Challenges in fluid, hybrid, and kinetic simulation of Heliophysics phenomena

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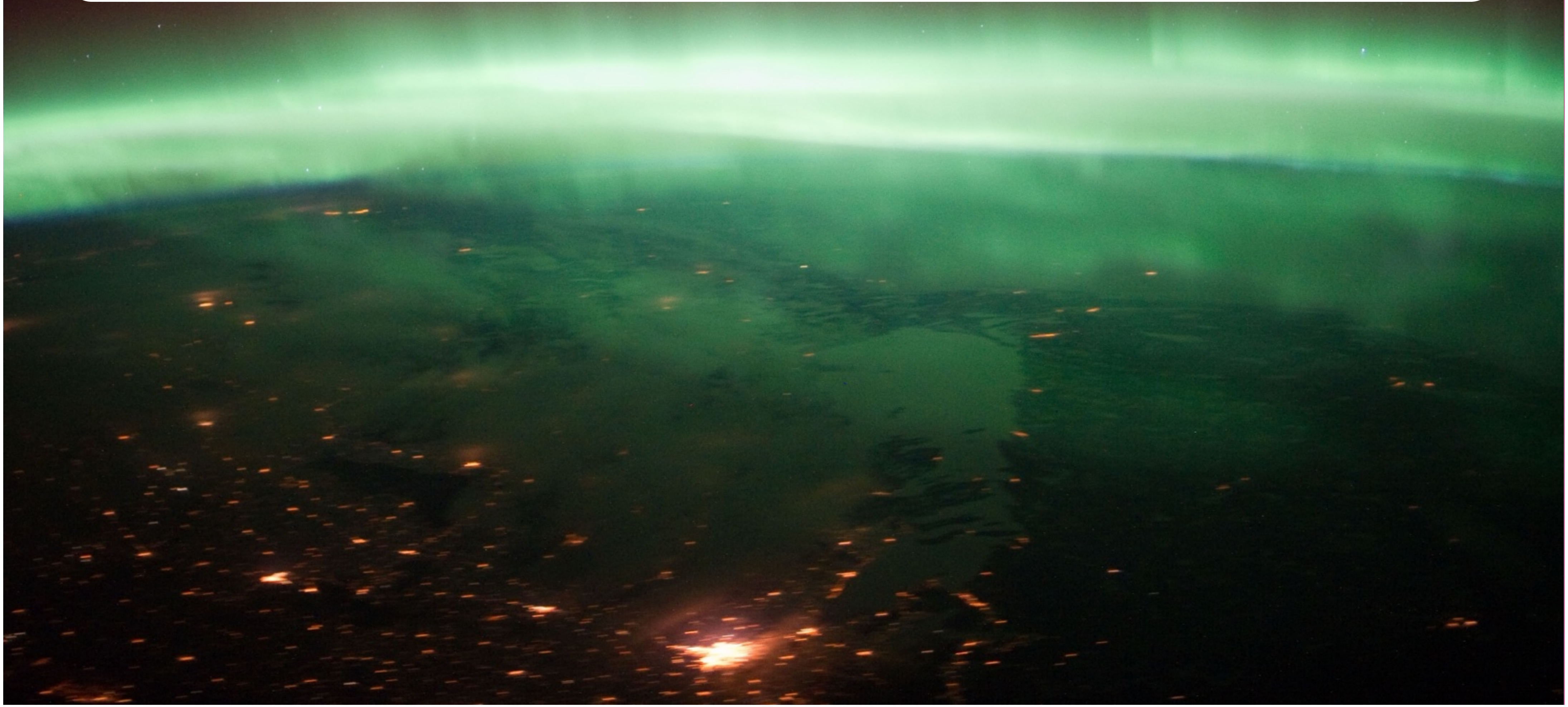
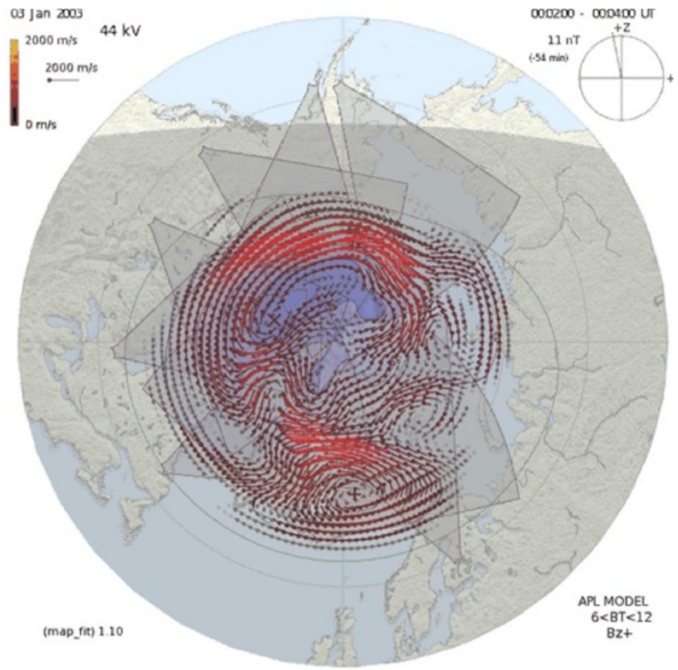
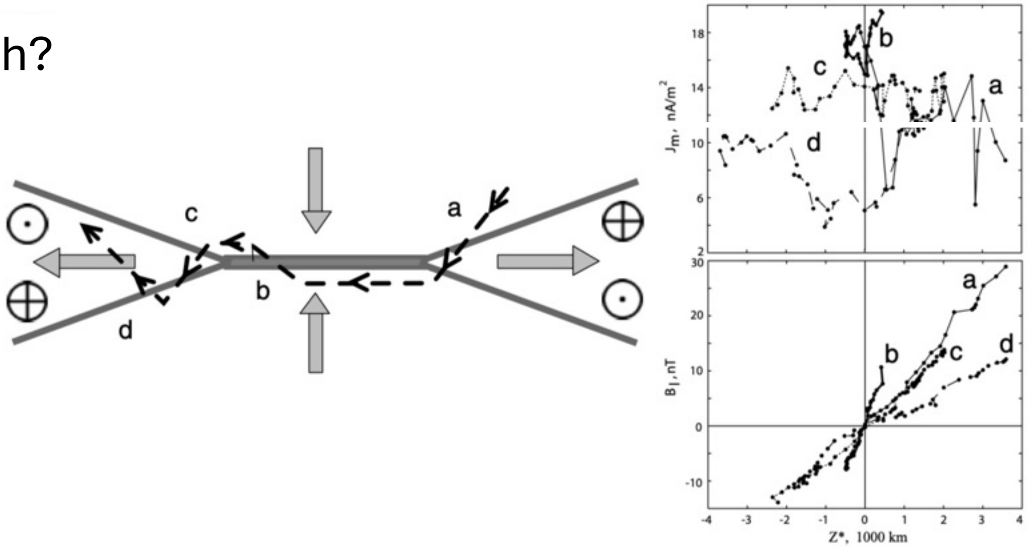
- **About nomenclature: *scales***
- Brief reminder of what are fluid, hybrid, and kinetic descriptions
- Modelling space plasmas with different plasma descriptions
- Example of scale coupling
- Challenges and future of modelling



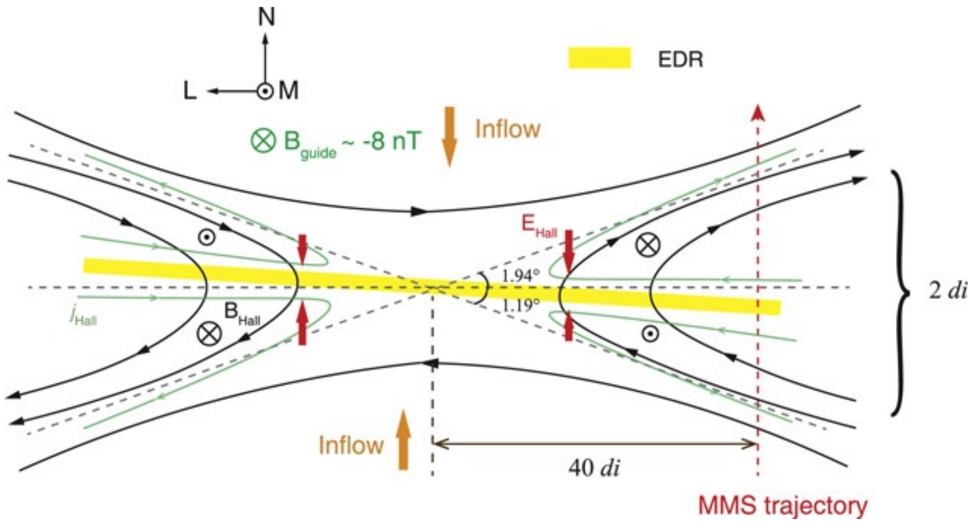
- **What do “scales” mean? / Observations**
    - Nomenclature: Large – meso – micro. OR: Fluid – ion – electron.
        - Dimension OR physics? Or both?



SuperDARN radar observations of ionospheric plasma circulation



Cluster observations of current sheet structure around reconnection region (Runov et al., 2005)



MMS observations of electron-only reconnection (Huang et al., 2021)

- **What do “scales” mean? / Simulations**
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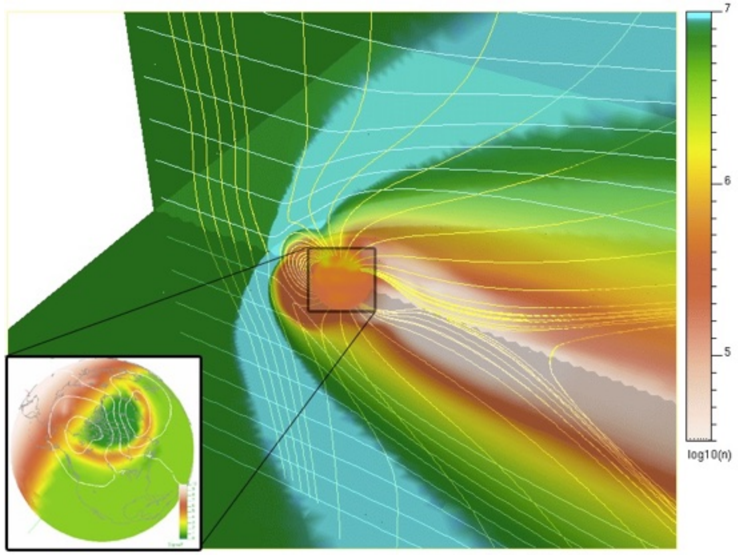
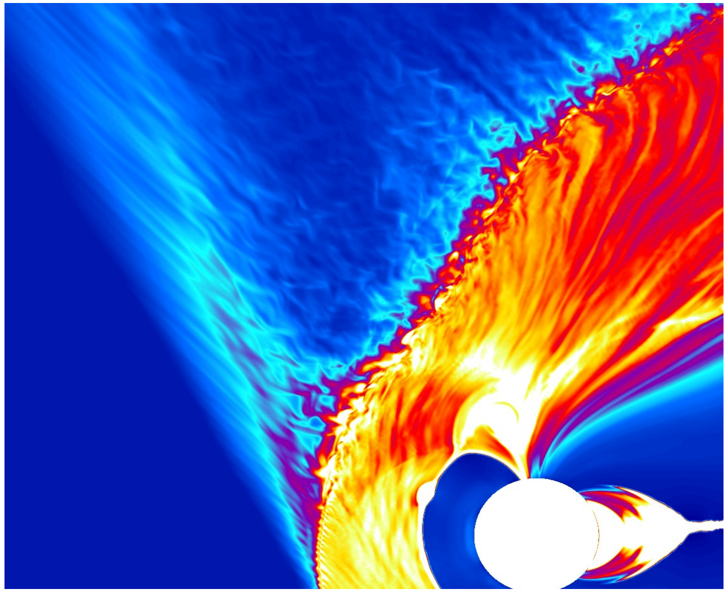
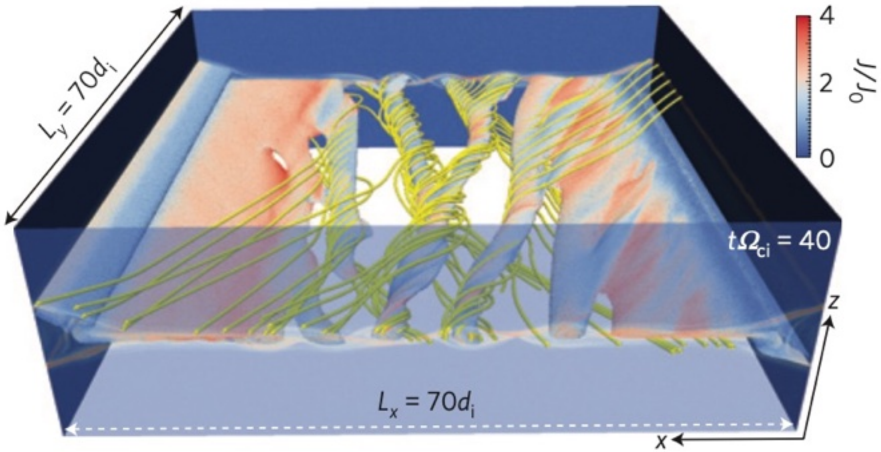
    - Dimension OR physics? Or both?



GUMICS-5 MHD simulation of magnetosphere – ionosphere coupling



Vlasiator simulation of foreshock – magnetosheath interaction



Fully kinetic simulation of reconnection (Daughton et al. 2011)

If we were able to make a global magnetospheric simulation

- At “electron scales” (i.e., fully kinetic global simulation), would that be a large-scale simulation? Or a small-scale simulation? Or a meso-scale simulation?
  - Answer is: YES.
- At “fluid scales” (i.e., MHD simulation), would that be a large-scale simulation? Or a small-scale simulation? Or a meso-scale simulation?
  - Answer is: large-scale (or fluid-scale) simulation

Logical deduction of the above is therefore

- In modelling, *scales* are very much a concept based on MHD
- Division to *scales* becomes obsolete when moving beyond MHD
  - Ion-kinetic global simulations are inherently producing ion-kinetic physics at the global scale, even though using the definition of micro – meso – large *scales* they would be meso- or micro-scale.
  - Satellite observations have always been at electron or ion *scales*, because it is the nature which is being observed. (Is it even possible to make fluid-scale observations?)

➔ **Hence, in modelling, people should not anymore talk about fluid, meso or micro *scales*, but fluid, hybrid, kinetic *physics*, whatever the dimension of the problem is.**

What is scale-coupling?

- Phenomena, in which dimensionally large features emerge from electron or ion kinetic physics
  - Prime example: Plasma eruptions (substorms, flares, CMEs)
  - Or: Reconnection initiated by electron or ion physics
- Or phenomena in which large features drive consequences detected in electrons or ions
  - For example: Reconnection driven by external conditions

We do not fundamentally understand scale coupling

- Observations: There are great satellites and satellite constellations, and ground-based instruments, but we can never cover the entire region of interest with observations
- Simulations: Nowadays we have large-scale ion-hybrid simulations, but kinetic (explicit) electrons will be impossible also in the foreseeable future
  - Seem Markidis' work with implicit schemes
- ➔ How to reconcile?

