RUHR-UNIVERSITÄT BOCHUM

RUB

# *Multiphysics simulations of collisionless plasmas*

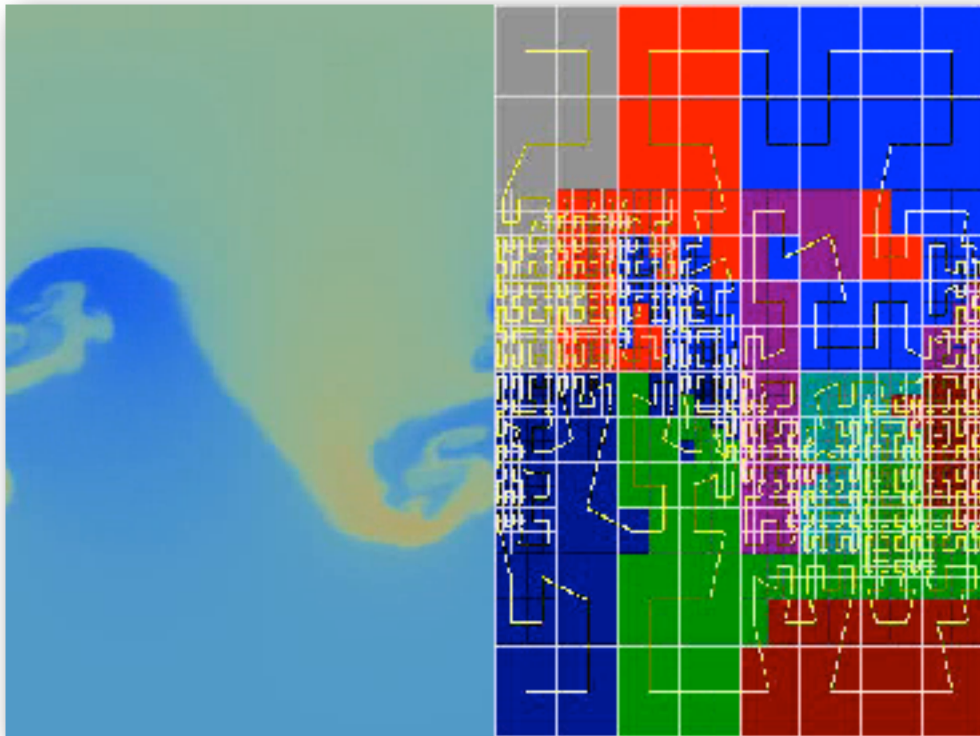
## Numerical Methods in MHD

Dundee 07. Sept. 2018

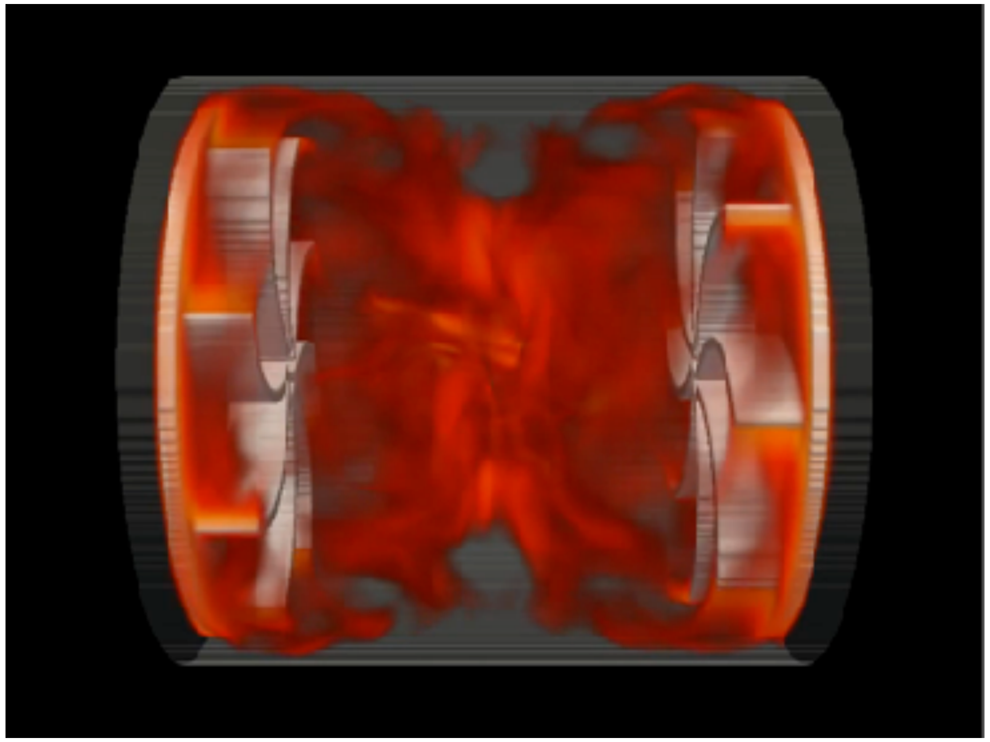
Rainer Grauer, Simon Lautenbach, Thomas Trost
TP I RUB

# What are we doing in Bochum ?

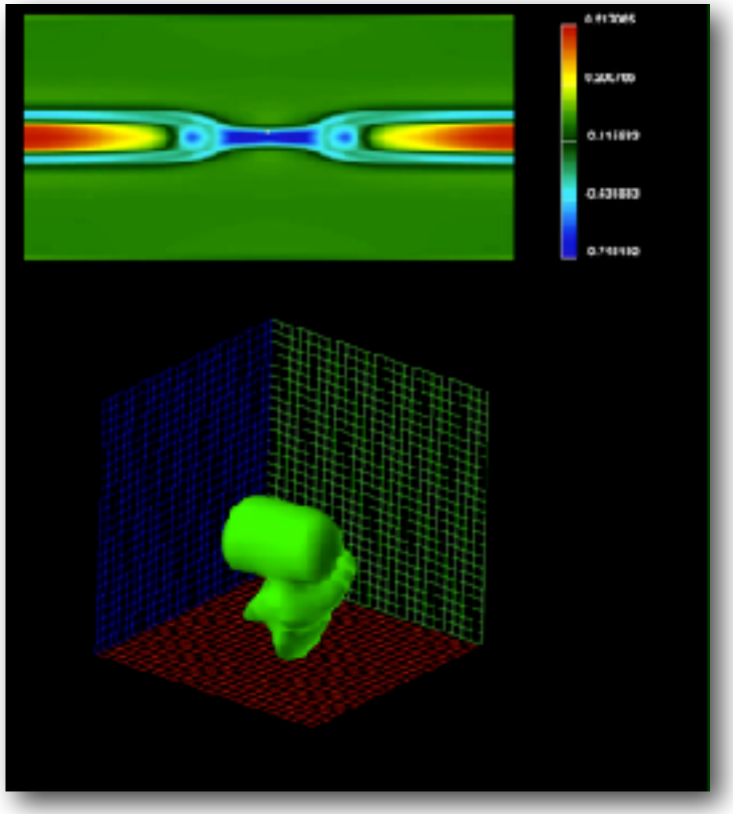
Numerical Methods



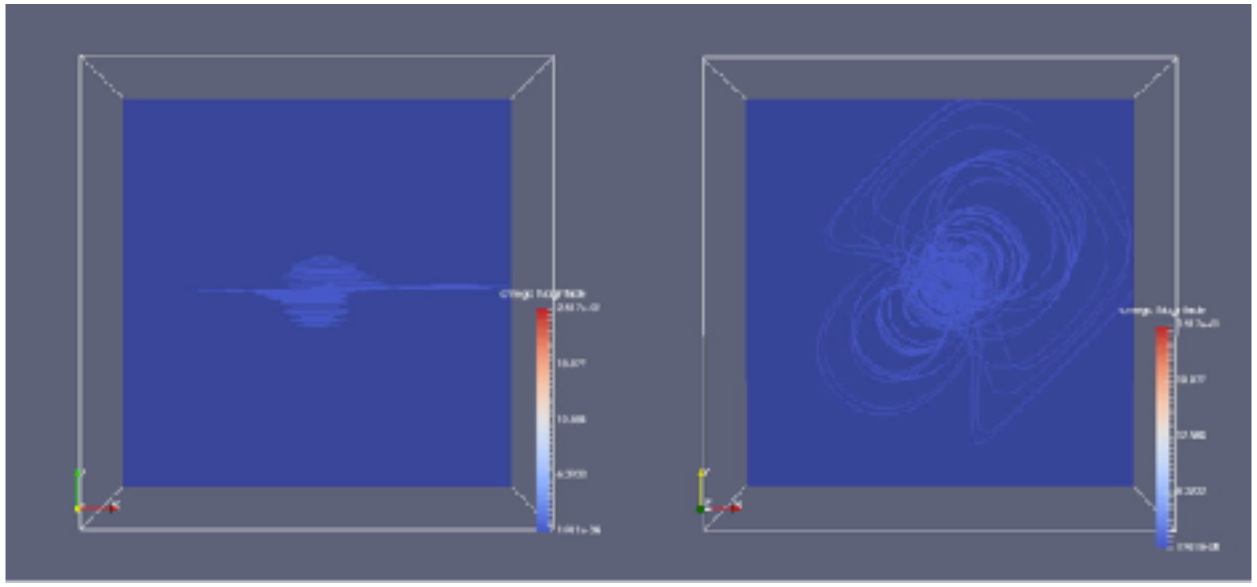
Dynamos



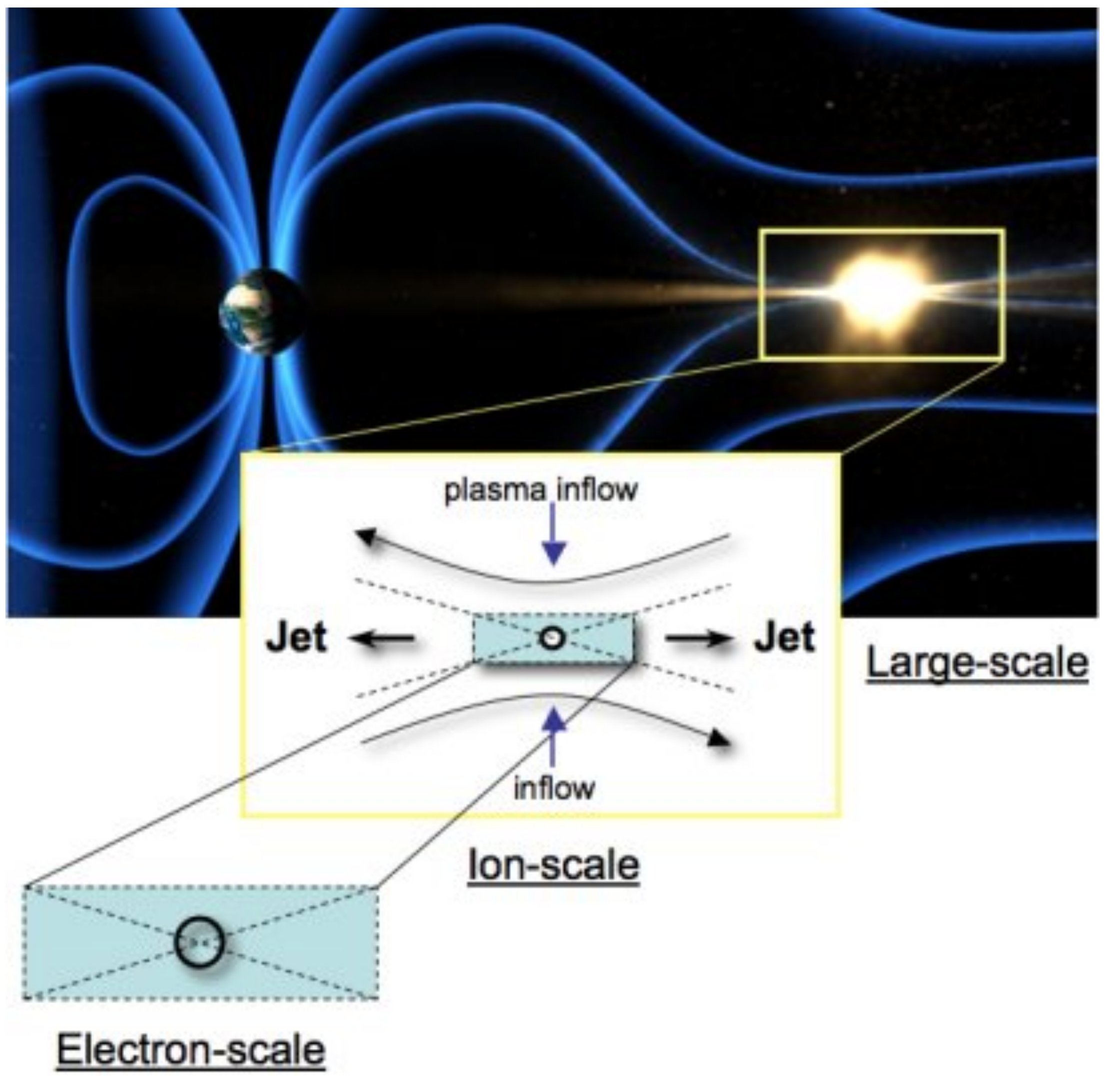
Vlasov Simulations



Instantons in turbulence



# Plasma = physics of scales



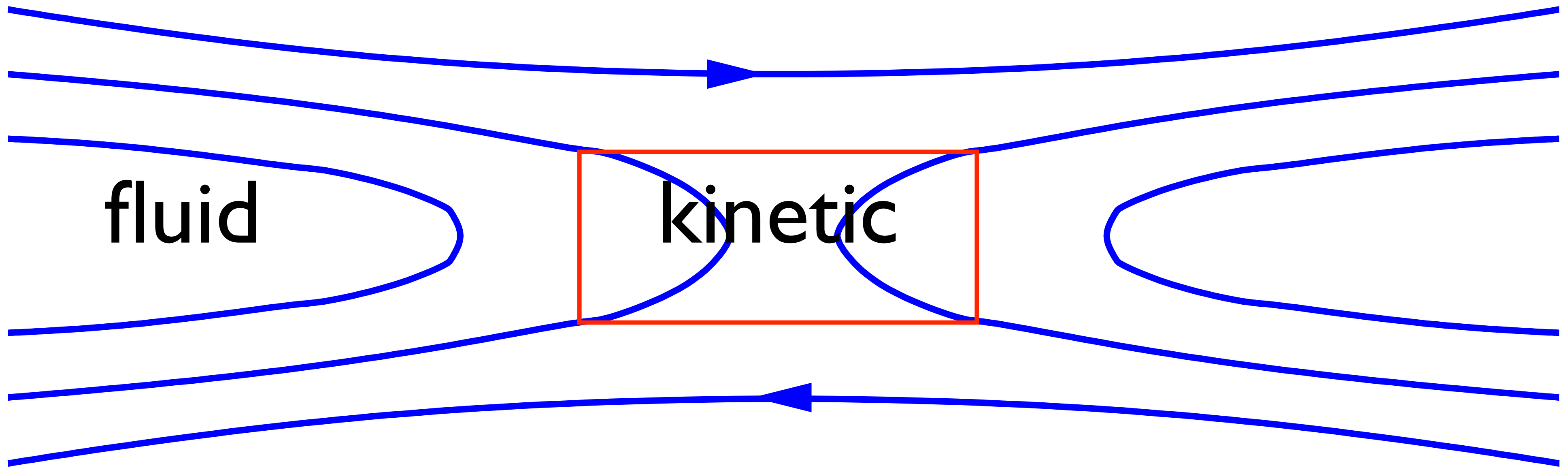

from G. Lapenta ISSS10

| | | spatial scales | time scales |
|---|---|---|---|
| | global scale: | $10^6$ km | hours |
| | system scale: | $10^5$ km | minutes |
| | ion scales $\rho_i$, $d_i$: | $10^3$ km | seconds |
| | $d_e$: | 10 km | $10^{-3}$ s |
| electron scales | $\rho_e$: | 1 km | $10^{-4}$ s |
| | $\lambda_e$: | 100 m | $10^{-5}$ s |

