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Institute for Theoretical Physics I, Faculty of Physics and Astronomy
Numerics Group, Faculty of Mathematics

Multi-Physics Simulations in Space Plasma Physics

Conceptualization and Implementation with the `muphyII` framework

Simon Lautenbach

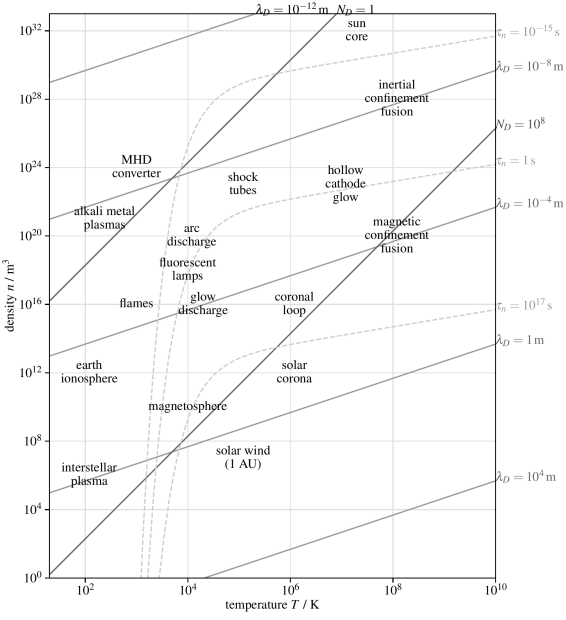
15th International Symposium for Space Simulations *August 3, 2024*

Session Outline

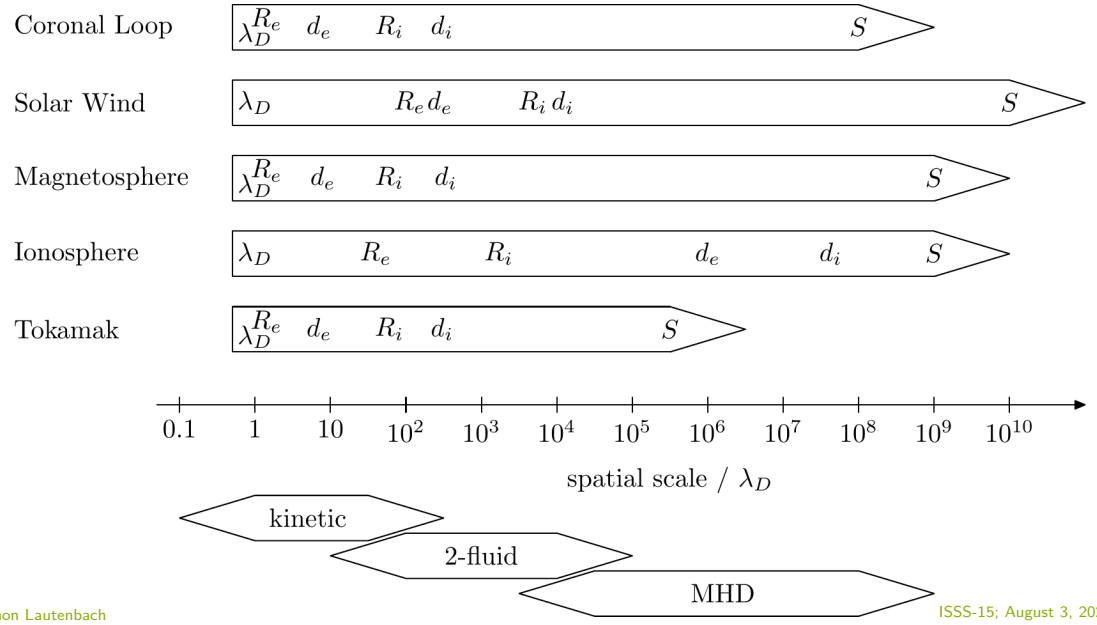
- Multi-Physics Plasma Modelling
  - Motivation
  - Plasma Physics Models
  - Model Implementations
  - Model Coupling
- Hands-on: Multi-Physics Plasma Modelling with the muphy2 framework
  - muphy2 Framework Implementation
  - Simple Examples

Multi-Physics Plasma Modelling

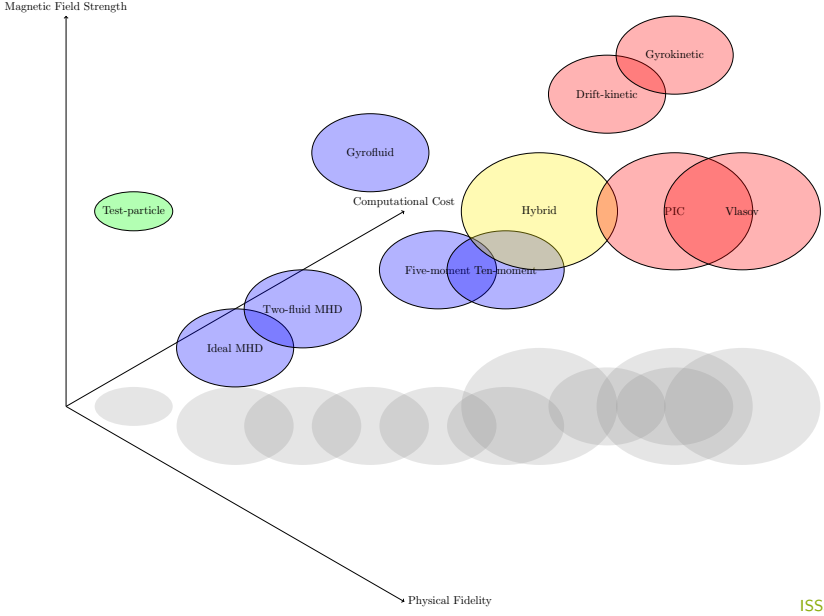
Space Plasma Parameters



Separation of Scales



The Range of Plasma Models



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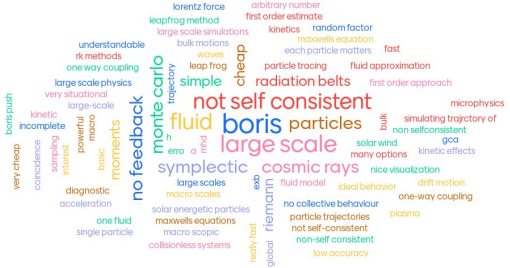
Mentimeter

What springs to your mind about test particle methods?

114 responses



Test-particle Methods

Evolve particle trajectories in prescribed fields

Advantages:

- Extremely computationally efficient
- Useful for studying single-particle dynamics
- Can provide insights into particle behavior in complex field geometries

Disadvantages:

- No self-consistency (fields don't evolve with particles)
- Misses collective effects
- Cannot capture plasma self-organization or instabilities

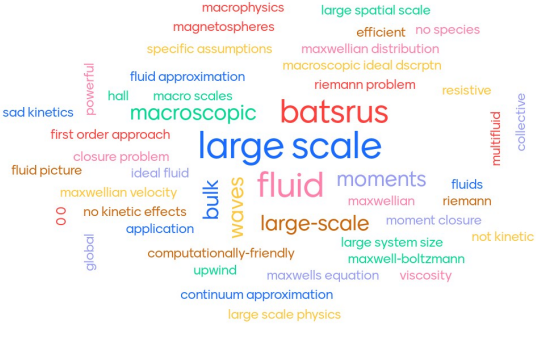
Common Improvements:

- Incorporate simple field solvers for partial self-consistency

Mentimeter

What springs to your mind about MHD?

64 responses



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Magnetohydrodynamics

Single-fluid model treating plasma as a perfectly conducting fluid

Advantages:

- Computationally efficient for large-scale phenomena
- Captures basic plasma dynamics and equilibria
- Well-suited for studying macroscopic instabilities

Disadvantages:

- Ignores kinetic effects and separate species dynamics
- Assumes infinite conductivity
- Cannot resolve small-scale phenomena or high-frequency waves

Common Improvements:

- Include resistivity for finite conductivity effects
- Add Hall terms for better small-scale physics
- Incorporate two-fluid effects for improved species separation

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Mentimeter

What springs to your mind about multi-moment fluid models?

47 responses

26

Multi-moment two-fluid

Evolves density, momentum, and energy for each species

Advantages:

- Captures separate evolution of electron and ion fluids
- Includes basic kinetic effects through heat flux
- More complete than standard two-fluid MHD

Disadvantages:

- Limited description of pressure tensor anisotropy
- Misses higher-order kinetic effects
- Closure problem for heat flux

Common Improvements:

- Add higher-order moments for improved energy transport modeling
- Develop improved closure schemes based on kinetic theory
- Couple with reduced kinetic models for specific particle populations

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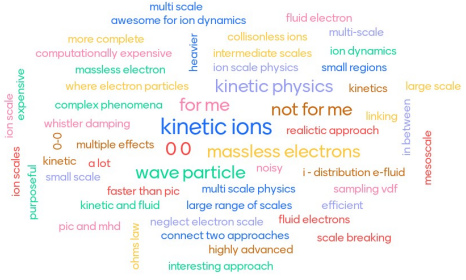
Mentimeter

What springs to your mind about hybrid models?

62 responses



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Hybrid

Kinetic ions with fluid electrons

Kinetic ions with fluid electrons using full Maxwell equations

Advantages:

- Captures ion kinetic effects
- More efficient than full kinetic
- Good for ion-scale phenomena

Disadvantages:

- Misses electron kinetic effects
- Challenging to implement efficiently
- Limited by fluid electron description

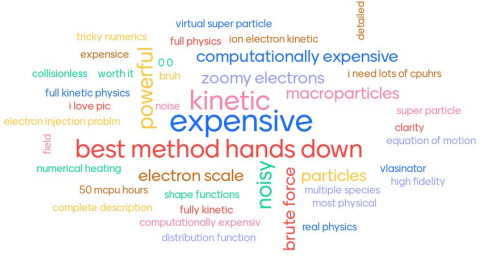
Common Improvements:

- Implement delta-f method for electrons to capture some kinetic effects
- Couple with local fully kinetic solvers in regions of interest
- Develop improved electron fluid models

Mentimeter

What springs to your mind about PIC models?

65 responses



Particle-In-Cell

Fully kinetic particle-in-cell method coupled with Maxwell's equations

Advantages:

- Captures full range of kinetic phenomena
- Intuitive particle representation
- Flexible for complex geometries

Disadvantages:

- Computationally expensive
- Suffers from numerical noise
- Challenging for high dynamic range problems

Common Improvements:

- Implement adaptive particle weighting to reduce noise
- Develop implicit methods for improved efficiency
- Couple with reduced models for multi-scale simulations

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Mentimeter

What springs to your mind about continuous Vlasov models?

