Implicit Particle-in-Cell Simulations of Magnetic Reconnection

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Outline

- PDC – Lindgren– Exascale supercomputers.
- Particle-in-Cell simulations. Limitations of common Particle-in-Cell codes.
- Implicit Particle-in-Cell method and iPIC3D code.
- 3D simulations of magnetic reconnection.
- Plasmoid chain PIC simulations.
- Conclusions.

PDC – KTH

PDC is the High Performance Computing (HPC) center at KTH.

- It provides computing resources (6 supercomputers) for Swedish **academic** research.
- It hosts the **fastest Swedish supercomputer** (Lindgren), and it explores **novel approaches for HPC in both hardware and software** (GPU clusters and programming, low power solutions for HPC, efficient cooling systems, new programming approaches for parallel computing, automatic optimization).
- It provides **application experts** to help users in running and optimizing parallel codes.
- It organizes **courses for parallel computing** http://www.pdc.kth.se/education)

Lindgren – Fastest Supercomputer in Sweden

36,384 cores supercomputer.

Theoretical peak performance: **0.305 Peta (10^{15}) FLOP** (~ 5,000 MacBook pro).

Physically located at KTH main campus.

How to Apply for Computing Time on Lindgren ?

Up to 80,000 core hours/month (Middle-sized computing time allocation)
Fill the form at: http://www.shpc.net/snac/medium/submit/pdc/

Requirements:

- Project title and abstract.
- You can use your codes, that need to be parallel, or use the ones present at PDC.
- Need a rough estimate of the resources you need, and estimate of how efficient is the code (we can help with that).

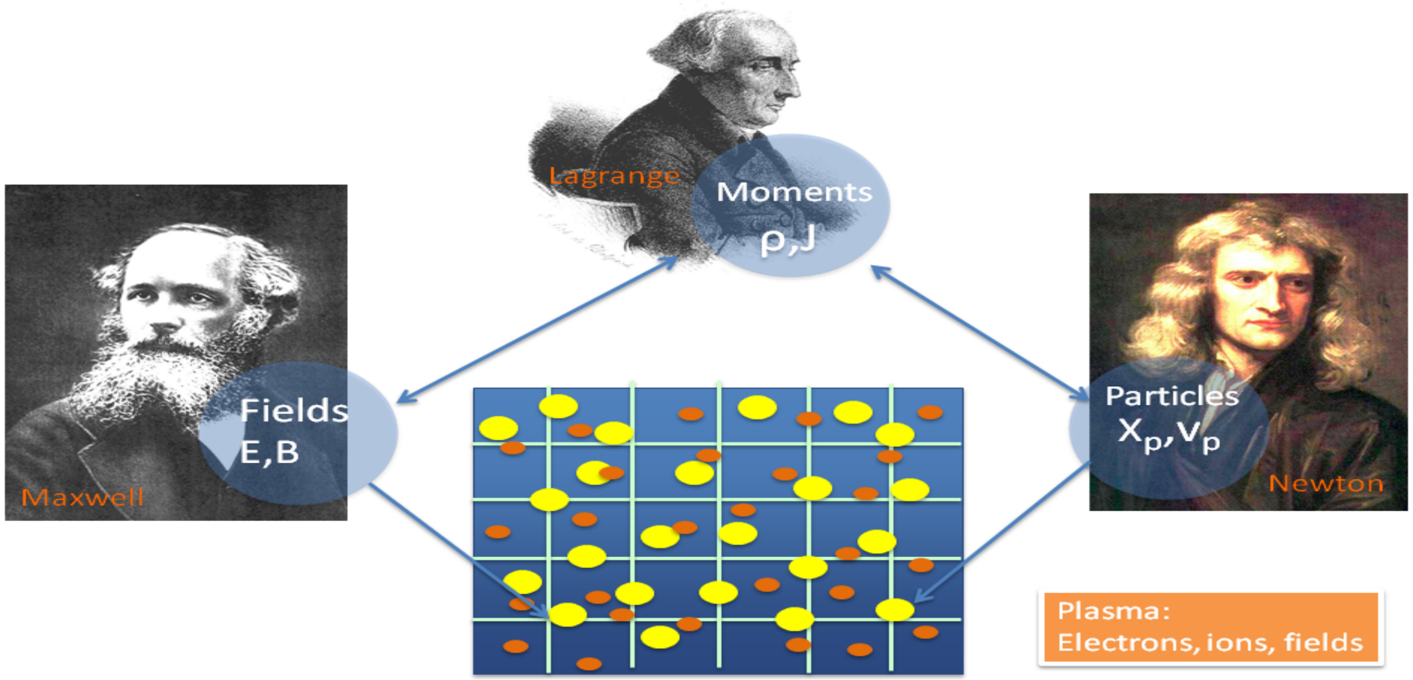
Where we are in the world? TOP500 list November 2011 (www.top500.org)

