Kinetic Plasma Simulations

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Current deposition can take as much time as the mover (sometimes more). More optimized deposits exist (Umeda 2003).

Higher order schemes possible (Esirkepov 2001, Umeda 2004) Charge conservation makes the whole Maxwell solver local and hyperbolic (like nature intended!). Static fields can be established dynamically.
Charge and current deposition

Charge-conservative deposition without Poisson solver:
initial state must satisfy Poisson equation
usually start with E=0, or drift E field (non-divergent)
initially 0 charge density means electrons must be on top of ions;
can have more elaborate states with initial Poisson solve.

Charge-conservative deposition dynamically establishes static EM fields.

What happens if we start with charge imbalance?

Other alternatives:
solve Poisson equation to correct E field after non-conservative deposition. Then can use simple volume weighting.
Electromagnetic codes

Special sauce

Particle shape should be smoothed to reduce noise. We use current filtering after deposition to reduce high frequency aliases.

Higher order FDTD schemes (4th spatial order) work better at reducing unphysical Cherenkov instability.

Boundary conditions

Periodic is simple -- just copy ghost zones and loop particles. Should not forget particle charge on the other side of the grid!

Conducting BCs: set E field parallel to boundary to 0. Boundary has to lie along the grid.

Outgoing BCs: match an outgoing wave to E, B fields at boundary (Lindman 1975).
Electromagnetic codes

Numerical dispersion is anisotropic (best along grid diagonal)
Phase error for short wavelengths
Causes numerical Cherenkov radiation (when relativistic particles move faster than numerical speed of light)
Electromagnetic codes

Filtering of current

Filtering can be used to
1) improve agreement w/theory at long wavelengths $k \delta x \to 0$ (this is called “compensation”)
2) improve overall accuracy and reduce noise at short wavelengths, $k \delta x \to \pi$ (this is “smoothing” or “attenuating”)

In Fourier code: this can be done in k-space. In finite-difference code — in grid-space. “Digital filtering” (Hamming 77)

$$\phi_j \text{ with } \frac{W \phi_{j-1} + \phi_j + W \phi_{j+1}}{1 + 2W}$$

NB: can’t filter in-place.

see Birdsall & Langdon 1991, Appendix C.
Electromagnetic codes

Filtering of current

Fourier transform:

\[ \phi_{\text{filtered}}(k) = \sum_{j=1}^{N} W \phi_{j-1} + \phi_j + W \phi_{j+1} e^{i k \chi_j} \frac{1}{1 + 2W} \]

\[ \phi_f(k) = \frac{1 + 2W \cos k \Delta x}{1 + 2W} \phi_0(k) = SM_W(\theta) \phi_0(k), \quad \theta \equiv k \Delta x \]

\( W < 0.5 \), or SM reverses sign

\( W = 0.5 \), SM always positive, approaches 0

Application of filter N times:

\( \cos^{2N} (\theta/2) \)

three point: \( \frac{1}{4} (1, 2, 1) \)

five point: \( \frac{1}{16} (1, 4, 6, 4, 1) \)

seven point: \( \frac{1}{64} (1, 6, 15, 20, 15, 6, 1) \)

\( W = 0.5 \) is “binomial” filter. \( W = -1/6 \) is “compensator”

Filter can be called many times — optimization is essential
Field boundary conditions: a few examples

Periodic

![Diagram of periodic boundary conditions]

Perfectly conducting walls

![Diagram of perfectly conducting walls]

Absorbing layer (open boundary)

![Diagram of absorbing layer]

\[
\frac{\partial E}{\partial t} + \sigma E = c \nabla \times B - 4\pi J
\]

\[
\frac{\partial B}{\partial t} + \sigma^* B = -c \nabla \times E
\]

Multi-D generalization: Perfectly Matched Layer (see Bérenger 1994-1996)
Electromagnetic codes

Boundary conditions

Perfectly matched layer (Berenger 1994) -- works like absorbing material with different conductivity for E and B fields). Also, Lindman 1975, transmitting wall (works quite well).

Moving window: simulation can fly at c to follow a fast beam. In this case, outgoing plasma requires no conditions.

