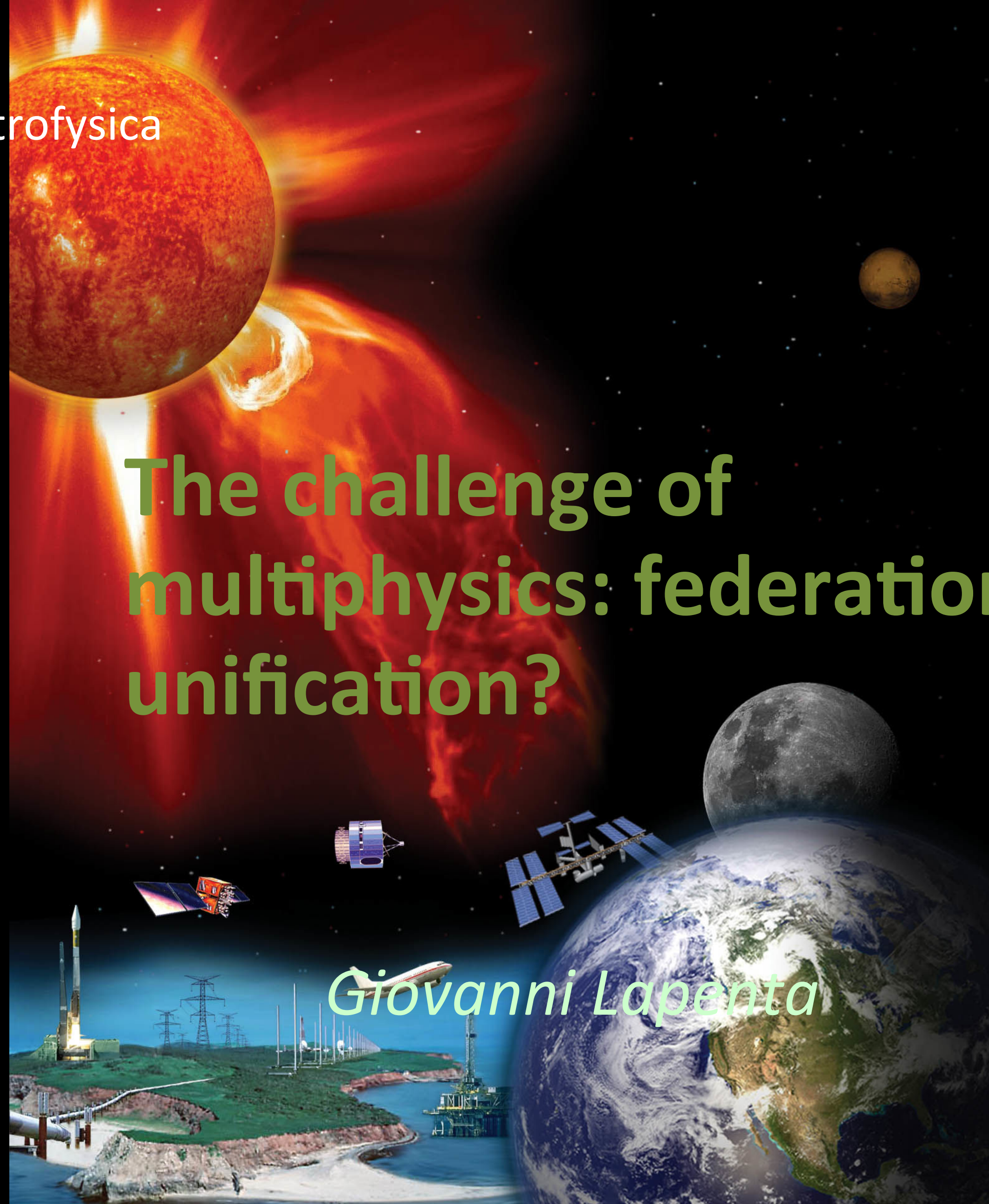
Centrum voor Plasma-Astrofysica
KU Leuven

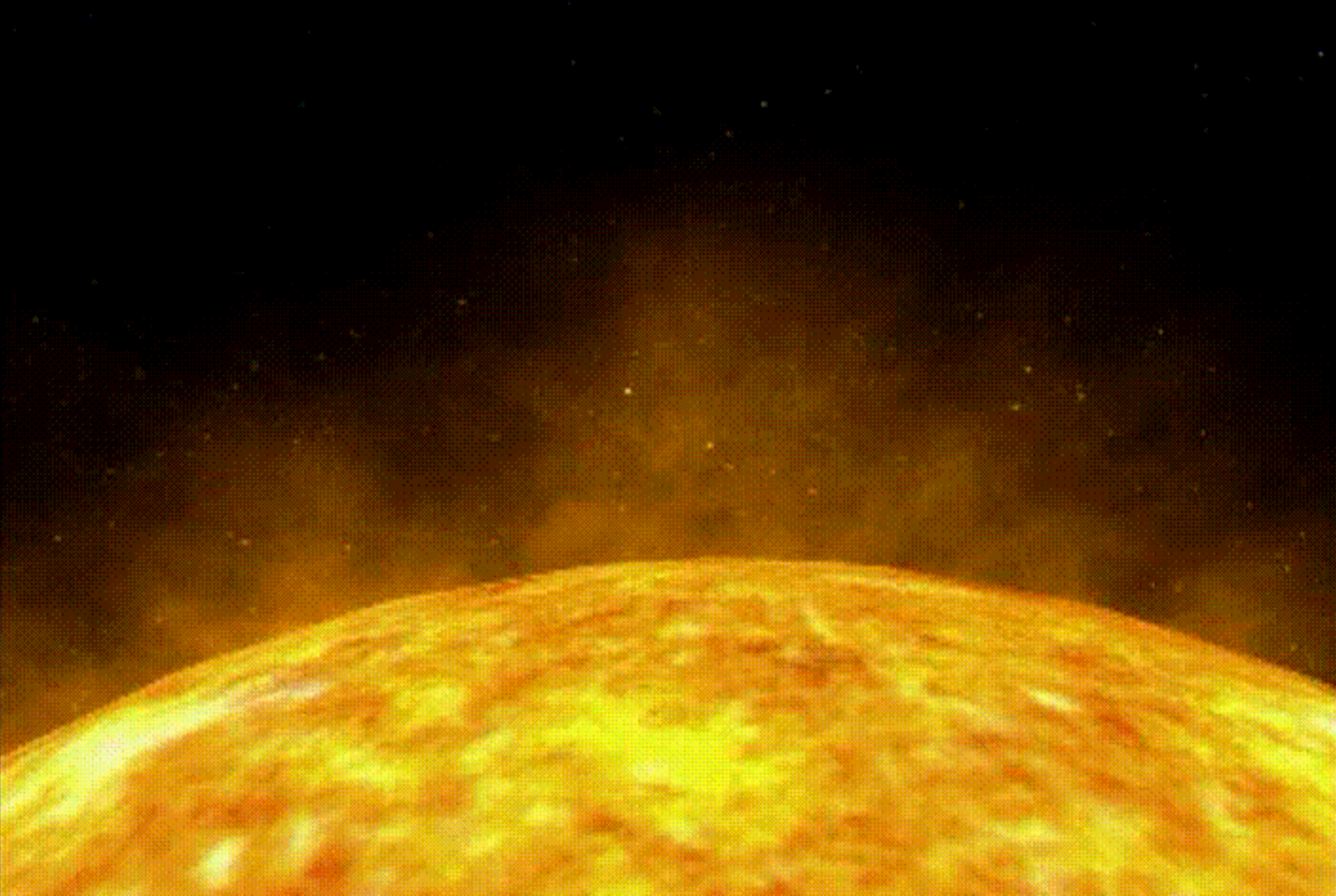
The challenge of multiphysics: federation or unification?



Giovanni Lapenta

Funding from:
BOF & GOA (KU Leuven),
EC (Swiff, Soteria),
NASA (MMS Mission),
Intel Exascience Lab.

Space Weather



Co-Design and space weather at KU Leven

KATHOLIEKE UNIVERSITEIT LEUVEN

Space Weather projects

Soteria

- First ever EC-FP7 funded project on space weather
- Started 2008
- End this year
- Cordinator: G. Lapenta

Swiff

- FP7 project on the space weather call
- To run till 2014
- Cordinator: G. Lapenta

eHeroes

- FP7 project
- From the 2011 call
- Kick-off in Rome in March 2012
- To run till 2015
- Cordinator: G. Lapenta

HPC projects

- DEEP
- Intel Exascience Lab (ExaScience Lab, Intel Labs Europe, EXASCALE COMPUTING)
- Hybrid Computing

SPACECAST · CASSIS · MMS NASA · esa space situational awareness

Outline

KATHOLIEKE UNIVERSITEIT LEUVEN

Challenges of space weather:

- multiscale
- Multiphysics

Federation of models

Unification of models

Ongoing efforts at KU Leuven

Outline

KATHOLIEKE UNIVERSITEIT LEUVEN

Challenges of space weather:

- multiscale
- multiphysics

Federation of models

Unification of models

Ongoing efforts at KU Leuven

Importance of Space Weather Simulation

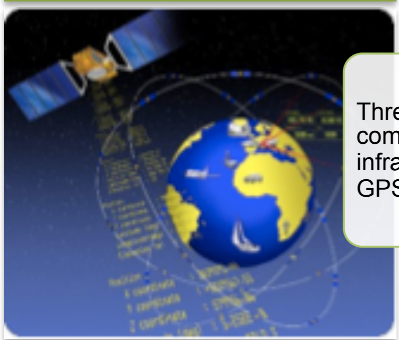
KATHOLIEKE UNIVERSITEIT LEUVEN

Societal Impact:

Science

Natural Phenomena

Technology in Space



Threats to communication infrastructure, GPS

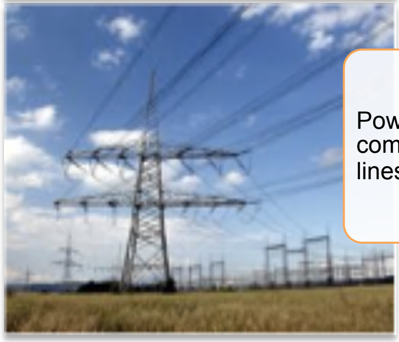
Humans in Space

Threats to life and missions

Ground effects

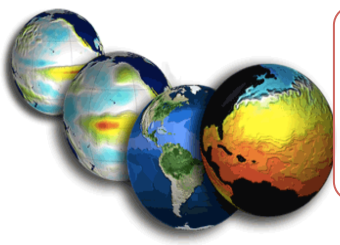
Pipelines

Ground effects



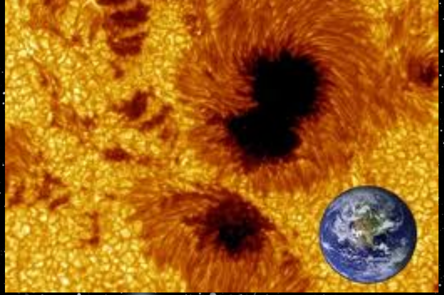
Power grid and communication lines

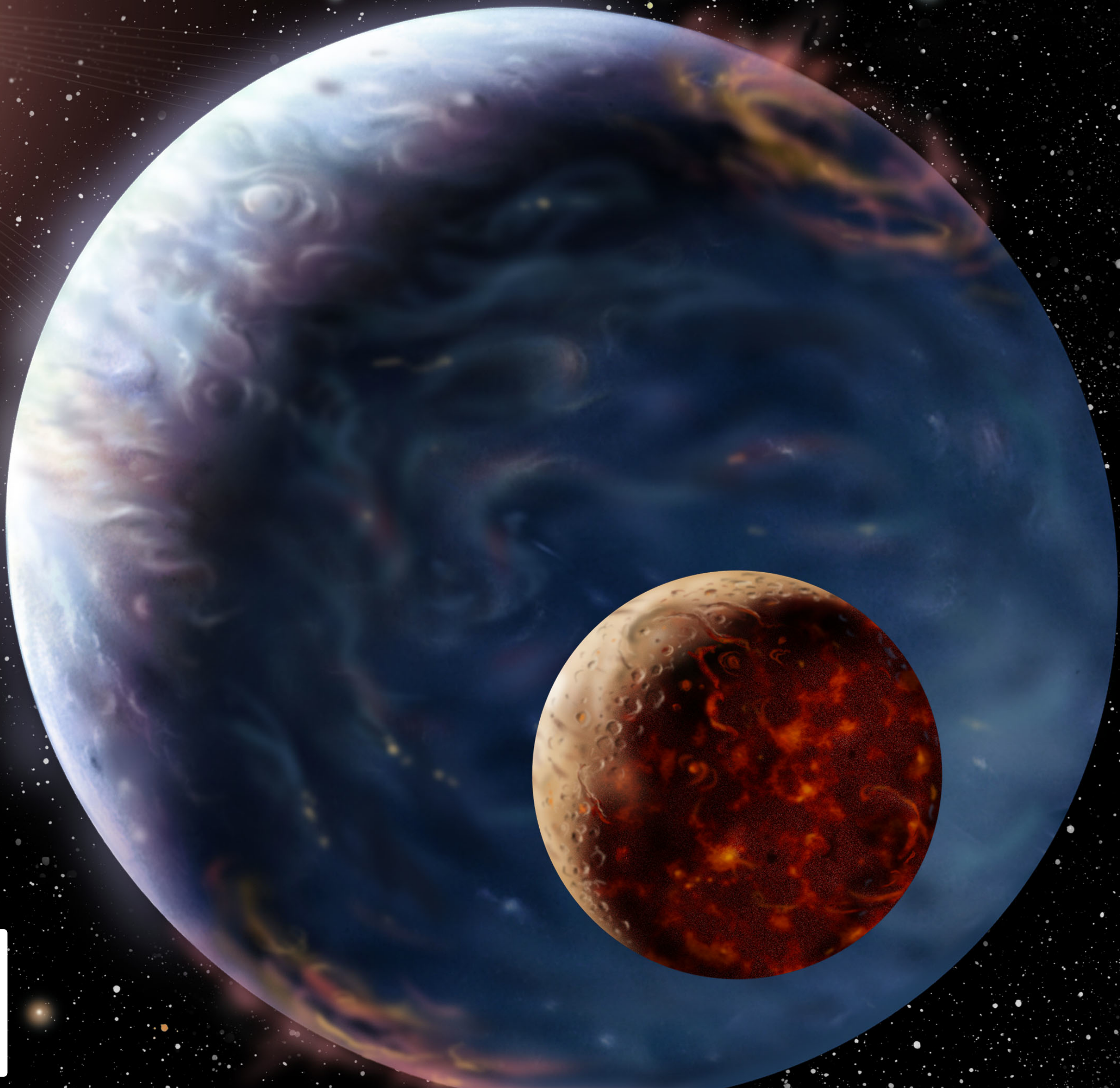
Impact on Earth Climate



Relative importance of CO_2 and solar drives

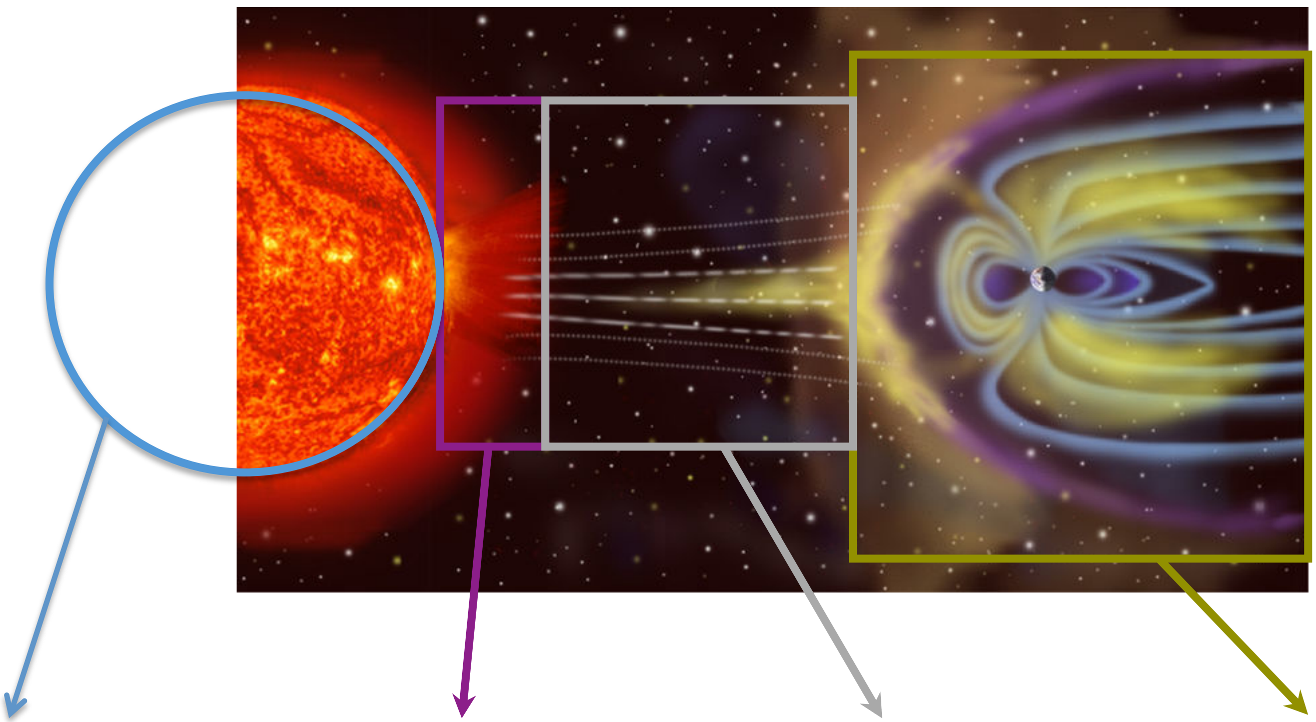
Challenges





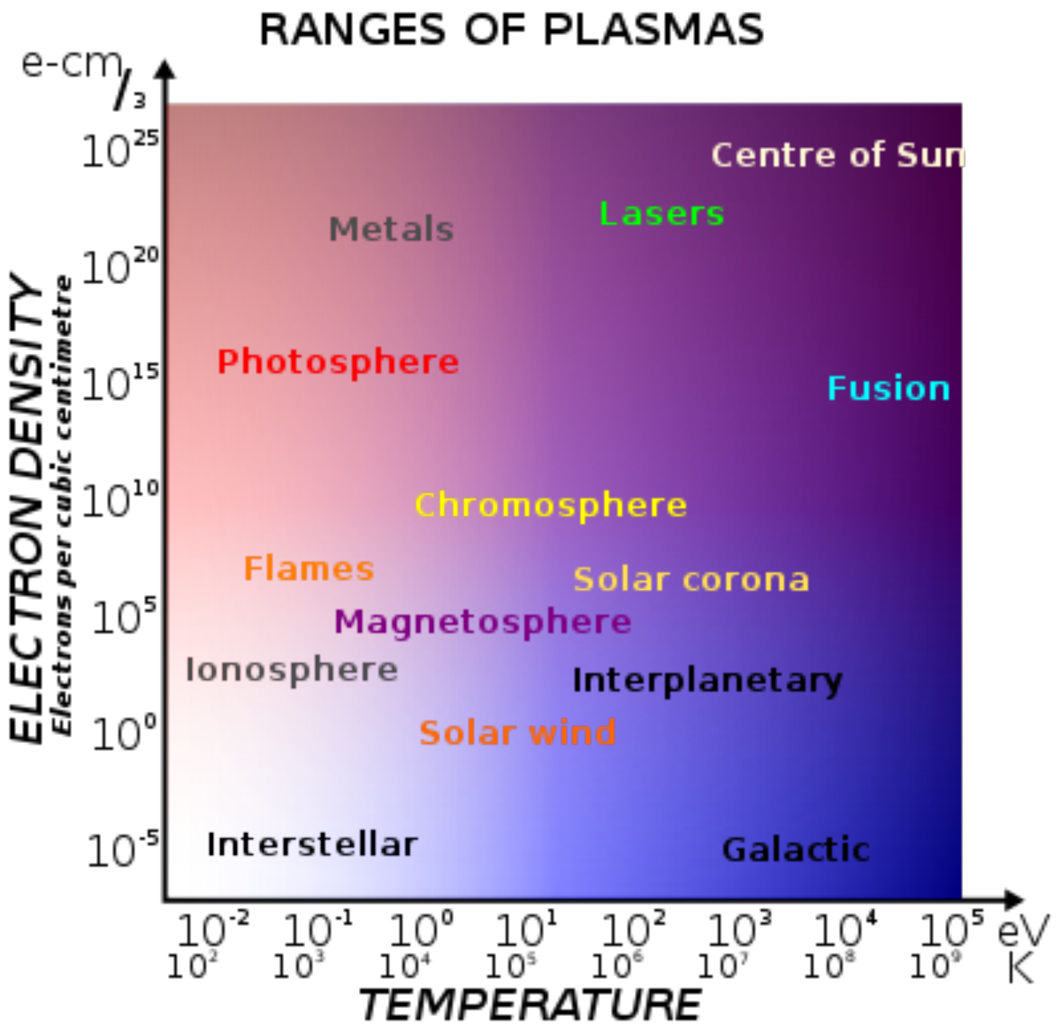
- Challenge of Space Weather
  - Multiple scales
  - Multiple physics

