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# Progress with Near-Field Pellet / SPI Models and Coupling to M3D-C1 and NIMROD

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# Talk Overview

- New developments of the FronTier pellet code
- New developments of the Lagrangian particle/SPI model
- Simulation results
- Coupling of LP pellet code to NIMROD / M3D-C1

# Our Research Objectives

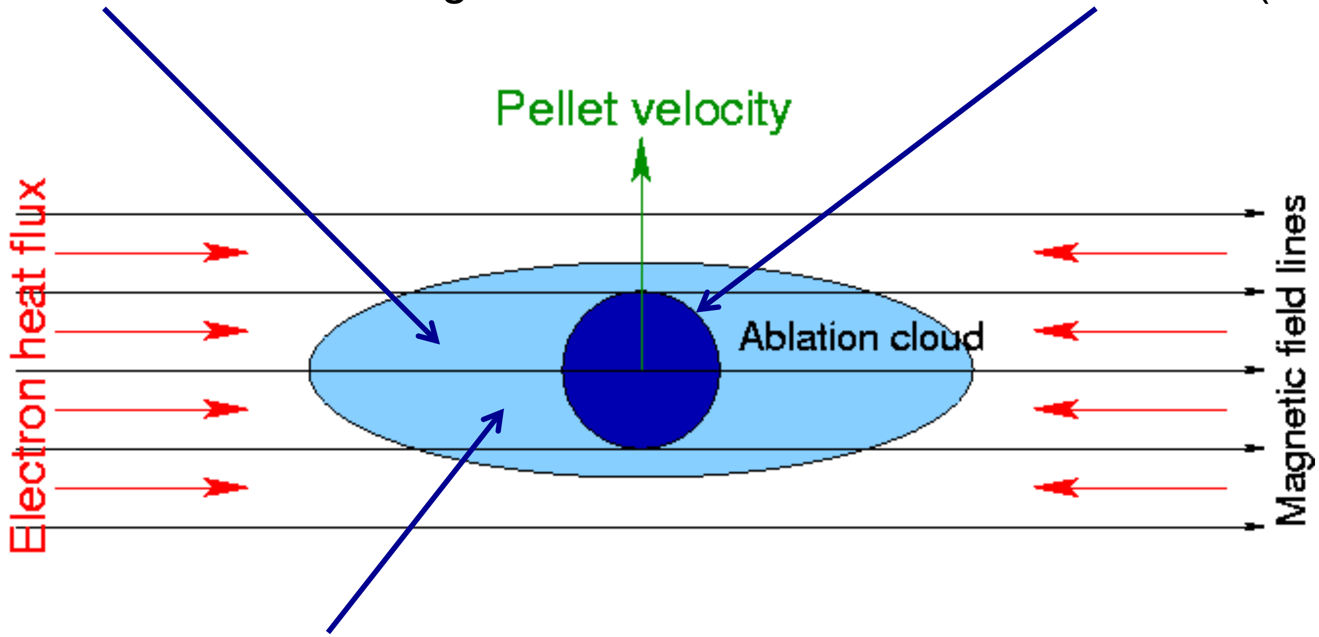
- **Improved local models** for pellet ablation simulation (SBU)
- FronTier, 2D axisymmetric code
- Full 3D Lagrangian Particle code for single pellets and SPI (simulations of hundreds of fragments in 3D
- Bring codes to the level capable of not only predicting the ablation rate but also correctly distributing ablated material in tokamak plasma via improved models

- **Perform multiscale coupling** of local pellet / SPI model based on Lagrangian particles with M3D-C1 and NIMROD
  - Study propagation of the ablated material using coupled codes

# Traditional Physics Models for Local Pellet / SPI Codes

- 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

# New Physics Models

- Improved boundary conditions at the ablated material – plasma interface

 - In the past, expansion of the ablation cloud into the vacuum was balance only by the Lorentz force

 - At present, the interface is also a contact discontinuity of the Riemann problem -> the pressure at the cloud boundary is corrected

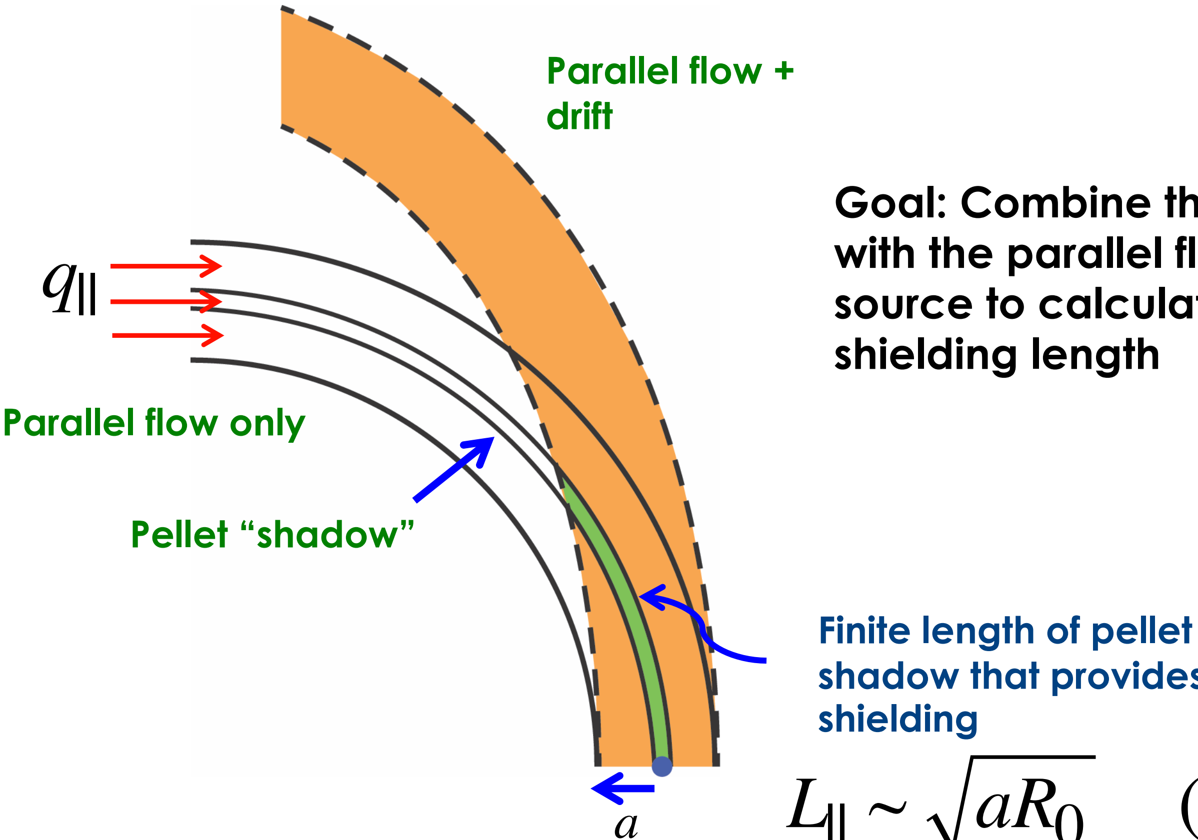
 - In the future, Ampere's law and Faraday's law will also be used to restrict the motion of the background plasma across the magnetic field lines

