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Progress on simulations of pellets and SPI with detailed near-field models and coupling to M3D-C1/NIMROD

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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
- Coupling of LP pellet code to NIMROD / M3D-C1

Introduction: Overview of Main Approaches to Pellet Modeling

Local or near-field 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 or far-field 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

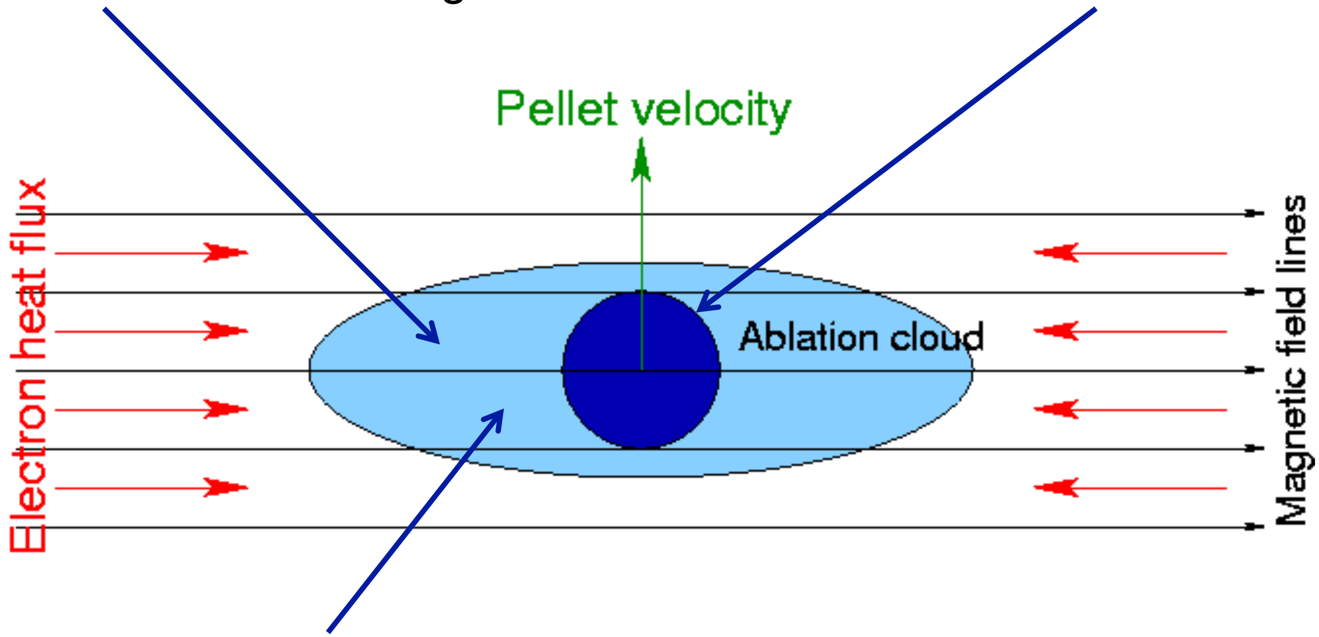
- Develop **improved local models** for pellet ablation simulation (SBU)
  - 2D axisymmetric and full 3D
  - Suitable for both single pellets and SPI (simulations of hundreds of fragments in 3D)
  - Two codes are currently used: FronTier and Lagrangian Particle code