Space weather: Chain of events



Solar Interior → Solar atmosphere → Interplanetary space → Earth Environment

Multiple scales are present in many plasmas



Multiscale: Example of scales involved

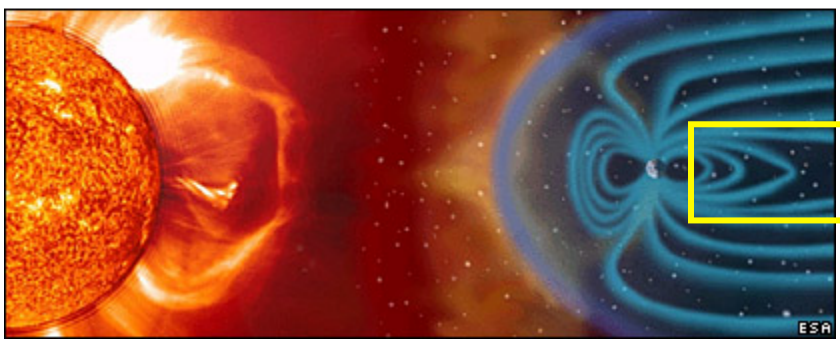
KATHOLIEKE UNIVERSITEIT LEUVEN

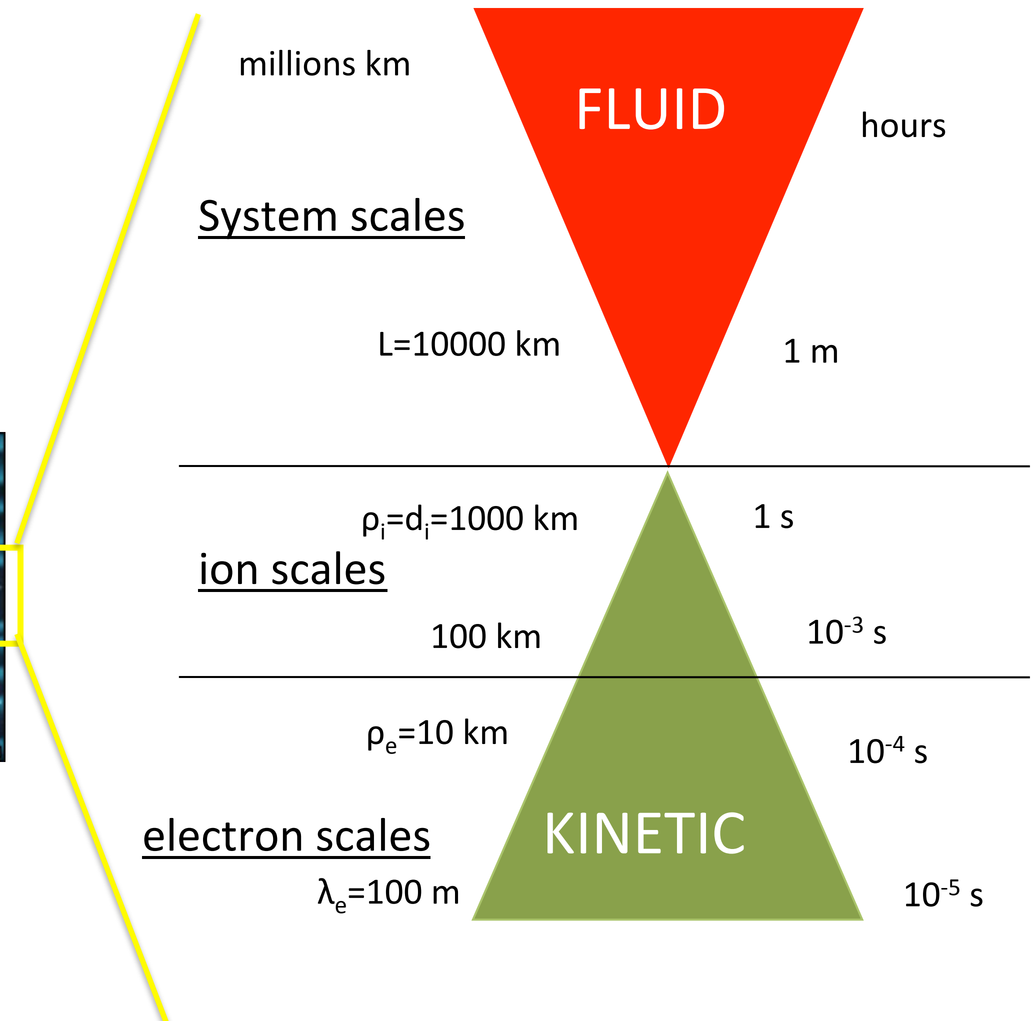
Overall event duration: hours to days

AU = 150 million Km (1.49 10^8 km)

Solar Radius = 6.9 10^5 km

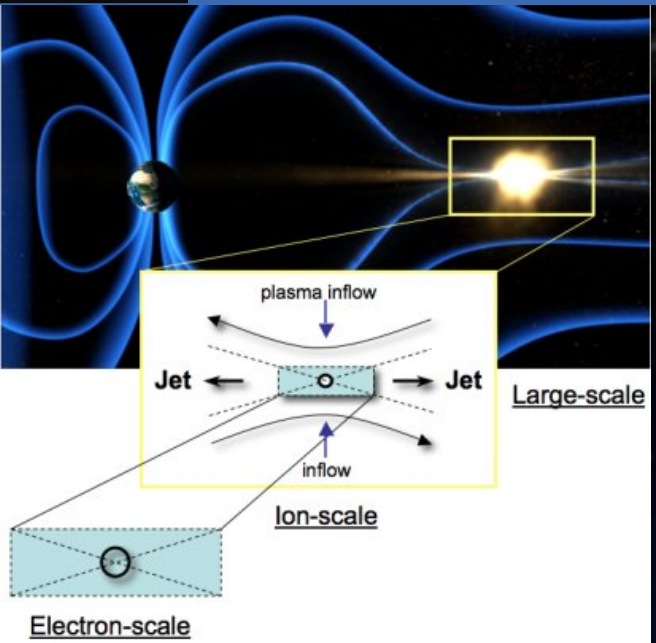
Earth Radius = 6.4 10^3 km

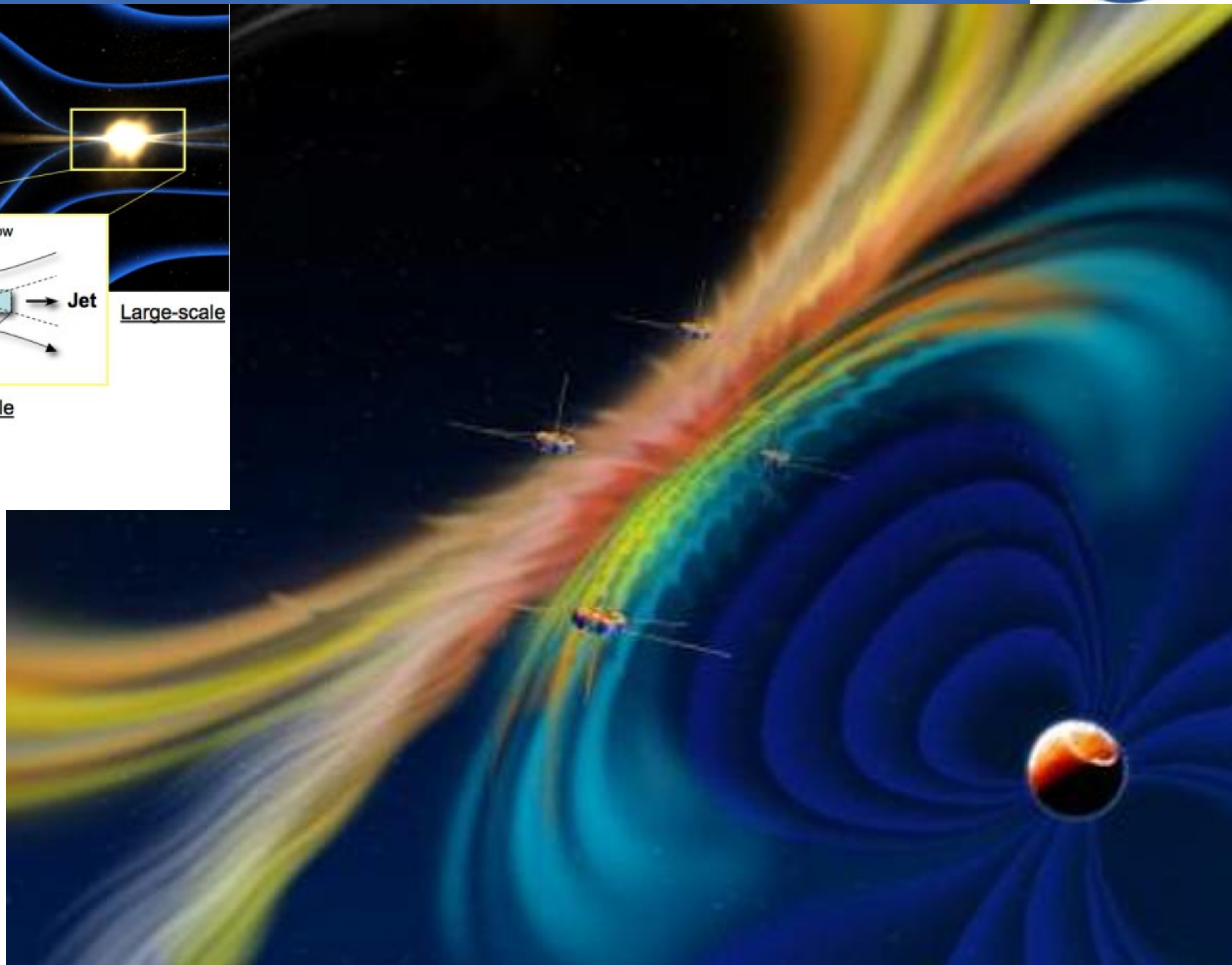




Magnetospheric multiscale mission

KATHOLIEKE UNIVERSITEIT LEUVEN



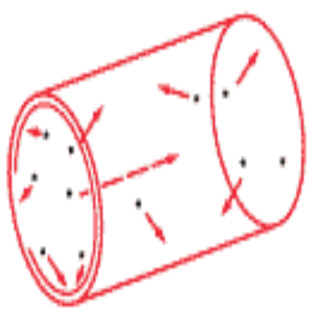


Multiphysics: A plasma and its models

KATHOLIEKE UNIVERSITEIT LEUVEN

GAS

PLASMA



Motion of charged particles without magnetic field.

Motion of charged particles with magnetic field.

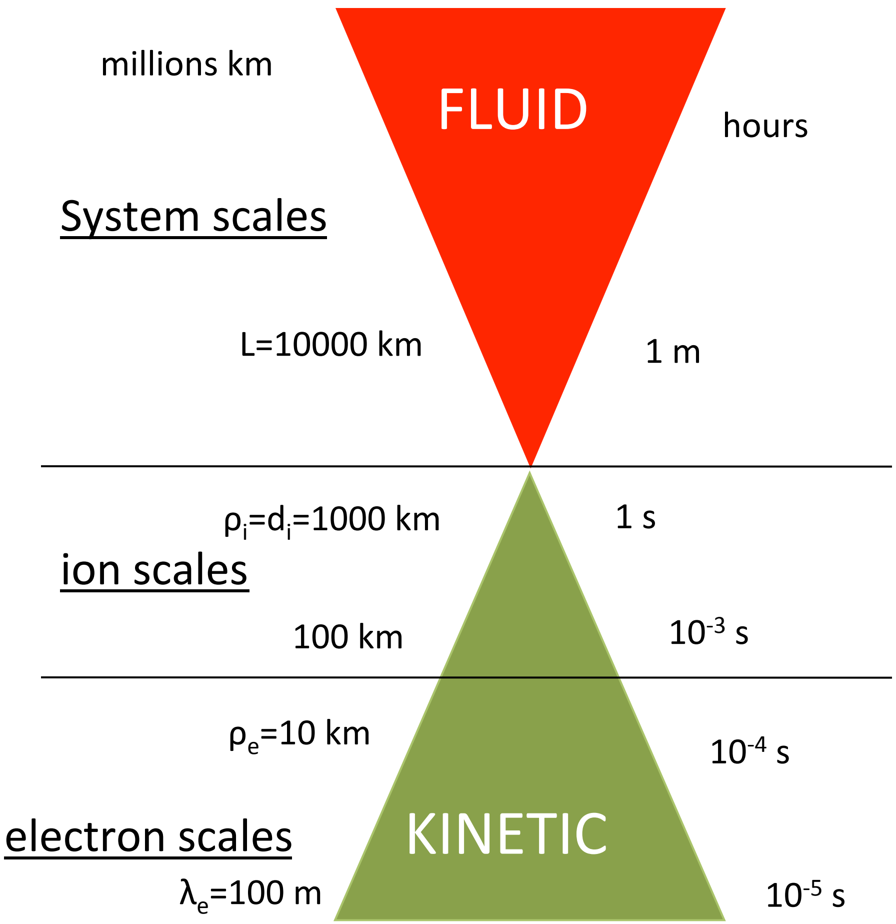
Kinetic approach: study the distribution function (probability of finding a particle with a given velocity in a given point at a given time):

$$\{x_p, v_p\} \qquad f(\mathbf{x},\mathbf{v},t)$$

Fluid approach: study local averages (density, average speed, temperature, ….)

$$n(\mathbf{x},t), \mathbf{U}(\mathbf{x},t), T(\mathbf{x},t)$$

Different physics models at different scales



Fluid models

- computation effort manageable even at large scales
- miss the small scale physics
- adjustable parameters reduce the predictive value

Kinetic models

- first principles: include all physics, in particular what we do not yet understand
- surprisingly simple to conceive and implement in computers
- not economical at large scale

Outline

KATHOLIEKE UNIVERSITEIT LEUVEN

Challenges of space weather:

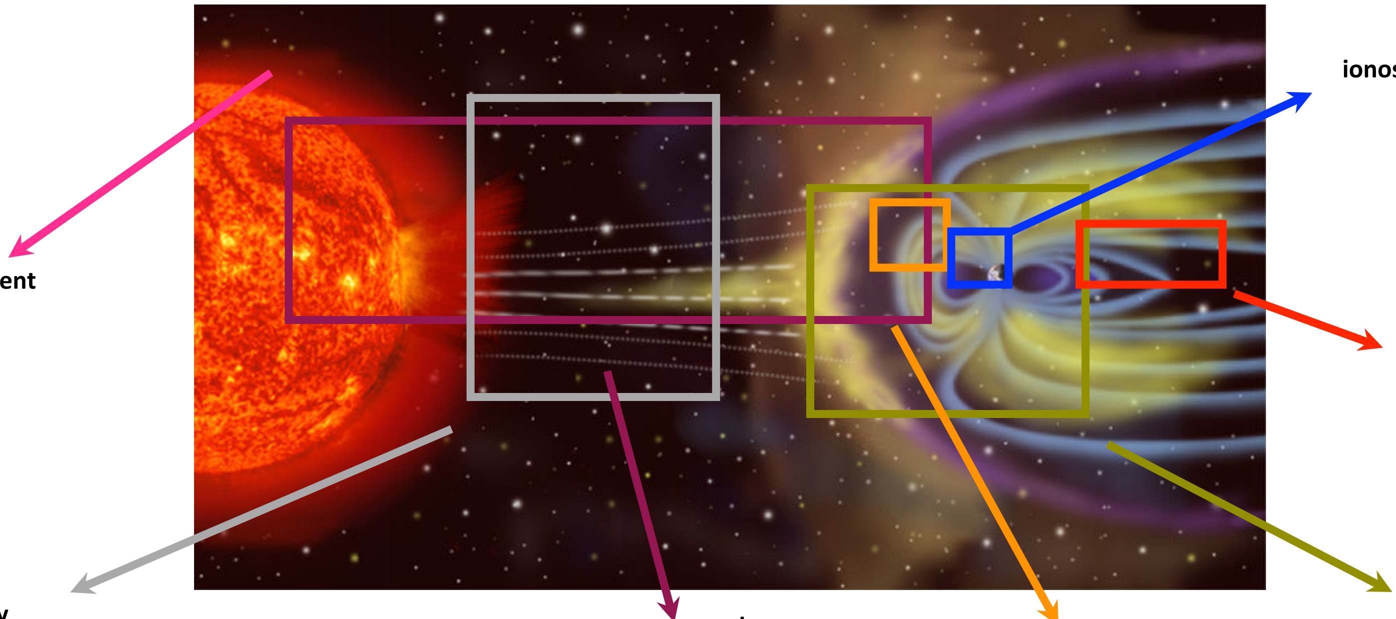
- multiscale
- Multiphysics

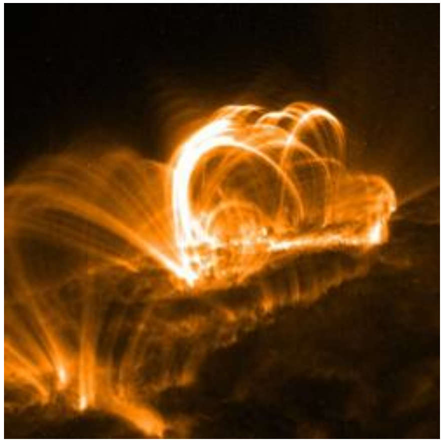
Federation of models

Unification of models

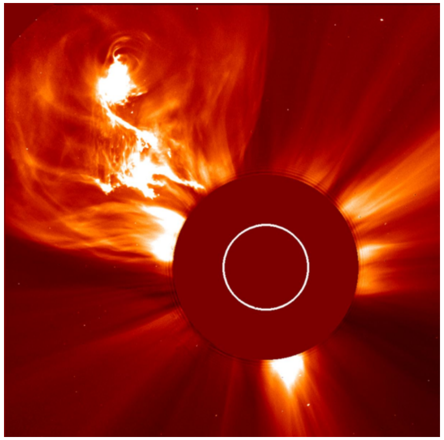
Ongoing efforts at KU Leuven

Federation of Models





TRACE September 2005



LASCO September 2002

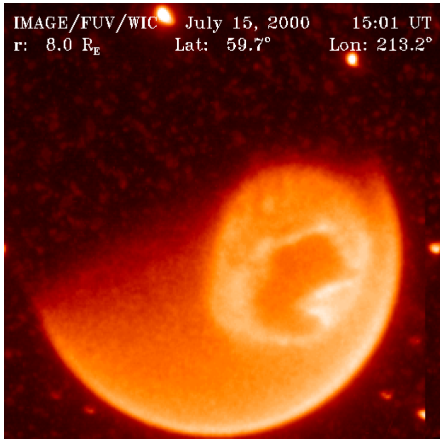
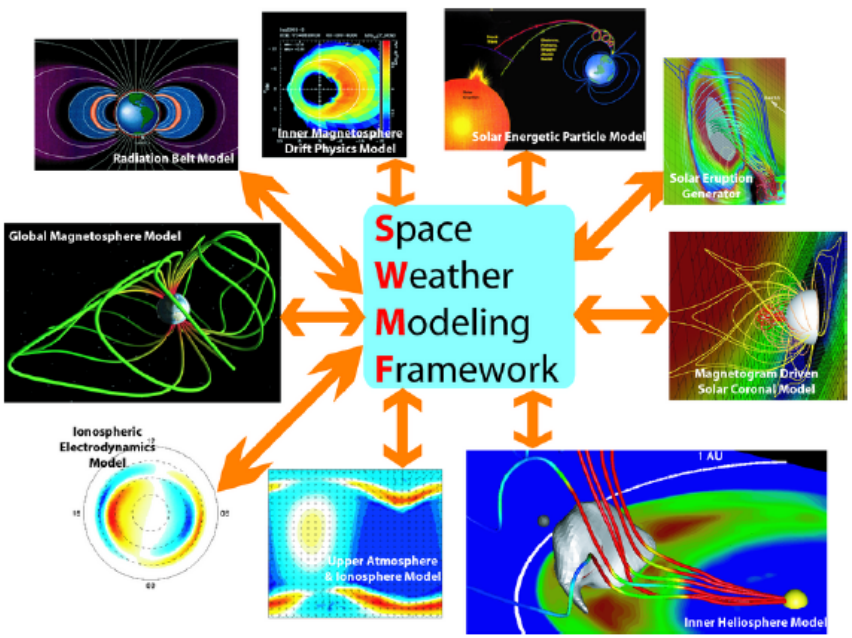
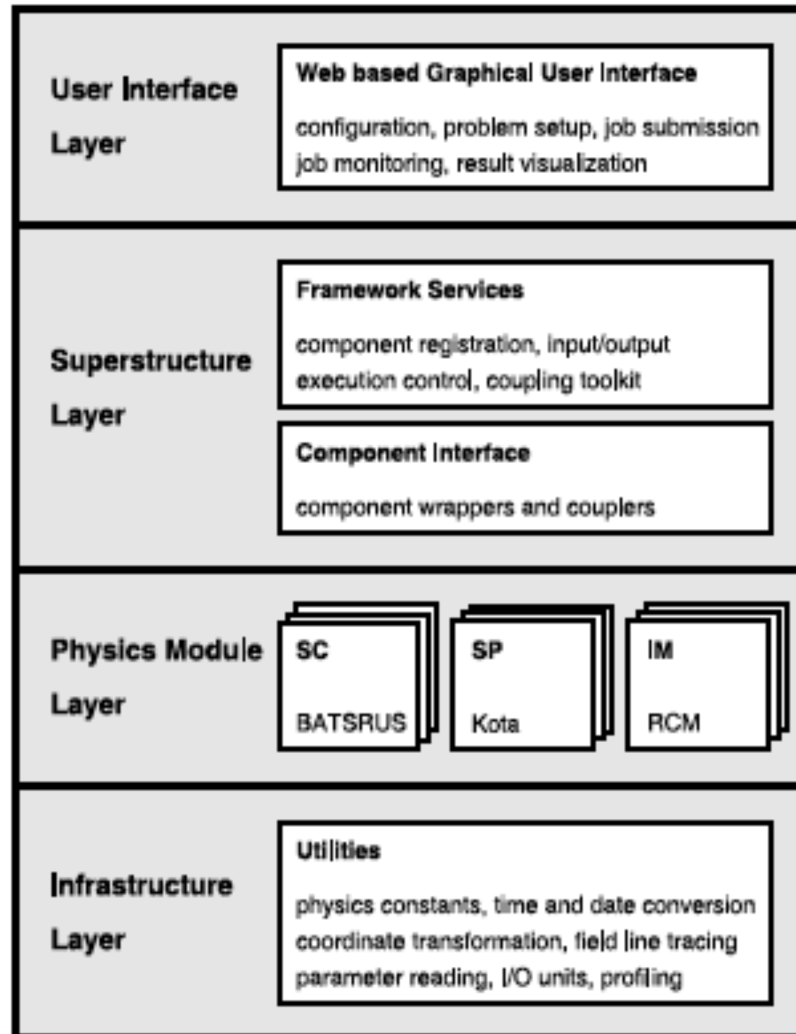


