Structure and Shear Modulus of the Neutron Star Crust

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Outline

Simulations

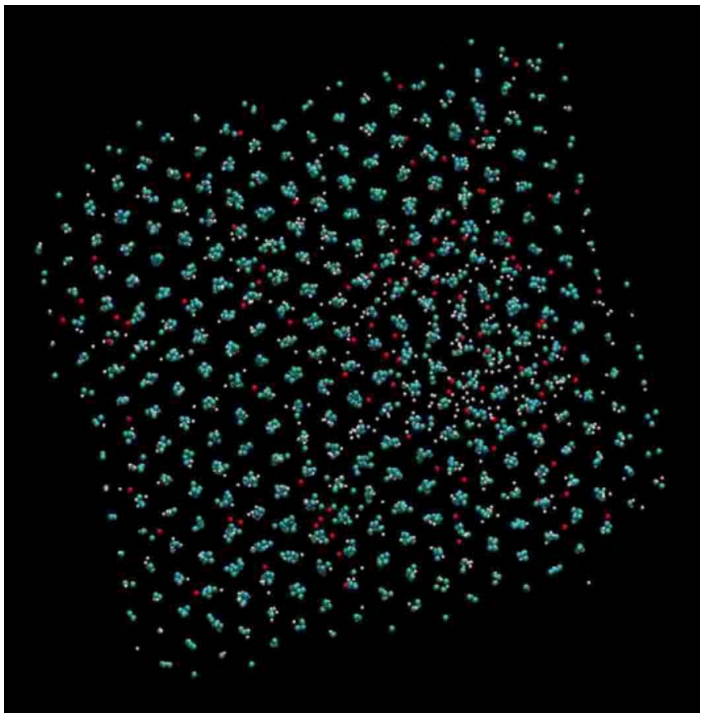

Figure: Horowitz, Caballero, Berry (2009)

- MD simulations can be used to model a variety of microphysical processes
  - Shear modulus, shear speed
  - Breaking strain
  - Bulk modulus
  - Shear viscosity
  - Thermal conductivity
  - Electrical conductivity
  - Diffusion coefficients
  - Heat capacity
  - Pycnonuclear and electron capture reaction rates
  - Phase diagram (melting point and chemical separation) (André's talk)
  - ...

Molecular Dynamics

- We use a screened Yukawa potential, $V(r) \propto \frac{e^{-r/\lambda}}{r}$
- λ is the Thomas-Fermi screening length, $\lambda^{-1} = 2\alpha^{1/2} k_F / \pi^{1/2}$
- Atoms are completely pressure ionized so $n_e = Zn$ and the electrons form a degenerate Fermi gas
- Simulations are characterized by the Coulomb Parameter

$$\Gamma \equiv \frac{PE}{KE} = \frac{Z^2 e^2}{aT}, \tag{1}$$

where inter-ion spacing

$$a = \left(\frac{3}{4\pi n}\right)^{1/3}. \tag{2}$$

MD code

- Our potential is very long range, so MD simulations are essentially $\mathcal{O}\left(N^2\right)$
- We need scalable code that can run on many nodes
- Hybrid OpenMP/MPI scheme
  - MPI
    - One MPI rank per node
    - Copies data between nodes
  - OpenMP
    - Four (Big Red) to twelve (Kraken) OpenMP threads per node
    - Computes forces and updates positions and velocities

Shear Modulus: Method 1

- Use Kubo formalism and compute correlations of free energy change under virtual deformations D_m with $m = 1, \ldots, 6$
- $D_{1,2,3}$ are stretching and $D_{4,5,6}$ are shearing deformations
- The magnitude of the deformation is given by ϵ and the angle-averaged shear modulus

$$\mu_{eff} = \frac{1}{5}\left(\frac{2}{9}\sum_{m=1}^{3} f_m + \sum_{m=4}^{6} f_m\right), \tag{3}$$

where

$$f_m = \frac{1}{V}\left\{\left\langle \frac{d^2V}{d\epsilon^2}\right\rangle - \frac{1}{T}\left[\left\langle \frac{dV}{d\epsilon}^2\right\rangle - \left\langle \frac{dV}{d\epsilon}\right\rangle^2\right]\right\}. \tag{4}$$

Shear Modulus: Method 1

- Finite size effects are large due to the long tail of our screened potential
- Ogata et al. used a standard Coulomb potential whereas we use a Yukawa
- Screening gives $\sim 10\%$ reduction in shear modulus

