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Study of neon and deuterium pellet ablation rates in the presence of grad B drift and cloud rotation

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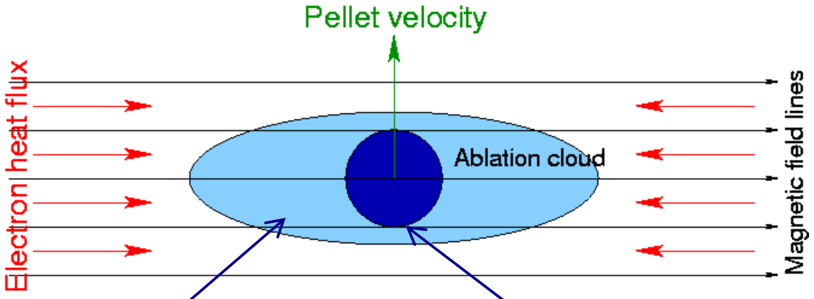
Talk overview

- Successful resolution of disagreements between FronTier and Lagrangian particle codes
- Study of ablation rates of neon pellets in the presence of grad B drift
- Simulation of cloud charging and rotation
- Update on multiscale coupling
- Summary and future work

Introduction: local models and codes for pellet ablation

Local Model



- Phase transition (ablation model) for pellet surface

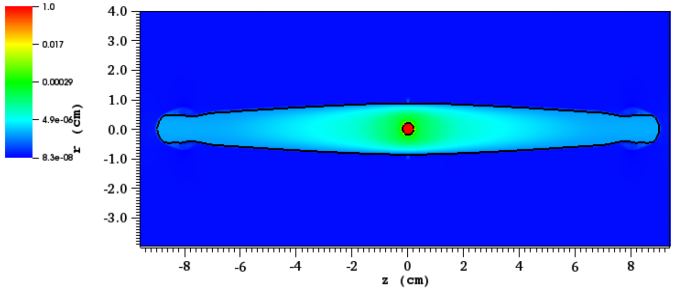
- Kinetic model for the electron heating
- Low magnetic Re MHD equations
- EOS with atomic processes, radiation
- Grad B drift models for ablated material
- Pellet cloud charging models

Local Codes

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

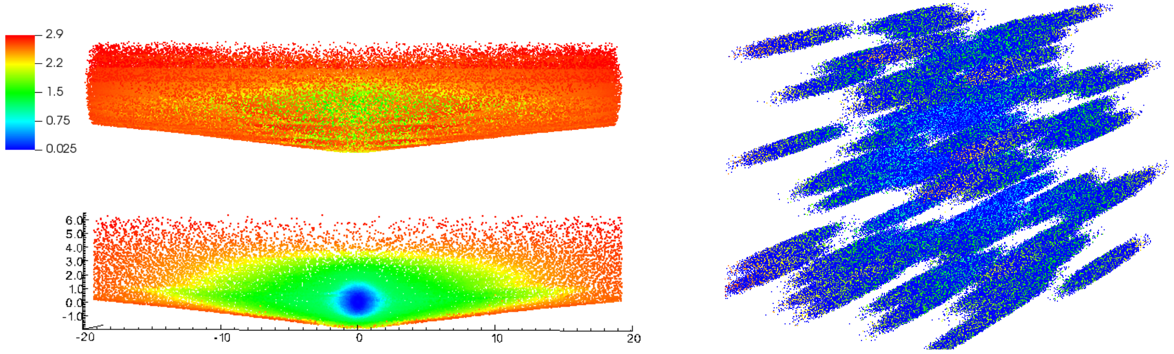
FT simulation of neon pellet in 2T magnetic field



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.
- Supports many SPI fragments in 3D
- Parallelized using P4EST library (parallel forest of K-trees)
- R. Samulyak, X. Wang, H.-S. Chen, J. Comput. Phys., 362 (2018), 1-19.

LP simulation of neon pellet in 2T magnetic field with grad B drift (left) and SPI fragments (right)



Resolution of discrepancies between FronTier and Lagrangian Particle Codes

At the pre-DPP CTTS meeting, we reported that

- FronTier and Lagrangian particle codes were in reasonably good agreement on ablation rates for simulations of the pellet ablation with spherically-symmetric heat source and the directional heating at zero B field
- Even when the ablation rates in FT and LP were close, we observed a significant disagreement in the distribution of states (higher ablation cloud density and lower velocity in LP compared to FT)
- Large inter-particle noise and discrepancy between density and particle number density were observed in LP
- LP code predicted much smaller reduction of pellet ablation rates in magnetic fields of increasing strength compared to the FT code

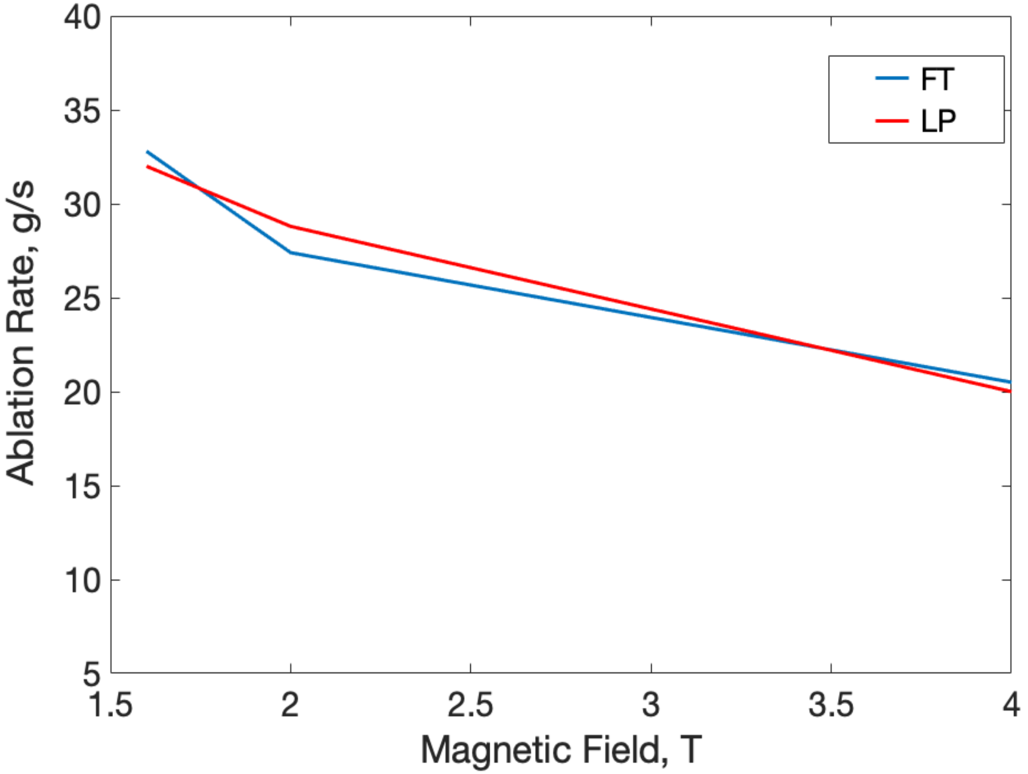
In Feb. 18 talk to CTTS, we presented important code updates

- FronTier: explicit tracking of ablation cloud / plasma interface with new Riemann solver led to improved states at the interface (e.g. velocity discontinuity
- Lagrangian Particles: new massively parallel code, kinetic electron heating algorithms let to elimination of noise, better accuracy, and significantly improved agreement with FT

