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Modeling and Simulation of Ablation of Single Pellet and SPI

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Talk Overview

- Introduction and research objectives

- Main Physics Models and Algorithms

- Simulations of single pellet injection with FronTier and Lagrangian Particle Code
  - Verification of Scaling laws
  - Hydro and MHD simulations, ablation rates

- Progress on simulation of SPI

- Ideas for coupling to NIMROD / M3D-C1

Introduction: Overview of Main Approaches to Pellet Modeling

Local pellet ablation studies [Parks, Kuteev, Ishizaki, Samulyak,…]:
- Small length scales studies compared to the tokamak scale
- Resolution of all relevant physics processes on the pellet surface and in the ablation cloud
- 1D (spherically symmetric) theoretical models, 1D and 2D (spherically and cylindrically symmetric) numerical simulations
- Resolution of details of pellet ablation and computation of ablation rates
- Spherically and cylindrically symmetric approximations are not applicable to SPI

Global pellet ablation studies [V. Izzo, Fil, Kolemen, D. Hu, C. Kim]:
- Use typical MHD codes / tokamak transport codes with the addition of analytic source terms
- Compute transport of ablated material in the entire tokamak
- Analytic source terms are not very accurate (3D effects, MHD, interaction / screening of fragments in SPI affect ablation rates)

Our Research Objectives

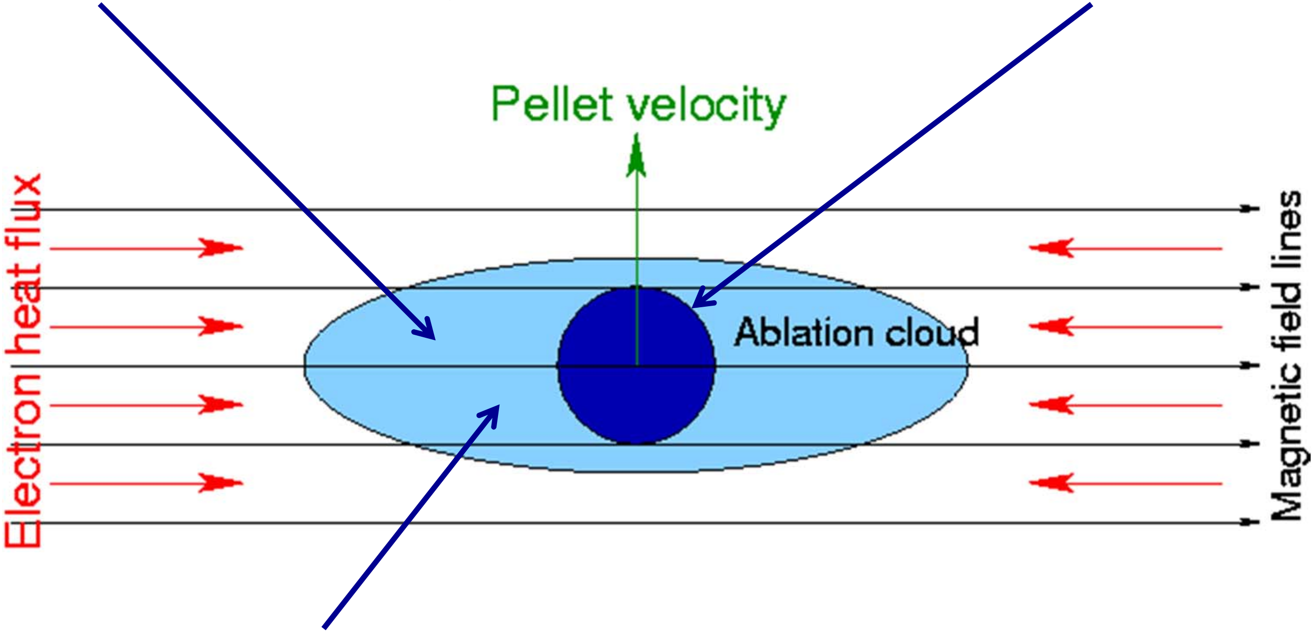
- Develop **improved local models** for pellet ablation simulation (SBU)
  - 2D axisymmetric and full 3D
  - Suitable for both single pellets and SPI (simulations of hundreds of fragments in 3D)
  - Two codes are currently used: FronTier and Lagrangian Particle code

- Develop **improved global models** for pellets and SPI (SBU in collaboration with PPPL and GA)
  - Perform multiscale coupling of local pellet / SPI model based on Lagrangian particles with M3D-C1 and NIMROD

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 and tabular EOS based on solution of Saha equations)
- Radiation model
- Electric conductivity model

Simulation Codes. (1) FronTier

- All physics models outlined above are implemented in two pellet ablation codes: **FronTier** and **Lagrangian Particle** code

- **FronTier**: a grid based Eurerian code with explicit tracking of material interfaces (pellet ablation surface)
- Pellet ablation code based on FronTier developed 10+ years ago
- Excellent agreement with (improved) Neutral Gas Shielding model by P. Parks and scaling laws
- Simulations of fueling (DT) pellets and the influence of geometry, atomic processes, plasma properties, and magnetic field on ablation rates
- Not optimal for 3D SPI simulations
- Not optimal for coupling with tokamak MHD codes
- Currently FronTier is used for single pellet simulations and for verification / code comparison with Lagrangian particle approach