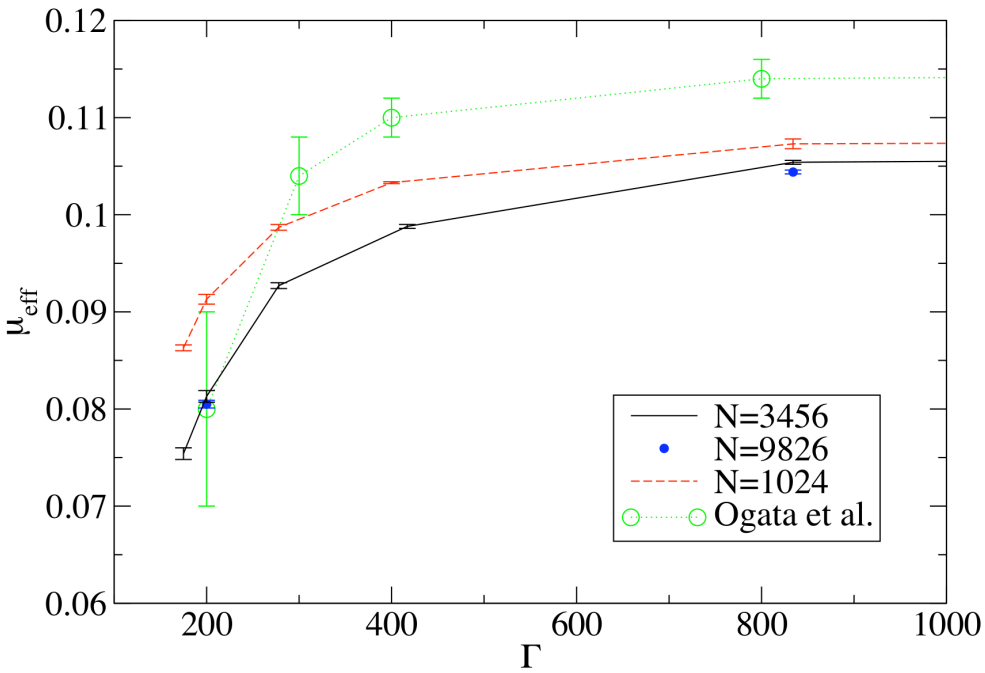

Figure: Horowitz, Hughto (2008)

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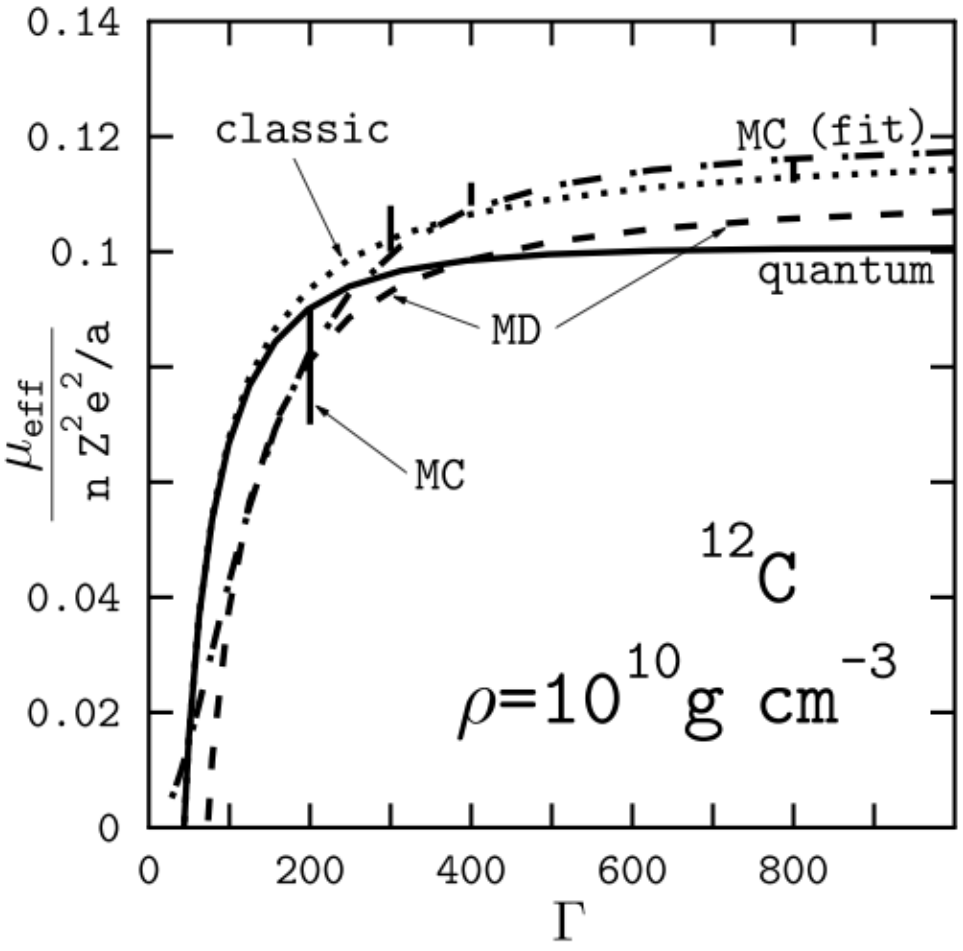


