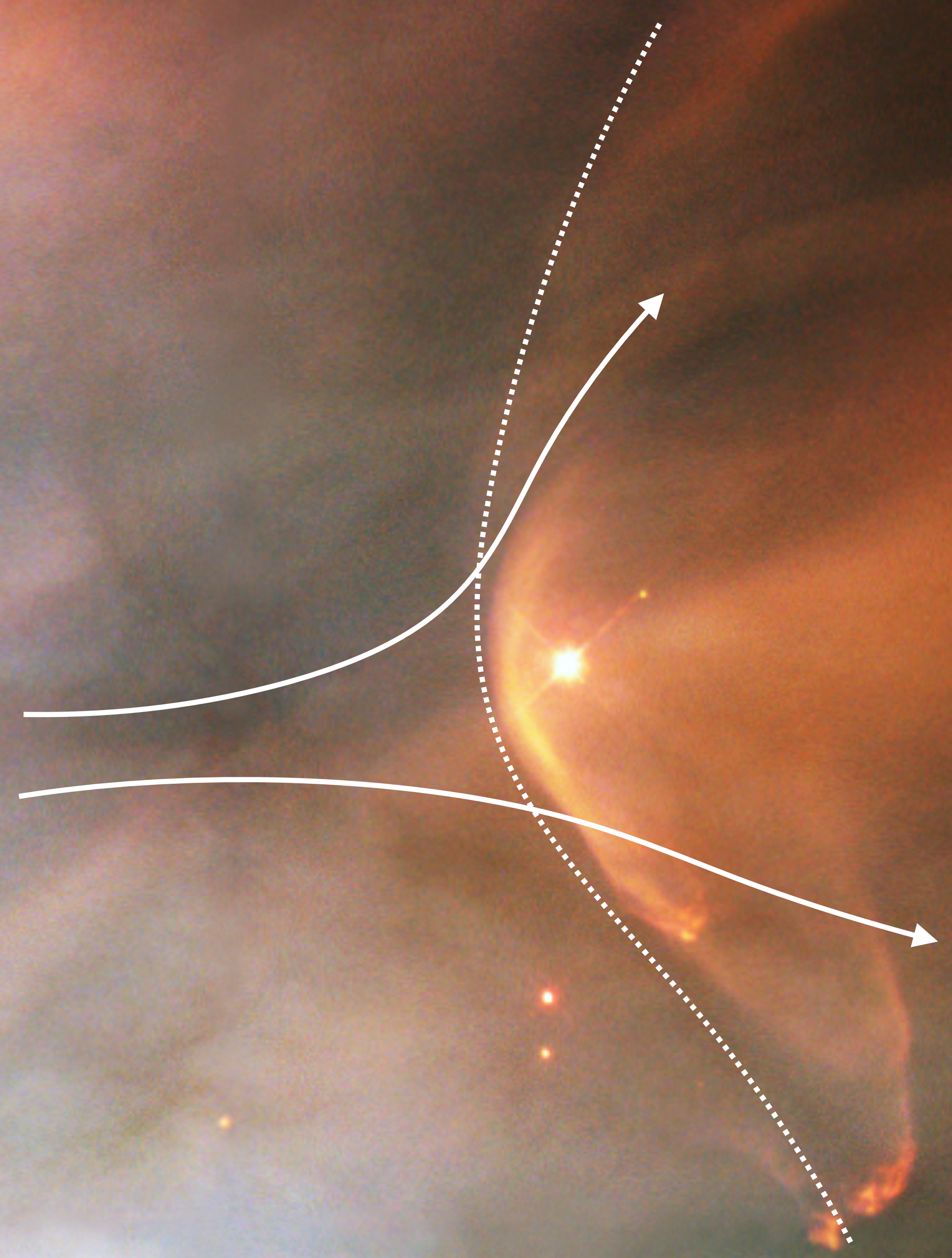
Parallel Hybrid Particle-In-Cell code with Adaptive Mesh Refinement



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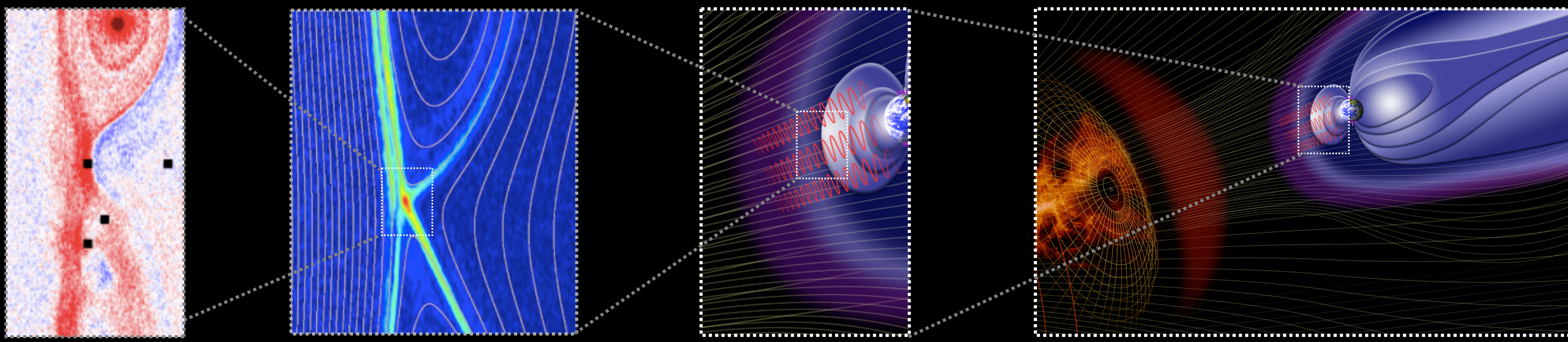
Plasmas à Paris

LERMA

THE MULTISCALE CHALLENGE



10 Km | 500 Km | 100000 Km | 1 Million Km

Fully Kinetic
fully kinetic physics, but small domains, short durations

Fluid « MHD »
Global scale system
But no kinetic physics

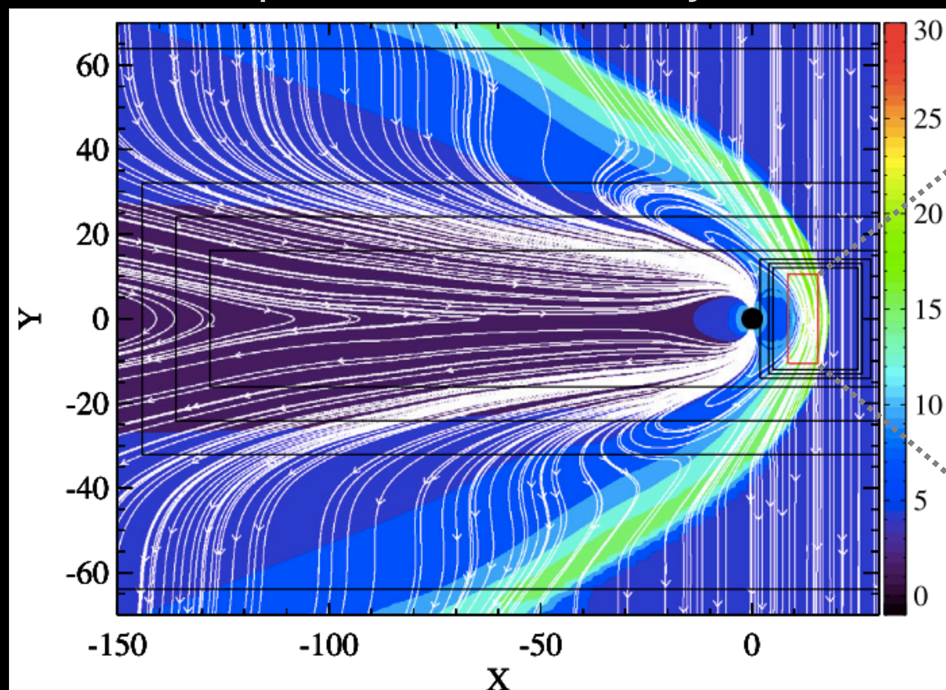
ω_{ce}^{-1} ρ_e — ω_{ci}^{-1} ρ_i — L,T

Solar corona : $\delta_e = 20cm$ $\delta_i = 10m$ $L = 10^9 m$

(insane)

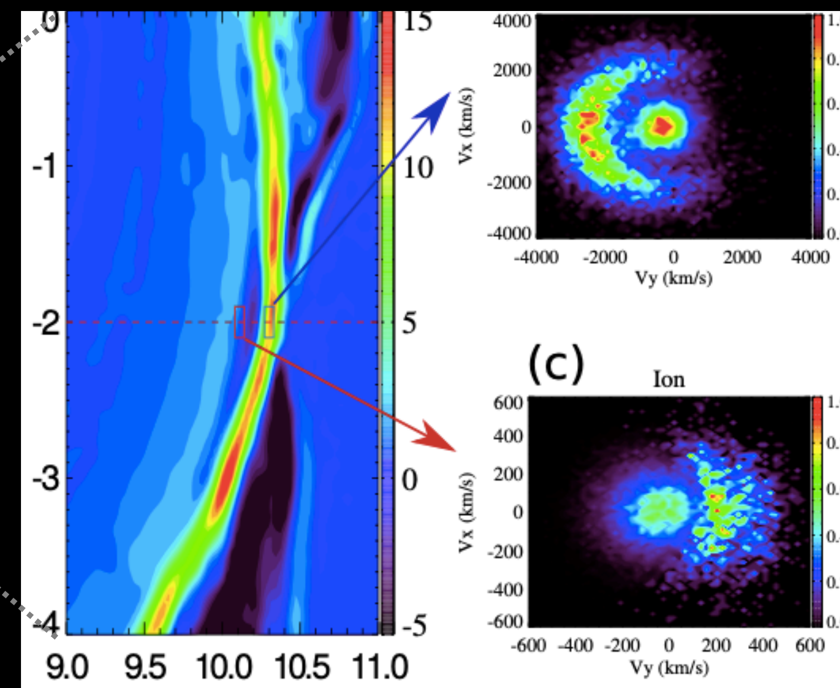
Coupling MHD with fully kinetic models

Global MHD model coupled
with implicit full PIC two-ways



[Daldorff et al. 2014]

Embedded full PIC domain with iPIC



[Yuxi Chen et al 2017]

Full-PIC

Fluid « MHD »

ω_{ce}^{-1}

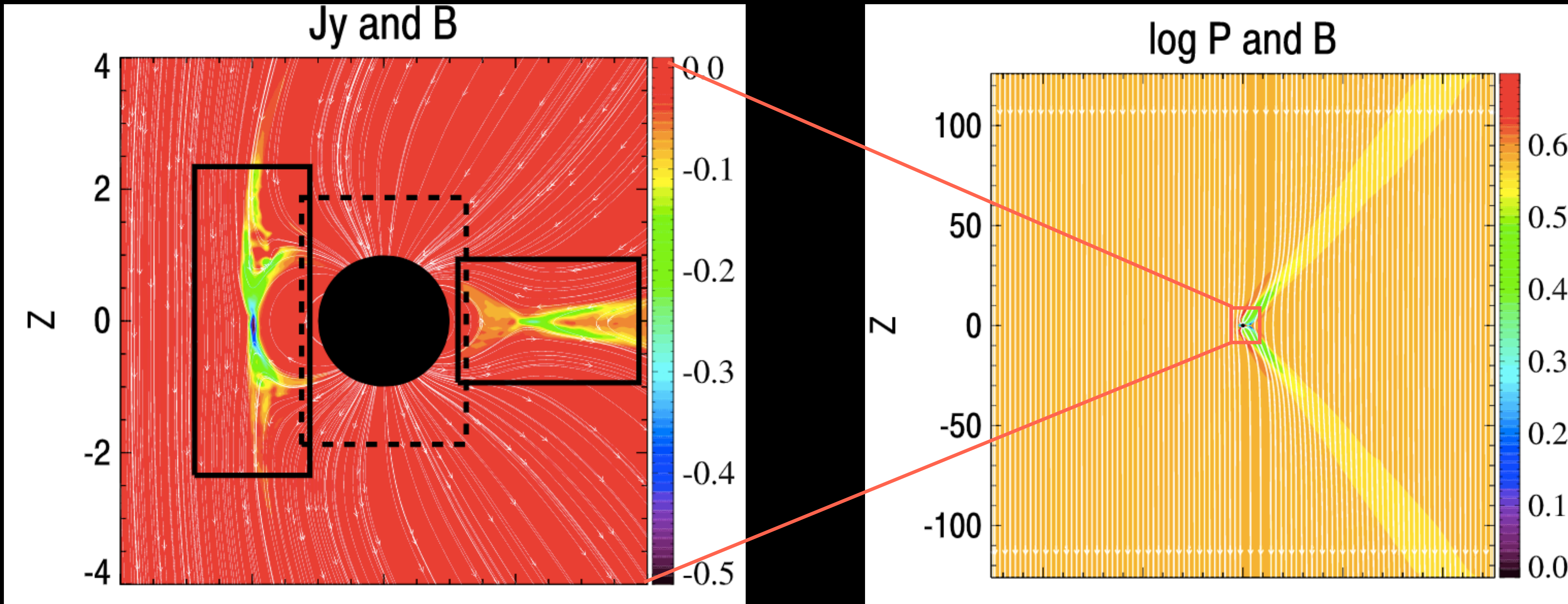
ρ_e

L,T

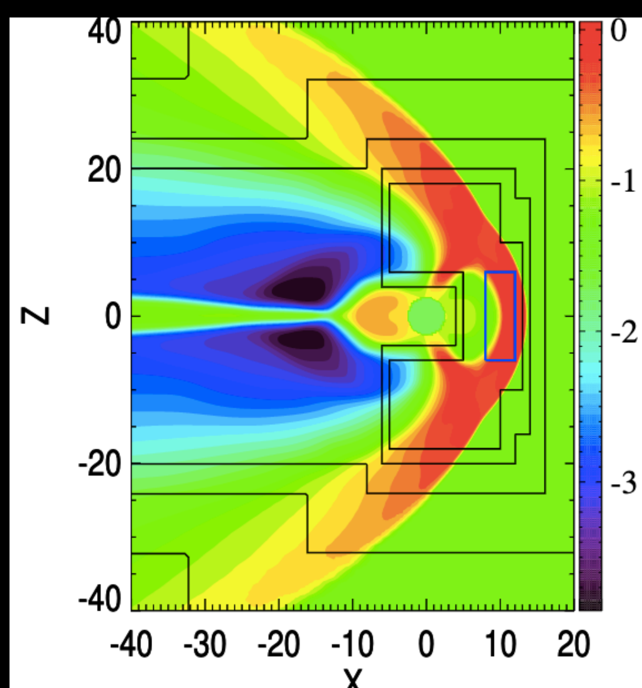
Kinetic domain position is fixed

Full-PIC is quite heavy : limited spatial domain : no global kinetic ions

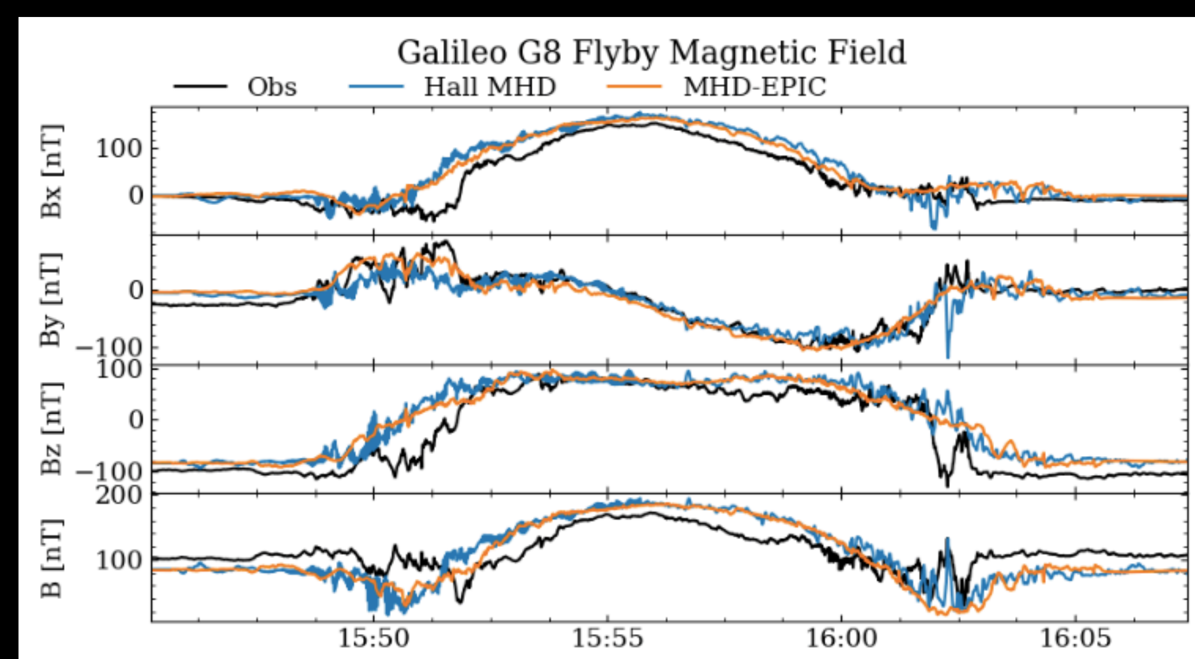
Coupling MHD with fully kinetic models



[Toth et al 2014]