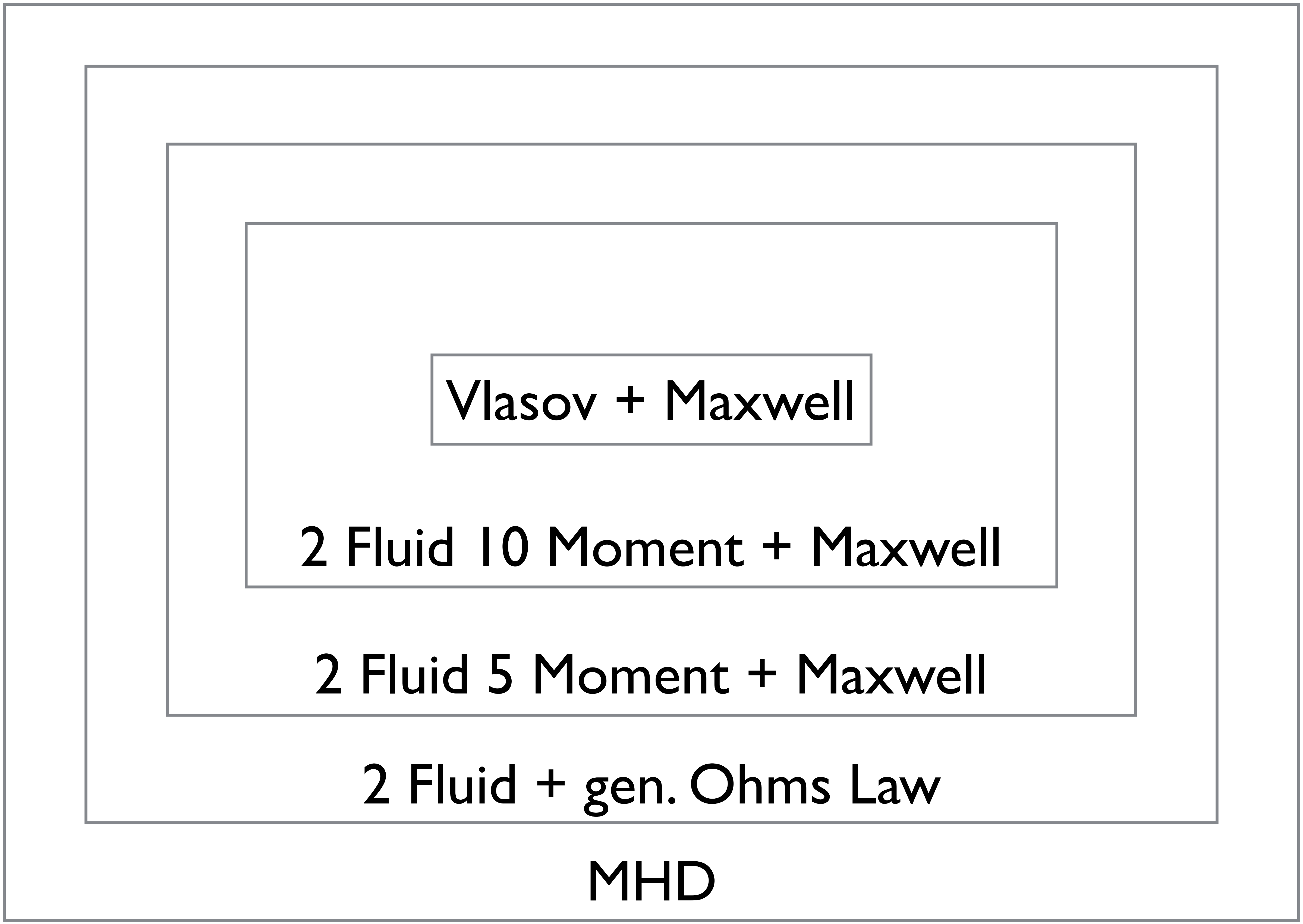
# Coupling of different plasma models

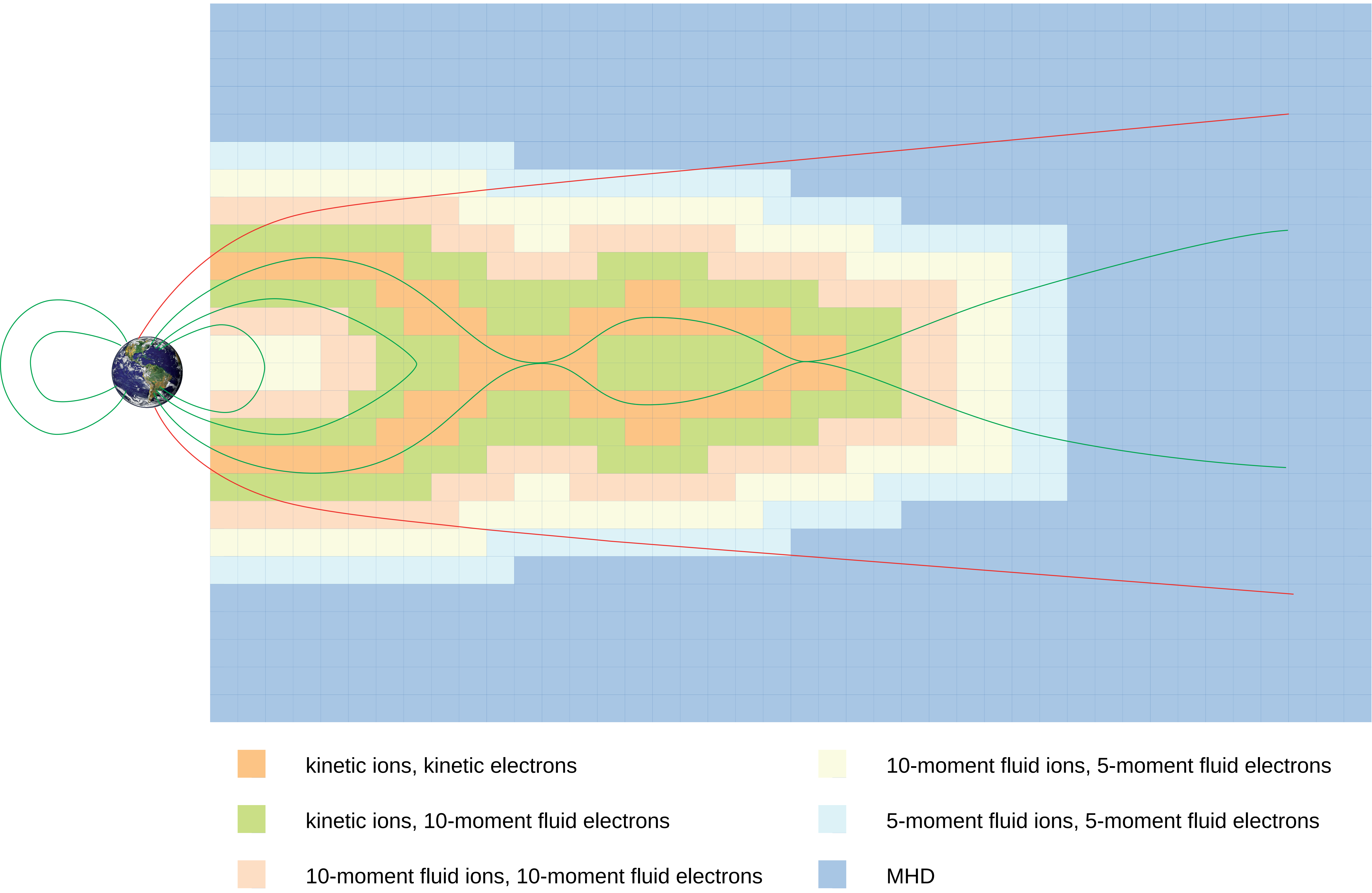
## Motivation

- fluid description
  MHD, Hall-MHD, 5- or 10 moment 2 Fluid
- kinetic description
  PIC, Vlasov
- Coupling fluid and kinetic simulations



# Dream:


Vlasov + Maxwell
2 Fluid 10 Moment + Maxwell
2 Fluid 5 Moment + Maxwell
2 Fluid + gen. Ohms Law
MHD


kinetic ions, kinetic electrons
kinetic ions, 10-moment fluid electrons
10-moment fluid ions, 10-moment fluid electrons
10-moment fluid ions, 5-moment fluid electrons
5-moment fluid ions, 5-moment fluid electrons
MHD

# Very active field (we are not alone)

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## Development of Multi-hierarchy Simulation Model for Studies of Magnetic Reconnection

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**Abstract.** The multi-hierarchy simulation model for magnetic reconnection is developed, where both micro and macro hierarchies are expressed consistently and simultaneously. Two hierarchies are connected smoothly by shake-hand scheme. As a numerical test, propagation of one-dimensional Alfvén wave is examined using the multi-hierarchy simulation model. It is found that waves smoothly pass through from macro to micro hierarchies and *vice versa*.

**AMS subject classifications**: 82D10, 93B40, 76W05

**Key words**: Multi-hierarchy, magnetic reconnection, MHD, particle-in-cell.

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Journal of Computational Physics 227 (2007) 1340–1352

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## Multi-scale plasma simulation by the interlocking of magnetohydrodynamic model and particle-in-cell kinetic model

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Available online 25 September 2007

**Abstract**

Many kinds of simulation models have been developed to understand the complex plasma systems. However, these simulation models have been separately performed because the fundamental assumption of each model is different and restricts the physical processes in each spatial and temporal scales. On the other hand, it is well known that the interactions among the multiple scales may play crucial roles in the plasma phenomena (e.g. magnetic reconnection, collisionless shock), where the kinetic processes in the micro-scale may interact with the global structure in the fluid dynamics. To take self-consistently into account such multi-scale phenomena, we have developed a new simulation model by directly interlocking the fluid simulation of the magnetohyrdodynamics (MHD) model and the kinetic simulation of the particle-in-cell (PIC) model. The PIC domain is embedded in a small part of MHD domain. The both simulations are performed simultaneously in each domain and the bounded data are frequently exchanged each other to keep the consistency between the models. We have applied our new interlocked simulation to Alfvén wave propagation problem as a benchmark test and confirmed that the waves can propagate smoothly through the boundaries of each domain.


MHD ⟷ PIC

Degond P, Dimarce G, Mieussens L.
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MHD–PIC connection model in a magnetosphere–ionosphere coupling system.
*Journal of Plasma Physics* 72 (2006) 945–948

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*Journal of Geophysical Research: Space Physics* 122 (2017) 10,336–10,355.

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Two-way coupling of magnetohydrodynamic simulations with embedded particle-in-cell simulations.
*Computer Physics Communications* 221 (2017) 81–94.

Lautenbach S., Grauer R.
Multiphysics simulations of collisionless plasmas
arXiv:1805.05698 (2018)

## What are we doing different?

Daldorff, Toth, Gombosi, Lapenta, Amaya, Markidis,Brackbill 2014:

implicit PIC + MHD, buffer zone, Maxwellian

Our approach:

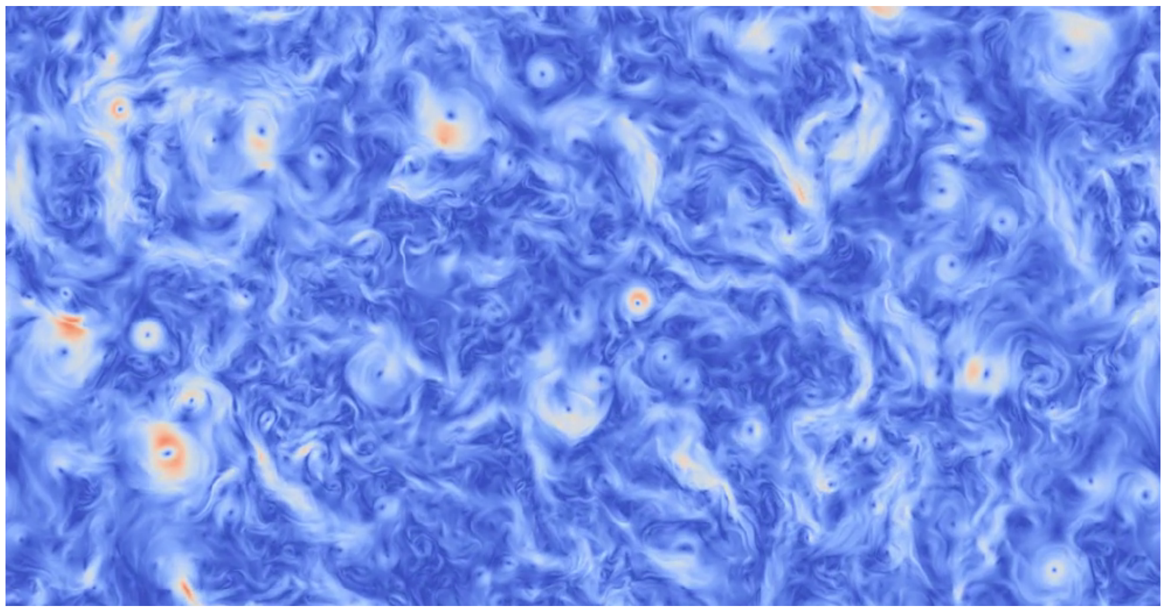
several models, no buffer zone, no assumption on Maxwellian form

+ adaptive and criteria

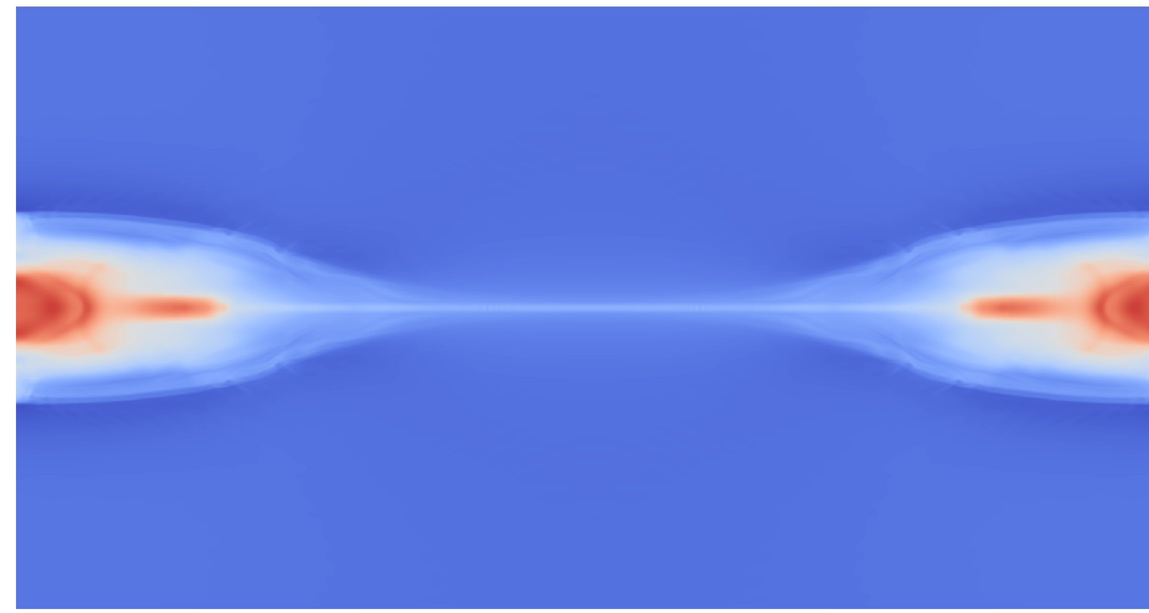
status: proof of principle, not really mature

# Suitable situations for adaptive modelling

In which situations can adaptive modelling be applied?



turbulence: ✗



magnetic reconnection: ✓

Phenomena must...

... be localized.

... occur in a specific plasma regime.

# Ingredients

Hyperbolic fluid equations:

- CWENO — Kurganov, Levy 2000
- 5- and 10-moment equations — Hakim, Loverich, Shumlak 2006, Johnson, Rossmanith 2010; Wang, Hakim, Germaschewski, Bhattacharjee 2015

Vlasov:

- semi-Lagrangian PFC — Filbet, Sonnendrücker, Bertrand 2001
- Boris push + back-substitution — Schmitz, Grauer 2006
- CUDA

Explicit Maxwell solver:

- Yee
- FDTD

Sub-cycling

- Maxwell (factor 4)
- reduced speed of light ($c = 20\ v_{alfven}$)

Coupling:

- kinetic -> fluid
- fluid -> kinetic
- refinement criteria

# Models

$$\rho_s = m_s \int \mathrm{d}^3 v f_s \qquad \text{(mass density)}$$

$$\mathbf{u}_s = \frac{m_s}{\rho_s} \int \mathrm{d}^3 v \mathbf{v} f_s \qquad \text{(velocity)}$$

$$\mathsf{E}_s = \frac{1}{2} m_s \int \mathrm{d}^3 v \mathbf{v}\mathbf{v} f_s \quad \text{(energy tensor)}$$

$$\mathsf{Q}_s = \frac{1}{2} m_s \int \mathrm{d}^3 v (\mathbf{v} - \mathbf{u}_s)(\mathbf{v} - \mathbf{u}_s)(\mathbf{v} - \mathbf{u}_s) f_s \quad \text{(heat flux tensor)}$$

$$\mathsf{P}_s = 2\mathsf{E}_s - \rho_s \mathbf{u}_s \mathbf{u}_s$$

$$p_s = \frac{1}{3} \operatorname{tr} \mathsf{P}_s$$

$$\mathcal{E}_s = \operatorname{tr} \mathsf{E}_s$$

5-moment model:

$$
\begin{aligned}
\partial_t \rho_s &= -\nabla \cdot (\rho_s \mathbf{u}_s) \\
\partial_t (\rho_s \mathbf{u}_s) &= -\nabla \cdot \Big(\rho_s \mathbf{u}_s \mathbf{u}_s\Big) - \frac{1}{3}\nabla\Big(2\mathcal{E}_s - \rho_s \mathbf{u}_s^2\Big) + \frac{q_s}{m_s}\rho_s\Big(\mathbf{E} + \mathbf{u}_s \times \mathbf{B}\Big) \\
\partial_t \mathcal{E}_s &= -\frac{1}{3}\nabla \cdot \Big(\big(5\mathcal{E}_s - \rho_s \mathbf{u}_s^2\big)\mathbf{u}_s\Big) + \frac{q_s}{m_s}\rho_s \mathbf{u}_s \cdot \mathbf{E} - \nabla \cdot \mathbf{Q}_s
\end{aligned}
$$

$$
\mathbf{Q} = \begin{pmatrix} Q_{xxx} + Q_{xyy} + Q_{xzz} \\ Q_{xxy} + Q_{yyy} + Q_{yzz} \\ Q_{xxz} + Q_{yyz} + Q_{zzz} \end{pmatrix}
$$

10-moment model:

$$
\begin{aligned}
\partial_t \rho_s &= -\nabla \cdot (\rho_s \mathbf{u}_s) \\
\partial_t (\rho_s \mathbf{u}_s) &= -\nabla \cdot \mathrm{E}_s + \frac{q_s}{m_s}\rho_s(\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) \\
\partial_t \mathrm{E}_s &= -\nabla \cdot \big[3\,\mathrm{Sym}(\mathbf{u}_s \mathrm{E}_s) - 2\rho_s \mathbf{u}_s \mathbf{u}_s \mathbf{u}_s\big] + \frac{2q_s}{m_s}\,\mathrm{Sym}\Big(\rho_s \mathbf{u}_s \mathbf{E} + \mathrm{E}_s \times \mathbf{B}\Big) + \mathrm{R}_{\mathrm{iso},s} - \nabla \cdot \mathrm{Q}_s
\end{aligned}
$$

$$
\mathrm{R}_{\mathrm{iso},s} = \frac{1}{\tau_s}\left(\frac{1}{3}(\mathrm{tr}\,\mathrm{P}_s)\mathbb{1} - \mathrm{P}_s\right) \quad \text{with} \quad \tau_s = \tau_0\sqrt{\frac{\det \mathrm{P}_s}{\rho_s^5}}
$$

Vlasov equation

$$\partial_t f_s + \mathbf{v} \cdot \nabla_{\mathbf{r}} f_s + \frac{q_s}{m_s} \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} \Big) f_s = 0$$

Maxwell's equations

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

$$\partial_t \mathbf{E} = c^2 \left( \nabla \times \mathbf{B} - \mu_0 \sum_s \frac{q_s \rho_s}{m_s} \mathbf{u}_s \right)$$

compressible MHD

in conservation form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left( \mathbf{v}\rho\mathbf{v} + \mathbf{I}(p + \frac{\mathbf{B}^2}{2}) - \mathbf{BB} \right) = 0$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left( \mathbf{v}(e + p + \frac{\mathbf{B}^2}{2}) - \mathbf{B}(\mathbf{v} \cdot \mathbf{B}) \right)$$

$$\frac{\partial B}{\partial t} + \nabla \cdot (\mathbf{vB} - \mathbf{Bv}) = 0$$

$$p = (\gamma - 1) \left( e - \frac{1}{2}\rho\mathbf{v}^2 - \frac{1}{2}\mathbf{B}^2 \right)$$

# compressible MHD

## Riemann solvers

examples: Godunov, PPM, HLL(*), wave-propagation

- very good resolution of shocks
- very bad in smooth regions

## ENO-schemes

- shock resolution not as good as from Riemann solvers,
- much better resolution of waves in smooth regions
- very easy!!!