Figure: Baiko (2011)

Shear Modulus: Method 2

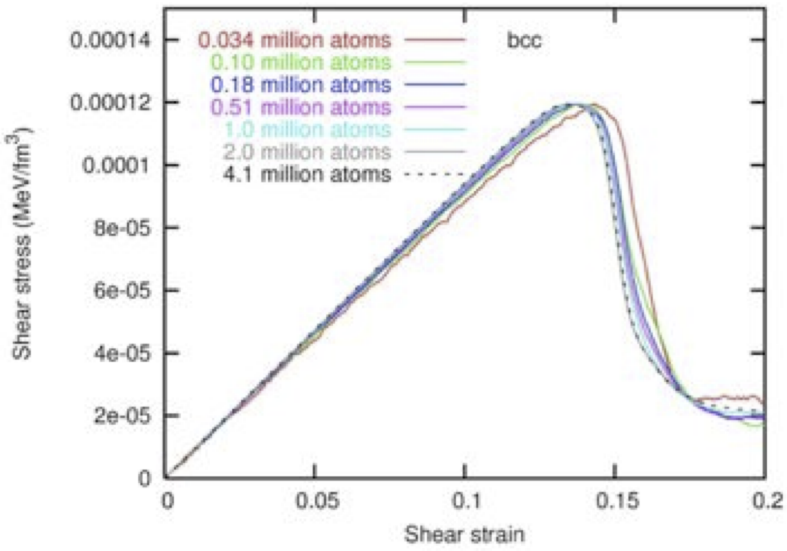


Figure: Horowitz, Kadau (2009)

- Physically shear the system
- Slope of stress vs. strain is the shear modulus
- This method also allows for a breaking strain calculation at the same time
- This method is more efficient for large systems (pasta)

Solid Diffusion

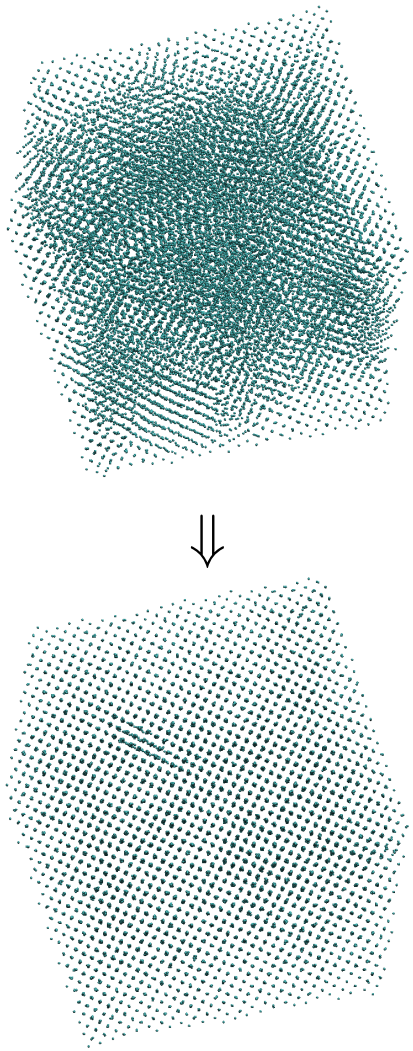
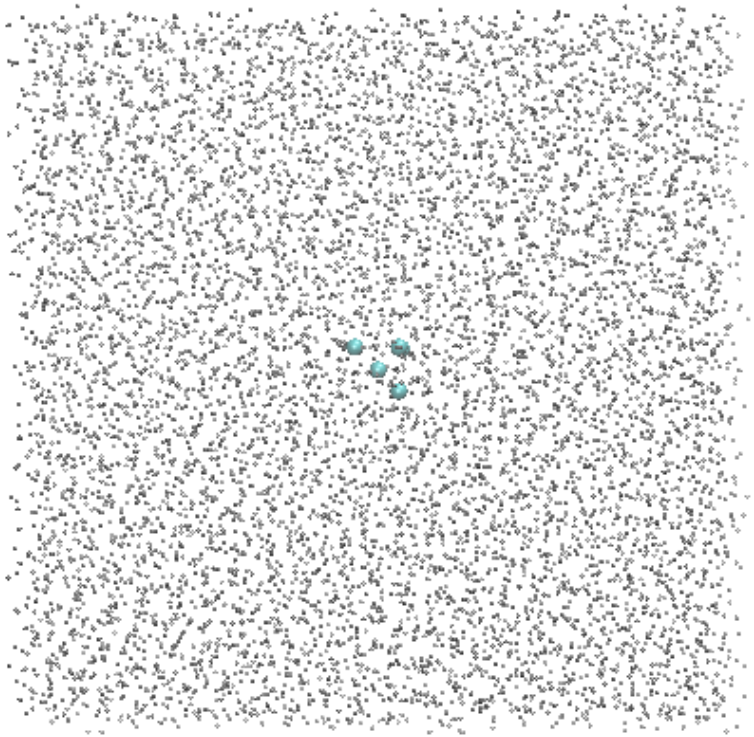


