Simulation of Pellet Ablation using FronTier and Lagrangian Particle Codes

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Talk Overview

- Update on Physics Models and Apgorithms
  - Conductivity
  - Radiation
  - Improved surface ablation algorithm
  - Corrected coupling of WENO solver with Neon EOS

- Simulations of single pellet injection woth FronTier
  - Verification of Scaling laws
  - Hydro and MHD simulations, ablation rates

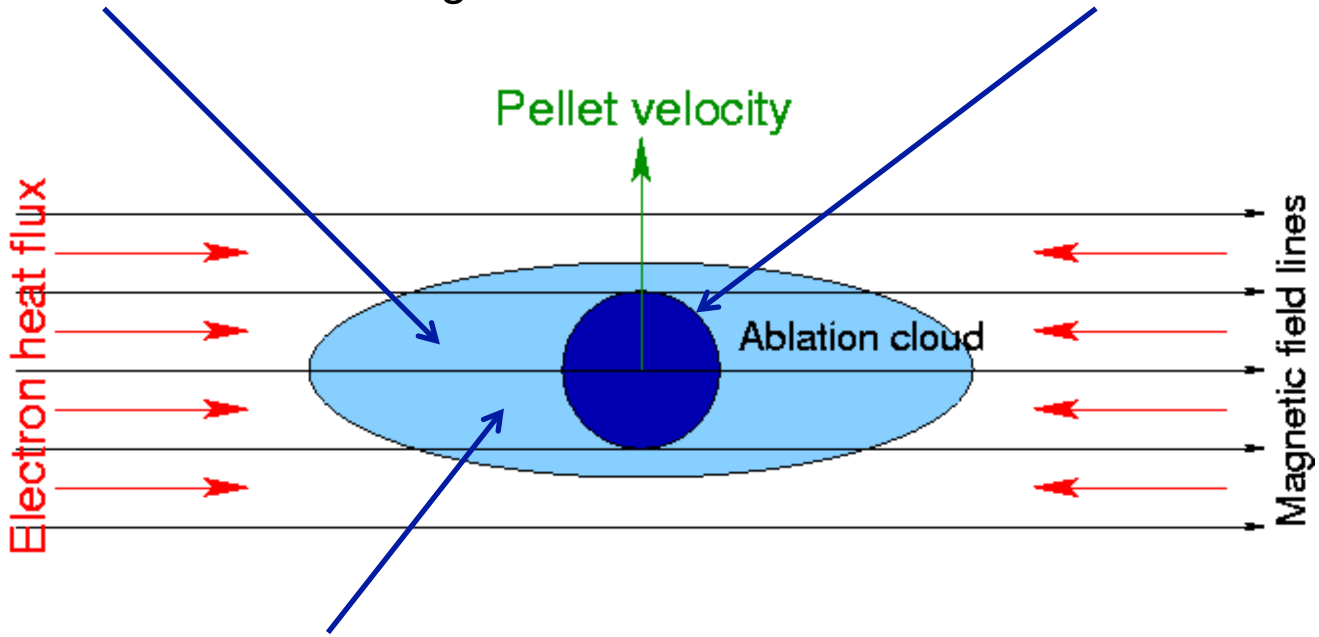
- Progress on simulation of SPI
  - 3D Lagrangian Particle code for multiple pellet fragments
  - Hydro and MHD simulations, ablation rates
  - Ideas for coupling to NIMROD / M3D-C1

Update on Physics Models and Algorithms

Physics Models for Pellet Simulations

- Kinetic model for the interaction of hot electrons with ablated gas

- Explicitly tracked pellet surface
- Phase transition (ablation model)



- Low Magnetic Re MHD equations
- Equation of state with atomic processes (Zeldovich Average Ionization Model)
- Radiation model
- Conductivity models
- Pellet cloud charging models

Radiation models

The photon mean free path in the ablation channel is much longer compared to the channel diameter and length

- The exception is the narrow region near the pellet surface, but the radiation coming from this region is very low
- Radiation model in thin optical limit is a good approximation

Two models were compared in our simulations:

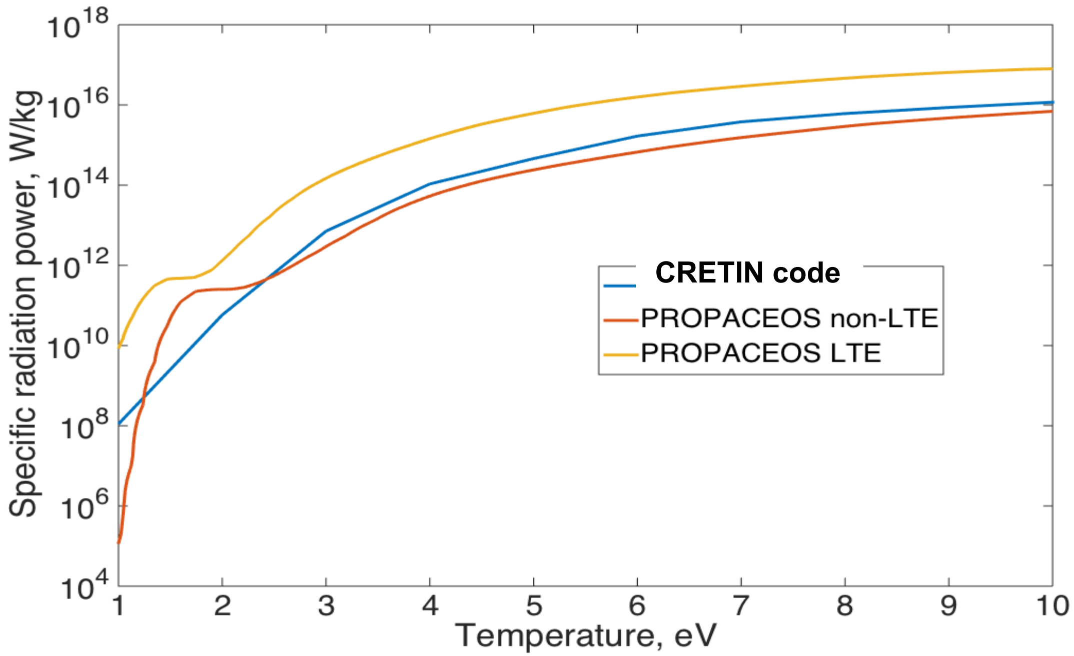
- Radiation model based on **CRETIN code** (P. Parks provided tabulated data)
- Radiation model implemented in software from Prism Computational Sciences (**PROPACEOUS tables**)

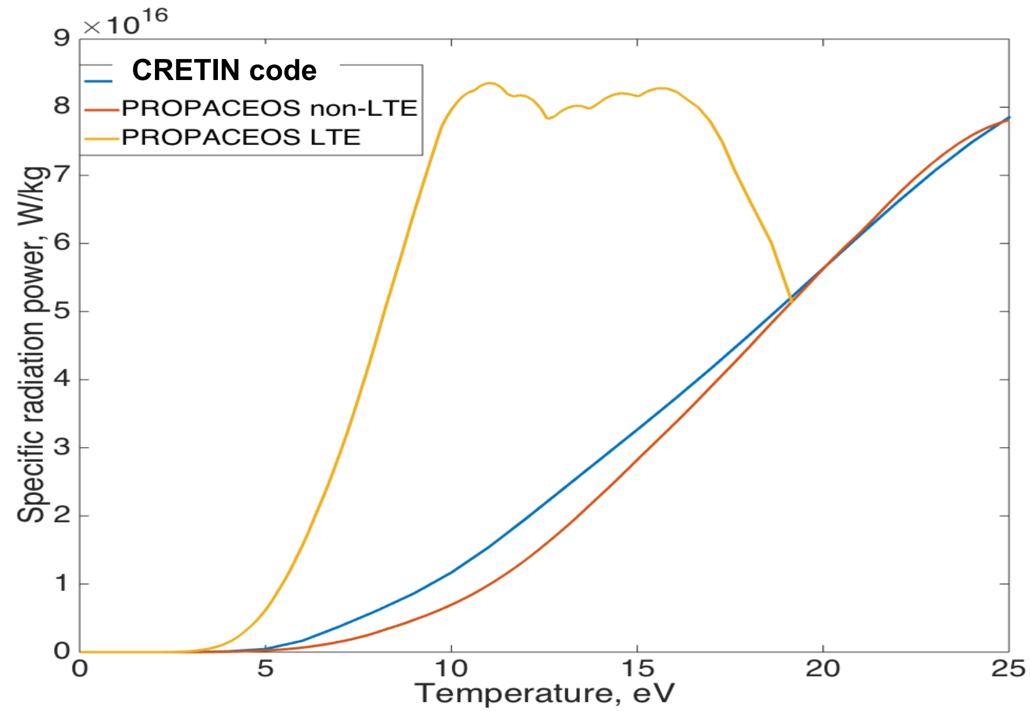
$$\frac{de}{dt} = -4\sigma T_e^4 \chi_{Plank}$$

