Hybrid modeling of plasmas

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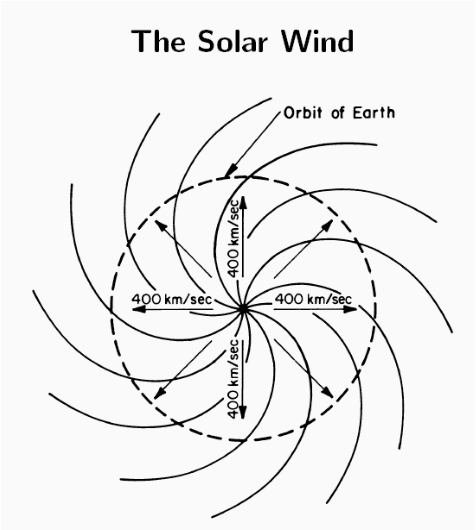
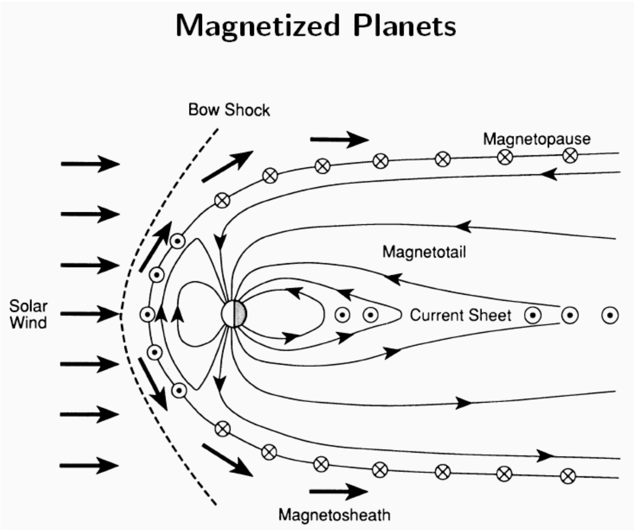
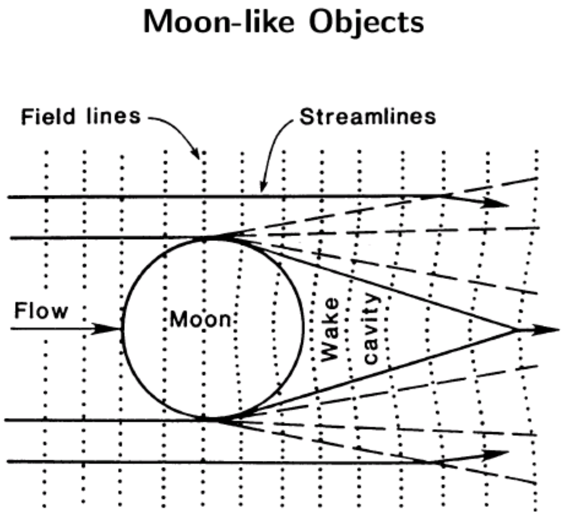
Outline

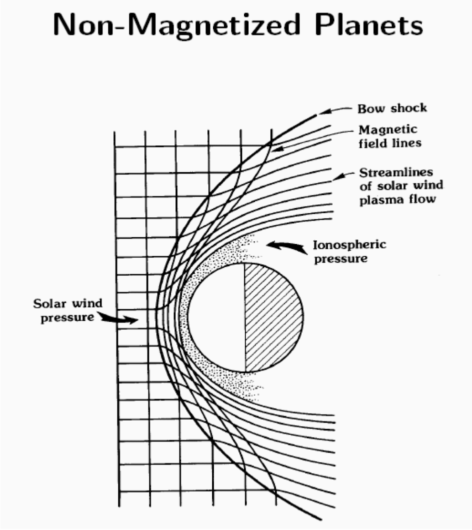
- Background and motivation
- Space plasma modeling
    - Fluid
    - Particle
    - Hybrid
- Hybrid model
    - Algorithm
    - Results
        - Energy conservation
        - Temporal and spatial scales
        - Moon, Mars

Interactions between the solar wind and solar system objects









[Kivelson and Russell]

The MHD Equations

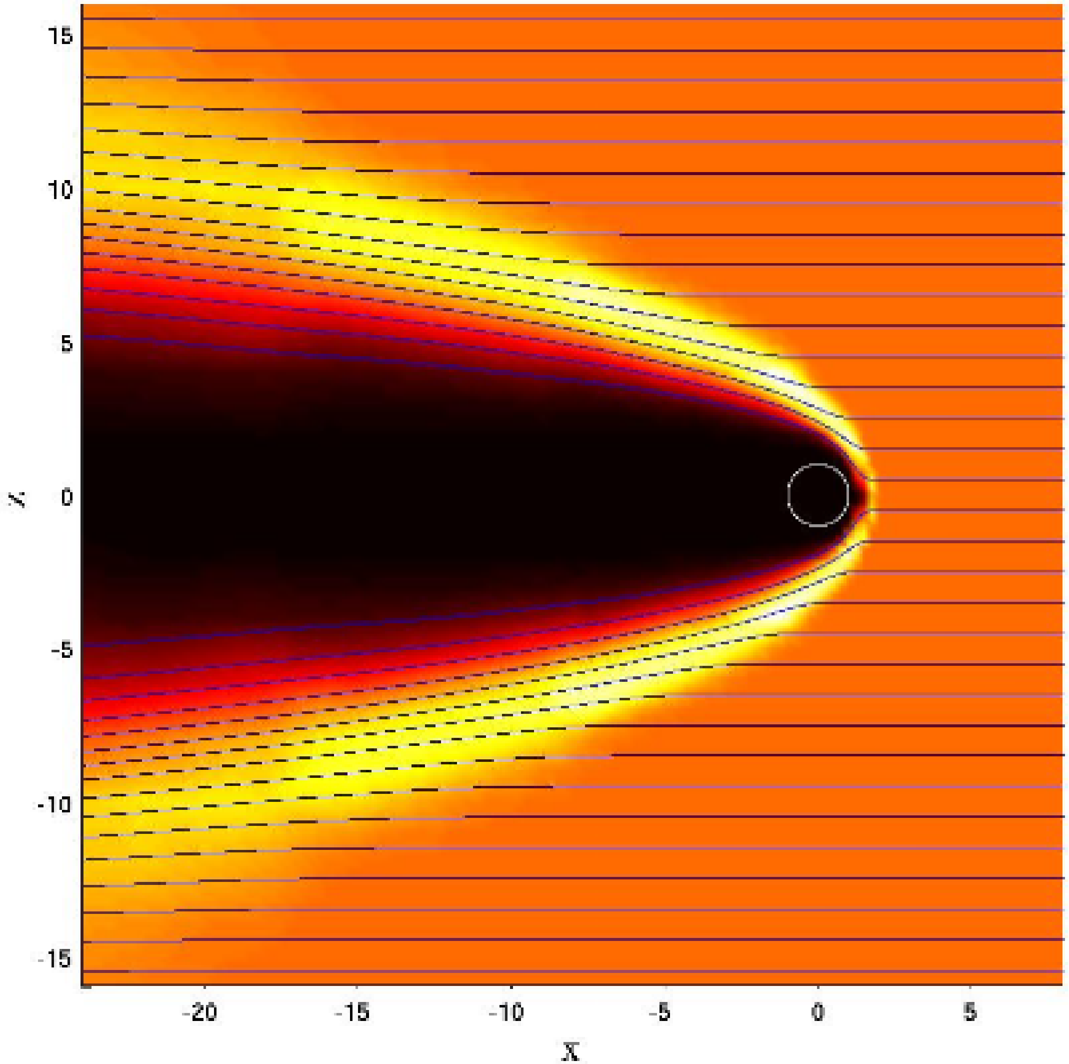
The MHD equations on conservative form are

$$\begin{cases} \dfrac{\partial \rho}{\partial t} & = & -\nabla \cdot (\rho u), \\ \dfrac{\partial \rho u}{\partial t} & = & -\nabla \cdot \left(\rho u u + (p + \frac{1}{2}|B|^2) I - BB\right), \\ \dfrac{\partial B}{\partial t} & = & -\nabla \cdot (uB - Bu), \\ \dfrac{\partial e}{\partial t} & = & -\nabla \cdot \left[(e + p + \frac{1}{2}|B|^2) u - (B \cdot u) B\right]. \end{cases}$$

$$e = \frac{1}{2}\rho|u|^2 + \frac{p}{\gamma - 1} + \frac{1}{2}|B|^2, \qquad \rho, p > 0, \quad \nabla \cdot B = 0$$

$$\phi_t + \nabla \cdot f(\phi) = 0, \qquad \phi = (\rho, \rho u, B, e)^T$$

MHD Model for Mars



Solar wind flow around Mars [Ma et al., 2002]

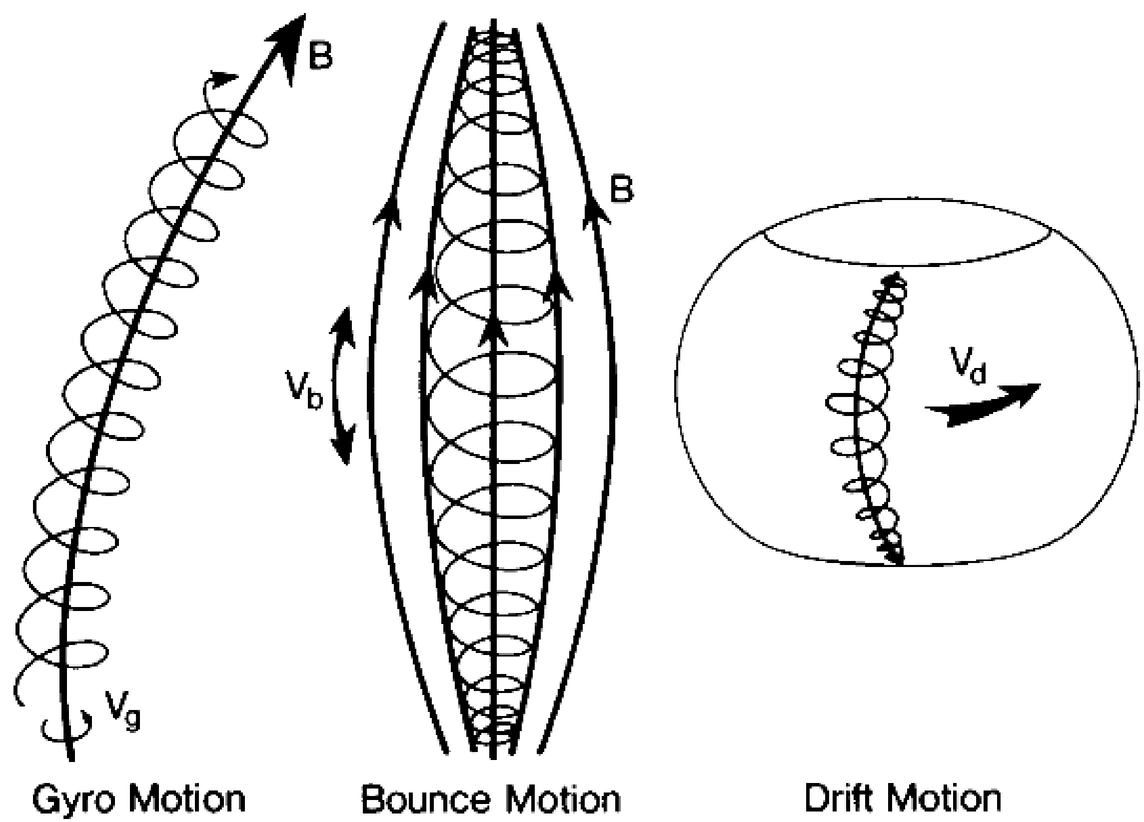
Comments on MHD

- Three-dimensional grid
- Can use well known methods for hydrodynamics
- The magnetic field is *frozen in* to the fluid from $\mathbf{E} = -\mathbf{u} \times \mathbf{B}$
- Assumes a Maxwellian velocity distribution.
  Velocity space distribution is parametrized by the bulk velocity and the temperature
- No kinetic effects
  Assumes infinitely small gyro radius

...several of the basic concepts on which the theories are founded, are not applicable to the condition prevailing in cosmos. They are «generally accepted» by most theoreticians, they are developed with the most sophisticated mathematical methods and it is only the plasma itself which does not «understand», how beautiful the theories are and absolutely refuses to obey them. ...