- Models for the polarization ExB and grad B drift of the ablation cloud based on works of Rozhansky, Parks, and Baylor
- At present, we have been evaluating these ideas using a stand-alone 2D solver for the potential that drives the drift of the ablated material across magnetic field lines

$$\tau \frac{\partial \nabla_\perp^2 \Phi}{\partial t} + \nabla_\perp \tau \cdot \frac{\partial \nabla_\perp \Phi}{\partial t} + \frac{\tau}{B}\{\Phi, \nabla_\perp^2 \Phi\} + \frac{\nabla_\perp \tau}{B} \cdot \{\Phi, \nabla_\perp \Phi\} = 0$$

- Models on ExB and grad B drift will be added to the Lagrangian code in the future
- One consequence of this approach will be self-consistent calculation of the ablation channel length

# Parallel Flow With grad-B drift Leads to finite Shielding Length




**Goal: Combine the toroidal drift physics with the parallel flow with moving pellet source to calculate the effective shielding length**

$$L_{||} \sim \sqrt{aR_0} \quad \text{(estimate)}$$

$R_0$ = 6 m for ITER, = 1.6 m for DIII-D

Self-consistent calculation of the ablation channel length will be implemented in the LP code.

# FronTier Code Updates

- **FronTier**: a grid based Eurerian code with explicit tracking of material interfaces (pellet ablation surface)

- Implicit tracking of the interface between the ablation cloud and the vacuum plasma has also been used as a first step to enforce plasma - cloud boundary conditions

- The major recent improvement of the FronTier code was re-formulation of the pellet interface boundary conditions from ghost points to WENO fluxes

  - Fixed pellet temperature T = 20K

  - Ablated material normal velocity: $$\rho_v u_v = q_{\pm} \cos\theta / E_s$$

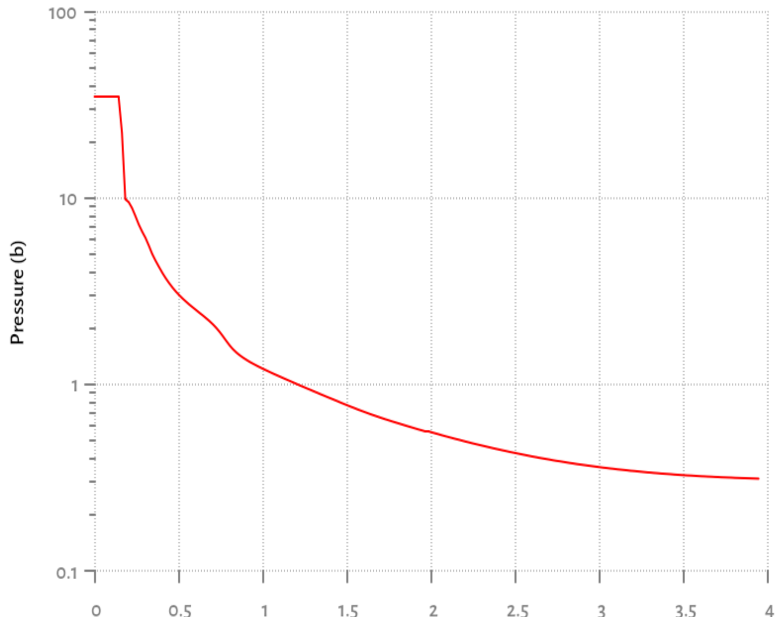
  - EOS (density – temperature – internal energy constraint)

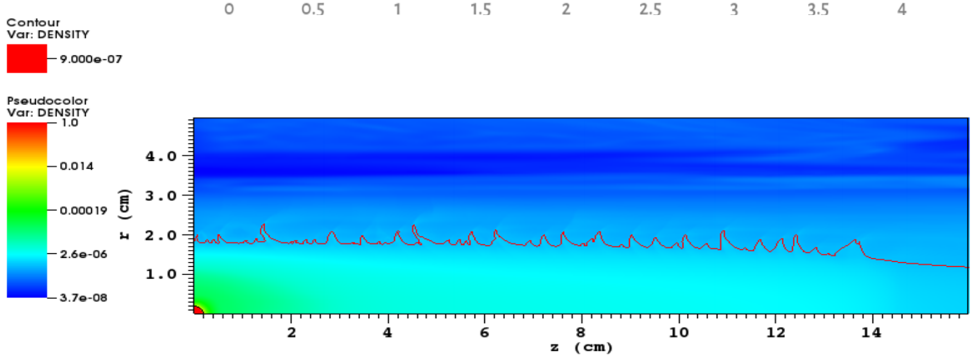
  - Riemann wave curve: $$\frac{\partial \rho}{\partial t} + (u-c)\frac{\partial \rho}{\partial n} - \rho c\left(\frac{\partial u}{\partial t} + (u-c)\frac{\partial u}{\partial n}\right) = \Gamma \frac{\partial q_{\pm}}{\partial z}$$

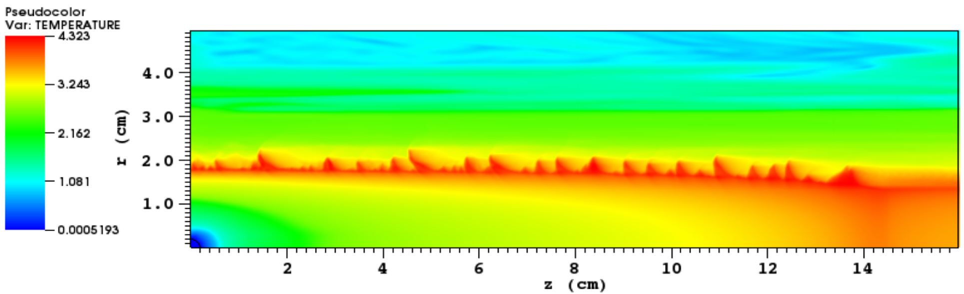
  - This implementation fixed the previously observed sensitivity to initial T.