χ_{Plank} is Plank's emission opacity

PROPACEOS tables provide this in tabular form

Comparison of Radiation Models

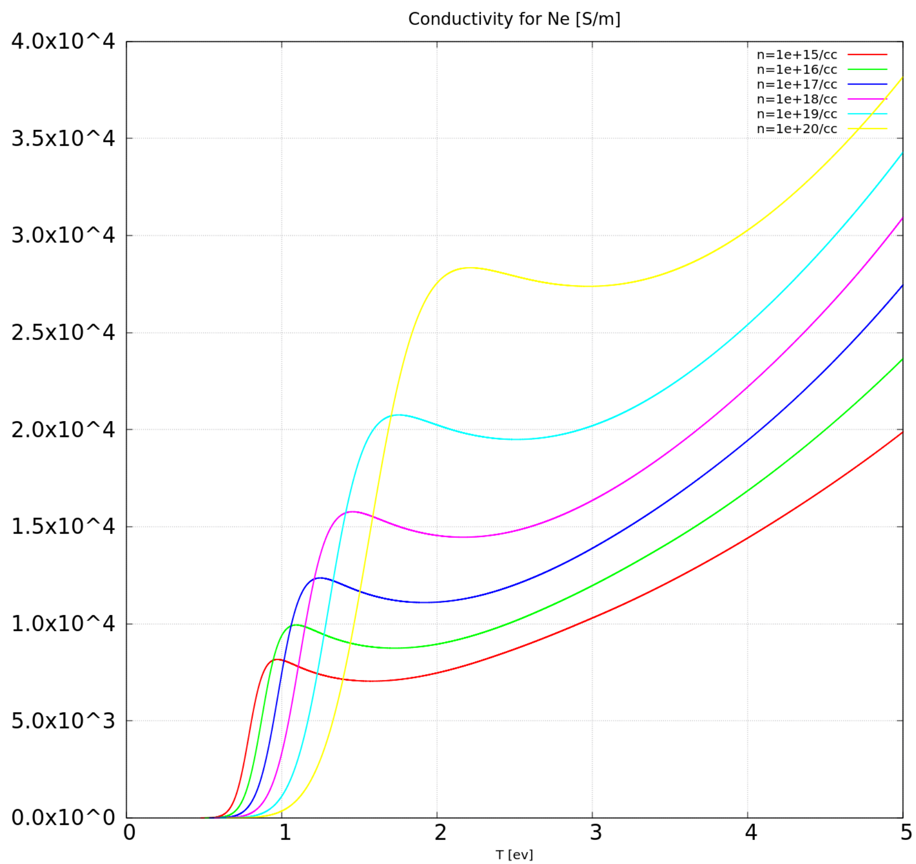




Electric conductivity model for high-Z materials

P. Parks (Jan. 2017)

$$\sigma_{\perp} = \frac{9700 T_e^{3/2}}{\left(Z_{eff} \ln \Lambda_{ei} + 0.00443 T_e^{2.245} \frac{n^0}{n_e} \right)}$$



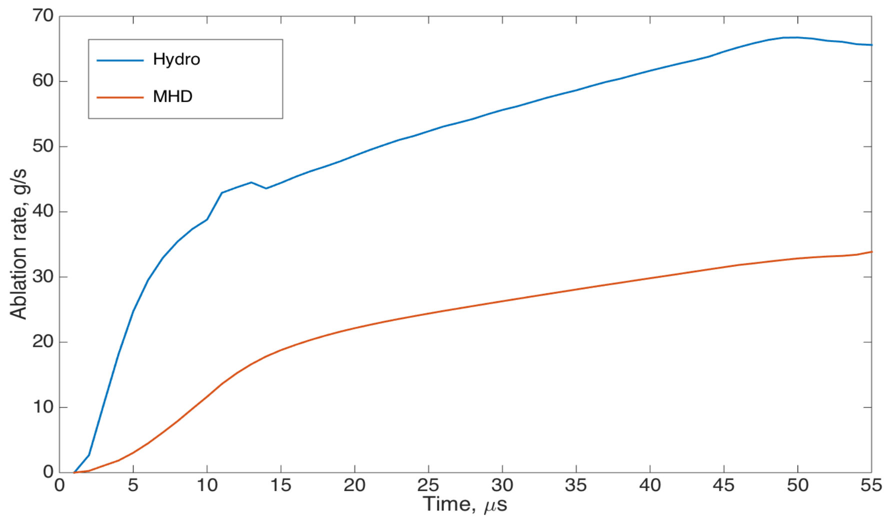
Improvement of Pellet Ablation Surface Boundary Conditions

The following boundary conditions are used:

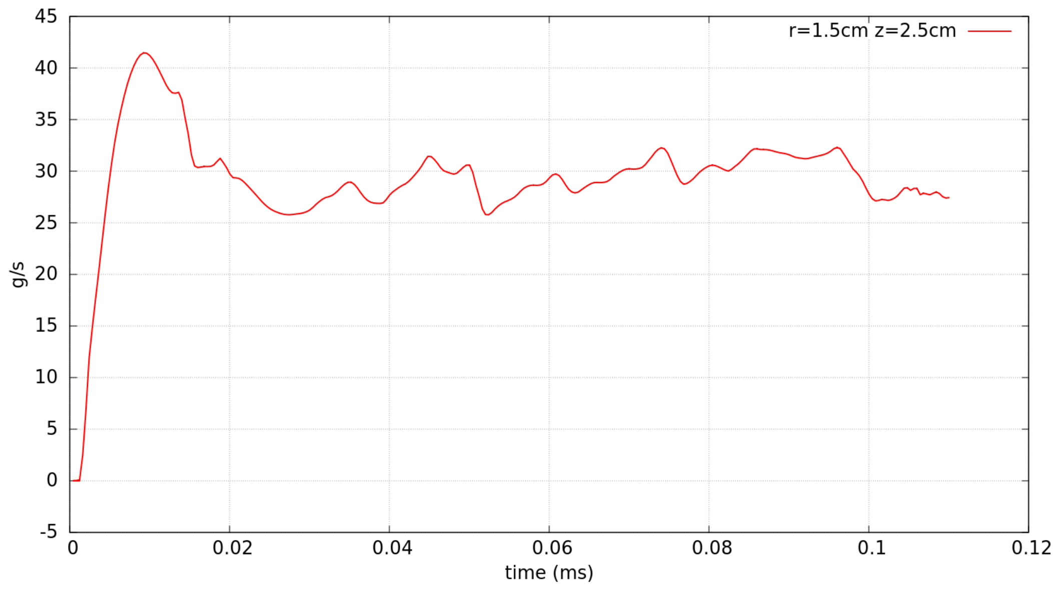
- Fixed pellet T = 20K
- Ablated vapor normal velocity: $\rho_v u_v = q_{\pm} \cos\theta / E_s$
- EOS (density – temperature – internal energy constraint)
- Riemann wave curve: $\frac{\partial \rho}{\partial t} + (u-c)\frac{\partial \rho}{\partial n} - \rho c\left(\frac{\partial u}{\partial t} + (u-c)\frac{\partial u}{\partial n}\right) = \Gamma \frac{\partial q_{\pm}}{\partial z}$
- In addition, we tested simpler subsonic outflow boundary conditions used in NASA codes. Simulations results are very close
- The current improvement deals with situations when these BC's do not apply
  - Initial supersonic outflow: fixed BCs' are used
  - Zero mass flux (along pellet equator): BC's are obtained using neighboring states

