

# Nuclear Pasta Observables

Matt Caplan  
Indiana University

Institute for Nuclear Theory  
August 1, 2016



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

**NUCLEI**  
Nuclear Computational Low-Energy Initiative

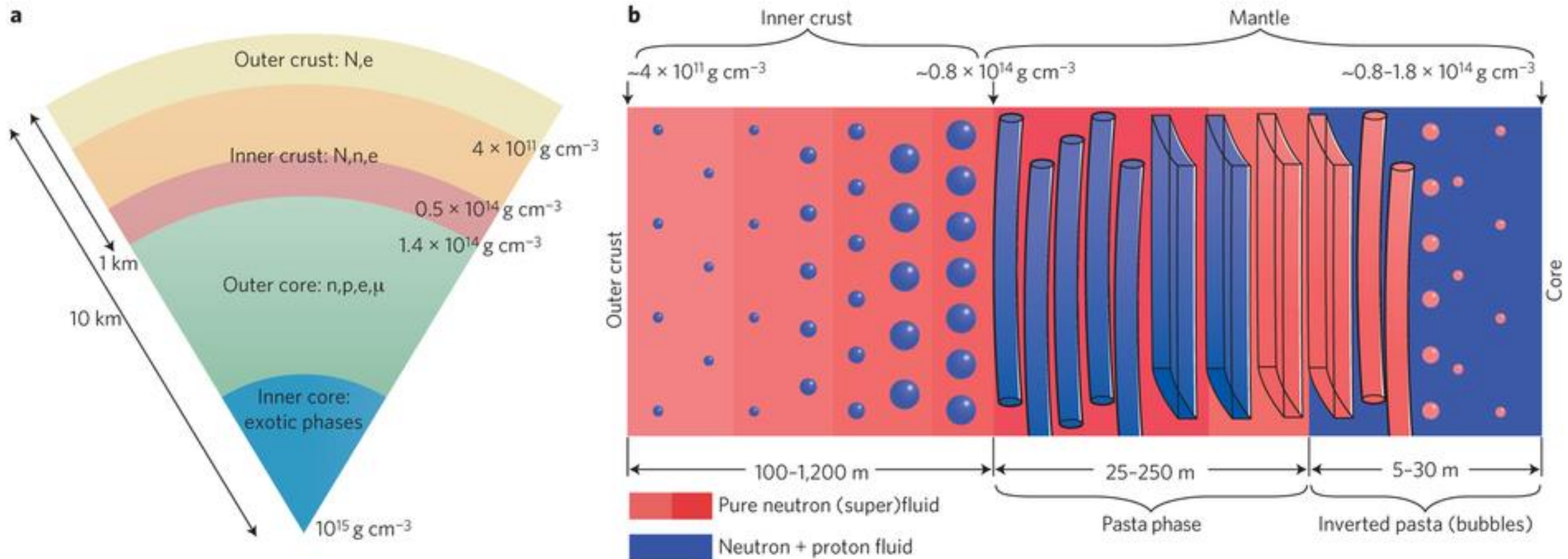


**INDIANA UNIVERSITY**

# Neutron stars



- The crust is a crystalline lattice, while the core is uniform nuclear matter, like a nucleus. What's in between these two phases?



# Non-Spherical Nuclei



- 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

Shape of Nuclei in the Crust of Neutron Star

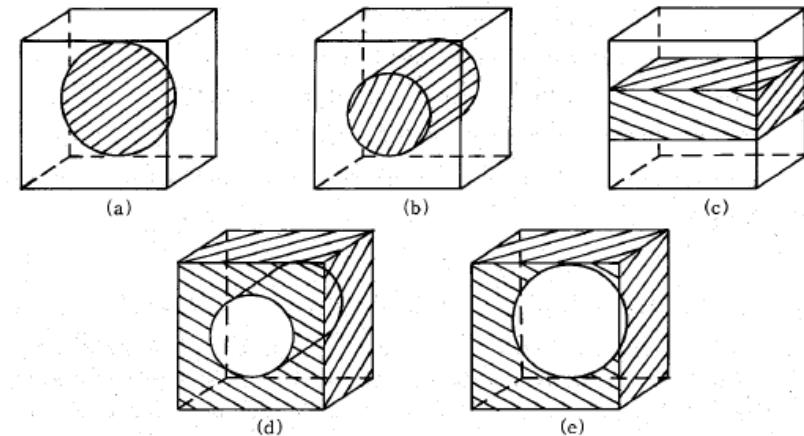
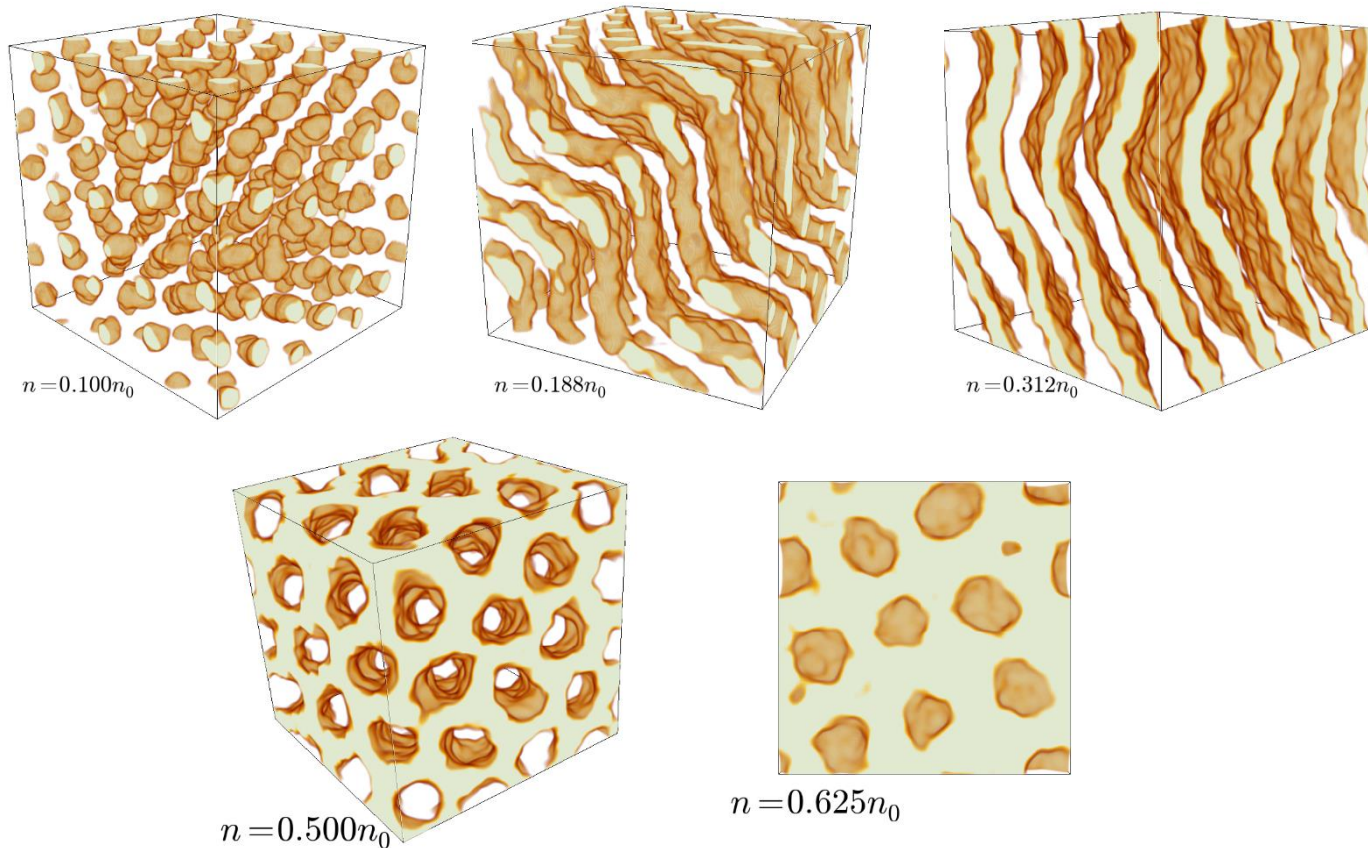


Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole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

# Nuclear Pasta



*Shape of Nuclei in the Crust of Neutron Star*

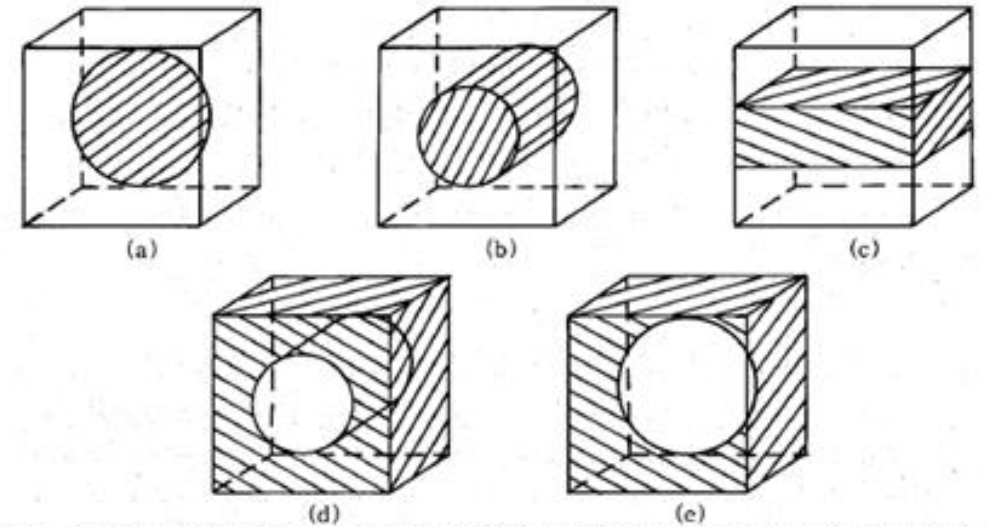


Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole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

# Classical Pasta Formalism



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

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

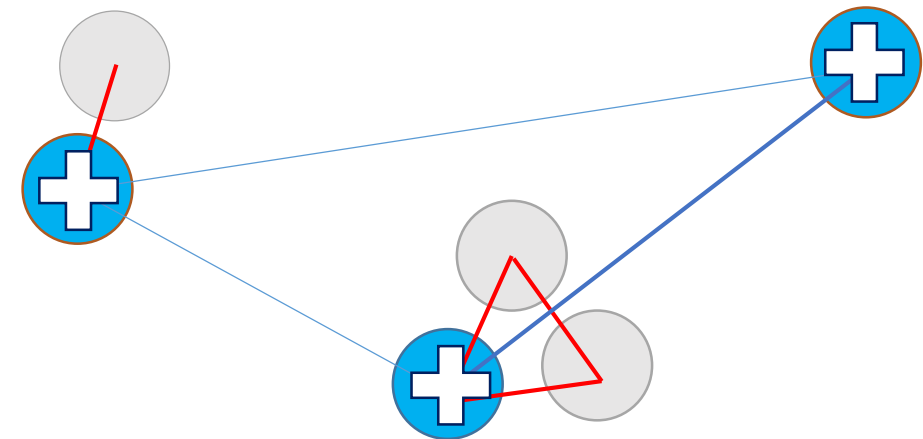
$$V_{nn}(r_{ij}) = a e^{-r_{ij}^2/\Lambda} + [b + c] e^{-r_{ij}^2/2\Lambda}$$

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

$a$	$b$	$c$	$\Lambda$	$\lambda$
110 MeV	-26 MeV	24 MeV	1.25 fm <sup>2</sup>	10 fm

- Short range **nuclear** force
- Long range **Coulomb** force

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



# Classical Pasta Formalism



- Classical Molecular Dynamics IUM Red II

Density

NSE!

$\Lambda$	$\lambda$
1.25 fm <sup>2</sup>	10 fm

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

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

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

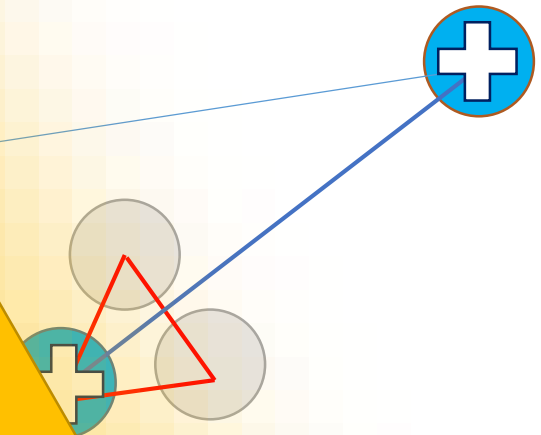


range **nuclear** force  
range **Coulomb** force

Nucleus	Monte-Carlo $\langle V_{tot} \rangle$ (MeV)
<sup>16</sup> O	-7.56 ± 0.01
<sup>40</sup> Ca	-8.75 ± 0.03
<sup>90</sup> Zr	-9.13 ± 0.0
<sup>208</sup> Pb	-8.2 ± 0.0

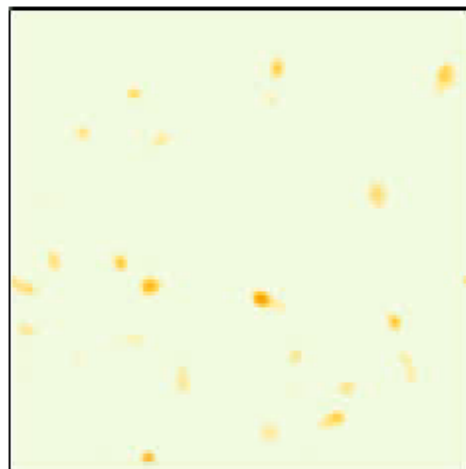
Proton Fraction

Temperature





Gold Nucleus  
For Scale



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

# Pass around the 3D printed cubes



- I always forget so I made a slide to remind myself that I have them.





# Classical and Quantum MD



- We can use the classical pasta to initiate the quantum codes
- Classical structures remain stable when evolved via HF

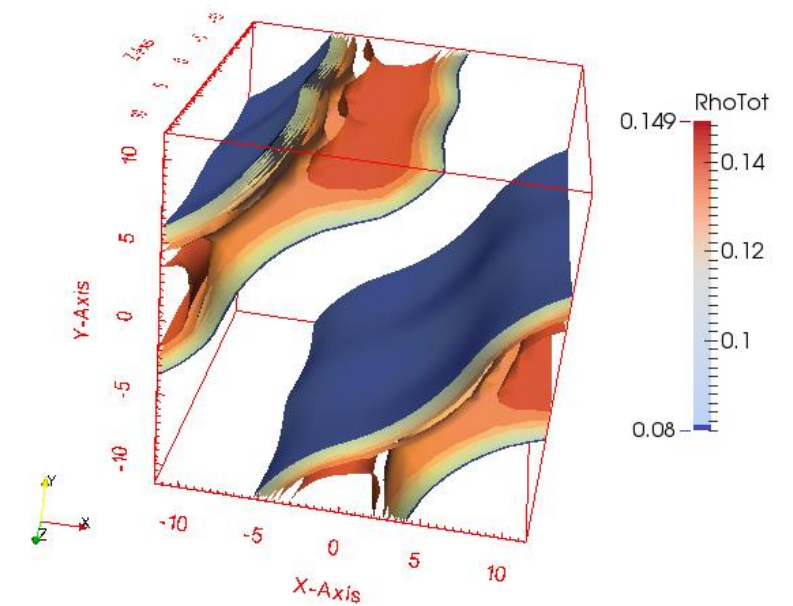
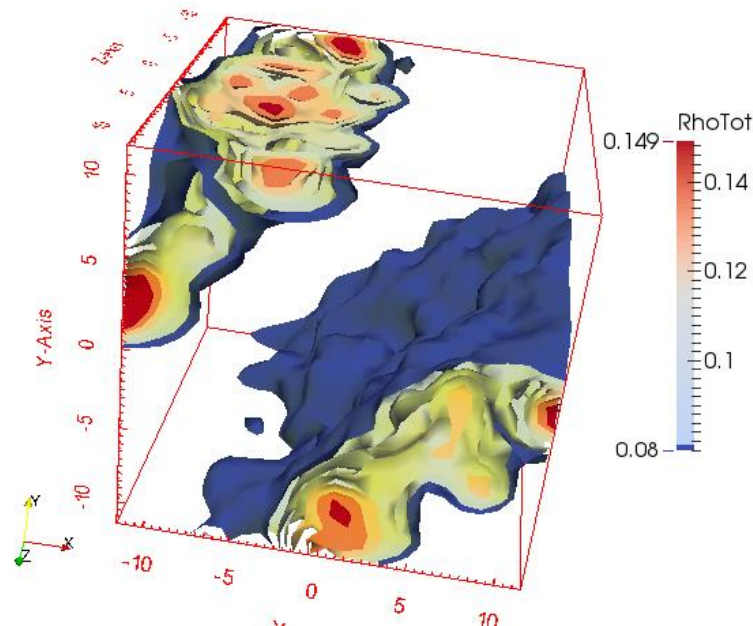
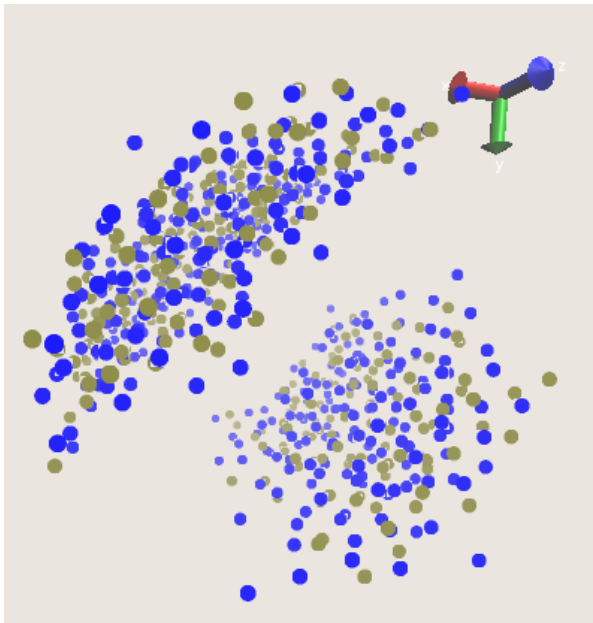
**Classical Points**