Hannes Alfven, *Plasma physics, space research and the origin of the solar system*, Nobel Lecture, December 11, 1970

Ion motion



Particle Models

- Lorentz force
$$\mathbf{a} = q/m(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$
moves ions and electrons

- Fields on a grid $(\mathbf{E}, \mathbf{B})$

- Get fields by solving the Maxwell equations: Poisson's equation, Faraday's and Ampère's laws
$$\nabla \cdot \mathbf{E} = \rho/\epsilon_0, \qquad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$
$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{j} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right), \qquad \text{and } \nabla \cdot \mathbf{B} = 0.$$

- Charge distribution on grid: Particle-in-cell, Cloud-in-cell,. . .

Comments on Particle Models

- Macro particles used
- Few particles gives Monte Carlo type statistical fluctuations
- Adaptivity by split and join
- Gyrofrequency $\sim qB/m$. Problem for electrons. Gyrocenter approximation possible.
- Error from the assignment of charges to the grid

Hybrid Models

- Ions as particles, electrons as a massless fluid

- Infinite conductivity: $\mathbf{E} = -\mathbf{U}_e \times \mathbf{B}$.
  Magnetic field frozen in to the electron fluid

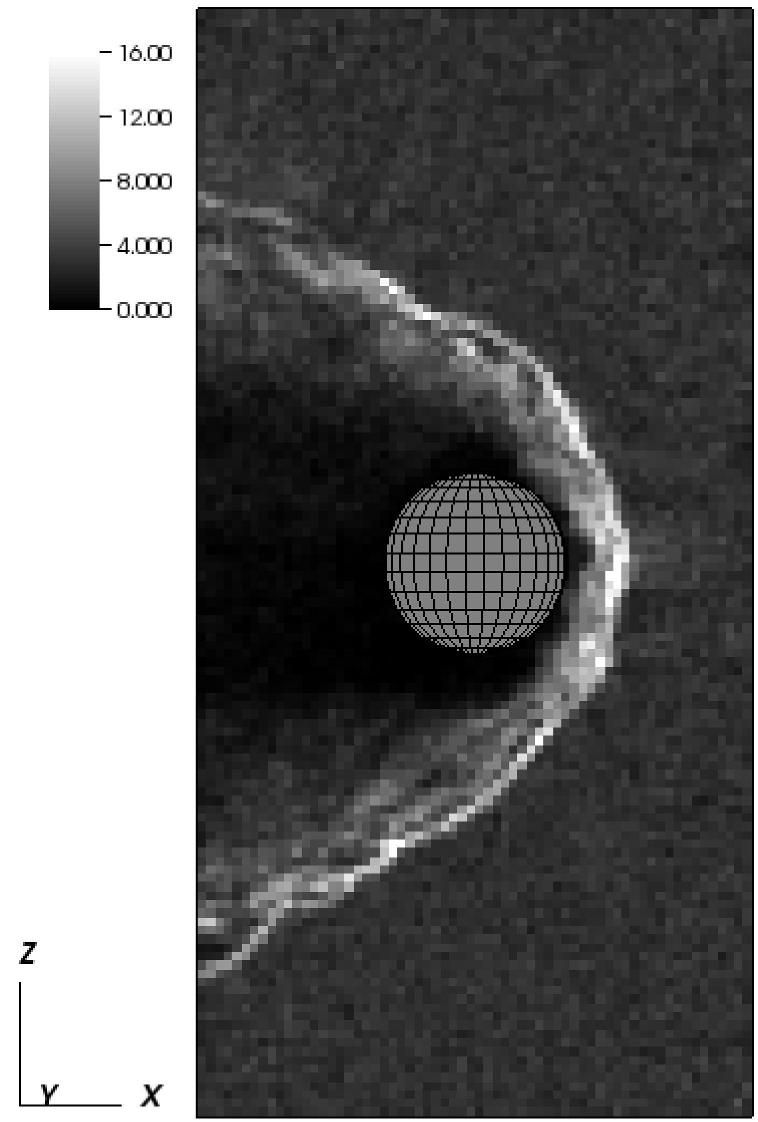
- Lorentz' force on ions is

$$\mathbf{a}_i = q/m(\mathbf{E} + \mathbf{v}_i \times \mathbf{B}) = q/m(\mathbf{v}_i - \mathbf{U}_e) \times \mathbf{B}$$

- Grid values: $\mathbf{B}$ and $\mathbf{U}_e$
  $\mathbf{U}_e$ such that $\mu_0 \mathbf{j} = \nabla \times \mathbf{B}$, and

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{U}_e \times \mathbf{B})$$

Hybrid model for Mars



Kinetic Models

- View the problem as the flow of a phase space fluid:
  Solve the Vlasov equation (and field equations)

- A six-dimensional problem:
  Needs adaptivity

Ion production- and loss processes

- Charge-exchange
- Photoionization of neutrals
- Electron impact ionization

Equations

- Full particle model. Electrons and ions as particles
  - Need to resolve the electron time and spatial scales
- Hybrid model. Particle ions, fluid electrons
  - Resolve ion time and spatial scale
- Magnetohydrodynamics (MHD).
  - Temporal and spatial scales larger than ion scales

The Hybrid Model

- Particle ions, massless e⁻ fluid
- ***B***-field on a grid

Definitions

We have N_I ions at positions $\mathbf{r}_i(t)$ [m] with velocities $\mathbf{v}_i(t)$ [m/s], mass m_i [kg] and charge q_i [C], $i = 1, \ldots, N_I$. By spatial averaging[1], we can define the charge density $\rho_I(\mathbf{r}, t)$ [Cm^{-3}] of the ions, their average velocity $\mathbf{u}_I(\mathbf{r}, t)$ [m/s], and the corresponding current density $\mathbf{J}_I(\mathbf{r}, t) = \rho_I \mathbf{u}_I$ [Cm^{-2}s^{-1}]. Electrons are modelled as a fluid with charge density $\rho_e(\mathbf{r}, t)$, average velocity $\mathbf{u}_e(\mathbf{r}, t)$, and current density $\mathbf{J}_e(\mathbf{r}, t) = \rho_e \mathbf{u}_e$. The electron number density is $n_e = -\rho_e/e$, where e is the elementary charge. If we assume that the electrons are an ideal gas, then $p_e = n_e k T_e$, so the pressure is directly related to temperature (k is Boltzmann's constant).

The trajectories of the ions are computed from the Lorentz force,

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{v}_i}{dt} = \frac{q_i}{m_i}\left(\mathbf{E} + \mathbf{v}_i \times \mathbf{B}\right), \quad i = 1, \ldots, N_I$$

where $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$ is the electric field, and $\mathbf{B} = \mathbf{B}(\mathbf{r}, t)$ is the magnetic field.[2]

Hybrid approximations

Winske and Yin (2001) presents a brief overview of hybrid codes. A more complete survey can be found in Pritchett (2000). Most hybrid solvers for global simulations have the following assumptions in common.

1. Quasi-neutrality, $\rho_I + \rho_e = 0$, so that given the ion charge density, the electron charge density is specified by $\rho_e = -\rho_I$.

2. Ampere's law whithout the displacement current (also called the Darwin approximation, or the nonradiative limit) provides the total current, given $\mathbf{B}$, by

$$\boxed{\mathbf{J} = \mu_0^{-1} \nabla \times \mathbf{B},}$$

Ampere's law

   where $\mu_0 = 4\pi \cdot 10^{-7}$ [Hm^{-1}] is the magnetic constant ($\epsilon_0 \mu_0 c^2 = 1$), and from the total current we get the electron current, $\mathbf{J}_e = \mathbf{J} - \mathbf{J}_I$, and thus the electron velocity, since the quasi-neutrality implies that $\mathbf{u}_e = \mathbf{J}_e / \rho_e = (\mathbf{J}_I - \mathbf{J})/\rho_I$.

3. Massless electrons, $m_e = 0$, lead to the electron momentum equation

$$\boxed{n_e m_e \frac{d\mathbf{u}_e}{dt} = \mathbf{0} = \rho_e \mathbf{E} + \mathbf{J}_e \times \mathbf{B} - \nabla p_e + \mathcal{C}}$$

e- momentum eq:n

   where the force terms $\mathcal{C}$ can be due to electron-ion collisions, electron-neutral (Terada et al., 2002) or anomalous, i.e. representing electron-wave interactions (Bagdonat and Motschmann, 2002). This provides an equation of state (Ohm's law) for the electric field

$$\boxed{\mathbf{E} = \frac{1}{\rho_I} \left[(\mathbf{J} - \mathbf{J}_I) \times \mathbf{B} - \nabla p_e + \mathcal{C} \right],}$$

Ohm's law

   with $\mathbf{J}$ from Ampere's law. So the electric field is not an unknown. Whenever it is needed, it can be computed.

4. Faraday's law is used to advance the magnetic field in time,

$$\boxed{\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}.}$$

Faraday's law

5. The electron pressure is isotropic (p_e is a scalar, not a tensor).

Electron Pressure

For the electrons, the remaining degree of freedom is the pressure, p_e. Note that p_e only affects the ion motions through the electric field. The evolution of the magnetic field is not affected since we have $\nabla \times \nabla p_e = 0$ in Faraday's law. There are several ways to handle the electron pressure,

1. Assume p_e is constant, or zero (Kallio and Janhunen, 2003).
2. Assume p_e is adiabatic (small collision frequency). Then the electron pressure is related to the electron charge density by $p_e \propto |\rho_e|^\gamma$, where $\gamma = 5/3$ is the adiabatic index (Bagdonat and Motschmann, 2002; Lipatov, 2002).
3. Solve the massless fluid energy equation,

$$\frac{\partial p_e}{\partial t} + \mathbf{u}_e \cdot \nabla p_e + \gamma p_e \nabla \cdot \mathbf{u}_e = (\gamma - 1)\, \eta |\mathbf{J}|^2,$$

   (Richardson and Chapman, 1994; Lipatov, 2002)

Hybrid equations

If we store the magnetic field on a discrete grid $\mathbf{B}_j$, the unknowns are $\mathbf{r}_i$, $\mathbf{v}_i$, and $\mathbf{B}_j$ (supplemented by p_e on a grid, if we include the electron energy equation). The time advance of the unknowns can then be written as the ODE

$$\frac{d}{dt}\begin{pmatrix} \mathbf{r}_i \\ \mathbf{v}_i \\ \mathbf{B}_j \end{pmatrix} = \begin{pmatrix} \mathbf{v}_i \\ \frac{q_i}{m_i}(\mathbf{E} + \mathbf{v}_i \times \mathbf{B}) \\ -\nabla_j \times \mathbf{E} \end{pmatrix} \tag{1}$$

where $\nabla_j \times$ is a discrete rotation operator, and the electric field is

$$\mathbf{E}_j = \frac{1}{\rho_I}\left(-\mathbf{J}_I \times \mathbf{B}_j + \mu_0^{-1}(\nabla_j \times \mathbf{B}_j) \times \mathbf{B}_j\right) - \nabla p_e + \mathcal{C}.$$