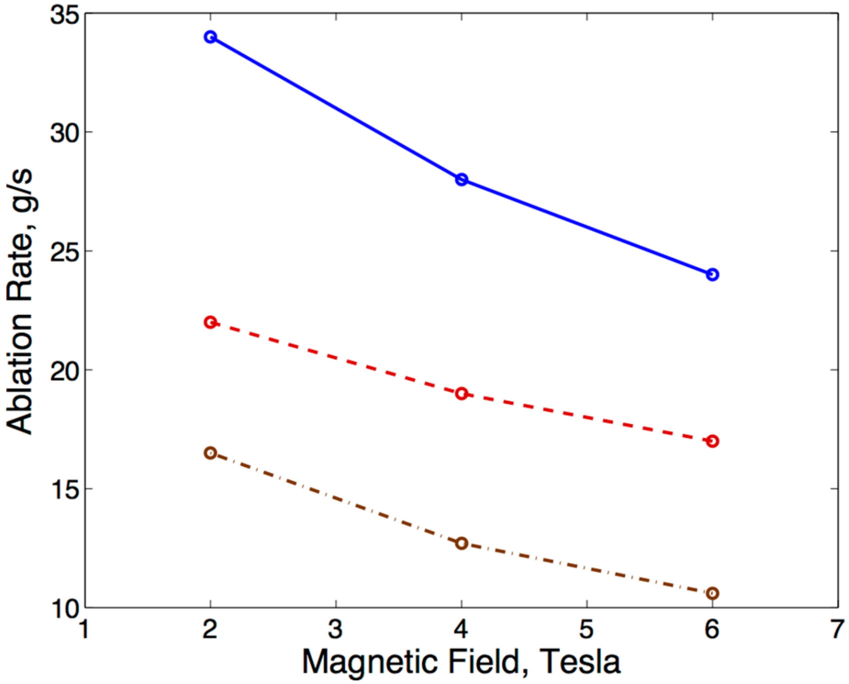
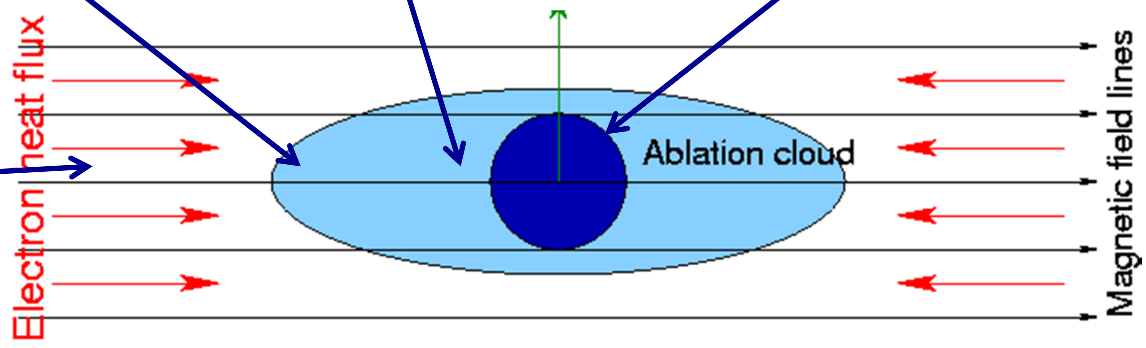


Figure: Solid line: n_e = 1.e14, t_p (pedestal travel time) = 10 microseconds
Dashed line: n_e ~ 1.e13, t_p = 10 microseconds
Dash-dotted line: n_e ~ 1.e13, t_p = 5 microsec.

Pellet / SPI model based on Lagrangian particles

- A new pellet model has been developed based on Lagrangian Particle (LP) method and software for hydrodynamics
- Lagrangian treatment of ablated material – eliminated numerical difficulties caused by hot background plasma (see schematic below)
- Ablated material can be tracked during long time / distances
- Optimal and continuously adapting resolution results in small computing time
- LP is usable for hundreds of fragments in 3D
- Significantly reduced stability conditions for Lagrangian flows
- Lagrangian approach provides a natural platform for coupling with global MHD codes



Ablated material far away from the pellet: T ~ 10 eV, low density

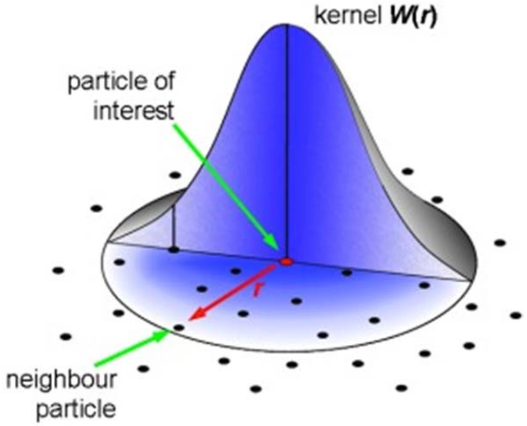
High-density cloud near the pellet: T ~ 1 - 2 eV

Pellet surface: T ~ 20 K

Background plasma: T ~ 2 keV, ‘vacuum’ density compared to ablation cloud

Main Ideas of the Method of Lagrangian Particles. Introduction to SPH

- Motivation: improve accuracy of Smooth Particle Hydrodynamics (SPH).



In SPH, density is computed using particle distribution as

$$\rho(\mathbf{r}) = \sum_b m_b W(\mathbf{r} - \mathbf{r}_b, h)$$

$$A(\vec{r}) = \int A(\vec{r}\,')\,\delta(\vec{r} - \vec{r}\,')\,d\vec{r}\,' \longrightarrow A^W(\vec{r}) = \int A(\vec{r}\,')\,W(\vec{r} - \vec{r}\,', h)\,d\vec{r}\,'$$

$$\longrightarrow A_i^W = \sum_j \frac{m_j}{\rho_j} A_j W_{ij}(h) \longrightarrow \nabla A_i^W$$

- SPH is a popular Lagrangian method for hydrodynamics, but it is known to be inaccurate
  - Traditional SPH has very low accuracy of derivatives (zero-order, non-convergent)
  - SPH derivative are accurate and convergent only if particles are placed on a rectangular mesh (due to cancellation of cross-terms)
  - Accuracy rapidly decreases if particles even slightly deviate from the mesh
  - The chain above is not based on rigorous approximation theory

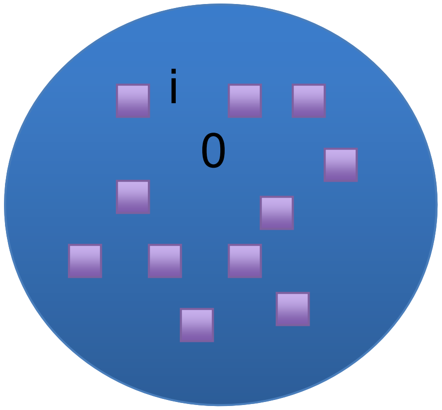
Computing Derivatives in Lagrangian Particles: Local Polynomial Fitting (Generalized Finite Differences)