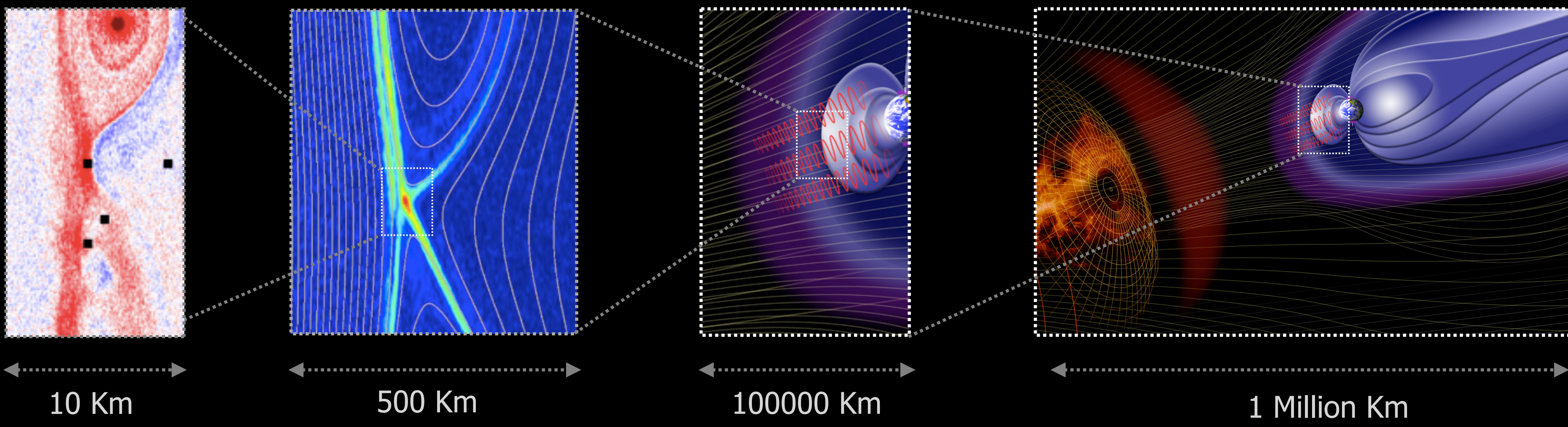


[Chen et al 2017]



[Zhou et al 2020]

Filling the gap between small and large scales



Fully kinetic

Fluid « MHD »

ω_{ce}^{-1} ρ_e

ω_{ci}^{-1} ρ_i

L,T

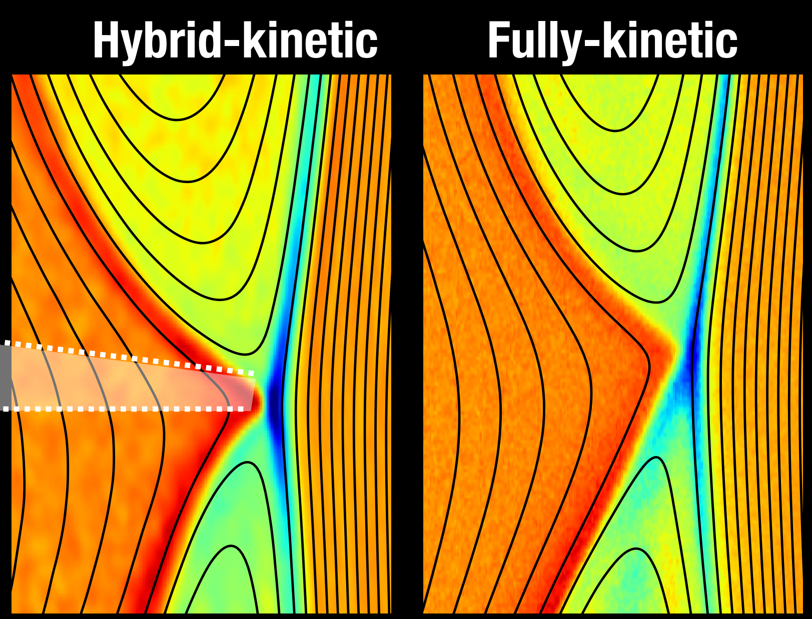
Hybrid kinetic

include ion kinetics but a fluid electron model

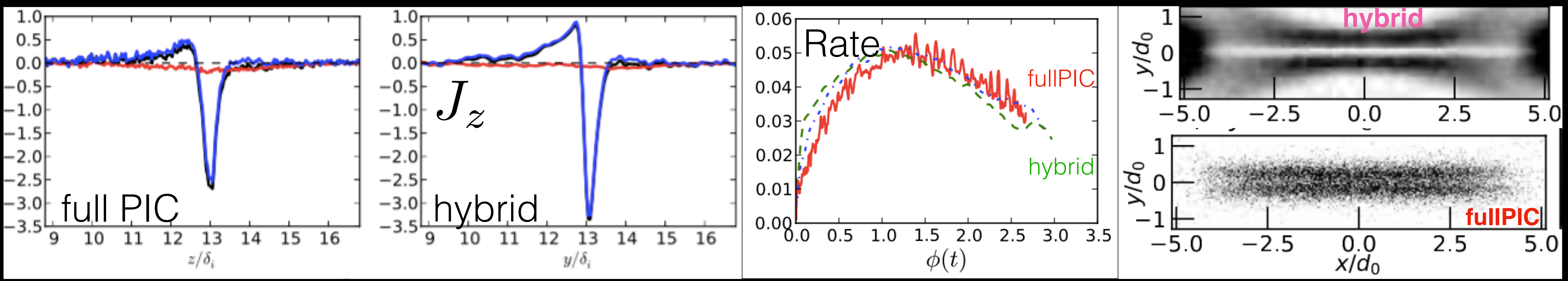
Hybrid kinetic capture reconnection dynamics pretty well

$\sim 100\ km$ $\qquad$ $\sim 10\ km$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left(-\mathbf{v}_i \times \mathbf{B} + \frac{\mathbf{j} \times \mathbf{B}}{ne} - \frac{\nabla P_e}{ne} - \nu \nabla^2 \mathbf{j} \right)$$



[Aunai et al. 2013]



[Sladkov et al. 21]

- Hall currents, ion acceleration/heating, collisionless mixing
- Reconnection rate
- Misses X-line electron scale mechanisms, fully kinetic instabilities
- Depends on the electron closure equation

$$\partial_t \mathbf{P} = -\mathbf{V}_e.\boldsymbol{\nabla}\mathbf{P} - \mathbf{P}\boldsymbol{\nabla}.\mathbf{V}_e - \mathbf{P}.\boldsymbol{\nabla}\mathbf{V}_e - (\mathbf{P}.\boldsymbol{\nabla}\mathbf{V}_e)^T$$
$$-\frac{e}{m}[\mathbf{P} \times \mathbf{B} + (\mathbf{P} \times \mathbf{B})^T] - \frac{1}{\tau}[\mathbf{P} - \frac{1}{3}\mathrm{Tr}(\mathbf{P})\mathbf{1}]$$

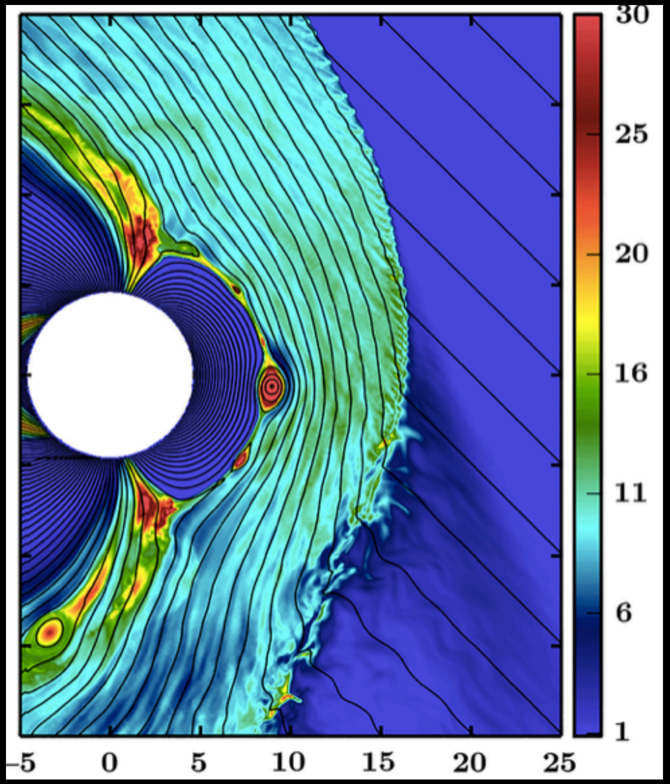
GLOBAL VLASOV (EULERIAN 6D) HYBRID KINETIC MODEL

Started in ~2010

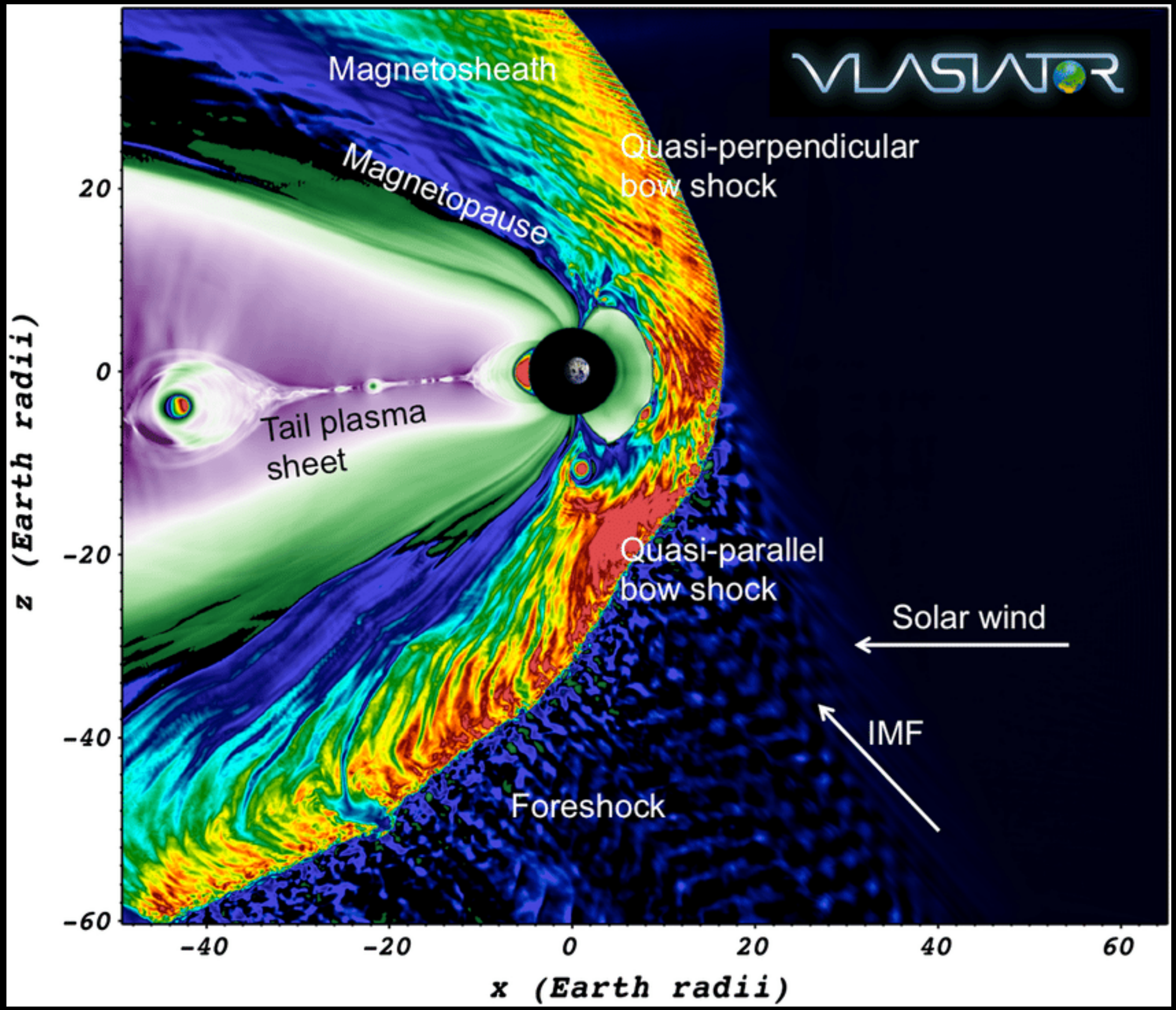
Advantage : noise free compared to PIC

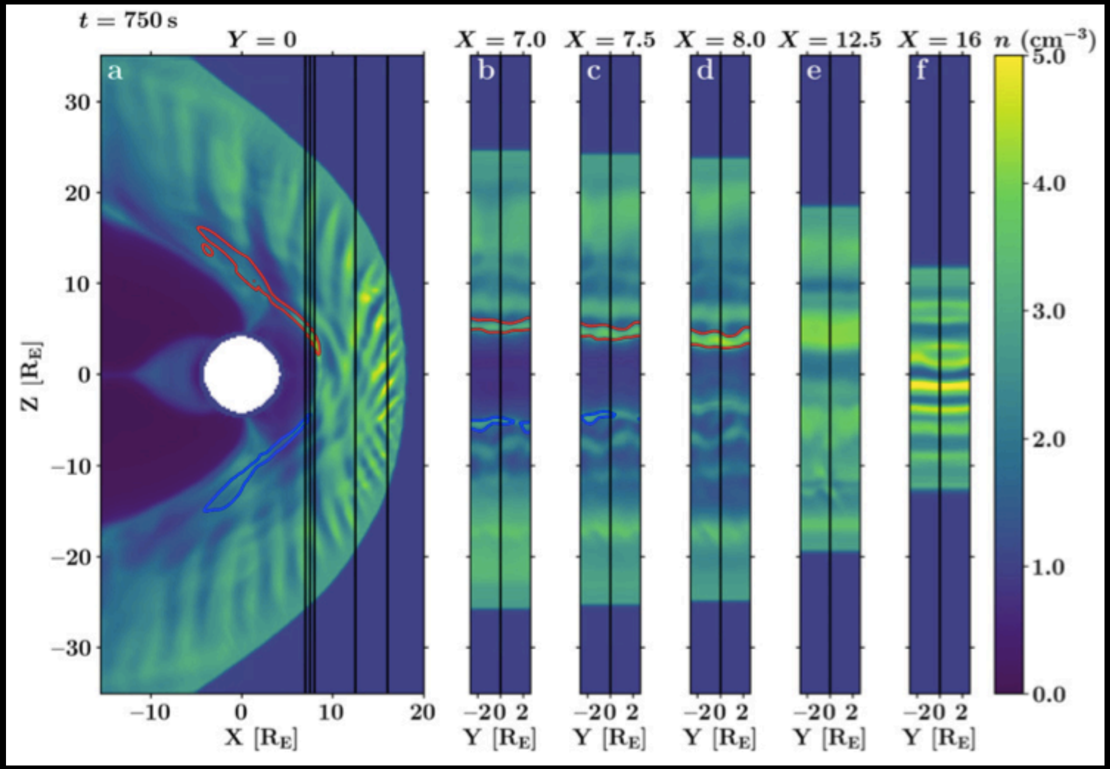
Drawback : complex and computationally heavy : 2021 first spatial 3D

2D vlasiator run



[S. Hoilijoki et al. 2017]



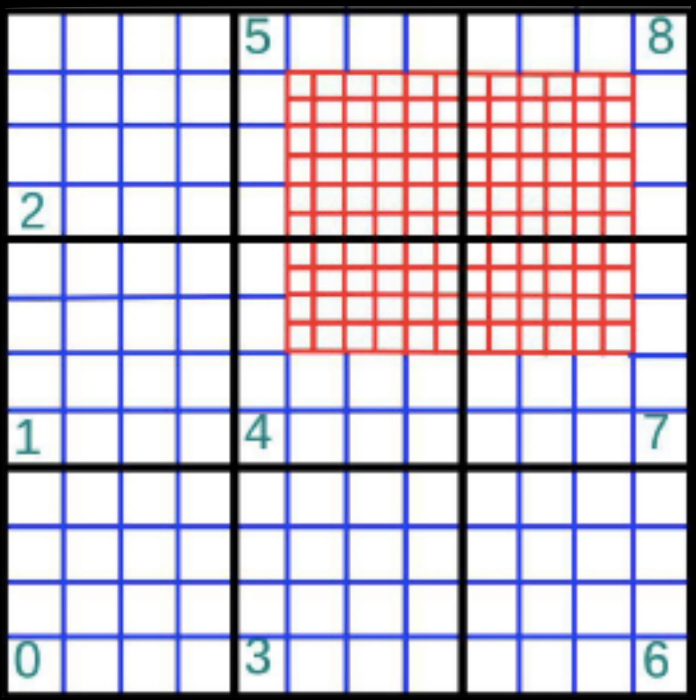


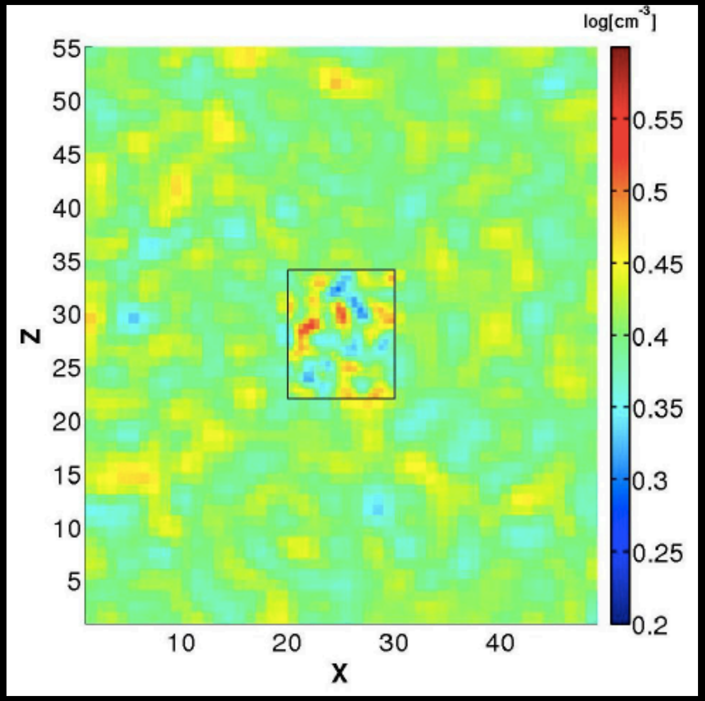
[Kempf et al. 2020]