- 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

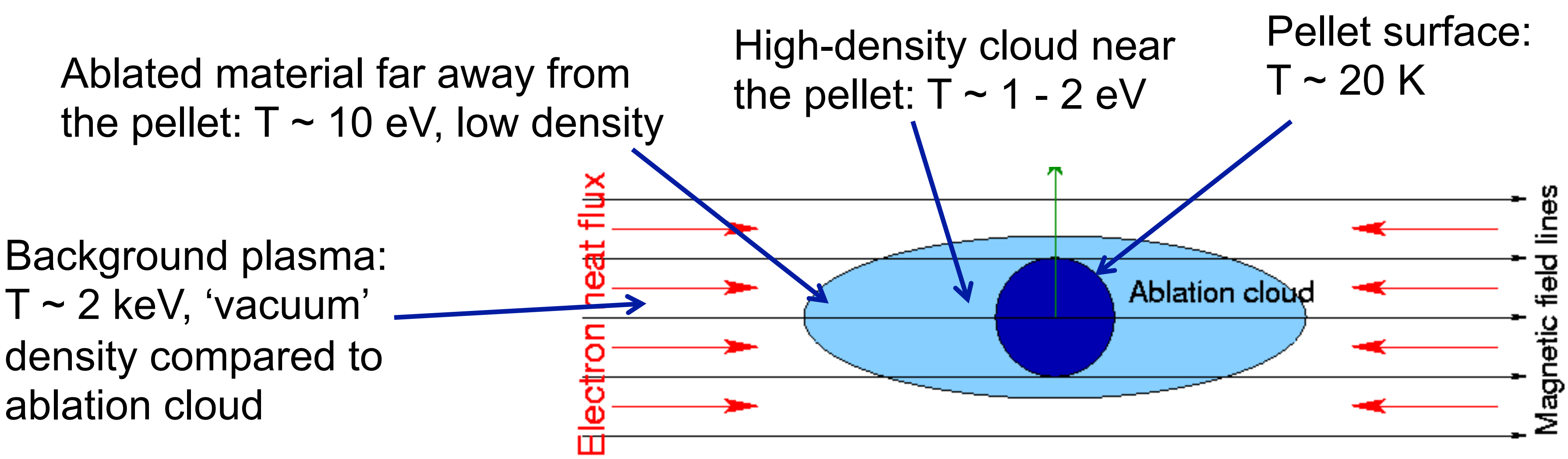
Simulation Codes. (1) FronTier

- 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

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



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

Typical Simulation Parameters:

- Background electron density: 1.e14 1/cc – electrostatic shielding = 1.0682×10^{13}/cc
- 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: 2 - 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

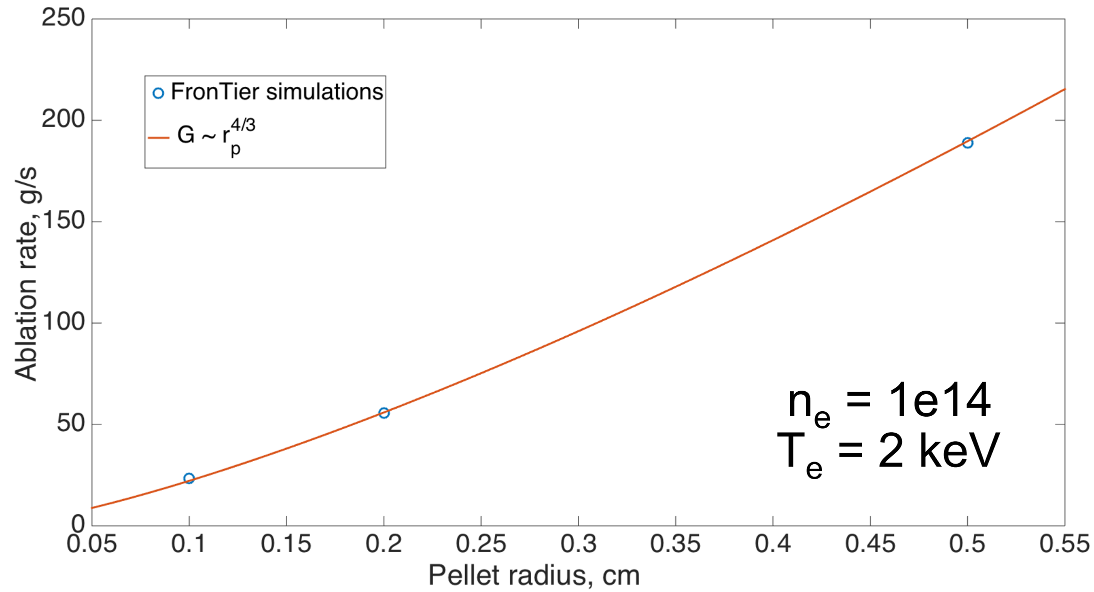
Verification of Scaling Laws for Neon Pellet

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 :