- 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* neighbors:

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

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

New Lagrangian Particle Method

- LP proposes new and consistent way to discretize equations based on general principles of approximation theory (without using smoothed kernels). It does not just improve differential operators of SPH
- Replacing SPH derivatives with very accurate GFD (generalized finite difference) derivatives produces an unconditionally unstable code!
    - Why bad derivatives lead to a stable discretization and accurate derivatives lead to an unstable scheme?
    - The answer is in the hidden Hamiltonian property of SPH: Inaccurate SPH discretization of Euler equations is identical to accurate Lagrange / Hamilton equations for this particle system (interacting via isentropic potential energy)
- The method has been extensively verified and successfully compared with other codes for test problems involving complex hydro flows

Reference: R. Samulyak, X. Wang, H.-S. Chen, Lagrangian Particle Method for Compressible Fluid Dynamics, J. Comput. Phys., 362 (2018), 1-19.

Lagrangian Particle Method: 1D illustration

- Equations of compressible hydrodynamics can be written as $U_t + A(U)U_x = 0,$

$$U = \begin{pmatrix} V \\ u \\ P \end{pmatrix}, \quad A(U) = V \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & K & 0 \end{pmatrix}, \quad K = \left(P + \frac{\partial e}{\partial V}\right) \Big/ \frac{\partial e}{\partial P}$$

- Performing matrix diagonalization, we obtain three advection equations

$$U_t + R\Lambda R^{-1}U_x = 0,$$

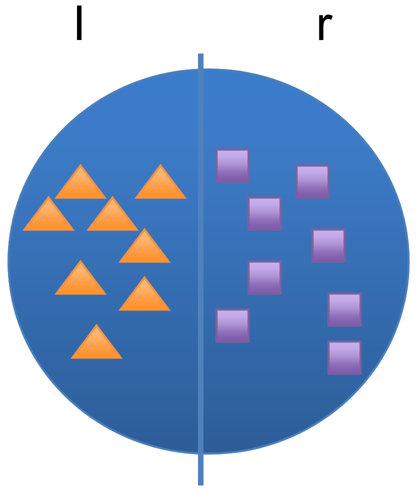
$$R^{-1}U_t + \Lambda R^{-1}U_x = 0,$$

$$\Lambda = V \begin{pmatrix} 0 & & \\ & \sqrt{K} & \\ & & -\sqrt{K} \end{pmatrix} \quad R^{-1} = \begin{pmatrix} 1 & 0 & \frac{1}{K} \\ 0 & -\frac{1}{2\sqrt{K}} & -\frac{1}{2K} \\ 0 & \frac{1}{2\sqrt{K}} & -\frac{1}{2K} \end{pmatrix}$$

Upwind Lagrangian Particle Method

- Advection equations can be transformed as follows. Adding the subscripts l and r to the spatial derivatives

$$
\begin{aligned}
V_t &= \frac{V}{2}\left(u_{xr}+u_{xl}\right) - \frac{V}{2\sqrt{K}}\left(P_{xr}-P_{xl}\right), \\
u_t &= \frac{V\sqrt{K}}{2}\left(u_{xr}-u_{xl}\right) - \frac{V}{2}\left(P_{xr}+P_{xl}\right), \\
P_t &= -\frac{VK}{2}\left(u_{xr}+u_{xl}\right) + \frac{V\sqrt{K}}{2}\left(P_{xr}-P_{xl}\right).
\end{aligned}
$$



■ : RHS neighbors

▲ : LHS neighbors

- First order discretization of temporal derivatives of the state (V, u or P) at the location of particle j

$$\frac{\mathrm{state}_j^{n+1}-\mathrm{state}_j^{n}}{\Delta t}$$

- Moving the particles

$$\frac{x^{n+1}-x^{n}}{\Delta t} = \frac{1}{2}\left(u^{n}+u^{n+1}\right)$$

- The above yields a first order scheme. 2nd order LP method has been implemented in 2D and 3D in an unsplit way. Higher-order approximations are in progress.

Simulations of Single Pellets and SPI using FronTier and Lagrangian Particle Pellet Codes

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
  - T_e ramped up from 100 eV to 2 keV

- Magnetic field: 6T

- MHD in low magnetic Reynolds number approximation
- Averaged ionization EOS model with radiation losses or
- Tabular EOS based on Saha equation solver
- Improved pellet surface ablation boundary conditions leading to fast convergence

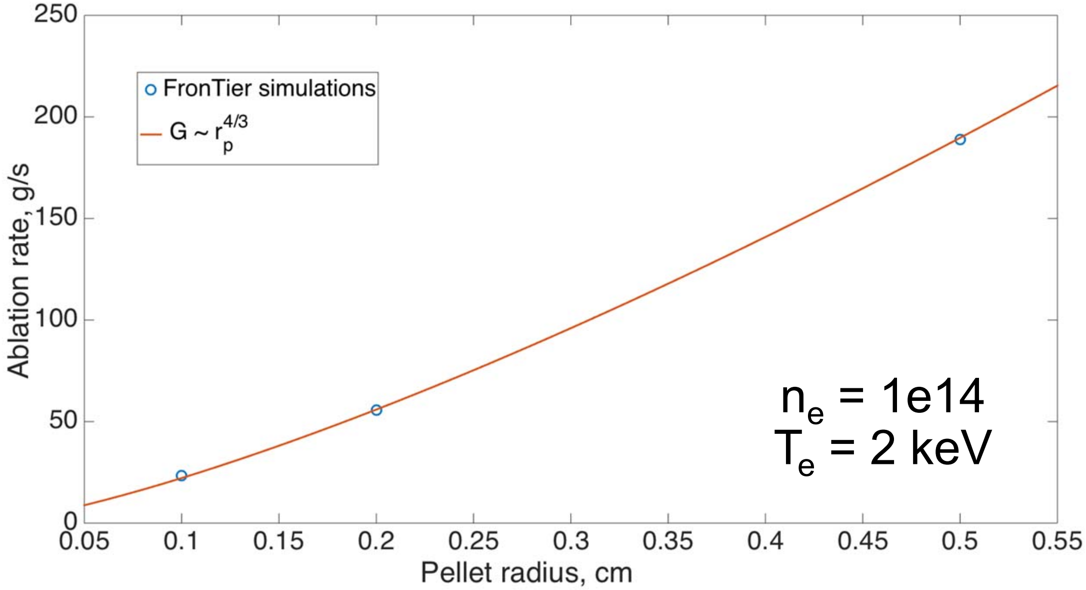
Verification of Scaling Laws for Neon Pellet

