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Implicit and Hybrid Techniques for the Simulation of High-Density Electrode Plasmas for Pulsed Power Applications

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Topics

- Motivation for Implicit/Hybrid Modeling
- PIC algorithm advances including Magnetic Implicit with Poisson Correction.
- Fast fluid technique and Particle Migration Hybrid.
- OpenMP threading.
- Application to Simplified Convolute geometry to assess speed up and accuracy.
- Summary and Conclusions

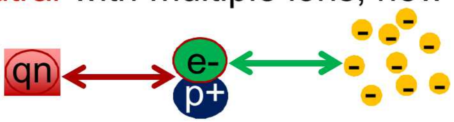
Motivation for Implicit/Hybrid Power Flow Simulation

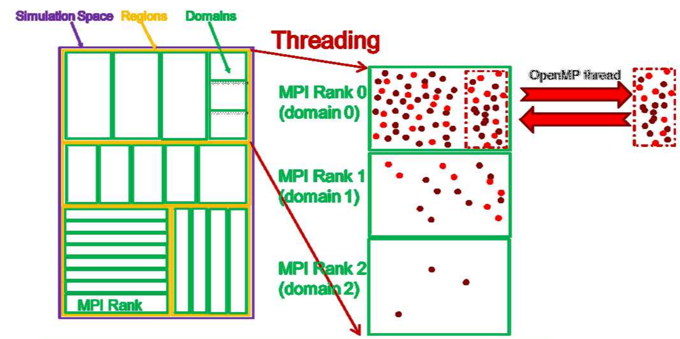
- Power flow, charged particle emission, current sheaths:
  - Non-neutral, nonMaxwellian, turbulent, nonlinear instability growth.
  - < 10^{15} cm^{-3} density -> Fully Kinetic physics.
- Evolving Contaminant Plasmas:
  - Non-neutral physics such as bipolar flow, nonlinear instability growth.
  - Detailed chemistry: Breakdown, charge exchange, etc.
  - < 10^{19} cm^{-3} density -> Multi Fluid through kinetic (hybrid).
- MITL Metal Substrate:
  - Mostly quasi-neutral with *kinetic impacts*.
  - EOS, solid density -> Single Fluid or Multi Fluid (hybrid).
- Liner Evolution:
  - Mostly quasi-neutral with EOS, maybe with Hall like physics.
  - Magnetized Shocks, mix.
  - >> solid density, but features such as laser heating, *beams* and *fusion product transport* requiring kinetic effects -> Hybrid.

All regimes can benefit from some hybrid description, PIC techniques being developed in the Chicago and LSP codes offer a integrated method to model both kinetics and fluids!

Chicago* is a FDTD Toolkit of Field/Particle Advanced Techniques for Plasma Simulation

- Fully electromagnetic and relativistic.
- 3D orthogonal grid 1st or 2nd order (partial-cell conformal boundaries with particles*) surfaces.
- ***All*** plasma descriptions use PIC techniques, and can be combined in ***Particle Migration Hybrid*** operation.
- Kinetic, multi-fluids (inertia and charge separation).
- Quasi-neutral with multiple ions, new Hall implementation.#





Chicago uses a two-level spatial decomposition *plus* multiple threads/domain.

MITL Sheaths

Electrode plasmas

HEDP plasmas

Solution technique	Speed	$\lambda_{Debye}/\Delta x$	$\omega_c \Delta t$	$\omega_p \Delta t$	Use/Comments
Explicit mom. conserving	fast	< 1	< 2	< 2	No particle self force. Must resolve Debye length.
Explicit energy conserving	fast	>> 1	< 1—2	< 1—2	Best energy and momentum conservation with second order CIC.
Direct Implicit	slower	>> 1	< 1	>> 10	Cyclotron orbit growth. Best conservation with Poisson Correction on, CIC.
Magnetic Implicit	slower	>> 1	< 3-12	>> 10	Accurate orbits. Limited o moderate ω_c with large ω_p.
Multi-Fluids	faster	>> 1	< 1-12	>> 10	Lagrangian or Eulerian. EOS/Radiation available. Better long time conservation. Implicit, CIC.
Quasi–Neutral (Resistive MHD)	fast	>> 1	>> 1	>> 1	EOS, Radiation, Kinetic ions available. Hall physics tested in 2D. No electron inertia.