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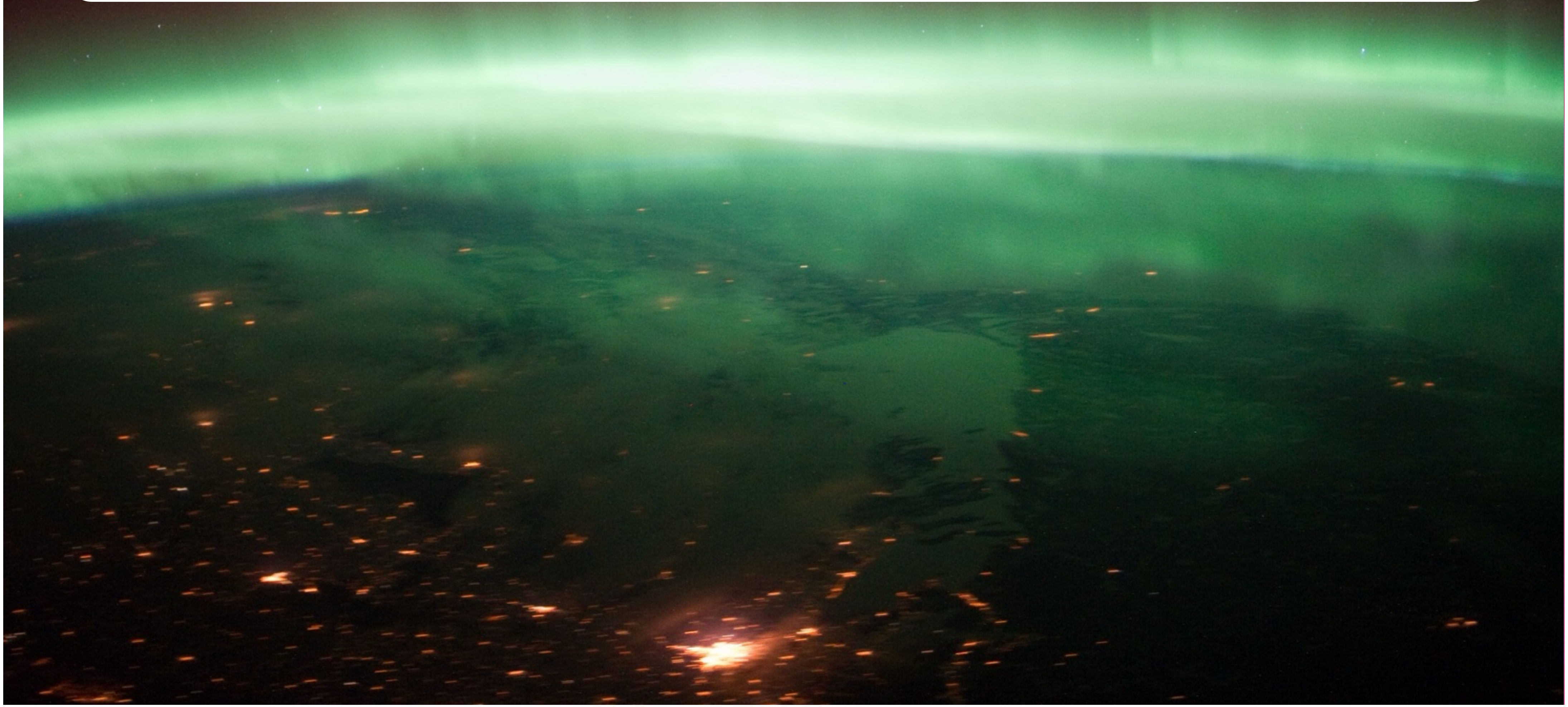
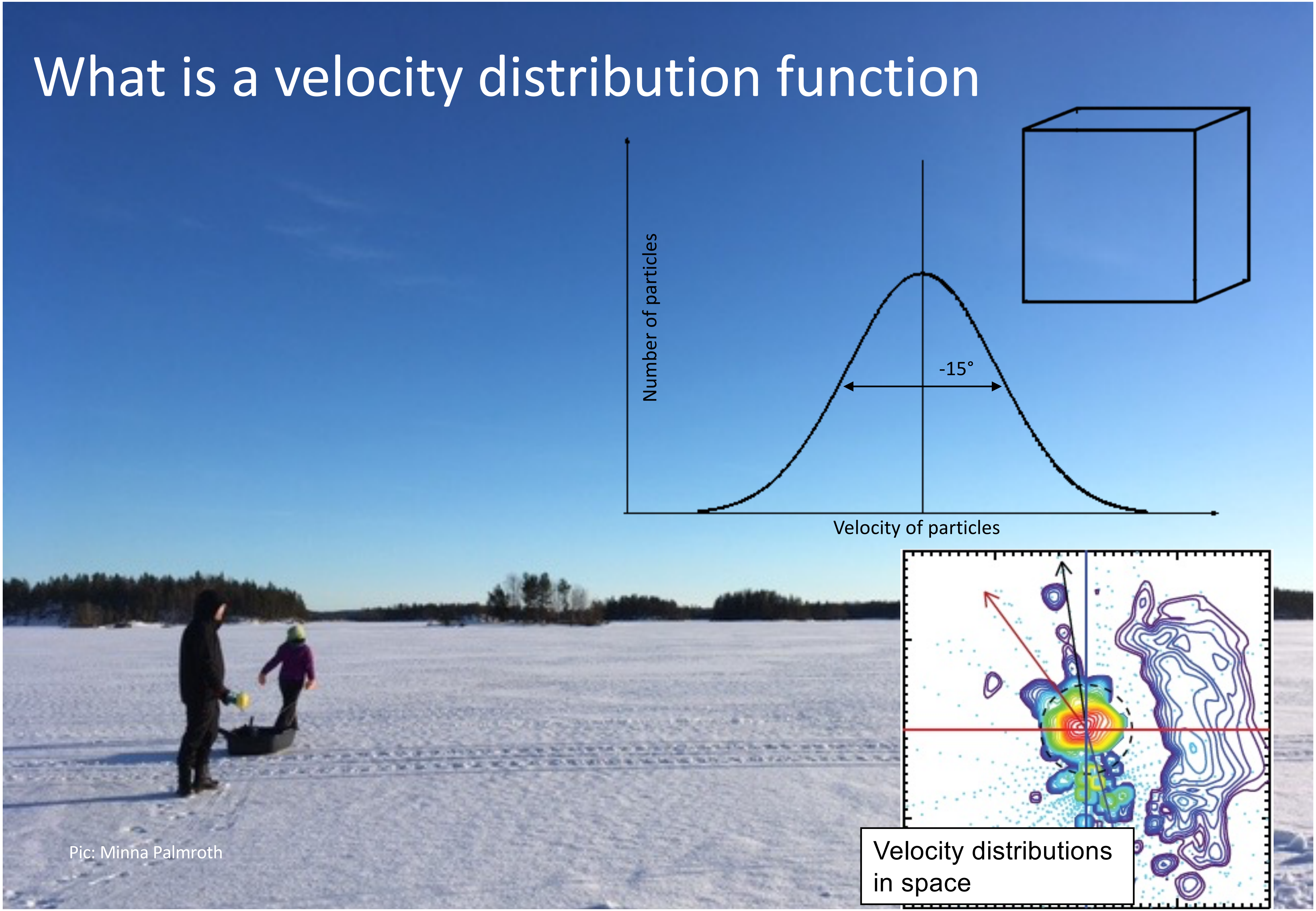


Different levels of plasma description

- Exact microphysical description
  - follow all particles and calculate the resulting fields
  - practically impossible in plasma
  - useful in strong external fields, e.g., acceleration of individual particles in predescribed fields
- Kinetic theory
  - consider particle distribution functions
  - Boltzmann and Vlasov equations
- Macroscopic theory
  - calculate macroscopic variables (density, flux, pressure, temperature,…) from the kinetic theory
  - several different approaches, e.g., magnetohydrodynamics (MHD)

What is a velocity distribution function



Distribution function

- All you need in plasma physics: all collective descriptions start from the distribution function, and then make some assumptions relevant to the problem at hand

- **Example, billiards**: When does a ball hit the pocket?
    - **Exact particle description, two balls**: Know the velocity and the angle at which the que ball is hit, the friction, etc, predict the pocket at which the ball lands at time *t*
    - Increase the number of balls? The description is most useful for the final shot.

Distribution function

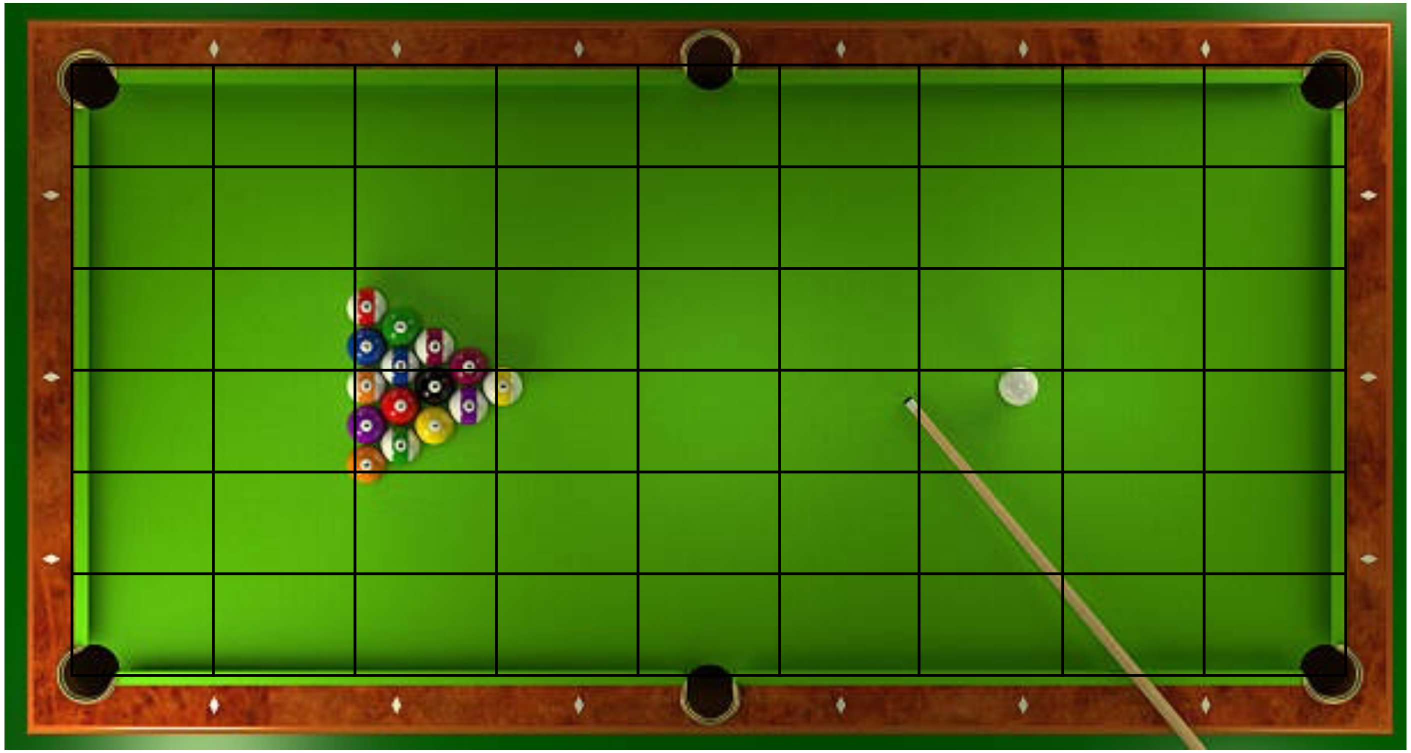
- All you need in plasma physics: all collective descriptions start from the distribution function, and then make some assumptions relevant to the problem at hand

- **Example, billiards**: When does a ball hit the pocket?
  - **Fluid description**: All balls are tied to each other. You don't have individual balls, but a collection. Average velocity of the collection is known at any given time and place.
  - Pocketing? Perhaps you only know when 1/4th of the total density has vanished.

Distribution function

- All you need in plasma physics: all collective descriptions start from the distribution function, and then make some assumptions relevant to the problem at hand

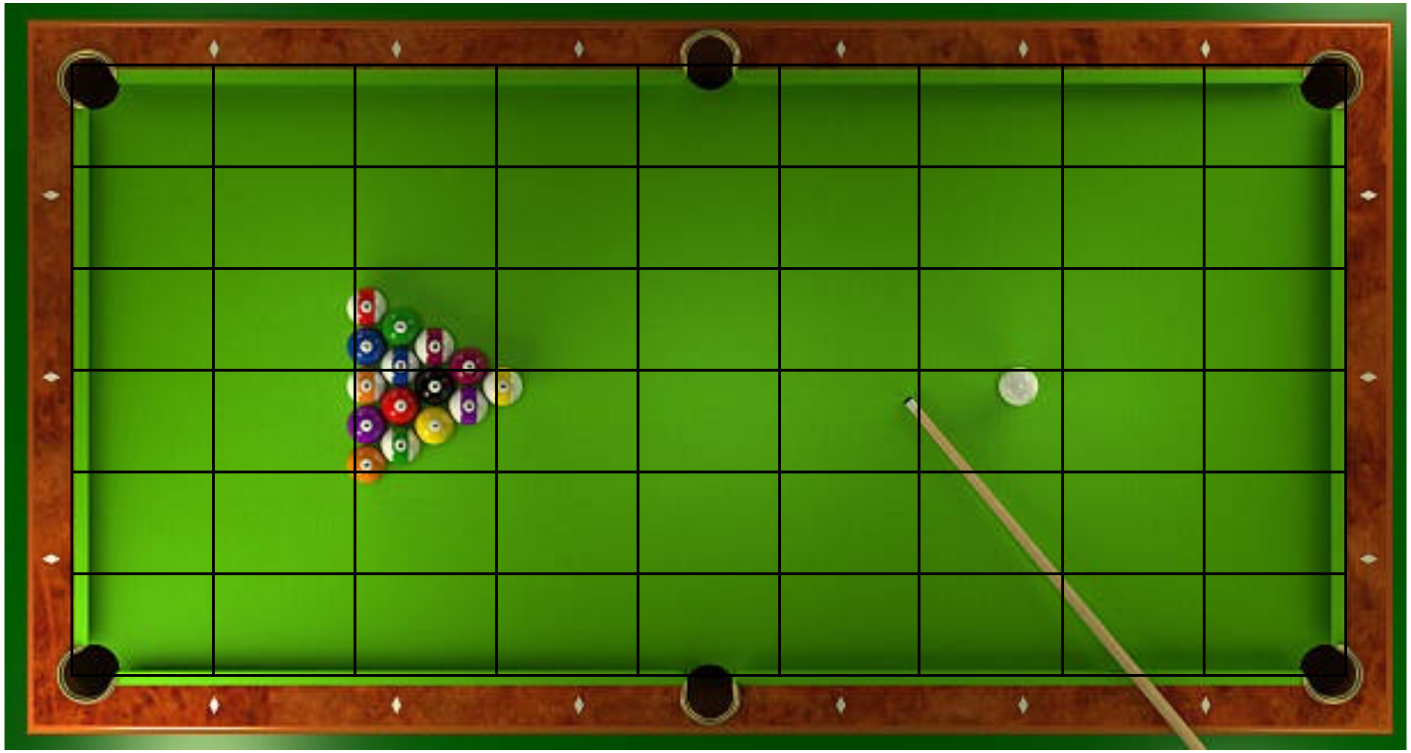
- **Example, billiards**: When does a ball hit the pocket?
  - **Kinetic description**: Make a grid, record the number of balls and their velocity vector in all grid points at all times. Do not follow individual balls.
  - Pocketing? Record the number of balls in pocket grids. Powerful, but costly.



Distribution function

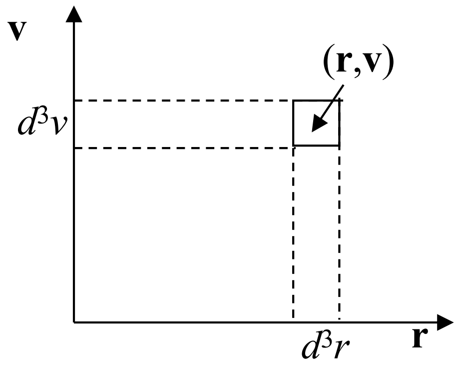
- All you need in plasma physics: all collective descriptions start from the distribution function, and then make some assumptions relevant to the problem at hand

- **Example, billiards**: When does a ball hit the pocket?
  - **Kinetic particle-in-cell description**: Make a grid, create collection of (macro)particles, follow them. At each time *t* reconstruct a distribution function in each grid point.
  - Pocketing? Record a macro particle in pocket grids. Less costly. Detection of pocketings?