47 responses

30

Vlasov

Solves Vlasov equation for distribution function coupled with Maxwell's equations

Advantages:

- Fully kinetic with low numerical noise
- Captures full range of plasma phenomena
- Excellent conservation properties

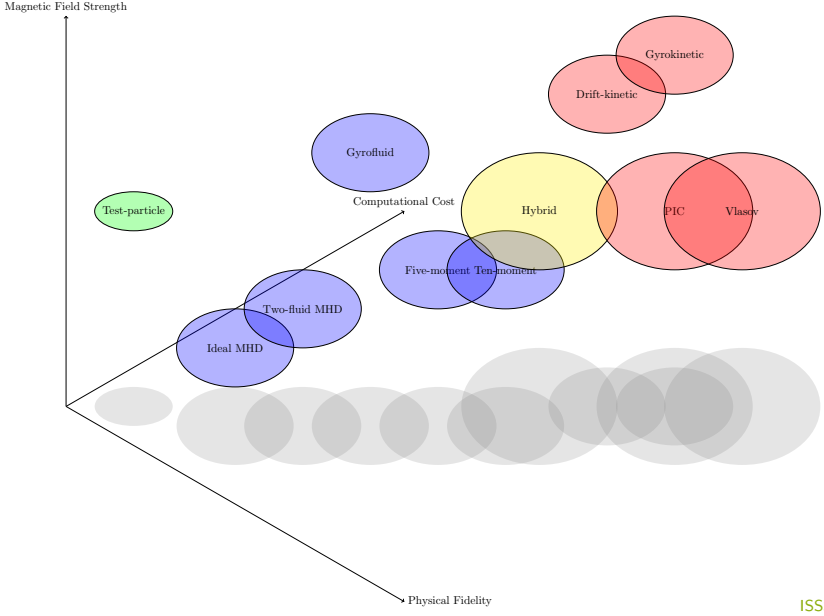
Disadvantages:

- Extremely computationally expensive
- Challenging to implement efficiently
- Suffers from curse of dimensionality

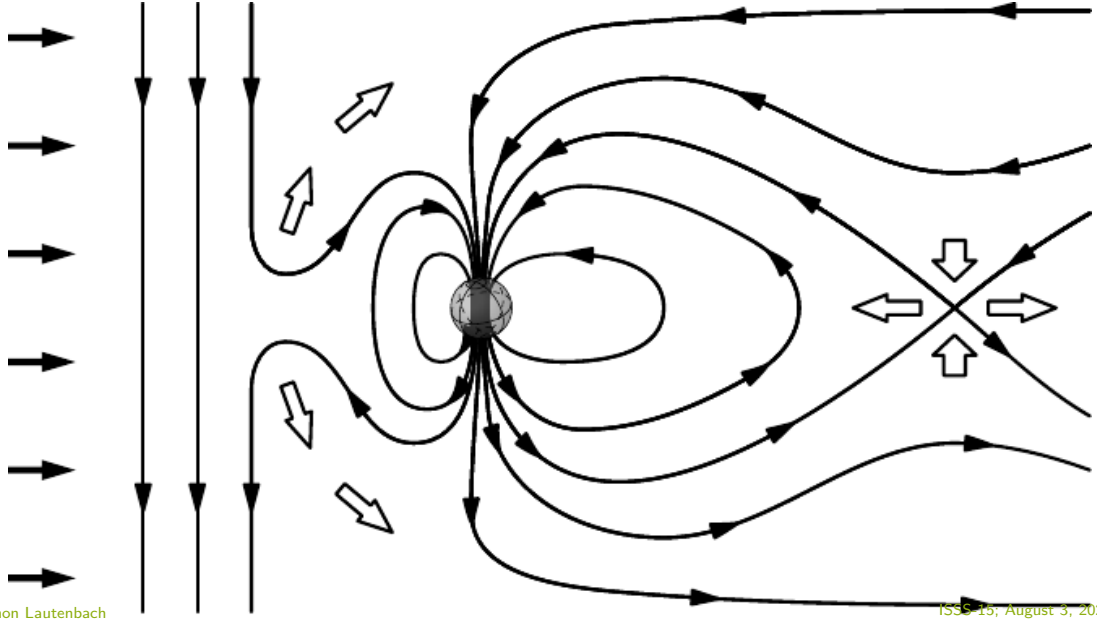
Common Improvements:

- Implement adaptive mesh refinement in phase space
- Develop semi-Lagrangian methods for improved efficiency
- Couple with reduced models for multi-scale simulations

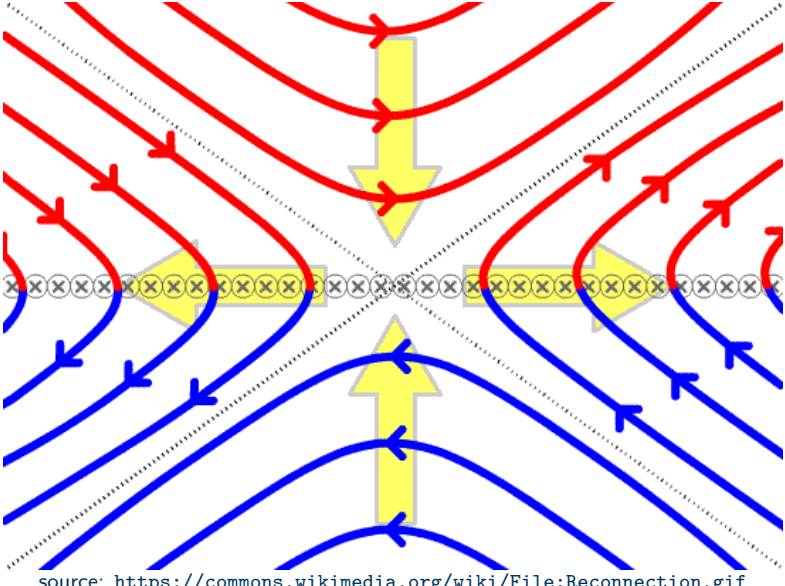
The Range of Plasma Models



Localization of 'Activity'

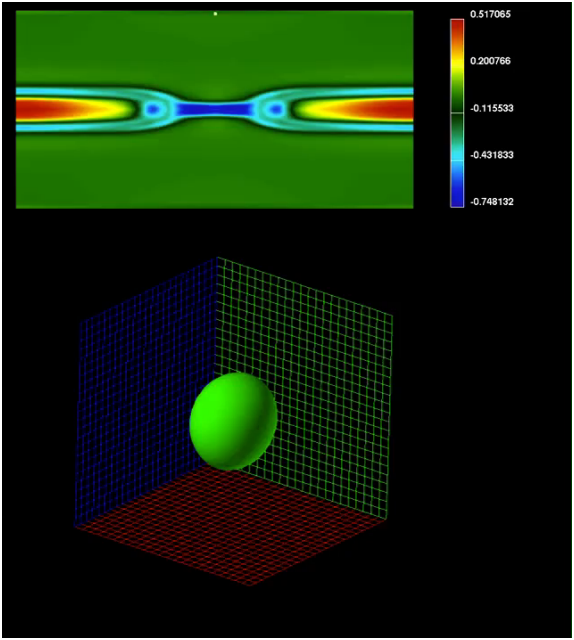


Magnetic Reconnection

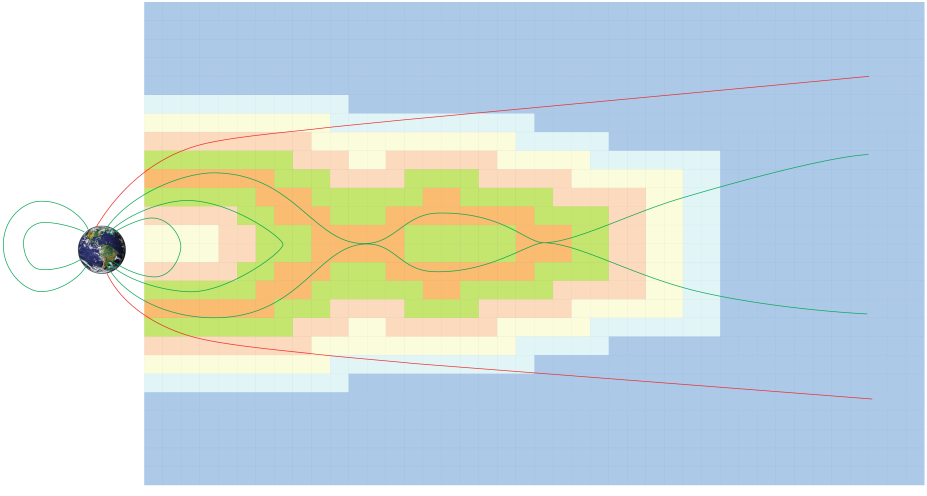


source: https://commons.wikimedia.org/wiki/File:Reconnection.gif
author: ChamouJacoN

Magnetotail Reconnection VDF



Multi-Physics Approach



Kinetic-Fluid Coupling: Histroy

Early efforts to couple kinetic Boltzmann descriptions to fluid models include

- Patrick Le Tallec and François Mallinger (1997). "Coupling Boltzmann and Navier–Stokes Equations by Half Fluxes". In: *Journal of Computational Physics* 136.1, pp. 51–67
- S. Tiwari and A. Klar (1998). "An adaptive domain decomposition procedure for Boltzmann and Euler equations". In: *Journal of Computational and Applied Mathematics* 90.2, pp. 223–237
- Stéphane Dellacherie (2003). "Kinetic-Fluid Coupling in the Field of the Atomic Vapor Laser Isotopic Separation: Numerical Results in the Case of a Monospecies Perfect Gas". In: *AIP Conference Proceedings* 663.1, pp. 947–956
- Pierre Degond, Giacomo Dimarco, and Luc Mieussens (2010). "A multiscale kinetic–fluid solver with dynamic localization of kinetic effects". In: *Journal of Computational Physics* 229.13, pp. 4907–4933
- Thierry Goudon et al. (2013). "Asymptotic-preserving schemes for kinetic-fluid modeling of disperse two-phase flows". In: *Journal of Computational Physics* 246, pp. 145–164
- Sudarshan Tiwari et al. (2013). "Coupled solution of the Boltzmann and Navier–Stokes equations in gas–liquid two phase flow". In: *Computers & Fluids* 71, pp. 283–296

Kinetic-Fluid Coupling: Histroy

In the context of space plasma physics: Static kinetic regions:

- Fixed-region 1D MHD-PIC coupling:
  Tooru Sugiyama and Kanya Kusano (2007). "Multi-scale plasma simulation by the interlocking of magnetohydrodynamic model and particle-in-cell kinetic model". In: *Journal of Computational Physics* 227.2, pp. 1340–1352
- Two-way HMHD-PIC interface coupling using iPIC3D and BATS-R-US:
  Lars K. S. Daldorff et al. (2014). "Two-way coupling of a global Hall magnetohydrodynamics model with a local implicit particle-in-cell model". In: *Journal of Computational Physics* 268, pp. 236–254
- Two-way MHD-PIC interface coupling using iPIC3D and MPI-AMRVAC:
  K. D. Makwana, R. Keppens, and G. Lapenta (2017). "Two-way coupling of magnetohydrodynamic simulations with embedded particle-in-cell simulations". In: *Computer Physics Communications* 221, pp. 81–94
- One-way MHD-iPIC3D coupling in global simulations:
  Raymond J. Walker et al. (2019). "Embedding particle-in-cell simulations in global magnetohydrodynamic simulations of the magnetosphere". In: *Journal of Plasma Physics* 85.1, p. 905850109
  Giovanni Lapenta et al. (2020). "Multiscale MHD-Kinetic PIC Study of Energy Fluxes Caused by Reconnection". In: *Journal of Geophysical Research: Space Physics* 125.3, e2019JA027276

Kinetic-Fluid Coupling: Histroy

In the contect of space plasma physics: Adaptive kinetic regions:

- Adaptive two-way MHD-PIC (AMPS, BATS-R-US)
  Yinsi Shou et al. (2021). "Magnetohydrodynamic with Adaptively Embedded Particle-in-Cell model: MHD-AEPIC". In: *Journal of Computational Physics* 446, p. 110656
- Adaptive two-way MHD-PIC (FLEKS, BATS-R-US) global simulations
  Xiantong Wang, Yuxi Chen, and Gábor Tóth (2022a). "Global Magnetohydrodynamic Magnetosphere Simulation With an Adaptively Embedded Particle-In-Cell Model". In: *Journal of Geophysical Research: Space Physics* 127.8, e2021JA030091
  Xiantong Wang, Yuxi Chen, and Gábor Tóth (2022b). "Simulation of Magnetospheric Sawtooth Oscillations: The Role of Kinetic Reconnection in the Magnetotail". In: *Geophysical Research Letters* 49.15, e2022GL099638

Kinetic-Fluid Coupling: Histroy

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Two-fluid/Maxwell and kinetic coupling :

- One-way bulk coupling two-fluid/Maxwell with PIC:
  Stefano Markidis et al. (2014). "The Fluid-Kinetic Particle-in-Cell method for plasma simulations". In: *Journal of Computational Physics*. Frontiers in Computational Physics 271, pp. 415–429
- Two-way coupling two-fluid/Maxwell with Vlasov M. Rieke, T. Trost, and R. Grauer (2015). "Coupled Vlasov and two-fluid codes on GPUs". In: *Journal of Computational Physics* 283, pp. 436–452
- Adaptive two-way coupling two-fluid/Maxwell with Vlasov
  Simon Lautenbach and Rainer Grauer (2018). "Multiphysics Simulations of Collisionless Plasmas". In: *Frontiers in Physics* 6
- Application to mid-size problems
  F. Allmann-Rahn et al. (2024). "The *muphy*II code: Multiphysics plasma simulation on large HPC systems". In: *Computer Physics Communications* 296, p. 109064

Two-Way MHD-PIC Coupling

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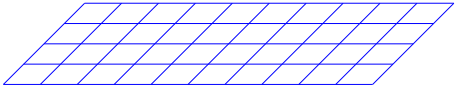
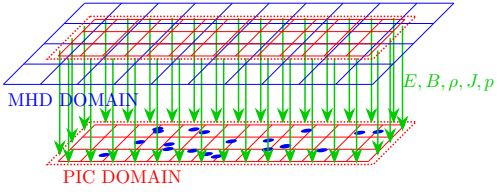
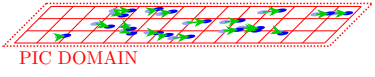
1. ADVANCE MHD SIMULATION $t^n \rightarrow t^{n+1}$



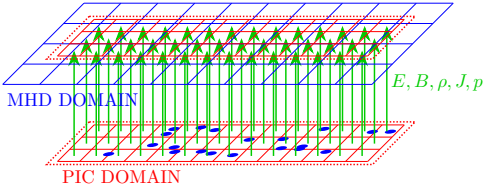
2. PROVIDE BOUNDARY CONDITIONS TO PIC REGION



3. ADVANCE PIC SIMULATION $t^n \rightarrow t^{n+1}$



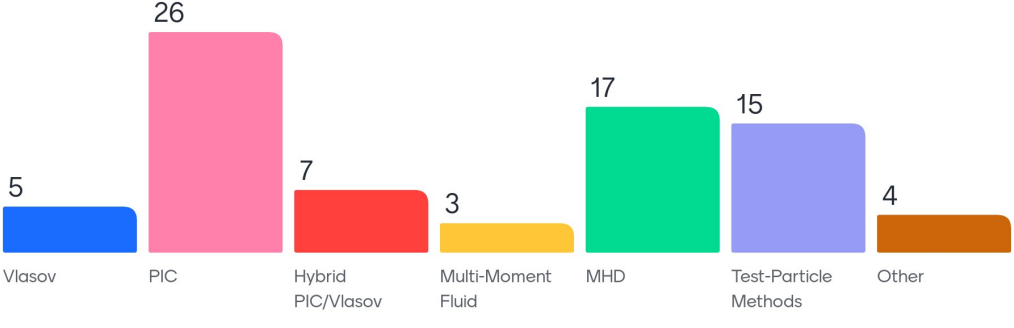
4. CORECT MHD SIMULATION WITH PIC REGION VALUES



Plasma Model Equations

Mentimeter

Which models do you use in your research?



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Kinetic Model (Vlasov-Maxwell)

The *Vlasov equation* describes the evolution of a distribution $f_s(\mathbf{x}, \mathbf{v}, t)$ of interacting charged particles:

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

The electromagnetic fields are governed by *Maxwell's equations*:

$$\partial_t \mathbf{E} = c^2(\nabla \times \mathbf{B} - \mu_0 \mathbf{J}) \qquad \nabla \cdot \mathbf{E} = \frac{\rho_c}{\varepsilon_0}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E} \qquad \nabla \cdot \mathbf{B} = 0$$

Fluid Model ("10-moment" Fluid-Maxwell)

The moments $\int v^{(k)} \langle \cdot \rangle \mathrm{d}v$ of the Vlasov equation constitute the *fluid moment hierarchy*

$$\partial_t \mu_s^{(k)} = -\nabla \cdot \mu_s^{(k+1)} + \frac{q_s}{m_s} \operatorname{sym}\left(\mu_s^{(k-1)} \mathbf{E} + \mu_s^{(k)} \times \mathbf{B} \right)$$

where the electromagnetic fields are governed by *Maxwell's equations*.

The first three moments are given by the following ten equations:

$$\begin{aligned} \partial_t n_s &= -\nabla \cdot (n_s \mathbf{u}_s) \\ m_s \partial_t (n_s \mathbf{u}_s) &= n_s q_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) - \nabla \cdot \mathbb{P}_s \\ \partial_t \mathbb{P}_s &= q_s \left(n_s \operatorname{sym}[\mathbf{u}_s \otimes \mathbf{E}] + \frac{1}{m_s} \operatorname{sym}[\mathbb{P}_s \times \mathbf{B}] \right) - \nabla \cdot \mathbb{Q}_s \end{aligned}$$

To close the hierarchy, an expression for the heat flux divergence $\nabla \cdot \mathbb{Q}_s$ has to be found.

10-moment Fluid Closure

- Hammet-Perkins 1990:

$$\mathbb{Q}_s = -n_{0,s}\frac{2}{\sqrt{\pi}}v_{\mathrm{th},s}\mathcal{H}\mathbb{T}_s$$

- Snyder-Hammett-Dorland 1997:

$$\mathbb{Q}_{\parallel,s} = -n_{0,s}\frac{2}{\sqrt{\pi}}v_{\mathrm{th},\parallel,s}\mathcal{H}\mathbb{T}_{\parallel,s}$$

$$\mathbb{Q}_{\perp,s} = -n_{0,s}\frac{1}{\sqrt{\pi}}v_{\mathrm{th},\parallel,s}\mathcal{H}\left(T_{\perp,s} - T_{\perp,0,s}\left(1 - \frac{T_{\perp,0,s}}{T_{\parallel,0,s}}\right)\frac{|\mathbf{B}|}{B_0}\right)$$

- Sulem-Passot 2015

$$\mathbb{Q}_{\parallel,s} = -n_{0,s}\frac{2}{\sqrt{\pi}}v_{\mathrm{th},\parallel,s}\mathcal{H}\mathbb{T}_{\parallel,s}$$

$$\mathbb{Q}_{\perp,s} = -n_{0,s}\left(1 - \frac{T_{\parallel,0,s}}{T_{\perp,0,s}}\right)\frac{\hat{\mathbf{b}}}{\Omega_e m_e}\cdot\left(\nabla\times\frac{\mathbf{B}}{B_0}\right)$$
$$- n_{0,s}\frac{1}{\sqrt{\pi}}v_{\mathrm{th},\parallel,s}\mathcal{H}\left(T_{\perp,s} - T_{\perp,0,s}\left(1 - \frac{T_{\perp,0,s}}{T_{\parallel,0,s}}\right)\frac{|\mathbf{B}|}{B_0}\right)$$

10-moment Fluid Closure

To approach the Hilbert transform $\mathcal{H} \sim ik_\parallel/|k_\parallel|$, it is (conceptually) decomposed into $ik_\parallel \sim \partial_\parallel$ and $1/|k_\parallel|$. For the latter, approximations include:

- Sharma-Hammett-Quataert-Stone 2006: $1/|k_\parallel| := 1/k_L = \text{const.}$
- Passot-Henri-Laveder-Sulem 2014: $1/|k_\parallel| := \mathcal{F}^{-1}\left(1/\sqrt{\mathbf{k}\cdot\langle\hat{\mathbf{b}}\hat{\mathbf{b}}\rangle\cdot\mathbf{k}}\right)$

Another caveat lies in the generalization of the parallel derivative.
Options include a Laplacian diffusion characteristic:

$$\nabla\cdot\mathbb{Q}_s = -\frac{\chi}{k_{L,s}} n_s v_{\text{th},s}\nabla^2\mathbb{T}_s$$

or a symetrization of the temperature gradient:

$$\nabla\cdot\mathbb{Q}_s = -\frac{\chi}{k_{L,s}} n_s v_{\text{th},s}\nabla\cdot\text{sym}\,\nabla\mathbb{T}_s$$

Hybrid Model (Vlasov-Fluid-Maxwell)