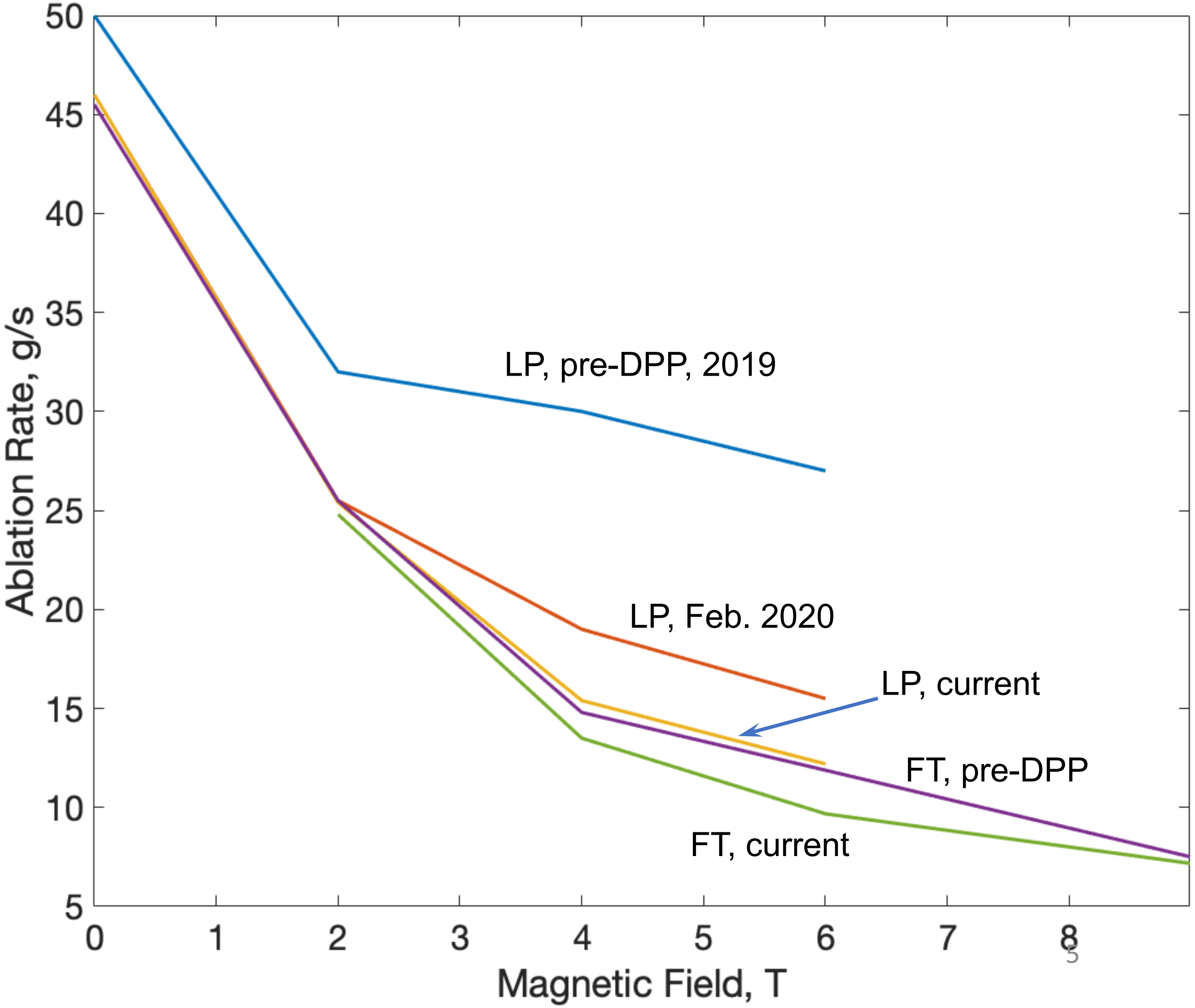
Since then, the agreement has been further improved: if the same approximations are used, both codes give essentially the same results

Resolution of discrepancies between FronTier and Lagrangian Particle Codes

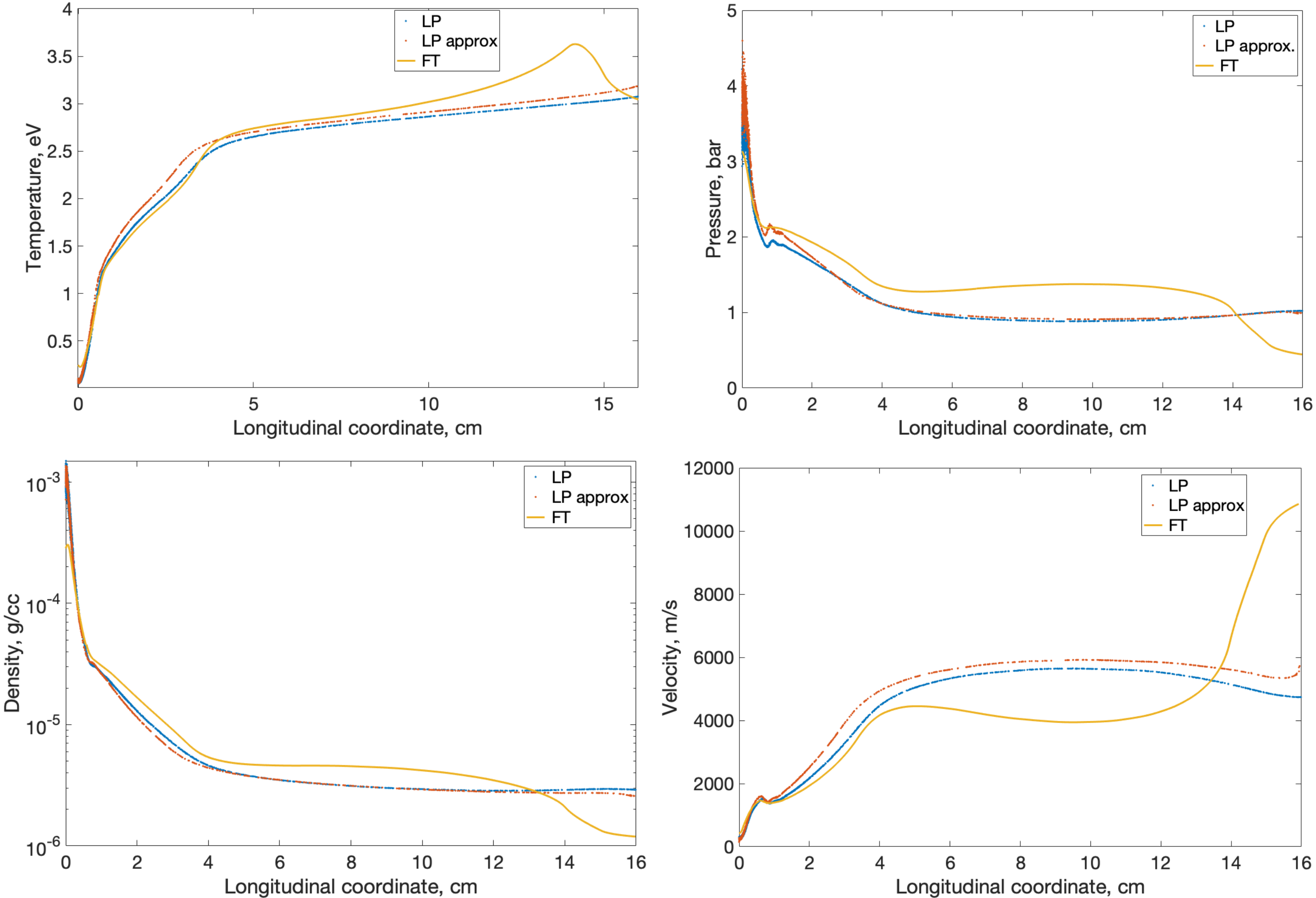
Ablation rates of Deuterium (D2) pellets



Ablation rates of neon pellets



Comparison of States in FronTier and Lagrangian Particle Codes, B = 2T



FronTier, for the reason of numerical stability, ramps down the electron heating at the end of the cloud. This causes a rapid drop of temperature and pressure, and the large pressure gradient drives the flow in the far field.

