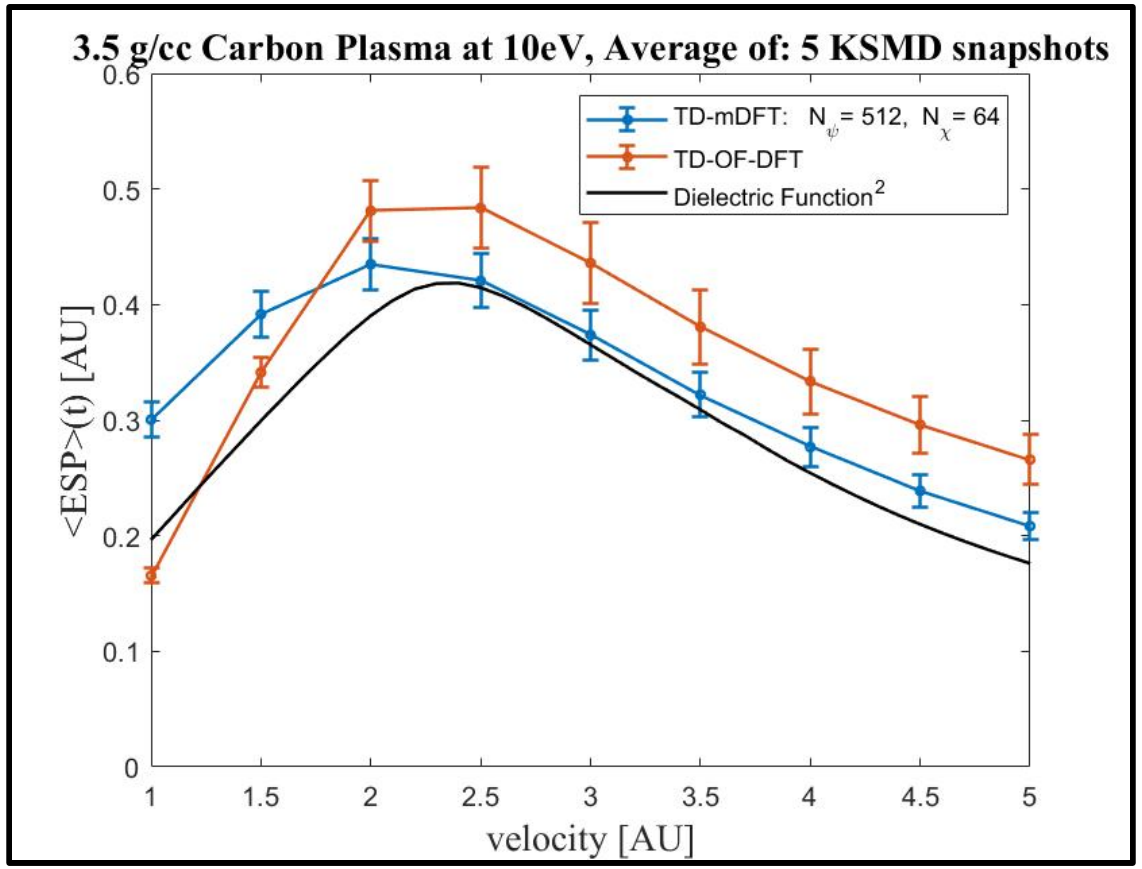
Investigating the Stopping Power of Warm Dense Plasmas using Time-Dependent Mixed Density-Functional Theory (TD-mDFT)



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Summary

Our studies show that TD-mDFT, when converged to TD-dDFT, can provide first-principles answers to electronic stopping power of warm dense plasma

- **The warm dense plasma regime is difficult to model due to strong coupling and electron degeneracy effects**

- **The newly developed time-dependent mixed density-functional theory (TD-mDFT) approach can be used to calculate dynamic plasma properties, such as electron stopping power, in a wide range of temperatures and densities**

- **These preliminary studies have proved that TD-mDFT can be applied to a wide range of dynamic properties for astrophysics and ICF applications**

TD-mDFT offers a more precise and computationally efficient method of modeling dynamic properties of warm dense plasma

TD-DFT is a more accurate approach to calculating electronic stopping power in warm dense matter (WDM) than many analytical models

