The Efficacy
for Non-

A Special Thar

San Jose

* 33,000 students (5,500 g
* Minority serving institutio
* Nationally ranked for SM

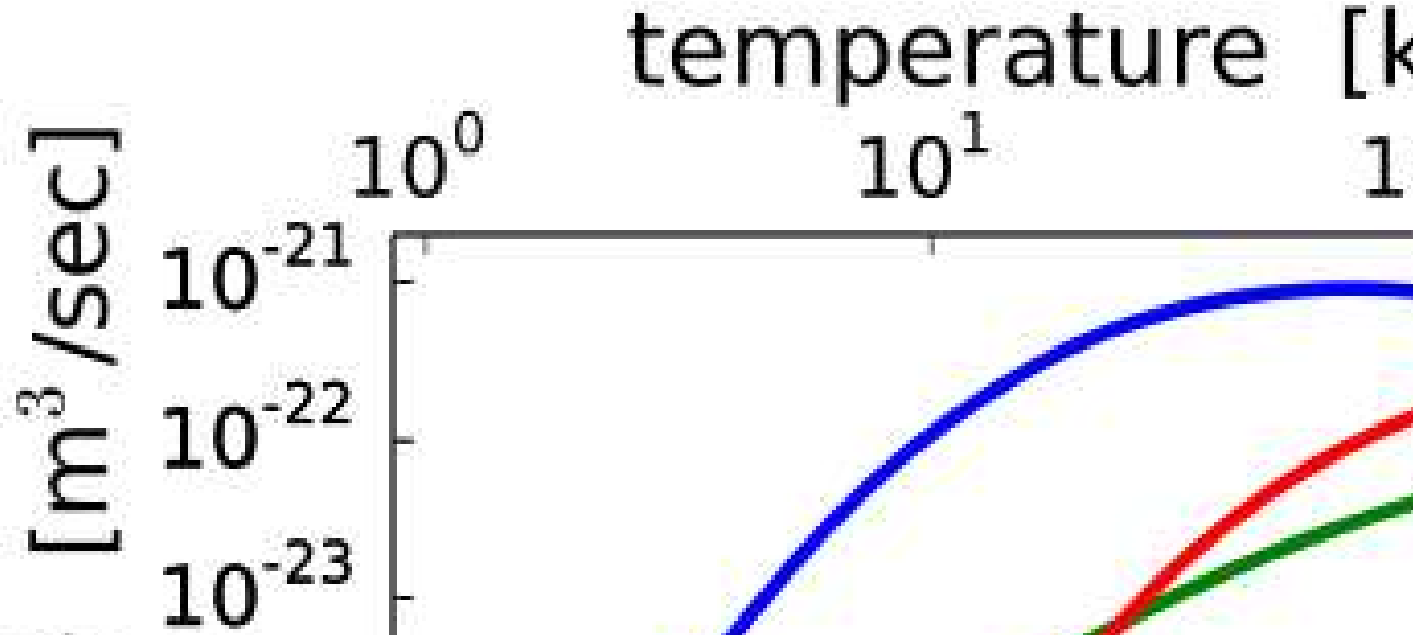
I. Modelir

II. Calculat
converg

III. Verificat

Why is Transport Im

* The pursuit of fusion require



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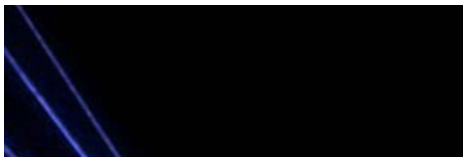

Why is Transport Im

* The pursuit of fusion require
* Consequently, our HEDP fac
  continued to probe increasi
* The resulting plasmas are b

How does Microph

* HED Plasmas are often well-

Example: $$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}$$

$$\rho_i \left(\frac{\partial \mathbf{u}}{\partial t} \right.$$

How does Microph

* Hydro equations express co
micro-physics is contained i

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}$$

$$\left(\frac{\partial \mathbf{u}}{\partial t} \right.$$

How does Microph

* Equilibrium statistical mecha
  "equation of state" quantit

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}$$

$$\left(\frac{\partial \mathbf{u}}{\partial t} \right.$$

How does Microph

* The non-equilibrium proces
are captured through the re

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}$$

$$\left(\frac{\partial \mathbf{u}}{\partial t} \right.$$

I. Modelin

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How do we <u>obta</u>

* HEDP experiments are
  models are required.

