Large-scale PIC-MCC simulation of low-temperature plasmas

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Why is Particle-In-Cell good for ExB plasma simulation?

- Particle-In-Cell with Monte Carlo Collisions (PIC-MCC) is a simulation model for plasmas that includes kinetic effects
    - *Can reproduce essential physics* (non-Maxwellian electrons, collisions, plasma-surface interaction)
- PIC-MCC requires high spatial and temporal resolution for numerical stability
    - Simulations often require large computers and long run times
- For most low-temperature plasmas (LTPs), the electrostatic (ES) approximation is valid (Poisson solve, not explicit time integration of Ampere’s and Faraday’s laws)
    - Often allows for much longer time steps (factor ten or hundred)
    - Time step still limited by either plasma oscillation or electron cell-transit time
- For many LTP applications, device sizes are large compared to Debye length
    - Many cells are needed to resolve Debye sphere throughout device
- PIC simulations are therefore often large
    - need lots of memory and long run times,
- but can be made to *scale well*
    - takes advantage of many (~10^4) processors on distributed-memory computer (cluster)

List of contemporary PIC codes (courtesy of J.-L. Vay)

● - Electrostatic Capable

Table 1. List of simulation PIC codes for the modeling of plasma accelerators.

Code	Type	Website/reference	Availability/license
ALaDyn/PICCANTE	EM-PIC 3D	http://aladyn.github.io/piccante	Open/GPLv3+
Architect	EM-PIC RZ	https://github.com/albz/Architect	Open/GPL
Calder	EM-PIC 3D	http://iopscience.iop.org/article/10.1088/0029-5515/43/7/317	Collaborators/Proprietary
Calder-Circ	EM-PIC RZ^+	http://dx.doi.org/10.1016/j.jcp.2008.11.017	Upon Request/Proprietary
CHIMERA	EM-PIC RZ+	https://github.com/hightower8083/chimera	Open/GPLv3
ELMIS	EM-PIC 3D	http://www.diva-portal.org/smash/record.jsf?pid=diva2%3A681092&dswid=-8610	Collaborators/Proprietary
EPOCH	EM-PIC 3D	http://www.ccpp.ac.uk/codes.html	Collaborators/GPL
FBPIC	EM-PIC RZ^+	https://fbpic.github.io	Open/modified BSD
HiPACE	QS-PIC 3D	http://dx.doi.org/10.1088/0741-3335/56/8/084012	Collaborators/Proprietary
INF&RNO	QS/EM-PIC RZ	http://dx.doi.org/10.1063/1.3520323	Collaborators/Proprietary
LCODE	QS-PIC RZ	http://www.inp.nsk.su/~lotov/lcode	Open/None
LSP	EM-PIC 3D/RZ ●	http://www.lspsuite.com/LSP/index.html	Commercial/Proprietary
MAGIC	EM-PIC 3D	http://www.mrcwdc.com/magic/index.html	Commercial/Proprietary
Osiris	EM-PIC 3D/RZ^+	http://picksc.idre.ucla.edu/software/software-production-codes/osiris	Collaborators/Proprietary
PHOTON-PLASMA	EM-PIC 3D	https://bitbucket.org/thaugboelle/ppcode	Open/GPLv2
PICADOR	EM-PIC 3D	http://hpc-education.unn.ru/en/research/overview/laser-plasma	Collaborators/Proprietary
PIConGPU	EM-PIC 3D	http://picongpu.hzdr.de	Open/GPLv3+
PICLS	EM-PIC 3D	http://dx.doi.org/10.1016/j.jcp.2008.03.043	Collaborators/Proprietary
PSC	EM-PIC 3D	http://www.sciencedirect.com/science/article/pii/S0021999116301413	Open/GPLv3
QuickPIC	QS-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/quickpic	Collaborators/Proprietary
REMP	EM-PIC 3D	http://dx.doi.org/10.1016/S0010-4655(00)00228-9	Collaborators/Proprietary
Smilei	EM-PIC 2D	http://www.maisondelasimulation.fr/projects/Smilei/html/licence.html	Open/CeCILL
TurboWave	EM-PIC 3D/RZ	http://dx.doi.org/10.1109/27.893300	Collaborators/Proprietary
UPIC-EMMA	EM-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/upic-emma	Collaborators/Proprietary
VLPL	EM/QS-PIC 3D	http://www.tp1.hhu.de/~pukhov/	Collaborators/Proprietary
VPIC	EM-PIC 3D	http://github.com/losalamos/vpic	Open/BSD clause-3 license
VSim (Vorpal)	EM-PIC 3D ●	https://txcorp.com/vsim	Commercial/Proprietary
Wake	QS-PIC RZ	http://dx.doi.org/10.1063/1.872134	Collaborators/Proprietary
Warp	EM-PIC 3D/RZ^+ ●	http://warp.lbl.gov	Open/modified BSD