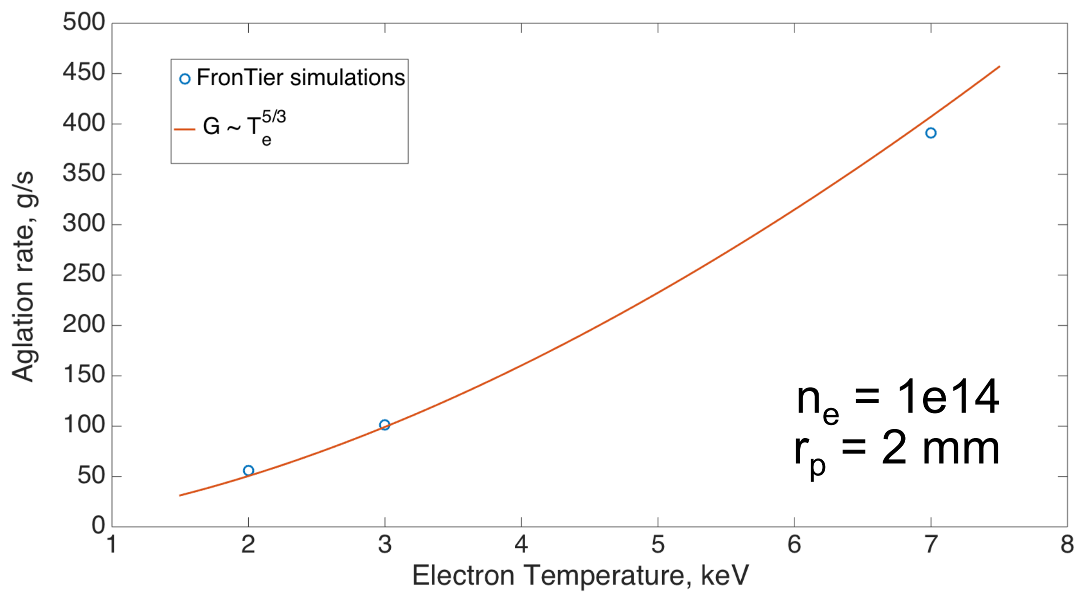
$$G(g/s), \quad T_e(eV), \quad n_e(1/cc), \quad r_p(cm)$$



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)

Ablation rates clarifications

- Ablation rate for Ne with ionization in 1D spherical symmetric case comparable to ideal gas case
  - Ionization significantly reduces temperature, sound speed, and the ablation flow speed
  - In terms of the ablation rate, **the influence of ionization is negligibly small**

- Ablation rates for D2 has been verified against pusblished results (Samulyak et al, *Nucl. Fus.*,2007) for new FT-LITE solver.

- In D2 case, it has been observed that dissociation is mainly responsible for the reduction of the ablation rate due to lower dissociation energy (4.5 eV < 13.6 eV for ionization)

- If only ionization is considered, the ablation rate is negligibly smaller than for the ideal case.

EOS Issues

- Atomic processes / ionization:
    - The previously used Zeldovich average ionization model is not very robust (results depend on initial settings) and very slow (nonlinear solvers); it is not accurate at low T
    - tabular EOS with thermodynamic data obtained from solving Saha system.
    - We built a tabular EOS with thermodynamic data obtained from solving the coupled Saha system; bi-cubic interpolation
    - Achieved **6 – 8 x** code speedup with new EOS (no nonlinear equation to solve at each time step for each point)
    - We built tables for neon and deuterium. Non-equilibrium EOS data sets can be used as well

- 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
    - Conclusion: non-ideal EOS has negligibly small effect on pellet ablation properties and the ablation rate compared to the ideal EOS model

