# Molecular Dynamics Simulations of Neutron Star Crusts

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NUCLEI
Nuclear Computational Low-Energy Initiative

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# Crust Structure

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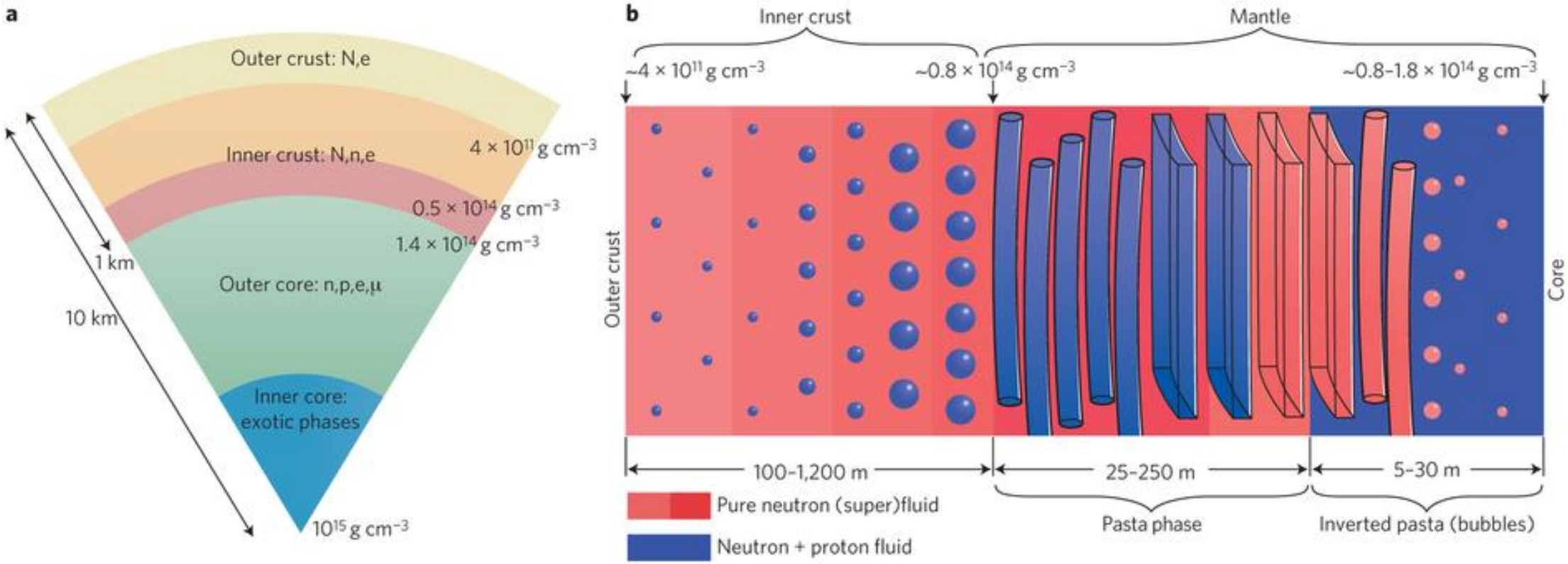


- What is the structure and composition of the crust?
  What are its properties?

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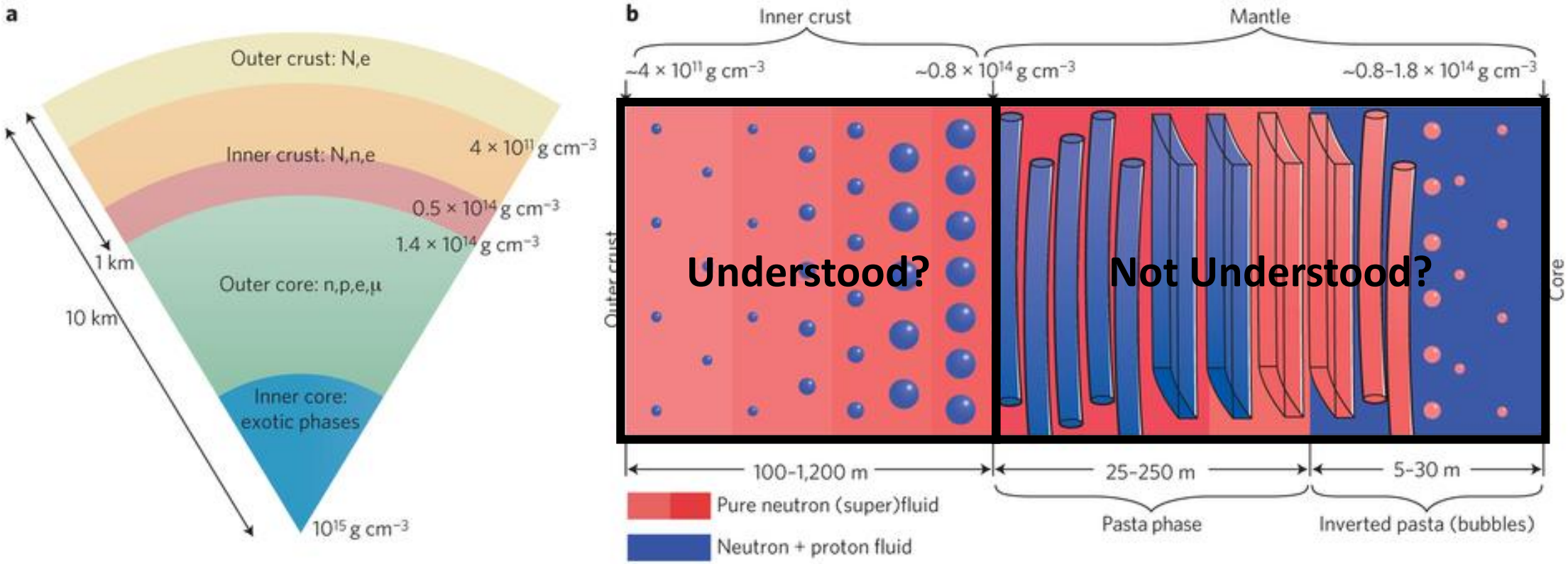


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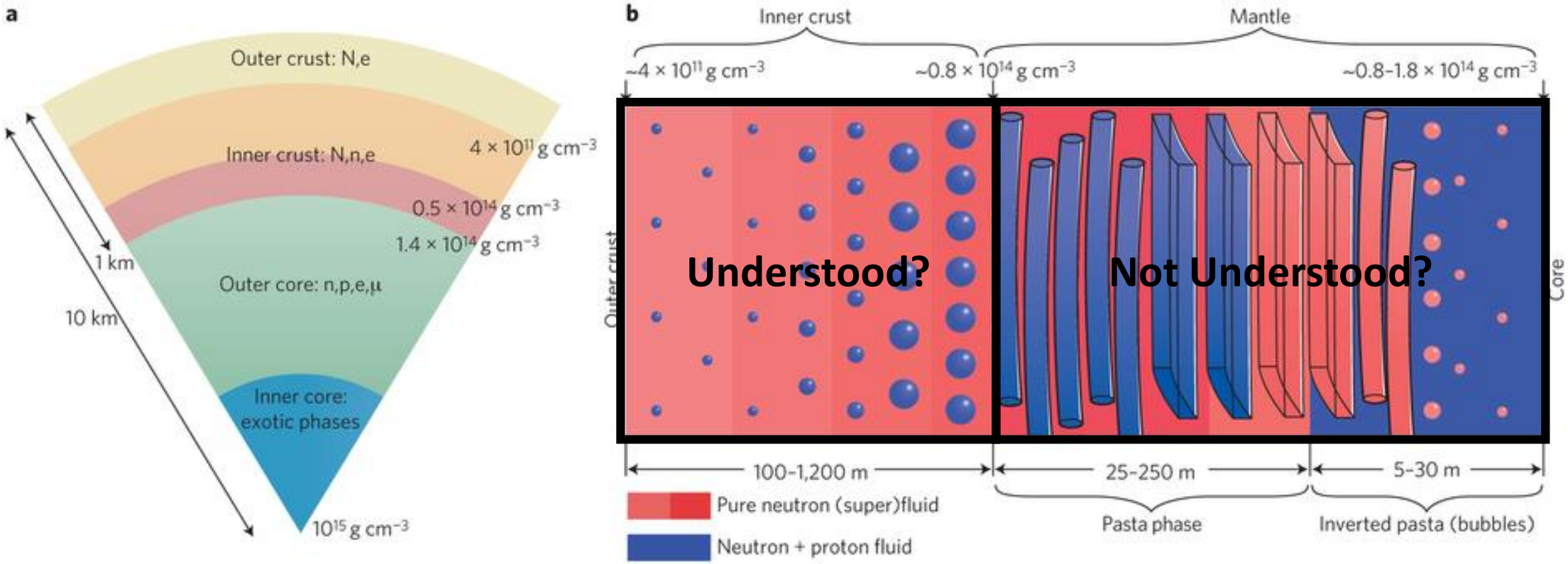


- How can we study the properties of matter when it is undergoing a nuclear phase transition in the inner crust?

# Molecular Dynamics

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- Simulate materials at the particle level with some chosen interaction
- **Outer crust**, for example, is studied using a Coulomb repulsion

$$V(r_{ij}) = \frac{Z_i Z_j e^2}{r_{ij}} \exp(-r_{ij}/\lambda)$$

and the TF screening length: $\lambda = \frac{\pi^{1/2}}{(4\alpha k_F)^{1/2}(k_F^2 + m_e^2)^{1/4}} \sim \frac{1}{2k_F}\sqrt{\frac{\pi}{\alpha}}$

- Frequently characterized by the plasma parameter:

$$\Gamma = \frac{Z^2 e^2}{akT}, \quad a = (3/4\pi n)^{1/3}$$

# Molecular Dynamics

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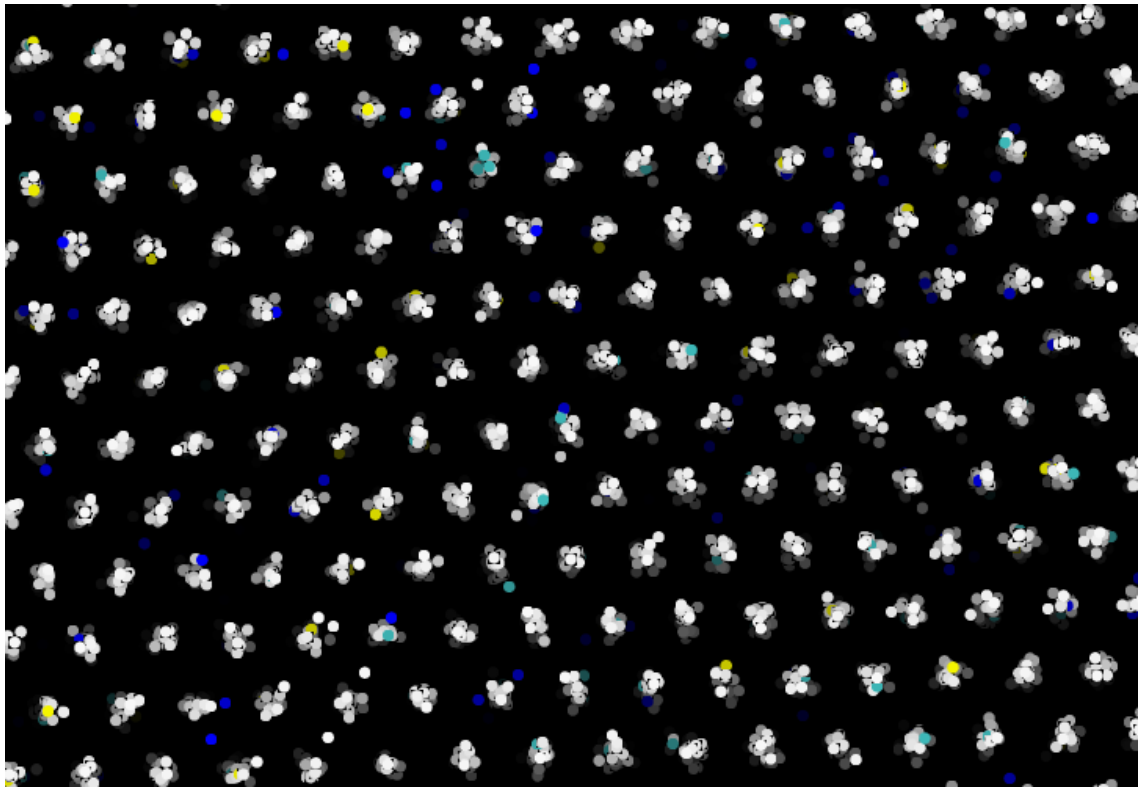
- Example: Simulate ions in a bcc lattice in the outer crust:

- Initialize: Give particles positions and velocities

  1. Calculate forces between all pairs of particles
  2. Update velocities using acceleration found in (1)
  3. Update positions of all particles

  Iterate for as long as desired



# Outer Crust (Breaking Strain)

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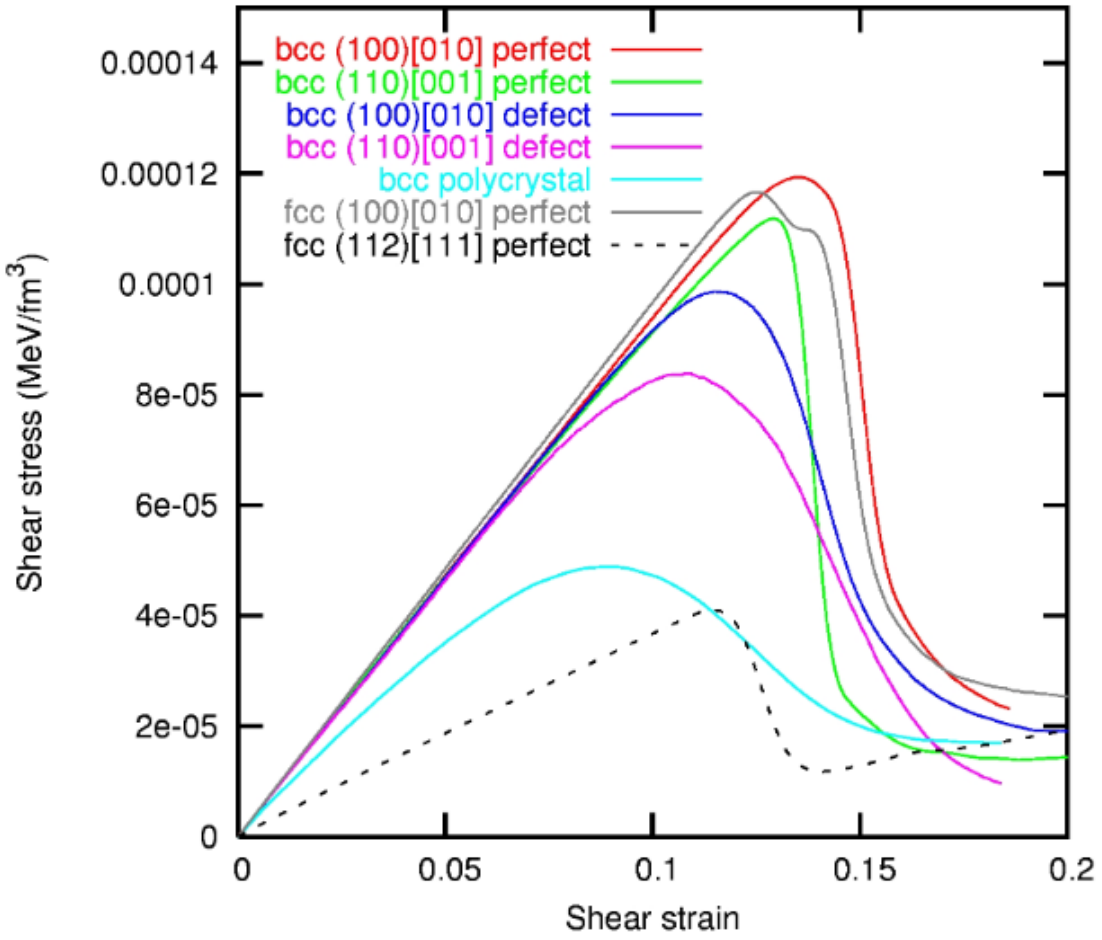
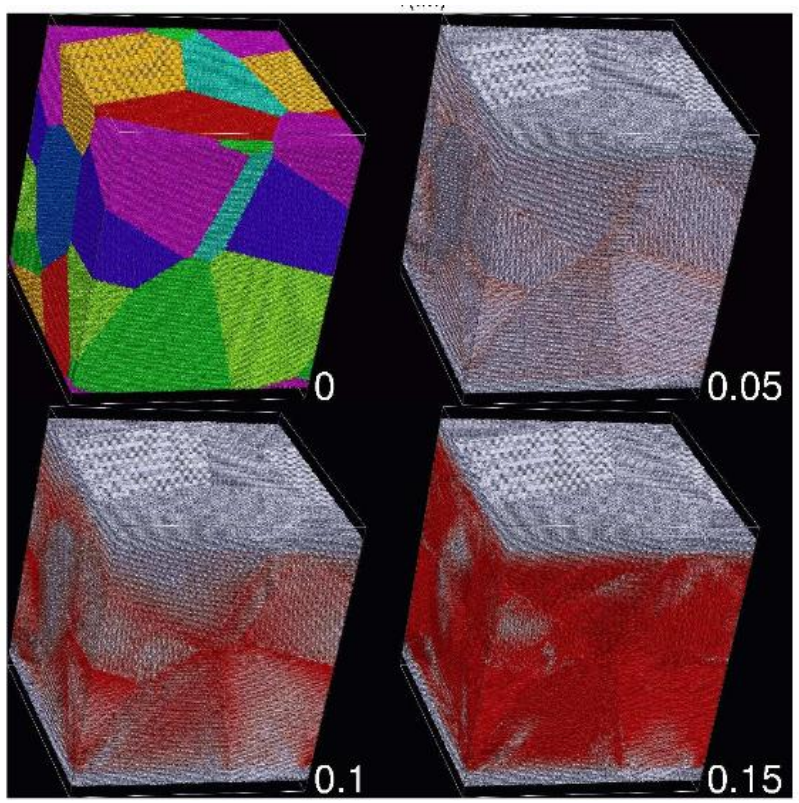
- Breaking strain of the outer crust is ~0.1 (Horowitz & Kadau 2009)



# Outer Crust (Shear Modulus)

- Six deformations tell you everything (3 each, tensile and shear)
- Expectation values can be used to find the elastic constants (assumed here to be isotropic)

$$f_m = \frac{1}{V}\Big\{\langle\frac{d^2V_{tot}}{d\epsilon^2}\rangle - \frac{1}{T}[\langle(\frac{dV_{tot}}{d\epsilon})^2\rangle - \langle\frac{dV_{tot}}{d\epsilon}\rangle^2]\Big\},$$

$$f_1 = f_2 = f_3 = 3b_{11} = 3(c_{11} - c_{12})$$

$$f_4 = f_5 = f_6 = c_{44}.$$

- $$\mu_{\text{eff}} = (2b_{11} + 3c_{44})/5.$$

- Important piece:

$$\mu_{\text{eff}} \approx (0.1106 - \frac{28.7}{\Gamma^{1.3}})(n\frac{Z^2e^2}{a}).$$

$$D_1: \quad u_{xx} = \epsilon + \frac{3}{4}\epsilon^2, \quad u_{yy} = u_{zz} = -\frac{\epsilon}{2}$$

$$D_2: \quad u_{yy} = \epsilon + \frac{3}{4}\epsilon^2, \quad u_{xx} = u_{zz} = -\frac{\epsilon}{2}$$

$$D_3: \quad u_{zz} = \epsilon + \frac{3}{4}\epsilon^2, \quad u_{xx} = u_{yy} = -\frac{\epsilon}{2}$$

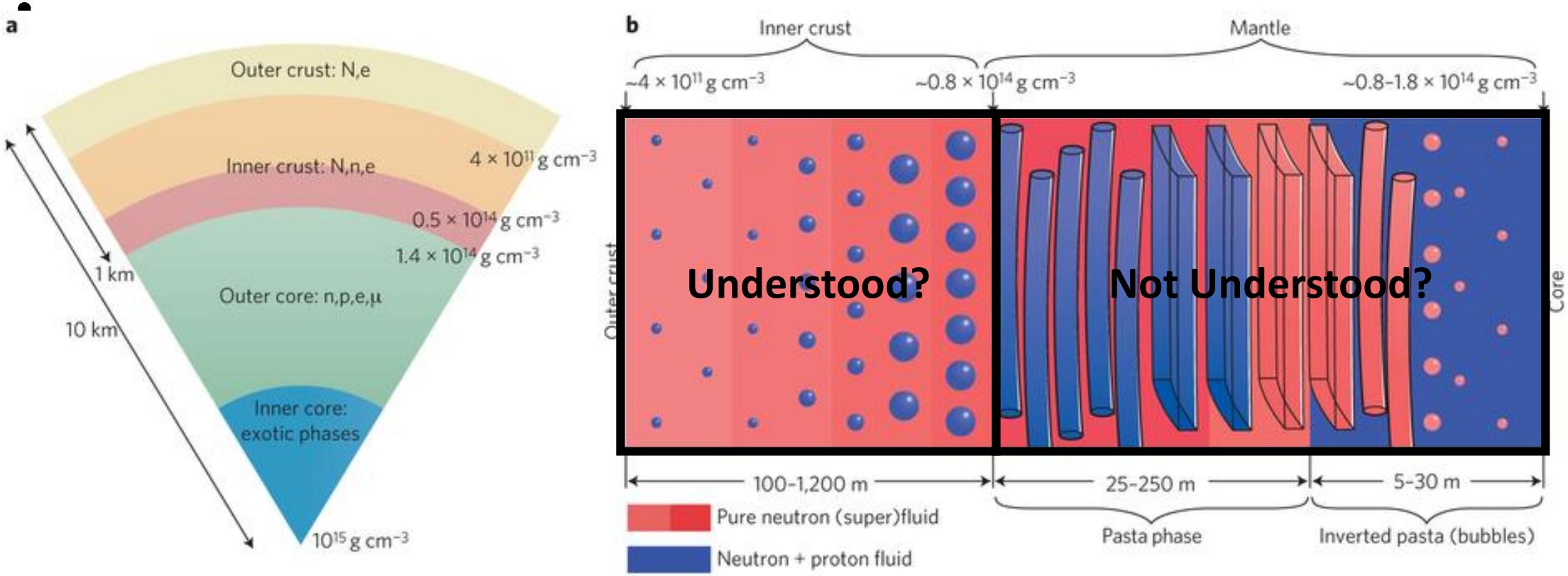
$$D_4: \quad u_{xy} = u_{yx} = \frac{\epsilon}{2}, \quad u_{zz} = \frac{\epsilon^2}{4}$$

$$D_5: \quad u_{yz} = u_{zy} = \frac{\epsilon}{2}, \quad u_{xx} = \frac{\epsilon^2}{4}$$

$$D_6: \quad u_{zx} = u_{xz} = \frac{\epsilon}{2}, \quad u_{yy} = \frac{\epsilon^2}{4}$$

(Strohmayer 1991) (Horowitz & Hughto 2008)

# Outer Crust (Shear Modulus)




- Important piece:

$$\mu_{\rm eff} \approx (0.1106 - \frac{28.7}{\Gamma^{1.3}})(n\frac{Z^2e^2}{a}).$$

(Horowitz & Hughto 2008)

# Inner Crust

- Though it may only be ~100 m thick, the pasta layer may contain up to half of the crust mass. Thus, important for understanding production of gravitational waves from the crust
- What is the shear modulus and breaking strain of the inner crust, specifically, through the pasta layer?
  - At the top, should be large (ions)
  - At the bottom, should be small (core)

# Non-Spherical Nuclei

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- First theoretical models of the shapes of nuclei near $n_0$
  - 1983: Ravenhall, Pethick, & Wilson
  - 1984: Hashimoto, H. Seki, and M. Yamada
- *Frustration*: Competition between proton-proton Coulomb repulsion and strong nuclear attraction
- Nucleons adopt non-spherical geometries near the saturation density to minimize surface energy

Pethick and Potekin 1998

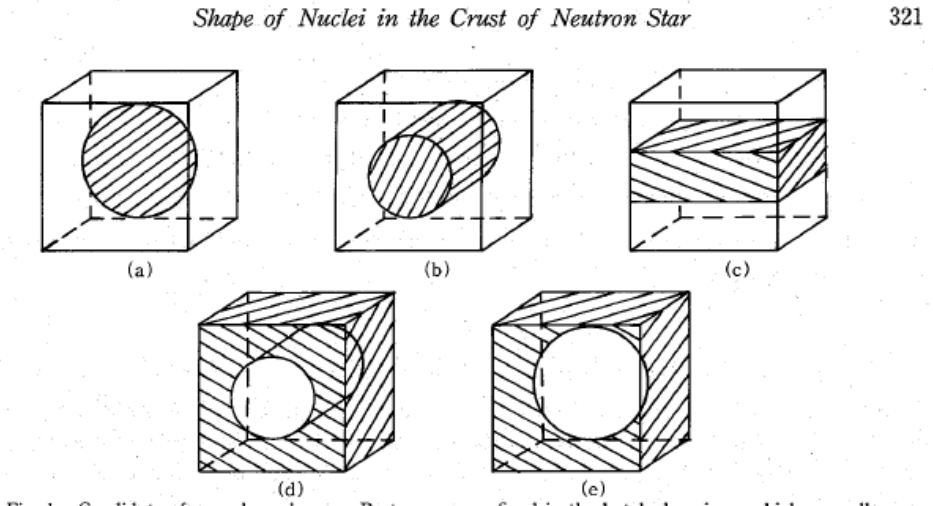

Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole space, and thereby the nuclei are joined to each other except for the spherical nuclei (a).