We use CWENO-type schemes.

Main reason: **easy** !!!

# Semi-discrete central schemes, CWENO

Nessyahu and Tadmor (1990)
Kurganov and Levy (2000)

# Why central schemes?

- no (aproximate) Riemann solver necessary
- dimension by dimension approach makes sence
- high order
- monotone, WENO, TVD depends on the reconstruction
- **easy** for complex problems

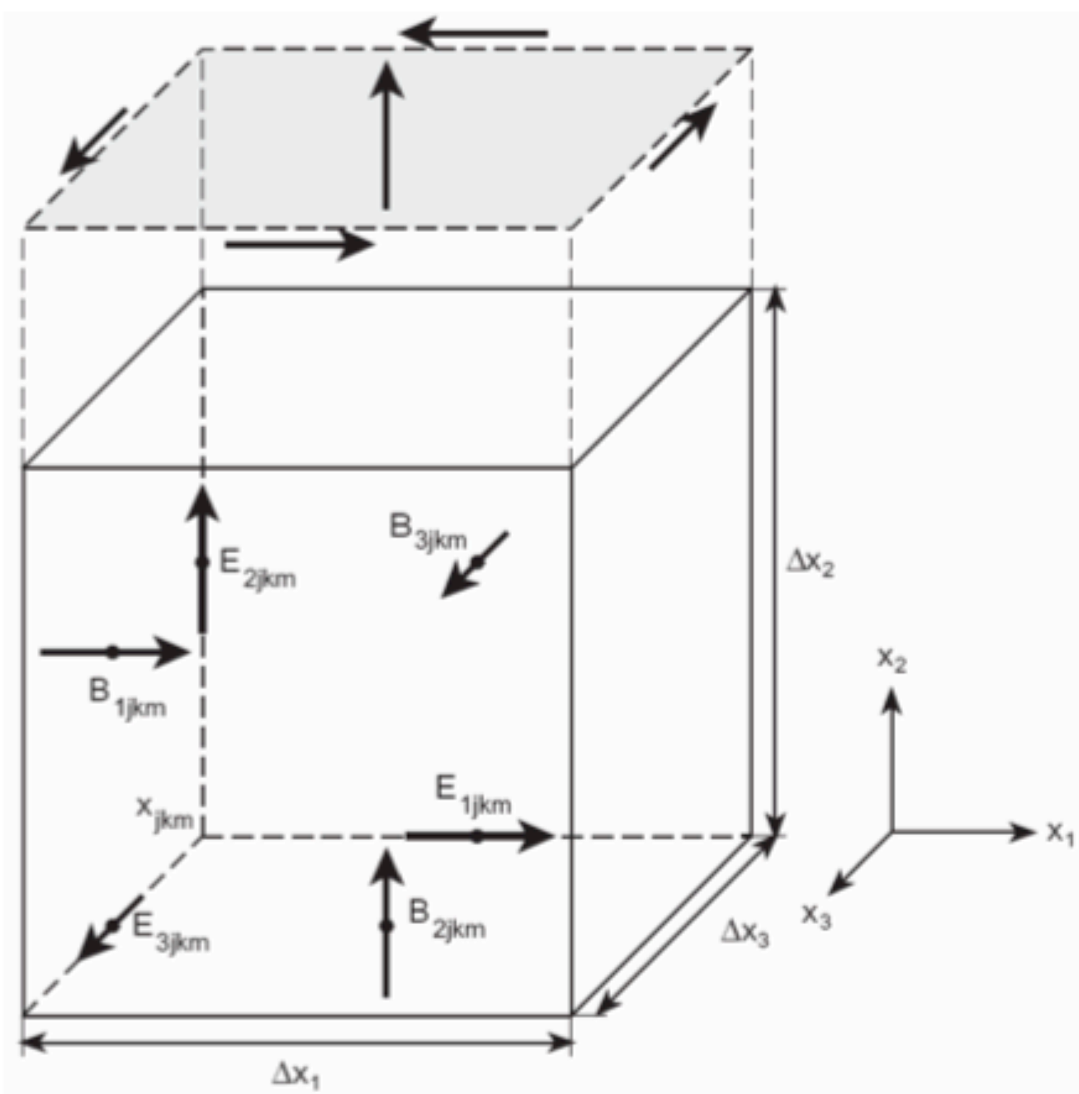
low Mach number limit ok

# Maxwell Solver: FDTD and Yee mesh (1966)

*inspired by lectures by A. Spitkovsky*

$$\partial E/\partial t = c(\nabla \times B) - 4\pi J\,, \qquad \nabla \cdot E = 4\pi\varrho\,, \quad \nabla \cdot B = 0$$

$$\partial B/\partial t = -c(\nabla \times E)\,, \qquad \frac{d}{dt}\gamma m\mathbf{v} = q(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B})$$




FDTD: second order in space and

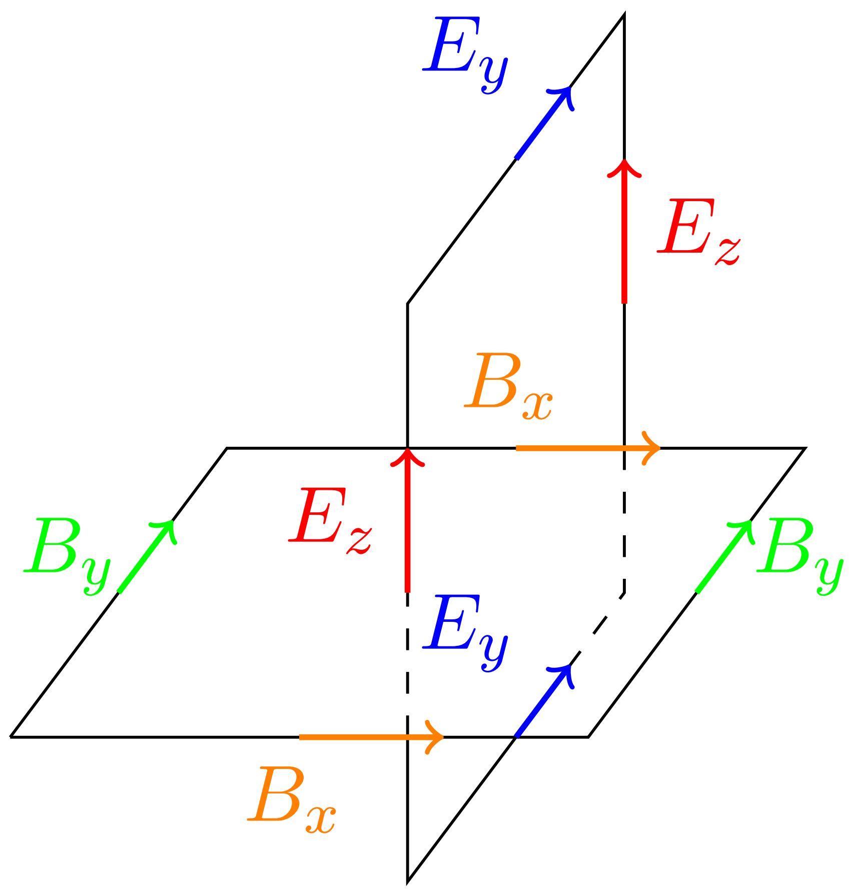
$$E^{n+1/2} = E^{n-1/2} + \Delta t[c(\nabla \times B^n) - 4\pi J^n]$$

$$B^{n+1} = B^n - c\Delta t \nabla \times E^{n+1/2}$$

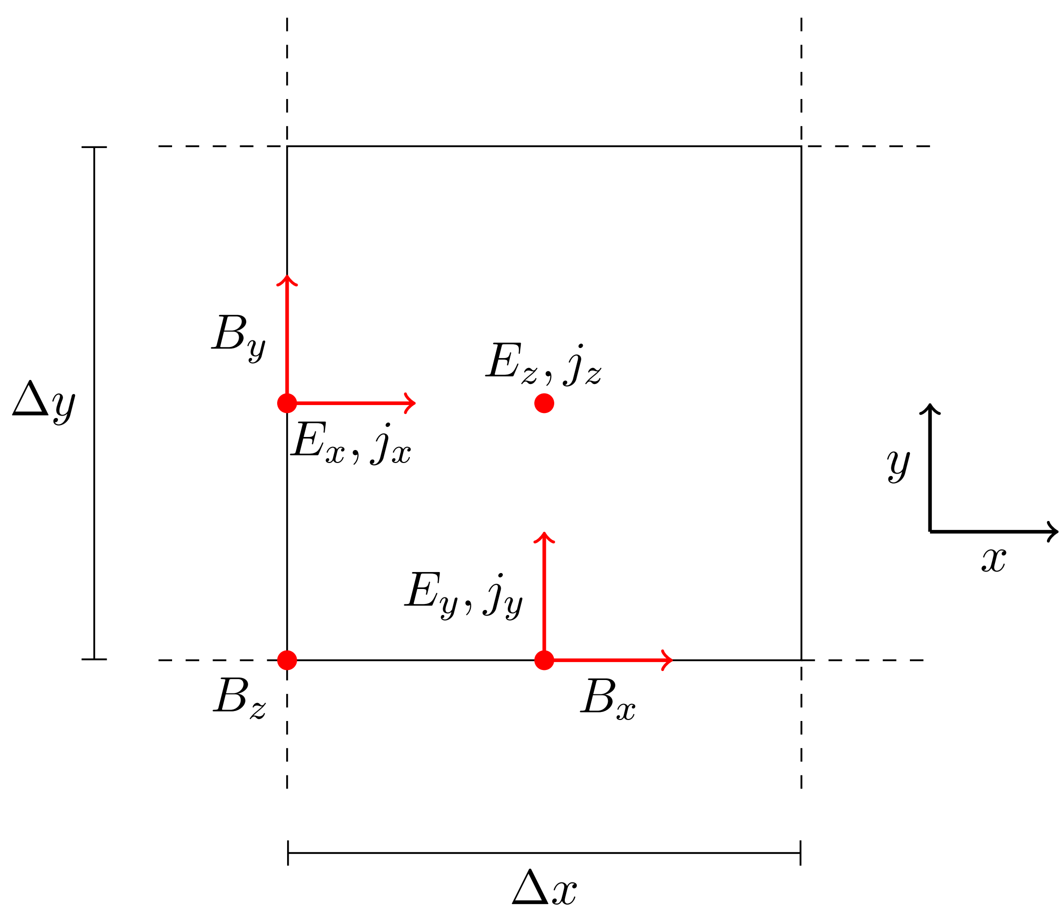
Yee mesh: div B

# Yee mesh motivated by integral form:

$$\partial_t \int_\Sigma \mathbf{B} \cdot \mathrm{d}\mathbf{S} = -\oint_{\partial\Sigma} \mathbf{E} \cdot \mathrm{d}\mathbf{l}$$
$$\partial_t \int_\Sigma \mathbf{E} \cdot \mathrm{d}\mathbf{S} = -c^2 \int_\Sigma \mathbf{j} \cdot \mathrm{d}\mathbf{S} + c^2 \oint_{\partial\Sigma} \mathbf{B} \cdot \mathrm{d}\mathbf{l}$$




## 2D by projection



# Coupling FDTD- and CWENO Method

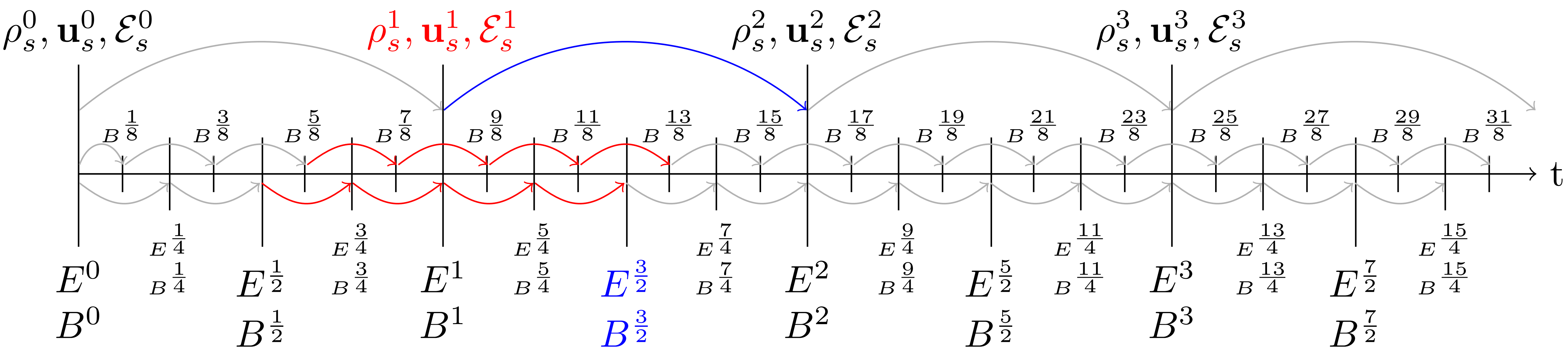
Fluid: strongly stable TVD Runge Kutta (Shu-Osher 1988)

$$v' = v^n + \frac{\Delta t}{6} f\left(v^n, t^n\right)$$

$$v'' = v' + \frac{\Delta t}{6} f\left(6v' - 5v^n, t^n + \Delta t\right)$$

$$v^{n+1} = v'' + \frac{2\Delta t}{3} f\left(\tfrac{3}{2}v'' - \tfrac{1}{2}v^n, t^n + \tfrac{1}{2}\Delta t\right)$$

subcycling and interpolation



Ok, now we have a fluid code !