Semi-analytic formula (Parks) based on NGS model:

$$G \sim \left(\frac{T_e}{2000}\right)^{5/3} \left(\frac{r_p}{0.2}\right)^{4/3} \left(\frac{n_e}{10^{14}}\right)^{1/3}$$

$$units:$$

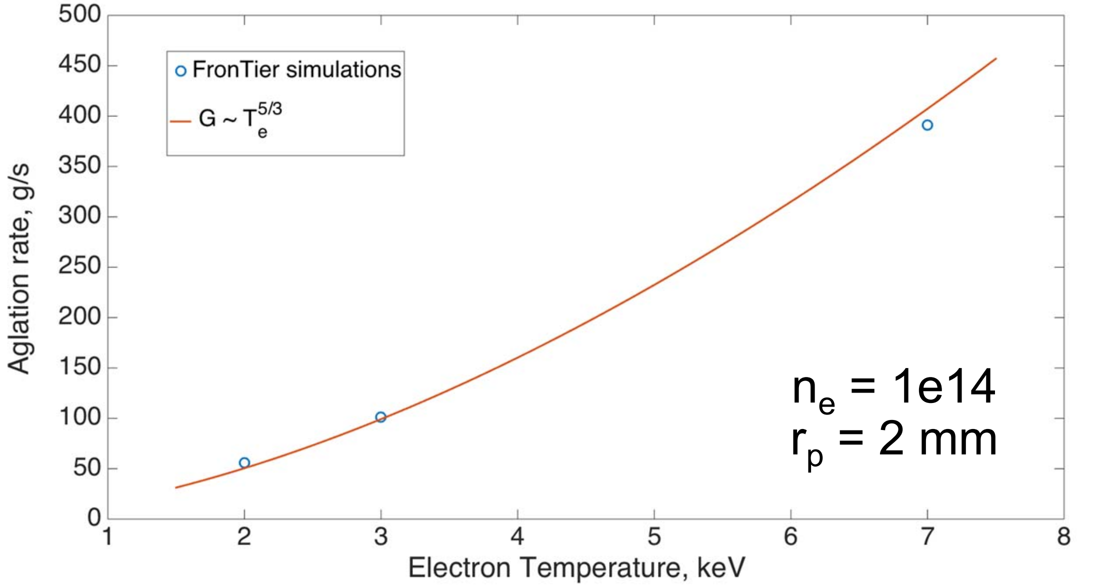
$$G(g/s), \quad T_e(eV), \quad n_e(1/cc), \quad r_p(cm)$$



For the canonical case, the ablation rate is:

- Theory: 52.9 g/s
- FronTier: 53.4 g/s (1D)
- LP: 54 g/s (3D simulation)

- Excellent agreement of theory and simulations using both codes



Verification using D_2 pellets

$$\gamma = 7/5,\ I_* = 7.5\ \text{eV},\ r_p = 2\ \text{mm},\ T_{e\infty} = 2\ \text{keV},\ n_{e\infty} = 10^{14}\ \text{cm}^{-3}$$

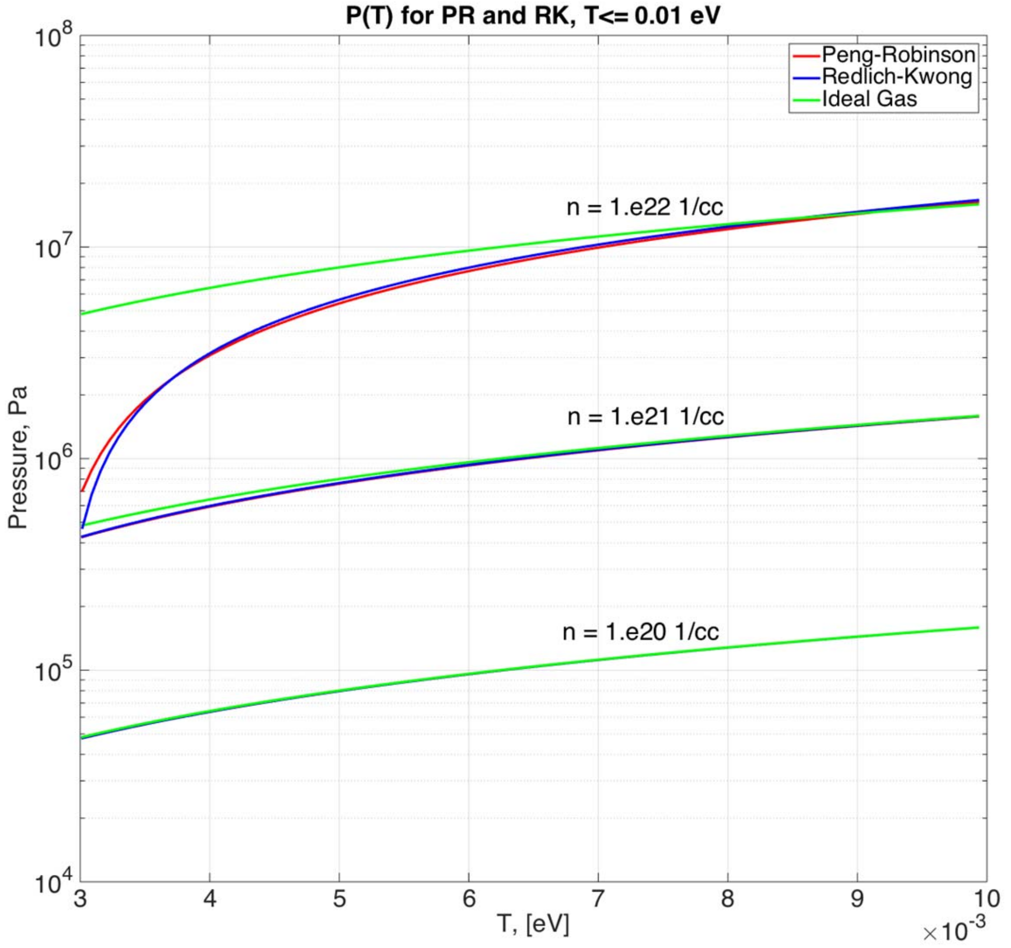
(No atomic processes included and no electrostatic shielding)

