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PIC and PIC/Fluid modeling in Chicago: Algorithms and Key Computational Issues for modeling on Z today

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Presented at the ZFSP Breakout Session (Beyond Resistive MHD Theory)

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Both algorithmic and computational techniques are stressed in Z power flow and load PIC simulation

- Volumes are large and sheaths are small.
- Plasma densities range from near vacuum to above solid density.
- Characteristic plasma frequencies are high pulses can be long.
- Pulsed power, power flow and load dynamics are closely coupled.

Here we discuss methodologies being employed in the new code CHICAGO.

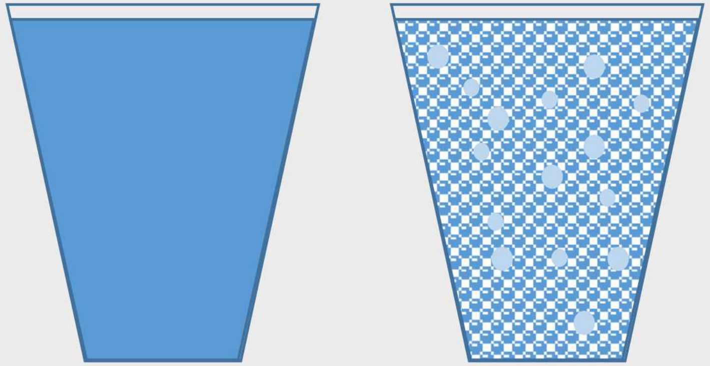
Problem: Typical MHD is fast but approximate, PIC is accurate but slow

- Traditional plasma simulation programs make use of fluid continuum, magneto hydrodynamics (MHD) approximations which are computationally fast, but inadequate in many situations, and its assumptions can be invalid; Electromagnetic Particle-in-Cell (PIC) simulation is adequate for more situations, but is much slower;
- Techniques to bridge the divide between MHD and PIC have been slow to develop;
- Existing physics simulation codes, magneto hydrodynamics (MHD) and Electromagnetic Particle-in-Cell (PIC codes) lack:
  - Advances in high-level physics, material data bases,
  - Parallel algorithms,
  - Use of modern HPC computing technology required for adequate solutions;

The pitfalls of these codes have several negative quantitative impacts, including:

Typical MHD Code:

- Assumes velocity distribution.
- Assumes small MFP, no mix.
- Transport coefficients break down at critical phases, temperatures, and time scales in plasma evolution;
- Many knobs.

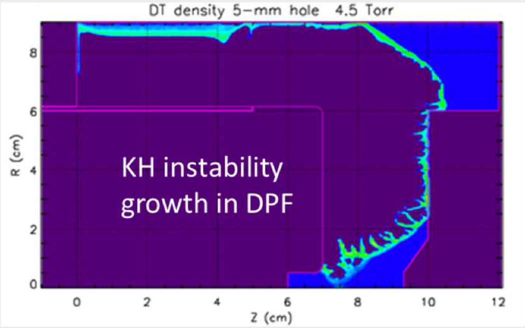


Typical PIC Code:

- Limited to low density, energetic plasmas in order to resolve Debye length.
- Requires many particles per cell.
- Slow to obtain results.

CHICAGO developed to bridge gap between PIC and MHD for high power fusion, Z power flow, and diode plasmas.

- PIC methods are applied to particles using several different descriptions or equations of motion.
  - Kinetic, multi inertial fluids, quasi-neutral MHD-like fluid with increasing level of approximation.
  - Because all species are particles, migration from one EOM to another is seamless.
  - Interactions between all particle descriptions can be treated with fluid-like or binary methods.
  - Charge-conserving EOS/radiation physics.
  - The particle number per cell of all descriptions is controlled with Adaptive Particle Management technique.



- Advanced Monte Carlo treatments for gas breakdown, ionization.
  - PICMC including excitation, ionization, attachment, recombination
  - Energetic electron interactions in gas/solids (ITS).
  - Photon transport including molecular photo ionization and emission.

- Advanced partial-cell method yields second-order accuracy for curved conducting boundaries including charged particles.

- Combines both MHD and PIC codes and adds advanced physics, state-of- the-art hardware, accelerators (such as GPUs and Intel Xeon Phi), and algorithms;

Novel hybrid/implicit algorithms developed to reduce computational time when physics valid

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

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

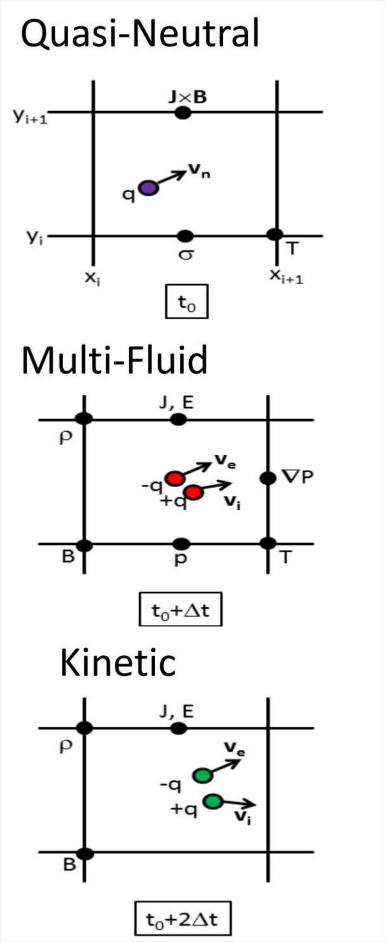
$$\nabla \cdot (1+\langle S \rangle) \cdot \nabla \psi_{err} = \rho^0_{n+1} - \nabla \cdot (1+\langle S \rangle) \cdot E'_{n+1} = \rho_{err}, \qquad \text{Poisson Correction}$$

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

- PIC fluids have equations of motion and energy. Macroparticles carry internal energy, EOS, radiation..
- Advanced *Multi-Ion* Quasi-Neutral PIC algorithm includes effects from kinetic and multi-fluid particles.

$$n_K m_K \frac{Dv_K}{Dt} = \left(\frac{\bar{Z}_K n_K}{n_e}\right) J_{MHD} \times B + e\bar{Z}_K n_K (\bar{v}_K - v_+) \times B$$
$$-\left[\nabla P_K + \left(\frac{\bar{Z}_K n_K}{n_e}\right)\left(\nabla P_e - \sum_K \bar{Z}_K \frac{m_e}{m_K} \nabla P_K\right)\right] + \beta_o \bar{Z}_K n_K \nabla T_e \left(1 - \frac{(n_e)_L}{n_e} F_\beta\right)$$
$$-n_K m_K \sum_{M'} \nu_{KM'} (v_K - v_{M'}) - n_K m_K \nu_{Ke} (v_K - v_+) + \bar{Z}_K n_K m_e \sum_{M'} \nu_{eM'} (v_{M'} - v_+)$$
$$-n_e m_e \left[\left(\frac{\bar{Z}_K n_K}{n_e}\right) \sum_{M'} \nu_{eM'} - \nu_{eK}\right] (v_e - v_+)$$

- Seamless *migration* between particles of one EOM to another



Particle Migration

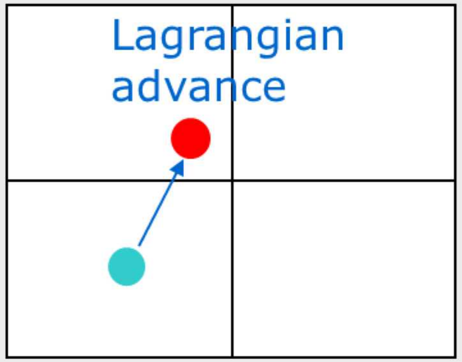
PIC Multi-Fluids are treated similarly to kinetic with the exception of additional EOM and energy equation terms*

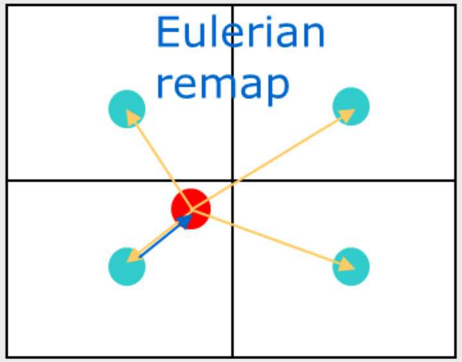
The momenta of electron and ion macroparticles are advanced by the Lagrangian force equations

$$\frac{d\vec{v}_e}{dt} = Q_e \frac{e}{m_e}\left(\vec{E} + \frac{\vec{v}_e}{c}\times\vec{B}\right) - \frac{\nabla P_e}{n_e m_e} - \nu_{ei}\left(\vec{v}_e - \vec{V}_i\right),$$
$$\frac{d\vec{v}_i}{dt} = Q_i \bar{z}_i \frac{e}{m_i}\left(\vec{E} + \frac{\vec{v}_i}{c}\times\vec{B}\right) - \frac{\nabla P_i}{n_i m_i} - \nu_{ie}\left(\vec{v}_i - \vec{V}_e\right), \quad (1)$$

$$\frac{dT_e}{dt} = \left(\frac{3\bar{Z}_i}{2m_i C_v}\right)\frac{2}{3}\left[-\frac{P_e \nabla\cdot\vec{V}_e}{n_e} + \frac{\nabla\cdot(\kappa_e \nabla T_e)}{n_e} + m_{ei}\nu_{ei}\left(\vec{V}_i - \vec{V}_e\right)^2 + \mu_{ei}(T_i - T_e) + \frac{m_i}{\bar{Z}_i}\left(\dot{E}_e\right)_{\mathrm{rad}}\right],$$
$$\frac{dT_i}{dt} = \frac{2}{3}\left[-\frac{P_i \nabla\cdot\vec{V}_i}{n_i} + \frac{\nabla\cdot(\kappa_i \nabla T_i)}{n_i} + m_{ie}\nu_{ie}\left(\vec{V}_i - \vec{V}_e\right)^2 + \mu_{ie}(T_i - T_e)\right]. \quad (4)$$

1. PIC fluid position and velocities are advanced on the grid.
2. Currents, charges, susceptibilities, densities, energies, pressures, etc. are scattering to the grid where temperatures, pressure gradients, and momentum exchange between species are calculated and fields advanced.
3. Change in temperatures, internal energies, momentum, as well as Lorentz force, are gathered back to particles.





*D. R. Welch, et al., Phys. Plasmas **16**, 123102 (2009); C. Thoma, et al., Phys. Plasmas **18**, 103507 (2011).

Adding 2nd order Cloud-in-Cell shape* to existing trapezoidal shaped particle

New 1D density form factor

$$W_{i-1} = \frac{1}{2}(1+\Delta x^2) - \Delta x,$$

$$W_i = \frac{1}{2} - \Delta x^2 + \Delta x,$$

$$W_{i+1} = \frac{1}{2}\Delta x^2.$$

Original 1D density form factor

$$Wep_{i-1} = \frac{1}{2}(1-\Delta x),$$

$$Wep_i = \frac{1}{2},$$

$$Wep_{i+1} = \frac{1}{2}\Delta x.$$

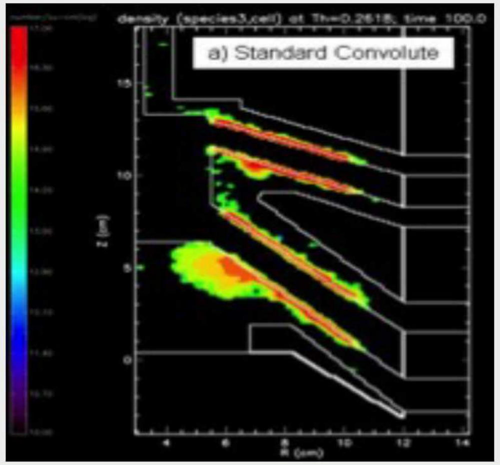
- In both shapes, the charge conservation is obtained by integrating the continuity equation.
- E field forces from the natural cell positions with linear weighting in the E direction and using form factors in the other two directions.
- The 2nd order shape can have a 1 to 2 orders of magnitude smaller energy error than the *Wep* shape.
- Rewrote all current, charge, susceptibility and collapse algorithms to accommodate new shape.