Combine kinetic ion physics with fluid electron modeling and Maxwell's equations:

$$\partial_t f_i = -\mathbf{v}_i \cdot \nabla_{\mathbf{x}} f_i - \frac{q_i}{m_i} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_i$$

$$\partial_t n_e = -\nabla \cdot (n_s \mathbf{u}_e)$$

$$m_e \partial_t (n_e \mathbf{u}_e) = n_e q_e (\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) - \nabla \cdot \mathbb{P}_e$$

$$\partial_t \mathbb{P}_e = q_e \left(n_e \, \mathrm{sym}[\mathbf{u}_e \otimes \mathbf{E}] + \frac{1}{m_e} \mathrm{sym}[\mathbb{P}_e \times \mathbf{B}] \right) - \nabla \cdot \mathbb{Q}_e$$

$$\nabla \cdot \mathbb{Q}_e = -\frac{\chi}{k_{L,e}} n_e v_{\mathrm{th},e} \nabla^2 \mathbb{T}_e$$

$$\partial_t \mathbf{E} = c^2 (\nabla \times \mathbf{B} - \mu_0 \mathbf{J}) \qquad \nabla \cdot \mathbf{E} = \frac{\rho_c}{\varepsilon_0}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E} \qquad \nabla \cdot \mathbf{B} = 0$$

Isotropic Fluid ("5-moment" Fluid-Maxwell)

In the fluid equations, assume isotropy and vanishing heat flux

$$\begin{aligned}
\partial_t n_s &= -\nabla \cdot (n_s \mathbf{u}_s) \\
m_s \partial_t (n_s \mathbf{u}_s) &= n_s q_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) - \nabla \cdot \mathcal{P}_s \\
\partial_t \mathcal{E}_s &= q_s n_s \mathbf{u}_s \cdot \mathbf{E} - \frac{1}{N} \nabla \cdot \left(\mathbf{u}_s ((N+2)\mathcal{E}_s - m_s n_s u_s^2) \right)
\end{aligned}$$

$$\begin{aligned}
\partial_t \mathbf{E} &= c^2 (\nabla \times \mathbf{B} - \mu_0 \mathbf{J}) & \nabla \cdot \mathbf{E} &= \frac{\rho_c}{\varepsilon_0} \\
\partial_t \mathbf{B} &= -\nabla \times \mathbf{E} & \nabla \cdot \mathbf{B} &= 0
\end{aligned}$$

Magnetohydrodynamic Fluid (MHD-Ohm)

$\partial_t \mathbf{E}/c^2 \ll \mu_0 \mathbf{J}$ $\Rightarrow$ Maxwell's equations become

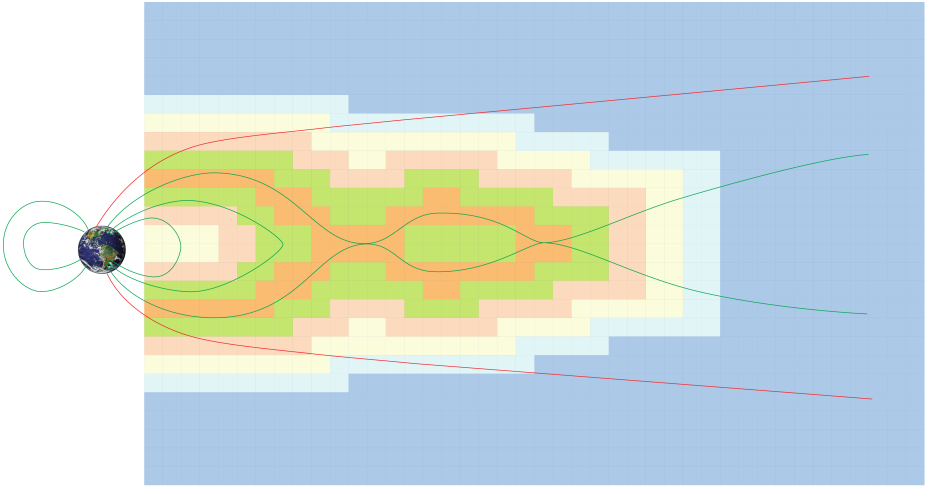
$$\mathbf{J} = \frac{1}{\mu_0} \nabla \times \mathbf{B}$$
$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Need generalized Ohm's law

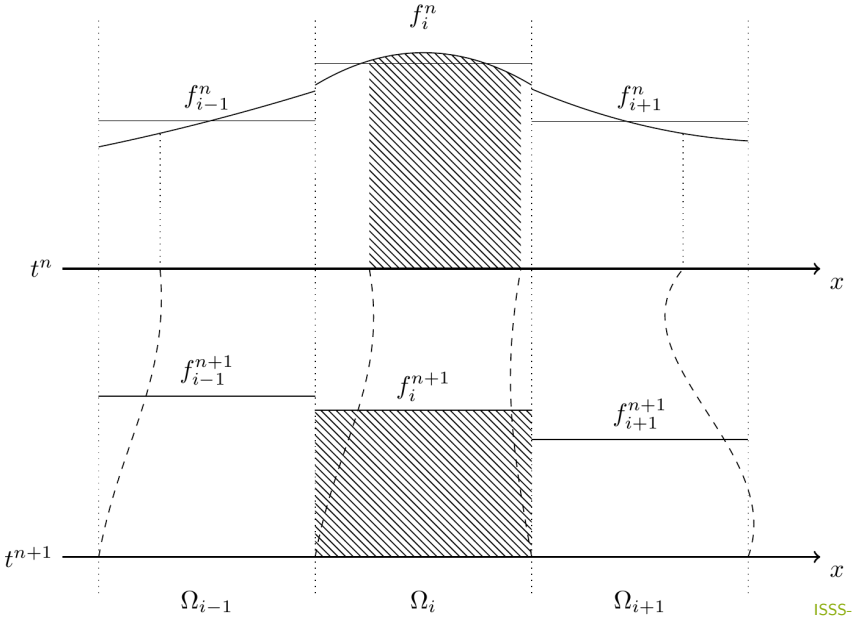
$$\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \frac{1}{q_0 n} \mathbf{J} \times \mathbf{B} - \frac{1}{q_0 n} \nabla \cdot \mathbb{P}_e - \frac{m_e}{q_0} \mathrm{d}_t \mathbf{u}_e$$

Couling Plasma Solvers

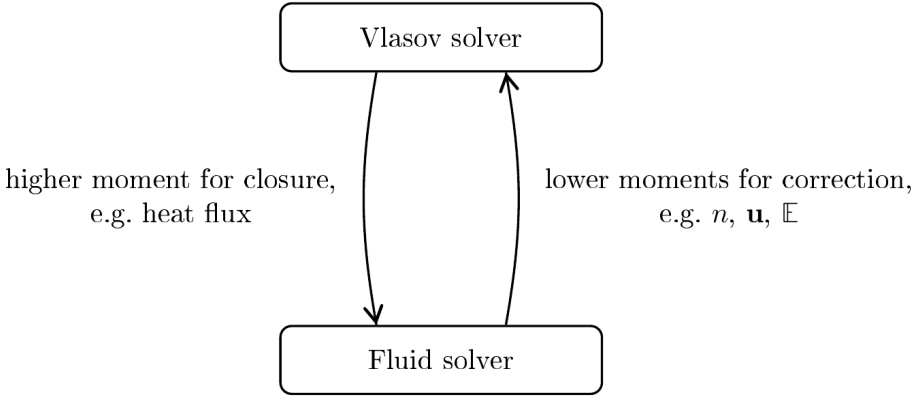
Multi-Physics Approach

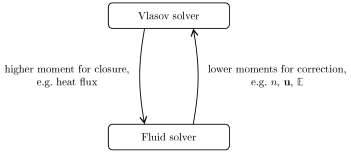


PFC (Vlasov)


f_i^n
f_{i-1}^n
f_{i+1}^n
t^n
x
f_{i-1}^{n+1}
f_i^{n+1}
f_{i+1}^{n+1}
t^{n+1}
x
Ω_{i-1}
Ω_i
Ω_{i+1}

Moment-Matched PFC





Algorithm 1: Time stepping of the moment fitting Vlasov-Maxwell solver as it is implemented

Initialize with a half step of the Maxwell solver
Time Step
  Calculate third moment $\mathcal{Q}^t$ from f^t
  Full Vlasov leapfrog step to advance to f^{t+1}
  Calculate $\mathcal{Q}^{t+1}$ from f^{t+1}
  Interpolate to get $\mathcal{Q}^{t+1/2}$
  Full Runge-Kutta fluid step (input $\mathcal{Q}$ at appropriate times)
  Moment Fitting
    Calculate moments n_V, $\mathbf{u}_\mathrm{V}$, $\mathcal{P}_\mathrm{V}$ from f
    Calculate ten-moment Maxwellian $f_\mathrm{M,V}$ from n_V, $\mathbf{u}_\mathrm{V}$, $\mathcal{P}_\mathrm{V}$
    Multiply the fluid solver's moments n_F, $\mathbf{u}_\mathrm{F}$, $\mathcal{P}_\mathrm{F}$ by $n_\mathrm{V}/n_\mathrm{F}$ to ensure conservation of f
    Calculate ten-moment Maxwellian $f_\mathrm{M,F}$ from the fluid solver's moments
    Exchange ten-moment Maxwellians: $f = f - f_\mathrm{M,V} + f_\mathrm{M,F}$
    Limit f
  end
  Full step of the Maxwell solver

Conservative Vlasov-Fluid Coupling

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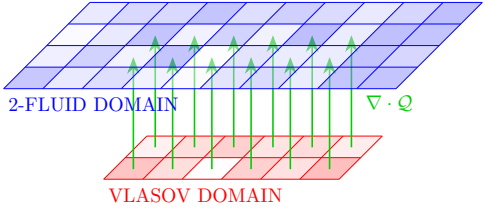
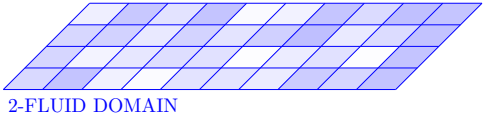
1. ADVANCE VLASOV SIMULATIONS $t^n \to t^{n+1}$