# Non-Spherical Nuclei

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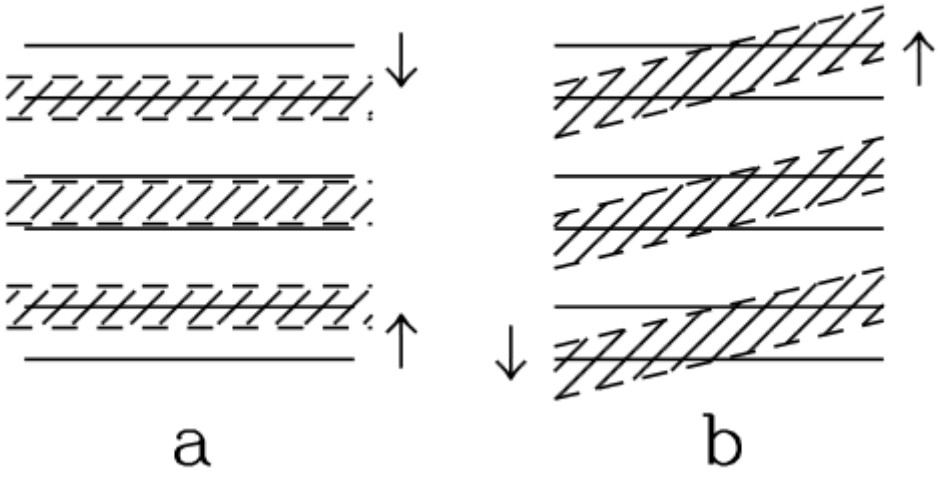
- Energy deformation of a liquid crystal (plate spacing and bending)

$$E_d = \frac{B}{2}\left[\frac{\partial u}{\partial z} - \frac{1}{2}(\nabla_\perp u)^2\right]^2 + \frac{K_1}{2}(\nabla_\perp^2 u)^2,$$

(Pethick and Potekin 1998)




- Properties more characteristic of a liquid crystal. Can we understand a ‘unit cell’ of this material, and generalize to a larger sample?
- Use molecular dynamics again to study the elastic properties of crustal material

# Classical Pasta Formalism

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- **Classical Molecular Dynamics** with IUMD on Big Red II

$$V_{np}(r_{ij}) = a e^{-r_{ij}^2/\Lambda} + [b - c] e^{-r_{ij}^2/2\Lambda}$$

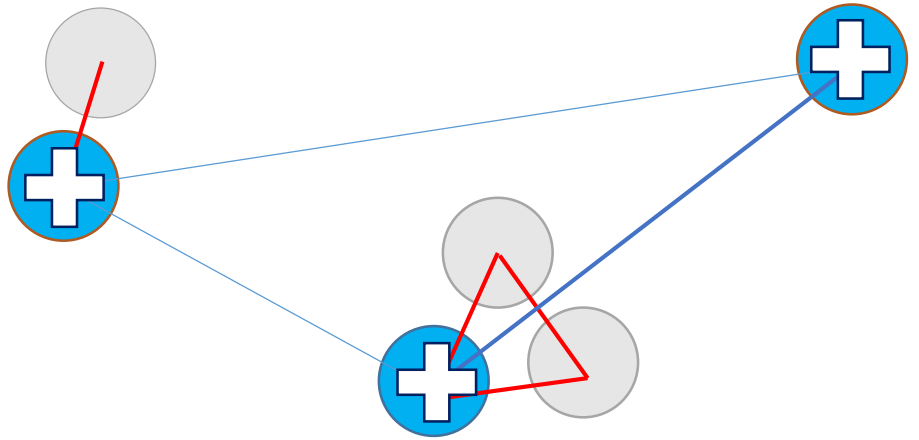
$$V_{nn}(r_{ij}) = a e^{-r_{ij}^2/\Lambda} + [b + c] e^{-r_{ij}^2/2\Lambda}$$

$$V_{pp}(r_{ij}) = a e^{-r_{ij}^2/\Lambda} + [b + c] e^{-r_{ij}^2/2\Lambda} + \frac{\alpha}{r_{ij}} e^{-r_{ij}/\lambda}$$

| $a$ | $b$ | $c$ | $\Lambda$ | $\lambda$ |
|---|---|---|---|---|
| 110 MeV | -26 MeV | 24 MeV | 1.25 $fm^2$ | 10 fm |

- Short range nuclear force
- Long range Coulomb force

| Nucleus | Monte-Carlo $\langle V_{tot} \rangle$ (MeV) | Experiment (MeV) |
|---|---|---|
| $^{16}O$ | -7.56±0.01 | -7.98 |
| $^{40}Ca$ | -8.75±0.03 | -8.45 |
| $^{90}Zr$ | -9.13±0.03 | -8.66 |
| $^{208}Pb$ | -8.2 ±0.1 | -7.86 |



# Nuclear Pasta

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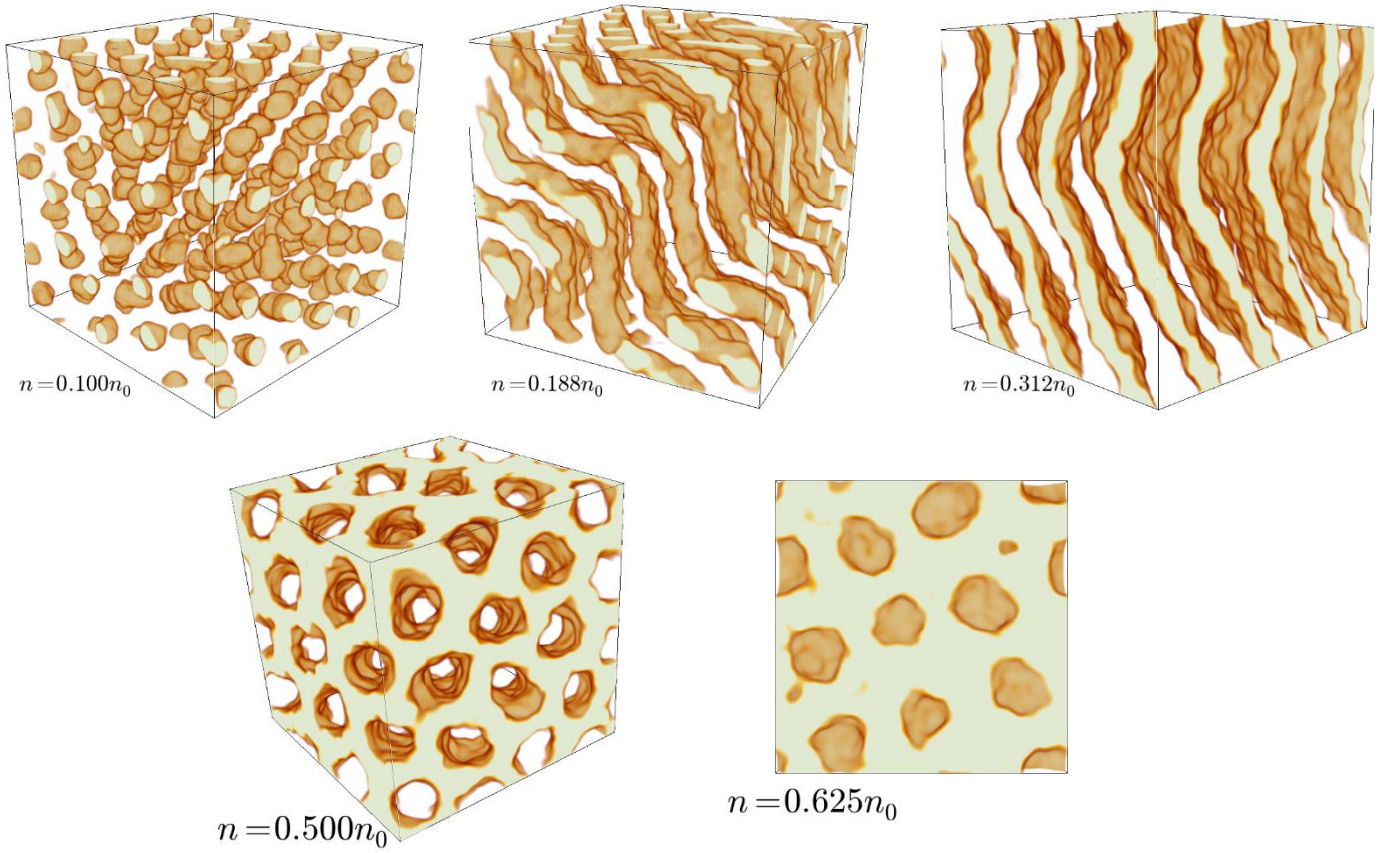


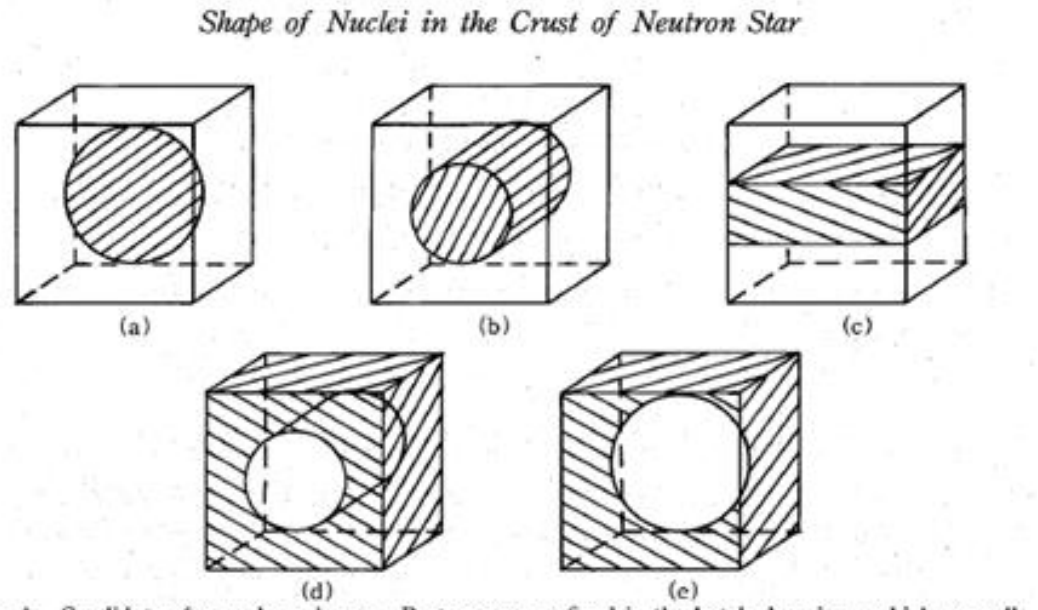


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Gold Nucleus
For Scale

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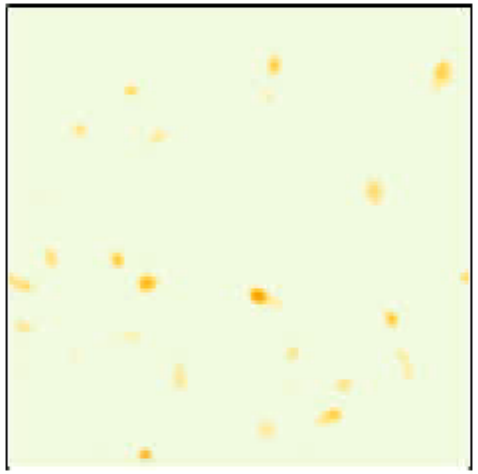