- Currently FronTier is used for single pellet simulations and for verification / code comparison with Lagrangian particle approach (not optimal for 3D SPI simulations / coupling with tokamak MHD codes)

# Improved boundary conditions at the ablated material – plasma interface




- The ablation channel edge should correspond to a drop in the pressure profile, delimiting cold ablated neon material and hot background plasma
- However, our profiles show a ”flat” pressure profile across the radial direction (at z=0 cm in this plot)
- To mitigate the influence of the pressure increase in vacuum due to streaming electrons we used implicit tracking as a density level function ($2.5x10^{16}$ /cc)
- This leads to small surface perturbations which do not grow

# Update of Equations for Kinetic Heating Model

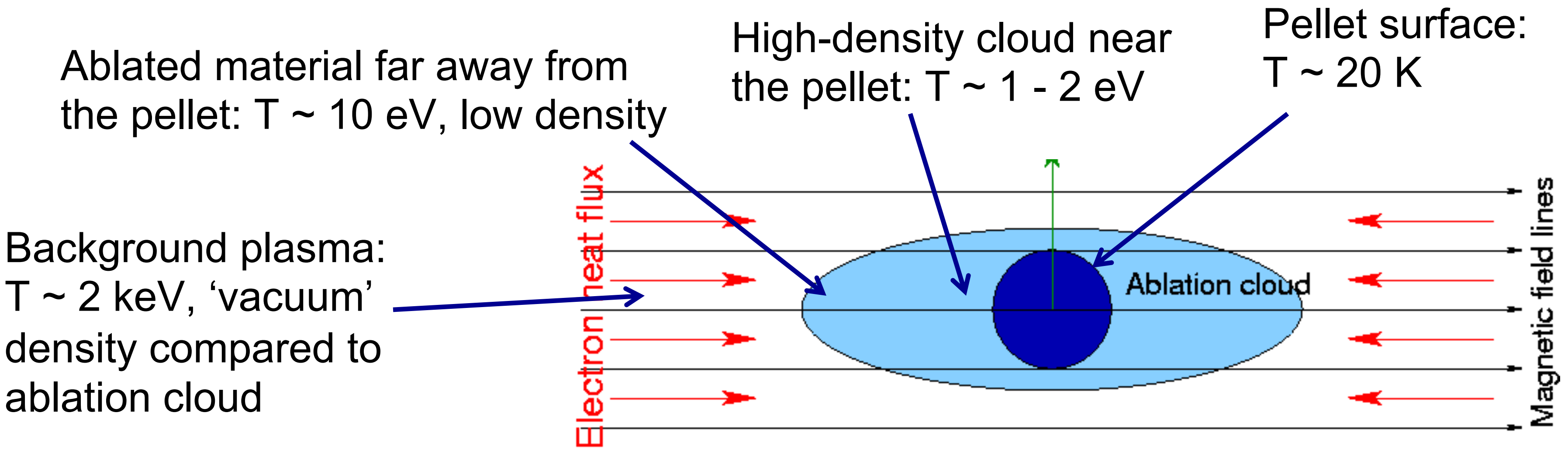
- Implemented updates to the kinetic electron heating models provided recently by Paul Parks
- The effective stopping thickness for the energy flux is improved as well as the reduction of electron density due to electrostatic shielding (is not a global constant in the new model)
- The new model increases the ablation rate by approximately 20%
- For the standard spherically-symmetric case with 2 mm radius neon pellet, Te = 2 keV, ne = 1.e14 1/cc

G(old model) = 54.5 g/s
G(new model) = 64.43 g/s (theory)    65.3 (FT simulations)

# Updates on Pellet / SPI code based on Lagrangian Particles

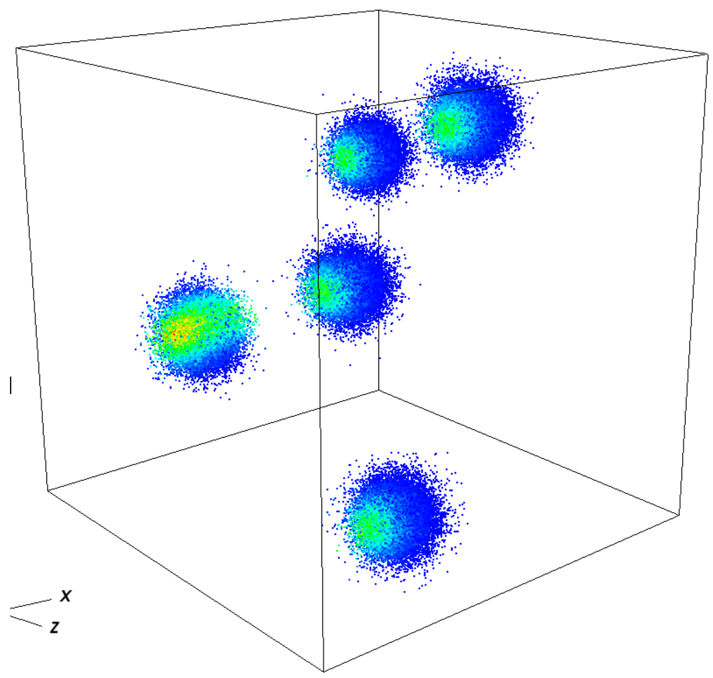
# Pellet / SPI model based on Lagrangian particles

- Lagrangian treatment of ablated material – eliminates 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

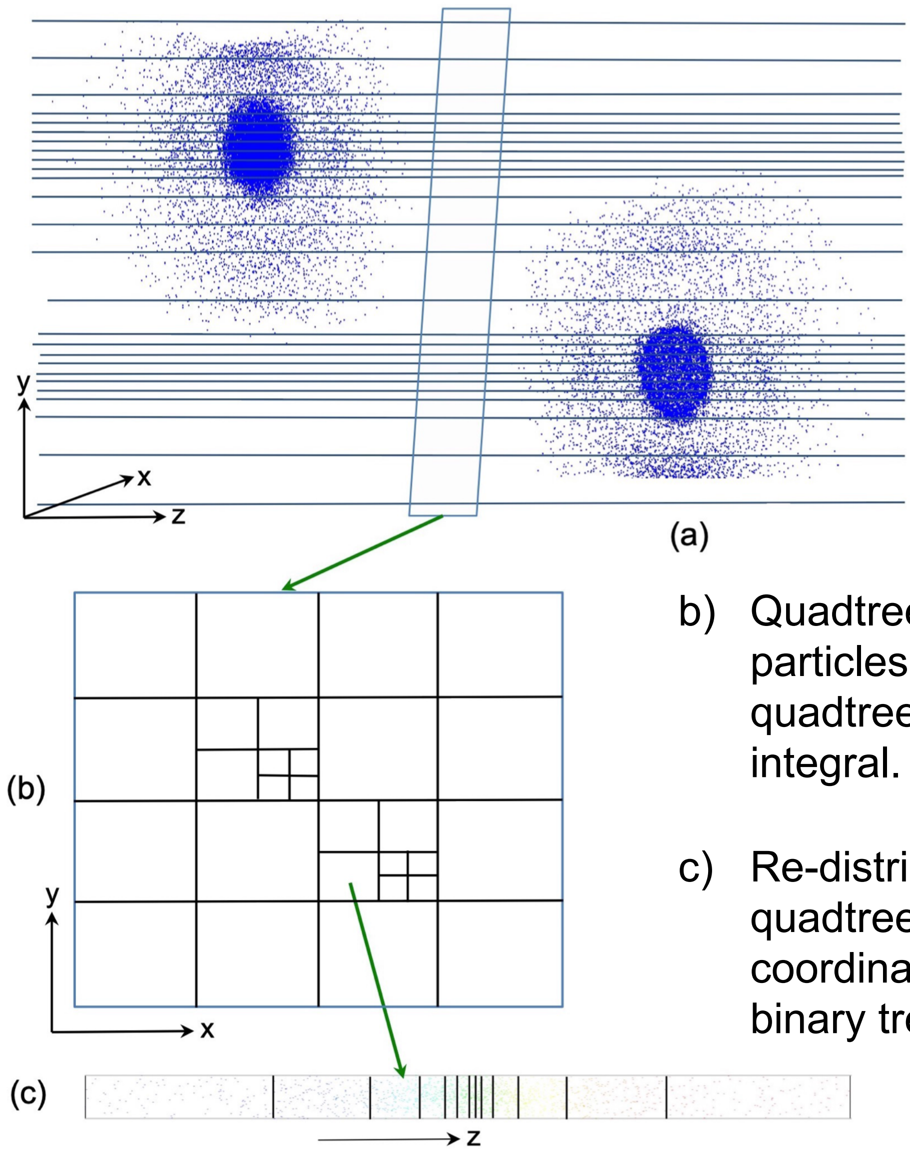


# Significant improvement of kinetic electron heating algorithms for SPI

How to compute line density integrals for highly non-uniform and dynamic particle systems in the most accurate and efficient way?