* D. R. Welch, N. Bennett, T. C. Genoni, D.V. Rose, C. Thoma, C. Miller, and W. A. Stygar, *Electrode contaminant plasma effects in 10^7-A Z pinch accelerators,* Phys. Rev. Accel. Beams **22,** 070401 (2019).. # C. Thoma, et al., manuscript submitted (2019).

Direct Implicit* has allowed relaxed frequency constraints by integrating over fast plasma oscillation.

$$x^{n+1} = x^n + \frac{\Delta t}{c} p^{n+1/2}$$

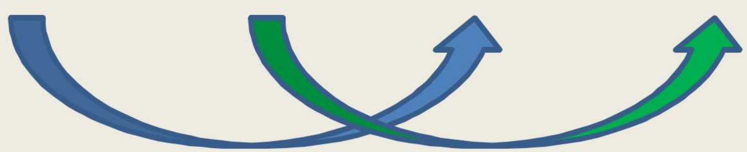
$$p^{n+1/2} = p^{n-1/2} + \frac{\Delta t}{2m}\left(E^{n-1} + E^{n+1} + \frac{p^{n-1/2} + p^{n+1/2}}{\gamma c} \times B^n\right)$$

$$E^{n+1} = E^n + \frac{\Delta t}{2} \nabla \times (B^n + B^{n+1}) - \Delta t J^{n+\frac{1}{2}} - S \cdot E^{n+1}$$

$$B^{n+1} = B^n - \frac{\Delta t}{2} \nabla \times (E^n + E^{n+1})$$

Solve for future fields via matrix inversion.
Fluctuations in E reduced by
$1+1/2\ \omega_p^2$

Time Step	n-1	n-1/2	n	n+1/2	n+1
EM fields	E,B		E,B		E,B
Particles	X	P	X	P	X



DI has a wide temporal stencil, and problems at high $\omega_c \Delta t$.

*Cohen, Langdon, Friedman, J. Comp. Phys. **46** , 15 (1982);
D. R. Welch, et al., Nucl. Inst. Meth. Phys. Res. A **464**, 134 (2001).

Magnetic Implicit* algorithm further relaxes constraints and enables realistic power flow, diode simulations.

Time Step	n	$n+1/2$	$n+1$
Fields	E,B	B'	E,B
Position	x	x'	x
Momentum	p	p'	p

MI calculates all particle attributes and EM fields at full time steps after initial half step advance for centering. *Energy conserving* with *2nd order cloud* gives superior results:

$$\omega_p \Delta t >> 1 \text{ and } \omega_c \Delta t < 10$$

2 Step Particle advance

- 1st step pushes x and p with E^n and $B^{n+1/2}$ and $\langle \boldsymbol{S} \rangle$ constructed at x' .

$$\langle \boldsymbol{S} \rangle = \frac{\rho \Delta t q}{2\gamma_{n+1/2} m} \langle \boldsymbol{T} \rangle \left(I - \mathbf{v}_{n+1/2} \mathbf{v}_{n+1/2} \right),$$

- 2nd step after fields are advanced to n+1, x and p are pushed from n to n+1 positions. Corrects for errors in mirror force and transverse magnetic field gradient drift.

$$p^{n+1} = p^n + \frac{q\Delta t}{2m} \left[\left(E^n + E^{n+1} \right) + \frac{\left(p^n + p^{n+1} \right)}{\gamma^{n+1/2} c} \times B^{n+1/2} \right],$$

$$x^{n+1} = x^n + \Delta t \left(\frac{p^n + p^{n+1}}{\gamma^n + \gamma^{n+1}} + \Delta v_{drift} \right).$$

Implicit EM advance with Poisson correction

- For calculation of susceptibility $\langle \boldsymbol{S} \rangle$ and magnetic rotation matrix $\langle \boldsymbol{T} \rangle$ at x', *B* is advanced ½ step with explicit Faraday's Law ,

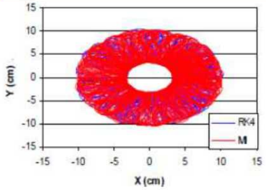
$$\frac{B^{n+1/2} - B^n}{\Delta t} = -\frac{1}{2} \nabla \times E^n.$$