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
				10 Peta FLOP		12 MW!
1	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect / 2011 Fujitsu	705024	10510.00	11280.38	12659.9
2	National Supercomputing Center in Tianjin China	NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050 / 2010 NUDT	186368	2566.00	4701.00	4040.0
3	DOE/SC/Oak Ridge National Laboratory United States	Cray XT5-HE Opteron 6-core 2.6 GHz / 2009 Cray Inc.	224162	1759.00	2331.00	6950.0
	…	Lindgren		0.23 Peta FLOP		
44	KTH - Royal Institute of Technology Sweden	Cray XE6, Opteron 12 Core 2.10 GHz, Custom / 2011 Cray Inc.	36384	237.20	305.63	

What is Future? The Advent of Exascale Computing

- Exascale HPC will reach **10^{18} FLOPS** (100 x fastest supercomputer now). These computers are expected in **2018**. Our role at PDC is to prepare programming tools for next generation supercomputer for efficient use of computing resources.
- PDC is part of the **EC FP7 CRESTA** (Collaborative Research Exascale Systemware Tools and Applications) to study the next exascale supercomputers.
- PDC is leading the CRESTA work-package for development tools (**languages/compilers/ runtime systems/ autotuners/ performance analysis/debuggers**).

Particle-in-Cell Method



The Particle-in-Cell (PIC) method solves **the Vlasov-Maxwell** system by using **computing particles**.
The **distribution function** is represented by a **statistical sample of particles**. At each computational cycle, particles positions and velocities are calculated by solving **Newton equation**, charge and current densities are interpolated into grid points, and **Maxwell equations** are solved on the grid.

PIC Simulations for Magnetic Reconnection

- PIC simulations are the most fundamental approach for modeling magnetic reconnection. They describe correctly **kinetic effects**, such as wave-particle interactions.
- PIC method is well suited for parallel computing. Magnetic reconnection simulations require **parallel supercomputers**, unless a smart algorithm is used.
- Many computational groups simulate magnetic reconnection with parallel PIC codes. Typically, each group supports the development of a **PIC code**, that is not open-source.

Supercomputers used for Space Physics Magnetic Reconnection PIC Simulations

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Very few examples:

7	**Pleiades** NASA/Ames Research Center/NAS United States	SGI Altix ICE 8200EX/8400EX, Xeon HT QC 3.0/Xeon 5570/5670 2.93 Ghz, Infiniband / 2011 SGI	111104	1088.00	1315.33	4102.0	Lapenta – Markidis – Newman
8	**Hopper** DOE/SC/LBNL/NERSC United States	Cray XE6, Opteron 6172 12C 2.10GHz, Custom / 2010 Cray Inc.	153408	1054.00	1288.63	2910.0	Karimabadi-Daughton – Drake - Swisdak - Shay
10	**Roadrunner** DOE/NNSA/LANL United States	BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband / 2009 IBM	122400	1042.00	1375.78	2345.0	Daughton-Bowers
11	**Kraken** National Institute for Computational Sciences/University of Tennessee United States	Cray XT5-HE Opteron Six Core 2.6 GHz / 2011 Cray Inc.	112800	919.10	1173.00	3090.0	Pritchett

Largest PIC magnetic reconnection simulations!

