# Astromaterial Science

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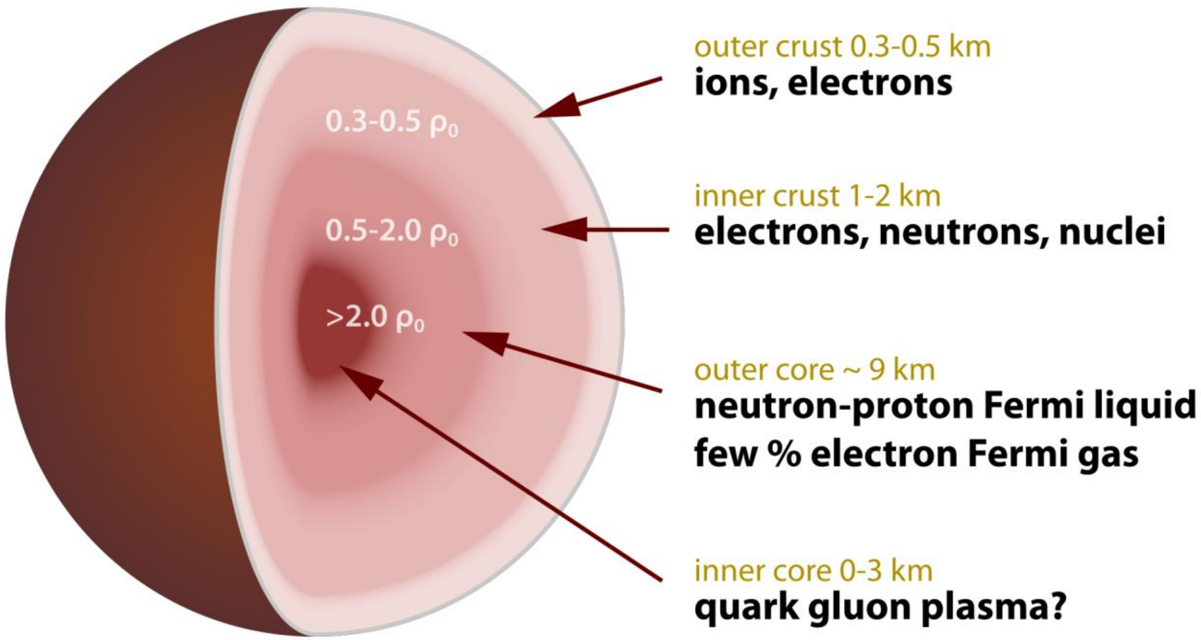
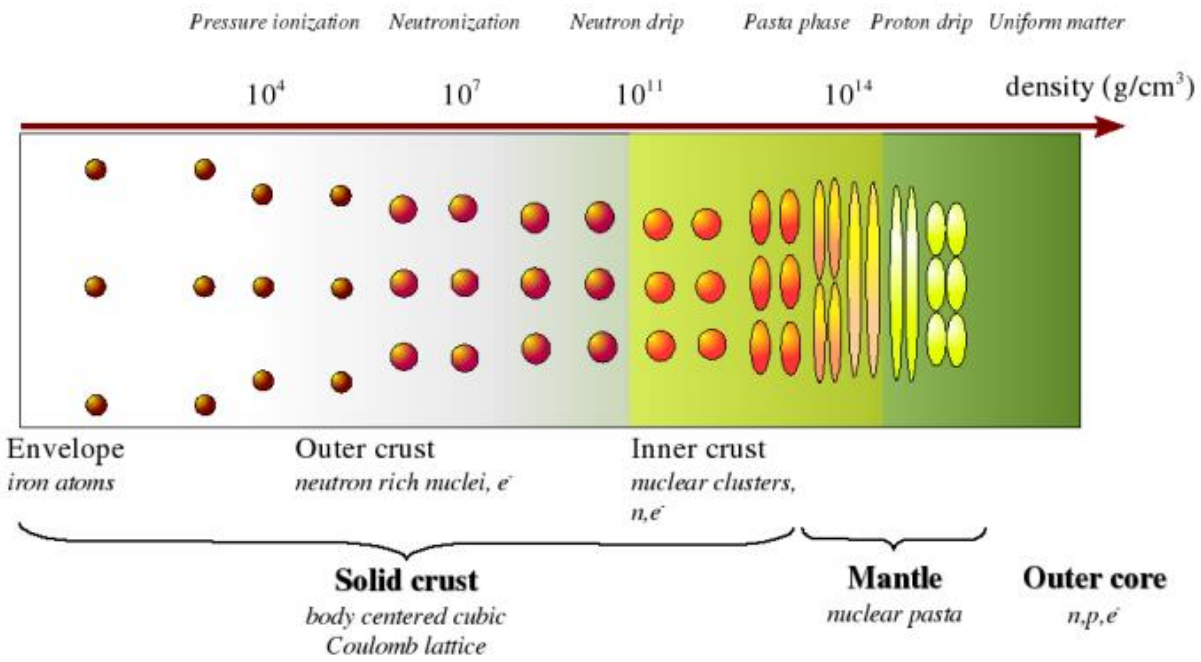
U.S. DEPARTMENT OF ENERGY | Office of Science
NUCLEI Nuclear Computational Low-Energy Initiative
INDIANA UNIVERSITY

# Neutron Star Structure

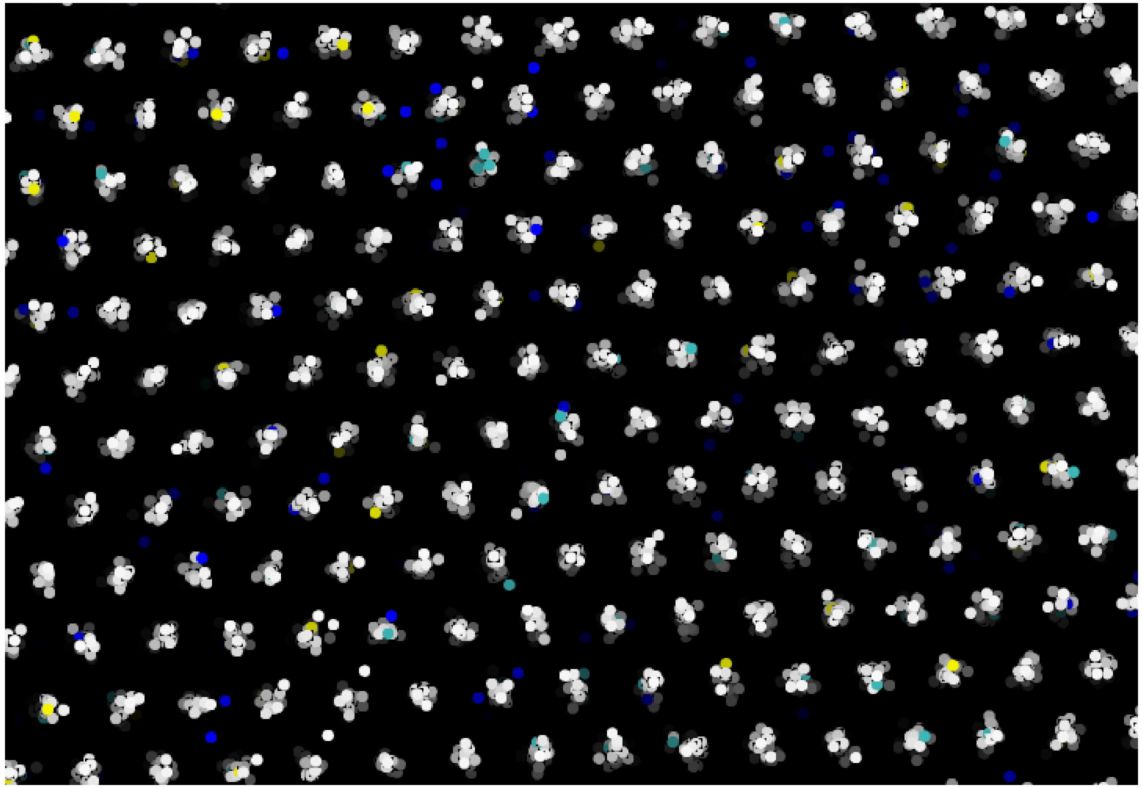
- What's inside a neutron star?



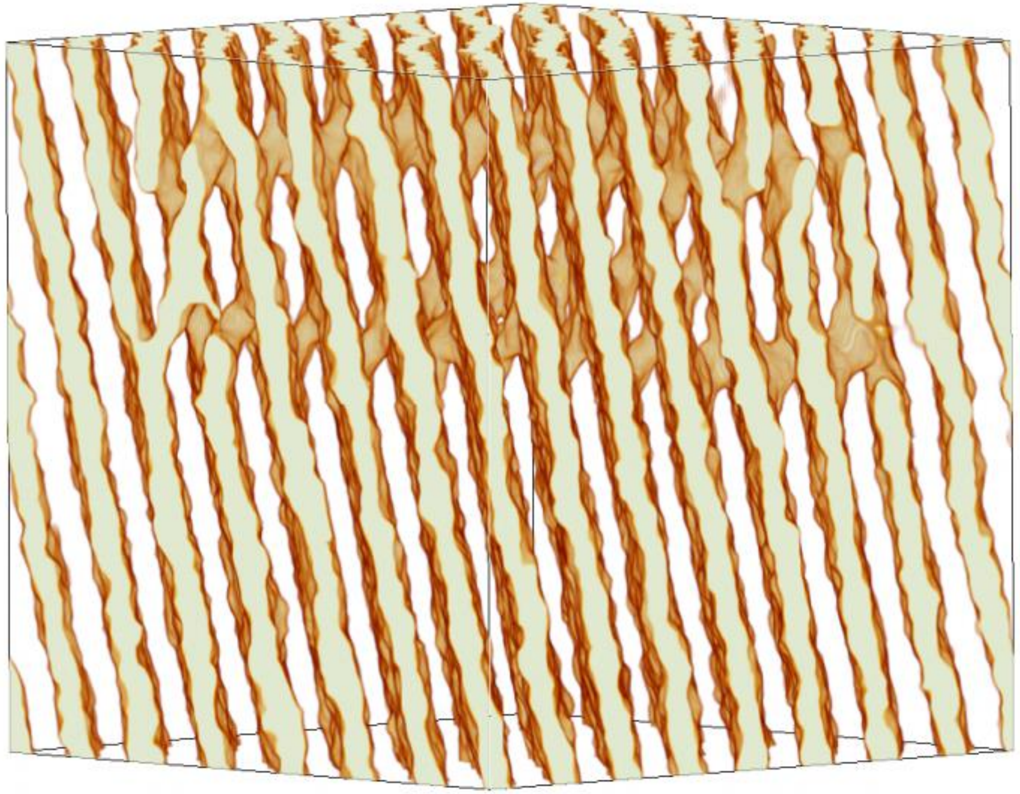



# Astromaterials

- Stars freeze. But not all stars. Only parts of some stars freeze.



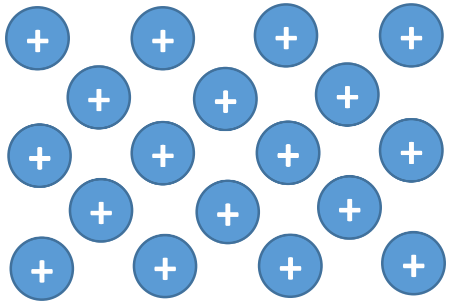
HARD

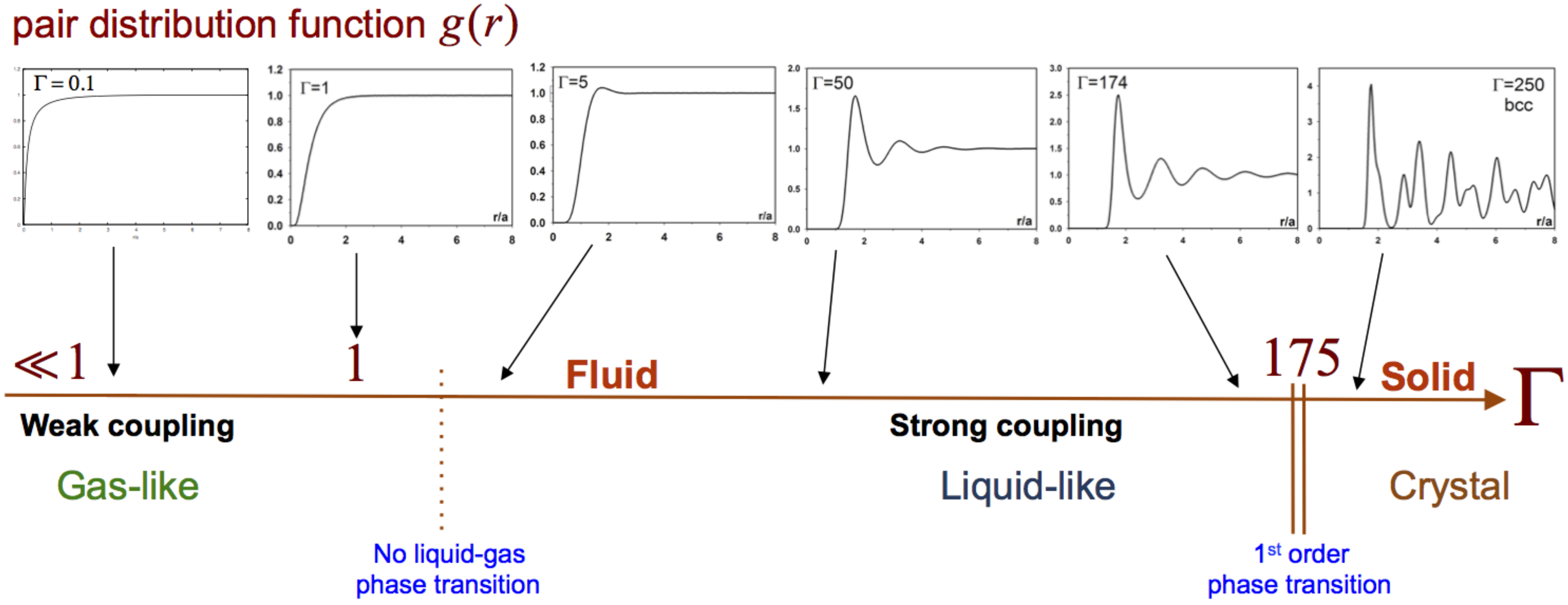


SOFT

# Hard Astromaterials

- "Coulomb Crystal" – Fully ionized nuclei embedded in a degenerate electron gas
- Simplest example: One component plasma