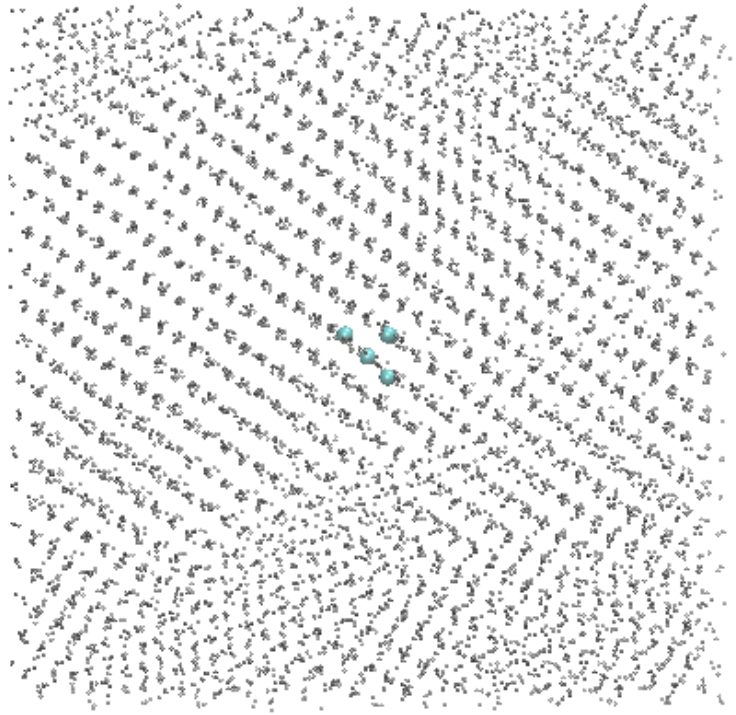
Figure: Hughto et al. (2011)

- Completely pressure-ionized ions have soft $1/r$ cores
- Diffusion is very fast in solid systems
- Fast enough that quenched systems can initially freeze with many different domains but then evolve into few-domain crystals in very short timescales
- This fast diffusion suggests that NS crusts are remarkably good crystals with few defects