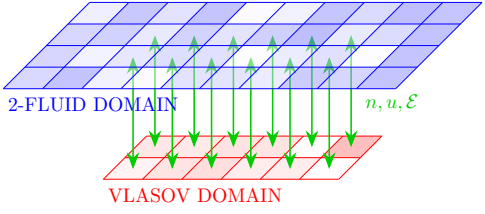
2. PROVIDE KINETIC FLUID CLOSURE FROM VLASOV DISTRIBUTION FUNCTION



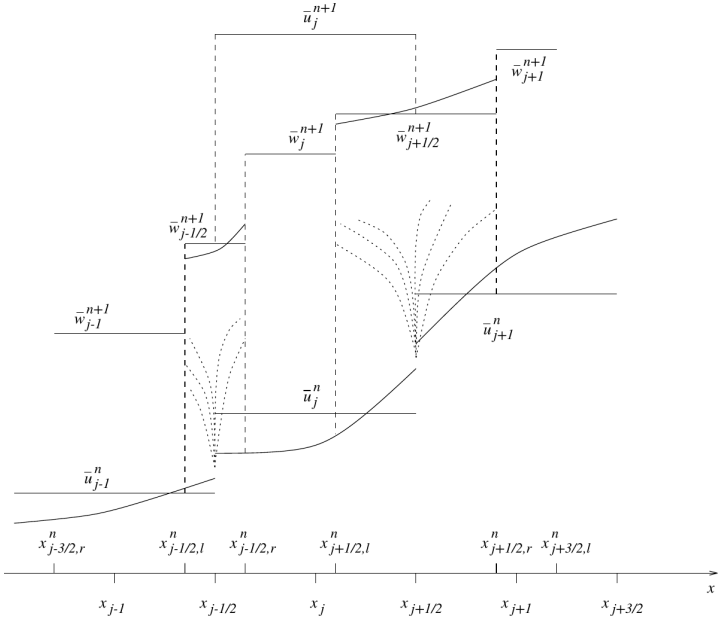
3. ADVANCE 2-FLUID SIMULATIONS $t^n \to t^{n+1}$



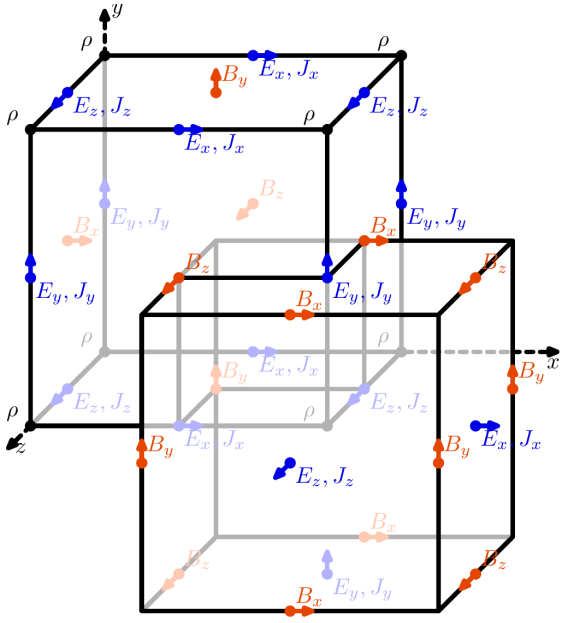
4. MATCH CONSERVATIONAL PROPERTIES



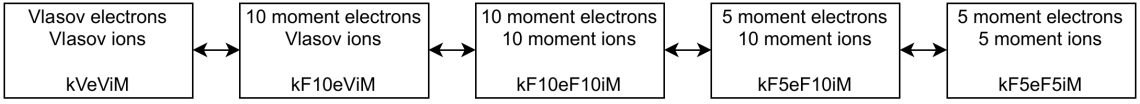
CWENO (Fluid)


$\bar{u}_j^{n+1}$
$\bar{w}_{j+1}^{n+1}$
$\bar{w}_j^{n+1}$
$\bar{w}_{j+1/2}^{n+1}$
$\bar{w}_{j-1/2}^{n+1}$
$\bar{w}_{j-1}^{n+1}$
$\bar{u}_{j+1}^{n}$
$\bar{u}_j^{n}$
$\bar{u}_{j-1}^{n}$
$x_{j-3/2,r}^{n}$
$x_{j-1/2,l}^{n}$
$x_{j-1/2,r}^{n}$
$x_{j+1/2,l}^{n}$
$x_{j+1/2,r}^{n}$
$x_{j+3/2,l}^{n}$
x
x_{j-1}
$x_{j-1/2}$
x_j
$x_{j+1/2}$
x_{j+1}
$x_{j+3/2}$

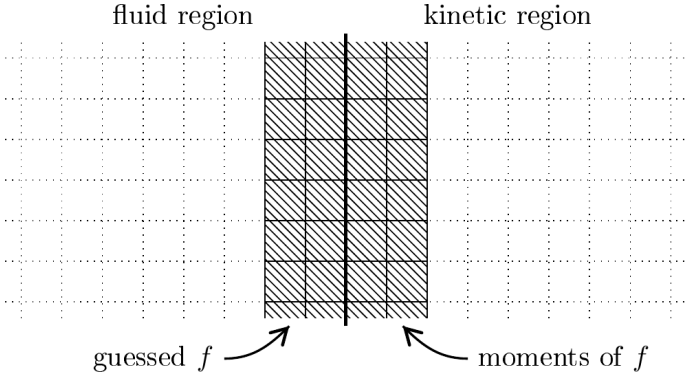
FDTD (Maxwell)



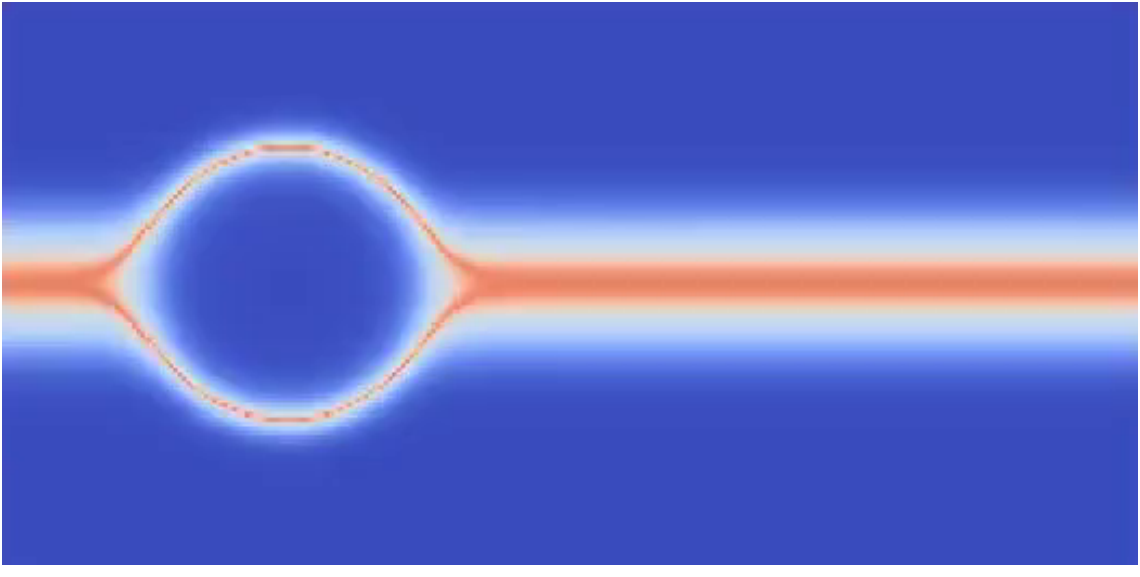
Model Coupling



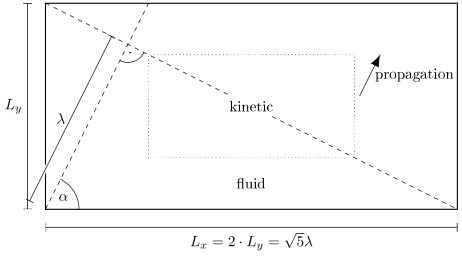
Vlasov-Fluid Interface Coupling

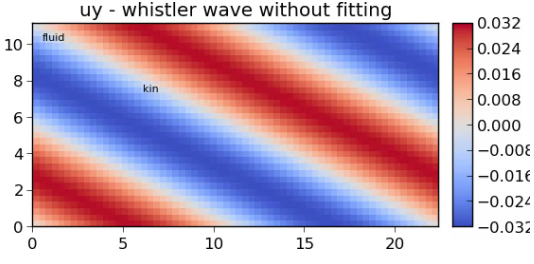


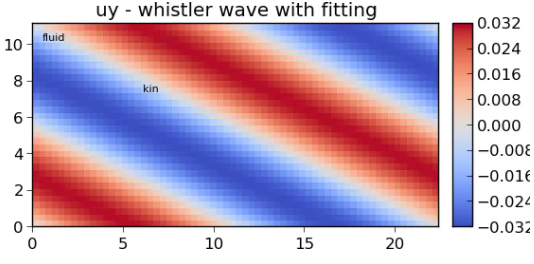
Vlasov-Fluid Interface Coupling: Static Coupling



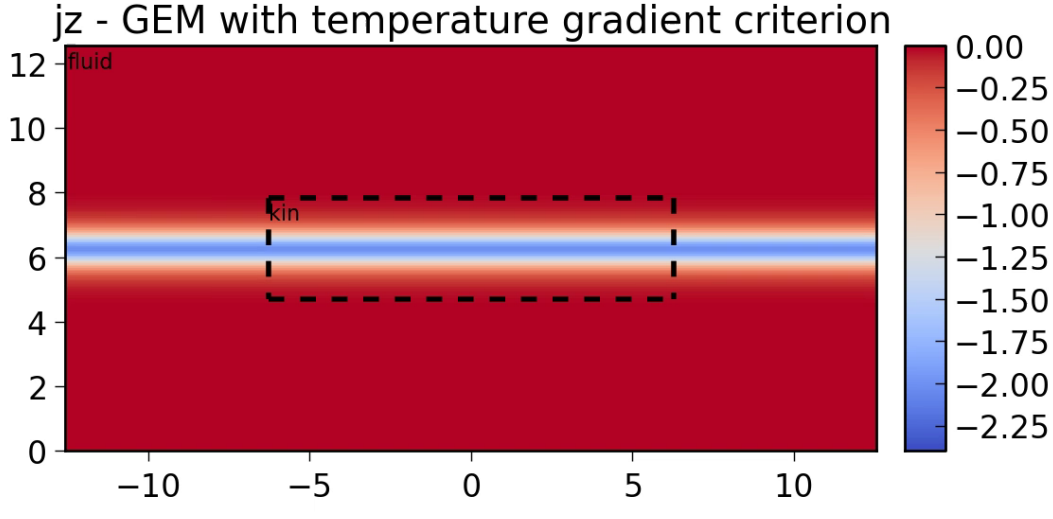
Vlasov-Fluid Interface Coupling: Dissipation Characteristics



