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Near-field models and simulations of the ablation of pellets and SPI fragments

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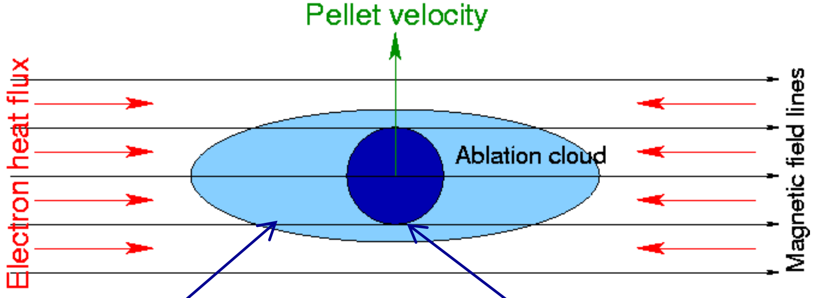
Multiple scales of Pellet / Shuttered Pellet Ablation

- Ablation of pellets and SPI fragments in tokamaks is intrinsically a multiscale problem with spatial scales ranging from millimeters (dense clouds near cryogenic pellets) to 10x meters (expansion of ablated material along magnetic field lines), as well as multiple time scales
- A two-level approach is adopted

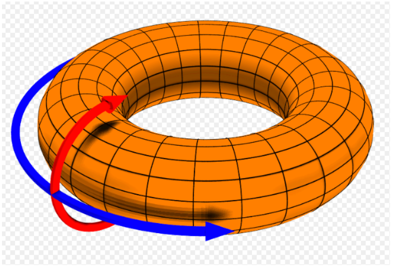
Local Model



- Phase transition (ablation model) for pellet surface

- Kinetic model for the electron heating of ablated gas
- Low magnetic Re MHD equations
- EOS with atomic processes
- Radiation and Conductivity models
- Pellet cloud charging models
- grad B drift models for ablated material

Global Model

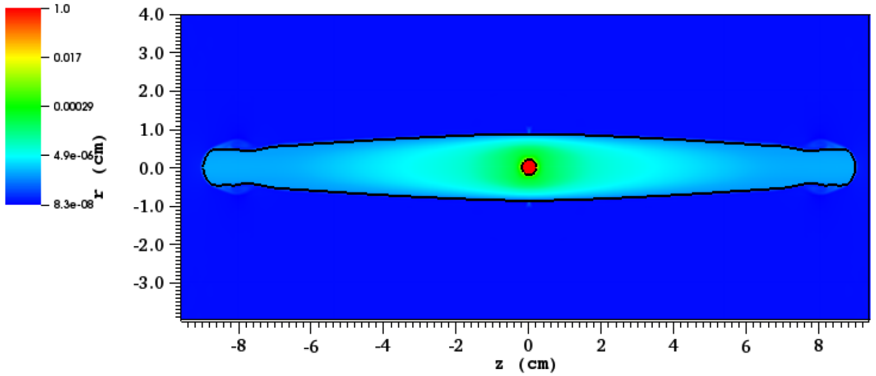


- Extended-MHD
  – Fluid equations for density, momentum, and temperature
  – Faraday-Ampere-Ohm's Law
- Impurity dynamics
  – Continuity eqs. for each charge state
  – Coupled by ionization/recombination
  – Calculates radiated power

Codes that implement Local Pellet Physics Models

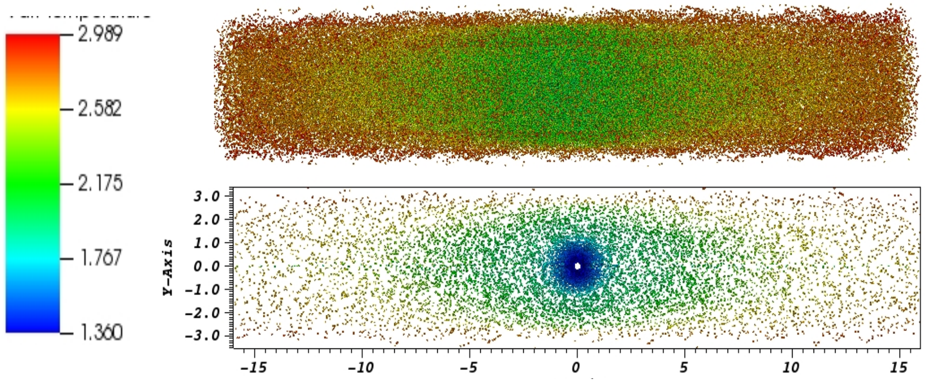
FronTier (FT)

- Hybrid Lagrangian-Eulerian code with explicit interface tracking
- Both pellet surface and ablation cloud – plasma interface are explicitly tracked
- 2D axisymmetric simulation of the ablation of single neon or deuterium pellets, computing ablation rates