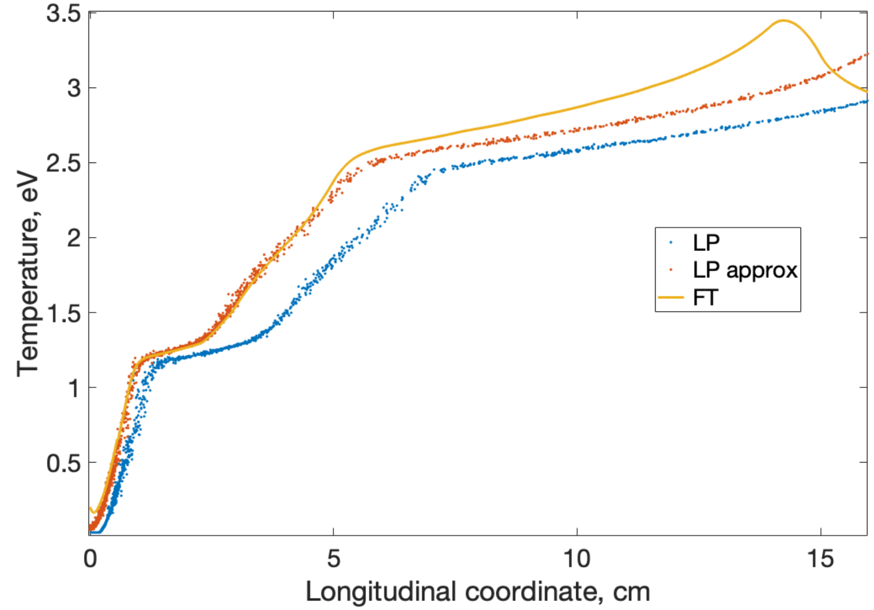
LP does not make such approximations and the flow in the far field is much more realistic.

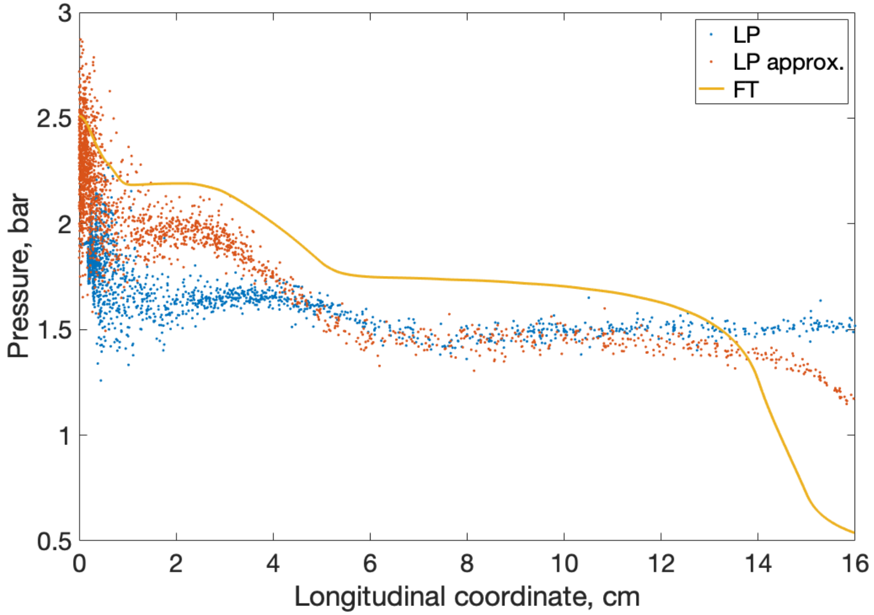
The numerical artifact in the FronTier far field may be responsible for a small difference in the ablation rate.

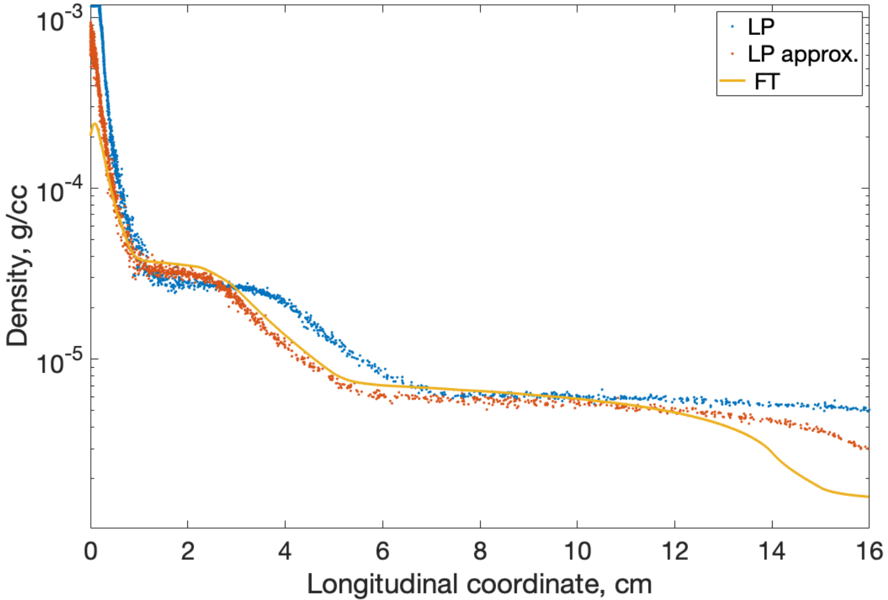
Red dots: LP's approximation of the outflow that is closer to FT.

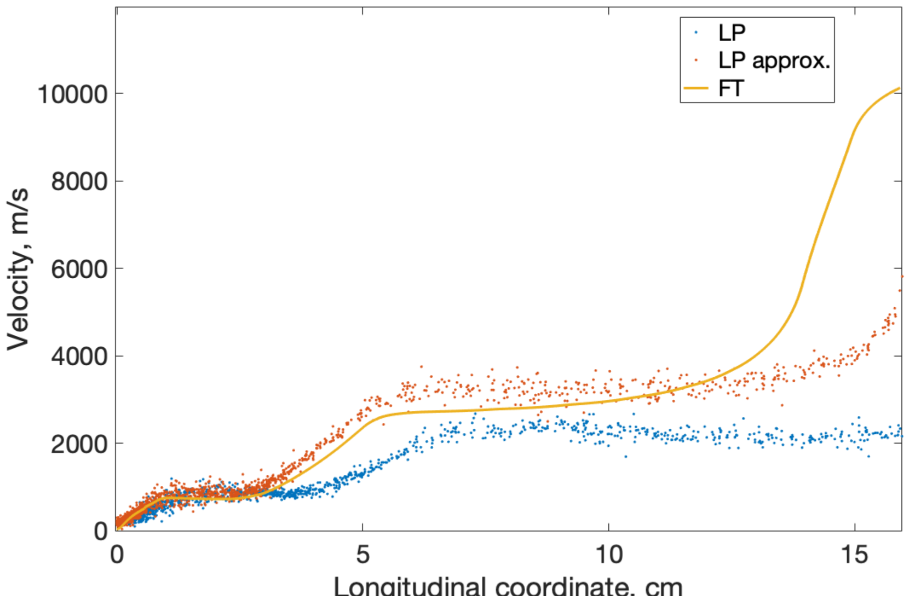
Blue dots: Better approximation of the outflow conditions (more important for 6T, see next slide)

Comparison of States in FronTier and Lagrangian Particle Codes, B = 6T









States along the axis of symmetry of the ablation cloud

Solid line: FT

Red dots: LP’s approximation of the outflow that is closer to FT.

