#### Kinetic Simulations of Astrophysical Plasmas Anatoly Spitkovsky (Princeton)



## Contents

Plasma physics on computers How PIC works Electrostatic codes Charge assignment and shape factors Discretization effects Electromagnetic codes FDTD and Yee mesh Particle movers: Boris' algorithm Conservative charge deposition Boundary conditions Applications and examples

# **PIC cycle**



# **Electromagnetic codes**

#### Charge and current deposition



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

Charge conservation makes the whole Maxwell solver local and hyperbolic (like nature intended!). Static fields can be established dynamically.

#### **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**

#### **Boundary conditions**

Perfectly matched layer (Berenger 1994) -- works like absorbing material with different conductivity for E and B fields)

Moving window: simulation can fly at c to follow a fast beam. 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.

#### 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).

# **Electromagnetic codes**

#### Optimization

Main time expense: the mover and the deposition.

Both involve moving data to and from memory, hence cache optimization is essential.

Single precision vs double.

#### Data analysis

Nontrivial, as one can easily generate terabytes of data (in 3D) Saving every particle is VERY expensive, so one chooses which information to discard, or do analysis on-the-fly. E.g., fluid quantities can be reconstructed from particles (like taking moments of the distribution function).

Test-particle trajectories can be useful (or confusing).

Visualization: What do you do with 100 billion particles? Treat simulations as experiments?

# Notes on PIC

There is no "subscale" physics with PIC -- we resolve the smallest scales! Converse is expense...

Usually deal with non-clumped flows, hence AMR usually not used. 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...

#### Laser-plasma interaction and plasma based accelerators Laser driver:



#### Beam driver:



# 30 September 2004 International weekly journal of science

**Dream beam** 

The dawn of compact particle accelerators

Offshore tuna ranches A threat to US waters?

The Earth's hum Sounds of air and sea

technology feature RNA interference

Protein folding Escape from the ribosome

Human ancestry One from all and all from one

#### Engineering:

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

Lightning-oil tank interaction!



### Astrophysics:

Any problem with multivalued, anisotropic or otherwise strange distribution function.

Collisionless shocks (solar wind, interstellar medium, relativistic jets): structure and the physics of shock mediation

Particle acceleration: when, where, how?

Cosmic ray propagation and field generation

Reconnection

**Dissipation of turbulence** 

Case study: Wind-magnetosphere interaction in double pulsar binary J0737. (*How to use PIC as a bad MHD code*)

Simulation of a macroscopic system with PIC (AS & Arons 2004). Possible if the size of the system is > 50 skindepths.





#### Shock and magnetosheath of pulsar B



Similar to the interaction between Earth magnetosphere and solar wind.

#### Shock and magnetosheath of pulsar B: effects of rotation



Shock modulated at  $2\Omega$ Reconnection once per period Cusp filling on downwind side Density asymmetries  $R_m$ ~50000 km

### 3D magnetosphere



## 3D magnetosphere



#### 3D magnetosphere



## Simulations of Relativistic Shocks

Anatoly Spitkovsky

In collaboration with: Jon Arons & Phil Chang (Berkeley), Uri Keshet (IAS), Boaz Katz (Weizmann), Lorenzo Sironi & Mario Riquelme (Princeton)

## The physics of collisionless shocks

Shock: sudden change in density, temperature, pressure that decelerates supersonic flow

Thickness ~mean free path in air: mean free path ~micron



On Earth, most shocks are mediated by collisions



Astro: Mean free path to Coulomb collisions in enormous: 1000pc in supernova remnants, ~Mpc in galaxy clusters *Mean free path > scales of interest* 

shocks must be mediated without direct collision, but through interaction with collective fields

collisionless shocks

## The physics of collisionless shocks

Shock: sudden change in density, temperature, pressure that decelerates supersonic flow