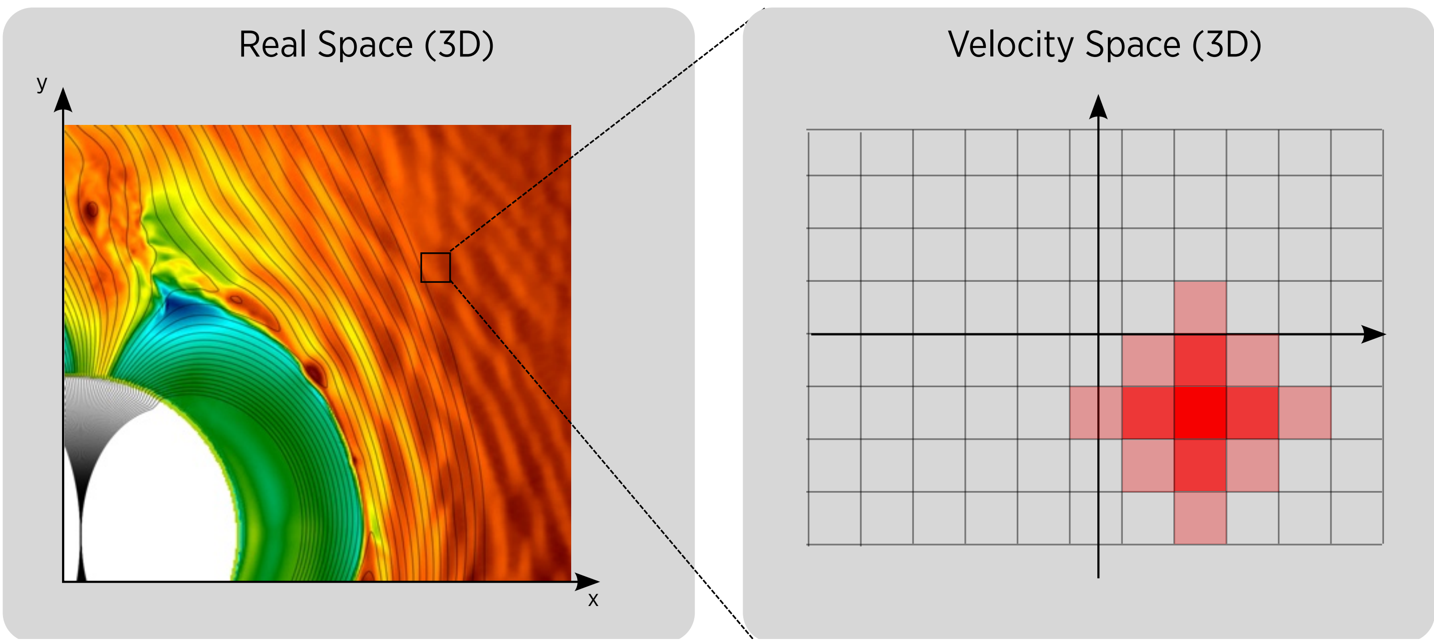
Distribution function

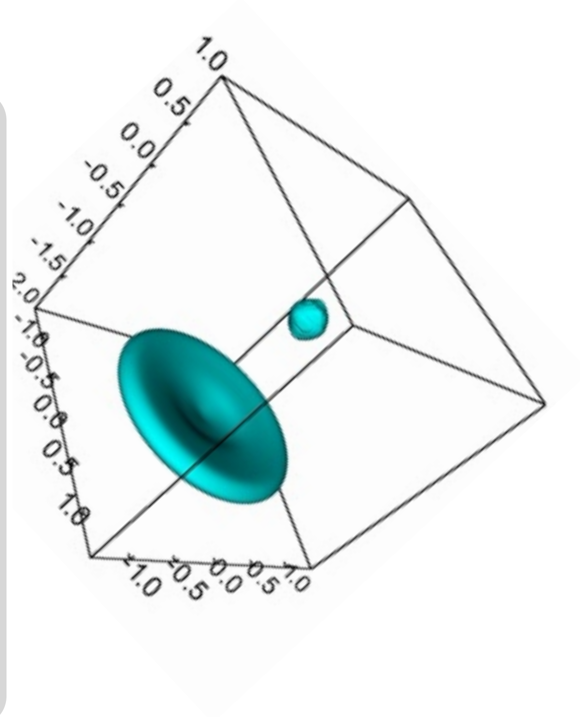
Distribution function *f*(**r**,**v**,*t*) is defined in 6D phase space



In a 3-dimensional real space ***r****(t)*, each position has an additional 3D velocity space ***v****(t)*

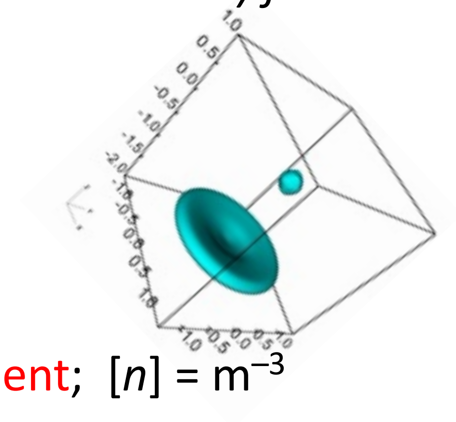
The units of *f* :
volume^{-1} x (volume of velocity space)$^{-1}$
= s^{3}m^{-6}





From f to average bulk parameters

How to get macroscopic, measurable parameters (density, temperature etc) from a known distribution function?



A physical quantity related to the given probability distribution is defined as a velocity moment of this distribution

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

Density is the zeroth moment; [n] = m^{-3}

The first moment:

$$\mathbf{\Gamma}_\alpha(\mathbf{r}, t) = \int \mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3 v$$

Particle flux; $[\Gamma] = \mathrm{m}^{-2}\,\mathrm{s}^{-1}$

$$\mathbf{V}_\alpha(\mathbf{r}, t) = \frac{\int \mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3 v}{\int f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3 v}$$

Average velocity = flux/density, [V] = m s^{-1}

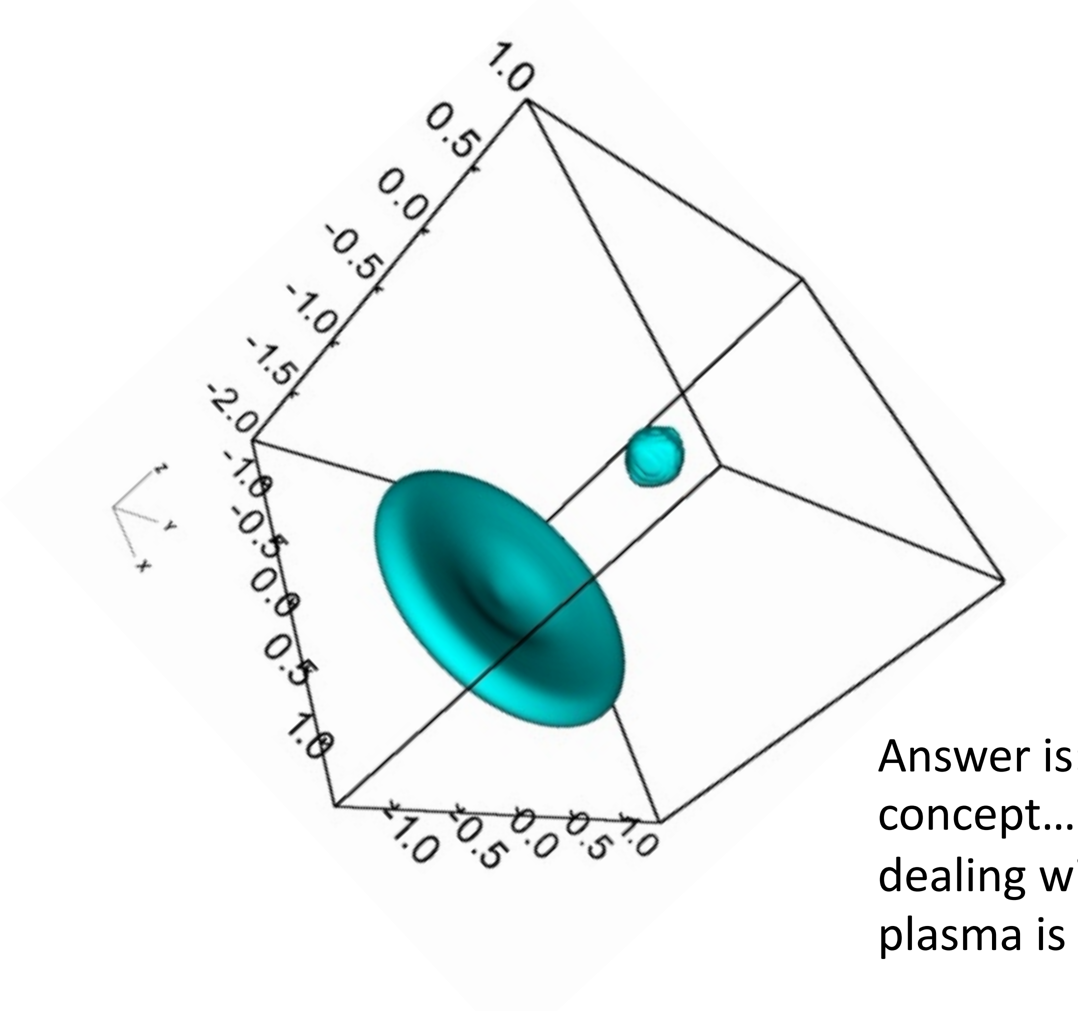
Second moment,
Pressure tensor

$$\mathcal{P}_\alpha(\mathbf{r}, t) = m_\alpha \int \underbrace{(\mathbf{v} - \mathbf{V}_\alpha)(\mathbf{v} - \mathbf{V}_\alpha)}_{\text{dyadic product} \rightarrow \text{tensor}} f_\alpha(\mathbf{r}, \mathbf{v}, t) d^3 v$$

3rd moment → heat flux (temperature x velocity), etc. to higher orders…

Example

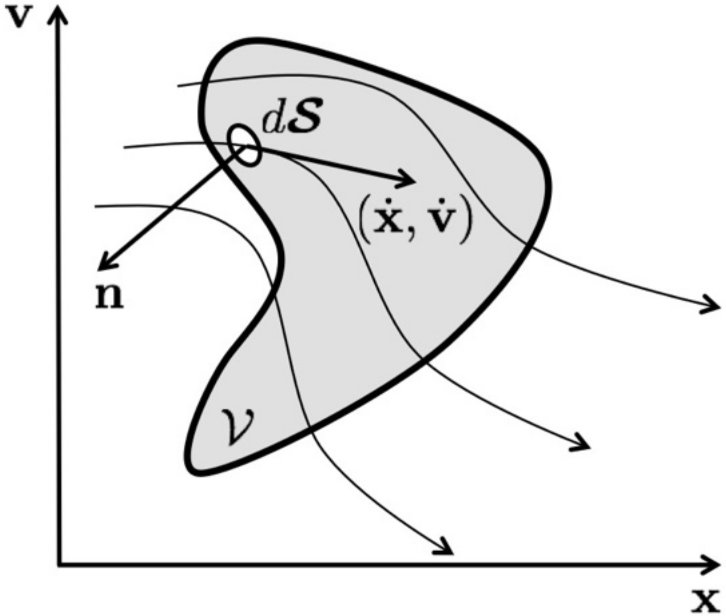
If temperature of the plasma is understood by the width of the distribution function, what is the temperature of this distribution function?



Answer is: Temperature is a difficult concept… It is the width only when dealing with Maxwellians (and space plasma is almost never Maxwellian)

Motion of *f*: Vlasov and Boltzmann equations

equation(s) of motion for *f*



Each infinitesimal plasma element moves in phase space according to

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad ; \quad \frac{d\mathbf{v}}{dt} = \frac{\mathbf{F}}{m}$$

Let *V* be some fixed phase space volume (6D) containing

$$N = \int_V f(\mathbf{r}, \mathbf{v}, t) d^3r d^3v$$ particles

1) Rate of change of particles in a fixed volume

$$\boxed{\frac{dN}{dt} = \int_V \frac{\partial f}{\partial t} d^3r d^3v}$$

2) As particles are not created nor destroyed, the rate of change is due to flux of particles through the surface of the volume.

Let's define the number flux of particles as **U***f*. Then rate of change through surface ***S***

$$\frac{dN}{dt} = -\oint \mathbf{U} f \cdot d\mathbf{S} \quad \Rightarrow \quad \int [\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{U} f)] d^3r d^3v = 0$$

$$\Uparrow$$

$$\oint \mathbf{F} \cdot d\mathbf{S} = \int_V \nabla \cdot \mathbf{F} dV$$

Conservation law, independent V

$$\boxed{\Rightarrow \quad \frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{U} f) = 0}$$

If **F** $\neq$ **F(v)** $\quad \frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{U}) = 0 \quad \Rightarrow \quad \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$

Coulomb force and gravitation OK, but the magnetic force is $\propto \; q(\mathbf{v} \times \mathbf{B})$

Fortunately $\quad \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{v} \times \mathbf{B}) = 0$

$$\Rightarrow \quad \boxed{\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = 0}$$

Vlasov equation (VE)

Compare with the Boltzmann equation in statistical physics (BE)

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t}\right)_c$$

Boltzmann derived $\quad (\partial f / \partial t)_c$ for strong short-range collisions

In plasmas most collisions are long-range small-angle collisions.
They are taken care by the average Lorentz force term

$$\boxed{\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t}\right)_c}$$

large-angle collisions only
e.g., charge vs. neutral

VE is often called collisionless Boltzmann equation

Ludwig Boltzmann

Macroscopic plasma description

Macroscopic plasma theories are fluid theories at different levels

- single fluid (magnetohydrodynamics MHD)
- two-fluid (multifluid, separate equations for electron and ion fluids)
- hybrid (fluid electrons with kinetic ions)

Macroscopic equations can be obtained by taking velocity moments of Boltzmann / Vlasov equations

$$\int \mathbf{v}^n \left(\frac{\partial f_\alpha}{\partial t} + \mathbf{v}\cdot\frac{\partial f_\alpha}{\partial \mathbf{r}} + \frac{q_\alpha}{m_\alpha}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\frac{\partial f_\alpha}{\partial \mathbf{v}}\right) d^3v = \int \left(\frac{\partial f_\alpha}{\partial t}\right)_c d^3v$$

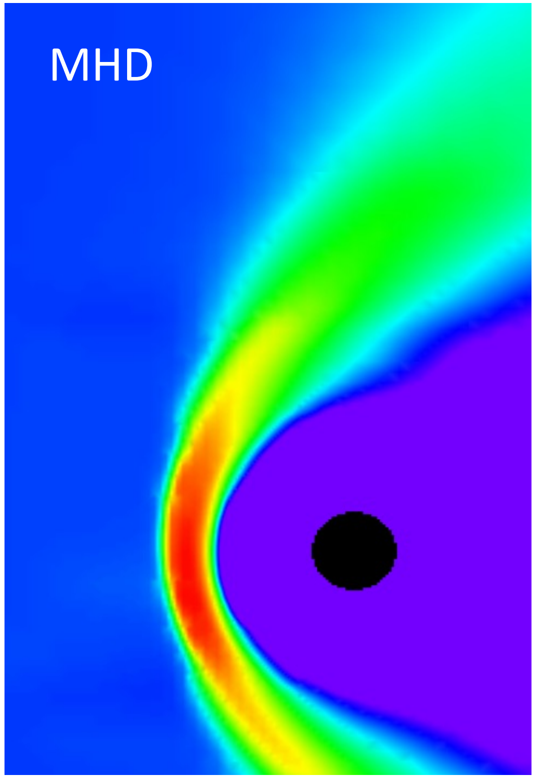
order n order $n+1$

Taking the n^{th} moment of BE/VE introduces terms of order n +1 !
This leads to ***a closure problem***, open chain of equations that must be terminated by applying some form of physical intuition.

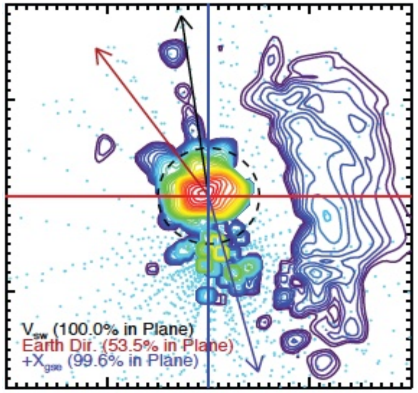
Brief reminder of what are fluid, hybrid, and kinetic descriptions: Summary

- Distribution function is key.
  - It’s moments give all measurable plasma parameters
- Fluid description:
  - Underlying assumption is that the distribution function is Maxwellian. Single value for fluid temperature. No particles. Average parameters.
- Kinetic description:
  - All particle species are described by an own distribution function everywhere. Distribution function moments give feedback to long-range forces, which feedback to the distributions for all species.
- Hybrid description:
  - Some species are described by a distribution function. Some are fluid.