IMAGE July 2000

Software-based federation

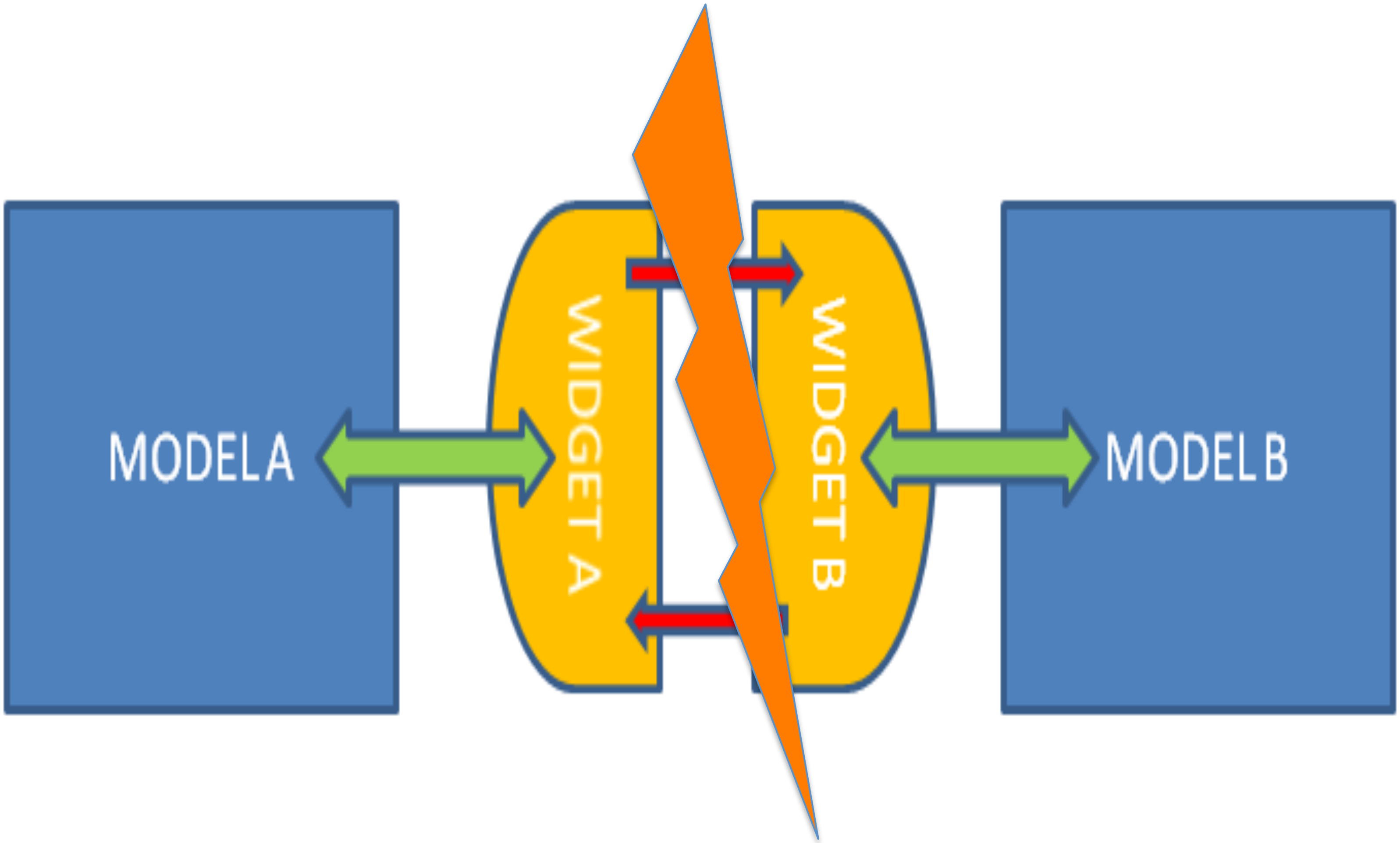
- US efforts: CISM amd SWMF (see Gombosi – next talk)
- EU: the SSA initiative



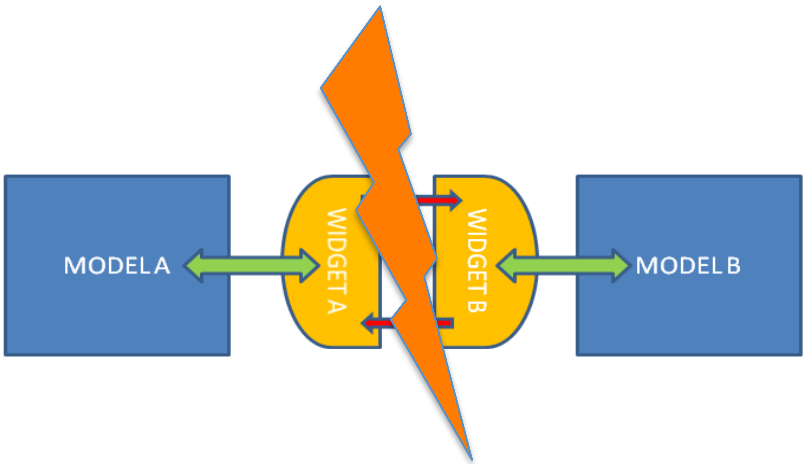


Toth et al., JGR, 110, A12226 (2005)

Need to understand coupling before plugging two codes

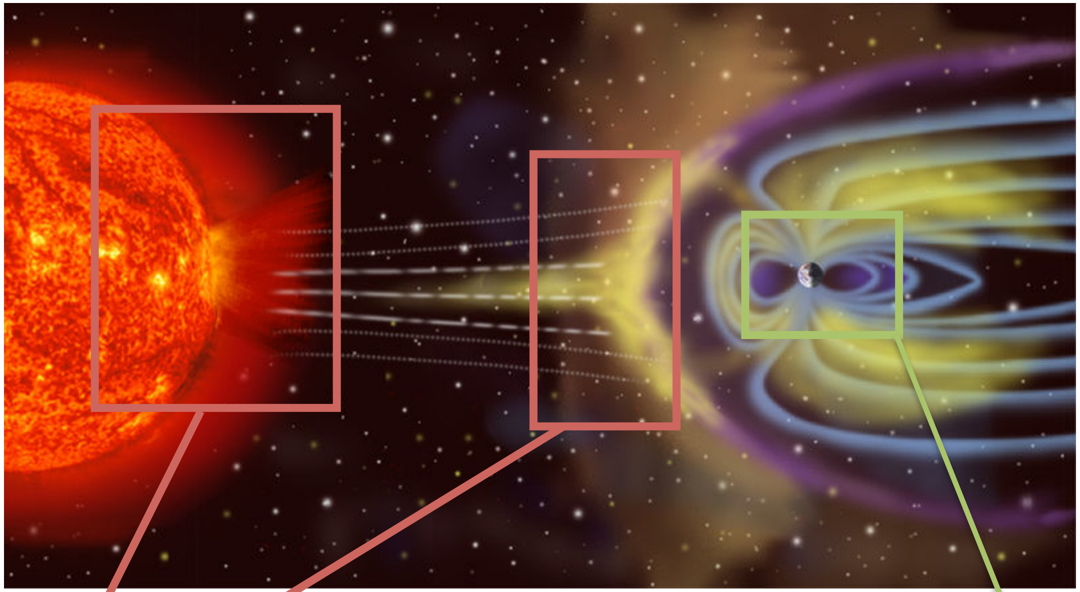


Understanding coupling first



- Resolution in space and time
- Units, geometric representation
- Computational complexity
- Compatible assumptions, approximations, physical ingredients
- Level of statistical noise
- Coupling across interface or across an overlap domain

Lessons: critical points to address

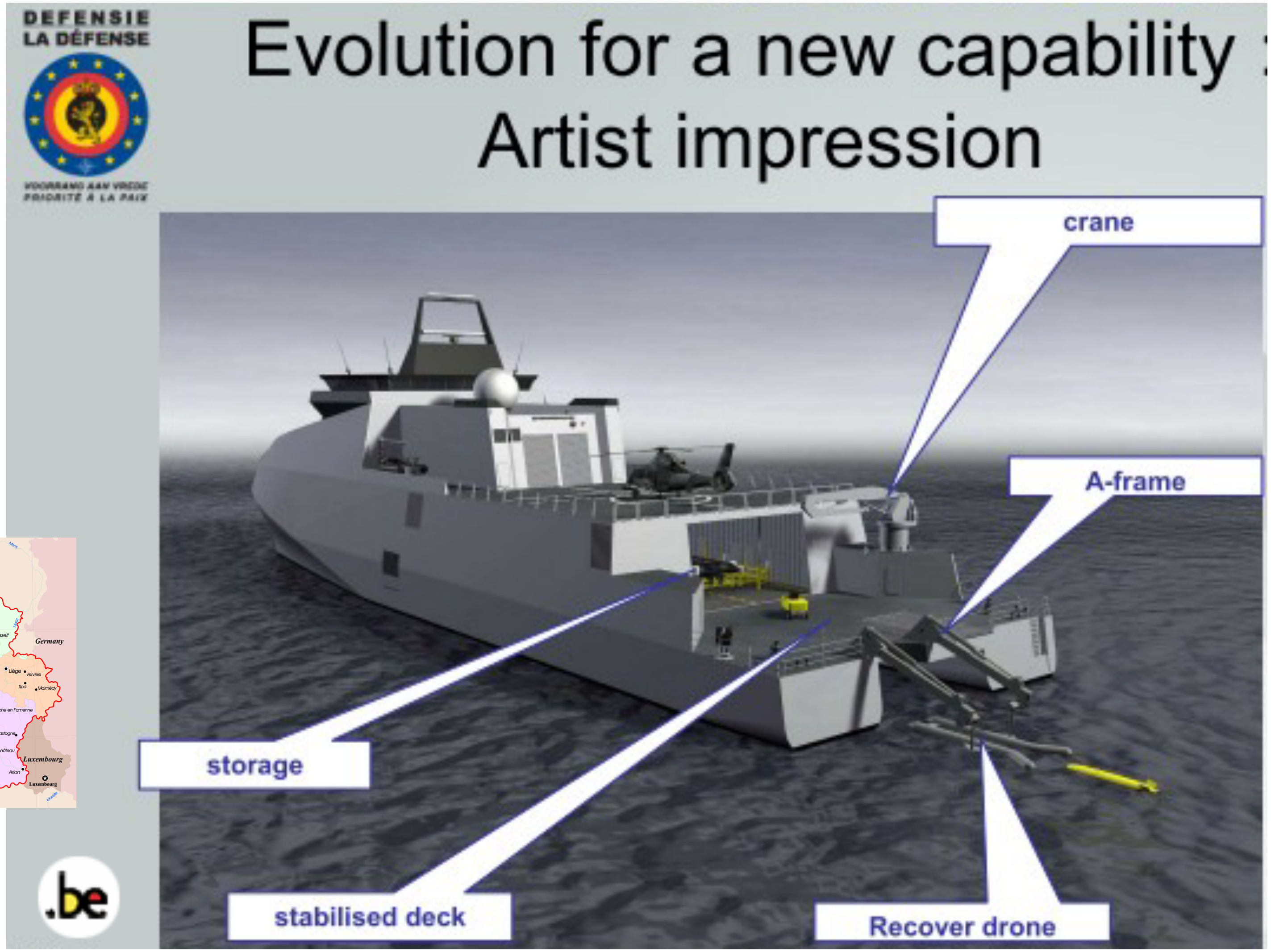


Critical points: reconnection, shocks, need multiphysics approach

Ionosphere-Magnetosphere: different physics and different resolution

Federation of models: a common problem in simulation

KATHOLIEKE UNIVERSITEIT LEUVEN
Claude Archer – Belgian Naval Research



High Level Architecture (HLA) - IEEE/NATO standards

Outline

KATHOLIEKE UNIVERSITEIT LEUVEN

Challenges of space weather:

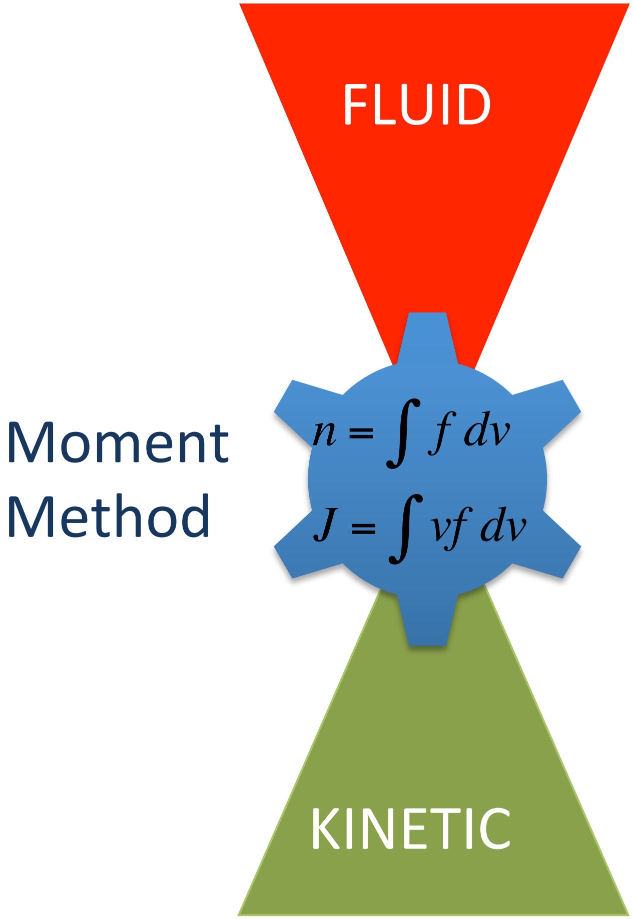
- multiscale
- Multiphysics

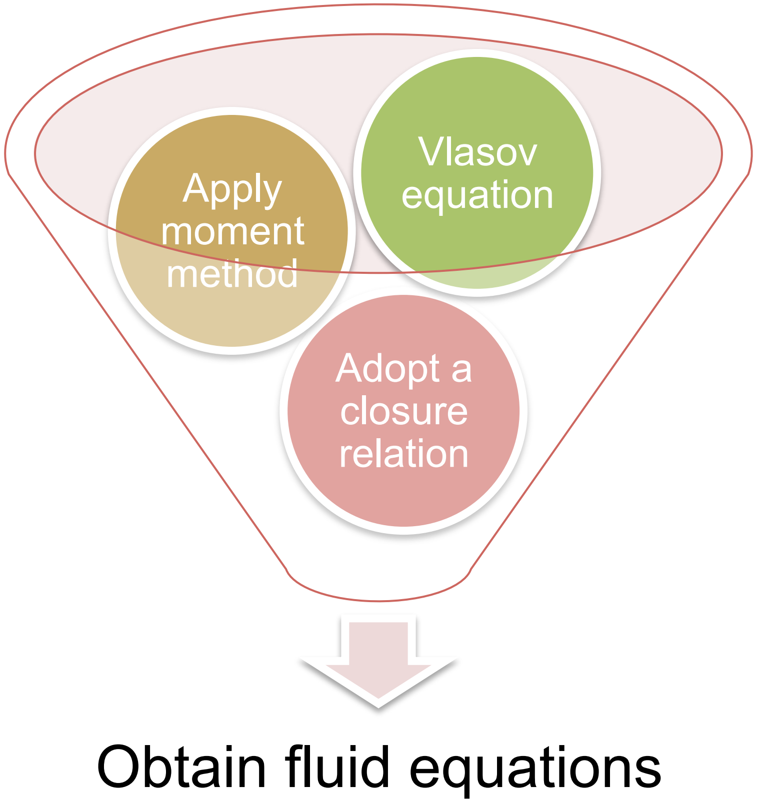
Federation of models

Unification of models

Ongoing efforts at KU Leuven

Unification approach: the moment method





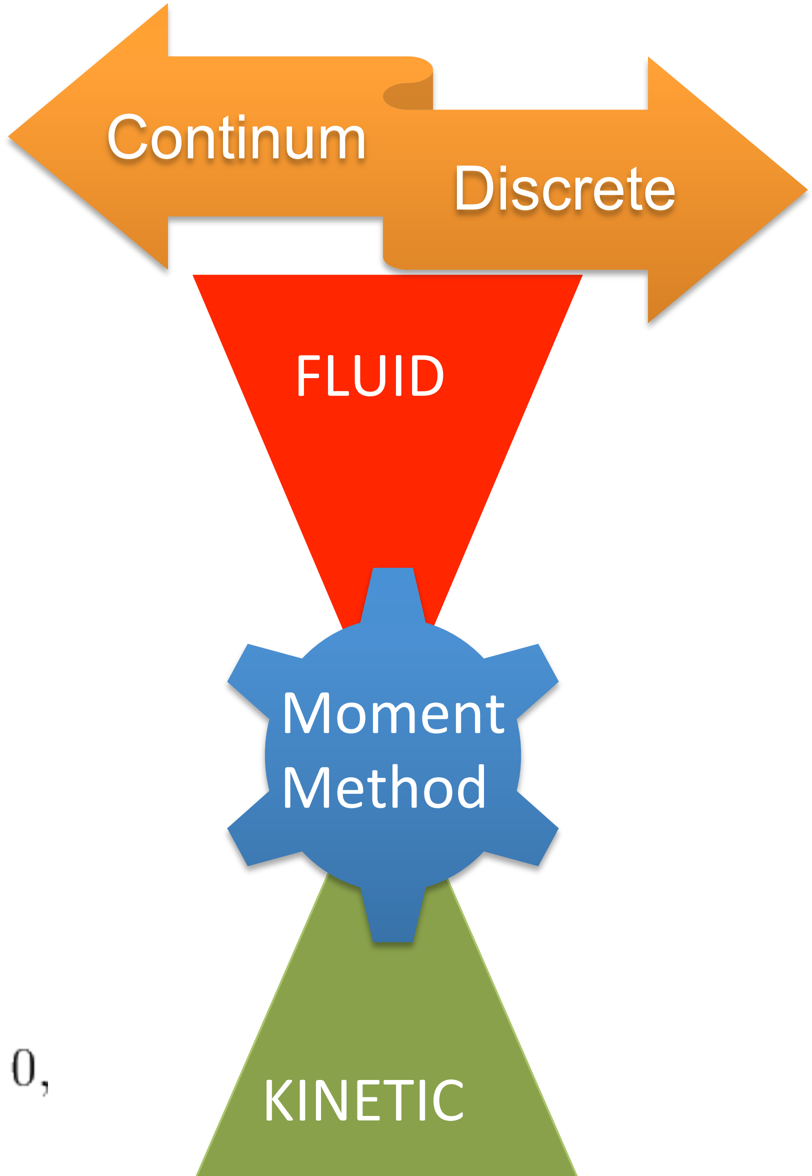
Moment method: From theory to practice

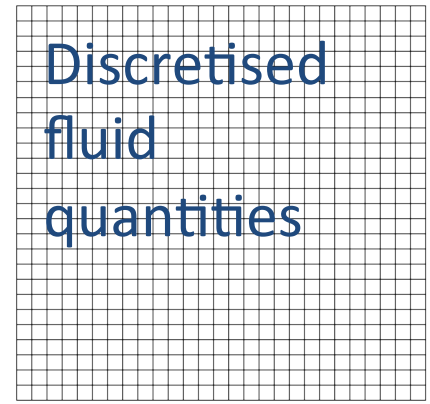
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0.$$

$$n = \int f\, dv$$

$$J = \int vf\, dv$$

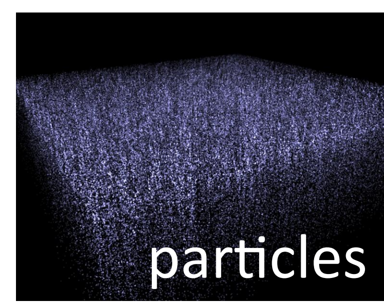
$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{\vec{F}}{m} \cdot \frac{\partial f}{\partial \vec{v}} = 0,$$