Let’s do Vlasov

# Vlasov simulations

collisionless Plasma: Vlasov equation

$$\frac{\partial f_k}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_k + \frac{q_k}{m_k} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_k = 0$$

$+$ Maxwell, $k = e, i$

important: positive conservative scheme, semi-Lagrangian, Boris, backsubstitution method

(Filbet, Sonnendrücker, Bertrand 2001)

## Darwin-Approximation

CFL-condition too restrictive

$\Longrightarrow$ Darwin approximation

electric field split into *longitudinal* and *transversal* part

$$\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T \quad \text{mit } \nabla \cdot \mathbf{E}_T = 0 \text{und } \nabla \times \mathbf{E}_L = 0$$

Maxwell equations

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \times \mathbf{B} = \mu_0 \left( \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j} \right) \qquad \nabla \cdot \mathbf{B} = 0$$

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Maxwell equations with Darwin approximation

$$\nabla \times \mathbf{E_T} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{E_L} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \times \mathbf{B} = \mu_0 \left( \varepsilon_0 \frac{\partial \mathbf{E_L}}{\partial t} + \mathbf{j} \right) \qquad \nabla \cdot \mathbf{B} = 0$$

no timestep restriction by the speed of light, but 8 elliptic equations

# Semi-Lagrangean scheme

Consider $\partial_t f + \partial_x \left( v(t,x) f \right) = 0$

The characteristics of this PDE are given by:

$$\begin{aligned} \frac{dX}{ds}(s) &= v(s, X(s)) \\ X(t) &= x \end{aligned}$$

Denote the solution as $X(s,t,x)$

Since $\frac{df}{ds} = 0$ (r.h.s. of the PDE), we have

$$\int_{x_1}^{x_2} f(t,x)dx = \int_{X(s,t,x_1)}^{X(s,t,x_2)} f(s,x)dx$$

With this we can update the cell-average of $f$ in the $i$th cell:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(t^{n+1},x)dx = \int_{X(t^n,t^{n+1},x_{i-\frac{1}{2}})}^{X(t^n,t^{n+1},x_{i+\frac{1}{2}})} f(t^n,x)dx$$

Let $\bar{f}_i^n$ denote the cell-average in the $i$th cell at time $t^n$.

$$\bar{f}_i^{n+1} = \bar{f}_i^n + \Phi_{i-\frac{1}{2}} - \Phi_{i+\frac{1}{2}}$$
$$= \bar{f}_i^n + \int_{X(t^n, t^{n+1}, x_{i-\frac{1}{2}})}^{x_{i-\frac{1}{2}}} f(t^n, x)\mathrm{d}x - \int_{x_{i+\frac{1}{2}}}^{X(t^n, t^{n+1}, x_{i+\frac{1}{2}})} f(t^n, x)\mathrm{d}x$$

Strategy:

- Follow the Characteristics ending at the cell borders backwards in time and find their footpoint
- Reconstruct the integral of $f$ from the footpoint to the cell border
- Update with $\bar{f}_i^{n+1} = \bar{f}_i^n + \Phi_{i-\frac{1}{2}} - \Phi_{i+\frac{1}{2}}$

This will lead to a conservative scheme.

Developed by *Filbet, Sonnendrücker, Bertrand (JCP 2001)*
PFC = *Positive Flux-Conservative*

Let's consider the simple second-order scheme for positive velocities: Approximate the primit function of $f$ in the interval $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ (again, $\bar{f}_i$ denotes the cell average):

$$F(x) = \int_{-\infty}^{x} f(x)\mathrm{d}x$$

by

$$\tilde{F}(x) = w_{i-1} + (x - x_{i-\frac{1}{2}})\bar{f}_i + \frac{1}{2}(x - x_{i-\frac{1}{2}})(x - x_{i+\frac{1}{2}})\frac{\bar{f}_{i+1} - \bar{f}_i}{\Delta x}$$

Now we can reconstruct $f$ itself:

$$\tilde{f}(x) = \frac{\mathrm{d}F}{\mathrm{d}x}(x) = \bar{f}_i + (x - x_i)\frac{\bar{f}_{i+1} - \bar{f}_i}{\Delta x}$$

However this scheme can cause negative reconstructed $\tilde{f}$. To avoid this, one can introduce a slope-limiter $\epsilon$ to ensure that the reconstruction lies between $0$ and $f_\infty$:

$$\epsilon_i = \begin{cases} \min(1; 2\bar{f}_i/(\bar{f}_{i+1} - \bar{f}_i)) & \text{if } \bar{f}_{i+1} > \bar{f}_i \\ \min(1; -2(f_\infty - \bar{f}_i)/((\bar{f}_{i+1} - \bar{f}_i)) & \text{if } \bar{f}_{i+1} < \bar{f}_i, \end{cases}$$

to obtain

$$f_h(x) = \bar{f}_i + \epsilon_i (x - x_i) \frac{\bar{f}_{i+1} - \bar{f}_i}{\Delta x}$$

Let's denote the distance from the footpoint of the characteristic to the cell-boundary by $\alpha$. Integrating $f_h$ then gives the flux through the boundary at $x_{i+\frac{1}{2}}$:

$$\begin{aligned} \Phi_{i+\frac{1}{2}} &= \int_{x_{i+\frac{1}{2}-\alpha}}^{x_{i+\frac{1}{2}}} f_h(x) \mathrm{d}x \\ &= \alpha \left( \bar{f}_i + \frac{\epsilon_i}{2} \left(1 - \frac{\alpha}{\Delta x}\right) (\bar{f}_{i+1} - \bar{f}_i) \right) \end{aligned}$$

Some remarks:

- This scheme can be extended to higher orders. We use the third order one.
- A similar derivation produces the scheme for negative velocities.
- The length of the characteristics can be arbitrarily large with only a minor change in the derivation.
- The accuracy in time depends only on how good the characteristics can be calculated.

# The Vlasov equation

$$\partial_t f_s + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0$$

We want to solve this PDE using a one-dimensional semi-Lagrangian scheme.
Why? Becase one-dimensional schemes can have fancy limiters, conservation-properties and efficient implementations that are difficult to generalise to higher dimensions.
Remember: The Vlasov equation is a conservative, hyperbolic PDE in 6 dimension (plus time)

One way to do this is *splitting*.

# Splitting

Consider $\partial_t f = \mathcal{A}f + \mathcal{B}f$, where $\mathcal{A}$ and $\mathcal{B}$ are linear operators (with no time dependance).

The formal solution to this is

$$f(t) = \exp\big((\mathcal{A} + \mathcal{B})t\big) f_0$$

If $\mathcal{A}$ and $\mathcal{B}$ commute, we can also write:

$$f(t) = \exp(\mathcal{B}t) \exp(\mathcal{A}t) f_0$$

This means we can just solve $\partial_t f = \mathcal{A}f$, use the result as an initial value for $\partial_t f = \mathcal{B}f$ and still get the correct solution!

# Godunov splitting

What happens when $\mathcal{A}$ and $\mathcal{B}$ do *not* commute?
Let's look at the *Zassenhaus* formula (A variation on *Baker-Campbell-Hausdorff*):

$$\exp\left((\mathcal{A}+\mathcal{B})t\right) = \exp\left(\mathcal{B}t\right)\exp\left(\mathcal{A}t\right)\exp\left([\mathcal{A},\mathcal{B}]\frac{t^2}{2}\right)\exp\left(\mathcal{O}(t^3)\right)$$

So now we have:

$$f(t) = \exp(\mathcal{B}t)\exp(\mathcal{A}t)f_0 + \mathcal{O}(t^2)$$

We still get an approximate solution accurate to first order in time.
This is called *Godunov* splitting or *Lie-Trotter* splitting

# Strang splitting

Can we do better?

A scheme accurate to second order in time is the *Strang-Splitting*:

$$f(t) = \exp(\mathcal{B}t/2)\exp(\mathcal{A}t)\exp(\mathcal{B}t/2)f_0 + \mathcal{O}(t^3)$$

By manipulating the *Baker-Campbell-Hausdorff* formula, splitting schemes of arbitrary order can be constructed.

However, the *Sheng-Suzuki theorem* states that all splitting schemes better than second order will have at least one negative exponent (i.e. negative time-steps).

# Strang splitting and the Vlasov equation

We will now use Strang splitting on the Vlasov equation:

$$\partial_t f_s + \underbrace{\mathbf{v} \cdot \nabla_{\mathbf{x}}}_{\mathcal{A}} f_s + \underbrace{\frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}}}_{\mathcal{B}} f_s = 0$$

$$f_s(t^{n+1}) = \exp(\mathcal{B}t/2) \exp(\mathcal{A}t) \exp(\mathcal{B}t/2) f_s(t^n) + \mathcal{O}(t^3)$$

This means we update the velocity-part of $f_s$ over one half time-step,
then update the position-part over one full time-step,
then update the velocity-part again over one half time-step.

This is equivalent to the *Leapfrog* or *Strömer-Verlet* schemes in PIC simulations!

# The position update

We want to solve

$$\partial_t f_s + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = 0$$

Let's rewrite this equation to

$$\partial_t f_s + \partial_x v_x f_s + \partial_y v_y f_s + \partial_z v_z f_s = 0$$

Since $\mathbf{v}$ is just a variable and does not depend on $\mathbf{x}$, we can write this in a conservative form. Now we have three linear operators that all commute!

We can just solve each step seperately and the solution is still exact. By using a conservative numerical scheme, the conservation property of the Vlasov equation is kept.

# The velocity update

The velocity part is not that easy.

$$
\begin{aligned}
\partial_t f_s + \frac{q_s}{m_s}\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) \cdot \nabla_{\mathbf{v}} f_s = \\
\partial_t f_s + \frac{q_s}{m_s} \partial_{v_x} (E_x + v_y B_z - v_z B_y) f_s \\
+ \frac{q_s}{m_s} \partial_{v_y} (E_y + v_z B_x - v_x B_z) f_s \\
+ \frac{q_s}{m_s} \partial_{v_z} (E_z + v_x B_y - v_y B_x) f_s = 0
\end{aligned}
$$

We can still rewrite this in a conservative way, but the three operators do not commute because of the velocity in the $\mathbf{v} \times \mathbf{B}$ term.

# The velocity update

Can we use Strang splitting?

If we denote the individual operators by $\mathcal{V}_x$, $\mathcal{V}_y$, and $\mathcal{V}_z$ we will have

$$\begin{aligned} f(t^{n+1}) = & \exp(\mathcal{V}_x t/4) \exp(\mathcal{V}_y t/2) \exp(\mathcal{V}_x t/4) \\ & \times \exp(\mathcal{V}_z t) \\ & \times \exp(\mathcal{V}_x t/4) \exp(\mathcal{V}_y t/2) \exp(\mathcal{V}_x t/4) f(t^n) + \mathcal{O}(t^3) \end{aligned}$$

This means 7 steps for the velocity update and we have a numerically preferred direction.

# Backsubstitution

What we really want is:

- Just one step per operator
- No splitting error in time

Equations of motion:

$$\begin{aligned} \frac{d}{dt} m\mathbf{v} &= q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \\ \frac{d}{dt}\mathbf{x} &= \mathbf{v} \end{aligned}$$

looks implicit

leap-frog

$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}^n + \frac{1}{2}(\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}) \times \mathbf{B}^n\right)$$

Solution: Boris (1970) explicit

$$\mathbf{v}^{n-1/2} = \mathbf{v}^- - \frac{q\mathbf{E}^n}{m}\frac{\Delta t}{2}$$

$$\mathbf{v}^{n+1/2} = \mathbf{v}^+ + \frac{q\mathbf{E}^n}{m}\frac{\Delta t}{2}$$

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}$$

$$\mathbf{v}^- = \mathbf{v}^{n-1/2} + \frac{q\Delta t\mathbf{E}^n}{2m}$$

$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}^n$$

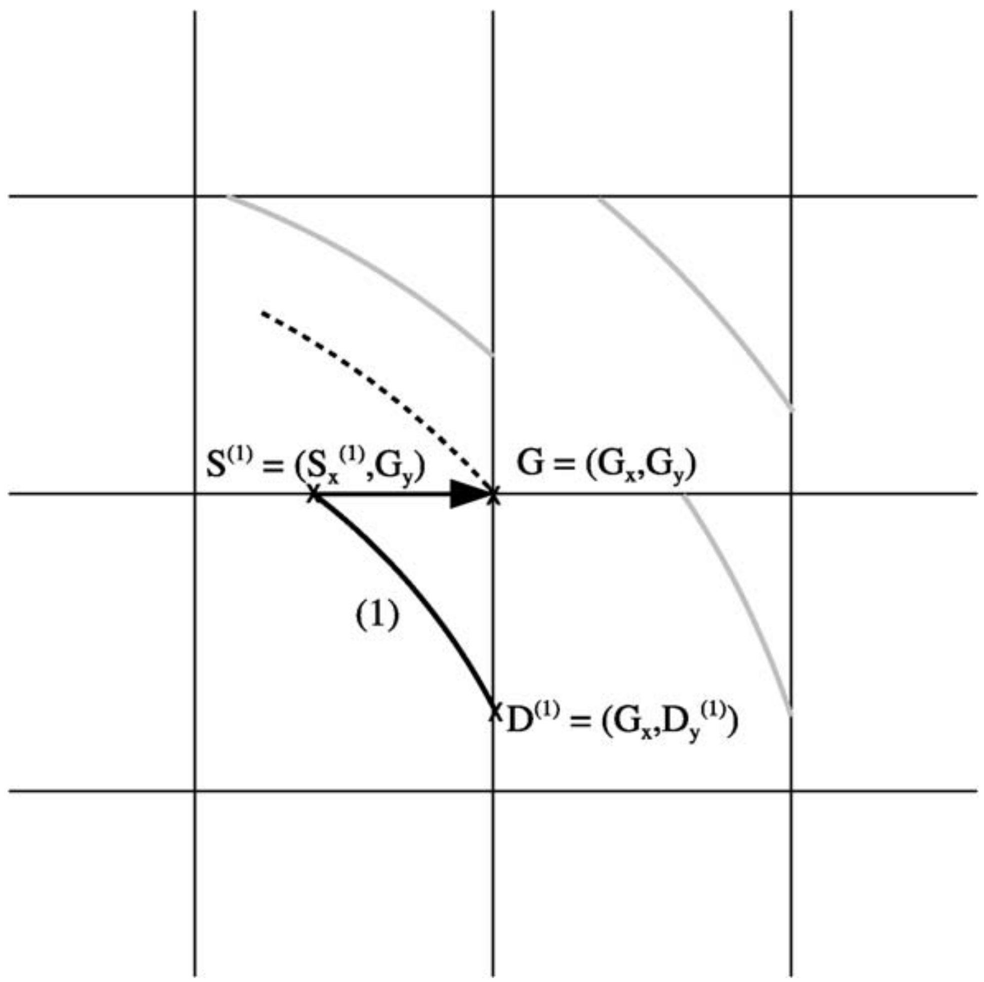
$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \frac{2\mathbf{t}^n}{1 + \mathbf{t}^n \cdot \mathbf{t}^n}$$

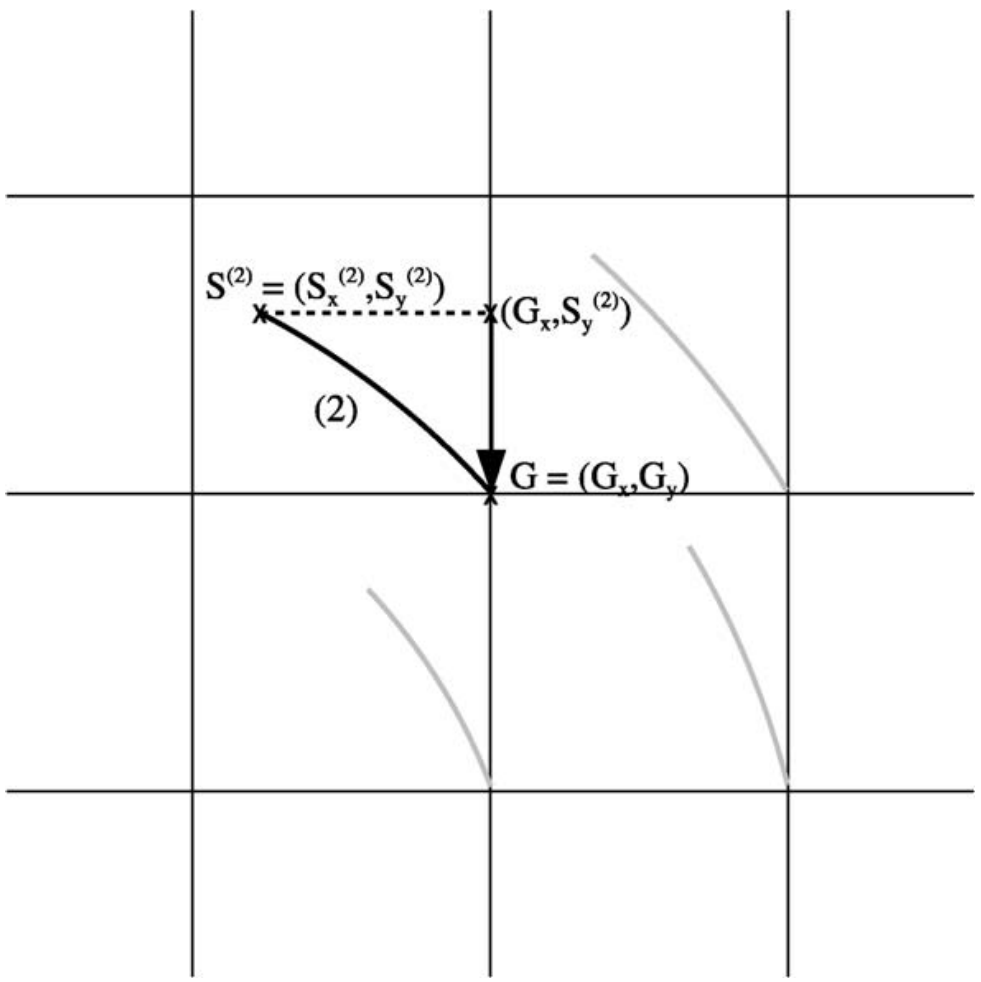
$$\mathbf{v}^{n+1/2} = \mathbf{v}^+ + \frac{q\Delta t\mathbf{E}^n}{2m}$$

with $\mathbf{t}^n = \frac{q\Delta t\mathbf{B}^n}{2m}$

So let's revisit what the semi-Lagrangian scheme does (for simplicity in 2D).
A full two-dimensional scheme would transport the value of f along the black characteristic.