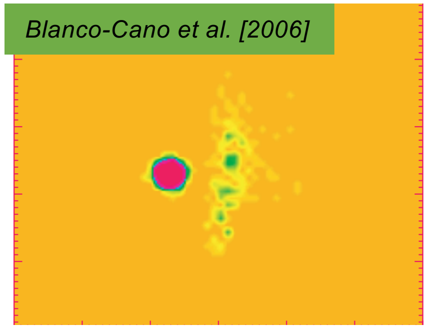
Everything depends on how to model the plasma distribution function



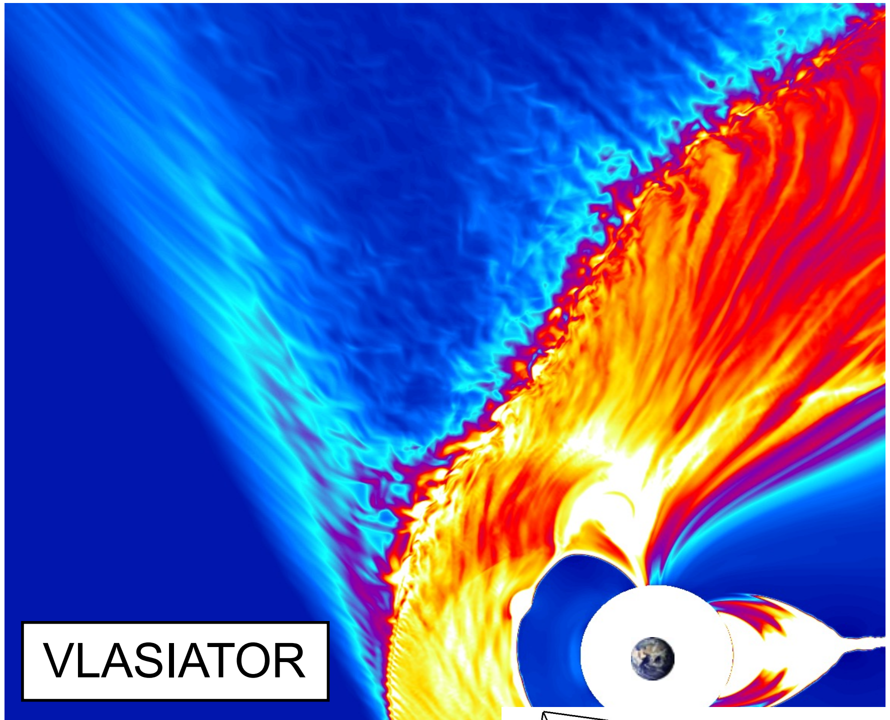
MHD: Distribution function is not modelled. Single value is used for temperature.



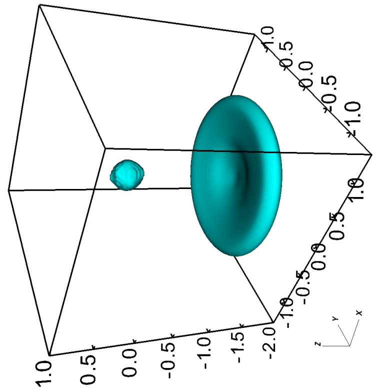
Observations (THEMIS spacecraft)



Particle-in-cell (PIC). Distribution is constructed from particle statistics.



Vlasiator: Distribution function is modelled perfectly. No assumptions.



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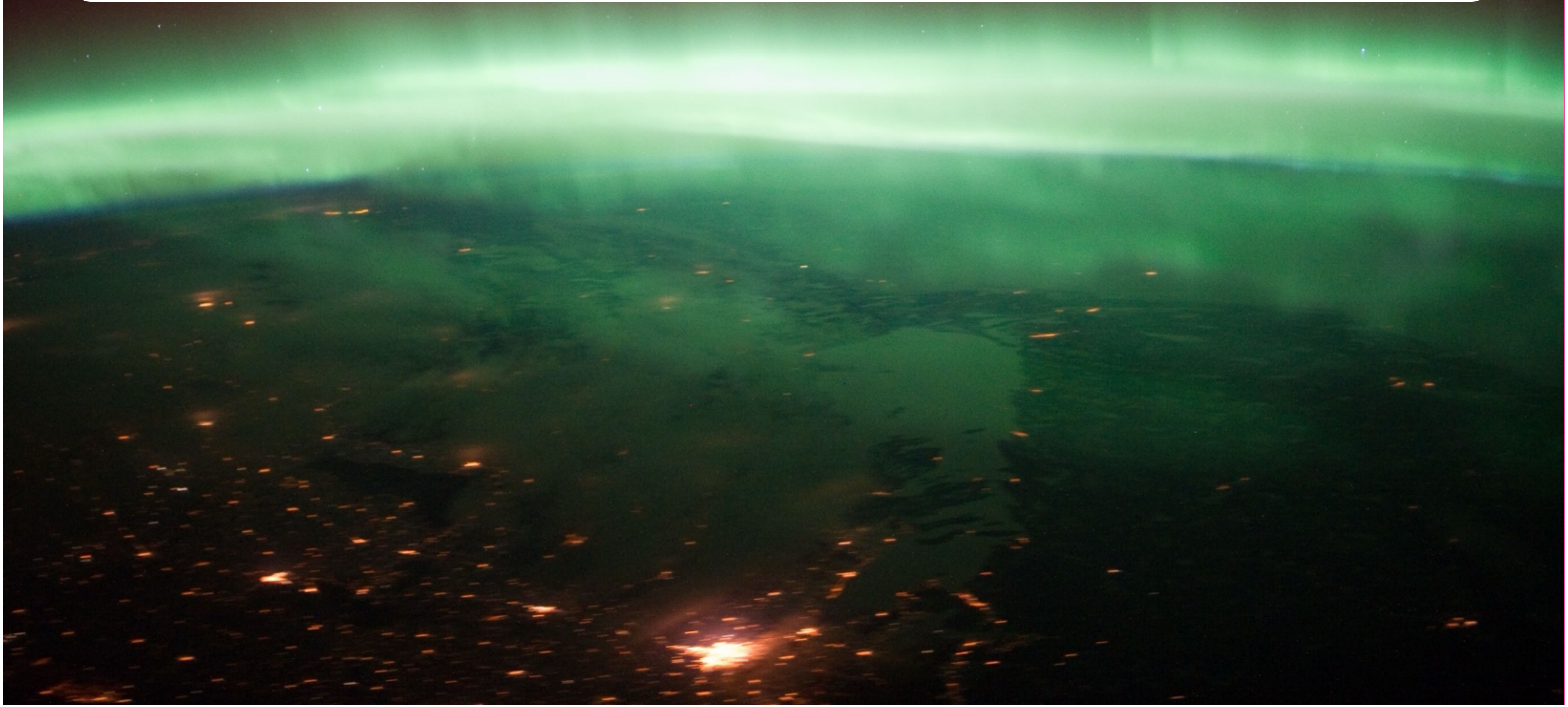
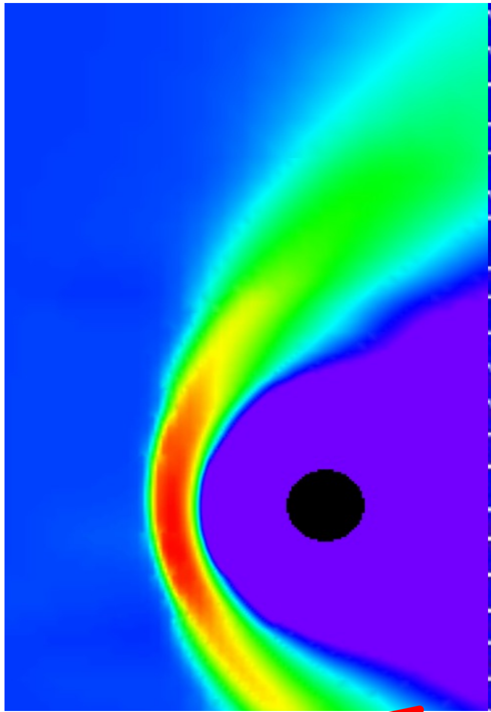


Principle of modelling

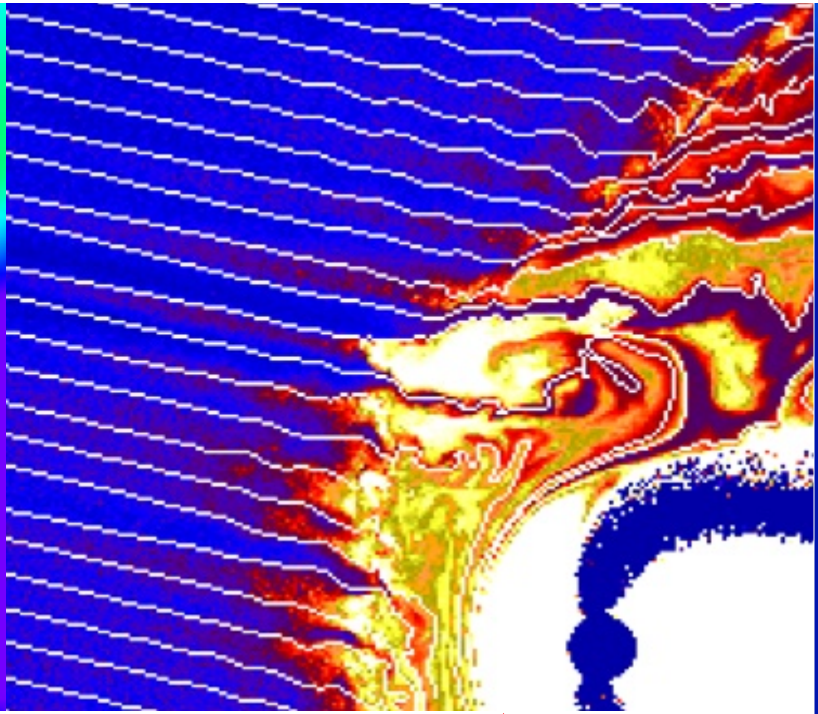
Terrestrial weather

- Divide the modelling volume into a grid
- Measure modelled parametres in cell centres (e.g. density velocity)
- Compute how much density goes to neighbour and update neighbour cell average
- Use hydrodynamics and partial differential equations (in this example; pick equations of your taste in your problem)
- Compute faster than density moves in reality ➔ **forecast**

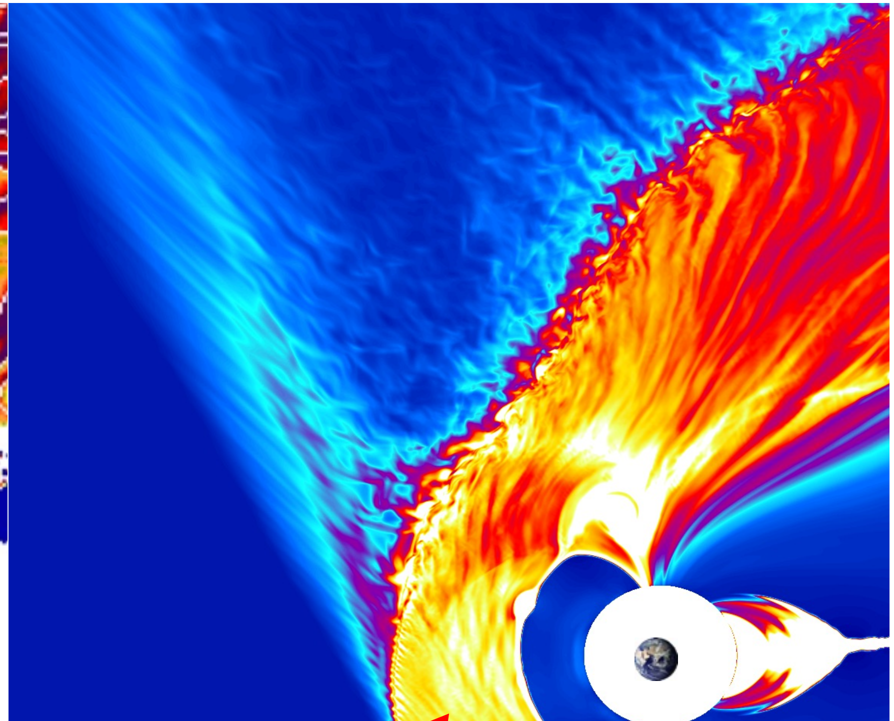
Global modelling techniques



GUMICS-4, FMI



Karimabadi et al., 2014



helsinki.fi/vlasiator

	Global fluid (MHD)	Hybrid particle-in-cell	Hybrid-Vlasov (Vlasiator)
Ions	Fluid	Particles	Distribution functions
Electrons	Fluid	Fluid	Fluid
Run time	Real-time to weeks	Weeks	Weeks – months
Scale of applications	Fluid scale (1000 km) Now: Solar system	Ion kinetic effects (10 – 1000 km) Global = Solar wind, magnetosphere (+ ionosphere)	

Computational MHD

Magnetohydrodynamics (MHD)

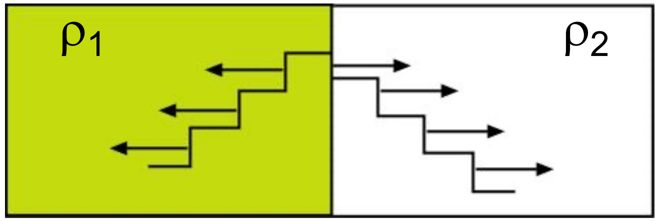
- Plasma as fluid

Riemann problem in MHD

- 8 waves: 8 eigenvalues of a closed equation set
    - Fast magnetosonic
    - Slow magnetosonic
    - Alfvén velocity
    - Bulk velocity (*entropy wave*)
    - 8th wave: zero ($\nabla \cdot \mathbf{B}=0$)

Finite volume method (FVM)

- Cell averages from neighbors
- Conservative



$$\frac{\partial u}{\partial t} + (\nabla \cdot \mathbf{F}) = 0 \quad \text{(continuity)}$$

$$u = \begin{pmatrix} \rho \\ \mathbf{p} = \rho\mathbf{v} \\ U \\ \mathbf{B} \end{pmatrix} \begin{matrix} \text{(mass)} \\ \text{(momentum)} \\ \text{(energy)} \\ \text{(magnetic field)} \end{matrix}$$

$$\mathbf{F} = \begin{pmatrix} \rho\mathbf{v} \\ \frac{\mathbf{pp}}{\rho} + P + \frac{B^2}{2\mu_0} - \frac{1}{\mu_0}\mathbf{BB} \\ (U + P - \frac{B^2}{2\mu_0})\frac{\mathbf{p}}{\rho} + \frac{1}{\mu_0}(\mathbf{B} \times \frac{\mathbf{p}}{\rho} \times \mathbf{B}) \\ \mathbf{vB} - \mathbf{Bv} \end{pmatrix}$$

$$U = \frac{P}{\gamma - 1} + \frac{1}{2}\rho\mathbf{v}^2 + \frac{\mathbf{B}^2}{2\mu_0}$$

Grand Unified Magnetosphere Ionosphere Coupling Simulation (GUMICS @FMI)

Ideal conservative MHD

- Riemann solver
- FVM discretization

Boundary conditions

- Input: Solar wind parameters
  - **B**, **v**, n, T (8 parameters)
- Dipole field
- Ionosphere (MHD inner shell at 3.7Re)

Output parameters

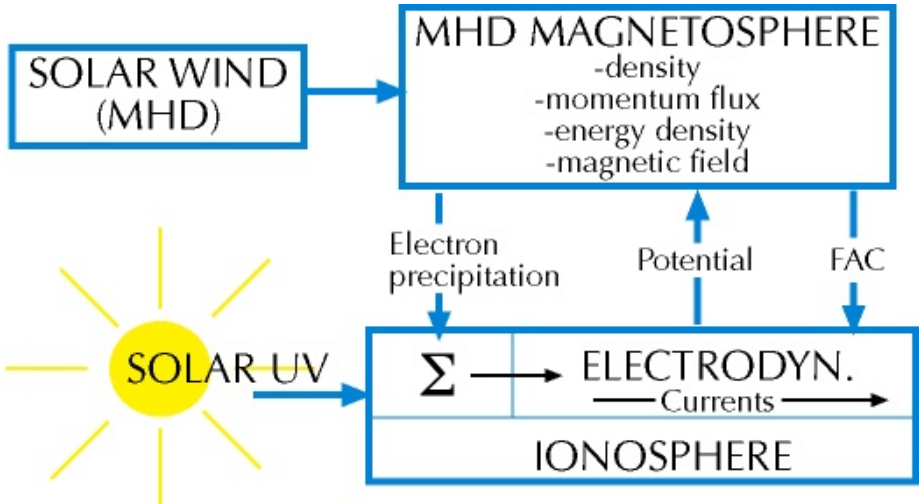
- Plasma parameters and the em field in space and time (min. ~1ms)