- *With significant scattering, numerical cooling can only be controlled by more particles.*

*T. Zh. Esirkepov, Comp. Phys. Comm. **135**, 133 (2001); T. D. Pointon, Comp. Phys. Comm. 179, 535 (2008).

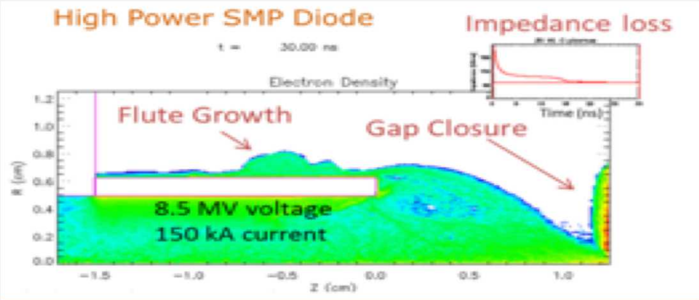
CHICAGO algorithms are being benchmarked on relevant plasma problems:

Z Convolute



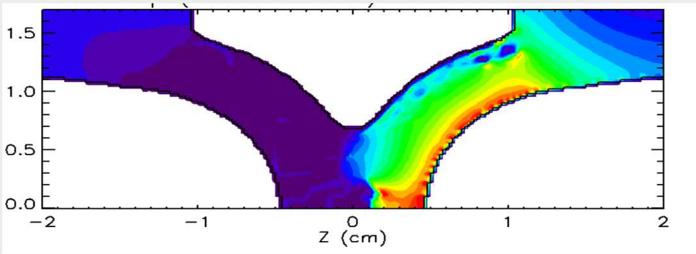
Electrode plasma simulations showing enhance current loss measured on Z.

Electron Beam Radiography



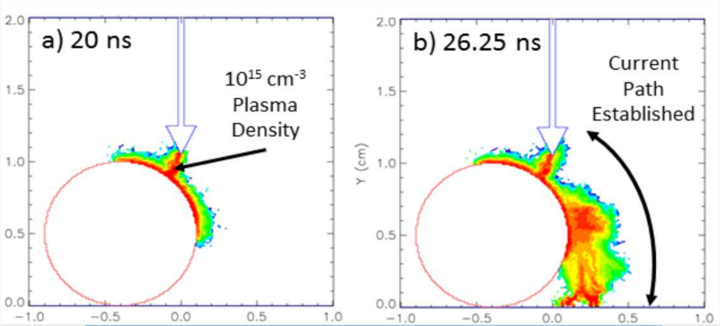
Electrode plasma evolution in extreme diode conditions reproduce dose measurements.

Gas-Filled Switches



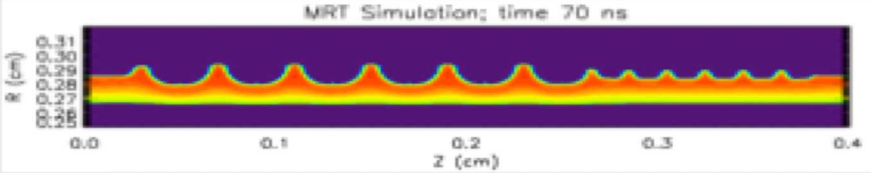
Realistic gas breakdown calculations for pulsed power give insight into switch inductance.

Lightning Arrestor Connectors



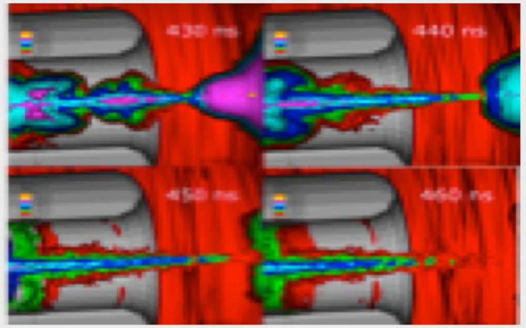
3D Streamer evolution along a dielectric in air.

Z Liner Implosions



Validated Magnetic Rayleigh-Tayler Group simulation.

Dense Plasma Focus



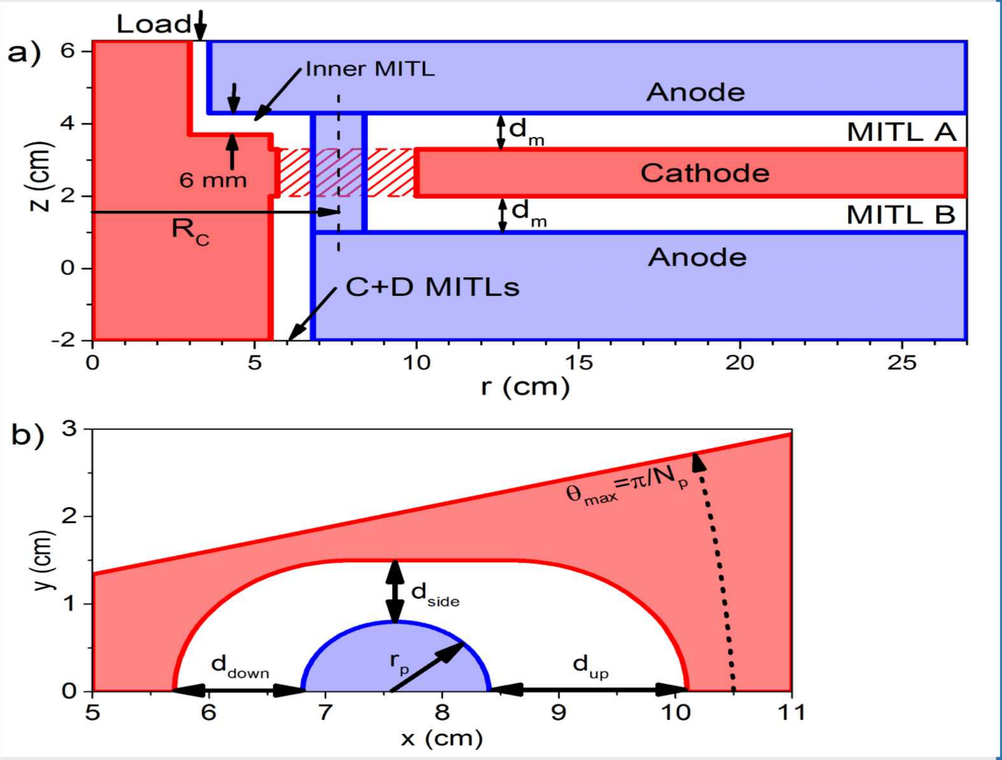
Hybrid simulation with validated neutron yield .

High Power Z Convolute Modeling:

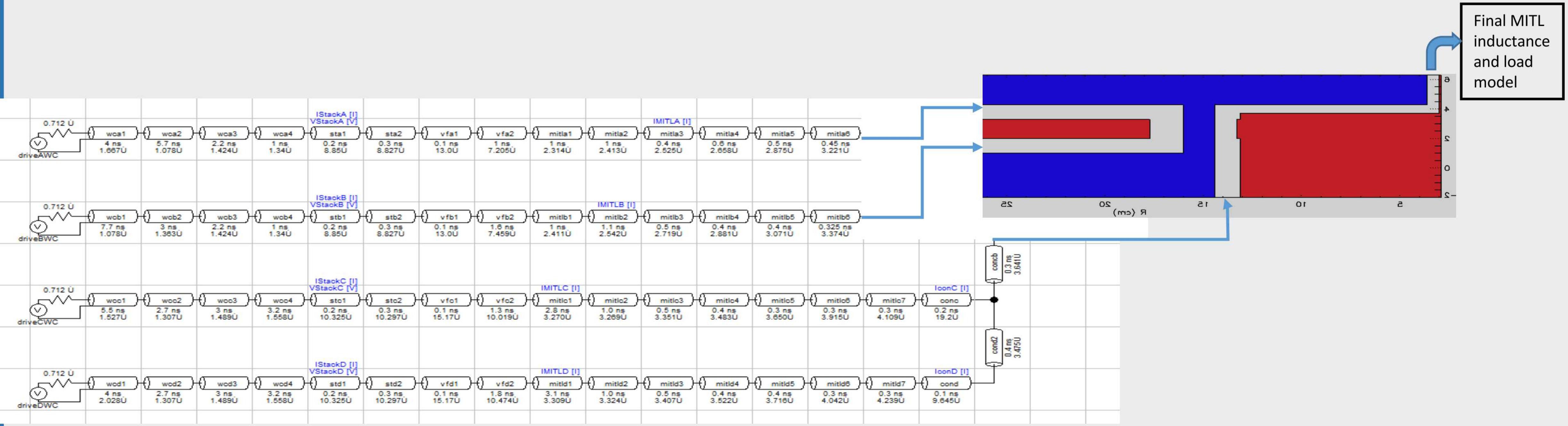
- The coupled Magnetically Insulated Transmission Line and Post-Hole Convolute on Z is a complex 3D structure in which charged particle emission and electrode plasmas dynamically evolve, leading to current loss.
- Over the past 20+ years, 3D EM PIC simulations have been used to aid in the design and analysis of this MITL/Convolute system.
- The time-dependent evolution of dense electrode plasmas is currently believed to be a significant component of the overall current losses on Z.
- New computational modeling developments in Chicago are already leading to new understanding of the various current loss mechanisms.

Require ~ 0.002 cm resolution in > 10000 cm^3 volume.
Must resolve $\omega_{ce}\,\Delta t < 10$ in 10-100 MA current device.