$$\Gamma = \frac{Coulomb}{Thermal}$$

Image Credit: LANL

# Hard Astromaterials

- "Coulomb Crystal" – Fully ionized nuclei embedded in a degenerate electron gas
- Simplest example:
  One component plasma
  - $Z$ = Ion Charge
  - $a$ = Ion sphere radius ($\sim n^{-1/3}$)
  - $T$ = Temperature

$$\Gamma = \frac{Coulomb}{Thermal} \qquad \Gamma = \frac{Z^2 e^2}{aT}$$

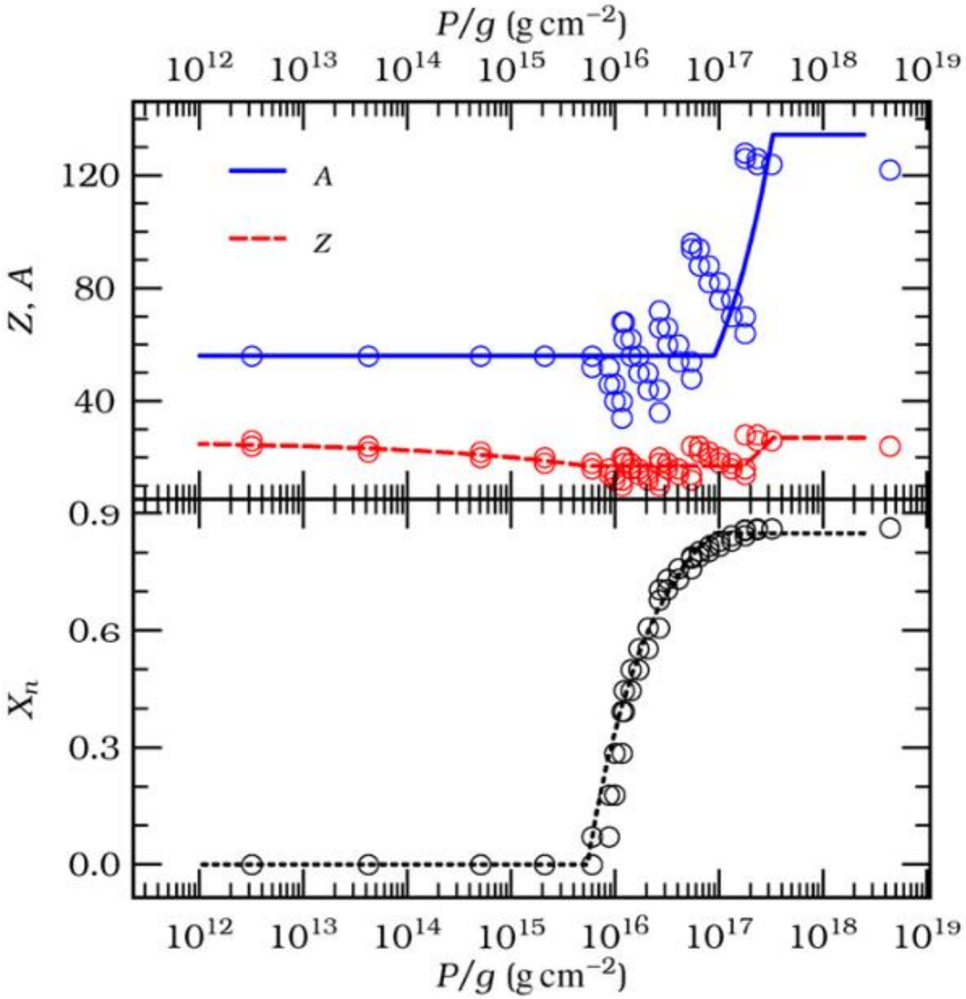
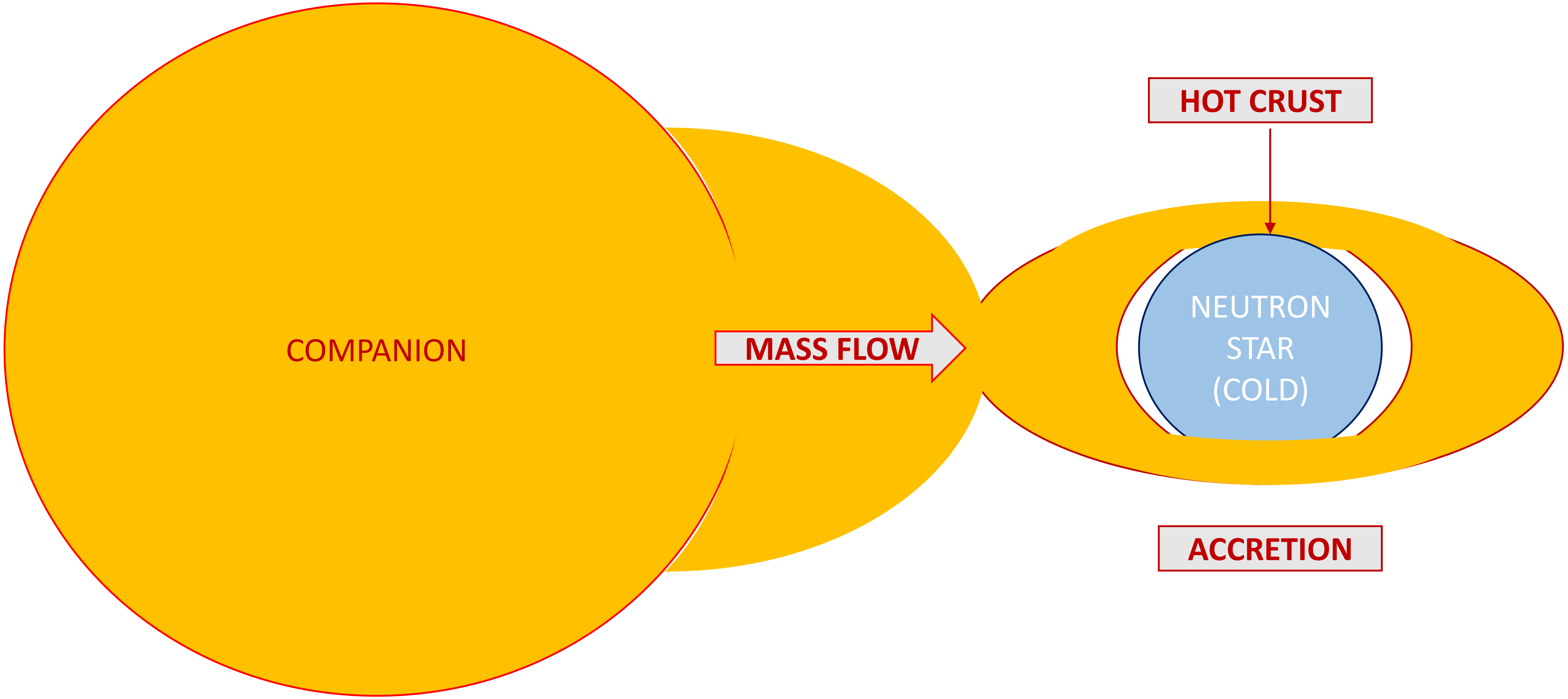


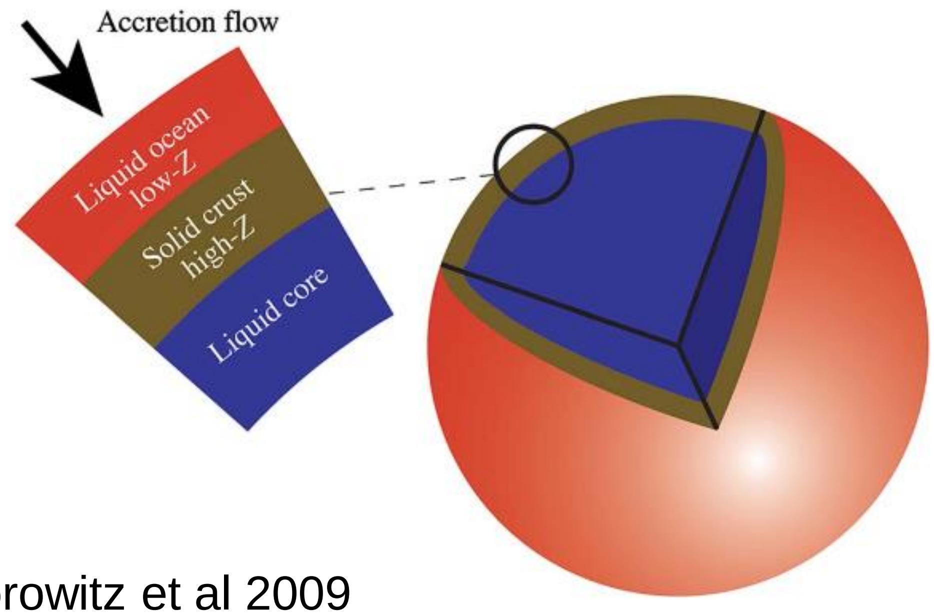

Image Credit: Brown & Cumming 2009

# Low Mass X-Ray Binaries



# X-ray bursts

- As matter accretes, it is compressed, buried, and heated
- Explosive nuclear burning produces a mix of heavy nuclei (rp-process)
- Phase separation sets crust composition



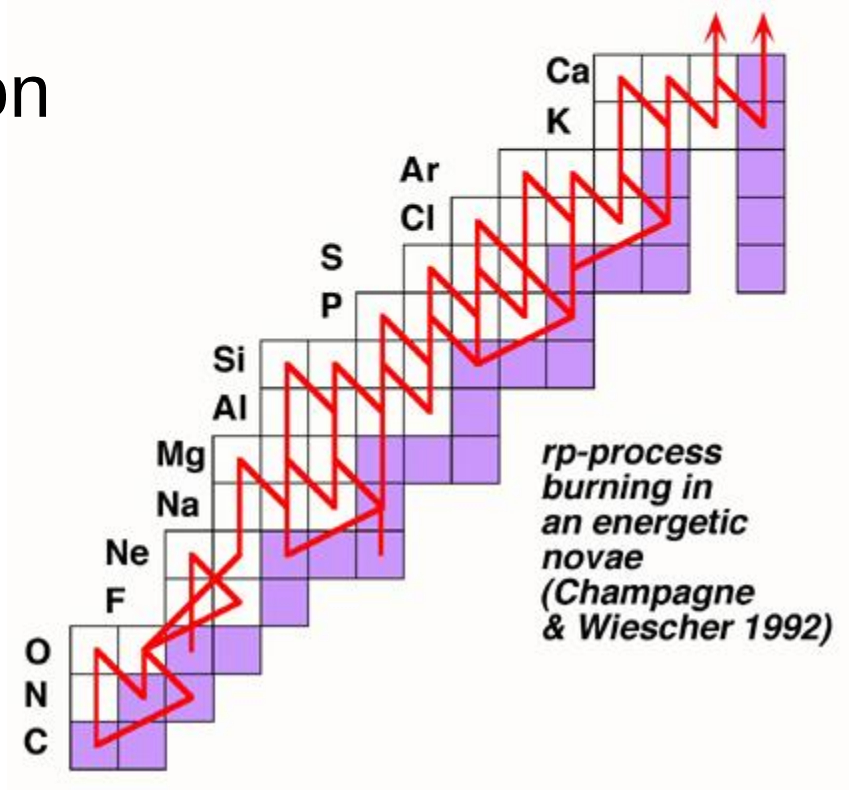
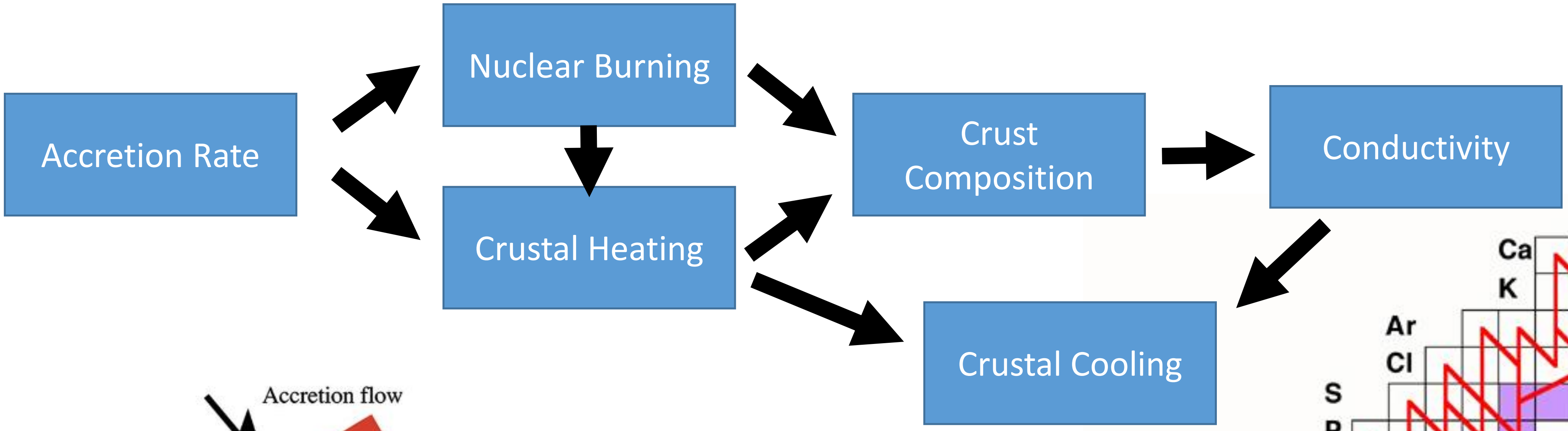
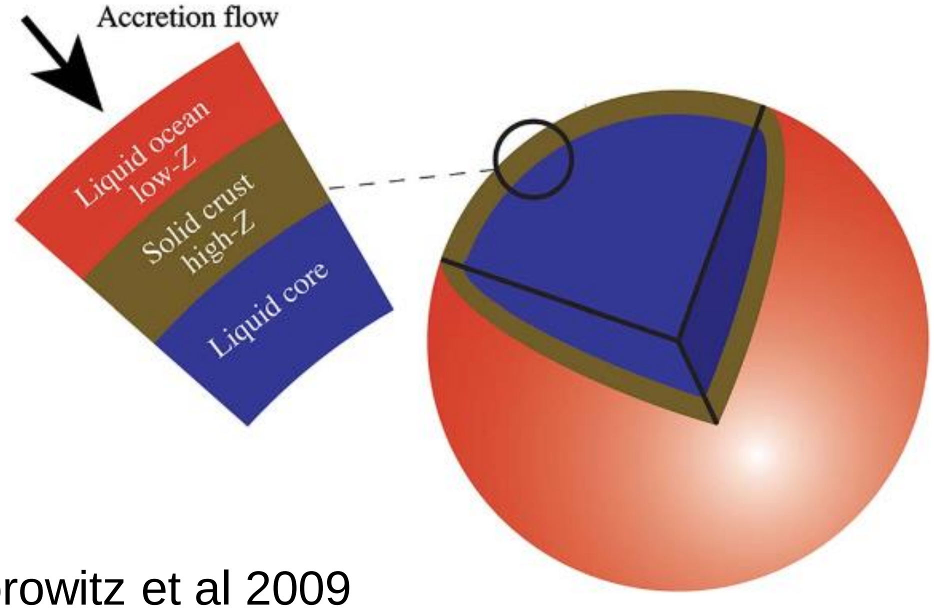