Blue dots: Better approximation of the outflow conditions

Comparison of Ablation Rates with FronTier and Lagrangian Particle Codes

Neon pellet, shielding length = 16 cm

B	G LP (g/s)	Reduction compared to B=0	G FT (g/s)	Reduction compared to B=0
2T	25.4	1.8	24	1.9
4T	15.4	3.0	14	3.3
6T	12.2	3.8	10	4.0

Deuterium (D2) pellet, shielding length = 16 cm

B	G LP (g/s)	G FT (g/s)
1.6T	32	32.8
2T	28.8	27.4
4T	20	20.5

In previous presentations, we also reported on good agreement of both FronTier and Lagrangian Particle simulations with spherically-symmetric initial data with theory

Benchmarking FronTier Spherically Symmetric Simulations with Theory

ne = 1e14/cc with electrostatic/albedo shielding for ideal EOS

Te = 2 keV

r_p(cm)	Theory	FronTier 1/27/20	% error
0.1	25.5245	25.60	+0.296
0.2	64.9295	64.53	-0.615
0.5	222.206	220.9	-0.588
0.7	348.814	347.3	-0.434

Te = 5 keV

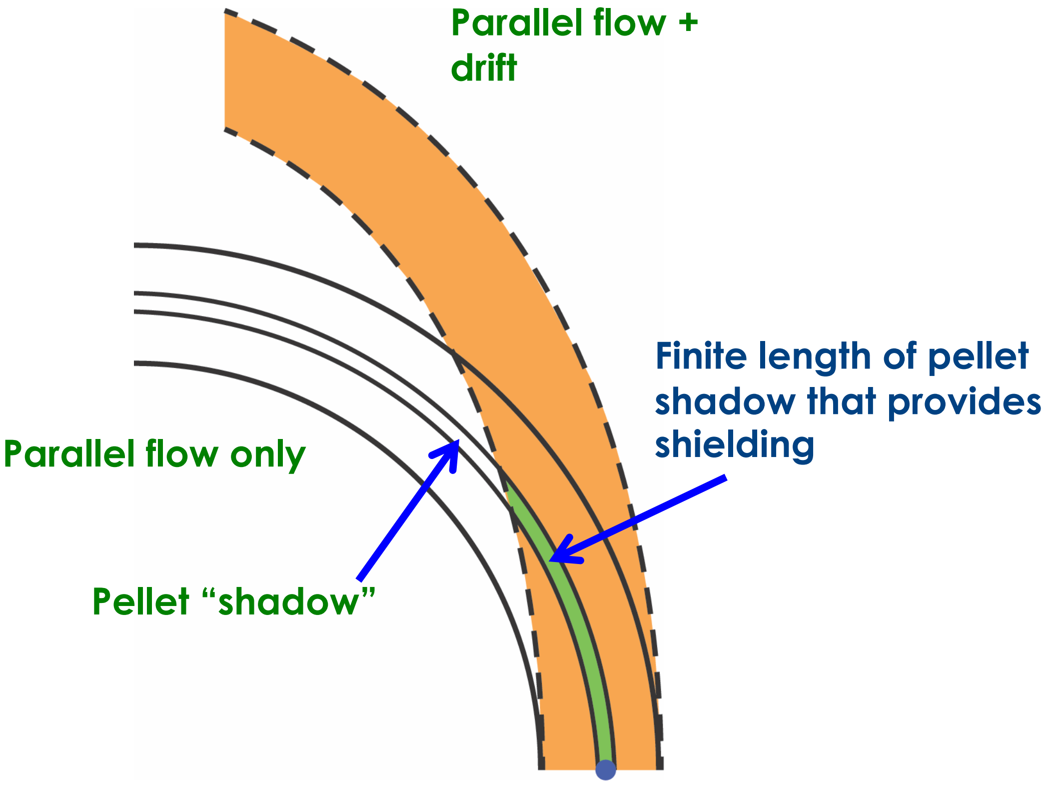
r_p(cm)	Theory	FronTier 1/27/20	% error
0.1	25.5245	25.60	+0.296
0.2	64.9295	64.53	-0.615
0.5	222.206	220.9	-0.588
0.7	348.814	347.3	-0.434

Te = 8 keV

r_p(cm)	Theory	FronTier 1/27/20	% error
0.1	116.815	117.0	+0.158
0.2	297.469	295.4	-0.695
0.5	1019.02	1013	-0.589
0.7	1600.07	1591	-0.567

Neon pellet ablation in the presence of grad B drift

Neon pellet ablation in the presence of grad-B drift



- In previous simulations, we assumed that the finite shielding length is an input parameter, set as 16 cm
- LP code is capable of computing the shielding length self-consistently

Grad-B drift model:

- We assume that the electrostatic potential is always uniform along the magnetic field. The equation for the horizontal grad-B drift velocity in the x (large-R) direction is governed by the formula [Parks 2000, Rozhansky 1995, 2004]

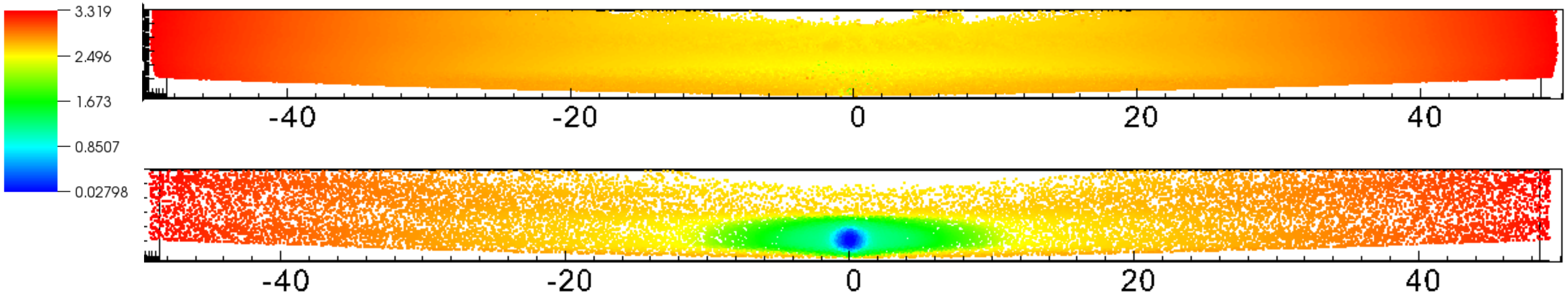
$$v_D \frac{dv_D}{dx} = J(x) = \frac{2\langle P - P_\infty \rangle}{R\langle \rho \rangle}$$

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

- These integrations are evaluated in the LP code with the kinetic heating algorithms
- The major radii of 1.6 m (DIII-D) and 6.2 m (ITER) are used in simulations