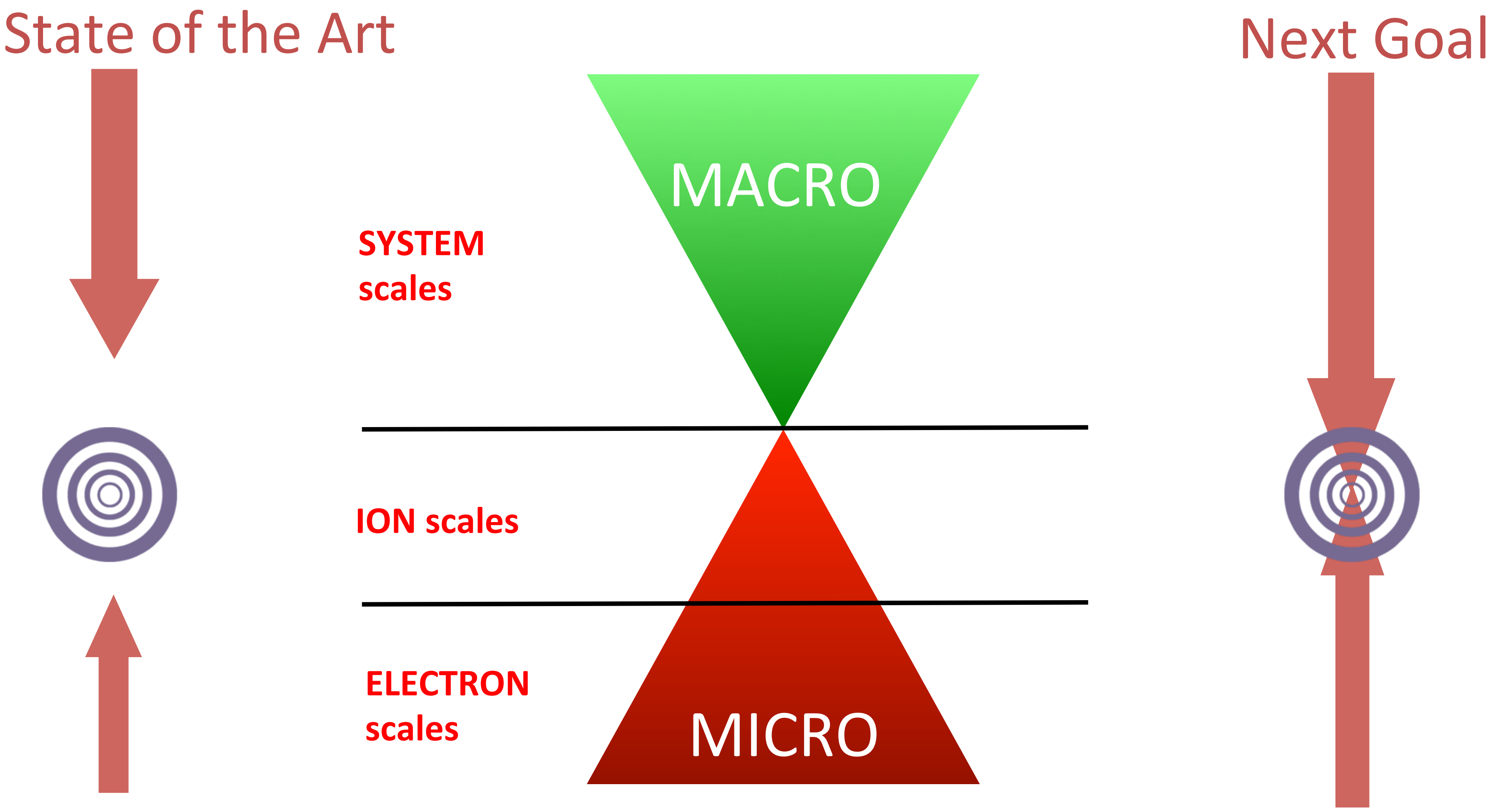


$$n_g = \sum_p S(x_p - x_g)$$

$$J_g = \sum_p u_p S(x_p - x_g)$$



Multiscale – Multiphysis: Unification approach



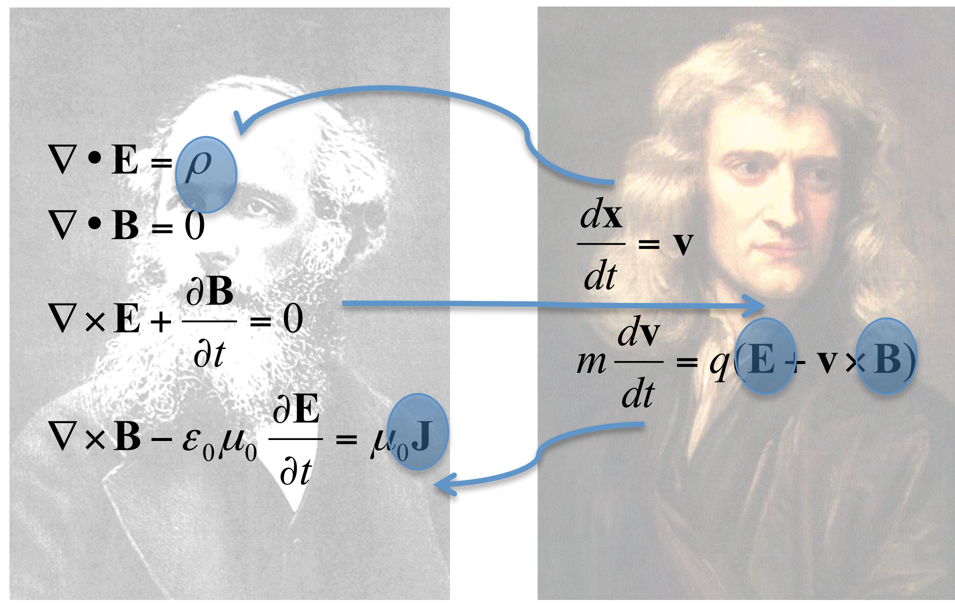
Unification: The core mathematical idea

KATHOLIEKE UNIVERSITEIT LEUVEN

Macro: Fields and Fluids

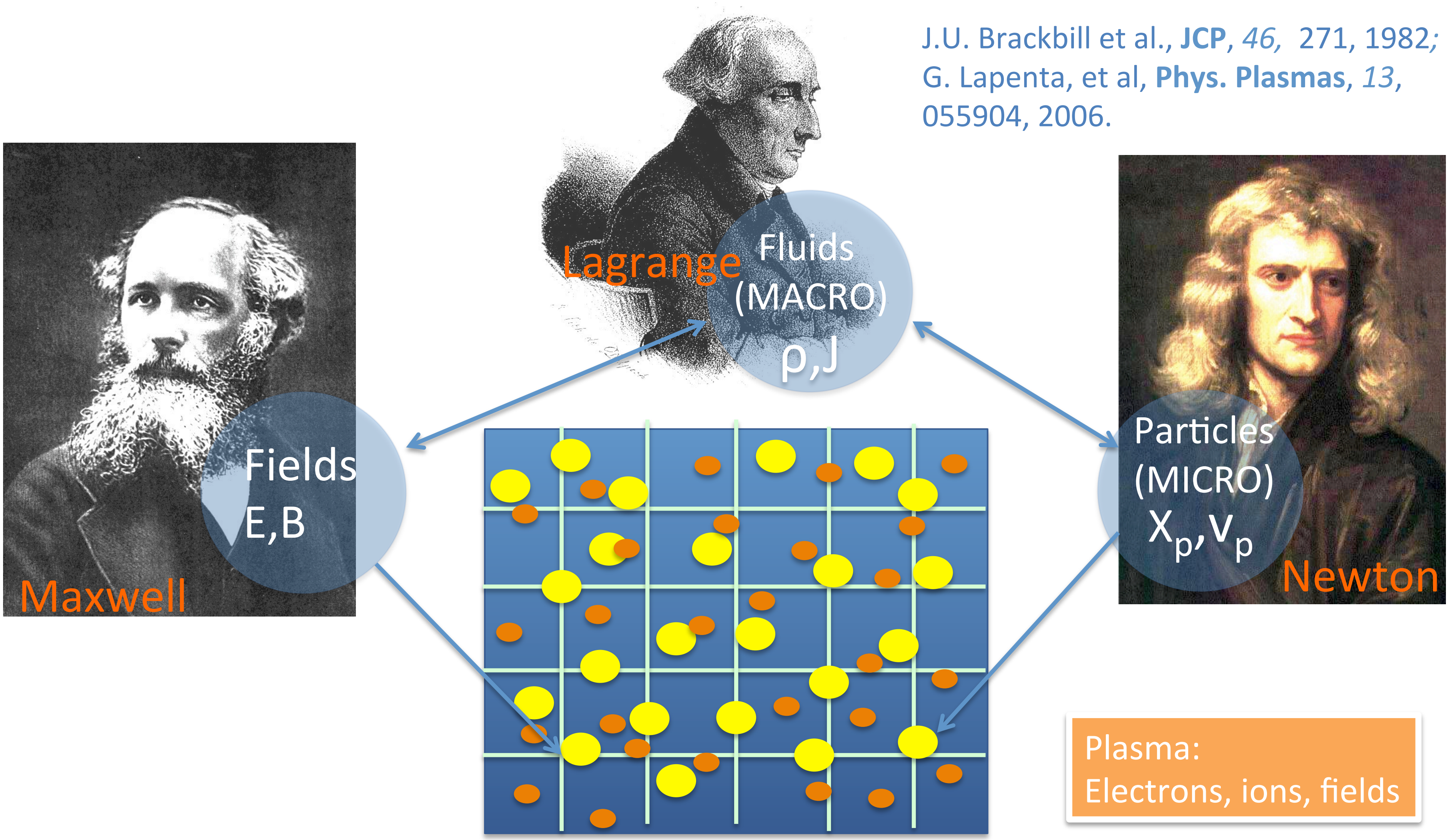
Micro: Particles and Fields

Mathematical and Software connection: Implicit moment method



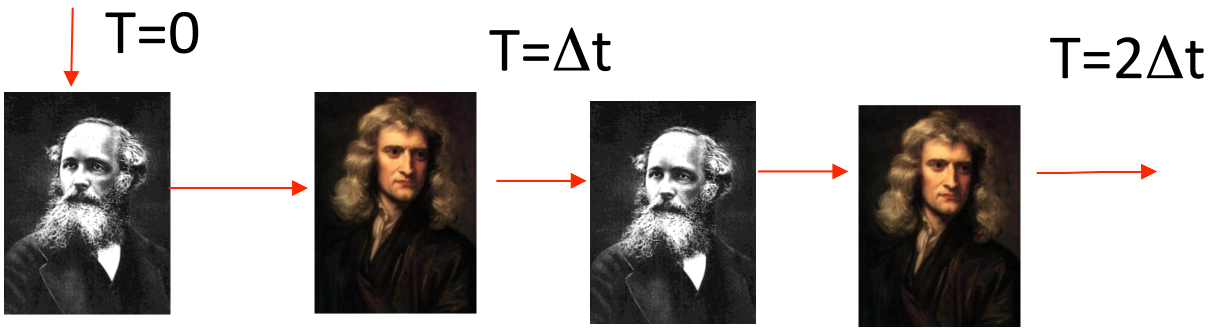
Implicit Moment Method: FLUID to KINETIC

J.U. Brackbill et al., **JCP**, *46*, 271, 1982; G. Lapenta, et al, **Phys. Plasmas**, *13*, 055904, 2006.



Plasma:
Electrons, ions, fields

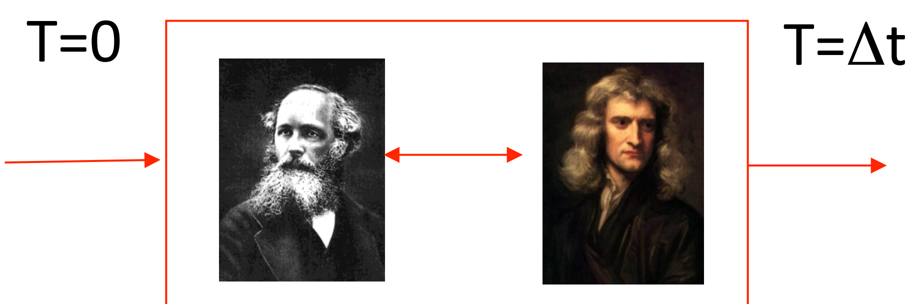
Explicit vs. Implicit



EXPLICIT

Operations:

1. Solve Newton equations in previous electromagnetic fields
2. Solve Maxwell equations with previous particle positions



IMPLICIT

Operations:

Over each time step, iteratively solve the two coupled equations until convergence

Advantages of the Implicit Approach

Explicit stability constraints

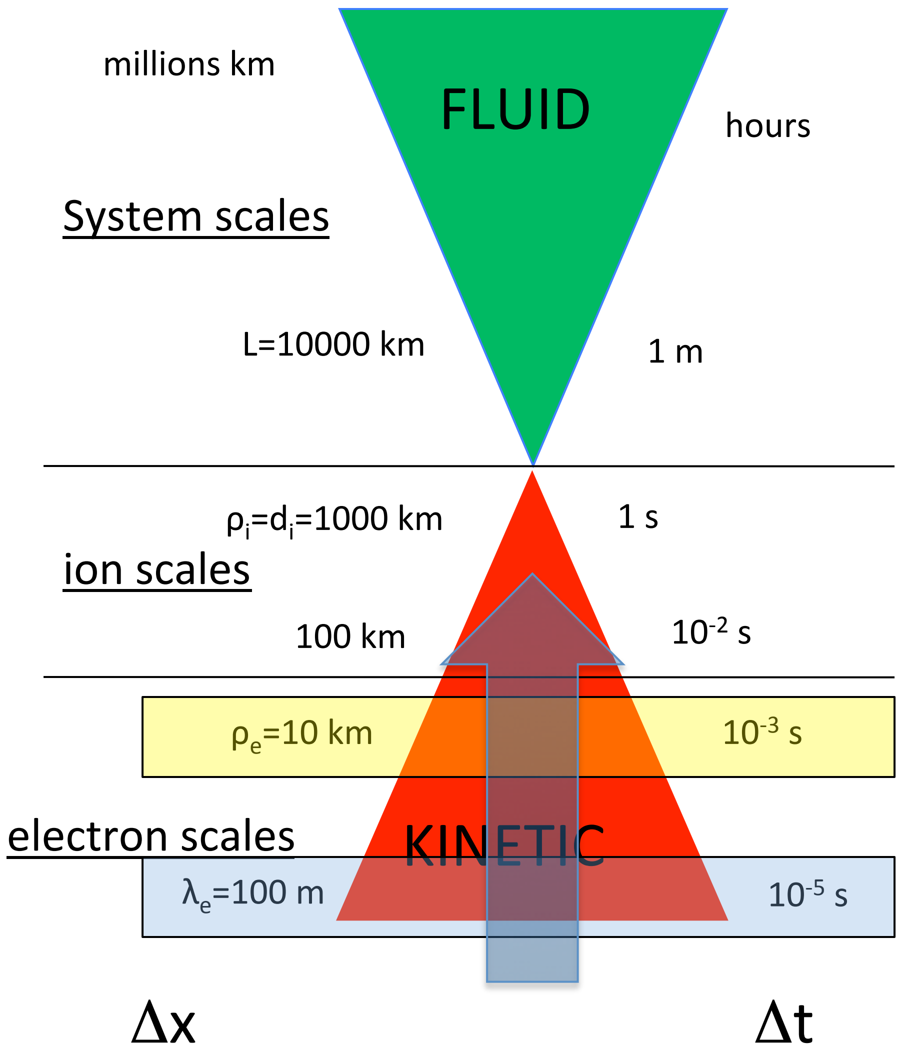
$$\omega_{fastest}\Delta t < 2$$

$$\Delta x < \lambda_{smallest}$$

$$c\Delta t < \Delta x$$

Implicit stability constraints

$$\frac{\Delta t\,\omega_{fastest}}{\Delta x / \lambda_{smallest}} < 1$$



Implicit Moment Method

Brackbill, Forslund (LANL)

Brackbill, Lapenta, (LANL)

Markidis, Lapenta (LANL-UIUC)

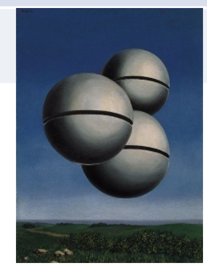
Markidis, Lapenta (Leuven)

Venus	Celeste	Parsek	iPIC
80's	90's - now	2005-2008	2008-now

Venere
(Sandro Botticelli)

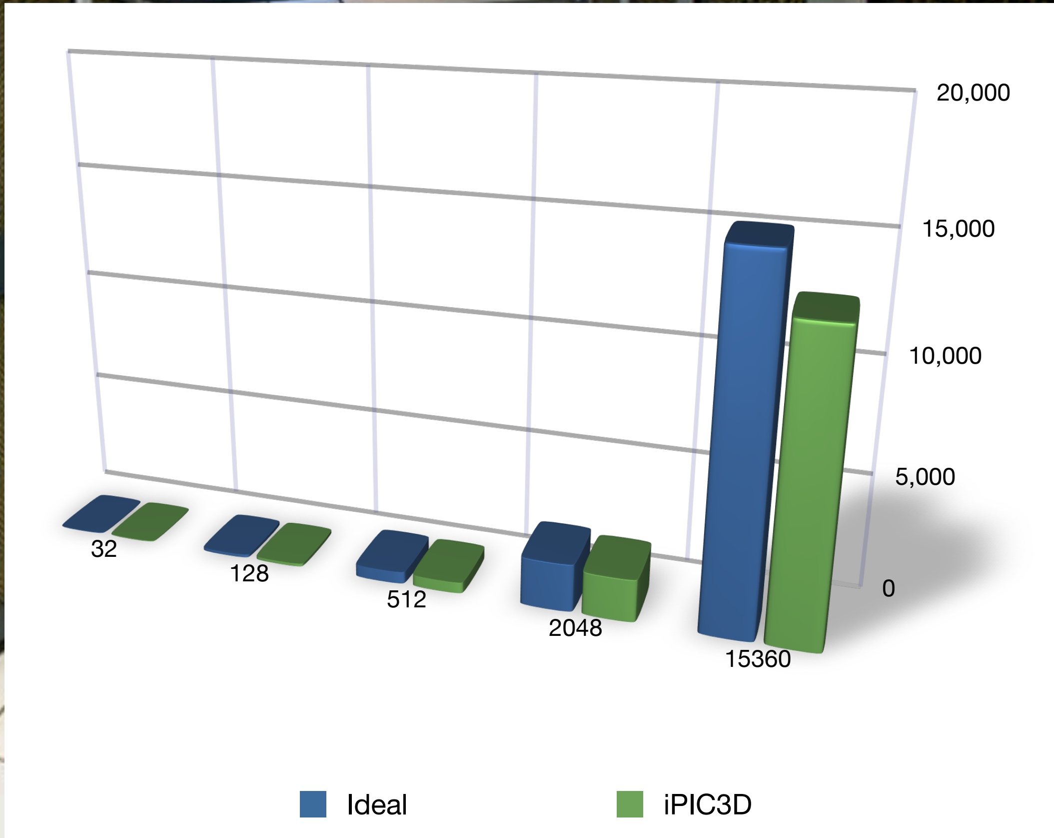
Starry Night
(Vincent Van Gogh)

Several Circles
(Vasily Kandinsky)



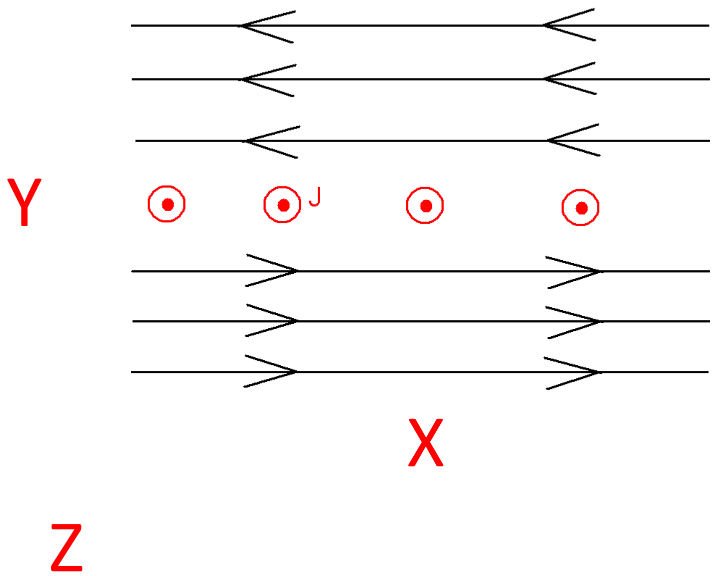
The Voice of Space
(René Magritte)

Performances of iPIC3D on Pleiades



Simulations at fixed initial load per core, done increasing the system size at constant resolution

Example: simulations for the MMS mission

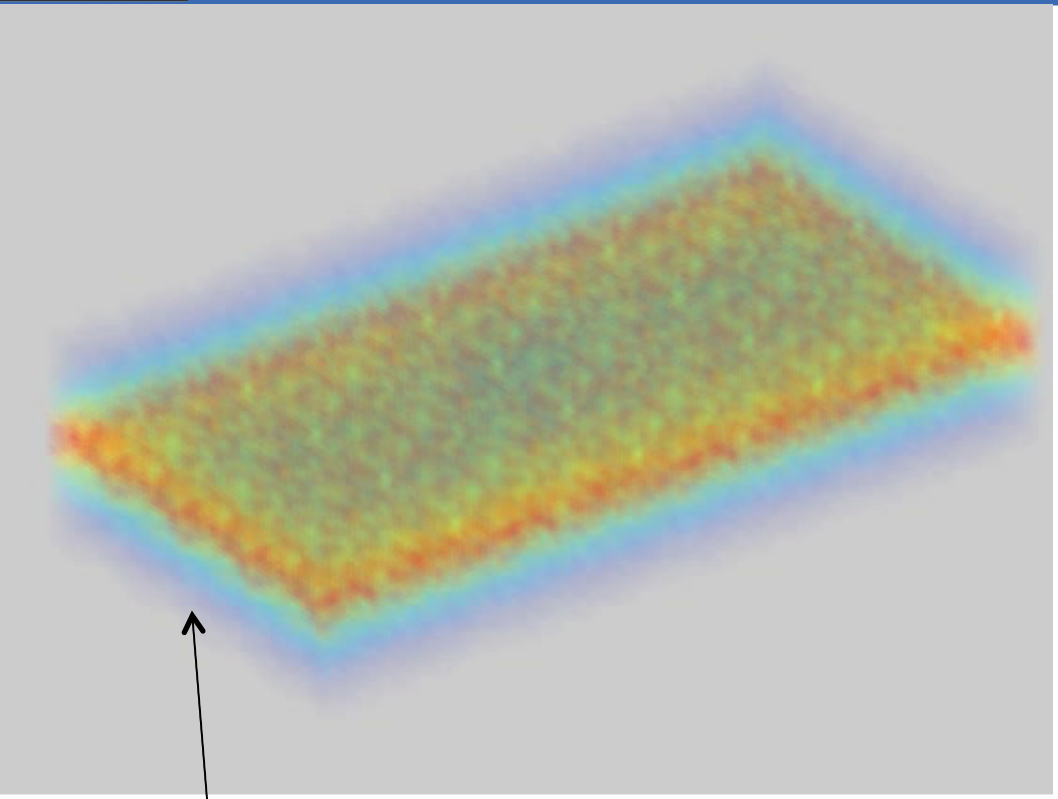


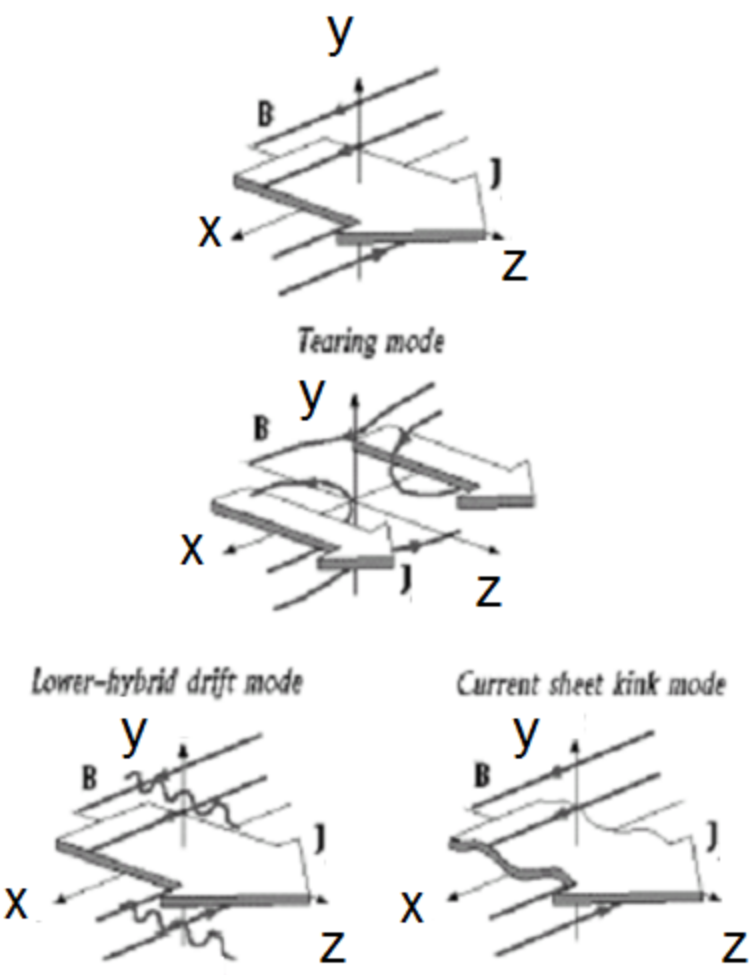
$$\mathbf{B} = B_0 \tanh(y/L)\hat{\mathbf{x}} + B_g \hat{\mathbf{z}}$$

$$p = p_b + p_0 \mathrm{sech}^2(y/L)$$

$$\beta = \frac{p}{B^2/8\pi} \rightarrow \beta(z=0) = \frac{p_b + p_0}{B_g^2/8\pi}$$