- **Methods of calculating electronic stopping power (ESP):**
  - **Theories based on homogeneous electron gas vs. Density Functional Theory (DFT) methods[1-7]**
  - **Kohn-Sham DFT (KS-DFT)**
    - **KS-DFT single particle Hamiltonian:**

$$\hat{H} = -\frac{\nabla^2}{2} + \int d\vec{r}^3 \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} + \hat{V}_{xc} + \hat{V}_{ext}$$

    - **Deterministic KS-DFT (dDFT) computational cost:** $\propto V^3T^3$
    - **Stochastic KS-DFT (sDFT) computational cost:** $\propto V/T$
      - **Stochastic (Hutchison) trace estimator[5,6,7]**
  - **Orbital Free (OF-DFT) computational cost is not dependent on temperature, but is more approximate[1,2,3]**

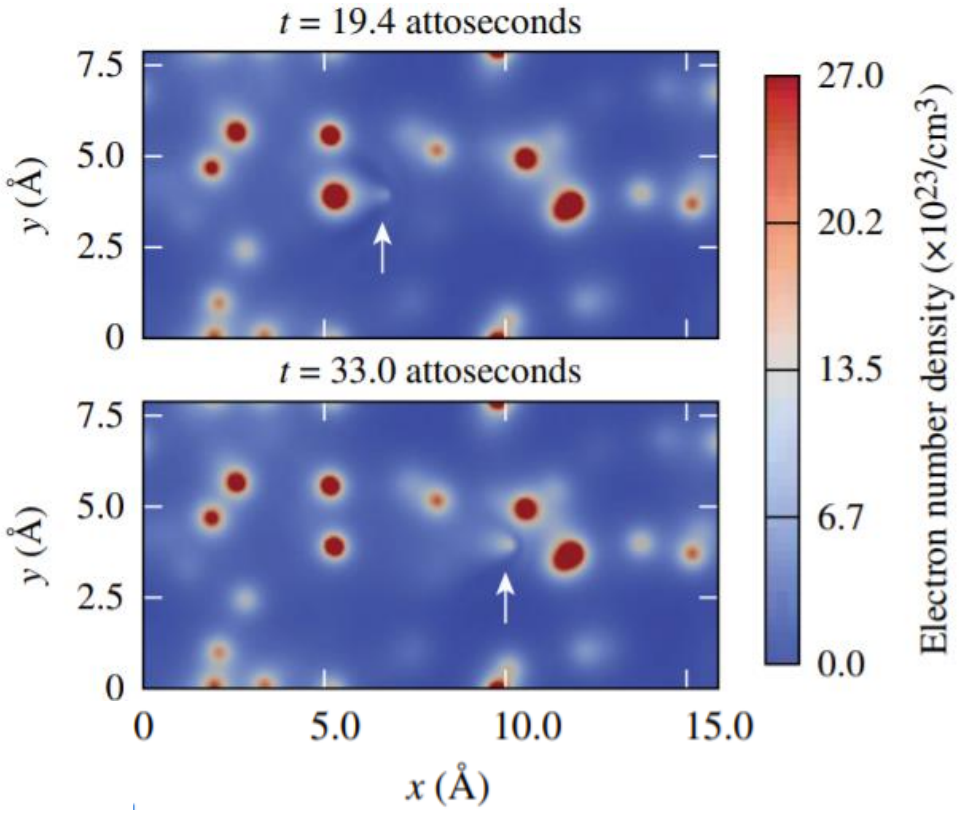
[1]Y. H. Ding, A. J. White, S. X. Hu, O. Certik, and L. A. Collins, Phys. Rev. Lett. 121, 145001 (2018).
[2]A. J. White, O. Certik, Y. H. Ding, S. X. Hu, and L. A. Collins, Phys. Rev. B 98, 144302 (2018).
[3]A.J. White and L. A. Collins, Phys. Rev. Lett. 125, 055002 (2020).
[4]M. Chen, R. Baer, D. Neuhauser, and E. Rabani J. Chem. Phys. 154, 204108 (2021).
[5] Y. Cytter, E. Rabani, D. Neuhauser, and R. Baer Phys. Rev. B 97, 115207 (2018).
[6]D. Yost, Y. Yao, and Y. Kanai, J. Phys. Chem. Lett. 11, 229−237 (2020).
[7]M.F. Hutchinson, Commun. Stat. Simul. Comput., 18:3, 1059-1076,(1989).