	G (g/s)	T_* (eV)	r_* (mm)	P_{sur}/p_*
Semi-analytic Parks[*]	119.1	3.5616	5.161	4.844 $p_* = 27.8$ bar
CAP[**] **code**	120.7	3.65	5.25	4.66
FronTier June 2018	119.2	3.580	5.18	5.13 $p_* = 27.7$ bar

[*] Parks, "The ablation rate of some low-Z pellets in fusion plasmas using a kinetic electron energy flux model"

[**] Ishizaki and Parks, Phys Plasmas **5**, 1968 (2004)

Influence of non-ideal EOS model



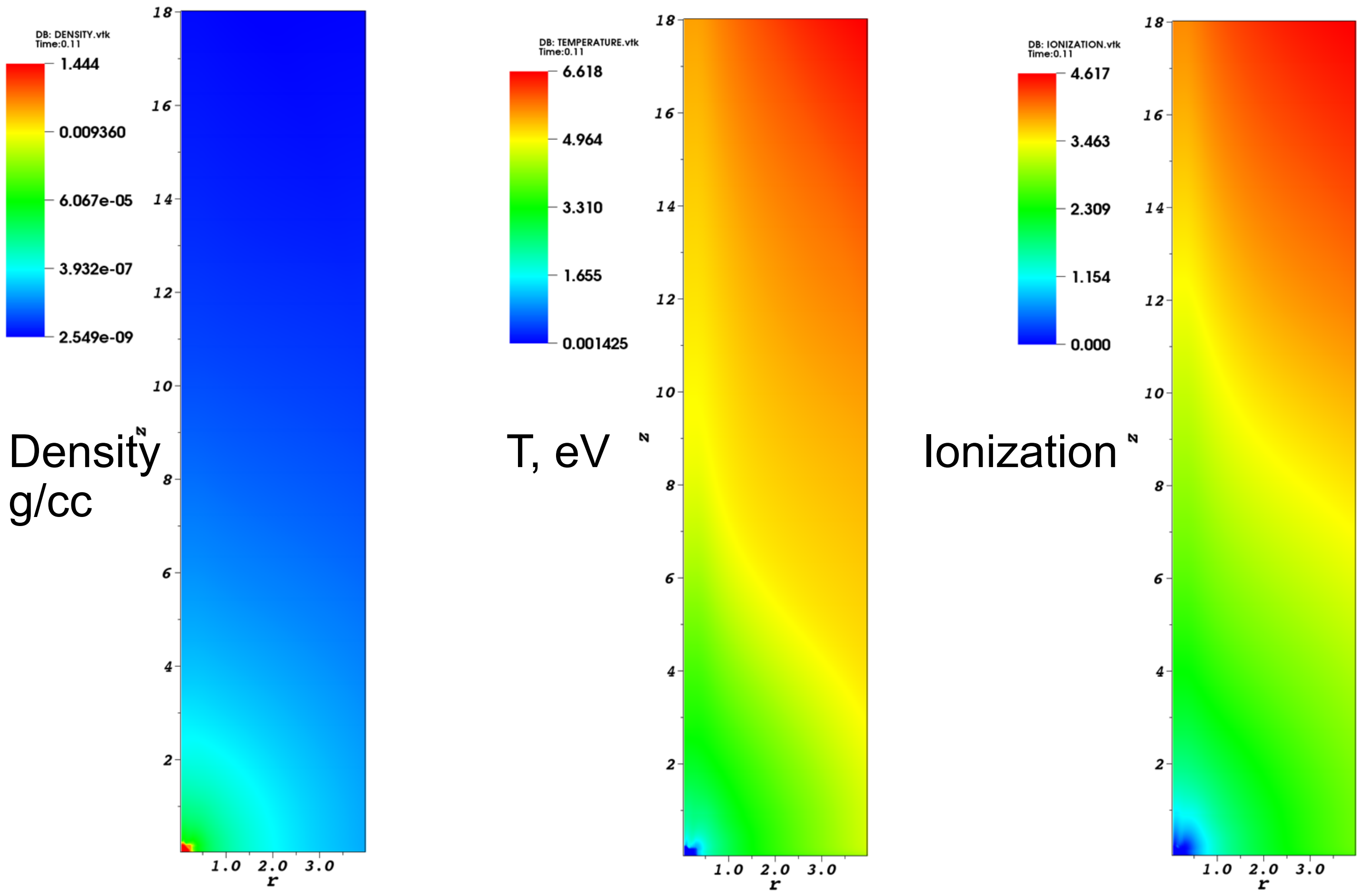
- To account for non-ideal properties of the ablated material in the cold, dense layer near the pellet, Redlich-Kwong and Peng-Robinson EOS models were implemented and tested

- RK and PR EOS models deviate from the ideal model only for densities larger than 1.e22 1/cc and T lower than 0.01 eV

- RK and PR EOS are practically identical

- Pellet simulations showed that it non-ideal EOS has negligibly small effect on pellet ablation properties and the ablation rate compared to the ideal EOS model