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Limitations of Common PIC Methods

- **Time step** must be a **fraction of the plasma period** (resolve electron oscillation). Typically, plasma period is well resolved in PIC simulations and the **timescale of ion dynamics are scaled down** by changing the mass ratio between ion and electron.
- **Grid spacing** that must be smaller than 2-3 Debye lengths. Because such small grid spacing, the total size of the simulation box is typically small (hundreds of grid points for each direction -> hundreds Debye lengths)

Collisionless magnetic reconnection develops over ion time scales (tens W_{ci}^{-1}) on spatial regions of tens of ion skin depths, and therefore it is very challenging to be simulated with conventional PIC methods.

Implicit Particle-in-Cell Methods

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To remove these limitations, implicit Particle-in-Cell numerical schemes were introduced at the beginning of the Eighties at LANL and LLNL.
Implicit PIC methods are **unconditionally stable methods**, and allow users to have grid spacings that **are tens of Debye lengths**.
Implicit PIC schemes **artificially damps waves that are not resolved by the time step** (i.e. if the time step is much larger than plasma period Langmuir waves are artificially damped)
These properties come at cost of an increased computational complexity and time.

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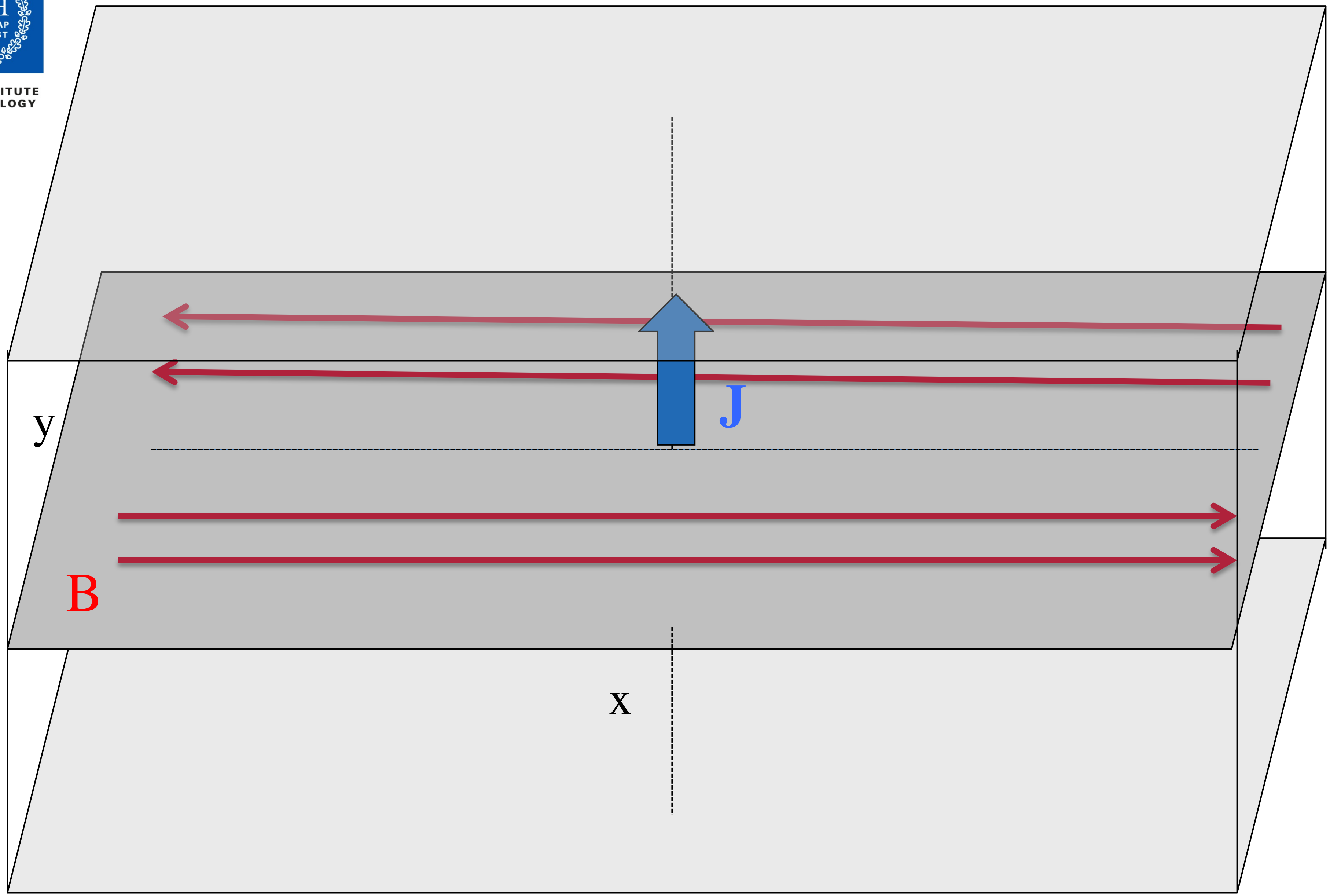
iPIC3D Code