EM = electromagnetic; QS = quasistatic; PIC = particle-in-cell; 3D = three-dimensional; RZ = axisymmetric; RZ^+ = axisymmetric with azimuthal Fourier decomposition.

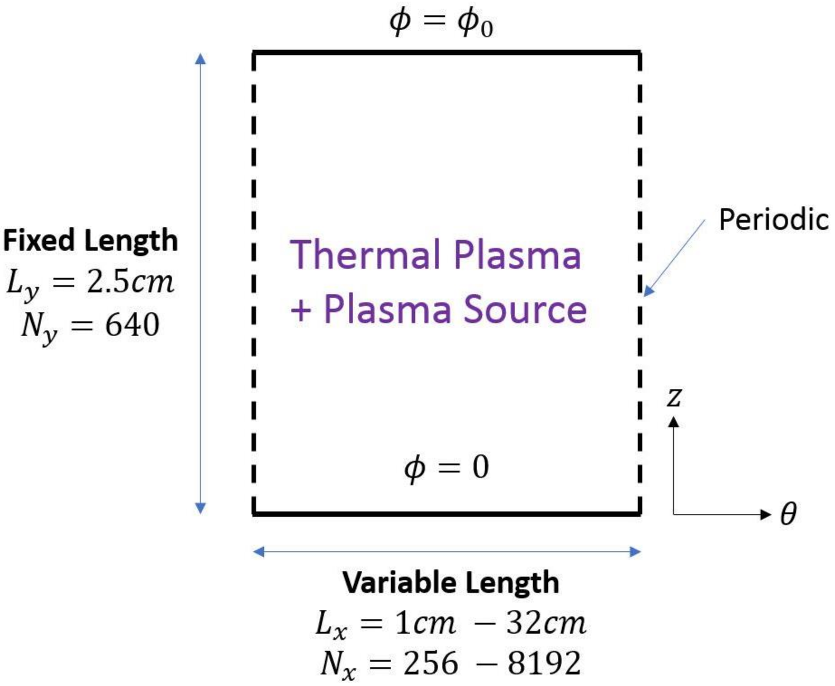
What makes a PIC-MCC code good for low-temperature plasma applications?

- Many PIC codes available, commercial and open source
- Routinely used for large-scale 3D simulations (10^4 - 10^5 processor cores)
- But not all of them suitable for LTP applications
- Ideal LTP PIC code needs
  - Poisson solve using Multi-Grid (MG) method (to achieve scalability on distributed-memory computer architectures)
    - Solve should be coupled to circuit model
  - State-of-the-art (or at least customizable) low-temperature specific models for
    - Collisions
    - Plasma-surface interaction

How to get the code to scale

- Evolving particles (due to influence of both Lorentz force and collisions) is straightforward to do in a scalable way
  - Thread and vectorize for best performance
- For electrostatic (or implicit electromagnetic) PIC, the *field solve is global, making it a scalability bottleneck*
- Scalable Poisson solve is a tough problem, but it has fortunately largely been solved and excellent *multigrid solver* libraries are available:
  - hypre and Trilinos from Lawrence Livermore national lab
  - PETSc from Argonne national lab (can be coupled with hypre)
- Communication over the network of ES potential and charge density data at grid points can also limit scalability
  - The *ratio of computation to communication should be high*, that is the local domain should have many interior grid points for each edge grid point
  - This is why 3D is hard (a square grid has higher fraction of interior points than a cube)
- Empirical evidence says code needs to be *“born parallel”* to scale well