3D Hydro Lagrangian Particle Simulations

- Hydrodynamic simulation of 2 mm neon pellet ablation

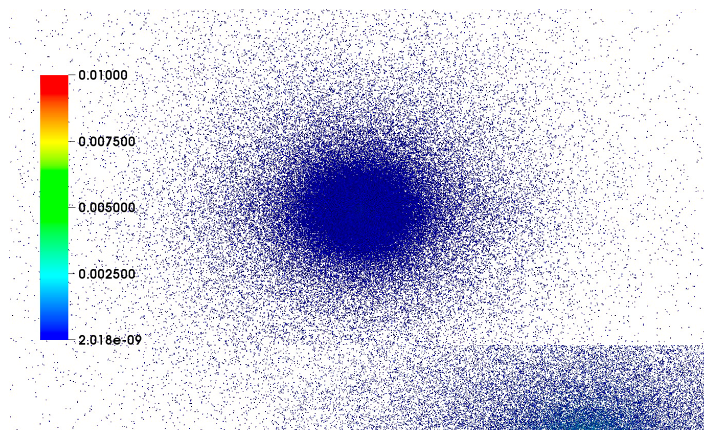
- Top: view from far-field

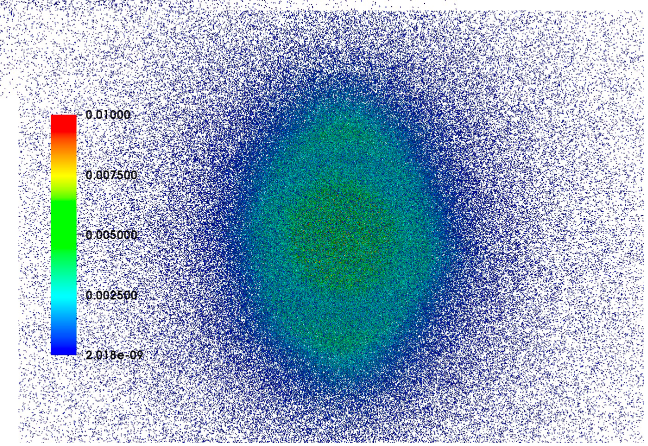
- Middle: zoom-in dense ablation cloud near the pellet surface

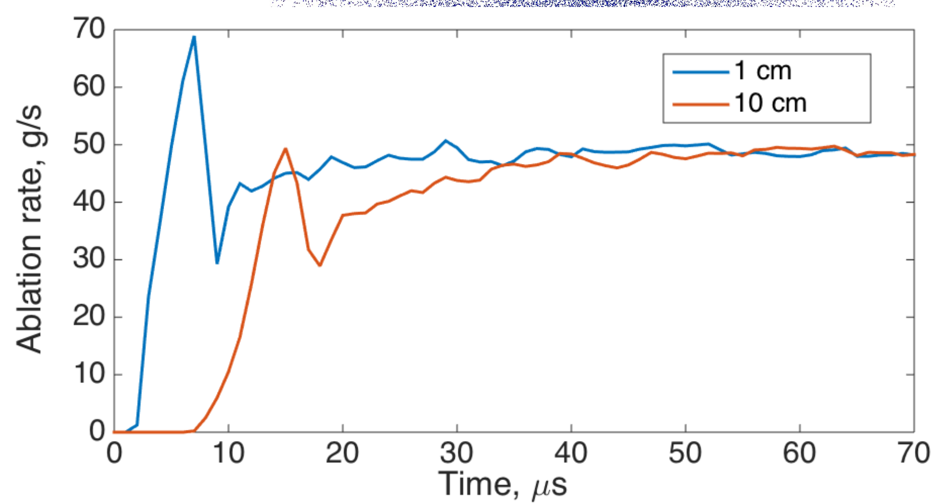
- Bottom: evolution of pellet ablation rateswith directional heating computed at various distances to the pellet. The ablation rate is reduced to 48 g/s

- Consistently with FronTier, very small effect of atomic processes on the ablation rate observed