Motivation

Electronic stopping power is important for WDM and high energy density physics (HEDP)

- **Warm dense matter: $\mathbf{Temp} \approx 5 - 40eV$**
  - **Introduce mixed DFT (mDFT): combination of low energy deterministic (ψ) orbitals and high energy stochastic (χ) orbitals[2]**
- **High energy proton projected into background carbon plasma**
  - **Change in energy measured**
- **Electronic stopping power formula:**

$$ESP = \left\langle \frac{dW_p}{dR_p} \right\rangle = -\langle F_p[\rho, R, t] \rangle$$



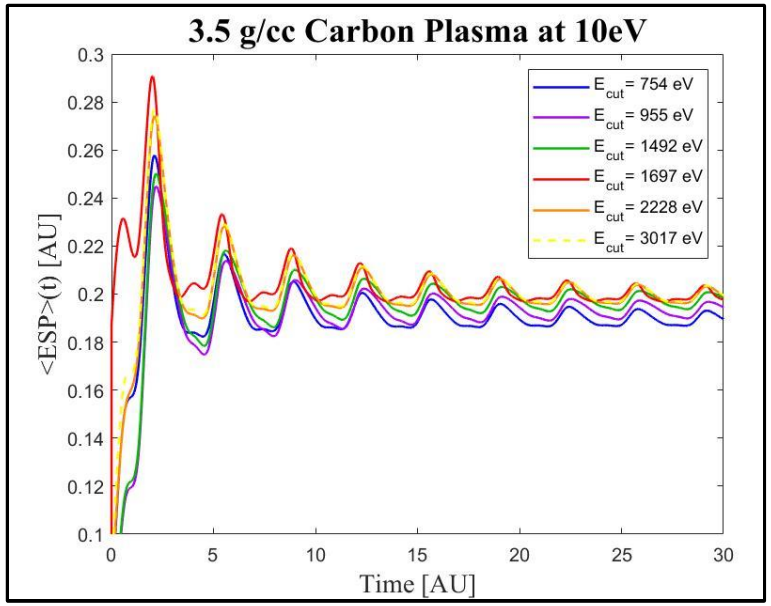
TD-DFT can be utilized to determine the electronic stopping power in WDM

[1]Y. H. Ding, A. J. White, S. X. Hu, O. Certik, and L. A. Collins, Phys. Rev. Lett. 121, 145001 (2018).

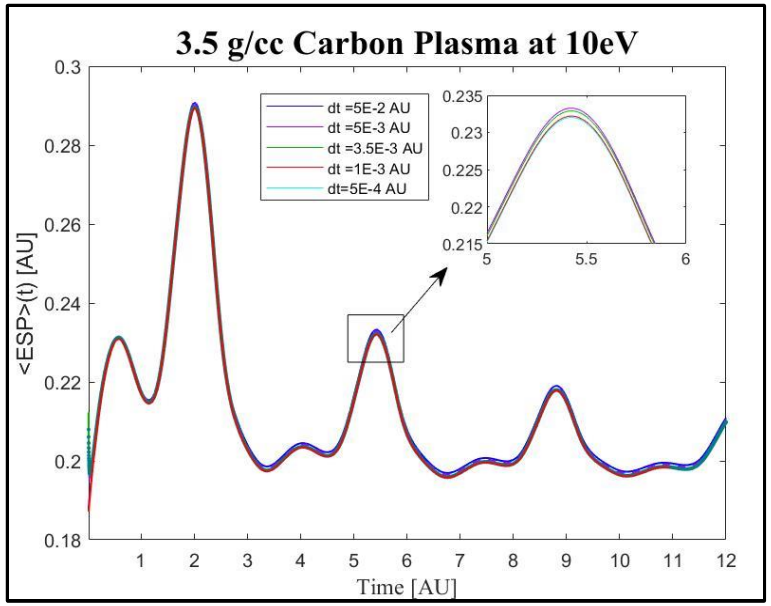
[2]A.J. White and L. A. Collins, Phys. Rev. Lett. 125, 055002 (2020).