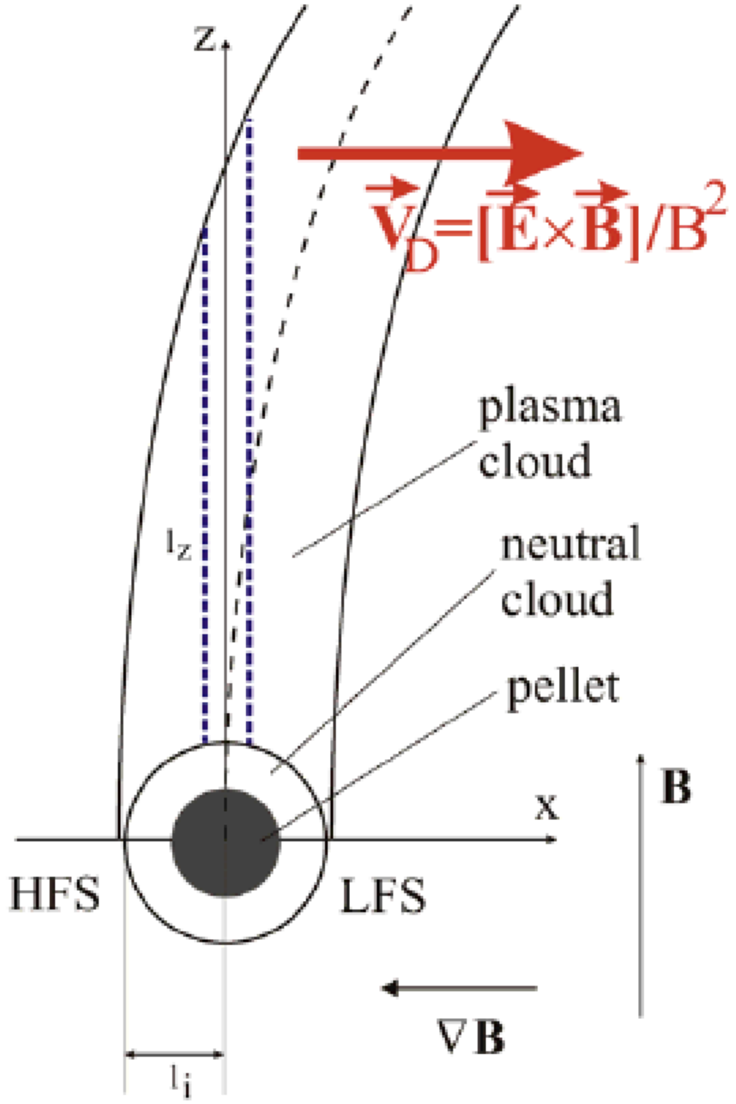
Lagrangian Particle code **(LP)**

- Highly adaptive 3D particle code
- Lagrangian treatment of ablation material eliminated numerous numerical difficulties associated with ambient plasma, fast time scales etc.
- Simulate SPI fragments in 3D
- Used for coupling with NIMROD and M3D-C1
- R. Samulyak, X. Wang, H.-S. Chen, J. Comput. Phys., 362 (2018), 1-19.
- X. Wang, R. Samulyak, J. Jiao, K. Yu, J. Comput. Phys., 316 (2016), 682 - 699.



- **Code agreement with certain classes of problems is important for our V&V program**
- The ablation rate = [electron energy flux on the pellet surface / vaporization heat] is effectively **0/0** compared to the order of magnitude of other processes. Small numerical errors in the pellet cloud may significantly change the ablation rate. The ablation rate is also sensitive to other aspects of numerical models (boundary conditions etc.)

New Physics Algorithm: Grad-B Drift Model for Lagrangian Particle Code



- In close proximity to the pellet, steady state flow with grad-B induced drift can be assumed
- Since the drift is independent of the z coordinate (the electrostatic potential is always assumed uniform along the magnetic field) the equation for the horizontal ExB drift velocity in the x (large-R) direction is governed by the formula [Parks 2000, Rozhansky 1995, 2004]

$$v_D \frac{dv_D}{dx} = \mathrm{J(x)} = \frac{2\langle P - P_\infty \rangle}{R\langle \rho \rangle}$$

where $\langle A \rangle \equiv \int_0^\infty A dz$.

Brief Summary of Results obtained with FronTier and Lagrangian Particle Codes

- Verification: comparison of 1D spherically symmetric FronTier simulations and full 3D LP with spherically symmetric initial conditions with theory
- 2D axisymmetric FronTier simulations and 3D LP simulations in magnetic field
  - No grad B drift model
  - To prevent cutting-off the electron heat flux from the pellet by ablation cloud expanding along magnetic field lines, a finite shielding length is imposed based on theoretical estimates
- 3D LP simulations of pellets and SPI in magnetic field with grad B drift
- Coupling of Lagrangian particle pellet / SPI code with NIMROD and M3D-C1
- Parallel flow problem

FT simulations of neon pellet ablation (spherical symmetry): clarification of the influence of atomic processes

No atomic processes (ideal gas, 2013 heat flux model):

$n_{e\infty} = 10^{14}$ /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

$n_{e\infty} = 4\times10^{14}$ /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, Saha EOS (2013 heat flux model):

$n_{e\infty} = 10^{14}$ /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%)

$n_{e\infty} = 4\times10^{14}$ /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%)

Neon pellet ablation (spherical symmetry)

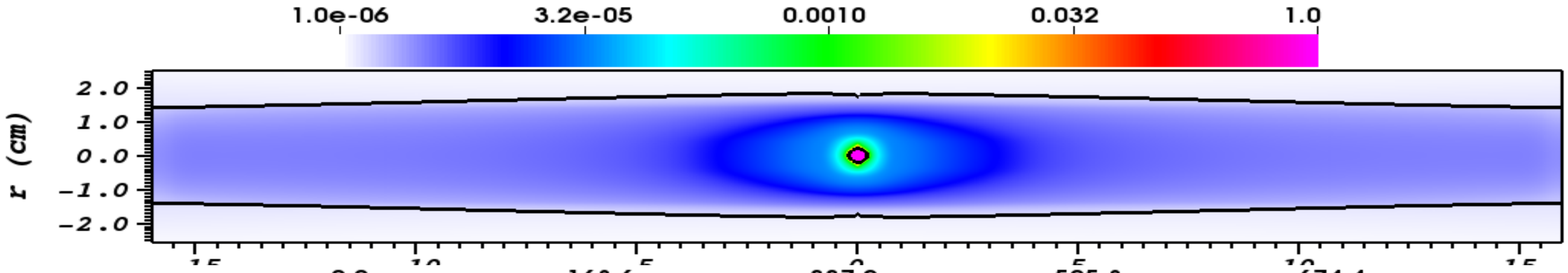
Theoretical predictions (2019 heat flux model):

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

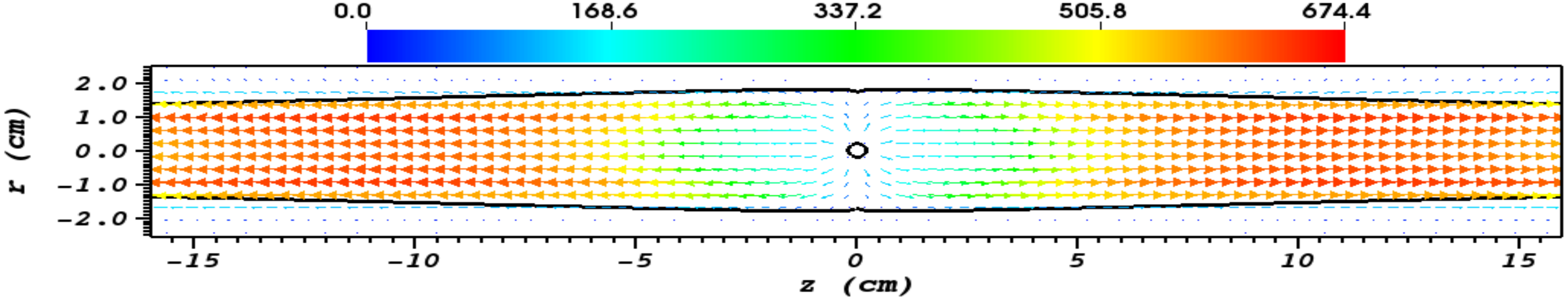
FronTier (2019 heat flux model):