Injection: particles can be injected from boundary, or created in pairs throughout the domain. We implemented moving injectors and expanding domains for shock problems. Subsonic inflows/outflows are hard (may need to re-inject some leaving particles)

Parallelization

We use domain decomposition with ghost zones that are communicated via MPI. In 3D we decompose in slabs in y-z plane, so all x-s are on each processor (useful for shocks). In 2D, can decompose both x and y. In 3D, y-z decomposition and slabs in x are used.
Particle boundary conditions: a few examples

- **Periodic**
- **Perfectly reflective walls**
- **Injection absorption**
Parallelization: Domain decomposition

PIC code are really demanding in computing resources => Need to parallelize the code!

A common practice is to use the Message Passing Interface (MPI) library and the domain decomposition technique.

**Example:** Consider a 2D mesh 9x9 cells and 9 CPUs.

**1D decomposition**

```
#1 #2 #3 #4 #5 #6 #7 #8 #9
```

**2D decomposition**

```
#1 #2 #3
#4 #5 #6
#7 #8 #9
```

Applicable to an arbitrary number of CPUs
Choice decomposition depends on the problem
Parallelization: Domain decomposition

MPI Communications

1D: Up to 2 / CPU

2D: Up to 8 / CPU

3D: Up to 26 / CPU

Example: 2D decomposition
Communications of CPU #5

Diagram showing the communication pattern for CPU #5 in a 2D decomposition.
PIC codes scale well to large number of CPUs.

The era of High-Performance Computing! Today $\sim 10^6$ CPUs

See [http://www.top500.org/](http://www.top500.org/)

**OSIRIS Code**

- Weak scaling
- Strong scaling
- Optimal

Efficiency @ 1.6m cores: 97% and 75%

**Zeltron Code**

Zeltron 3D on Mira, first 50 steps

1 MPI rank/core

- cells/core = $7^3$
- cells/core = $10^3$
- cells/core = $13^3$
- cells/core = $16^3$
- cells/core = $20^3$

- core-time/ptcl-step (μs)
Load balancing issues

Computing time (without communications): ~90% particles, ~10% fields

Many particles Processor #5 is slowing down all the others

Few particles Processor #9 is waiting for all the others
A specific example: a reconnecting layer

Density contrast \( \sim > 10! \)

Low-particle density

High-particle density

Some solutions:
- Appropriate domain decomposition
- Dynamical changes of the decomposition
- Varying particle weights
- Hybrid code: MPI-OpenMP
...
Hybrid parallelization: MPI-OpenMP

Example: 2 nodes, 4 processors per node. 1D decomposition

- Pure MPI:
  - Memory is shared within a node
  - The particle loop can be parallelized with OpenMP within a node => Bigger domain, better load balancing.

- MPI-OpenMP:
  - Node 1
  - Node 2
Optimization issues:
As we proceed to ever-denser systems with large number of slower cores per node, unique challenges to scaling are introduced.
This is at the time when formal FP throughput of the systems is increasing.
Memory bandwidth; vectorization pipeline; algorithmic issues

Main time hogs:
Mover (Lorentz force push) — trivially parallelizable
Deposit (current calculation on the grid) — algorithmic issues (possible solution: “private tiles of current array”)

Data locality? array of structures vs structure of arrays
p( x(n), y(n), z(n), vx(n), vy(n), vz(n)) vs p(n).(x,y,z,vx,vy,vz)
XOOPIC (2D RPIC, free unix version, Mac and Windows are paid through Tech-X);
VORPAL (1,2,3D RPIC, hybrid, sold by Tech-X)
TRISTAN (public serial version), 3D RPIC (also have 2D), becoming public now
OSIRIS (UCLA) 3D RPIC, mainly used for plasma accelerator research
Apar-T, Zeltron.
PIC-on-GPU — open source
LSP -- commercial PIC and hybrid code, used at national labs
VLPL -- laser-plasma code (Pukhov ~2000)
Reconnection research code (UMD, UDelaware)
Every national lab has PIC codes.
All are tuned for different problems, and sometimes use different formulations (e.g. vector potential vs fields, etc). Direct comparison is rarely done.
Public codes

http://ptsg.egr.msu.edu/

Download the software now.

