shocks look similar. The magnetized one is slower.

Ion acoustic speed in (a) : $2.2 \cdot 10^5 m/s$.

Fast magneto-sonic speed in (b) : $8.2 \cdot 10^5 \text{ m/s}$.

The latter speed exceeds the shock speed : (b) can thus not be a fast MHD shock.

Observation : the magnetic field was not in an equilibrium.



From: Particle-in-cell simulation study of a lower-hybrid shock : Dieckmann, M. E. et al Phys. Plasmas, 23, 062111 (2016).

The shock evolution

/e keep all plasma parameters unchanged.

- *Ie evolve the expansion over 227 ns* (14 nillion time steps).
- ime is given in $\omega_{lh}^{-1} = 0.4$ ns.
- h : lower-hybrid frequency.
- pace unit : $r_{qe} = 1.25 \cdot 10^{-4} m$
- on density is normalized to that of the ilute ions and 8 is the largest displayed alue.
- lagnetic field is normalized to 0.85 T.



The wave front



- Panel (a) shows the evolution of B_z(x,t) in reference frame of the downstream fram
- X* and t* are normalized to the electron thermal gyro-radius and lower-hybrid frequency downstream.
- Panel (b) is the frequency spectrum as a function of the position.
- Panel (c) is the dispersion relation of the l frequency waves downstream compares dispersion relation of the fast magneto-so mode to the coupled FMS/LH branch.

Initial condition for 2D simulation

- Periodic boundary conditions.
- $L_x = 6.4$ cm and $L_y = 12.8$ cm.
- Total of *3·10⁹* CPs.
- Magnetic field points along y.
- Ambient plasma temperature 2keV (electrons) and 160 eV (nitrogen).
- Dense plasma confined by circle 1.
- Density inside 1 is 10 times higher.
- Electrons inside 1 is 3 times hotter.
- Statistical resolution of ions changes across circle 2.



The shock evolution

- Jpper panel: magnetic pressure in units of electron thermal pressure.
- ower panel: ion density in units of ambient ion density (clamped to naximum value 5).



Summary

- I have discussed how we derived the kinetic equations for plasma.
- I have summarized Esirkepov's numerical scheme.
- Experimental results from my collaborators at QUB were presented.
- I have shown how I used 1D/2D PIC simulations to identify the observed structures.