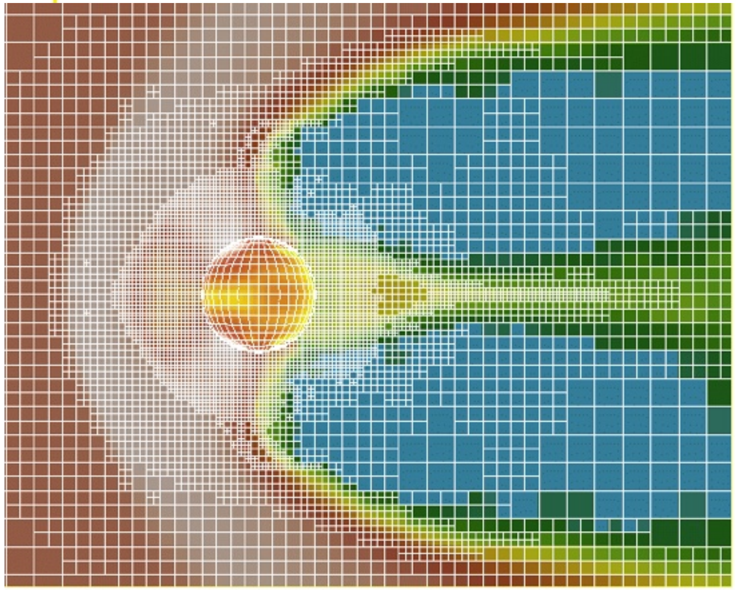
Adaptive (cell-by-cell) Cartesian grid

  - Max 8 Re resolution, min typically 0.25 Re

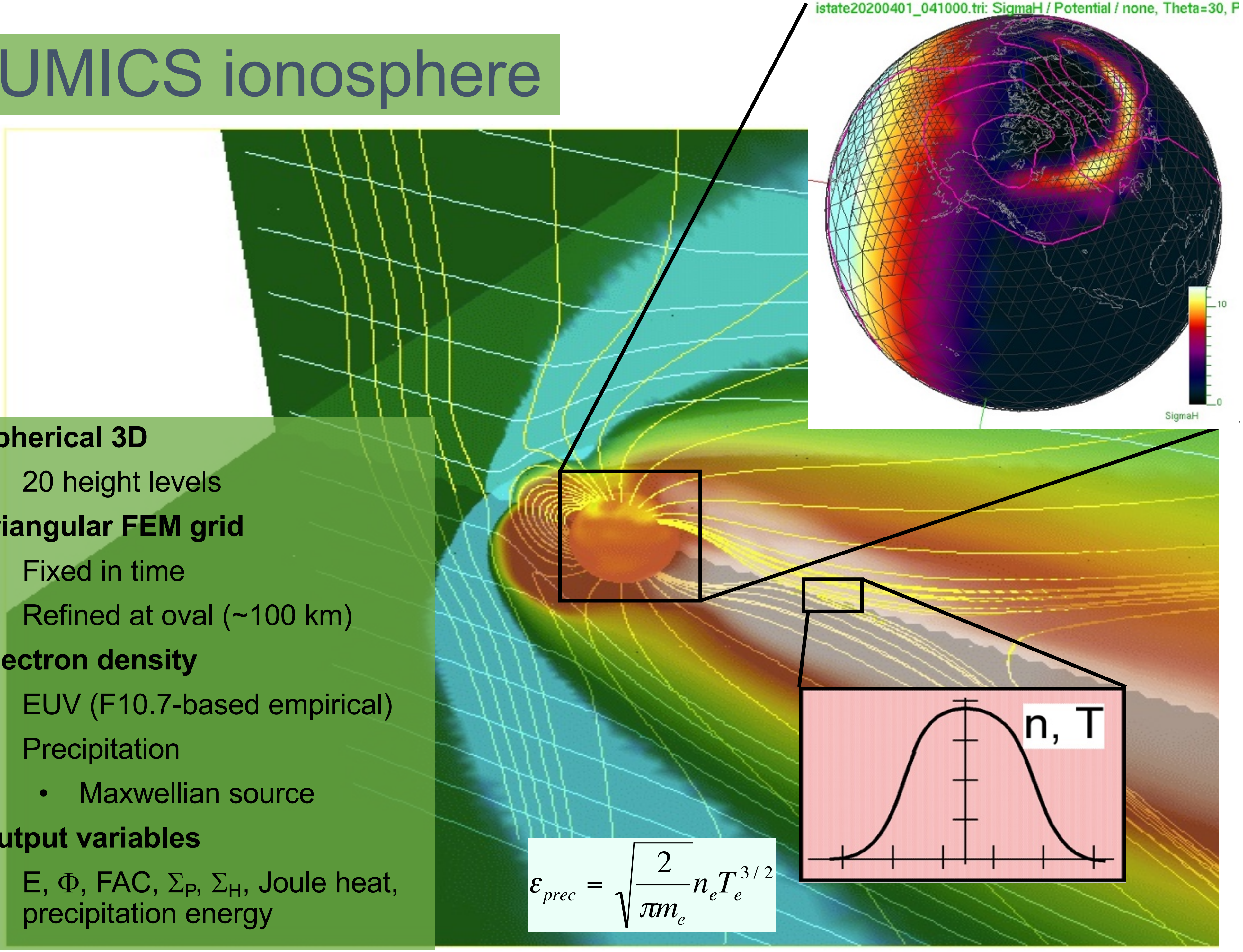
Subcycling (variable time step)

Other MHD codes, e.g.: LFM / GAMERA; BATS-R-US / SWMF





GUMICS ionosphere



Spherical 3D

- 20 height levels

Triangular FEM grid

- Fixed in time
- Refined at oval (~100 km)

Electron density

- EUV (F10.7-based empirical)
- Precipitation
  - Maxwellian source

Output variables

- E, Φ, FAC, Σ_P, Σ_H, Joule heat, precipitation energy

$$\varepsilon_{prec} = \sqrt{\frac{2}{\pi m_e}} n_e T_e^{3/2}$$

Similarities & differences to other global codes

Godunov-type solver (&BATS-R-US)
- Sharp stationary boundaries

1st order interpolation
- Others higher order

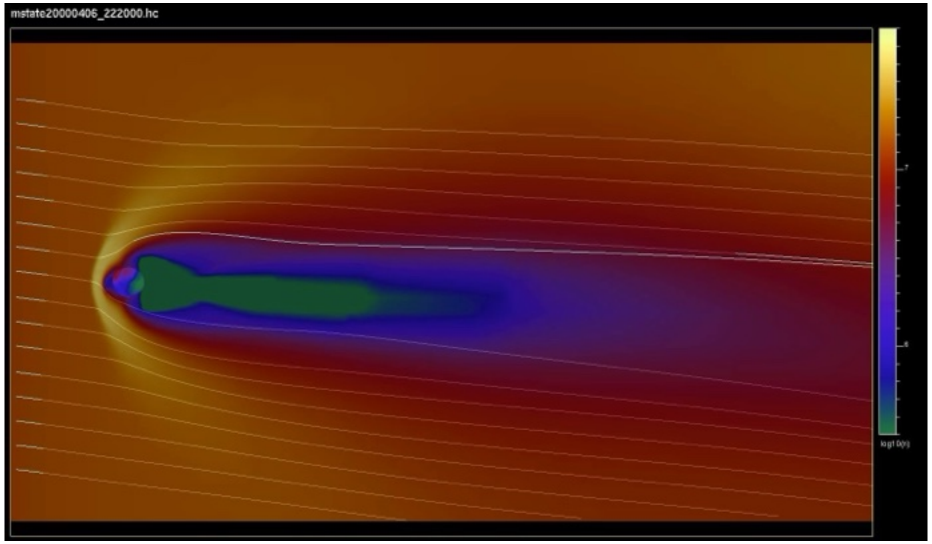
Cell-by-cell adaptive
- Others block-adaptive or non-adaptive

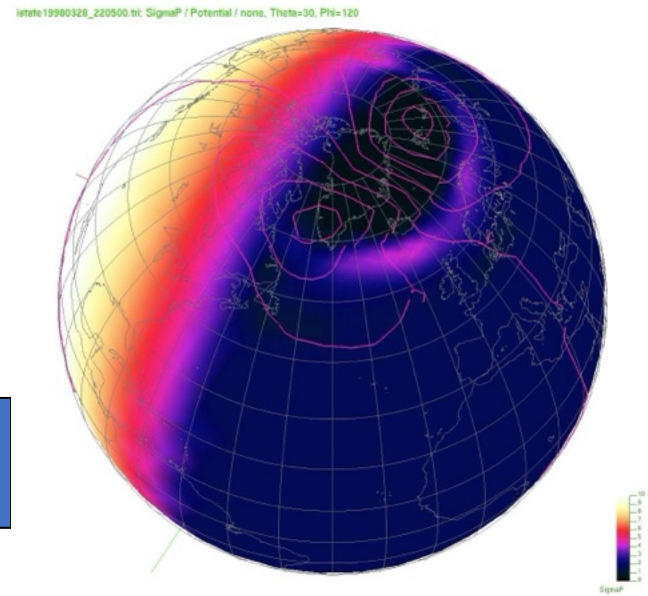
Knight relationship
- Parallel electric field between ionosphere and magnetosphere
- Implemented but often set to zero
  - Sub-grid scale physics

Not coupled to dedicated codes

No current-dependent resistivity

Storm on 2000/04/06





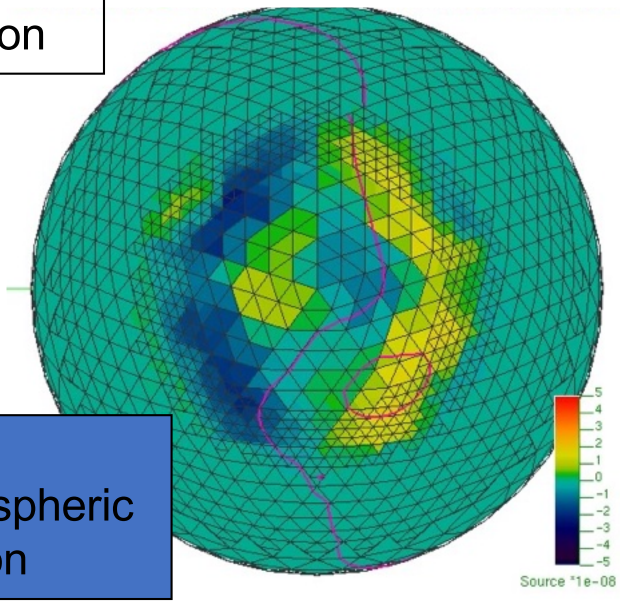
Substorm on 1998/03/28

General remarks: MHD & Inner magnetosphere

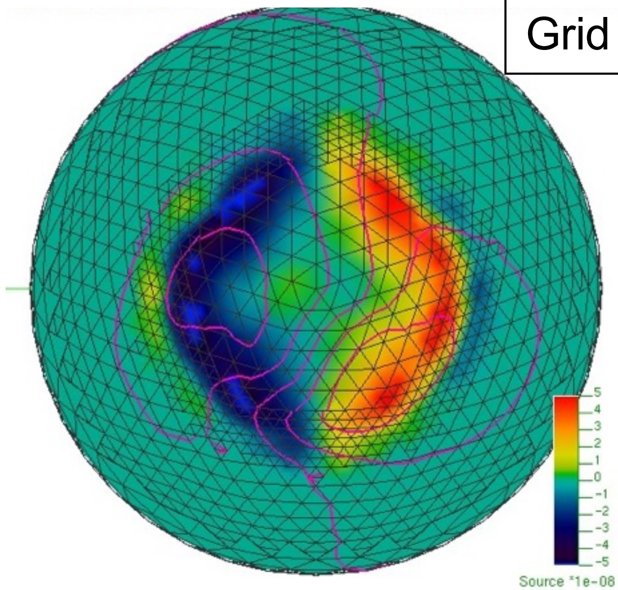
Inner magnetospheric physics not ideal MHD

- Overlapping plasma populations, different temperature
- Magnetospheric pressure gradient determines R2 FAC
    - Improve partly by refining the magnetospheric grid