- After 1st particle advance, fields advanced with implicit term for *J* at *n*+1

$$\frac{\partial E}{\partial t} = \nabla \times B - J - \langle S \rangle \cdot E'_{n+1} \quad \text{Implicit electromagnetics}$$

$$\nabla \cdot (1 + \langle S \rangle) \cdot \nabla \psi_{err} = \rho^0_{n+1} - \nabla \cdot (1 + \langle S \rangle) \cdot E'_{n+1} = \rho_{err}, \quad \text{Poisson Correction}$$

$$E_{n+1} = E'_{n+1} - \nabla \psi_{err}, \quad \text{Corrected field applied to particle in second push}$$



Benchmarked* against 4th order RK solution of complex Field Reversed Configuration orbits.

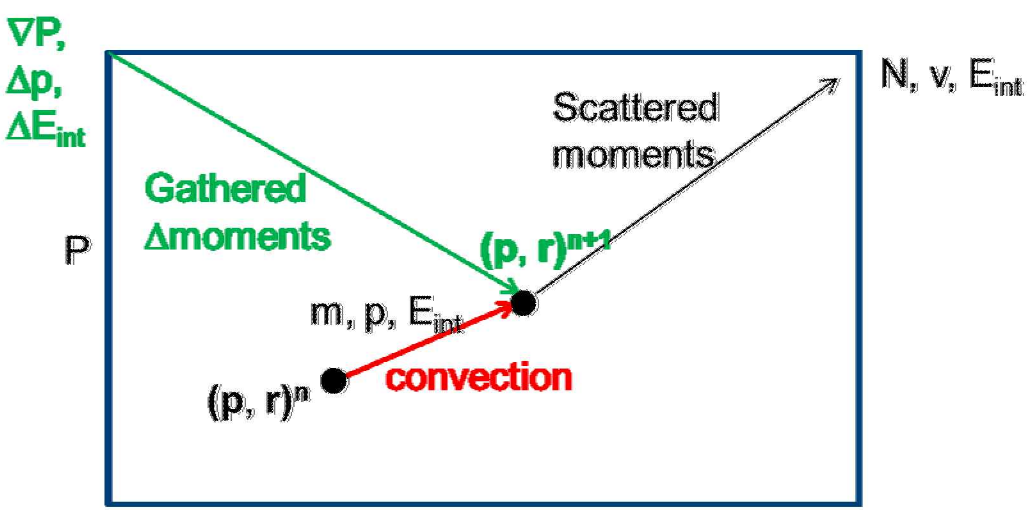
*T. C. Genoni, R. E. Clark and D. R. Welch, The Open Plasma Physics Journal **3**, 36 (2010).
D. R. Welch, et al., Phys. Rev. Accel. Beams **22,** 070401 (2019).

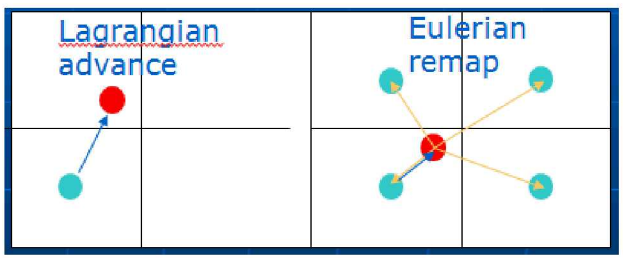
Basic PIC Fluid Technique* with optional EOS is computational faster with fewer particles.

- Lagrangian fluid macroparticles *convect moments* (charge, mass, momentum and energy) with little diffusion.
- Fluid moments scattered to grid where interactions, transport, etc. calculated.
- Δp, ΔE_{int} gathered back to particles.
- Pushed with collective velocity.
- More diffusive with Eulerian remap, but 1 particle per cell.

$$n_i \frac{dU_i}{dt} = -n_i T_i \nabla \cdot v_i + \sum_j \frac{2 m_j n_j}{m_i \tau_{ji}} (T_j - T_i) + \nabla \cdot \kappa \nabla T_i + \sum_j v_{ji} \frac{m_i m_j}{m_i + m_j} \left(\frac{p_i}{m_i} - \frac{p_j}{m_j} \right)^2 + \dot{R}$$

$$\frac{dp_i}{dt} = \frac{q}{m}(E + v_i \times B) - \frac{\nabla P_i}{n m_i} + \sum_j (p_i - p_j) \nu_{ij}$$





*J. U. Brackbill, Comp. Phys. Comm **48**, 25-38 (1988); D. R. Welch, Phys. Plasmas **16**, 123102 (2009); C. Thoma, Phys. Plasmas **18**, 103507 (2011).