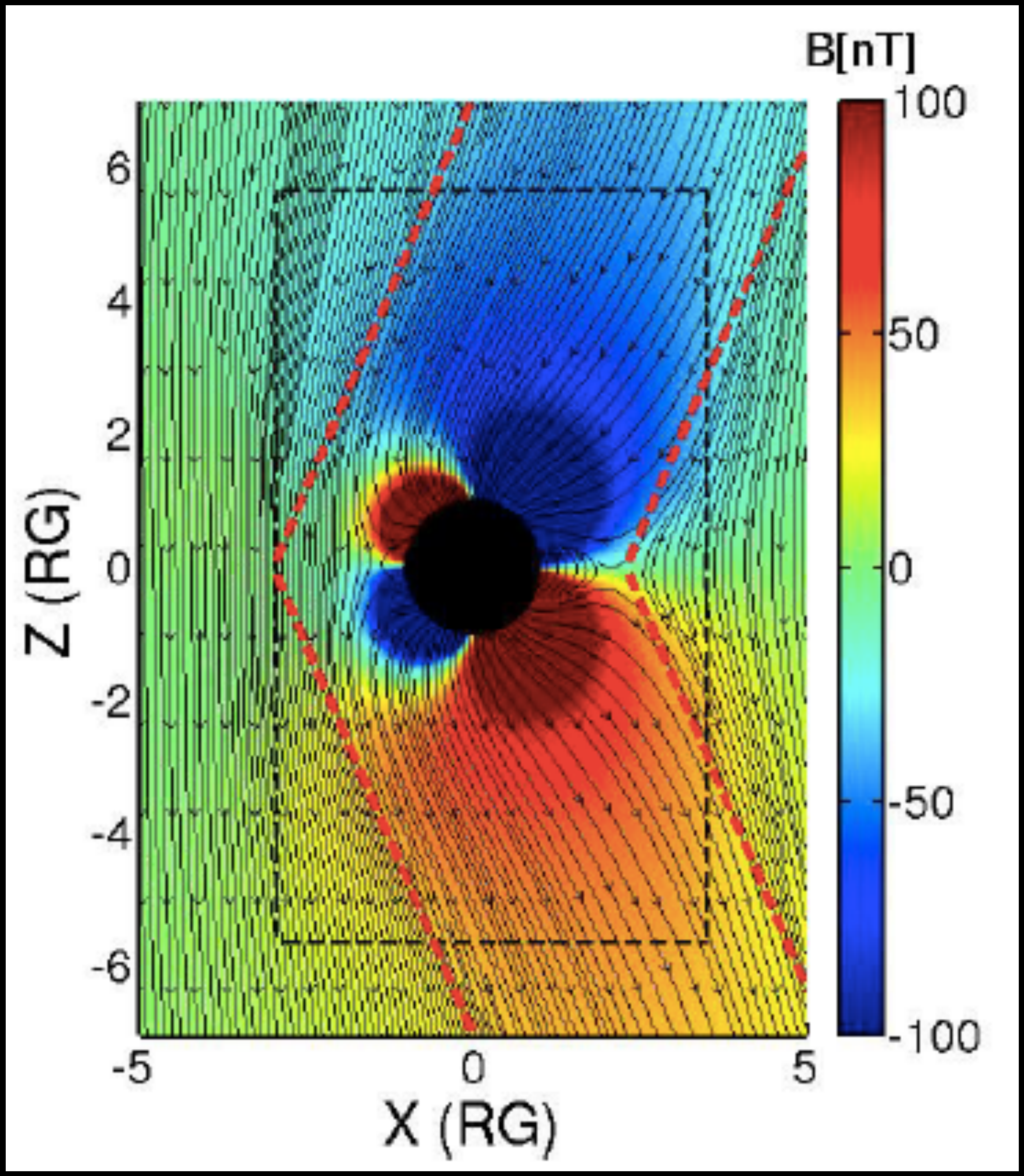
BEYOND « CLASSICAL » HYBRID PIC CODES

A first step : using a refined grid around a region of interest

[Leclercq et al. 2016]

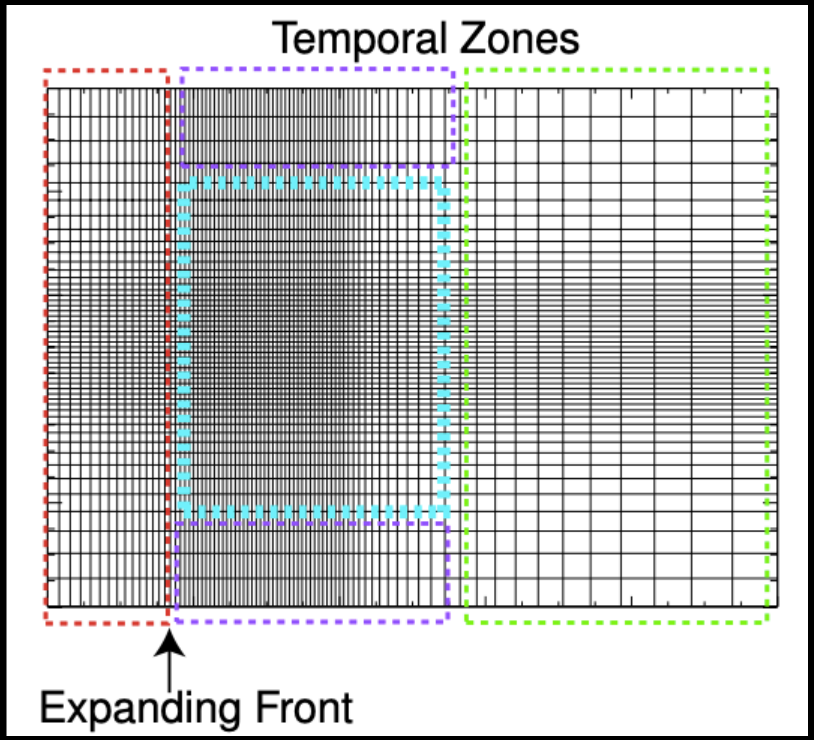




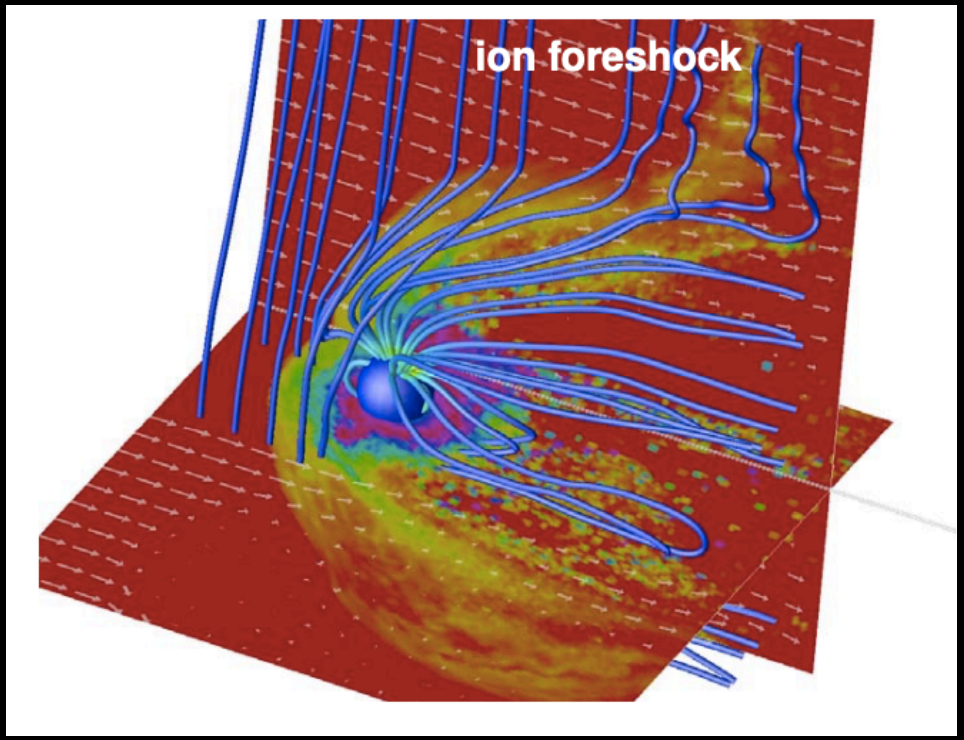


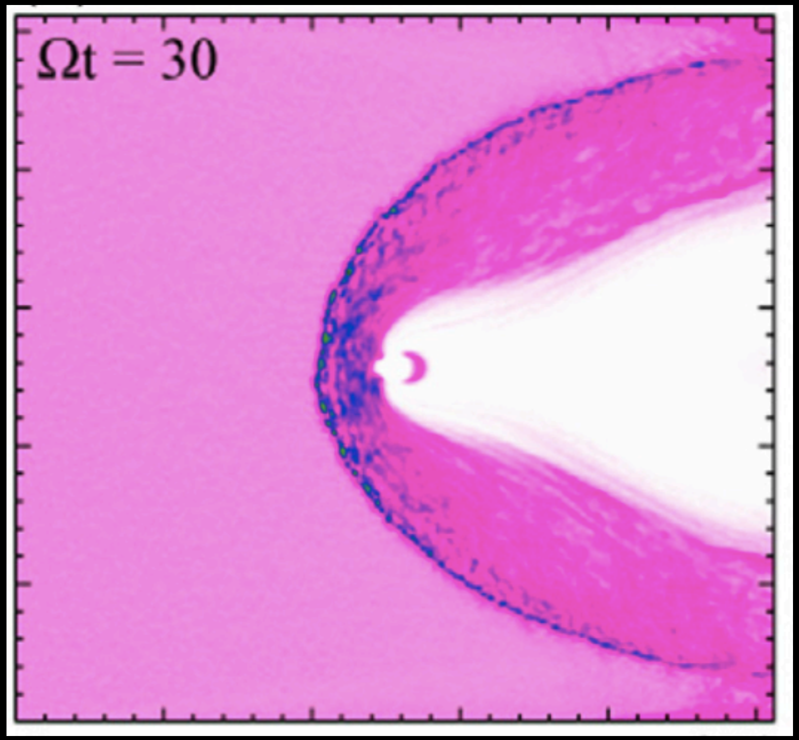
- Better than uniform grid
- *Home made* gridding
- Not adaptive

Global hybrid particle in cell



[Karimabadi et al. 2006]





[Omelchenko et al. 2012]

Time zones and stretched grids can address this issue but not so flexible

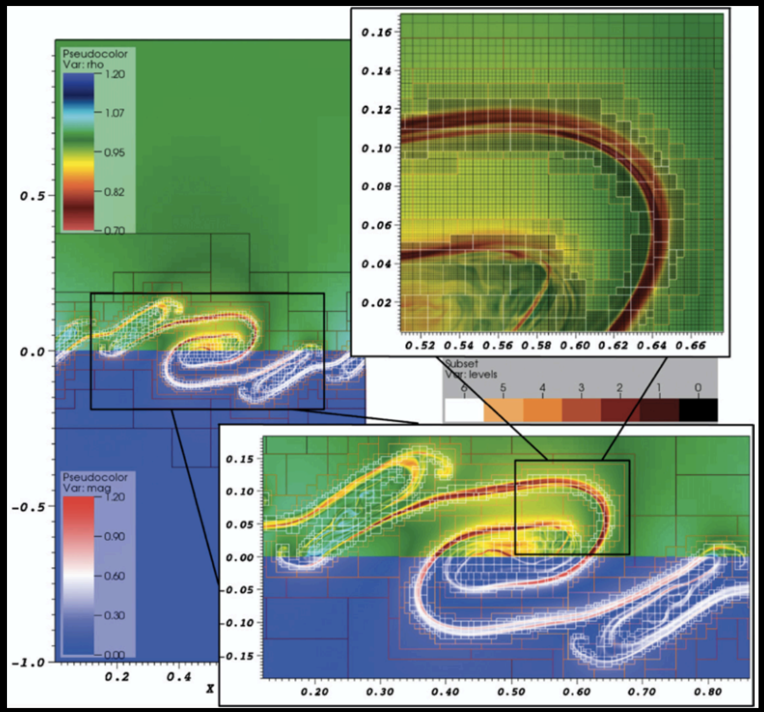
Discrete Event Simulations (DES)
Each node/particle evolved when needed

Adaptive Mesh Refinement (AMR) (in fluid codes…)

« finer mesh is more accurate, but more costly »

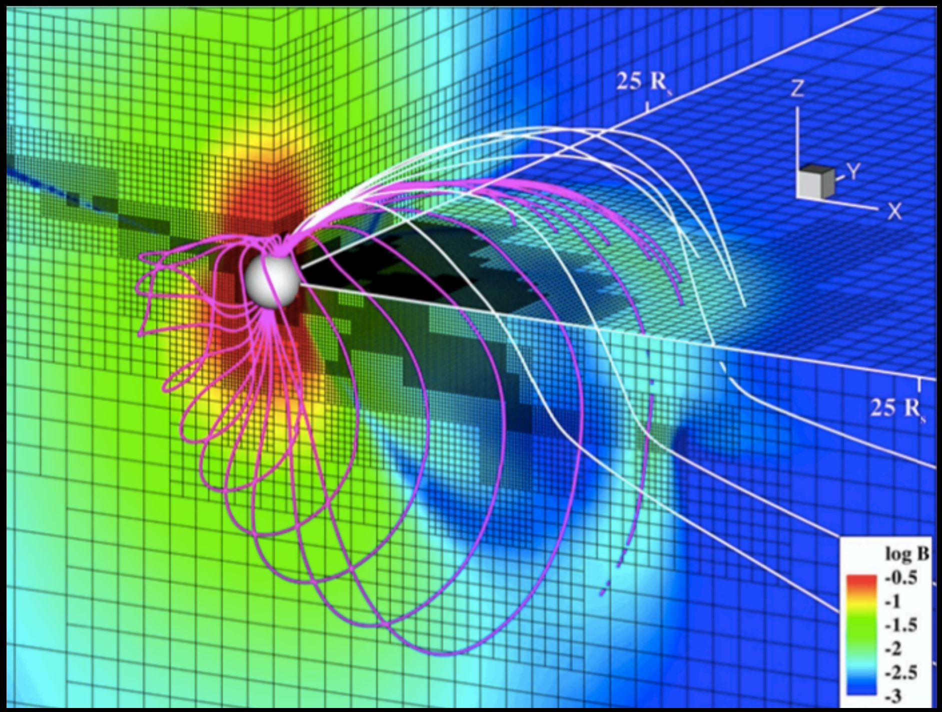
Refine the mesh where a certain set of criteria is met to provide a better accuracy of the solution in critical regions while keeping a coarser resolution in regions of less interest

PLUTO



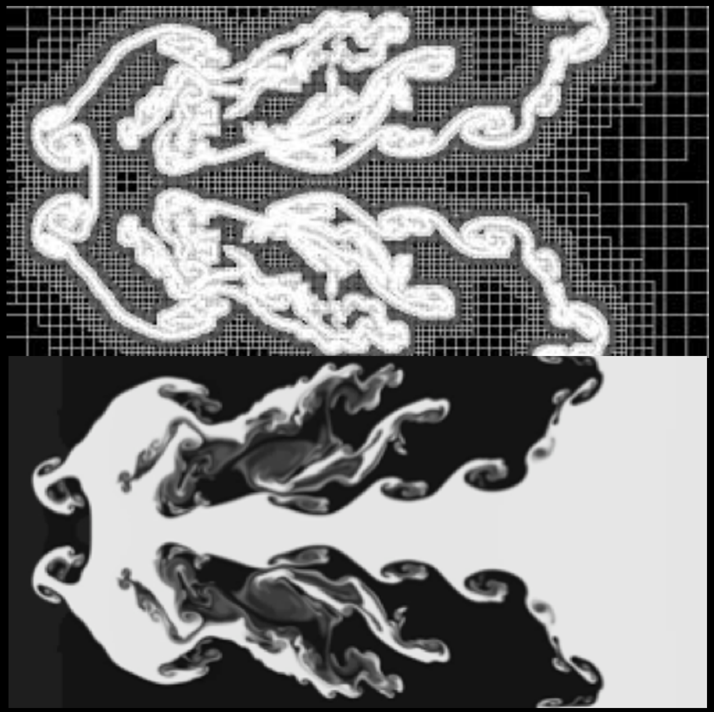
[Mignone et al. 2012]

BATSRUS



[Gombosi et al. 2003]

RAMSES

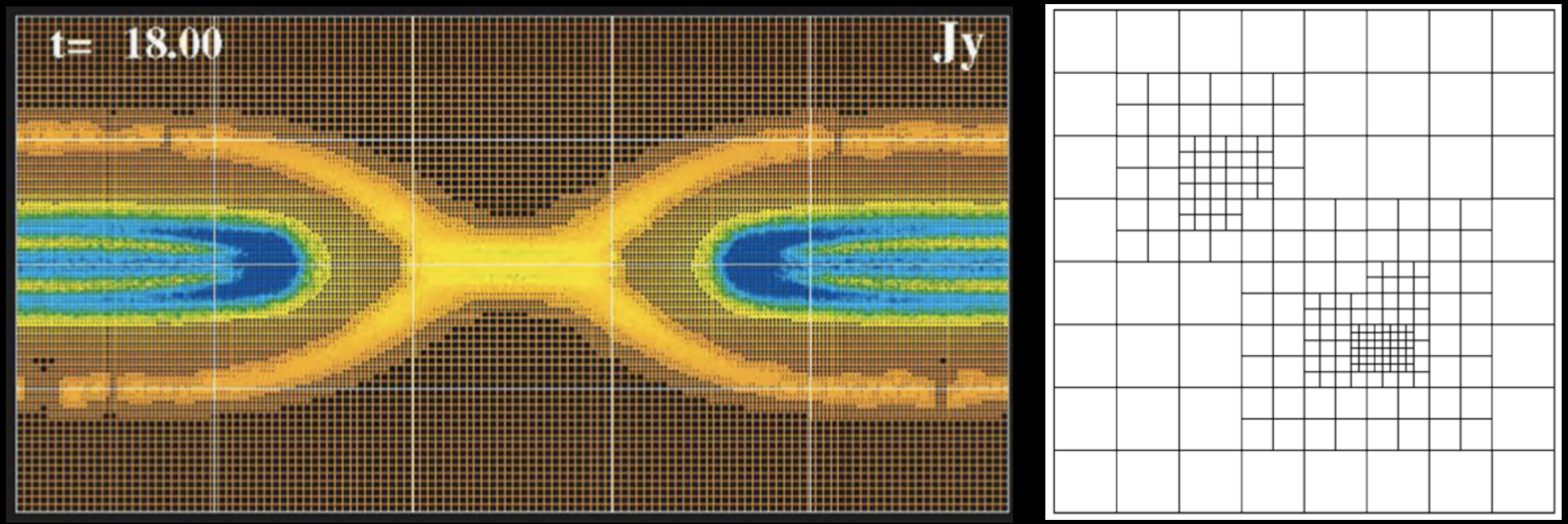


[Teyssier et al. 200..]