Image Credit: Horowitz et al 2009

# X-ray bursts



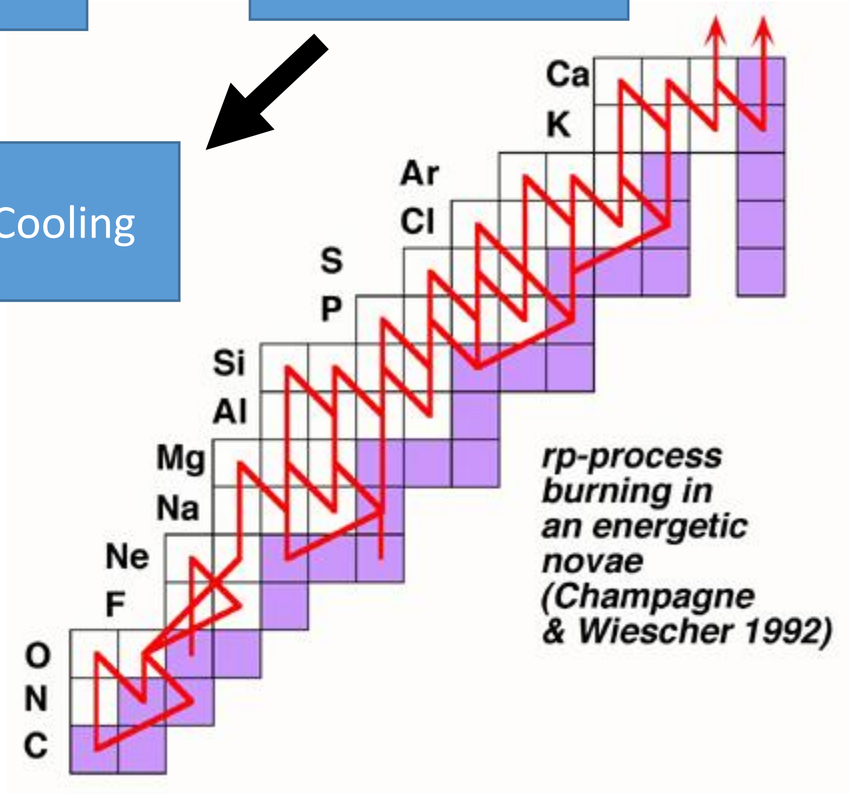




Image Credit: Horowitz et al 2009

# Multi-component Plasma

- Phase separation is now well studied (Mckinven et al 2016) for a variety of rp-ash compositions
- Liquid is enriched in light Z, solid is enriched in heavy Z.
- Use molecular dynamics to study crystal structure

$$\Gamma = \frac{\langle Z^{5/3}\rangle e^2}{T}\left[\frac{4\pi\rho_{ch}}{3}\right]^{1/3}$$

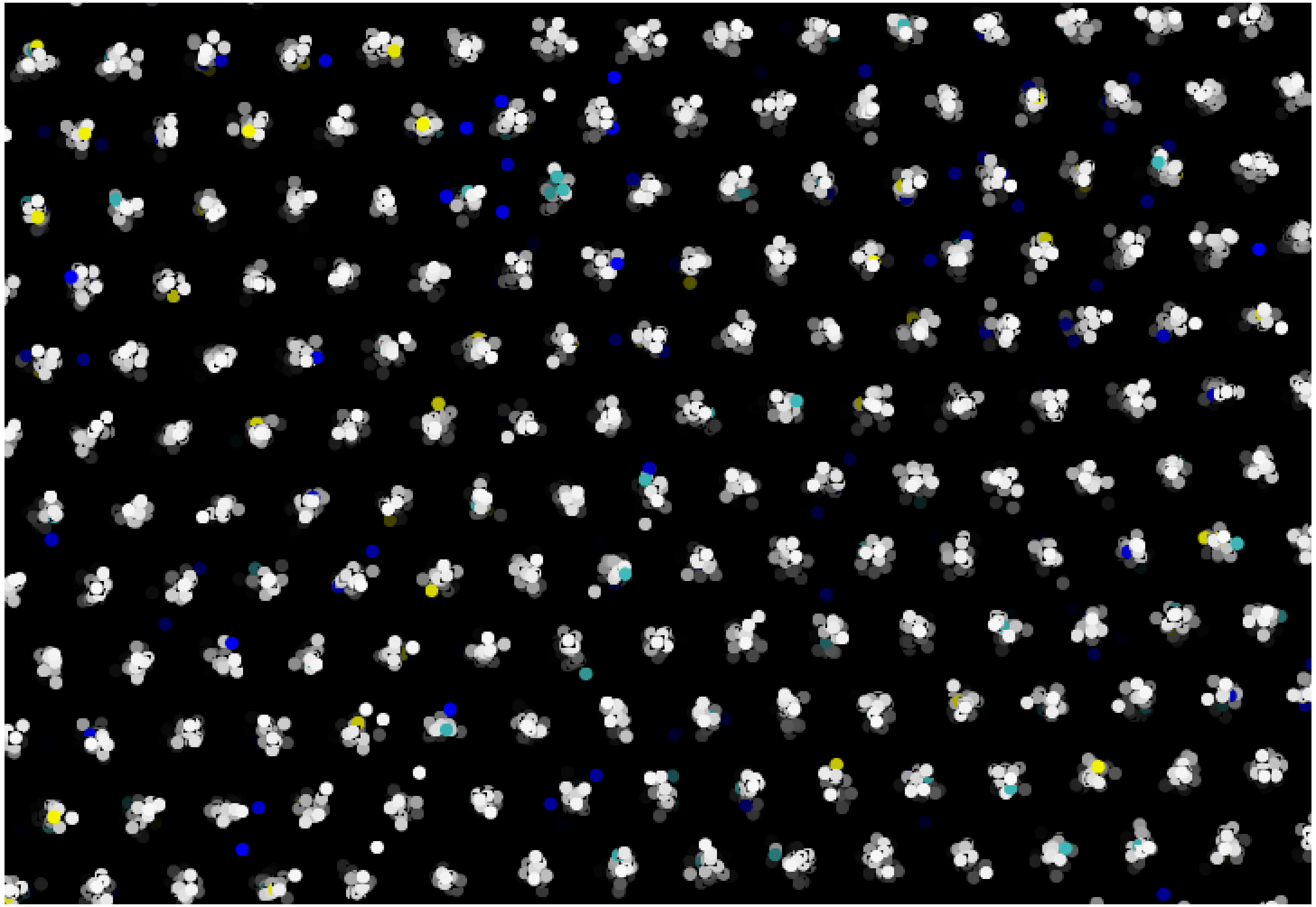
$$V_{ij}(r) = \frac{Z_i Z_j}{r} e^{-r/\lambda}$$

# Multi-component Plasma

$$\Gamma = \frac{\langle Z^{5/3}\rangle e^2}{T}\left[\frac{4\pi\rho_{ch}}{3}\right]^{1/3}$$

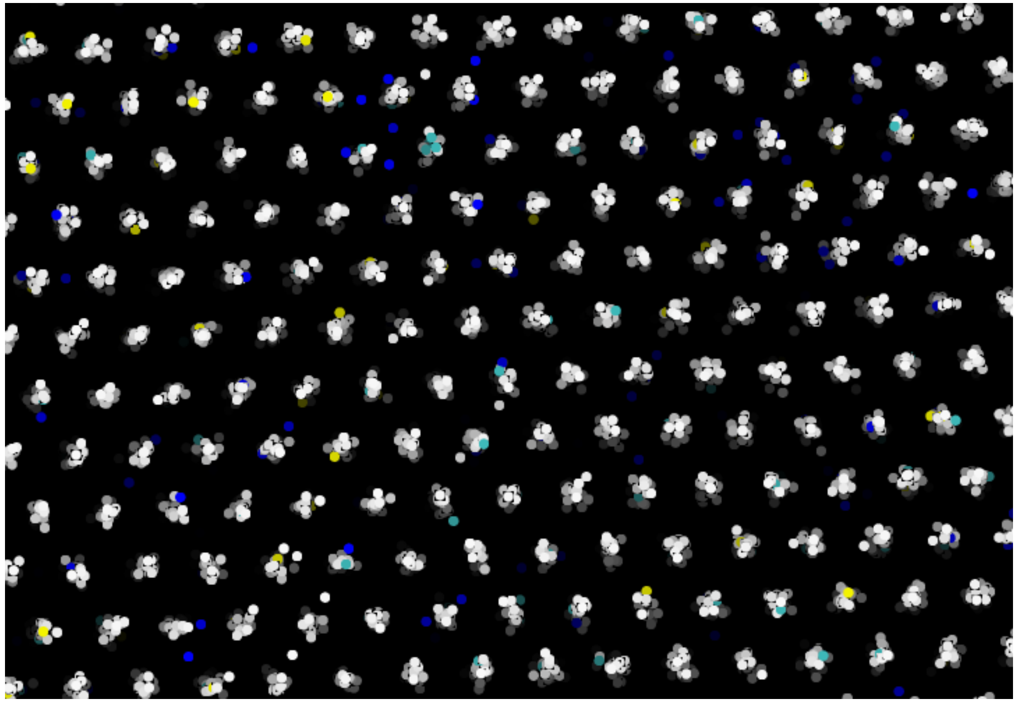
Impurity Parameter:

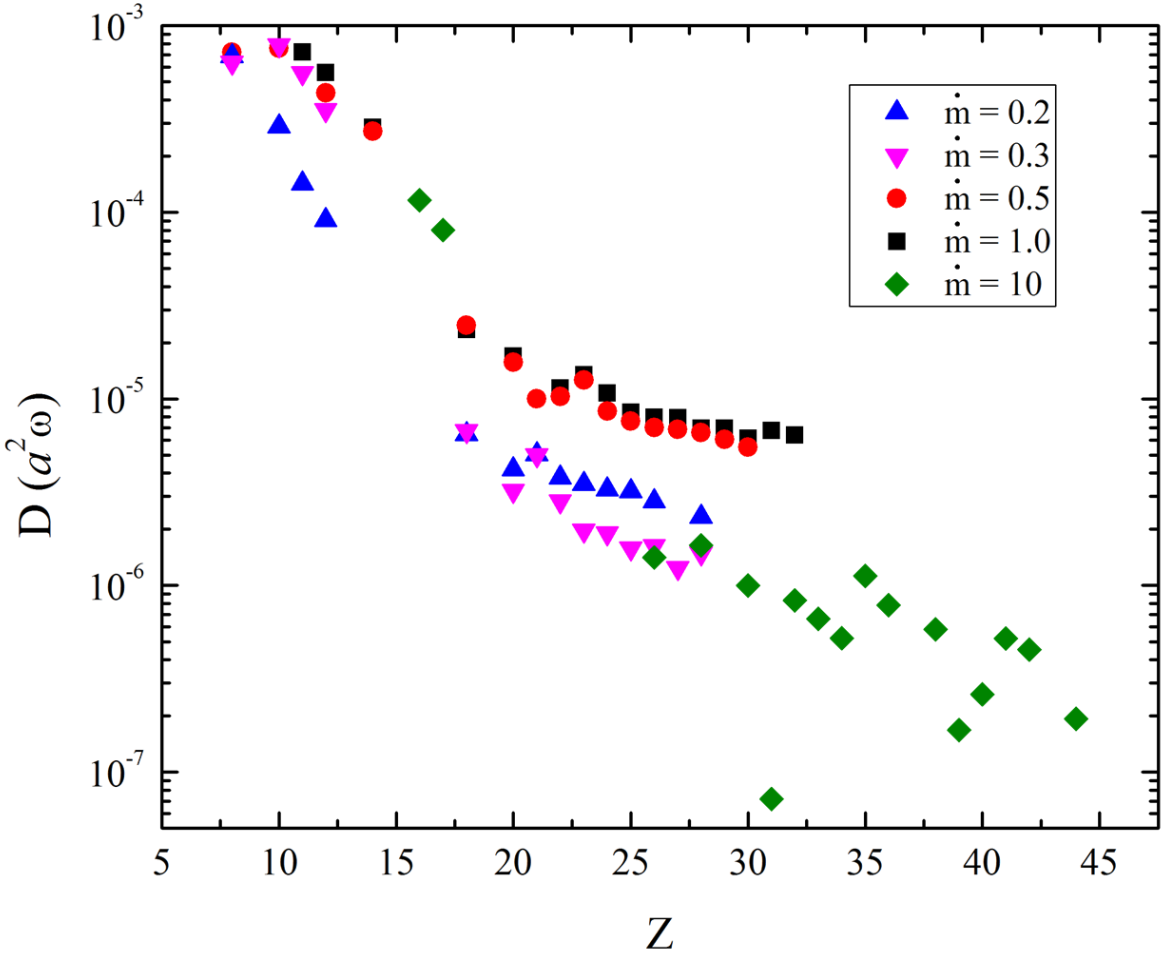
$$Q_{\mathrm{imp}} \equiv n_{\mathrm{ion}}^{-1}\sum_i n_i(Z_i - \langle Z\rangle)^2$$



# Molecular Dynamics

- Study the crystal structure by simulating it
- Low Z: Diffusive, Interstitial
- High Z: Nondiffusive, On lattice





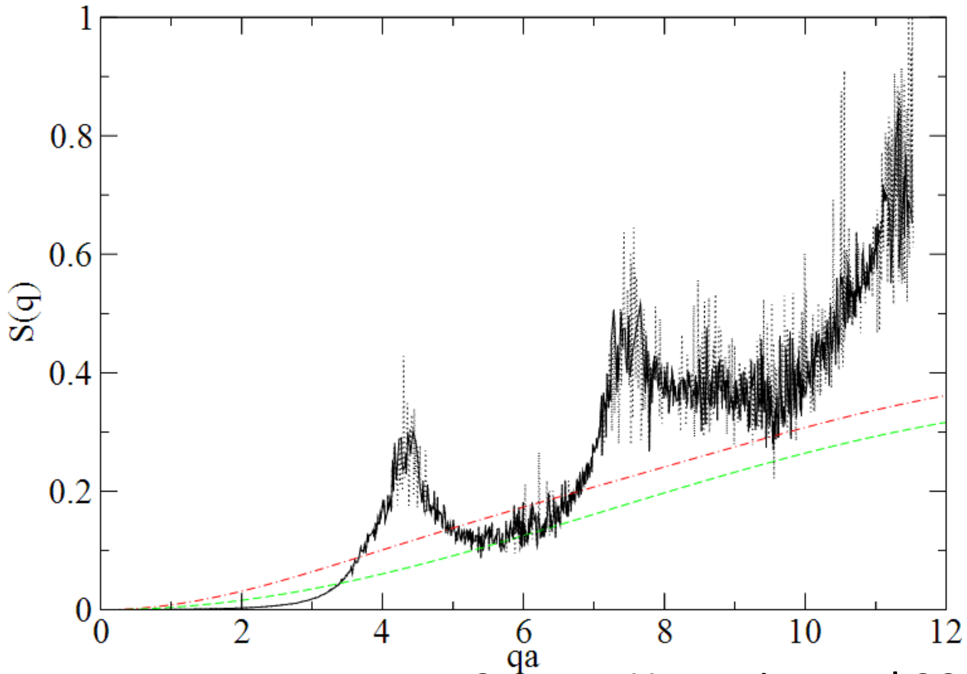
# Molecular Dynamics

- Calculate the static structure factor:

$$S(\mathbf{q}) = \langle \rho^*(\mathbf{q})\rho(\mathbf{q})\rangle - |\langle \rho(\mathbf{q})\rangle|^2$$

$$\rho(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \frac{Z_i}{\langle Z \rangle} e^{i\mathbf{q}\cdot\mathbf{r}_i}$$

- Integrate to obtain the Coulomb Log



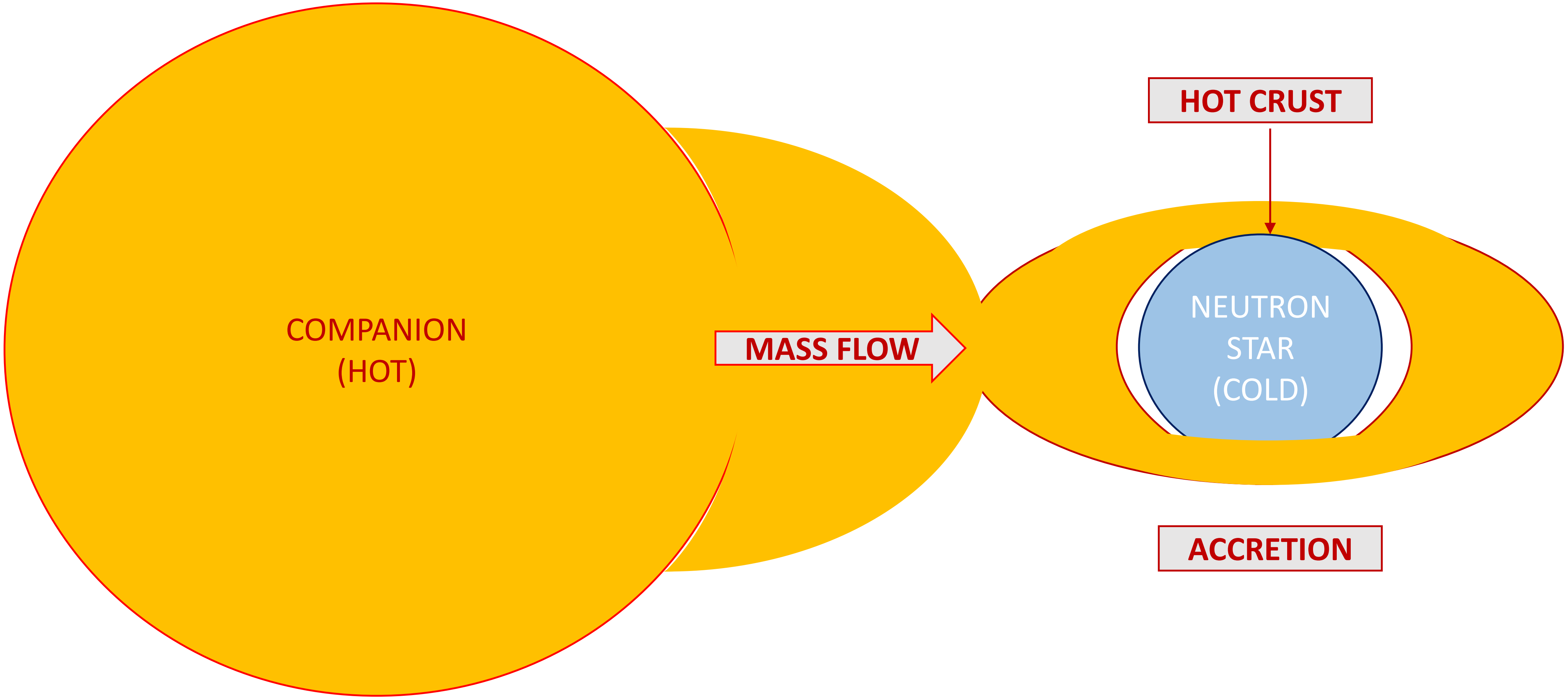

Source: Horowitz et al 2009

$$\Lambda = \int_{q_0}^{2k_F} \frac{dq}{q\epsilon(q,0)^2} S'(q)(1 - \frac{q^2}{4k_F^2})$$

$$K_e = \frac{\pi}{12} \frac{E_{F,e}\, k_B^2\, T c}{e^4} \frac{\langle Z \rangle}{Q_{imp}\Lambda_{eQ}}$$

$$\approx 4 \times 10^{19}\ \mathrm{erg\ s^{-1} cm^{-1} K^{-1}} \left[ T_8 \left( \frac{\rho_{14} Y_e}{0.05} \right)^{1/3} \frac{\langle Z \rangle}{Q_{imp}\Lambda_{eQ}} \right]$$

# Low Mass X-Ray Binaries



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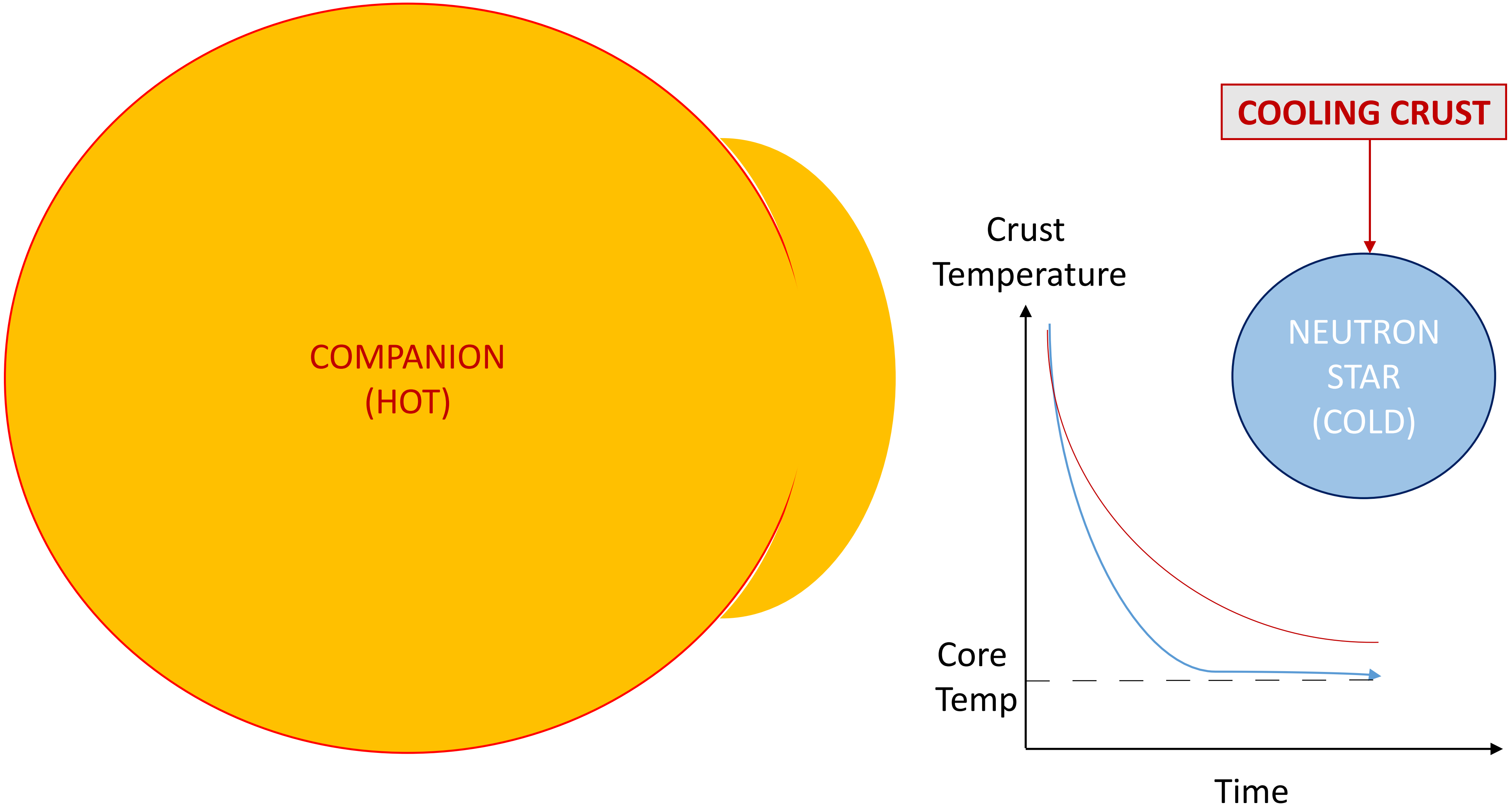


# Crust Cooling

- Observations of crust cooling of LMXBs require low impurity parameter in the crust (how does knowing the crystal structure change this?)