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

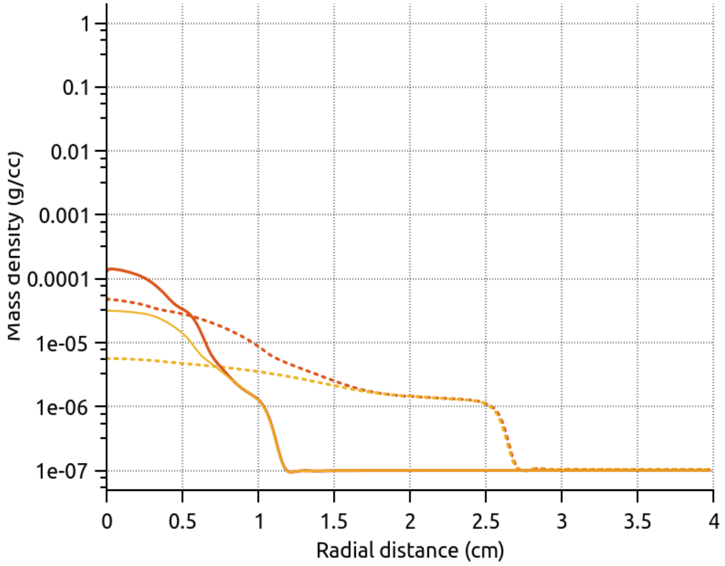
Lagrangian Particles: G = 64.0 g/s



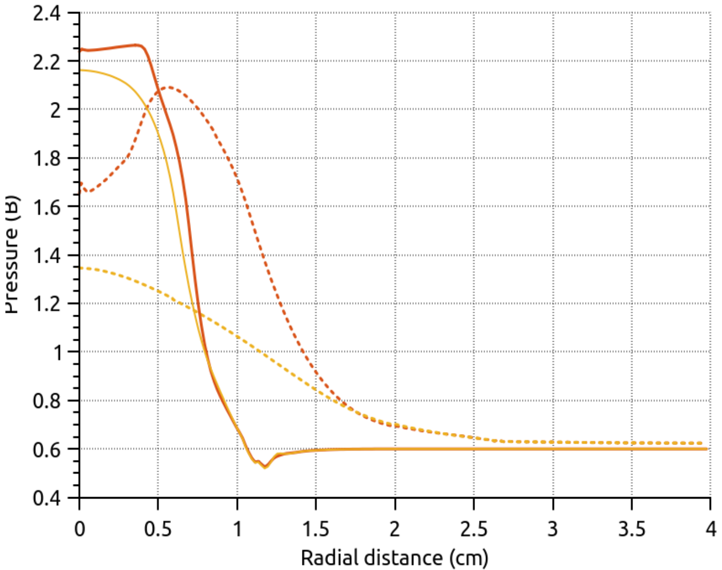
Density (g/cc)
2T



Velocity
(cm/ms=10 m/s)



Mass density (g/cc, left) and pressure (bar, right) for B=2T (dashed lines) and B=9T (solid lines) across z=0.5 (red) and z=3 cm (yellow) planes



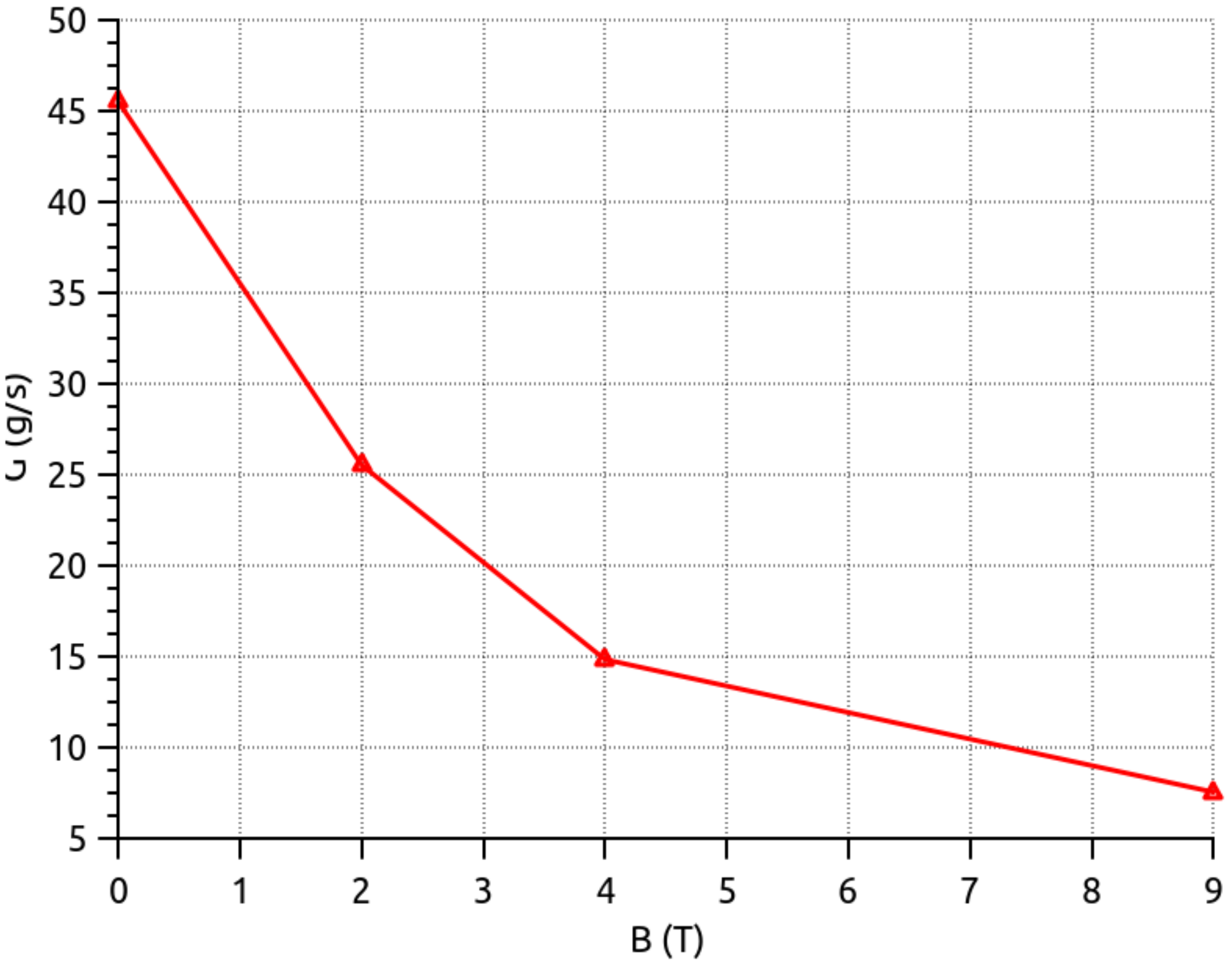
Effects of magnetic field strength on ablation rate

- In isotropic expansion (no atomic processes, no B field) only a thin layer of ablated gas around the pellet account for most of the shielding.

