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Fast and Accurate Transport Coefficients for Dense Plasma Applications

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Introduction

Mixing of high-Z ablator materials into thermonuclear fuel can spoil burn conditions. We compare existing microscopic models such as Kohn-Sham density functional theory molecular dynamics (KS-DFT-MD) and pair-potential molecular dynamics (PP-MD) and fit more accurate models to compute transport coefficients.

Instabilities in Inertial Confinement Fusion (ICF) Experiments

In ICF experiments, instabilities due to surface roughness of the shell, non-uniform heating, etc. make obtaining a net gain in energy difficult. These instabilties result in mixing which can be explained through molecular dynamics simulation.

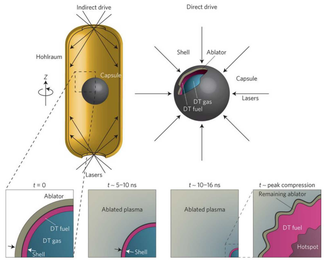


Figure 1: Indirect and direct drive ICF experimental setup. Note the instabilities depicted in the bottom right image which are a result in mixing.

Goal: Have an accurate description of the mixing process over the entire temperature range of the experiment.

Kohn-Sham Density Functional Theory MD v.s. Pair Potential MD

Correlation Functions

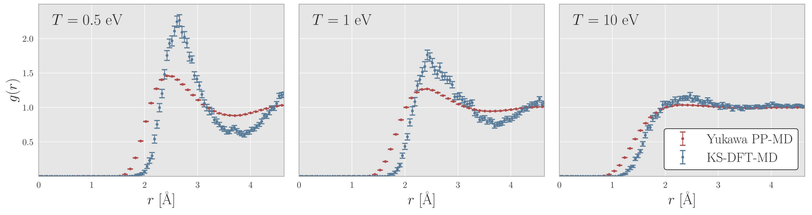


Figure 2: Radial distribution function for different temperatures.

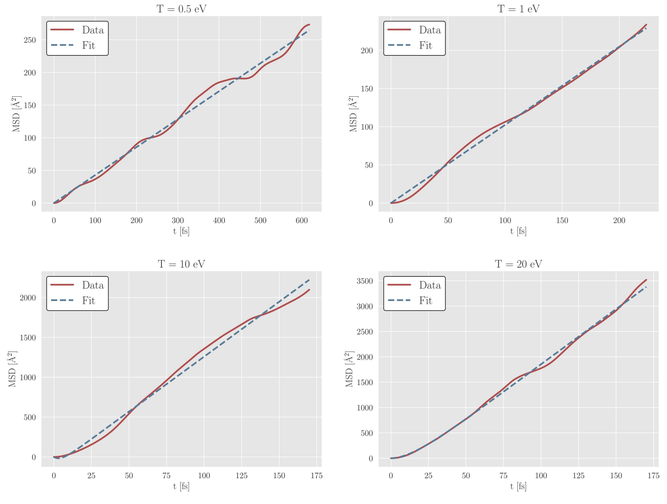


Figure 3: Mean-Squared Displacement over time for each simulation. Fits that capture the early time quadratic behavior and late time linear behavior have been added for computing self-diffusion coefficient.

Self-Diffusion Coefficient

Temp [eV]	PP-MD $\left[\frac{\text{Å}^2}{\text{fs}}\right]$	KS-DFT-MD $\left[\frac{\text{Å}^2}{\text{fs}}\right]$
0.5	$7.89e-3$	$1.42e-4$
1	$1.59e-2$	$3.40e-3$
10	$1.02e-1$	$4.91e-2$
20	$1.18e-1$	$7.23e-2$

Table 1: Self-diffusion transport coefficient for both methods. This was computed using the slope of the line in Figure 3.

Computation Time

Temp [eV]	PP-MD $\left[\frac{\text{sec}}{\text{particle}\times\text{time step}}\right]$	KS-DFT-MD $\left[\frac{\text{sec}}{\text{particle}\times\text{time step}}\right]$
5	$1.4e-4$	68.4
10	$1.1e-4$	57.6
20	$1.1e-4$	32.2

Table 2: PP-MD code uses a standard Yukawa interaction potential and KS-DFT-MD simulations are done with VASP [3].