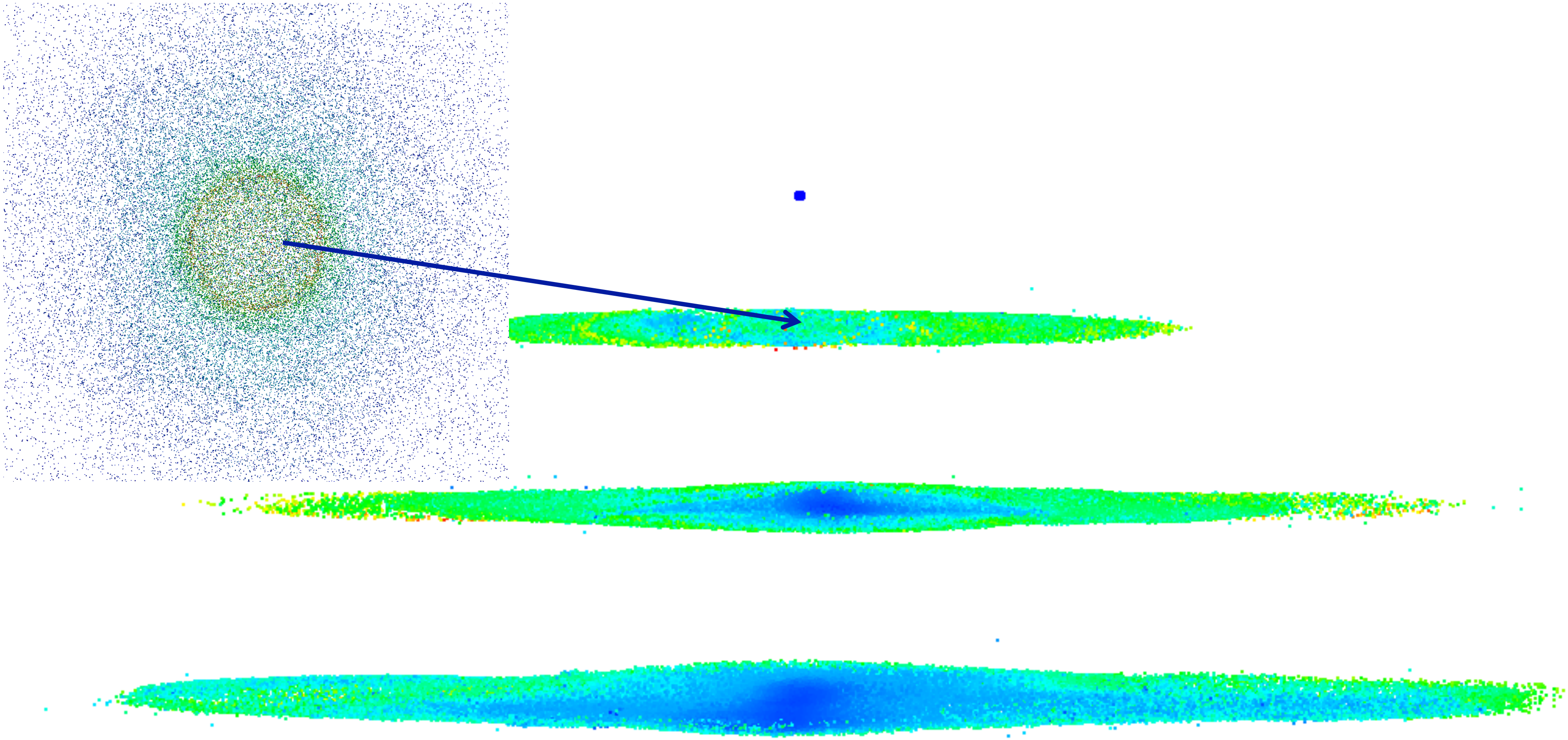
- Due to high level of adaptivity, 3D LP code runs much faster than 2D FronTier with the same resolution near the pellet





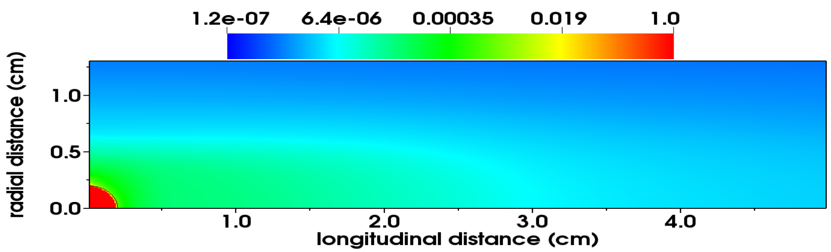


3D Lagrangian particle simulations of neon pellet

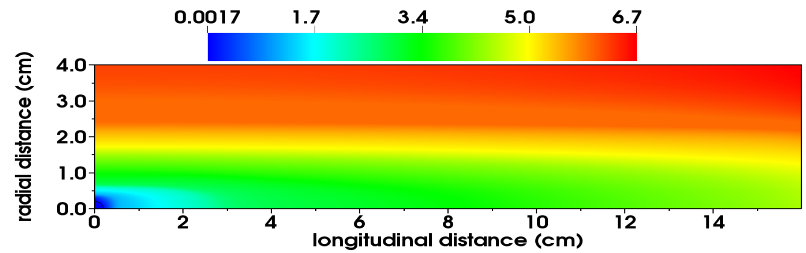


MHD simulation of the formation and evolution of pellet ablation cloud in 2T magnetic field using Lagrangian particles. Distributions of the ablated material are shown, from top to bottom, at the initial time, and 20, 40, and 60 μs. The ablation rate is reduced by factor 1.38.