Improvement of pellet ablation boundary conditions resulted in steady ablation rates:

Previous simulations showed increasing pellet ablation rate (perhaps very long transient oscillation)



In current FronTier simulations, a steady state (with some oscillations) is reached in short time



Verification: Comparison of Spherically Symmetric Simulations with Theory

- Spherically symmetric, no ionization, Maxwellian heat flux

$$G^{fit} = 67.08\left(\frac{T_e}{2000}\right)^{5/3}\left(\frac{r_p}{0.2}\right)^{4/3} n_{e14}^{1/3}$$

- units: $G(\mathrm{g/s})$ $T_e(\mathrm{eV})$ $r_p(\mathrm{cm})$ $n_e(10^{14}\mathrm{cm}^{-3})$

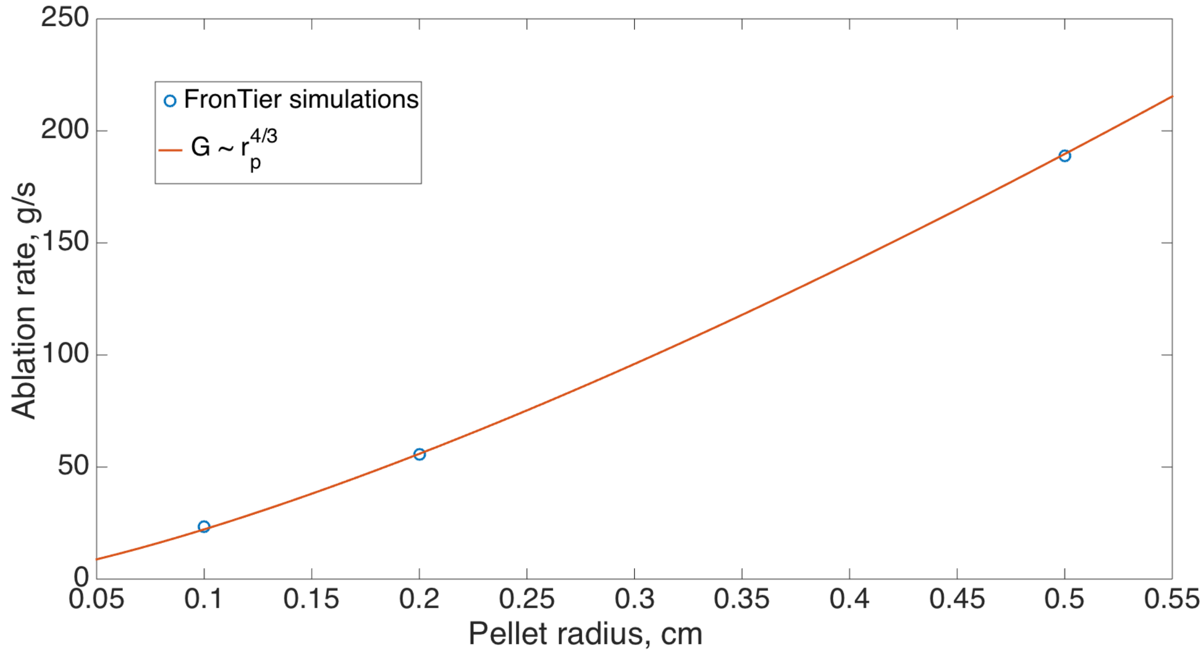
- Surface recession speed

$$\frac{dr_p}{dt} = -\frac{G}{4\pi r_p^2 \rho_0} \quad (\mathrm{cm/s}) \qquad \rho_0 = 1.444 \ g/\mathrm{cm}^3$$

- Example: $G^{fit} = 26.621 \quad for \quad r_p = 0.1, n_{e14} = 1, T_e = 2000$
  which is close to the Parks numerical transonic flow value G = 25.5 and updated analytic scaling expression G = 26.56

Verification of Scaling Laws for Neon Pellet

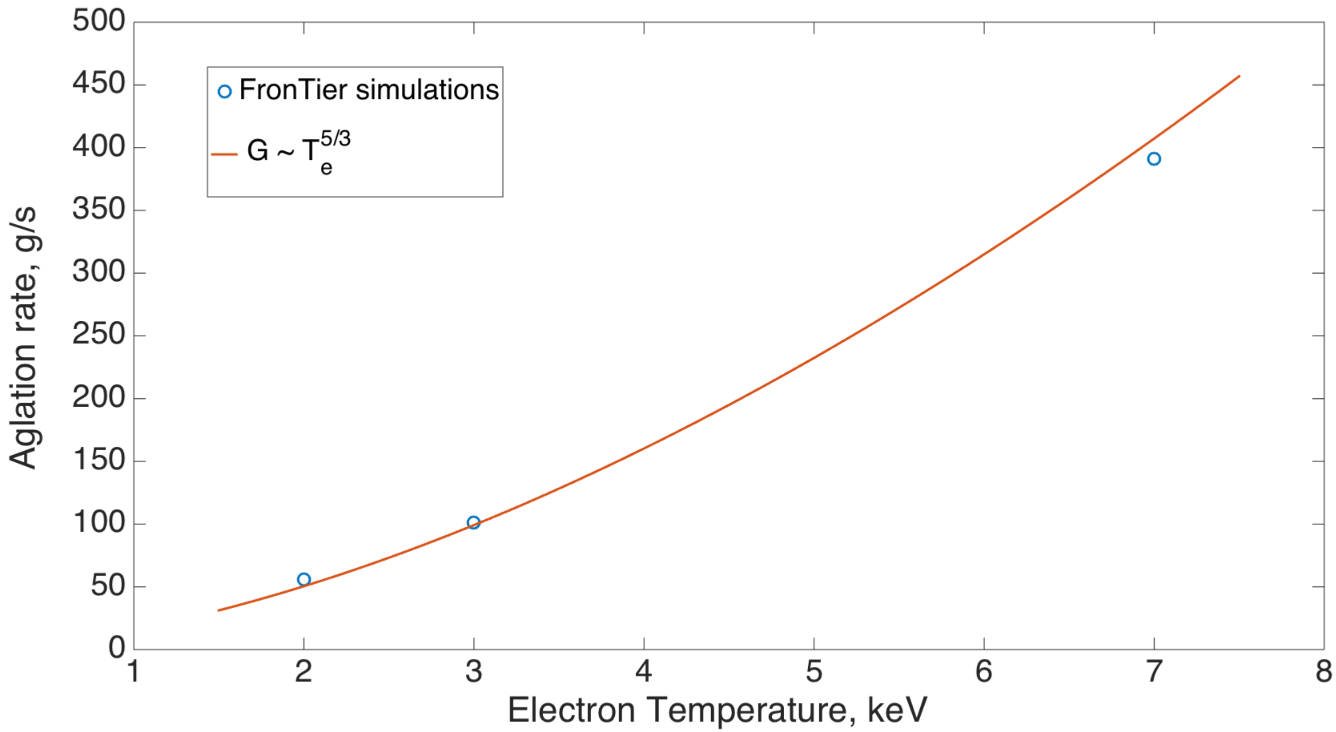
n_e = 1e14
T_e = 2 keV



n_e = 1e14 T_e = 2 keV	G (g/s)	Recession rate (cm/s)	Surface ablation Pressure (b)	T* (eV)	r*	r*/r_p
r_p = 0.1	23.5	130	52	3.14	0.275	2.75
r_p = 0.2	55.6	76.8	39	4.99	0.532	2.66
r_p = 0.5	189	41.8	28	9.6	1.34	2.68