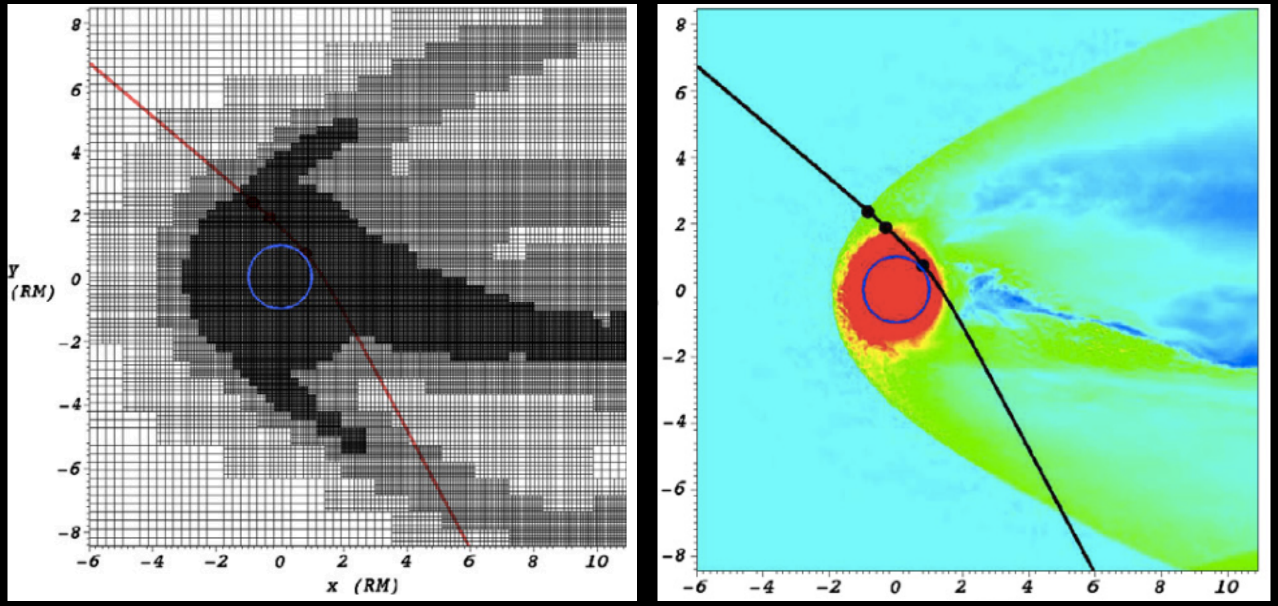
AMR is now a mainstream technology in MHD codes

AMR is rare in PIC codes

- Explicit full PIC code with tree (cell)-based AMR still needs mesh Debye-scale



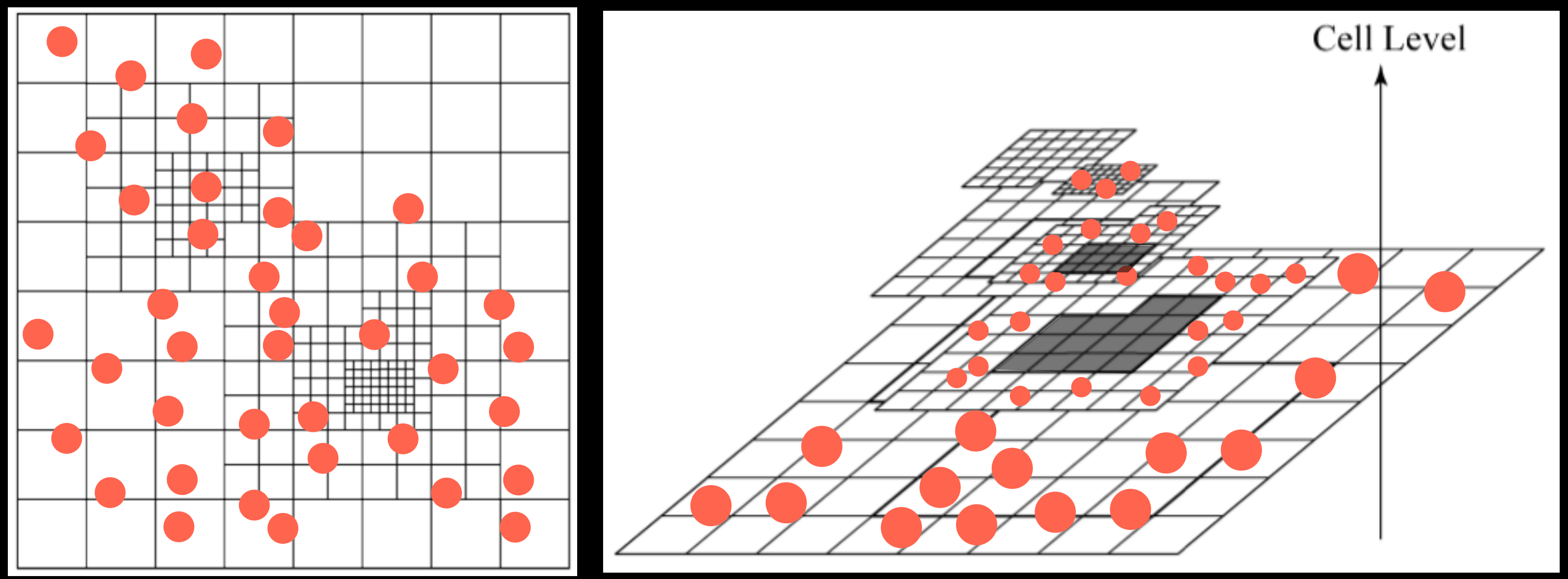
[Fujimoto et al. 2008]



[Muller et al. 2011]

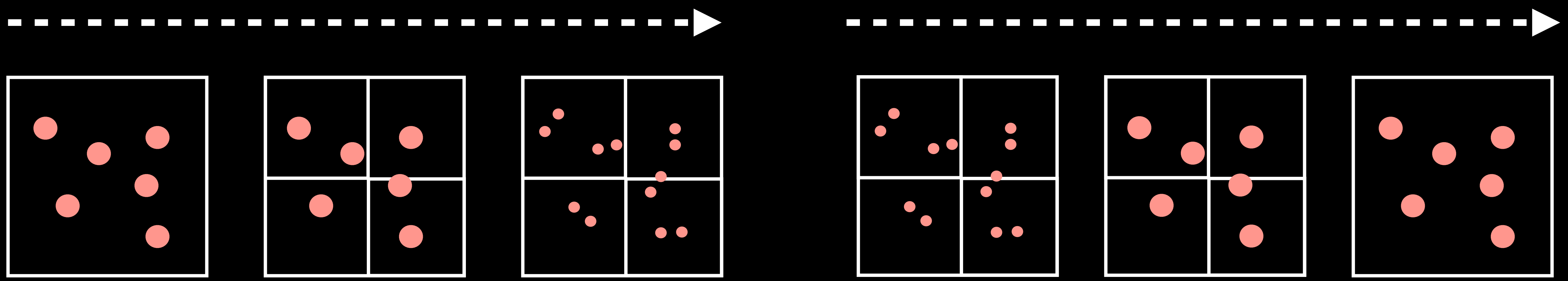
- Hybrid PIC with hybrid block AMR, since 2012 only used with fixed grids

AMR ONLY FOR FIELDS



[adapted from Fujimoto et al. 2008]

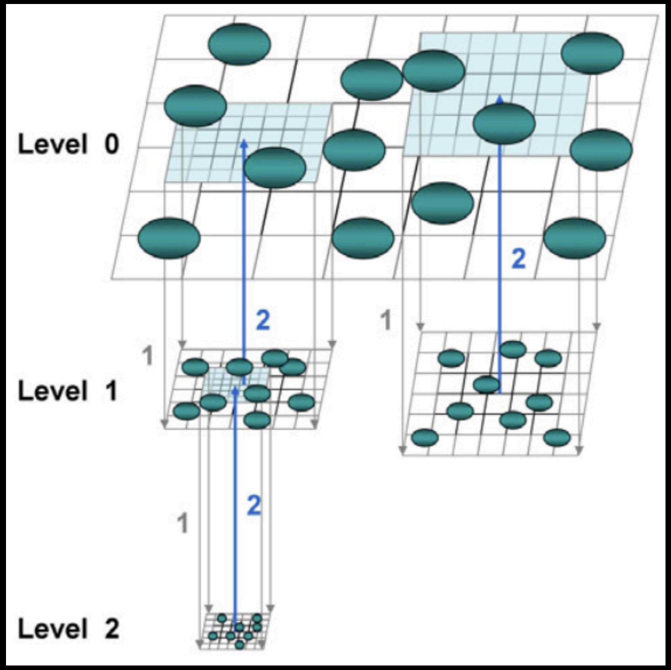
- Field equations are solved on each grid level
- However macroparticles only interact with the finest mesh at their location



- Split macroparticles for coarse to fine flux to keep noise constant
- Merging does not conserve the distribution function…

MULTI-DOMAIN-MULTI-LEVEL (MLMD) SOLVES AMR PIC ISSUES

Solve all equations (like fluid) on all levels : fields AND particles.
No need to merge macroparticles!

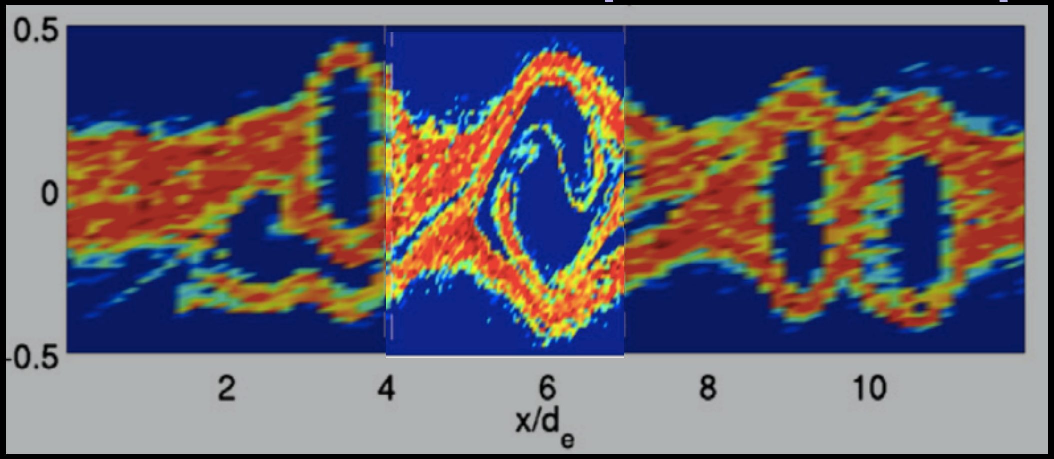


[Innocenti et al. 2013]

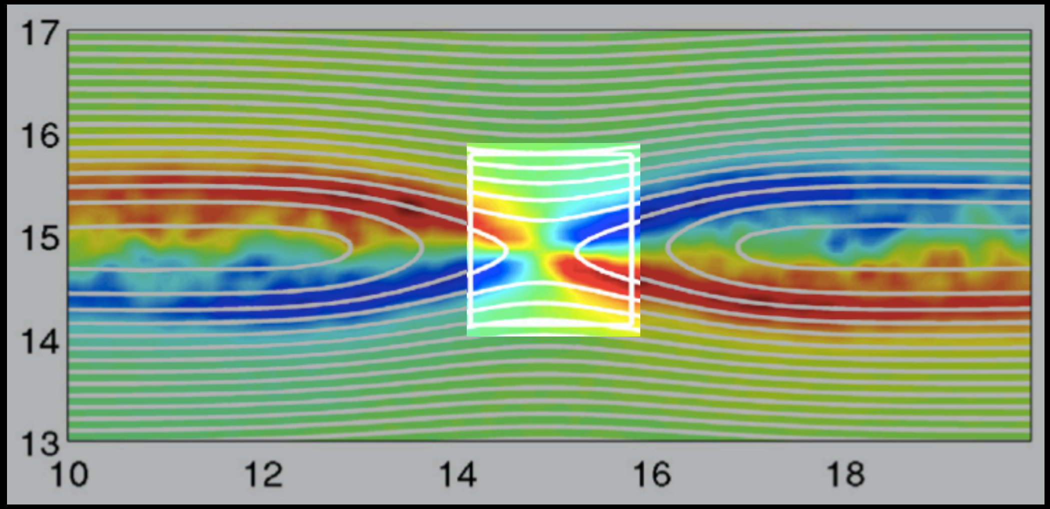
Levels are coupled through boundaries and synchronization but otherwise rather independent : opens the way to multi-formalisms.

Concept in 1D with implicit PIC

[Innocenti et al. 2013]

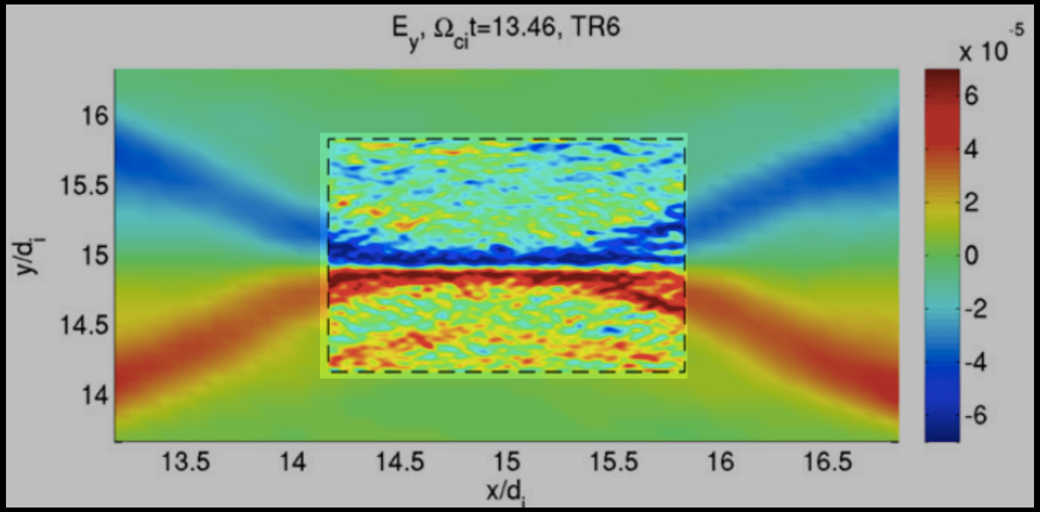


Generalized to 2D



[Beck et al. 2014]

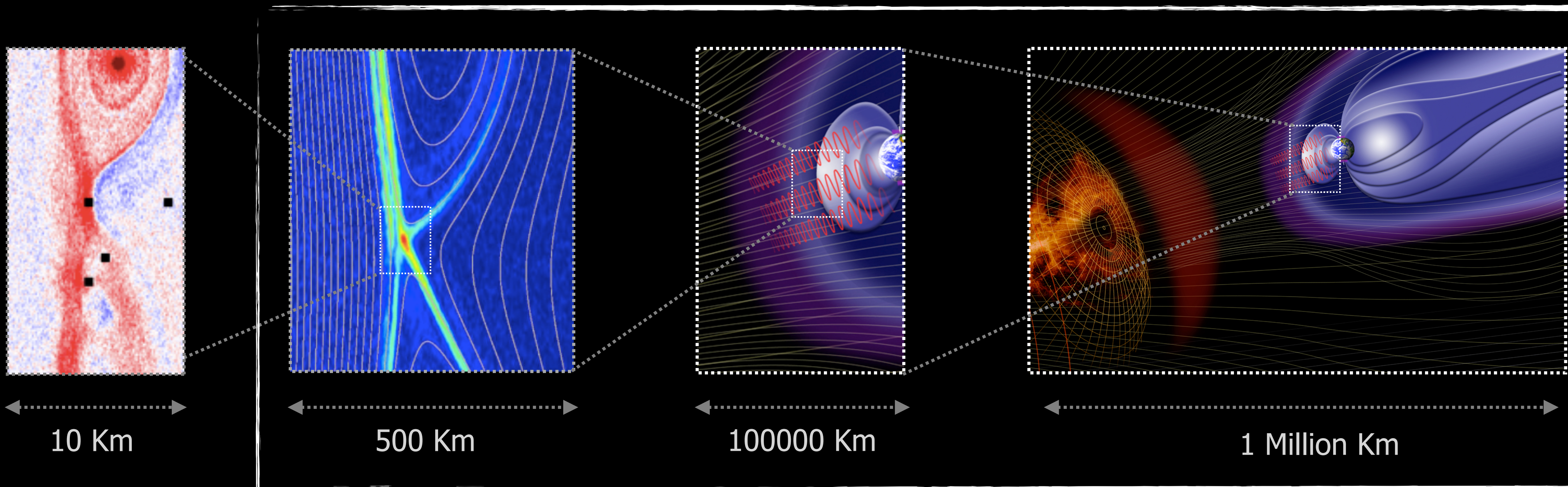
Time subcycling



[Innocenti et al. 2015]

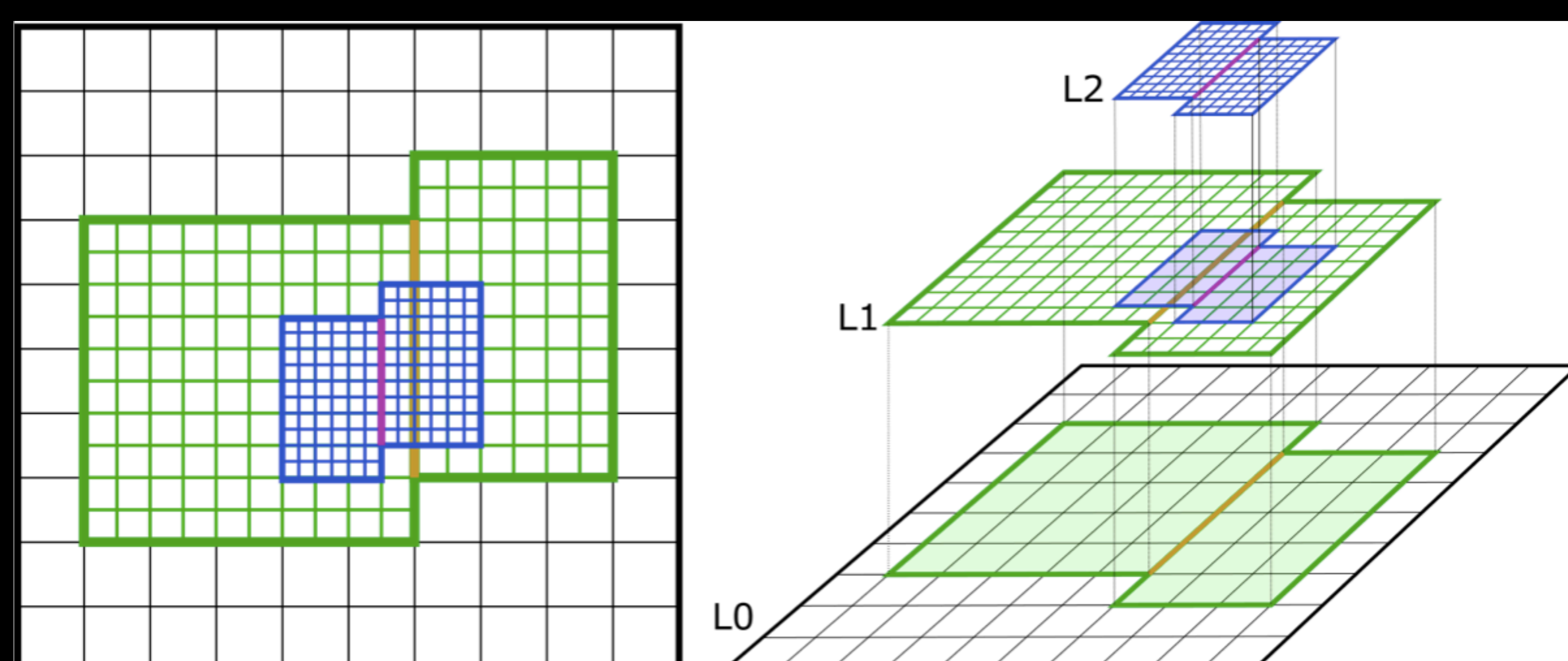
Unfortunately : home-made, limited to 1 (fixed) refined level (but with refined ratio>2)