* In radiation-hydrodynar
  potentially needs to be
  at *<u>every</u>* time step durin

How do we mod

How do we mod

Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_i m_i |\mathbf{v}_i|^2 + \frac{1}{2}\sum_{i,j} u_{ij}(\mathbf{r}_i, \mathbf{r}_j)$$

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BBGKY Hierarchy

$$\frac{\partial}{\partial t} f_s + \sum^{s} \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i} f_s + \sum^{s}$$

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Kinetic Equation (V, B, FP, BGK, LB, ..

$$\frac{\partial}{\partial t} f + \mathbf{v} \cdot \nabla_{\mathbf{r}} f = \mathcal{C}[f]$$

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Modified A

The problem with pla

* Coulombic interactions
  collision integrals.

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One Resolution:

* "b_{max} issue" resolved in

$$1) \quad f_3(\mathbf{r}_{1,2,3}, \mathbf{v}_{1,2,3}$$

$$2) \quad \int d\mathbf{v}_3 f_1(\mathbf{r}_3) =$$

Modified A

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An "Effective

* The end result?

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* The end result?

* Despite the simplicity, the *entire* calculation must be

So, we fit the c

Cross section fi

$$\phi_n(w) \approx \begin{cases} \phi_n^{\mathrm{SC}}(w), & w < 1 \\ \phi_n^{\mathrm{WC}}(w), & w > 1 \end{cases}$$

where the strongly coupled component is giv

$$\phi_n^{\mathrm{SC}}(w) = \frac{c_0 + c_1 \ln(w) + c_2 \ln^2(y) + c_3}{1 + c_4 \ln(w)}$$

Wha

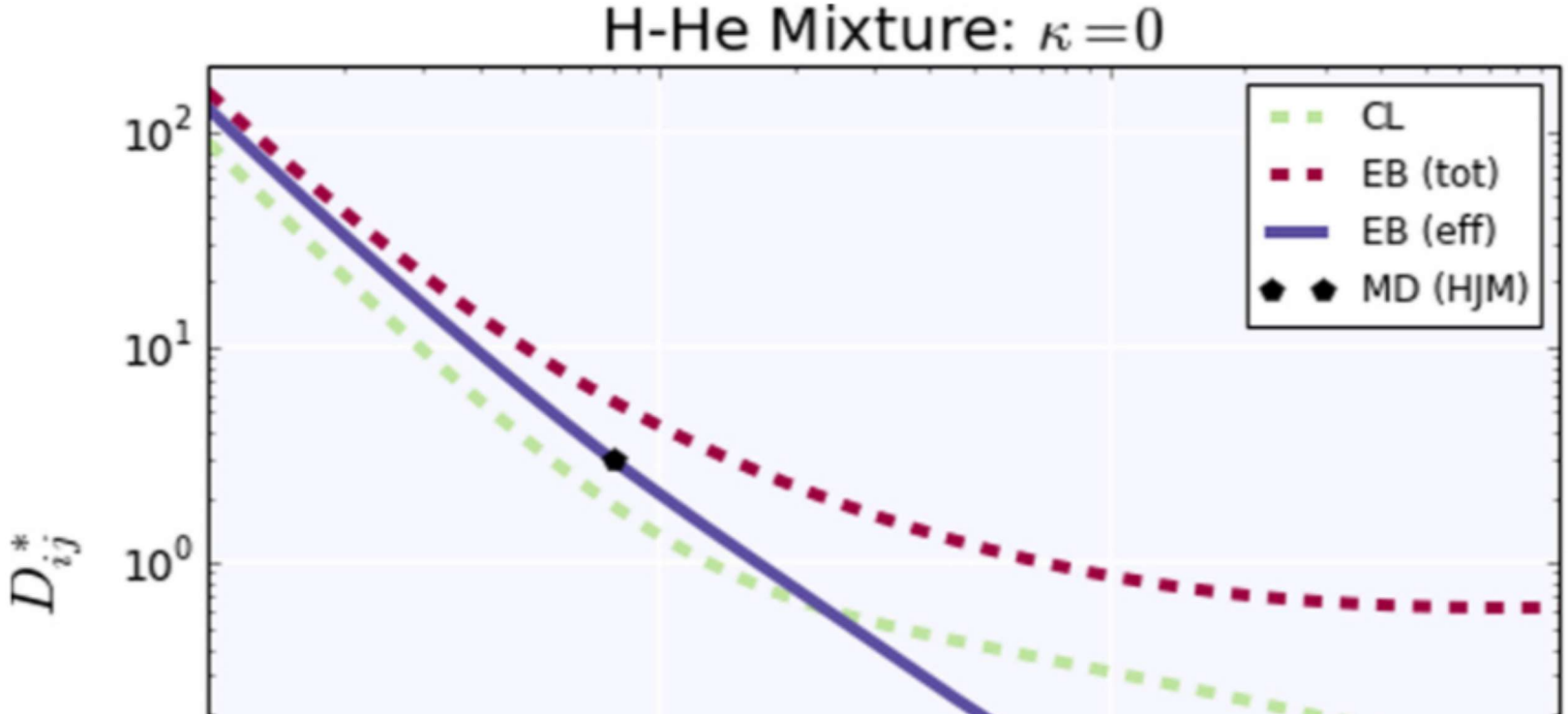
* This parameter is a "screeni
  theories to predict it (Debye