"Halfolute" model



The Reduced Bertha Circuit Model is in Excellent Agreement With the Chicago EM Cold Test Simulation

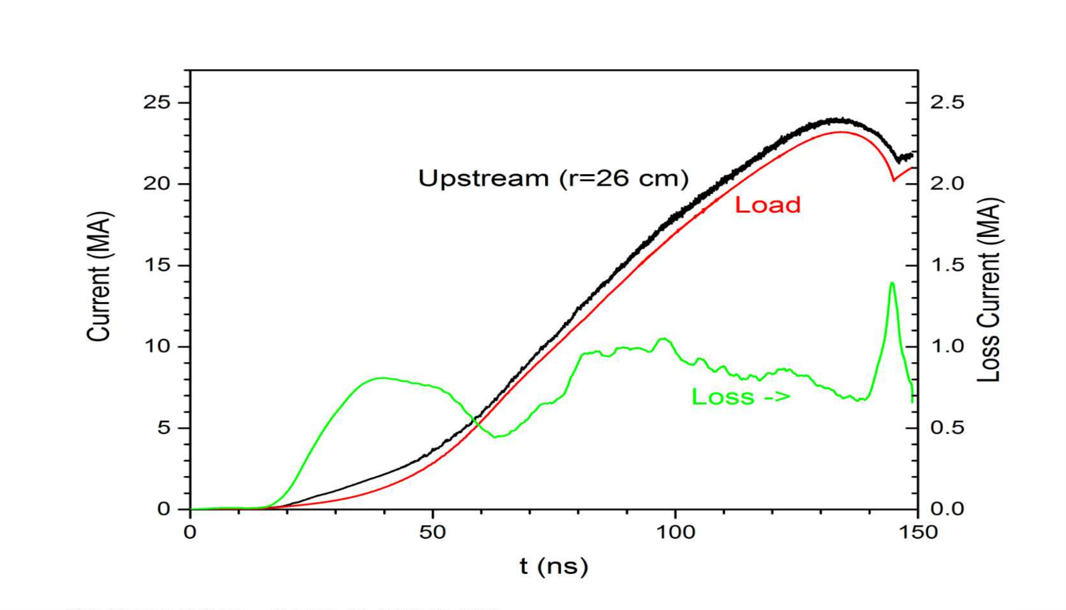


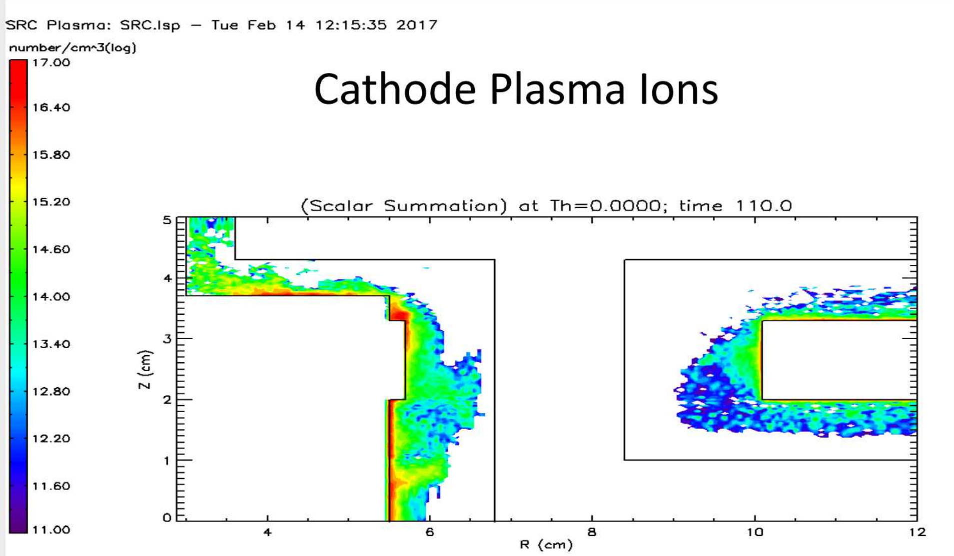
The final transmission line of the EM simulation is terminated by an equivalent transmission line model to give an accurate representation of the final MITL driving the MAGLIF load.

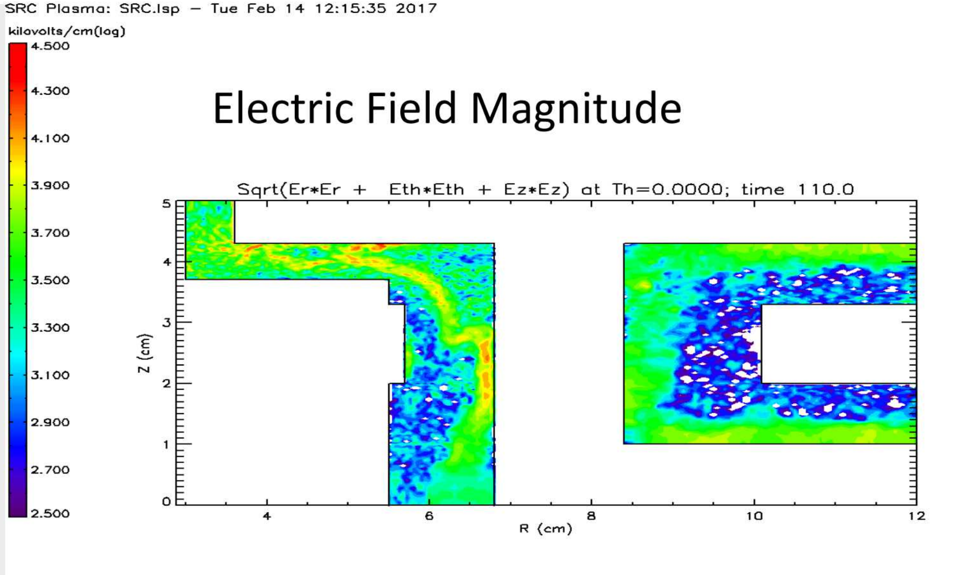
The circuit model uses 4 input voltage waveforms as inputs and these are provided by the **full** Bertha Z model.

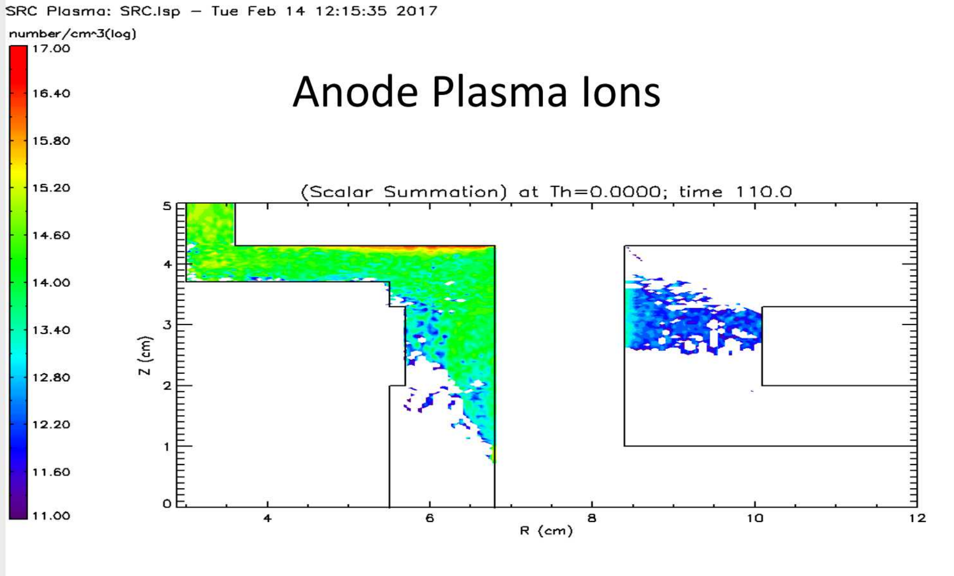
In the reduced Bertha model (Hutsel), the EM simulation volume is replaced by an equivalent circuit description with (optional) loss model functions.

The 3D EM CHICAGO simulations indicate the evolution of dense plasma that fills the AK gap on the downstream side of the post:



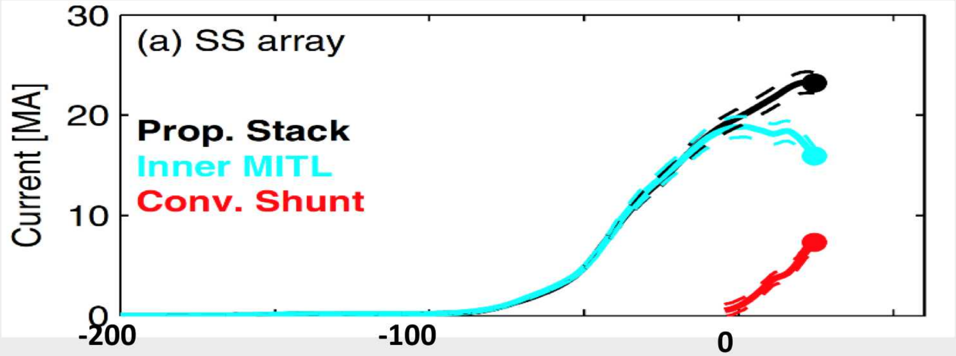


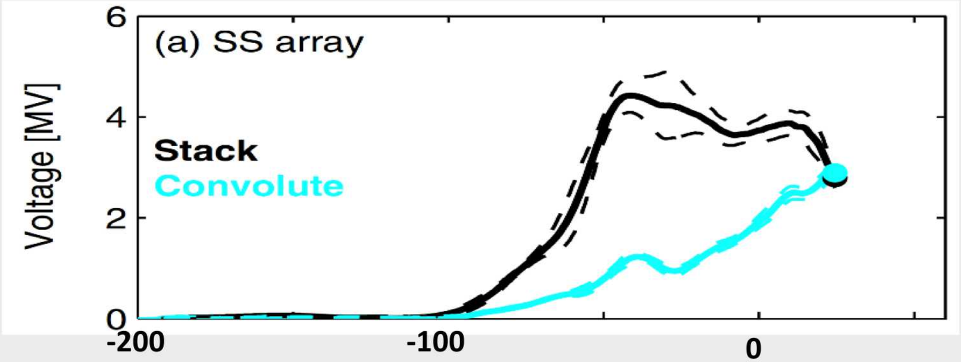




being used to model individual Z shots (validation): 70-mm SS wire array load.

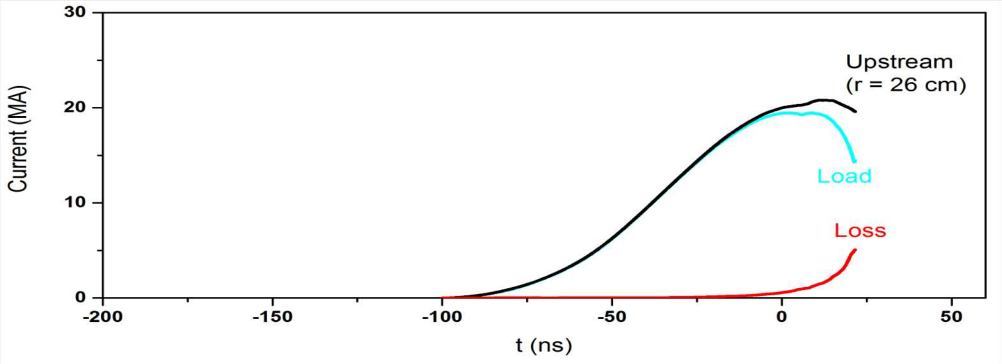
Shot 2082

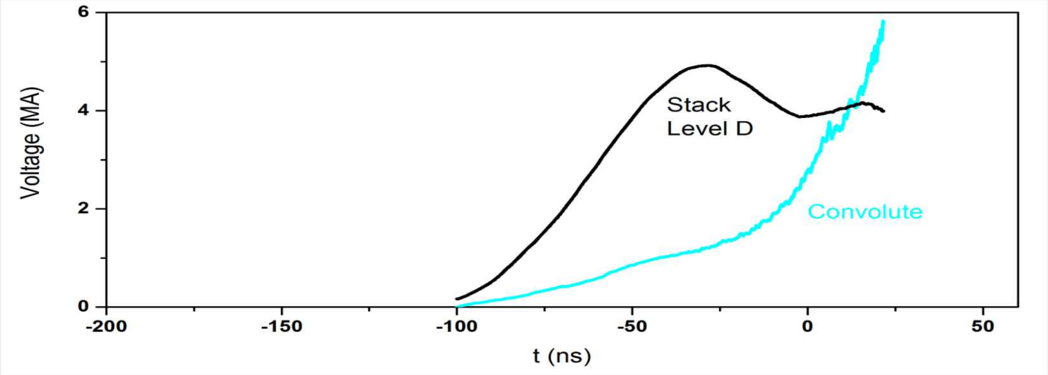




From Gomez *et. al* (2017).