PHARE: AMR Hybrid-PIC code



PHARE

Structured
Adaptive Mesh
Refinement



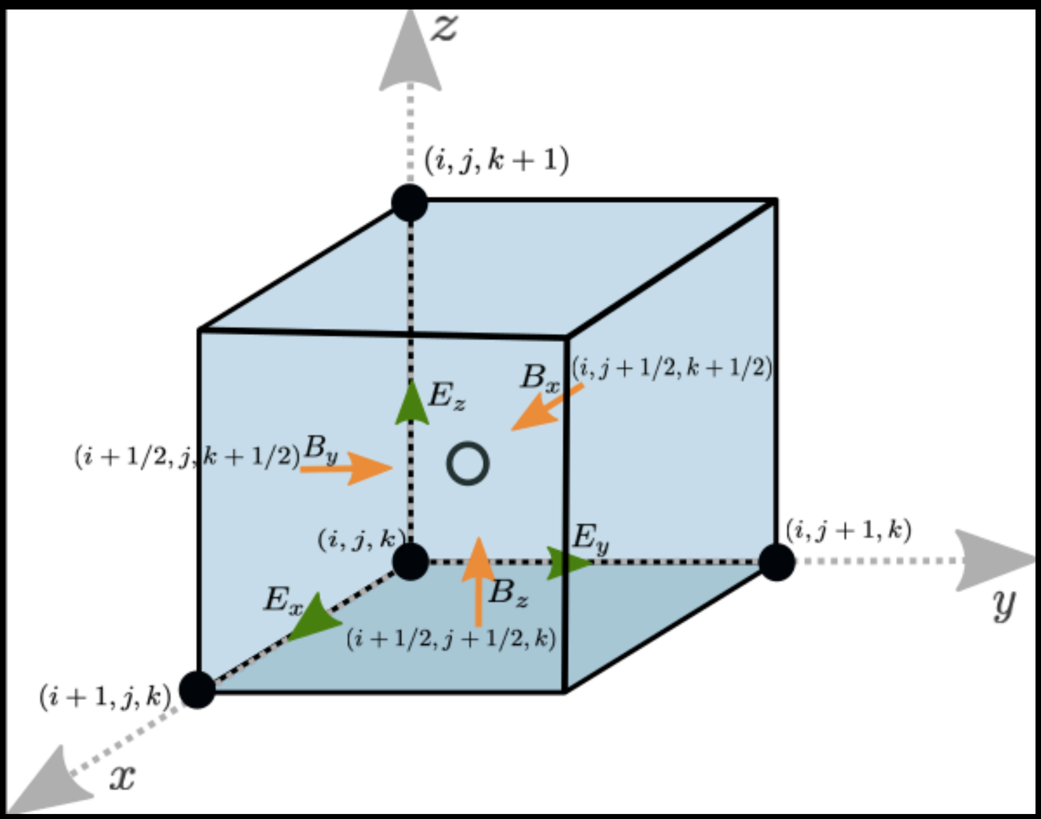
AMR Hybrid-PIC

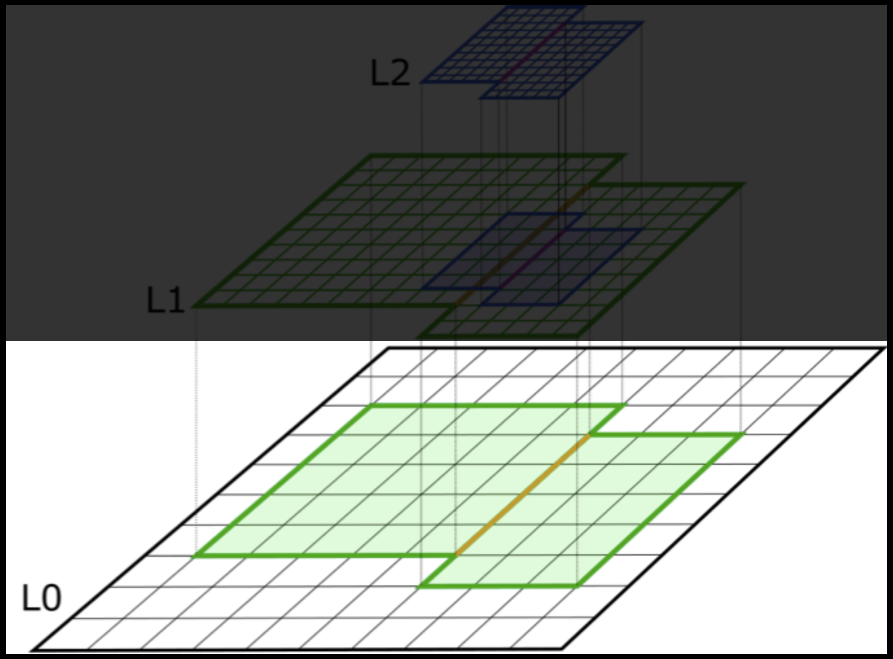
Hybrid or MHD?

SPATIAL DISCRETIZATION

Equations are discretized following the Yee layout [Yee 1966]

This conserves $\nabla \cdot \mathbf{B} = 0$ intrinsically





Iterated Crank-Nicholson
Predictor-Predictor-Corrector (PPC)
[Kunz al. 2014]

t

Prediction

$$\mathbf{B}_{p1}^{n+1} = \mathbf{B}^n - \Delta t \nabla \times \mathbf{E}^n$$

$$\mathbf{E}_{p1}^{n+1} = -\mathbf{u}^n \times \mathbf{B}_{p1}^{n+1} + \frac{\nabla \times \mathbf{B}_{p1}^{n+1}}{N^n} - \frac{\nabla \cdot \mathbf{P_e}}{N^n} + \eta \nabla \times \mathbf{B}_{p1}^{n+1} - \nu \nabla^2 \nabla \times \mathbf{B_{p1}^{n+1}}$$

$$(\mathbf{E}, \mathbf{B})^{n+1/2} =< (\mathbf{E}, \mathbf{B}) >_n^{n+1}$$

$$\mathbf{r}_{p1}^{n+1/2} = \mathbf{r}^n + \Delta t/2 \mathbf{v}^n$$

$$\mathbf{E}, \mathbf{B}\left(\mathbf{r_{p1}^{n+1/2}}\right) = \sum_{ijk} (\mathbf{E}, \mathbf{B}_{ijk})\, W\left(|\mathbf{r}_{ijk} - \mathbf{r}_{p1}^{n+1/2}|\right)$$

$$m_i \frac{d\mathbf{v}_{p1}^{n+1}}{dt} = e\left(\mathbf{v}^n \times + \mathbf{B}^{n+1/2} + \mathbf{E}^{n+1/2}\right)$$

$$N^{n+1} = \sum_p w_p \mathbf{v}_{p1}^{n+1} W\left(|\mathbf{r}_{ijk} - \mathbf{r}_{p1}^{n+1}|\right) \qquad u^{n+1} = \sum_p w_p \mathbf{v}_{p1}^{n+1} W\left(|\mathbf{r}_{ijk} - \mathbf{r}_{p1}^{n+1}|\right)$$

Prediction

$$\mathbf{B}_{p2}^{n+1} = \mathbf{B}^n - \Delta t \nabla \times \mathbf{E}^{n+1/2}$$

$$\mathbf{E}_{p2}^{n+1} = -\mathbf{u}^{n+1} \times \mathbf{B}_{p2}^{n+1} + \frac{\nabla \times \mathbf{B}_{p2}^{n+1}}{N^{n+1}} - \frac{\nabla \cdot \mathbf{P_e}}{N^{n+1}} + \eta \nabla \times \mathbf{B}_{p2}^{n+1} - \nu \nabla^2 \nabla \times \mathbf{B_{p2}^{n+1}}$$

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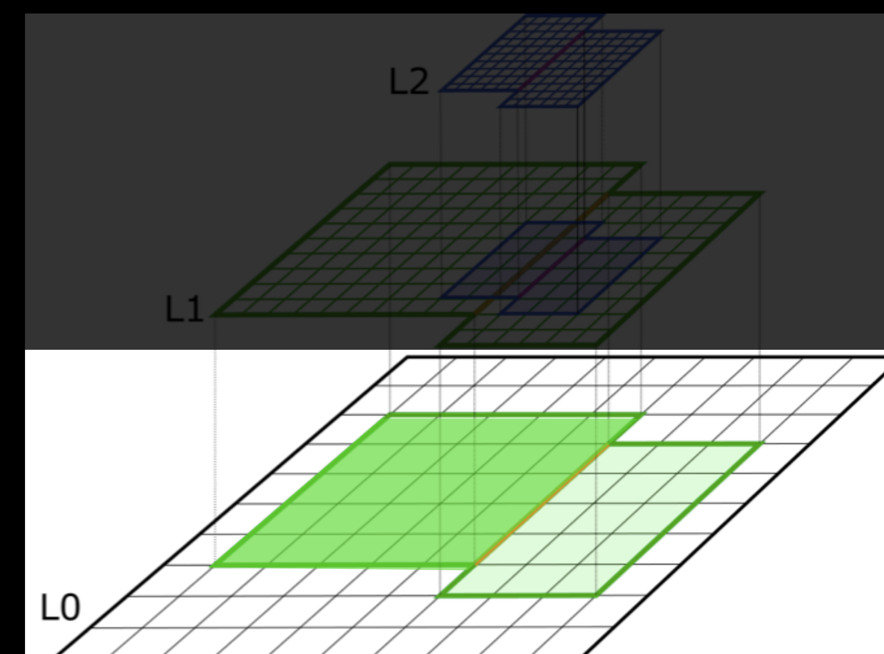
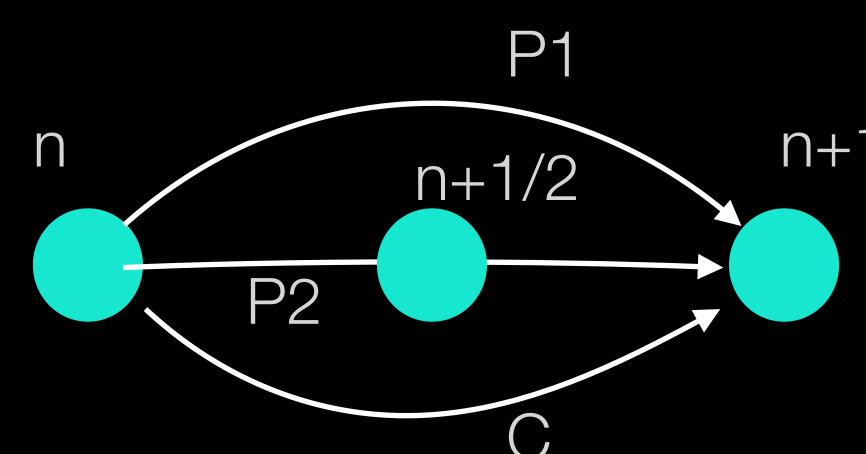
Correction

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

$$\mathbf{E}^{n+1} = -\mathbf{u}^{n+1} \times \mathbf{B}^{n+1} + \frac{\nabla \times \mathbf{B}^{n+1}}{N^{n+1}} - \frac{\nabla \cdot \mathbf{P_e}}{N^{n+1}} + \eta \nabla \times \mathbf{B}^{n+1} - \nu \nabla^2 \nabla \times \mathbf{B^{n+1}}$$

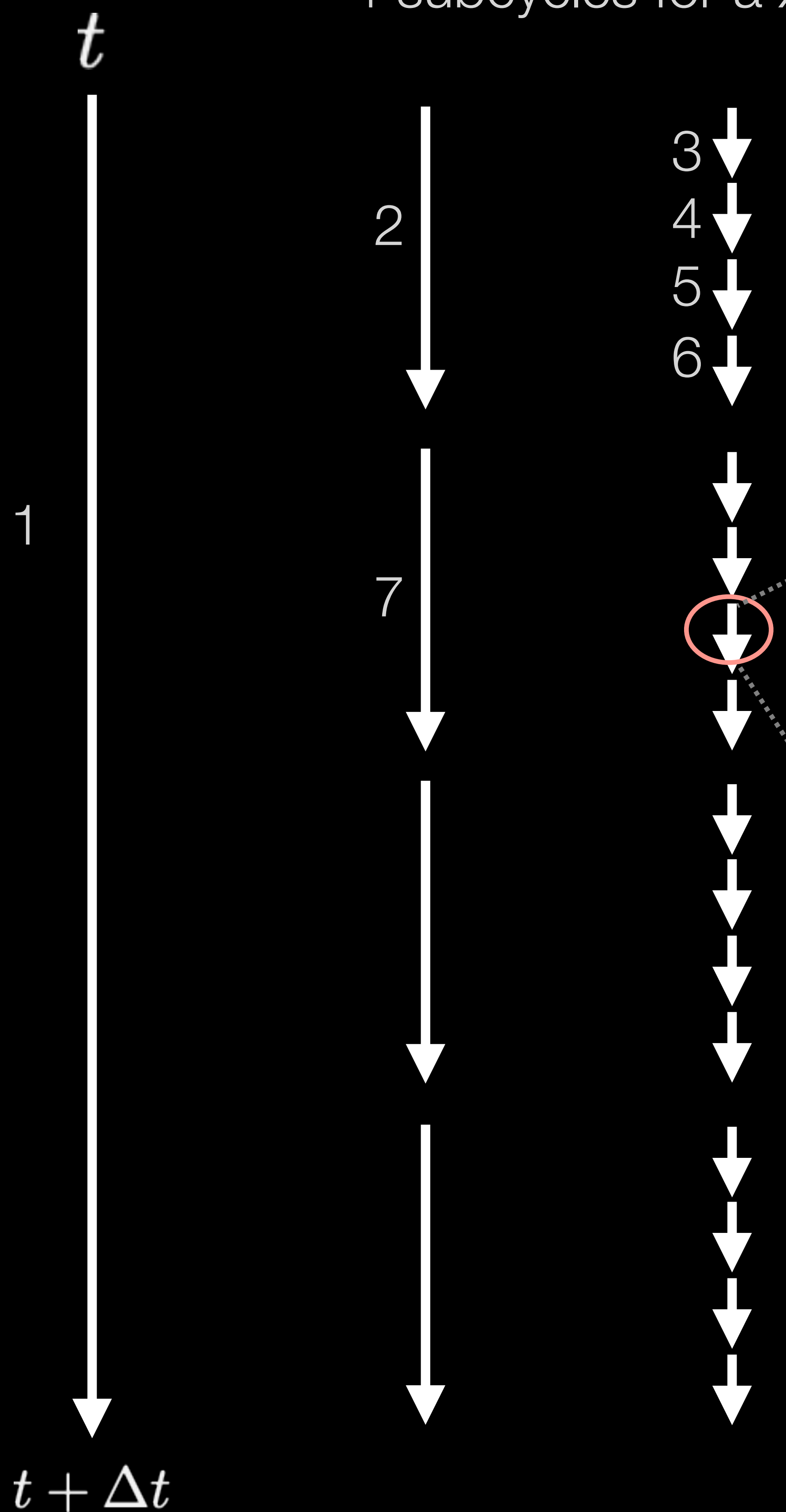
$t + \Delta t$





Recursive time stepping

4 subcycles for a x2 refinement ratio : whistler wave CFL



PPC step

Prediction

$$\mathbf{B}_{p1}^{n+1} = \mathbf{B}^n - \Delta t \nabla \times \mathbf{E}^n$$

$$\mathbf{E}_{p1}^{n+1} = -\mathbf{u}^n \times \mathbf{B}_{p1}^{n+1} + \frac{\nabla \times \mathbf{B}_{p1}^{n+1}}{N^n} - \frac{\nabla \cdot \mathbf{P_e}}{N^n} + \eta \nabla \times \mathbf{B}_{p1}^{n+1} - \nu \nabla^2 \nabla \times \mathbf{B_{p1}^{n+1}}$$

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Prediction

$$\mathbf{B}_{p2}^{n+1} = \mathbf{B}^n - \Delta t \nabla \times \mathbf{E}^{n+1/2}$$

$$\mathbf{E}_{p2}^{n+1} = -\mathbf{u}^{n+1} \times \mathbf{B}_{p2}^{n+1} + \frac{\nabla \times \mathbf{B}_{p2}^{n+1}}{N^{n+1}} - \frac{\nabla \cdot \mathbf{P_e}}{N^{n+1}} + \eta \nabla \times \mathbf{B}_{p2}^{n+1} - \nu \nabla^2 \nabla \times \mathbf{B_{p2}^{n+1}}$$