- XES1
- XPDP1
- XPDC1
- XPDS1
- XPDP2
- XOOPIC
- XIBC
- XGRAFIX

Our most recent, popular and well kept up codes are on bounded plasma, plasma device codes XPDP1, XPDC1, XPDS1, and XPDP2. The P, C, and S mean planar, cylindrical, or spherical bounding electrodes; the 1 means 1d 3v and the 2 means 2d 3v. These are electrostatic, may have an applied magnetic field, use many particles (like hundreds to millions), particle-in-cell (PIC), and allow for collisions between the charged particles (electrons and ions, + or -) and the background neutrals (PCC-MCC). The electrodes are connected by an external series R, L, C, source circuit, solved by Kirchhoff's laws simultaneously with the internal plasma solution (Poisson's equation). The source may be V(t) or I(t), may include a ramp-up (in time). XPDP2 is planar in x, periodic in y or fully bounded in (x,y), driven by one or two sources. (For detailed information, click here)
Beyond the standard electromagnetic PIC code

Non-Cartesian grid

Sometimes, it can be more interesting to use non-cartesian grid to take advantage of the symmetries of the system.

=> Simplifies the initial setup load balancing and boundary conditions

Cartesian Yee-mesh

Spherical Yee-mesh

Applications to plasmas around a central object.

Examples: pulsar magnetospheres, accreting systems

[Belyaev 15]

[Chen & Beloborodov 14]
Beyond the standard electromagnetic PIC code

Emission of non-thermal radiation

The frequency of the energetic radiation is often not resolved by the grid!

Example: Synchrotron radiation critical frequency: \[ \omega_{\text{syn}} \propto \gamma^2 \frac{qB}{mc} = \gamma^3 \omega_c \gg 1/\Delta t \]

Hence, photons must be added as a separate species.

Also, the radiation reaction force must be added in the equation of motion explicitly:

\[
\frac{dp}{dt} = q \left( E + \frac{v \times B}{c} \right) + g
\]

The radiation reaction force is then given by the Landau-Lifshitz formula (classical electrodynamics):

\[
g \approx \frac{2}{3} r_e^2 \left[ (E + \beta \times B) \times B + (\beta \cdot E) E \right] - \frac{2}{3} r_e^2 \gamma^2 \left[ (E + \beta \times B)^2 - (\beta \cdot E)^2 \right] \beta
\]

For inverse Compton scattering (isotropic external source in the Thomson regime):

\[
g = -\frac{4}{3} \sigma_T \gamma^2 U_{rad} \beta
\]

Applications to e.g., PWN, AGN jets

[See Cerutti+2013, 2016]
Beyond the standard electromagnetic PIC code

Pair creation, QED effects

The laser-plasma community is adding extra physics for the next generation of high-intensity laser that will reach a fraction of the critical field.

\[ E_{QED} = \frac{m_e^2 c^3}{e \hbar} \approx 4.4 \times 10^{13} \text{ G} \]

\[ \Rightarrow \text{QED effects and pair creation important} \]

Regime relevant to pulsars, magnetars \((B > B_{QED})\), and black hole magnetospheres.

PIC with pair creation start being used in astrophysics: Timokhin 2010, Chen & Beloborodov 2014, Philippov + 2015a,b.
Beyond the standard electromagnetic PIC code

Non-Euclidian metric

Application to e.g., black hole magnetospheres and pulsars.

The metric changes Maxwell equations, the effective size of the particles (current deposition), and the equation of motion.