Thickness ~mean free path in air: mean free path ~micron

On Earth, most shocks are mediated by collisions





Astro: Mean free path to Coulomb collisions in enormous: 1000pc in supernova remnants, ~Mpc in galaxy clusters *Mean free path > scales of interest* 

shocks must be mediated without direct collision, but through interaction with collective fields

collisionless shocks

## The physics of collisionless shocks

Shock: sudden change in density, temperature, pressure that decelerates supersonic flow

Thickness ~mean free path in air: mean free path ~micron

On Earth, most shocks are mediated by collisions





Astro: Mean free path to Coulomb collisions i enormous: 1000pc in supernova remnants, ~Mpc in galaxy clusters *Mean free path > scales of interest* 

shocks must be mediated without direct collision, but through interaction with collective fields

 $l_{Coul} = \frac{m_e^2 v^4}{8\pi n Z^2 e^4 l n \Lambda} \approx 1.4 \times 10^4 (\frac{T}{K})^2 (\frac{n}{cm^{-3}})^{-1} cm$ 

![](_page_22_Figure_0.jpeg)

Shocks span a range of parameters: nonrelativistic to relativistic flows

magnetization (magnetic/kinetic energy ratio)

composition (pairs/e-ions/pairs + ions)

![](_page_22_Figure_4.jpeg)

![](_page_23_Picture_0.jpeg)

#### SN 1006; age 1002 yrs

![](_page_23_Picture_2.jpeg)

Chandra X-ray observatory

![](_page_23_Picture_4.jpeg)

## Supernova Remnants

![](_page_23_Picture_6.jpeg)

Casiopea A

Age 300 yr (1670 AD)

Age 954 yr (1054 AD)

Crab Nebula

Age 436 yr (1572 AD)

Tycho

![](_page_23_Figure_12.jpeg)

#### G347.3 TeV $\gamma\text{-rays}$

Explosions release  $10^{51}$  ergs of energy

X-ray luminosity: 3.8x10<sup>36</sup> erg/s

Sun: 10<sup>33</sup> erg/s in optical

![](_page_23_Picture_17.jpeg)

#### Supernova Remnants

 $E_{SN} \sim 10^{51} ergs$   $E_{SN} \sim \frac{1}{2} M_{ej} v_{ej}^2$   $v_{ej} \sim 10^4 km/s$ 

Stages of evolution of supernova remnants

Free expansion ~ 200 yrs Blast wave -- Sedov-Taylor E=const solution 10^6 K Radiative shock -- momentum conserving Merge with ISM

![](_page_24_Figure_4.jpeg)

3% of the SNR energy is enough to explain energy density of galactic cosmic rays.

![](_page_24_Picture_6.jpeg)

![](_page_24_Figure_7.jpeg)

![](_page_24_Figure_8.jpeg)

Tycho

![](_page_24_Picture_10.jpeg)

## SN remnant: Cas A (3-70 kev; Chandra)

SNe II remnant

Age 300 yr (1670 AD)

![](_page_25_Picture_3.jpeg)

X-ray luminosity: 3.8x10<sup>36</sup> erg/s Mass of x-ray gas 10-15 solar mass.

# SN remnant: Cas A (3-70 kev; Chandra)

![](_page_26_Picture_1.jpeg)

# Shocking astrophysics

![](_page_27_Picture_1.jpeg)

![](_page_27_Figure_2.jpeg)

![](_page_27_Figure_3.jpeg)

March 27, 1994

April 3

Astrophysical collisonless shocks can:

- 1. accelerate particles
- 2. amplify magnetic fields (or generate them from scratch)
- 3. exchange energy between electrons and ions

![](_page_27_Figure_8.jpeg)

### Particle acceleration:

 $\Delta E/E \sim V_{shock}/C$ 

ľ

 $\overline{N(E)} \sim \overline{N_0} E^{-K(r)}$ 

- Original idea -- Fermi (1949) -- scattering off moving clouds. Too slow (second order in v/c) to explain CR spectrum, because clouds both approach and recede.
- In shocks, acceleration is first order in v/c, because flows are always converging (Blandford & Ostriker 78,Bell 78, Krymsky 77)
- Efficient scattering of particles is required. Particles diffuse around the shock. Monte Carlo simulations show that this implies very high level of turbulence. Is this realistic? Are there specific conditions?

