Introduction to TriForce: A multi-physics code for hybrid fluid-kinetic simulations

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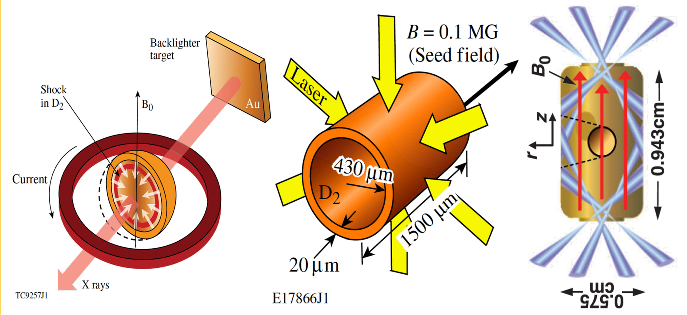
Summary

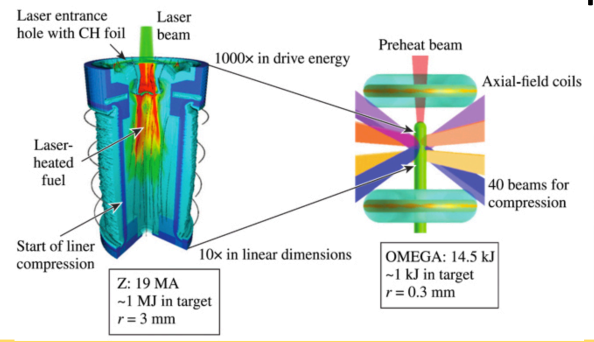
- `TriForce` is a C++ framework for open-source parallel 3D particle-based hybrid fluid-kinetic simulations.
- The code recovers results from both radiation magnetohydrodynamic and fully kinetic codes in those asymptotic limits, and will operate in between where both descriptions may co-exist and interact.
- We are strengthening the science base in support of several communities' efforts by developing and freely distributing our continually-validated code.
- It encourages first-of-a-kind cross-disciplinary collaboration between students and scientists in astrophysics, plasma, geoscience, atmospheric chemistry, computer science, and others.
- The hybrid method enables capabilities beyond either of the individual modeling methods alone, and is being used to investigate a range of topics such as controlled nuclear fusion, astrophysics, high-energy-density physics, and high-intensity lasers.
- The goal is to provide better predictive capability and access to advanced models for the benefit of the whole community.
- *Asterisks (*) denote development work still needed/in-progress*

Scientific motivation

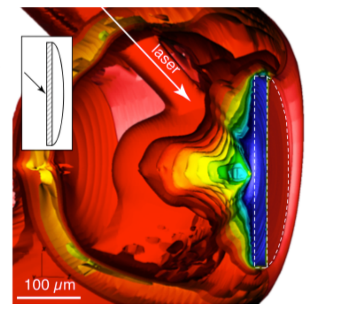
Direct and indirect inertial confinement fusion



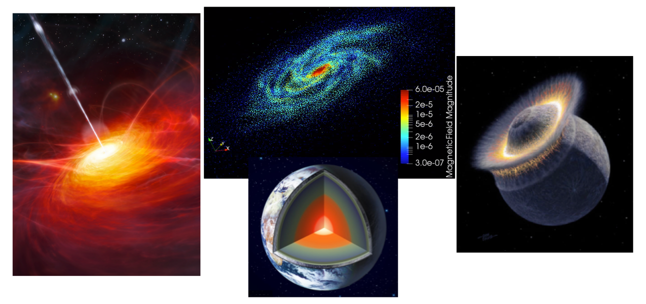
Magneto-inertial fusion



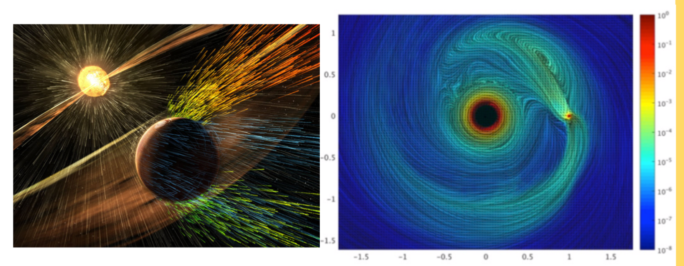
High-intensity lasers



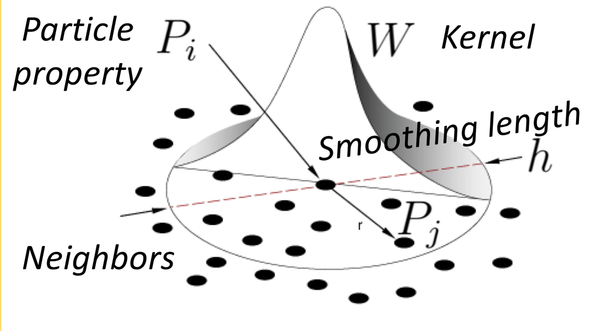
Astrophysics, multi-messenger astronomy, and high-energy-density physics