**Solution:** combination of quad-tree in the transverse direction with binary tree integration for each quad-tree cell.



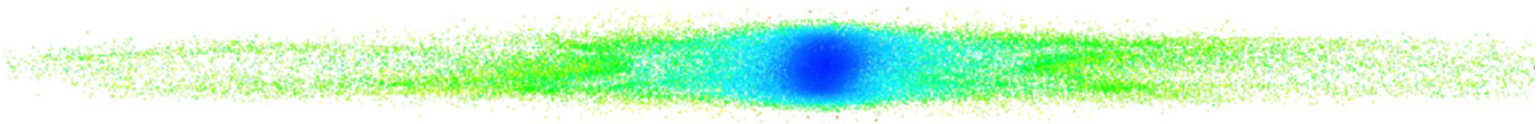

a) 3D distribution of Lagrangian particles in SPI simulation. Horizontal lines schematically depict plasma density integral paths, adaptively refined near pellet fragments.

b) Quadtree data structure, built using Lagrangian particles projected to a transverse plane. Each quadtree cell contains one path for the plasma density integral.

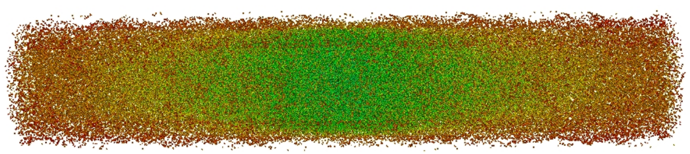
c) Re-distribution of Lagrangian particles in each quadtree cell to 3D using their saved longitudinal coordinate and line integration of density based on a binary tree in the longitudinal direction.

# 3D Lagrangian particle simulations of neon pellet: mitigated ViSit visualization software bug.

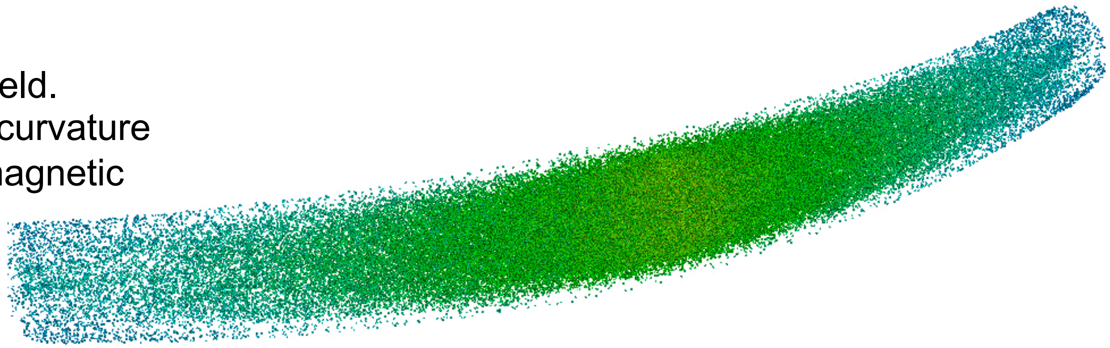
- Some plots were affected by ViSIT visualization software bug
- If we visualize a sequence of particle-based data files, LLNL visualization software ViSit allocates arrays based the 1st data file, let's say length N
- But the initial file has only small number of particles near the pellet!
- As new particles are created in the process, the system still visualized only N particles, randomly sampled – the cloud incorrectly/incompletely represented
- We now force the viz program to allocate large arrays, and now we see the full cloud.