Shot 2500



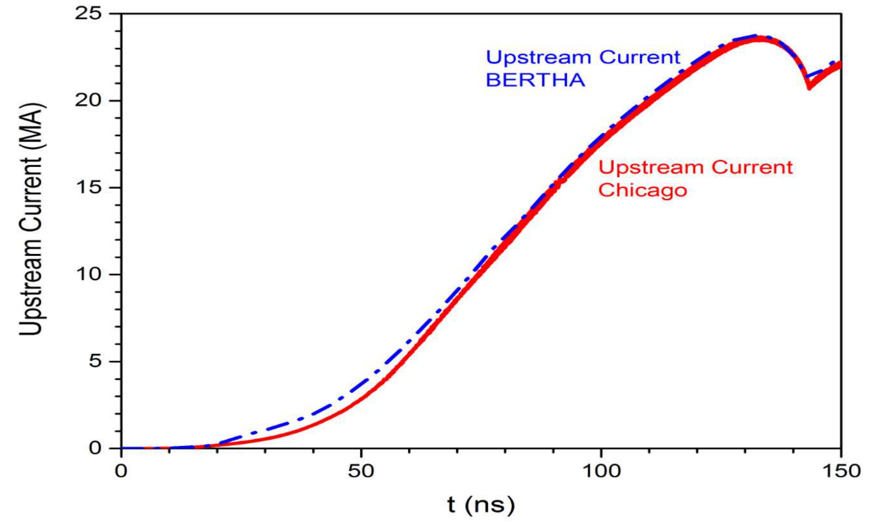


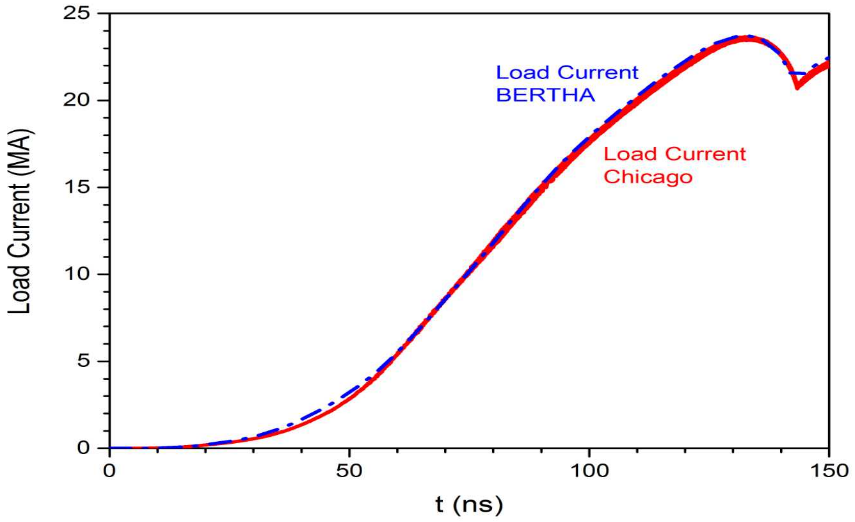
Chicago simulation with half-a-lute model.

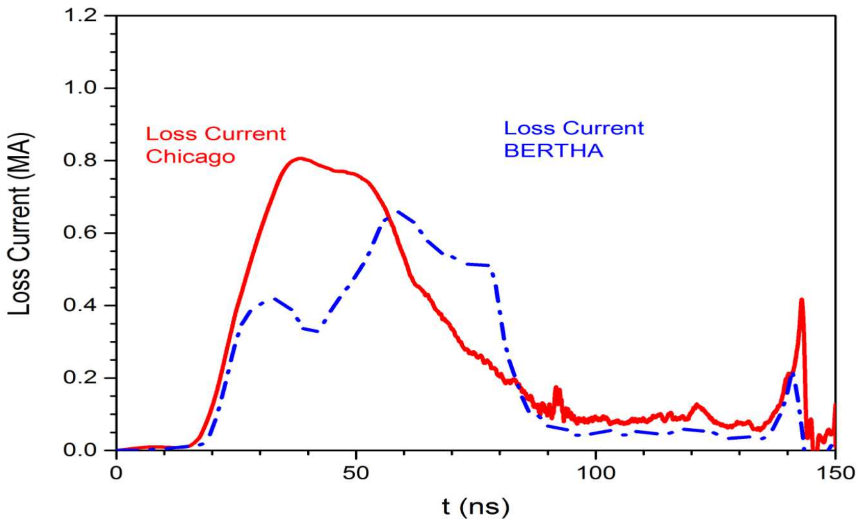
The simulation was run at 7×10^{-5} Torr, shot 2500 had a vacuum pressure of 2.6×10^{-5} Torr.

Direct comparisons between a physics-based circuit model of Z (Hutsel) and the Chicago simulations are being used to tune the circuit model loss mechanisms (Electron-ion simulation, dynamic load)

The load current peak and stagnation values from Chicago and Bertha agree to within 2%.







I_L (peak): Chicago 23.6 MA
Bertha 23.7 MA

I_L (stagnation): Chicago 21.0 MA
Bertha 20.9 MA

The loss current is < 0.8 MA.

The losses dominates early in time; i.e., when the load current is < 11 MA.

The losses are in reasonable agreement after 60 ns; i.e., after insulation is established in the outer MITLs.

Initial conditions were approximately that of a typical DPF plasma sheath

Simulations were initialized with a preformed plasma sheath.

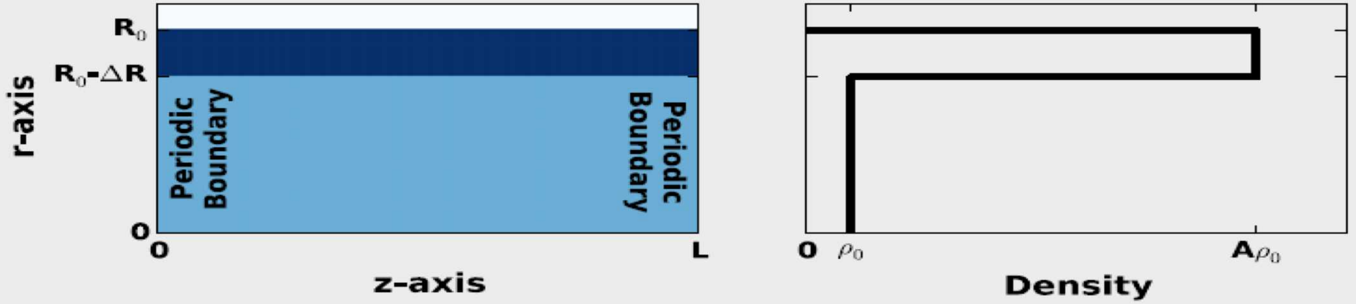
The drive current rose fast to a constant value.

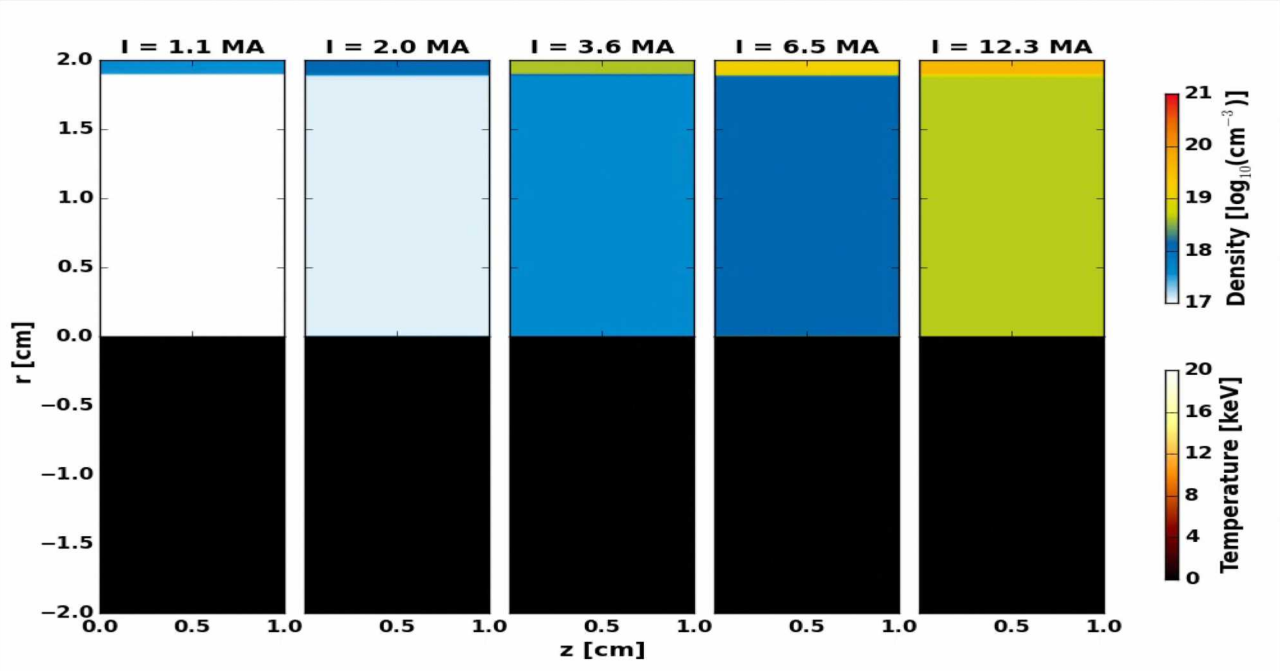
Current was scaled keeping the initial radius and drive parameter constant ($\frac{n_0 R^4}{I^2} = 5.25\times10^5 \, \frac{\mathrm{cm}}{\mathrm{A}}$).

MRT seed was applied by adding a random speckle to the density in the sheath region (±6%)

Simulations largely explain turnover in I^4 neutron yields in DPFs, Gas Pinches

D.T. Offermann, *et al.*, PRL, **116**, 195001 (2016).