Force Matching

Loss Function

In order to generate pair potentials from DFT calculations, we make use of the *force-matching* method [2] for which we minimize a loss function given by

$$Z(\alpha) = \left(3\sum_{k=1}^{M} N_k\right)^{-1} \sum_{k=1}^{M}\sum_{i=1}^{N_k} (\mathbf{F}_{ki}(\alpha) - \mathbf{F}^0_{ki})^2 \tag{1}$$

- M: Total number of atomic configurations
- N_k: Number of atoms in the k-th configuration
- $\mathbf{F}^0_{ik}$: Reference force on atom i in configuration k (obtained from DFT)
- $\mathbf{F}_{ik}(\alpha)$: Calculated force on atom i in configuration k due to parameters α

Data and Optimization Routines

Data:

- *Data Set*: 1,000 strided samples of each temperature
- *1 Large Training Set*: The entire data set
- *2 Small Training Sets*: 500 configuration each of strided samples

These datasets will be used in the following optimization routines.

Optimization:

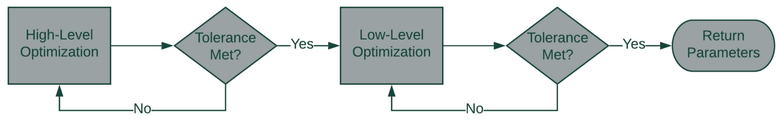


Figure 4: The software "Potfit"[1] was used to perform the optimization.

High-Level Optimization Routines:

- Simulated Annealing
- Genetic Algorithm

Low-Level Optimization Routine:

- Powell Least Squares Optimization

Analytic Potential Forms

We select four analytic potentials forms and perform the optimization:

Yukawa

$$u^Y(r) = \frac{Z^2e^2}{r}e^{-r/\lambda_{TF}}. \tag{2}$$

Short-Range Repulsion Yukawa [5]

$$u^{Y+SRR}(r) = \frac{a}{r^4} + \frac{Z^2e^2}{r}e^{-r/\lambda_{TF}}. \tag{3}$$

Exact Gradient-Corrected [4]

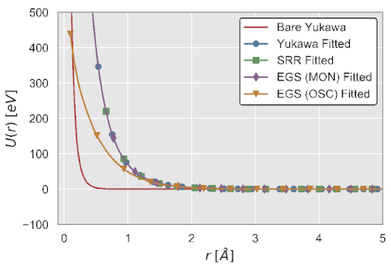
$$u^{EGS}_{\text{mon}}(r) = \frac{Z^2e^2}{2r}[(1+\alpha)e^{-r/\lambda_-} + (1-\alpha)e^{-r/\lambda_+}], \tag{4}$$

$$u^{EGS}_{\text{osc}}(r) = \frac{Z^2e^2}{2r}[\cos(r/\gamma_-) + \alpha'\cos(r/\gamma_-)]e^{-r/\gamma_+}. \tag{5}$$

The red terms are fit from KS-DFT-MD data.

Fitted Potentials

Analytic Potential Fits



Potential	RMS Error
Yukawa Fit	$1.35e+02$
SRR Yukawa Fit	$1.35e+02$
EGS MON Fit	$1.35e+02$
EGS OSC Fit	$9.08e+01$

Table 3: The RMS error computed after fitting the analytic potentials for $T = 0.5$ eV.

Figure 5: Fitted analytic potentials for $T = 0.5$ eV.

Screening Functions

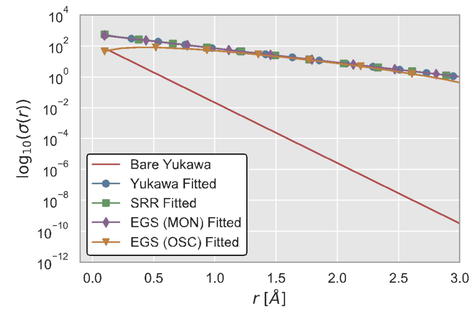


Figure 6: The screening functions for $T = 0.5$ eV. The screening function is given by $\sigma(r) = r\,u(r)$.

Bibliography

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Acknowledgements

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