* Molecular dynamics (MD) ca
  performed, and none quite

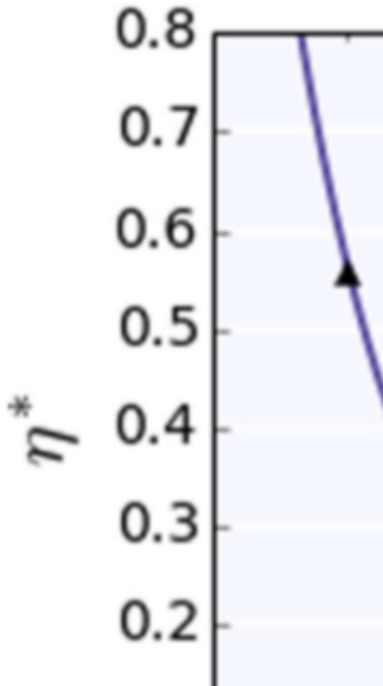
* Fi

Validation of Effe
Molecular

D_{ij}: inter-diffusivity*



η:



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How do we valid

1) High Fideli

- HFPCs are oft
- They are usua
- Multi-species
- Results can b
  processes.

Comparis

- Simulation data from the Charged-Particle T
  Coefficient Code Comparison Workshop*.
- Example: H at ρ = 1 g/cc, 0.2eV < T < 2keV
- 12 methods shown for ion viscosity (η), elec
  conductivity (σ) and thermal conductivity (κ

*P. E. Grabowski *et al*. (submitted)

Comparis

- Our method (**black**) compares well.
- Simple functional form of fits allows for ‘continuous’ calculations.
- Electronic transport (σ, κ) is shown to be captured despite classical approximations.

*P. E. Grabowski *et al*. (submitted)

Dyna

- Dynamic screening can be incorporated by adding a velocity dependence to the scree length (Zwicknagel *et al.*, 1999)

- This enables the calculation of quantities su stopping power.

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Ultracold Ne

UN Plasmas

- $n \sim O(10^9\ cm^{-3})$
- $T_i \sim O(1\ K)$
- $T_e \sim O(10^2\ K)$
- $Z = 1$

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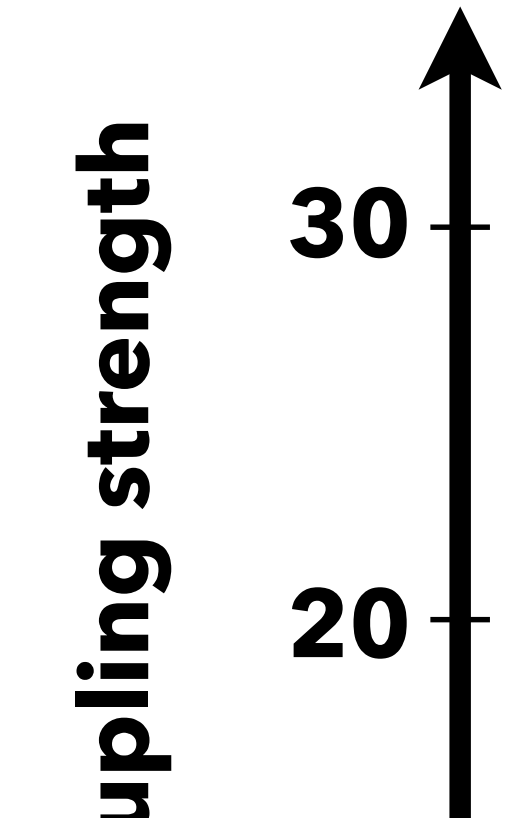