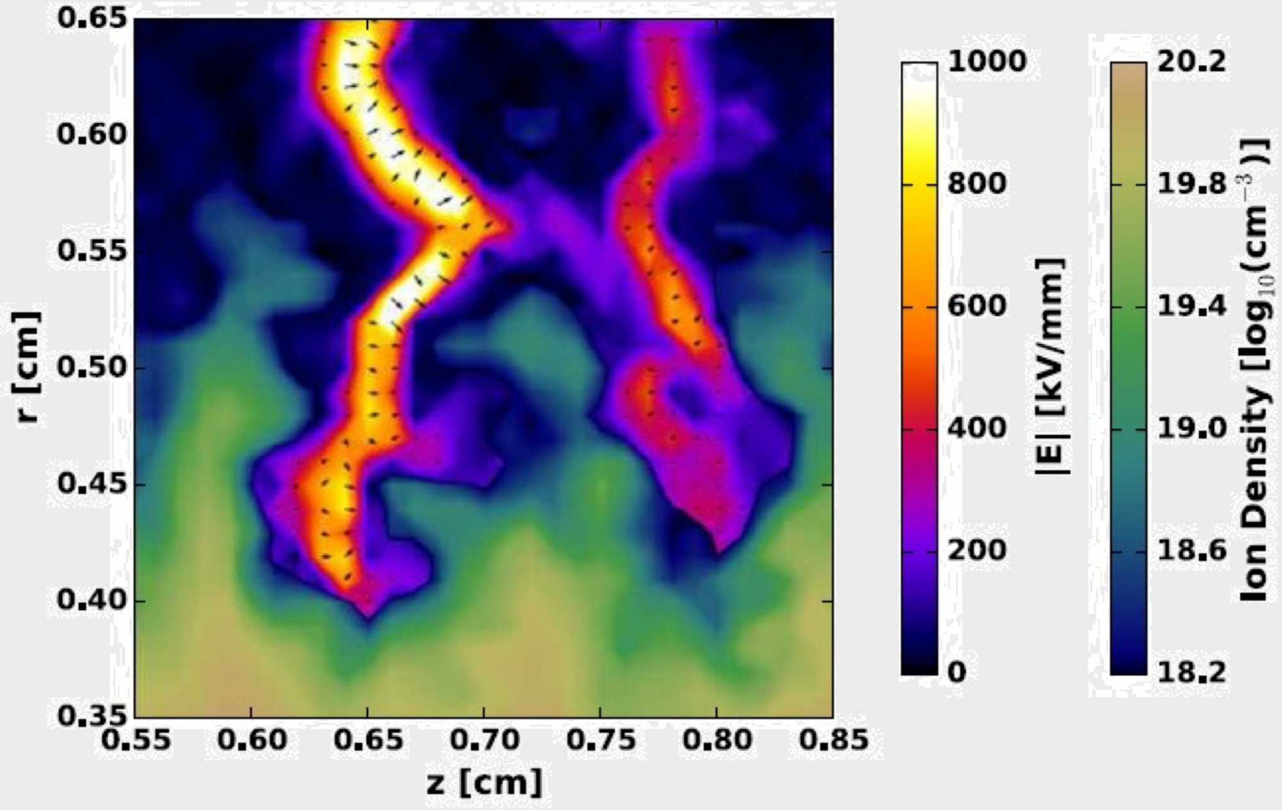


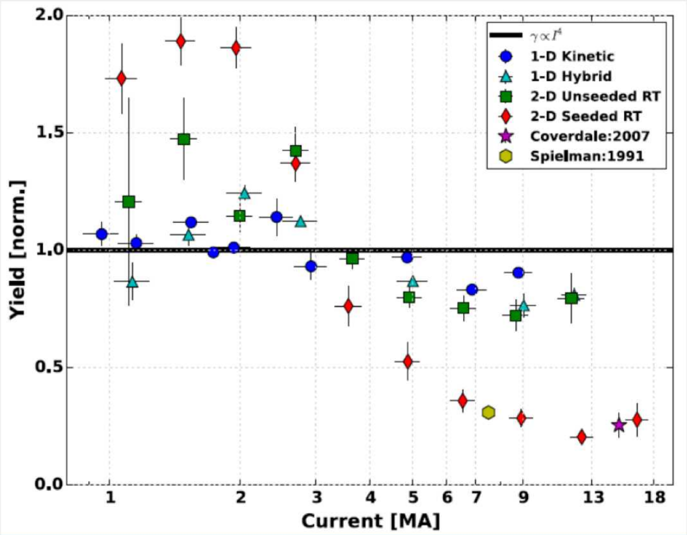


Advances Model Intense Electric Fields that drive ion beams in DPF and Zpinches → realistic neutron yield

Voss Scientific

- CHICAGO captures the induced electromagnetic fields which have the effect of producing high-energy ion beams;
- The ion beams contribute to as much as half of the total nuclear fusion in such plasma pinches;

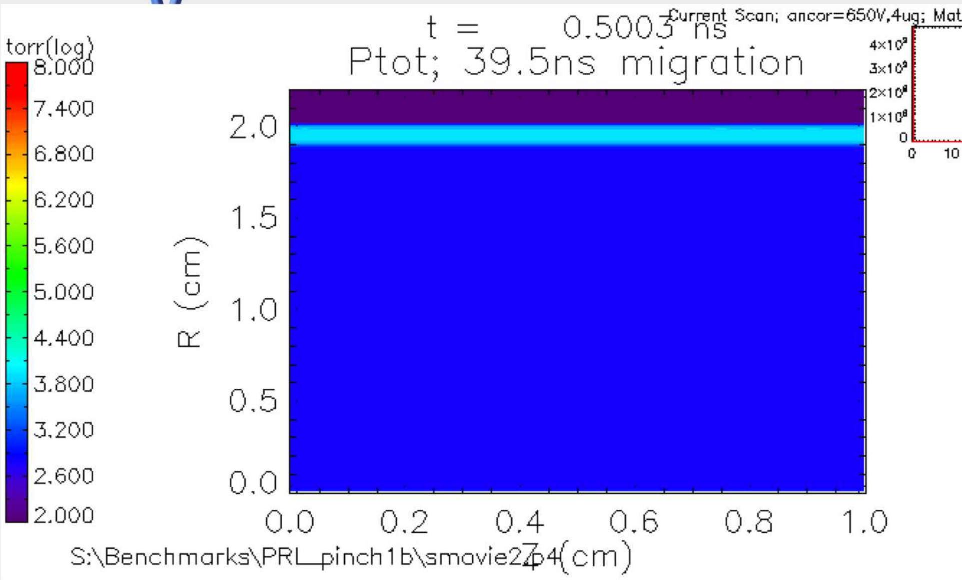




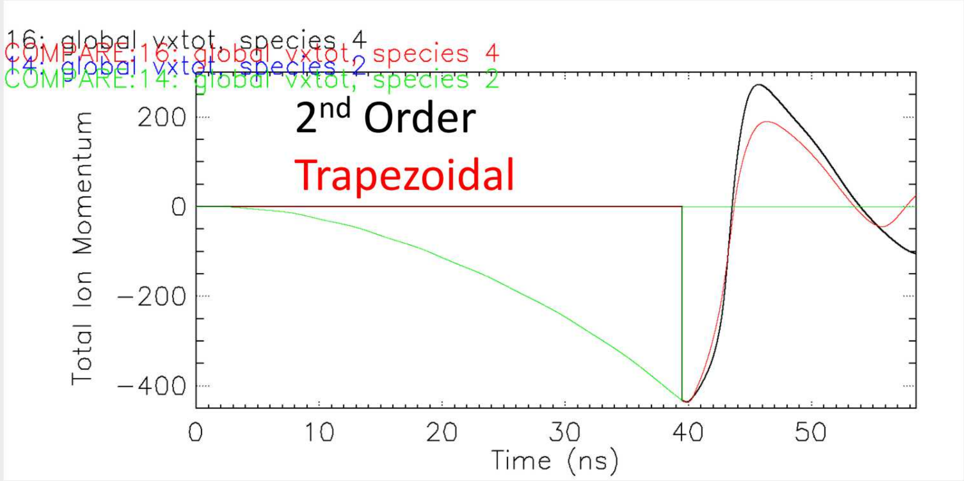
The intense electric fields seen in this simulation are responsible for a substantial contribution to fusion in plasma pinches. The ability of CHICAGO to capture this physics and the high speed with which it solves them made it possible to settle a nearly 50 year old debate explaining why some pinches perform better than others. The results have been published in: D.T. Offermann et al, Phys. Rev. Lett. 116, 195001, (2016).

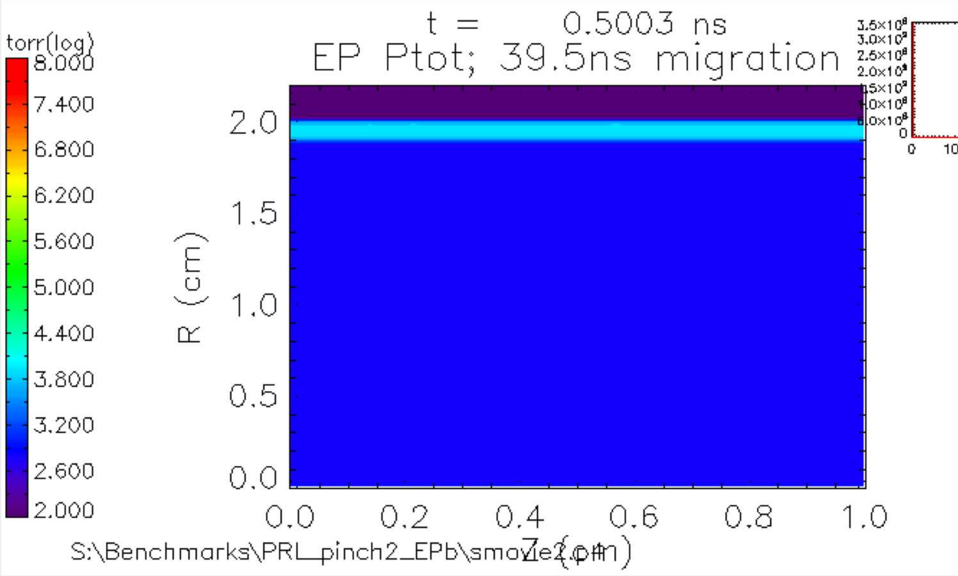
Voss Scientific

New Particle Form-Factor improves conservation by factor of 2 (< 10% of 13 kJ)