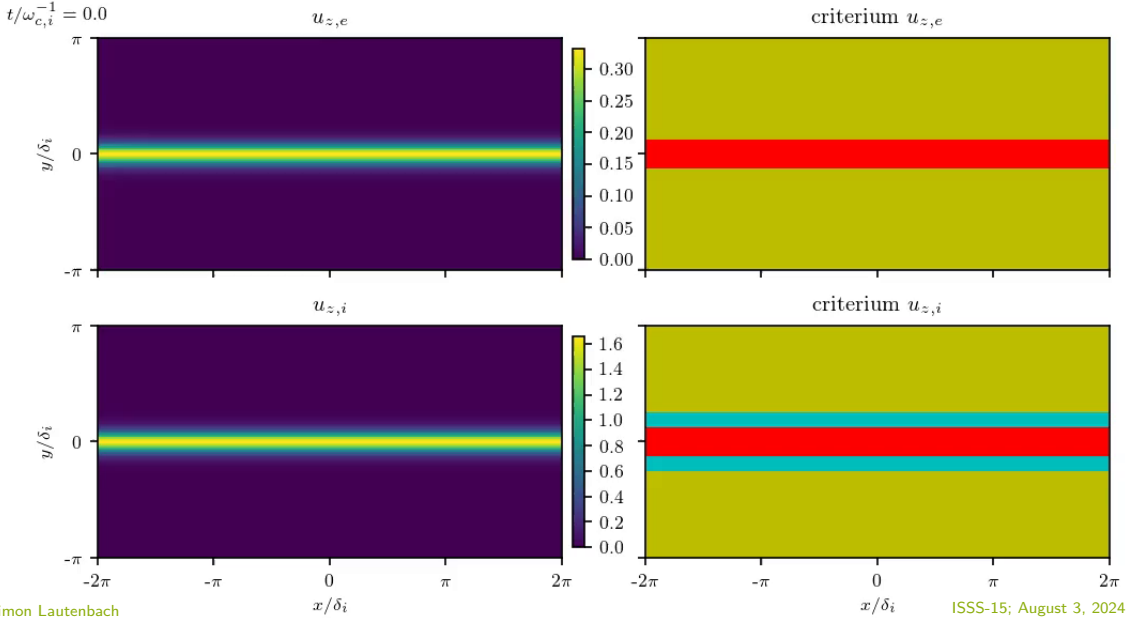




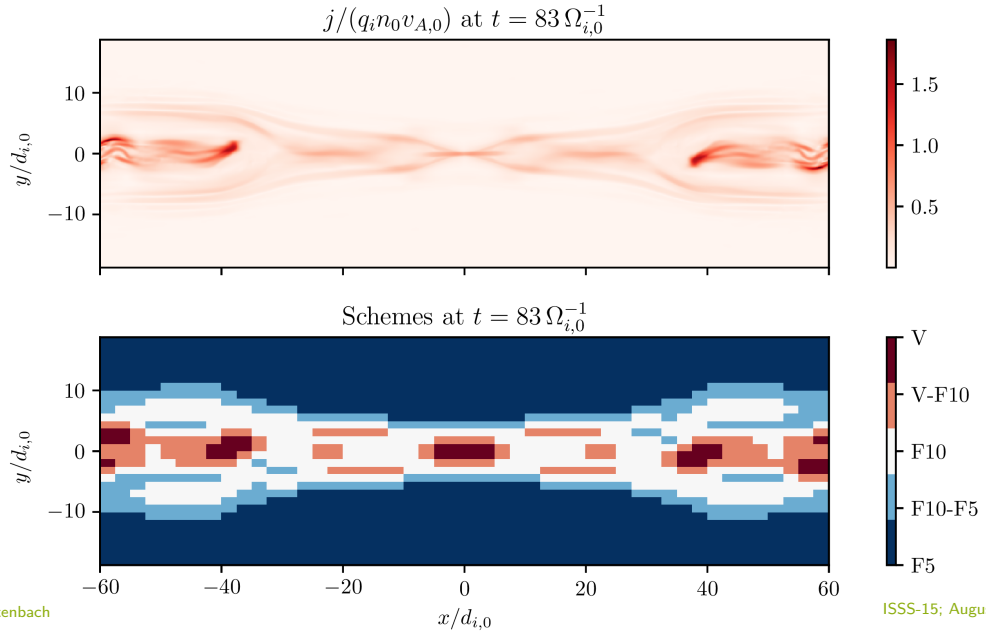
Vlasov-Fluid Interface Coupling: Dynamic Coupling



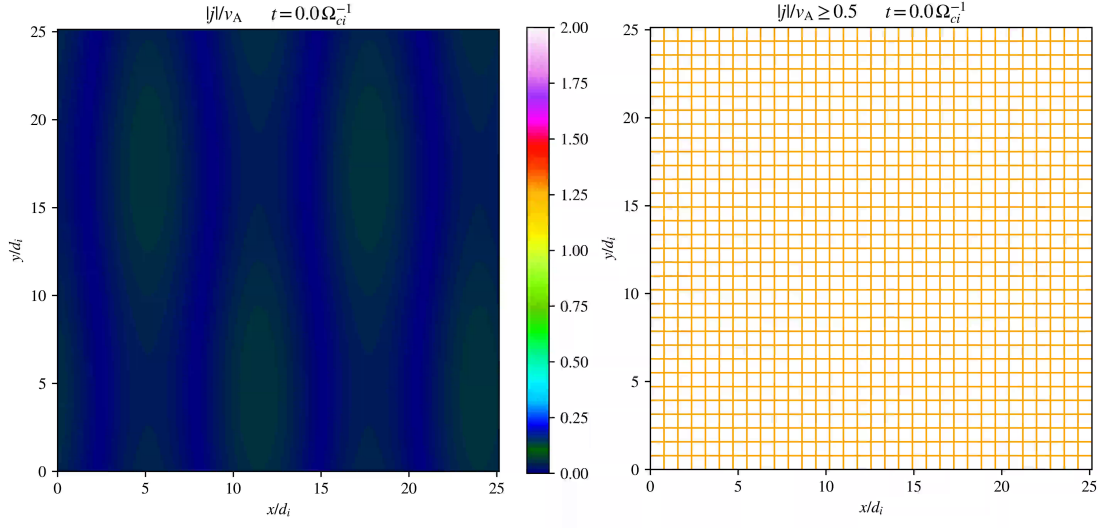
Refinement Criteria



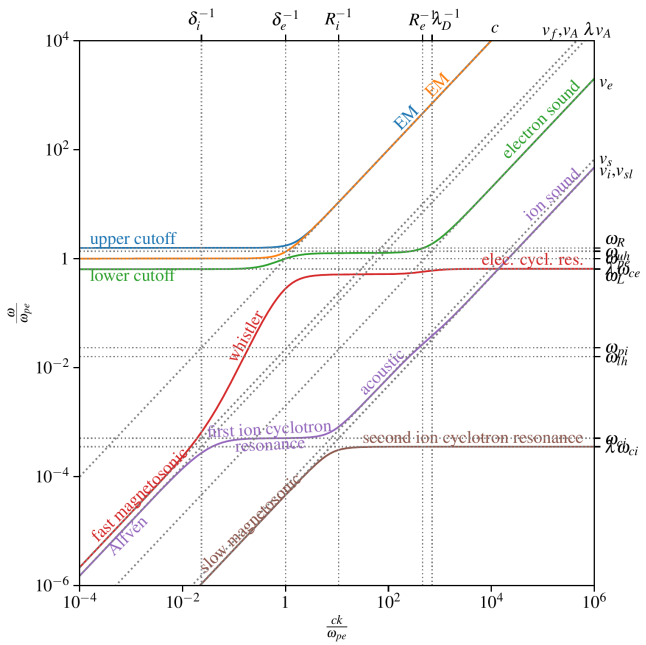
Coupling Complexity



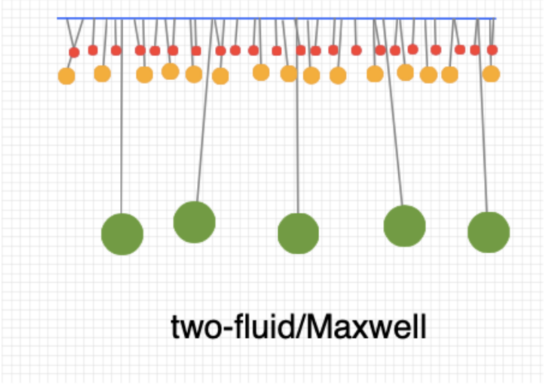
Domain Decomposition in Turbulent Environments

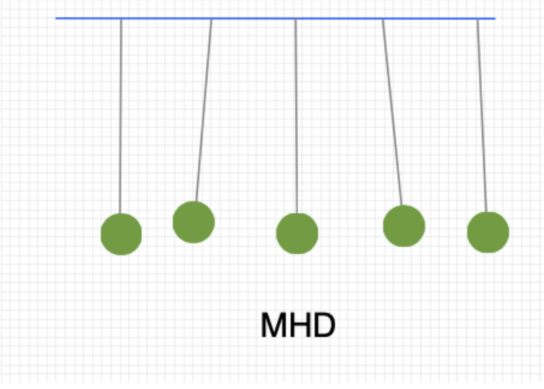


Maxwell-Ohm Coupling: EM Waves



Asymptotic-Preserving Fluid-Maxwell / MHD-Ohm Coupling





Asymptotic-Preserving Fluid-Maxwell / MHD-Ohm Coupling

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5-moment two fluid

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot \mathbf{p}_s = 0$$

$$\frac{\partial \mathbf{p}_s}{\partial t} + \nabla \cdot \left(\frac{\mathbf{p}_s \otimes \mathbf{p}_s}{\rho_s} + P_s \overleftrightarrow{\mathbf{I}} \right) = \left(\frac{L}{\delta_p} \right) \left(\frac{Z_s}{A_s} \right) (\rho_s \mathbf{E} + \mathbf{p}_s \times \mathbf{B})$$

$$\frac{\partial e_s}{\partial t} + \nabla \cdot \left((e_s + P_s) \frac{\mathbf{p}_s}{\rho_s} \right) = \left(\frac{L}{\delta_p} \right) \left(\frac{Z_s}{A_s} \right) \mathbf{p}_s \cdot \mathbf{E}$$

two temperature MHD

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{p} = 0$$

$$\frac{\partial \mathbf{p}}{\partial t} + \nabla \cdot \left(\frac{\mathbf{p} \otimes \mathbf{p}}{\rho} - \mathbf{B} \otimes \mathbf{B} + \left(P + \frac{\mathbf{B} \cdot \mathbf{B}}{2} \right) \overleftrightarrow{\mathbf{I}} \right) = 0$$

$$\frac{\partial e_s}{\partial t} + \nabla \cdot \left((e_s + P_s) \frac{\mathbf{p}_s}{\rho_s} \right) = \left(\frac{L}{\delta_p} \right) \left(\frac{Z_s}{A_s} \right) \mathbf{p}_s \cdot \mathbf{E}$$

$$\nabla \times \mathbf{B} = \mathbf{J} \text{ initially} \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \qquad \nabla \cdot \mathbf{B} = 0$$