**Folded with Gaussian**



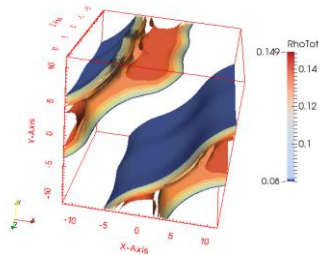
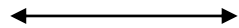
**Equilibrated  
Wavefunctions**



# Classical and Quantum MD



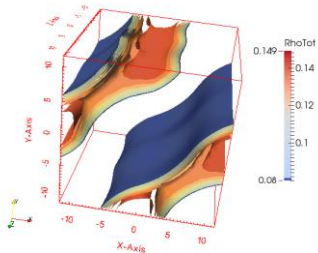
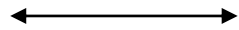
**800 nucleons**  
**24 fm**



# Classical and Quantum MD

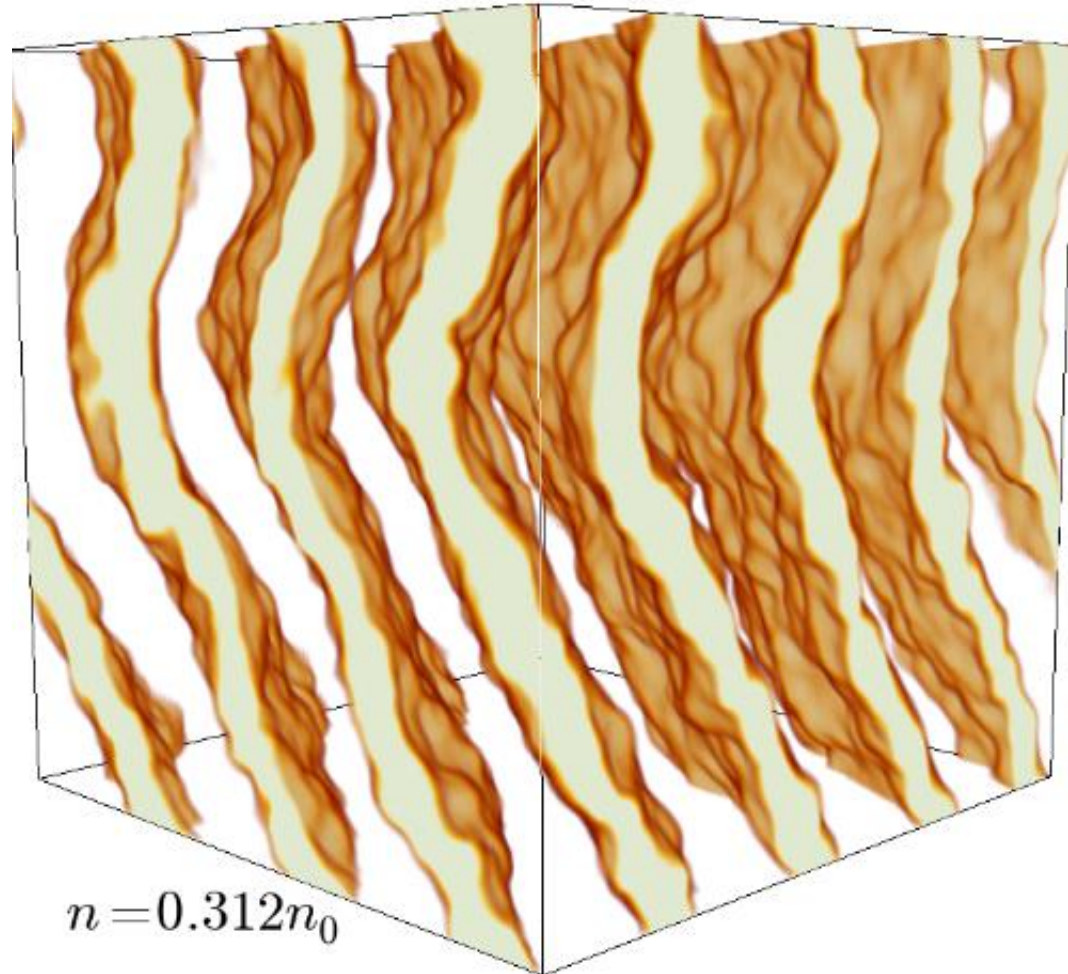


800 nucleons  
24 fm



100 fm

51,200 nucleons

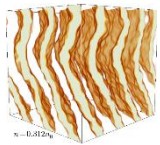


$$n = 0.312n_0$$

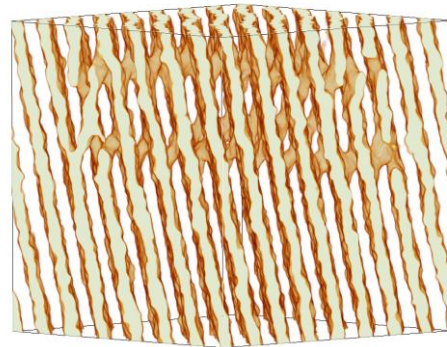
# Molecular Dynamics



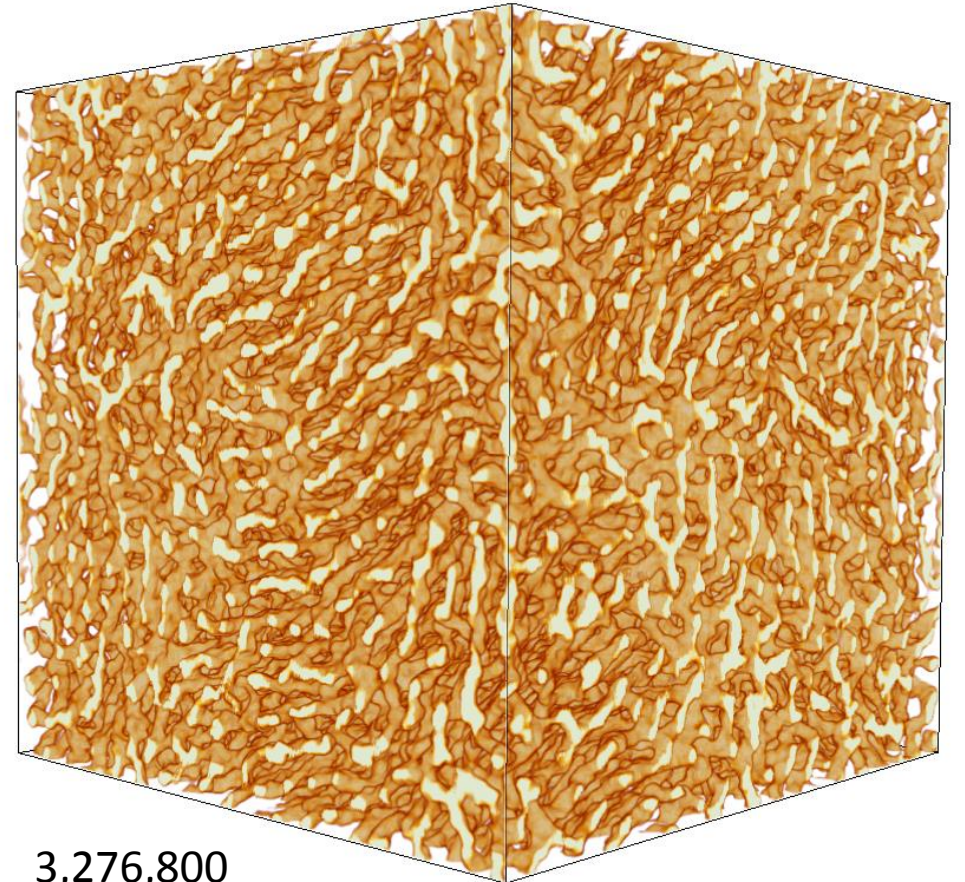
- We have evolved simulations of 409,600 nucleons, 819,200 nucleons, 1,638,400 nucleons, and 3,276,800 nucleons



51,200



409,600



3,276,800

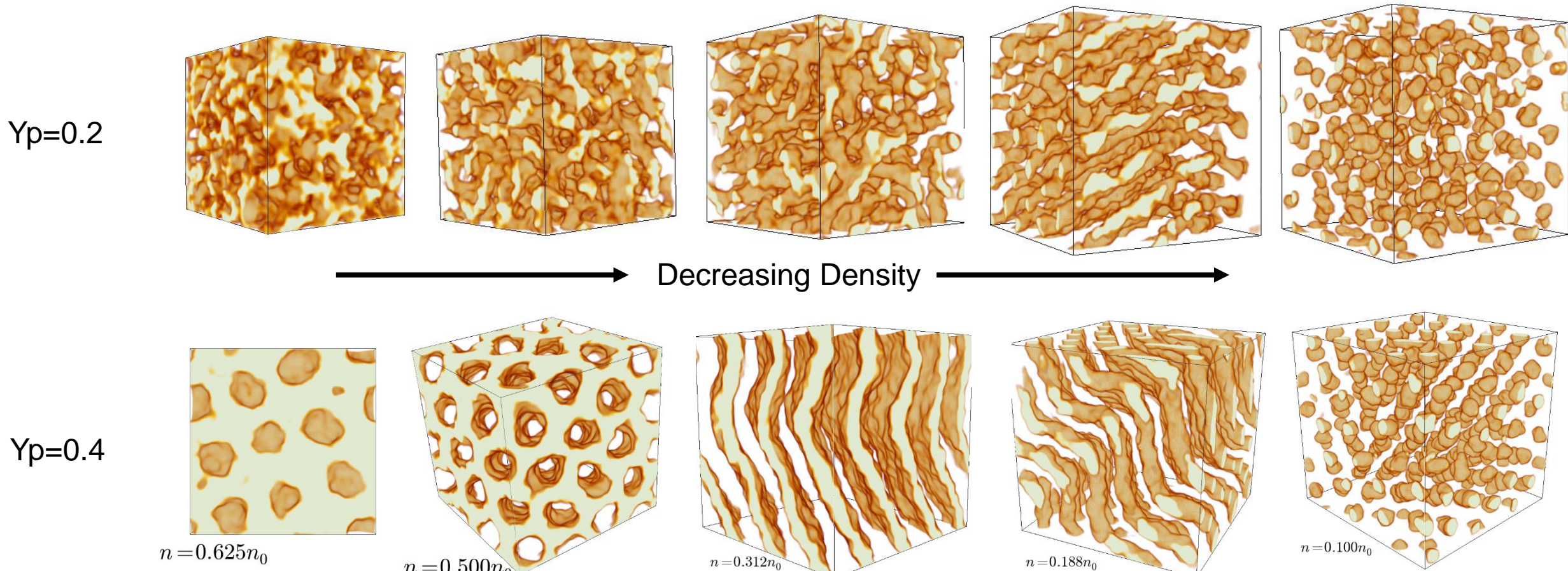
# Phase Diagrams



# Phase Diagrams



- Simulate pasta with constant temperature and proton fraction
- Observe phase transitions as a function of density



# “Thermodynamic” Curvature







- Use curvature as a thermodynamic quantity
- Discontinuities in curvature indicate phase changes

$V$	Volume
$A = \int_{\partial K} dA$	Surface Area
$B = \int_{\partial K} (\kappa_1 + \kappa_2) / 4\pi dA$	Mean Breadth
$\chi = \int_{\partial K} (\kappa_1 \cdot \kappa_2) / 4\pi dA$	Euler Characteristic

$$\int_M K dA + \int_{\partial M} k_g ds = 2\pi\chi(M)$$

$\chi(M) = 2 - 2g$

- Pieces + Cavities - Holes

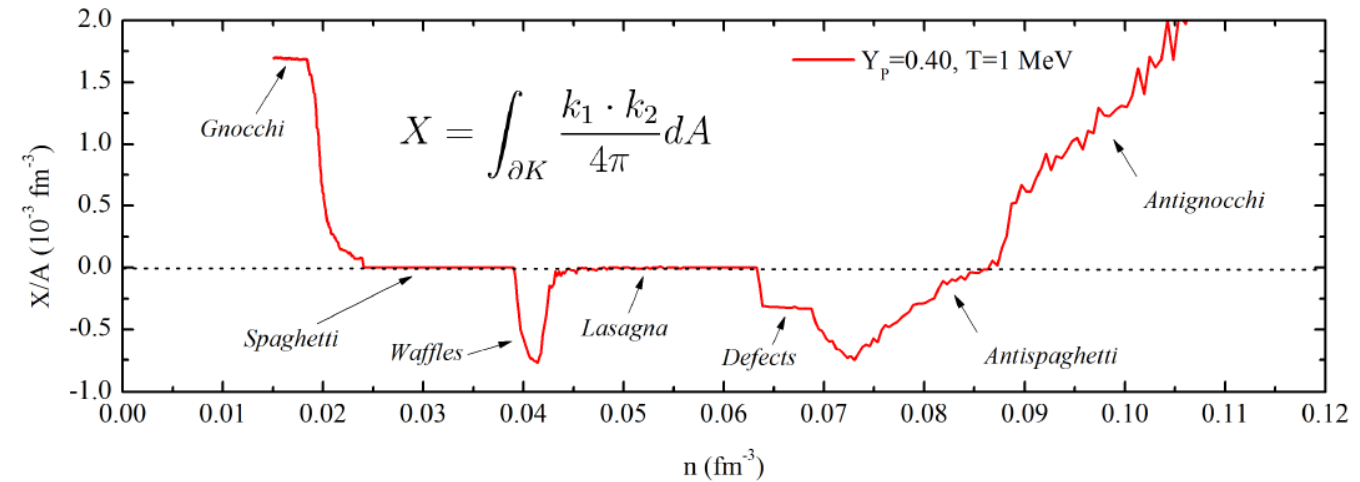
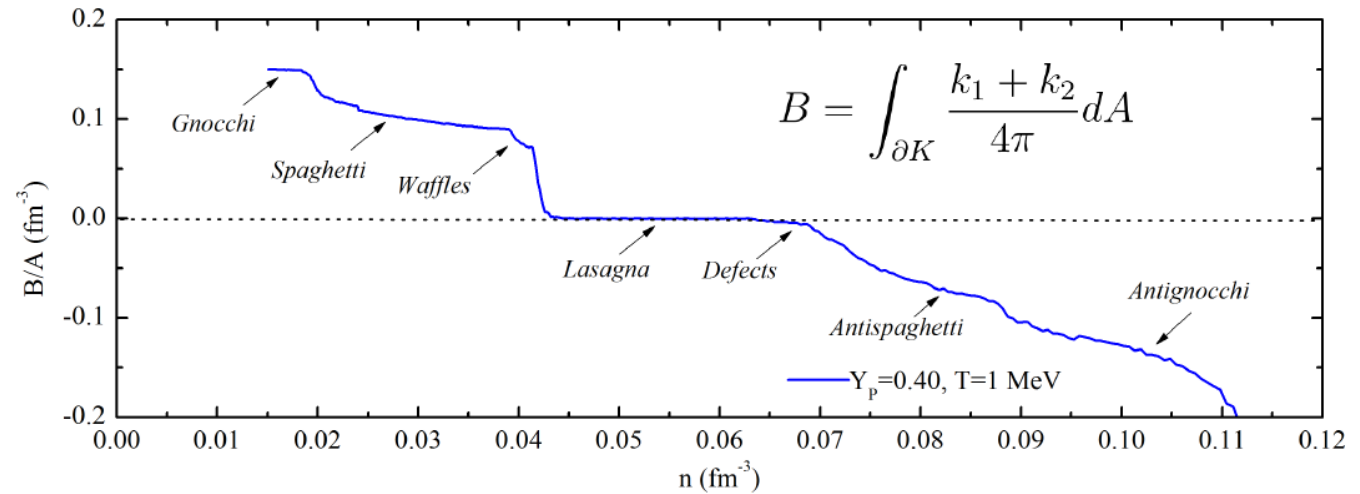
Sphere		2
Torus (Product of two circles)		0
Double torus		-2
Triple torus		-4