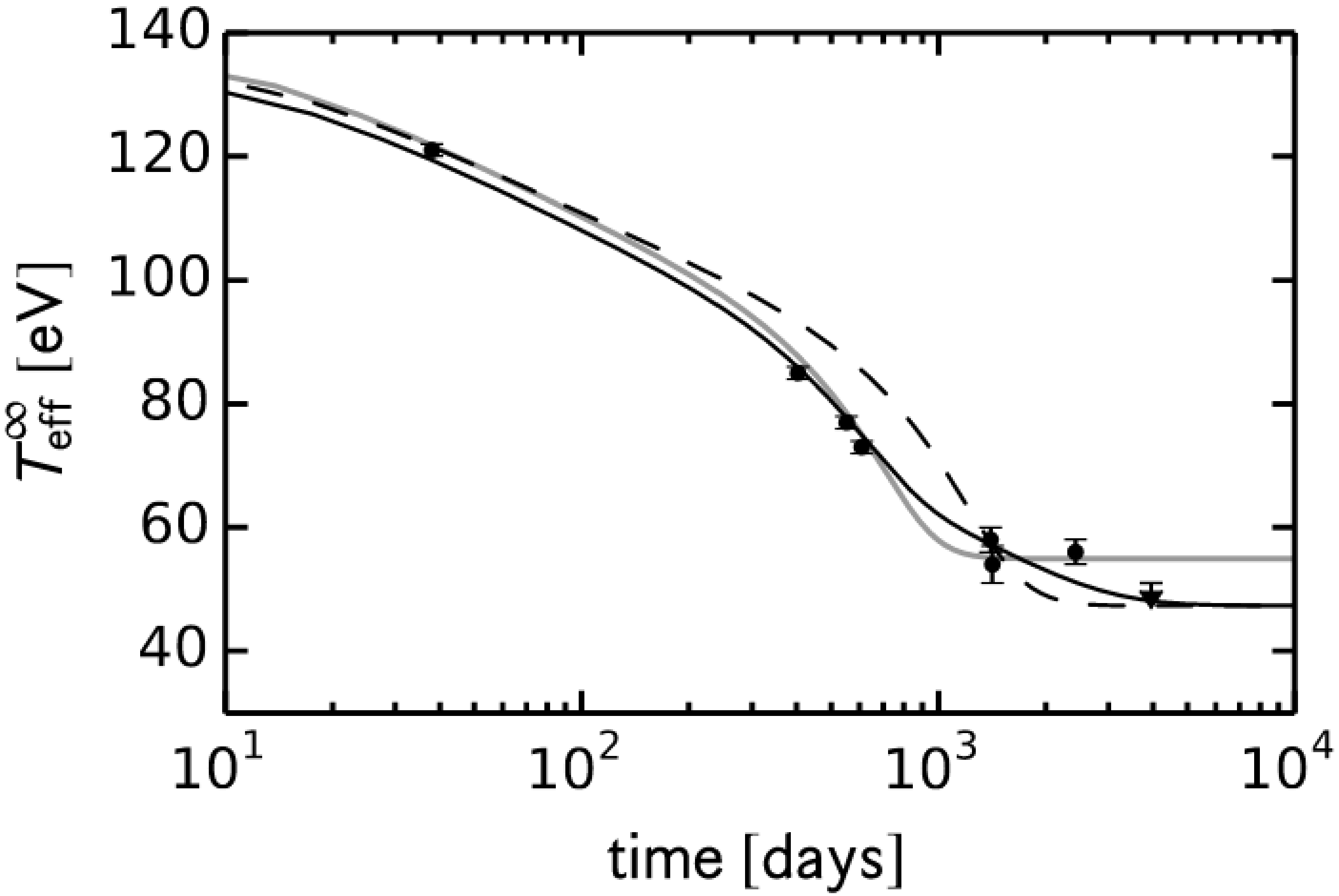
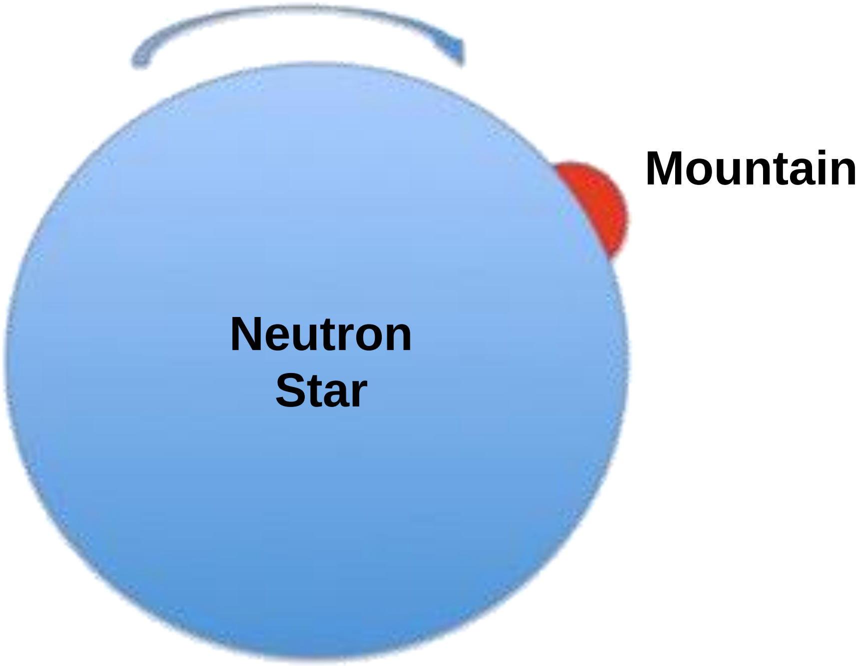



Image Credit: Deibel et al 2016

# Crust Breaking

- Shear modulus and breaking strain of crust could determine the maximum size of mountains which could be a persistent source of gravitational waves



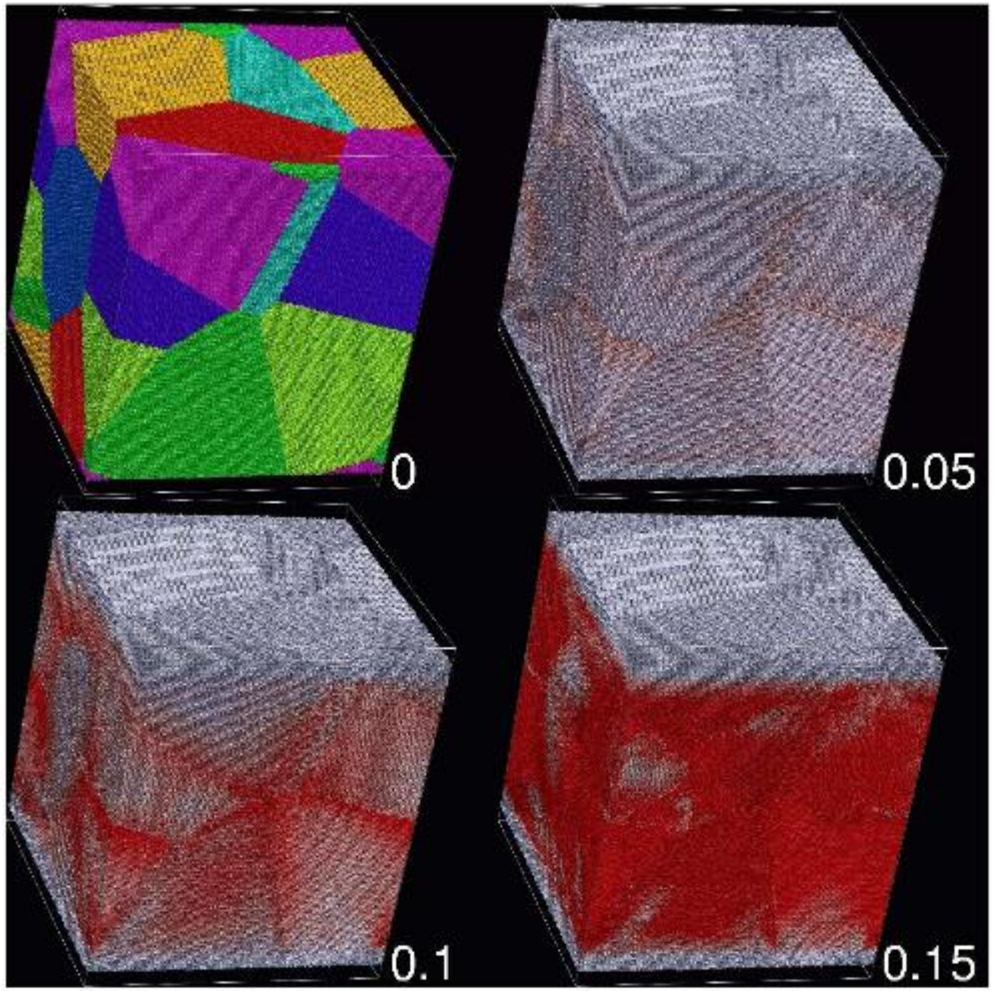




Image Credit: Horowitz et al 2009

# Soft Astromaterials

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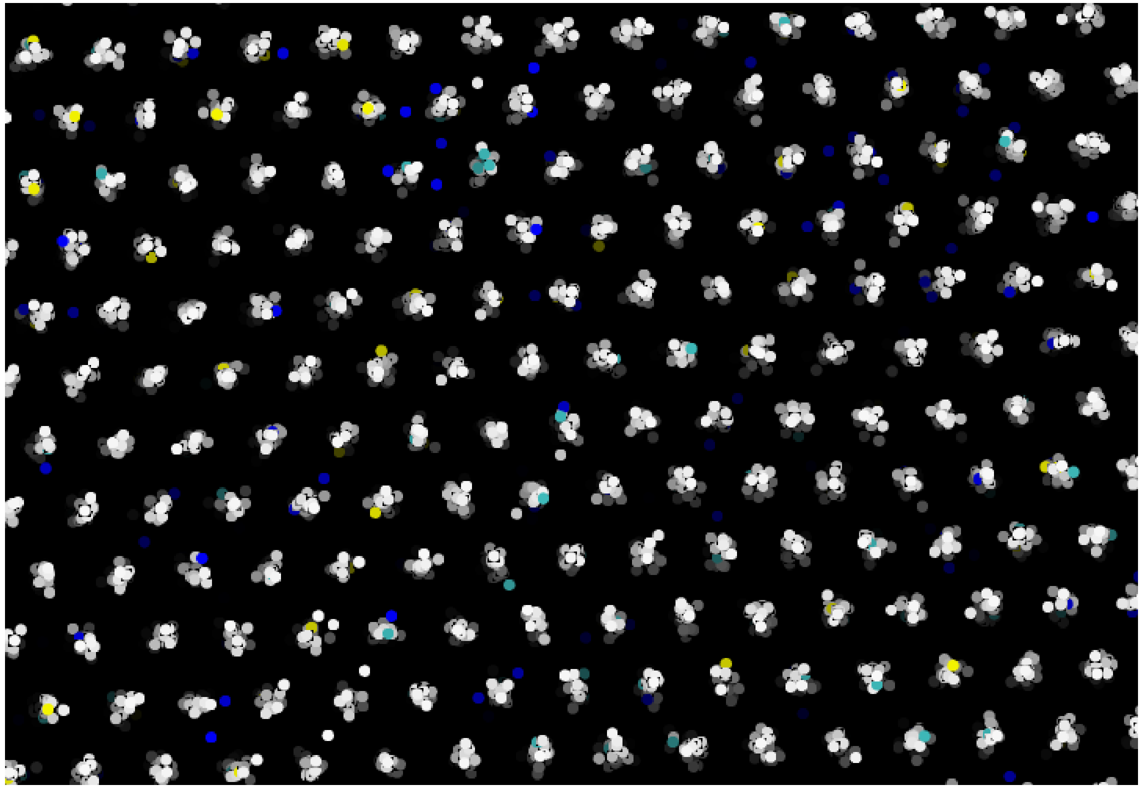
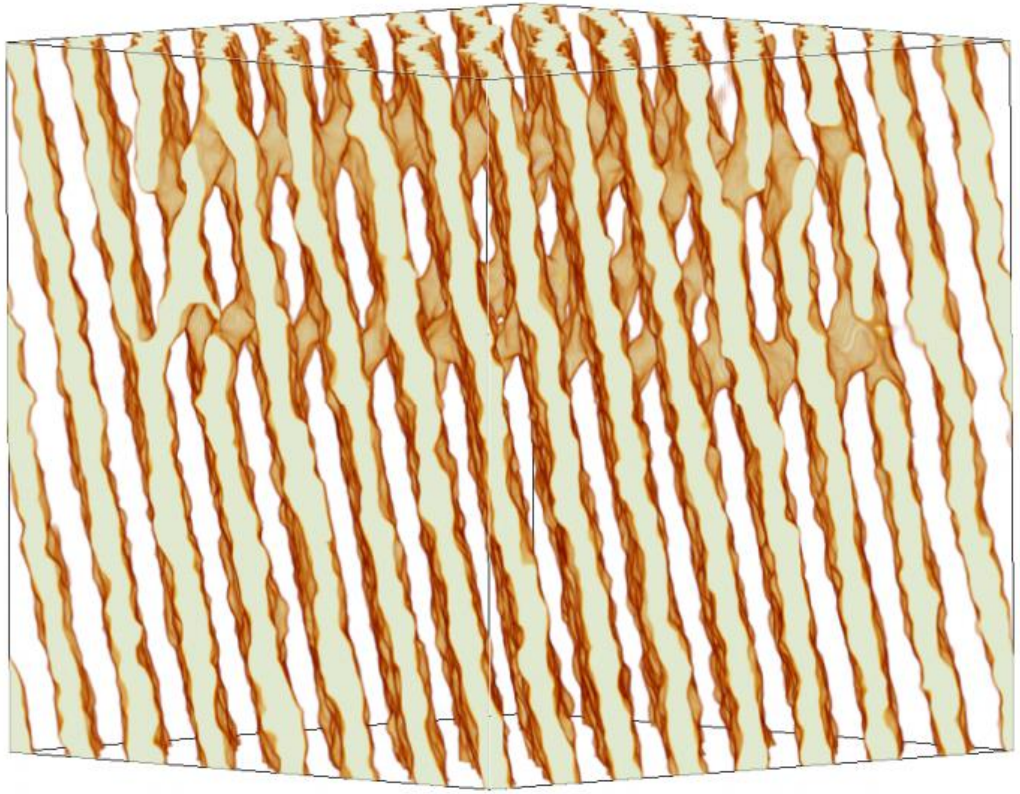


HARD



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# 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?