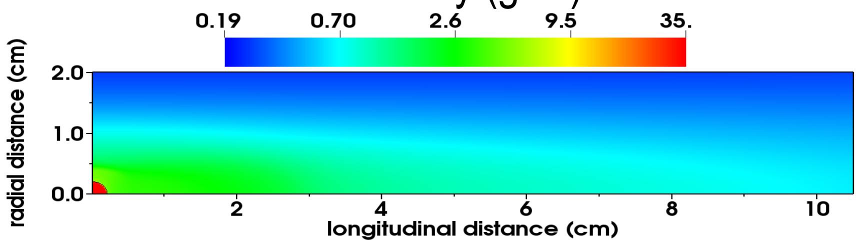
2D Axysymmetric FronTier MHD Simulation



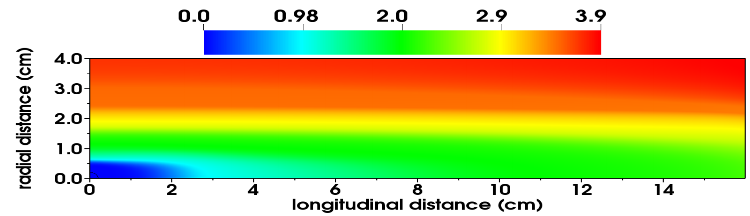
Density (g/cc)



Temperature (eV)



Pressure (bar)



Ionization

FronTier simulation of the ablation channel along magnetic field lines at 6T

- In the past, we reported difficulties with instabilities associated with the heating of vacuum (background plasma). To resolve these instabilities, density cutoffs were applied: the heat deposition and LF were reduced from max value to 0 as density reduces from 1e-7 g/cc to 1e-8 g/cc.

- Artificial cutoffs led to low accuracy (due to radial velocity profiles)
- All artificial cutoffs are completely eliminated in the improved version of the code. Numerical problems were resolved by improving the quality of WENO solvers.

Summary of Ablation Rates

	0T	2T	4T	6T
FT, G (g/s)	35	24.9	19.2	13.7
FT, G reduction	--	1.4	1.82	2.55

FronTier: 2D asisymmetric simulations with radiation

Lagrangian Particles: 3D simulations without radiation give the following ablation rates
0T: 40 g/s   2T: 29 g/s   Reduction: 1.38

We started to build pellet ablation rate database by computing ablation rated and ablation cloud properties for by varying the pellet size, magnetic field strength, plasma temperature and density.

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

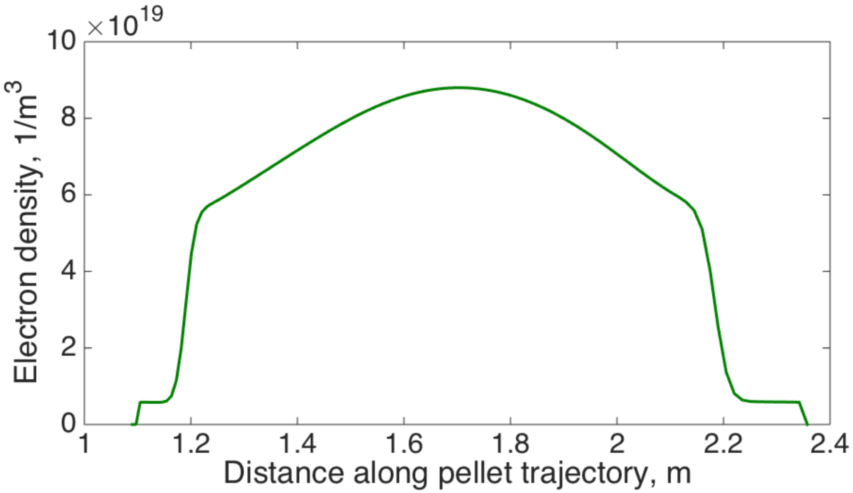
    - Global MHD and Pellet codes are linked and run in parallel on a supercomputer using different nodes / communicators (a light version of LP code will be used – stripped of all functions not relevant to the pellet ablation model).
        - LP pellet code can be implemented based on the current PIC module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