Tests for energy cutoff, number of atoms, and timestep for a proton projected at $v = 4\hat{z}\ AU$ into 3.5 g/cc carbon plasma at 10eV are used to determine the converged simulation cell

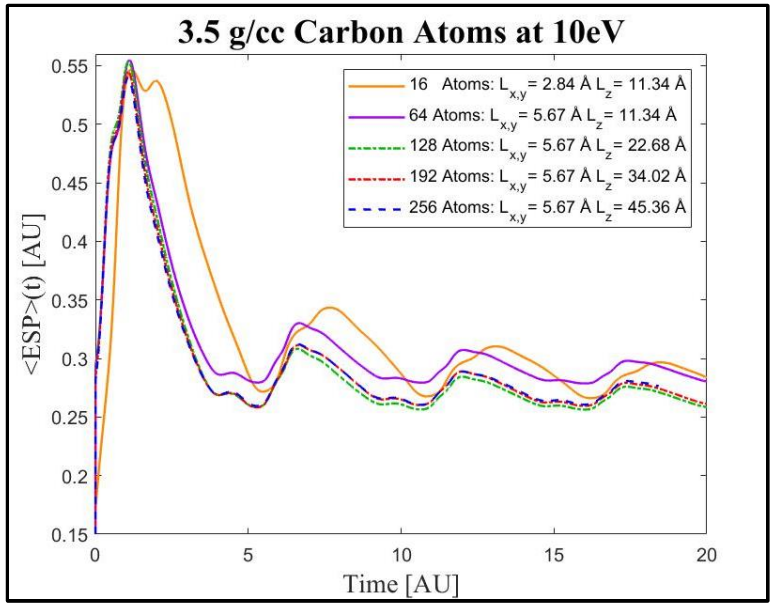
Energy Cutoff



Timestep



Box size / Number of atoms



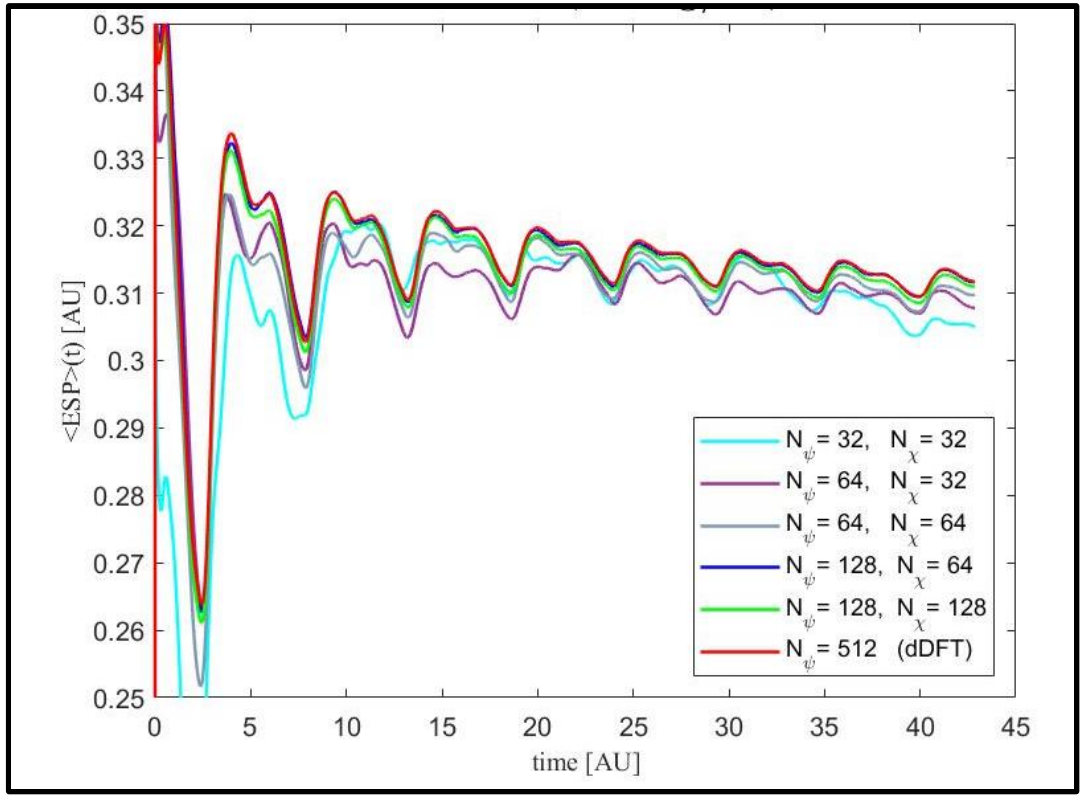
$$ESP[AU] \approx 1.94 \cdot ESP\left[\frac{MeV}{\mu m}\right]$$