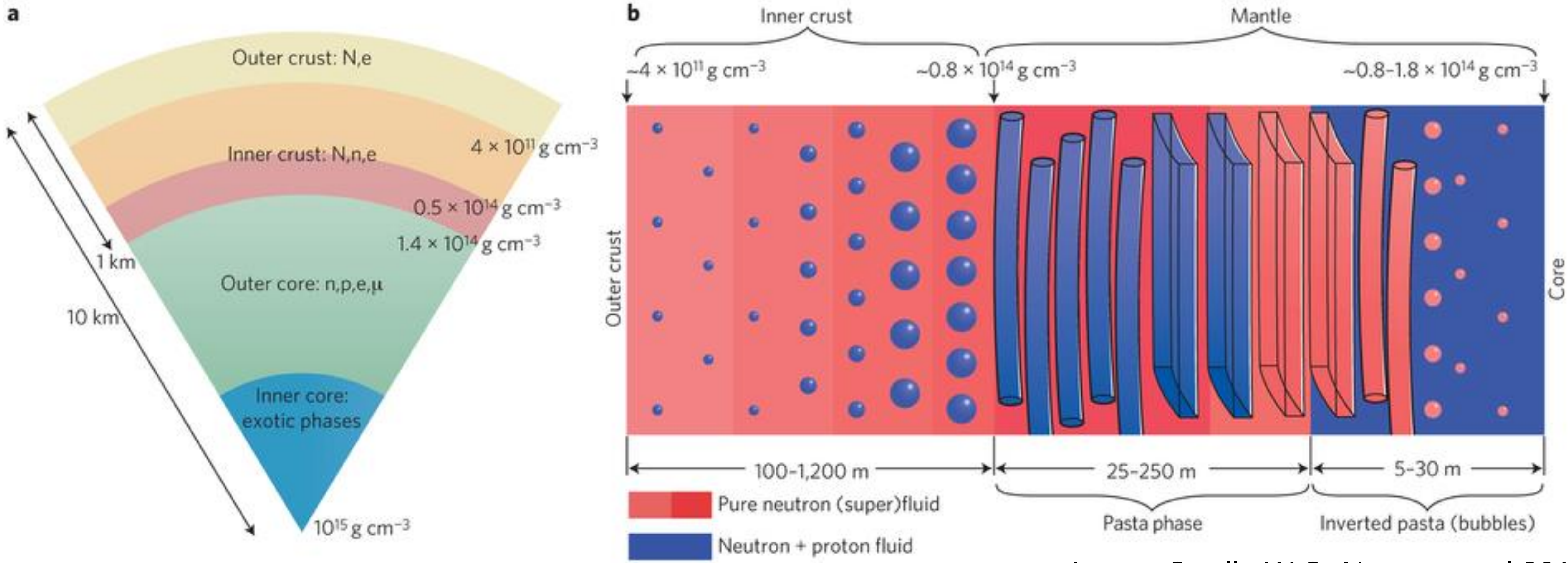



Image Credit: W.G. Newton et al 2012

# 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 321

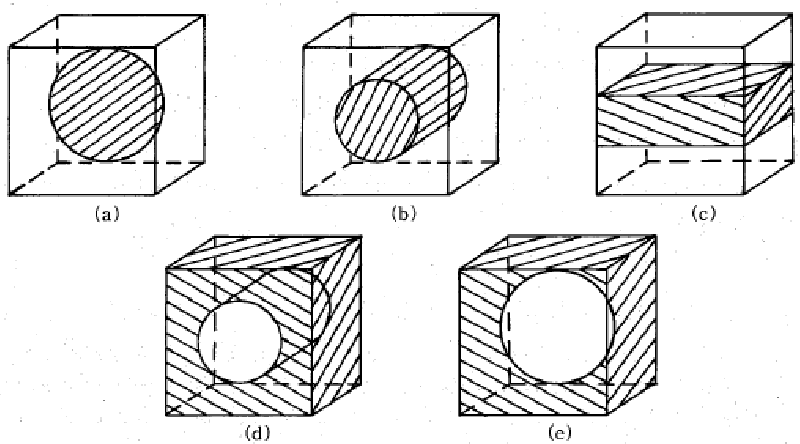
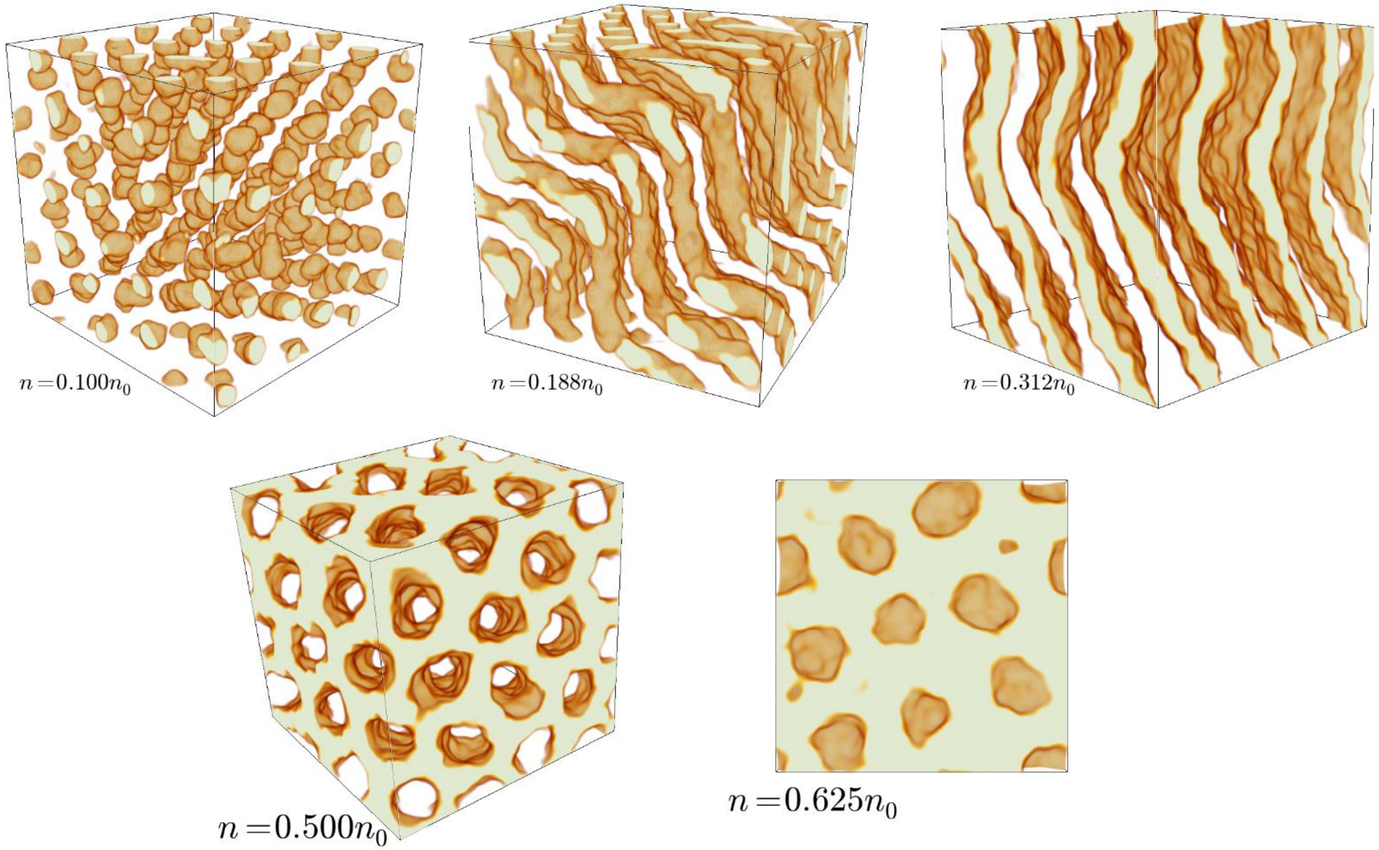
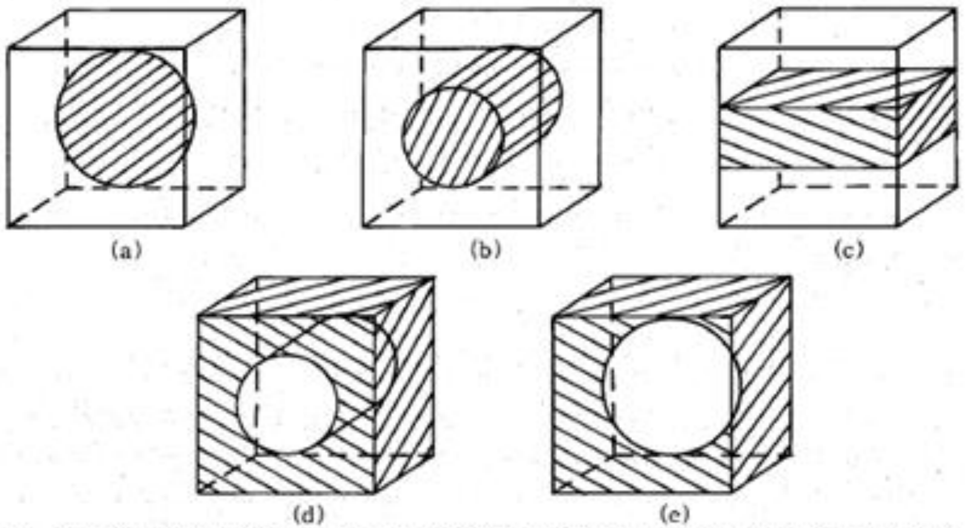



Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole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

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# Classical Pasta Formalism

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

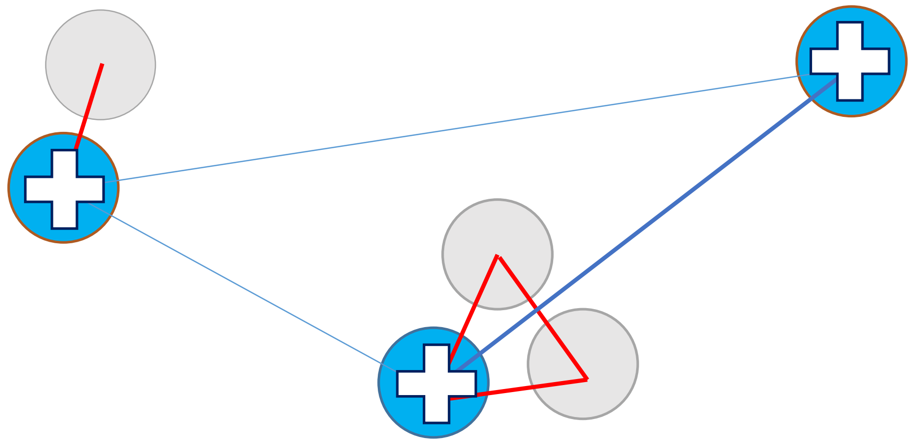
| $a$ | $b$ | $c$ | $\Lambda$ | $\lambda$ |
|---|---|---|---|---|
| 110 MeV | -26 MeV | 24 MeV | 1.25 fm$^2$ | 10 fm |

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

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

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

- 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 |

Horowitz et al. (2004) PhysRevC 69, 045804

# Classical Pasta Formalism

- **Classical Molecular Dynar** IUM Red II

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

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

| $\Lambda$ | $\lambda$ |
|---|---|
| $1.25\,\mathrm{fm}^2$ | $10\,\mathrm{fm}$ |

range nuclear force

nge Coulomb force

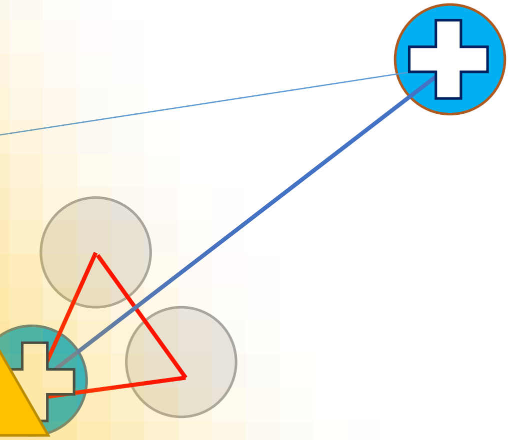
| Nucleus | Monte-Carlo $\langle V_{tot} \rangle$ (M |
|---|---|
| $^{16}$O | -7.56±0.01 |
| $^{40}$Ca | -8.75±0.03 |
| $^{90}$Zr | -9.13±0.[illegible] |
| $^{208}$Pb | -8.2 ±[illegible] |

Density

Proton Fraction

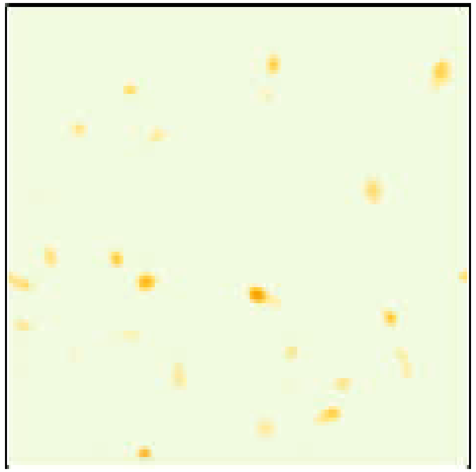
Temperature

NSE!