Old image of neon ablation cloud in 2T field

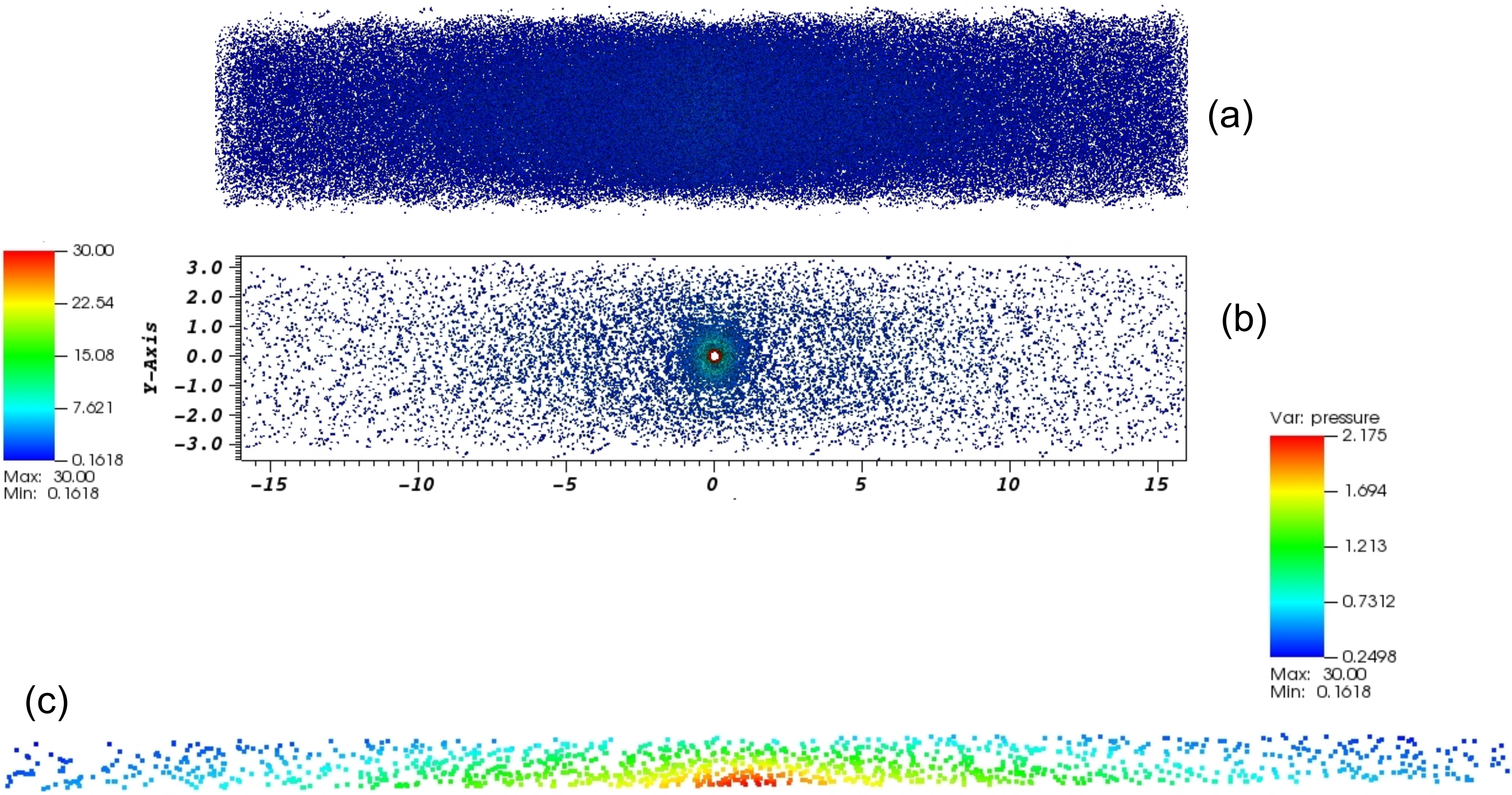


New images of neon ablation clouds in 2T field.
Top: 36 cm long channel, ignoring field line curvature
Bottom: 75 cm long channel along curved magnetic field lines



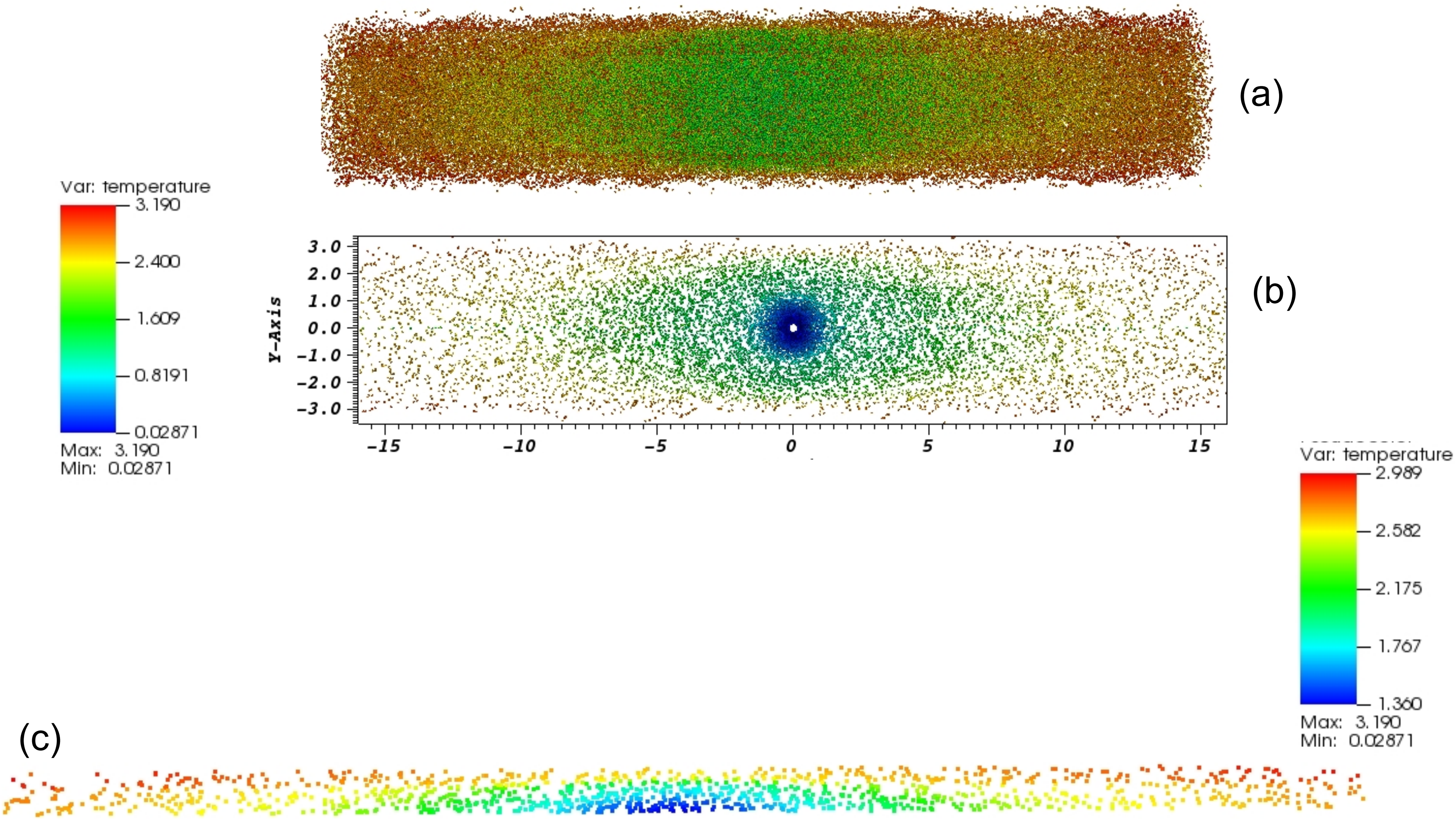
# Improvement of cloud – plasma interface condition in LP

Distribution of pressure (bar) in (a) 3D cloud, (b) 2D slice through the pellet center, (c) near-surface layer of particles



# Improvement of cloud – plasma interface condition in LP

Distribution of temperature (eV) in (a) 3D cloud, (b) 2D slice through the pellet center, (c) near-surface layer of particles



# New Simulation Results

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

**Typical Simulation Parameters:**

• Background electron density: 1.e14 1/cc (before: electrostatic shielding reduced it to $1.0682 \times 10^{13}$/cc; now computing the shielding is a part of the model
• 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
- Alternatively, real density and temerature profiles along the pellet trajectory are used

• Magnetic field: 2 - 6T

## Comparison of simulation results and with theoretical model

- Updated 2017 heat flux model
- spherically symmetric approximation, no atomic processes

**Theoretical model**

| G (g/s) | $r^*$ (cm) | $P^*$ (b) | $T^*$ (eV) |
|---|---|---|---|
| 64.44 | 0.595 | 6.1038 | 6.1923 |

**FronTier**

| G (g/s) | $r^*$ (cm) | $P^*$ (b) | $T^*$ (eV) |
|---|---|---|---|
| 63.77 | 0.593 cm | 6.096 | 6.212 |

**Lagrangian Particles: G = 62 g/s**

The new heat flux model results in a ~ 20% increase in the ablation rate

Good agreement with theoretical scaling laws

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

$$units:$$

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

# Influence of Atomic Processes on Ablation Rates

- 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 compared to the ideal case.