Example: For a Schwarzschild metric

\[ ds^2 = g_{\mu \nu} dx^\mu dx^\nu = -\alpha^2 dt^2 + \frac{dr^2}{\alpha^2 + r^2} + r^2 (d\theta^2 + \sin^2 \theta d\varphi^2) \]

Where \( \alpha = \sqrt{1 - \frac{r_g}{r}} \) is the “lapse function”

Maxwell equation as seen in a local frame (“FIDO” observers): [Thorne+1986]

\[ \frac{\partial E}{\partial t} = c \nabla \times (\alpha B) - 4 \pi \alpha J \quad \frac{\partial B}{\partial t} = -c \nabla \times (\alpha E) \]

See PIC implementation in \textit{EZeltron} by Philippov + 2015 for details.
A few words about hybrid PIC codes

An important limitation of full PIC methods is the **limited separation of scales**. Only microscopic systems can be modelled.

In particular, it's hard to model electron/ions plasmas with realistic mass ratio. Plasma frequency $\omega_p \propto \sqrt{m} \Rightarrow \omega_{pe}/\omega_{pi} = \sqrt{m_i/m_e} \approx 43$

Hence, **ion acceleration is hard to capture with PIC** (except in the ultra-relativistic limit).

**Hybrid code**: [e.g., see Winske+2003]

**Ions** are PIC particles: $m_i \frac{d v_i}{dt} = q \left( E + \frac{v_i \times B}{c} \right)$

**Electrons** are treated as a massless neutralizing fluid (method works for non-relativistic plasmas): $n_e m_e \frac{d V_e}{dt} = 0 = -e n_e q \left( E + \frac{V_e \times B}{c} \right) - \nabla \cdot P_e$

Hybrid codes


Hybrid Method: System Equations

- Electromagnetic Fields
  - Faraday’s Law
    \[ \frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} \]
  - Ampere’s Law
    \[ \nabla \times \vec{B} = \mu_0 \vec{J} = \mu_0 n_i q_i (\vec{V}_i - \vec{V}_e) \]
  - Electron momentum equation
    \[ \vec{E} = -\vec{V}_i \times \vec{B} - \frac{1}{n_i q_i} \nabla P_e - \frac{1}{\mu_0 n_i q_i} \vec{B} \times (\nabla \times \vec{B}) \]
  - Electric field is a “state” quantity

\[
\begin{align*}
\vec{E}_{i,j,k}^n &= -\vec{V}_{i,j,k}^n \times \vec{B}_{i,j,k}^n \\
&+ \frac{1}{n_{i,j,k}^n} (\nabla \times \vec{B}_{i+1/2,j+1/2,k+1/2}^n) \times \vec{B}_{i,j,k}^n \\
\vec{B}_{i+1/2,j+1/2,k+1/2}^{n+1/2} &= \vec{B}_{i+1/2,j+1/2,k+1/2}^n - \frac{\Delta t}{2} (\nabla \times \vec{E}_{i,j,k}^n), \\
\vec{B}_{i,j,k}^{n+1} &= \vec{B}_{i,j,k}^n - \Delta t (\nabla \times \vec{E}_{i+1/2,j+1/2,k+1/2}^{n+1/2})
\end{align*}
\]

Predictor-corrector method used to properly center B field in time. Requires two pushes of ions per time step.

Short-wavelength modes (whistler waves) run faster (omega \sim k^2) — need to truncate the mode
Hybrid codes


Dispersion relation for whistler and Alfven waves; note that whistler waves run away in hybrid approximation
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Applications and examples
No “subscale” physics – resolve the smallest scales! Converse is expense
Usually deal with non-clumped flows, hence AMR is not needed.
Some exceptions -- reconnection simulations.
FDTD conserves divergence of B to machine precision.

PIC issues:
• Particle discretization error
• Smoothing error (finite size particles)
• Statistical noise (granular force)
• Grid aliasing (grid assignment)
• Deterioration of quadrature in time integration
• Short-range forces (collisions) neglected

• Analysis of large-scale simulations is nontrivial

but the alternative is 6D Vlasov integration...
Outlook

PIC is a versatile robust tool for self-consistent solution of plasma physics.

- Electrostatic method is well understood, and analytical theory of numerical plasma exists.
- Electromagnetic model is more diverse, and many alternative formulations exist. Multidimensional theory of the simulation is not as well developed.
- Implicit methods are now common for large timestep solutions.
- Long term stability is an issue for largest runs.
- In astrophysics PIC has the potential to answer the most fundamental theoretical questions: particle acceleration, viability of two-temperature plasmas, dissipation of turbulence.
Applications

Laser-plasma interaction and plasma based accelerators

Laser driver:

Beam driver:
Applications

Engineering:
Gas discharges, plasma processing, film deposition. PIC with Monte-Carlo collisions and external circuit driving.