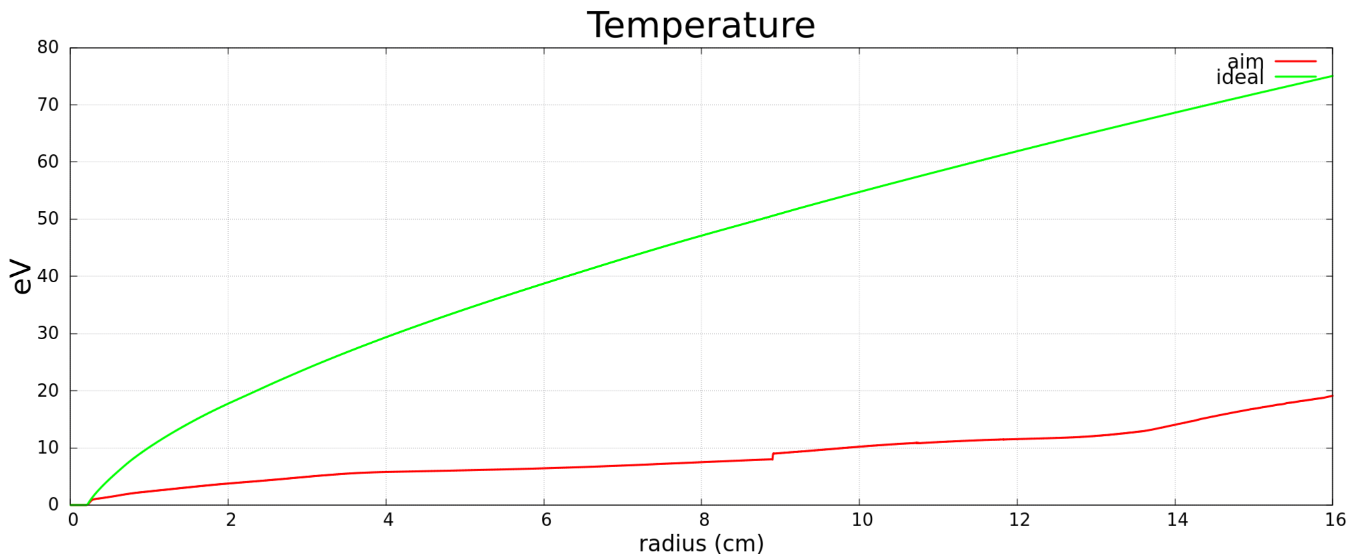
Verification of Scaling Laws for Ne Pellet

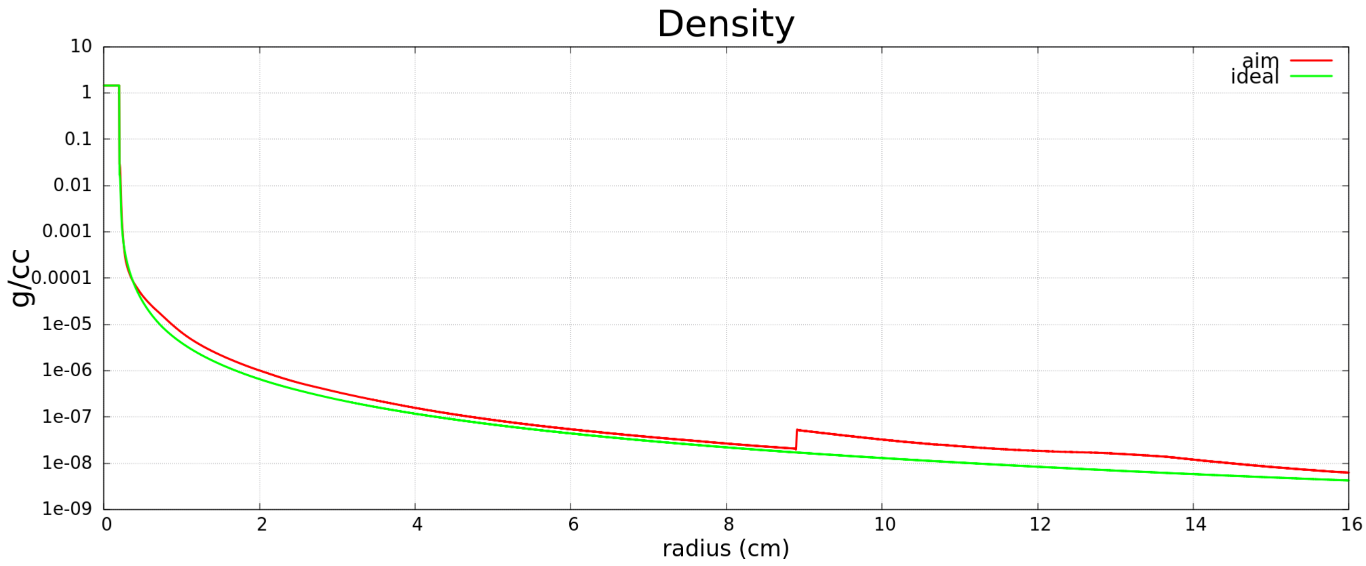
n_e = 1e14
r_p = 2 mm



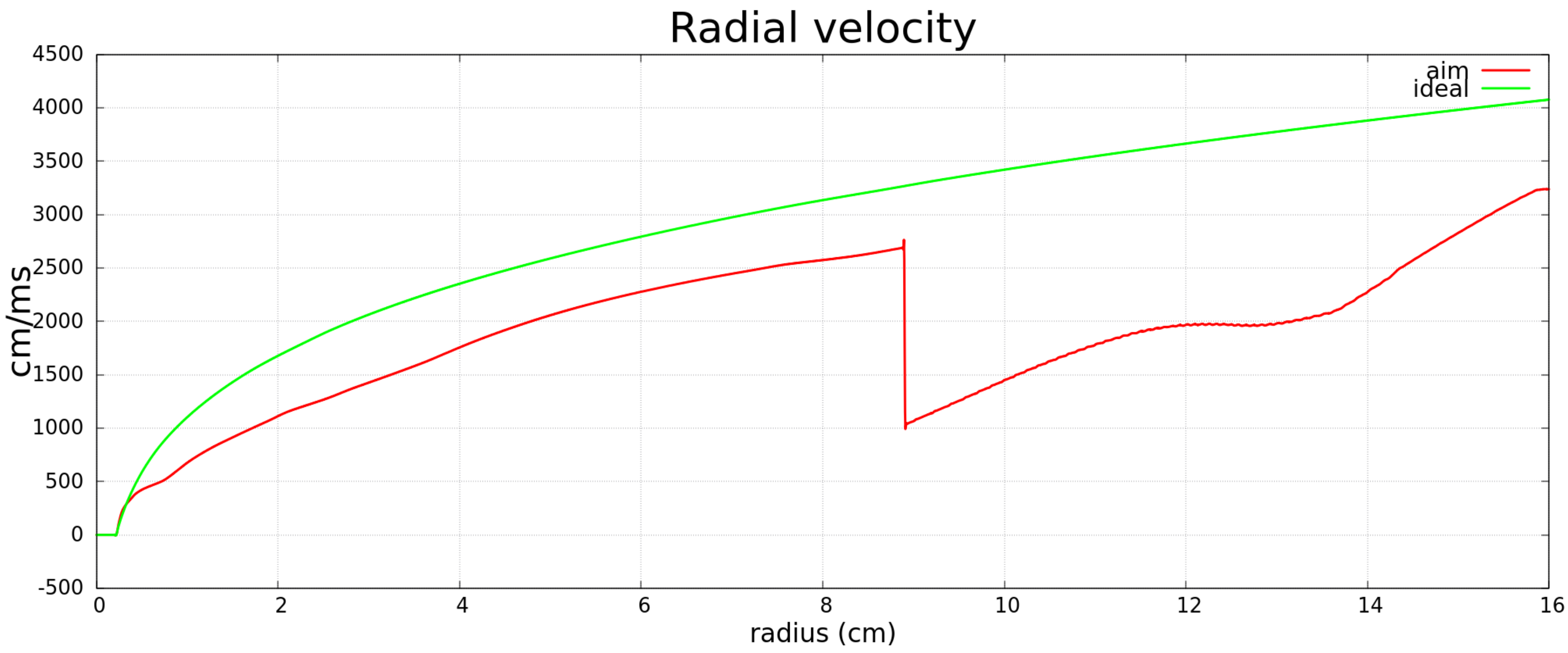
r_p = 0.2 n_e = 1e14	G (g/s)	Recession rate (cm/s)	Surface ablation Pressure (b)	T* (eV)	r*	r*/r_p
T_e = 3 keV	101.42	73.4	78	5.07	0.54	2.7
T_e = 7 keV	391	283	297	4.37	0.52	2.6