Planetary atmosphere evolution and exoplanet habitability



Introduction to smoothed particle hydrodynamics (SPH)



$$P_i(\mathbf{r}) = \int P_j(\mathbf{r}')\, W(\mathbf{r}-\mathbf{r}', h)\, d\mathbf{r}' \approx \sum_j \frac{m_j}{\rho_j} P_j(\mathbf{r}_j)\, W(\mathbf{r}-\mathbf{r}_j, h)$$

- Meshless approach to fluid dynamics
- Lagrangian particle-based description
- Well-suited for shear, mixing, and turbulence
- Commonly used outside of plasma physics
- Pros: No meshes to tangle, no rezoning, and *fast*!
- Cons: No logical connection between particles, must find neighbors as efficiently as possible…

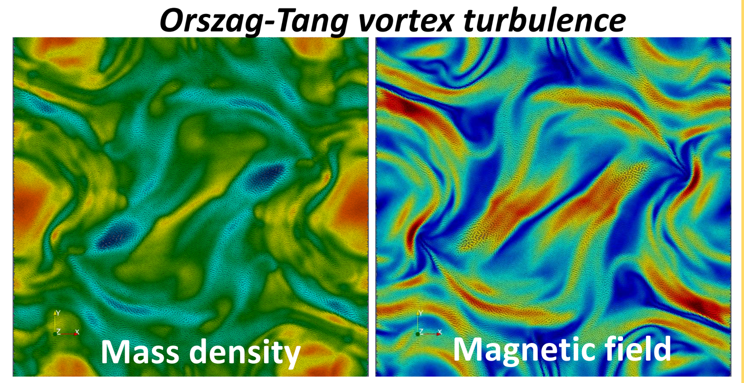
$$P = P_i + P_e + P_r \qquad \rho\frac{d\mathbf{v}}{dt} = -\nabla(P+Q) - \nabla\cdot\mathbf{\Pi} + \mathbf{J}\times\mathbf{B} + \mathbf{R}$$

$$\frac{3}{2}n_i k\frac{dT_i}{dt} + (P_i+Q)\nabla\cdot\mathbf{v} = \tau_{eq}^{-1}(T_e-T_i) - \nabla\cdot\mathbf{q}_i^T - \mathbf{\Pi_i}:\nabla\mathbf{v}$$

$$\rho\frac{\partial\epsilon_e}{\partial T_e}\frac{dT_e}{dt} + (P_e - \rho^2\frac{\partial\epsilon_e}{\partial\rho})\nabla\cdot\mathbf{v} = \tau_{eq}^{-1}(T_i-T_e) + \tau_{eq,r}^{-1}(T_r-T_e) - \nabla\cdot(\mathbf{q}_e^T+\mathbf{q}_e^F) - \mathbf{R}\cdot\mathbf{v}$$

$$4a_rT_r^3\frac{dT_r}{dt} + (P_r + a_rT_r^4)\nabla\cdot\mathbf{v} = \tau_{eq,r}^{-1}(T_e-T_r) - \nabla\cdot\mathbf{q}_r$$