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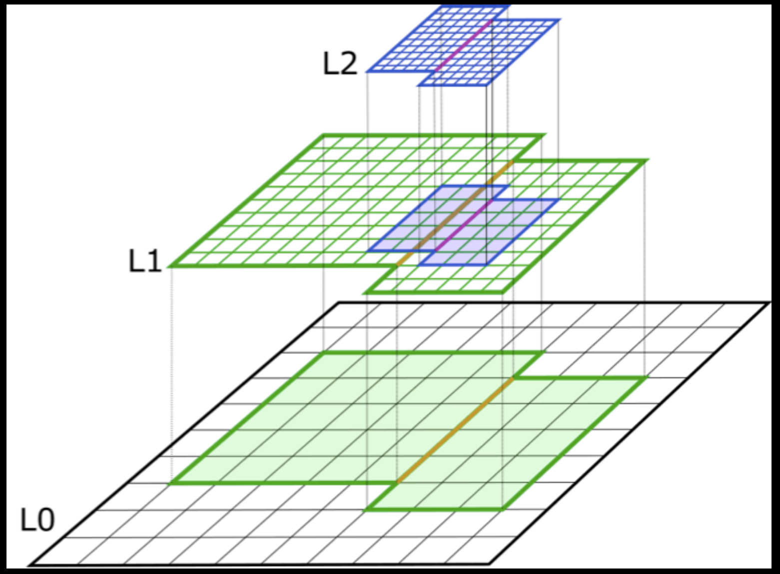
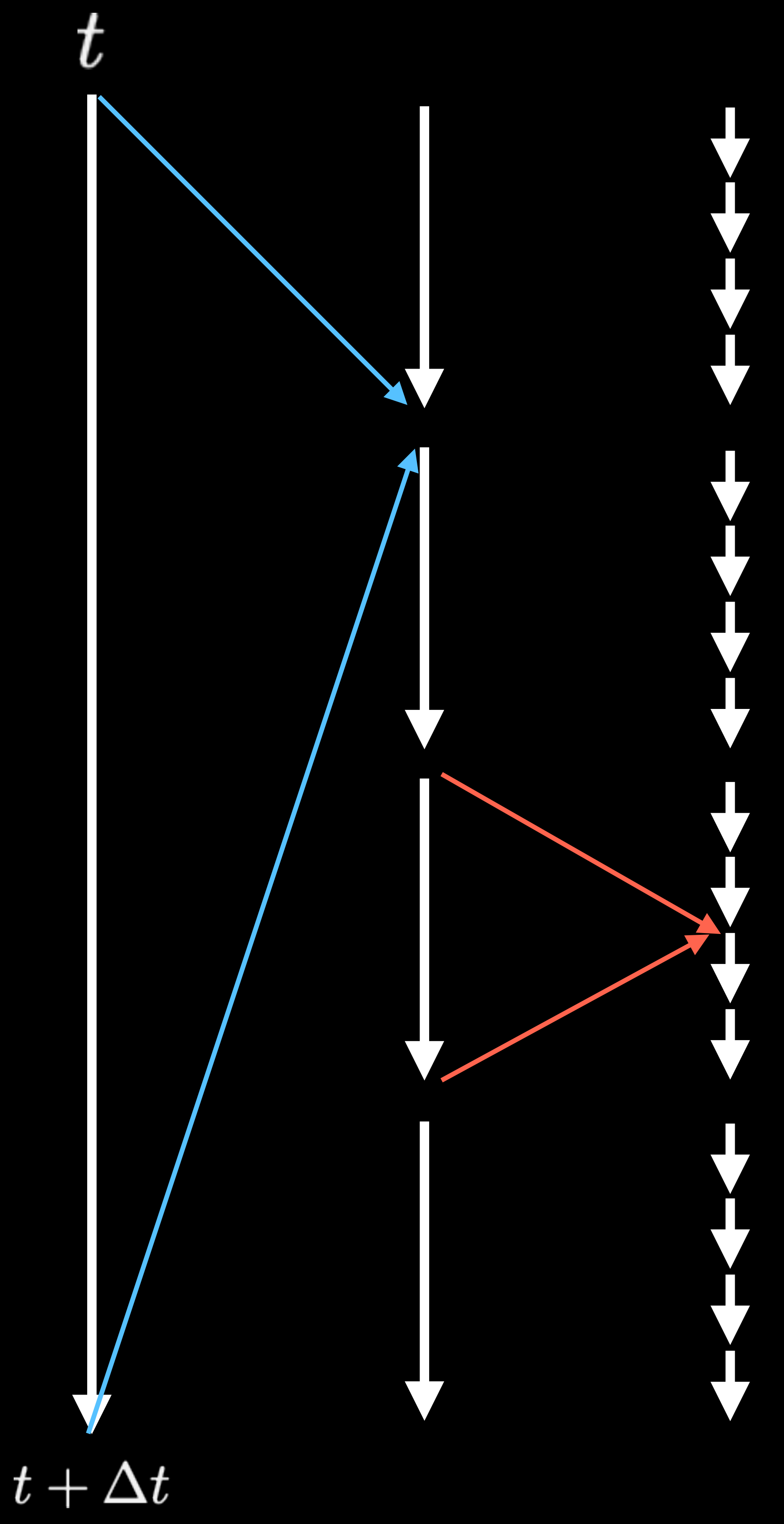
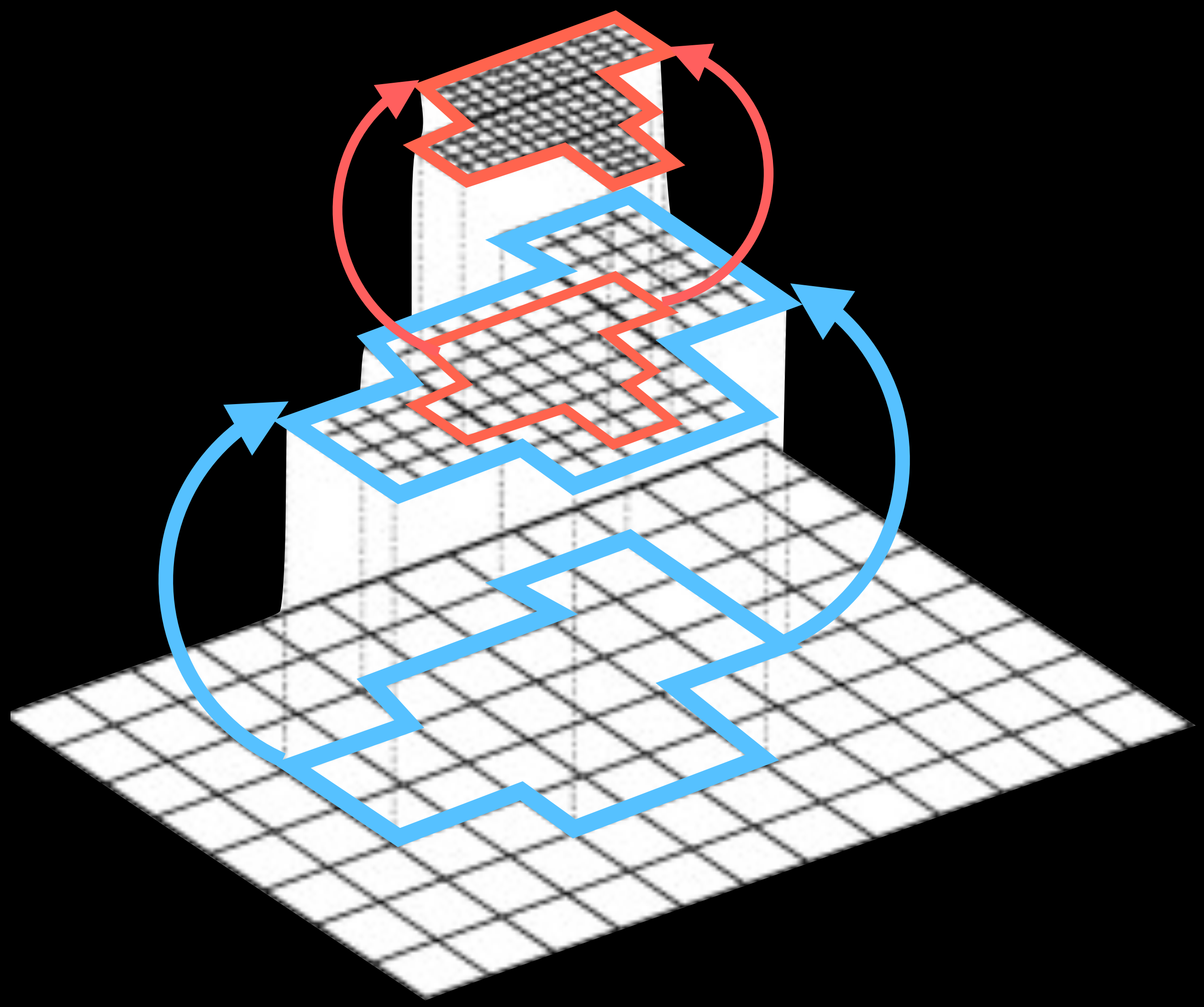


Third party AMR lib : LLNL/SAMRAI

Coarse region are evolved 4x less often than next finer

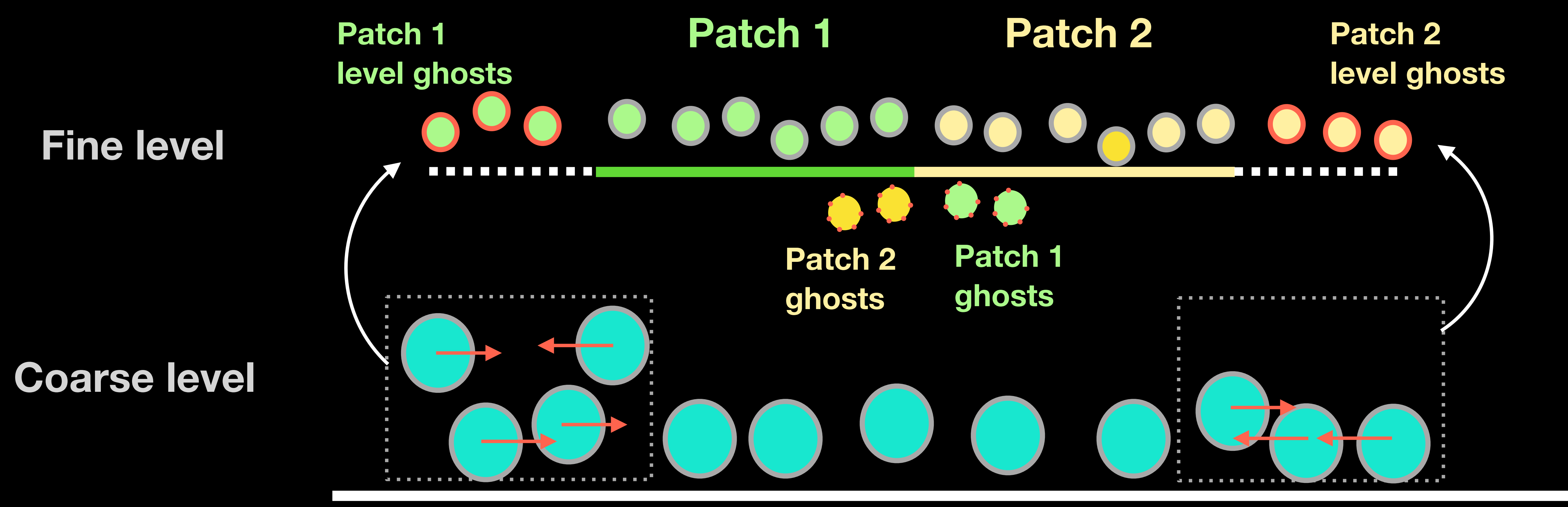
Coarse solution is time/space interpolated on fine boundaries

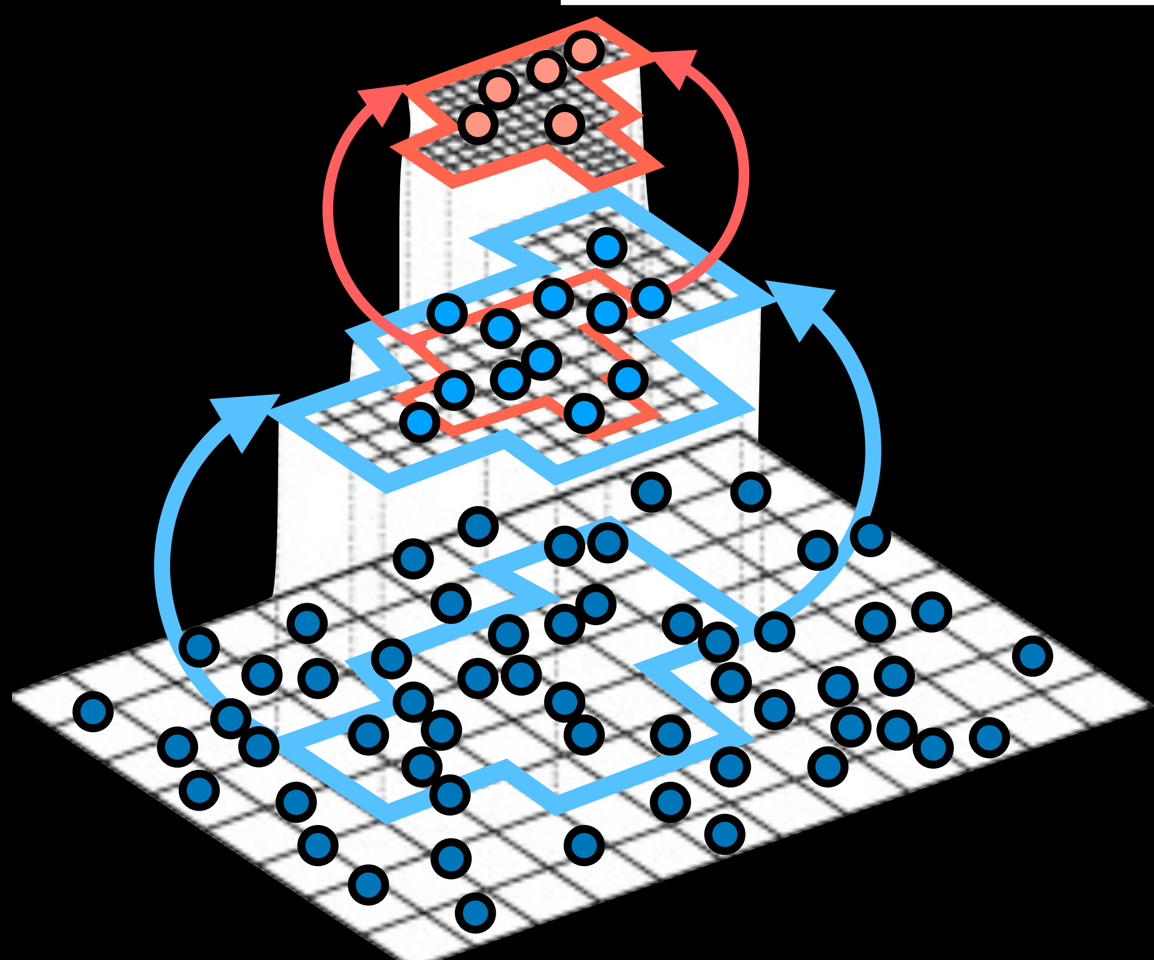


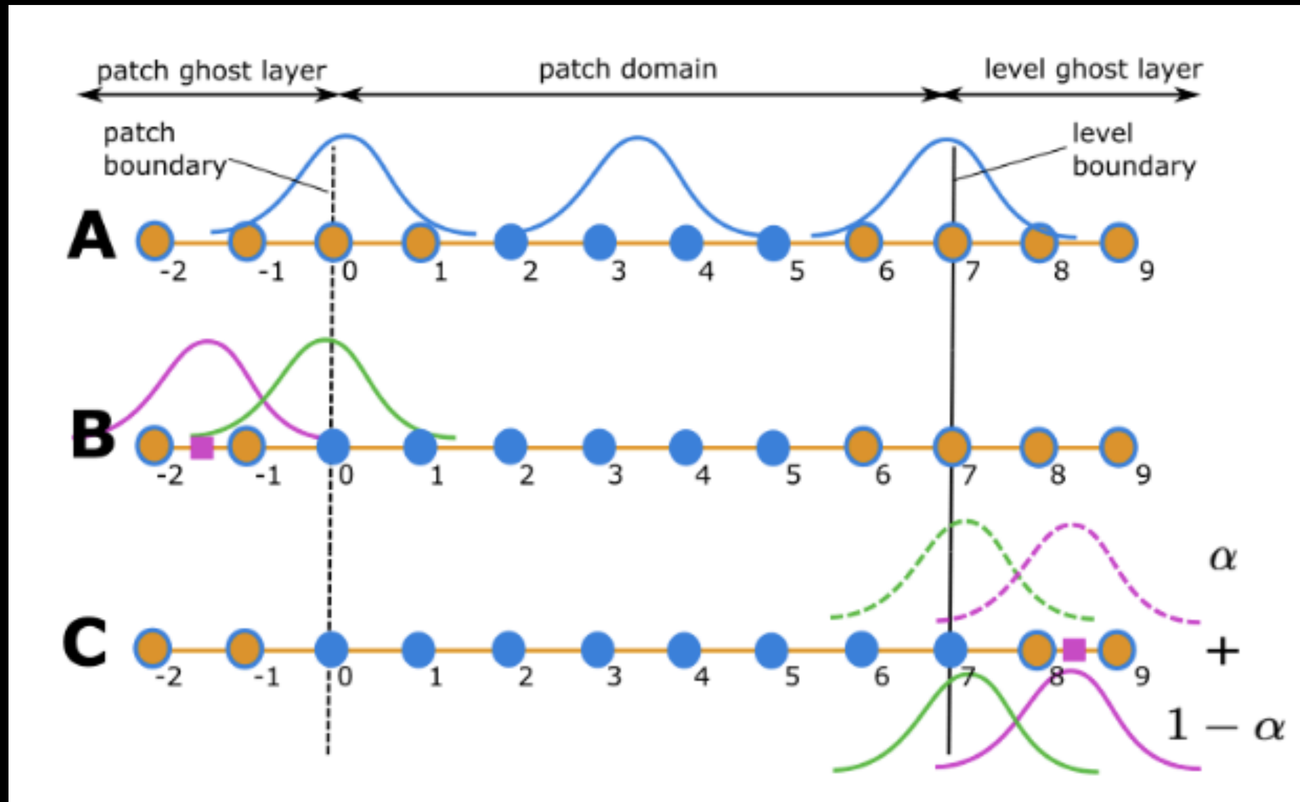


Coarse solution is linearly interpolated in time and then linearly interpolated in space on the refined grid.