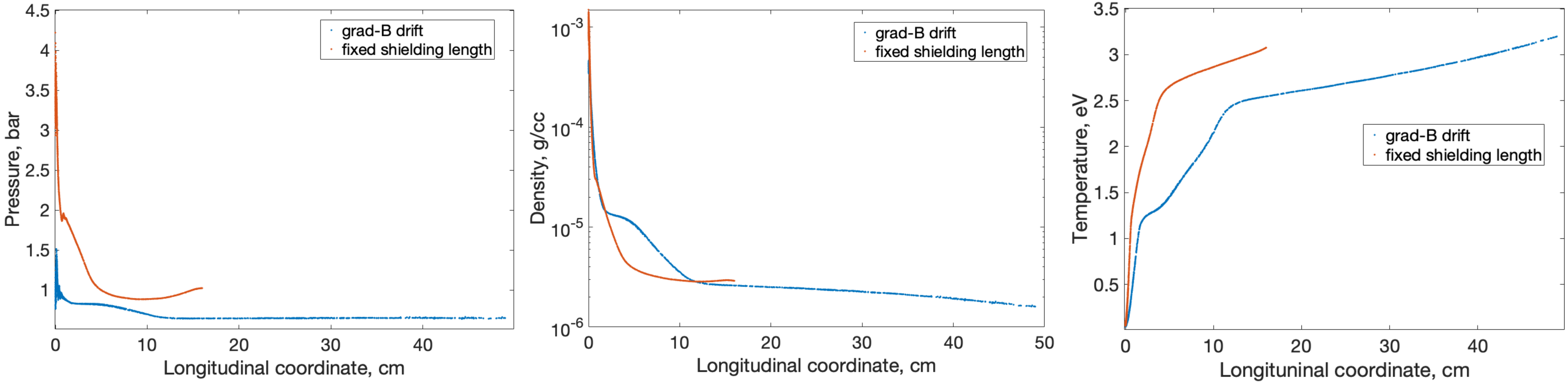
LP simulations in 2T field with grad-B drift

Domain = 100cm, massflowrate = 18 g/s, shielding length = 49cm



(a) Temperature distribution in full 3D cloud

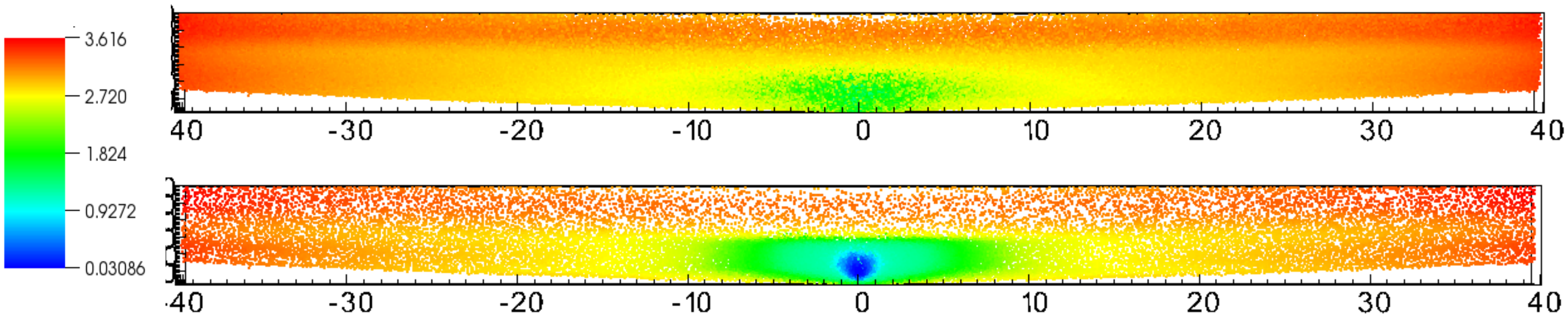
(b) Temperature distribution on 2D slice through pellet center



Distributions of pressure , density and temperature along magnetic field line through the pellet center for simulations with fixed shielding length and grad-B drift in 2T field.

LP simulations in 6T field with grad-B drift

Domain = 80cm, massflowrate = 16 g/s, shielding length = 27cm



(a) Temperature distribution in full 3D cloud

(b) Temperature distribution on 2D slice through pellet center

B	G (g/s) for fixed 16 cm shielding length	Shielding length with grad B drift	G (g/s) with grad B drift
2T	25.4	49 cm	18
6T	12.2	27 cm	16

Conclusion: grad B drift predicted unrealistically large shielding lengths. Model refinement was necessary.

Influence of the parallel flow Mach number on the grad B drift

- The grad-B drift model in the Lagrangian particle code was improved by including the effect of the parallel flow: $\langle P - P_\infty \rangle \; \Rightarrow \; \left\langle P\left(1+\frac{M^2}{2}\right) - P_\infty \right\rangle$ [P.B. Parks and L. R. Baylor "Effect of Parallel Flows and Toroidicity on Cross-Field Transport of Pellet Ablation Matter in Tokamak Plasmas", Physical Review Letters 94 125002 (2005)]

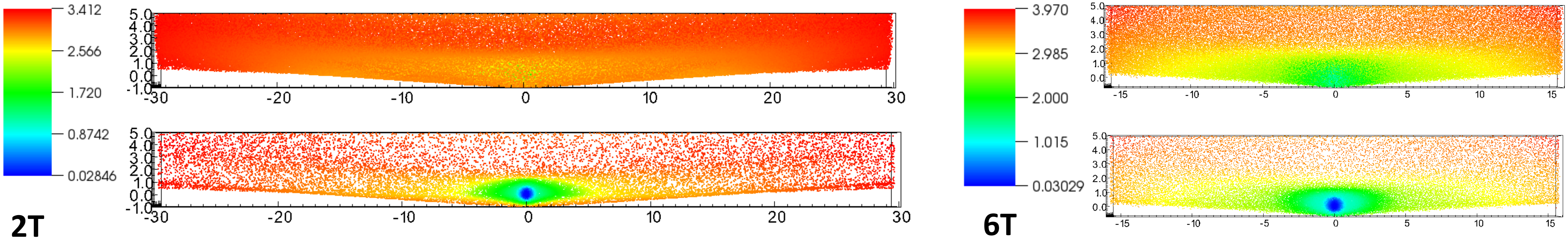
- Another potential factor affecting grad-B drift, the Alfvein wave drag, was estimated as non-essential

- The parallel flow Mach number has a significant effect on the grad B drift. Simulations predict much shorted shielding lengths:

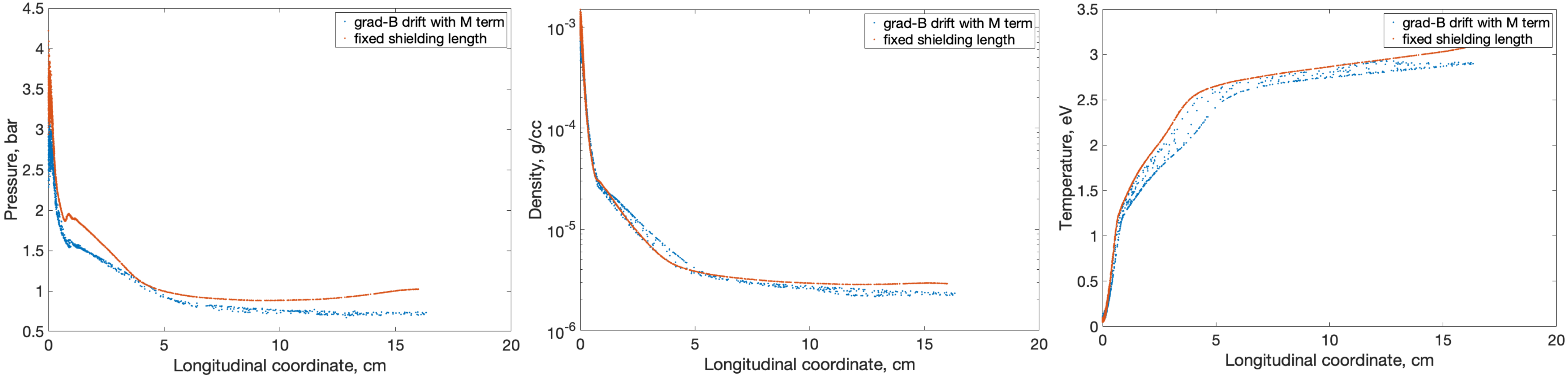
- For DIII-D major radius, the current shielding length in 2T field is 16.5 cm (49 cm was obtained without parallel flow term, 16 cm was used in fixed-length approximation)

- For 6T field, the new and old shielding lengths are 11 cm and 27 cm, correspondingly

Distributions of states in simulations with grad-B drift with Mach number term



Distributions of temperature in 3D ablation clouds (top) and on 2D slices through pellet centers for 2Tesla and 6 Tesla magnetic fields.



Distributions of pressure , density and temperature along magnetic field line through the pellet center for simulations with fixed shielding length and grad-B drift in 2T field. If the grad-B drift defined shielding length is the same as the fixed length, states are very close except states in grad-B drift simulations are not affected by the outflow boundary conditions (the domain extends beyond the shielding length).

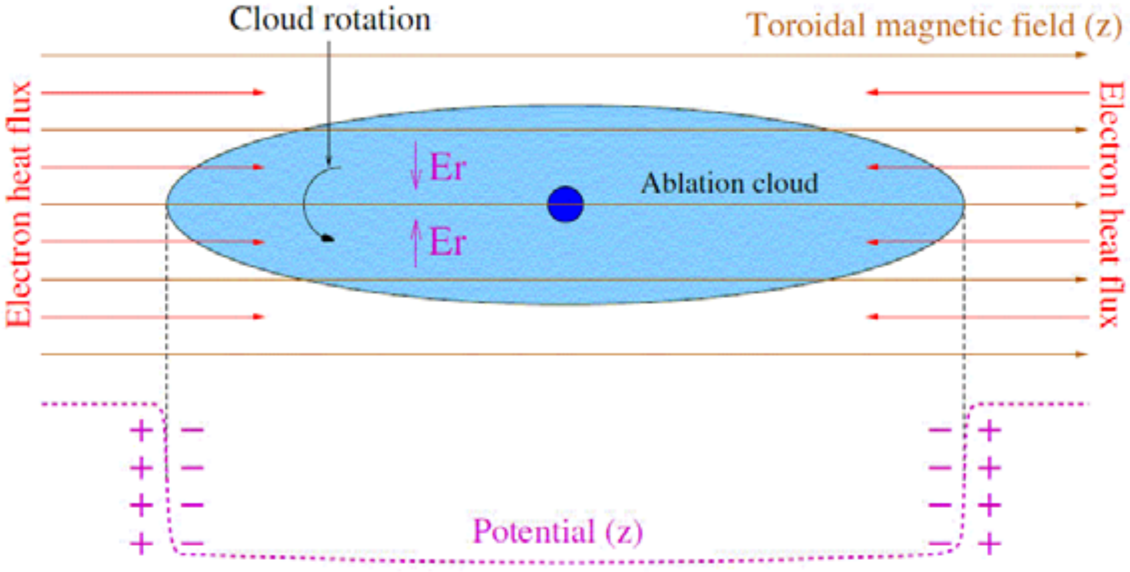
Dependence of ablation rates on magnetic field in the presence of grad B drift

B	G (g/s) 16 cm fixed shielding length	Shielding length with grad B drift, **R=1.6 (DIII-D)**	G (g/s) with grad B drift, **R=1.6 (DIII-D)**	Shielding length with grad B drift, **(R=6.2, ITER)**	G (g/s) with grad B drift, **(R=6.2, ITER)**
2T	25.4	16.5 cm	24.1	38 cm	21.5
6T	12.2	11 cm	20	27 cm	16

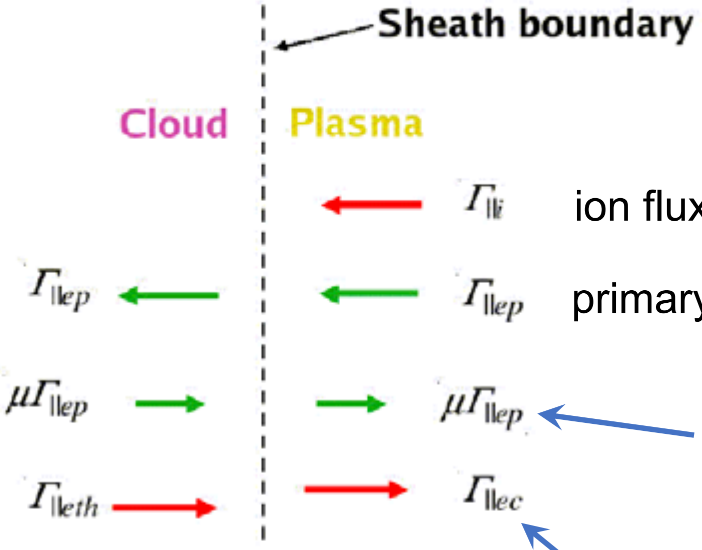
- With grad-B drift, we observe weaker reduction of the ablation rate in magnetic field compared to simulations with fixed shielding length
  - This effect is not only due to to different shielding length predicted by the grad-B drift: simulations of long plasma channels result in slightly different (improved) distribution of states as the numerical effect of outflow conditions is eliminated
  - Grad-B drift depends on the tokamak major radius
  - Grad-B drift in DIII-D (R_0 = 1.6 m) is stronger compared to ITER (R_0 = 6.2 m), all other factors assumed equal

- Any empirical G(B) fitting functions should be aware of the tokamak major radius

Pellet Cloud Charging and Rotation Model



(a) Potential distribution



(b) Sheath fluxes

ion flux

primary hot electron flux

attenuated hot electron flux that traversed the entire cloud length

cloud emitted electron flux

P.B.Parks, Plasma Phys. Controled Fusion, 1996.

P.B. Parks, T. Lu, and, R. Samulyak, “Charging and ExB rotation of ablation clouds surrounding refueling pellets in hot fusion plasmas”, Phys Plasmas 16 (2009) 060705.