2D runs to focus on current aligned modes





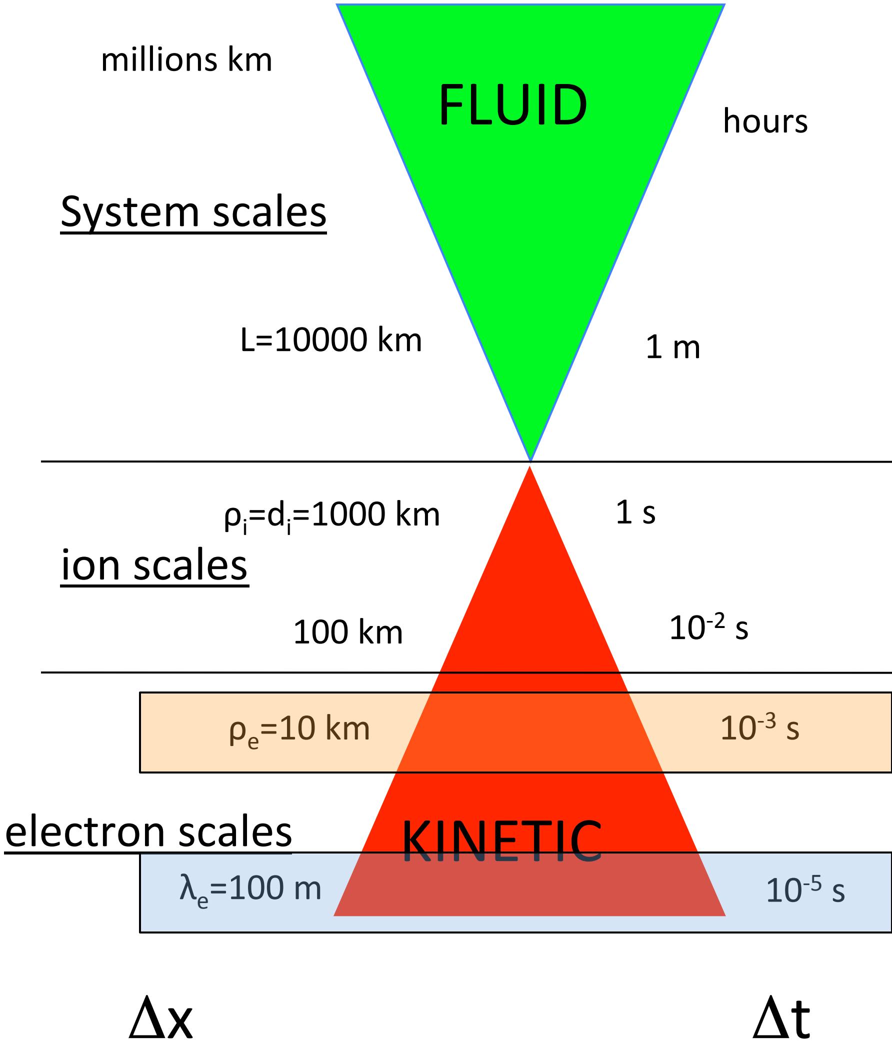
No initial perturbation, Bg=0

Timing considerations for 3D fully kinetic simulations - Implicit vs Explicit

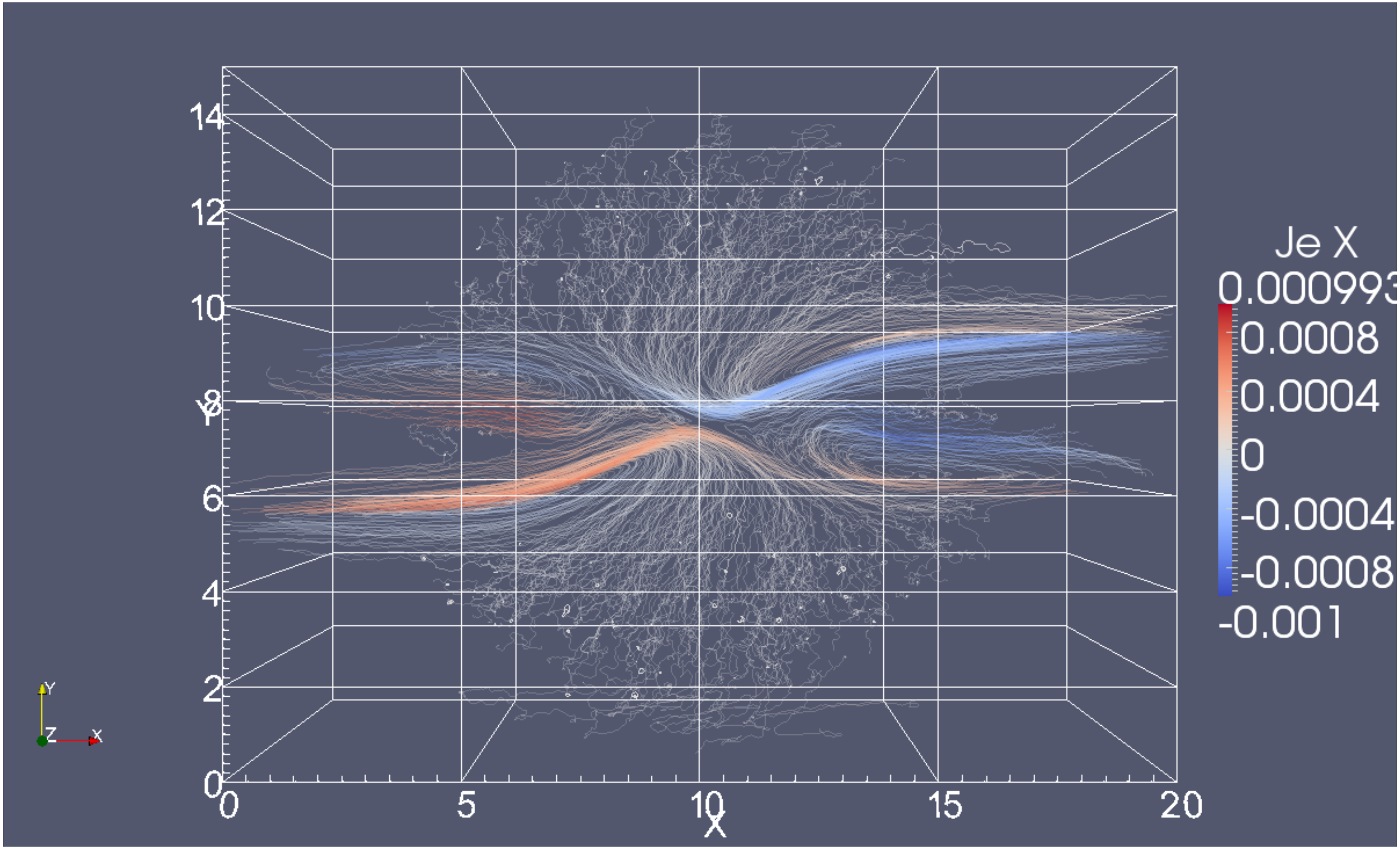
KATHOLIEKE UNIVERSITEIT LEUVEN

	Explicit	Implicit	Gain
Dx	λ_{De}=100 m	d_e=10 Km	100
Dy	λ_{De}=100 m	d_e=10 Km	100
Dz	λ_{De}=100 m	d_e=10 Km	100
Dt	$\omega_{pe}\Delta t$=0.1 or 10^{-5}s	$\omega_{pe}\Delta t$=100 or 10^{-3}s	1000
Tot			10^9

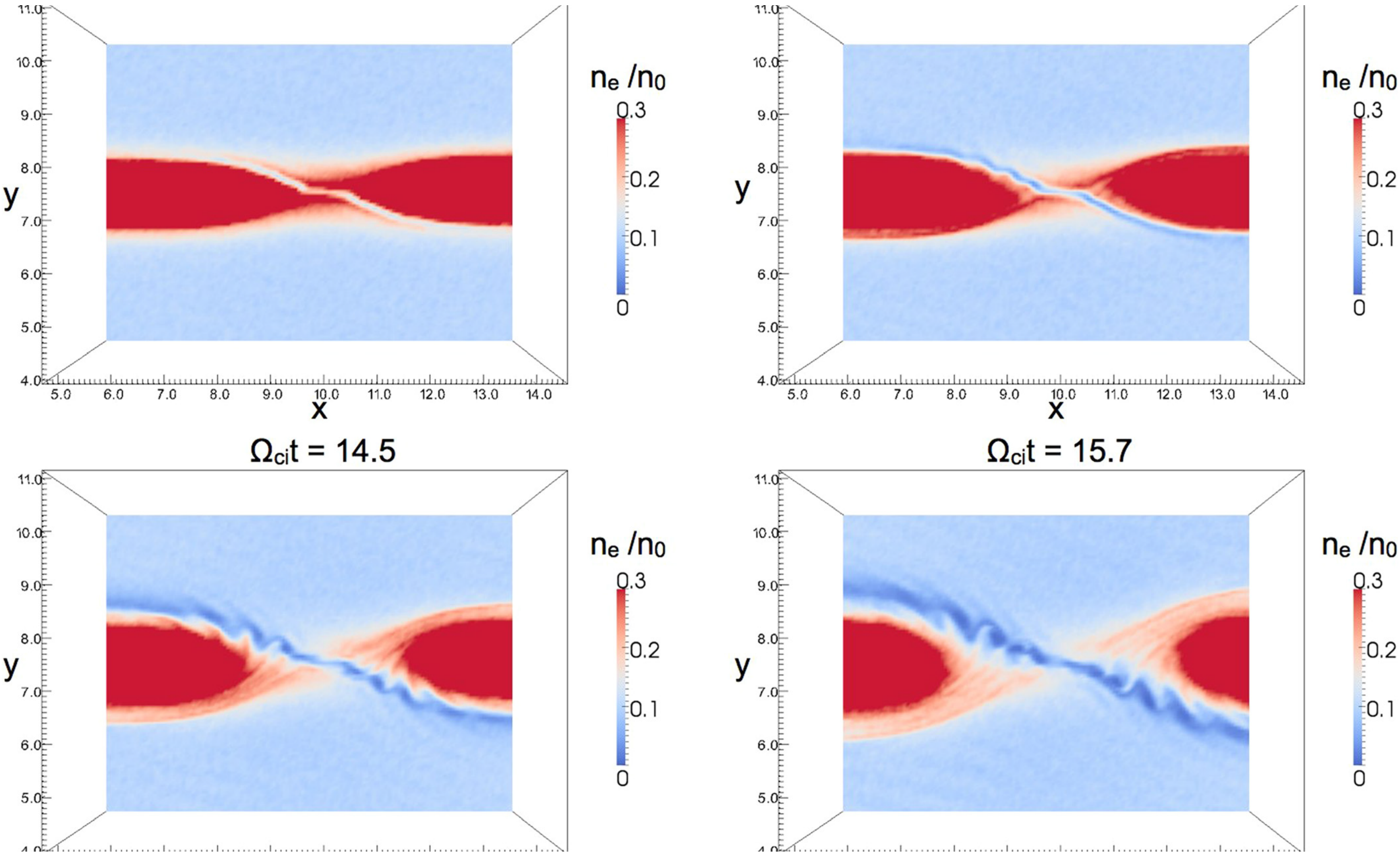
An implicit run that takes **1 day** would take: **2,800,000 years** with an explicit code



The reconnection jets are deflected

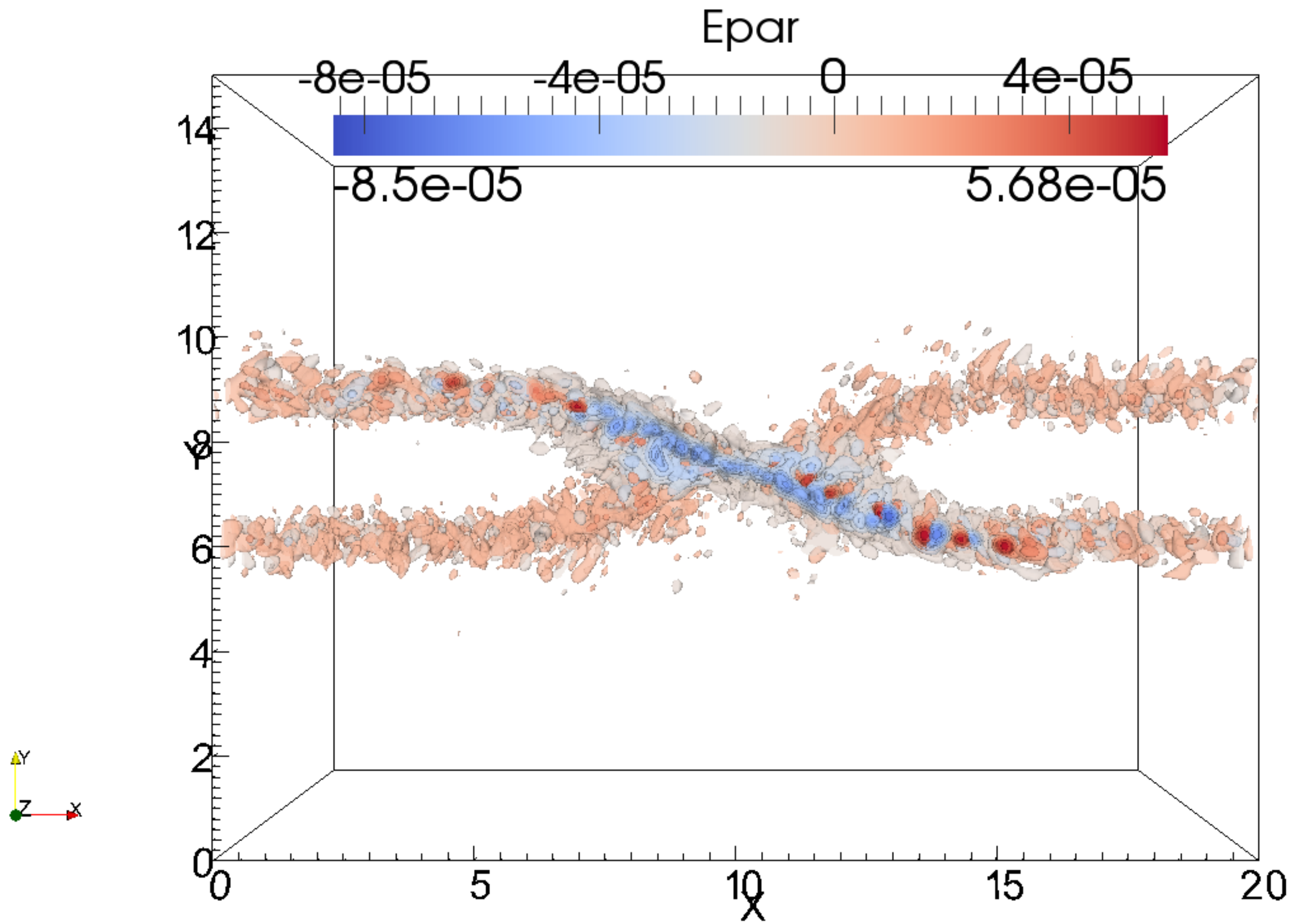


Separatrix regions are focus of instability



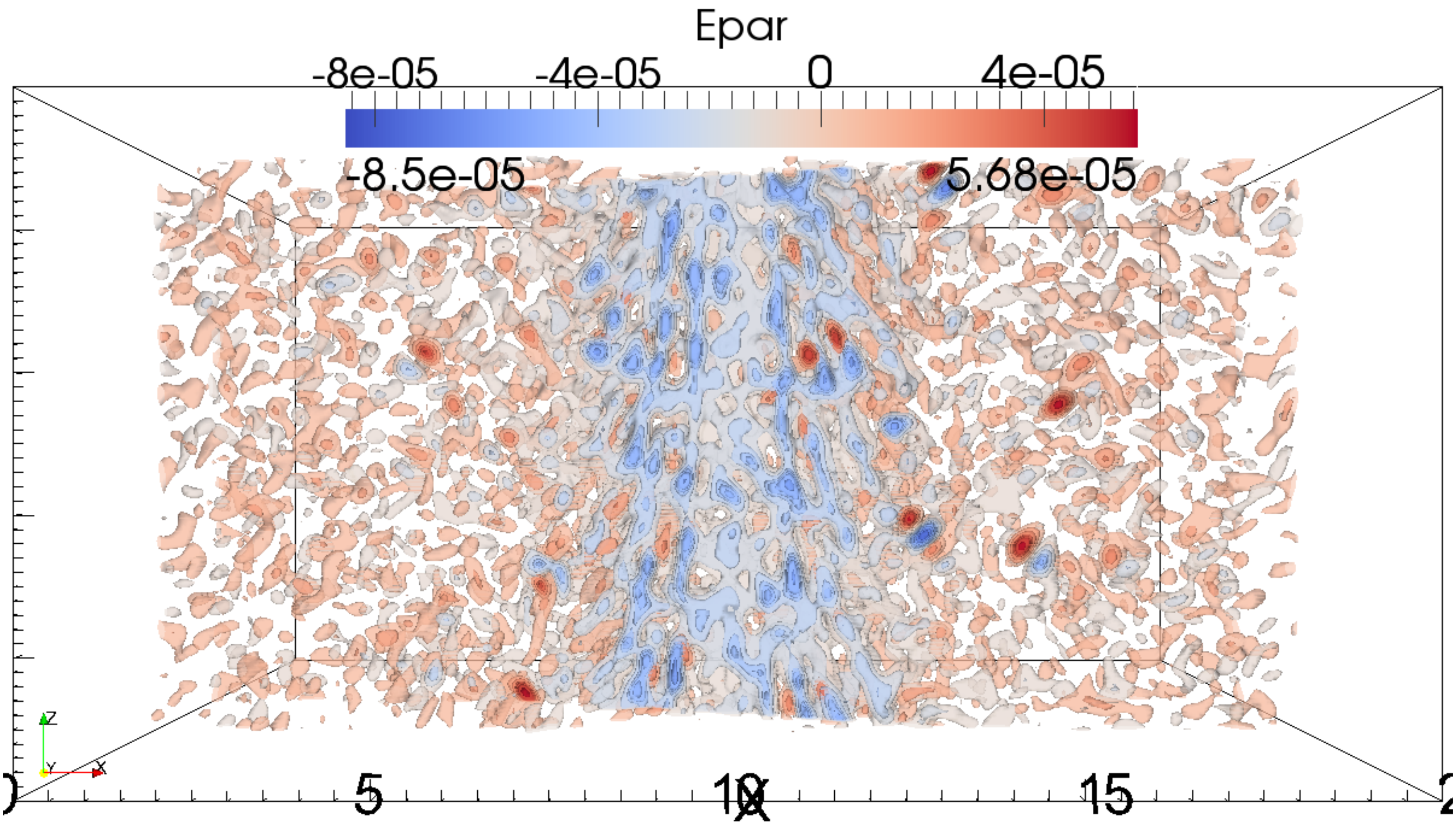
Strong electron flows cause parallel structures

KATHOLIEKE UNIVERSITEIT LEUVEN



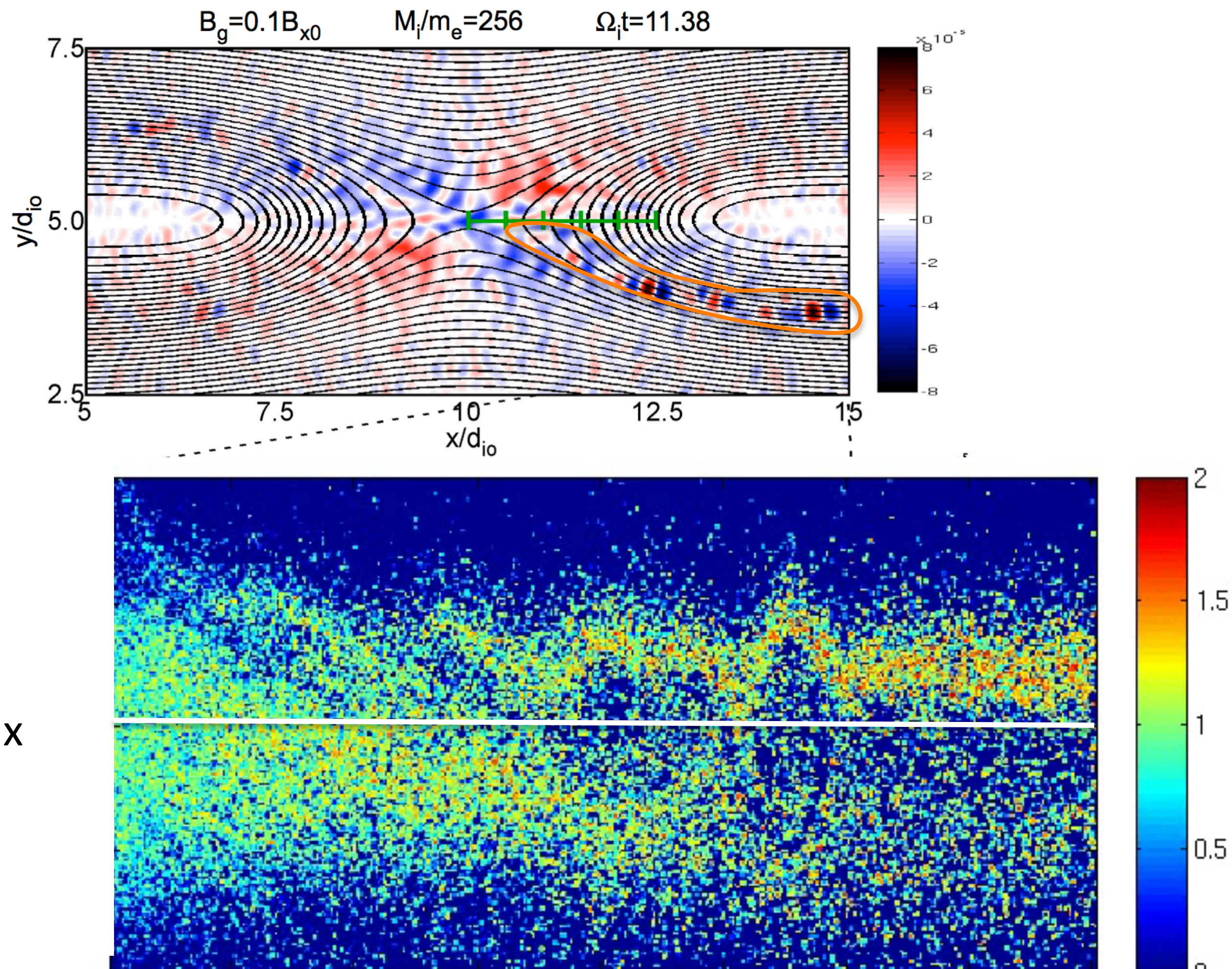
View from above

KATHOLIEKE UNIVERSITEIT LEUVEN



Electron Phase Space Dynamics for Bipolar Fields ($B_g = 0.1B_0$)