- **Implicit parallel code** developed by Markidis and Lapenta. It is parallel version of the **CELESTE code**, developed by Brackbill and Lapenta.
- It is written in C++/MPI and it scales (**good efficiency**) up to 16,000 cores.
- It has been ported to Lindgren and to many others supercomputers.
- **Prof. Lapenta created and manages a database of simulation results of 3D and 2D magnetic reconnection simulations from iPIC3D. Lot of data is already available for analysis.**

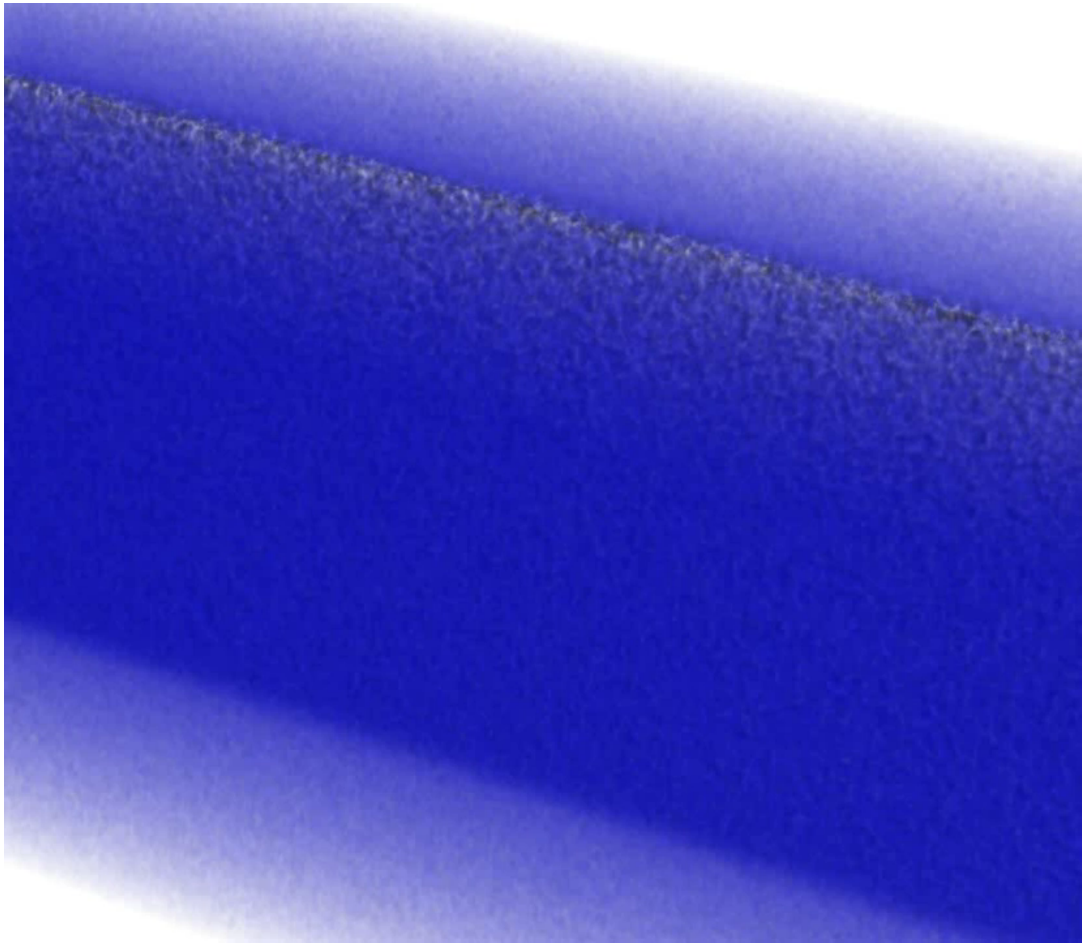
Results: Harris Current Sheet



Volume Plot of Intensity of Electron Current in Anti-Parallel Reconnection

Blue transparent -> low intensity.
White semi-transparent -> medium intensity.
Red opaque -> high intensity.

- Lower hybrid drift instability (LHDI).
- Onset of kink instability, triggered by LHDI
- Interchange instability at reconnection fronts. Ballooning instability?