# “Thermodynamic” Curvature



- Use curvature as a thermodynamic quantity
- Discontinuities in curvature indicate phase changes

$V$	Volume
$A = \int_{\partial K} dA$	Surface Area
$B = \int_{\partial K} (\kappa_1 + \kappa_2) / 4\pi dA$	Mean Breadth
$\chi = \int_{\partial K} (\kappa_1 \cdot \kappa_2) / 4\pi dA$	Euler Characteristic

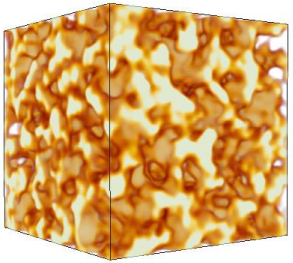




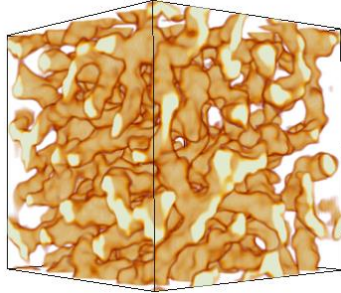
# Phases



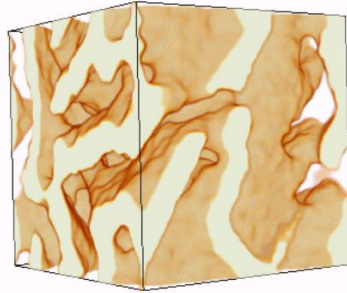
i-Antignocchi



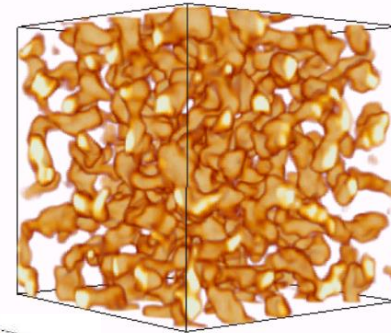
i-Antispaghetti



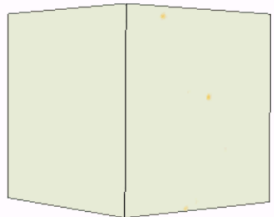
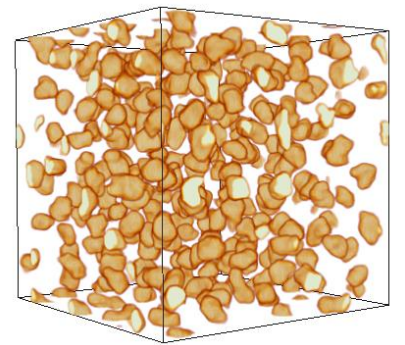
i-Lasagna



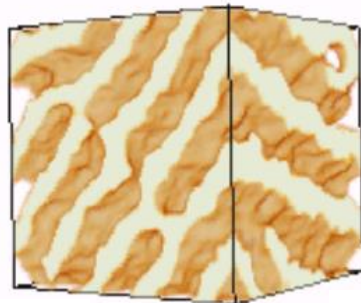
i-Spaghetti



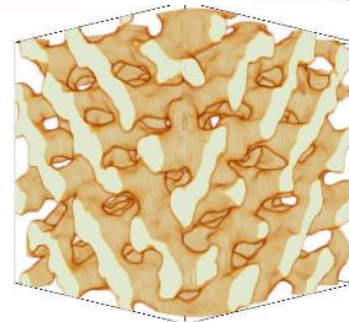
i-Gnocchi



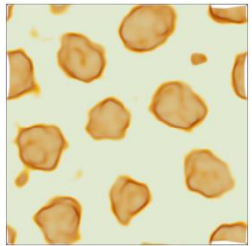
Uniform



Defects

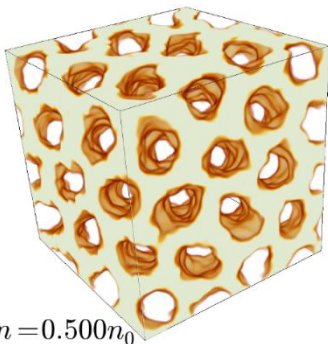


Waffles



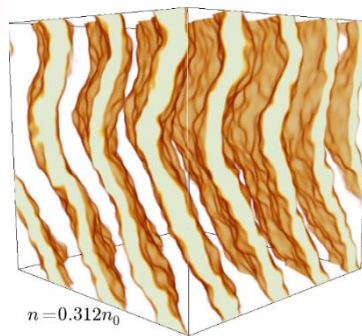
$$n = 0.625n_0$$

r-Antignocchi



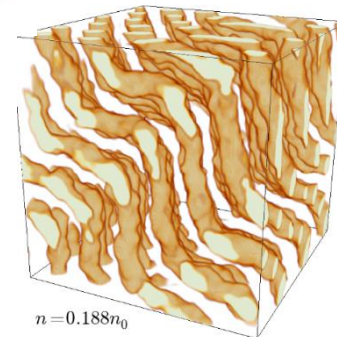
$$n = 0.500n_0$$

r-Antispaghetti



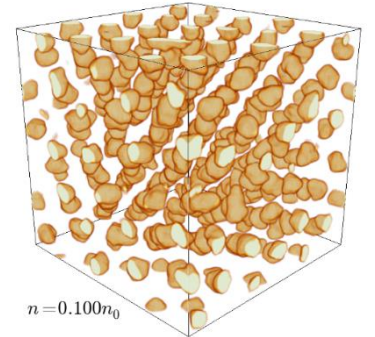
$$n = 0.312n_0$$

r-Lasagna



$$n = 0.188n_0$$

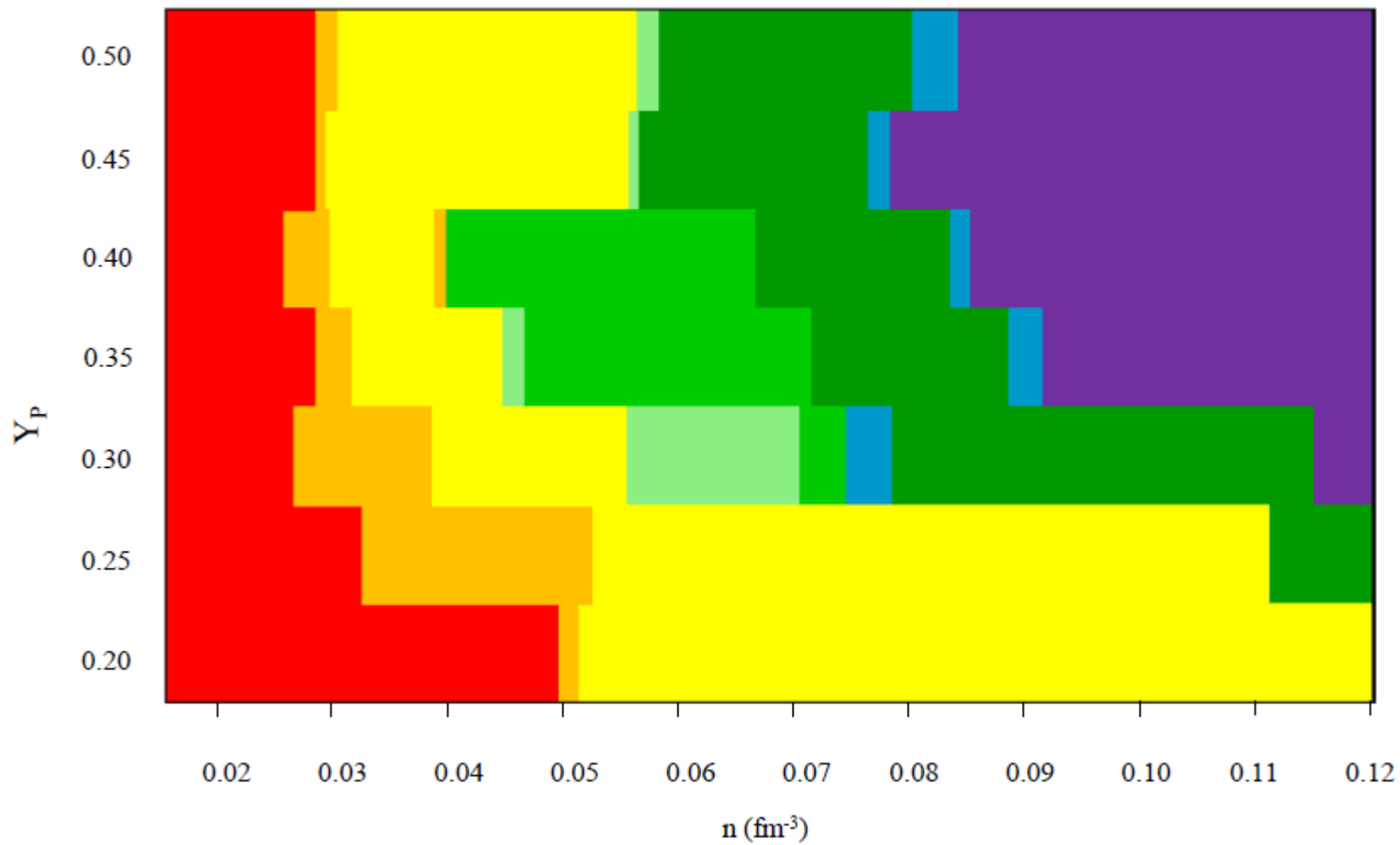
r-Spaghetti



$$n = 0.100n_0$$

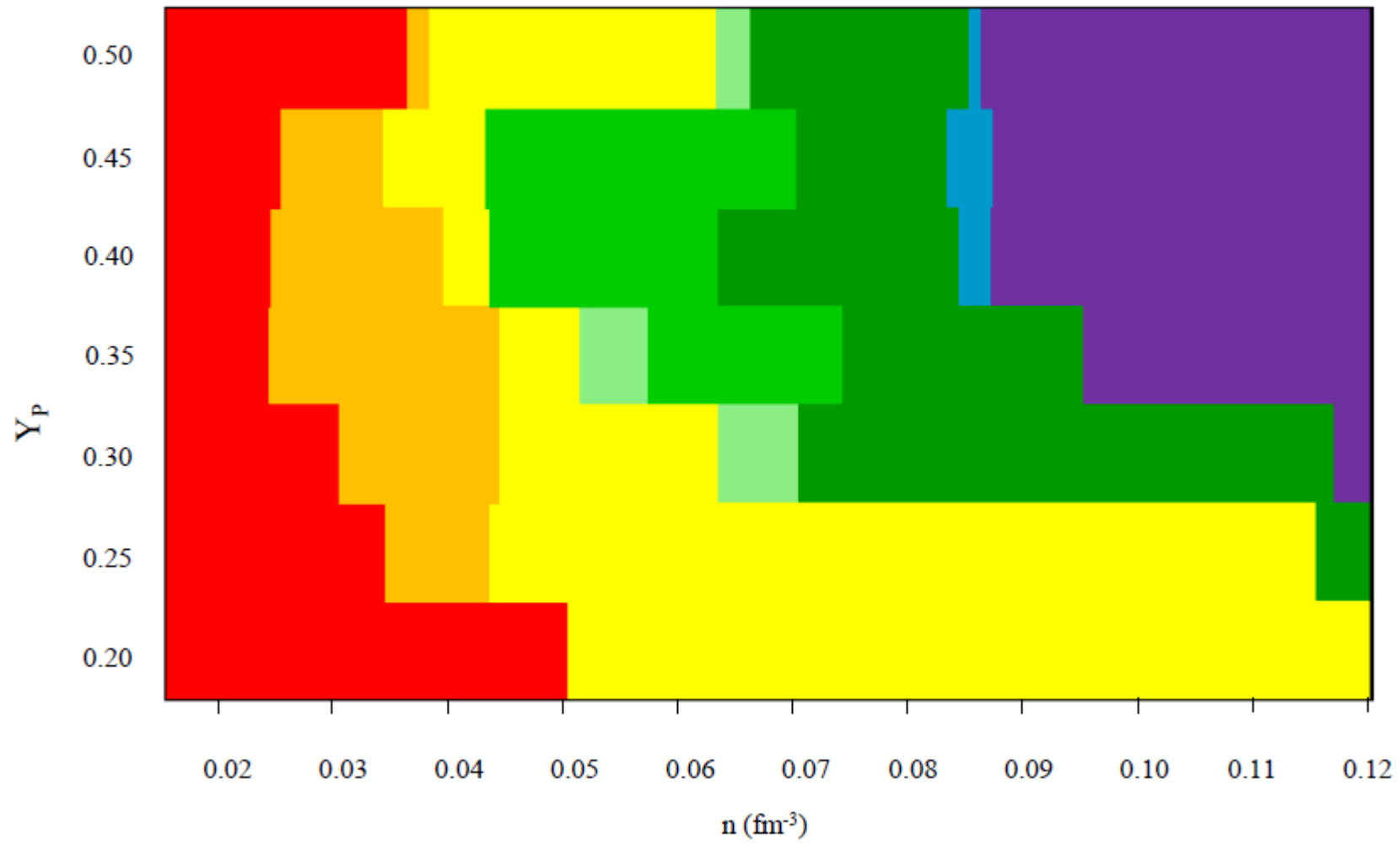
r-Gnocchi

T=0.8 MeV



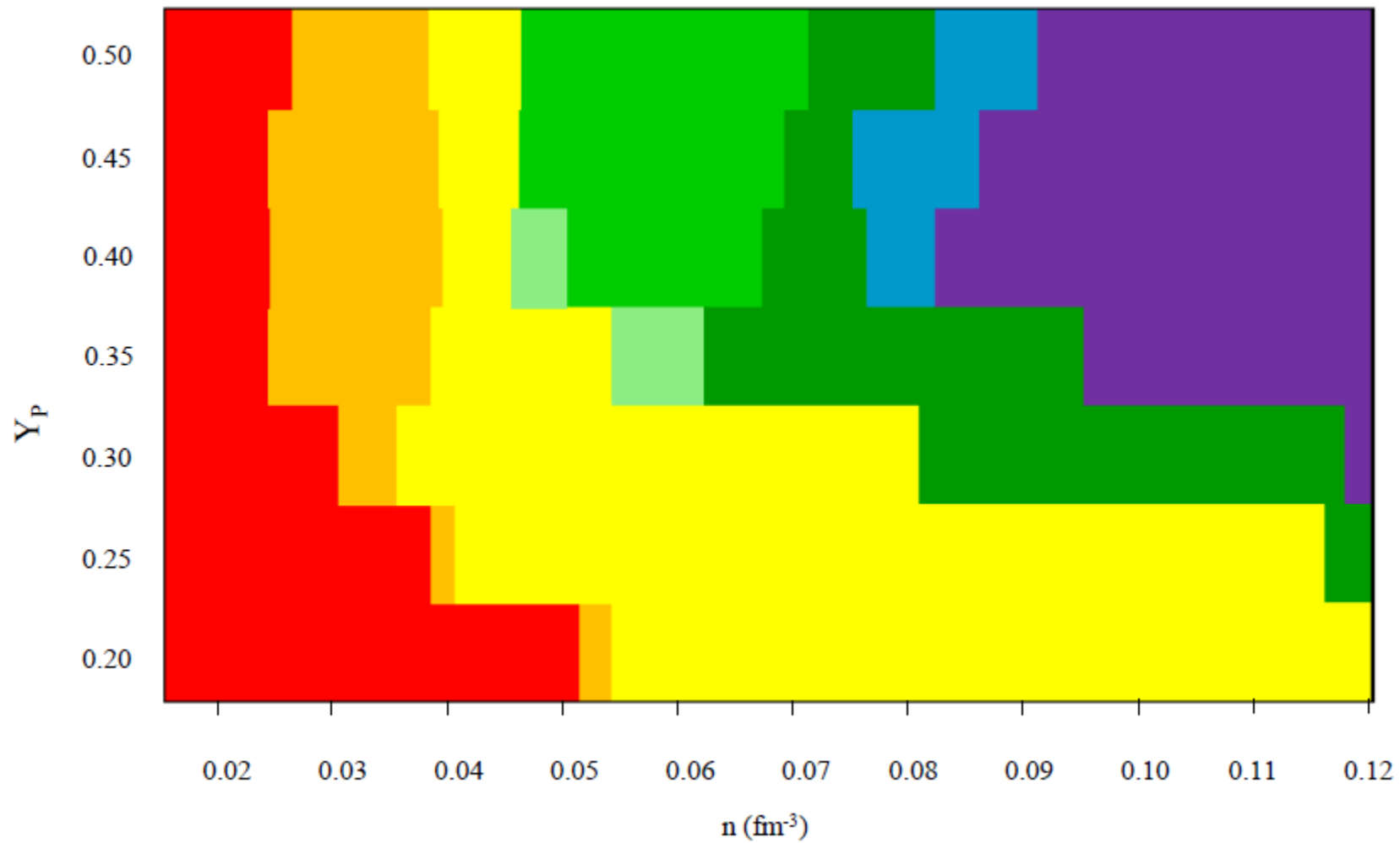
	$B < 0$	$B \sim 0$	$B > 0$
$\chi > 0$	■ sph b		■ sph
$\chi \sim 0$	■ rod-1 b	■ slab	■ rod-1
$\chi < 0$	■ rod-2 b	■ rod-3	■ rod-2