Algorithm

The unknown particle properties are $\mathbf{r}_i$ and $\mathbf{v}_i$; and the grid cell unknowns are $\mathbf{B}_j$, $\mathbf{J}_j$ and ρ_j. We denote time level $t = n\Delta t$ by superscript n. Given $\mathbf{B}_j^{n-1/2}$, $\mathbf{r}_i^{n-1/2}$ and $\mathbf{v}_i^n$, we do the following steps.

$$\mathbf{r}_i^{n+1/2} \leftarrow \mathbf{r}_i^{n-1/2} + \Delta t \mathbf{v}_i^n,$$

$$\mathbf{r}_i^n \leftarrow \frac{1}{2}\left(\mathbf{r}_i^{n+1/2} + \mathbf{r}_i^{n-1/2}\right)$$

At $\mathbf{r}_i^n$, deposit particle charges and currents

$$\rho_i \rightarrow \rho_j^n, \qquad \rho_i \mathbf{v}_i^n \rightarrow \mathbf{J}_j^n$$

$$\mathbf{B}_j^{n+1/2} \leftarrow \mathbf{B}_j^{n-1/2}, \rho_j^n, \mathbf{J}_j^n \qquad \text{according to CL} \tag{2}$$

At $\mathbf{r}_i^{n+1/2}$, deposit particle charge

$$\rho_i \rightarrow \rho_j^{n+1/2},$$

Estimate electric field at $n + 1/2$ using the currents at n

$$\mathbf{E}_j^* \leftarrow \mathbf{B}_j^{n+1/2}, \rho_j^{n+1/2}, \mathbf{J}_j^n, p_e$$

$$\mathbf{v}_i^{n+1/2} \leftarrow \mathbf{v}_i^n + \frac{\Delta t}{2}\frac{q_i}{m_i}\left(\mathbf{E}_j^* + \mathbf{v}_i^n \times \mathbf{B}_j^{n+1/2}\right)$$

At $\mathbf{r}_i^{n+1/2}$, deposit particle current

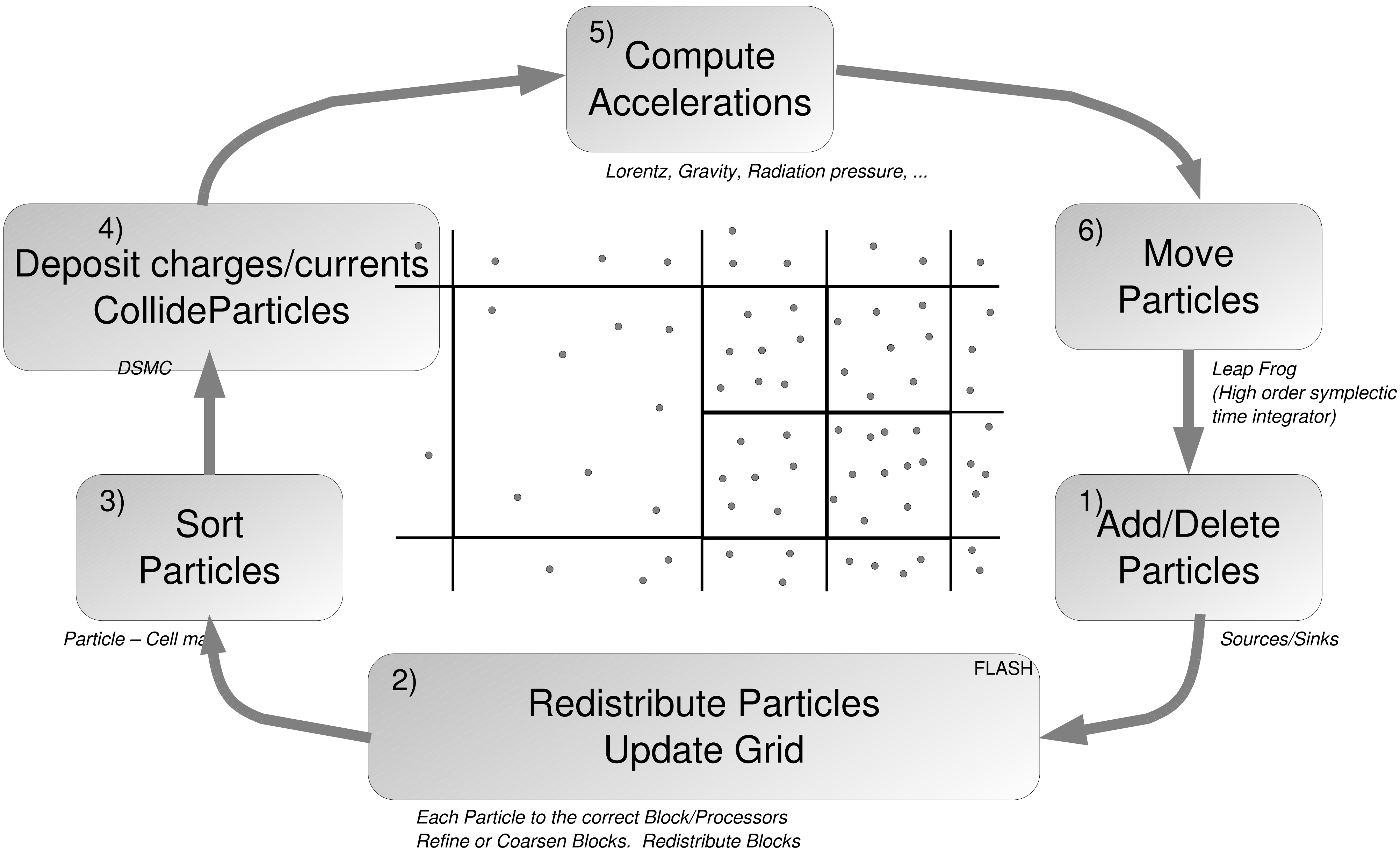
$$\rho_i \mathbf{v}_i^{n+1/2} \rightarrow \mathbf{J}_j^{n+1/2}$$

$$\mathbf{E}_j^{n+1/2} \leftarrow \mathbf{B}_j^{n+1/2}, \rho_j^{n+1/2}, \mathbf{J}_j^{n+1/2}, p_e$$

$$\mathbf{v}_i^{n+1} \leftarrow \mathbf{v}_i^n + \Delta t \frac{q_i}{m_i}\left(\mathbf{E}_j^{n+1/2} + \mathbf{v}_i^{n+1/2} \times \mathbf{B}_j^{n+1/2}\right)$$

Now we have $\mathbf{B}_j^{n+1/2}$, $\mathbf{r}_i^{n+1/2}$ and $\mathbf{v}_i^{n+1}$. Set $n \leftarrow n + 1$ and start over again.

Particle Simulation Cycle



Spatial discretization

- Standard 2nd order FD
- Non-staggered grid.
  Div(B) = 0 still conserved (Toth 2000)

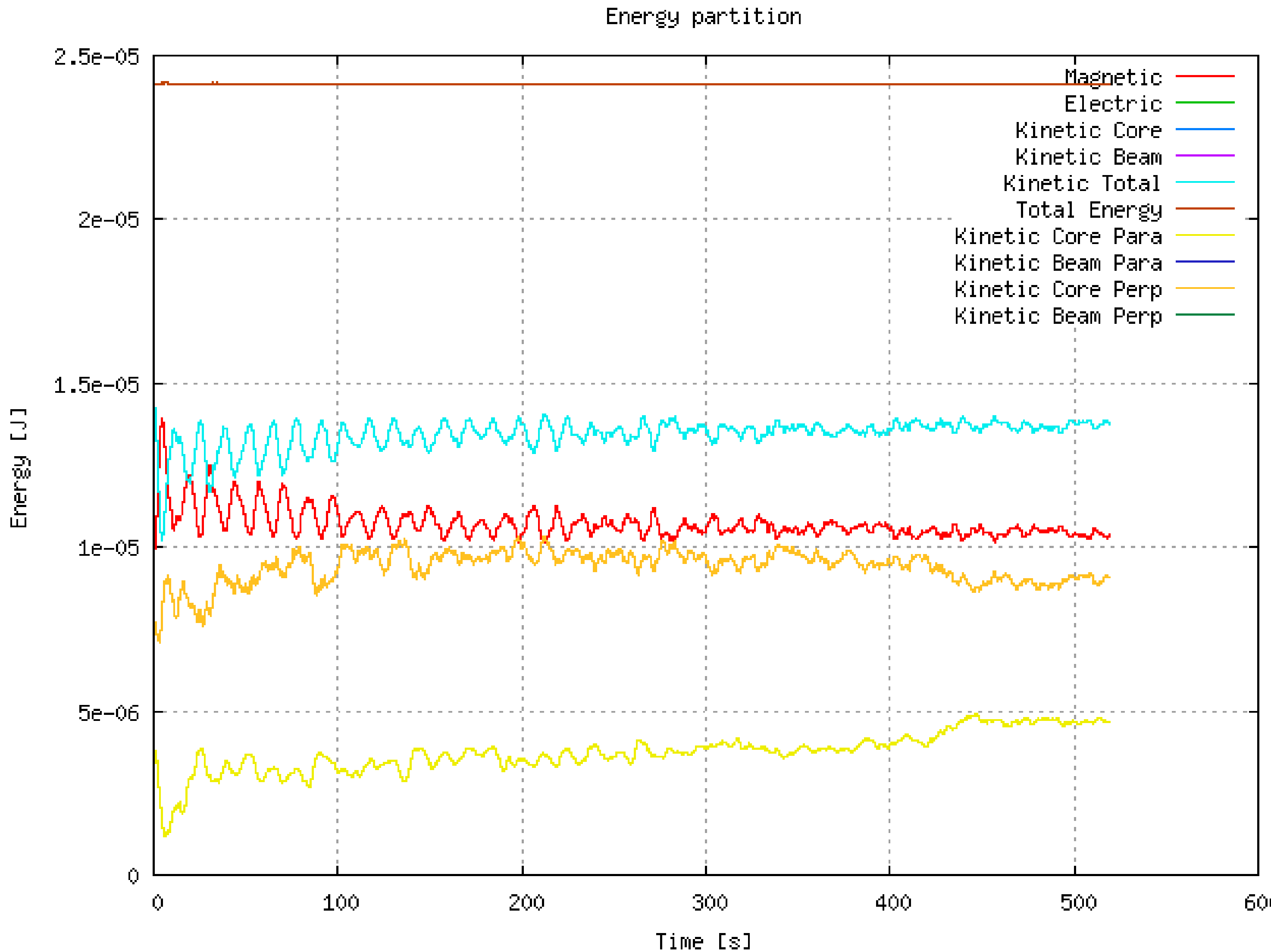
Cyclic Leapfrog B-field Update

The update of the magnetic field in (2) using cyclic leapfrog (CL) is done in m sub-time steps of length $h = \Delta t/m$. With the notation $\mathbf{B}_j^p \equiv \mathbf{B}_j\left((n+1/2)\Delta t + ph\right)$ we have the iteration

$$\begin{cases} \mathbf{B}_j^1 \leftarrow \mathbf{B}_j^0 - h\nabla \times \mathbf{E}_j^0, \\ \mathbf{B}_j^{p+1} \leftarrow \mathbf{B}_j^{p-1} - 2h\nabla \times \mathbf{E}_j^p, \qquad p = 1, 2, \ldots, m-1, \\ \tilde{\mathbf{B}}_j^m \leftarrow \mathbf{B}_j^{m-1} - h\nabla \times \mathbf{E}_j^m, \\ \mathbf{B}_j^{n+1/2} \leftarrow \frac{1}{2}\left(\mathbf{B}_j^m + \tilde{\mathbf{B}}_j^m\right) \end{cases}$$

Energy conservation

1D two stream instability



Energy conservation

Table 2: Energy errors (total energy) for quiet plasma runs at times T. Numbers in parentheses indicate that the parameter was not stated in the reference.

