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Six-dimensional Vlasov simulations with GPUs

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Introduction

The Vlasov equation describes the dynamics of charged particle motion with a six-dimensional distribution function f :

$$\partial_t f(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{v}, t) + \mathbf{a} \cdot \nabla_{\mathbf{v}} f(\mathbf{x}, \mathbf{v}, t) = 0$$

The acceleration \mathbf{a} is given by the Lorentz force:

$$\mathbf{a} = (q/m)(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t))$$

Vlasov eqn. is coupled with Maxwell's equations, which are solved using a separate field solver. Particle moments and Ohm's law are the necessary source terms:

$$\nabla \cdot \mathbf{E}(\mathbf{x}, t) = 0$$

$$\nabla \cdot \mathbf{B}(\mathbf{x}, t) = 0$$

$$\nabla \times \mathbf{E}(\mathbf{x}, t) = -\partial_t \mathbf{B}(\mathbf{x}, t)$$

$$\nabla \times \mathbf{B}(\mathbf{x}, t) = \mu_0 \mathbf{j}(\mathbf{x}, t)$$

$$n(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{v}, t) d^3 v$$

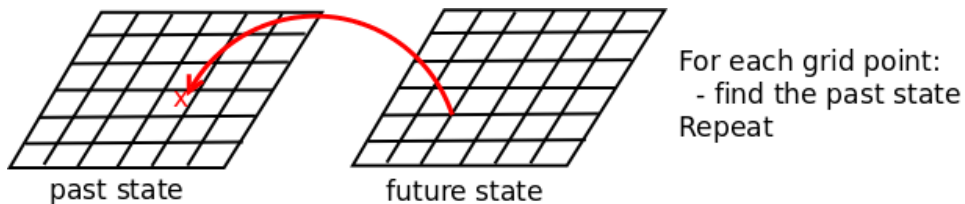
$$\mathbf{j} = q n(\mathbf{x}, t) \int f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d^3 v$$

$$\mathbf{E} = -\nabla V \times \mathbf{B}$$



Solving Vlasov: semi-Lagrangian

The Vlasov eq. is an equation for the motion of incompressible fluid. Often it is solved by using a semi-Lagrangian solver, which follows the characteristic curves (= "particle trajectories"):



In order to get good results, 6D cubic splines should be used for interpolation. **Memory requirements are quite heavy**, 4096 spline coefficients per grid point..

Lars Daldorff took a look into these algorithm, and in principle they should work with GPUs (matrix methods).



Solving Vlasov: FVM

The plan is to use a finite volume method (FVM) which are also used, e.g. for hydrodynamics. FVM schemes use volume averages instead of point values:

$$\partial_t f^{i,j,\dots} = -[F_x^{i+1} - F_x^i]/(\Delta x) - [F_y^{j+1} - F_y^j]/(\Delta y) - \dots$$

The fluxes, evaluated at cell faces, take on simple expressions:

$$F_x = v_x f(\mathbf{x}, \mathbf{v}, t)$$

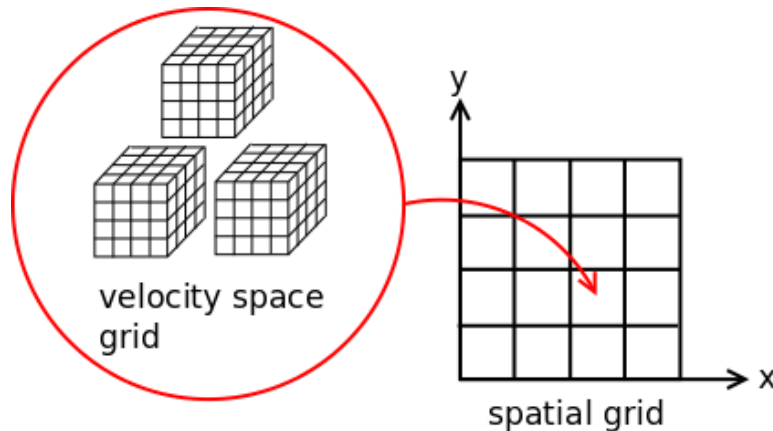
$$F_{v_x} = a_x(\mathbf{x}, \mathbf{v}, t) f(\mathbf{x}, \mathbf{v}, t)$$

However, FVM schemes are plagued by diffusion, and eventually adaptive mesh refinement is needed. In preparation the FVM scheme is implemented using a block cartesian grid.



Solving Vlasov: FVM

Spatial and velocity grids are separated: each spatial cell contains its own block-based velocity grid. Grids can be adapted separately if needed.



A leapfrog-type splitting scheme: first calculate the acceleration, then spatial translation.



Solving Vlasov: FVM

Acceleration:

1. Derivatives
2. Fluxes
3. Propagation
 - Send avgs to spat. Nbrs.

Neighbor data in same spatial cell but in different blocks → data available at every step.

Translation:

1. Derivatives
 - Send derivatives
2. Fluxes
 - Send fluxes
3. Propagation
 - Send averages

Neighbor data in corresponding velocity blocks but in different spatial cells.



On the problem

We estimate that the smallest possible velocity grid is 40^3 cells, i.e. 10^3 $4 \times 4 \times 4$ blocks.

GUMICS-4 uses about 300 000 spatial cells for the magnetosphere, we may need more (need to resolve gyro motion).

Few hours (in physical time) need to be simulated: time step is 0.1 s or less \rightarrow 180 000 time steps.

These numbers add up to $\sim 10^{15}$ calculated cells (5 hours). If a GPU propagates $20 \cdot 10^6$ cells per sec, 2000 GPU days are needed.

Memory requirement is ~ 200 GB.



Present status

A working single-GPU CUDA code exists:

- Rigorous testing on numerical algorithm need to be done
- Parallelization + I/O
- Can be optimized a bit more
- AMR