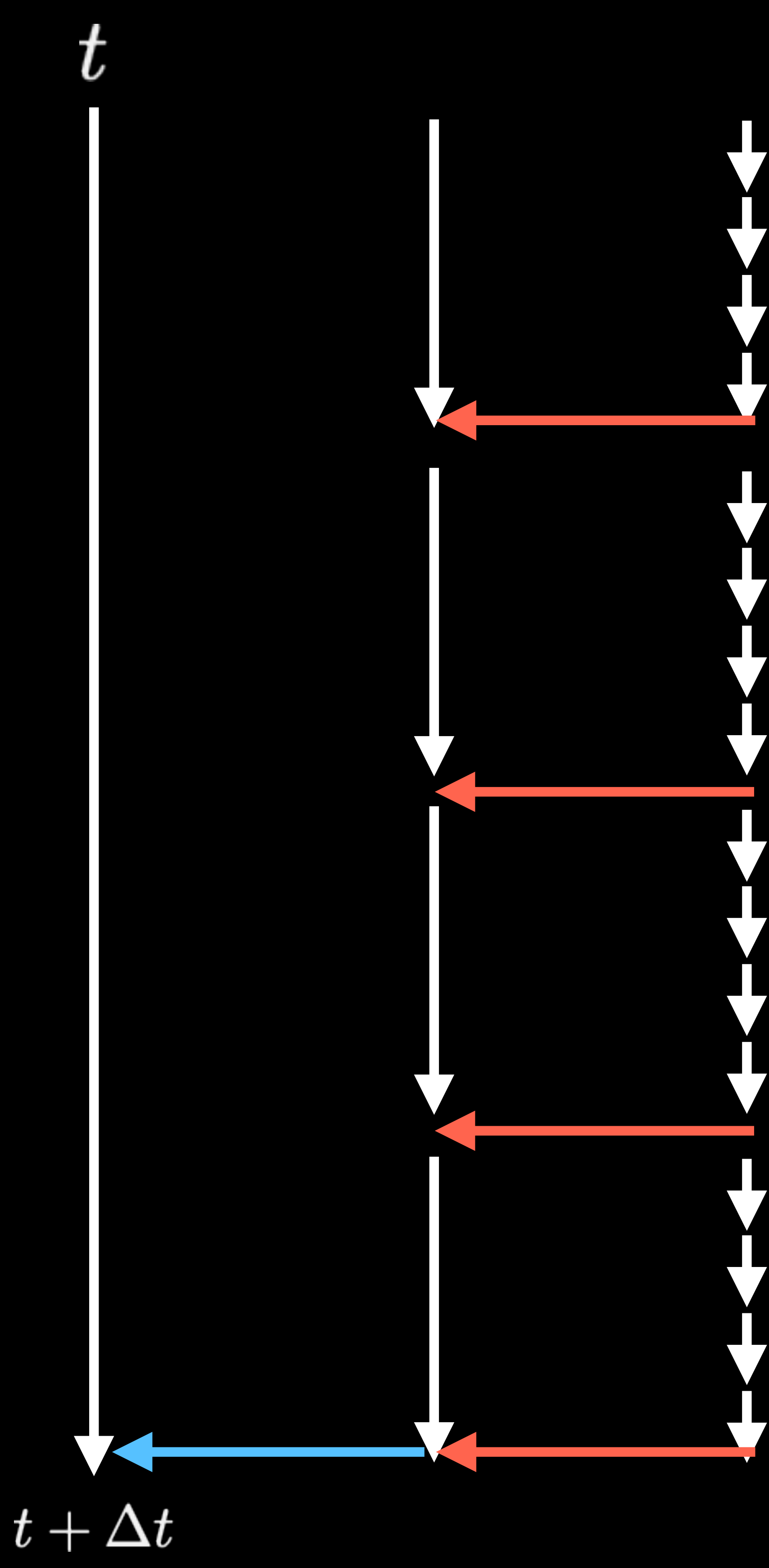
Coarse solution is time/space interpolated on fine boundaries



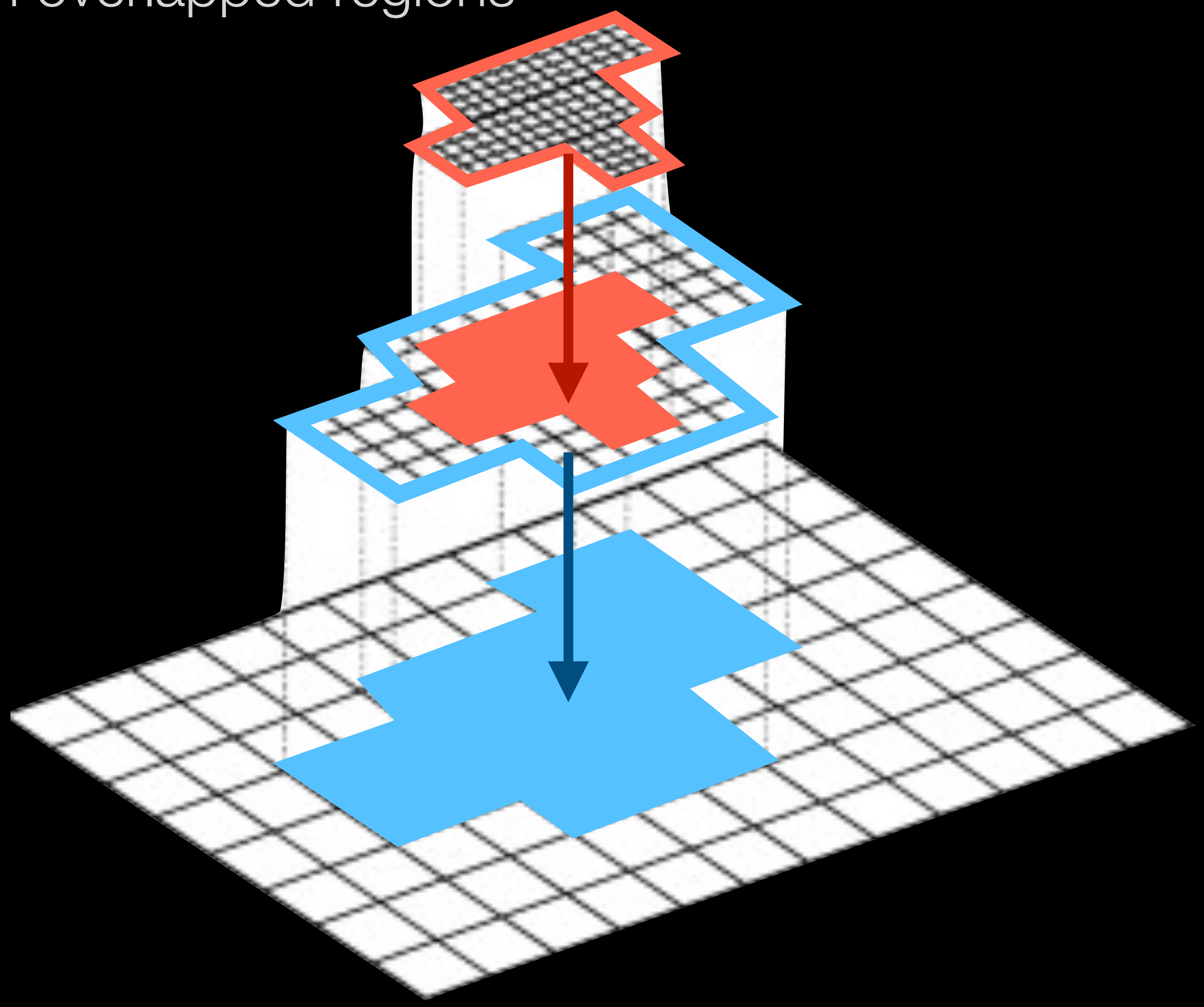


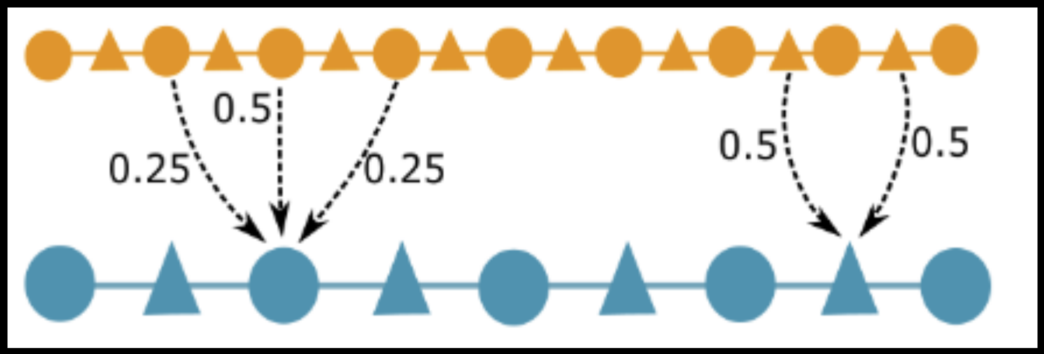


Fine solution are interpolated on the coarser underlying patches



Once a fine level has reached the next coarser time, the fine solution is coarsened and overwrites the coarse solution in overlapped regions





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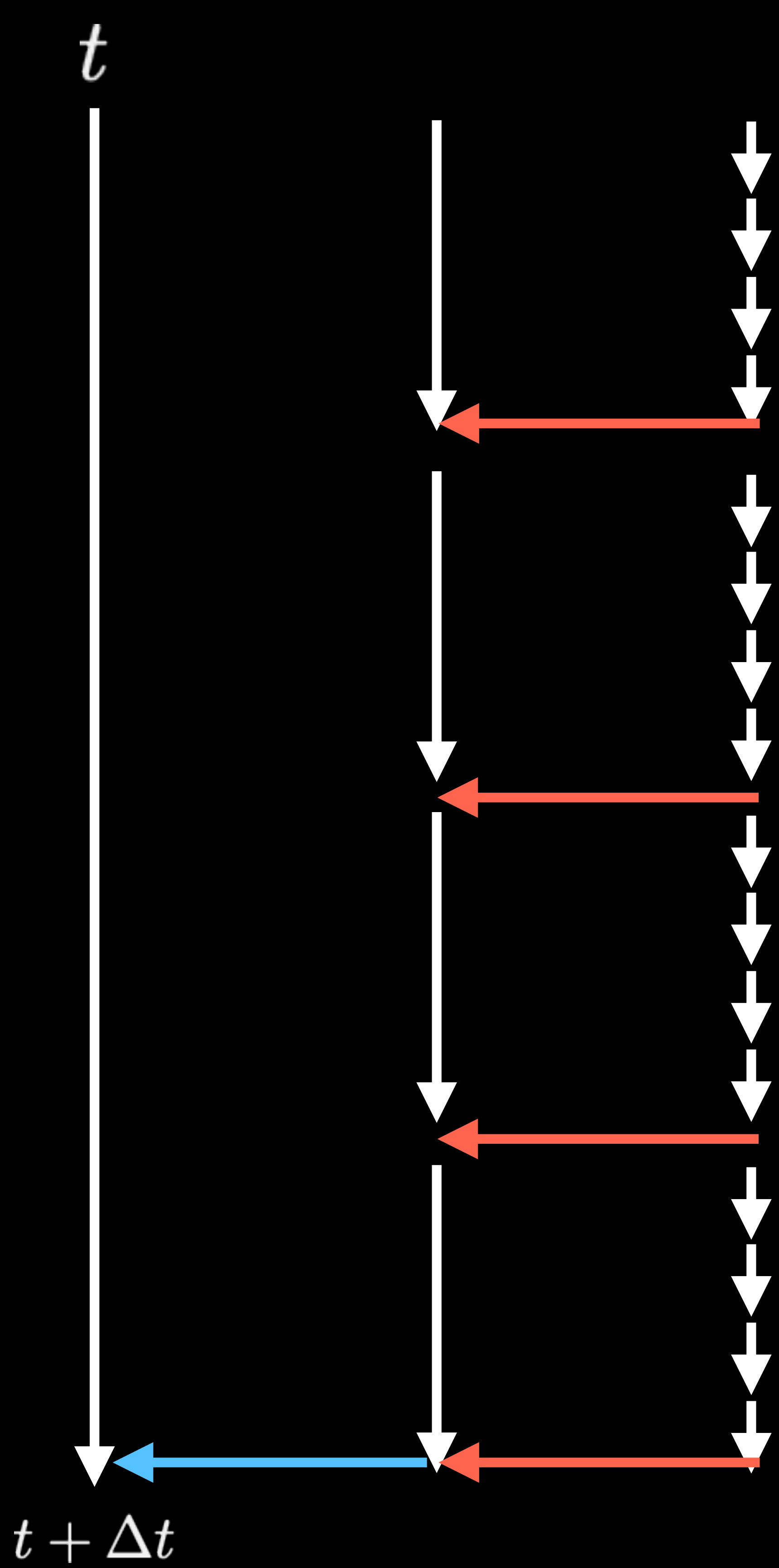

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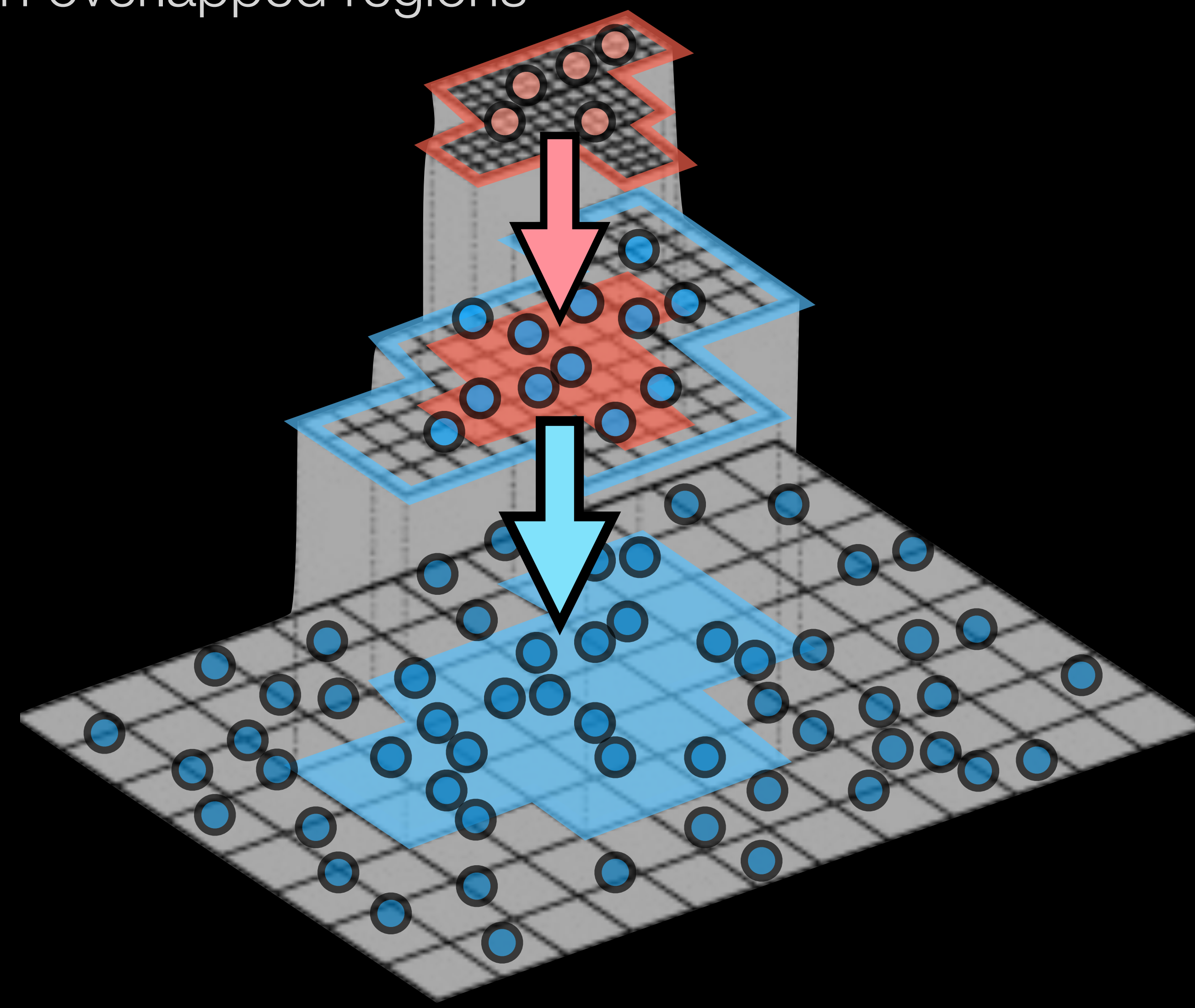
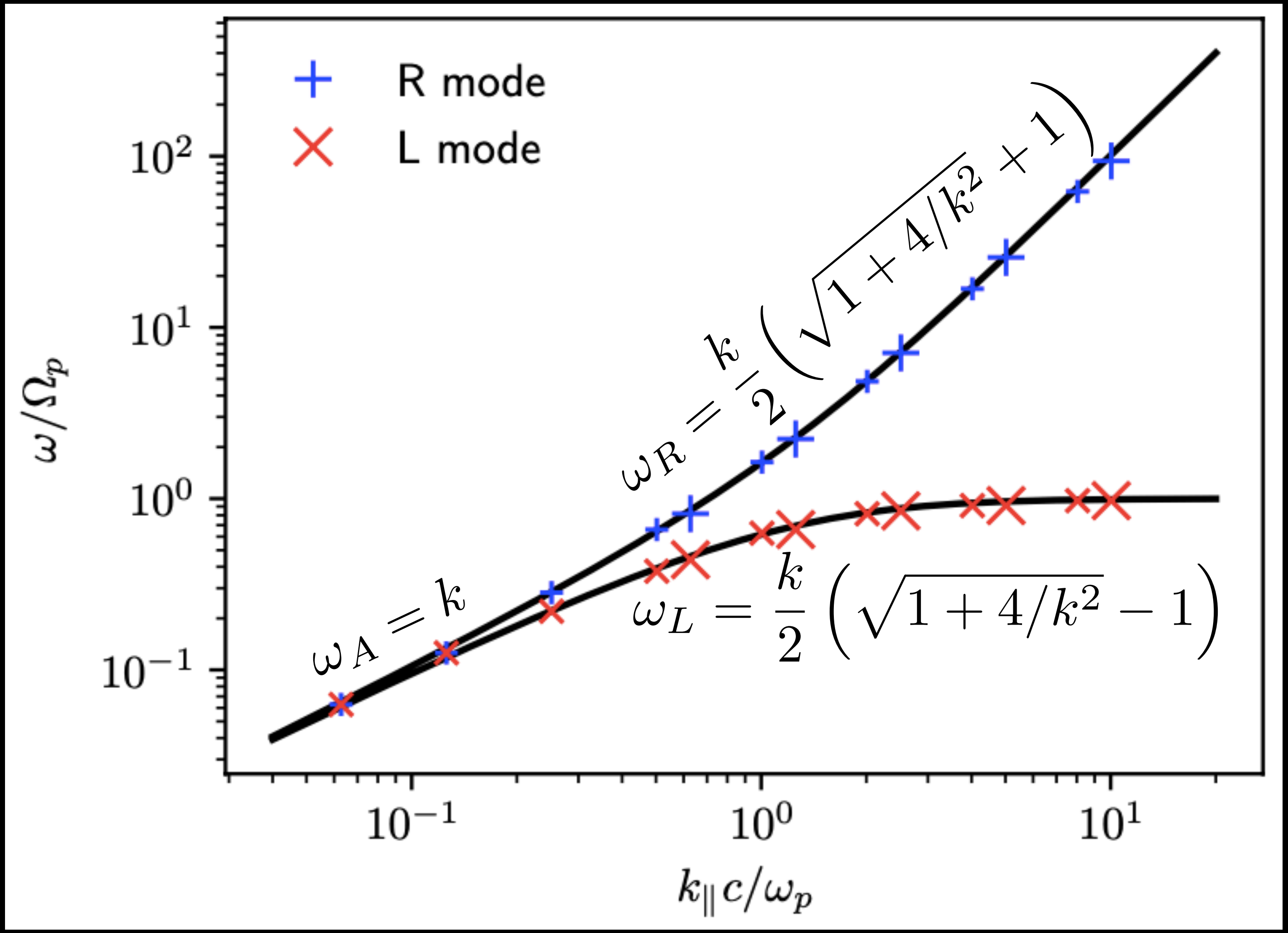