PIC representations of kinetic, multi-fluid, and quasi-neutral macroparticles can be combined → ***Particle Migration Hybrid***

- Advanced Implicit Method for kinetic/multi-fluid PIC.

$$\frac{\partial E}{\partial t} = \nabla \times B - J - \langle S \rangle \cdot E \quad \text{Implicit electromagnetics}$$

$$\nabla \cdot (1+\langle S \rangle) \cdot \nabla \psi_{err} = \rho^{0}_{n+1} - \nabla \cdot (1+\langle S \rangle) \cdot E'_{n+1} = \rho_{err}, \quad \text{Poisson Correction}$$

$$E_{n+1} = E'_{n+1} - \nabla \psi_{err}, \quad \text{Corrected field applied to particle in second push}$$

- PIC fluids have equations of motion and energy. Macroparticles carry internal energy.

$$\frac{dp_i}{dt} = \frac{q}{m}(E + v_i \times B) - \frac{\nabla P_i}{nm_i} + \sum_j (p_i - p_j)\nu_{ij}$$

- Advanced *Multi-Ion* Quasi-Neutral PIC algorithm includes effects from kinetic and multi-fluid particles.

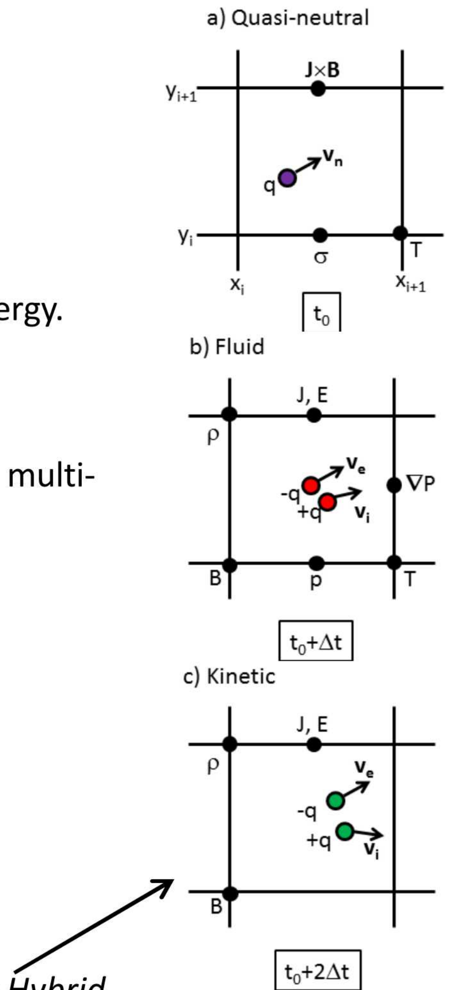
$$n_K m_K \frac{D\vec{v}_K}{Dt} = \left(\frac{\bar{Z}_K n_K}{n_e}\right)\vec{J}_{MHD} \times \vec{B} + e\bar{Z}_K n_K (\vec{v}_K - \vec{v}_+) \times \vec{B}$$

$$-\left[\nabla \tilde{P}_K + \left(\frac{\bar{Z}_K n_K}{n_e}\right)\left(\nabla \tilde{P}_e - \sum_K \bar{Z}_K \frac{m_e}{m_K} \nabla \tilde{P}_K\right)\right] + \beta_o \bar{Z}_K n_K \nabla T_e \left(1 - \frac{(n_e)_L}{n_e} F_\beta\right)$$

$$- n_K m_K \sum_{M'} \nu_{KM'} (\vec{v}_K - \vec{v}_{M'}) - n_K m_K \nu_{Ke} (\vec{v}_K - \vec{v}_+) + \bar{Z}_K n_K m_e \sum_{M'} \nu_{eM'} (\vec{v}_{M'} - \vec{v}_+)$$