- But from the longitudinal profiles we observe that MHD effects redistribute the ablated material along the channel.

- This leads to stronger shielding reducing the available energy for pellet ablation

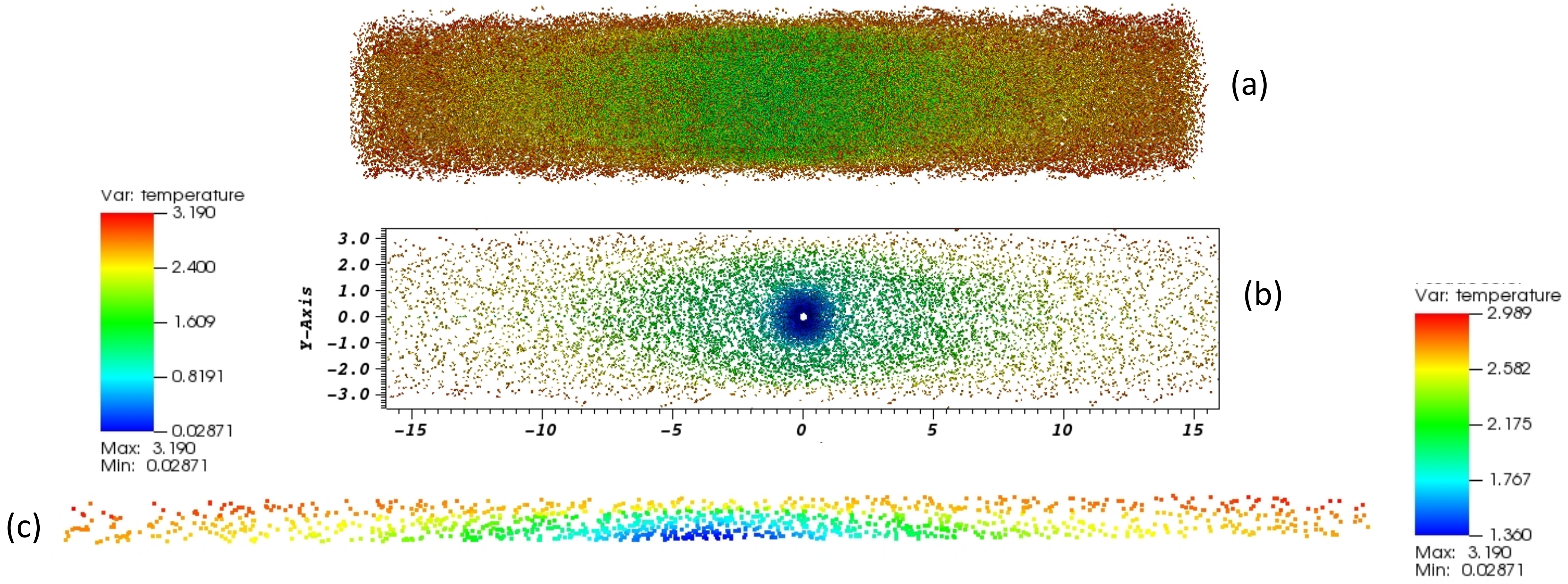
- As a results the ablation rate decreases with the strength of the magnetic field.



FT results: reduction of the steady state ablation rate with increasing B field strength

LP simulations of neon pellets by prescribing finite length of the ablation clouds (for comparison with FT), cont.

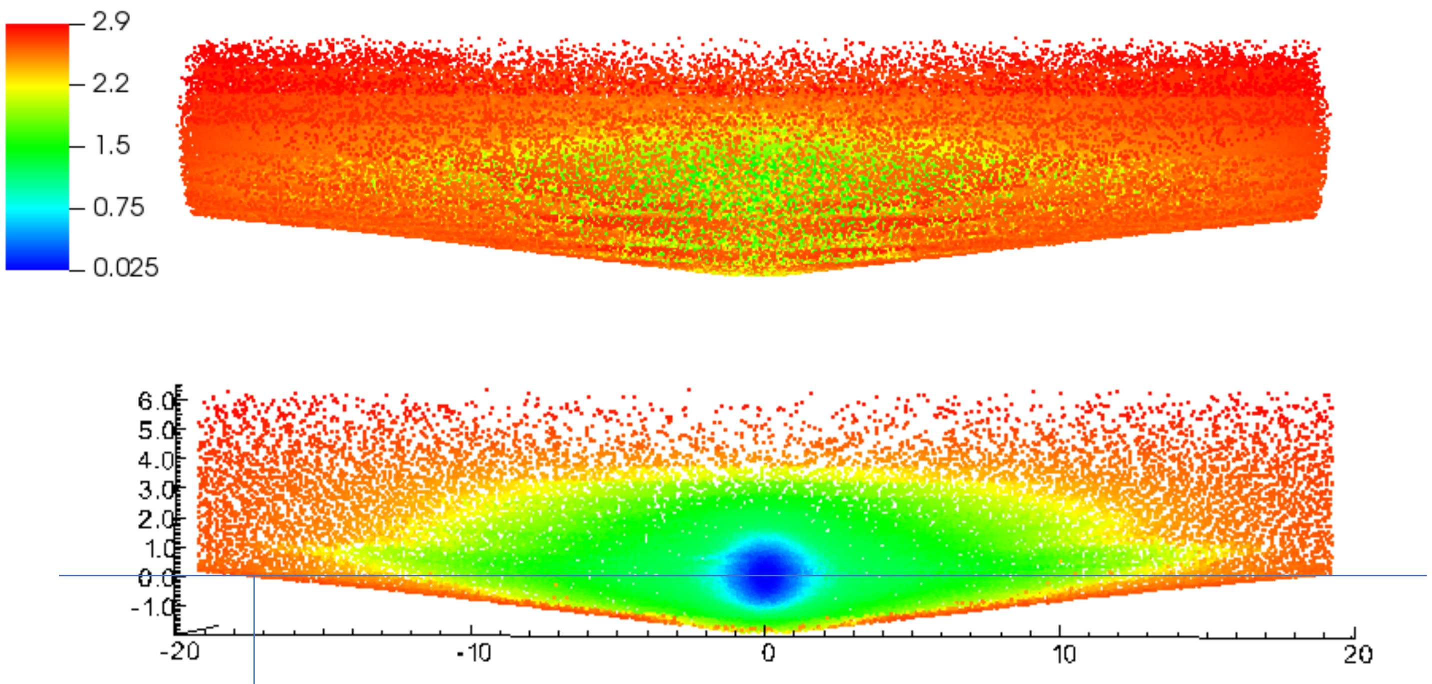
Distribution of temperature (eV) in (a) 3D cloud, (b) 2D slice through the pellet center, (c) near-surface layer of particles