Orszag-Tang vortex turbulence

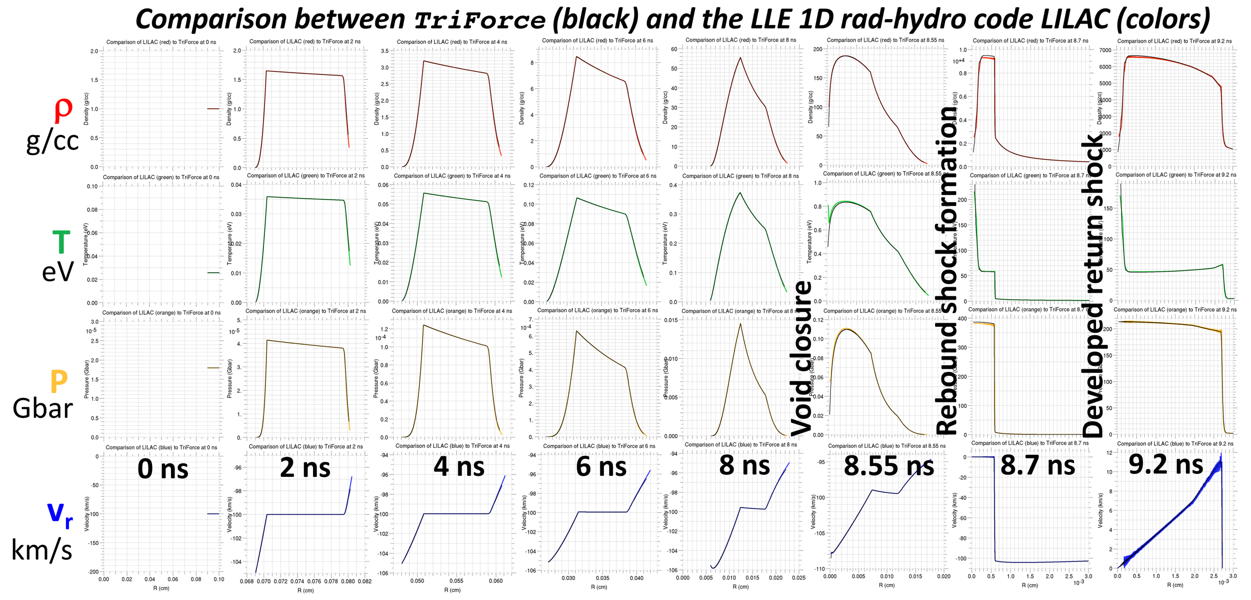


Shock capturing and adaptive particle methods

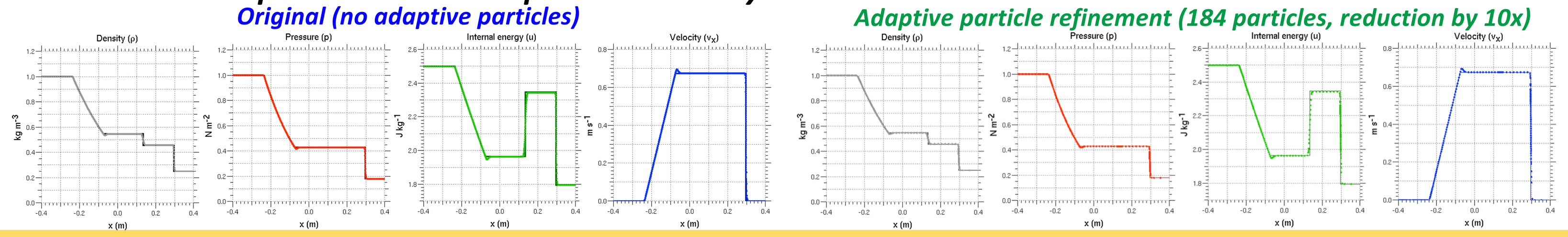
Comparison between TriForce (black) and the LLE 1D rad-hydro code LILAC (colors)

ICF-relevant implosion

- 1D spherical geometry
- Implosion of M~60 shell
- Outer radius = 1 mm
- Thin CH shell of 1 g/cc and Δr = 0.1 mm
- Initial temperature 298K
- Uniform v_r^{imp}=-100 km/s
- Central void
- Ideal gas EOS
- No radiation, laser, or fusion calculations