$E_{||}(x,y)$



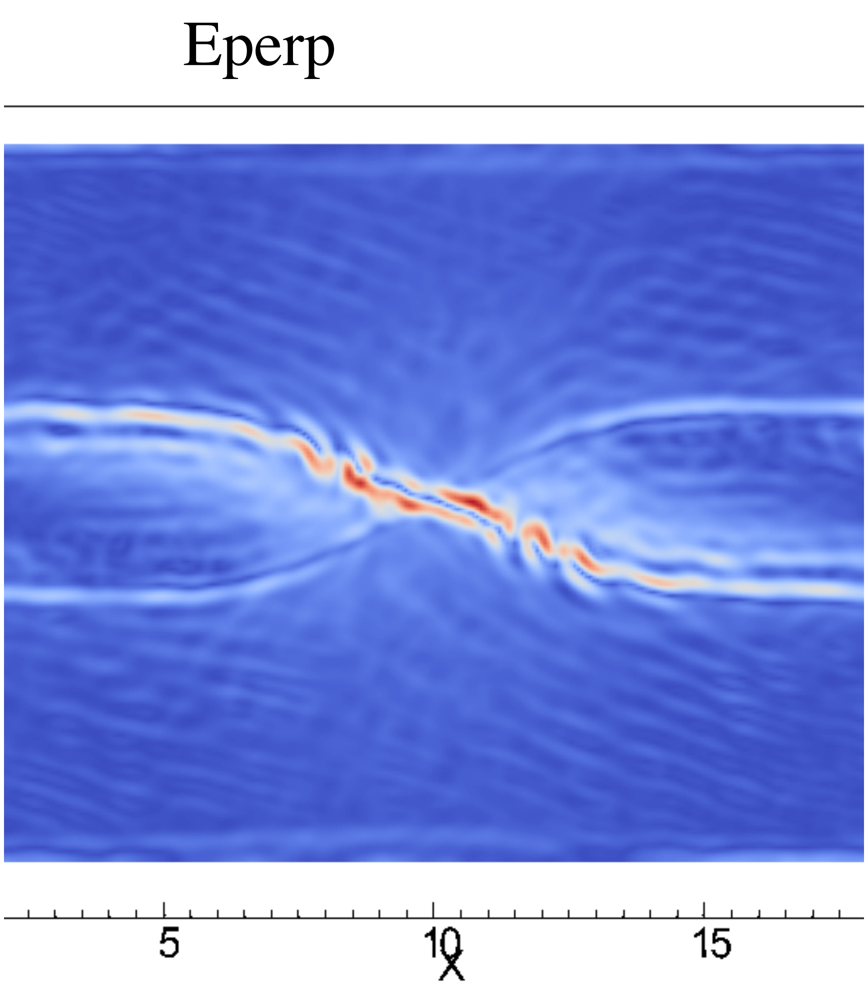
towards x-pt

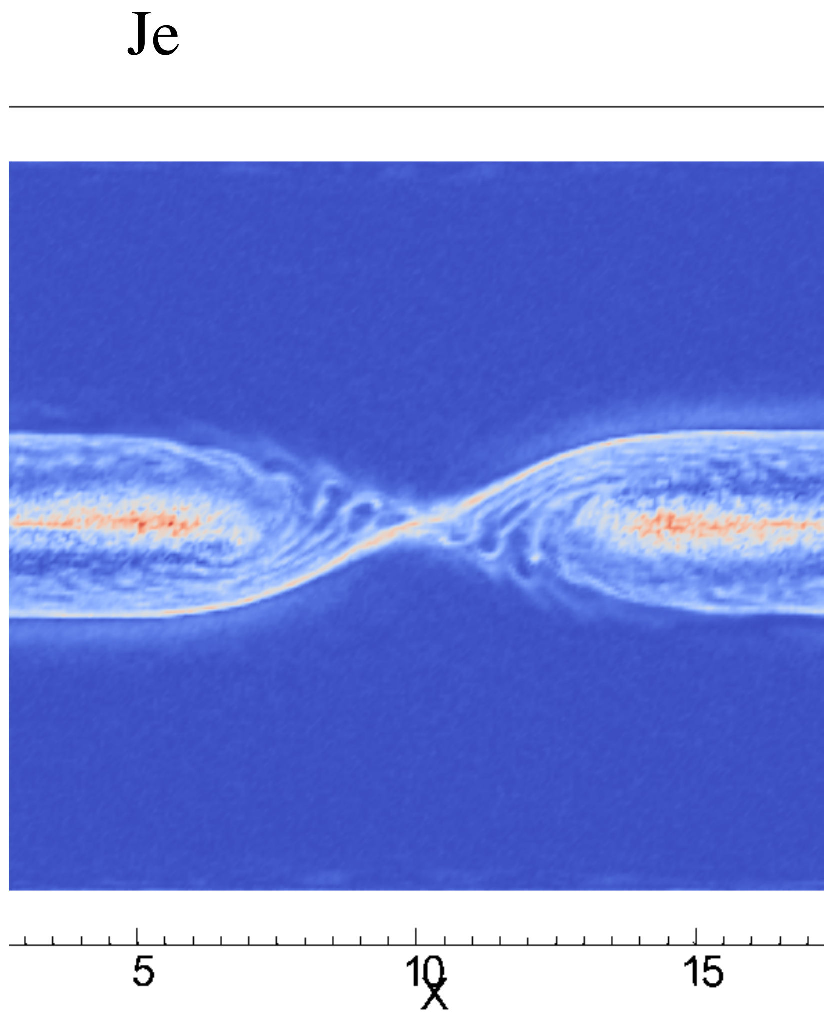
$v_{||}$

x

$11.5d_{i0}$ $15d_{i0}$

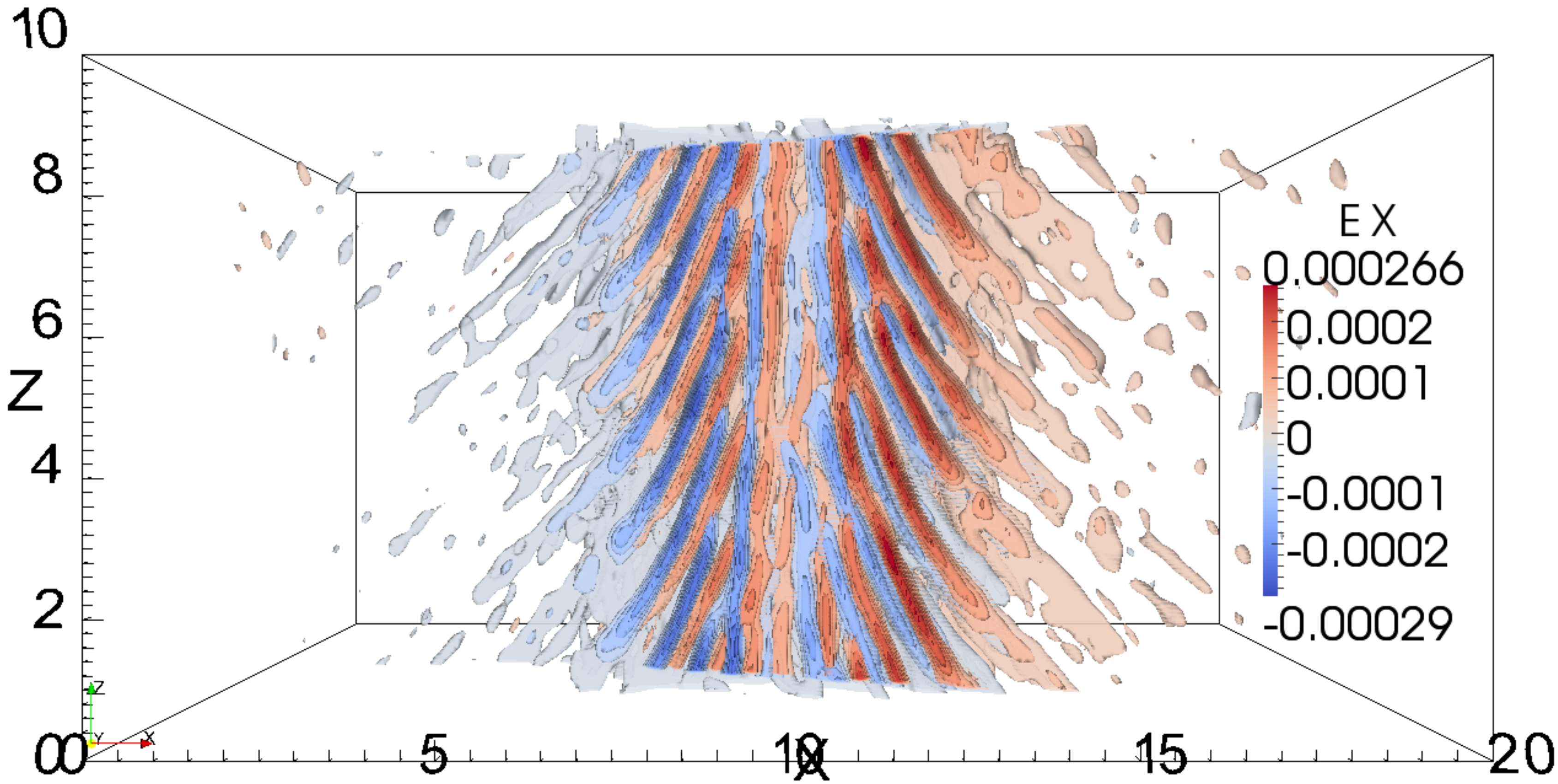
But there is another instability





And perpendicular structures

KATHOLIEKE UNIVERSITEIT LEUVEN



Outline

KATHOLIEKE UNIVERSITEIT LEUVEN

Challenges of space weather:

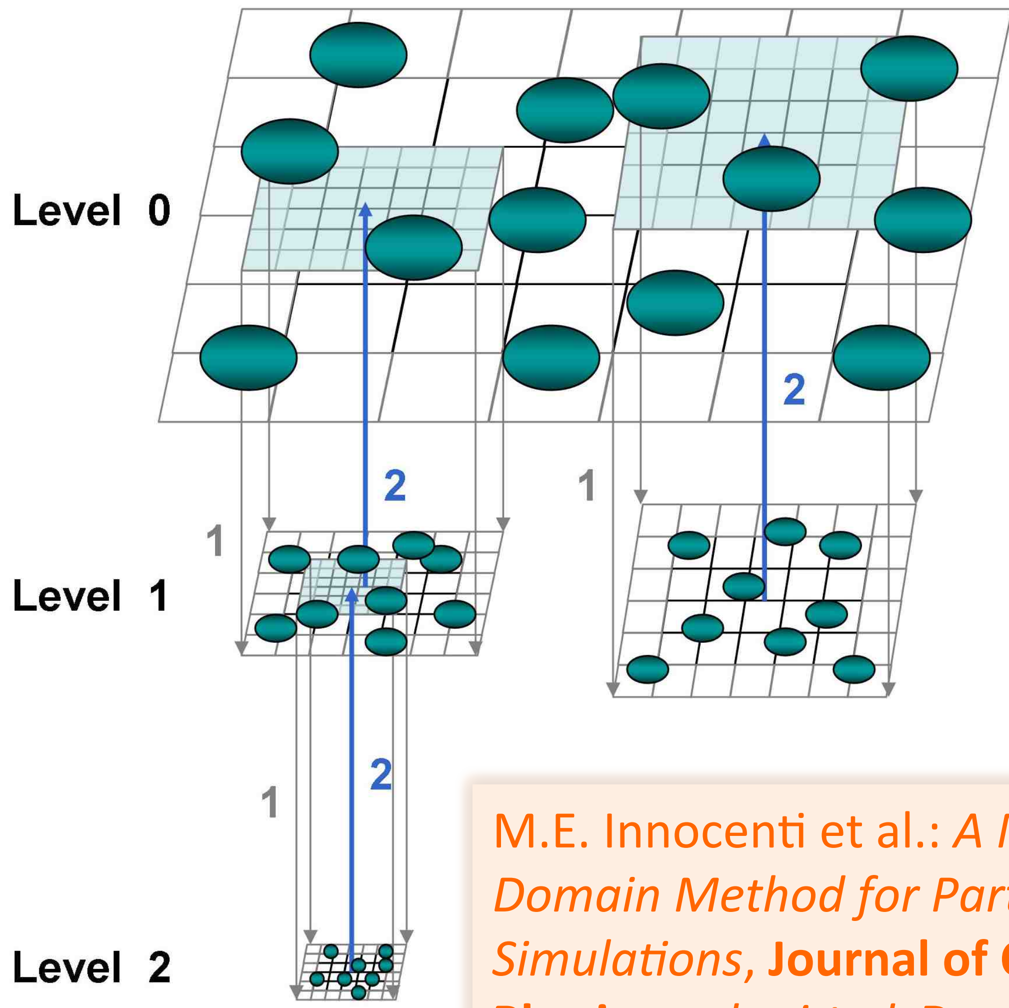
- multiscale
- Multiphysics

Federation of models

Unification of models

Ongoing efforts at KU Leuven

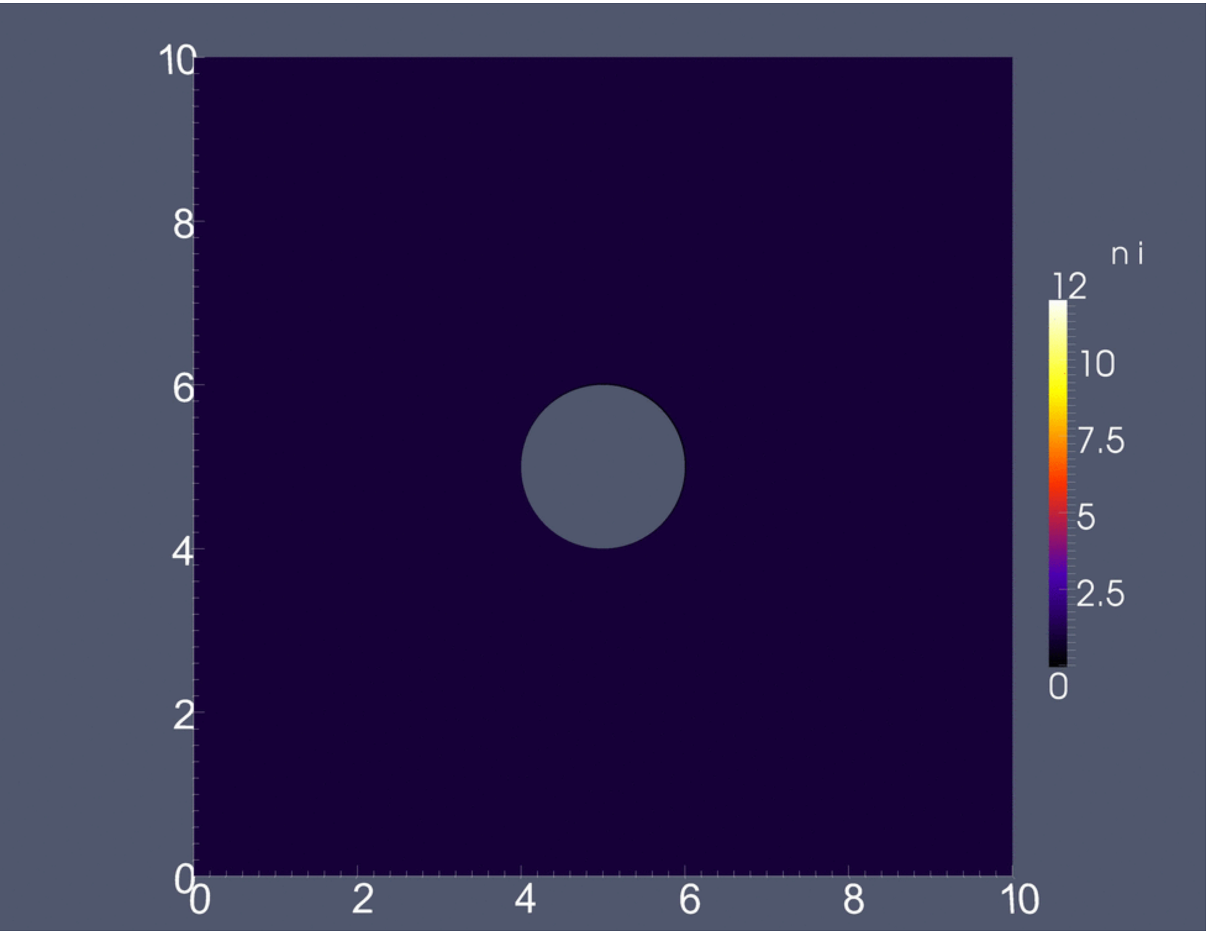
MultiLevel – MultiDomain Approach



M.E. Innocenti et al.: *A Multi Level Multi Domain Method for Particle In Cell Plasma Simulations*, **Journal of Computational Physics**, *submitted*, Dec. 2011, http://arxiv.org/abs/1201.6208.

Reference case: Earth Environment

KATHOLIEKE UNIVERSITEIT LEUVEN



Example: Mercury (S. Markidis with iPic3D)

Real Earth needs

Box:

100 R_E x 100 R_E x 100 R_E

Max load per processor:
- 16x16x16 cells
- 144 + 144 particles per cell(electron populations)
- 144 +144 particles per cell (ion populations)

Coupled with heliospheric models and observations

Earth Environment - State of the Art

KATHOLIEKE UNIVERSITEIT LEUVEN

Explicit PIC

- Resolution needed: electrostatic processes at electron scales: 100m (Debye length)
- Cells per dimension: 6,353,000
- Total processors needed: 6.2600e+16
- 63 million billions

Moment Implicit PIC

- Resolution needed: electromagnetic processes at electron scales: 10Km (inertial length)
- Cells per dimension: 63,530
- Total processors needed: 6.2600e+10
- 63 billions