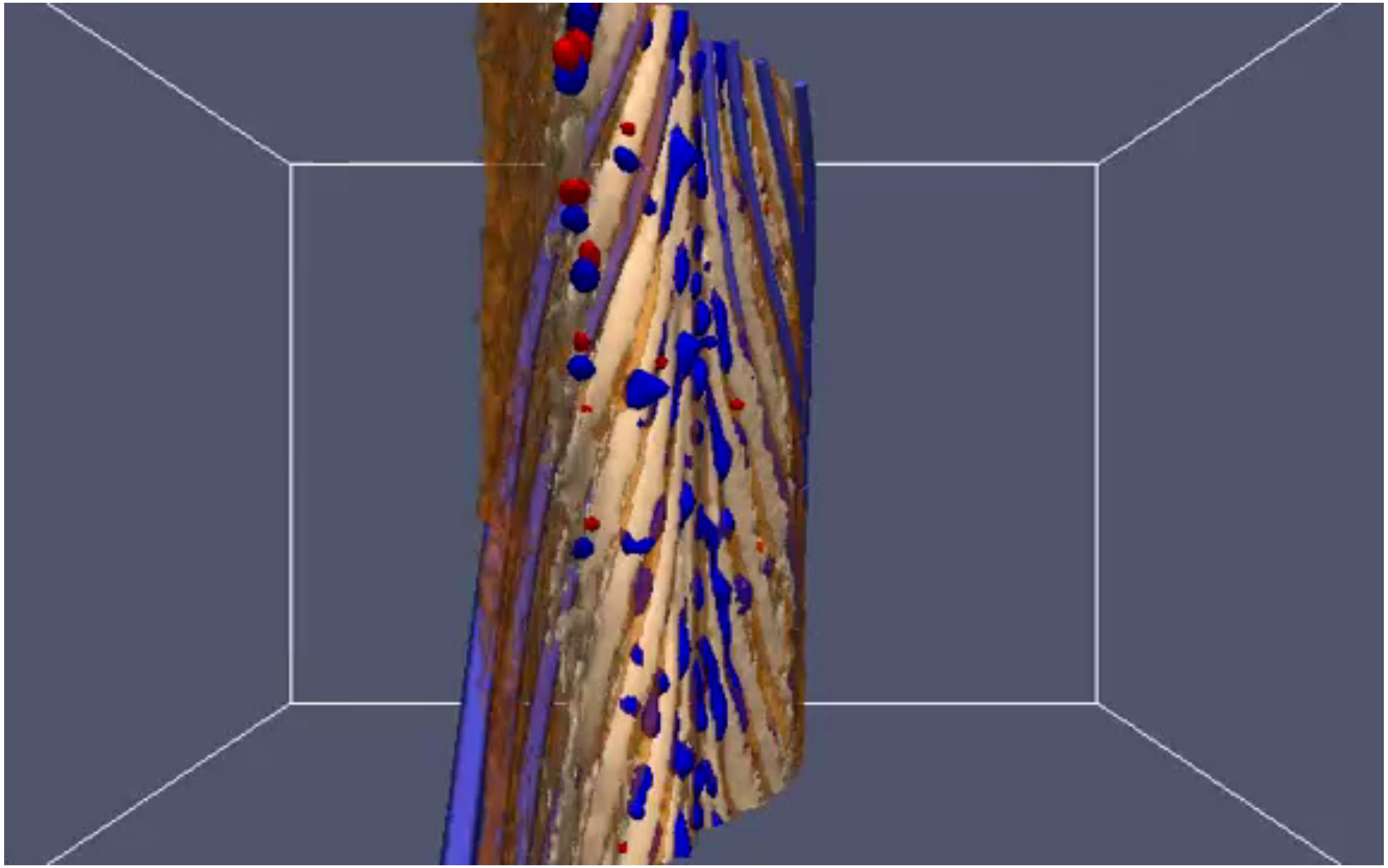


Guide Field Reconnection (a magnetic field is added along z) – Low Density Separatrix Structure at t = 14.5 W_{ci}^{-1}