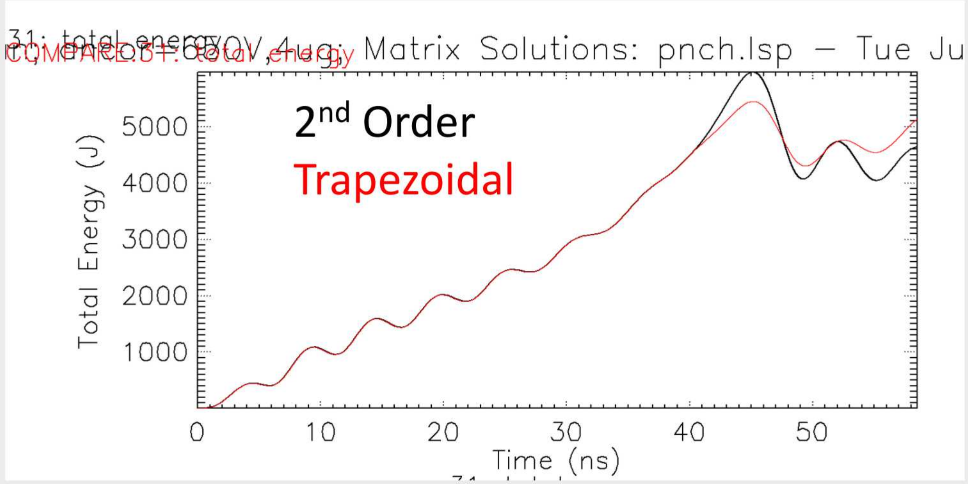


2nd order



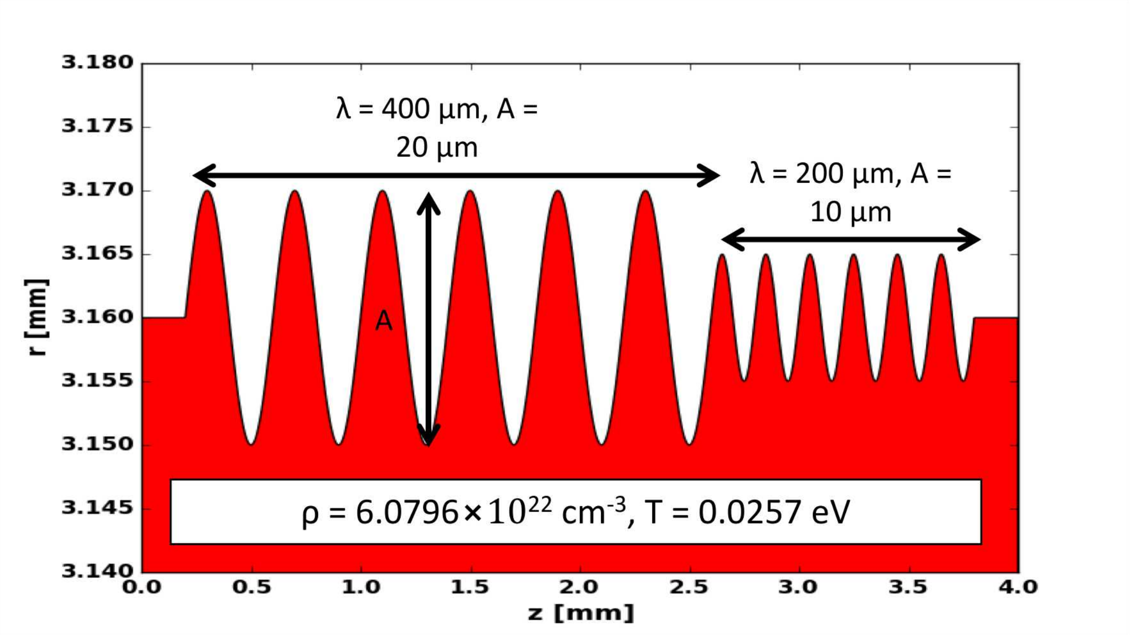


Trapezoidal



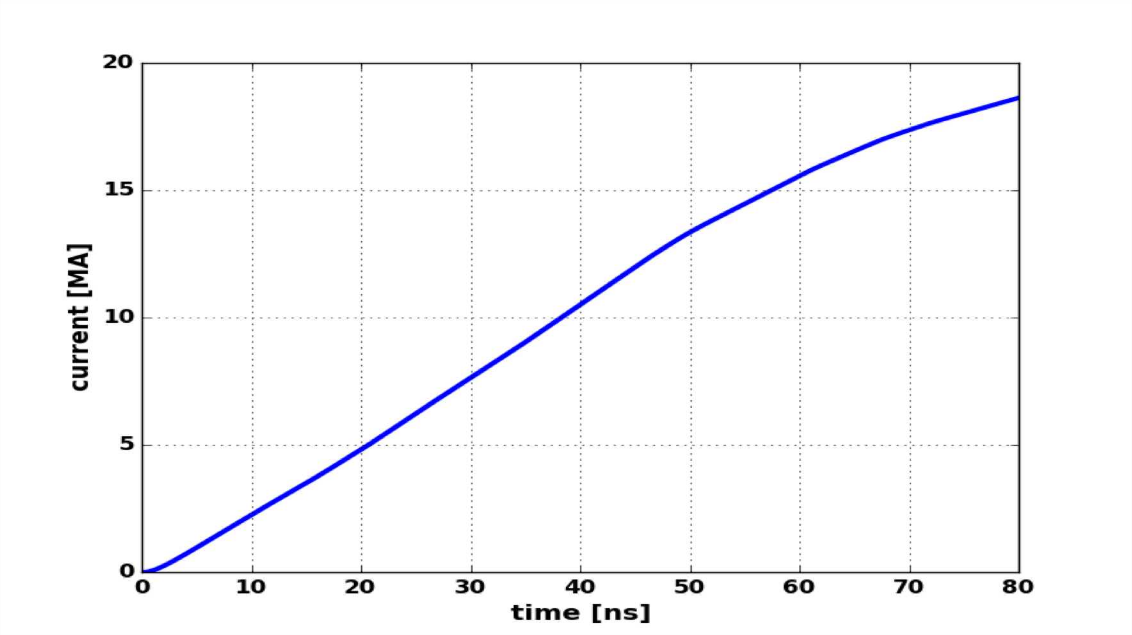
Perturbed Al liner was imploded by a 20 MA current drive for MRT study.*

An Al can with a wall thickness of 2.92 mm and OD of 6.32 mm



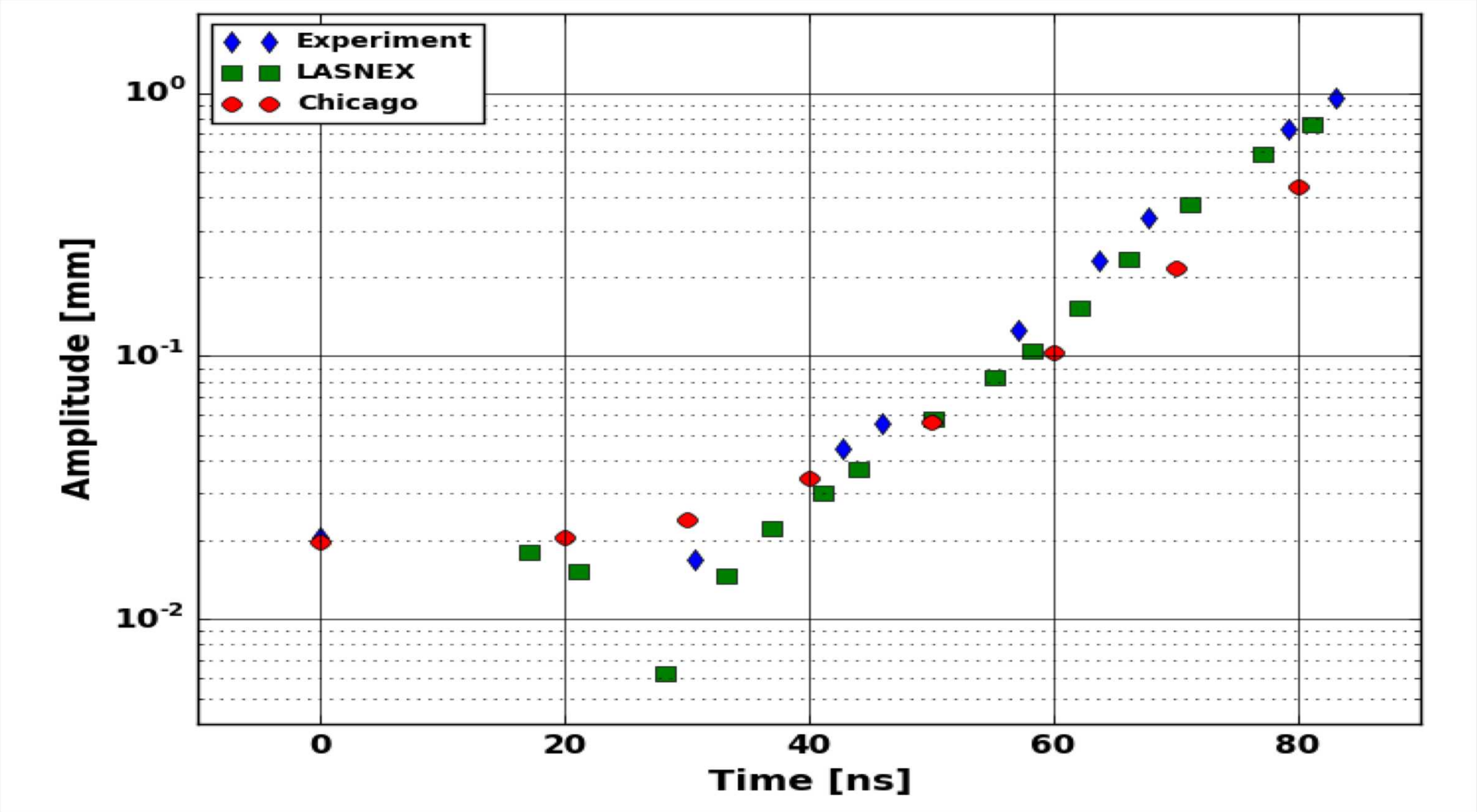
$$\Delta r = \frac{A}{2}\sin\left(\frac{2\pi z}{\lambda}\right)$$

Circuit was applied to provide a linear ramp to 20 MA in 80 ns



*D.B. Sinars, et al., Phys. Plasmas, **18**, 056301 (2011)

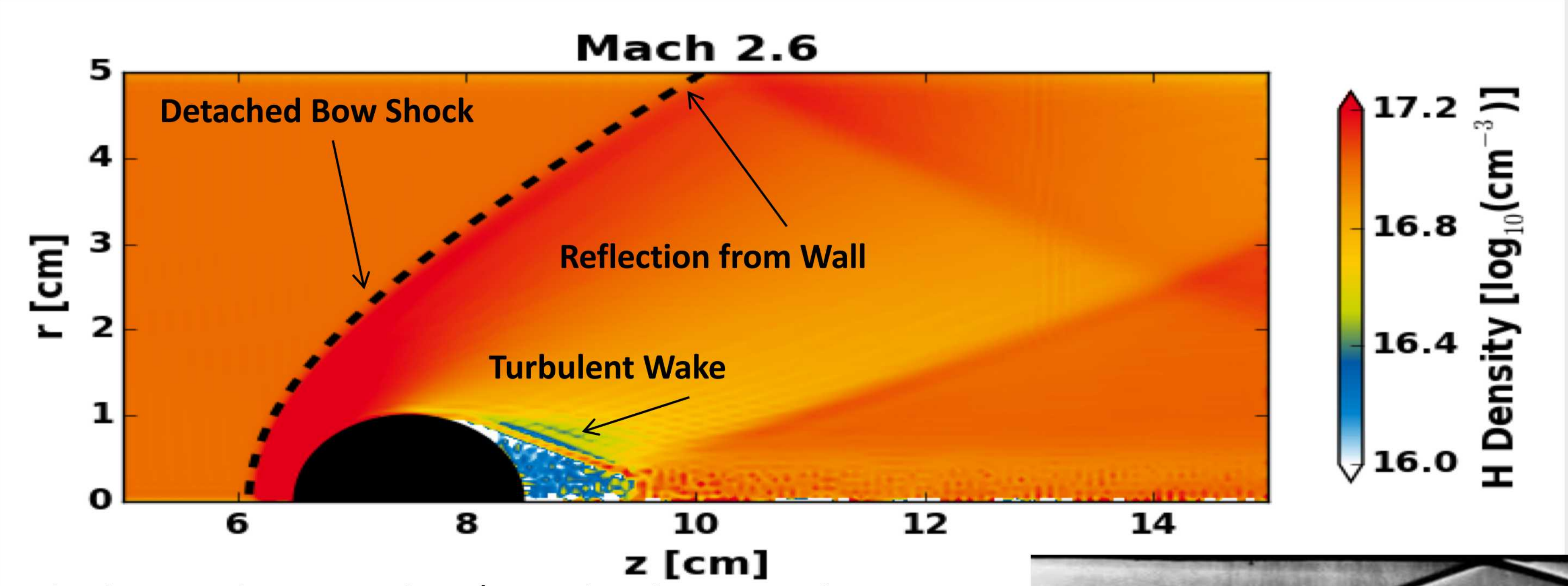
Quasi-Neutral Simulations exhibit agreement with experiments and other code results*

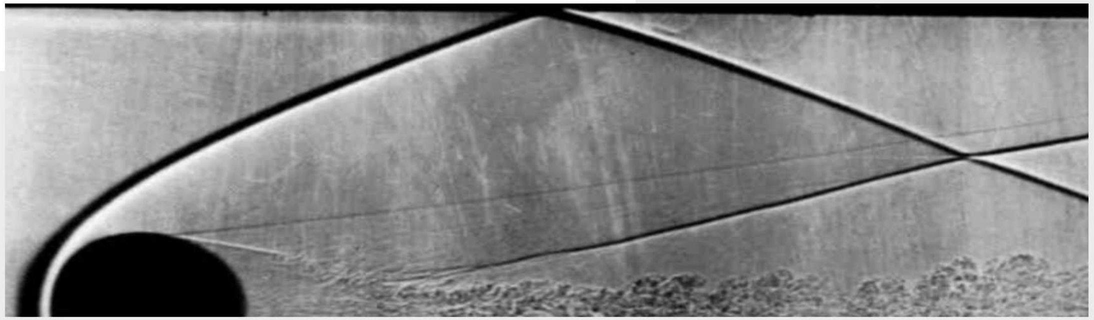


The amplitude of the MRT spikes vs time from the Chicago simulations are compared with experimental data and LASNEX simulations published in Sinars et al.