Pellet Cloud Charging and Rotation: Governing Equations

Normalized potential:

$$\Phi(r,z)=\Phi_{s0}(r)+\frac{e\Gamma_{\parallel ep}}{T_{e\infty}(eV)}\int_z^{\infty}\frac{\mu_{-}(r,z')-\mu_{-}(r,z')}{\sigma_{\parallel}(r,z')}dz'$$

Nonlinear equation for the sheath potential:

$$\exp(-\Phi_{s0})-\sqrt{\pi\Phi_{s0}}\,\mathrm{erfc}\left(\sqrt{\Phi_{s0}}\right)=\frac{\alpha}{1-\mu_s}$$

Attenuation coefficient:

$$\mu_{\pm}(u_{\pm})=\left[1+\left(\frac{u_{\pm}}{2}\right)^{1/2}-\frac{u_{\pm}}{4}+\frac{1}{2}\left(\frac{u_{\pm}}{2}\right)^{3/2}\right]\exp[-(u_{\pm}/2)^{1/2}]-\frac{u_{\pm}^2}{8}E_1[(u_{\pm}/2)^{1/2}]$$

Ohm's law:

$$J_r=-\sigma_{\perp}(-\partial\phi/\partial r+u_{\theta}B)$$

Hydro / Low magnetic Reynolds number MHD equations in the presence of cloud rotation:

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho u)=0 \quad ,$$

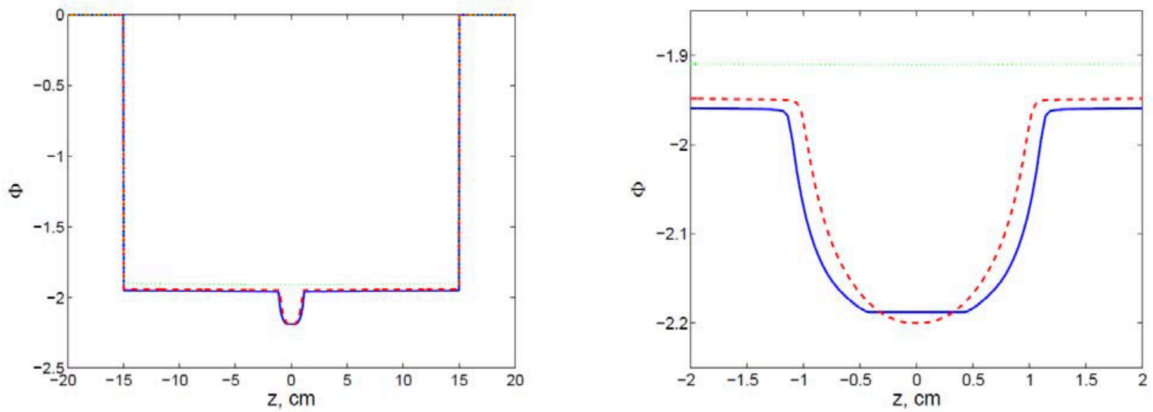
$$\rho\left(\frac{\partial u_r}{\partial t}+u_r\frac{\partial u_r}{\partial r}+u_z\frac{\partial u_r}{\partial z}\right)+\frac{\partial p}{\partial r}=J_{\theta}B+\rho\frac{u_{\theta}^2}{r} \quad ,$$

$$\rho\left(\frac{\partial u_z}{\partial t}+u_r\frac{\partial u_z}{\partial r}+u_z\frac{\partial u_z}{\partial z}\right)+\frac{\partial p}{\partial z}=0 \quad ,$$

$$\rho\left(\frac{\partial u_{\theta}}{\partial t}+u_r\frac{\partial u_{\theta}}{\partial r}+u_z\frac{\partial u_{\theta}}{\partial z}\right)=-J_rB-\rho\frac{u_r u_{\theta}}{r} \quad ,$$

$$\rho\left(\frac{\partial}{\partial t}+\boldsymbol{u}\cdot\nabla\right)e+p\nabla\cdot\boldsymbol{u}=\frac{1}{\sigma_{\perp}}(J_{\theta}^2+J_r^2)+\frac{J_{\parallel}^2}{\sigma_{\parallel}}-\nabla\cdot\boldsymbol{q_h}$$

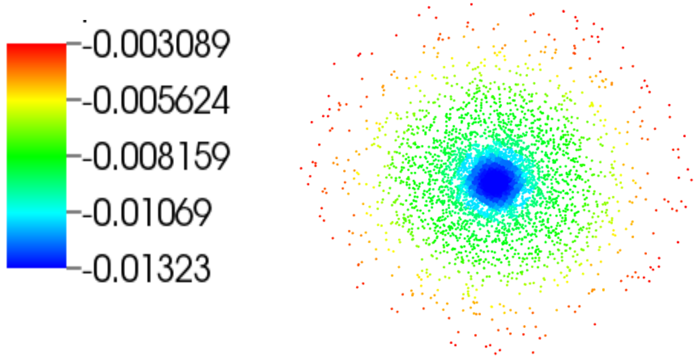
Equations are written in cylindrical coordinate system provide simpler explanation of the cloud rotation. In LP, they are implemented in Cartesian coordinates.



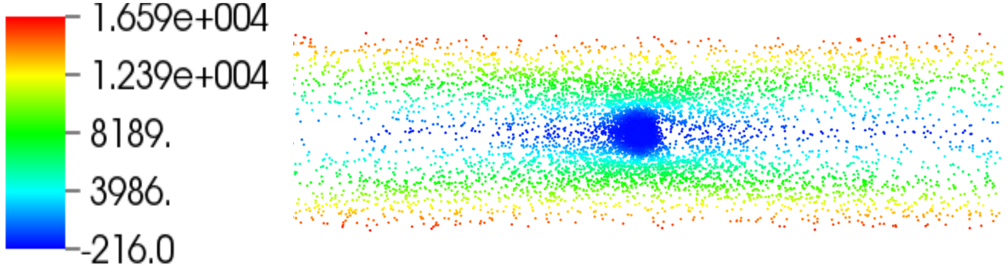
We showed [Parks, Lu, Samulyak 2009] that the potential is practically independent of the longitudinal coordinate except for a few mm layer around the pellet. In the present LP simulations, we assume that the potential depends only on the transverse coordinates.

Ablation of Deuterium Pellets with Cloud Rotation in 2T (work in progress)