Spherically symmetric: G = 64 g/s

0T: G = 50 g/s, 2T: G = 32 g/s, 6T: G = 27 g/s

Simulation of Neon Pellets with *grad B* drift



Temperature distribution in the pellet cloud in 2T magnetic field in the presence of grad B drift.
(a) 3D plot
(b) Longitudinal cross-section
(c) Transverse cross-section

Shielding length due to grad B drift is ~17.3 cm

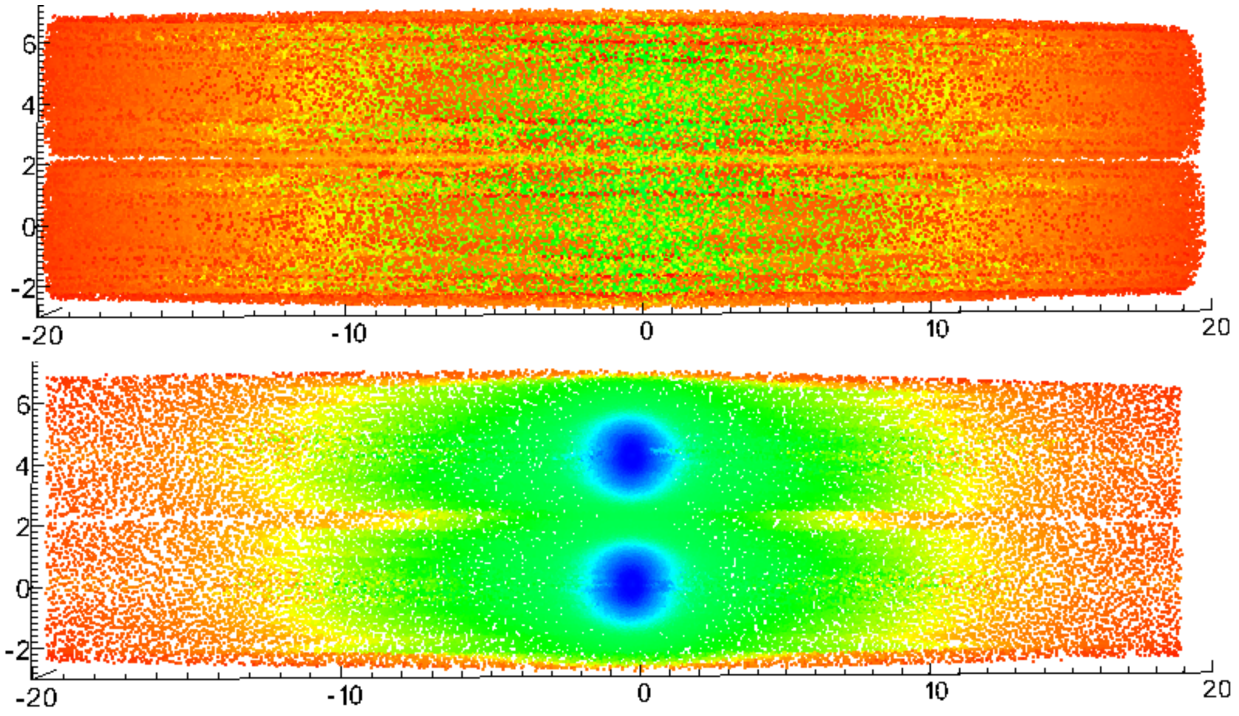
- Simulations that resolve grad B drift compute the pellet shielding length self-consistently
- For 2mm neon pellet in 2T magnetic field of DIII-D geometry, the computed shielding length is 17.3 cm
- Good agreement with previous theoretical estimates. In previous simulations with prescribed cloud length, the length was chosen in the range 16 – 18 cm
- Ablation rate is only slightly affected in simulations with grad B drift: the ablation rate increased by ~ 4% compared to the fixed length case

Simulation of SPI: estimates of sizes

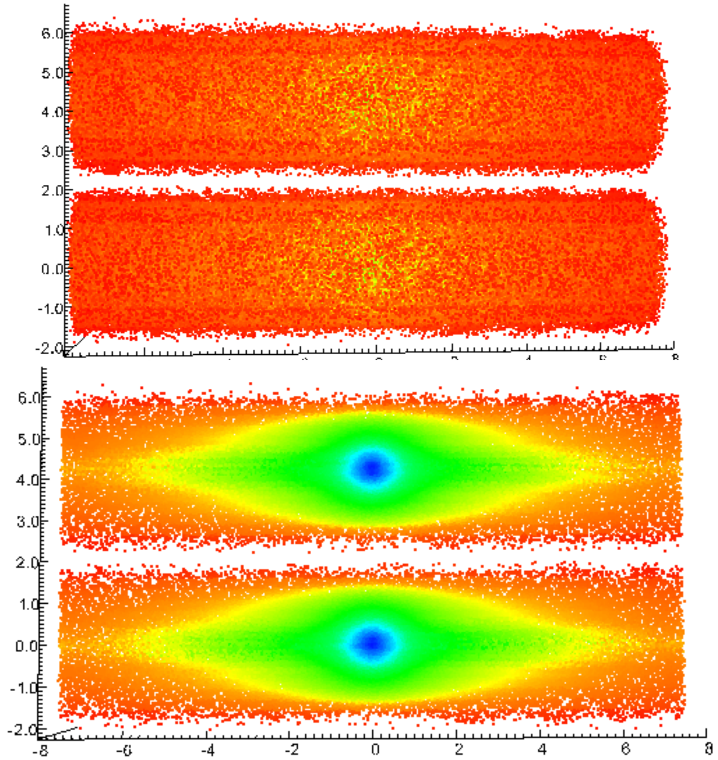
- Experimental image of the barrel with neon pellet fragments (Baylor, 2018) are shown
- Grad B drift is critical for interaction of SPI fragments

- For DIII-D, the total neon inventory is N_0 = 0.0213 moles
- This amount is contained in in a large pellet with r_{big} = *0.41 cm* (*W* = 20.183 amu is the atomic mass of neon and ρ = 1.444 g/cc is the mass density of frozen neon)
- The pellet is expected to shatter into *N* = 250 smaller fragments. Therefore, the radius of a spherical fragment is $r_{fragment}$ = 0.66 mm
- Assuming a uniform distribution of fragments throughout the cluster stream whose diameter is chosen as d = 30 cm, length L = 30 cm (with the volume of V = 21206 cc), we obtain the distance between fragments as ~4.4 cm