0.5 RE
Grid resolution

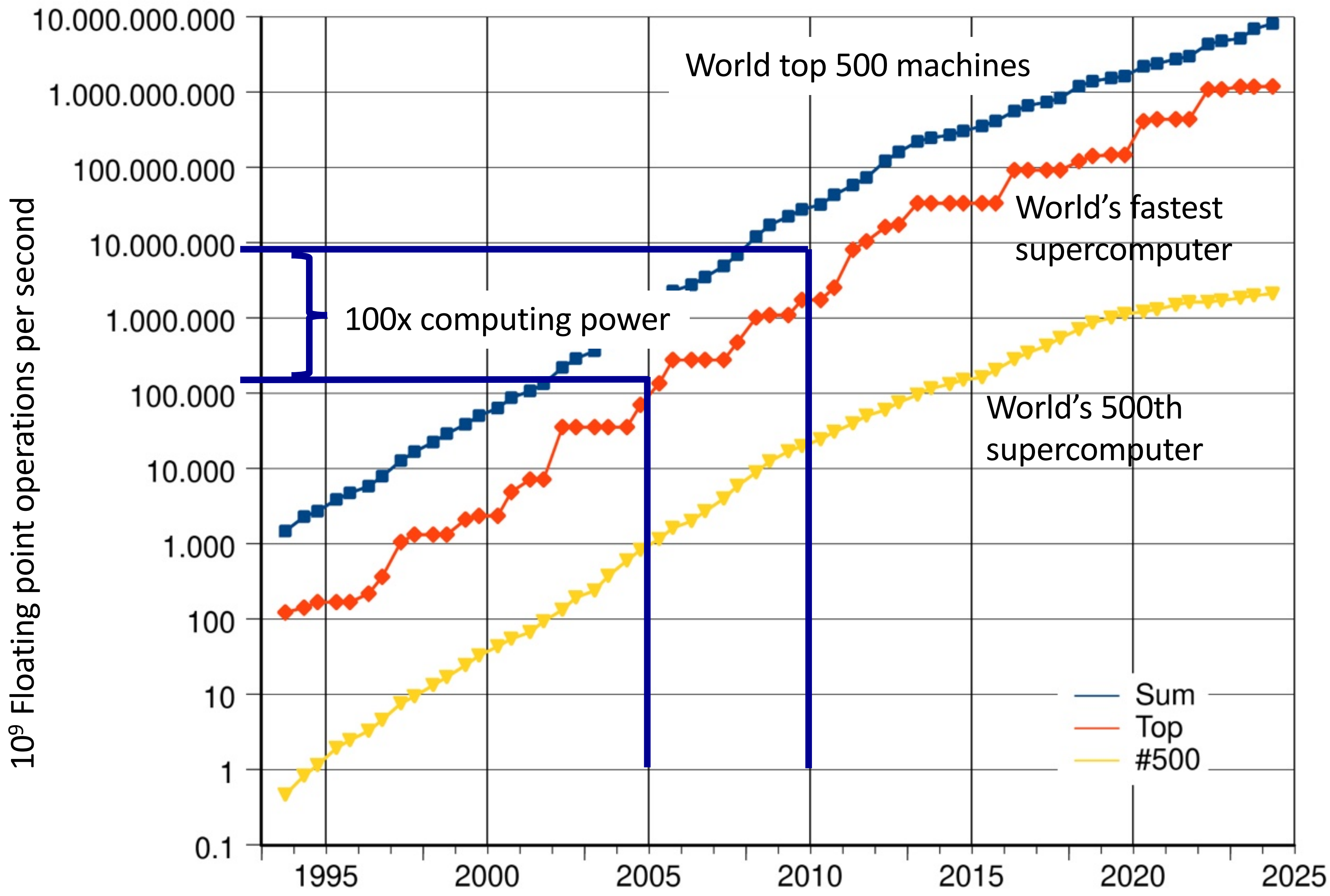


0.25 RE
Grid resolution

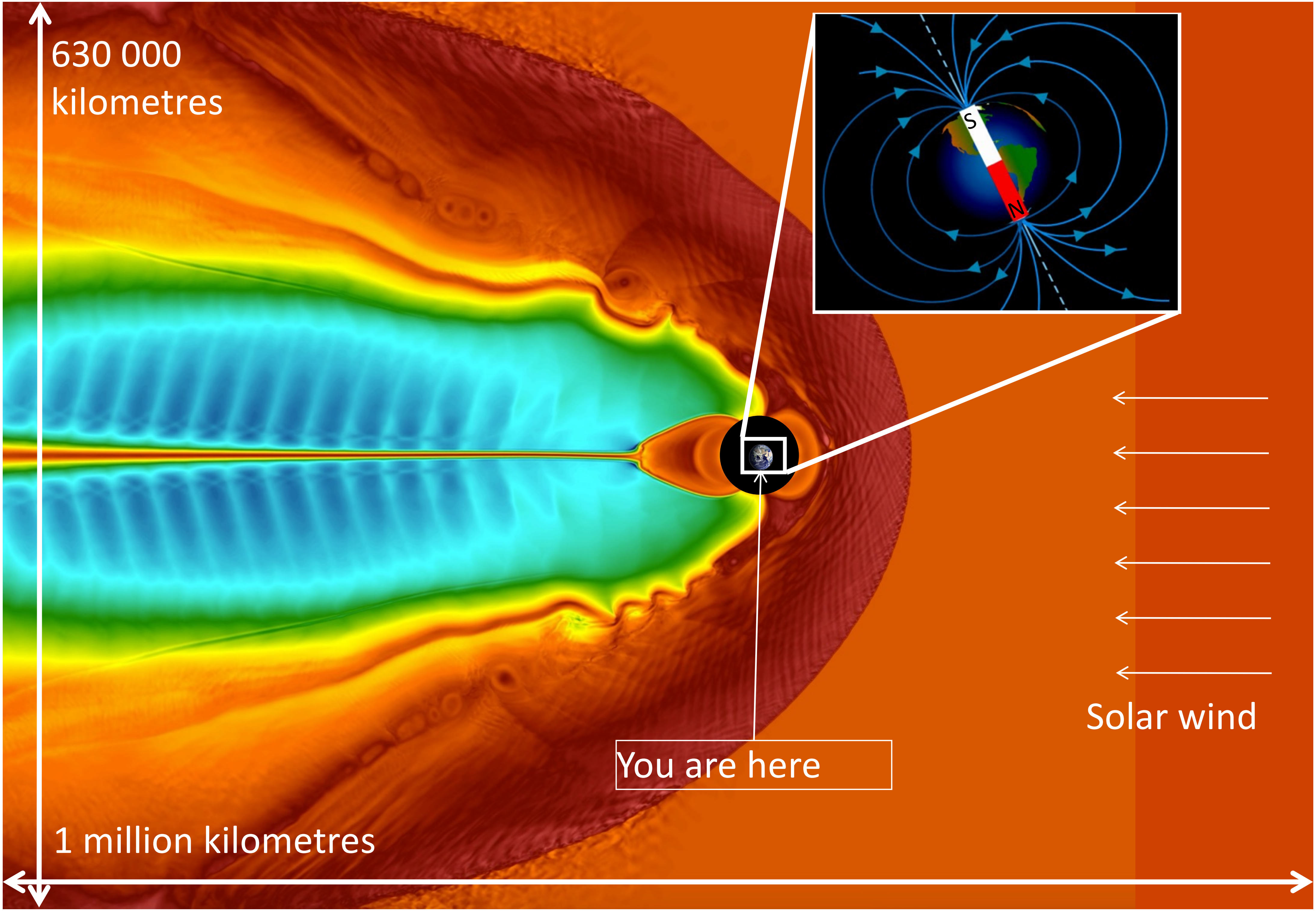


Same run
different magnetospheric
grid resolution

This is why several global MHD simulations couple to a dedicated inner magnetosphere like RCM



Picture: Wikipedia


630 000
kilometres
S
N
You are here
Solar wind
1 million kilometres

VLASIATOR

- Global ion-kinetic plasma physics beyond MHD
- Electrons are massless charge-neutralising fluid.

2D or 3D real space (R)

- Divide real space into grid cells
- Compute **E**, **B** fields
- Input to 3D velocity space
- Ohm's law: Hall + electron pressure gradient

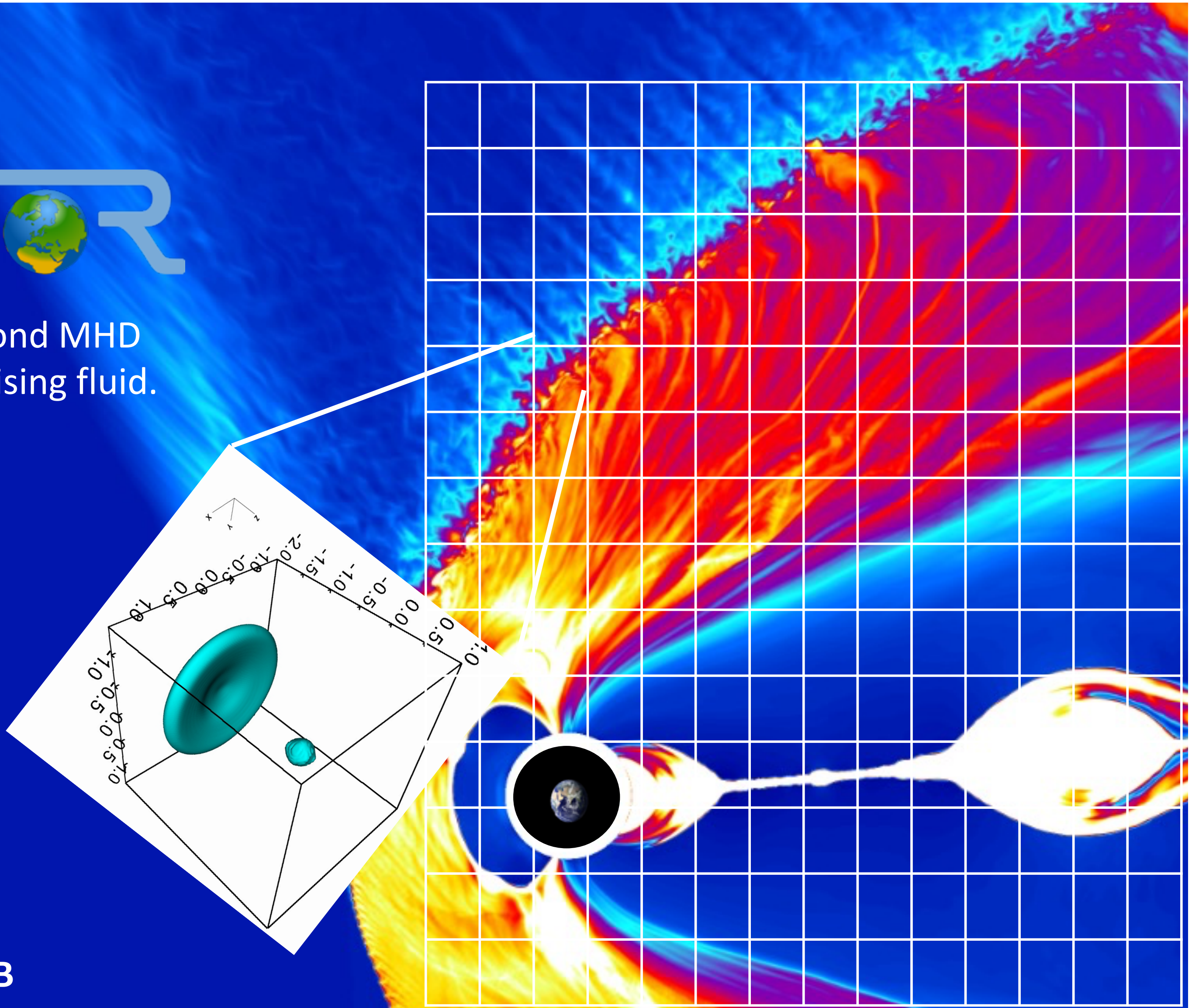
3D velocity space (V)

- Each R space cell contains a 3D velocity space
- Propagate and modify ion distribution function using Vlasov equation
- Couple back to real space to update **E**, **B** field

Self consistent

Noise-free multi-temperature physics

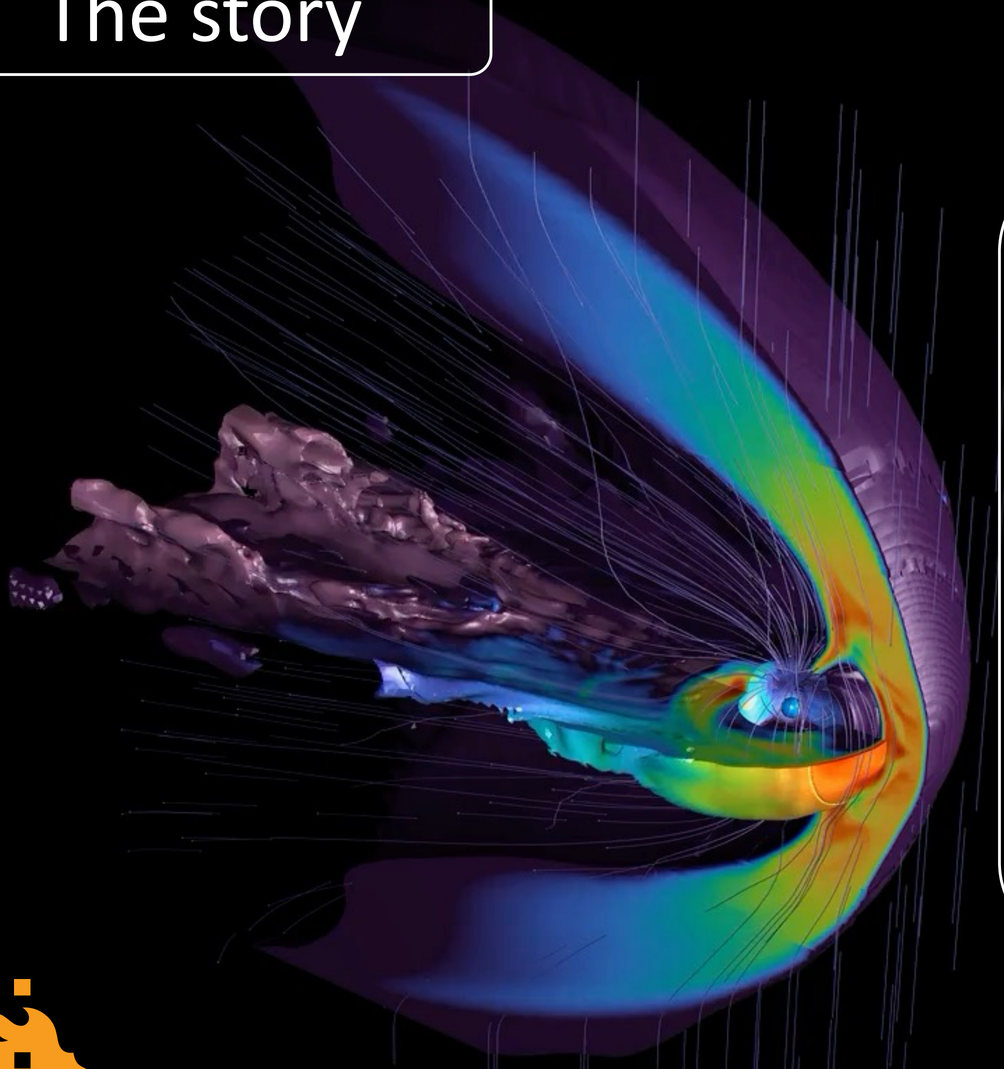
- **Total number of cells: 10^{12}**
- **Over 10^5 timesteps**



More information: http://helsinki.fi/vlasiator

Contact PI: *Minna.Palmroth@helsinki.fi*

The story



2007: First ERC grant (Starting)
2011: 6D Test-Vlasov in MHD fields
2012: Access to Europe's supercomputers
- First 5D runs (2D3V)

2015: Second ERC grant (Consolidator)
2019: Towards 6D (AMR)
- First preliminary run @CSC

2021: (Jan 13)
- First 6D production run @HLRS
- Around 15 MCPUh
- Data per run: ~30 T

2022: Dynamic ionosphere added

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

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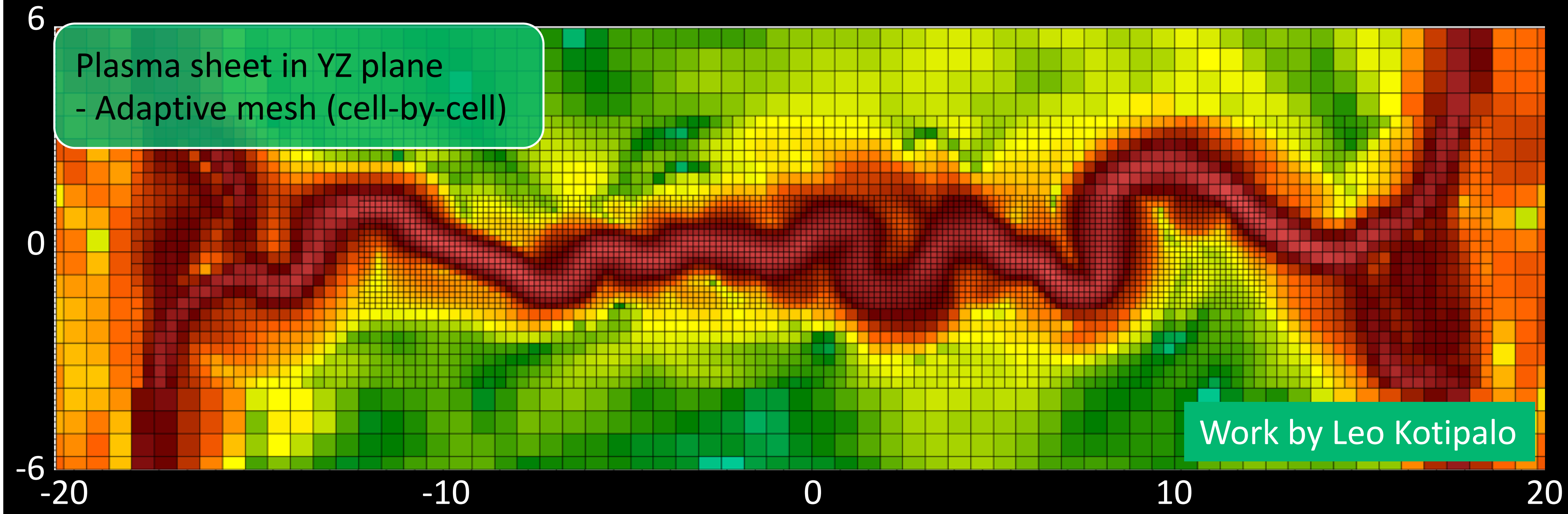
Enabling 6D: In a nutshell



- Subgrid functions for VDFs on coarse grid
- LUMI: Top 8 (world), Top 2 (Europe)
- Velocity space → GPU
  - By M. Battarbee
- Part of European Centre of Excellence in Code development (EuroHPC).
- See more: Palmroth et al. LRCA 2018, 2025