Reference	dim.	particles per cell	Δx δ_i	Δt Ω_i^{-1}	T Ω_i^{-1}	error Ref.	error Here
Matthews (1994)	1	16	0.5	0.1	100	9%	0.9%
					300	47%	3%
	2	32	0.5	0.1	100	2.6%	0.9%
					300	14%	3%
Brecht and Ledvina (2006)	3	4	(1.54)	0.0056	112	<1%	0.25%

Spatial and Temporal Scales

If we want solutions of the discrete equations to be accurate approximations of the solutions to the continuous equations, a necessary condition is that the discretisation resolves all relevant spatial and temporal scales. The smallest spatial scale for solar wind conditions is the ion inertial length (the ion skin depth) $\delta_i = c/\omega_{pi}$, where ω_{pi} is the ion plasma frequency, $\omega_{pi}^2 = n_i q_i^2/(\epsilon_0 m_i)$, n_i the ion number density, q_i the ion charge, m_i the ion mass, and $\epsilon_0 \approx 8.854 \cdot 10^{-12}$ [Fm^{-1}] the vacuum permittivity. The ion inertial length is associated with the $\mathbf{J} \times \mathbf{B}$ term in Ohm's law (the Hall term) that describe whistler dynamics. The fastest temporal scale is also associated with whistler dynamics. The whistler wave spectrum is cutoff at the electron cyclotron frequency, but due to the assumption of massless electrons it is unbounded, and the frequency scales like $\omega/\Omega_i = (kc/\omega_{pi})$ for large k (Pritchett, 2000). Here $\Omega_i = q_i B/m_i$ is the ion gyrofrequency. This gives the CFL constraint

$$\Delta t < \Omega_i^{-1} \left(\frac{\Delta x}{\delta_i} \right)^2$$

If we compare the ion inertial lengths for planets given in Table 1 with published global simulations of the solar wind interaction we find that no simulations has been made with a spatial resolution comparable to δ_i, e.g., for Mars the most resolved simulations has $\Delta x > 2\,\delta_i$. Also, the average number of ions per cell is at most about 10, clearly not enough to resolve the velocity space distribution. Local hybrid simulations have much higher resolution, e.g., $\Delta x = 0.25\,\delta_i$ and 60 ions per cell (Karimabadi et al., 2004).

Work Estimate for Different Solar System Objects

Table 1: Typical solar wind parameters at different solar system objects from Slavin and Holzer (1981), and the resulting spatial and temporal scales for hybrid simulations of the interaction between the objects and the solar wind. The assumed solar wind velocity is 430 km/s. Also shown are the object sizes, volumes, and the relative number of arithmetic operations required.

Object	n_i cm^{-3}	B nT	δ_i km	Ω_i^{-1} s	L 10^6 m	T s	L δ_i	L^3 $10^5\delta_i^3$	TL^3 $10^5\Omega_i\delta_i^3$
Mercury	73	46	27	0.2	4.9	11	184	62	3100
Venus	14	10	61	1.0	12	28	200	79	2200
Moon	7	6	86	1.7	3.5	8	41	0.7	3.1
Mars	3.0	3.3	131	3.1	6.8	16	52	1.4	7.0
Phobos	3.0	3.3	131	3.1	0.022	0.05	0.2	$5 \cdot 10^{-8}$	$8 \cdot 10^{-10}$

Solar wind density

Solar wind magnetic field

Ion inertial length

Proton gyro-period

Object size

Solar wind traversal time

~Number grid cells

~Arithmetic operations

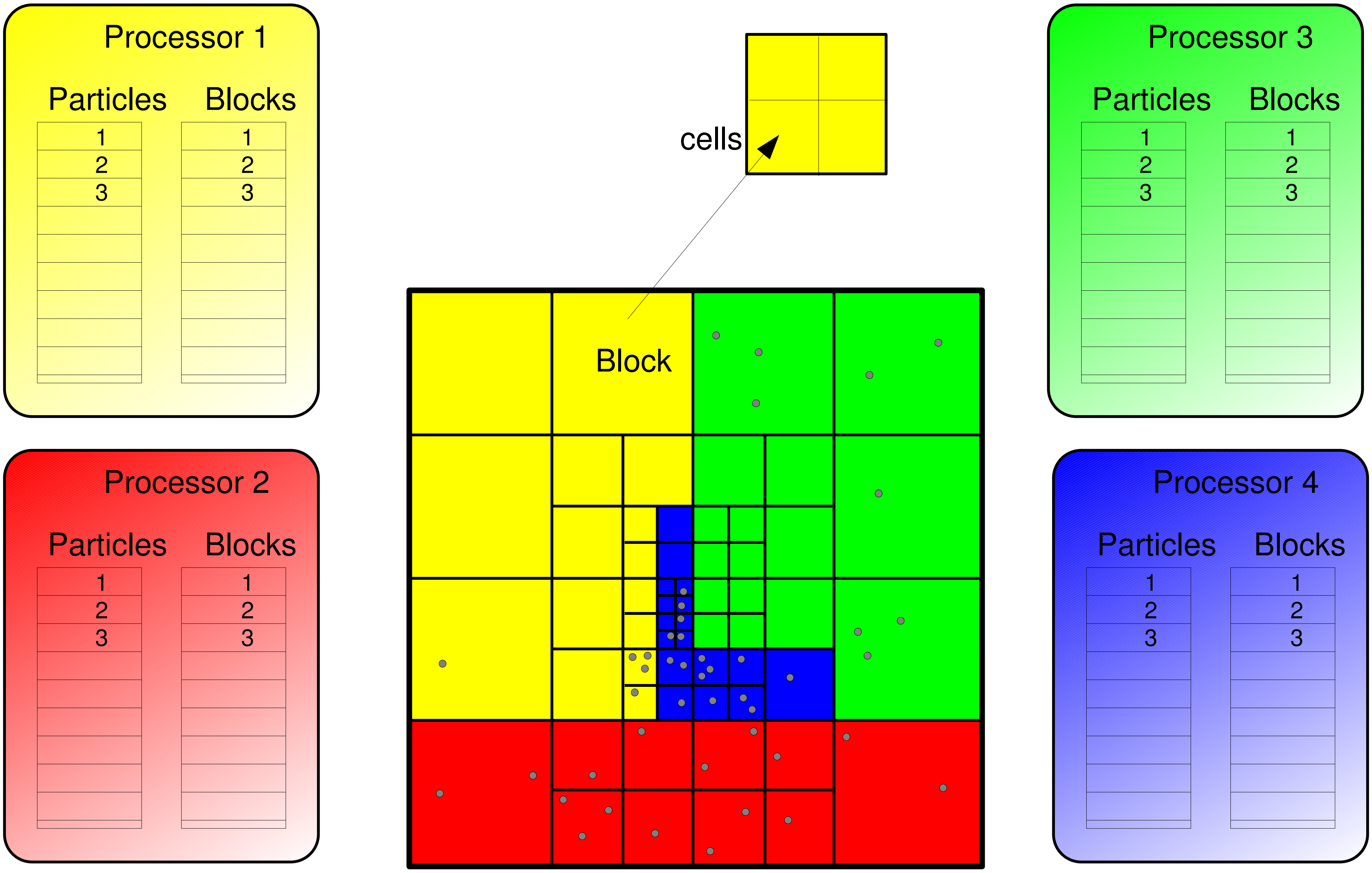
Outstanding questions regarding hybrid models

- How does the accuracy depend on the spatial resolution, in relation to the ion inertial length, δ_i?
- How does the accuracy depend on the number of particles per cell?
- How does the accuracy depend on spatial smoothing of charge density, currents, and fields?

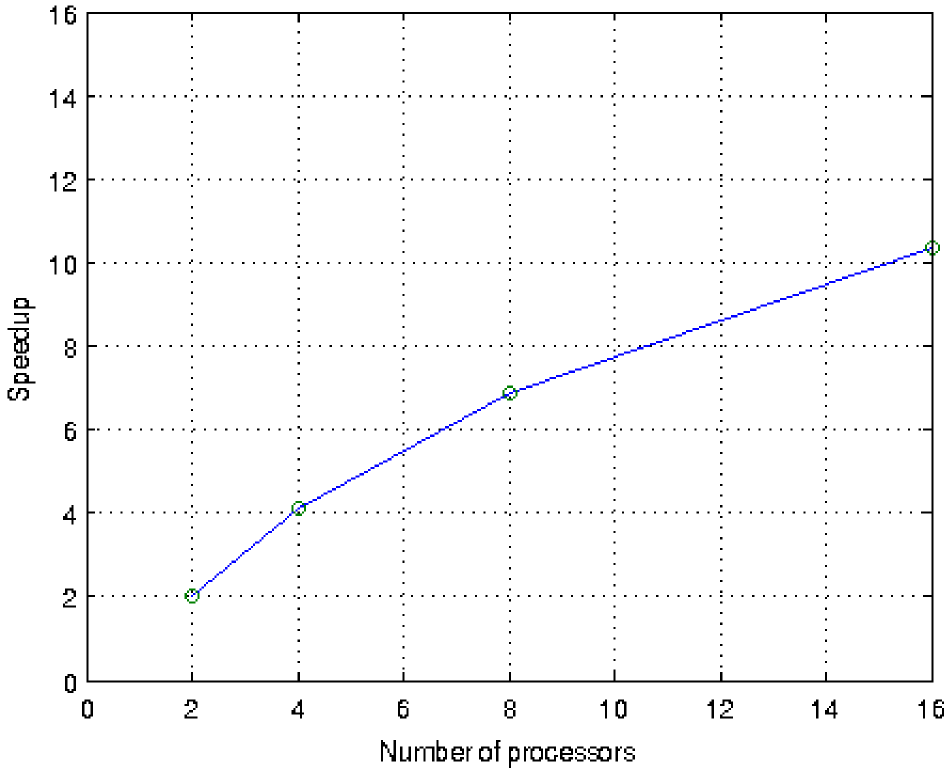
The FLASH Code

- Magnetohydrodynamic (MHD) solver that can include particles
- From University of Chicago
- General compressible flow solver
- Adaptive (Paramesh) and parallel (MPI)
- Open source, Fortran 90
- Add boundary conditions and sources for solar system objects - solar wind simulations
  (Mercury, Venus, earth, moon, Mars, ...)
- Investigations:
  - A comet (MHD with a photoion source)
  - Mars' exosphere (particles)
  - Exoplanet exosphere
  - Moon, Phobos, Mars hybrid models