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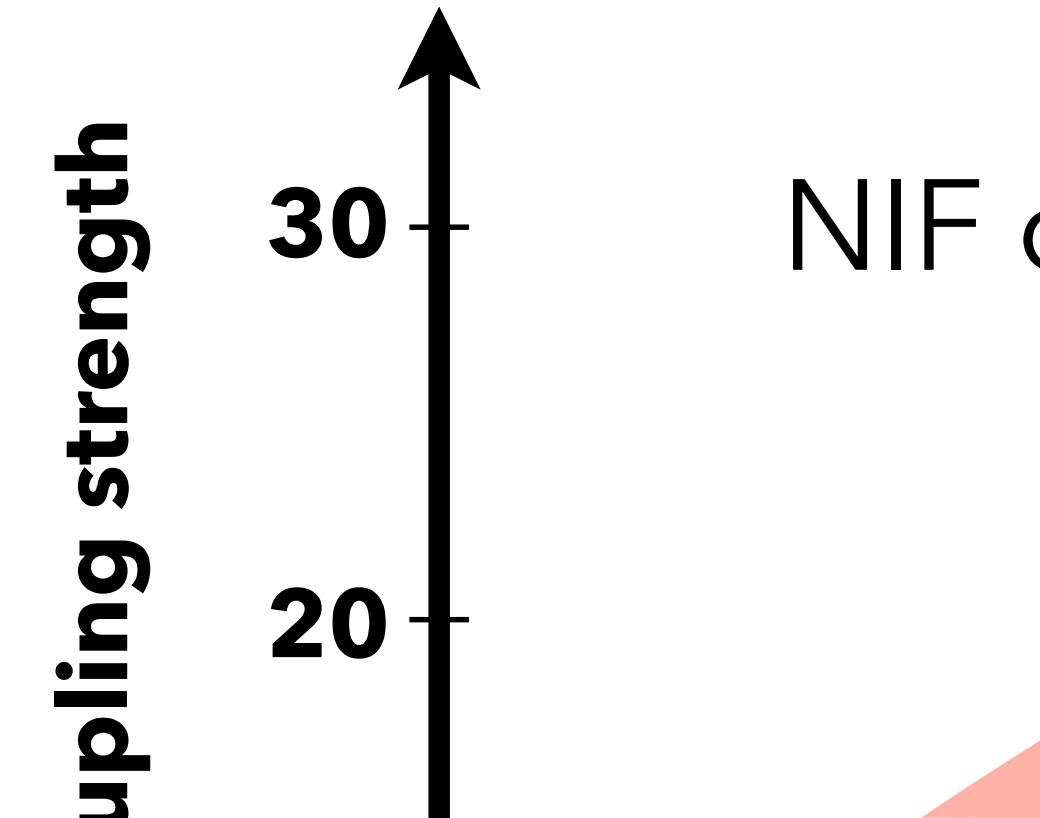

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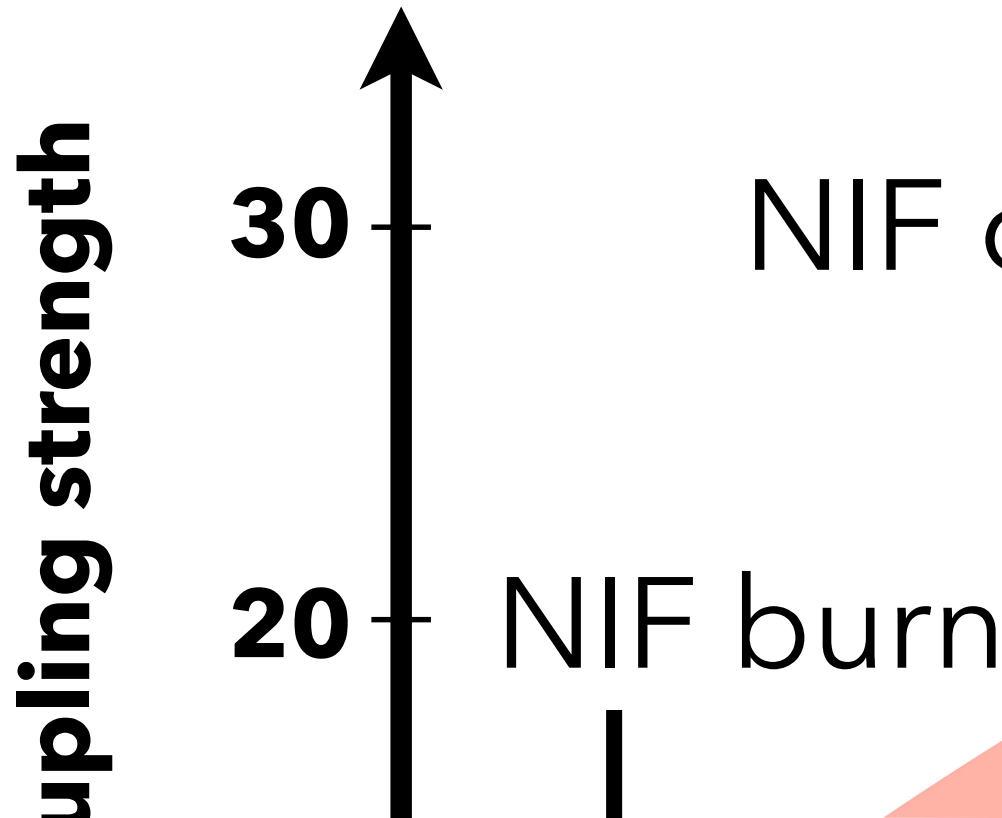