$$n = 0.1200 \mathrm{fm}^{-3}$$

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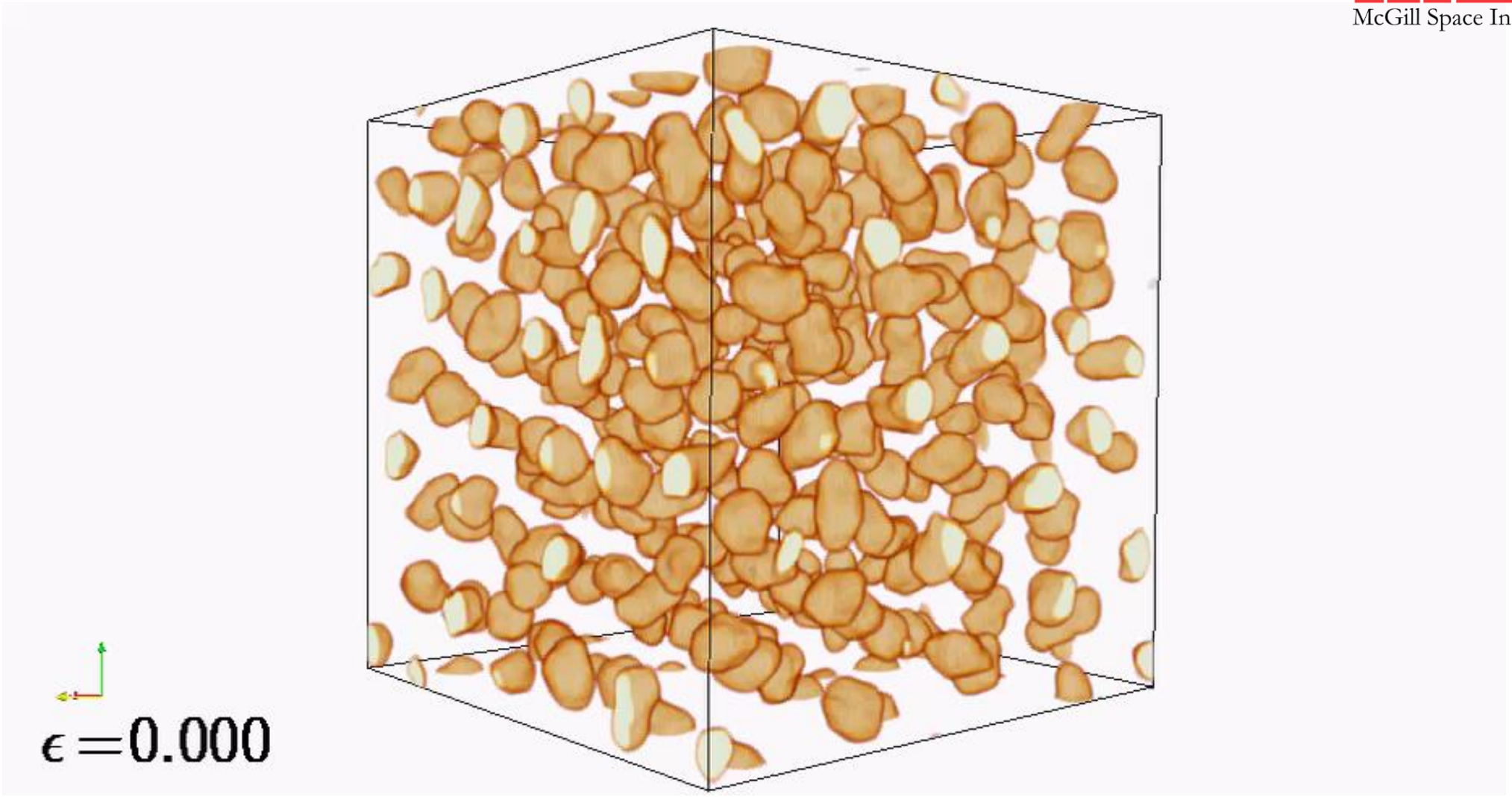

# Deforming Pasta

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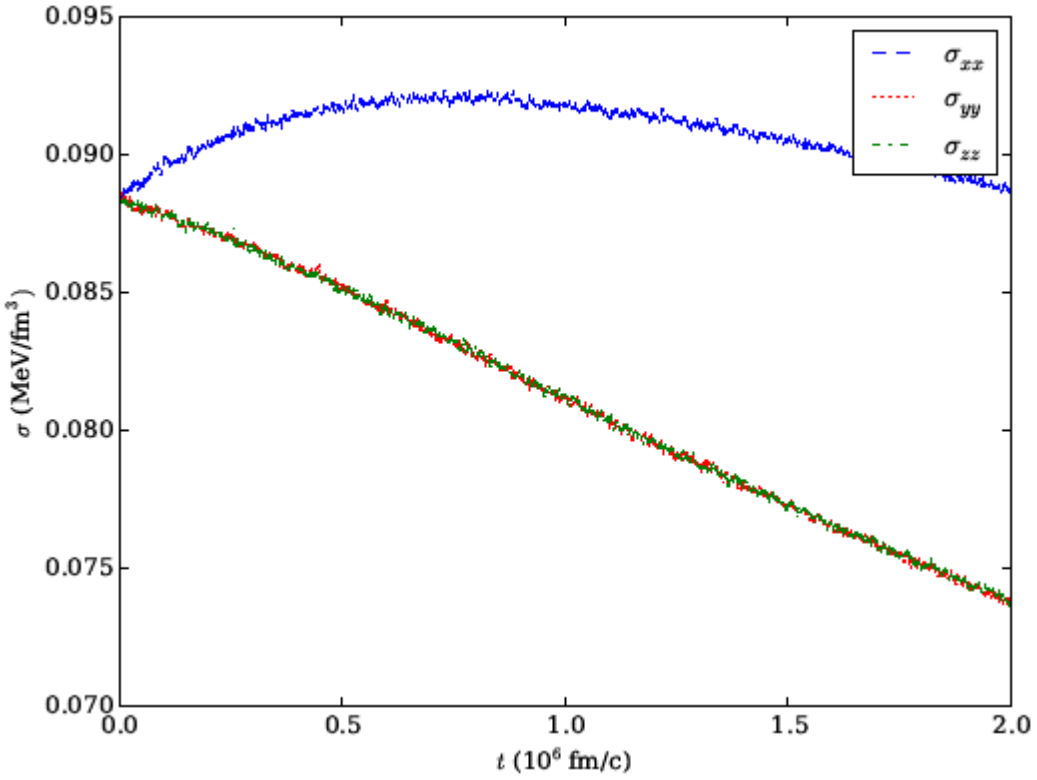
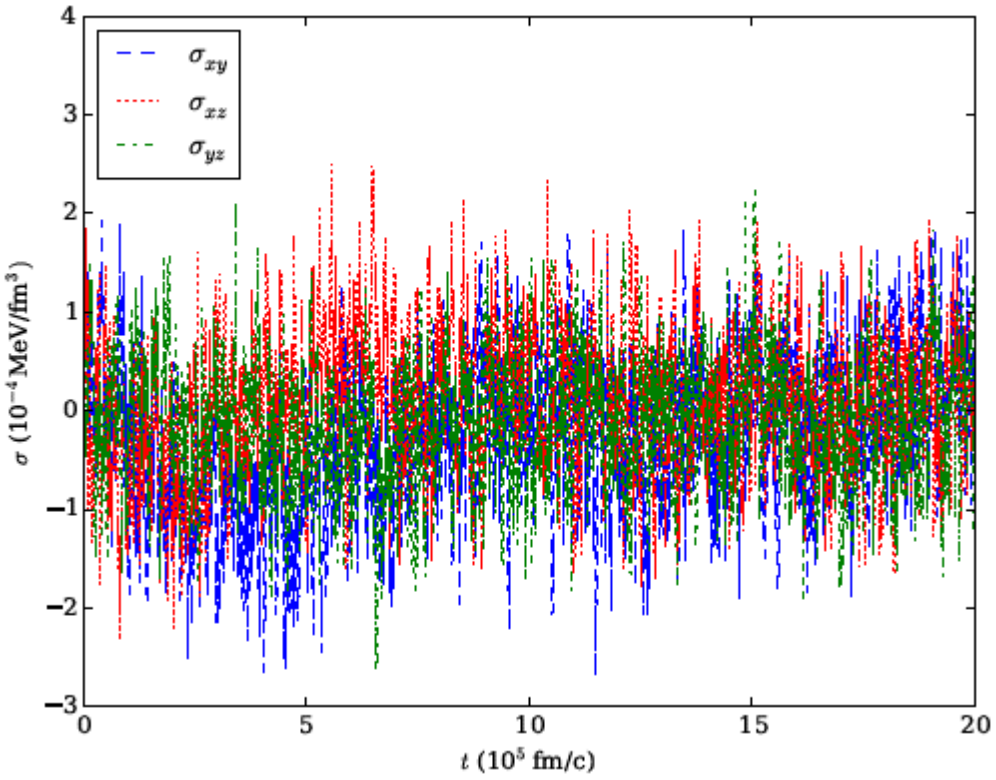
- Deformations of ‘gnocchi’ in the pasta model seem to reproduce the elastic response of a small Coulomb crystal

**TENSILE STRESSES**




**SHEAR STRESSES**



# Deforming Pasta

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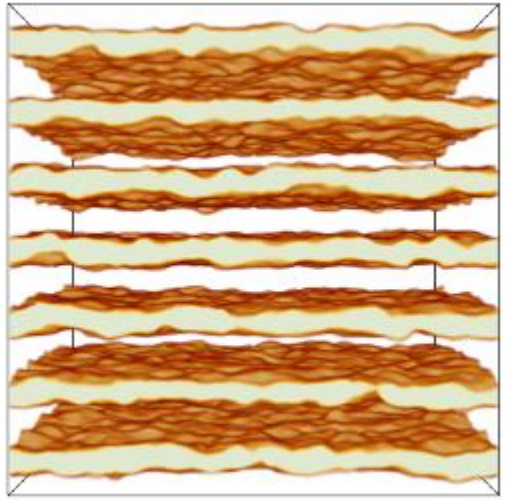
- Consider a tensile deformation that increases the separation between plates
- Periodic boundary, $Y_P$=0.4, 102,400 nucleons, n=0.05 $fm^{-3}$
- Previous work has initialized pasta that is parallel with the boundaries (using external potentials when equilibrating to force the pasta into certain regions)
- Can strain the pasta and calculate elastic properties from the response

(Schneider et al 2016)



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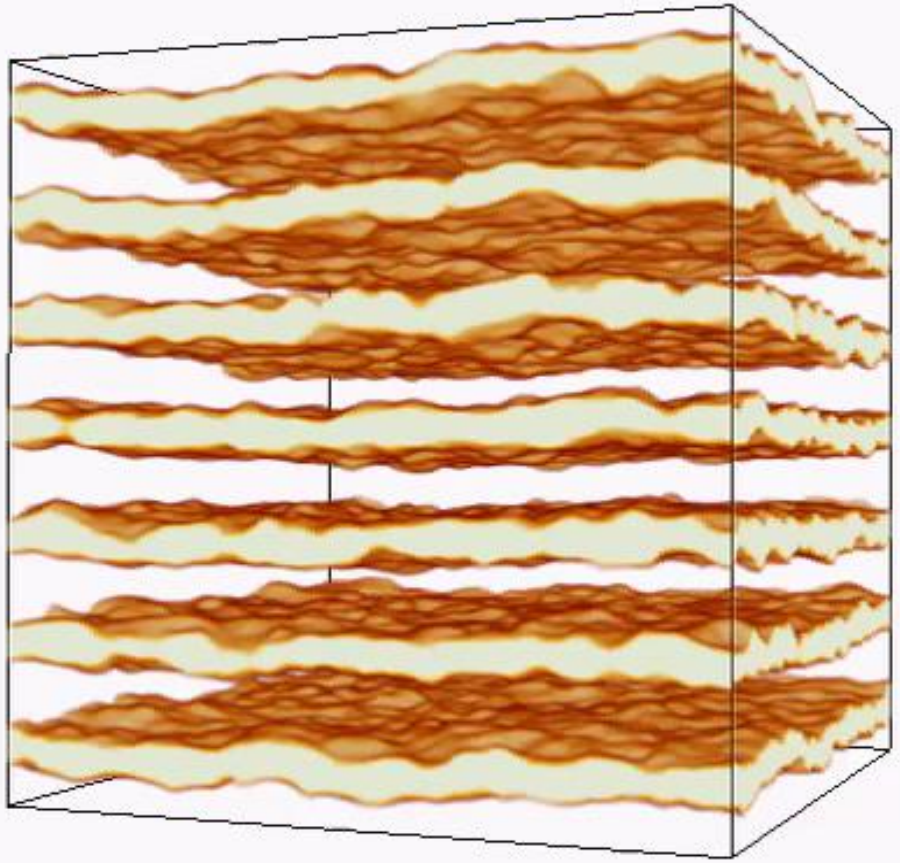