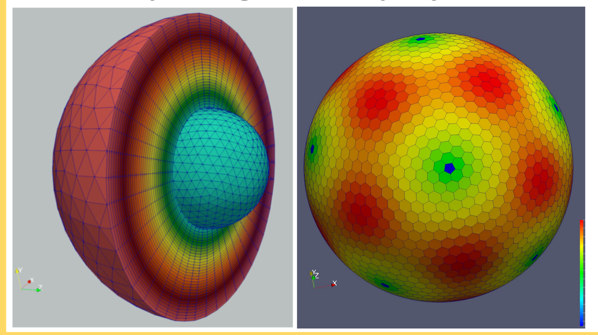


Sod shock tube problem with comparison to analytic result

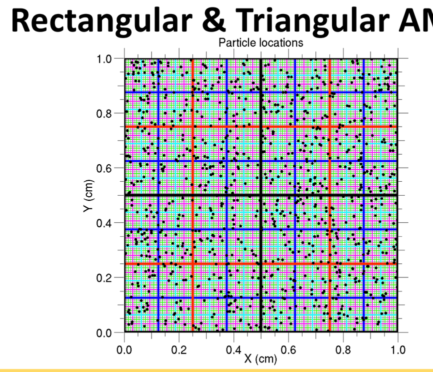


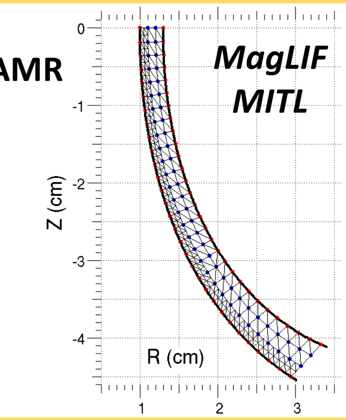
Integration of advanced meshes

Nonpolar geodesic polyhedra



Rectangular & Triangular AMR





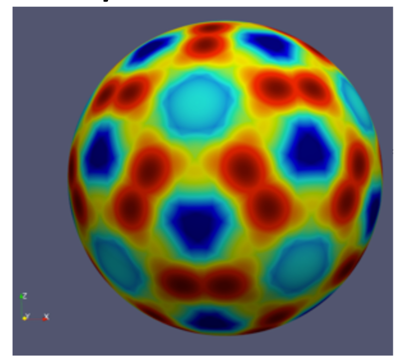
Material constitutive models

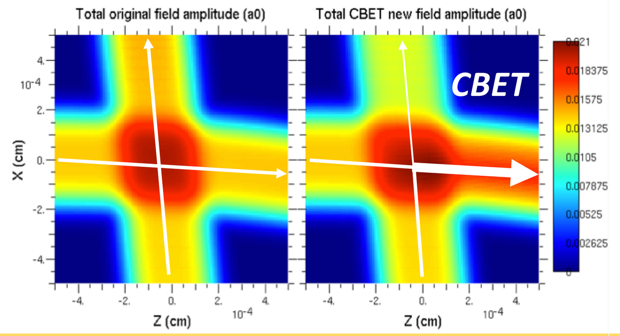
- Equation of state
  Analytic, tabular (FPEOS, LEOS, SESAME)
- Electrical resistivity
  Spitzer, tabular (QLMD)
- Opacity and <Z>
  Analytic, tabular (Astrophys., Prism)
- Material strength
  Elastic-plastic, Steinberg-Guinan/-Lund
- Viscosity
  Real and artificial
- Surface tension
- Molecular dynamics*

Laser propagation and absorption

- Low-noise bundled ray tracing
- Complex ray tracing
- Inverse projection
- Cross-beam energy transfer (CBET)
- Wave-based launcher

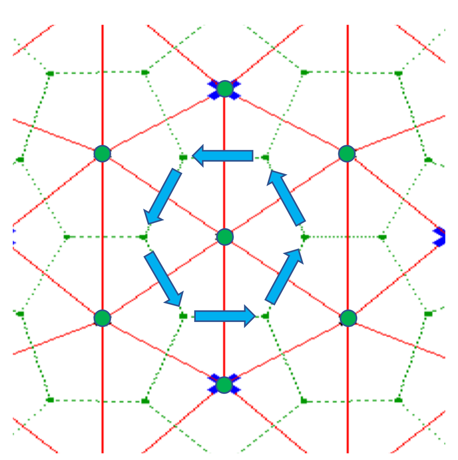
Imprint resolution





Electromagnetic fields

- Explicit or implicit time advance
- Rectangular or triangular mesh option

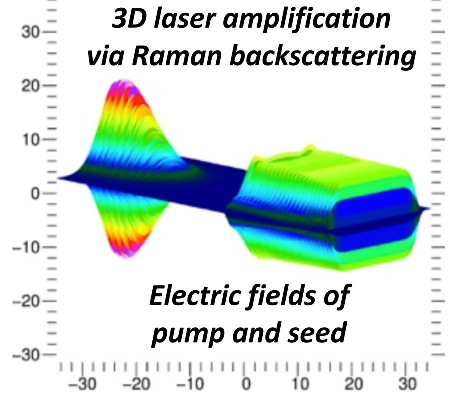


$$\nabla\cdot\mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \nabla\cdot\mathbf{B} = 0$$

$$\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{B} = \mu_0\left(\mathbf{J} + \epsilon_0\frac{\partial\mathbf{E}}{\partial t}\right)$$