$$1\text{Å} \approx 1.89\ AU$$

Figures: Rolling average electronic stopping power, $< \mathrm{ESP} > (\mathrm{t})$, with respect to time using TD-OF-DFT

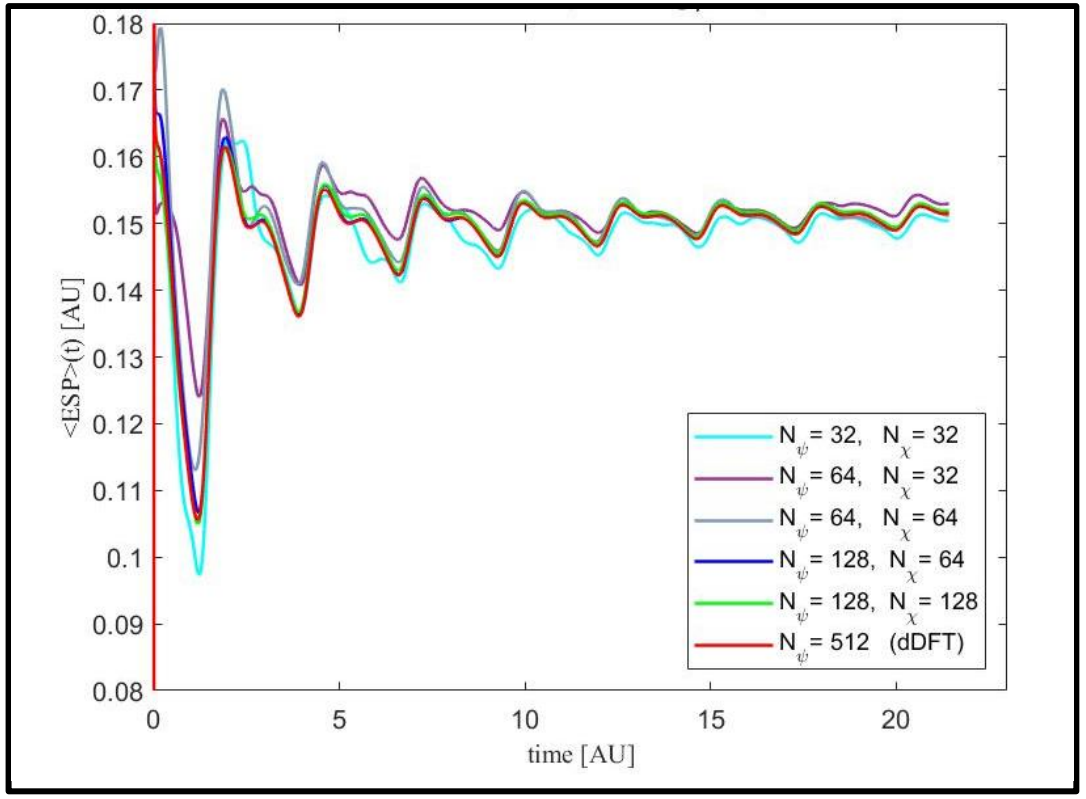
Small simulation cell comparison of TD-mDFT calculations to TD- dDFT for electronic stopping power for a single proton stopped by bulk carbon atoms