$\epsilon = 0.000$

# Stresses

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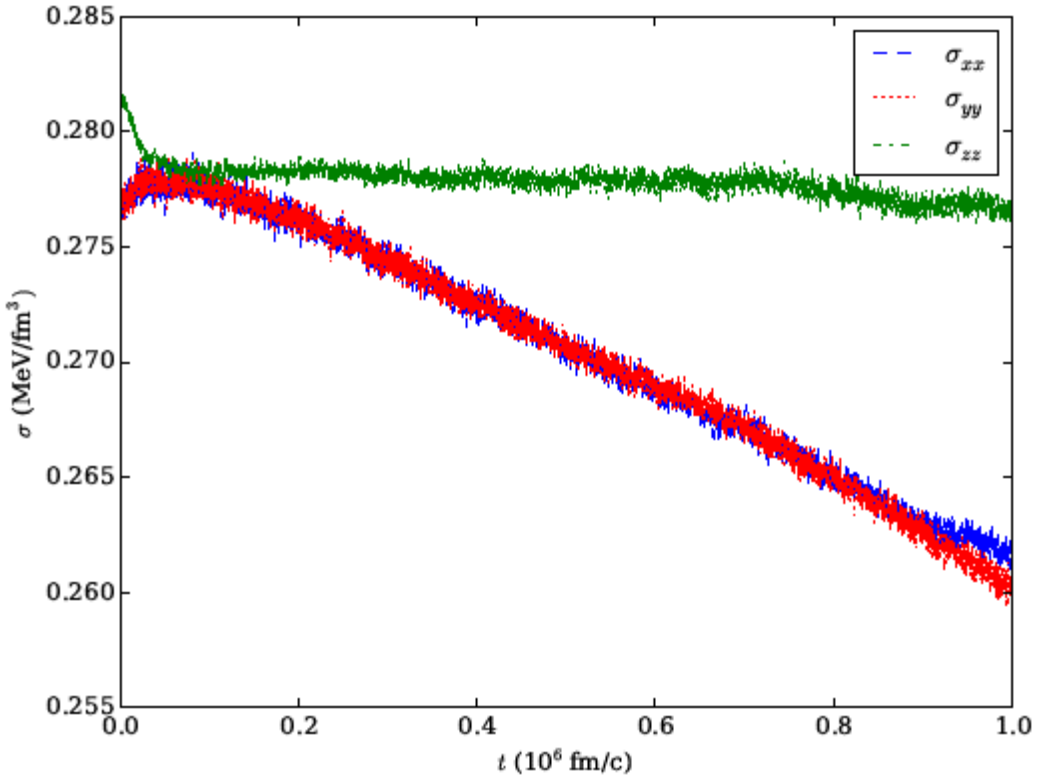
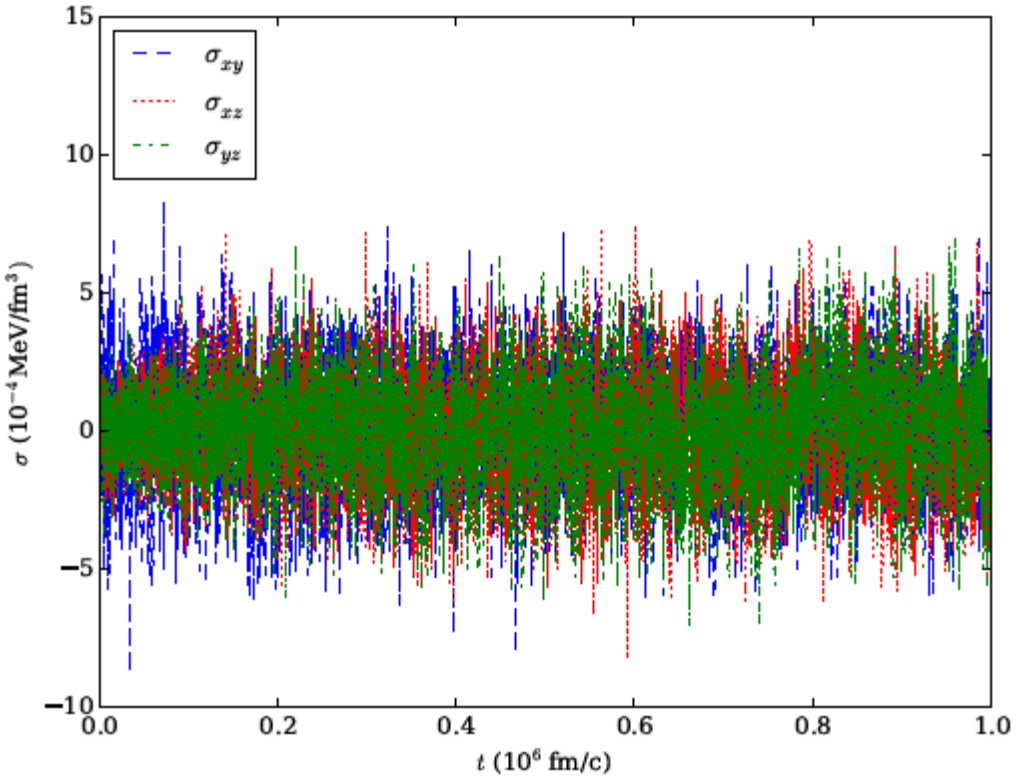
- Tensile Stress




Shear Stress



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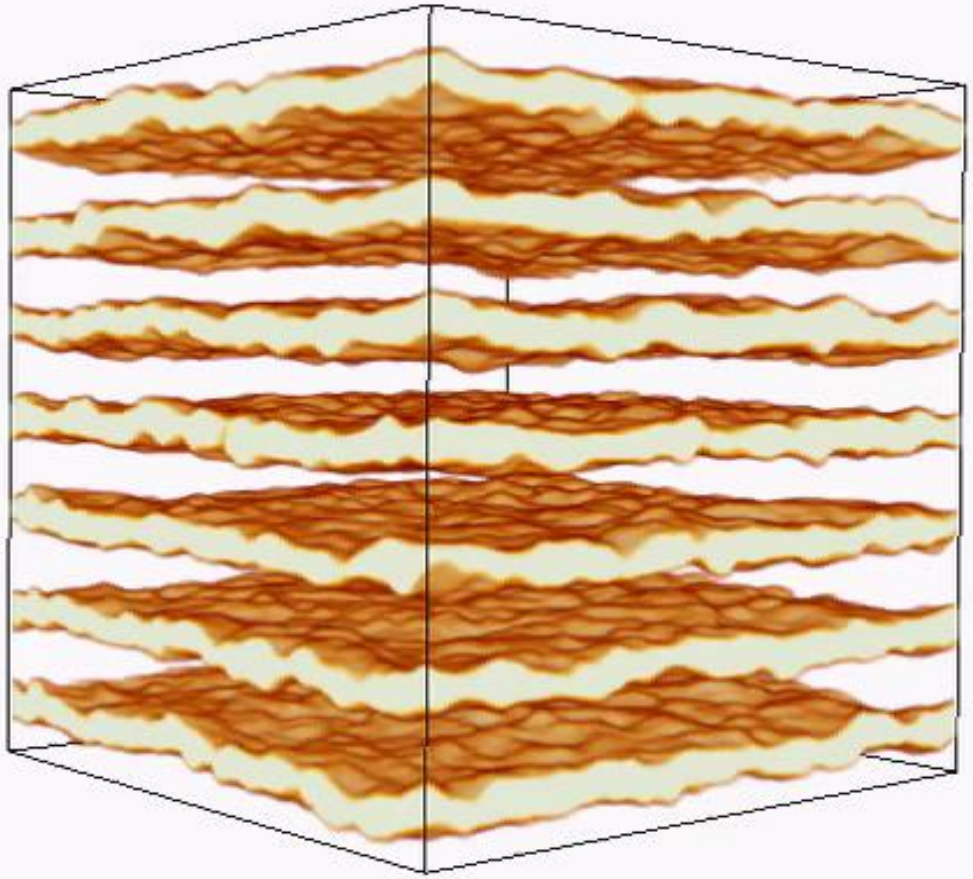

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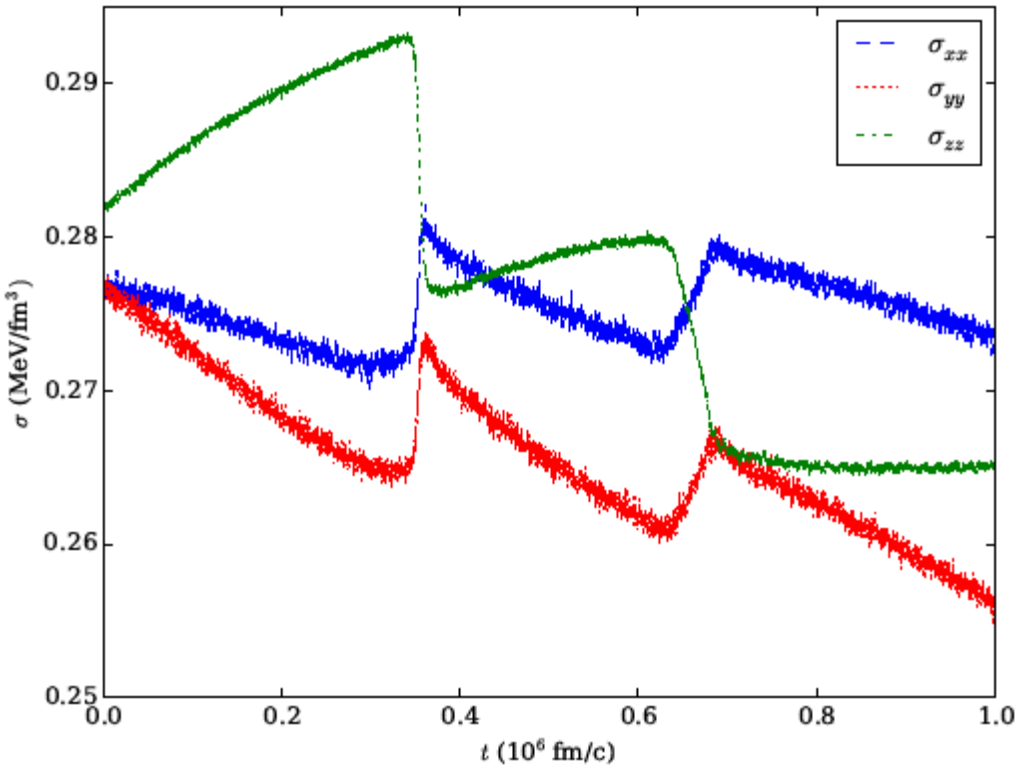


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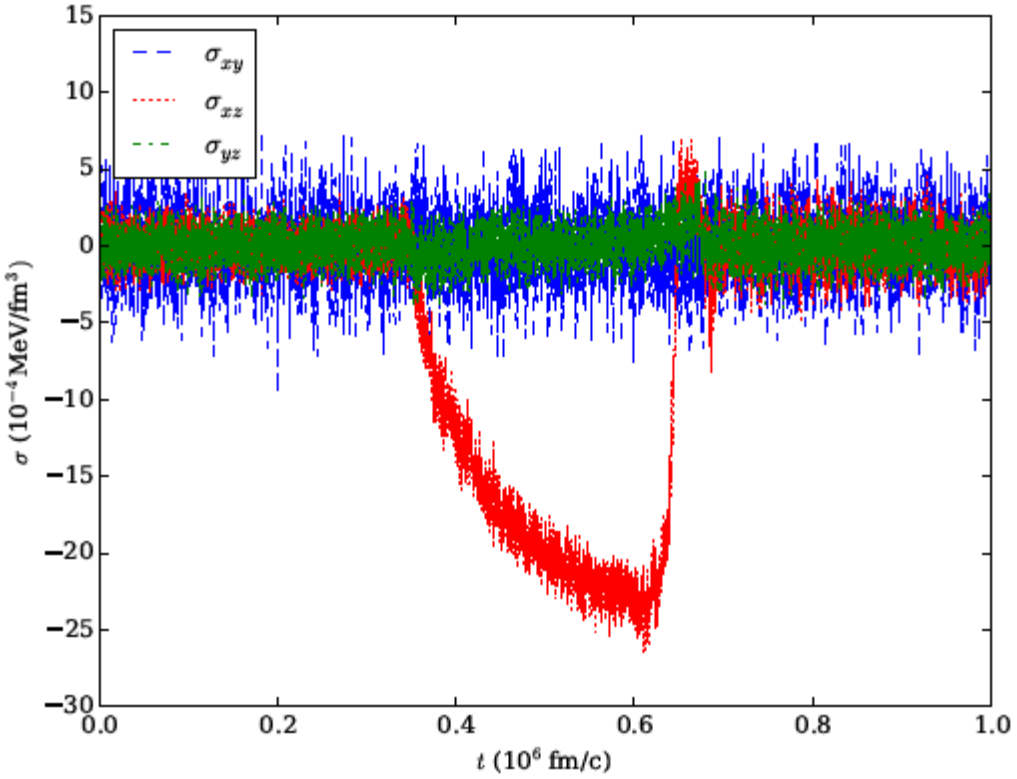