Influence of ionization





Influence of ionization



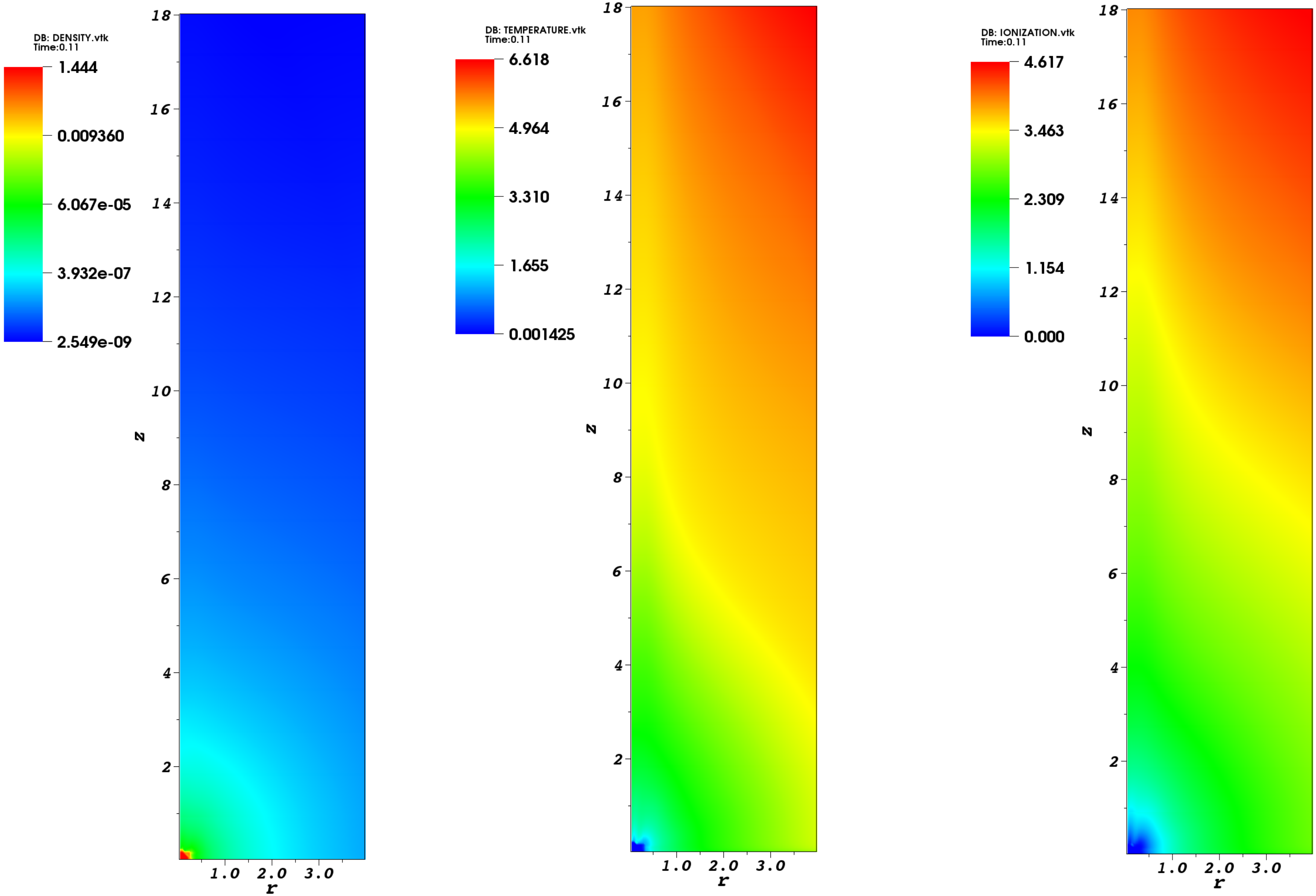
- Including atomic processes significantly changes the pressure and temperature, but the density and velocity changes compensate each other, leading to practically unchanged ablation rate
- Results of LP simulations confirm this statement

Cylindrically Symmetric Hydrodynamic Simulations (no JxB forces)

- Pellet radius = 2 mm
- Te = 2 keV
- Ne = 1.e14 with electrostatic shielding
- Averaged ionization EOS model with radiation losses

- Improved boundary conditions lead to fast convergence, approximately steady-state ablation rates (with some oscillations, but without global increase)

Density, Temperature, and Ionization at 110 microseconds

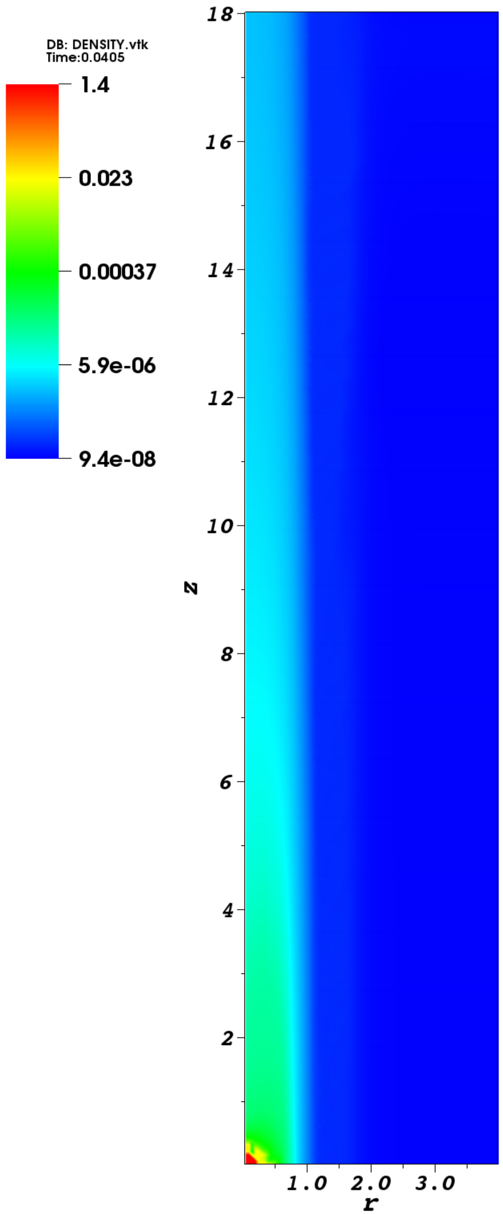


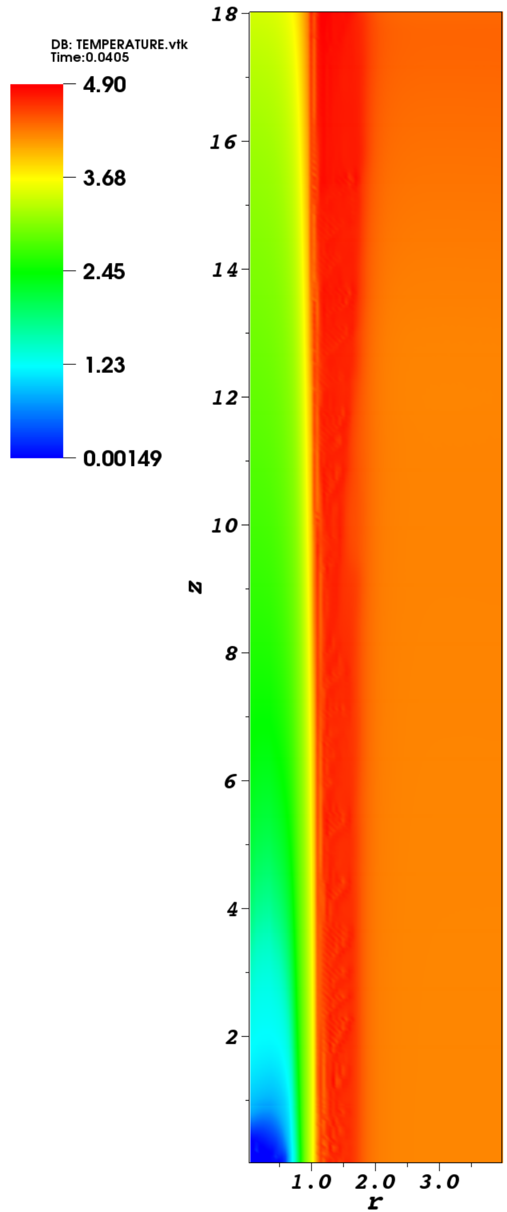
Cylindrically symmetric MHD simulations

Simulation Parameters:

- Background electron density: 1.e14 1/cc – electrostatic shielding
- Electron Temperature: 2 keV
- Pellet radius: 2 mm
- "Warm-up time" (time during which the pellet crosses the pedestal: 10 microseconds
  - Effective n_e ramped up from 0 to 1.068e13
  - Te ramped up from 100 eV to 2 keV
- Magnetic field: 6T
- MHD in low magnetic Reynolds number approximation

Density and Temperature in the Ablation Channel





To mitigate instabilities in far field that arise early in the simulation,we introduce a density cutoff on the heat deposition and LF. This cutoff starts at 1e-7 g/cc and the heat deposition and LF are reduced linearly (in log scale) to 0 at density=1e-8 g/cc. Using this technique we are able to run the code for 40 microsec.