Blue lines -> magnetic field lines

Orange and grey surfaces -> low density regions

Red and blue spheres -> bipolar electric field structures



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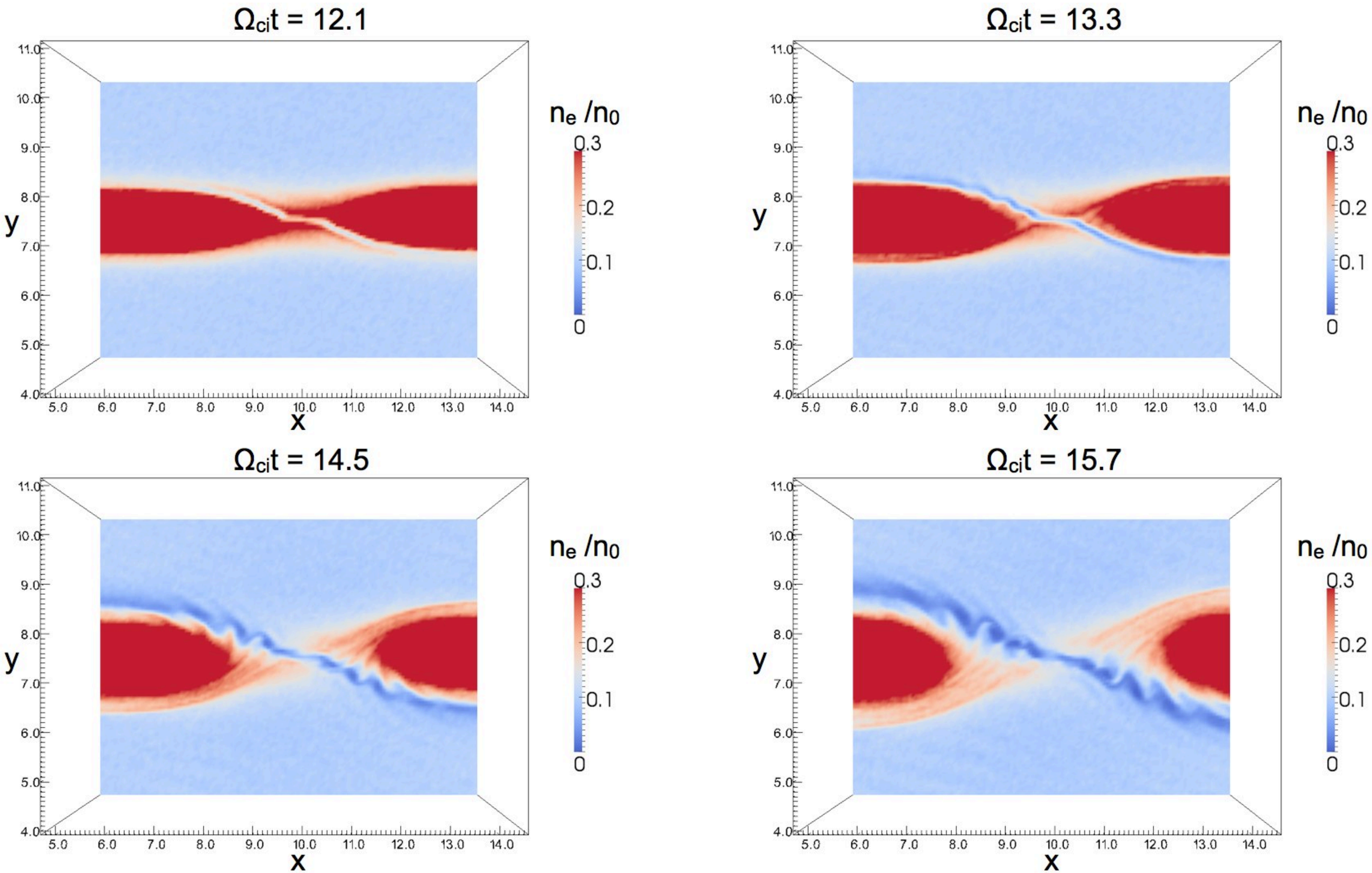
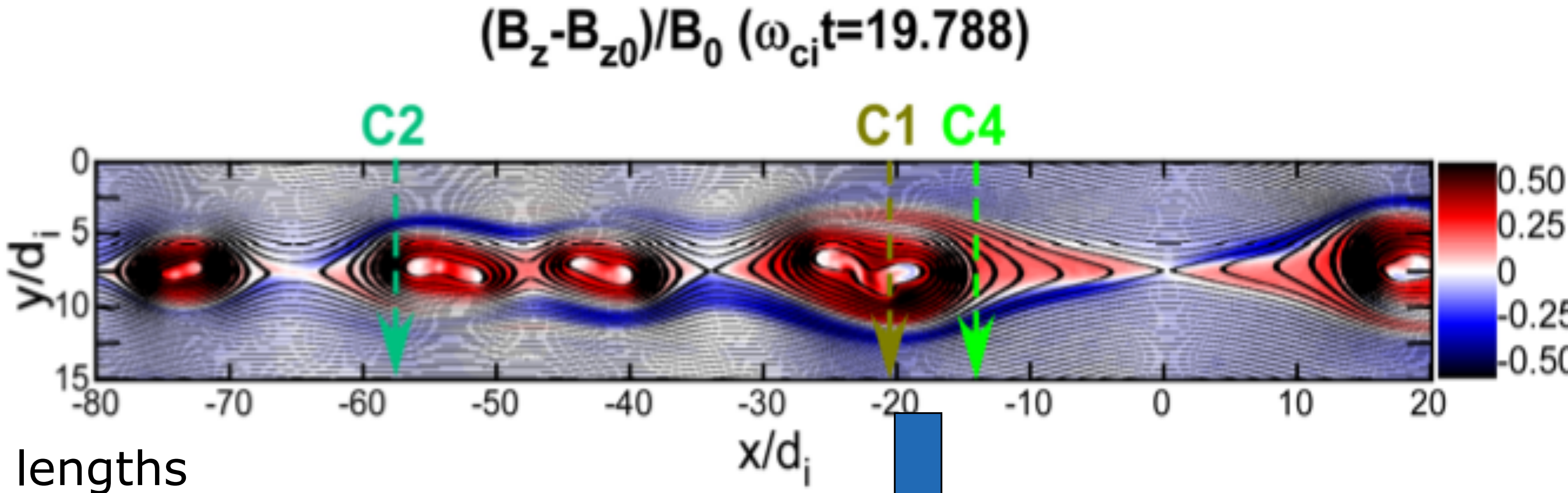
Vortices Structures on Reconnection Planes in Density and Electric field Plots