SPI Simulation: no grad B drift



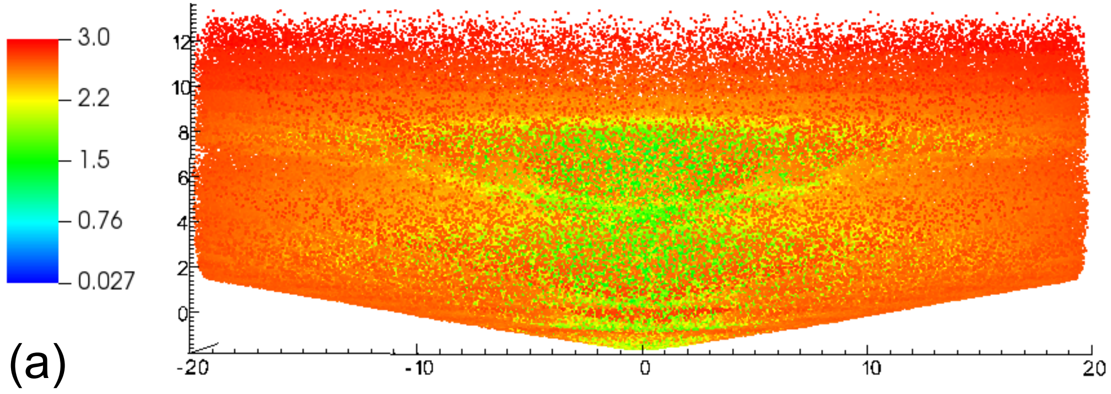
Ablation of large fragments (2 mm)

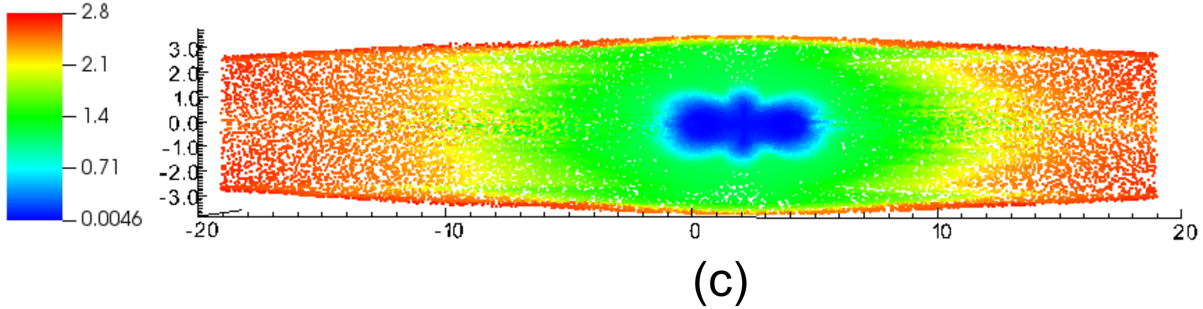


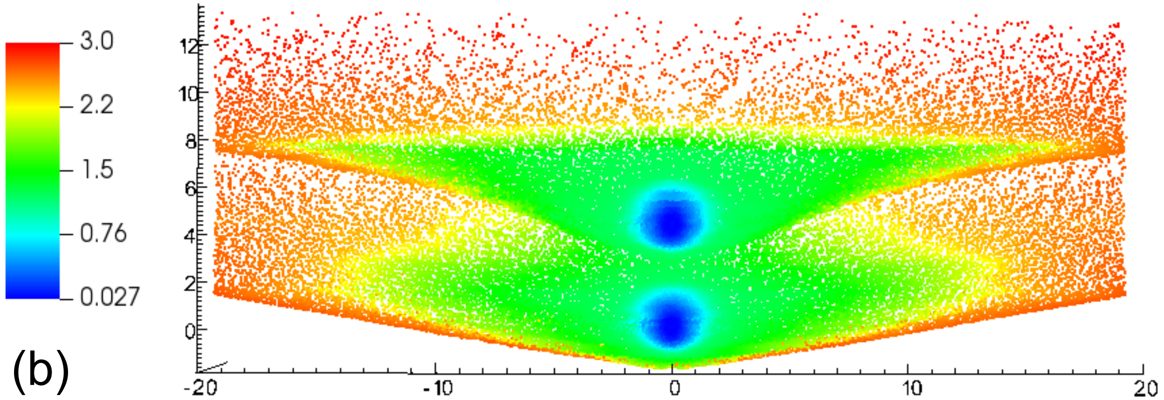
Ablation of small fragments (0.66 mm)

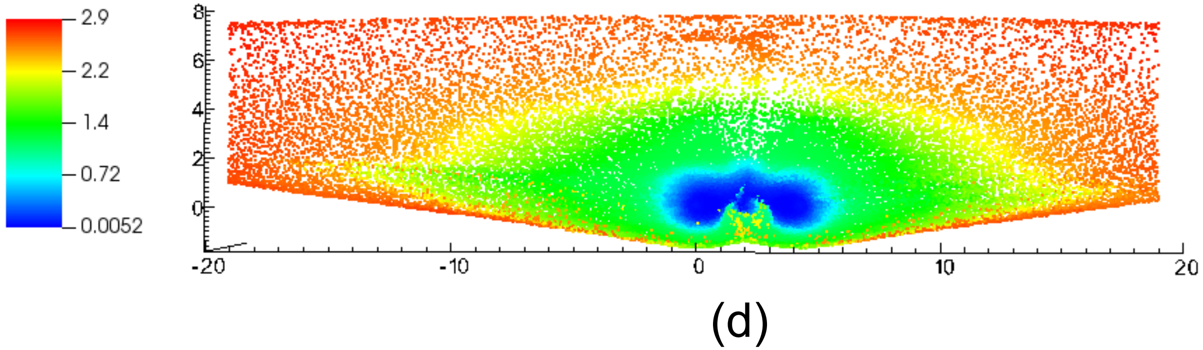
- Simulations without grad B drift show that ablation clouds of pellet fragments separated in the directions transverse to the magnetic field do not interact
  - Even for large fragments (r = 2mm), ablation clouds only touch each other)
  - The ablation rate of each fragment is not affected by the other fragment
  - Small (r = 0.66 mm) fragment create narrow ablation channels separated by ambient plasma

SPI Simulation with grad B drift









- In the presence of grad B drift, ablation cloud of SPI fragments interact with each other
- The ablation rate of the top fragment is slightly reduced compared to the bottom one. While the effect is small, it may be significant for large number of fragment
- Images on the right show SPI fragments located on the same magnetic field line. (c) No grad B drift. (d) grad B drift included
- For .66 mm fragments,
  - the top fragment ablation rate is reduced by ~ 9 % (a-b)
  - (c) 18% reduction compared to single fragment, (d) 15% reduction compared to single fragment (grad B drift)