would like to have: $$f^{\text{new}}(D_x, D_y) = f^{\text{old}}(S_x, S_y)$$




Splitting: $$f^{\text{inter}}(G_x, G_y) = f^{\text{old}}(S_x^{(1)}, G_y)$$

$f^{\text{old}}$ is lossed, only have $f^{\text{inter}}$

$$f^{\text{new}}(G_x, G_y) = f^{\text{inter}}(G_x, S_y^{(2)})$$

assuming correct interpolation $$f^{\text{inter}}(G_x, S_y^{(2)}) = f^{\text{old}}(S_x^{(2)}, S_y^{(2)})$$

$$\Longrightarrow \quad f^{\text{new}}(G_x, G_y) = f^{\text{old}}(S_x^{(2)}, S_y^{(2)}) \quad \checkmark$$

# Backsubstitution for the velocity update

The characteristics for the velocity update can be calculated by the *Boris* scheme. Define

$$\mathbf{k} = \frac{\Delta t}{2}\frac{q_s}{m_s}\mathbf{B} \qquad \mathbf{s} = \frac{2\mathbf{k}}{1+k^2}$$

Now the backward in time *Boris* scheme is given by:

$$\begin{aligned}
\mathbf{v}^{+} &= \mathbf{v}^{n+1} - \frac{\Delta t}{2}\frac{q_s}{m_s}\mathbf{E} \\
\tilde{\mathbf{v}} &= \mathbf{v}^{+} - \mathbf{v}^{+} \times \mathbf{k} \\
\mathbf{v}^{-} &= \mathbf{v}^{+} - \tilde{\mathbf{v}} \times \mathbf{s} \\
\mathbf{v}^{n} &= \mathbf{v}^{-} - \frac{\Delta t}{2}\frac{q_s}{m_s}\mathbf{E}
\end{aligned}$$

This formula has to be brought into this form:

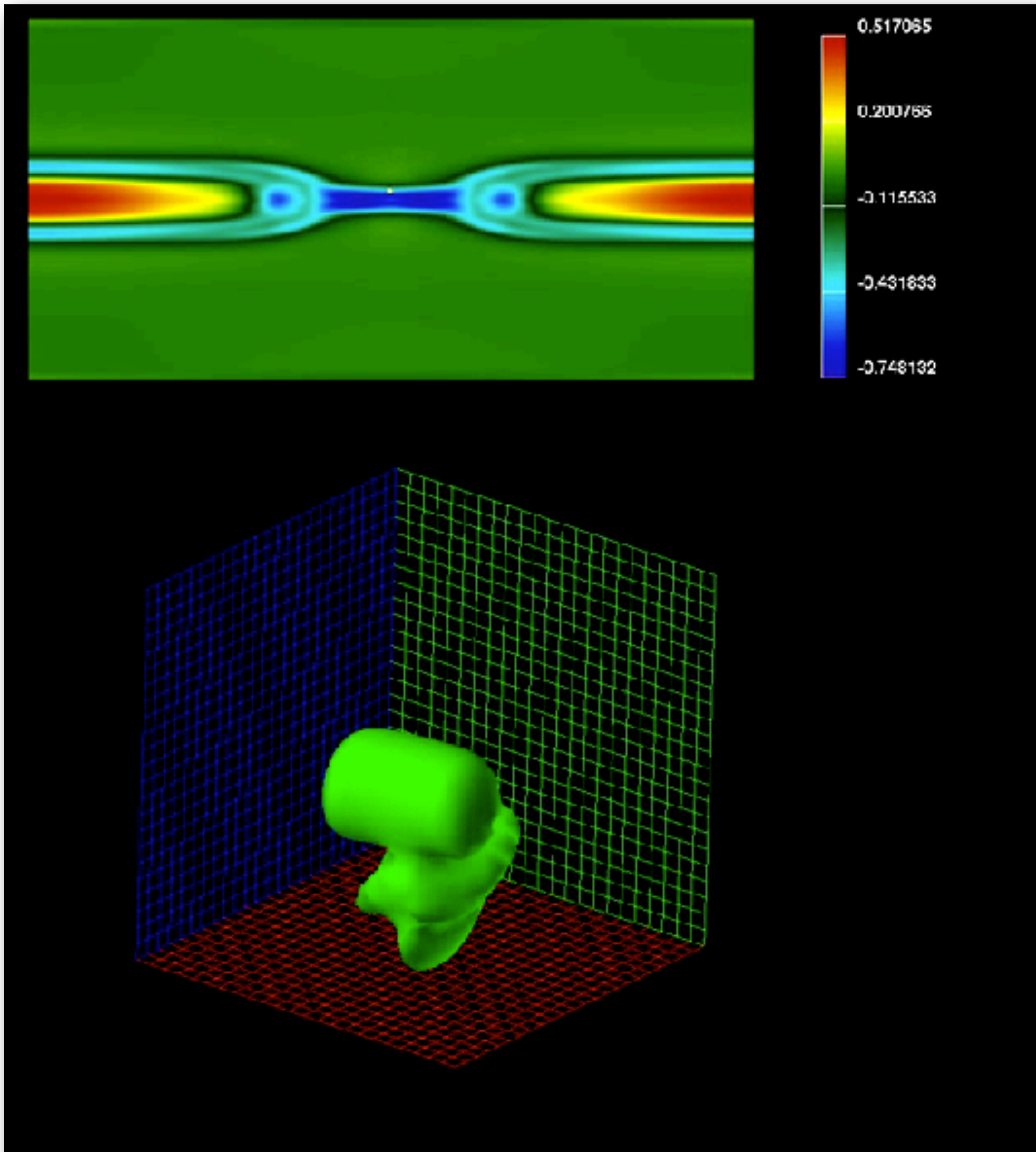
$$\begin{aligned}
v_x^n &= v_x^n(v_x^{n+1}, v_y^n, v_z^n) \\
v_y^n &= v_y^n(v_x^{n+1}, v_y^{n+1}, v_z^n) \\
v_z^n &= v_z^n(v_x^{n+1}, v_y^{n+1}, v_z^{n+1})
\end{aligned}$$

# Backsubstitution for the velocity update

$$v_x^n = v_x^n(v_x^{n+1}, v_y^n, v_z^n) \tag{1}$$
$$v_y^n = v_y^n(v_x^{n+1}, v_y^{n+1}, v_z^n) \tag{2}$$
$$v_z^n = v_z^n(v_x^{n+1}, v_y^{n+1}, v_z^{n+1}) \tag{3}$$

The last equation (3) is given simply by the $z$-component of Boris' scheme.
To find (2) we solve (3) for $v_z^{n+1}$ and substitute this into the $y$-component of Boris' scheme.
Equation (1) can be found by using the $x$-component of the *forward* in time Boris scheme and solving for $v_x^n$.

# Example: magnetic reconnection with DSDV I




Electron out of plane current

Electron distribution function

## New Code: DSDV II (Martin Rieke)

- full Maxwell Solver
- parallel CUDA

# Hardware and CUDA performance

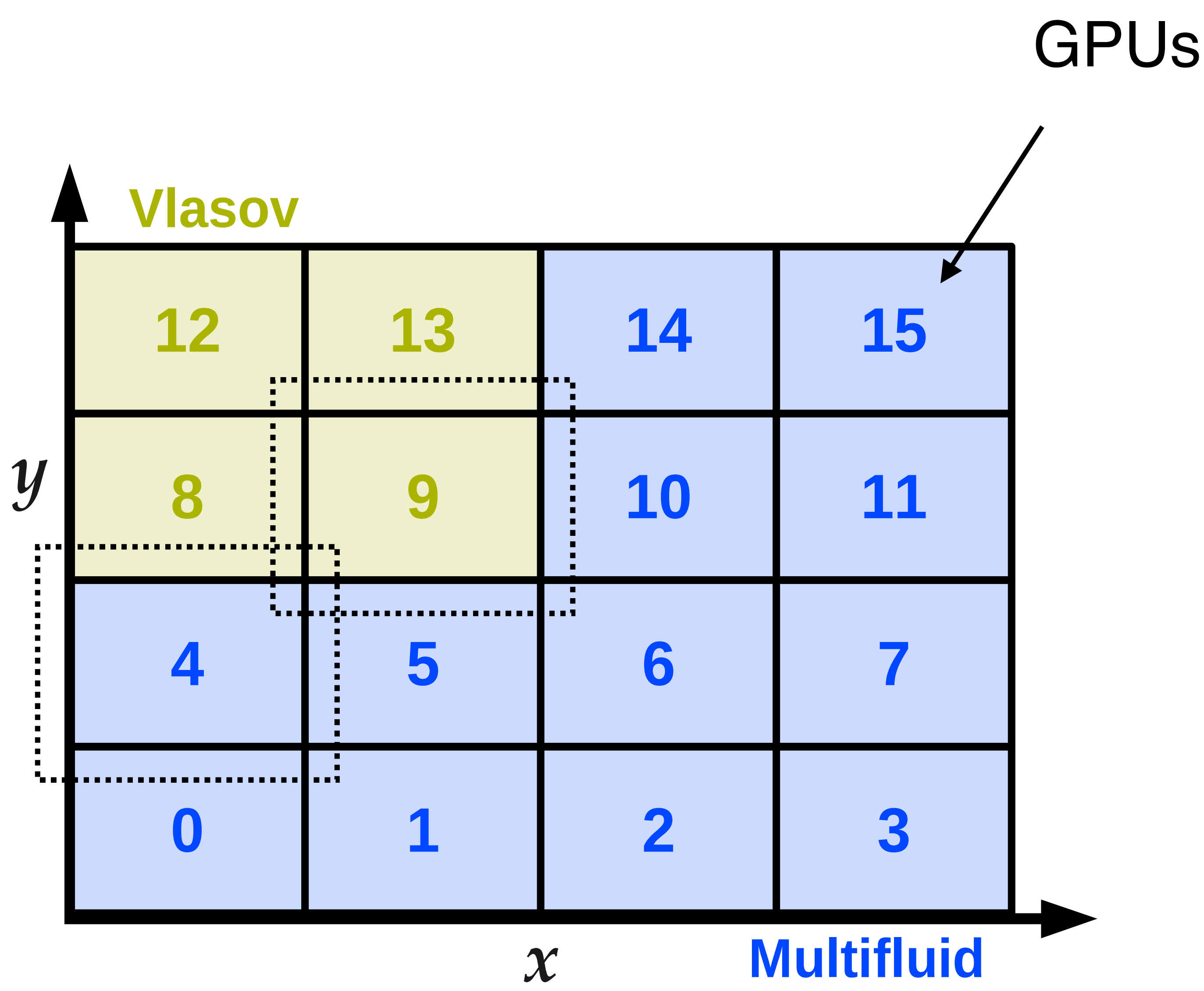
The *DaVinci-cluster* at the Ruhr-Universität Bochum consists of 17 nodes with a total of

- 16320 cores and 272 GB RAM on GPUs (68~NVidia Tesla S1070 cards with 240 cores and 4 GB RAM each)
- 136 respectively 272 (with HT) cores and 408 GB on CPUs (34 Xeon E5530 Quad Core CPUs (2.4 GHz) with 8 cores respectively 16 cores (with HT) and 12~GB RAM each)

| system | resolution | duration of run |
|---|---|---|
| CPUs (Schmitz, Grauer) | $256 \times 128 \times 30^3$ | $\sim 150$ h |
| GPUs (this work) | $256 \times 128 \times 32^3$ | $\sim 8$ h |

Comparison of the time necessary to simulate one quarter of the GEM setup until $t = 40\Omega_i^{-1}$.

# Basic idea




- Domain is subdivided into mostly autonomous blocks
- In each block, one physical model is applied
- Communication via exchange of boundary conditions

Parallelization: space-filling Hilbert-curve

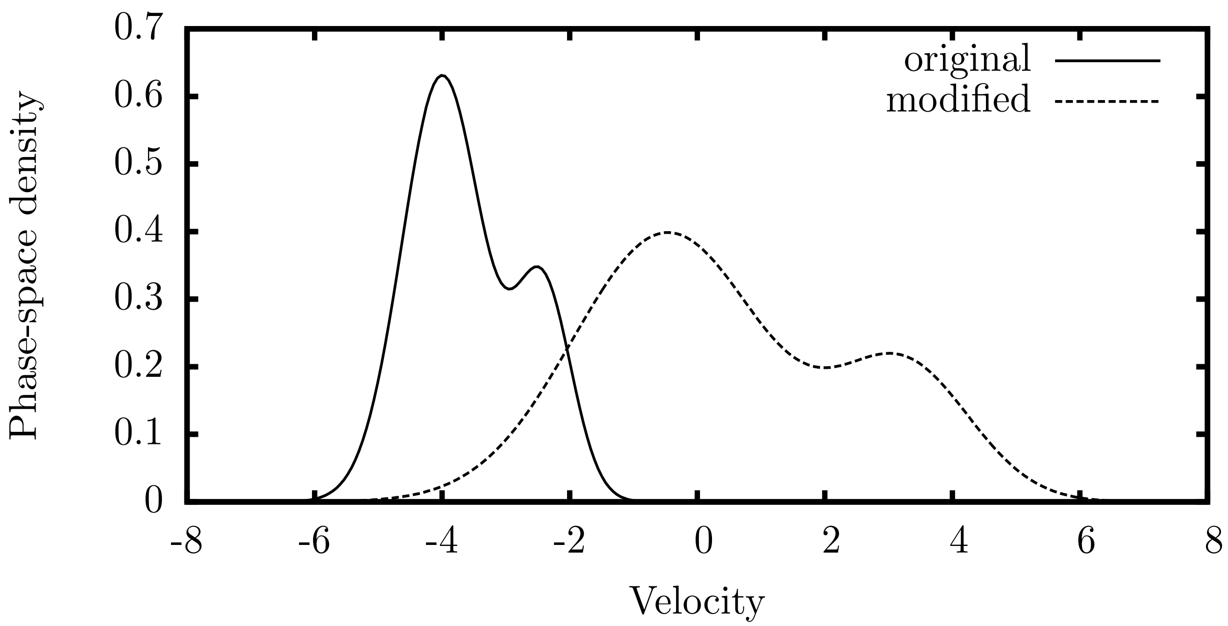
# Fitting moments

kinetic region → fluid region:

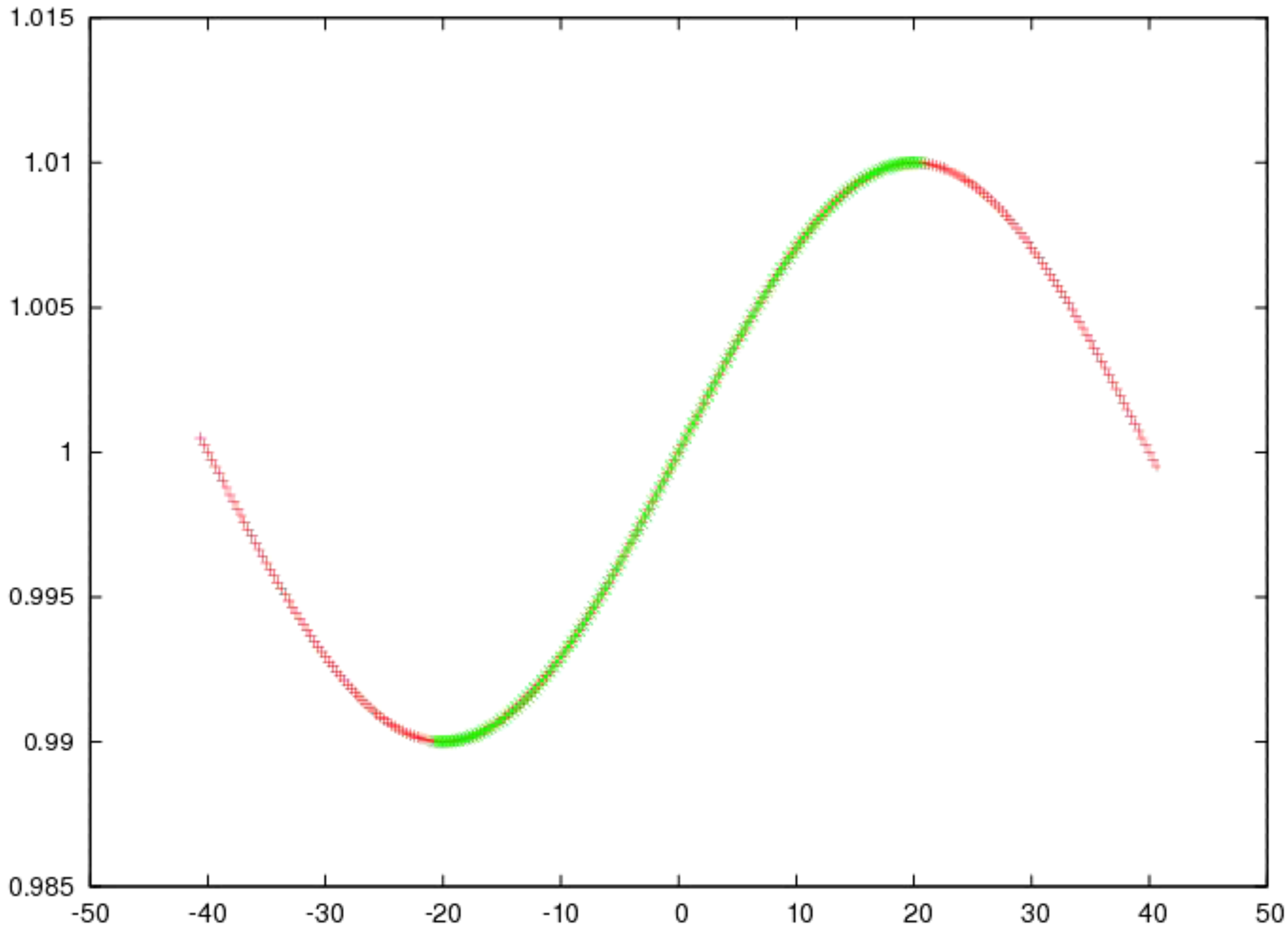
- Calculating moments via simple integration

fluid region → kinetic region:

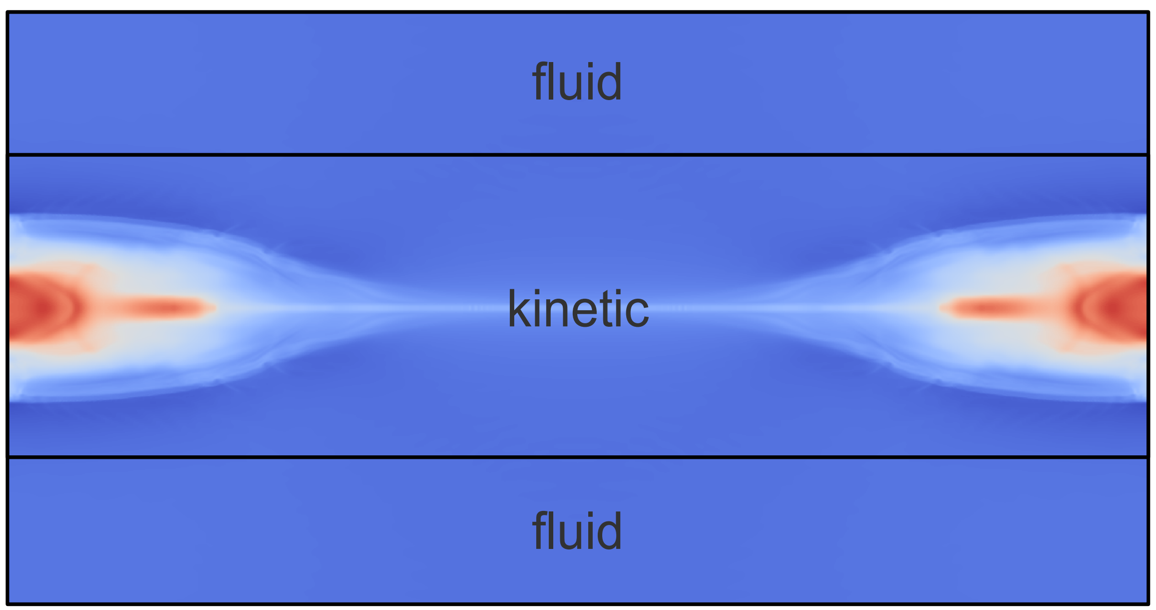
- Lack of sufficient information
- Extrapolation of shape of pdf into outer region
- Fitting of moments by advection step with suitable velocity field



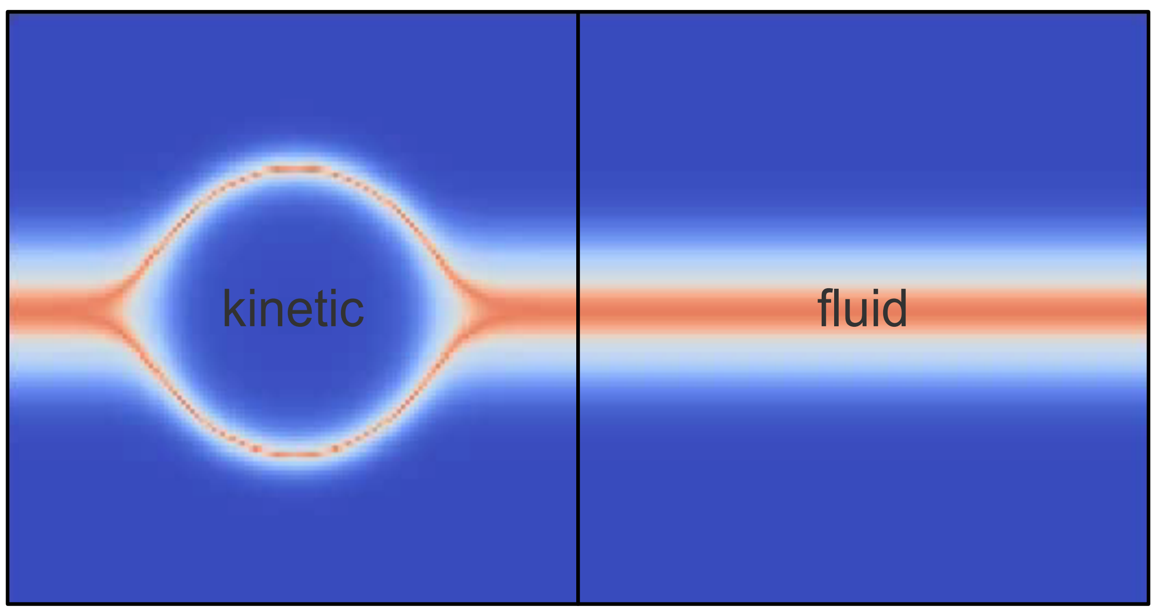
# Ion Sound Waves



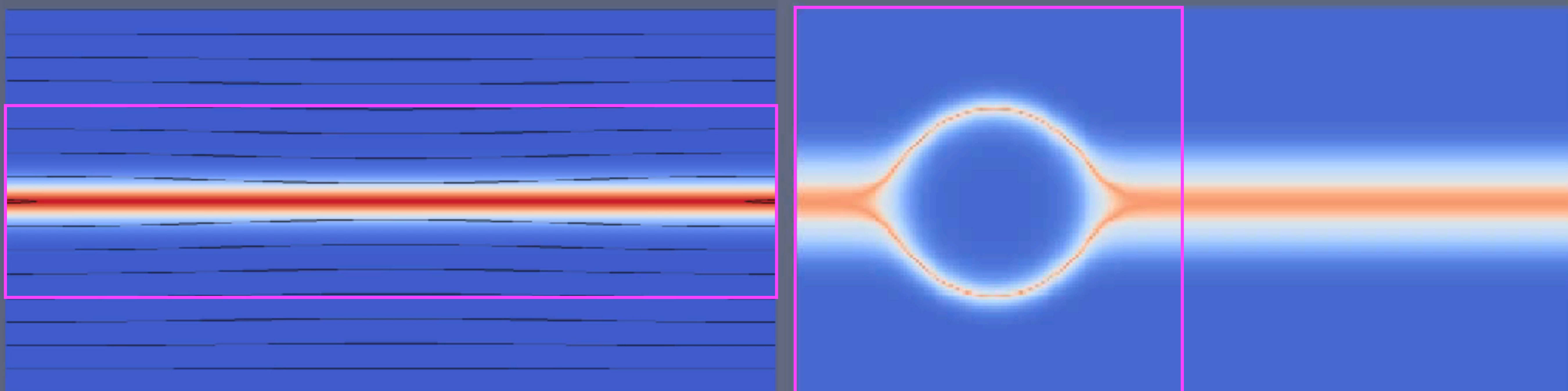
# First Results




GEM challenge (reconnection)




ion hole



Where is fluid and where is the kinetic region ?

# Issues and ToDo's

numerical errors act differently in fluid and kinetic codes:

numerical dissipation in Vlasov leads to **heating**

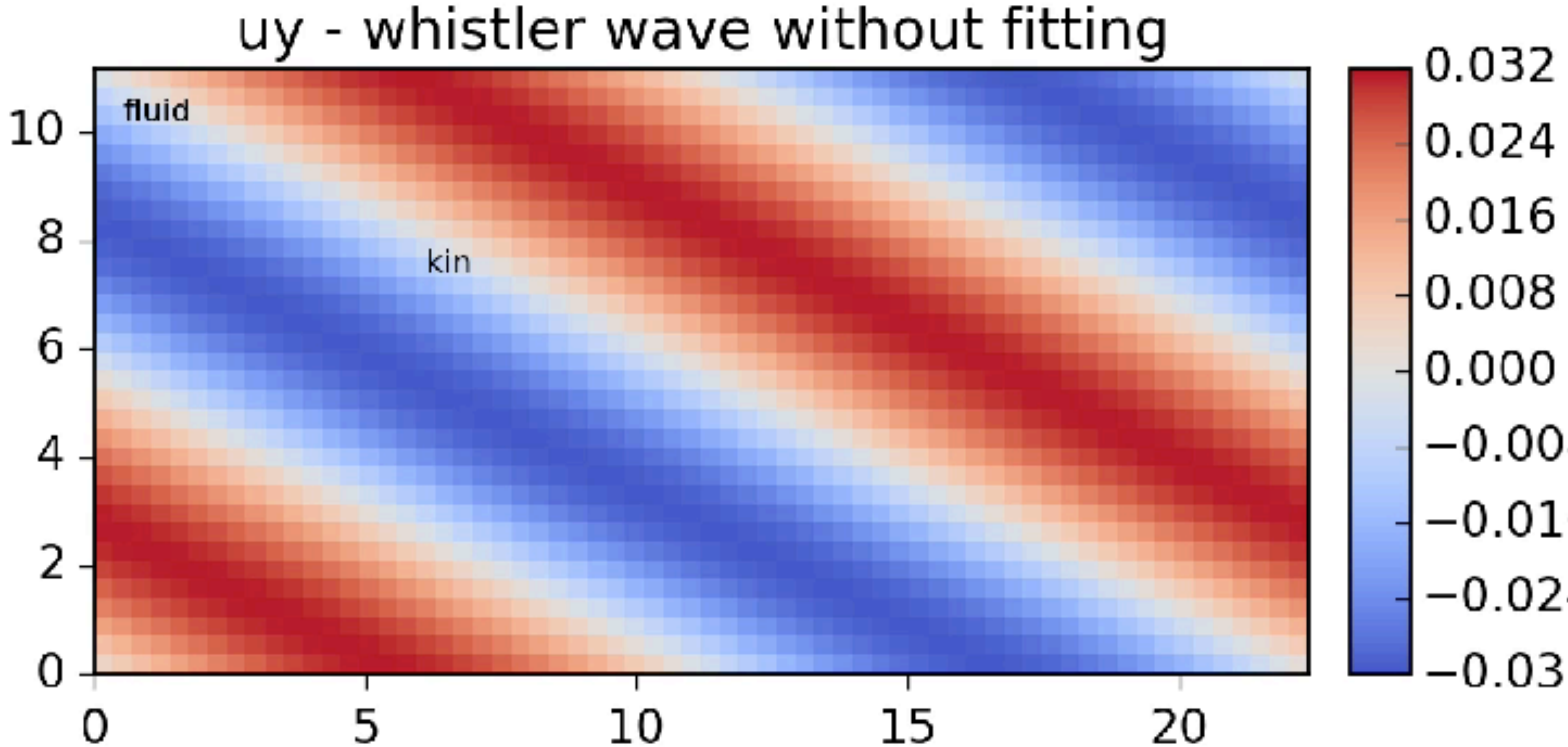
numerical dissipation in fluid leads to **cooling**

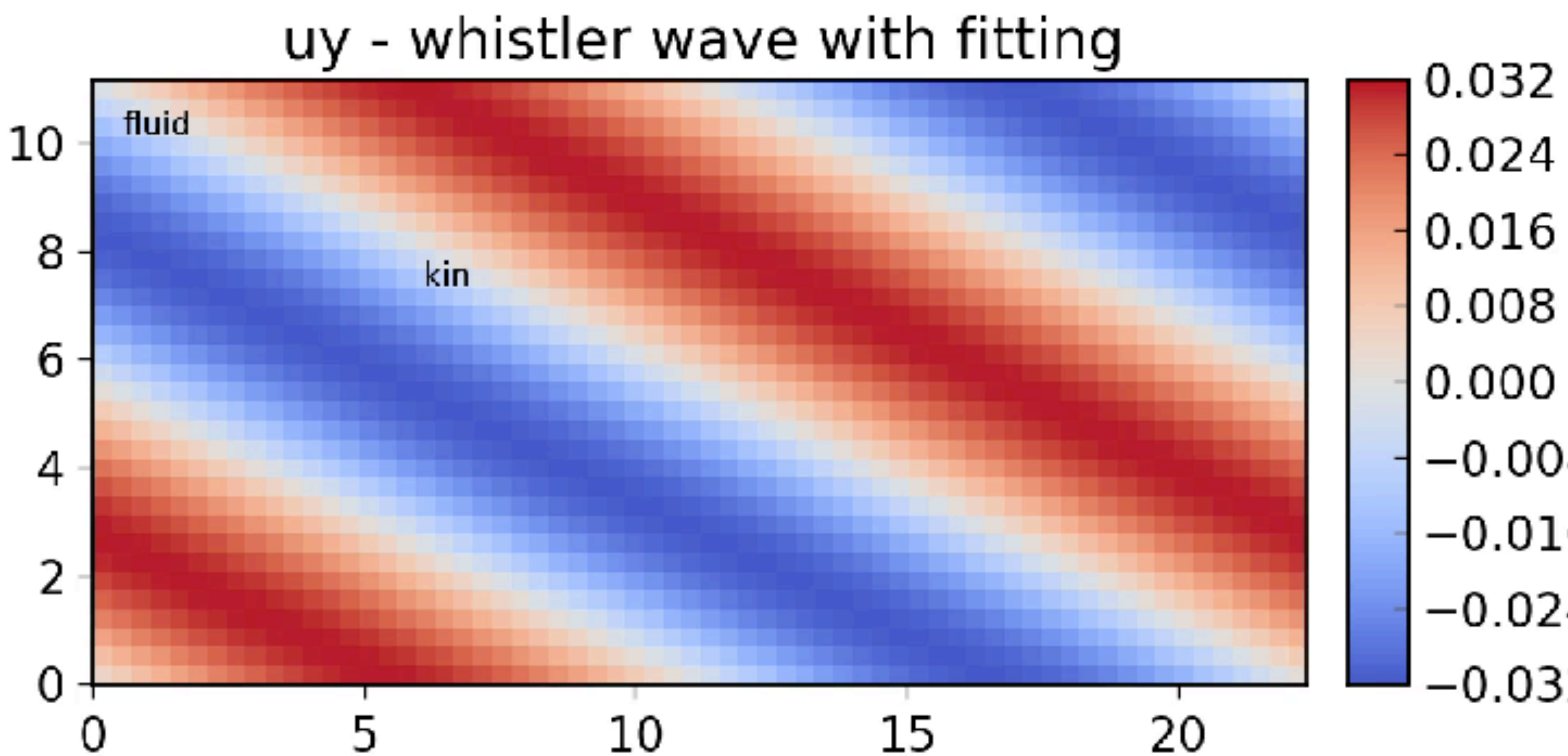
***Strategy:***

errors are "*smaller*" in fluid than in Vlasov, thus

- in the kinetic region solve fluid equations with heat flux Q from Vlasov
  if there were no numerical errors: fluid = Vlasov
- trust fluid
  adjust distribution function with the fluid moments

Example: Whistler wave (Daldorff, Toth, Gombosi, Lapenta, Amaya, Markidis,Brackbill JCP 2014)


uy - whistler wave without fitting
fluid
kin
0
2
4
6
8
10
0
5
10
15
20
0.032
0.024
0.016
0.008
0.000
−0.008
−0.016
−0.024
−0.032


uy - whistler wave with fitting
fluid
kin
0
2
4
6
8
10
0
5
10
15
20
0.032
0.024
0.016
0.008
0.000
−0.008
−0.016
−0.024
−0.032

# Adaptive Multiphysics Simulations

## Criterion

Consider 1D:

$$
\begin{aligned}
\partial_t \overline{\mu}_k =& -\partial_x \overline{\mu}_{k+1} + \frac{k\overline{\mu}_{k-1}}{\mu_0}\partial_x \overline{\mu}_2 \\
=& \left(\frac{k_\mathrm{B}}{m}\right)^{\frac{k+1}{2}} \left(-(k!!)\partial_x (nT^{\frac{k+1}{2}}) + k(k-2)!!\,T^{\frac{k-1}{2}}\partial_x(nT)\right) \\
=& -\left(\frac{k_\mathrm{B}}{m}\right)^{\frac{k+1}{2}} \left(\frac{n(k-1)(k!!)}{2} T^{\frac{k-1}{2}}\partial_x T\right) \\
=& -\frac{p}{m}\left(\frac{k_\mathrm{B}}{m}\right)\left(\frac{(k-1)(k!!)}{(\sqrt{2})^{k-1}} v_\mathrm{th}^{k-3}\partial_x T\right)
\end{aligned}
$$