Impact of UNP

UNPs

Experiments

Roberts Group (CSU)

Bergeson Group (BYU)

Impact of UNP

UNPs

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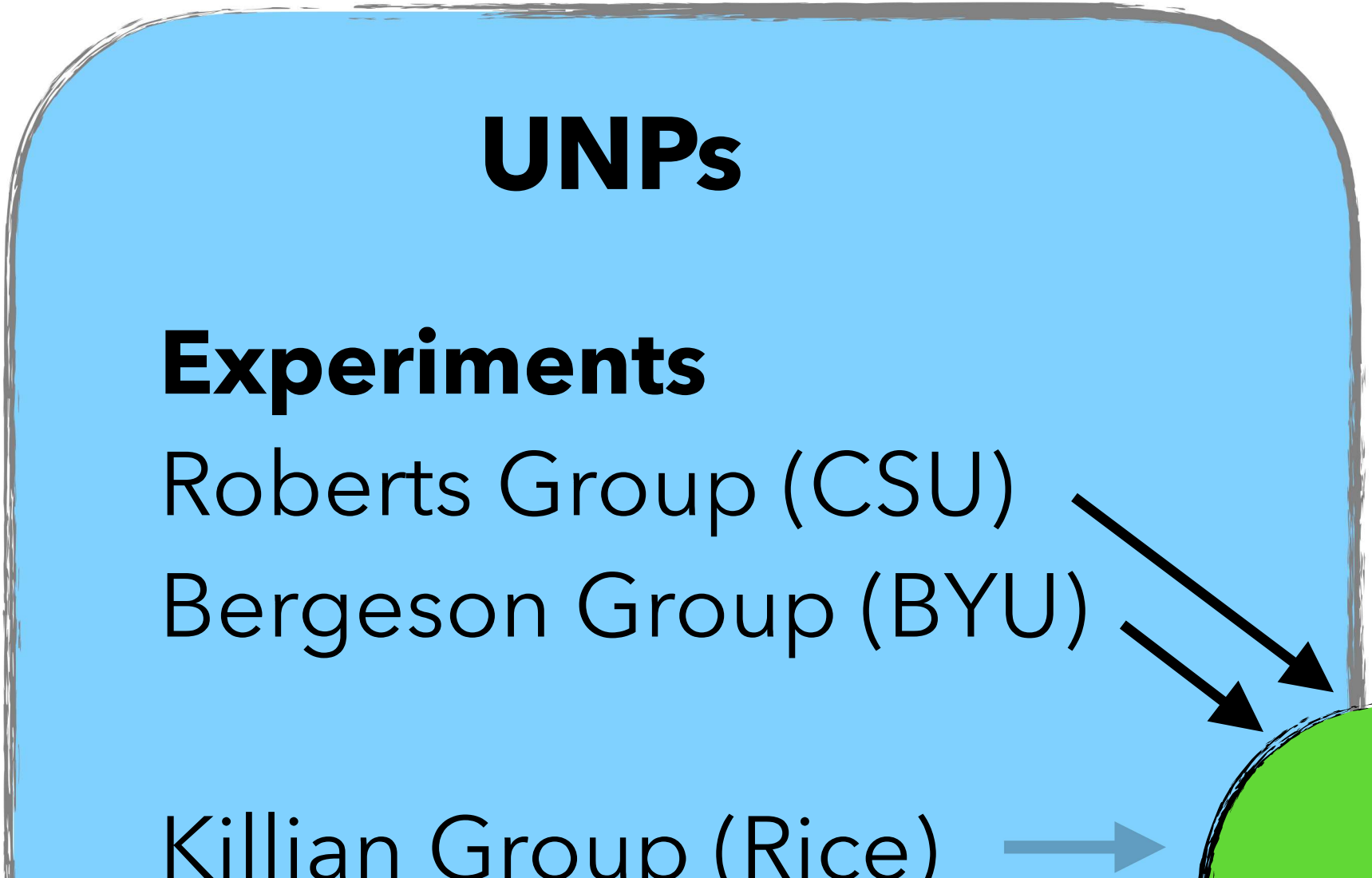
Killian Group (Rice)