High-performance computing

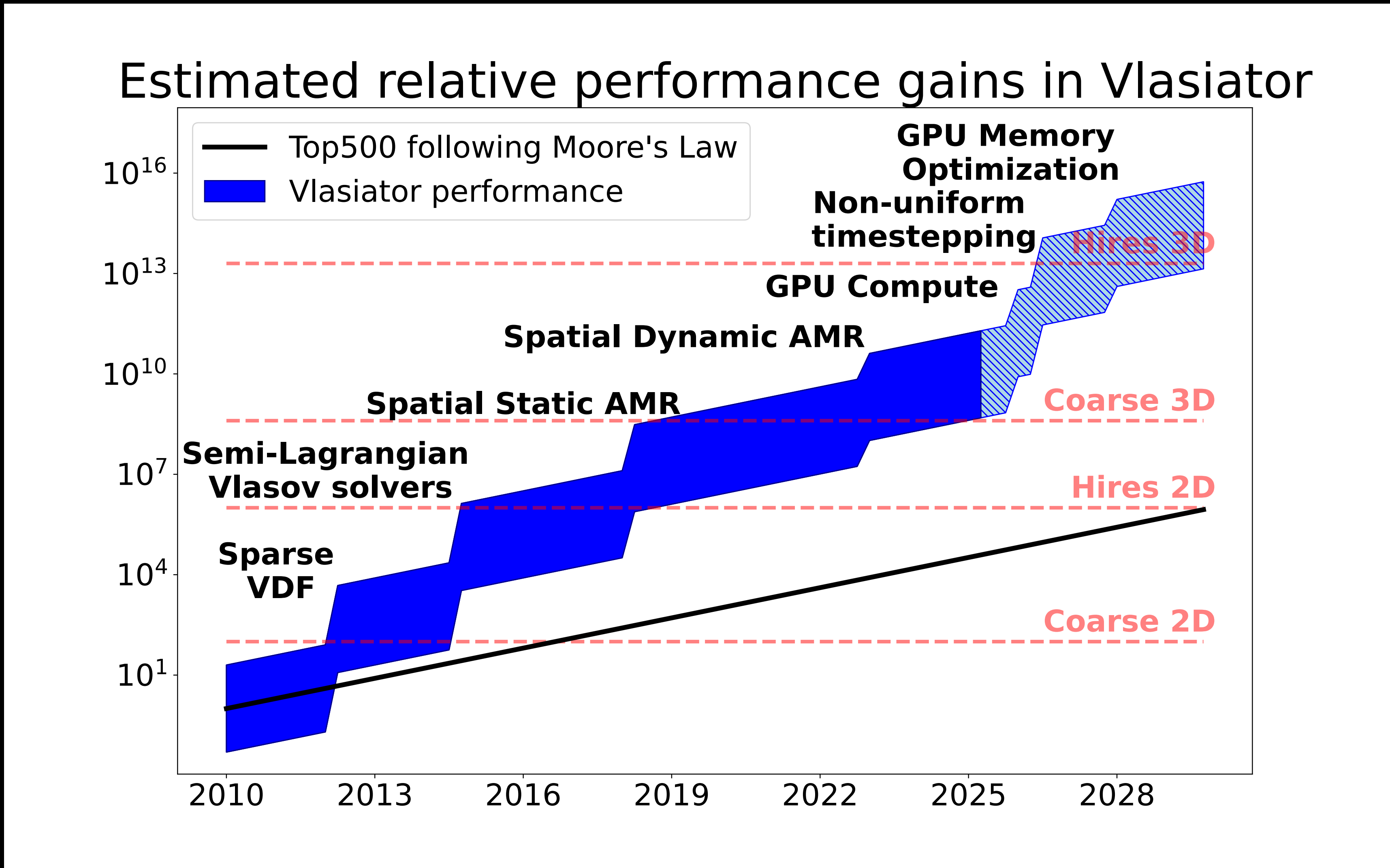


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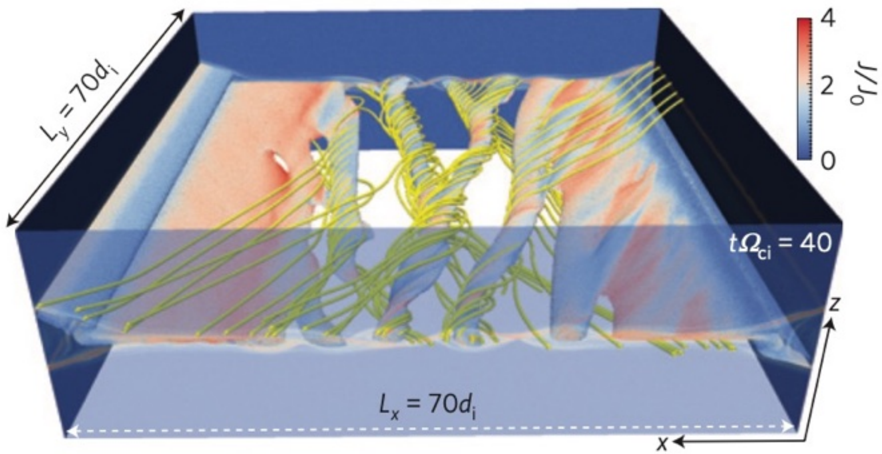
Image by Y. Pfau-Kempf

Fully kinetic simulations (kinetic electrons)

- **Explicit schemes: local geometries**
  - Electron kinetic physics occurs in ~100-1000x smaller scales ➔ real space resolution, time steps
- **Implicit schemes: Mercury (e.g., Lapenta et al. JGR 2022)**
  - See e.g. Lavorenti PhD thesis https://theses.hal.science/tel-04611766v1 about the different schemes
  - Or attend International School/Symposium in Space Simulations (ISSS-16) or similar
- **Treating velocity space either through Vlasov (gridded *f*) or through PIC (follow macroparticles)**
  - Own *f* for each population, all influence fields
  - Needs to assume something for the electron and ion mass ratio

Self consistent

Fully kinetic simulation of reconnection (Daughton et al. 2011)



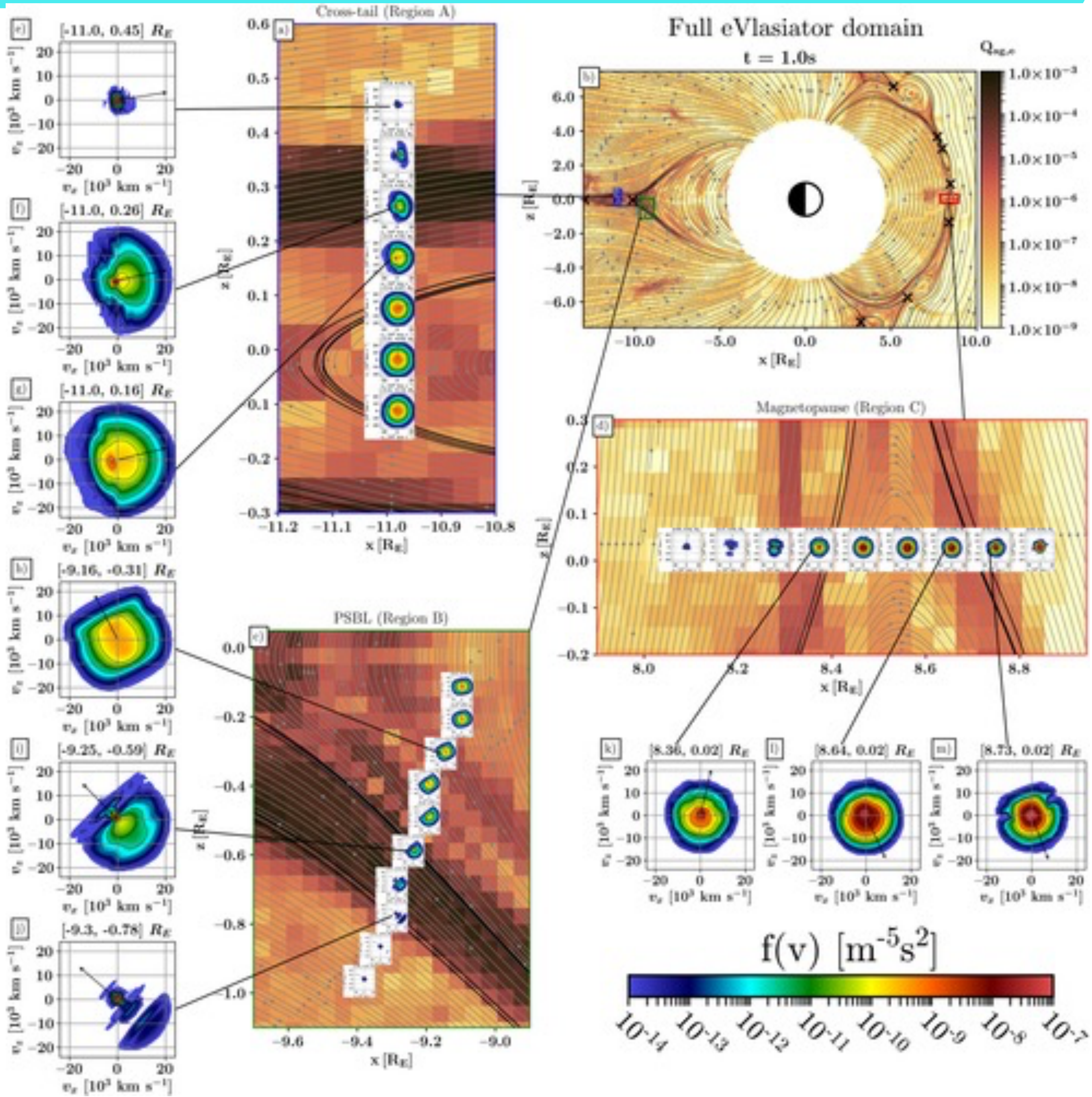
Or: eVlasiator – electron kinetics in hybrid-Vlasov dynamics

Electron distributions globally (Battarbee et al., 2021: https://doi.org/10.5194/angeo-2020-31)

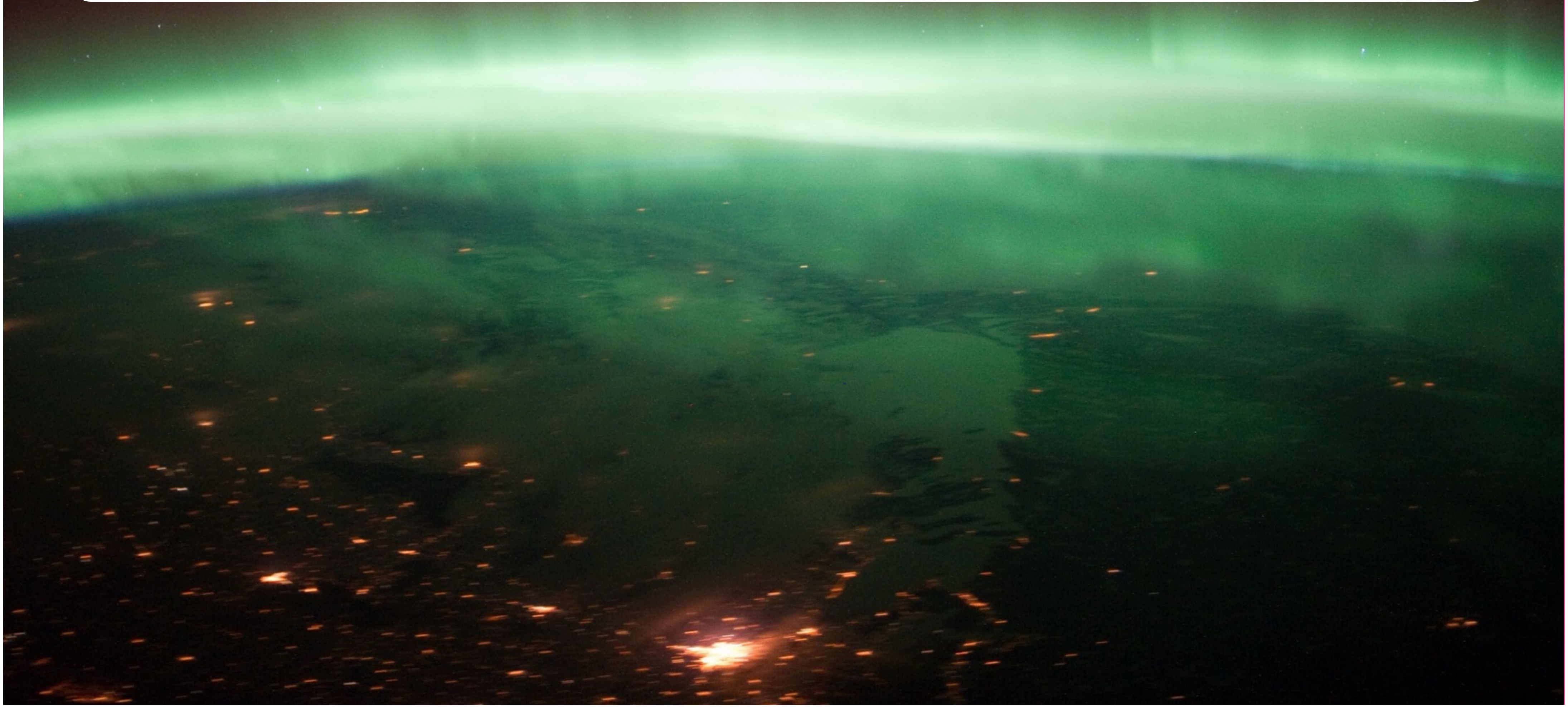
- Based on ion-determined em-fields

Agreement with spacecraft (MMS): Alho et al., GRL https://doi.org/10.1029/2022GL098329)

- Suggests that many (most) elecron VDF features are based on ion-scale em-fields!

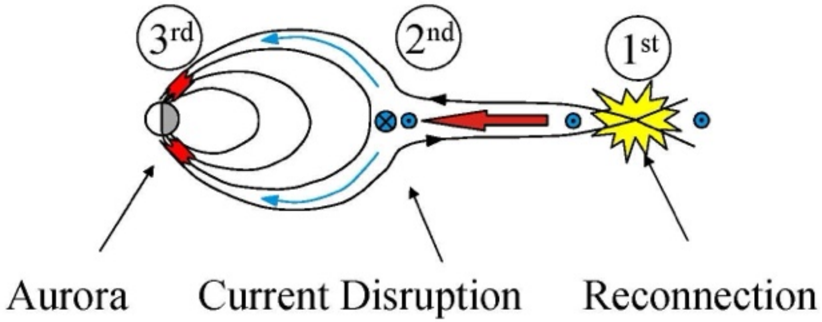


- About nomenclature: *scales*
- Brief reminder of what are fluid, hybrid, and kinetic descriptions
- Modelling space plasmas with different plasma descriptions
- Example of scale coupling
- Challenges and future of modelling



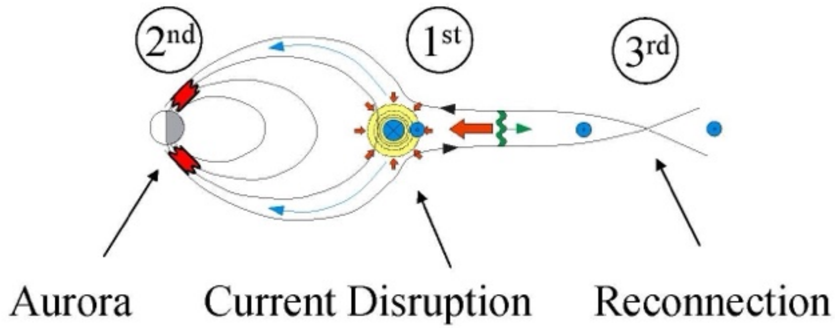
Broad review on plasmoid ejection scenarios

Near-Earth Neutral line
e.g., Baker+, *JGR*, 1996



- **Reconnection** launches a plasmoid tailward
- … and fast flows earthward
- Dipolarisation disrupts the magnetotail current

Current disruption
e.g., Lui, *JGR*, 1996



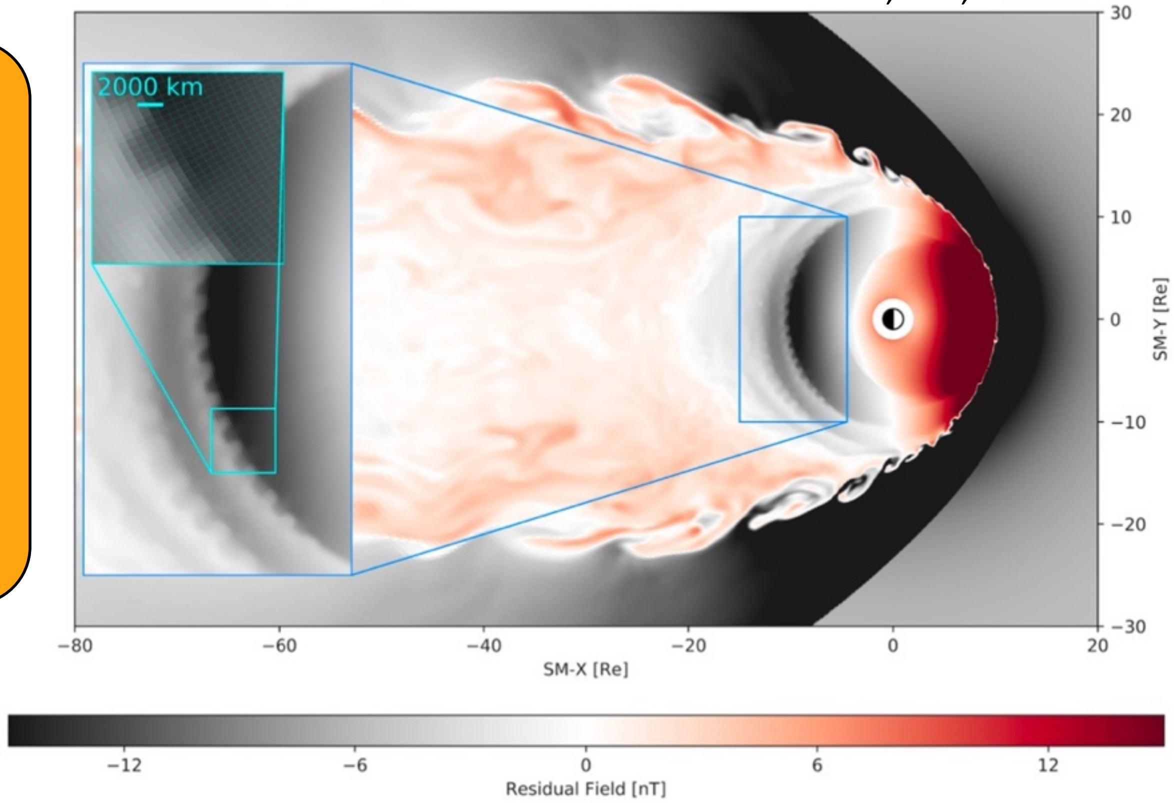
- A 3D plasma **instability** grows in transition region
- … disrupts the magnetotail current
- … launches waves that trigger reconnection
- plasmoid release, fast flows, and dipolarization