Maxwell

$$-\frac{1}{(\omega_p \tau)^2} \left(\frac{L}{\delta_p} \right)^2 \frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} = \left(\frac{L}{\delta_p} \right) \mathbf{j}$$

$$\frac{1}{(\omega_p \tau)^2} \frac{L}{\delta_p} \nabla \cdot \mathbf{E} = \rho_c$$

Ohm

$$\rho \mathbf{E} + \mathbf{p} \times \mathbf{B} = \left(\frac{A_i}{Z_i} \right) \left(\left(\frac{\delta_p}{L} \right) \nabla P_e + \mathbf{j} \times \mathbf{B} \right)$$

Transition Strategies

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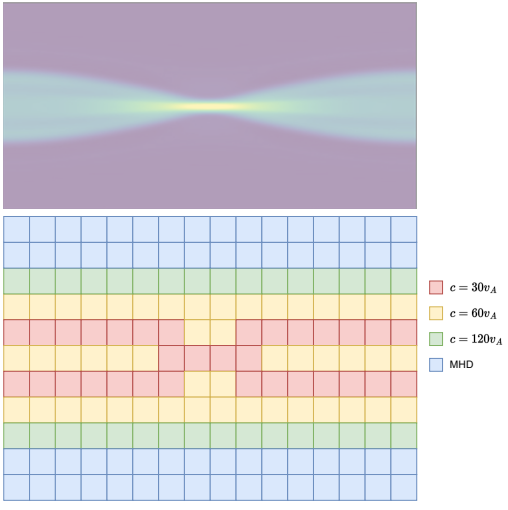
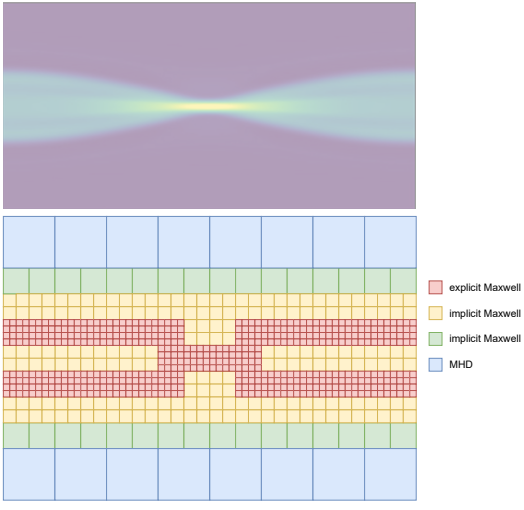
speed of light $c \to \infty$



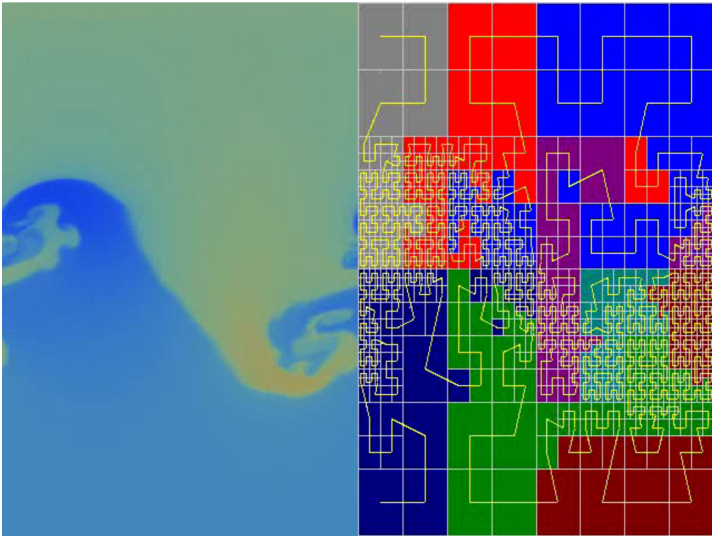
single-scale approach

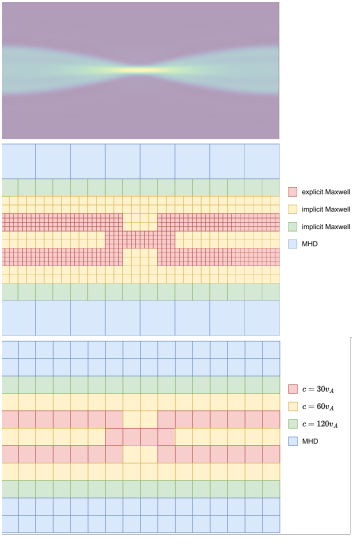
system scale $\to \infty$



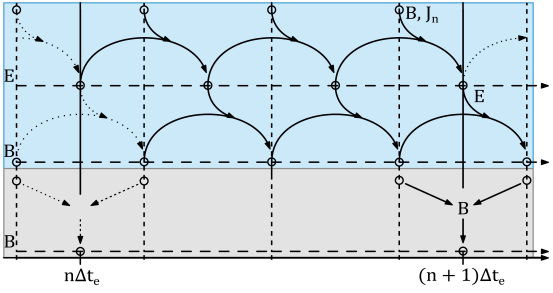
multi-scale approach

Transition Strategies

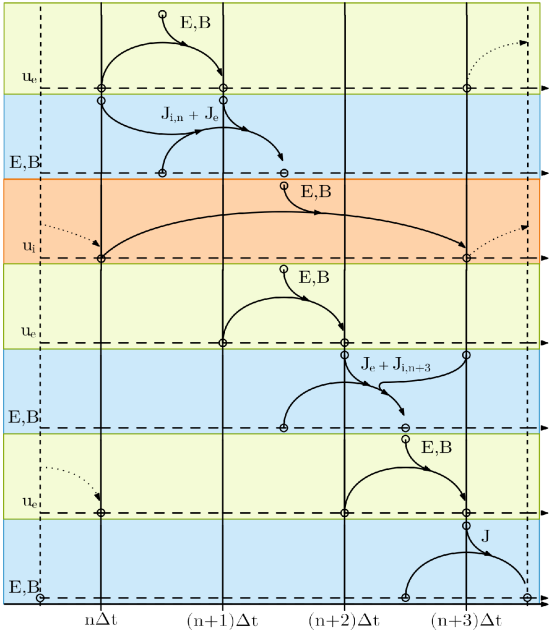




Maxwell Subcycling



Electron Subcycling



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Mentimeter

Model coupling takeaway impressions

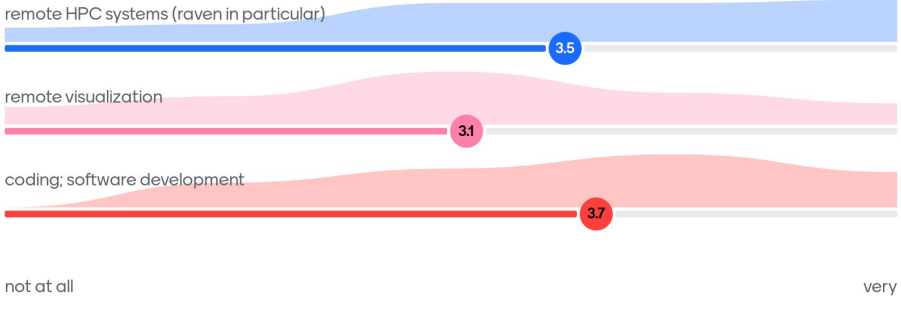
55 responses

33

The muphy2 framework

Mentimeter

How comfortable are you with using ...



43

Block-centric Design

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class Block

+ struct Block_id
+ struct Parameter
+ class *Scheme
+ class Boundary

loop_cycle
update_scheme
load_balancing

struct Block_id

+ my_id
+ neighbour_ids[]
+ my_coords
+ my_scheme_id
+ neighbour_scheme_ids{}

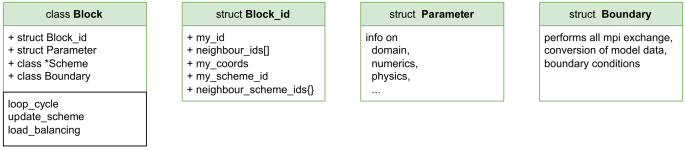
struct Parameter

info on
domain,
numerics,
physics,
...

struct Boundary

performs all mpi exchange,
conversion of model data,
boundary conditions

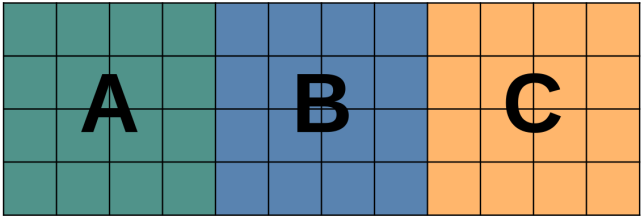
Block-centric Design

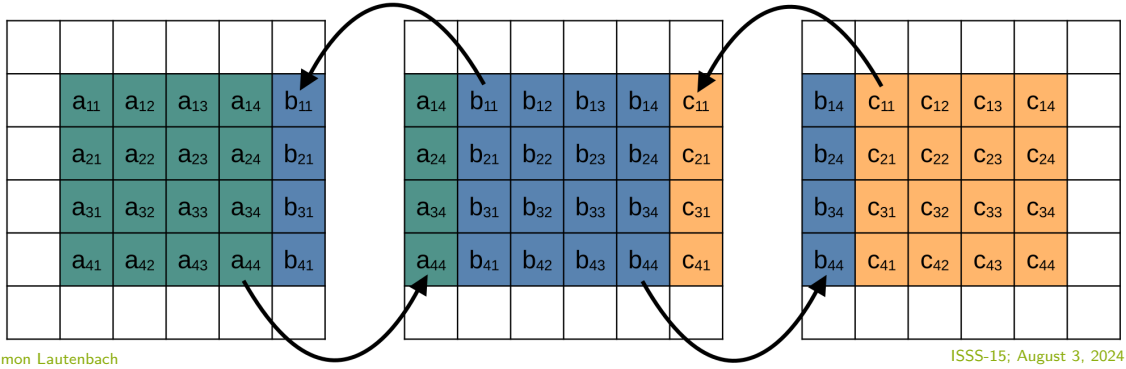



```
1  class Block {
2    public:
3    Block();
4    ~Block();
5
6    void loop_cycle(real &t);
7
8    real get_t_begin();
9    real get_t_end();
10
11   private:
12   void update_scheme();
13   void load_balancing();
14
15   Block_id block_id_;
16   Parameter parameter_;
17   Mpi_boundary boundary_;
18   scheme::Scheme *scheme_;
19
20   MPI_Comm comm3d_;
21
22   ...
23 }
```

```
1  struct Block_id {
2    int my_id,
3    neighbour_ids[6],
4    my_coords[3],
5    my_scheme_id,
6    neighbour_scheme_ids[6],
7    compute_node = -1,
8    selected_device = -1;
9  };
```