Coarse particles evolve with electromagnetic fields constantly updated by the fine solution and stay synchronized

VALIDATION OF THE HYBRID SOLVER : WAVE DISPERSION

Dispersion diagram of parallel waves



Small and large crosses represent 1D and 2D

whistler and ion cyclotron waves

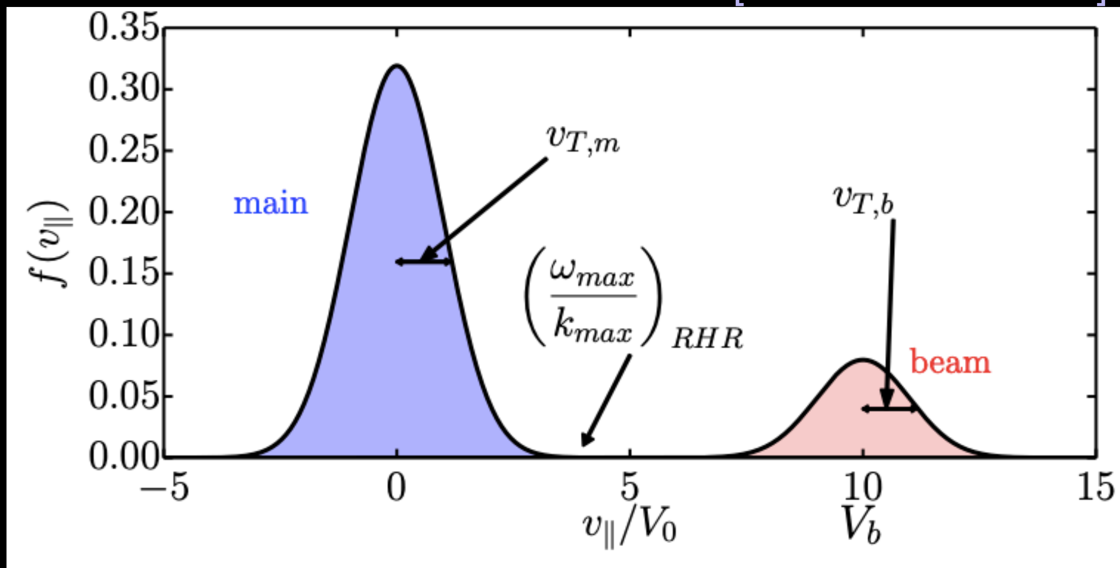
$$\omega_{L,R} = \frac{k}{2}\left(\sqrt{1+4/k^2}\pm 1\right)$$

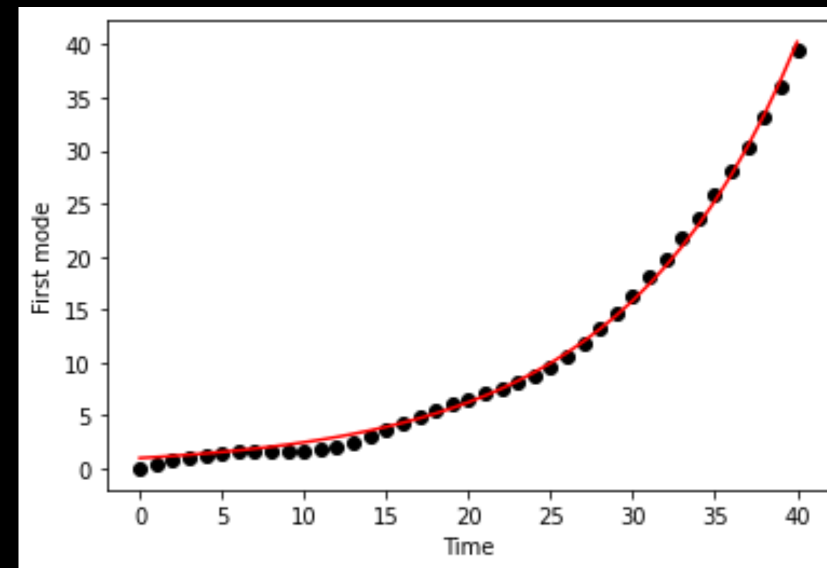
Alfvén waves

$$\omega_A = k$$

1D VALIDATION : RIGHT HAND ION STREAMING INSTABILITY

[Nicolas et al. 2018]





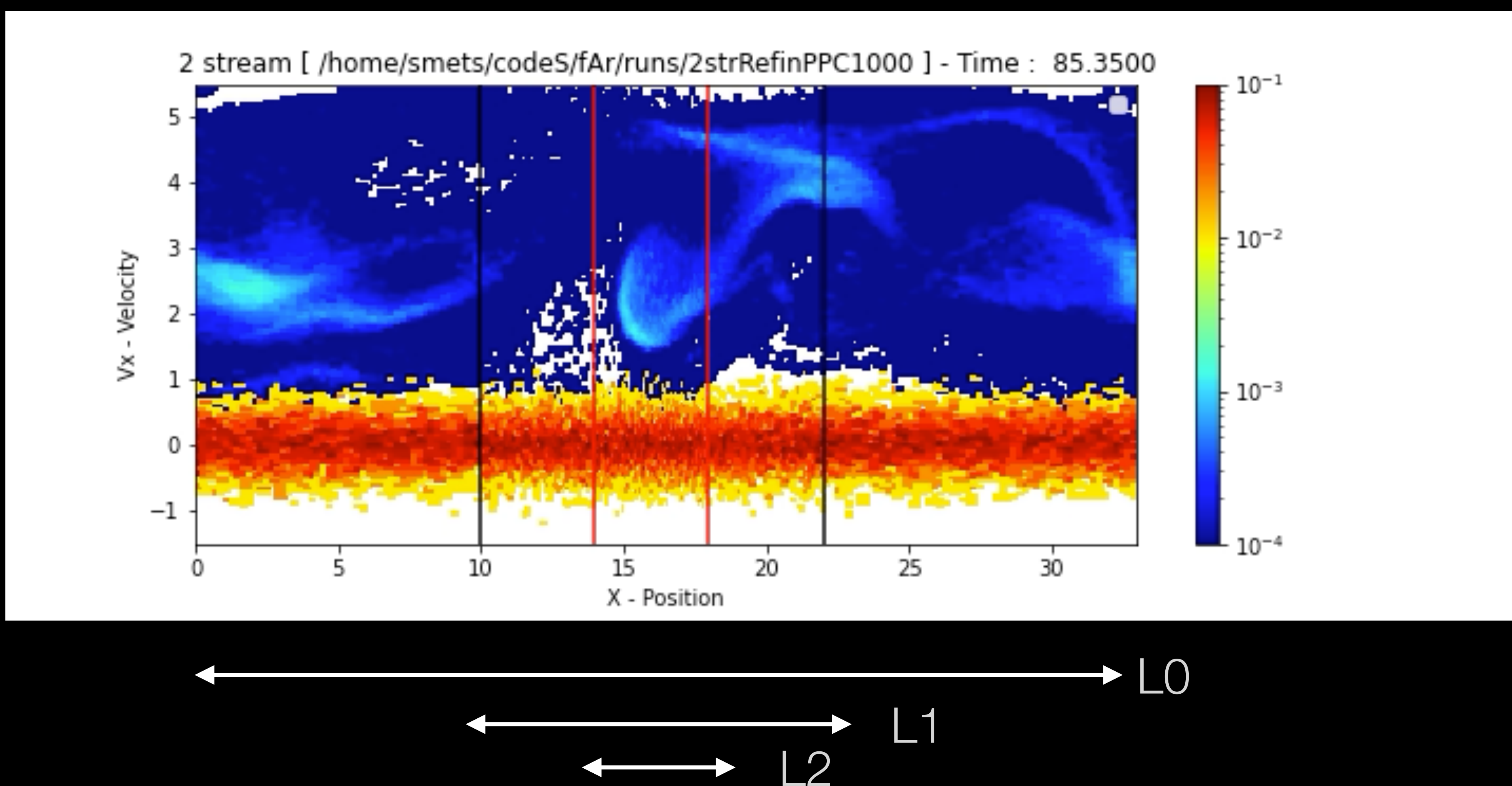
$T_i = T_e = 0.1 \quad V_b = 5$

$n_m = 1 \quad n_b = 0.01$

Linear theory $\gamma_{th} \approx 0.09$

Model :

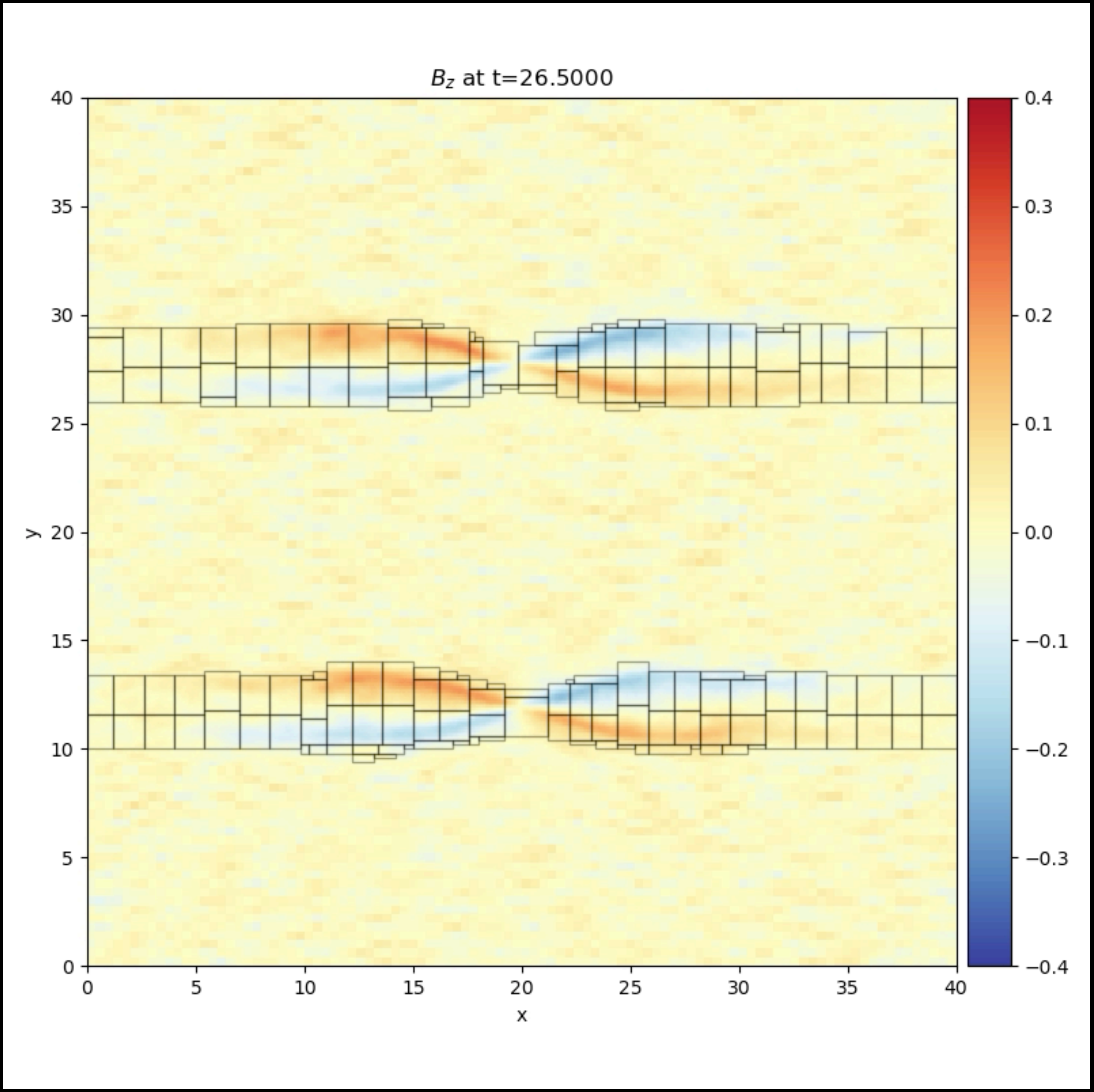
$\gamma_{sim} \approx 0.0908 \pm 0.0053$



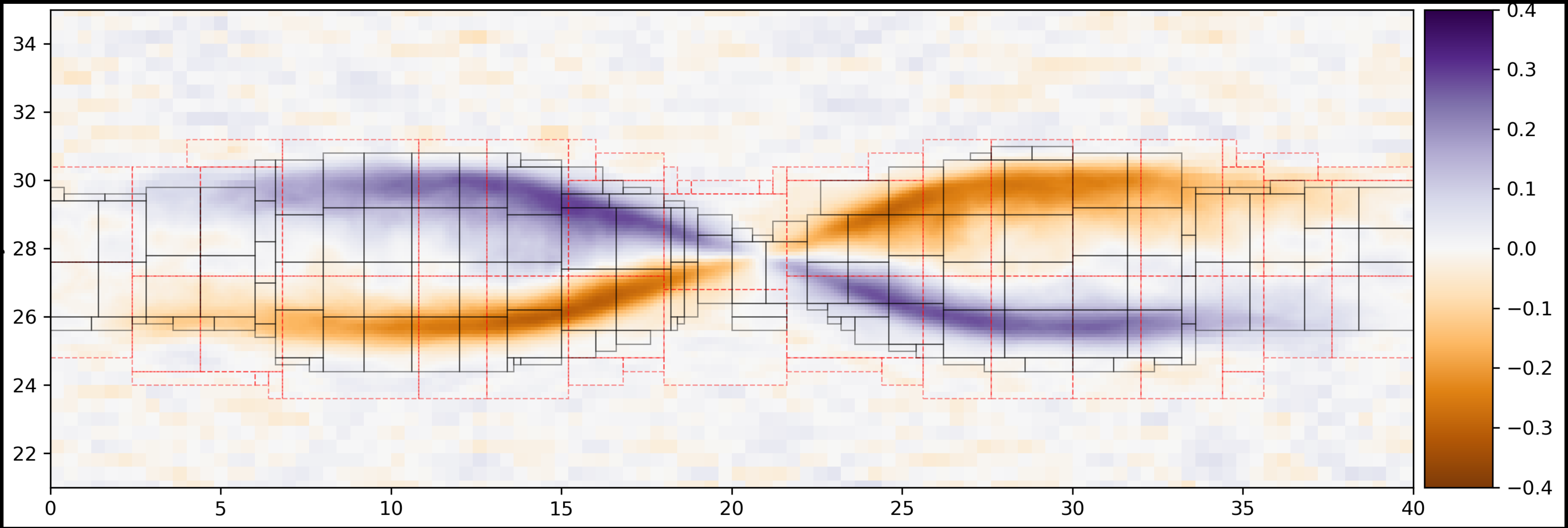
Phase space diagram

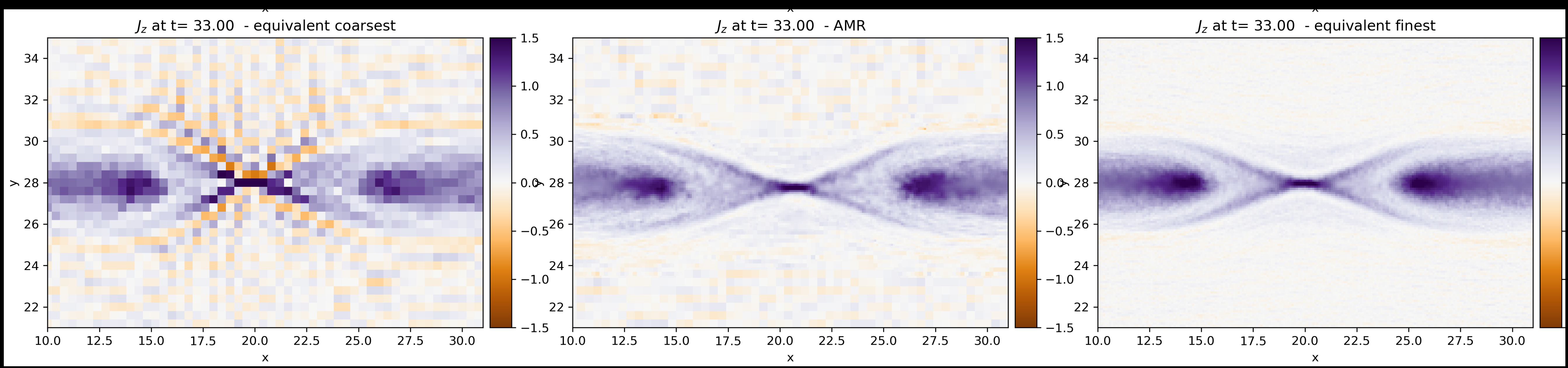
Structures cross level boundaries without any issue (ouf !)

2D MAGNETIC RECONNECTION



2D MAGNETIC RECONNECTION





[Aunai et al. in prep]

A CODE FOR THE COMMUNITY

100% open source	High perf. Abstractions	Ergonomy	Tested

- Aim at **high performance** while maintaining a **super user friendly** (python) interface
- Target users: simulation **experts and non experts** (observers, students…), classes
- Extensive unit (>1000) and functional tests at each merge and nightly builds to get a **robust code** that **can be upgraded and maintained**