$v_p = 2.0\hat{z}$ AU



N_ψ = Number of deterministic orbitals
N_χ = Number of stochastic orbitals

$v_p = 4.0\hat{z}$ AU

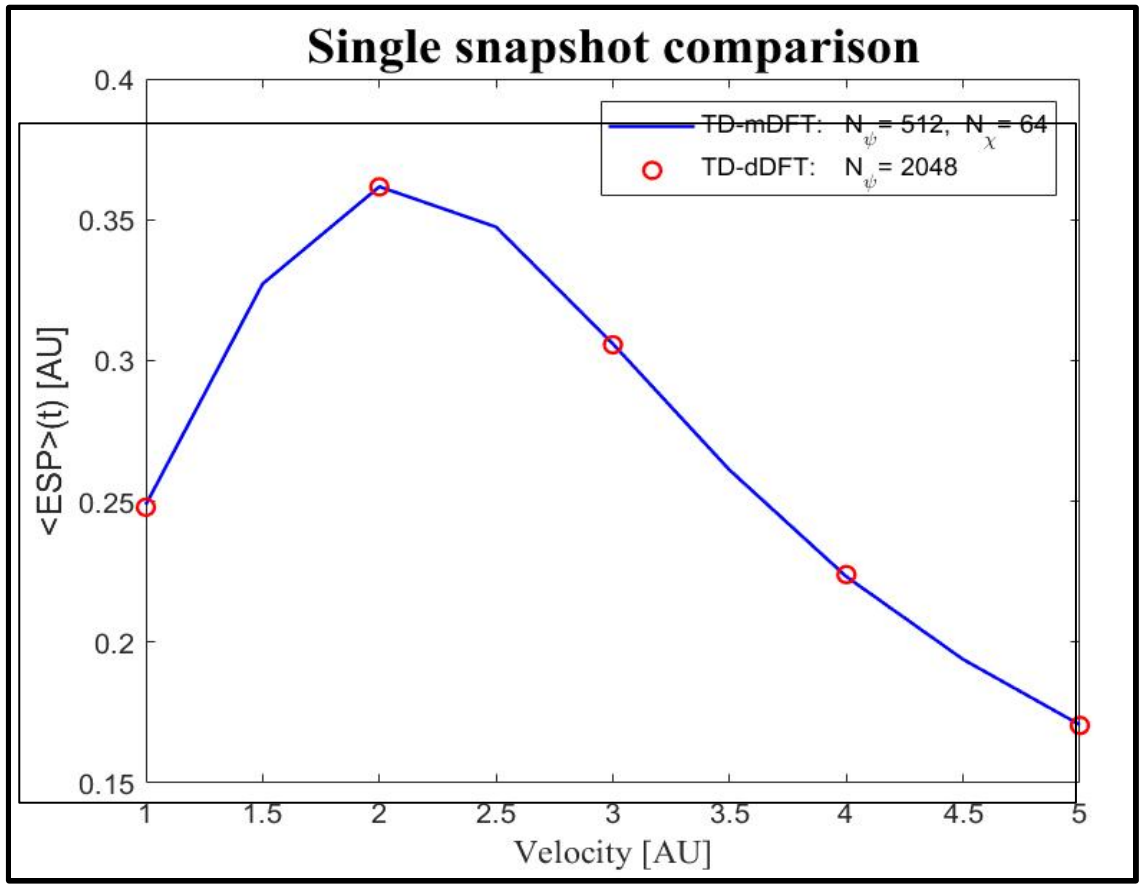


Simulation box: 32 atoms at 3.5 g/cc and 10eV

For a single snapshot, the converged TD-mDFT calculations for electronic stopping power converge well compared to purely TD-mDFT

Production Run: $3.5\ \mathrm{g/cc}, 10\mathrm{eV}$ carbon plasma

- **Single snapshot comparison between TD-mDFT : $N_\psi = 512,\ \psi_\chi = 64$ and purely TD-dDFT : $N_\psi = 2048$**
- **Due to computational cost of TD-dDFT only calculate ESP for 1 snapshot and a few projectile velocity values**
- **TD-mDFT well converged with TD-dDFT**