Data Distribution

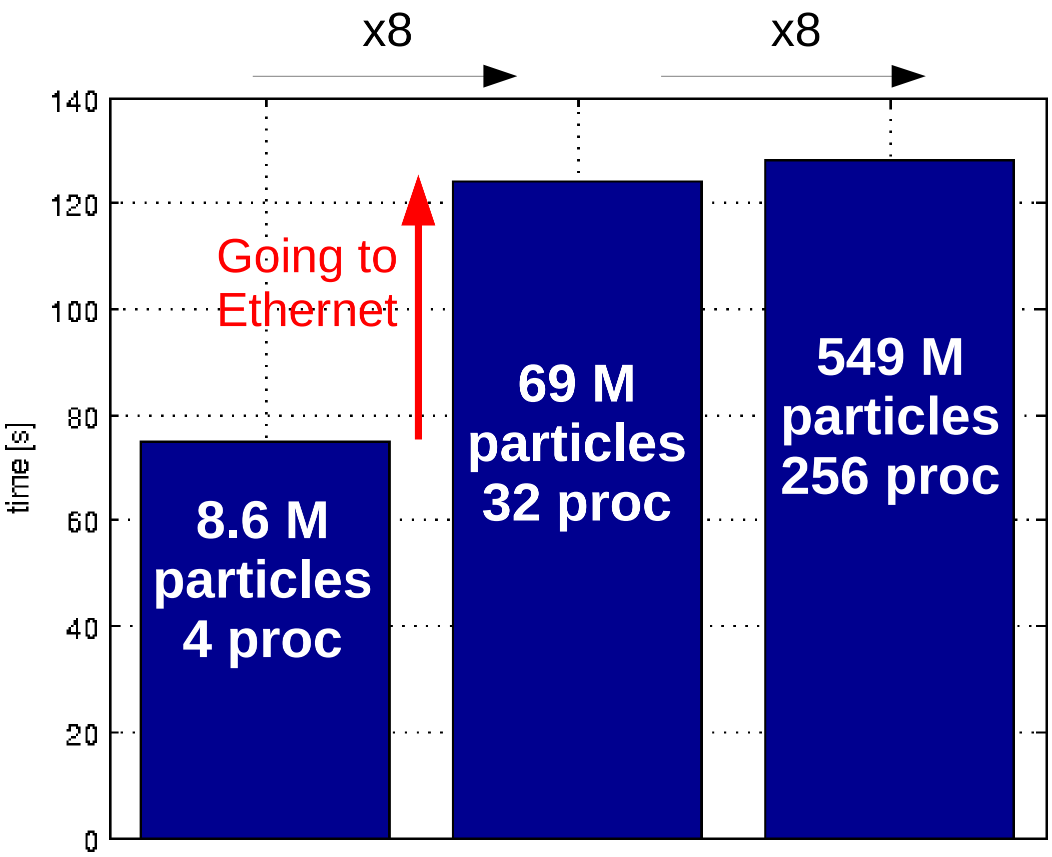


Timings: Constant size problem



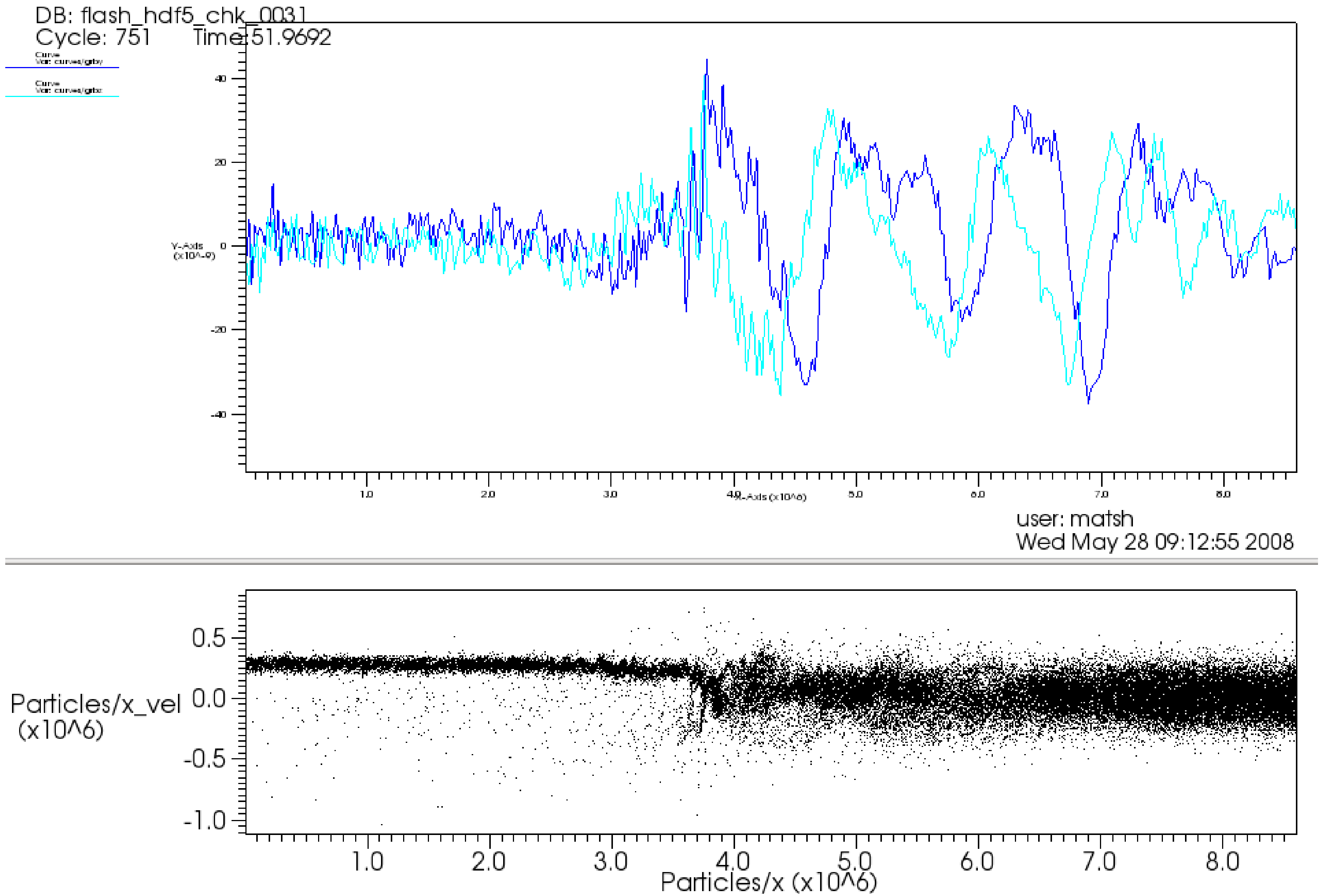
A simulation box with typical Mars solar wind conditions containing 8.6 M particles

Timings: Increasing problem size

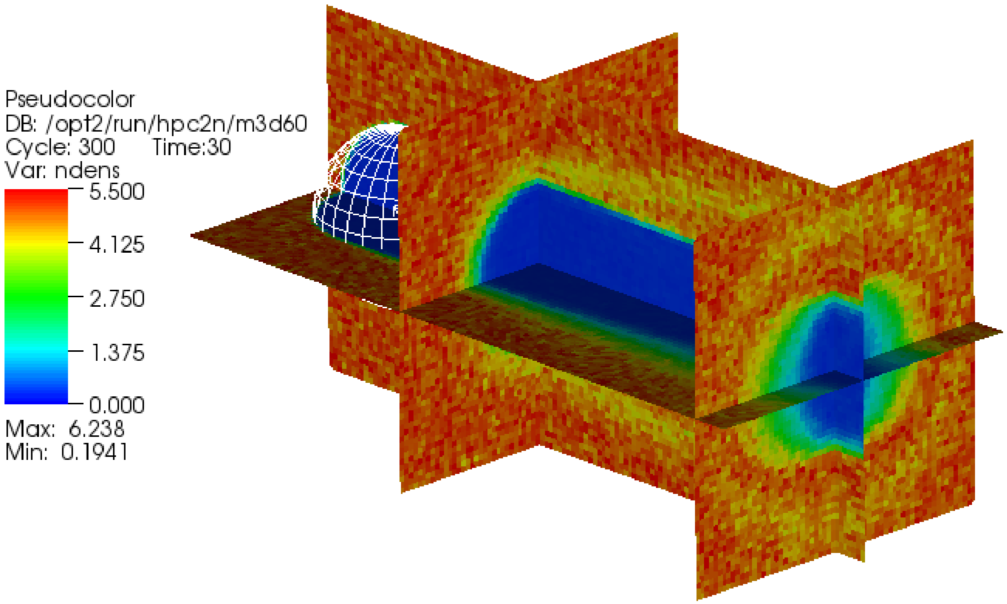


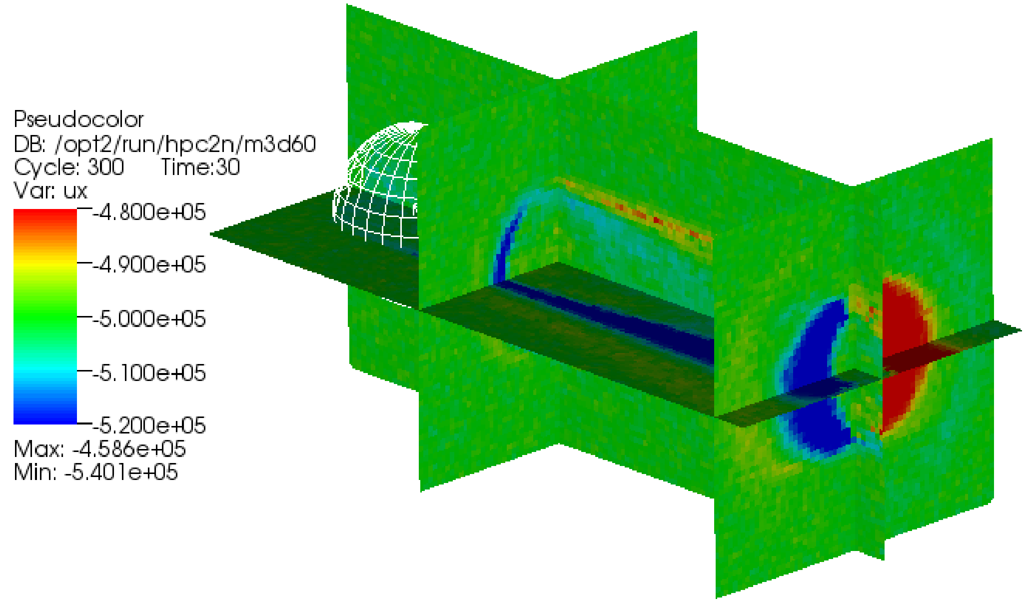
All runs were done at LUNARC, Lund University, Sweden, on a 1008 core cluster of Intel Xeon 5160 (3.0 GHz) with four cores and 4 GB memory per node, connected by GigaBit Ethernet.