Modelling requirements

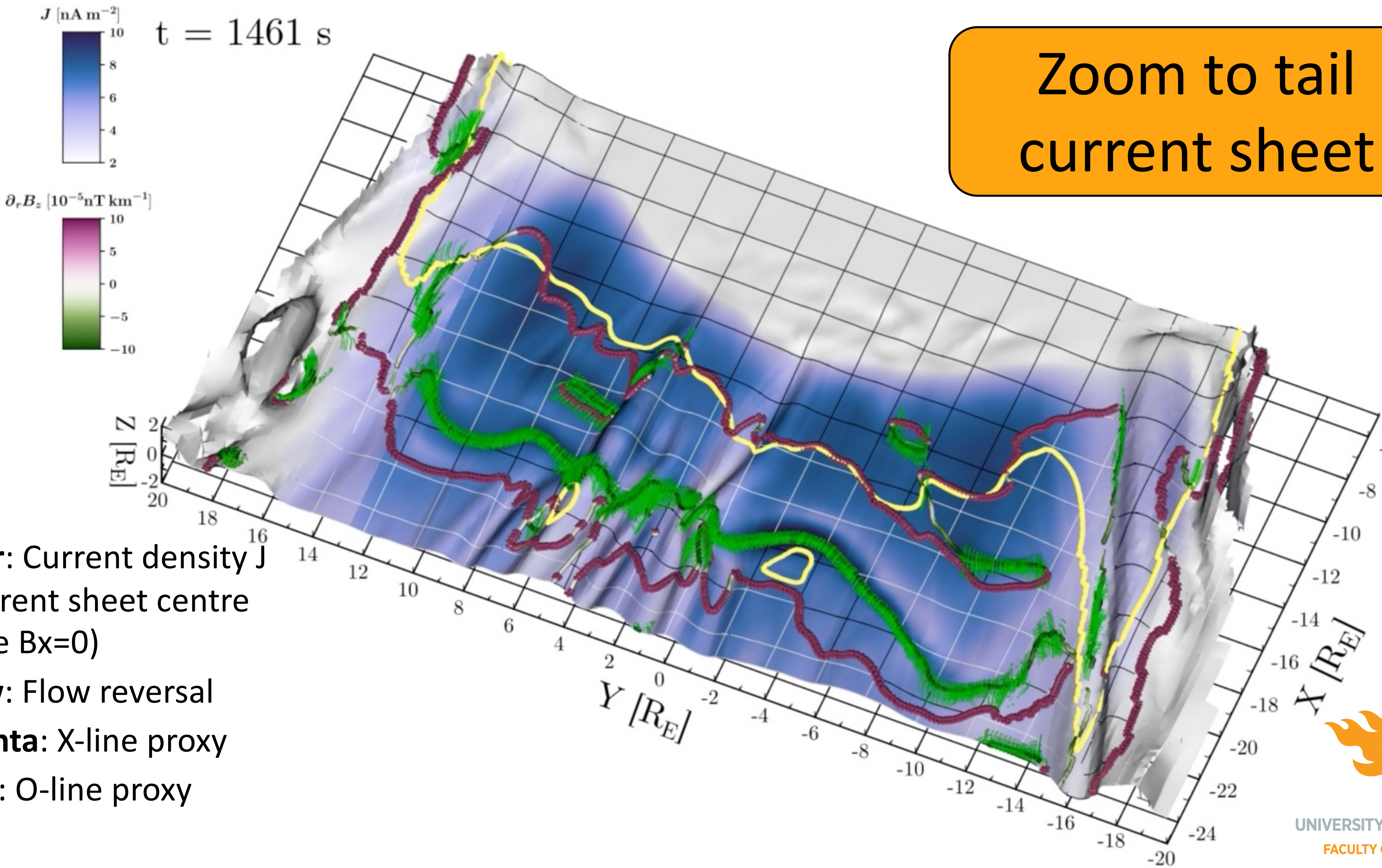
Modelling requirements
- Tail driven by dayside input ➔ *Global*
- NENL ➔ *Reconnection*
- CD ➔ *3D kinetic instabilities & drifts*

Modelling efforts so far
- **3D Global MHD**:
    - reconnection
    - MHD instabilities, no drifts
- **3D Hybrid-kinetic:**
    - Now available

Sorathia+, *GRL*, 2020



Zoom to tail current sheet



- **Colour**: Current density J on current sheet centre (where Bx=0)
- **Yellow**: Flow reversal
- **Magenta**: X-line proxy
- **Green**: O-line proxy

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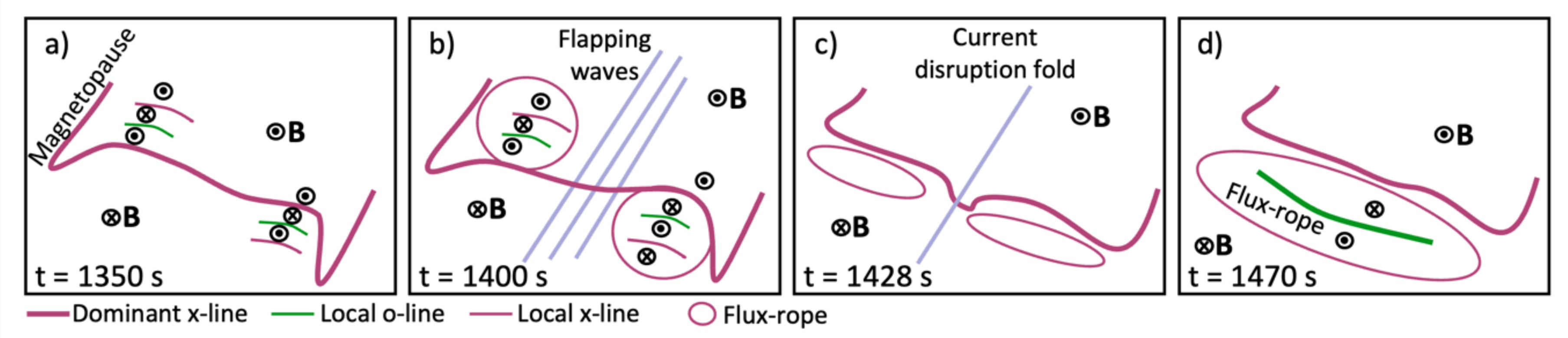
From Palmroth et al. Nature Geosci 2023. Visualisation: Markku Alho

Ion kinetic instabilities and reconnection work together to release the plasmoid via plasma sheet flapping



Vlasiator suggests reconciliation:

✓ **NENL**: Reconnection – current disruption – plasmoid

✗ **BUT**: Current disruption not in the same local time as reconnection **AND NOT** due to fast flows

✓ **CD**: Current disruption @ transition region – spreads outwards – large-scale reconnection – plasmoid

✗ **BUT**: CD caused by flapping, which is caused by reconnection

VLASIATOR **scenario**:

- Two reconnection sites @flanks move to centre: **plasmoid**
- Centre disrupts the current due to current sheet flapping

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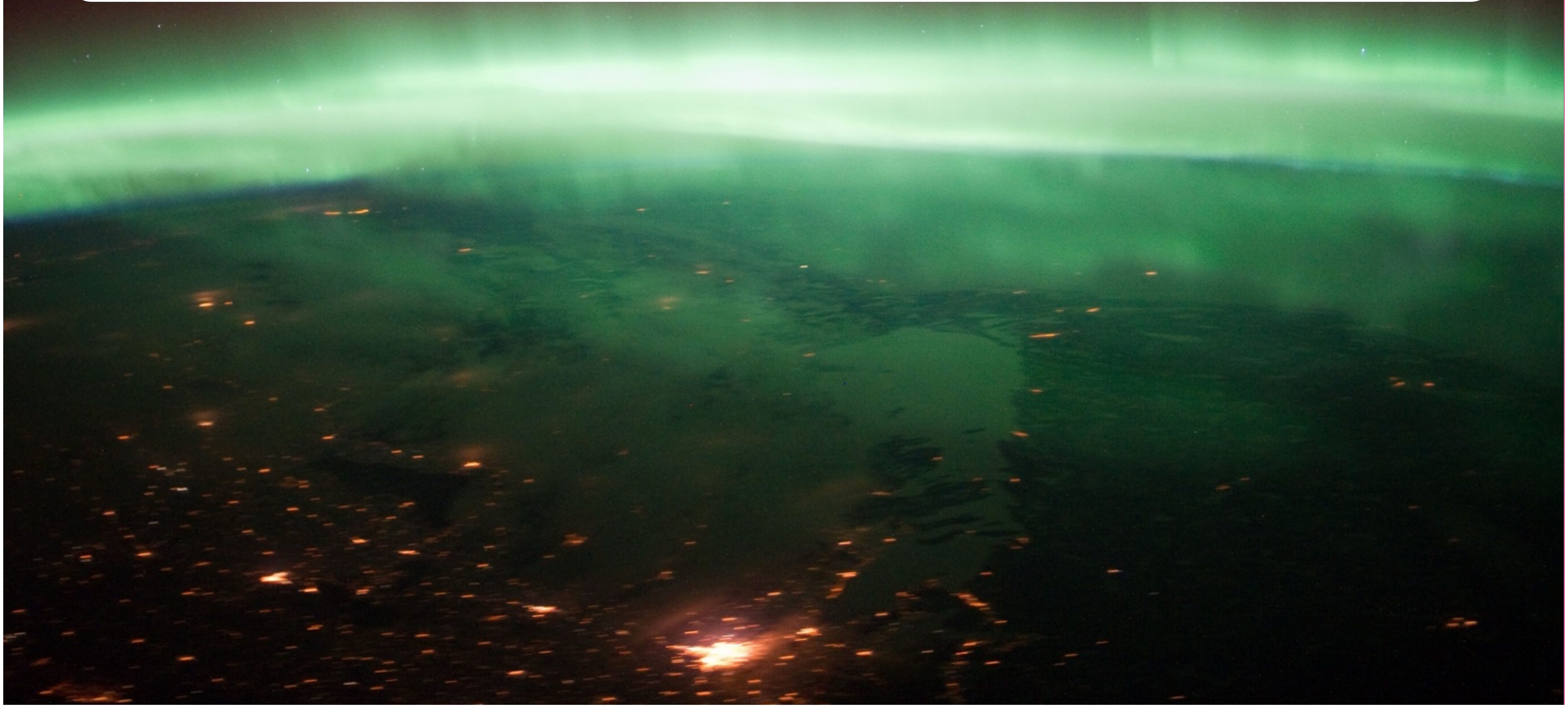


Trends in HPC (relative to space physics)

Read also: https://blog.purestorage.com/perspectives/5-trends-shaping-the-future-of-high-performance-computing/

- **Europe has an exascale strategy (EuroHPC)**
- **Future is in heterogeneous computing**
- **GPU Computing will increase** (portability is key)
- **HPC accessibility will increase**
  - Tools, performance profiling, etc.
- **AI will be used to improve HPC**
- **Modern data storage will be a critical investment**

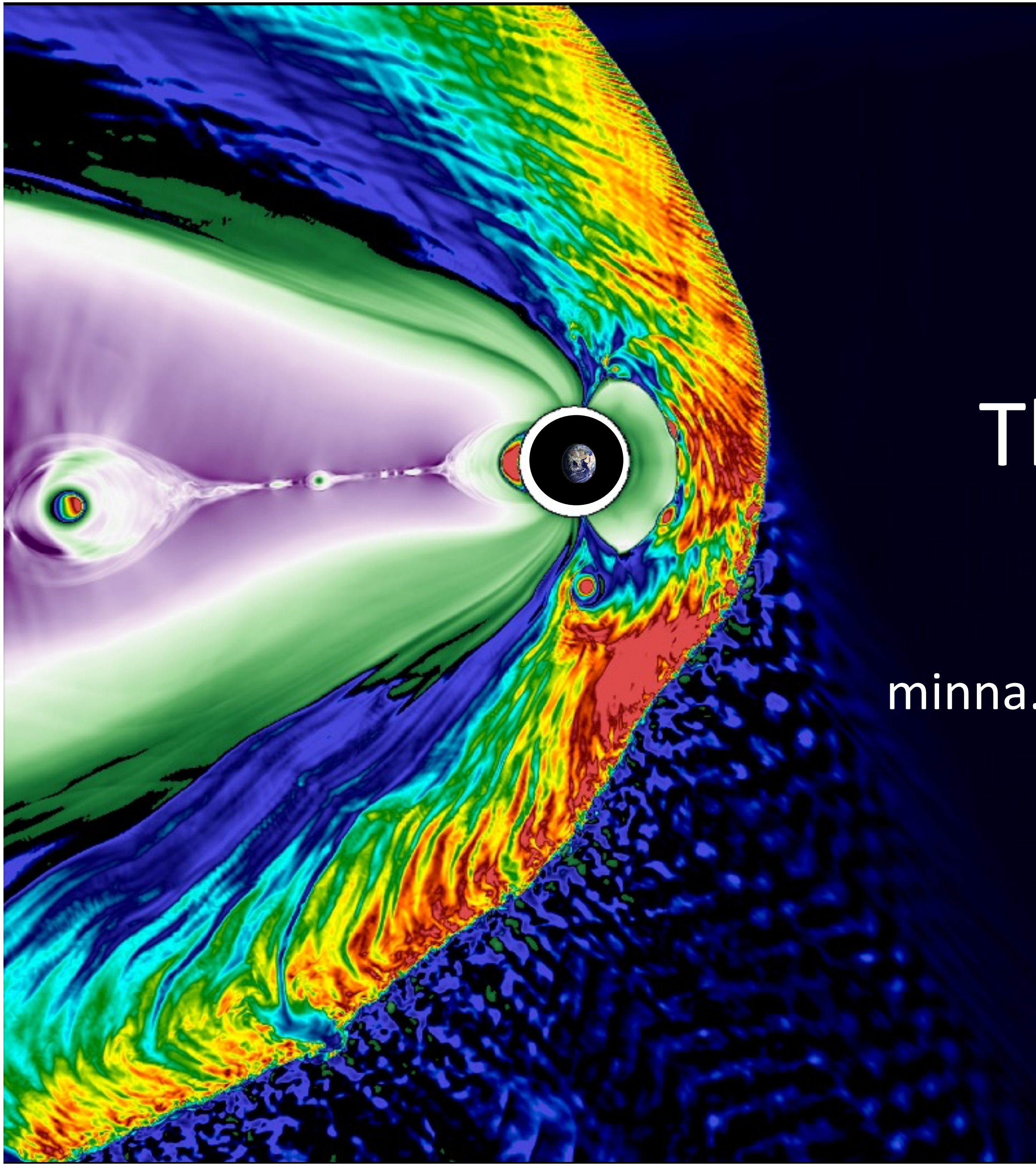
Trends:
Portability and future technologies

- Vlasiator currently runs on AMD-64, ARM, RISCV, and PowerPC
- CPU + GPU architectures (with NVIDIA and AMD)
- Ongoing development for scalable vector architectures and European accelerator project (EPAC)
- Sufficient portability for future architectures
  - This was always our strategy!
- Quantum computing? Forward propagation of a physical system isn't suitable on Quantum.

Vlasiator running on Aarch64 (64bit ARM) on our Lead Developer's mobile!
Credits: Urs Ganse & Eleanna Asvestari

In summary

- Economic use of space is skyrocketing.
- Our modern way of life is critically dependent on space-based services.
  - ➔ **There is an increasingly strong need to model geospace accurately.**
- Computing resources are massively increasing
  - **BUT**: Their use requires special skills in heterogeneous HPC
  - ➔ **Only those who take up the challenge will be able to use them**
- Future need and massive resources will allow versatile first-principles modelling and AI-based fast data analysis.
  - Skills to develop: HPC, GPU, ML
- BTW we are hiring again soon.



Thank you!

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minna.palmroth@helsinki.fi