Now consider heat flux

$$
\partial_t q = -\frac{3}{2}\frac{k_\mathrm{B}}{m} p \partial_x T,
$$

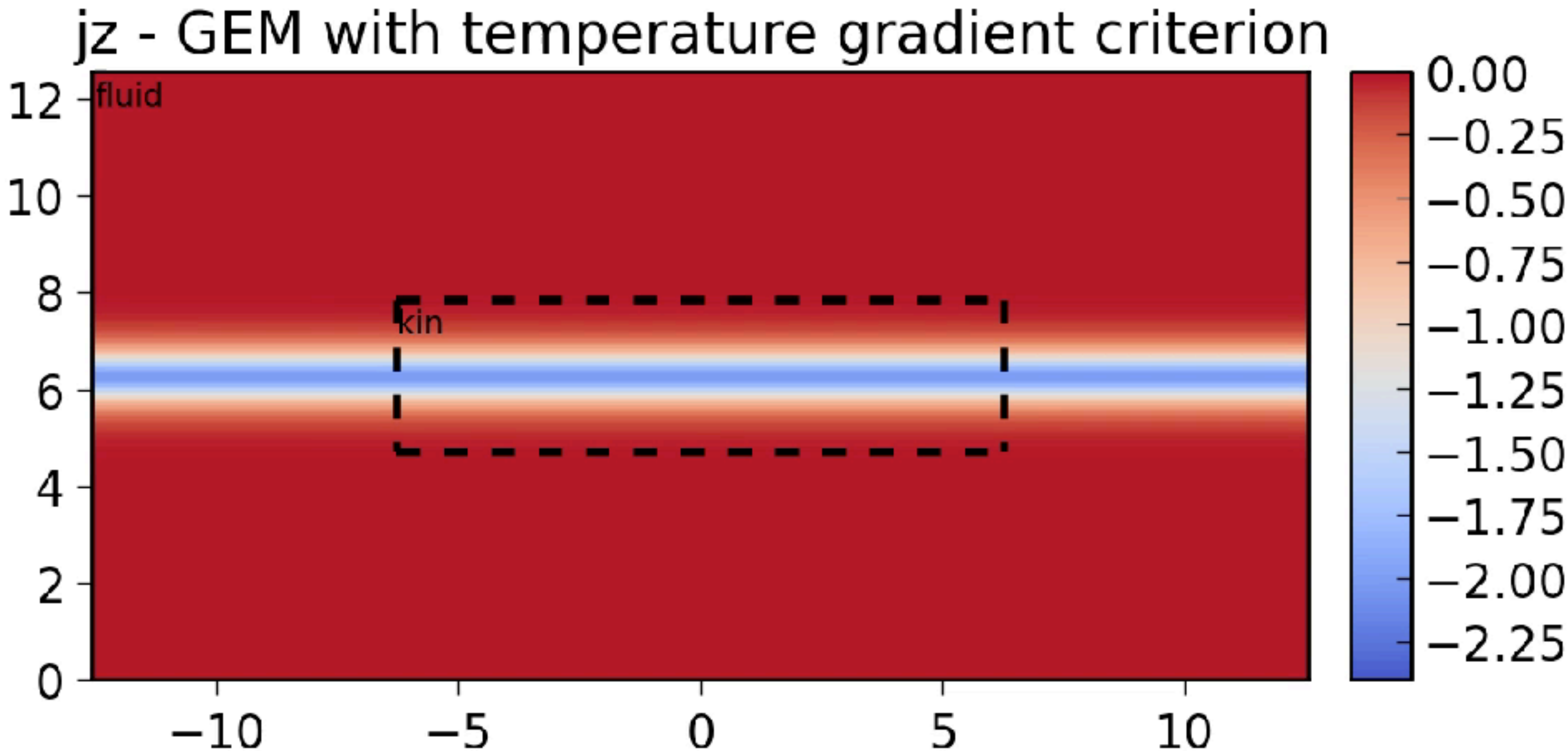
3d:

$$
\begin{aligned}
\mathrm{tr}\left(\partial_t \mathrm{Q}\right) = -\frac{3}{2} n \left(\frac{k_\mathrm{B}^2}{m}\right) \Big\{ & T_{xx}\partial_x T_{xx} + T_{yy}\partial_y T_{yy} + T_{zz}\partial_z T_{zz} \\
& + T_{xy}\left(\partial_y T_{xx} + \partial_x T_{yy}\right) + T_{yz}\left(\partial_z T_{yy} + \partial_y T_{zz}\right) + T_{xz}\left(\partial_z T_{xx} + \partial_x T_{zz}\right) \Big\}
\end{aligned}
$$

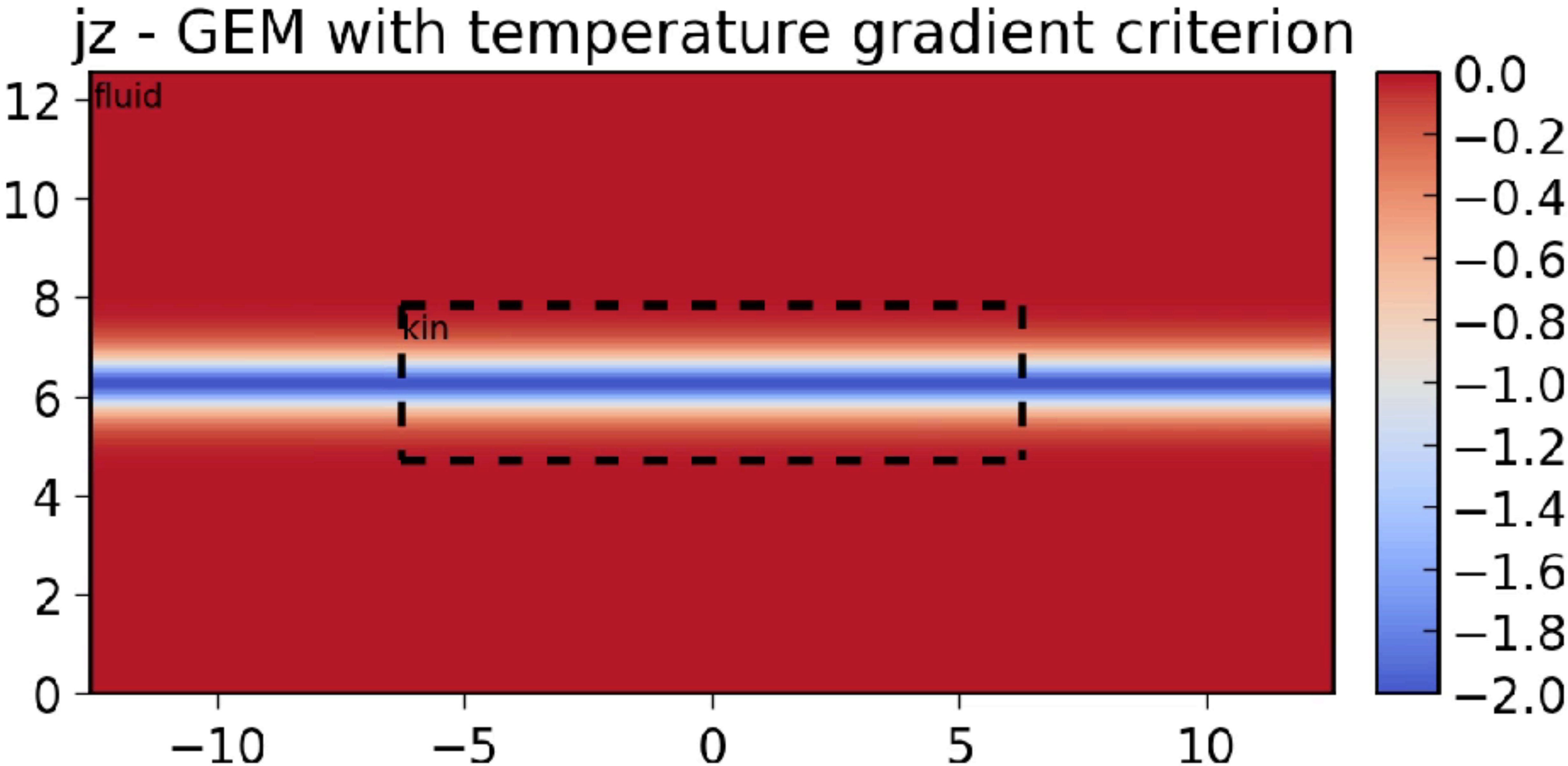
Assume isotropic temperature:

$$
\mathrm{tr}\left(\partial_t \mathrm{Q}\right) = -\frac{3}{2}\frac{k_\mathrm{B}}{m} p(\partial_x T + \partial_y T + \partial_z T),
$$

# Adaptive Multiphysics Simulations



# Adaptive Multiphysics Simulations



# Issues and ToDo's

- other models (Landau fluid?)
- better subcycling
- 3D
- Newton challenge
- shocks
- MHD

# 2D Simulations: GEM Setup

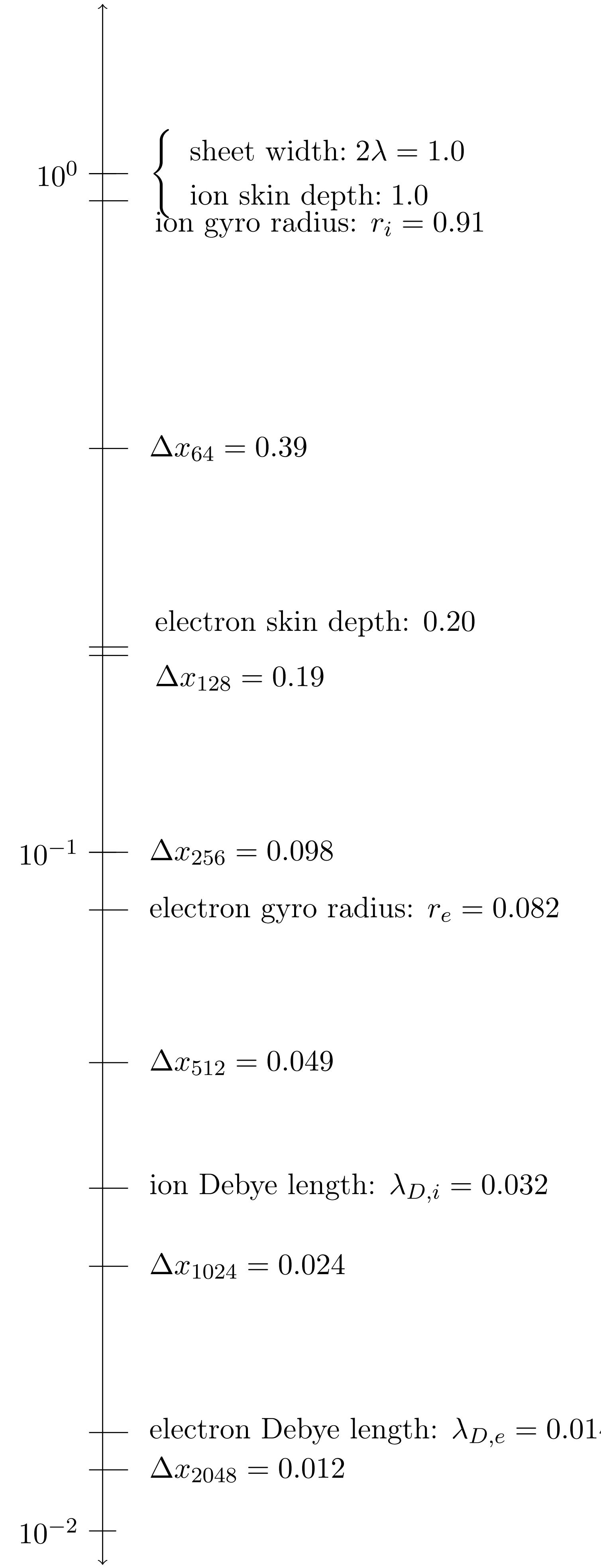
## Parameters:

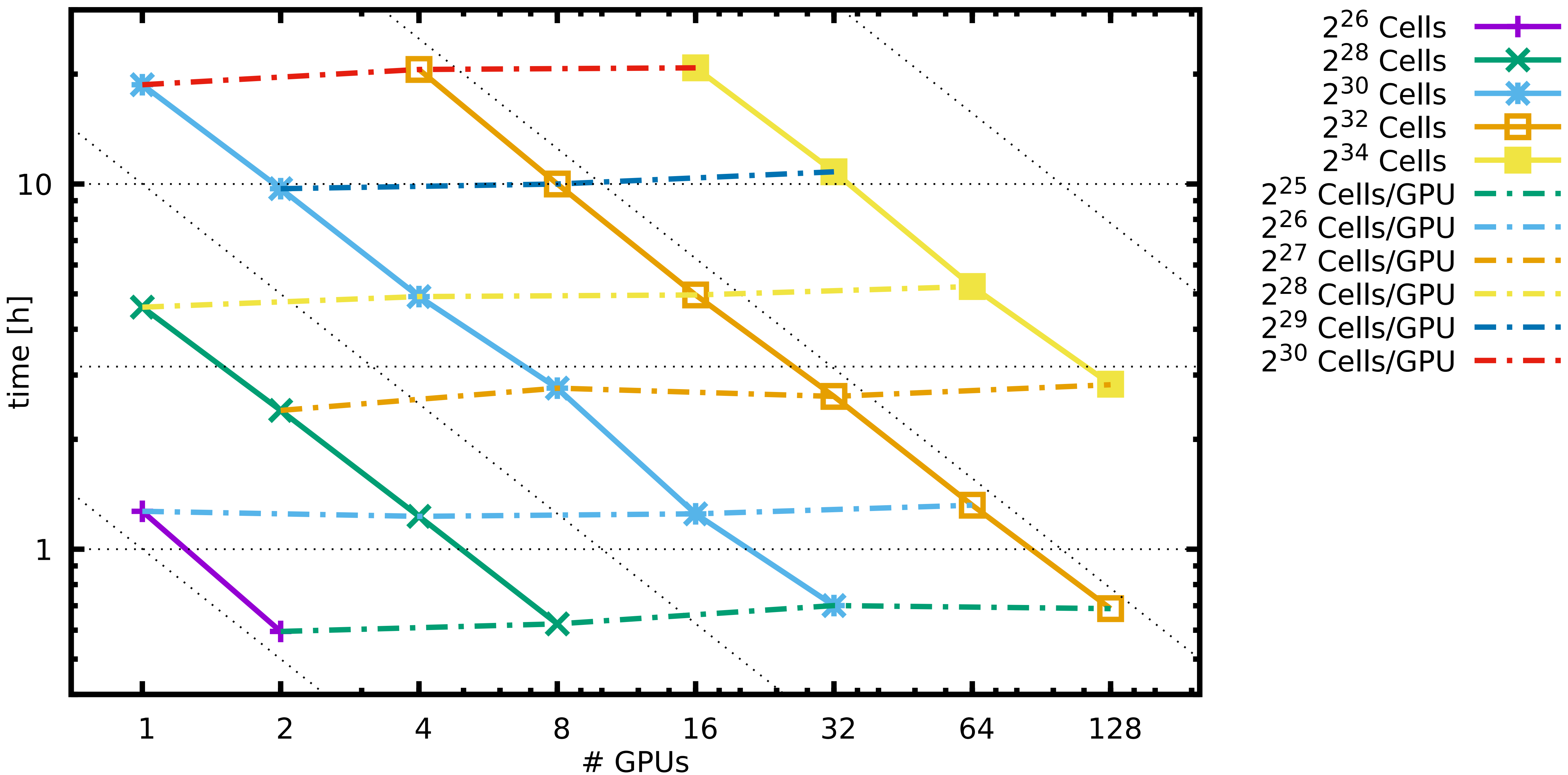
$\frac{m_i}{m_e} = 25$ | $\frac{T_i}{T_e} = \sqrt{\frac{m_i}{m_e}} = 5$ | $\lambda = 0.5$

$n_0 = 1$ | $n_\infty = 0.2$ | $B_0 = 1$

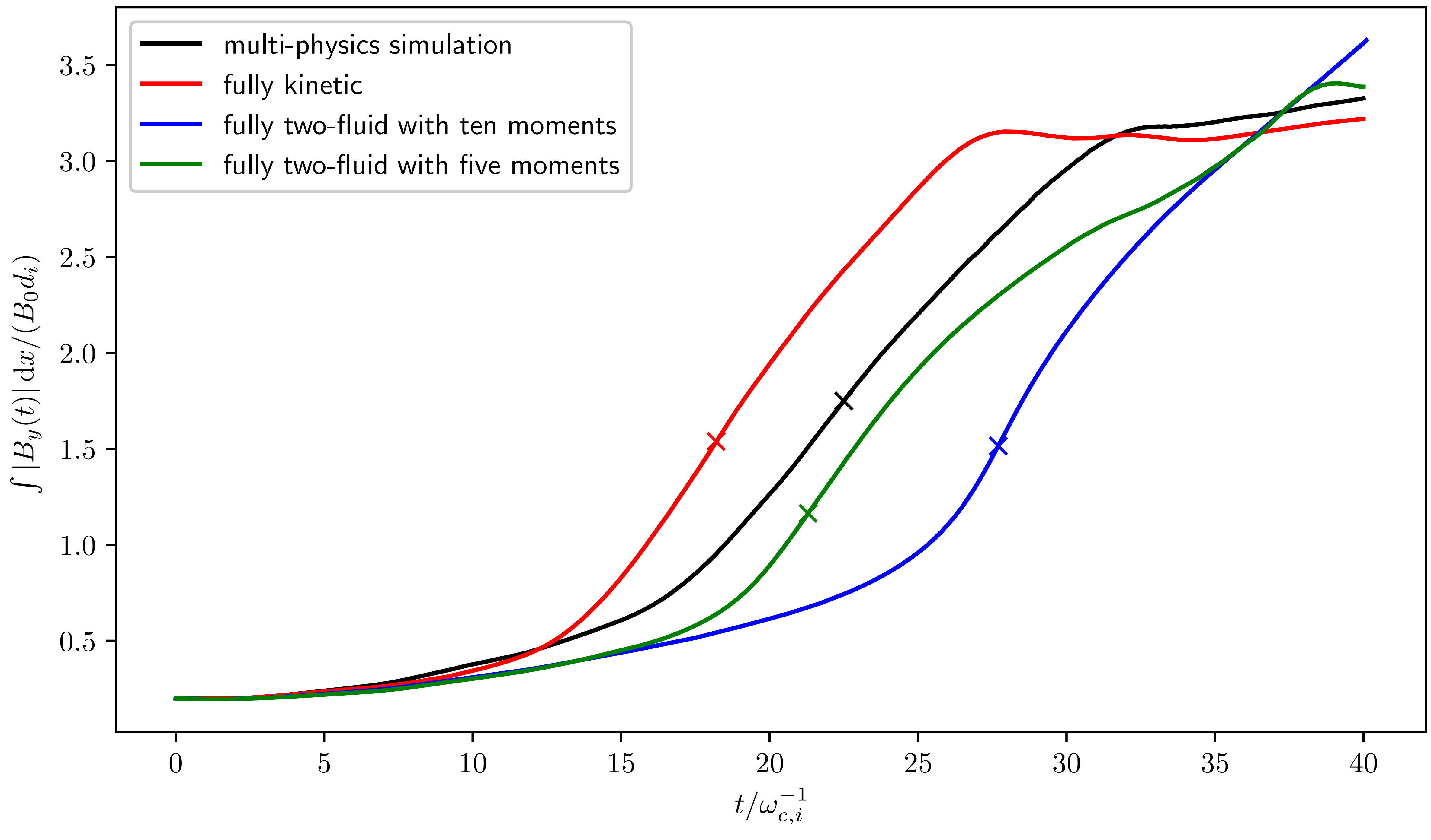
$\psi_0 = 0.1$ | $L_x = 8\pi$ | $L_y = 4\pi$

| Name | Expression | Electrons | Ions |
|---|---|---|---|
| thermal velocity | $v_{\text{th},s} = \sqrt{2T_{0,s}}\sqrt{\frac{m_i}{m_s}}$ | 2.0 | 0.91 |
| plasma frequency | $\omega_{\text{p},s} = c\sqrt{\frac{m_i}{m_s}}\sqrt{n_{0,s}}$ | 100 | 20 |
| gyro frequency | $\Omega_s = \frac{m_i}{m_s} B_0$ | 25 | 1 |
| Larmor radius | $r_s = \sqrt{2T_{0,s}}\sqrt{\frac{m_s}{m_i}}\frac{1}{B_0}$ | 0.082 | 0.91 |
| Debye length | $\lambda_{\text{D},s} = \frac{1}{c}\sqrt{\frac{T_{0,s}}{n_{0,s}}}$ | 0.014 | 0.032 |
| skin depth/inertial length | $\delta_s = \sqrt{\frac{m_s}{m_i}}\frac{1}{\sqrt{n_{0,s}}}$ | 0.2 | 1 |