*D.B. Sinars, et al., Phys. Plasmas, **18**, 056301 (2011)

Simulations of a supersonic sphere in a hydrogen plasma were performed



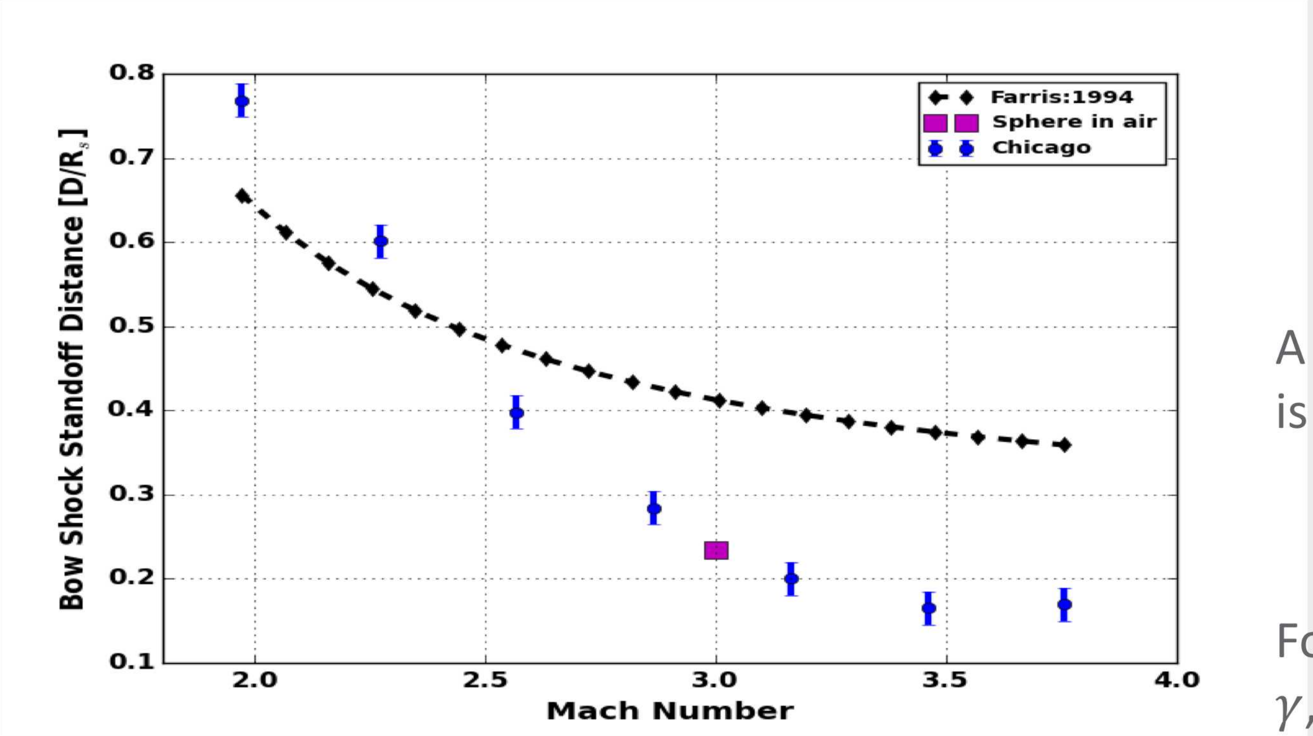


Shadowgraph image of a 9/16 inch sphere traveling in air at Mach 3.

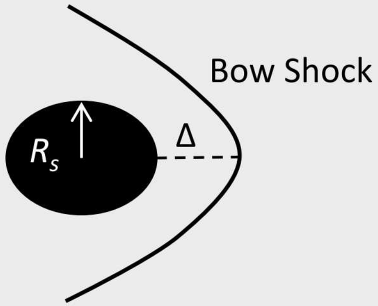
Photograph from U.S. Army Ballistic Research Laboratory, reprinted in M. Van Dyke, *An Album of Fluid Motion.*

M. Van Dyke, *An Album of Fluid Motion*, The Parabolic Press, Stanford, California(1982)

The standoff distance of the bow shock vs Mach number is compared



M.H. Farris and C.T. Russell, J. Geophys. Res., **99**, 17689 (1994)



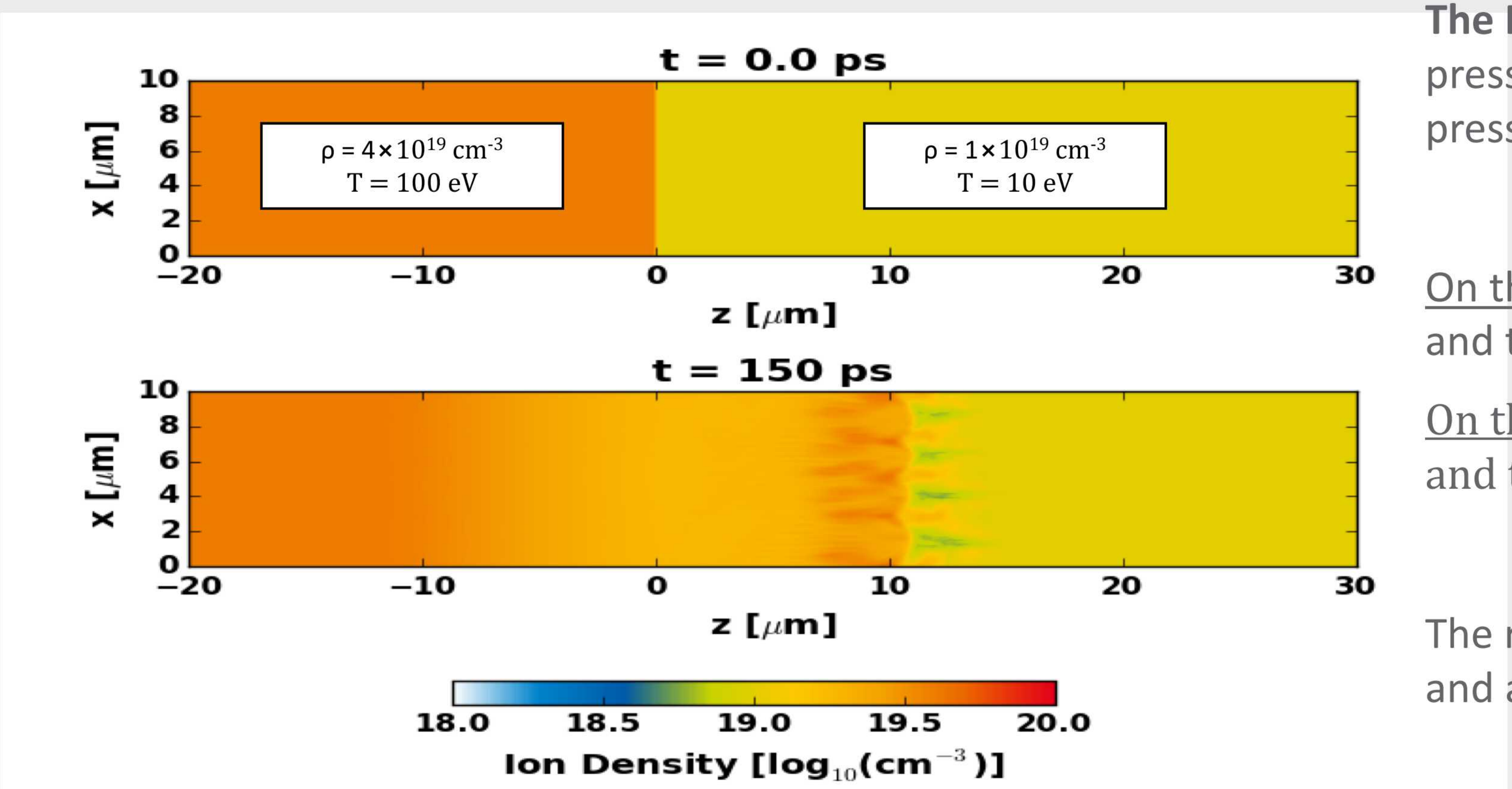
A semi-empirical model for the standoff distance is given in Farris *et al*.

$$\Delta = 1.1\, R_s \frac{(\gamma - 1)M^2 + 2}{(\gamma + 1)M^2 - 1}$$

For monatomic ideal gas, the Adiabatic constant, γ, is 5/3.

A data point measurements of a sphere in air at Mach 3 is also shown.

Simulations of the Riemann shock tube were performed



The Riemann shock tube problem: A high pressure fluid is initially in contact with a low pressure fluid and then released.

On the left side, the temperature is 100 eV and the density is 4×10^{19} cm^{-3}.

On the right side, the temperature is 10 eV and the density is 1×10^{19} cm^{-3}.

The result is a shock that travels to the right and a rarefaction of the high density region.

Chicago simulations compared with published LSP and Hydra results

Comparison of LSP and Hydra shock tube simulation

(C. Bellei *et al.*)

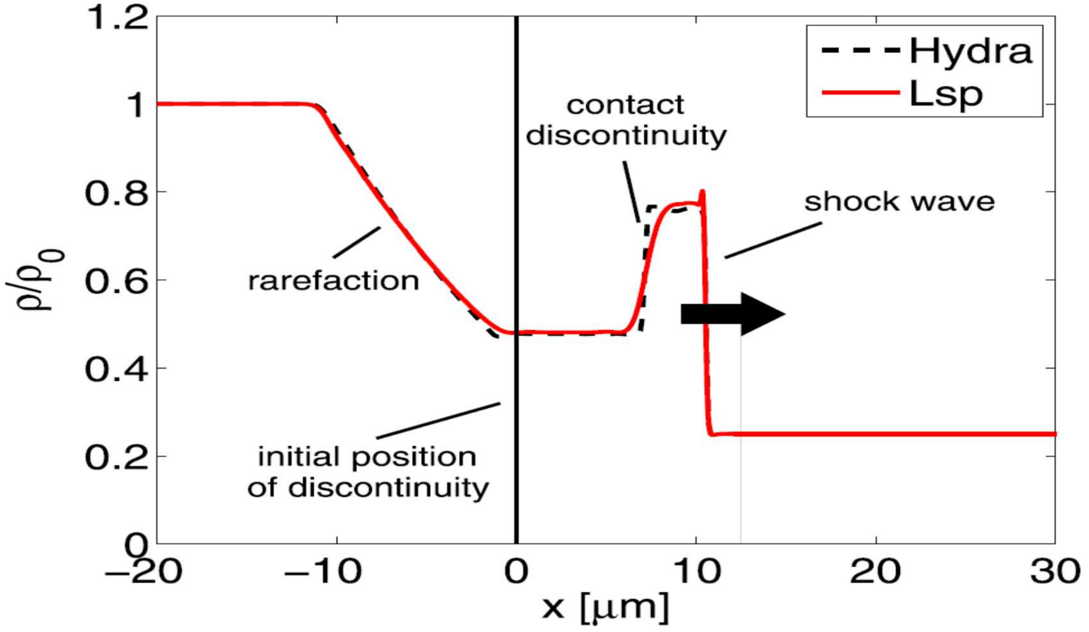
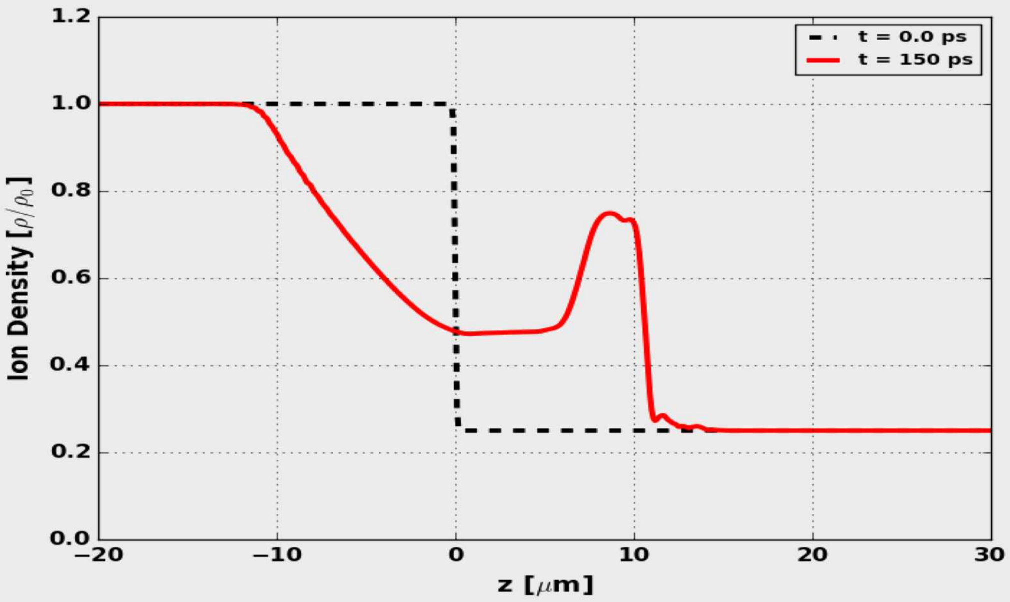


FIG. 3. Comparison of Hydra solution vs. (fluid) Lsp solution of the Riemann problem discussed in the text. When Lsp is run in fluid mode, the solution is close to the expected gas dynamics solution.