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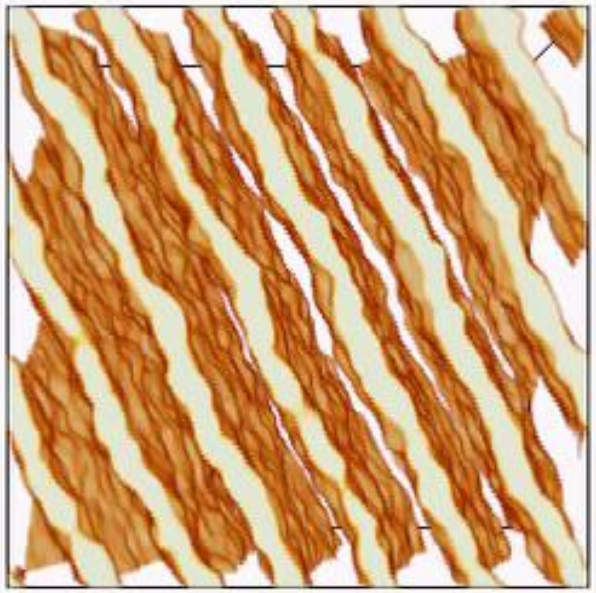

$\epsilon_y = 0.000$

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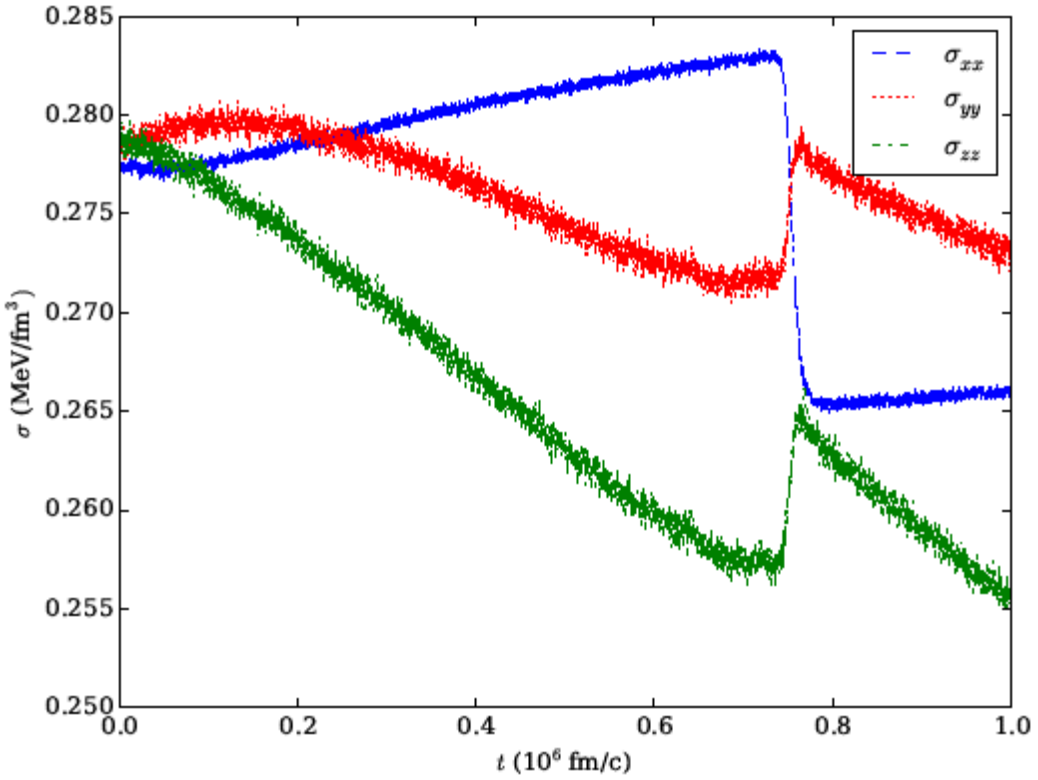
- Tensile Stress

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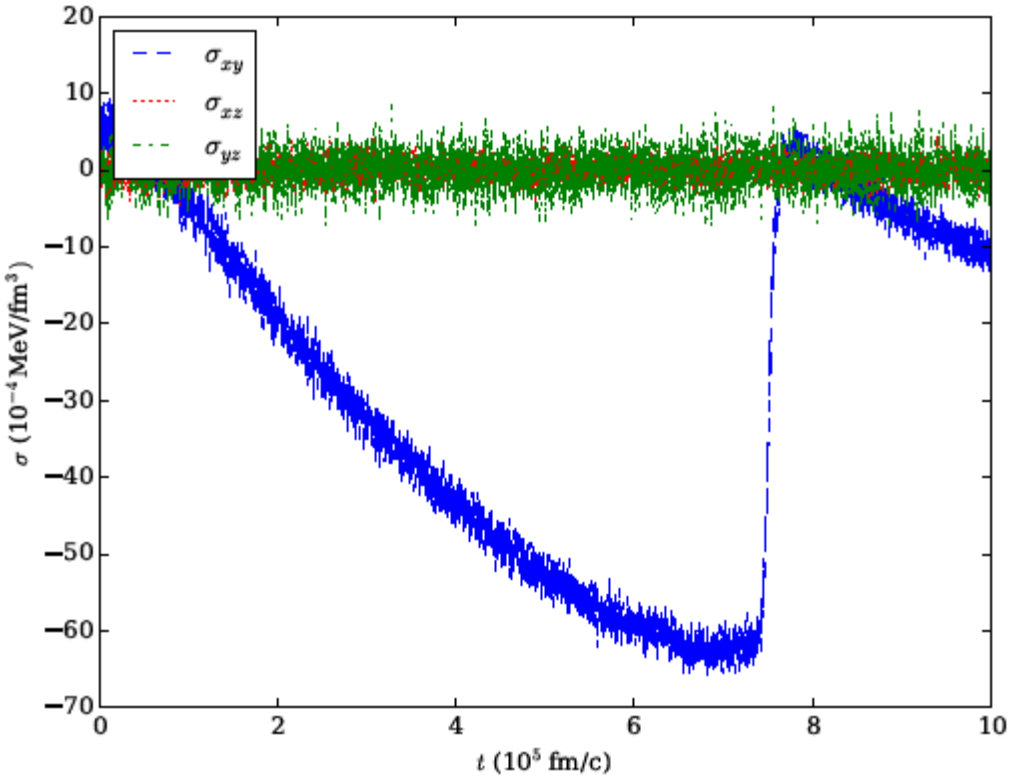

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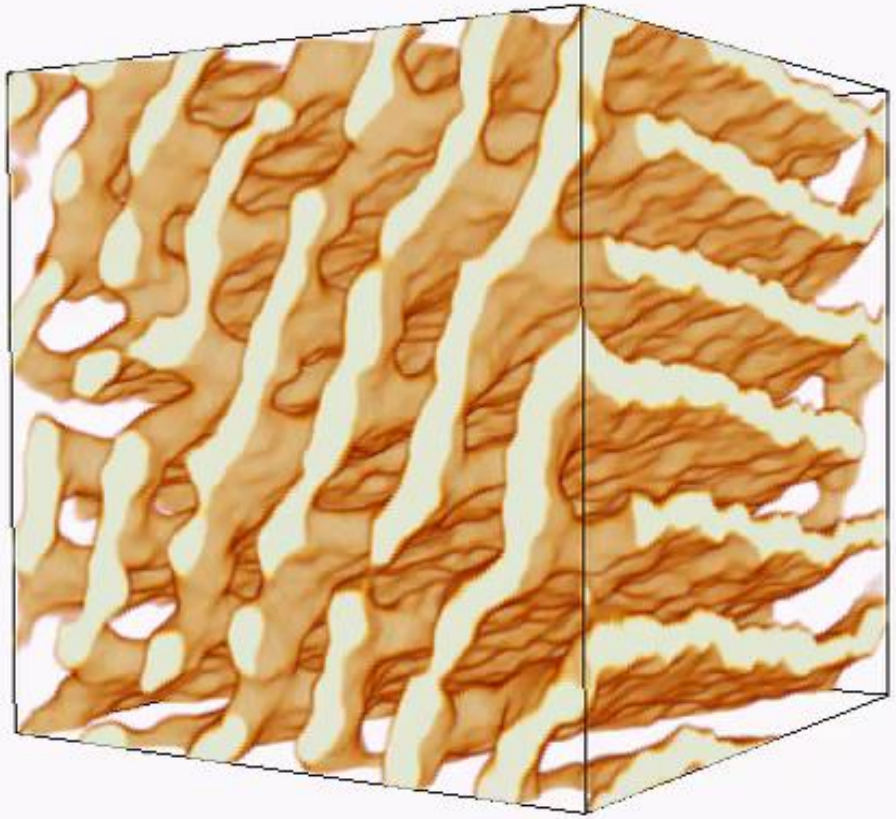

# Stresses

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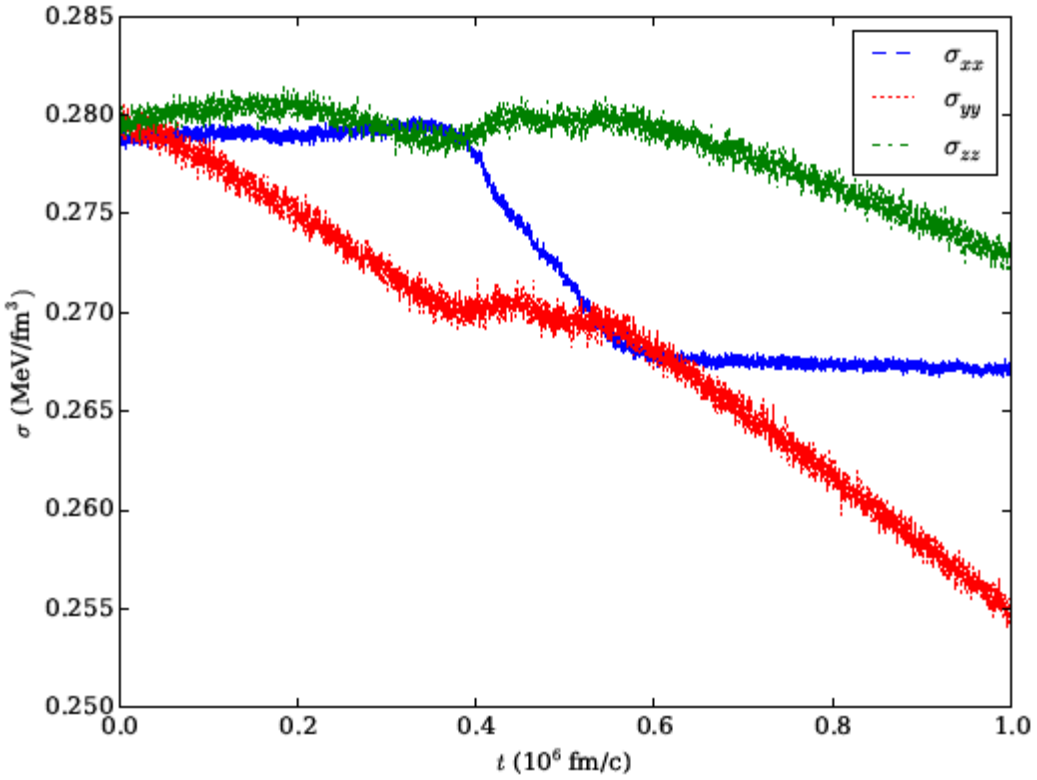
- Tensile Stress