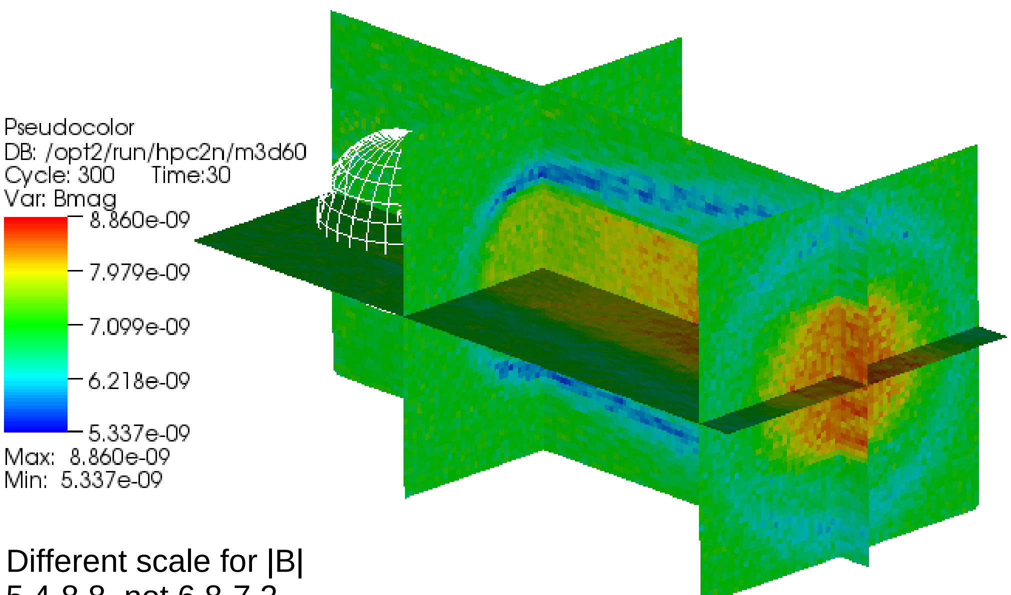
collisionless shock

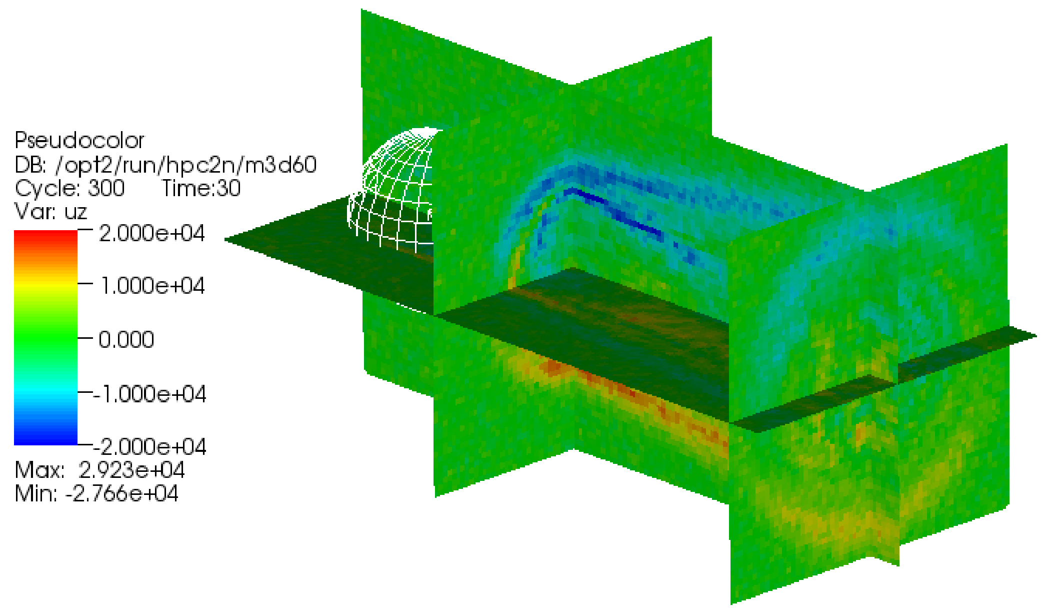


The Moon

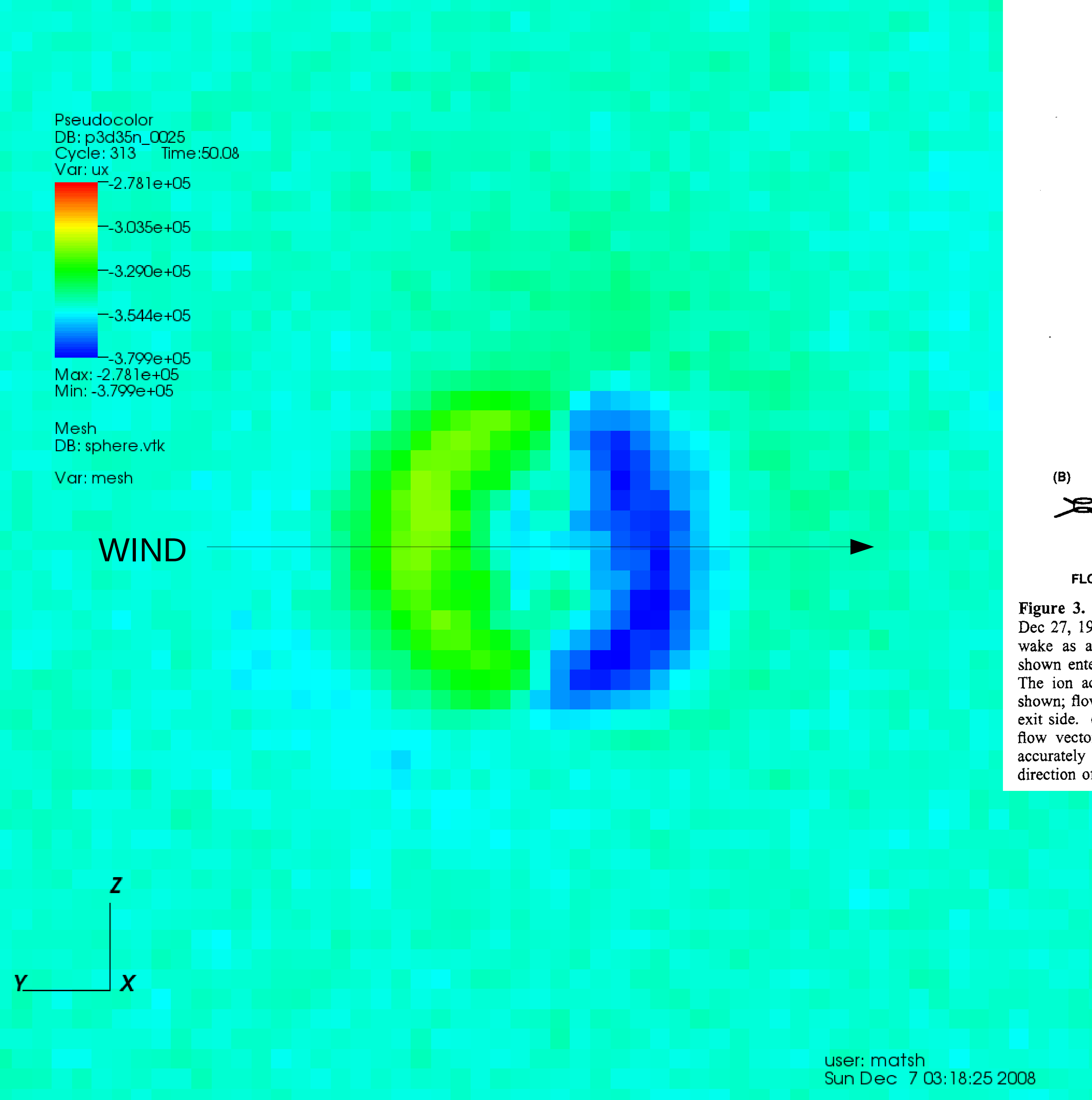








Different scale for |B|
5.4-8.8, not 6.8-7.2
(3.4, not 0.4 range)



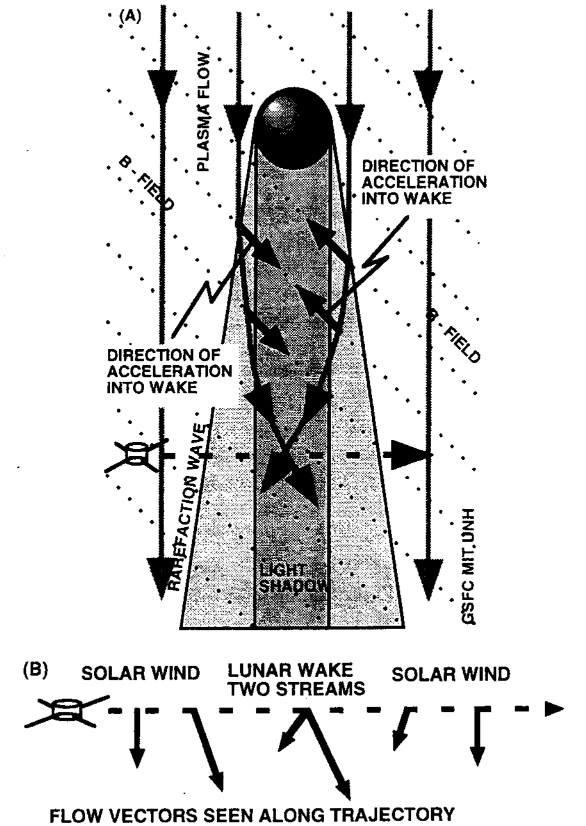
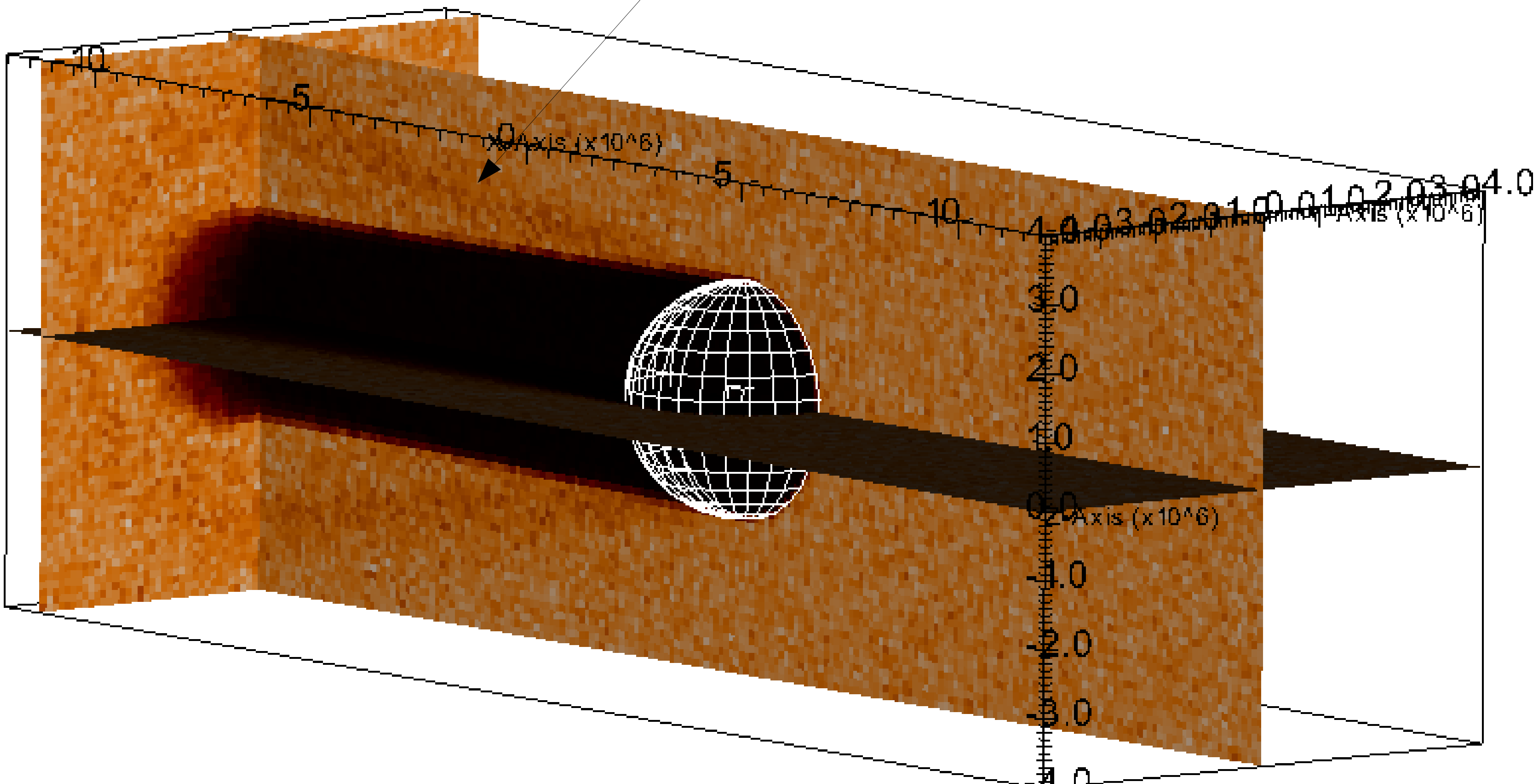


Figure 3. (a) The schematic representation of lunar wake on Dec 27, 1994. Region of plasma depletion propagates out from wake as a rarefaction wave. Streamlines of plasma flow are shown entering the wake from the satellite entry and exit side. The ion acceleration is directed along magnetic field lines as shown; flow speeds up on the entry side and slows down on the exit side. **(b)** Illustrative schematic to show behavior of the ion flow vectors measured as Wind crossed the wake. Does not accurately show the actual changes in relative magnitude or direction of vectors.