Ablation rate: ~25 g/s.

Higher resolution runs are in progress to study the convergence

Models for SPI

Implementation of Pellet / SPI code based on Lagrangian Particles

- Completed development of pellet ablation model based on Lagrangian particle (LP) code
- Advantages:
  - Lagrangian treatment of ablated material – eliminated numerical difficulties caused by hot background plasma. Ablated material can be tracked during long time / distances
  - Optimal and continuously adapting resolution
  - Small computing time: 3D LP simulations with higher resolution near pellet are much fasted compared to 2D FronTier simulations
  - LP is usable for hundreds of fragments in 3D
- Ionization EOS and MHD in LP have been recently added to the code and tested
- R. Samulyak, X. Wang, H.-S. Chen, Lagrangian Particle Method for Compressible Fluid Dynamics, J. Comput. Phys., 362 (2018), 1-19.

Main Ideas of Lagrangian Particle Method

- New method. Motivation for development: improve accuracy of SPH which has ZERO convergence order (for original SPH)
- We keep only one idea of SPH: each particle represents a Lagrangian fluid cell
- We completely avoid using artificial smooth kernels of SPH by proposing new particle-based discretization methods
- Key novel features of our method:
    - Accuracy: derivatives based on local polynomial fits (optimal coefficients of a local stencil are found via least squares)
    - Stable particle-based upwind and directionally unsplit methods were designed
        - High order methods
    - Scalability on modern supercomputer architectures
    - Lagrangian Particle code accurately reproduced numerous classical problems: Rayleigh-Taylor and Kelvin-Helmholtz in stabilities, triple-point (shock-vortex) problem, explosions / splashes etc.
- Complementary method: Adaptive Particle-in-Cloud (AP-Cloud). AP-Cloud is an adaptive and artifact-free replacement for the traditional PIC method (J. Comput. Phys, 2016)

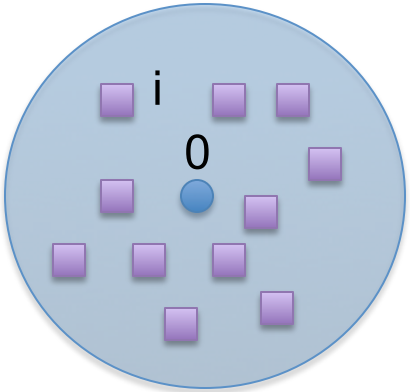
Computing Derivatives.
Local Polynomial Fitting (Generalized Finite Differences)

- In 2D at the vicinity of a point 0, the function value in the location of a point i can be expressed as

$$U_i = U_0 + h_i \left.\frac{\partial U}{\partial x}\right|_0 + k_i \left.\frac{\partial U}{\partial y}\right|_0 + \frac{1}{2}\left(h_i^2 \left.\frac{\partial^2 U}{\partial x^2}\right|_0 + k_i^2 \left.\frac{\partial^2 U}{\partial y^2}\right|_0 + 2h_i k_i \left.\frac{\partial^2 U}{\partial x \partial y}\right|_0 \right) + \dots$$

- Second order approximation

$$\tilde{U} = U_0 + h_i\theta_1 + k_i\theta_2 + \frac{1}{2}h_i^2\theta_3 + \frac{1}{2}k_i^2\theta_4 + h_i k_i \theta_5$$

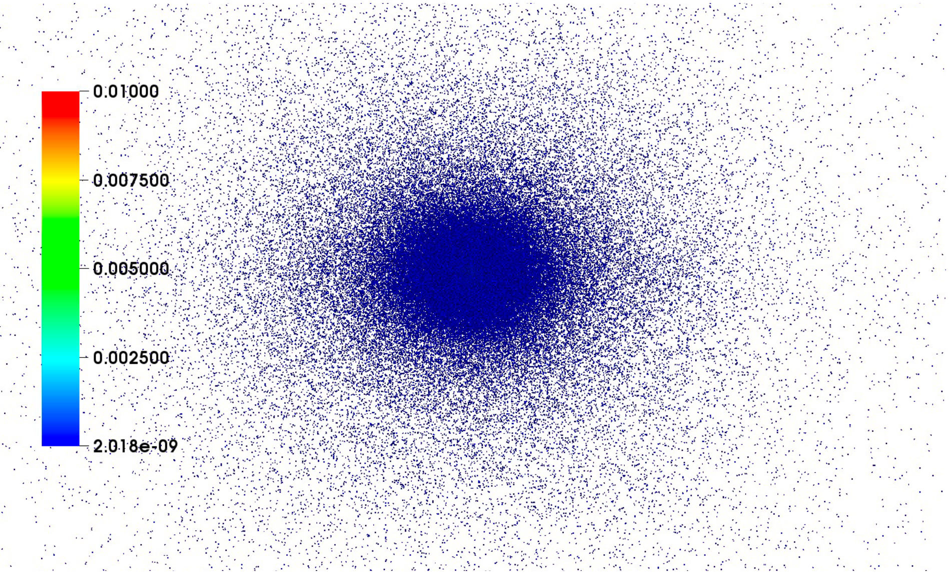


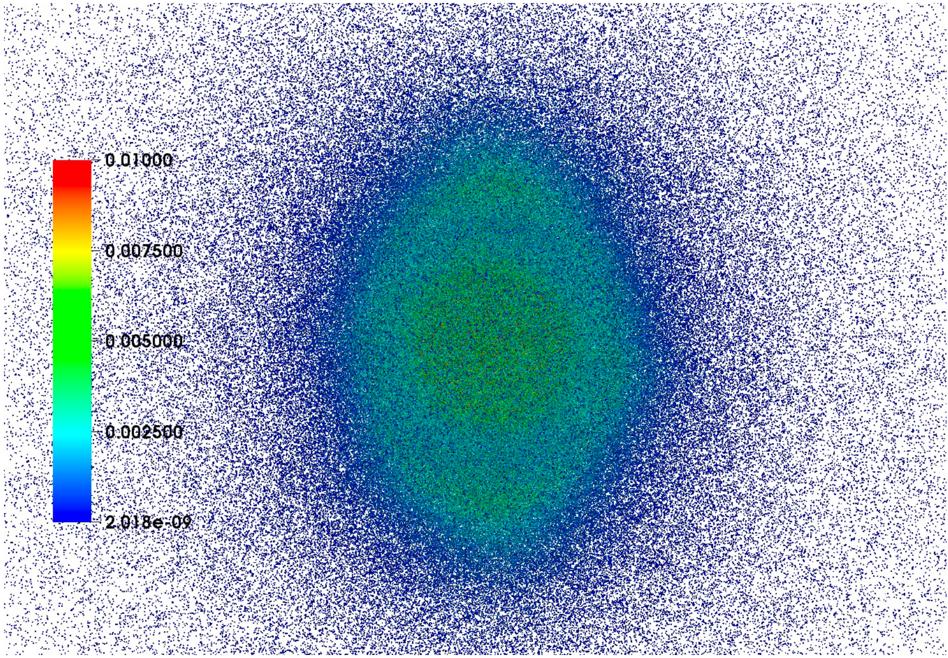
- Using *n* neighbours:

$$\begin{bmatrix} h_1 & k_1 & \frac{1}{2}h_1^2 & \frac{1}{2}k_1^2 & h_1k_1 \\ h_2 & k_2 & \frac{1}{2}h_2^2 & \frac{1}{2}k_2^2 & h_2k_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ h_n & k_n & \frac{1}{2}h_n^2 & \frac{1}{2}k_n^2 & h_nk_n \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \end{bmatrix} = \begin{bmatrix} U_1 - U_0 \\ U_2 - U_0 \\ \vdots \\ U_n - U_0 \end{bmatrix}$$