Horowitz et al. (2004) PhysRevC 69, 045804

Gold Nucleus
For Scale

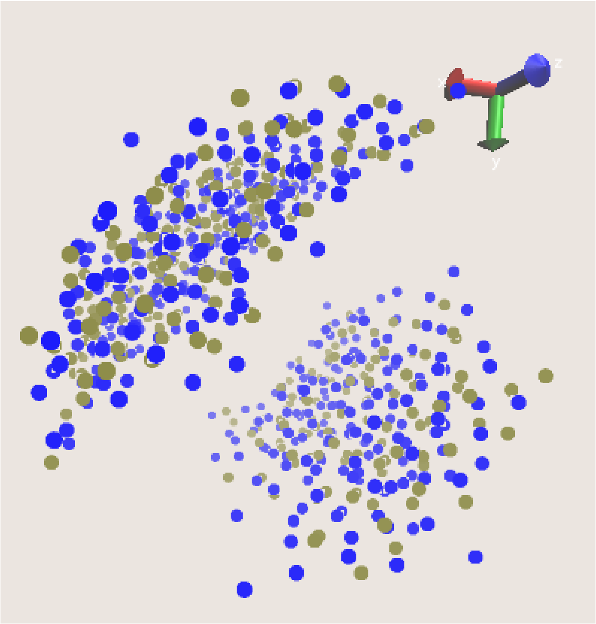


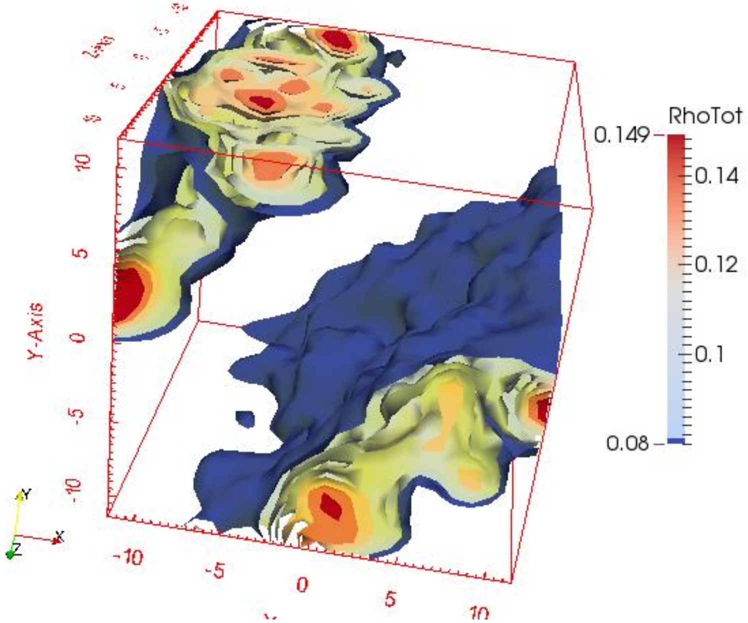
$$n = 0.1200 \mathrm{fm}^{-3}$$

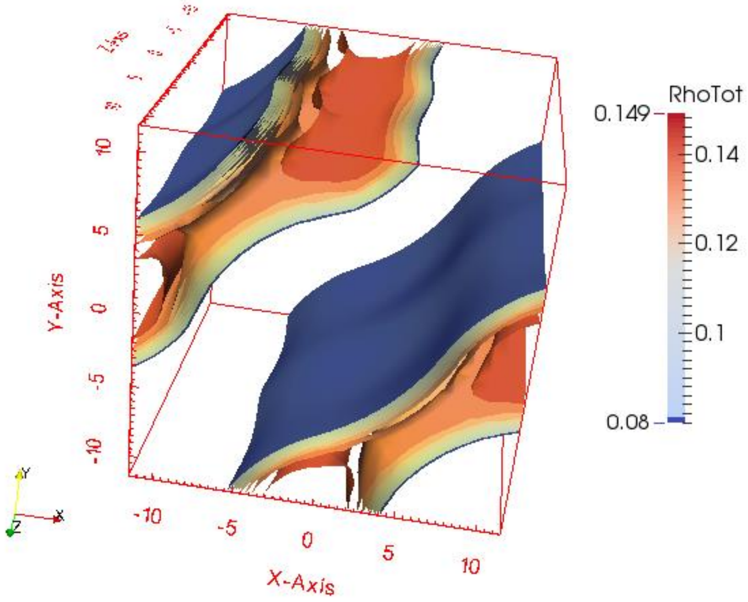
# Classical and Quantum MD

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

**Classical Points** → **Folded with Gaussian** → **Equilibrated Wavefunctions**

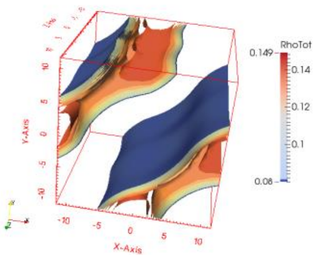




# Classical and Quantum MD

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



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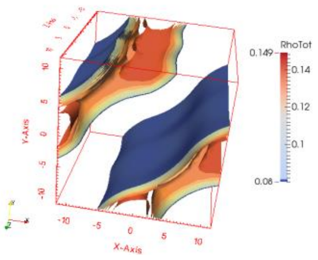
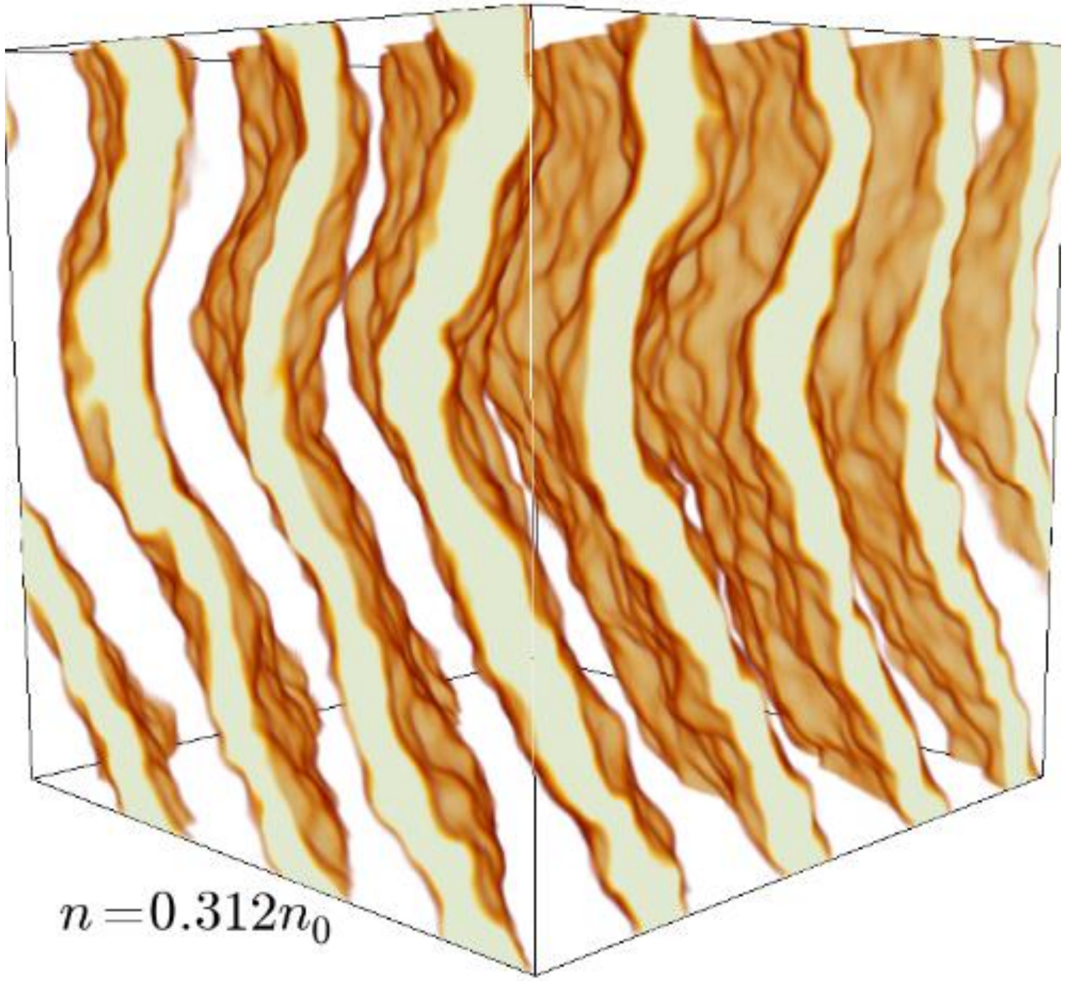


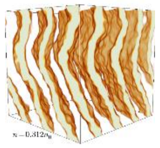
**100 fm**

**51,200 nucleons**

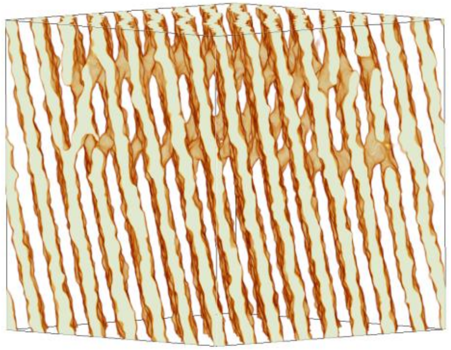


# Molecular Dynamics

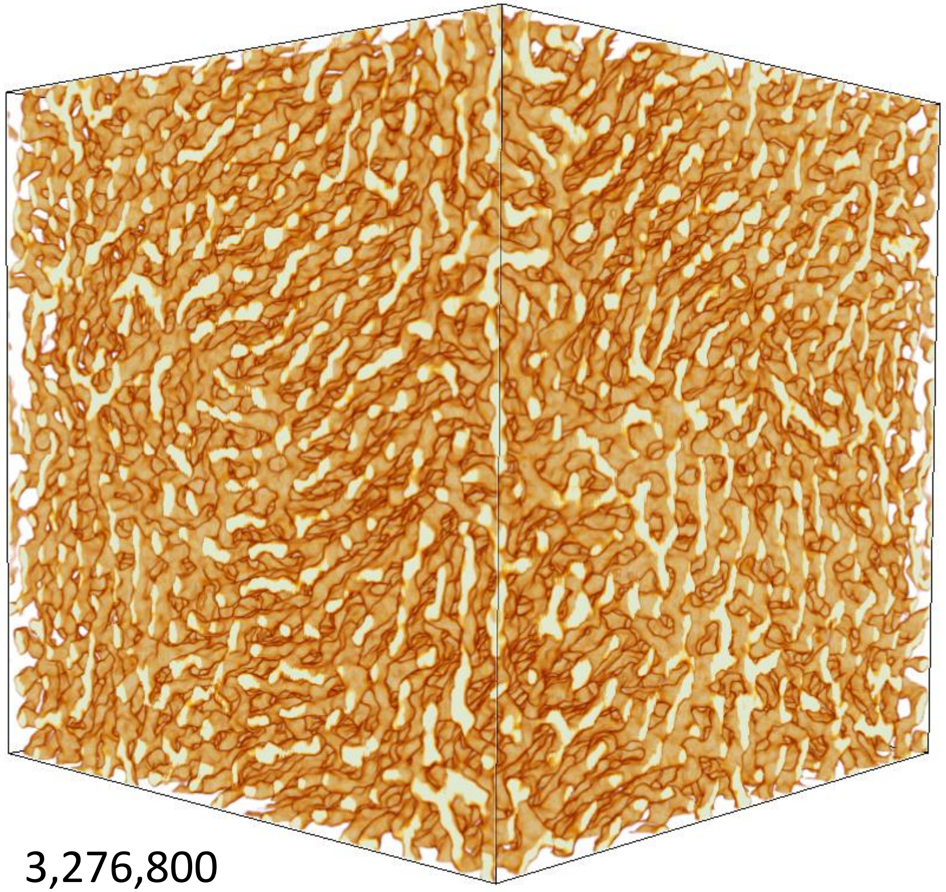
- We have evolved simulations of 409,600 nucleons, 819,200 nucleons, 1,638,400 nucleons, and 3,276,800 nucleons