T=1.0 MeV



	$B < 0$	$B \sim 0$	$B > 0$
$\chi > 0$	■ sph b		■ sph
$\chi \sim 0$	■ rod-1 b	■ slab	■ rod-1
$\chi < 0$	■ rod-2 b	■ rod-3	■ rod-2

T=1.2 MeV



	$B < 0$	$B \sim 0$	$B > 0$
$\chi > 0$	■ sph b		■ sph
$\chi \sim 0$	■ rod-1 b	■ slab	■ rod-1
$\chi < 0$	■ rod-2 b	■ rod-3	■ rod-2

Soft Matter

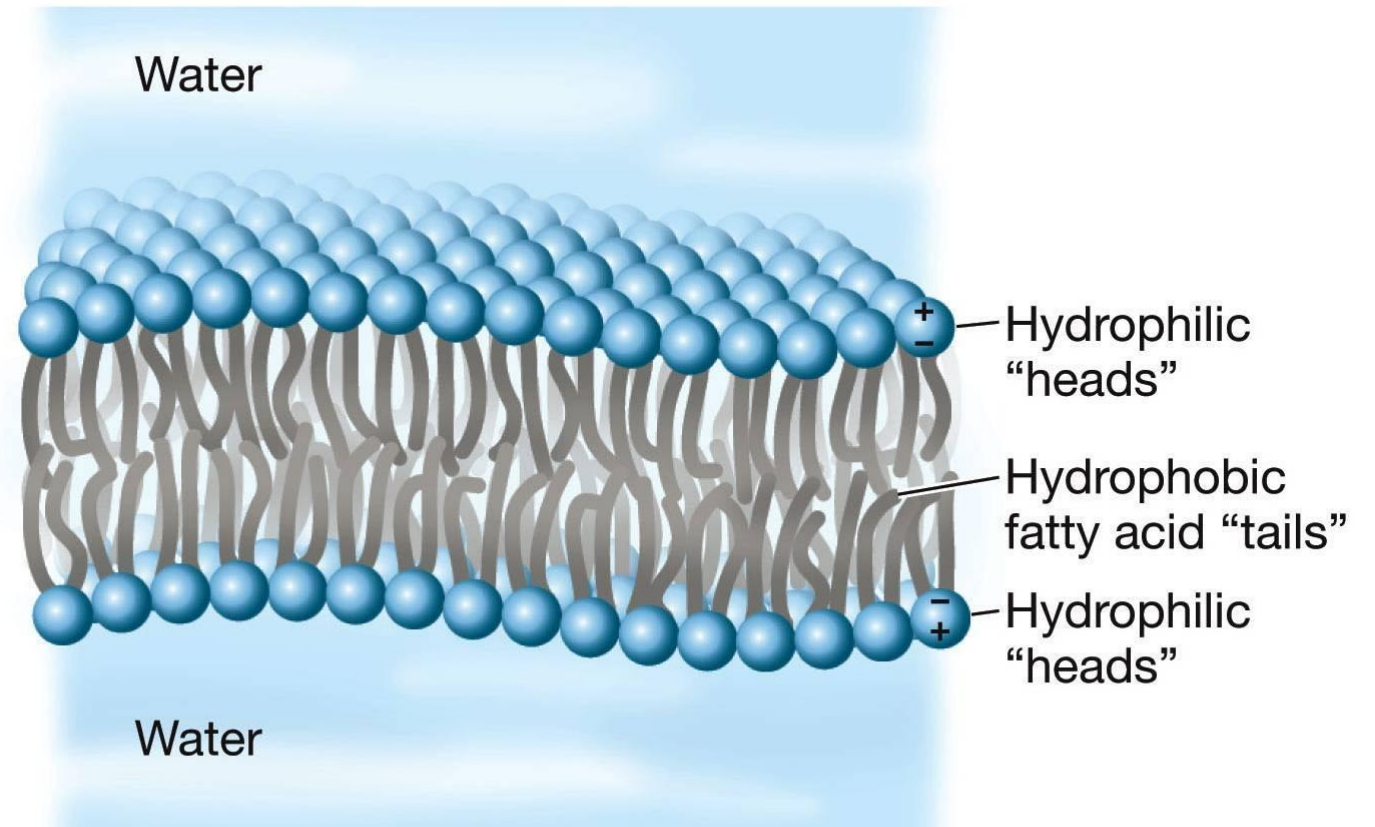


# Self Assembly

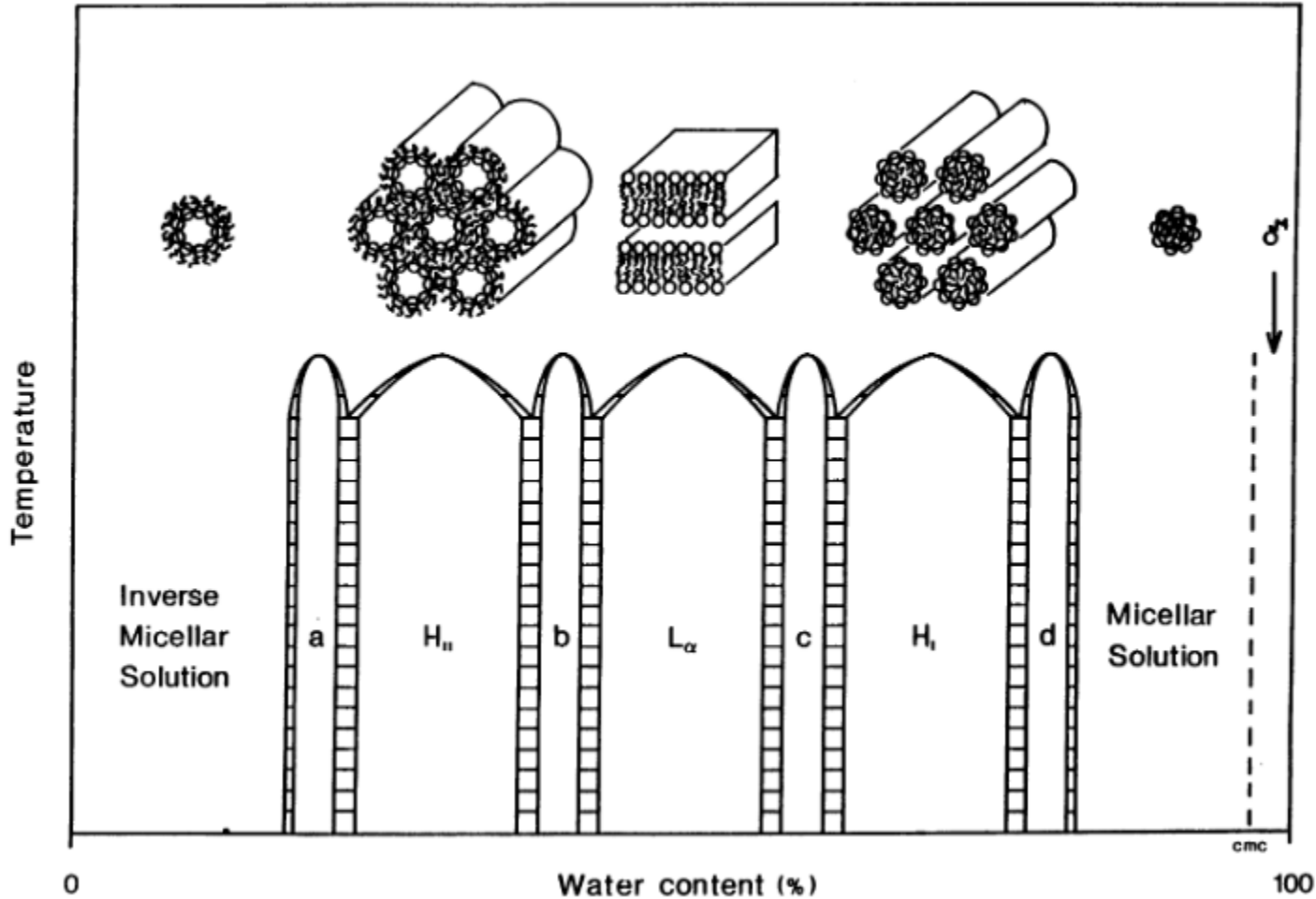


## (B) Phospholipid bilayer

- Well studied in phospholipids: hydrophilic heads and hydrophobic tails self assemble in an aqueous solution



# Self Assembly



*Shape of Nuclei in the Crust of Neutron Star*

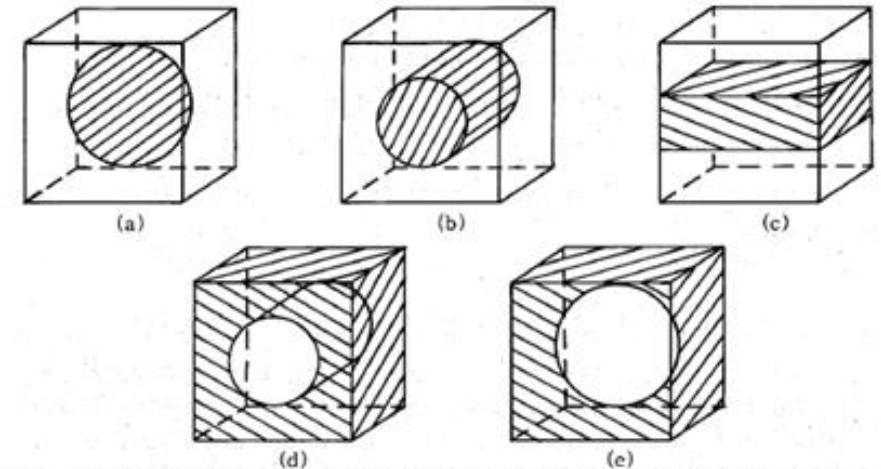
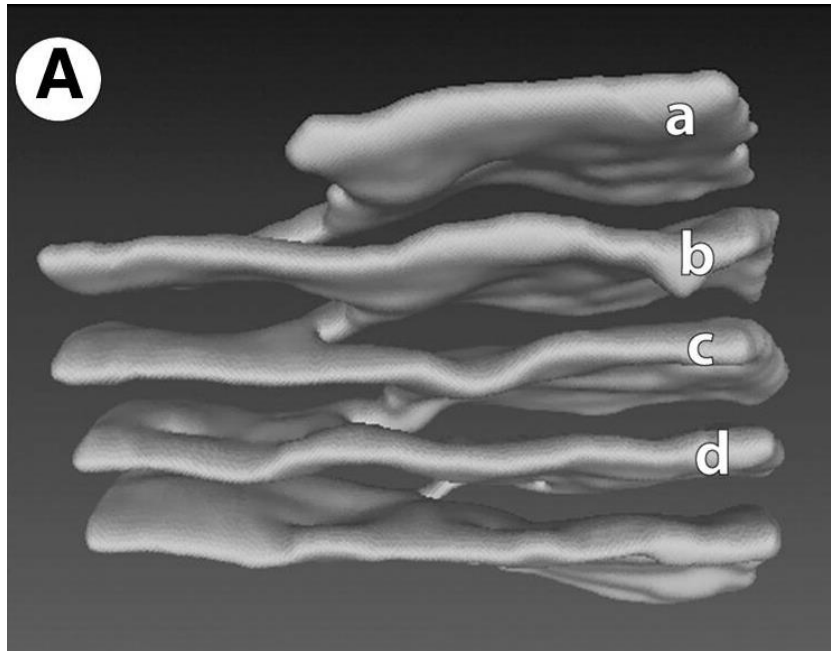


Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole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

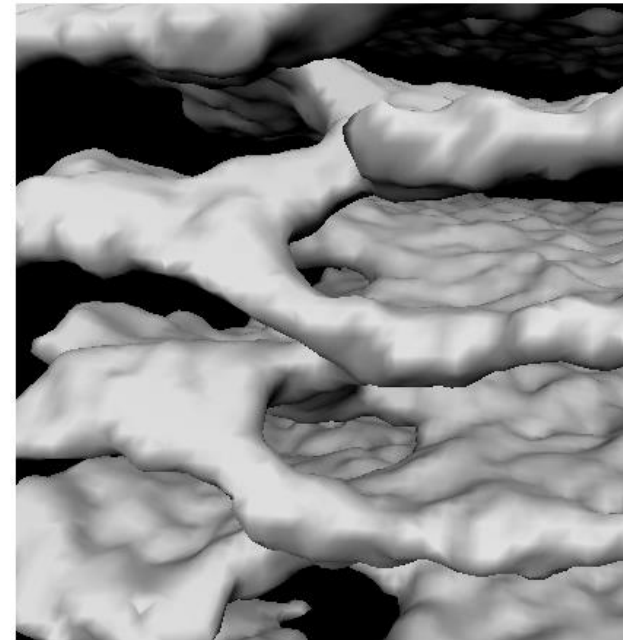
# Self Assembly



- Left: Electron microscopy of helicoids in mice endoplasmic reticulum



Terasaki et al, Cell 154.2 (2013)



Horowitz et al, PRL.114.031102 (2015)

- Right: Defects in nuclear pasta MD simulations

Parking Garage Structures in astrophysics and biophysics (arXiv:1509.00410)



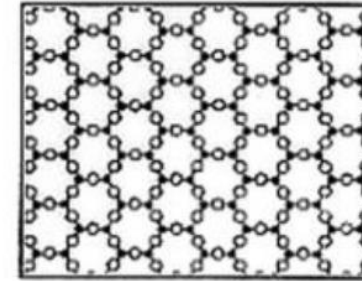
# Caloric Curve



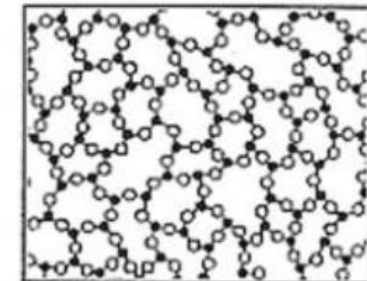
- Glass transition – impure substance forms an amorphous solid when quenched

- Solid:

- Long Range Order
- Nondiffusive
- First order phase transition



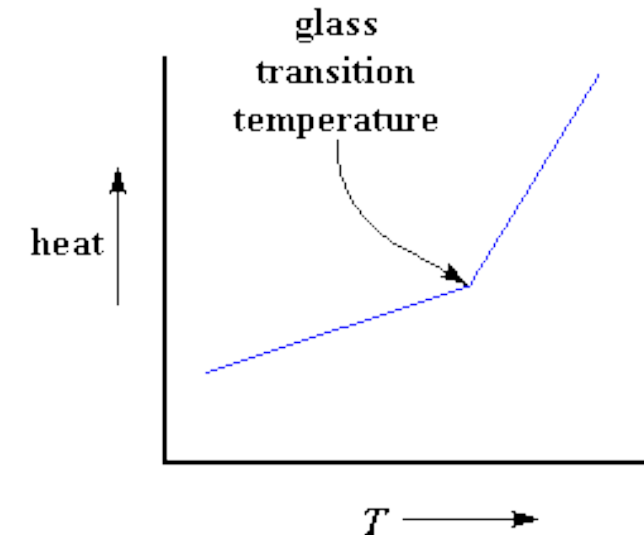
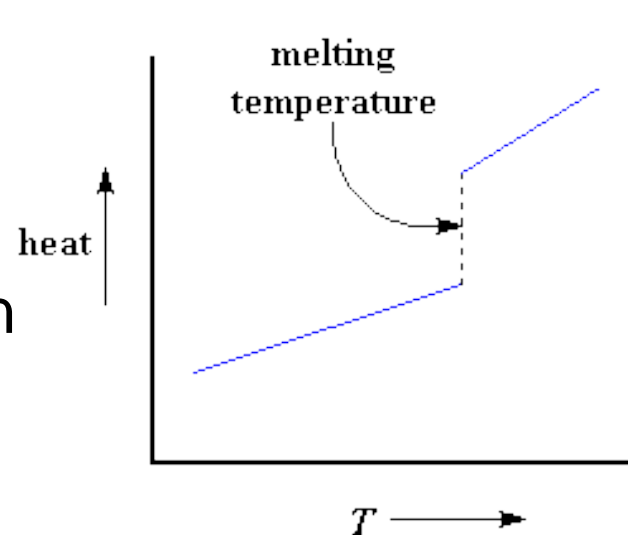
Crystal  
(e.g. quartz)



Glass  
(e.g. silica glass)

- Glass:

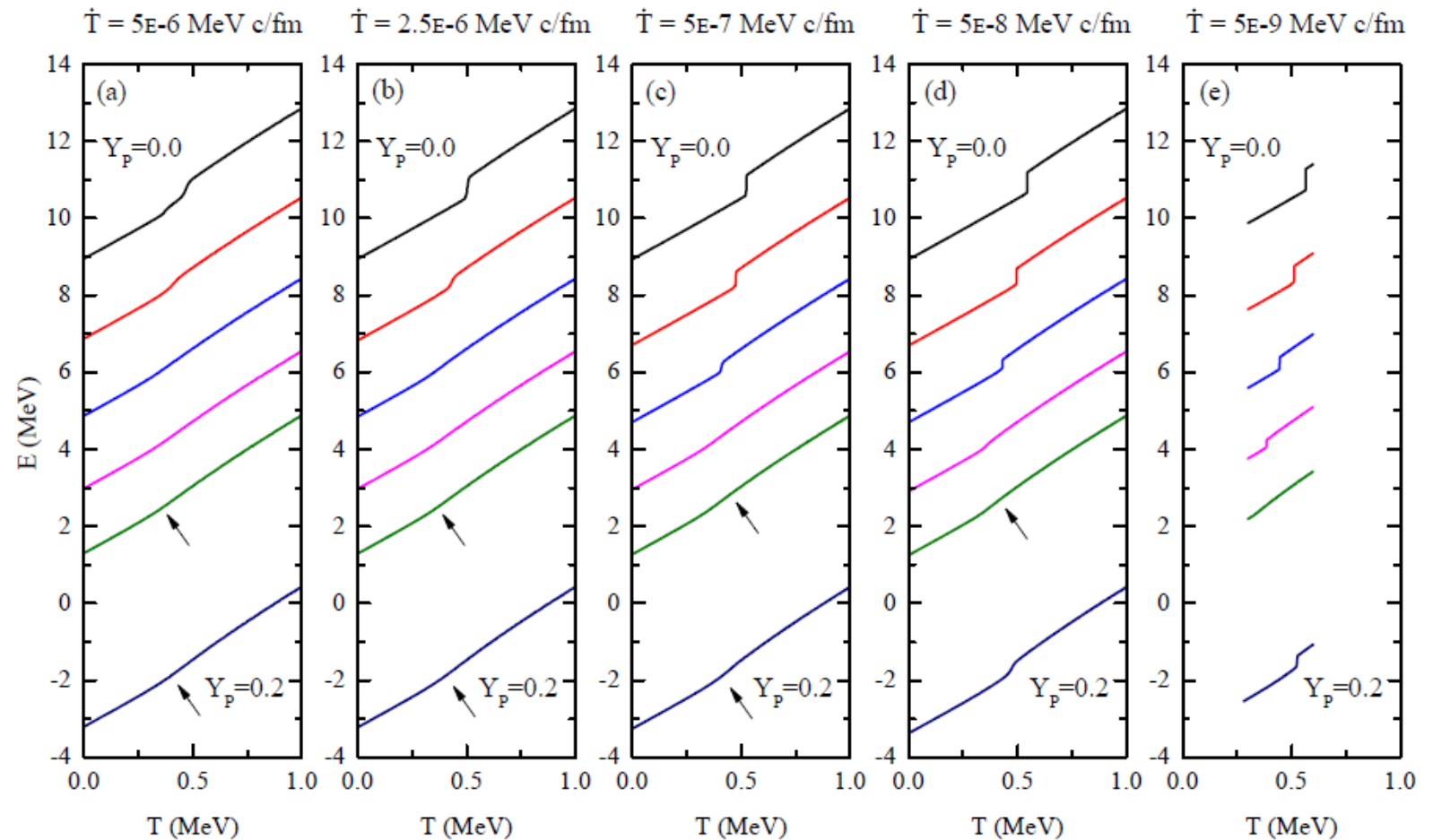
- Short range order
- Low diffusion
- Second order phase transition



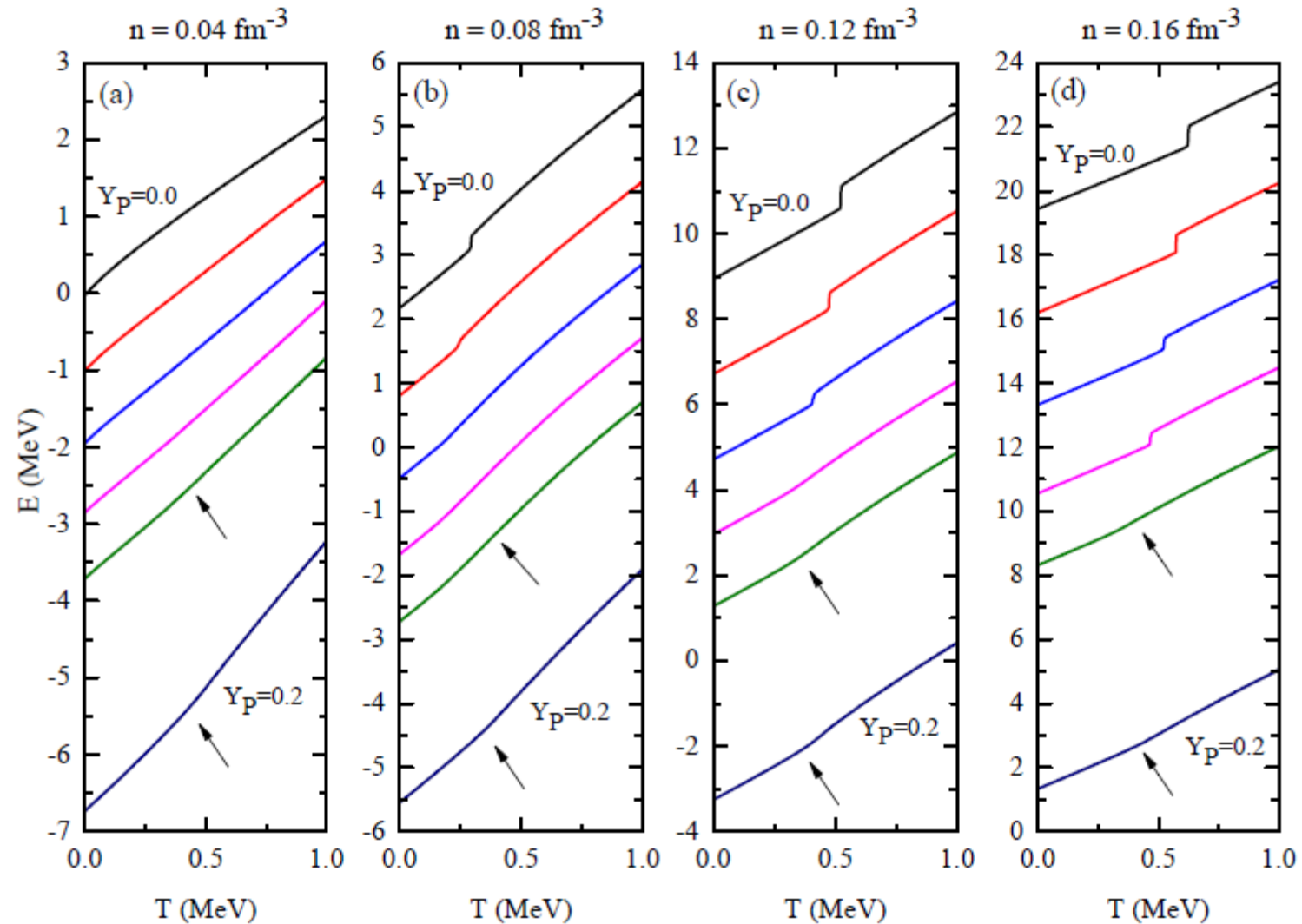
# Quench Rate



- Cooling quickly and cooling slowly
- Proton fractions:  $Y_p = 0.0 - 0.2$
- Density:  $n = 0.12 \text{ fm}^{-3}$



# Glassy Systems



Caplan et al (In Prep)

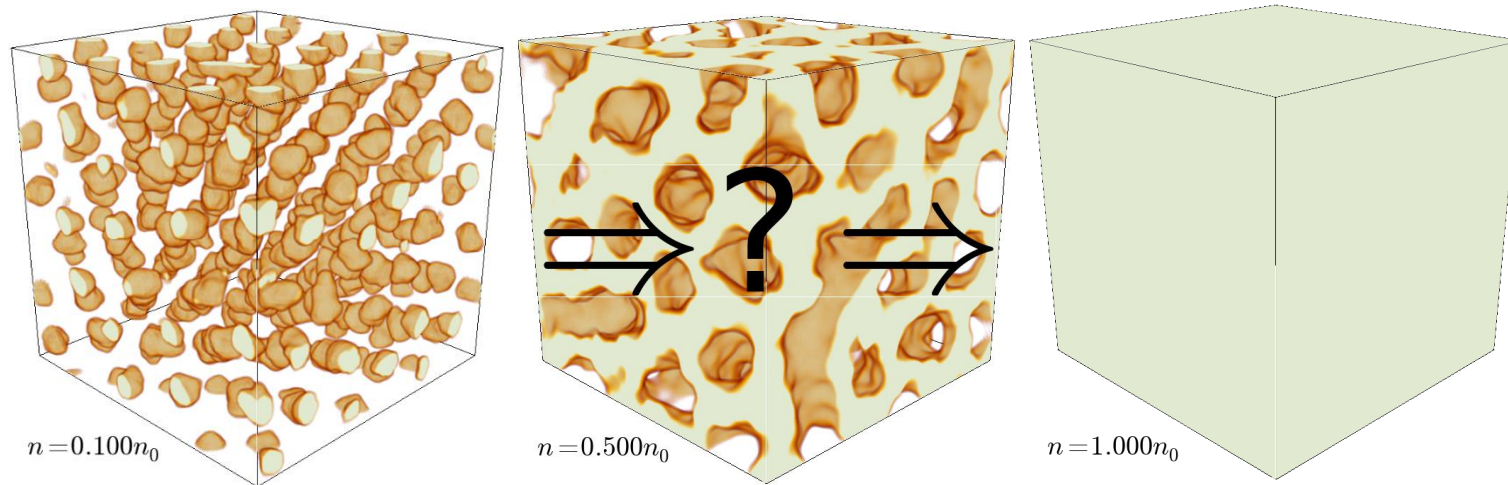
Observables



# Nuclear Pasta



- Important to many processes:
  - **Thermodynamics**: Late time crust cooling
  - **Magnetic field decay**: Electron scattering in pasta
  - **Gravitational wave amplitude**: Pasta elasticity and breaking strain
  - **Neutrino scattering**: Neutrino wavelength comparable to pasta spacing
  - **R-process**: Pasta is ejected in mergers



# Lepton Scattering

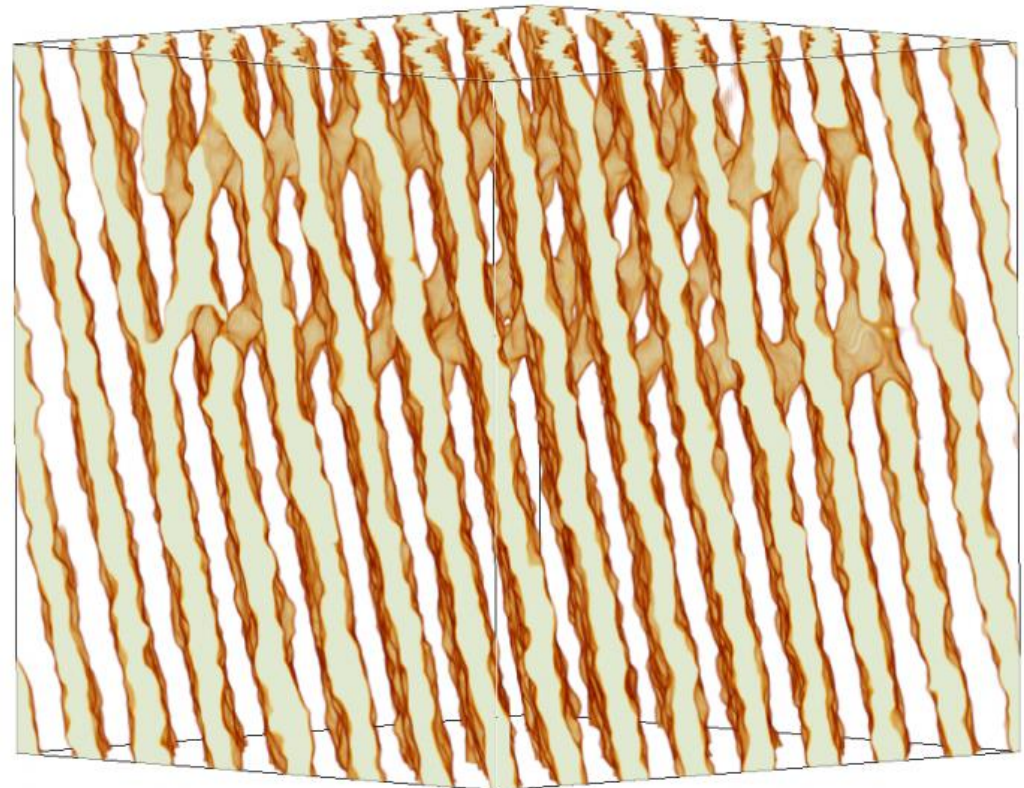
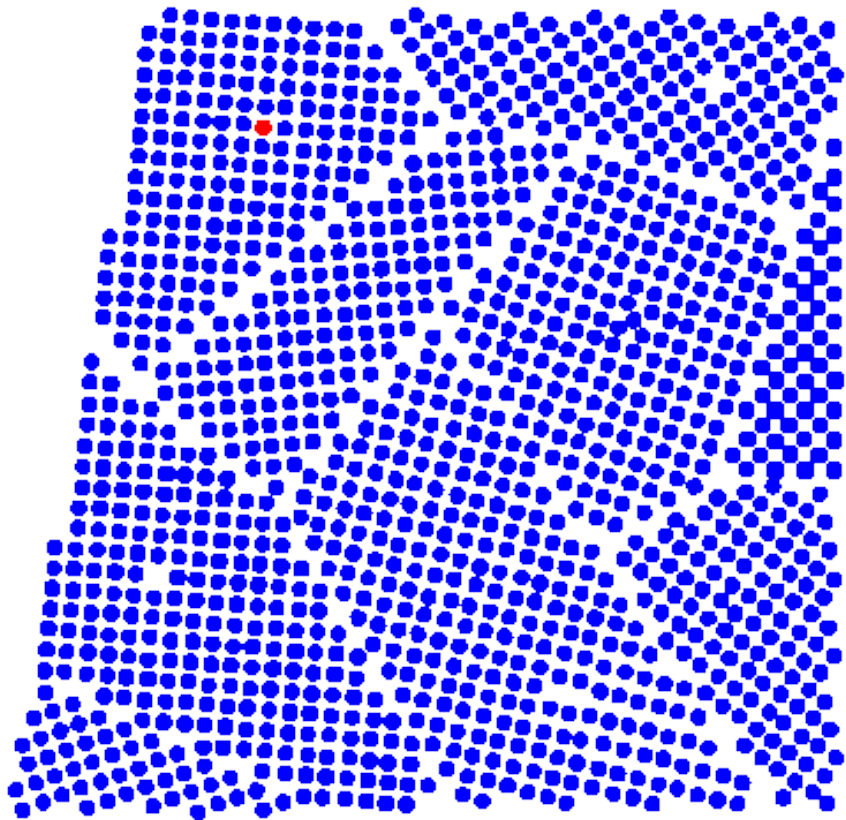


- Supernova: Hot, proton rich
  - Neutrino scattering?
- Neutron Stars: Cold, proton poor
  - Electron scattering?