Solve using QR to obtain derivatives **convergent to prescribed order**

3D Hydro Lagrangian Particle Simulations

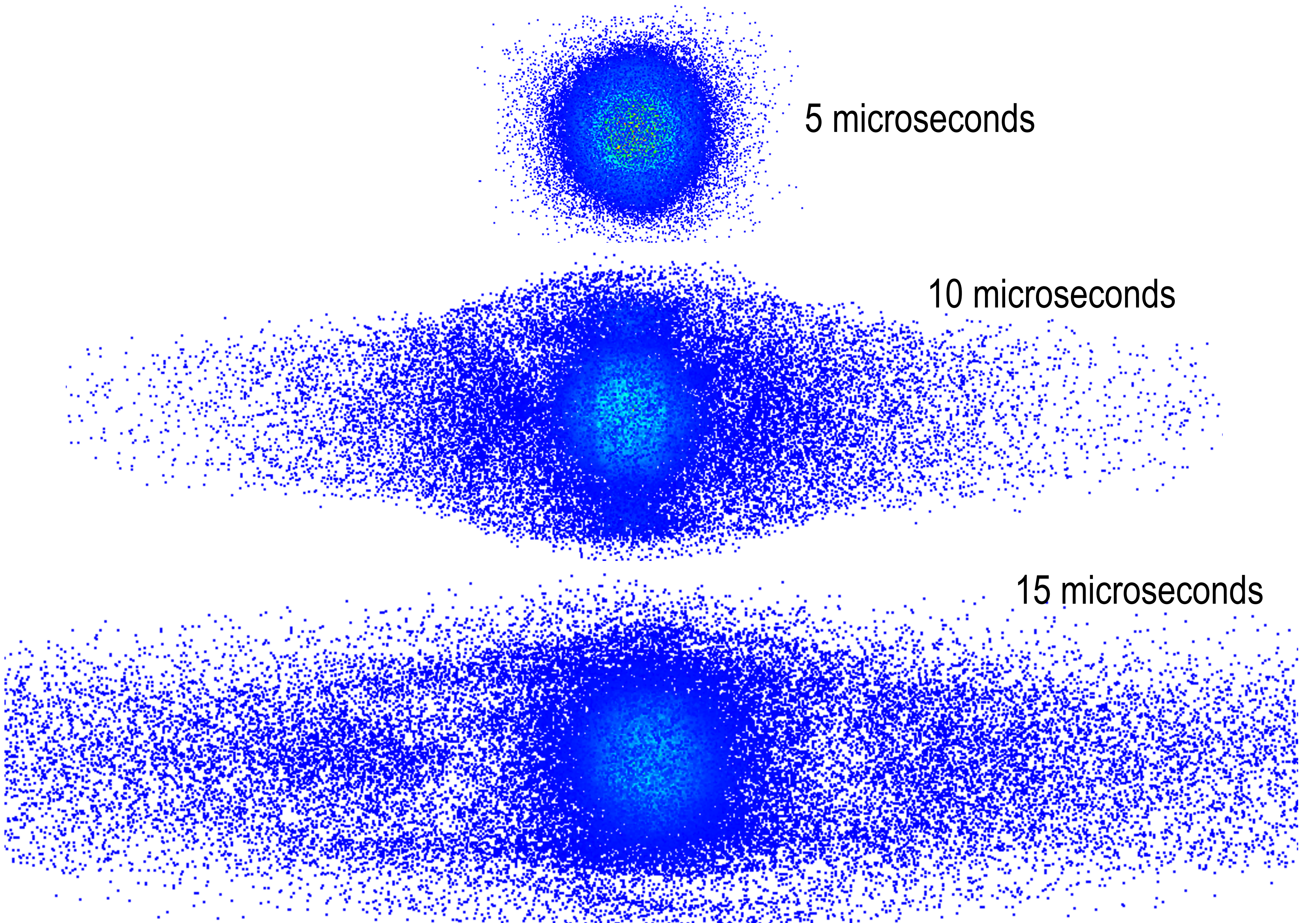




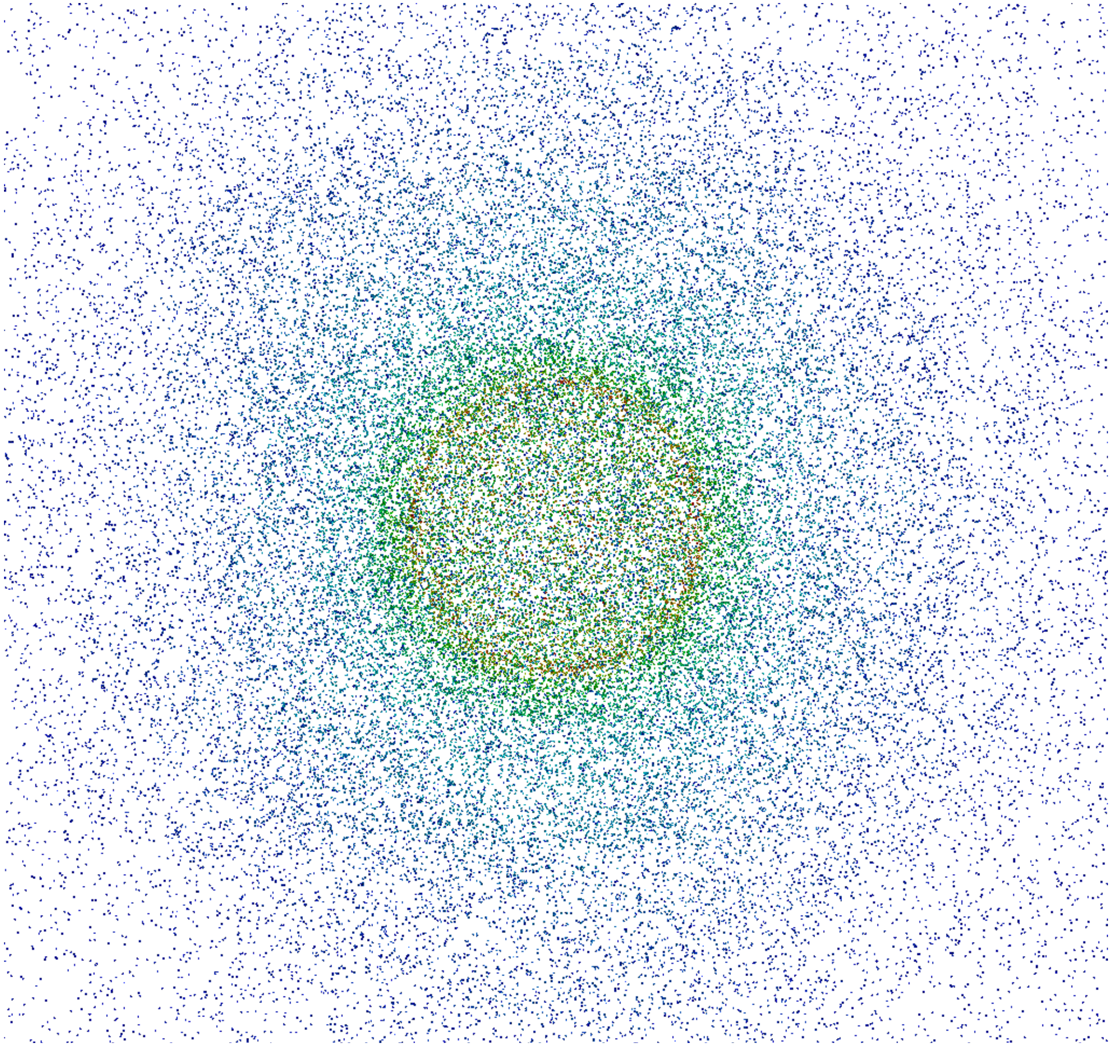
- LP hydro simulations of 2mm radius neon pellet (Left: view from far-field; Right: zoom-in cloud)

- 3D LP code runs much faster than 2D FronTier with the same resolution near the pellet