Impact of UNP



SM Transpo

- Python-based (link here)
- Easy to install with `pip` and can
  - `$ pip install plasma-p`

```
from plasma_properties import transport

Am = 1.9944235e-23 # Atomic mass of element [g]
rho_i = 1 # Mass density [g/cc]
T = 0.2 # Temperature [eV]
```

1) Impo

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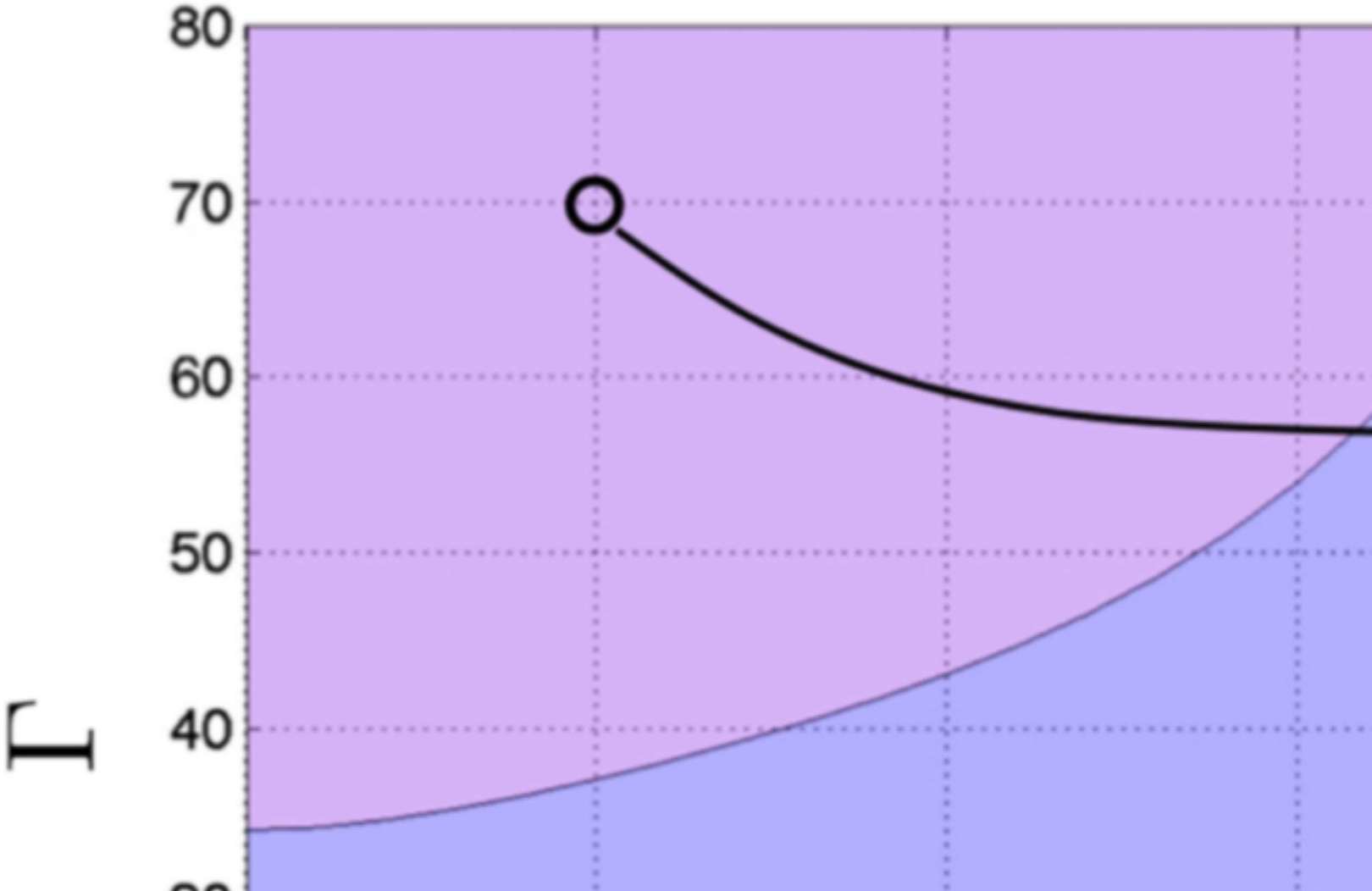
When do th



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- The linearization of the DFT calculatio
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$T = 100\ eV$ $T =$

When do th

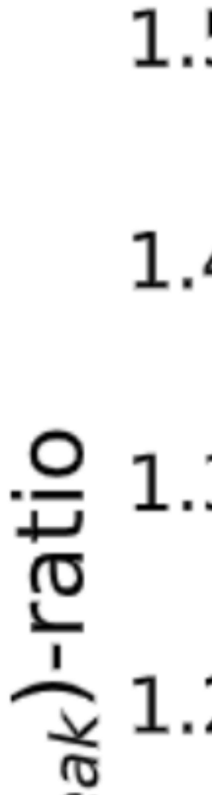
* RDF data from 46 simulations u
and all results were repeated with

* Ratios of RDF peak heights wer

* Feature engineering and selec

When do th

* The results indicate that no one parameter can predict accuracy, rather it must be a combination.