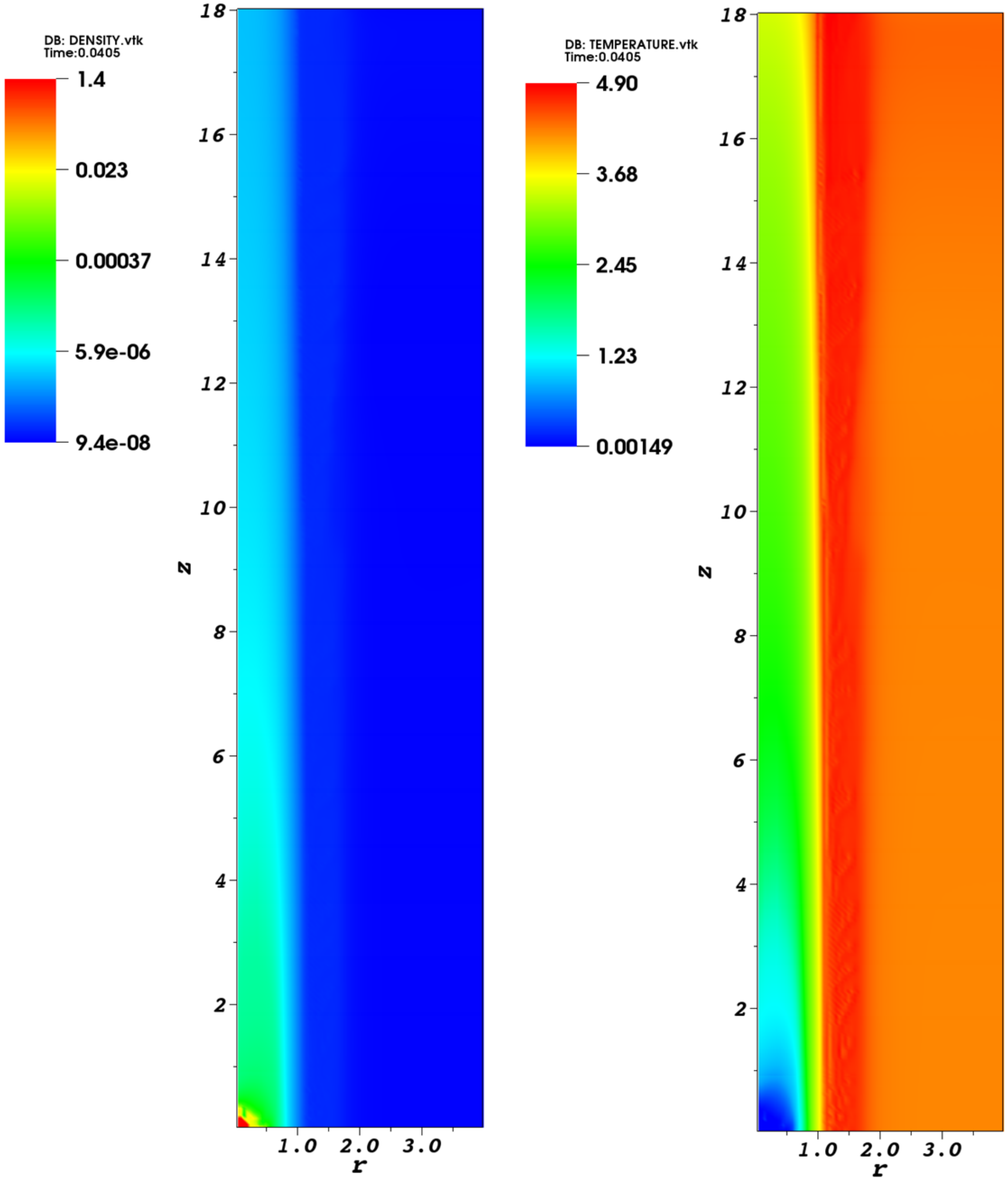
2D FronTier hydro simulations of neon pellet



Density, Temperature, and Ionization at 100 microseconds

- In hydro simulations, the role of magnetic field is reduced to directing the electron heat flux along magnetic field lines
- Simulations study the influence of geometry and atomic processes on the ablation rate
- Ionization reduces temperature and velocity, but it increases density, resulting in a similar ablation rate

2D FronTier MHD Simulatins: 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 Lorentz Force (LF).

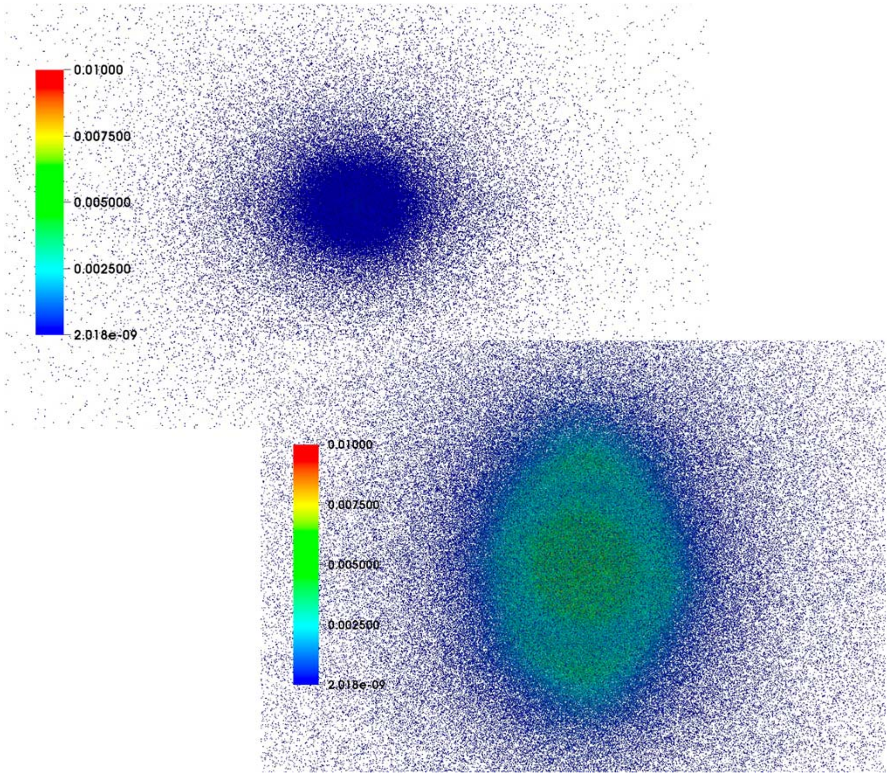
This cutoff starts at 1e-7 g/cc and the heat deposition and LF are reduced to 0 at density=1e-8 g/cc.