![](_page_28_Figure_6.jpeg)

## Shocking astrophysics

![](_page_29_Picture_1.jpeg)

#### Open issues:

What is the structure of collisionless shocks? Do they exist? How do you collide without collisions?

Particle acceleration -- Fermi mechanism? Other? Efficiency?

Generation of magnetic fields? GRB/SNR shocks, primordial fields?

Equilibration between ions and electrons?

Turns out that all questions are related, and particle acceleration is the crucial link

Understanding conditions when particles are accelerated can constrain astrophysical models

## Particle-in-Cell (PIC) method

Most fundamental way to treat plasma physics without (m)any approximations price: have to resolve tiny and fast scales (plasma skin depth and plasma freq.) to be interesting, simulations have to be large

![](_page_30_Figure_2.jpeg)

PIC method (aka PM method):

Collect currents at cell edges
Solve fields on the mesh (Maxwell's eqs)
Interpolate fields to particle positions
Move particles under Lorentz force

Commonly used in accelerator/plasma physics, and now starting to be accepted in astrophysics

*The code*: relativistic 3D EM PIC code *TRISTAN-MP* ; grids up to 1024^2x10000 Optimized for large-scale simulations with more than 20e9 particles. 100x100x1000 c/ $\omega_p$ Noise reduction, improved treatment of ultra-relativistic flows. Works in both 3D and 2D configurations. Most of the physics is captured in 2D *Most of our results are now starting to be confirmed by independent groups* 

## **Problem setup**

![](_page_31_Figure_1.jpeg)

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. (in these simulations we do not model the formation of contact discontinuity)

We verified that the wall plays no adverse effect by comparing with a two-shell collision.

# Setup

![](_page_32_Figure_1.jpeg)

$$\sigma \equiv \frac{B^2/4\pi}{(\gamma - 1)nmc^2} = \frac{1}{M_A^2} = \left(\frac{\omega_c}{\omega_p}\right)^2 \left(\frac{c}{v}\right)^2 = \left[\frac{c/\omega_p}{R_L}\right]^2$$

Simulation is done in the "downstream" frame, where a shock is moving on the grid Vary: B field and orientation, speed of the flow, composition

## Relativistic pair shocks

#### *Shock structure for* σ=0.1

#### **Shock structure for** σ=0

![](_page_33_Figure_3.jpeg)

Magnetized shock is mediated by magnetic reflection, while the unmagnetized shock -- by field generation from filamentation instability. Transition is near  $\sigma$ =1e-3 (A.S. 2005)

#### **Unmagnetized pair shock**

#### Magnetic field generation: Weibel instability

Field cascades from  $c/\omega_p$  scale to larger scale due to current filament merging

![](_page_34_Figure_3.jpeg)

50

decay and inverse cascade (Chang, AS, Arons 08).

150

100

c/om\_p

## Weibel instability

![](_page_35_Figure_1.jpeg)

Weibel (1959) Moiseev & Sagdeev (1963) Medvedev & Loeb (1999)

Electromagnetic streaming instability. Works by filamentation of plasma Spatial growth scale -- skin depth, time scale -- plasma frequency

$$L \approx c / \omega_{pe} = 10 \text{ km } \sqrt{\gamma / n_0 [\text{cm}^{-3}]}$$
$$T \approx 1 / \omega_p = 30 \text{ } \mu \text{s } \sqrt{\gamma / n_0 [\text{cm}^{-3}]}$$
## Relativistic pair shocks: no initial B field

*Establishment of a self-propagating shock structure for*  $\sigma$ =0







### 3D shock structure: long term



Secondary Weibel instability stops the bulk of the plasma. Pinching leads to randomization.