When do th

* If we use the normalized mean ionization state, we can see a similar trend.

$$\zeta = \frac{\langle Z \rangle}{Z}$$

Adding b

* We can explore the leading order effe
  form:

$$v_p(r) =$$

* The corresponding pair interaction wi

Adding b

* MD simulations with this “empty-core correction” and compared to the high-fidelity physics code (HFPC) dataset.

* In almost every case, the empty-core

Adding b

* We can also recompute the error metric of the *g(r)* peak ratios for the new potential.

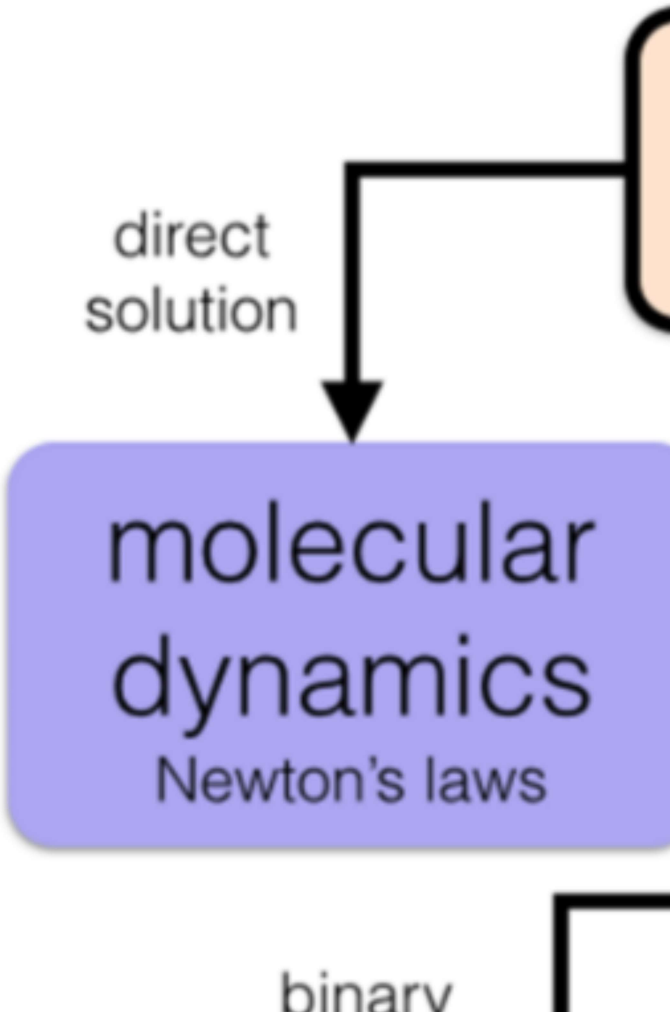
Conclu

* Simple screening models
  structure have been valid
  HFPC simulations over a

* The Thomas-Fermi-Yukaw
  fidelity physics codes wh


Tha

Ba



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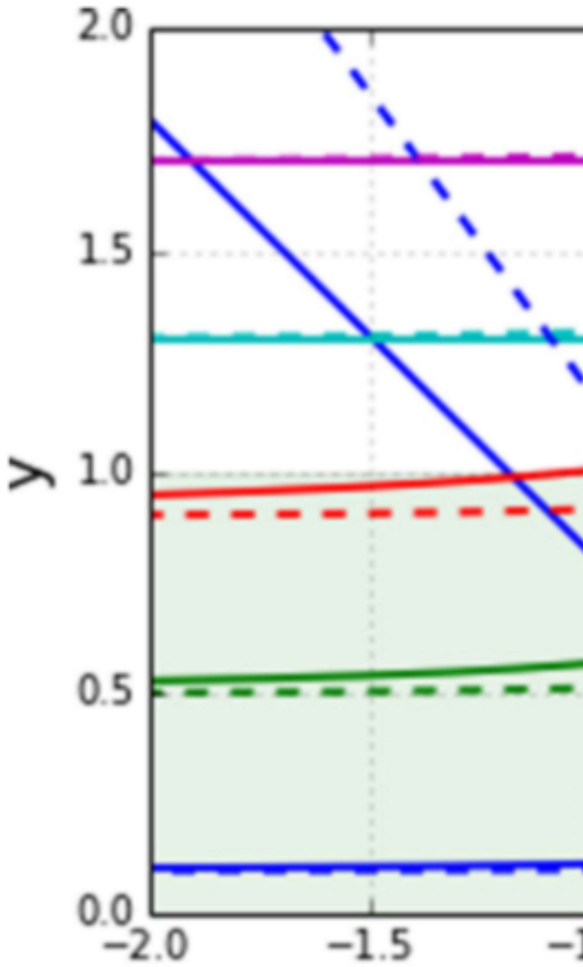