Chicago simulation using parameters in C. Bellei et al.



C. Bellei, et al., Phys. Plasmas, **20**, 012701 (2013)

Memory Management is key issue in code performance

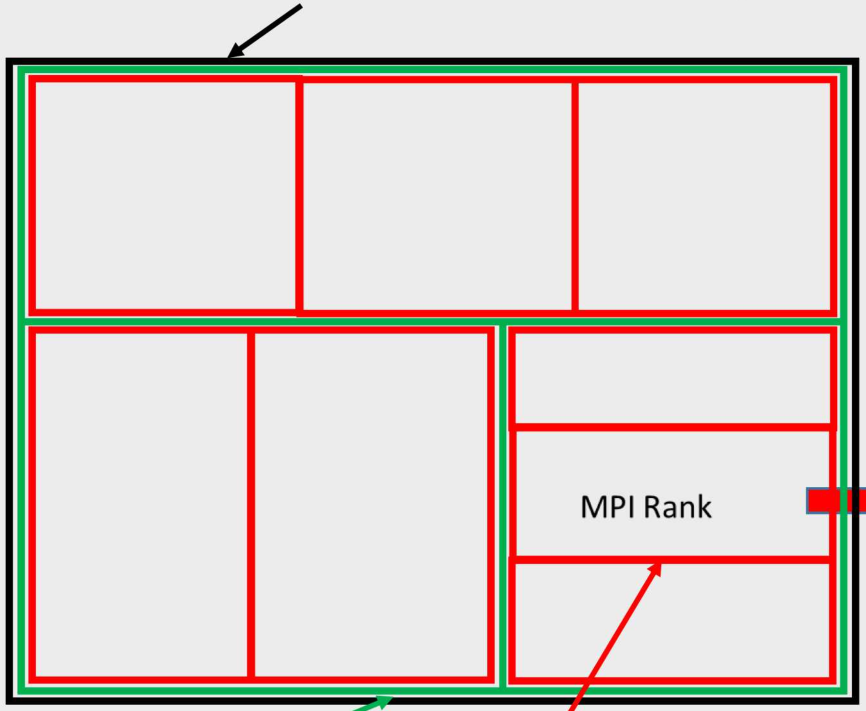
- Particle and grid quantity loads frequently are not uniform within volume. So a strictly volume decomposition can have severe bottle necks.
- Memory conflicts in shared memory with multiple threads can slow down processes.
- GPU threads are even more memory limited.
- Voss is developing an OpenMP library THRIL for agile task and data sharing.

THRIL Library Description

- Tile: A cache-line or GPU-memory sized construct containing all writable data for a subdomain.
  - Each MPI rank is assigned a distributed-memory domain.
  - Each domain is assigned a set of shared-memory tiles.
  - Multiple tiles per OpenMP thread are created to enable task sharing.
  - Data structures within each tile are blocked to include structures and included arrays and substructures in one data block. Each block is cache-aligned to avoid false sharing.
  - Blocking also optimizes data copying for GPU use.
- Tiles and threads are created at initialization, and persist through the entire simulation.
  - Effectively, an MPI-like execution model with agile data sharing.
  - This reduces fork-join overhead.
  - Data is shared by the allocation of data structures before entering the parallel section. All local variables are created within the parallel section.

Decomposition Scheme with Threads/Tiles:

Simulation Volume is broken into Regions/Domains

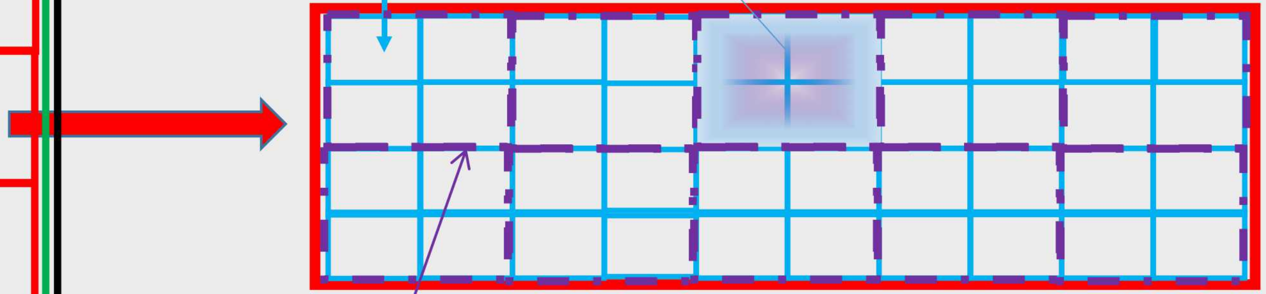


Region Boundary

Domain Boundary
(1 domain = 1 MPI Rank)

OpenMP or GPU threads process
both particle and field calculations within available Tiles.

Grid cells

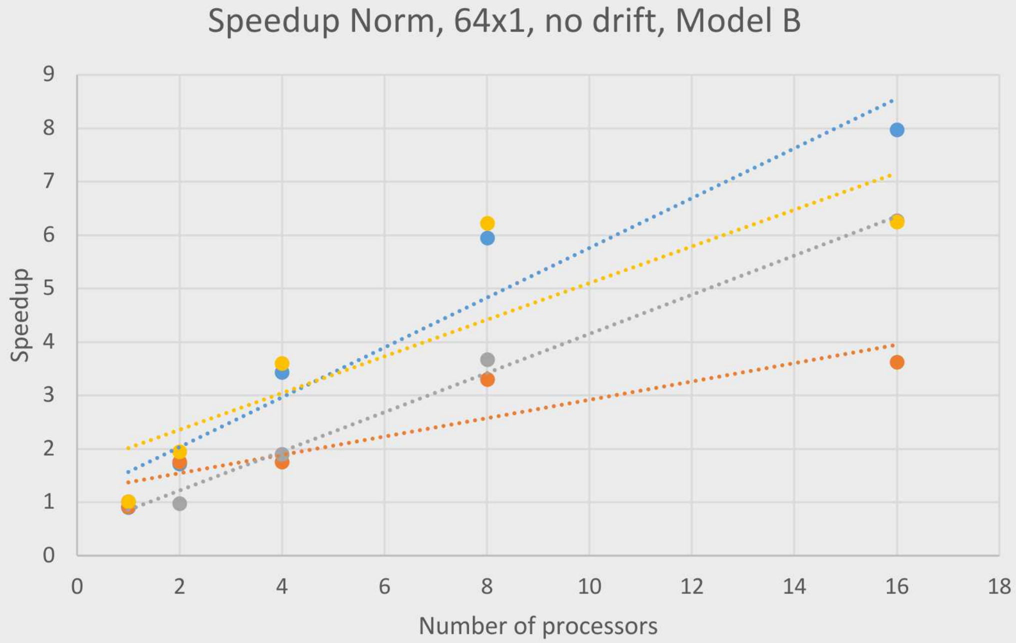


Tiles will have a fixed size determined by size of efficient memory transfer. (likely 2x2x2 or 3x3x3). Threads attached to domain will grab tiles based on their load.

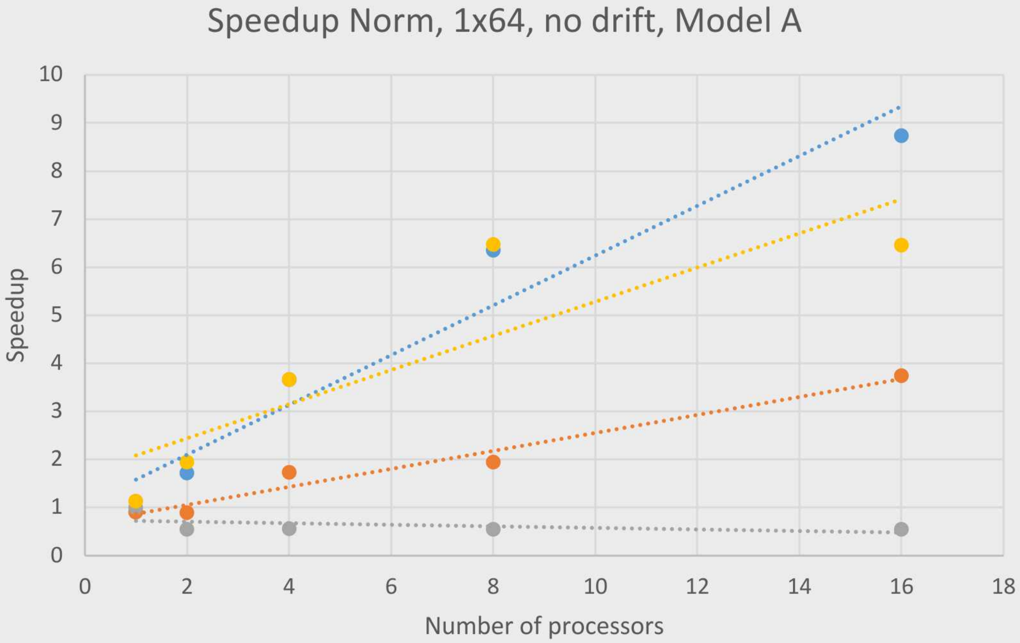
Load Balancing can be accomplished by adjusting domain volumes and number of threads per MPI Rank according to computational load.

THRIL outperforms MPI in CHICAGO

- For the model shown below, the particles were distributed along the entire y axis, but only one cell wide, providing maximal and no parallelism except as the particles move for the fixed MPI decomposition.
- The ability of the shared-memory tiling method to adapt to different particle distributions is its greatest advantage over fixed-rank decompositions.
- Similar results are seen for the models with nonzero drift velocity, i.e., a heavy communication load.



MPI can ideally balance



MPI cannot balance at all.

Many challenges left in Z simulation

- Problem size, duration, resolution requirements are challenging.
- Fast fluid modeling, both quasi-neutral and multi-fluid, is extremely useful when the assumptions are valid.
- Shear number of plasma periods to simulate requires improved accuracy in implicit kinetic mode.
- Efficient and task and memory management critical for speed with PIC.