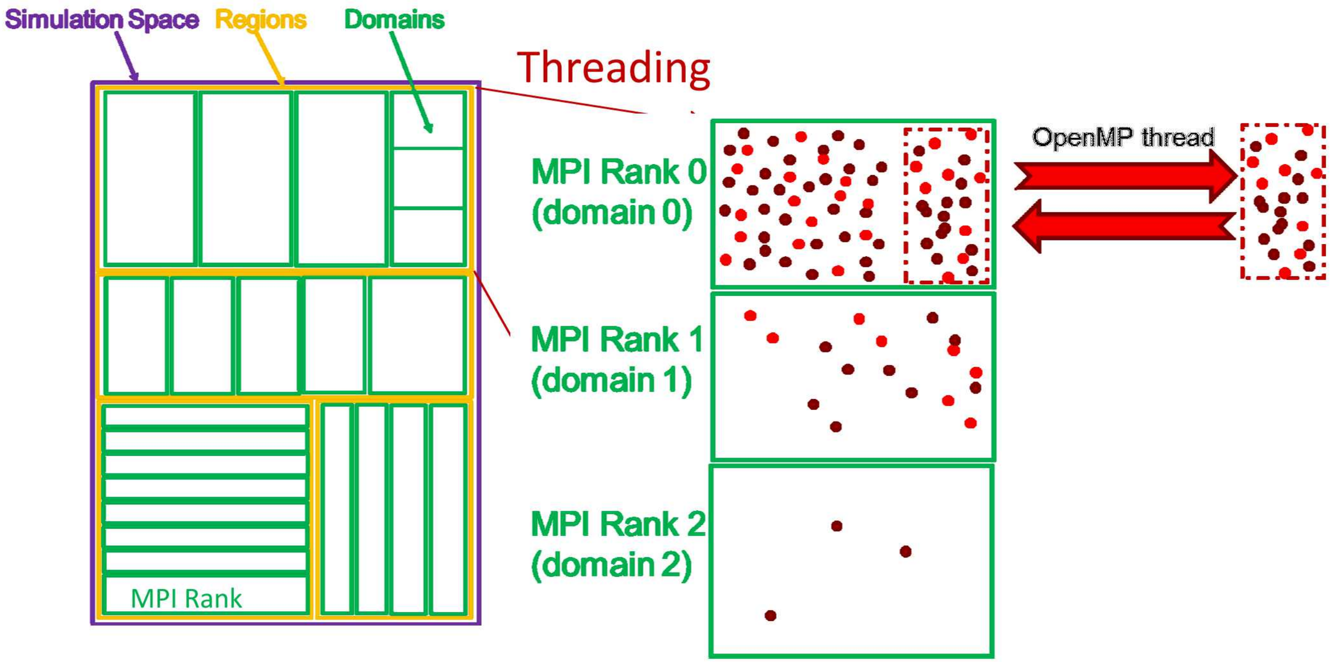
$$- n_e m_e \left[\left(\frac{\bar{Z}_K n_K}{n_e}\right)\sum_{M'} \nu_{eM'} - \nu_{eK}\right](\vec{v}_e - \vec{v}_+)$$

- Seamless *migration* between particles of one EOM to another (*Particle Migration Hybrid, PMH*). Particles may migrate wholesale or particle by particle based on energy, perveance, Mach number, etc.



Particle Migration Hybrid

New 3 level decomposition for parallel execution in Chicago with regions, domains, and threads.



Threads advance a portion of particles in a domain and scatter currents/charge to grid.

Multiple threads can be used per domain. GPU threading in development.

Threads are executed on additional CPU cores --- must be allocated at run-time.

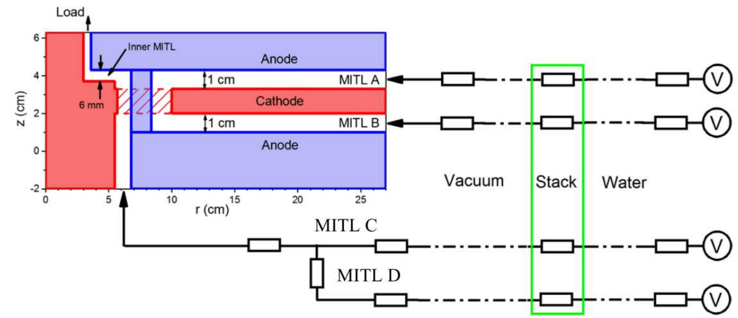
Load Balancing accomplished by adjusting domain volumes and number of threads per MPI Rank according to computational load.