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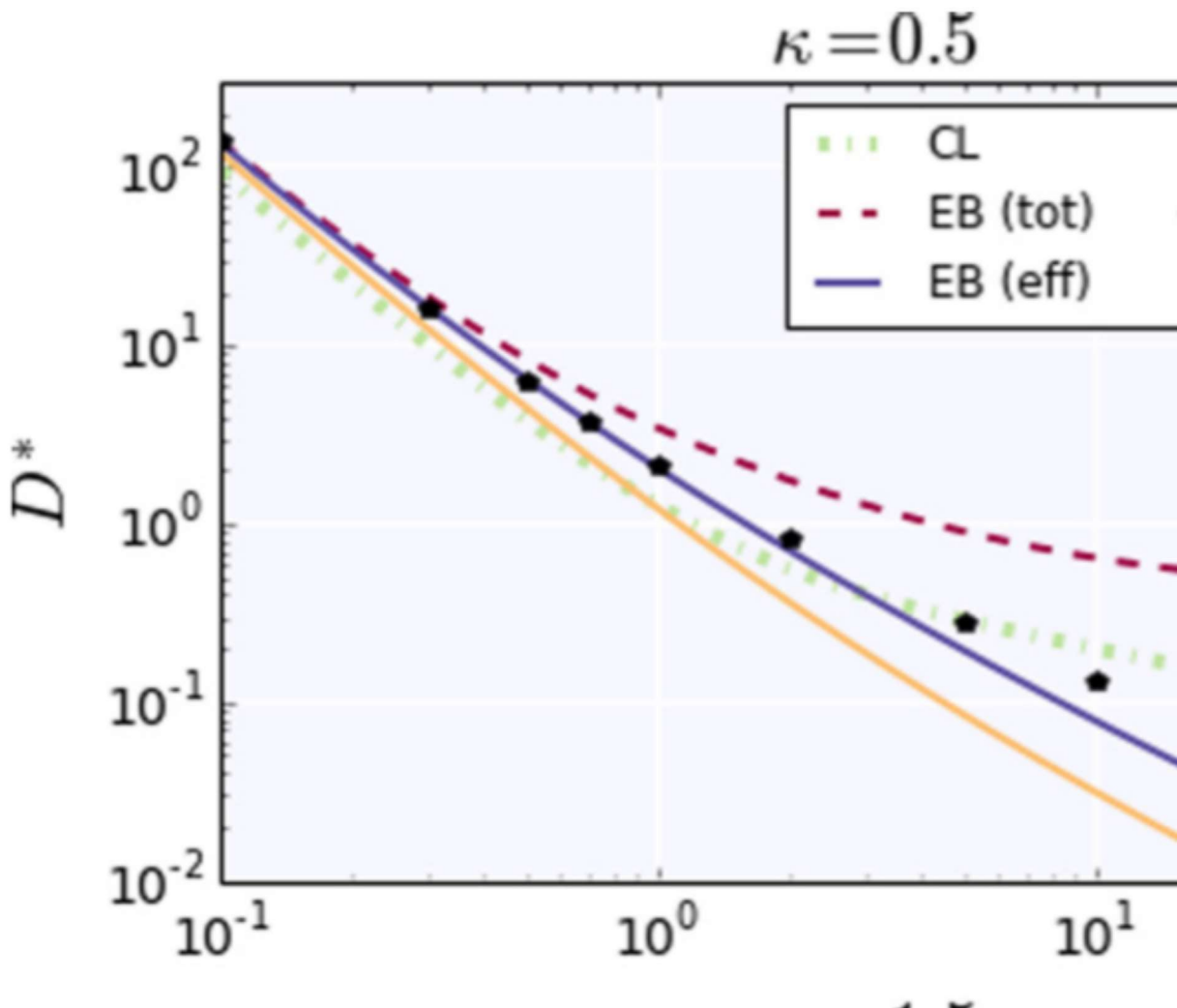

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