Lightning-oil tank interaction!
Applications

Astrophysics:
Collisionless shocks (solar wind, interstellar medium, relativistic jets), wind-magnetosphere interactions, pulsar magnetospheres. Rapid reconnection, particle acceleration.

Case study: Wind-magnetosphere interaction in double pulsar binary J0737. Attempt to simulate macroscopic system with PIC. Possible if the size of the system is > 50 skindepths.

“Caution is required, but one can be paralyzed by a conservative attitude into missing profitable applications”
Birdsall & Langdon (1991)
Shock and magnetosheath of pulsar B

Similar to the interaction between Earth magnetosphere and solar wind.
Shock modulated at $2\Omega$

Reconnection once per period

Cusp filling on downwind side

Density asymmetries

$R_m \sim 50000$ km
3D magnetosphere
3D magnetosphere
3D magnetosphere -- nonorthogonal rotator
3D magnetosphere -- nonorthogonal rotator
3D magnetosphere: fieldlines
Counterstreaming (Weibel) INSTABILITY


\[ B \]

\[ x \]

\[ y \]

\[ z \]

\[ J \]

\[ J \]

\[ B \] – field is generated ...

... current filamentation ...

For electron streams...

\[ \Gamma_{\text{max}} \simeq \frac{\omega_p^2}{\gamma} \]

\[ k_{\text{max}} \simeq \frac{1}{\sqrt{2} \gamma \perp c^2} \]
Counterstreaming instabilities
Counterstreaming instabilities
Counterstreaming instabilities
Simulations of Collisionless Shocks
Numerical simulation of collisionless shocks

Particle-in-cell method:
- Collect currents at the cell edges
- Solve fields on the mesh (Maxwell’s eqs)
- Interpolate fields to particles positions
- Move particles under Lorentz force

Code “TRISTAN-MP”:
- 3D (and 2D) cartesian electromagnetic particle-in-cell code
- Radiation BCs; moving window
- Charge-conservative current deposition (no Poisson eq)
- Filtering of current data
- Fully parallelized (512proc+) domain decomposition
- Routinely work with upto 10 billion+ particles

Simulation setup:
Relativistic $e^\pm$ or $e^-$ ion wind ($\gamma = 15$) with B field ($\sigma = \omega_c^2 / \omega_p^2 = B^2 / (4\pi n_\gamma mc^2) = 0-10$)
Reflecting wall (particles and fields)
Upstream $c/\omega_p = 10$ cells, $c/\omega_c > 5$ cells;
Problem setup

Simulation is in the downstream frame. If we understand how shocks work in this simple frame, we can boost the result to any frame to construct astrophysically interesting models. Disadvantage -- upstream flow has to move over the grid -- potential long term instabilities.

Use reflecting wall to initialize a shock

"Shock" is a jump in density & velocity
**Why does a shock exist?**

Particles are slowed down either by instability (two-stream-like) or by magnetic reflection. Electrostatic reflection is important for nonrelativistic shocks and when ions are present.

---

**Weibel instability** *(Weibel 1959)*

Spatial growth scale $c/\omega_p$; timescale $10/\omega_p$

\[
L \approx \frac{c}{\omega_{pe}} = 10 \text{ km} \sqrt{\gamma/n_0 [\text{cm}^{-3}]} \\
T \approx \frac{1}{\omega_p} = 30 \mu\text{s} \sqrt{\gamma/n_0 [\text{cm}^{-3}]} 
\]
Evolution of field energy through the 3D shock structure, including the precursor.

50x50x1500 skindepths. Current merging (like currents attract). Secondary Weibel instability stops the bulk of the plasma. Pinching leads to randomization.
3D unmagnetized pair shock: magnetic energy
Unmagnetized pair shock

Steady state counterstreaming leads to self-replicating shock structure