## 3D unmagnetized pair shock: magnetic energy



## **Counterstreaming instabilities**



## **Counterstreaming instabilities**



## **Counterstreaming instabilities**



## Unmagnetized pair shock: particle trajectories



color: magnetic energy density



Unmagnetized shock: shock is driven by returning particle precursor (CR!)

Steady counterstreaming leads to self-replicating shock structure

*x- px momentum space* 

x- py momentum space

Shock structure for σ=0 (AS '08)

# Unmagnetized pair shock:

downstream spectrum: development of nonthermal tail!



A.S. 2008, ApJ, 682, L5

## Unmagnetized pair shock: particle trajectories

Nonthermal tail develops,  $N(E) \sim E^{-2.4}$ . Nonthermal contribution is 1% by number, ~10% by energy. Well fit by low energy Maxwellian + power law with cutoff.

Same process is seen in the 3D data as well. Easy to have  $\Delta B/B >>1$  when B=0!

Injection works self-consistently from the thermal distribution.



Particles that are accelerated the most, graze the shock surface

## Unmagnetized pair shock: particle trajectories

Nonthermal tail develops,  $N(E) \sim E^{-2.4}$ . Nonthermal contribution is 1% by number, ~10% by energy. Well fit by low energy Maxwellian + power law with cutoff.

Same process is seen in the 3D data as well. Easy to have  $\Delta B/B >>1$  when B=0!

Injection works self-consistently from the thermal distribution.



Particles that are accelerated the most, graze the shock surface

## Transition between magnetized and unmagnetized shocks:



# Transition between magnetized and unmagnetized shocks:



B field

## Transition between magnetized and unmagnetized shocks:



B field

Acceleration:  $\sigma < 10^{-3}$  produce power laws,  $\sigma > 10^{-3}$  just thermalize

## Magnetized pair shocks: acceleration

### Pair shocks: $\sigma=0.1$ , $\gamma=15$ ; Find p-law index near -2.3 (Sironi & AS 2009)



 $\beta_{sh}/cos\theta < 1$  -- subluminal Self-turbulence is not enough to exceed superluminal constraint



In upstream frame need:  $\theta_{upstream} < 32^{\circ}/\gamma$  for acceleration

Observe transition between subluminal and superluminal shocks. Shock drift acceleration is important near transition.

Perpendicular shocks are poor accelerators.

# Acceleration mechanisms: "Fermi" vs shock-drift

Drift acceleration becomes increasingly important for higher obliquities.



## Acceleration mechanisms: "Fermi" vs shock-drift

Drift acceleration becomes increasingly important for higher obliquities.



### Relativistic Electron-ion shocks

We explored electron-ion shocks up to mass ratio of 1000.



#### A.S. 2008, ApJ, 673, L39

#### Relativistic Electron-ion shocks

We observe electron-ion energy exchange in the shock. Electrons come close to equipartition with the ions. *Behaves like pair shock!* This helps to explain the high electron energy fraction inferred in GRB afterglows.

Fermi acceleration proceeds very similarly in unmagnetized e-ion shocks

Perpendicular e-ion shocks do heating, but not significant acceleration.







Electron heating is related to electron oscillation in ion filaments, and the longitudinal instability of the filaments.



## Pair shocks: magnetic field evolution

Can Weibel shocks generate enough field for downstream synchrotron emission?

Returning particles cause filamentation far in the upstream region and cause growth of the scale and amplitude of the upstream field.

This affects the rate of decay of the field in the downsream (longer wavelengths decay slower).

1% magnetization is not unreasonable (Keshet, Katz, A.S., Waxman 2008).



we see growth of field energy and scale with time near shock, and slower decay downstream at 10<sup>4</sup> skindepths

## Pair shocks: magnetic field evolution



## Field evolution: Without high energy particles:

#### With high energy particles:

Scale growth is caused by accelerated particles. Larger field accelerates more particles -bootstrapping!