- New results show that ionization processes do affect the ablation rate if tokamak plasma properties are more extreme (much higher $T_e$ and $n_e$)

The ablation rate in the 1D spherically symmetric approximation with and without atomic processes for different pellet sizes and plasma parameters (using 2013 heat flux model from Parks):

No atomic processes (ideal gas):

| $n_{e\infty} = 10^{14}$ /cc | $T_{e\infty}$ = 2 keV | $T_{e\infty}$ = 5 keV |
|---|---|---|
| $r_p$ = 2 mm | 52.33 g/s | 248 g/s |
| $r_p$ = 5 mm | 181 g/s | 834 g/s |

With atomic processes:

| $n_{e\infty} = 10^{14}$ /cc | $T_{e\infty}$ = 2 keV | $T_{e\infty}$ = 5 keV |
|---|---|---|
| $r_p$ = 2 mm | 53.5 g/s (+2.2%) | 254 g/s (+2.4%) |
| $r_p$ = 5 mm | 178 g/s (-1.6%) | 851 g/s (+2%) |

The ablation rate in the 1D spherically symmetric approximation with and without atomic processes for different pellet sizes and plasma parameters (using 2013 heat flux model from Parks):

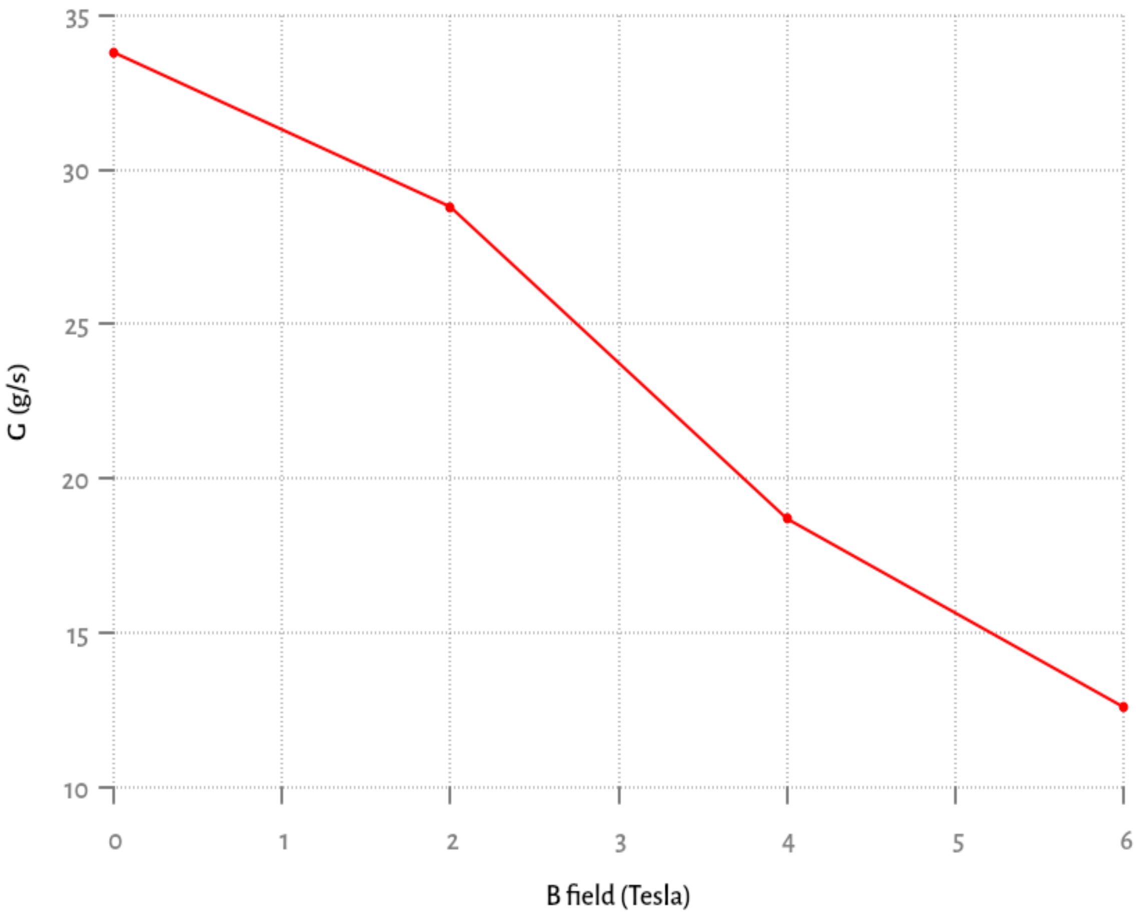
No atomic processes (ideal gas):

| $n_{e\infty} = 4x10^{14}$ /cc | $T_{e\infty}$ = 2 keV | $T_{e\infty}$ = 5 keV |
|---|---|---|
| $r_p$ = 2 mm | 127 g/s | 582 g/s |
| $r_p$ = 5 mm | 439 g/s | 2033 g/s |

With atomic processes:

| $n_{e\infty} = 4x10^{14}$ /cc | $T_{e\infty}$ = 2 keV | $T_{e\infty}$ = 5 keV |
|---|---|---|
| $r_p$ = 2 mm | 110 g/s (-13.4%) | 356 g/s (-38.8%) |
| $r_p$ = 5 mm | 334 g/s (-24%) | 1629 g/s (-20%) |

# Ablation rate reduction in magnetic field (new kinetic model)




Reduction factor compared to 0T case (no MHD forces):

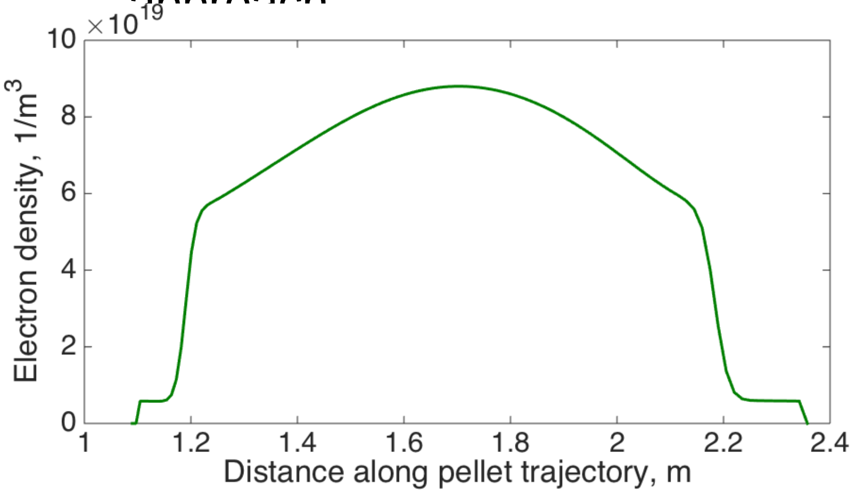
- 1.17 for 2T
- 1.8 for 4T
- 2.68 for 6T