Distributed Memory Parallelism





Distributed Memory Parallelism

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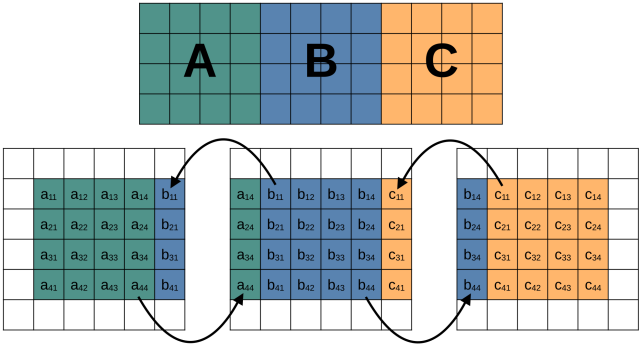
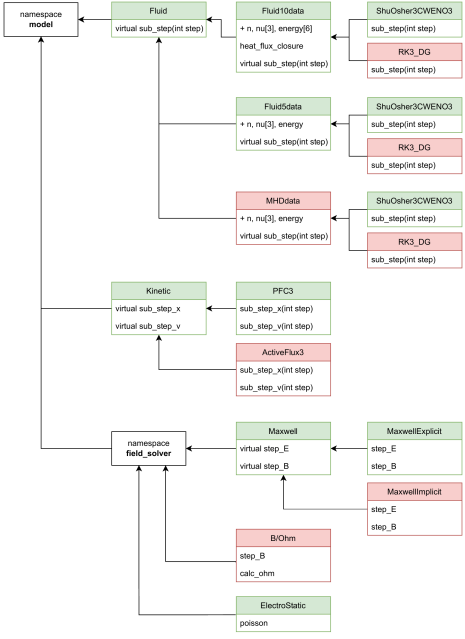
```
1  class Mpi_boundary {
2    public:
3    Mpi_boundary(const MPI_Comm& comm3d, const int* neighbour_ranks,
4    const int* my_coords, const Parameter& parameter);
5    ~Mpi_boundary();
6
7    real mpi_min(real local_value);
8    int mpi_min(int local_value);
9    real mpi_max(real local_value);
10   int mpi_max(int local_value);
11   real mpi_sum(real local_value);
12   int mpi_sum(int local_value);
13
14   // ... (other methods)
15
16   private:
17   const MPI_Comm& comm3d_;
18   const int* neighbour_ranks_,
19   * my_coords_;
20   const Parameter& p_;
21
22   int tags_[6] = {0,1,2,3,4,5};
23   MPI_Status status_[12];
24   MPI_Request requests_[12];
25 };
```



Model Layout



Example Model: Vlasov

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```
1  namespace model {
2
3    class Vlasov : public Model {
4      public:
5      Vlasov(const Parameter& parameter, const Species& species);
6      ~Vlasov();
7
8      int get_model_id();
9      real get_max_dt();
10
11     // wrappers for fortran functions
12     void step_x(const real dt);
13     void step_y(const real dt);
14     void step_z(const real dt);
15     void step_vx(const real dt, const real& E, const real& B, bool include_boundary_cells=false);
16     void step_vy(const real dt, const real& E, const real& B, bool include_boundary_cells=false);
17     void step_vz(const real dt, const real& E, const real& B, bool include_boundary_cells=false);
18
19     real* f;
20
21     private:
22     const Parameter& parameter_;
23     const Species& species_;
24   };
25
26 } // namespace model
```

Language Paradigm

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C++

- high-level
- general purpose language
- great for complex and dynamic data structures
- gives numerous chances to ruin performance
- it takes a lot of programming experience to write "good" C++ programs

→ **use for framework**

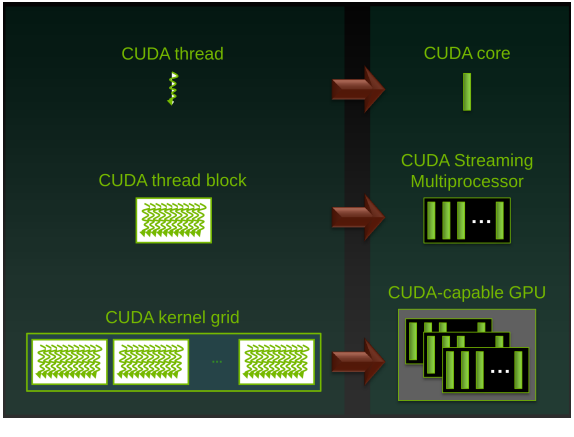
Fortran90

- low-level
- domain-specific language
- excels at array processing
- lacks flexibility
- it takes only a little programming experience to write "fast" Fortran90 programs

→ **use for numeric kernels**

OpenACC

More Science, Less Programming



Shared Memory Parallelism

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```
1   subroutine step_x_vlasov_pfc(f,dimX,dimV,BD,dx,dv,v_b,dt,dimensionality_x)
2     ...
3     ! cell update
4
5     !$acc data present(f)
6     !$acc parallel
7     !$acc loop gang collapse(3)
8     do vz = 1,dimV(3)
9       do vy = 1,dimV(2)
10        do vx = 1,dimV(1)
11          !$acc loop vector collapse(2)
12          do z = -BDZ,dimX(3)+BDZ
13            do y = -BDY,dimX(2)+BDY
14              ...
15
16              !$acc loop seq
17              do x = 0,dimX(1)+1
18                ...
19              enddo
20              f(dimX(1),y,z,vx,vy,vz) = f(dimX(1),y,z,vx,vy,vz) + flux_minus_1 - flux_current
21            enddo
22          enddo
23        enddo
24      enddo
25    enddo
26    !$acc end parallel
27    !$acc end data
28  end subroutine step_x_vlasov_pfc
```

Combining Models: Example Scheme

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```
1   namespace scheme {
2     // ten moments fluid electrons, Vlasov fluid ions, Maxwell
3
4     class F10eViM : public Scheme {
5       public:
6       F10eViM(const Block_id &block_id, Mpi_boundary &mpi_boundary, const Parameter &parameter);
7       ~F10eViM();
8
9       int get_scheme_id();
10      void init();
11      void step();
12      real get_dt(int species = 0);
13      void set_dt(real dt) { dt_ = dt; };
14      void output(real t, int output_number, bool output_vtk);
15      int evaluate_criterion();
16      void replace_dealloc_old_models(model::Model* plasma_model[],
17      model::Model* electromagnetic_model);
18      void calc_alloc_converted_model(model::Model*& model_out,
19      int species, int target_scheme_id);
20      void send_model_data(real* out_buffer, int receiver_id);
21      void receive_model_data(real* in_buffer, int sender_id);
22      int get_data_size();
23
24      // for electron subcycling
25      int get_substeps() { return electron_substeps_; };
26      int get_substep_counter() { return electron_substep_counter_; };
27      void set_substeps(int substeps) { electron_substeps_ = substeps; };
28      void set_substep_counter(int substep_counter) { electron_substep_counter_ = substep_counter; };
29
30      private:
31      void heat_flux_closure(model::Fluid10 *fluid, const real *ten_moments_tmp, real *source);
32      void exchange_plasma_solvers(real* data_e, real* data_i, bool runge_kutta_only=false);
```

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Directory Structure:

```
.
|-- bin
|   |-- machinefiles
|   `-- Makefile
|-- framework
|-- physics
|   `-- plasma
|       |-- converters
|       |-- criteria
|       |-- models
|       |-- output
|       |-- schemes
|       |-- scripts
|       `-- setup
|           `-- initial_conditions
`-- README.md
```

Key Components:

- `bin`: Contains machine-specific files and Makefile
- `framework`: Core framework code
- `physics`: Physics-specific modules
- `README.md`: Documentation

Problem Setup


```
1       subroutine setup_whistler_wave(n_e,n_i,u_e,u_i,E,B,dimX,BD,dx,xb_loc)
2         use definitions
3         implicit none
4
5         integer, intent(in) :: dimX(3), BD(3)
6         real(kind=PRC), intent(in) :: dx(3), xb_loc(3)
7         real(kind=PRC), intent(inout),
    ↪   dimension(-BD(1):dimX(1)+BD(1),-BD(2):dimX(2)+BD(2),-BD(3):dimX(3)+BD(3)) :: n_e, n_i
8         real(kind=PRC), intent(inout),
    ↪   dimension(-BD(1):dimX(1)+BD(1),-BD(2):dimX(2)+BD(2),-BD(3):dimX(3)+BD(3),3) :: u_e, u_i, E, B
9
10        integer :: x, y, z
11        real(kind=PRC) :: xVal, yVal, zVal
12        real(kind=PRC) :: kw, cw, db, du, cosa, sina, beta
13
14        kw = 0.62831853_PRC
15        cw = 1.169_PRC
16        db = 0.05_PRC
17        du = 0.05845_PRC
18        cosa = 0.44721_PRC
19        sina = 0.89443_PRC
20        beta = 0.9978_PRC
21
22        n_e = 1._PRC
23        n_i = 1._PRC
24
25        do z = -BD(3),dimX(3)+BD(3)
26          zVal = xb_loc(3) + (z+0.5_PRC)*dx(3)
27          do y = -BD(2),dimX(2)+BD(2)
28            yVal = xb_loc(2) + (y+0.5_PRC)*dx(2)
29            do x = -BD(1),dimX(1)+BD(1)
30              xVal = xb_loc(1) + (x+0.5_PRC)*dx(1)
```

Initial Conditions Configuration File

RUHR UNIVERSITÄT BOCHUM RUB

```
1   void Parameter::init() {
2     // GEM
3     default_scheme = kF10eF10iM;
4     output_directory = "YOUR_OUTPUT_PATH/";
5     noutputs_vtk = 40;
6     noutputs_csv = 40;
7
8     // time
9     t_end = 40.;
10
11    // physical parameters
12    nspecies = 2;
13    species = new Species[nspecies];
14    species[kElectron].q = -1.;
15    species[kIon].q = 1.;
16    species[kElectron].m = 0.04;
17    species[kIon].m = 1.;
18    species[kElectron].T0 = 1. / 12.;
19    species[kIon].T0 = 5. / 12.;
20    c0 = 20.;
21    mu0 = 1.;
22    eps0 = 1./(c0*c0);
23
24    // setup specific
25    setup = "harris_sheet";
26    setup_var["n_bg"] = 0.2;
27    setup_var["T_bg_e"] = species[kElectron].T0;
28    setup_var["T_bg_i"] = species[kIon].T0;
29    setup_var_bool["drifting_background"] = true;
30    setup_var_bool["sine_perturbation"] = true;
31    setup_var["lambda"] = 0.5;
32    setup_var["psi"] = 0.1;
```

Hands-on