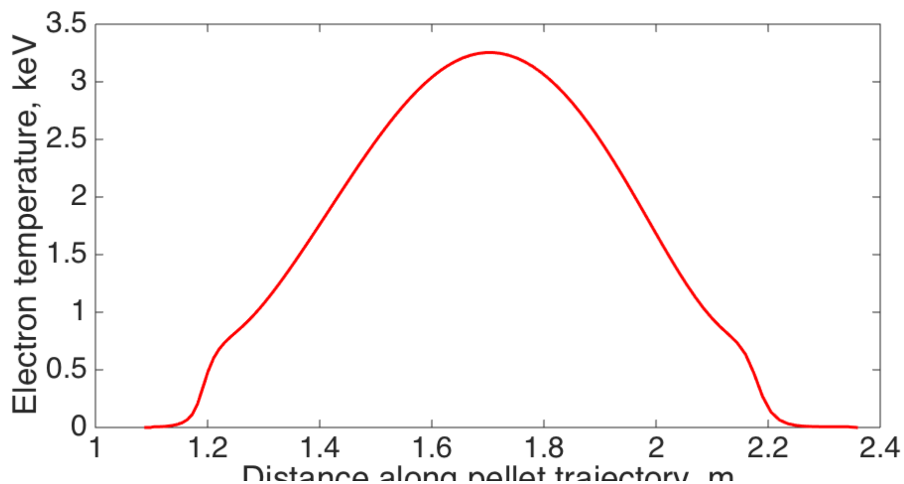
    - Data exchange is performed at the time step of the global MHD code

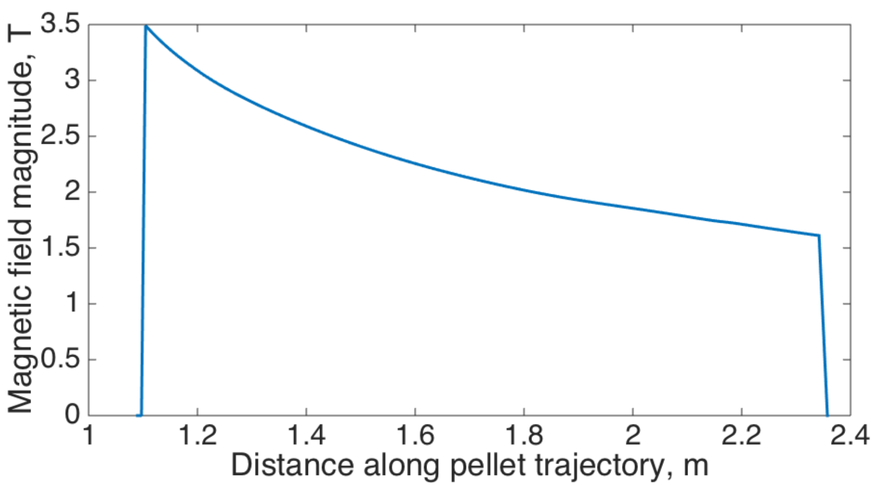
    - Pellet code data is represented in terms of basis functions of the global code and corresponding coefficients are sent to the global MHD code

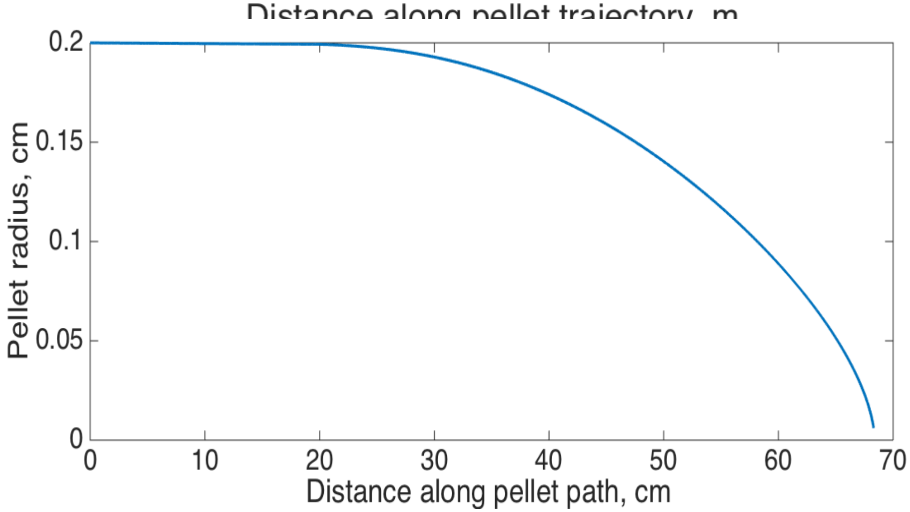
Pellet ablation simulation using data from M3D-C1