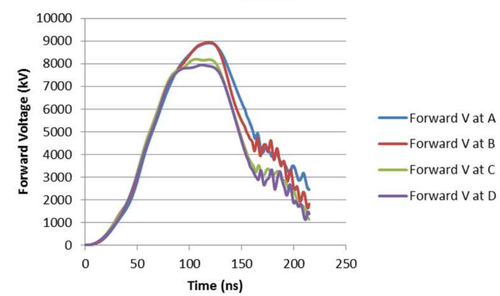
Demonstration in simplified convolute.

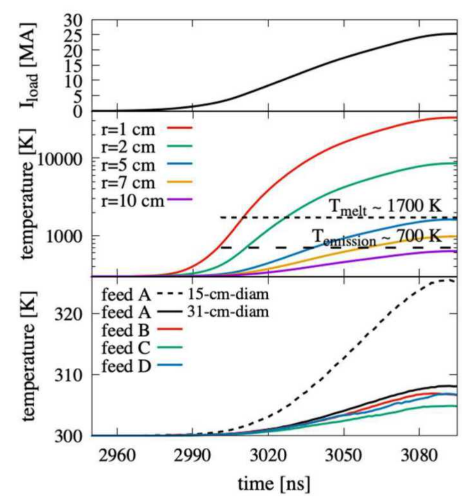
- Simulation Volume/Grid.
  - -1.94—6.34 cm; 457 radial cells (200 μm minimum)
  - 0--π/12; 20 azimuthal cells (uniform)
  - 2.9—27 cm; 289 axial cells (100 μm minimum)
- Simulation Boundaries.
  - Driven by 4 level Z circuit.
  - Load is a 4.86-nH inductor (inner MITL) to a short.
- Simulation Decomposition – 272 domains
  - 68 regions, 4 domain/region, 1 or2 threads per domain.
- SS Electrode material Heating – Ohmic (Knoepfel) and charged particle Impact.

$$\Delta T(t) \approx \frac{1.273\,\mu_0\, j^2(t)}{2c_v}$$

- Plasma Generation and interactions.
  - Space charge limited emission off A and K.
  - Contaminant plasma desorption from A and K.
    - Temkin H_2O thermal desorption: $p = 10^{-5}$ Torr vacuum, $8\text{x}10^{15}$ cm^{-2} = 1 ML, .83-1.0 eV binding energy, Staged fragmentation and ionization of water into $3e^-$, $2H^+$, O^+.
    - Fully general binary scattering between all particles.