# Defects



- In the same way that crystals have defects, pasta does too!
- Electrons don't scatter from *order*, they scatter from *disorder*

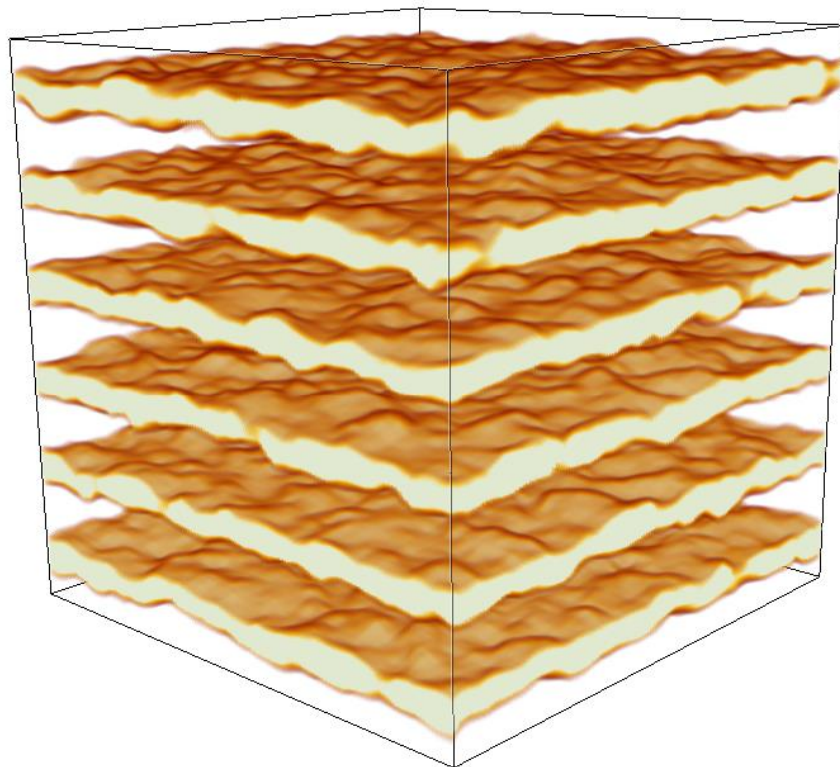


- Horowitz et al, PRL.114.031102 (2015)

# Pasta Defects

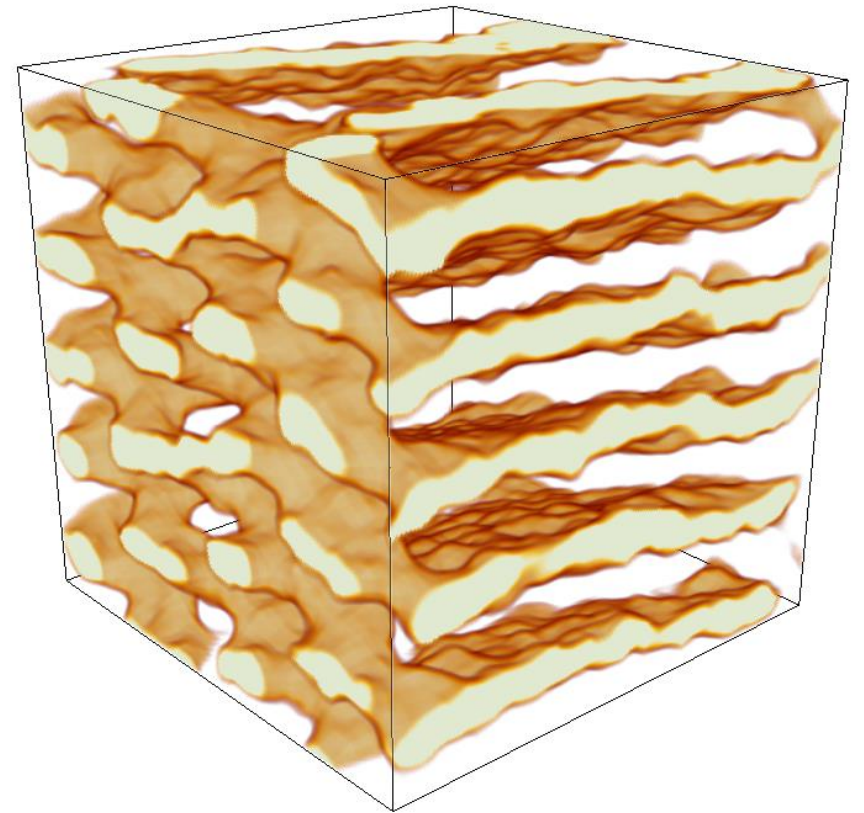


- Defects act as a site for *scattering*



← Perfect

Defects →

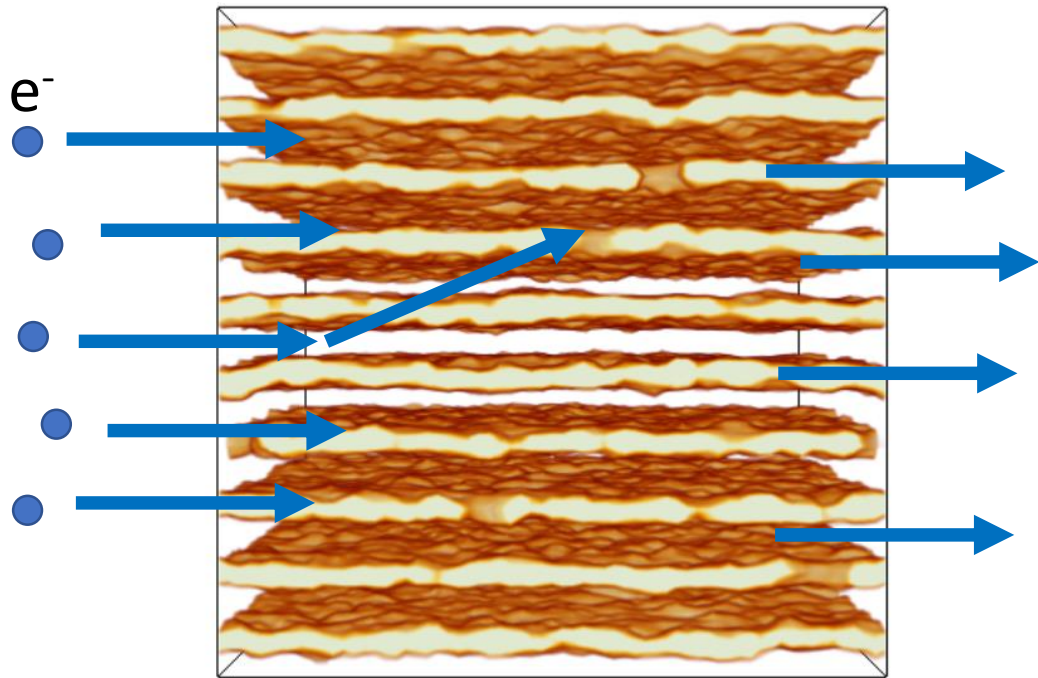




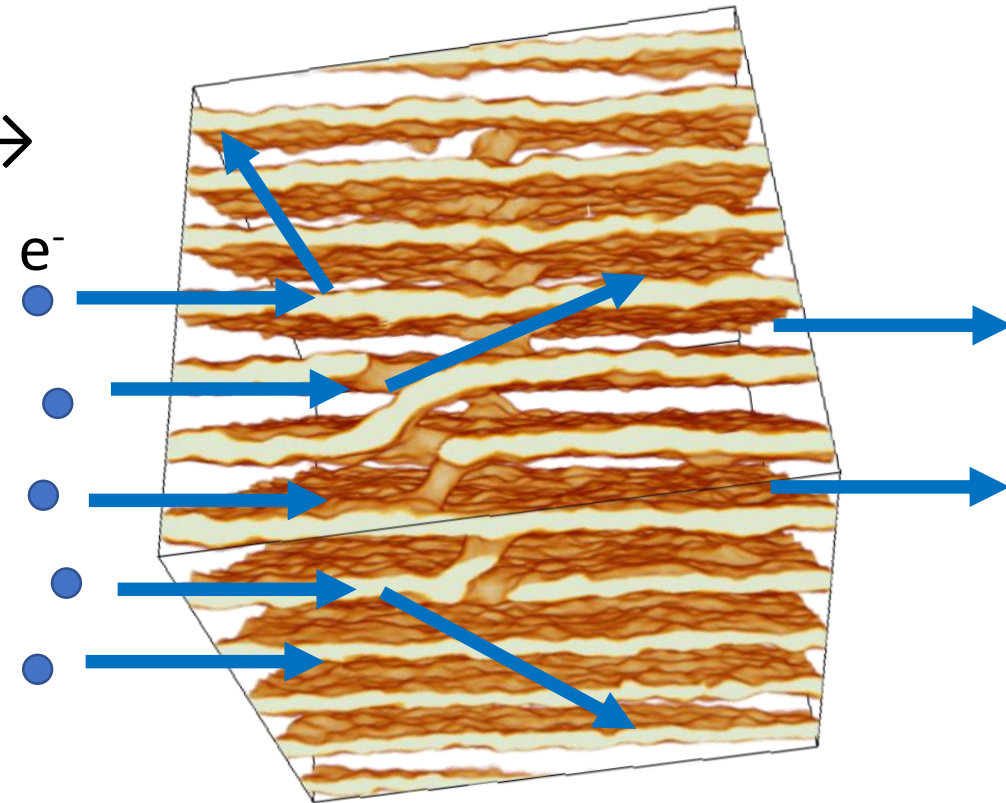
# Pasta Defects



- The magnetic field decays within about 1 million years, consistent with observations (Pons et al 2013)



← Perfect Defects →



# Lepton Scattering



- Lepton scattering from pasta influences a variety of transport coefficients:

- Shear viscosity:

$$\eta = \frac{\pi v_F^2 n_e}{20\alpha^2 \Lambda_{ep}^\eta},$$

- Electrical conductivity:

$$\sigma = \frac{v_F^2 k_F}{4\pi\alpha \Lambda_{ep}^\sigma} \quad \Lambda_{ep}^\eta = \int_0^{2k_F} \frac{dq}{q\epsilon^2(q)} \left(1 - \frac{q^2}{4k_F^2}\right) \left(1 - \frac{v_F^2 q^2}{4k_F^2}\right) S_p(q)$$

- Thermal conductivity:

$$\kappa = \frac{\pi v_F^2 k_F k_B^2 T}{12\alpha^2 \Lambda_{ep}^\kappa} \quad \Lambda_{ep}^\kappa = \Lambda_{ep}^\sigma = \int_0^{2k_F} \frac{dq}{q\epsilon^2(q)} \left(1 - \frac{v_F^2 q^2}{4k_F^2}\right) S_p(q).$$

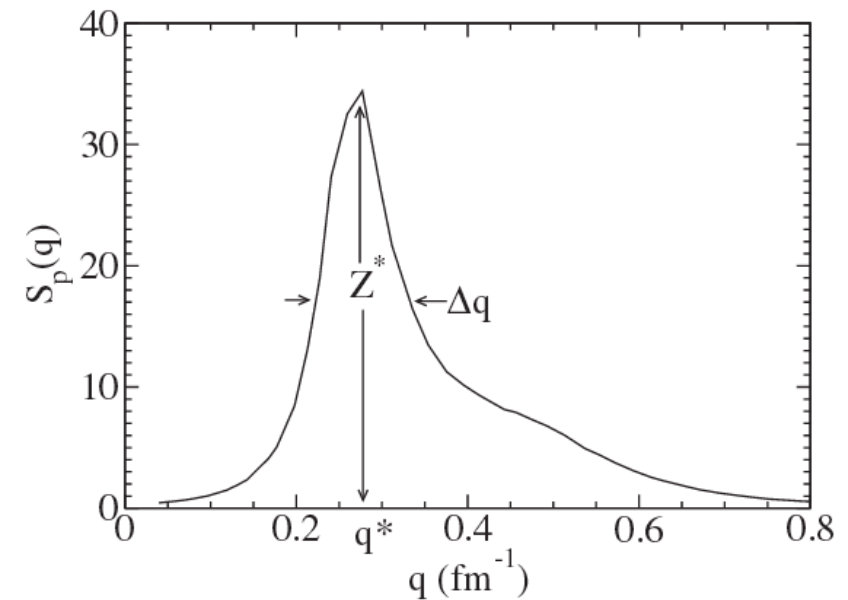
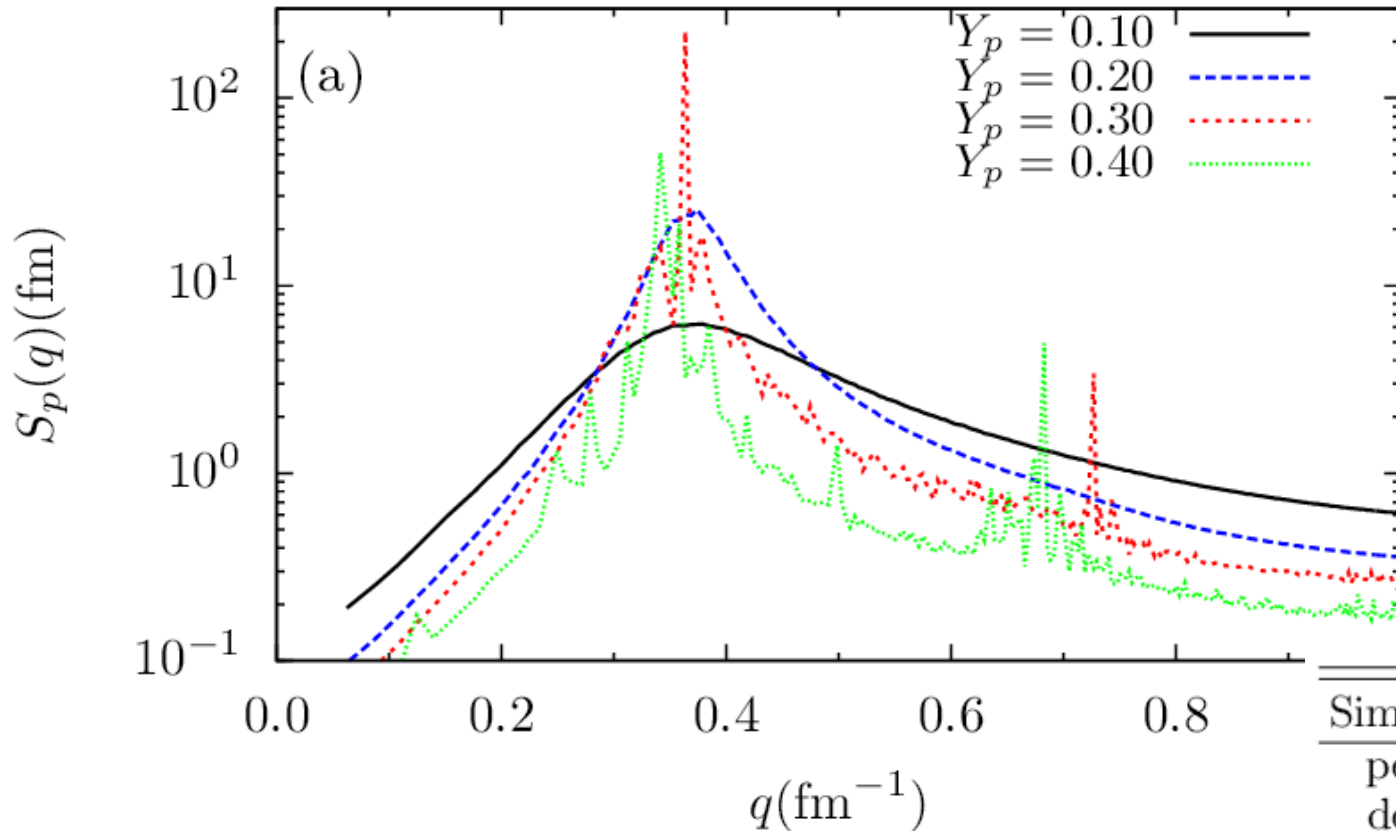
# Lepton Scattering



$$S_i(\mathbf{q}) = \langle \rho_i^*(\mathbf{q}, t) \rho_i(\mathbf{q}, t) \rangle_t - \langle \rho_i^*(\mathbf{q}, t) \rangle_t \langle \rho_i(\mathbf{q}, t) \rangle_t$$

$$\rho_i(\mathbf{q}, t) = N_i^{-1/2} \sum_{j=1}^{N_i} e^{i\mathbf{q} \cdot \mathbf{r}_j(t)}$$

$$\Lambda_{ep} \approx \frac{\Delta q^* Z^*}{q^*}$$



Simulation	$\bar{n}$ ( $\text{fm}^{-3}$ )	$\bar{\kappa}$ ( $10^3 k_B \text{ MeV}/\text{fm}$ )	$\bar{Z}^*$
perfect	87.7	6.66	5.5
defects	55.5	4.15	50.2