3D laser amplification via Raman backscattering

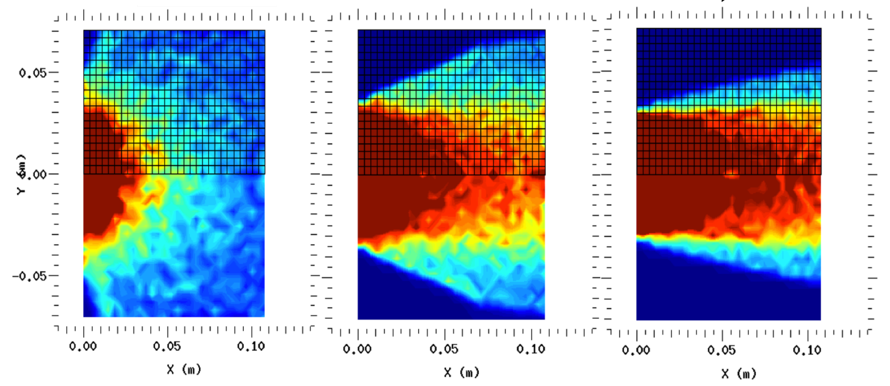


Electric fields of pump and seed

Kinetic particle transport

- Explicit or implicit PIC (particle-in-cell) push
- Standard scatter/gather operations are used to interact with meshless SPH particles

Increasing **B** field

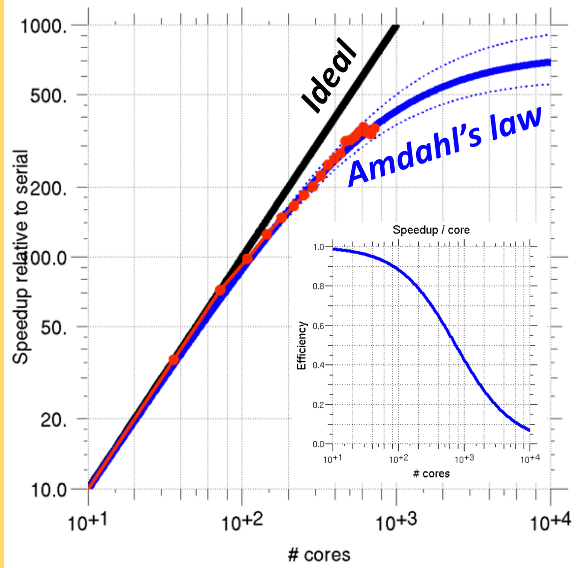


Magnetized charged particle transport

Parallelism

CPUs (mpi)

Strong scaling: p~0.9987



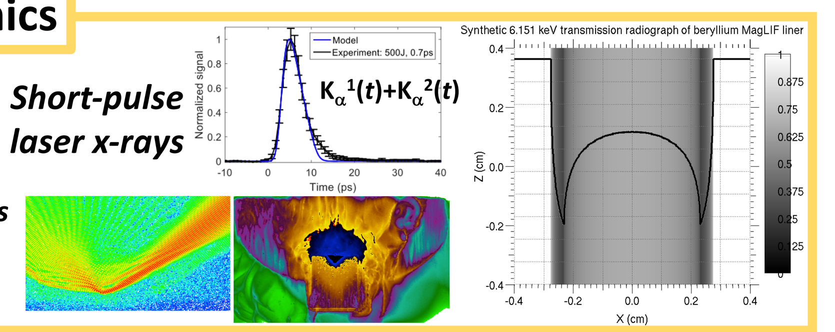
GPU version in development

I/O: parallel HDF5

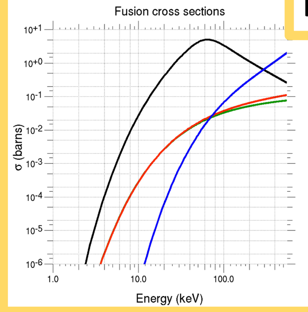
Radiation and atomics

- 3-T or Multi-group diffusion
- Particle-based Monte Carlo
- Generalized collisional-radiative*
  Spectrum of in-line and post-proc. options
- Synthetic diagnostics
  e.g. x-ray emission, backlighting, etc.