# B field amplification

CR accelerating shocks can cause a current of protons to propagate through the upstream. Bell (04, 05) found an MHD instability of CRs flying through magnetized plasma.

The interaction is nonresonant at wavelength << Larmor radius of CRs.

We simulated this instability with PIC in 2D and 3D (Riquelme and A.S. 08)

Saturation is due to plasma motion (V<sub>A</sub>~ V<sub>d,CR</sub>), or CR deflection; for SNR conditions expect ~10 field increase.

#### Bell's nonresonant CR instability



Cosmic ray current J<sub>cr</sub>=en<sub>cr</sub>v<sub>sh</sub>

# B field amplification

CR accelerating shocks can cause a current of protons to propagate through the upstream. Bell (04, 05) found an MHD instability of CRs flying through magnetized plasma.

The interaction is nonresonant at wavelength << Larmor radius of CRs.

We simulated this instability with PIC in 2D and 3D (Riquelme and A.S. 08)

Saturation is due to plasma motion ( $V_A \sim V_{d,CR}$ ), or CR deflection; for SNR conditions expect ~10 field increase.



#### Bell's nonresonant CR instability



 $k_{max} C = 2\pi J_{cr}/B_0$  $\gamma_{max} = k_{max} V_{Alfven,0}$ 

Need magnetized plasma:  $\omega_{ci} >> \gamma_{max}$ 

## B field amplification: 3D runs

#### Bell's nonresonant CR instability

(Riquelme and A.S. arXiv:0810.4565)



#### Field amplification of ~10 in SNRs can be due to Bell's instability

## B field amplification

#### Bell's nonresonant CR instability



## PIC simulations of shocks



## Shocking astrophysics

Open issues: What is the structure of collisionless shocks? Do they exist? How do you collide without collisions?

Particle acceleration -- Fermi mechanism? Other? Efficiency?

Equilibration between ions and electrons?

Generation of magnetic fields? GRB/SNR shocks, primordial fields?



# Shocking astrophysics

Open issues:

What is the structure of collisionless shocks? Do they exist? How do you collide without collisions?

Particle acceleration -- Fermi mechanism? Other? Efficiency?

Equilibration between ions and electrons?

Generation of magnetic fields? GRB/SNR shocks, primordial fields?



# Astrophysical implications: Pulsar Wind Nebulae (PWNe)



Shock acceleration in PWN implies low magnetization shock.  $\sigma$ =0.001-0.01 is inferred from modeling of the nebulae. This is a "transition" regime between magnetized and unmagnetized shocks -- expect Weibel instability to dominate the shock.

Equatorial shock occurs where the current sheet lies -- hence expect a weakly magnetized "equatorial wedge" -- consistent with shock physics.

At the moment pair composition could be ok, although other arguments suggest the presence of pair-ion plasma (A.S. & Arons 04).

Alternative -- reconnecting flow at the termination shock (Lyubarsky & Petri 07)

## **Astrophysical Implications**



9

#### Gamma Ray Bursts

Very low magnetization  $\sigma$ =10<sup>-8</sup> shocks can operate even in electron-ion plasma.

Electron heating to near equipartition with the ions implies that high electron energy fraction ( $\varepsilon_e$ =0.1) is not unreasonable. Magnetic fields near ( $\varepsilon_B$ =0.01) could also be generated. Can we see thermal component?

#### AGN and other jets

High magnetization perpendicular pair flows are unlikely to generate nonthermal particles through Fermi acceleration. Other physics needed? Not pure pair flows? Sheath flow?

#### Supernova Remnants

We see field amplification due to streaming CRs: Bell's instability is part of the amplification puzzle.

Parallel shocks are more likely to accelerate particles than perpendicular shocks (e.g. SN1006?).