Simulation Studies of Parallel Flow Problem

Schematic: deuterium plasma column interacting with background plasma electrons

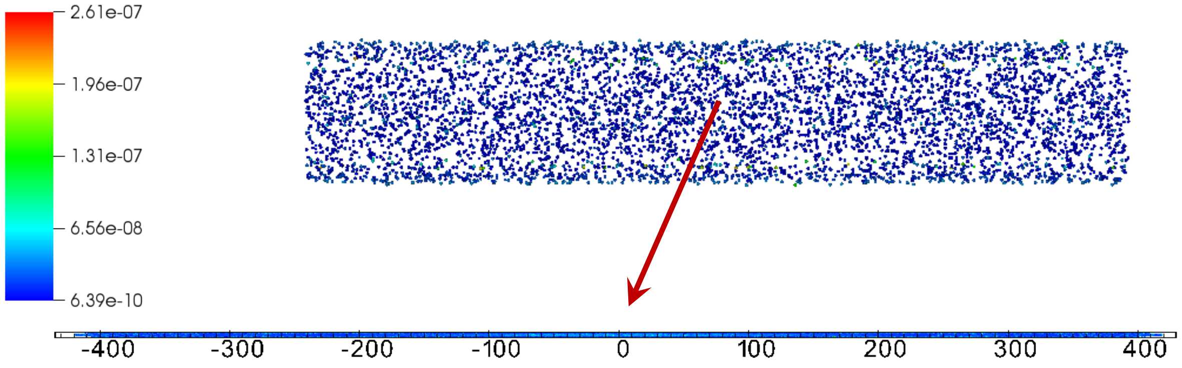
- Simulations of plasma column in magnetic field (no pellet ablation / particle source)
- Simulation purpose: study of the propagation of ablated material along magnetic field lines
- Compare with 1D PRL code simulations
- Study possible mechanisms leading to soliton-like signals in recent experiments

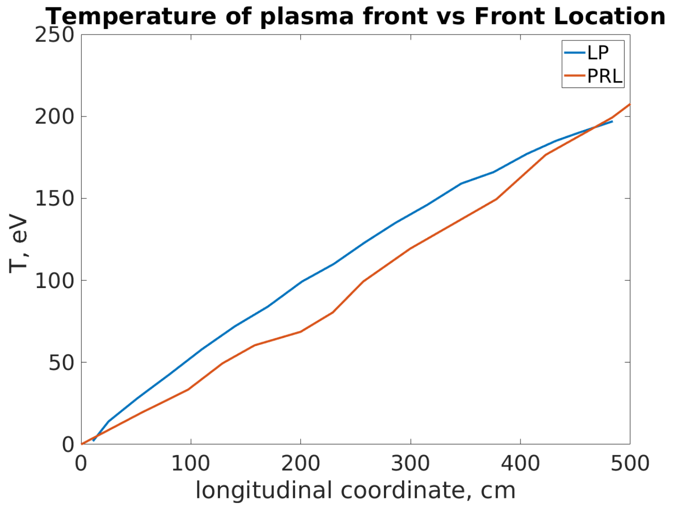
Deuterium column:
ne = ni = 4x10^16 /cc
Te = 2 eV
half-length of cloud = 10.8 cm

Background plasma:
Te_inf = 500 eV
ne = 4x10^13 1/cc, reduced to 6.4x10^12 1/cc by the electrostatic shielding

Simulation Studies of Parallel Flow Problem

- Understanding of long-range propagation of ablated material along magnetic field lines is a high-priority task
- 3D Lagrangian particle simulations of a plasma column expansion up to 10 m in length are in very good agreement with 1D PRL code results in terms of expansion distances and longitudinal profiles of thermodynamic states

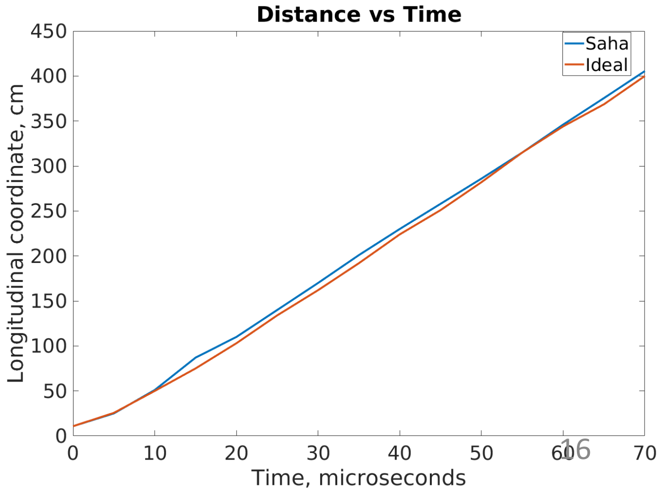




Top: temperature in the front part of plasma column vs the front location using 3D LP with Saha EOS and 1D PRL with ideal gas EOS. Bottom: front of plasma location in time.

Work in progress:

- A set of 1D equations was developed that incorporate changing magnetic field
- These equations are being implemented in 1D version of the Lagrangian Particle code
- 1D simulations will be compared with full 3D Lagrangian particle simulations of parallel flow in changing magnetic field



Multiscale coupling of Lagrangian particle pellet ablation code with NIMROD / M3D-C1:

- Lagrangian particle approach is beneficial for coupling with global tokamak codes:
    - No need for overlapping domain decomposition typical for grid-based codes
    - Lagrangian treatment of ablated material leads to conservative extraction of ablation flow data.

- Stage 1: Loose coupling. Pre-compute pellet / SPI ablation data and use them as source terms in global MHD codes. The current source terms incorporate information obtained from FT and LP simulations. Work on a detailed pellet ablation database G(B,Ne,T,rp) is undeway.