Short-pulse laser x-rays

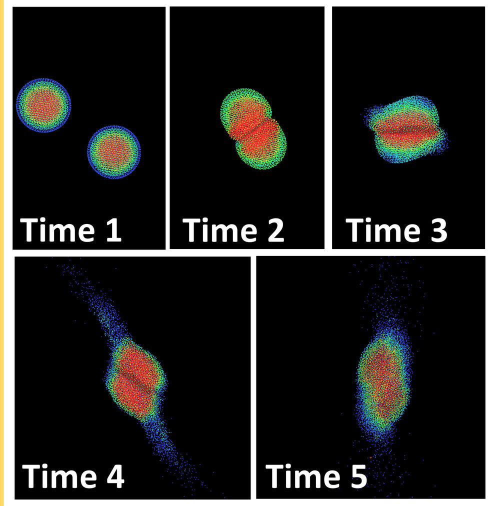


Nuclear fusion

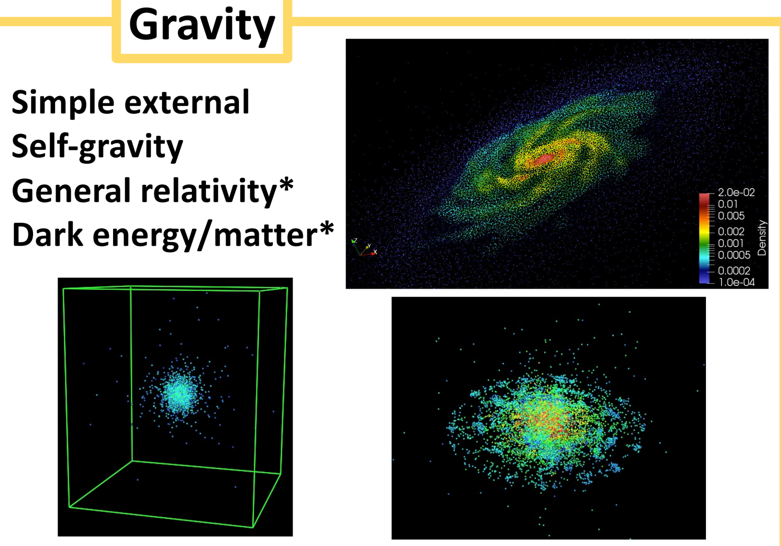


- *D+T → n+He⁴*
- *D+D → p+T*
- *D+D → n+He³*
- *D+He³ → p+He⁴*

Gravity



- Simple external
- Self-gravity
- General relativity*
- Dark energy/matter*



Ideal, resistive, and extended magnetohydrodynamics

Generalized Ohm's law:

- A primary goal is to improve fundamental understanding via the direct comparison of MHD to implicit electromagnetic field solutions

$$\overbrace{\underbrace{\mathbf{E}+\mathbf{v}\times\mathbf{B}}_{\text{Ideal}}-\boldsymbol{\eta}\cdot\mathbf{J}}^{\text{Resistive}} = \frac{1}{en_e}(\mathbf{J}\times\mathbf{B} - \nabla P_e - \nabla\cdot\mathbf{\Pi_e} - n_e k_b\boldsymbol{\beta}\cdot\nabla T_e + \frac{m_e}{e}[\frac{\partial\mathbf{J}}{\partial t} + \nabla\cdot(\mathbf{Jv}+\mathbf{vJ})])$$

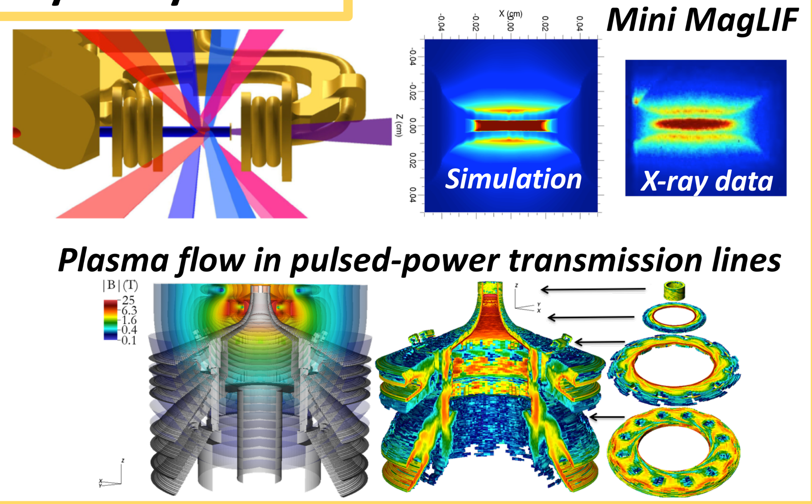
Extended (RHS)