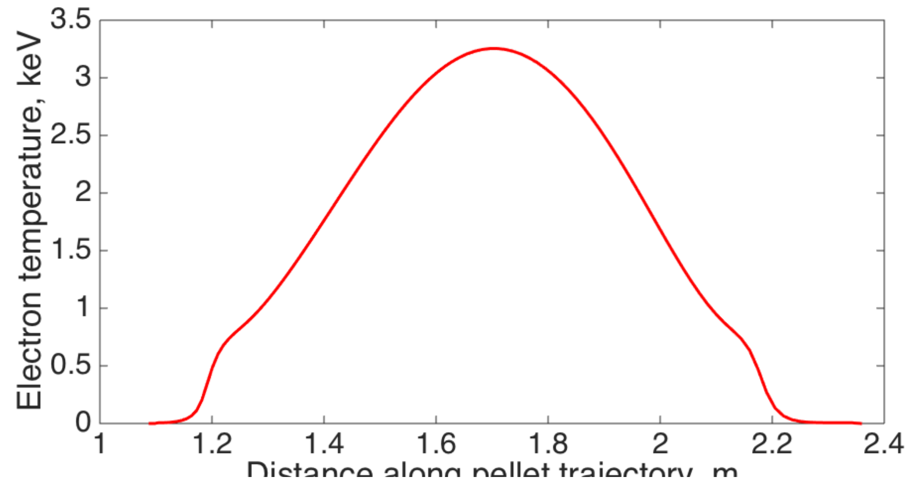
FronTier results. Lagrangian particles give good agreement in the hydro case and 2T case.

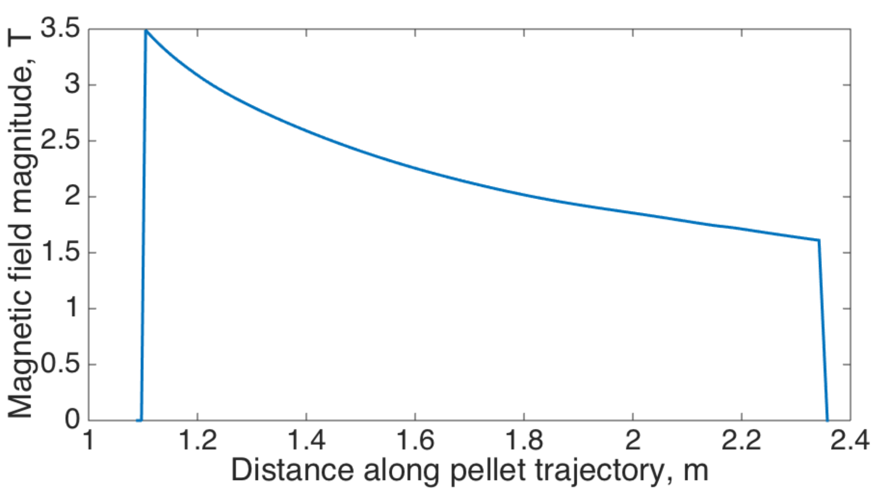
Current work aims to remove sensitivity to the pellet phase transition boundary conditions setting in the LP code.

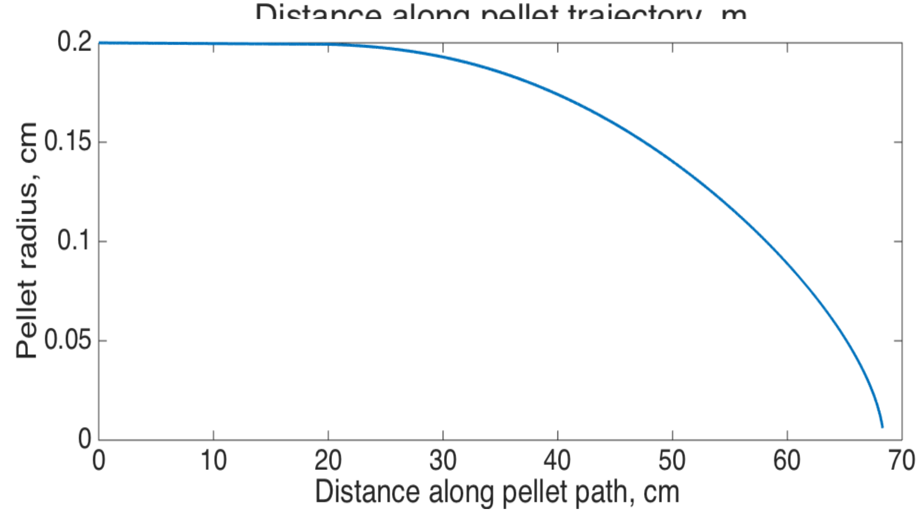
# Pellet ablation simulation using data from M3D-C1

- 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



# Coupling of the Lagrangian Particle Pellet / SPI code to NIMROD and M3D-C1

# Coupling of Lagrangian Particle Pellet / SPI code with NIMROD / M3D-C1

- Lagrangian particle approach is 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.

- **Conservative and consistent mass transfer.** Particles representing the ablated material can be labeled. If a set of particles is deposited from the SPI model to a tokamak code at a given time, the corresponding particle labels are changed, preventing them from being deposited again at the next data exchange step, thus eliminating double-counting or missing of some portion of the ablated material.

# Coupling of Lagrangian Particle Pellet / SPI code with NIMROD / M3D-C1 (cont.)

- **Stage 1: Loose coupling**. Pre-compute pellet / SPI ablation data and use them as source terms in global MHD codes
    - FronTier and LP codes currently provide coefficients of the reduction of the rate computed by NGS semi-analytic model

- **Stage 2: Strong coupling**

    - Phase I: one-directional data transfer from LP code to NIMROD / M3D-C1
    - Phase II: two-directional data exchange:
    - 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

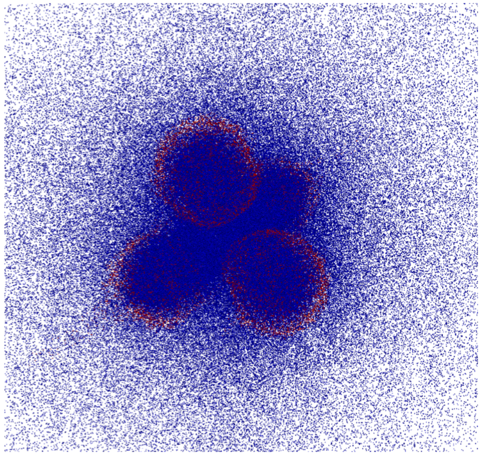
    - Pellet code data is represented in terms of basis functions of the global code and corresponding coefficients are sent to the global MHD code

# Coupling Algorithm (1)

- The data exchange between the Lagrangian particle SPI code and a tokamak code will be performed at every time step of the tokamak code, with the typical value of 0.5 - 1 microsecond.
- It corresponds to multiple time steps of the SPI code

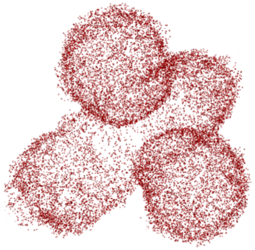
- At any given time, the SPI code will operate with local values (or distributions) of the electron temperature and density, and the magnetic field obtained from the tokamak code.