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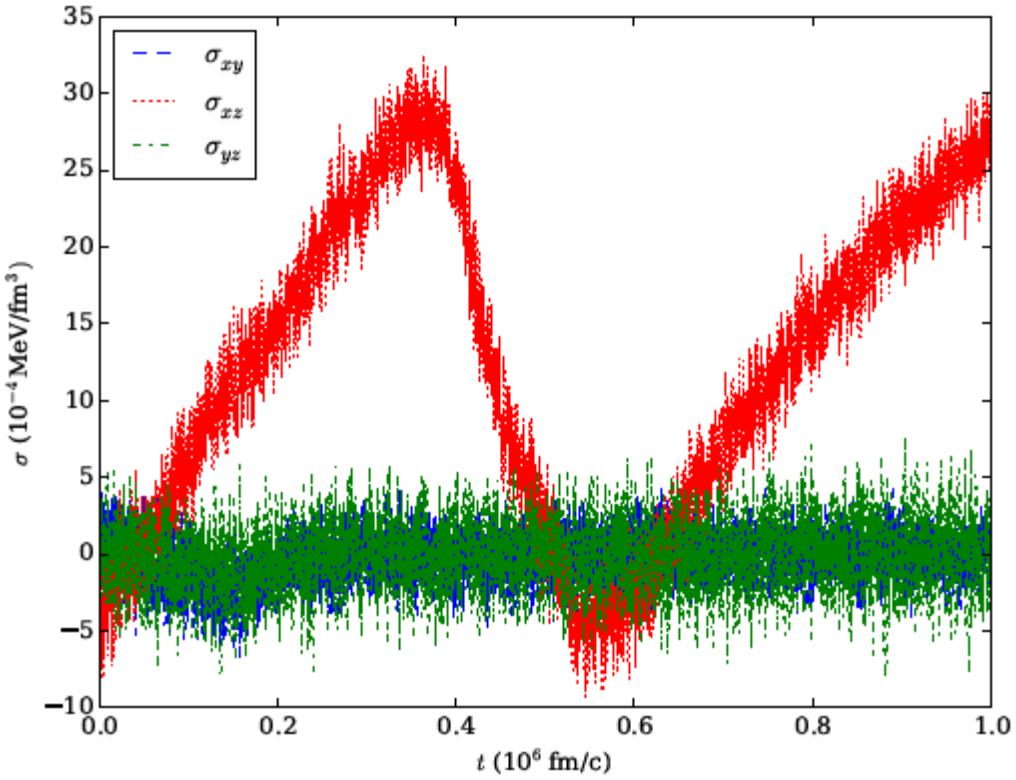

# Pasta Stresses

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- I’ve shown you ‘unit cells’ of ‘perfect pasta,’ maybe analogous to a small monocrystalline sample of a bcc lattice. Can we generalize this, like when we study the angle averaged properties of a polycrystalline bcc lattice in the outer crust?

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- Possibly? Pasta bending and defects may form ‘domains’ with local orientations (see Will Newton’s talk).

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- Possibly? Pasta bending and defects may form 'domains' with local orientations (see Will Newton's talk).

- **Can we create a 'polycrystalline' sample of nuclear pasta?**

# Polycrystalline Pasta

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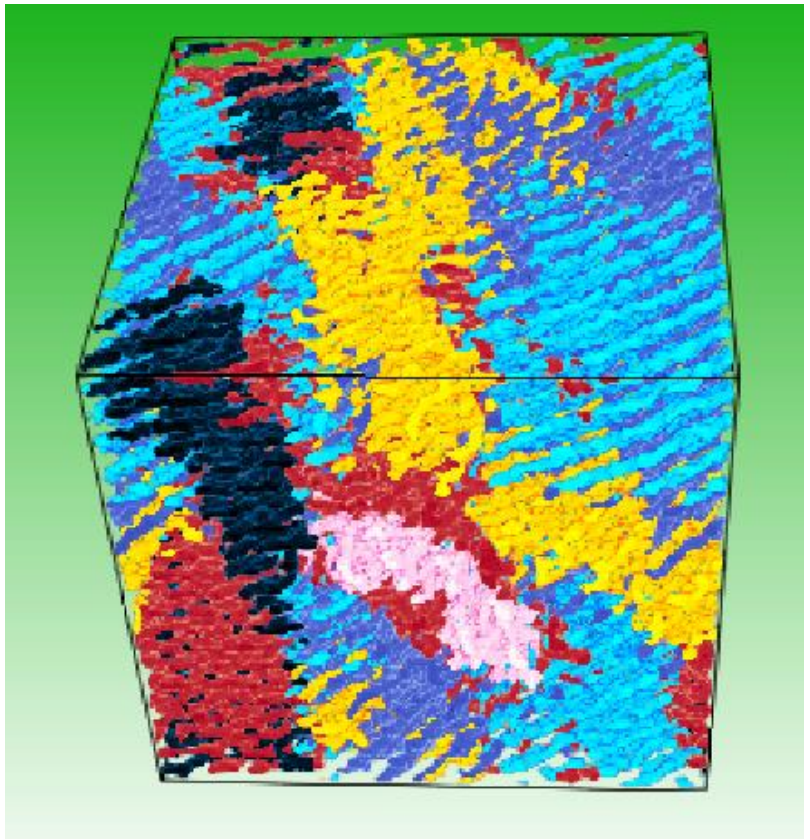
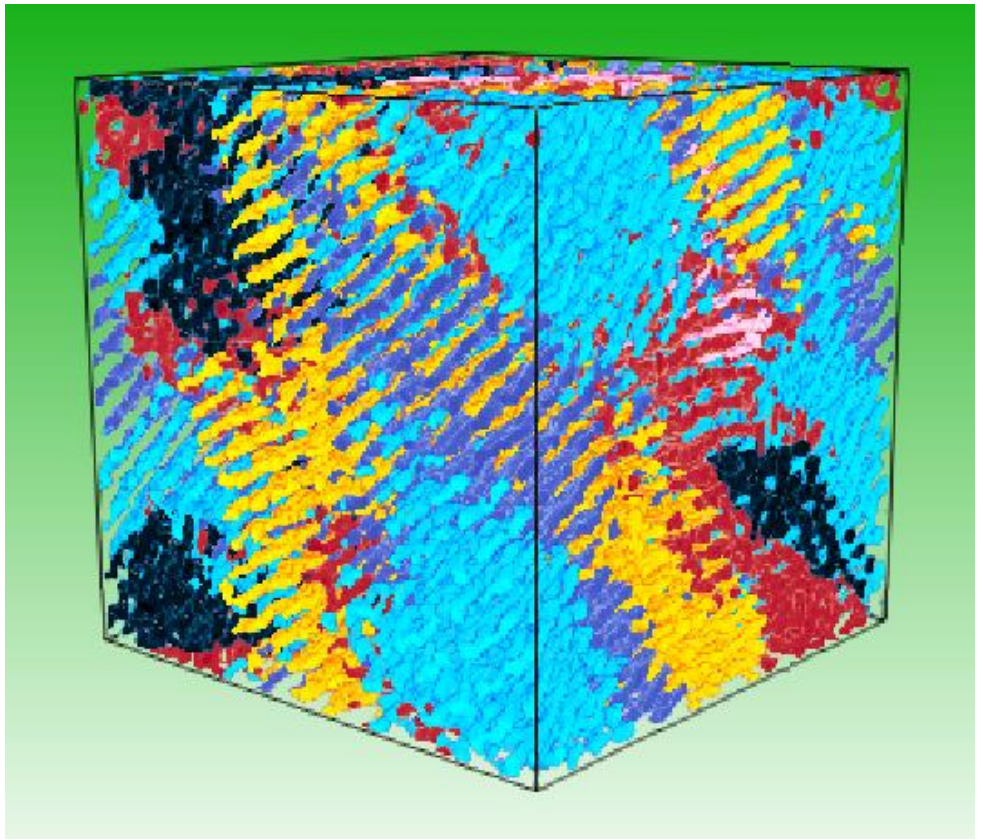
- Simulations with 3,276,800 nucleons do not equilibrate to form parallel plates with a single domain.





# Polycrystalline Pasta

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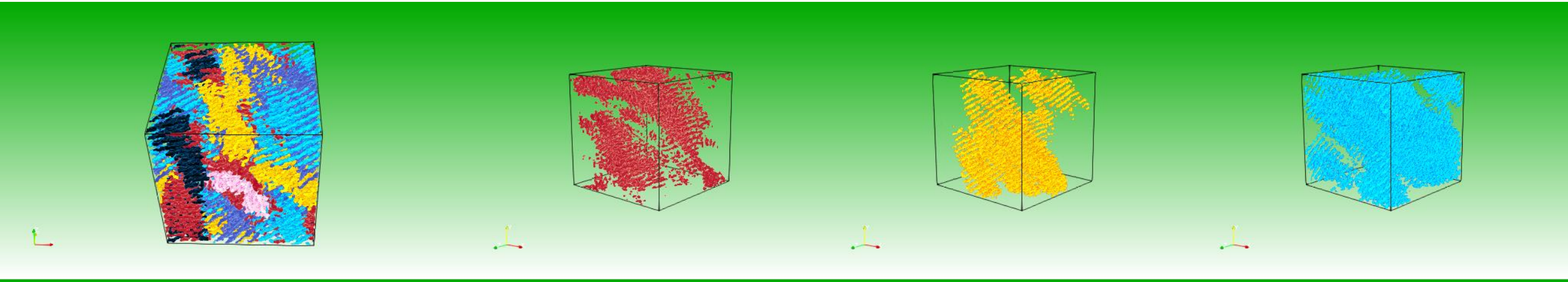
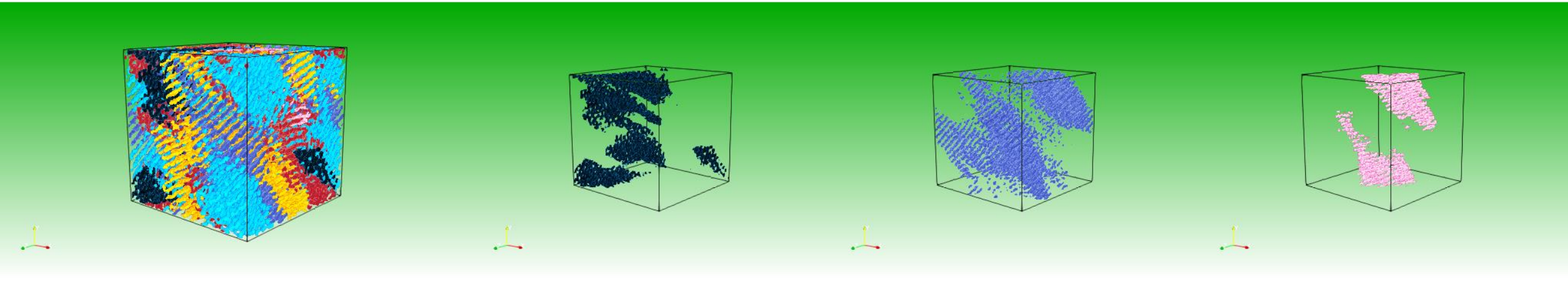
- Can deform this configuration, analogous to Horowitz 2009





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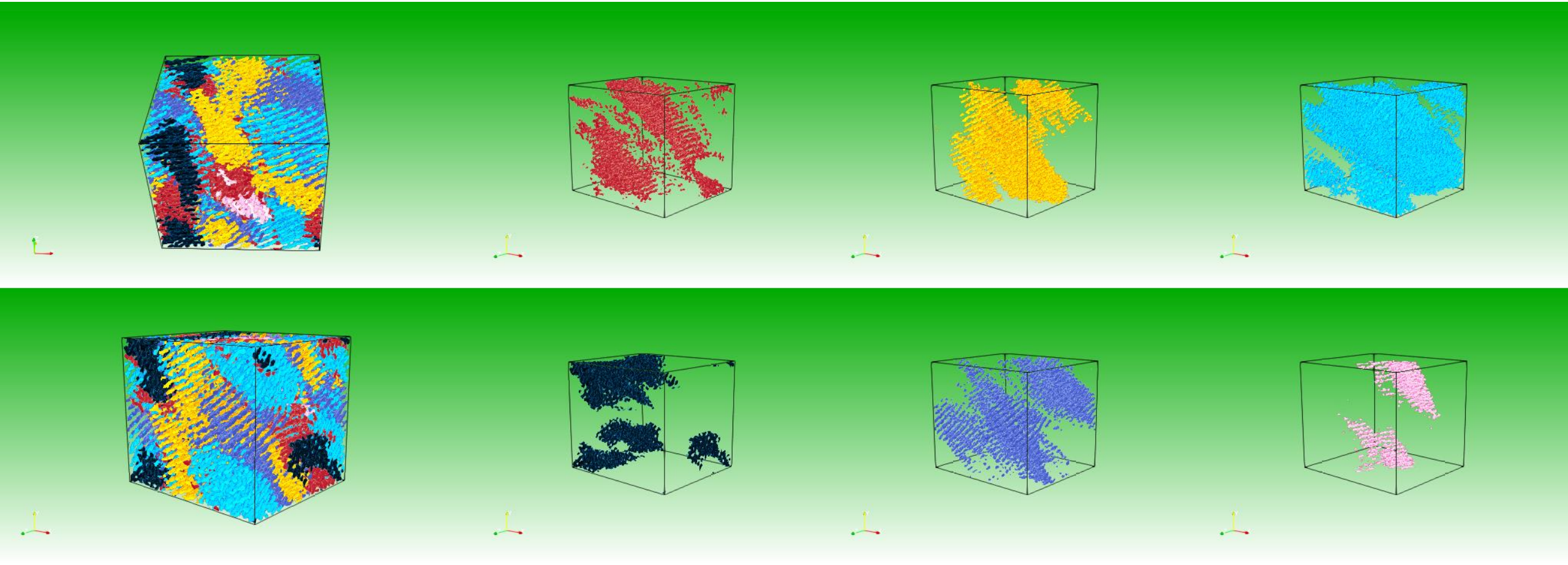