- Stage 2: Strong coupling

    - Global MHD and LP Pellet / SPI codes will run in parallel on a supercomputer using different nodes / communicators

    - Data exchange will be performed at the time step of the global MHD code (which is >> LP time step)

    - Pellet code data is currently represented by particle states data files; in the future, in terms of basis functions of the global code and the corresponding coefficients will be sent to the global MHD code

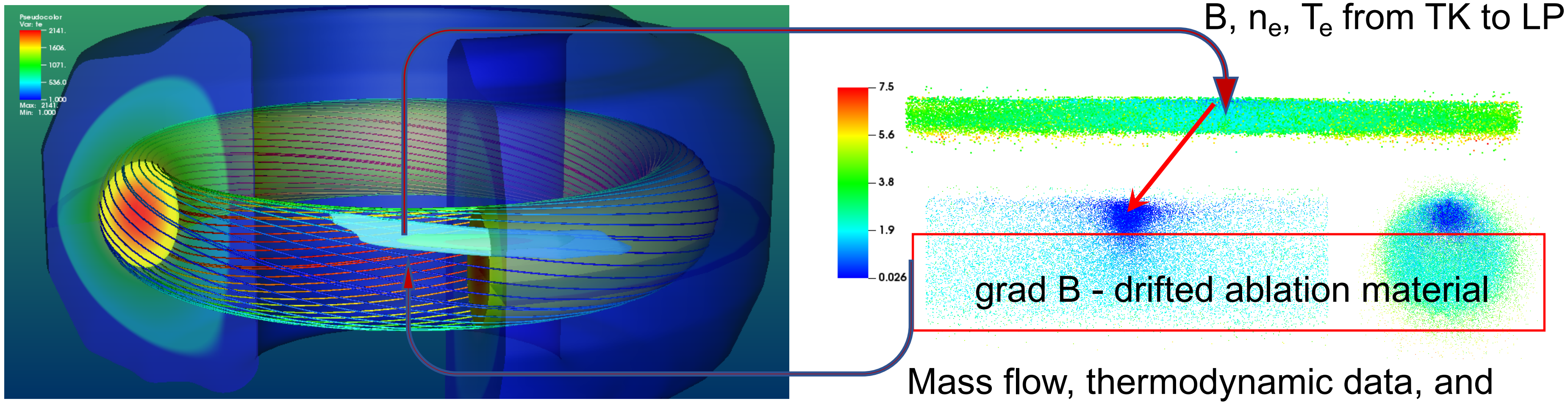
    - We have developed a coupling approach that has a well-defined, physics-based separation of scales

Multiscale coupling of Lagrangian Particle Pellet / SPI code to NIMROD and M3D-C1

NIMROD simulation domain showing ablated material obtained from LP code

LP simulation of pellet ablation cloud

B, n_e, T_e from TK to LP



Mass flow, thermodynamic data, and energy sinks from LP to TK

- **Grad B drift provides physics-based separation of scales for coupling**

- LP code evolves self-consistently the entire ablation cloud that provides pellet shielding
- grad B drift model in the LP code propagates ablated material across magnetic field lines, establishing the cloud shielding length. Ablated material that drifted beyond the main ablation cloud is transferred to the tokamak code, together with thermodynamic data and energy sinks. Particle representation ensures conservative mass transfer
- LP code obtains the magnetic field and electron density and temperature from the tokamak code

- LP data input has been successfully incorporated in NIMROD

Towards resolution of disagreements between FronTier and Lagrangian particle simulations in magnetic fields

- FronTier and Lagrangian particle codes are in good agreement for simulations of the pellet ablation with the spherically-symmetric heat source and the directional heating at zero magnetic field
- LP code predicts smaller reduction of pellet ablation rates in magnetic fields of increasing strength compared to the FT code
- In magnetic fields, LP obtains higher density clouds that react weaker to the magnetic field

- 3D LP is also in good agreement with 1D PRL code for the parallel field flow problem: propagation of ablated material along magnetic field lines over distances of 10 m

- **We understood theoretical reason for these results and how to resolve the disagreements**

Redundancy in LP equations: 1D Lagrangian Hydrodynamics

$$U_t + A(U)U_x = 0,$$

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

For example, using the ideal gas EOS, $e = \dfrac{PV}{\gamma - 1}$ $K = \left(\frac{c}{V}\right)^2$

Consider 1st order upwind equations (for simplicity)

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

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

$$\boxed{V_t = \frac{V}{2}(u_{xr} + u_{xl}) - \frac{V}{2\sqrt{K}}(P_{xr} - P_{xl})},$$

$$u_t = \frac{V\sqrt{K}}{2}(u_{xr} - u_{xl}) - \frac{V}{2}(P_{xr} + P_{xl}),$$

$$P_t = -\frac{VK}{2}(u_{xr} + u_{xl}) + \frac{V\sqrt{K}}{2}(P_{xr} - P_{xl}).$$

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

Current algorithm:

- Density (specific volume) is evolved by the 1st PDE
- Particles are moved according to the last equation
- **The new number density of particles must be consistent with the density obtained from the PDE**
- The number density of particles is not consistent with PDE-predicted density in the presence of B field

Redundancy in LP equations

- Two approaches can be used in the LP code:

(1) Evolve the density using the PDE and update locations of particles

(2) Ignore the 1st PDE, and obtain density from particle number density

- Both approached have been tested in the past an very similar results have been obtained for classic hydrodynamic problems; PDE density update was slightly better from the stability point of view and was selected for the production code
- PDE density update is not consistent in with the particle number density in the presence of the Lorentz force
  - PDE's predict new states but the motion of particles is restricted by the Lorentz force. After the particle motion, their number density disagrees with the PDE-predicted density
  - Agreement in the case of the parallel flow problem is due to the fact that the motion is effectively 1D
  - Density inconsistency is present only if the Lorentz force has a nontrivial action
- **Particle number density is a more fundamental quantity**
- In the classic literature on grid-based Lagrangian methods, the PDE for density is used in the analysis of Richtmyer and Morton
- The classic Lamb's Hydrodynamics operates with Jacobians of new Lagrangian coordinates with respect to old Lagrangian coordinates. This is similar to the density update by the particle number density
- We are working on changing the algorithm to use only the particle number density

Summary and Future Work

- Detailed physics model for pellet ablation based on front tracking (2D axisymmetric), and 3D pellet / SPI code based on Lagrangian particles have been further improved
    - Recent improvements of physics models and numerical algorithms (explicit tracking of ablation cloud in FT, grad B model in LP, improved adaptive K-tree algorithms)
    - Verification: good agreement of theoretical predictions and simulations using both codes for spherically-symmetric and zero-B cases

- Performed FT and LP simulations that quantify the influence of plasma parameters and tokamak magnetic fields on the ablation rate of neon pellets. Parallel ablation flow / long range expansion

- Started 3D simulations of SPI; grad B drift is critical for the interaction of ablation flows of individual fragments

- Developed a multiscale coupling method of with M3D-C1 and NIMROD
    - Well-defined, physics-based separation of scales
    - LP data input has been successfully incorporated in NIMROD

- Understood the reason for FT / LP disagreements on ablation rates in magnetic fields

- Future work:
    - Continue V&V; resolve FT / LP disagreements; perform runs with fully coupled codes
    - New physics: DT / neon mixtures, kinetic heating by runaway electrons