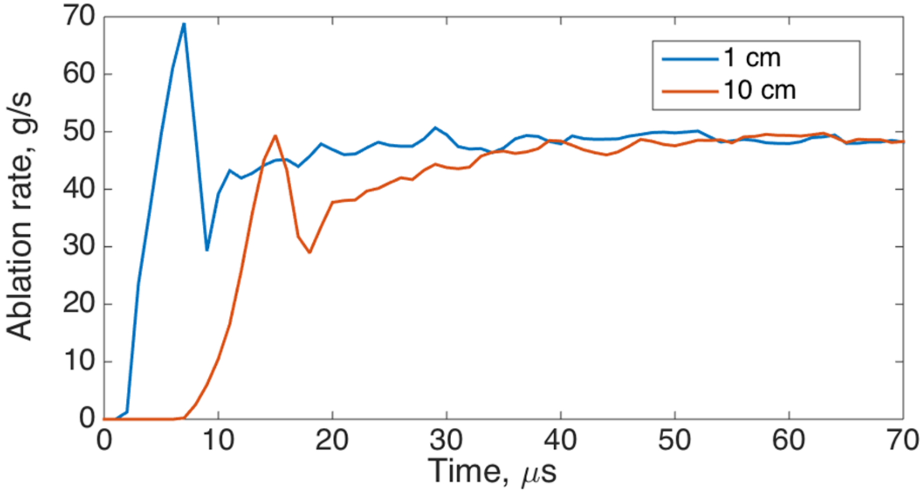
Using this technique we are able to run the code for 40 microsec.

Ablation rate: ~27 g/s.

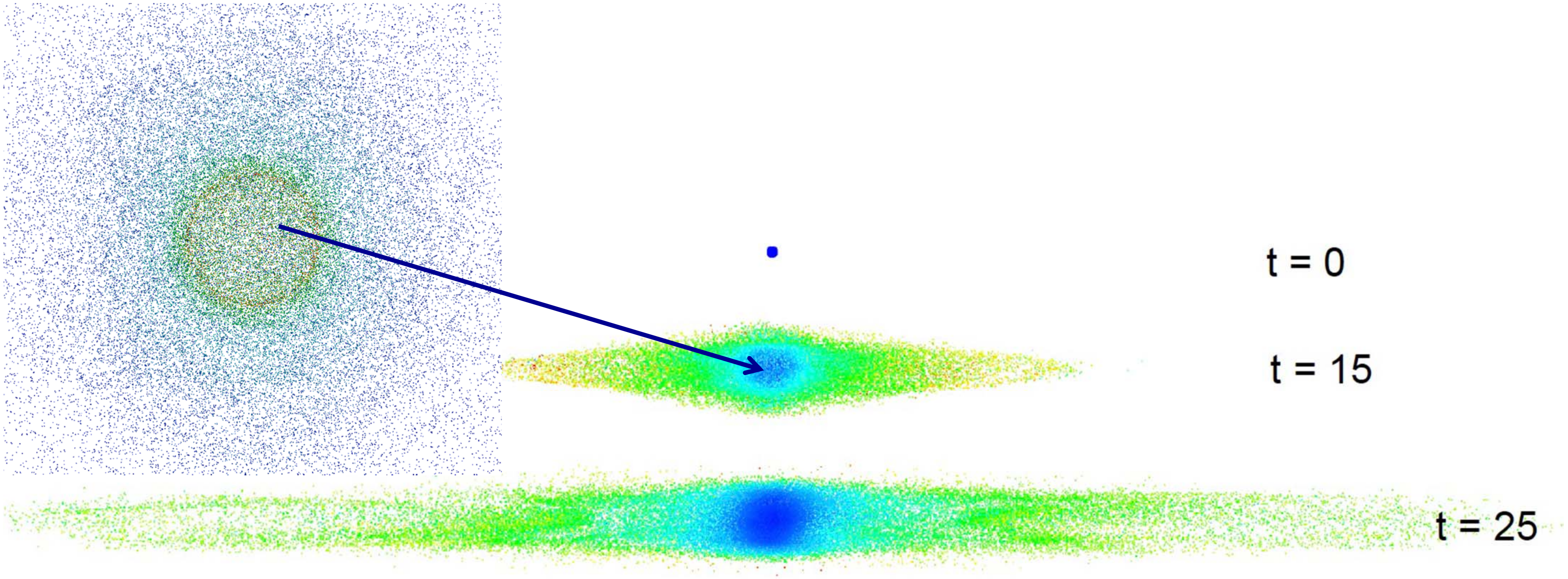
3D Hydro Lagrangian Particle Simulations

- Hydrodynamic simulation of 2 mm neon pellet ablation
- Top: view from far-field
- Middle: zoom-in dense ablation cloud near the pellet surface
- Bottom: evolution of pellet ablation rateswith directional heating computed at various distances to the pellet. The ablation rate is reduced to 48 g/s
- Consistently with FronTier, very small effect of atomic processes on the ablation rate observed
- Due to high level of adaptivity, 3D LP code runs much faster than 2D FronTier with the same resolution near the pellet