- At the data exchange step, the SPI code will send to the tokamak code a new fraction of the ablated material (counted from the previous exchange) that reached over 1 eV temperature (or some typical temperature specied by the tokamak code; temperatures below 1 eV, typical for states near the pellet surface, can not be resolved in a tokamak code)



Left: SPI ablation cloud

Right: Particles to be sent to the tokamak code.



# Coupling Algorithm (2)

- Particle labeling will prevent missing some of the ablated material or depositing it twice

- The deposition of the ablated material will also carry the information about thermodynamic states: density, temperature, velocity, and ionization states

- SPI code will also provide information on the total energy of hot electrons that was absorbed by the entire ablation cloud and the pellet since the last data exchange, thus providing an input on the cooling of hot electrons (notice that since the kinetic heating model will not be used in a global tokamak code, the electron cooling by the entire ablation cloud and not only the new portion of it must be computed)

- Particles sent to the tokamak code will not be discarded in the near-field SPI code and will continue contributing to the normal simulation process: the Lagrangian SPI code needs a fully developed cloud to compute the correct ablation rate

- New data on hot electrons and the magnetic field will be sent from the tokamak code to the SPI code

# Coupling Algorithm (3): Coupling to M3D-C1

- The algorithm described above is suitable for the coupling with M3D-C1 without major changes.
- The number of particles exchanged between the Lagrangian SPI code and M3D-C1 can be optimized. If the number of particles is too large (in the case of a very large numerical resolution of the Lagrangian SPI code), their number can be reduced for the data transfer.

# Coupling Algorithm (4): Coupling to NIMROD

- Coupling to NIMROD will be performed using the PIC module currently present in NIMROD

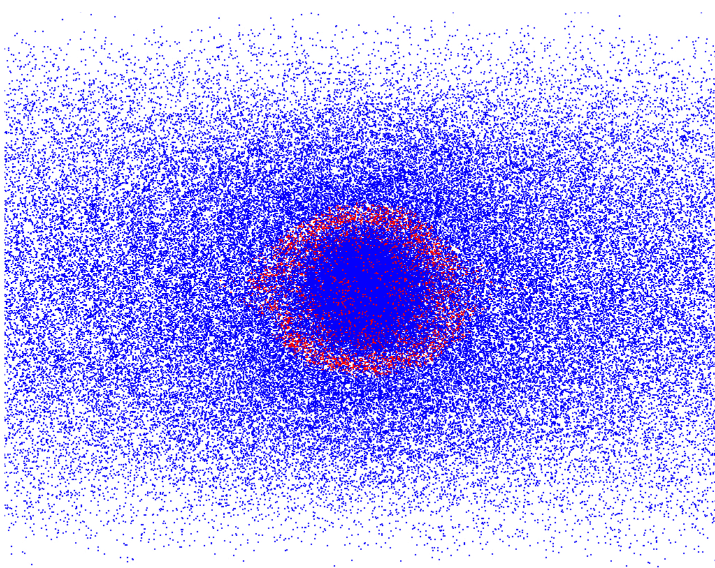
- The essential difference compared to the M3D-C1 coupling algorithms in the temperature data transfer method. NIMROD's PIC particles do not store thermodynamic states such as temperature. Instead, the temperature is represented by their thermal velocity distribution.

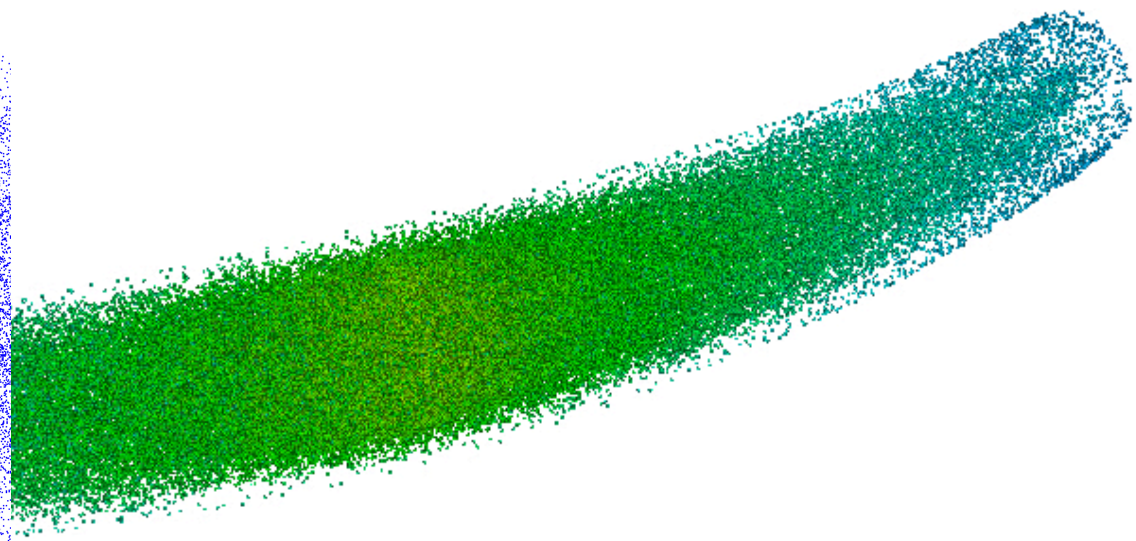
- As all Lagrangian particles of the SPI code move only with the hydrodynamic velocity, particles designated to the data transfer will be re-distributed in the following way.
- An optimal number of particles will be selected in the spatial domain in such a way that spatial gradients are sufficiently resolved.
- Each particle representing a Lagrangian fluid parcel in the SPI code will be replicated locally to create electrons and ions with a specific thermal velocity distribution corresponding to the temperature state of the original particle. Masses of all particles will also be changed to represent the correct local density.

# Example of the Data Exchange File

For each particle in the layer and the whole cloud, we provide

- x, y, z: coordinates
- Vx, Vy, Vz: velocities
- Temperature, density, and pressure
- electron heat deposition power density
- radiation power density
- number density of neutral atoms
- number density of 1+ ions, 2+, …, number density of fully (10+) ionized ions
- number density of electrons
- averaged ionization





# Summary and Future Work

- Improved several aspects of the 3D Lagrangian particle pellet/SPI code and the FronTier pellet code
    - Ablation boundary conditions at the pellet interface
    - Interface conditions at the ablation cloud – plasma interface
    - Kinetic heating models (both physics and numerical aspects)
    - Visualization (LP)

- Performed verification simulations and code comparison
    - Good 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 at typical conditions, consistent in both codes, is not well understood

- Computed ablation rate reductions in magnetic fields
- Obtained simulations of pellets using input from M3D-C1 code

# Summary and Future Work (cont.)

- Work on coupling with global tokamak MHD codes (M3D-C1 and NIMROD) has started
- Developed coupling algorithm
- Started work on data exchange with NIMROD

- Future work:
- Improve the sensitivity of LP to ablation phase transition boundary conditions at the pellet surface
- Complete code coupling
- Perform comprehensive FronTier – LP code comparisons for wide range of plasma parameters
- Perform simulations of multiple fragments
- Complete models for ExB and grad B drifts for the LP code
- Compare ExB and grad B drifts with NIMROD / M3D-C1 simulations