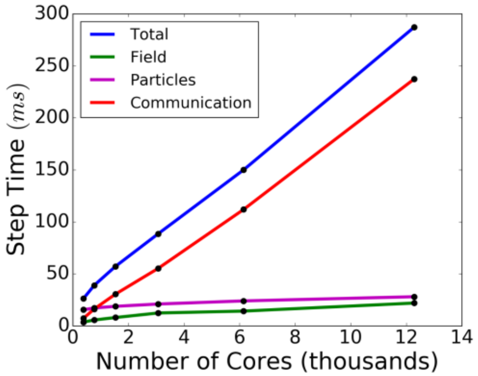
2D test problem for weak-scaling study (simulation size proportional to number of processor cores)



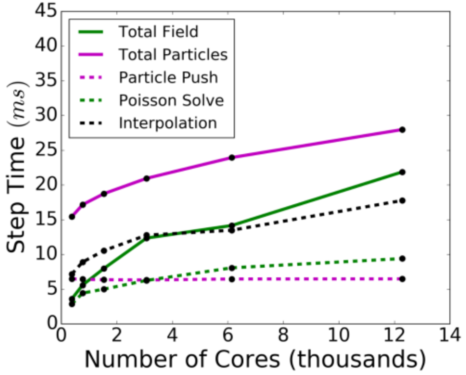
- Setup similar to Boeuf's 2D axial-azimuthal Hall thruster channel setup
- Vary azimuthal extent, with 16x24 = 384 processors per azimuthal cm
- Communication is domain decomposition for field solve and particle list decomposition for particles

Weak scaling results in 2D

Scaling problem from 1cm to 32cm azimuthal extent

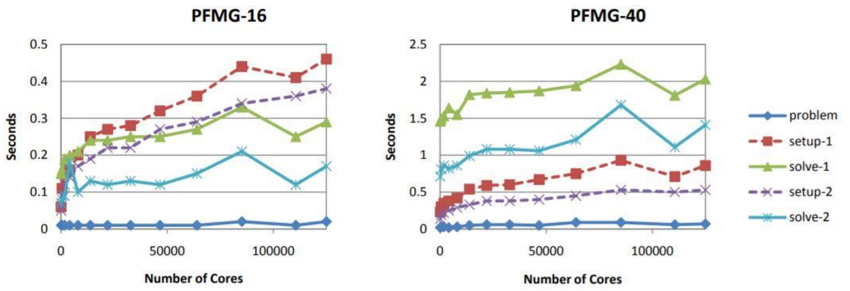


Detailed scaling behaviour

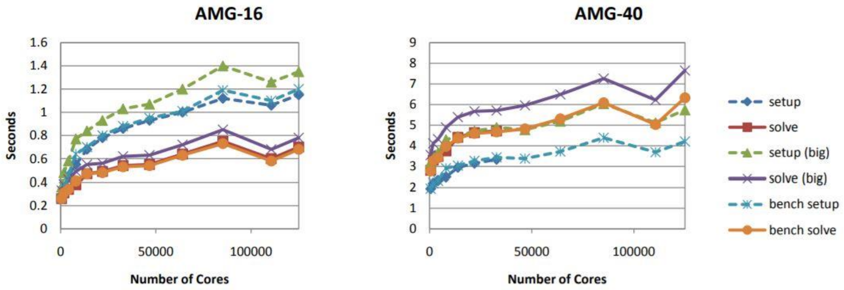


- Most importantly, the Poisson solve (Hypre Multi-Grid) scales very well
- Particle push scales perfectly
- Communication scaling is still poor, however this is expected
  - This is the final part of the core code to be systematically optimized
  - We will again perform numerical experiments to identify the best algorithm

Hypre 3D field-solve scaling results



Hypre Multi-Grid 3D Poisson Solve Weak Scaling. 16x16x16 and 40x40x40 boxes [1]



Hypre Algebraic Multi-Grid 3D Poisson Solve Weak Scaling. 16x16x16 and 40x40x40 boxes [1]

- The team at LLNL have done extensive scaling tests of Hypre for three-dimensional Poisson solves
- Shows excellent scaling beyond 10^5 cores and demonstrates that Multi-Grid is an ideal algorithm for large scale LTP simulation
- Algebraic Multi-Grid becomes favorable for complex geometries