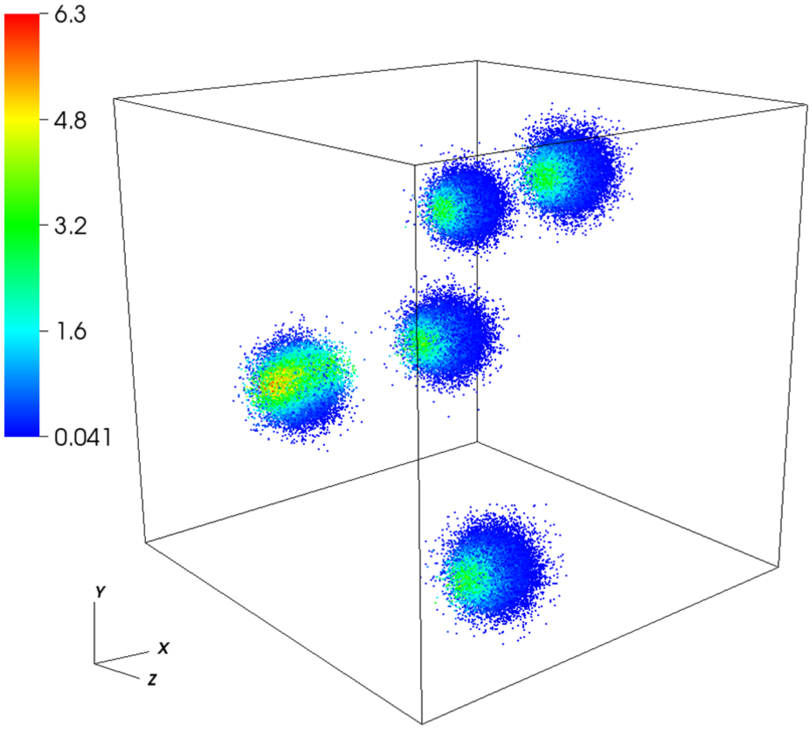
3D MHD Lagrangian Particle Simulations: evolution of ablation channel

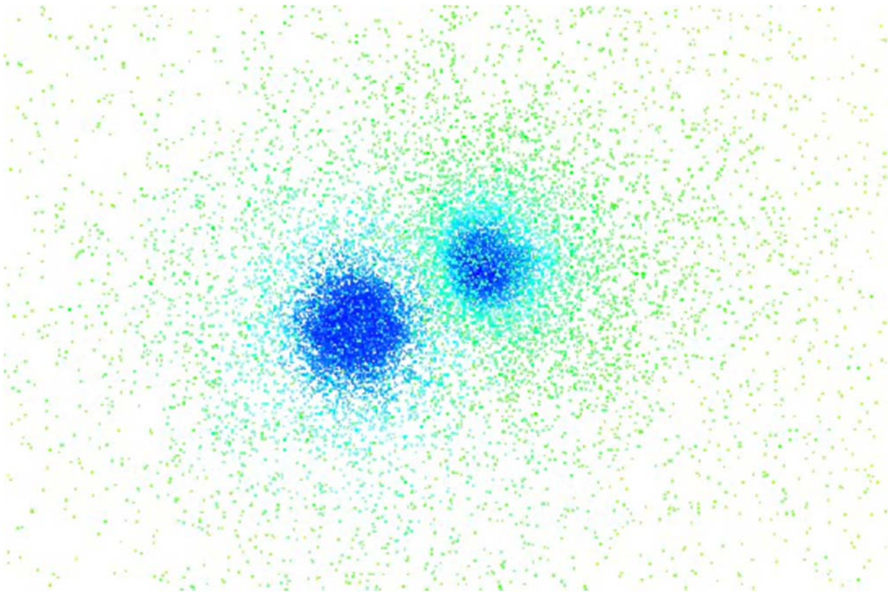


- MHD simulation of the formation and evolution of a pellet ablation cloud in 6T magnetic field
- Distributions of the ablated material are shown at the initial time (top image), at 15 microseconds (middle image), and 25 microseconds (bottom image)
- During the warm-up time, equal to 10 microseconds in the present simulations, the background electron density is linearly ramped-up to its maximum value, modeling the plasma pedestal
- Ablation rage is ~ 30 g/s

3D simulations of SPI using Lagrangian particle code

- Left image: distribution of the line density integral for the kinetic heating model
- Right image: ablation flow in the vicinity of two fragments
- Reduction of the ablation rate due to the partial screening of ablation clouds is currently being investigated





Global Pellet ablation code: ideas for coupling with NIMROD / M3D-C1:

- Lagrangian particle approach is very promising for coupling with global tokamak codes:
    - No need for overlapping domain decomposition typical for grid-based codes
    - No artificial plasma background is present in LP simulations – only ablated material is evolved. Easy to extract ablation flow data.

- Stage 1: loose coupling. Pre-compute pellet / SPI ablation data and use them as source terms in global MHD codes

- Stage 2: Strong coupling

    - Global MHD and Pellet codes are linked and run in parallel on a supercomputer using different nodes / communicators (a light version of LP code will be used – stripped of all functions not relevant to the pellet ablation model).
        - LP pellet code can be implemented based on the current PIC module in NIMROD

    - Data exchange is performed at the time step of the global MHD code

    - Pellet code data is represented in terms of basis functions of the global code and corresponding coefficients are sent to the global MHD code

Summary and Future Work

- Developed new Lagrangian particle pellet code for 3D simulations of SPI
- Improved numerous features in the FronTier-based pellet code
- Implemented new physics models in both codes:
    - Tabular EOS with atomic processes based on Saha solver
    - Zeldovich average ionization EOS model
    - Non-ideal EOS (Redlich-Kwong) for cold, dense gas
    - Radiation models
    - Improved pellet surface ablation model

- Performed verification simulations and code comparison
    - Excellent agreement of theoretical predictions and simulations using both codes for spherically-symmetric case

- Studied the influence of atomic processes, directional heating, and MHD forces on the ablation rate of neon pellets
    - Very small influence of atomic processes, consistent in both codes, is not well understood

- Started 3D simulations of SPI
- Work on coupling with global tokamak MHD codes (M3D-C1 and NIMROD) has started
- Future: comparison with experiments and code coupling