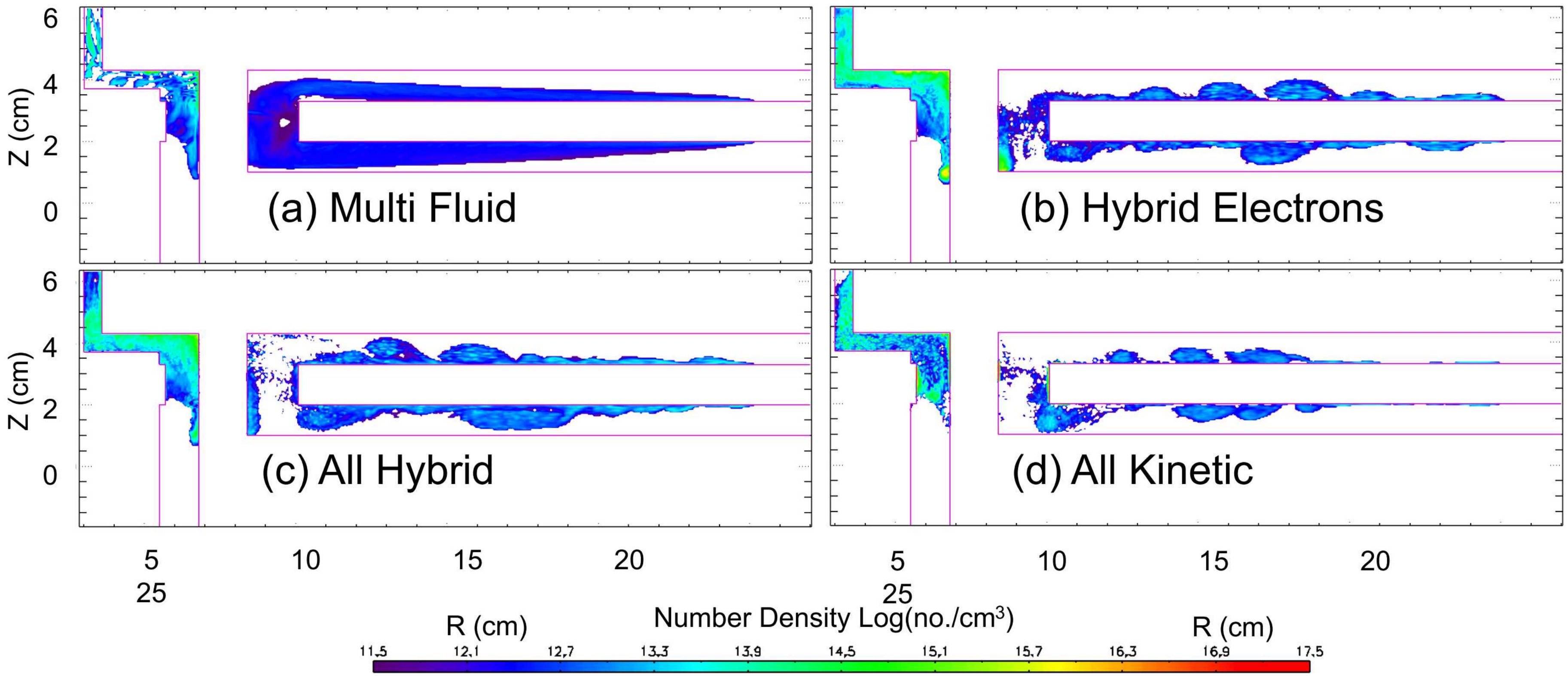


Fully kinetic, Multi-Fluid, Hybrid with Staged Ionization surface physics.

Multi Fluid shows smoother sheath behavior, hybrid closely resembles kinetic.

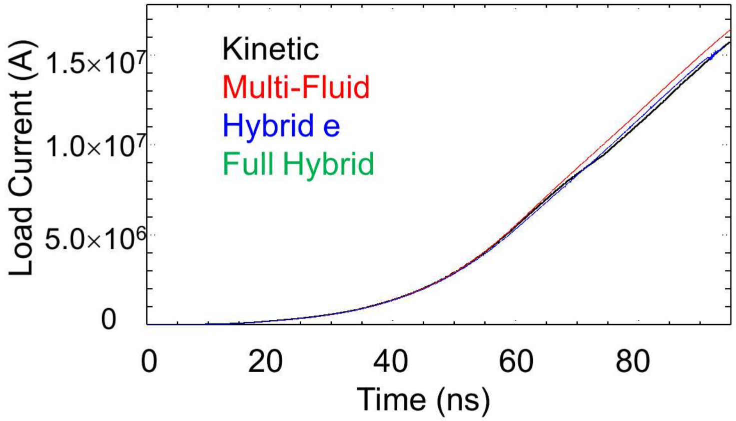
Two flavors of hybrid:

1. Hybrid electrons → only fluid electrons transition to kinetic.
2. Full Hybrid → all fluid electrons and ion species can transition to kinetic.

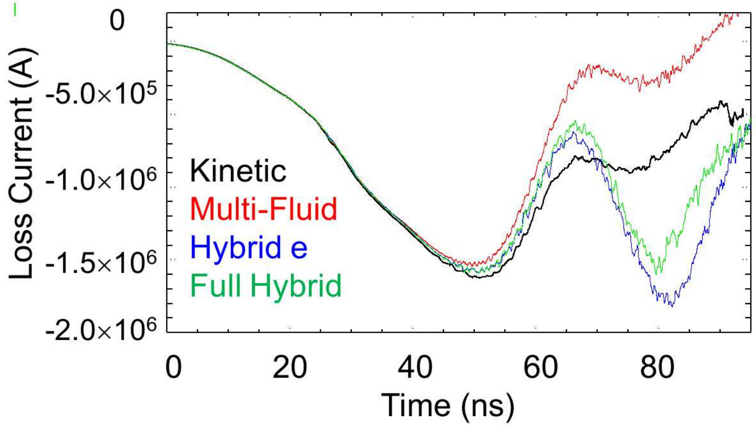


Plasma behavior with all fluids in inner MITL differs from kinetic/hybrid.