## Nonrelativistic shocks

New scales: speed is no longer c, so Debye and skin depth are different, thermal velocity no longer c.

Difficulties: longer runtimes (still resolve speed of light) Acceleration is intrinsically slower (vshock/c)^2

Injection problem -- how to pre-accelerate particles so their larmor radius exceeds the scale of the shock?

Two types of shocks -- quasi-parallel and quasi-perpendicular

We investigated quasi-perpendicular shocks (inclination angle 15 degrees), with mass ratios from 100 to 1000, and speeds from 3000 to 30000 km/s, Alfvenic Mach number from 3 to 100. For 1000km/s, B=25uG: Ma=18; 3000km/s->Ma=54 We are essentially in a realistic regime, albeit in 2.5D.



# Nonrelativistic shocks: shock structure

mi/me=400, v=18,000km/s, Ma=5



Shock foot, ramp, overshoot, returning ions, electron heating, whistler(?) waves.

# Nonrelativistic shocks: shock structure mi/me=100, v=18,000km/s, Ma=45



Shock foot, ramp, overshoot, returning ions, electron heating, whistler(?) waves, spectra.

# Nonrelativistic shocks: shock structure mi/me=100, v=18,000km/s, Ma=140



Shock foot, ramp, overshoot, returning ions, electron heating, whistler(?) waves, spectra.

# **Electron acceleration**

Whistler waves in the shock foot cause E II B.

 $\Gamma_{e}$ -1 (yellow line),  $\epsilon_{parallel}$  (green line), and  $\epsilon_{perpendicular}$  (red line)





 $\epsilon_i \equiv \int \frac{e}{m_e c^2} v_i E_i dt$
# **Electron acceleration**

Whistler waves in the shock foot cause E II B.

 $\Gamma_{e-1}$  (yellow line),  $\epsilon_{parallel}$  (green line), and  $\epsilon_{perpendicular}$  (red line)



ΙB

B

 $\epsilon_i \equiv \int \frac{e}{m_e c^2} v_i E_i dt$ 

We observe pre-acceleration of electrons to energies comparable to ion energies (injection)

# Parameter dependence

#### **Inclination angle**

#### **Mass ratio**



#### **Electron injection needs:**

Quasi-perpendicular shocks,  $45^{\circ} < \theta_{Bn} < 90^{\circ}$ Lower Alfvenic Mach numbers (to create whistlers),  $M_A < (m_i/m_e)^{1/2}$ 

### solar wind



Electron injection works better for lower Mach #s. Quasi-perpendicular Earth bow shocks observe strongest power laws.

# Application: magnetospheres

#### Astrophysics:

Nonneutral plasma physics in pulsar magnetospheres

Electric field on the surface extracts charges. Does magnetosphere form?

Expect to see this:





#### Astrophysics:

Nonneutral plasma physics in pulsar magnetospheres. Diocotron instability



#### Astrophysics:

Nonneutral plasma physics in pulsar magnetospheres. Diocotron instability

Space-charge limited flow dynamics in presence of pair formation needs to be addressed.





# Application: reconnection



#### BC arguments: periodic vs open

Daughton et al v Drake et al

Reconnection questions: Rate of reconection Partilce energization e-ion vs e-positron



#### Daughton & Karimabadi 07





#### Yin et al 08





## 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.

## Outlook

#### •Current results:

- ab-initio evidence for particle acceleration in shocks
- conditions for particle acceleration -- constraints on models!
- •measurements of ion-electron energy exchange in shocks
- •CR feedback and field amplification
- •Pulsars: instabilities that lead to charge transfer in the magnetosphere.
- •Reconnection: rate of reconnection, physics of the reconnection layer.



•Computational issues:

- optimization
- load balancing
- •visualization -- what to do with 100 billion particles?!!!
- treating simulations as experiments?
- •How to figure what is going on? Dispersion relations, test particle trajectories, reproducibility.