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 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)
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).
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<th>Rank</th>
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<th>$R_{\text{max}}$</th>
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Lindgren 0.23 Peta FLOP
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).
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 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

Very few examples:

<table>
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<th>Computer</th>
<th>Details</th>
<th>Users</th>
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Largest PIC magnetic reconnection simulations!
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.
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.
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
Vortices Structures on Reconnection Planes in Density and Electric field Plots

\[ \Omega_{\text{crit}} \] = 12.1

\[ \Omega_{\text{crit}} \] = 13.3

\[ \Omega_{\text{crit}} \] = 14.5

\[ \Omega_{\text{crit}} \] = 15.7
Plasmoid Chain Reconnection

Possibility of comparing observational data and simulation results

$Dt = 4.8 \text{ Wp}^{-1}$
$Dx = 277$ Debye lengths
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!