3D MHD Lagrangian Particle Simulations: development of ablation channel



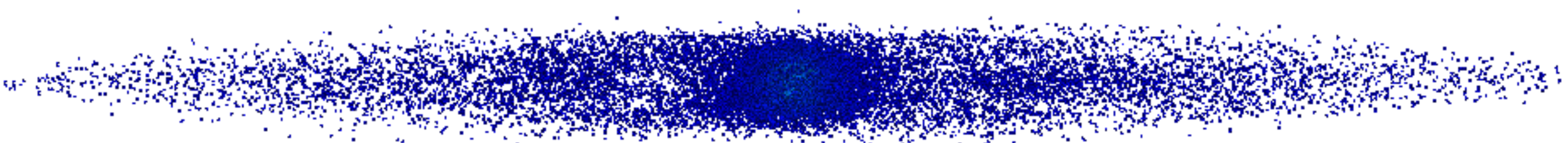
3D MHD Lagrangian Particle Simulations: development of ablation channel



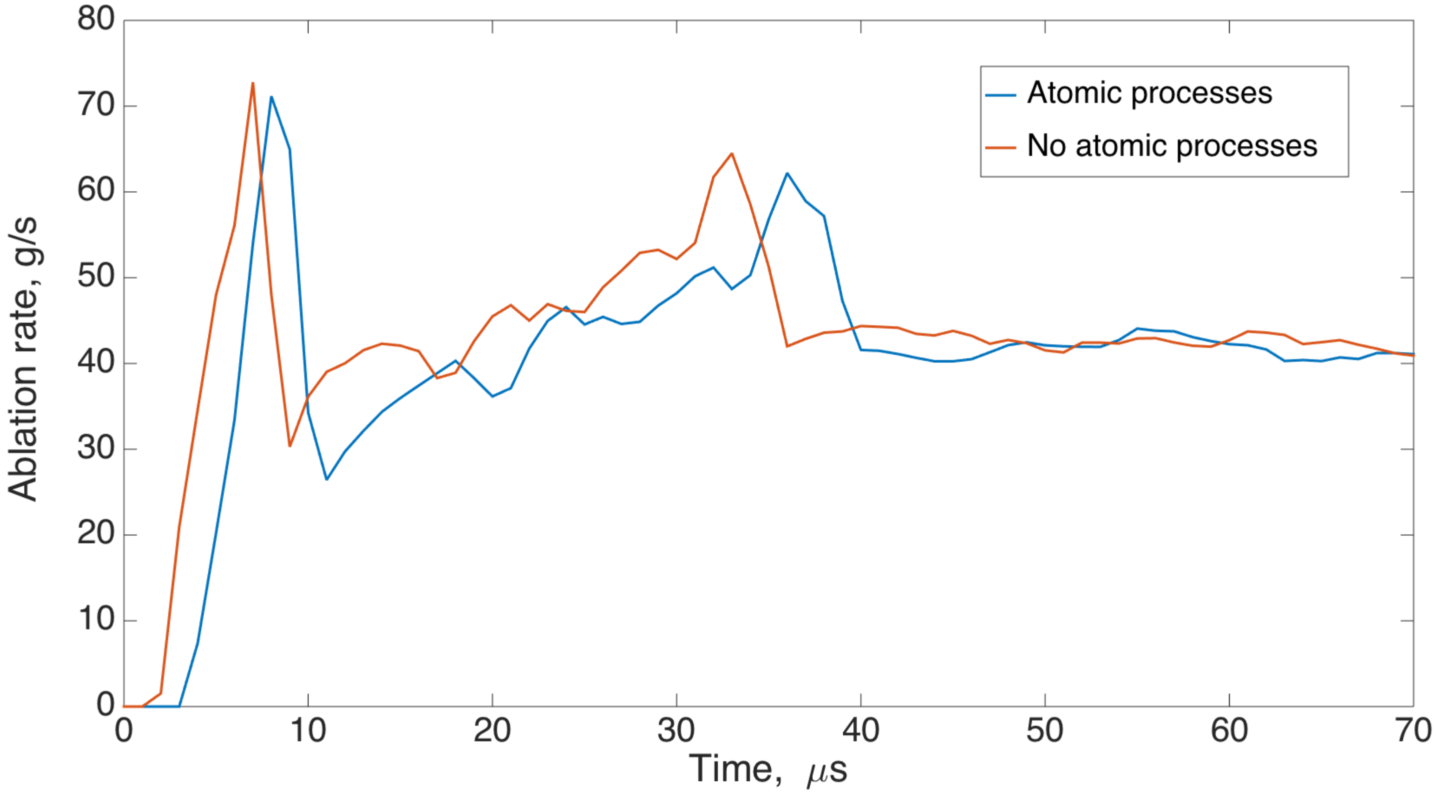
20 microseconds

Top: view from near-pellet

Bottom: view from far field



Ablation rate in LP simulations



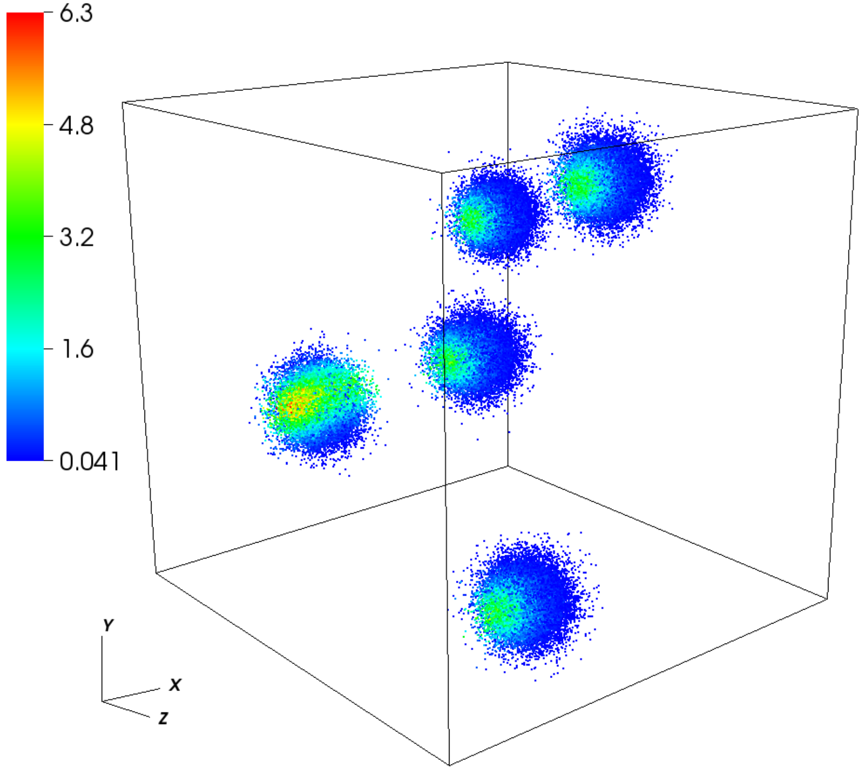
Ablation rates in LP

- Hydro, ideal gas: ~42 g/s (above, red)
- Hydro, average ionization model: ~ 41 g/s (above, blue)

- MHD, average ionization model: ~ 30 g/s
- Numerical convergence was fully reached for hydro simulations (with the increase of number of particles)

SPI simulation

- We have started simulations of multiple pellet fragments
- The density integral calculated on 5 initial pellet clouds. The integral direction is from right to left in x
- Colors show accumulation of integrated line density from one fragment to another



Code coupling ideas

- Lagrangian particle approach is a natural choice for coupling to global tokamak codes:
    - **Eulerian approach (FronTier) is not ideal for coupling**: the background plasma is part of simulation and, therefore, must have artificial properties in hydro simulations
    - Difficult to separate ablated material from background
    - Density cut-offs cause problems in simulations as well

    - **Lagrangian approach (LP):** the background plasma is not simulated (correct properties are assigned implicitly)
    - Ablated material can be tracked for large distances
    - Full 3D simulations

- With GA collaborators, we started working on the ideas for code coupling
    - LP will provide sources to NIMROD and M3D-C1 codes
    - Density, temperature, ionization etc. of sources will be presented in terms of the same sets of basis functions used by tokamak MHD codes