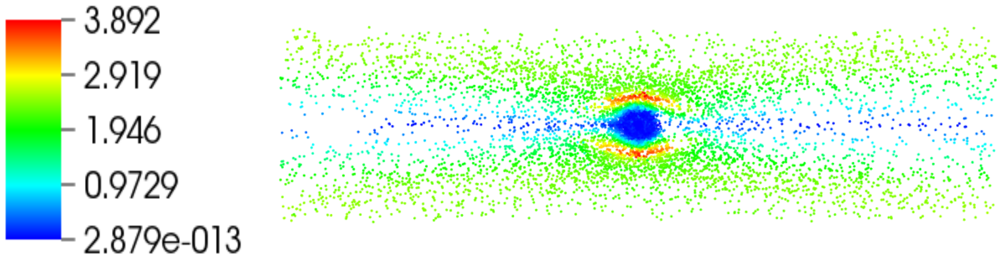
Potential



Rotational velocity



Rotational Mach number

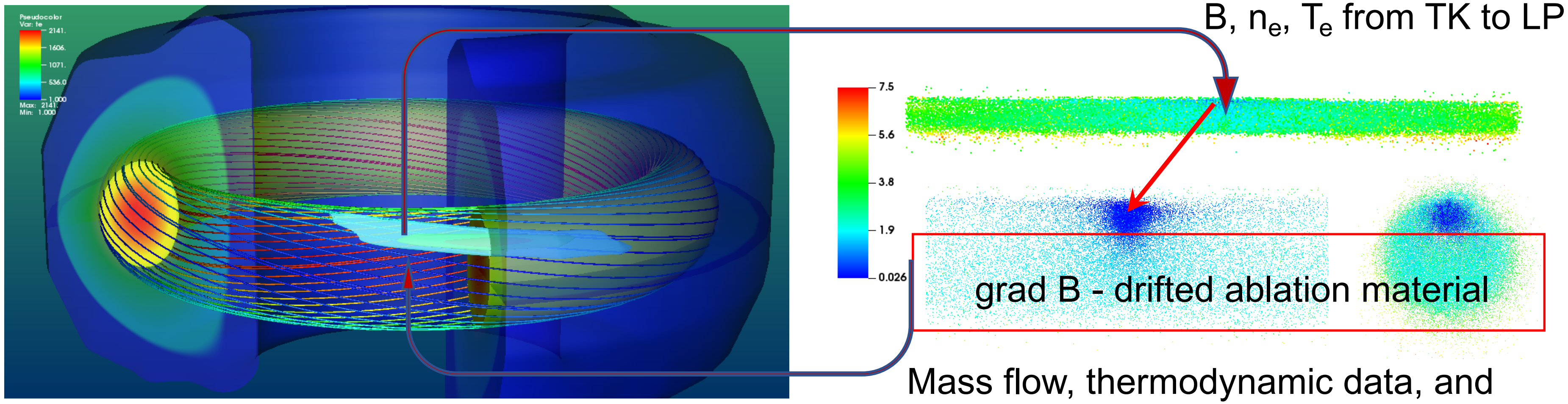


- Cloud rotation reaches supersonic values
- Density redistribution by centripetal force leads to the formation of low-density channel along the pellet axis
- Lower density channel along the pellet axis provides less shielding and affects the ablation rate
- We observe that the problem is very sensitive to fine details of the distribution of the potential and numerical resolution in the reduced density channel. More work is needed to report the ablation rate

Multiscale coupling: Introduction

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

Schematic of multiscale coupling

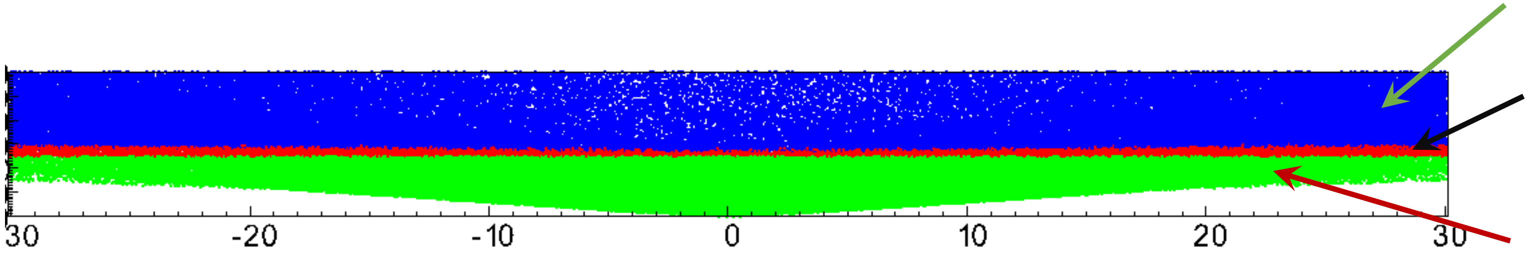
- **Grad B drift provides physics-based separation of scales for coupling**
- LP code evolves self-consistently the entire ablation cloud that provides pellet shielding
- grad B drift model in the LP code propagates ablated material across magnetic field lines, establishing the cloud shielding length. 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

Update on Multiscale coupling

- After improving the grad-B drift model, we generated data files for the next step in multiscale coupling
  - Files are uploaded to http://www.ams.sunysb.edu/~rosamu/Temp/Pellet_multiscale_coupling/
  - Particle data for the entire cloud, grad-B drifted layer, and file format description are uploaded

- For every particle, we record
  - local coordinates, velocity components
  - temperature, density, pressure
  - electron heat deposition power density, radiation power density
  - Number density of neutral atoms, number density of 1+, 2+, .. 10+ ions, electrons, and average ionization



Particles sent to NIMROD / M3D-C1 in past time steps

Particles being sent to NIMROD / M3D-C1 for the current time step

Particles in the main cloud that have not drifted yet beyond certain boundary

Schematic of particle labels in the LP code at any NIMROD / M3D-C1 time step

Summary and Conclusions

- Successfully resolved disagreements between FronTier and Lagrangian particle codes
  - If the same approximations are used, both codes give essentially the same results
  - Small differenced at high B are related to artifacts FT uses in the far field

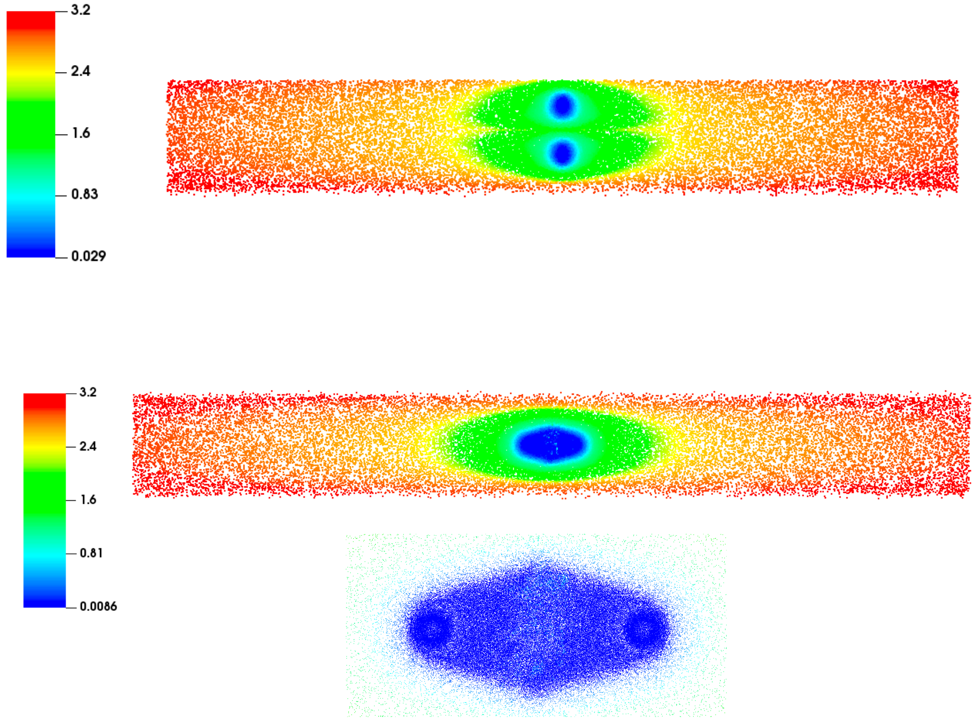
- Performed studies of ablation rates on neon pellets in the presence of grad B drift
  - Improved the grad-B grift model by parallel Mach number term
  - Simulations with grad-B grift show smaller reduction of the ablation rate magnetic fields
  - This effect strongly depends on the tokamak major radius and is less important for ITER compared to DIII-D

- Implemented cloud charging and rotation models in the Lagrangian particle code. More work is needed to finalize simulations

- Using improved grad-B drift model, obtained new data files for multiscale coupling

Future Work

- Complete cloud rotation simulations
- Single neon pellet validation
- SPI simulation. Implement a model for the reduction of plasma temperature in simulation with multiple fragments. We will use the dilution cooling model [P.B. Parks “A Theoretical Model for the Penetration of a Shattered Pellet Debris Plume” Invited Talk given at Theory and Simulation of Disruptions Workshop PPPL July 19, 2017].
- Complete multiscale coupling
- Combine grad-B drift with the cloud rotation (challenging)



Example of SPI simulations: two fragments placed across (top) and along (bottom) a magnetic field line.