Crust Cooling

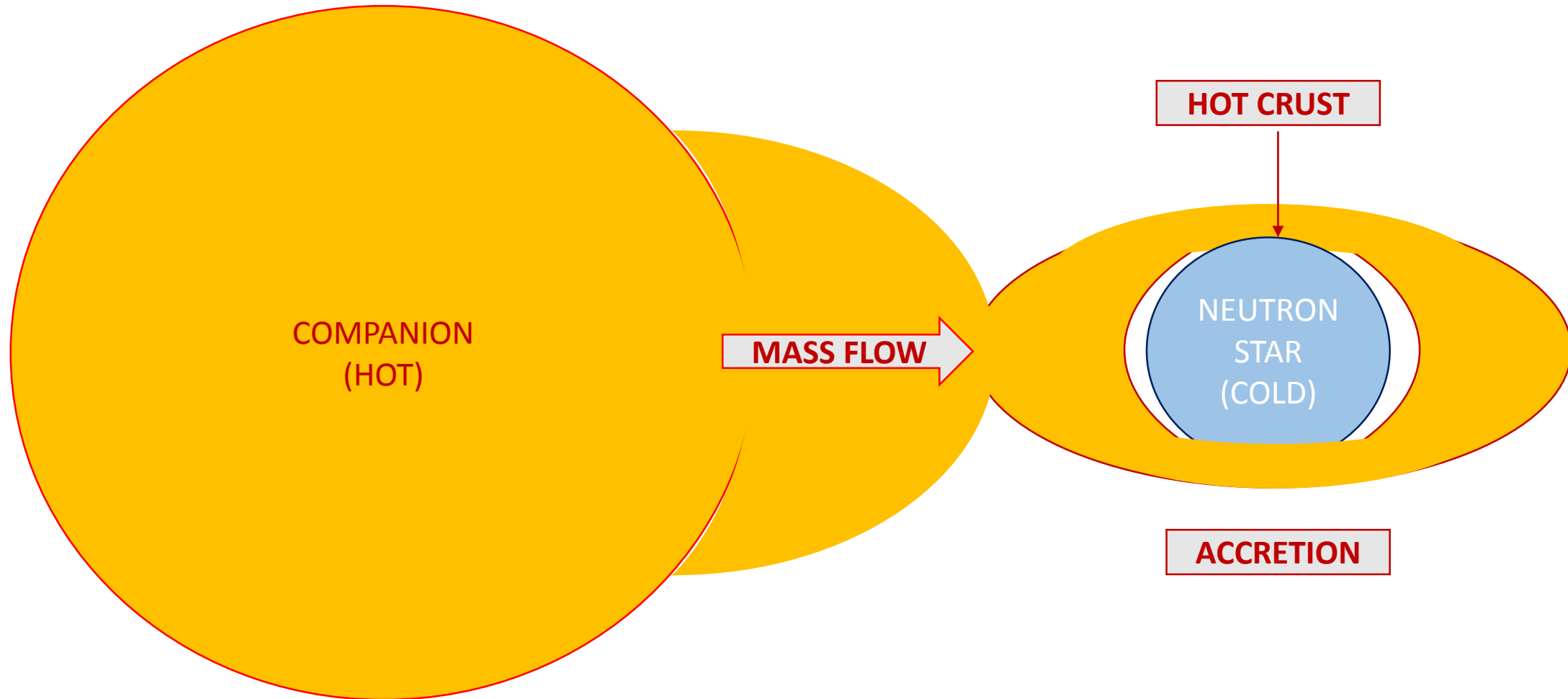


# Thermal Resistivity

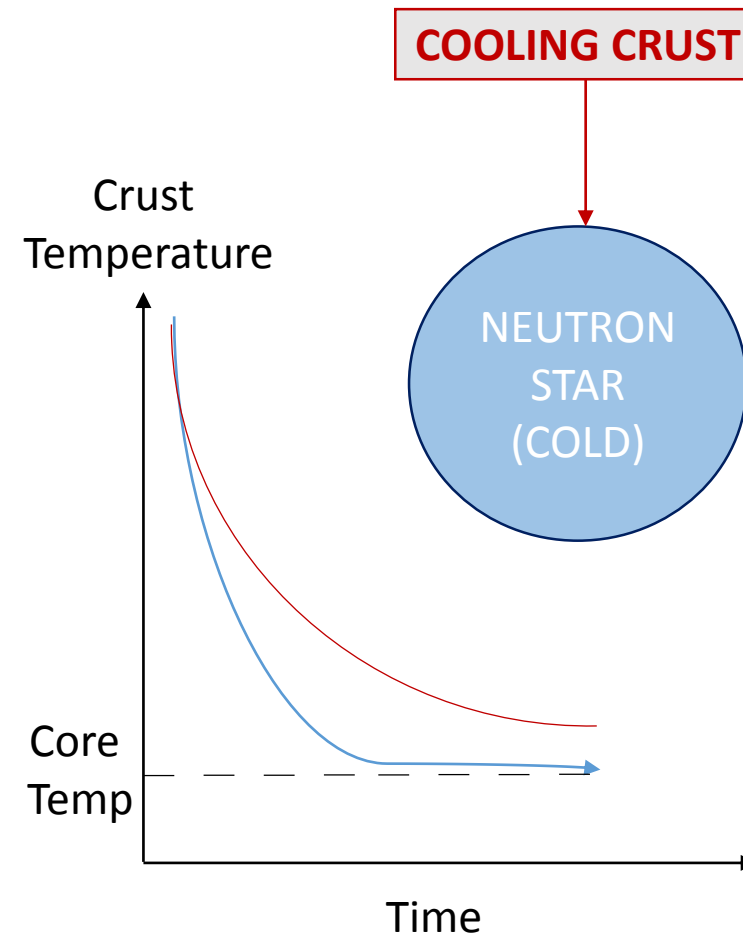
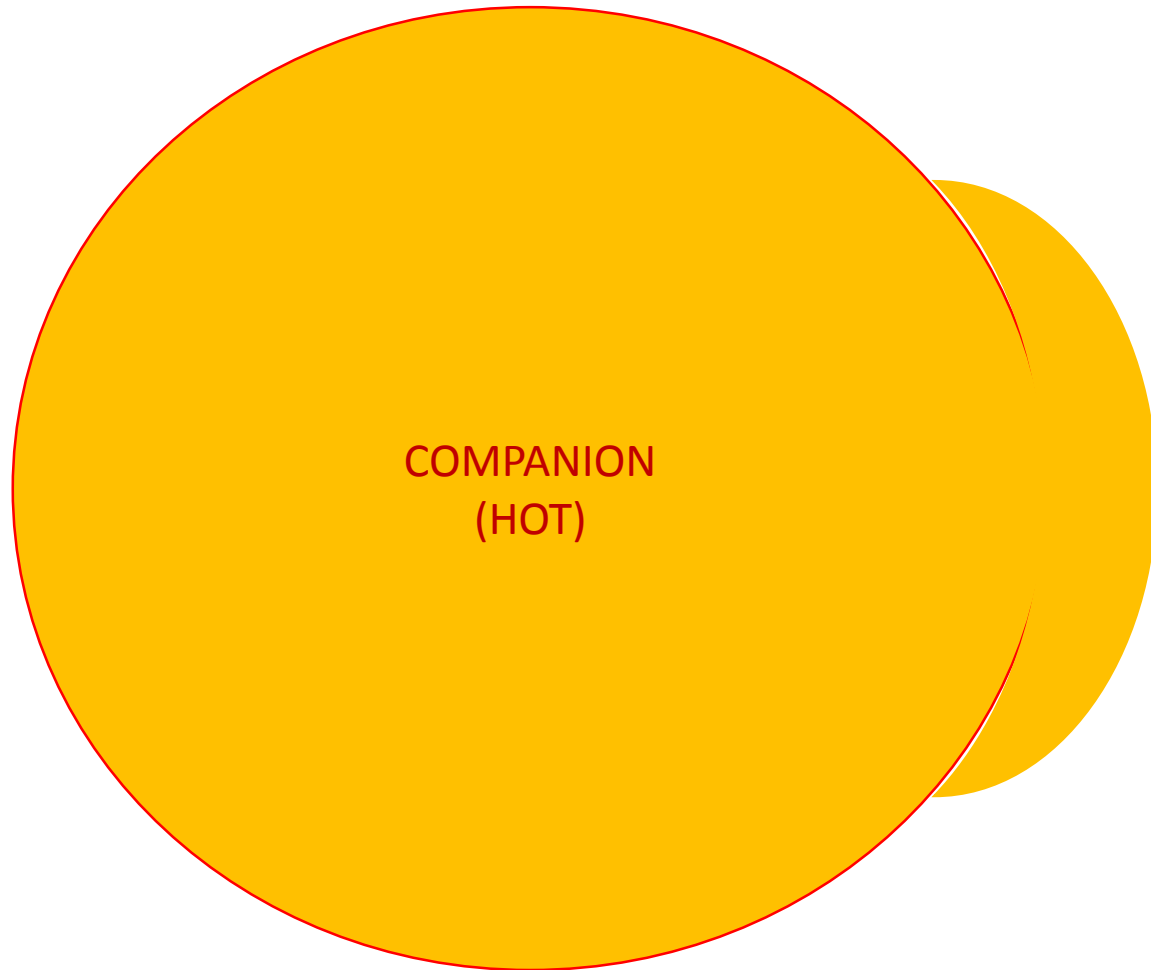


- So we've seen that pasta is electrically resistive...
- Electrons are a thermal carrier too! How does poor *thermal* conductivity effect the neutron star?

# Low Mass X-Ray Binaries



# Low Mass X-Ray Binaries



# Observables – Thermal Properties



- Guess an effective impurity parameter for defects and try to fit neutron star cooling curves
- Cooling curves: low mass X-ray binary MXB 1659-29

$$Q_{\text{imp}} \equiv n_{\text{ion}}^{-1} \sum_i n_i (Z_i - \langle Z \rangle)^2$$