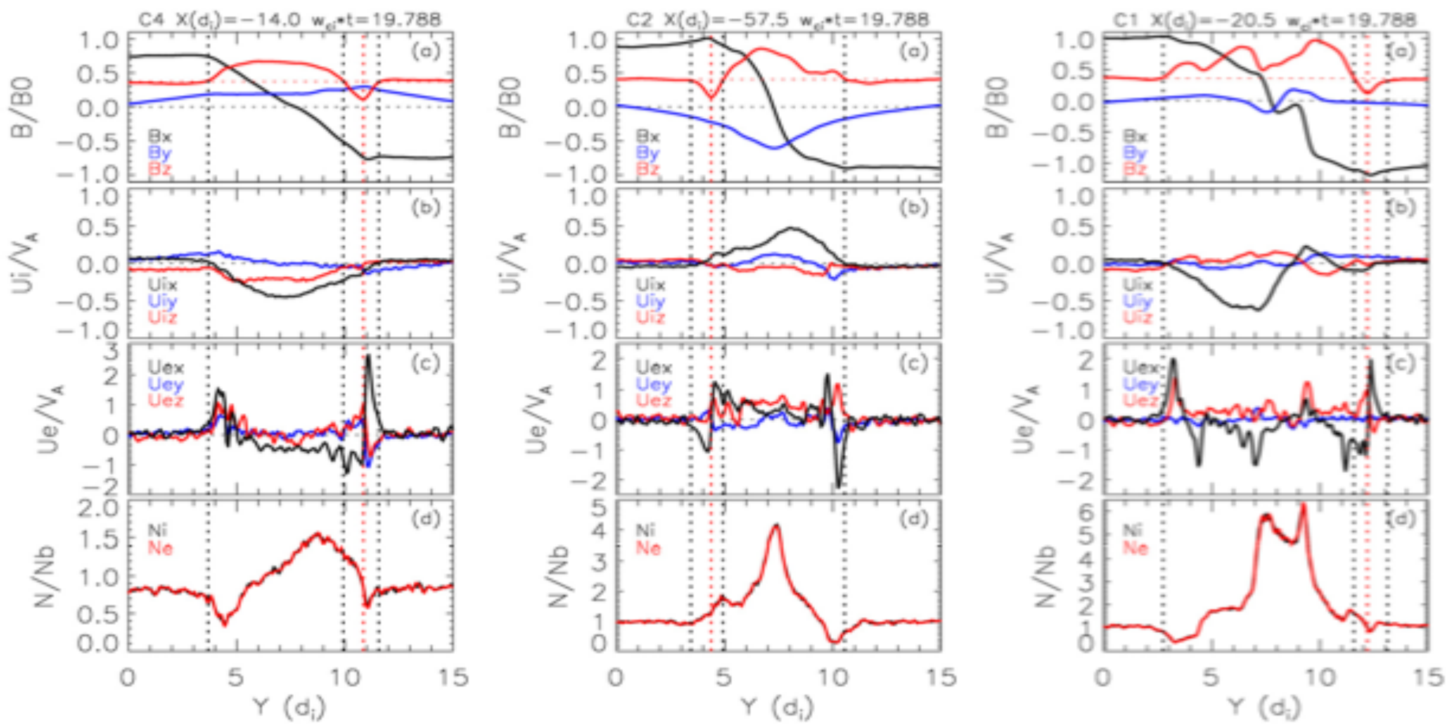


Plasmoid Chain Reconnection



Dt = 4.8 Wp^{-1}
Dx = 277 Debye lengths

C4 C2 C1



Possibility of comparing observational data and simulation results

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Conclusions

- Opportunities for computing time on Lindgren at PDC.
- Availability at PDC of an implicit Particle-in-Cell code, iPIC3D.
- Opportunities for comparing simulations results with observational data.
- Many simulations results from 3D/2D runs are available. Lots of data, something you are looking for might be there already!