Depletion of ions



Two stream instability in tail.
Good example of when Hybrid is needed

Current work: Resolving Mars' Ionosphere

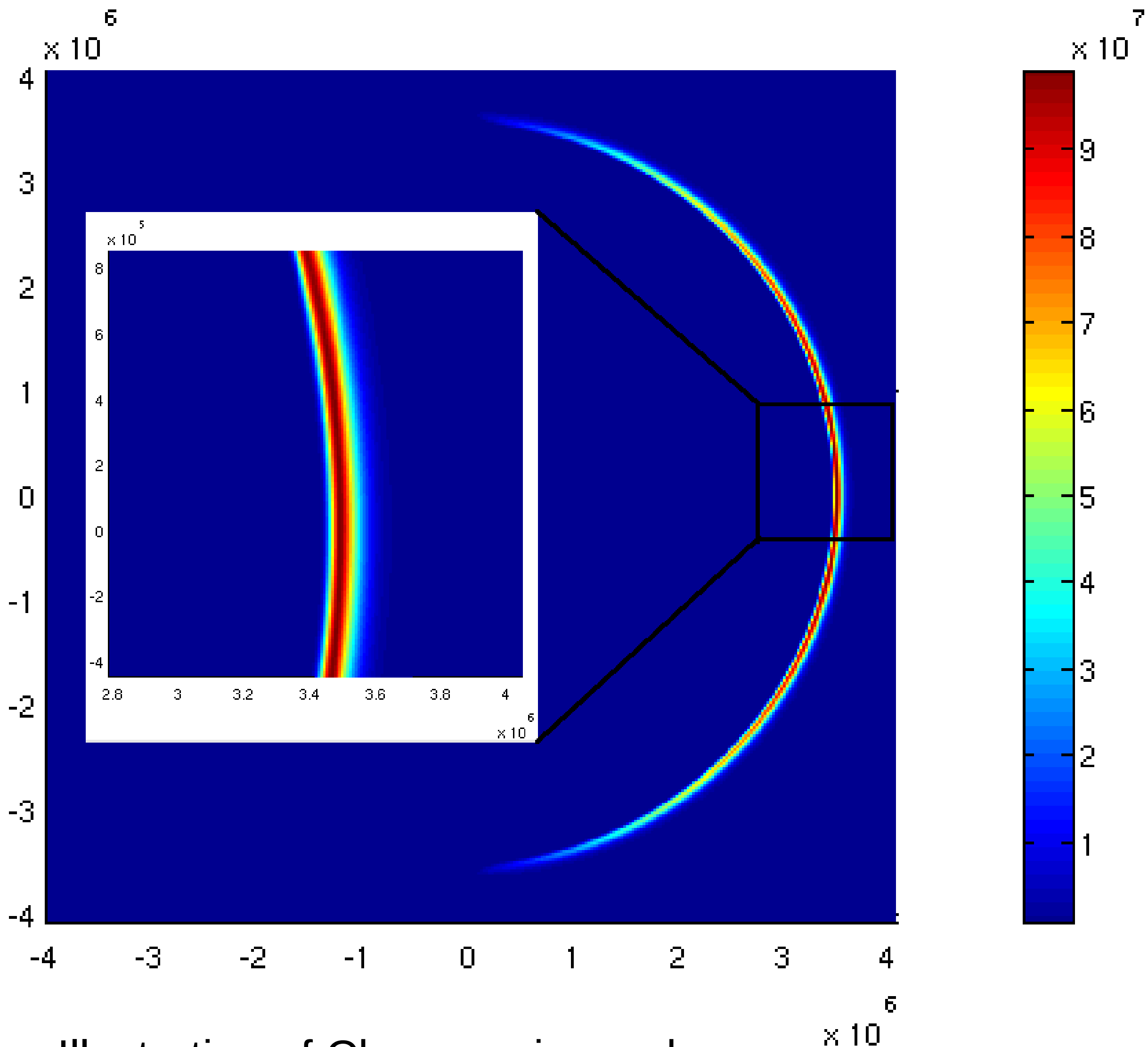


Illustration of Chapman ionosphere

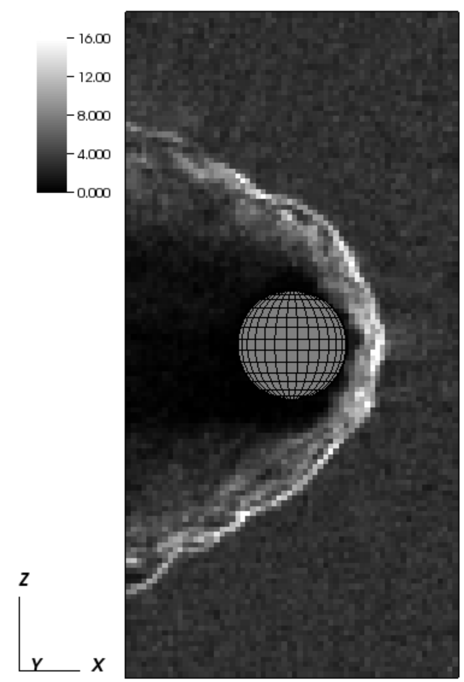
140000 cells with size $\delta_i = 131$ km