Summary of the current state of affairs for the Earth

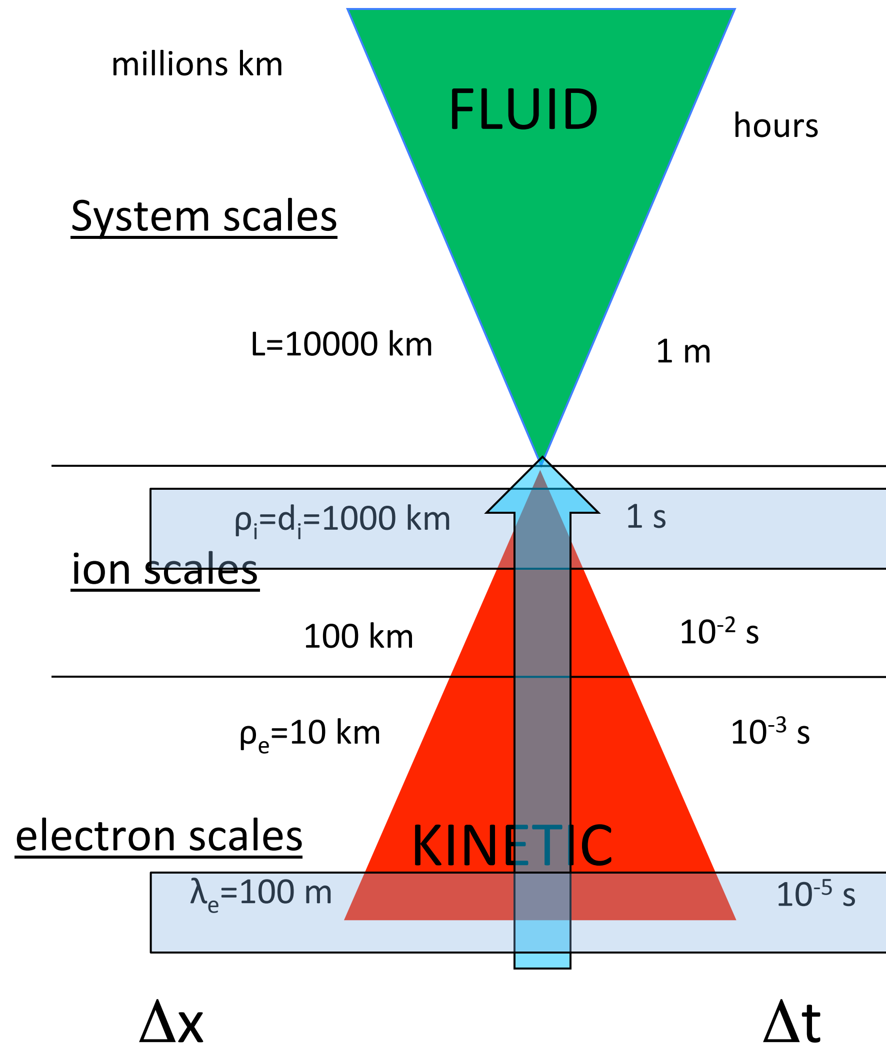
KATHOLIEKE UNIVERSITEIT LEUVEN

Explicit

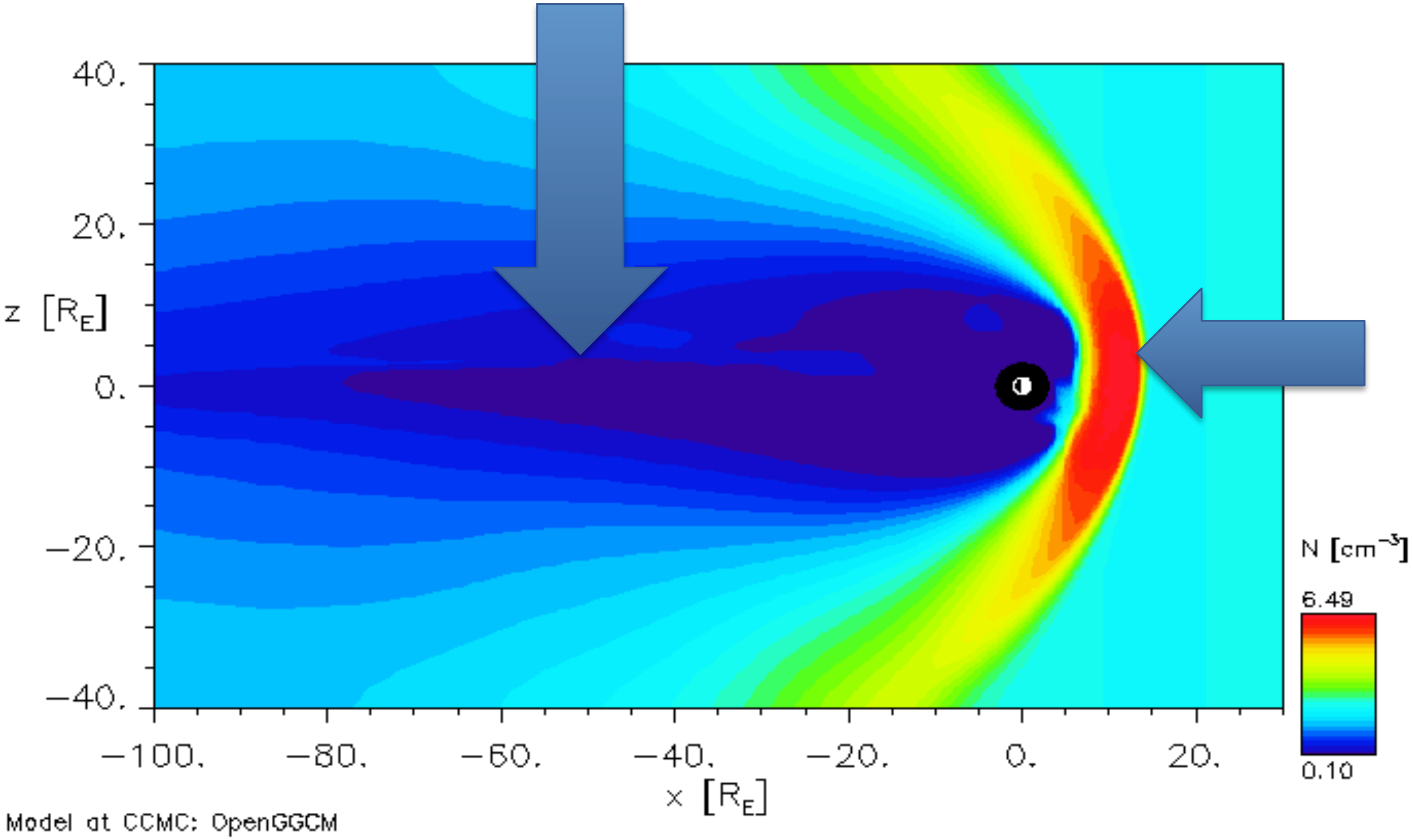
6.2600e+16 (63 million billion) processors	Not feasible

Implicit

63 billion processors	Still not feasible



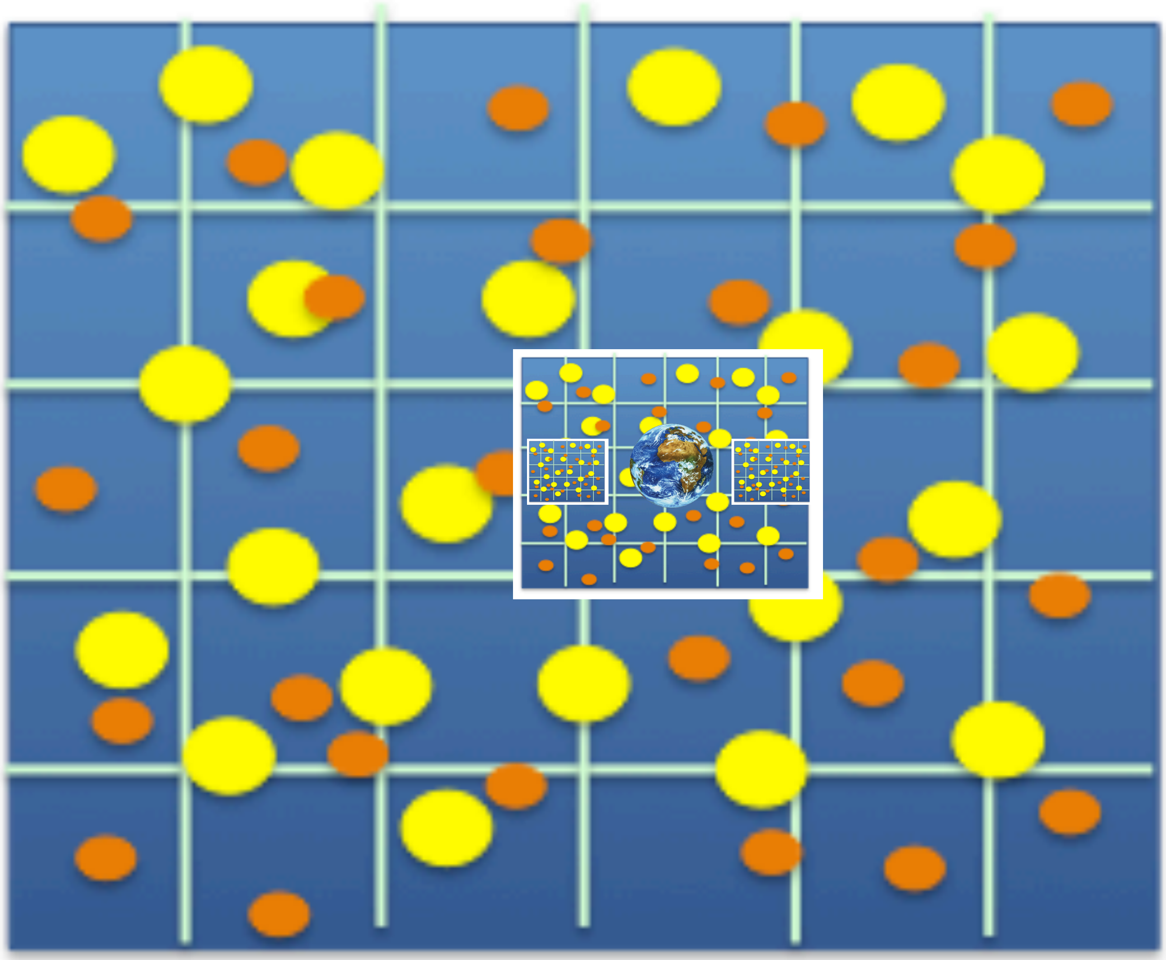
Resolution needed only in small areas



CCMC – NASA (Lapenta)

MultiLevel approach

KATHOLIEKE UNIVERSITEIT LEUVEN



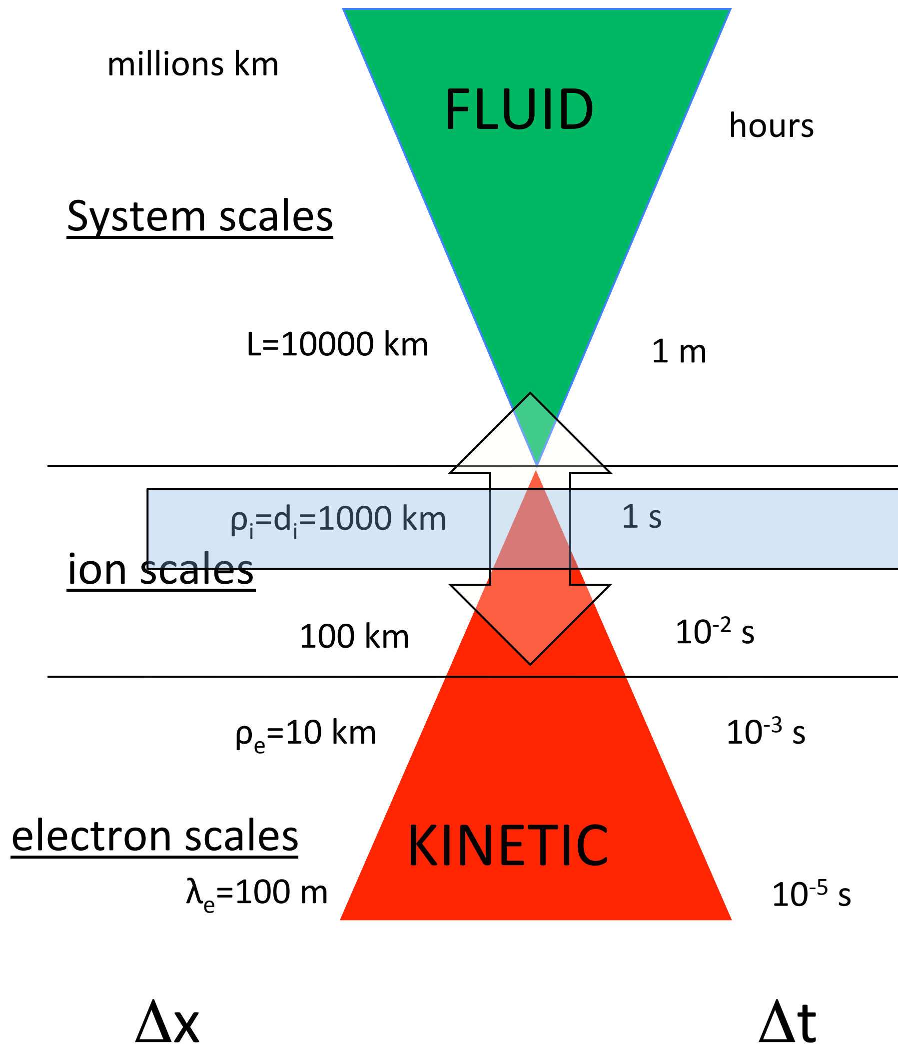
Beyond the State of the Art: Exascience Lab Earth Environment Model

KATHOLIEKE UNIVERSITEIT LEUVEN

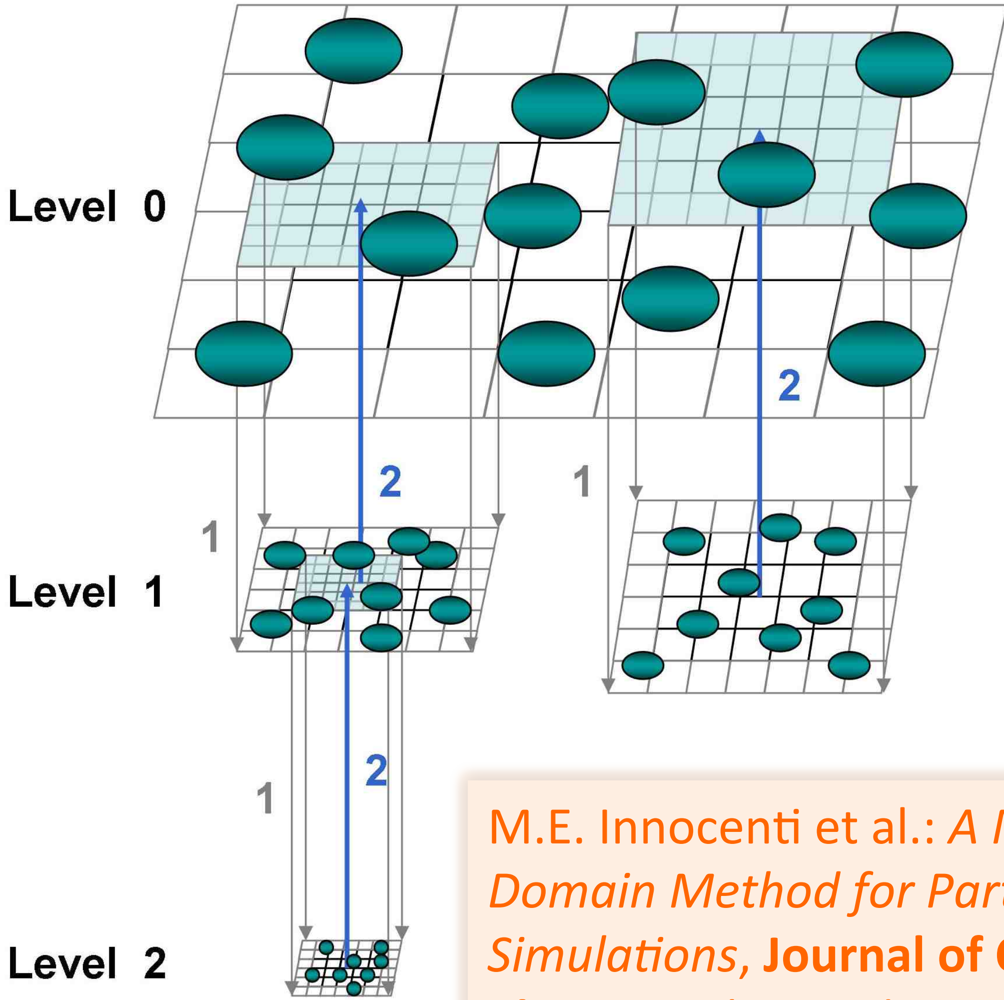
Explicit	
6.2600e+16 (63 million billion)processors	Not feasible

Implicit	
63 billion processors	Still not feasible

Implicit - Multilevel	
2 million processors	Feasible at EXASCALE



MultiLevel – MultiDomain Approach



M.E. Innocenti et al.: *A Multi Level Multi Domain Method for Particle In Cell Plasma Simulations*, **Journal of Computational Physics**, *submitted*, Dec. 2011, http://arxiv.org/abs/1201.6208.

MLMD: Some details

KATHOLIEKE UNIVERSITEIT LEUVEN

Each domain is an exact replica of the others, but scaled.

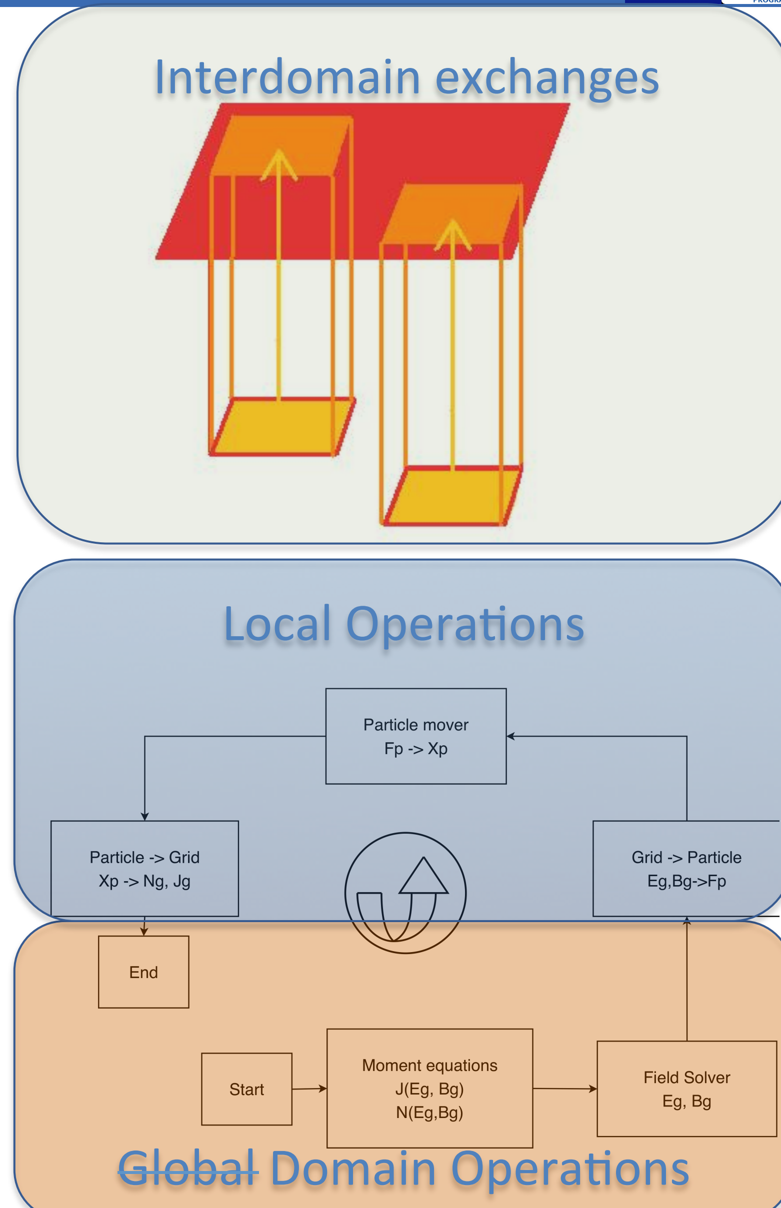
The operations are identical for the same physics module

Algorithm designed to minimize exchange of information

No global operation, all solvers operate on each domain

1D and 2D versions implemented on massively parallel computers

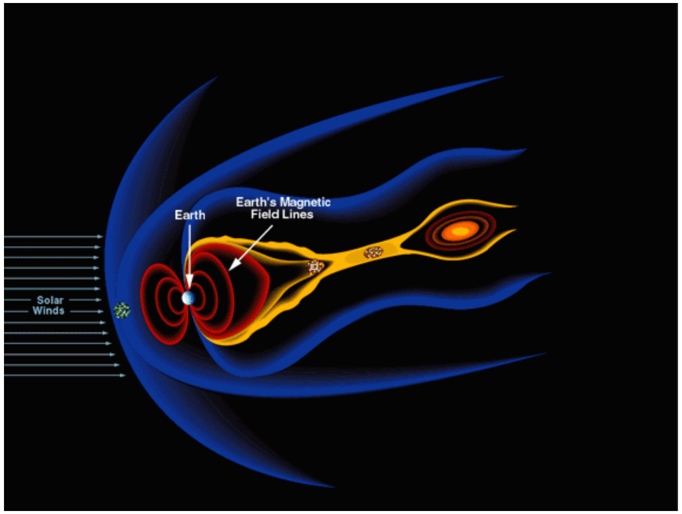
M.E. Innocenti et al.: *A Multi Level Multi Domain Method for Particle In Cell Plasma Simulations*, **Journal of Computational Physics**, *submitted*, Dec. 2011, http://arxiv.org/abs/1201.6208.

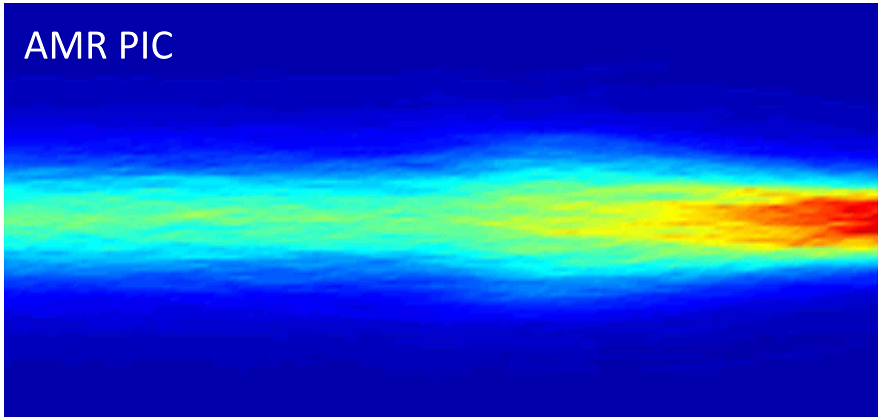


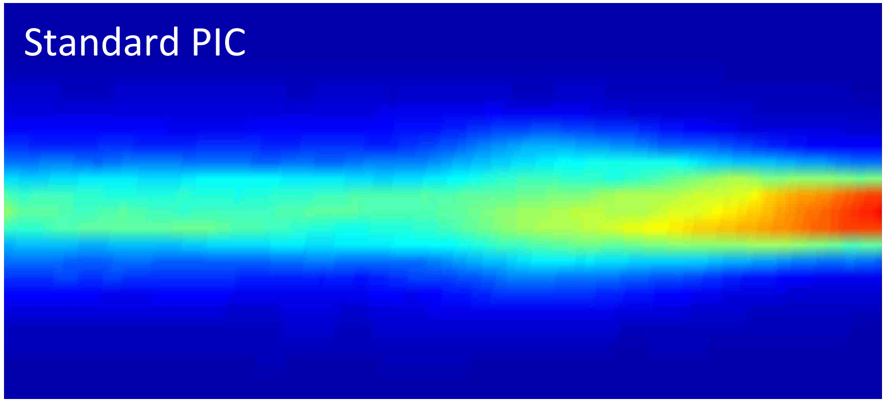
Example 1: AMR Kinetic Modeling of the Earth Magetotail

KATHOLIEKE UNIVERSITEIT LEUVEN

- ✓ Year 1 Profiling/ Parallel Performance
- ❑ Year 1 - Optimisation, with WP2
- ❑ Year 1-3 Visualization, with WP4
- ❑ Year 2 PIC for exascale (continuing)
- ◆ Year 3 AMR PIC (50% done)



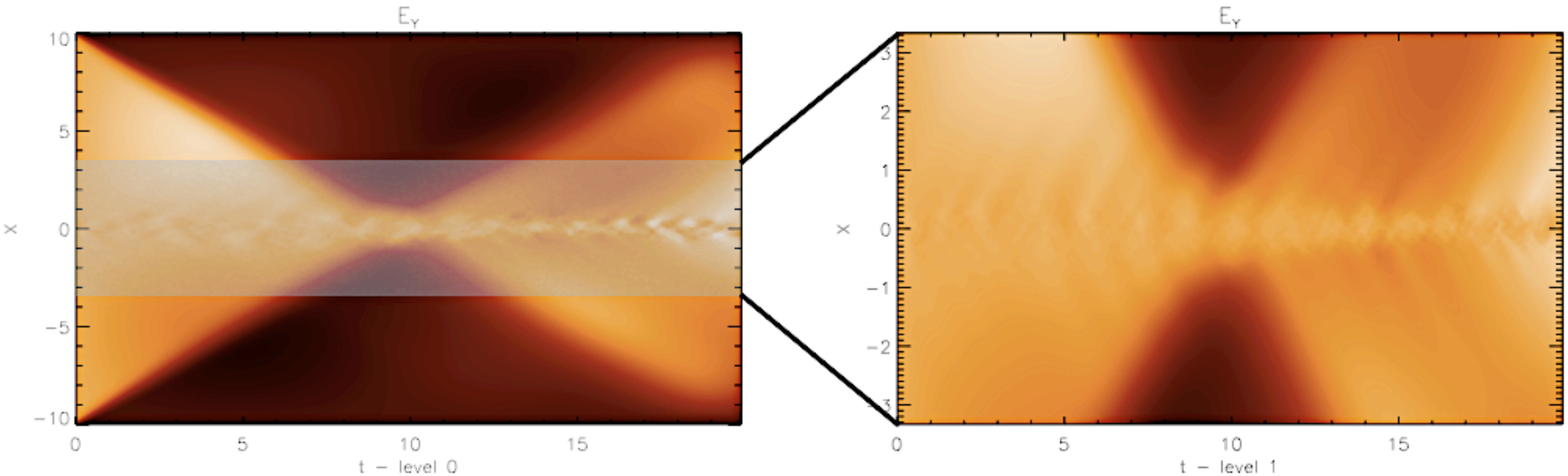




Example 2: shock collision

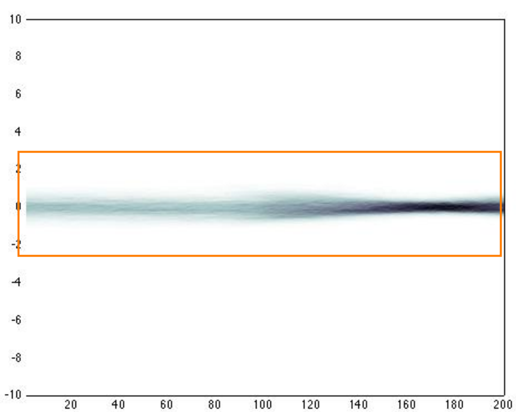
KATHOLIEKE UNIVERSITEIT LEUVEN

Ey



Jy

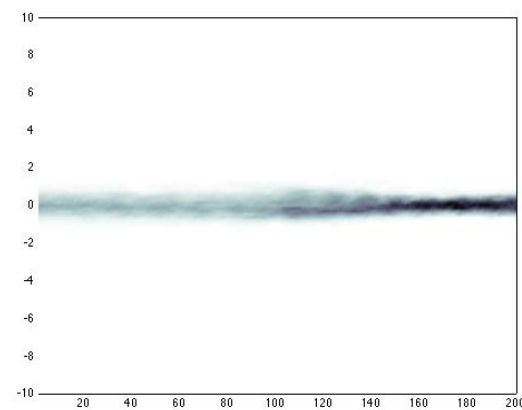
AMR eff 1280



Better resolution

Less noise

Regular 128



The need for Codesign

KATHOLIEKE UNIVERSITEIT LEUVEN

- Codesign
  - Algorithmic development
    - Implicit methods
    - Multilevel methods
  - Hardware Needs
    - Can the model be run on petascale?
    - Can the model be run on exascale?