- **Blue**: normal isotropic matter

$$Q_{\text{imp}} = 3.5$$

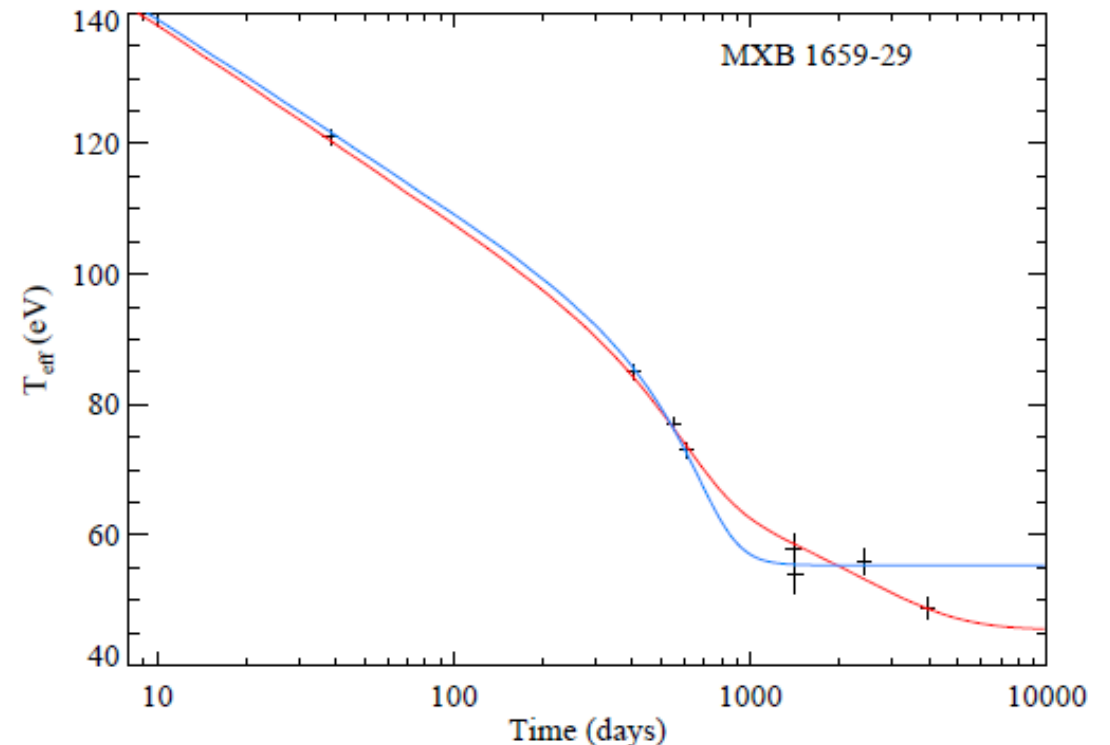
$$T_c = 3.05 \times 10^7 \text{ K}$$

- **Red**: impure pasta layer

$$Q_{\text{imp}} = 1.5 \text{ (outer crust)}$$

$$Q_{\text{imp}} = 30 \text{ (inner crust)}$$

$$T_c = 2 \times 10^7 \text{ K}$$





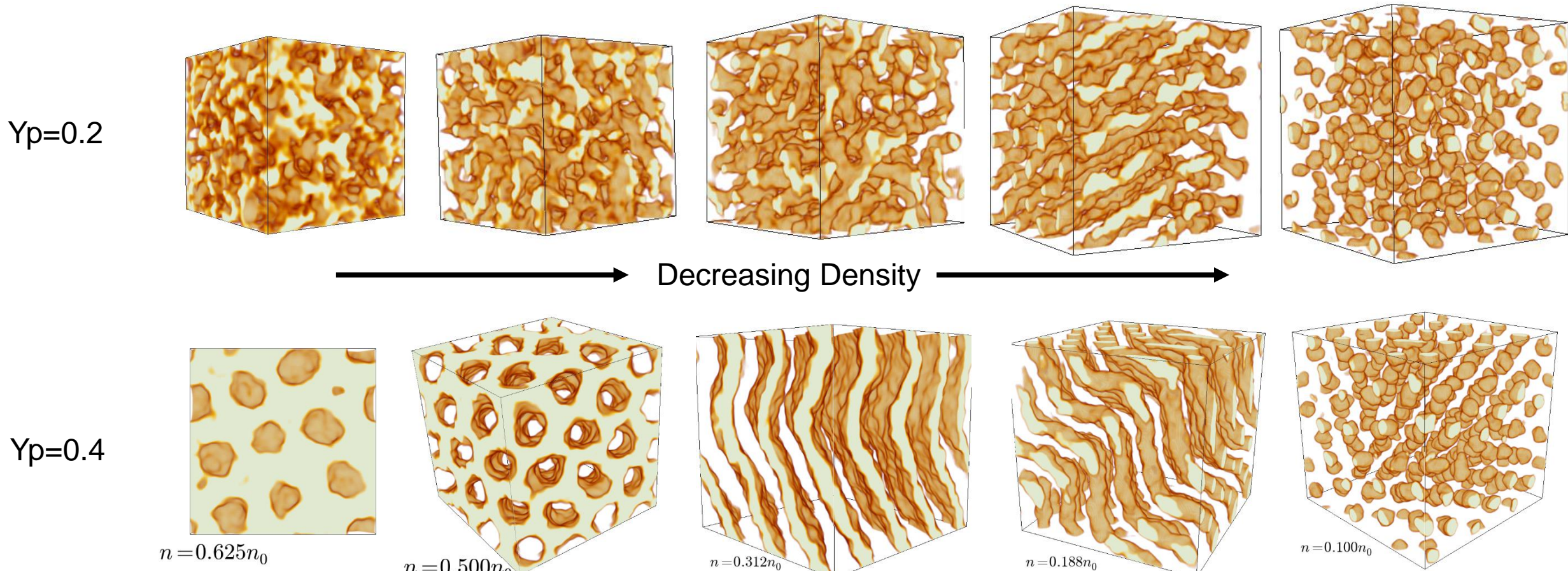
r-process

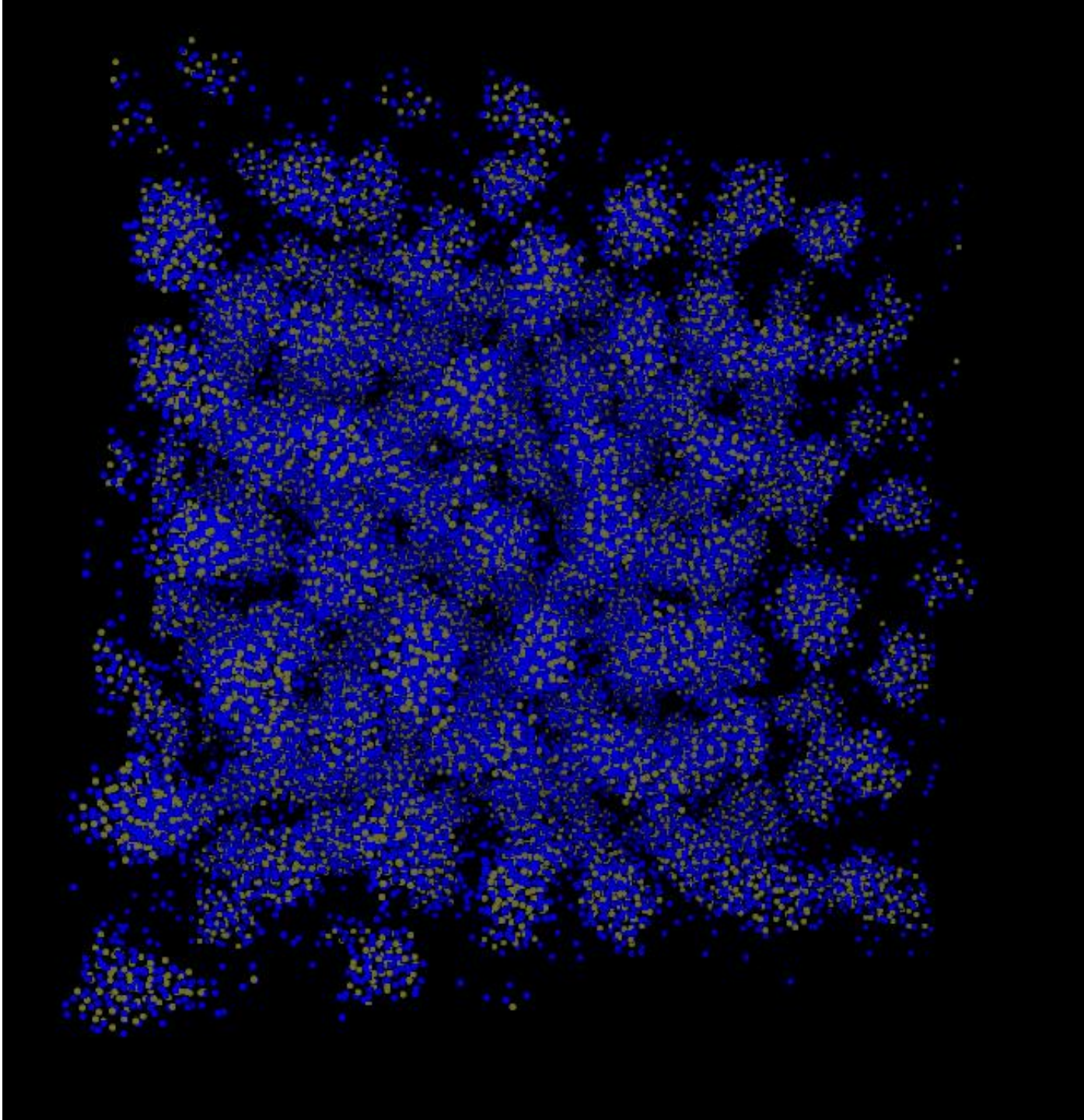


# Fragmentation



- Simulate pasta with constant temperature and proton fraction
- Observe 'nuclei' that form as pasta decompresses

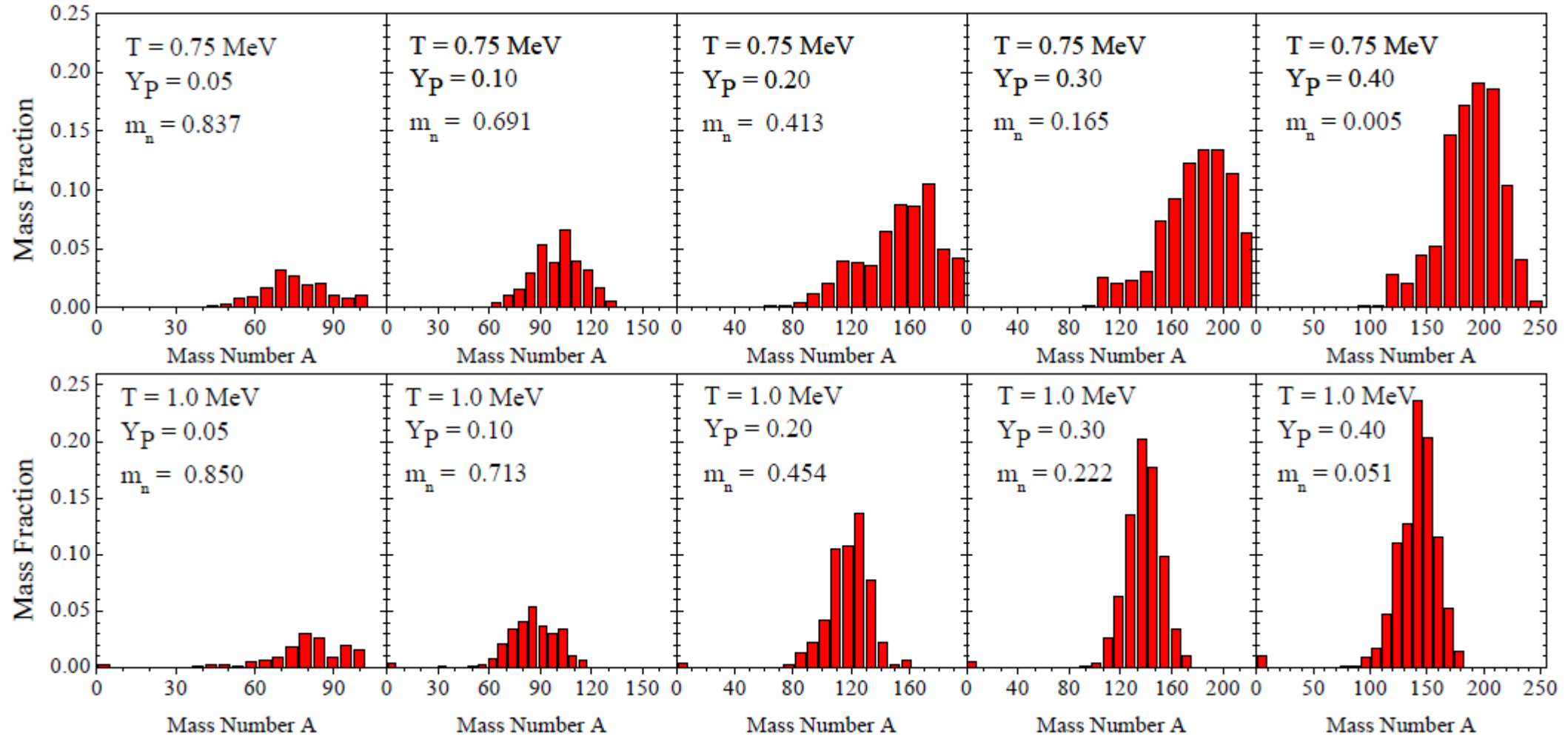




# Cluster Masses



Caplan (2015) Phys. Rev. C 91, 065802



# Nuclear Statistical Equilibrium



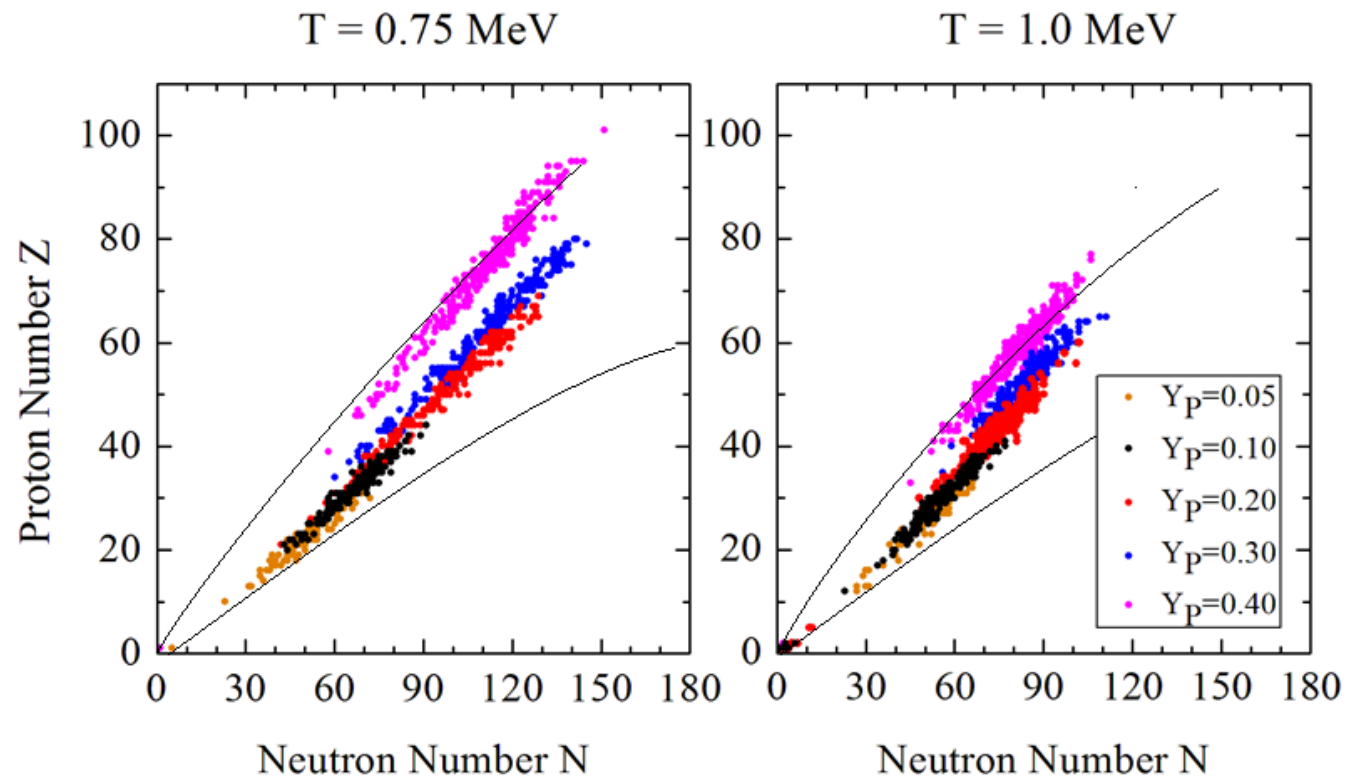
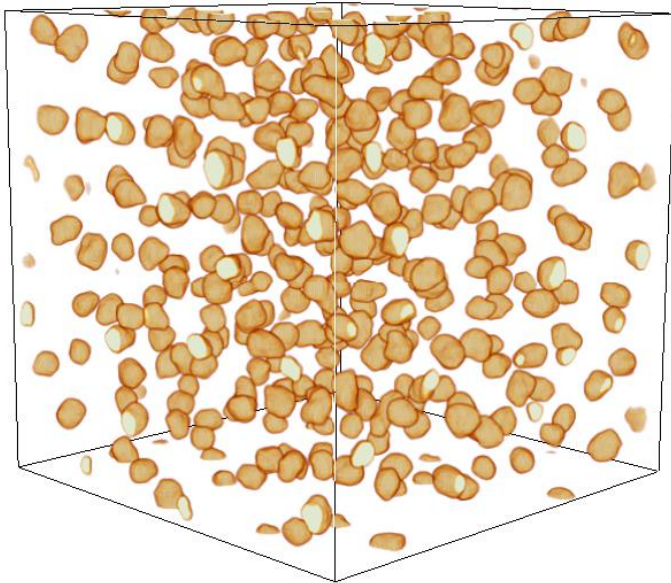
- Use a cluster algorithm to count A, Z of gnocchi
- Simulations at 1 MeV reproduce NSE for sufficiently slow evolution!

$Y_P$	$\log_{10} \dot{\xi}$	$M_{\text{free neutrons}}$	IUMD		$M_{\text{free neutrons}}$	NSE	
			$\bar{A} \pm \sigma_A$	$\bar{Z} \pm \sigma_Z$		$\bar{A}$	$\bar{Z}$
0.1	-5	0.6538	$90.12 \pm 24.20$	$26.25 \pm 7.69$	Unavailable		
	-6	0.6561	$94.08 \pm 18.01$	$27.57 \pm 5.69$			
	-7	0.6578	$99.18 \pm 17.42$	$29.20 \pm 5.57$			
0.2	-5	0.3748	$147.75 \pm 33.88$	$47.31 \pm 10.95$	0.3335	179.3	53.80
	-6	0.3731	$146.22 \pm 24.96$	$46.69 \pm 8.30$			
	-7	0.3704	$136.12 \pm 20.32$	$43.29 \pm 6.72$			
0.3	-5	0.1359	$186.47 \pm 73.19$	$64.75 \pm 24.59$	0.0475	184.4	58.07
	-6	0.1377	$175.13 \pm 34.48$	$60.94 \pm 12.16$			
	-7	0.1367	$166.74 \pm 34.71$	$57.95 \pm 12.44$			
0.4	-5	0.0109	$369.37 \pm 426.03$	$149.32 \pm 167.45$	0.0001	194.4	77.75
	-6	0.0121	$179.40 \pm 29.83$	$72.64 \pm 11.93$			
	-7	0.0115	$190.25 \pm 29.34$	$76.94 \pm 11.83$			
	-8	0.0111	$191.74 \pm 24.55$	$77.55 \pm 9.79$			

# Table of Nuclides



- Nuclear pasta simulations at constant proton fraction reproduce nuclear statistical equilibrium:
- Right distribution of isotopes and number of free neutrons for a given  $T$



# Summary



- Classical models give reasonable results, provided you stay in the range they are valid
- They can inform transport properties of the neutrino star crust, and be used to interpret neutron star observables.