Comparison of models shows similar peak losses and load currents.



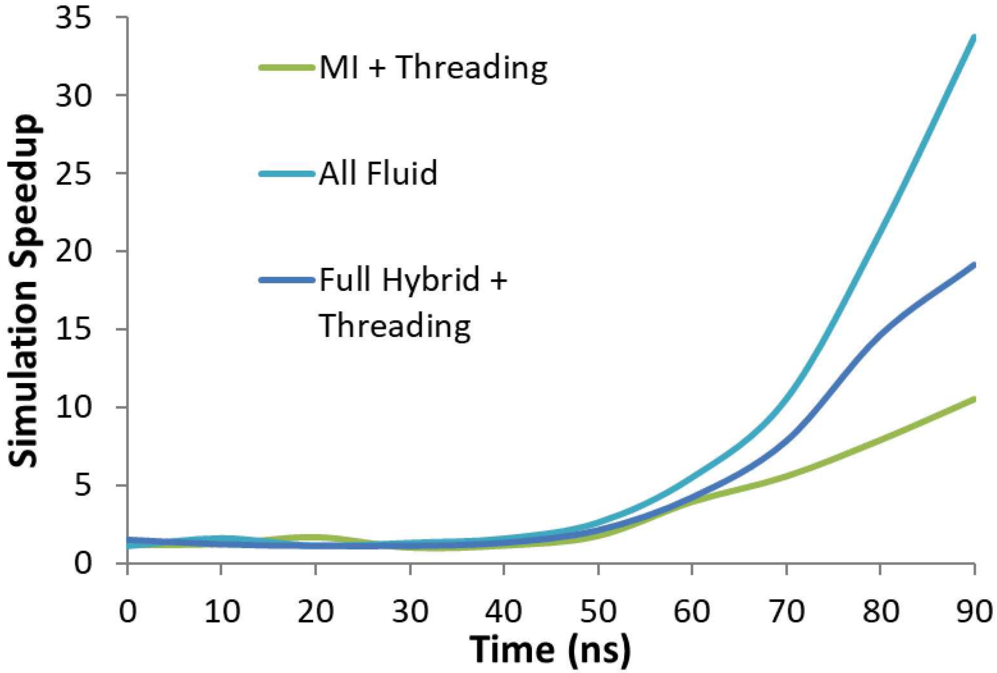
Current loss is difference of Stack and Load currents.



- Fluid simulation has no particle heating of electrodes, similar current sheath or “flow” losses, less current loss later (more turbulent transport).
- Investigating differences at 80 ns.

Speed up realized from new implicit MI algorithm, hybrid and threading.

Run	Total Time (h)	Average Speedup	Peak Speedup
DI 1 thread	314	1	1
MI 2 thread	63.49	5.0	10.5
All Fluid 1 thread	37.49	8.4	33.7
Full Hybrid 2 thread	49.03	6.4	19.1



Speedup with respect to DI 1 thread simulation.

1. MI algorithm yields 3x, threading 3x acceleration
2. Fluid/hybrid takes advantage of 9x larger times steps ($\omega_c \Delta t < 9$). Performs better at high currents.
3. Fluid speedup 34x, hybrid speedup 19x.

Summary

- Chicago and LSP have been upgraded with new implicit MI algorithm. Chicago has also been upgraded with new opnMP threading for more efficient computation. which has yield a 3—9x speed up from increases time step.
- A 3D representative Z convolute has been constructed and run with new configurations to gauge code performance and accuracy.
- Maximum speed up at high current:
  - New implicit technique is 3—9x.
  - Fully kinetic with threading is speed up 10x.
  - Hybrid technique with threading is 19x.
- We will integrating Tiling, OpenMP and GPU threads with goal of 100x speed up within 1 year.