Co-Design and space weather at KU Leven

Space Weather projects

Soteria
- First ever EC-FP7 funded project on space weather
- Started 2008
- End this year
- Cordinator: G. Lapenta

Swiff
- FP7 project on the space weather call
- To run till 2014
- Cordinator: G. Lapenta

eHeroes
- FP7 project
- From the 2011 call
- Kick-off in Rome in March 2012
- To run till 2015
- Cordinator: G. Lapenta

KATHOLIEKE UNIVERSITEIT LEUVEN

HPC projects

- DEEP
- Intel Exascience Lab (ExaScience Lab, Intel Labs Europe, EXASCALE COMPUTING)
- Hybrid Computing

SPACECAST · CASSIS · MMS NASA · esa space situational awareness

SWIFF: Space Weather Integrated Modelling Framework

KATHOLIEKE UNIVERSITEIT LEUVEN

SPACE-WEATHER INTEGRATED FORECASTING FRAMEWORK SWIFF

SEVENTH FRAMEWORK PROGRAMME

Collaborative Project
FP7- Space

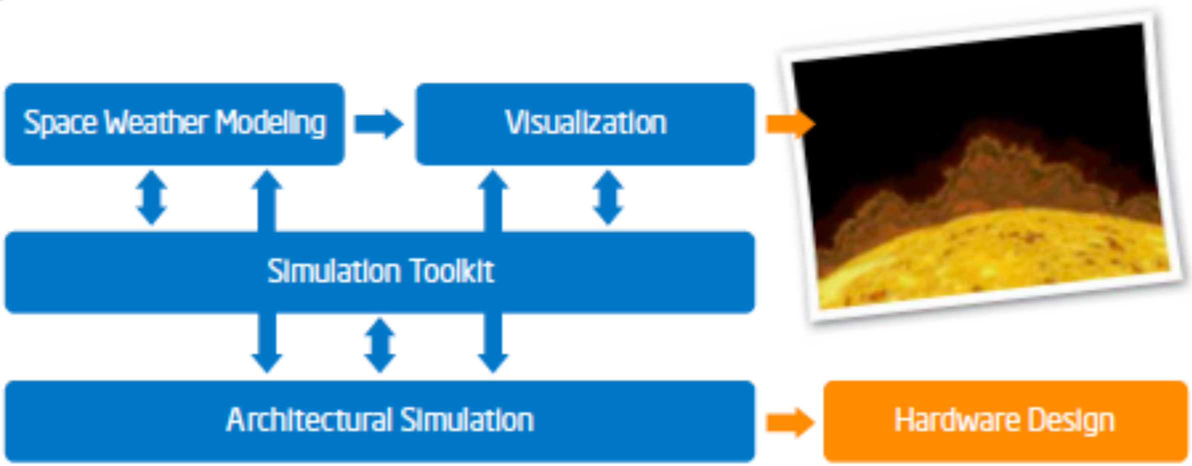
- Create a mathematical-physical framework to integrate multiple-physics (fluid with kinetic)
- Focus on coupling small-large scales
- Federation of models based on physical and amthematical understanding of the coupling
- Physics-based rather than software-based
- Founding approach: implicit, adaptivity and multilevel

Science Lead	Participant organisation name	Country
Coordinator: G. Lapenta	Katholieke Universiteit Leuven	Belgium
V. Pierrard	Belgian Institute for Space Aeronomy	Belgium
F. Califano	Università di Pisa	Italy
A. Nordlund	Københavns Universitet	Denmark
A. Bemporad	Astronomical Observatory Turin - Istituto Nazionale di Astrofisica	Italy
P. Travnicek	Astronomical Institute, Academy of Sciences of the Czech Republic	Czech Republic
C. Parnell	University of St Andrews	UK

Intel Exascience Lab (exascience.com)

KATHOLIEKE UNIVERSITEIT LEUVEN

ExaScience Lab
Intel Labs Europe
EXASCALE COMPUTING



iwt

imec

KATHOLIEKE UNIVERSITEIT LEUVEN

UNIVERSITEIT GENT

Vrije Universiteit Brussel

Universiteit Antwerpen

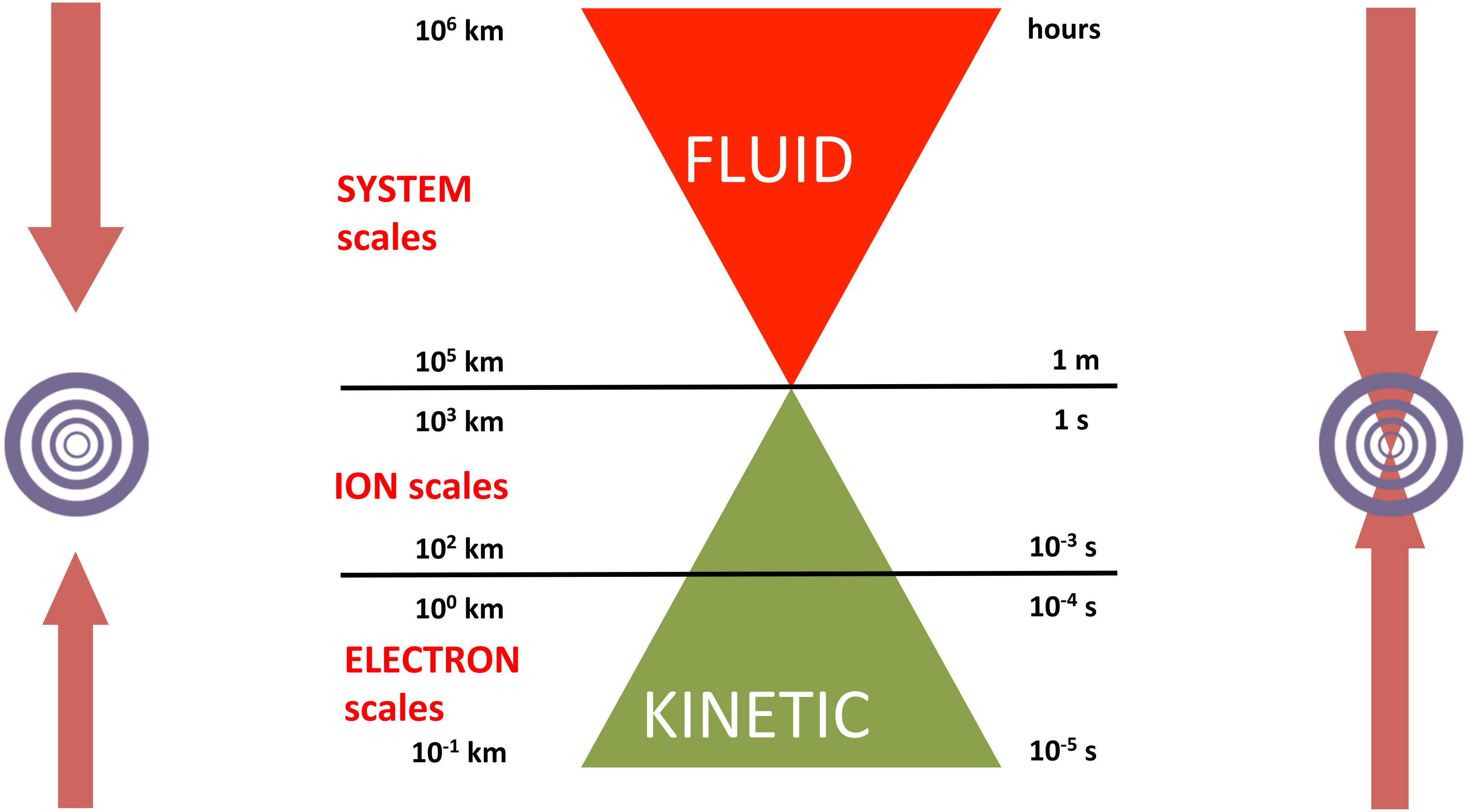
universiteit hasselt

intel

Goal of our effort

State of the Art

Our Goal



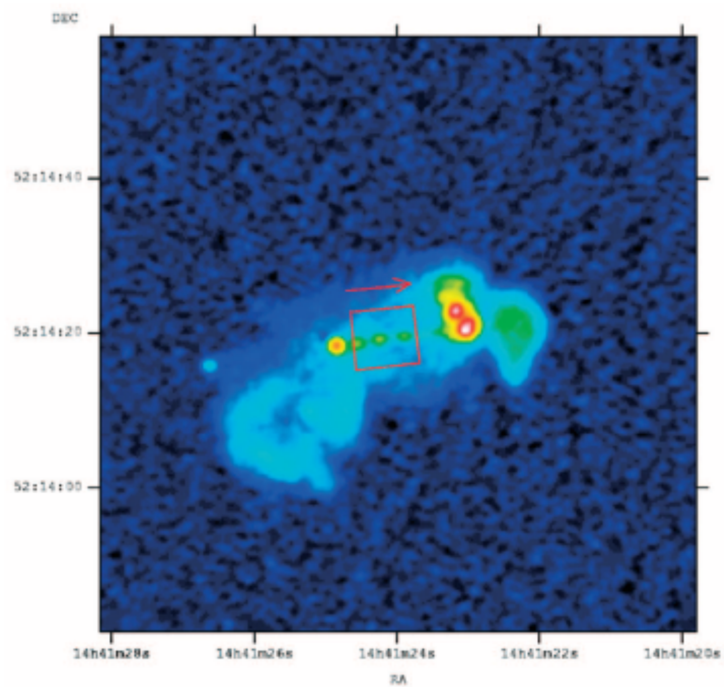
We want to bridge the micro-macro gap by unifying in a single mathematical approach fluid and kinetic physics

extra

Scales in extragalactic Jets

KATHOLIEKE UNIVERSITEIT LEUVEN

Jet in 3C303 (VLA: radio)



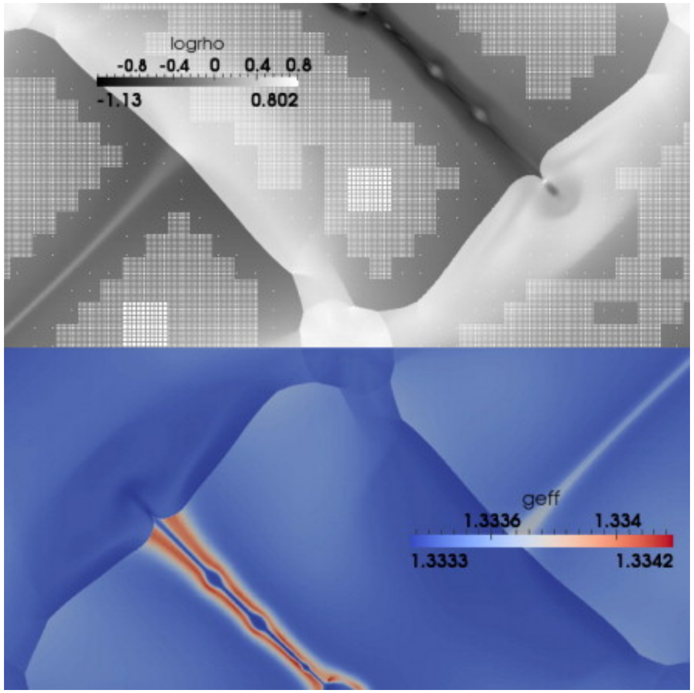
Kronberg, Lovelace, Lapenta, Colgate, ApJ Lett, 741, L15 (2011)

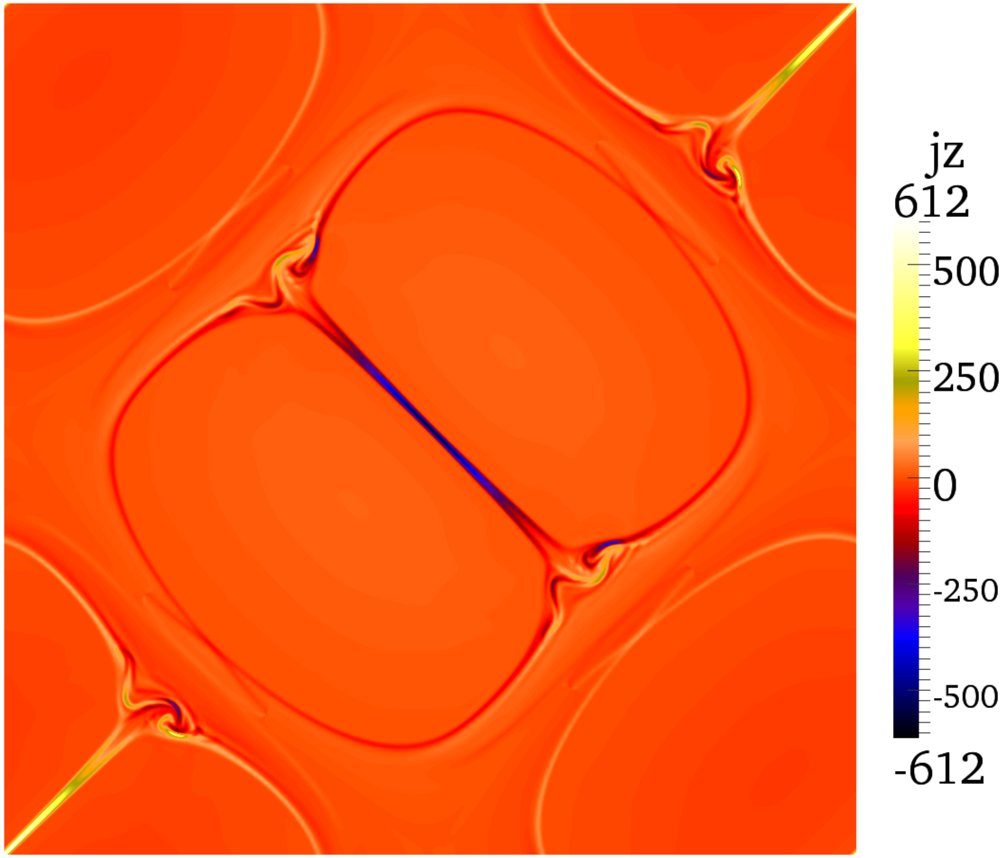
Typical Scales in 3C303

- Bulk speed $v_{bulk} \approx 0.7c$
- Plasma $\beta = 10^{-5}$
- Alfven speed $V_A \approx c$
- Thermal plasma: $T \approx 10^8$K, $n = 3 \cdot 10^{-5}$ cm^{-3}
- Jet length 60 kpc.
- Classical particles: $\rho_e \approx 10^{-13}$pc, $d_e \approx 8 \cdot 10^{-13}$pc, $\lambda_D \approx 4 \cdot 10^{-12}$pc
- Relativistic particles: $\rho_e \approx 10^{-2}$pc, $d_e \approx 3 \cdot 10^{-7}$pc

Example 2: AMR Modeling of Reconnection

KATHOLIEKE UNIVERSITEIT LEUVEN

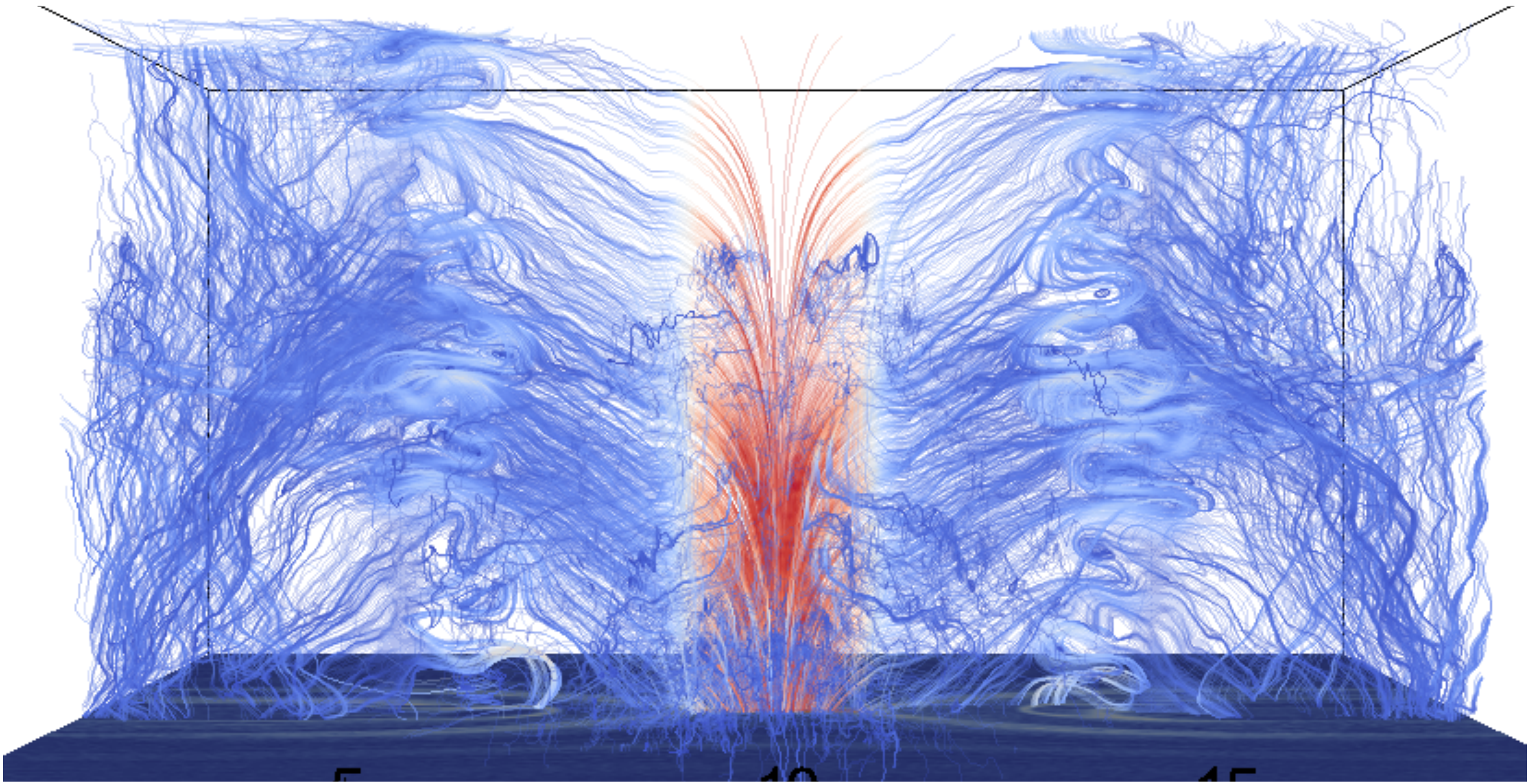




Keppens et al, JCP, 2012

The 3D flow is much more interesting

KATHOLIEKE UNIVERSITEIT LEUVEN



INTEGRATED SPACE-WEATHER FRAMEWORK SWIFF

SEVENTH FRAMEWORK PROGRAMME

MLMD: Some details

Each domain is an exact replica of the others, but scaled.

The operations are identical for the same physics module

Algorithm designed to minimize exchange of information

No global operation, all solvers operate on each domain

1D and 2D versions implemented on massively parallel computers

M.E. Innocenti et al.: *A Multi Level Multi Domain Method for Particle In Cell Plasma Simulations*, **Journal of Computational Physics**, *submitted*, Dec. 2011, http://arxiv.org/abs/1201.6208.