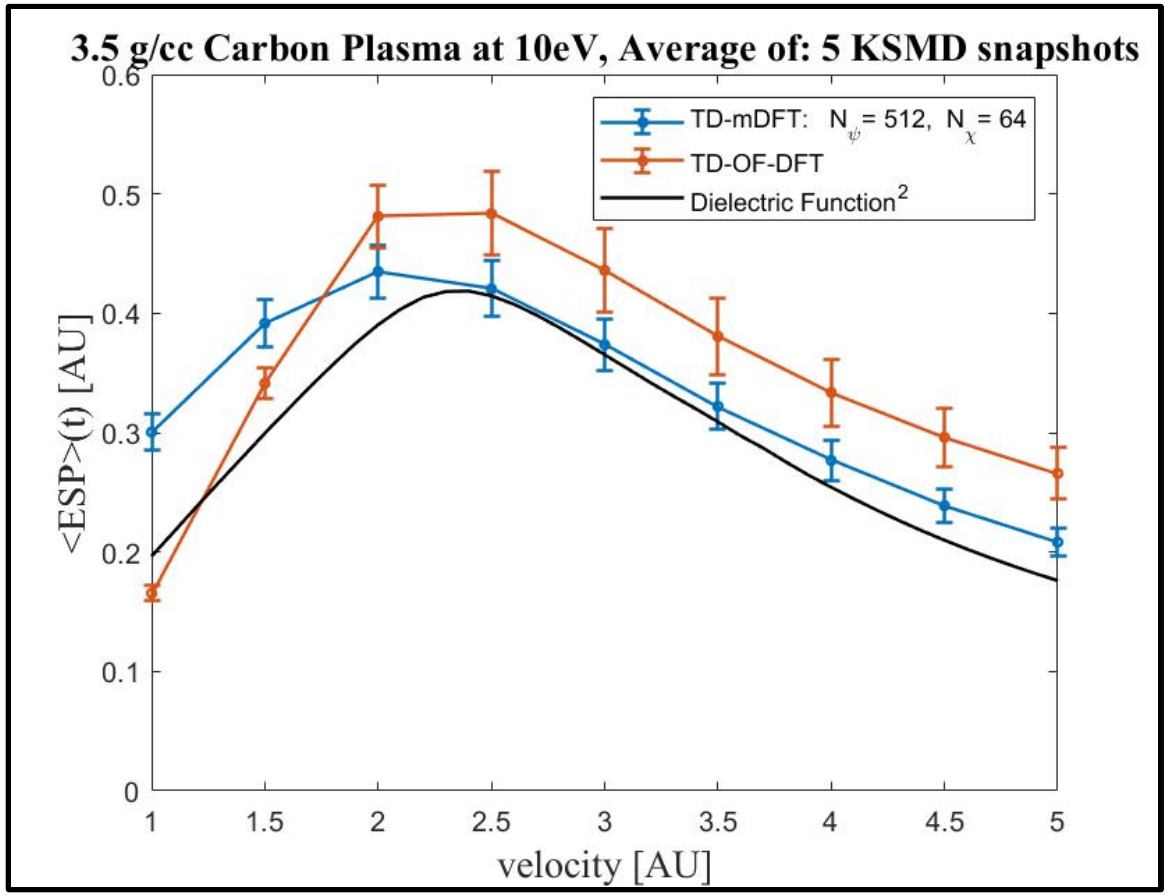


A single proton stopped by bulk carbon atoms.
Simulation box: 128 carbon atoms at 3.5 g/cc and 10eV

The converged TD-mDFT calculations for electronic stopping power give observable differences from TD-OF-DFT

Production Run: $3.5\ gcc, 10eV$ carbon plasma

- For each velocity increment: 5 distinct KSMD snapshots determine initial positions of background plasma, and are averaged over
- Comparison to TD-OF-DFT[1] and the analytical random phase dielectric function Method[2]
- Additional calculations in progress
- Standard error bars show relative error below 6.1% for all TD-mDFT velocity points



A single proton stopped by bulk carbon atoms. Simulation box: 128 carbon atoms at 3.5 g/cc and 10eV

[1] A. J. White, O. Certik, Y. H. Ding, S. X. Hu, and L. A. Collins, Phys. Rev. B 98, 144302 (2018).
[2] C. F. Clauser and N. R. Arista, Phys. Rev. E 97, 023202 (2018).

Outlook for future

- Continue stopping power calculations at higher temperatures and densities (20eV and 40eV)
  - Further prove that this time dependent mixed DFT method does in fact work irrespective of temperature and size of the system
  - Examine if this method can be used for alpha particle stopping in ICF hot spot
- Nonlocal electron stopping range calculations for ICF applications
- Apply mDFT method to other dynamic properties of WDM

TD-mDFT can be applied to any finite temperature, allowing for many unattainable calculations in WDM

Summary/Conclusions

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Thank You!