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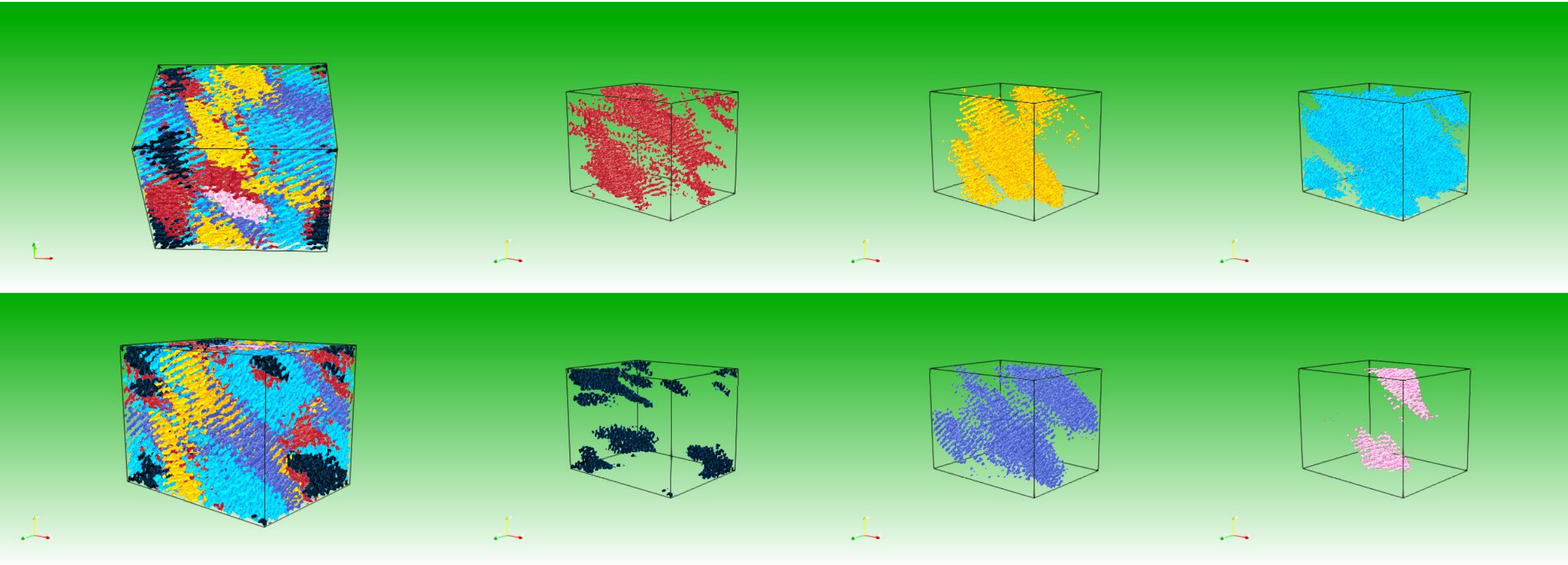
- Can deform this configuration, analogous to Horowitz 2009



# Polycrystalline Pasta

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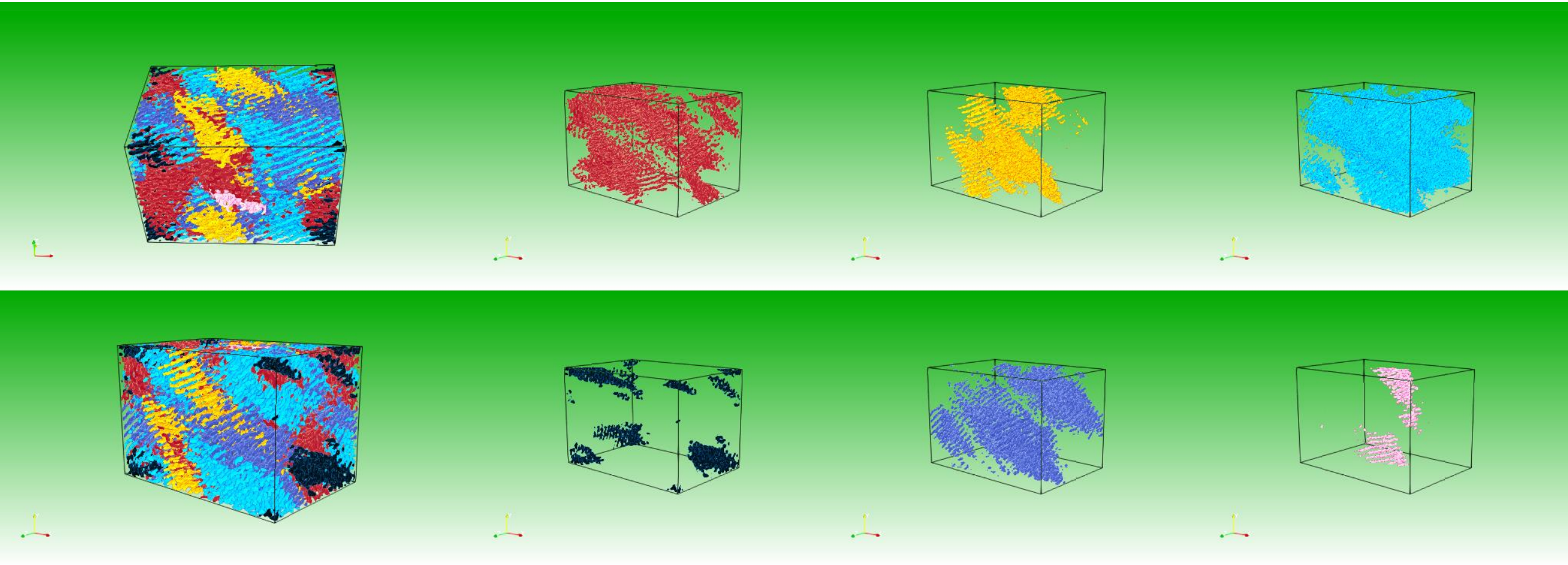
- Can deform this configuration, analogous to Horowitz 2009



# Stresses

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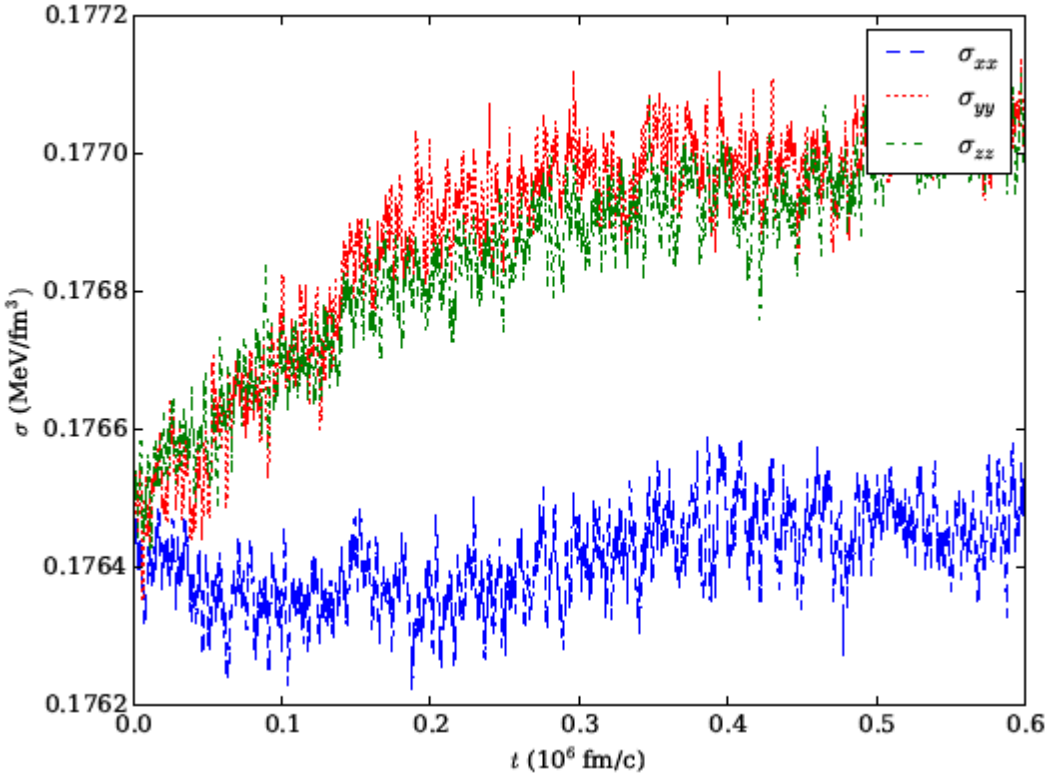
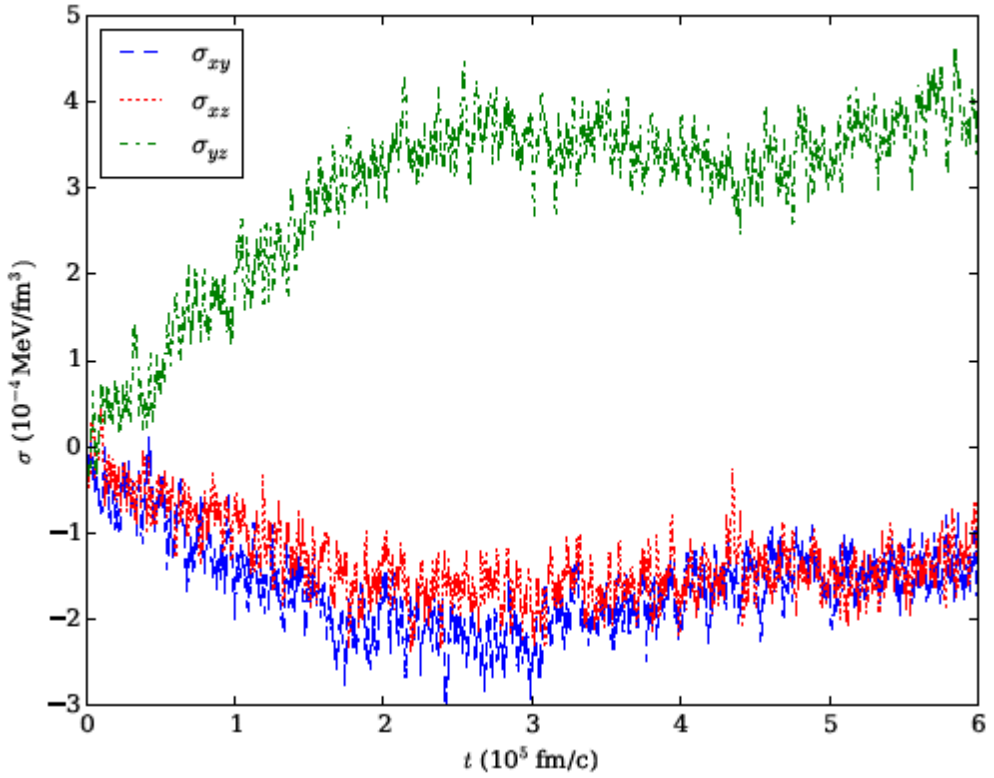
- Tensile Stress
  (Asssuming an induced shear strain of ~0.1, suggests $\mu_{eff}>10^{30}$ erg/cm$^3$

Shear Stress



# Molecular Dynamics Summary

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- **Result 1**: Pasta ‘unit cells’ can demonstrate a wide variety of elastic responses, which can be understood individually, but may be difficult to describe generally.
- **Result 2**: Pasta is very plastic and deforms readily. Compared to the outer crust, which may break at ($\varepsilon \sim 0.1$), domains of pasta can easily sustain large strains ($\varepsilon > 0.2$) without failure, while large multi-domain simulations show no sign of failure for $\varepsilon < 0.5$

- **Future Work:** Can we extract the shear modulus of pasta from molecular dynamics simulations of pasta deformations? Can we bridge the solid crust to the liquid core?