=>

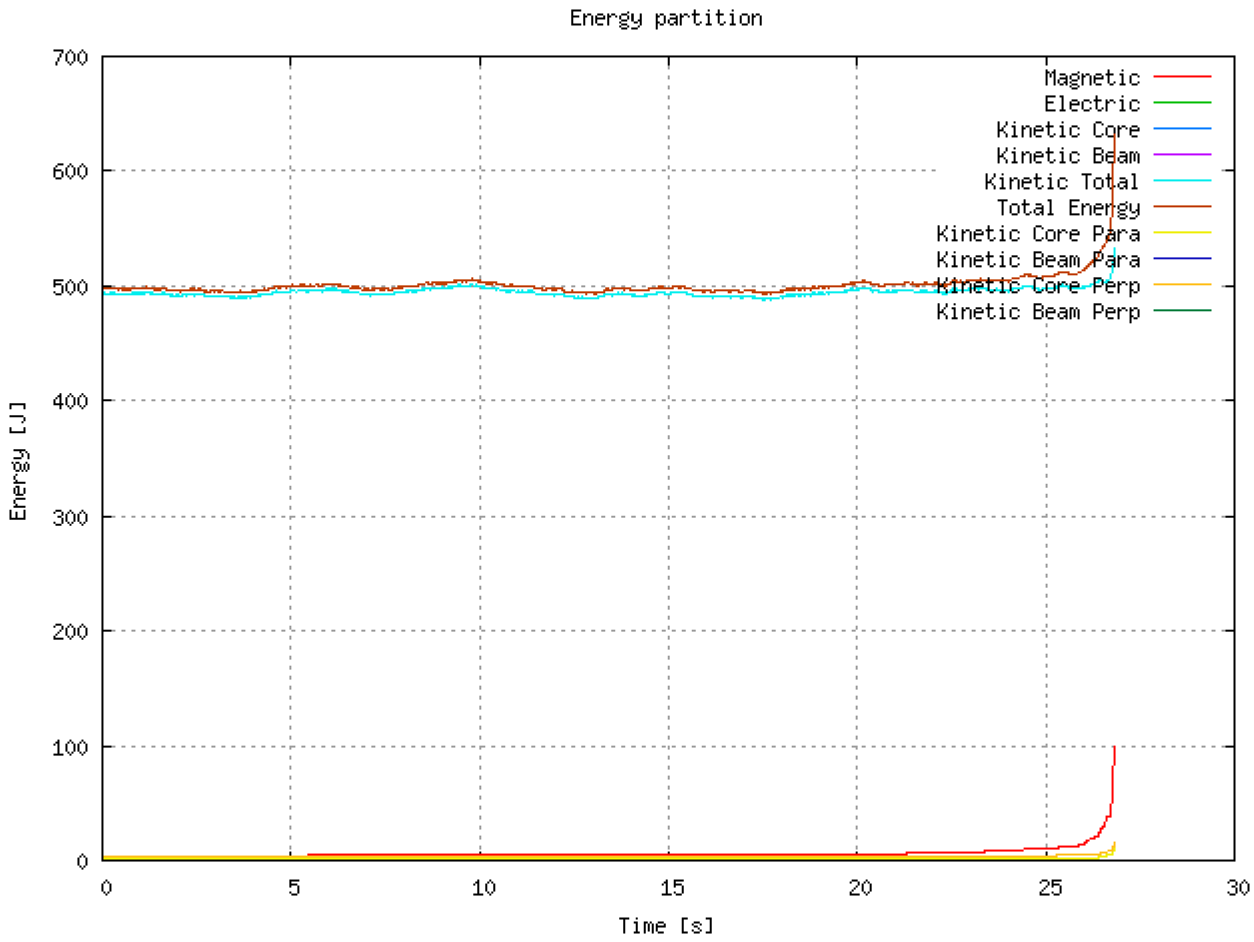
9M cells with size 33 km

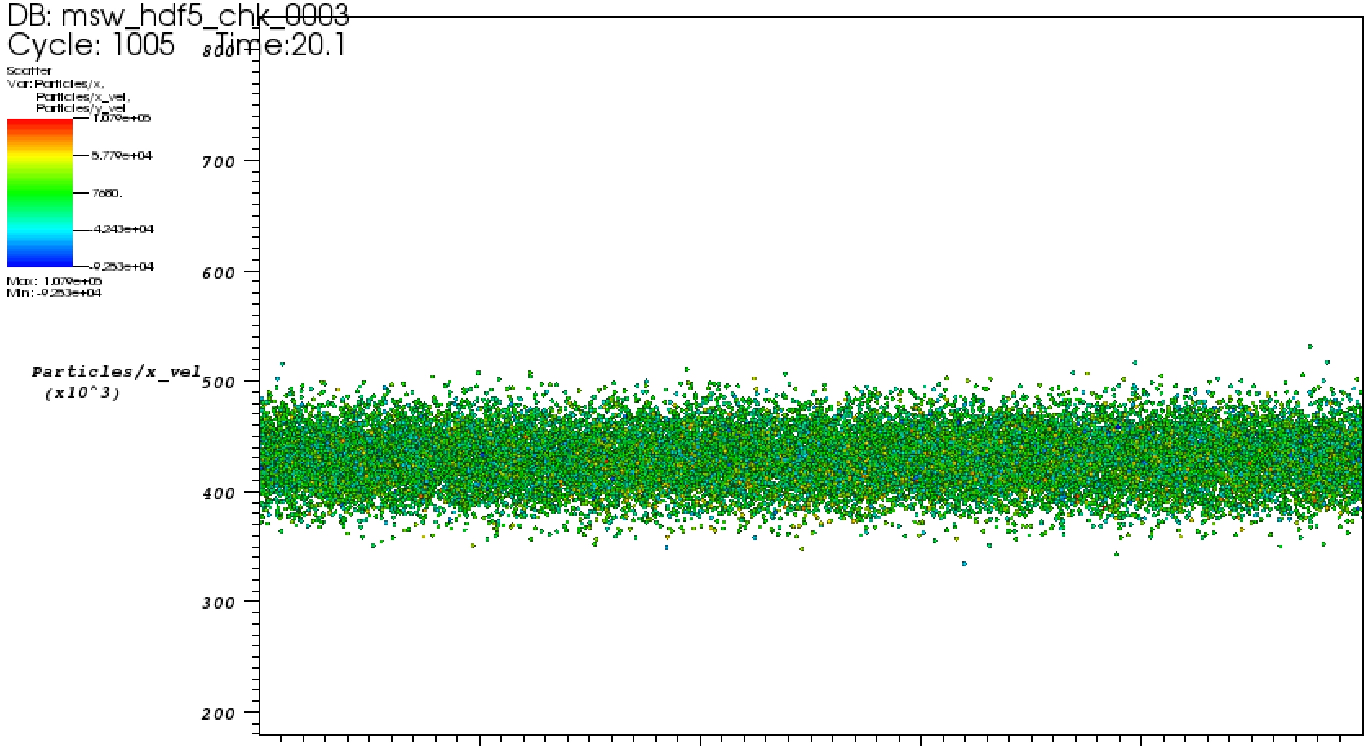
~ **900 M particles**

If we assume 100 particles/cell



Numerical instability example





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Scatter
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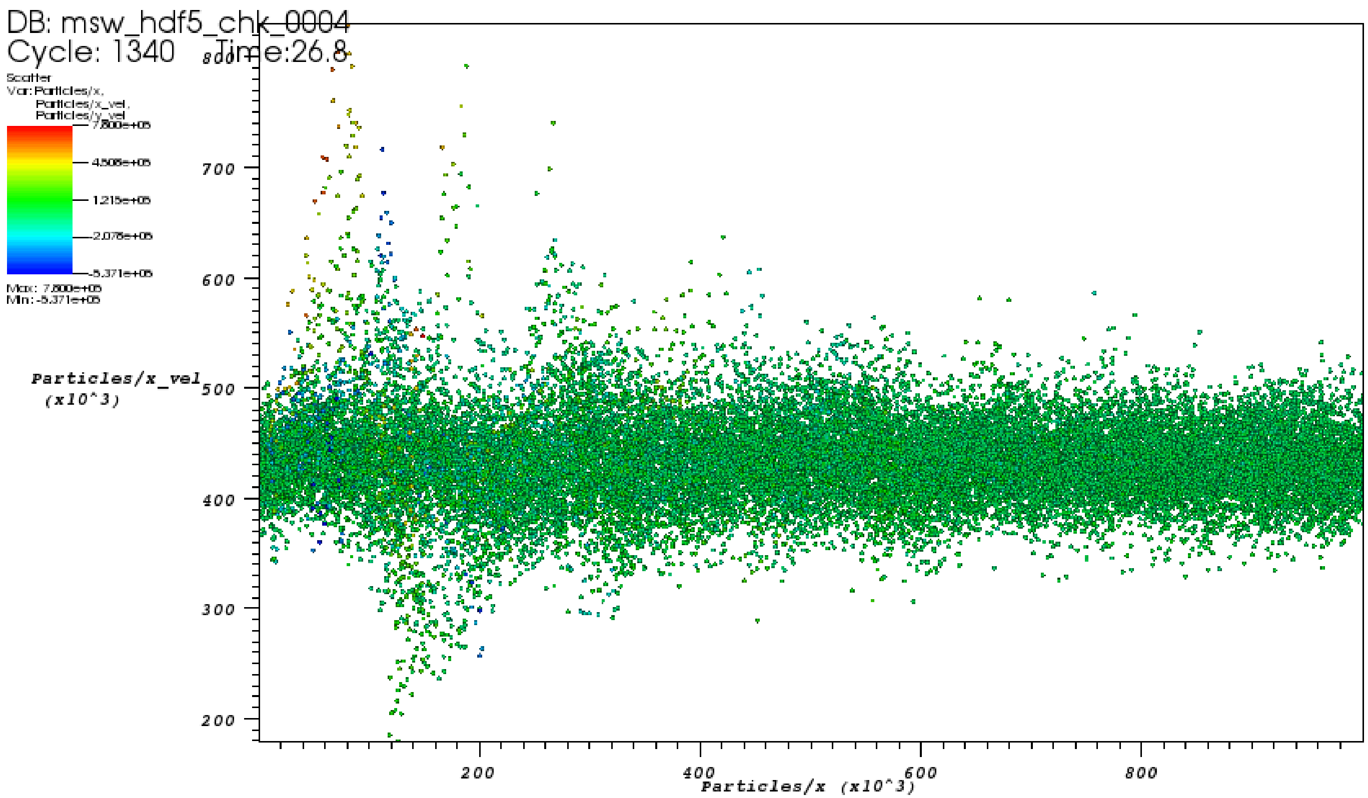
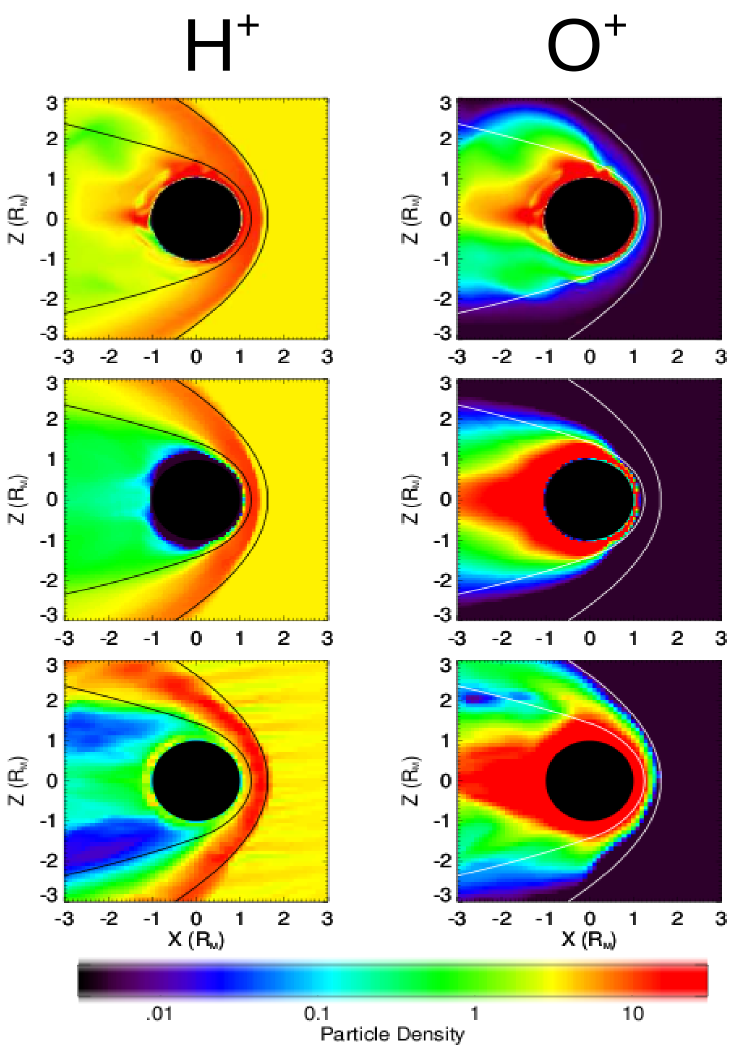
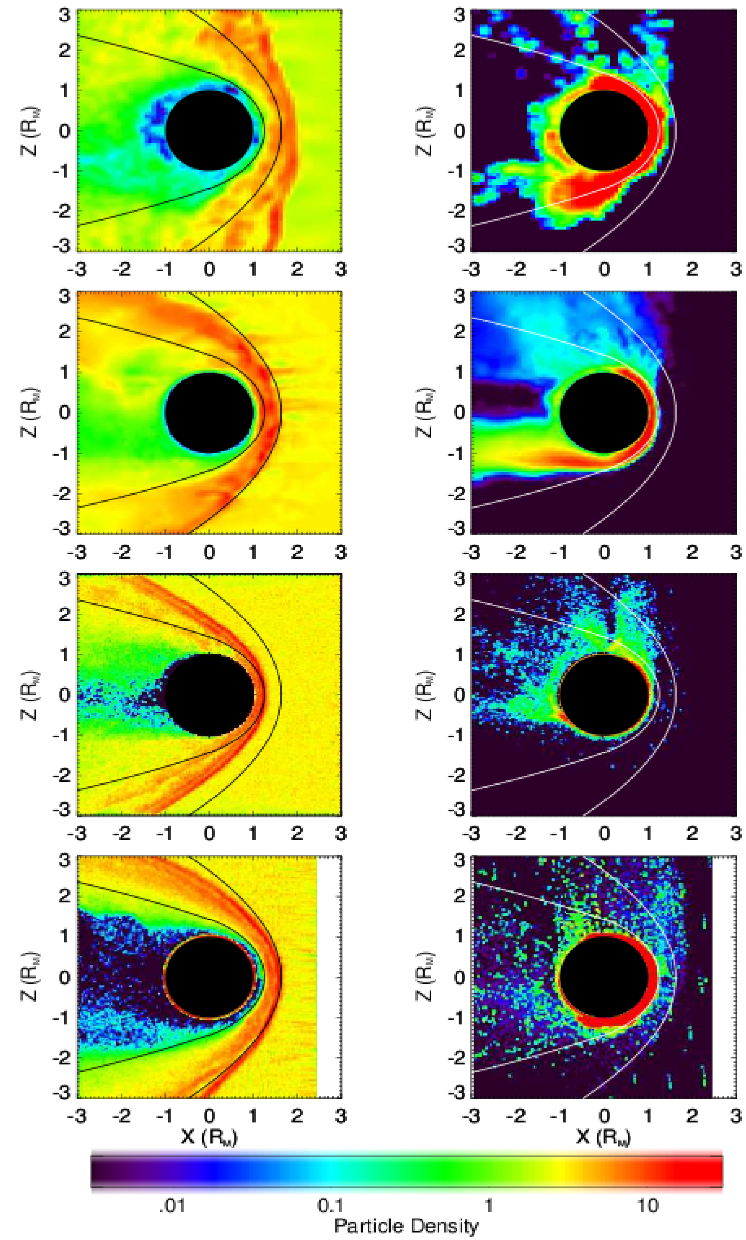
Particles/x_vel,
Particles/y_vel
1.079e+05
5.779e+04
7680.
-4.243e+04
-9.253e+04
Max: 1.079e+05
Min: -9.253e+04
Particles/x_vel
(x10^3)
800
700
600
500
400
300
200



DB: msw_hdf5_chk_0004
Cycle: 1340 Time:26.8
Scatter
Var: Particles/x,
Particles/x_vel,
Particles/y_vel
7.800e+05
4.508e+05
1.215e+05
-2.078e+05
-5.371e+05
Max: 7.800e+05
Min: -5.371e+05
Particles/x_vel
(x10^3)
800
700
600
500
400
300
200
200
400
600
800
Particles/x (x10^3)

Mars Model Intercomparison Densities





(Brain et al. Submitted to *Icarus*)

Two-dimensional cuts of H+ (left) and O+ (right) number densities in the noon-midnight (y = 0) plane. The nominal locations of the bow shock and MPB from (Trotignon et al., 2006) are indicated in black in each panel.

Summary

- Hybrid method. Much can be done regarding numerical analysis and algorithmic development.