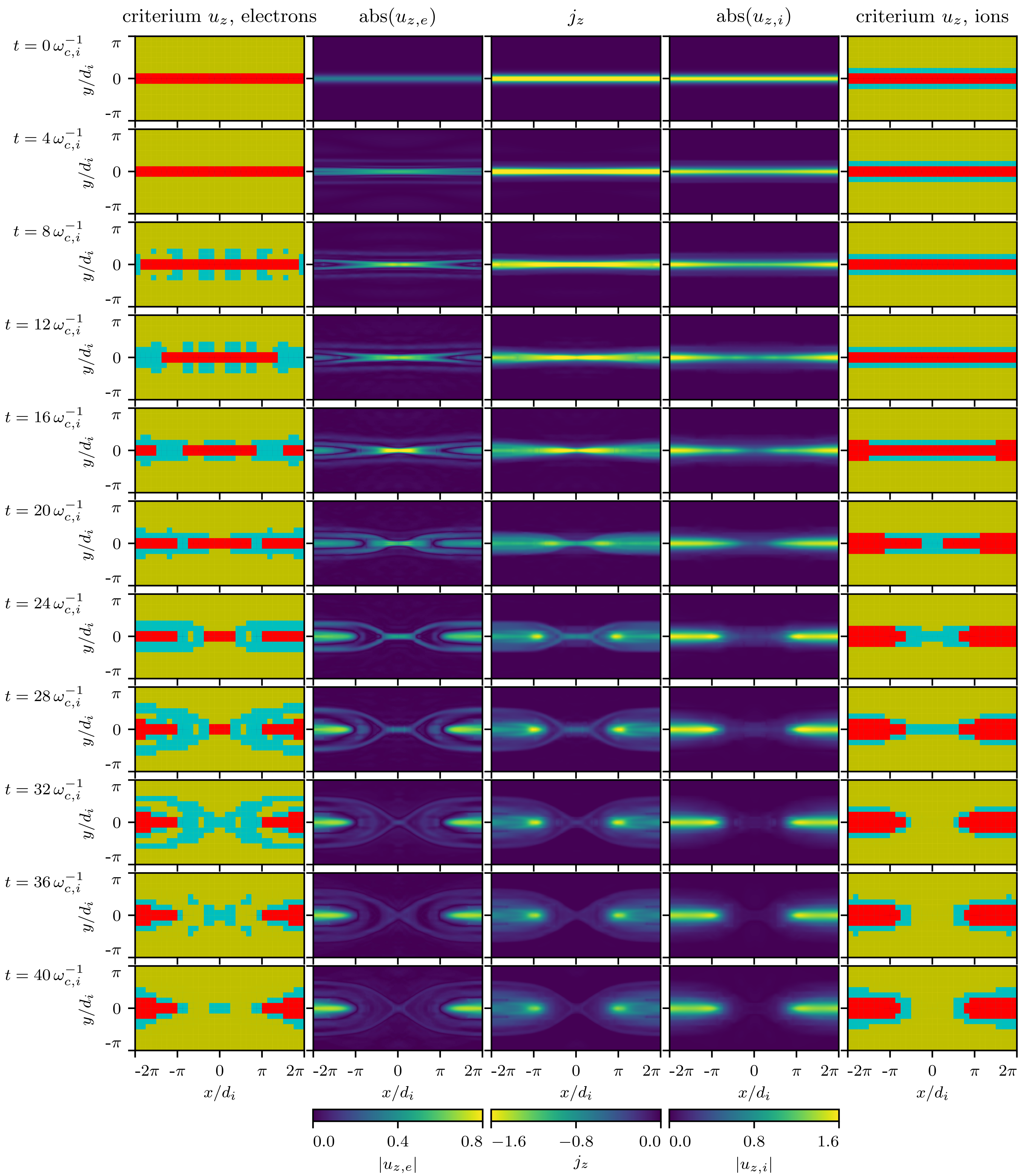




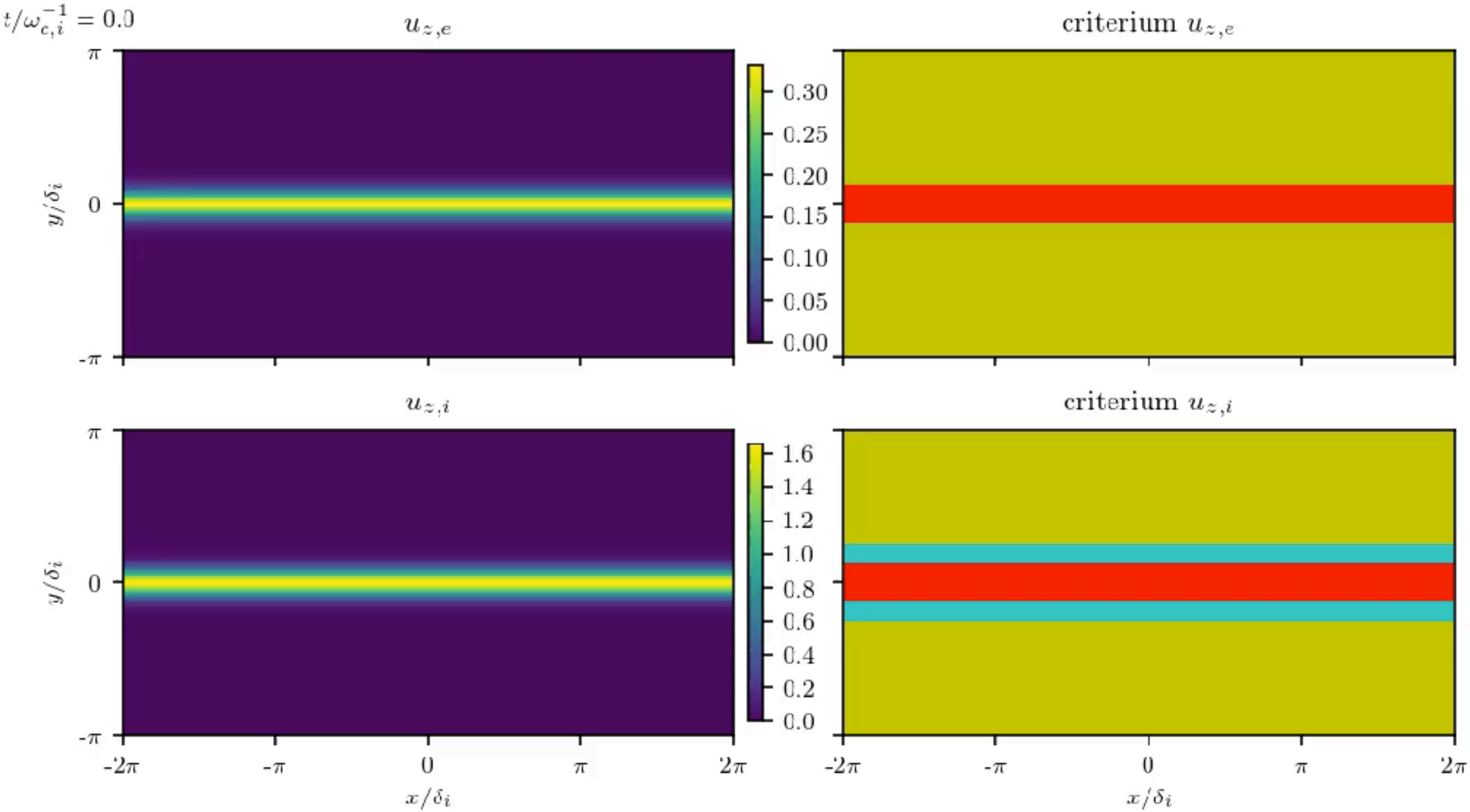
time [h]
10
1
1
2
4
8
16
32
64
128
# GPUs
$2^{26}$ Cells
$2^{28}$ Cells
$2^{30}$ Cells
$2^{32}$ Cells
$2^{34}$ Cells
$2^{25}$ Cells/GPU
$2^{26}$ Cells/GPU
$2^{27}$ Cells/GPU
$2^{28}$ Cells/GPU
$2^{29}$ Cells/GPU
$2^{30}$ Cells/GPU



multi-physics simulation
fully kinetic
fully two-fluid with ten moments
fully two-fluid with five moments
$\int |B_y(t)|\,\mathrm{d}x/(B_0 d_i)$
$t/\omega_{c,i}^{-1}$
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
5
10
15
20
25
30
35
40



criterium $u_z$, electrons
abs($u_{z,e}$)
$j_z$
abs($u_{z,i}$)
criterium $u_z$, ions
$t = 0\,\omega_{c,i}^{-1}$
$t = 4\,\omega_{c,i}^{-1}$
$t = 8\,\omega_{c,i}^{-1}$
$t = 12\,\omega_{c,i}^{-1}$
$t = 16\,\omega_{c,i}^{-1}$
$t = 20\,\omega_{c,i}^{-1}$
$t = 24\,\omega_{c,i}^{-1}$
$t = 28\,\omega_{c,i}^{-1}$
$t = 32\,\omega_{c,i}^{-1}$
$t = 36\,\omega_{c,i}^{-1}$
$t = 40\,\omega_{c,i}^{-1}$
$y/d_i$
π
0
-π
-2π
0
2π
$x/d_i$
0.0
0.4
0.8
$|u_{z,e}|$
−1.6
−0.8
0.0
$j_z$
0.0
0.8
1.6
$|u_{z,i}|$



$t/\omega_{c,i}^{-1} = 0.0$
$u_{z,e}$
criterium $u_{z,e}$
$u_{z,i}$
criterium $u_{z,i}$
$y/\delta_i$
$x/\delta_i$
π
0
-π
-2π
2π
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0

# Vision and advertisement: Tensor Networks

**Katharina Kormann**
A Semi-Lagrangian Vlasov Solver in Tensor Train Format
*SIAM J. Sci. Comput.*, 37(4), B613–B632

Lukas Einkemmer, Christian Lubich
A low-rank projector-splitting integrator for the Vlasov--Poisson equation
arXiv:1801.01103

matrix product states,
tensor networks

St. White 1992
U. Schollwöck 2005
J. I. Cirac, F. Verstraete, 2009
.
.
.
DMRG

tensor trains,
hierarchical Tucker

I. V. Oseledets 2008
W. Hackbusch 2009
L. Grasedyck 2013
.
.
.
ALS, MALS

Roman Orus *A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States* 2014

L. Grasedyck, D. Kressner, C. Tobler *A literature survey of low-rank tensor approximation technoques* 2013

2D: singular value decomposition SVD

diagonal

$$M^{m \times n} = U^{m \times m} \, \Sigma^{m \times n} \, (V^T)^{n \times n}$$

orthogonal matrix

2D: singular value decomposition SVD

diagonal

$$M^{m \times n} = U^{m \times r_1} \Sigma^{r_1 \times r_2} (V^T)^{r_2 \times n}$$

orthogonal matrix

only few singular values $r_1 \ll m$ , $r_2 \ll n$

tensors: example 4D

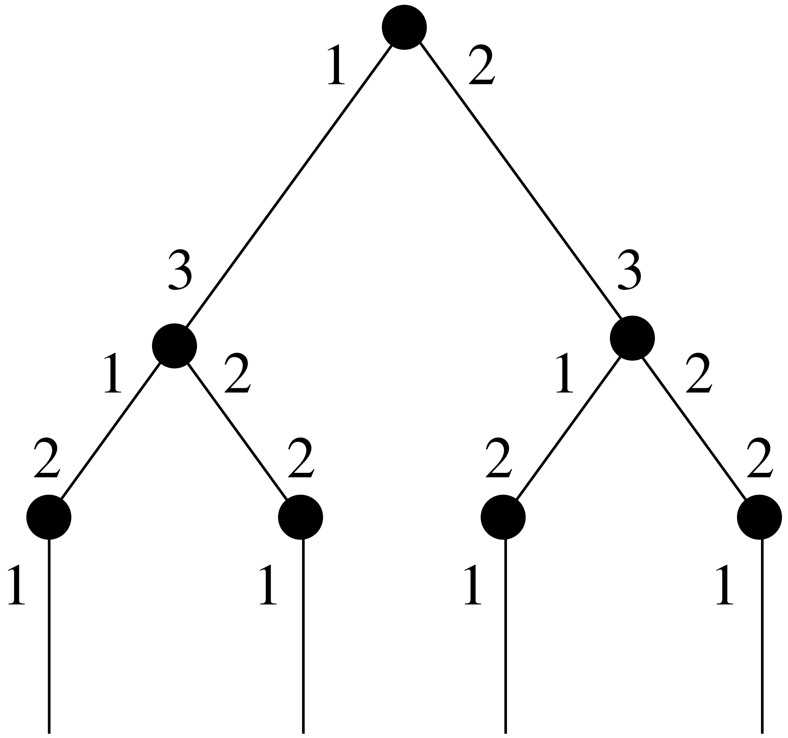
$$M^{d_1 \times d_2 \times d_3 \times d_4} \longrightarrow M^{d_1 \cdot d_2 \times d_3 \cdot d_4} = U_{34}^{d_3 d_4 \times r_{34}} \, U_{12}^{d_1 d_2 \times r_{12}} \, B_{1234}^{r_{34} \times r_{12}}$$

$$M = (U_{34} \otimes U_{12}) B_{1234}$$

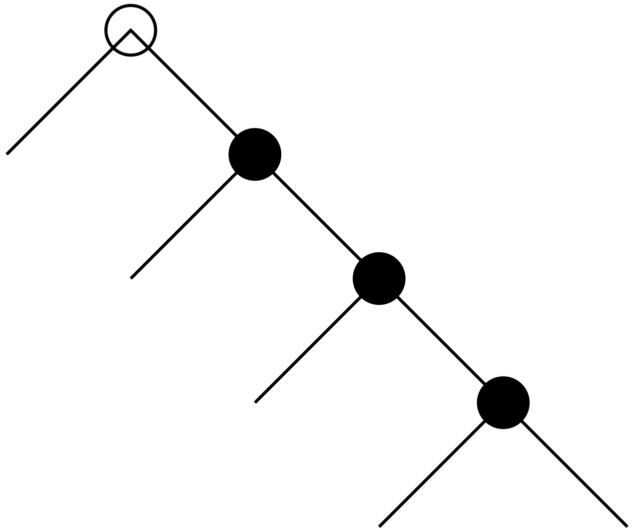
$$U_{12} = (U_2 \otimes U_1) B_{12} \qquad U_{34} = (U_4 \otimes U_3) B_{34}$$

$$M = (U_4 \otimes U_3 \times U_2 \otimes U_1)(B_{34} \times B_{12}) B_{1234}$$

hierarchical Tucker HT




tensor train TT



Now: not parallel, electrostatic with constant guide field

Master Student Florian Allmann-Rahn: parallelization with domain decomposition
in his Phd: generalisation to Maxwell

# Lot's of things to do

## Thank you

Rieke M, Trost T, Grauer R.
Coupled Vlasov and two-fluid codes on GPUs.
*Journal of Computational Physics* 283 (2015) 436–452

Lautenbach S., Grauer R.
Multiphysics simulations of collisionless plasmas
arXiv:1805.05698 (2018)