Nucleation: *Preliminary*

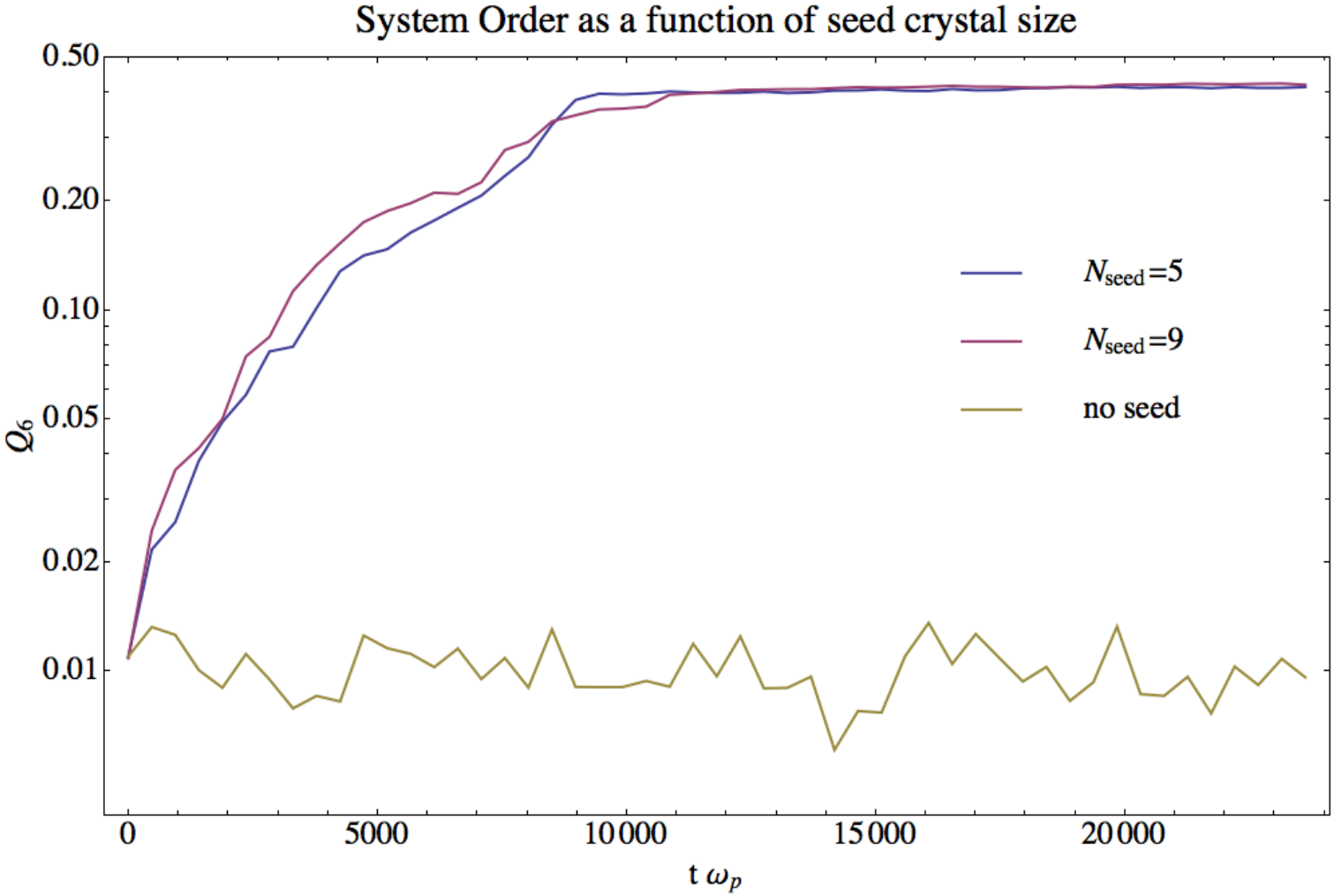
- Put a small (few ions) fixed seed crystal in a supercooled liquid
- Compute global bond order parameter Q_6 and test for crystallization





Nucleation: *Preliminary*

$\Gamma = 205, \Gamma_c = 177.6$



Very small seeds leads to crystallization

Crust cooling

- KS1731-260 accreted for $\gtrsim$ 12.5 years then crust was observed to cool
- Curve 5 is from an amorphous crust, while the others are from a crystalline crust
- There are strong observational and theoretical data pointing to a nearly perfect crystalline crust