Hall ~c/ω_pi | e⁻ pressure ~c/ω_pi | electrothermal ~c/ω_pi | e⁻ inertia ~c/ω_pe

Induction equation (magnetic field evolution):

$$\frac{\partial\mathbf{B}}{\partial t} = \nabla\times\mathbf{v}\times\mathbf{B} + \frac{\eta}{\mu_0}\nabla^2\mathbf{B} + \mathbf{J}\times\nabla\eta + \frac{1}{en_e}[k_b\nabla T_e\times\nabla n_e + \nabla\times(n_e k_b\boldsymbol{\beta}\cdot\nabla T_e - \mathbf{J}\times\mathbf{B})]$$

Advection | Diffusion | Diamagnetic/Biermann | Nernst/Seebeck | Hall

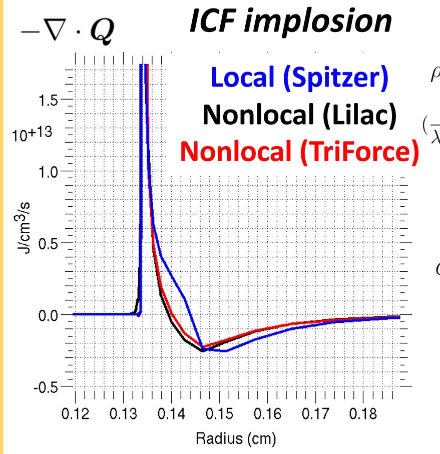


Plasma flow in pulsed-power transmission lines

Nonlocal thermal conduction

ICF implosion

Local (Spitzer)
Nonlocal (Lilac)
Nonlocal (TriForce)



Mod. SNB model

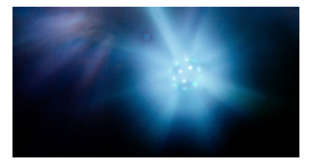
$$\rho C_{v,e}\frac{dT_e}{dt} = -\nabla\cdot\boldsymbol{Q_{SH}} + C_{nonlocal}$$

$$\left(\frac{1}{\lambda_g(r)} - \nabla\cdot\frac{\lambda_g'(r)}{3}\nabla\right)H_g(r) = -\nabla\cdot\boldsymbol{U_g}(r)$$

$$\boldsymbol{U_g}(r) = \boldsymbol{Q_{SH}}\frac{1}{24}\int_{E_{g-1}/k_bT_e}^{E_g/k_bT_e}\beta^4e^{-\beta}d\beta$$

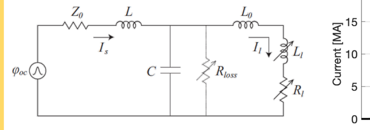
$$\lambda_g = 2(E_{g-\frac{1}{2}}/k_bT_e)^2\lambda_{mfp}^e$$

$$C_{nonlocal} = -\nabla\cdot\boldsymbol{Q_{nonlocal}} = \sum_g H_g^k/\lambda_g^k$$



Circuit model

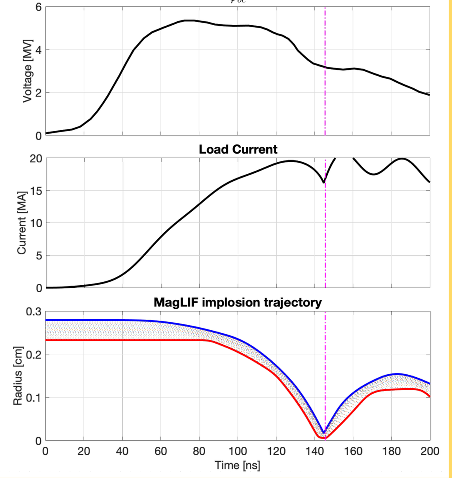
- Loads driven self-consistently by open-circuit voltage



$$\dot{I}_s = \frac{\varphi_{oc} - Z_0I_s - \varphi_c}{L}$$

$$\dot{\varphi}_c = \frac{I_s - I_l - \varphi_c/R_{loss}}{C}$$

$$\dot{I}_l = \frac{\varphi_c - \dot{L}_lI_l}{L_0+L_l}$$



Acknowledgments

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