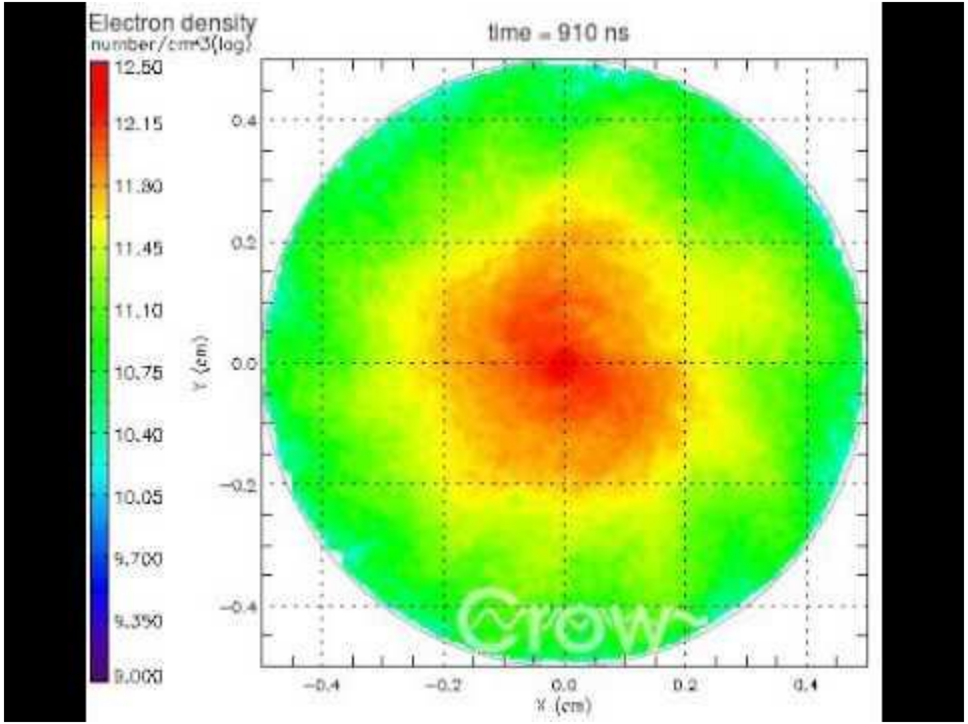
[1] Baker, Allison H., et al. "Scaling hypre’s multigrid solvers to 100,000 cores." *High-Performance Scientific Computing*. Springer, London, 2012. 261-279.

PIC-MCC simulations of LTP at PPPL

- Primarily two PIC-MCC codes are used at PPPL for LTP simulations:
  - PPPL-LSP, a modified version of LSP (updated ES solver, collision and circuit models)
    - 3D in principle, but Poisson solve severely communication bound in 3D
    - Used for 2D simulations of Penning discharge and various industrial plasmas
  - EDIPIC, by D. Sidorenko
    - Well validated collision models
    - Not 3D
    - Used for academic research as well as for various industrial plasmas
- New code under development by A. Powis
  - Used to produce scaling results presented in previous slide
- PPPL-LSP was used to simulate anomalous transport in Penning discharge
  - 2D simulation (axial derivatives assumed zero, Cartesian coordinates)
  - Electron beam injected on axis in axial direction (parallel to magnetic field)
  - 1000x1000 cells (either device size or relative permittivity was scaled)
  - Simulations advanced about one microsecond per day on 256 processor cores

PPPL-LSP simulation of spoke in Penning discharge

- Electron density contour from 2D electrostatic PIC simulation of Penning discharge
- A narrow electron beam is injected at the origin, in the normal direction parallel to a homogeneous magnetic field
- Electrons are magnetized, but ions are not
- A spoke-like rotating density perturbation forms that channels radial electron current



Summary

- PIC-MCC allows computer simulation that reproduces all the relevant physics of low-temperature plasmas (LTPs)
- Because it is necessary to resolve short length and time scales, PIC-MCC simulations tend to require large amounts of memory (RAM) and long run times
- However, if properly implemented PIC-MCC is highly scalable on distributed-memory clusters and supercomputers
- At PPPL, the codes PPPL-LSP and EDIPIC are routinely used for 2D LTP simulations using 10^2-10^3 processor cores
- A new code will be able to do 3D simulations using at least 10^4 cores