- We extract plasma and magnetic field states along pellet trajectory from M3D-C1 simulations data and use them in Lagrangian Particle simulations
- Preliminary result is obtained by combination of computed pellet steady-state ablation rates along the trajectory and scaling laws
- We are working towards a more efficient and self-consistent predictor-corrector approach



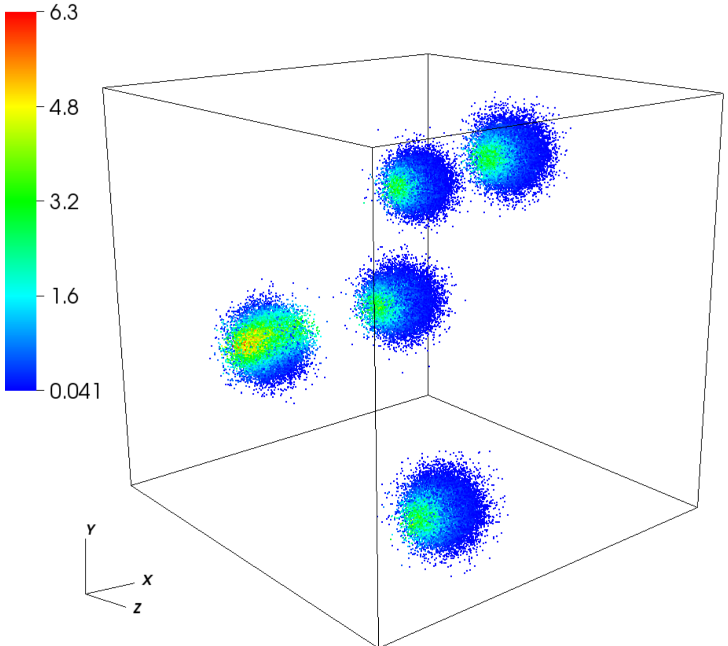


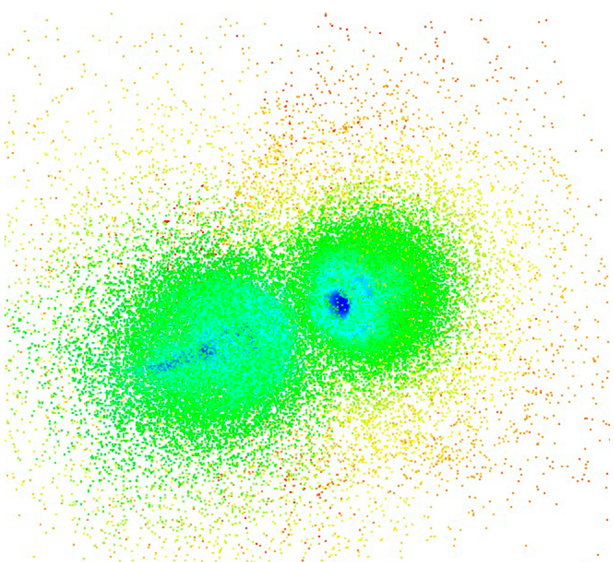




3D simulations of SPI using Lagrangian particle code

- Significantly improves accuracy of line density integrals for kinetic electron heating models
- Reduction of the ablation rate due to the partial screening of ablation clouds is currently being investigated
- Important theoretical issue: improvement kinetic models that account for cooling of electrons streaming through ablation clouds
- Left image: distribution of the line density integral for the kinetic heating model
- Right image: ablation flow in the vicinity of two fragments





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 EOS model, Non-ideal EOS (Redlich-Kwong)
    - 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
- Obtained simulations of pellets using input from M3D-C1 code
- Future: comparison with experiments and code coupling