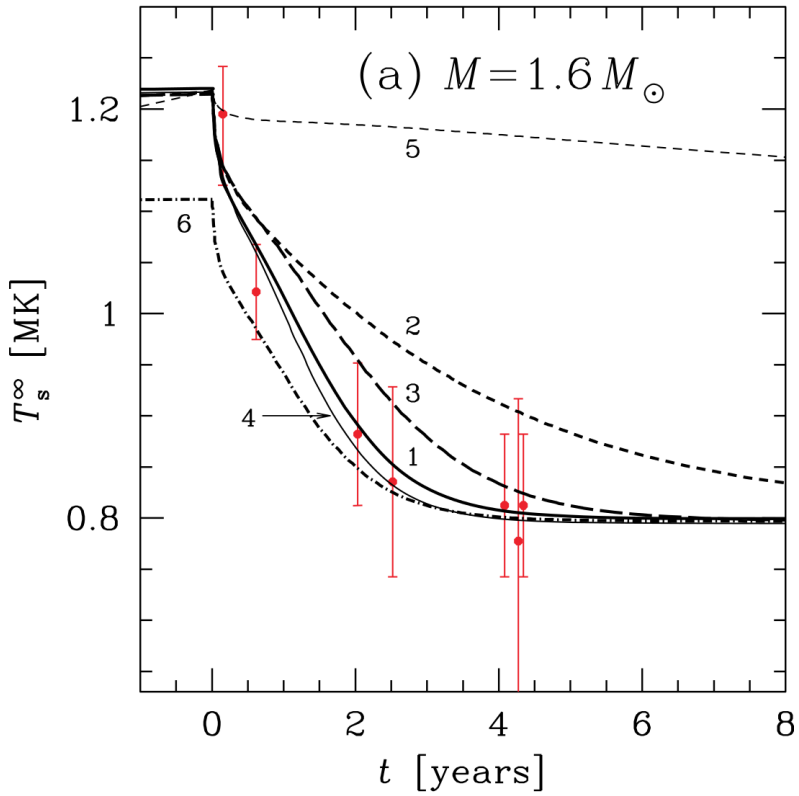


Figure: Shternin et al. (2007)

Future Work

- Shear modulus of pasta phases
- Solid diffusion with multicomponent systems
- Molecular dynamics with high magnetic fields

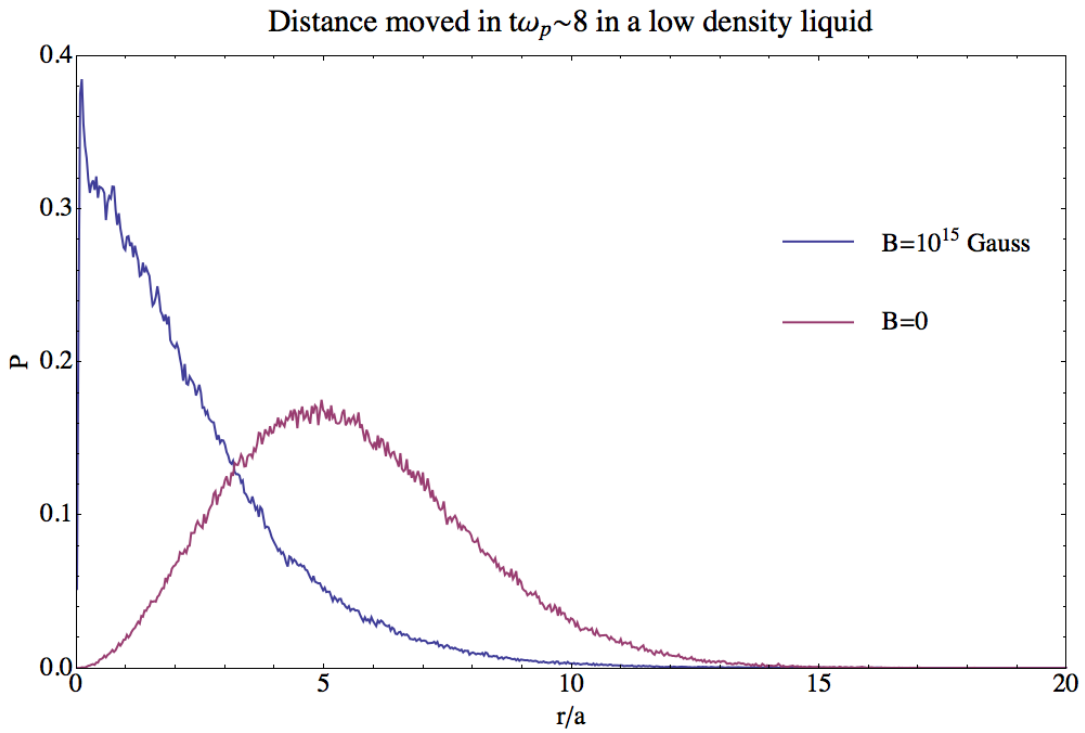


Figure: *Preliminary*

Summary

- Molecular dynamics simulations allow us to explore a range of different observables
- NS crust is a nearly perfect crystal
- High thermal conductivity
- High breaking strain
- Stay tuned for André's talk on phase diagrams
- IU Group: Chuck Horowitz, André da Silva Schneider, Don Berry, Justin Mason