51,200



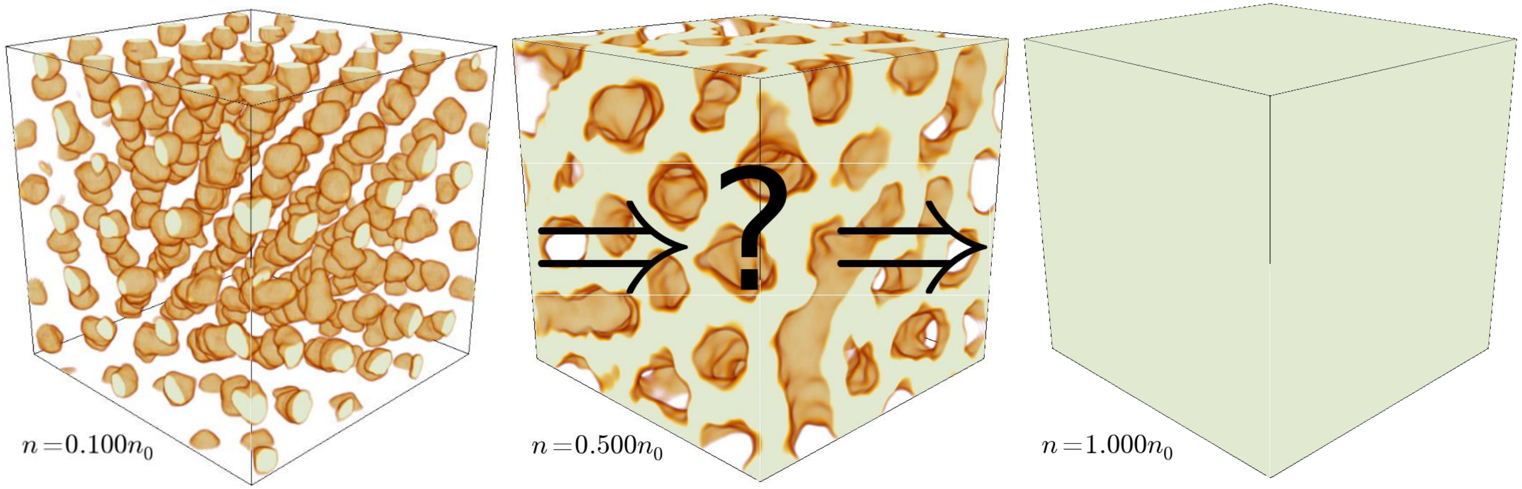
409,600



3,276,800

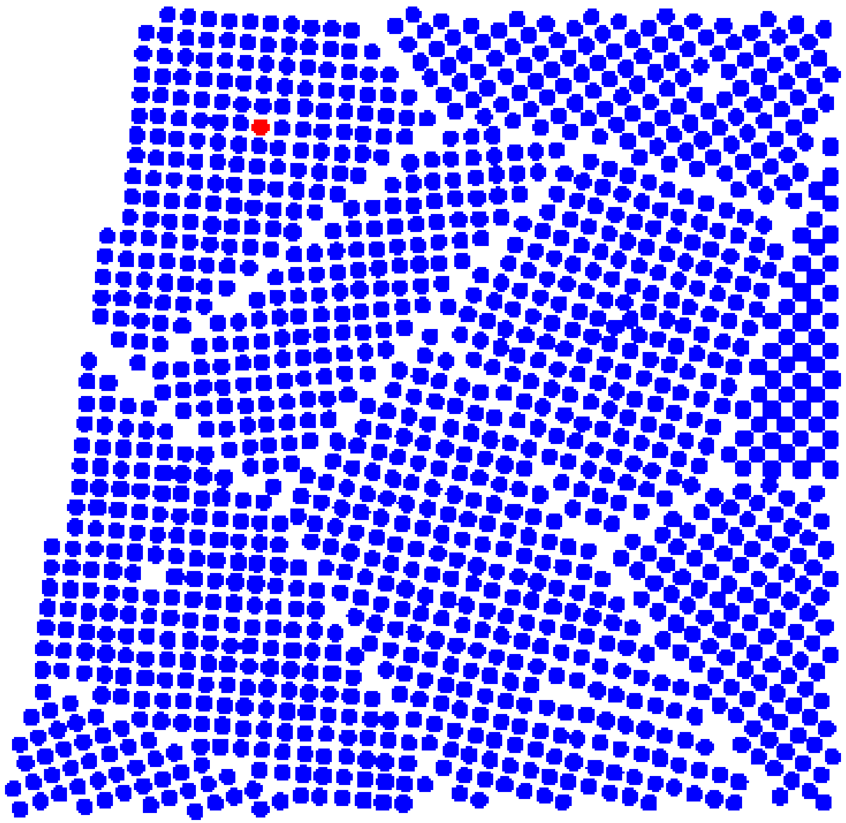
# Nuclear Pasta

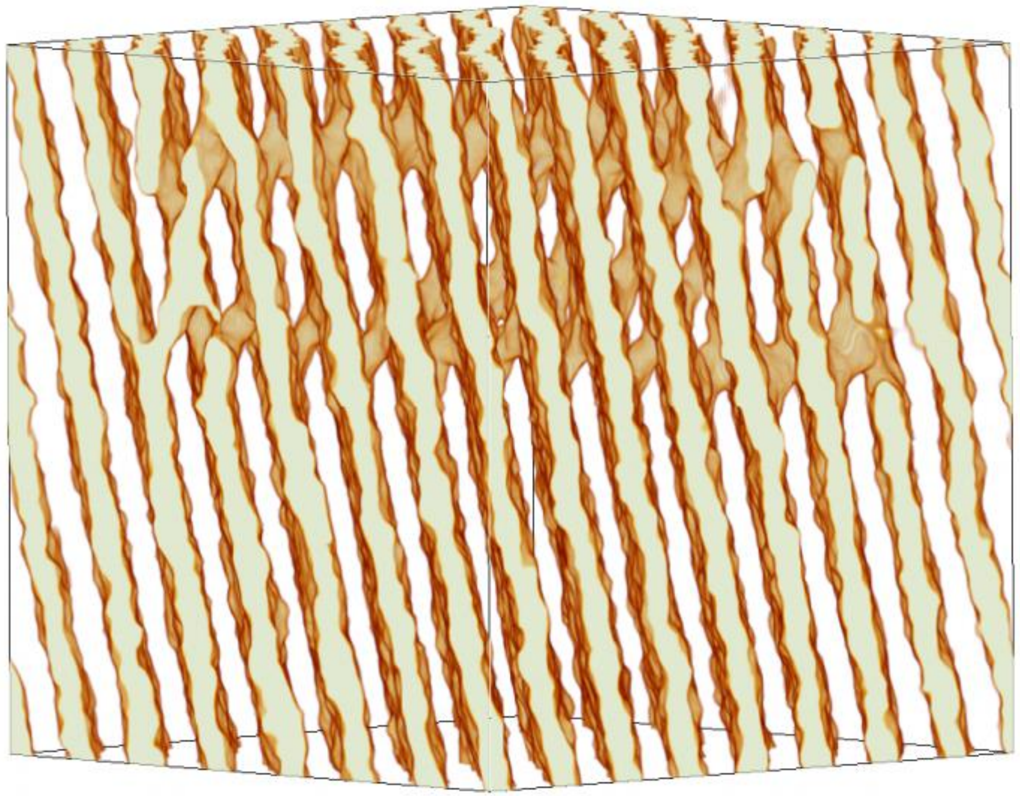
- Important to many processes:
  - Thermodynamics: Late time crust cooling
  - Magnetic field decay: Electron scattering in pasta
  - Gravitational wave amplitude: Pasta elasticity and breaking strain
  - Neutrino scattering: Neutrino wavelength comparable to pasta spacing
  - R-process: Pasta is ejected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



# Defects

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

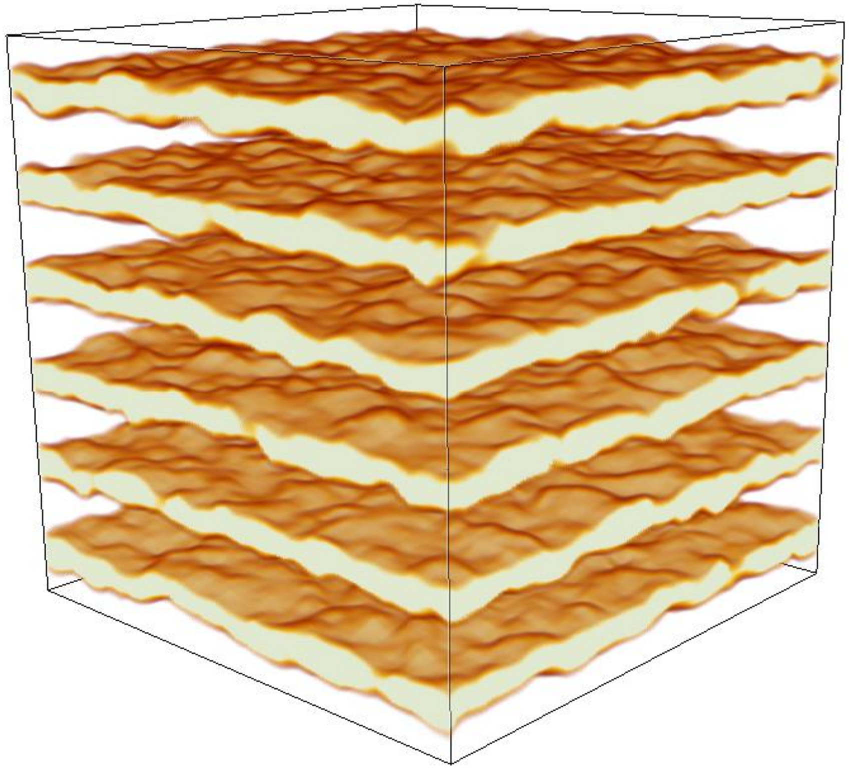




- Horowitz et al, PRL.114.031102 (2015)

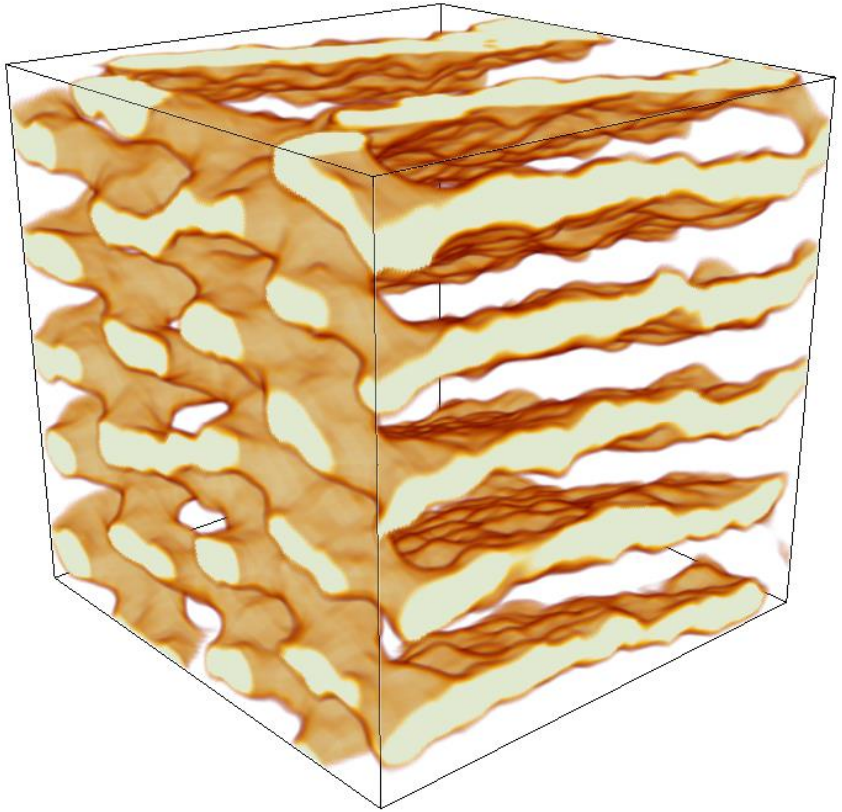
# Pasta Defects

- Defects act as a site for *scattering*



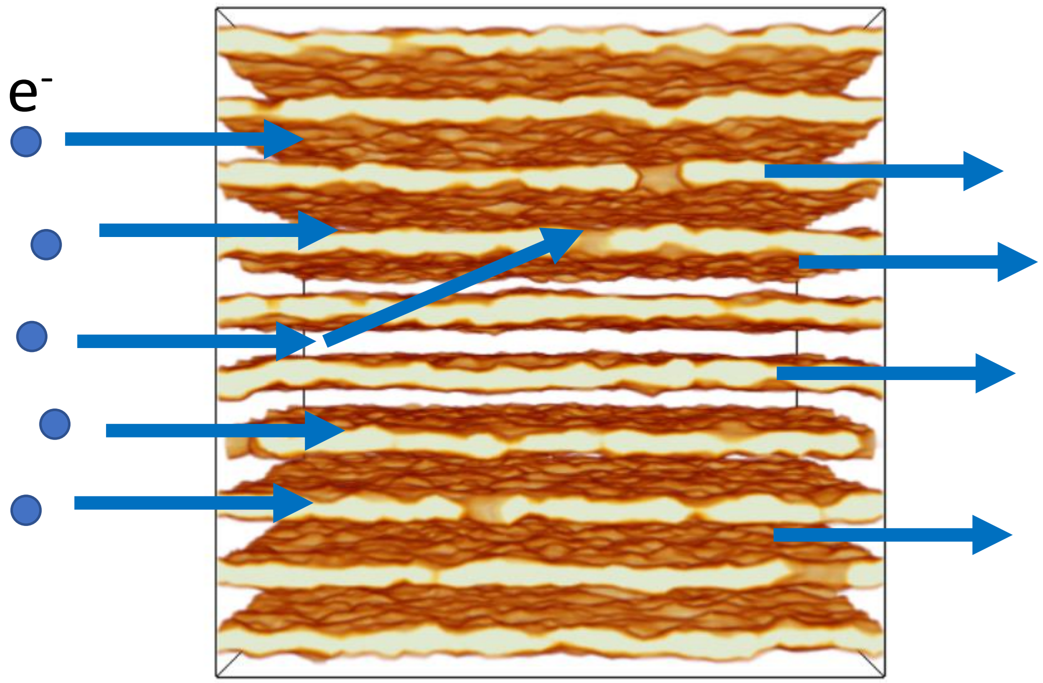
← Perfect

Defects →



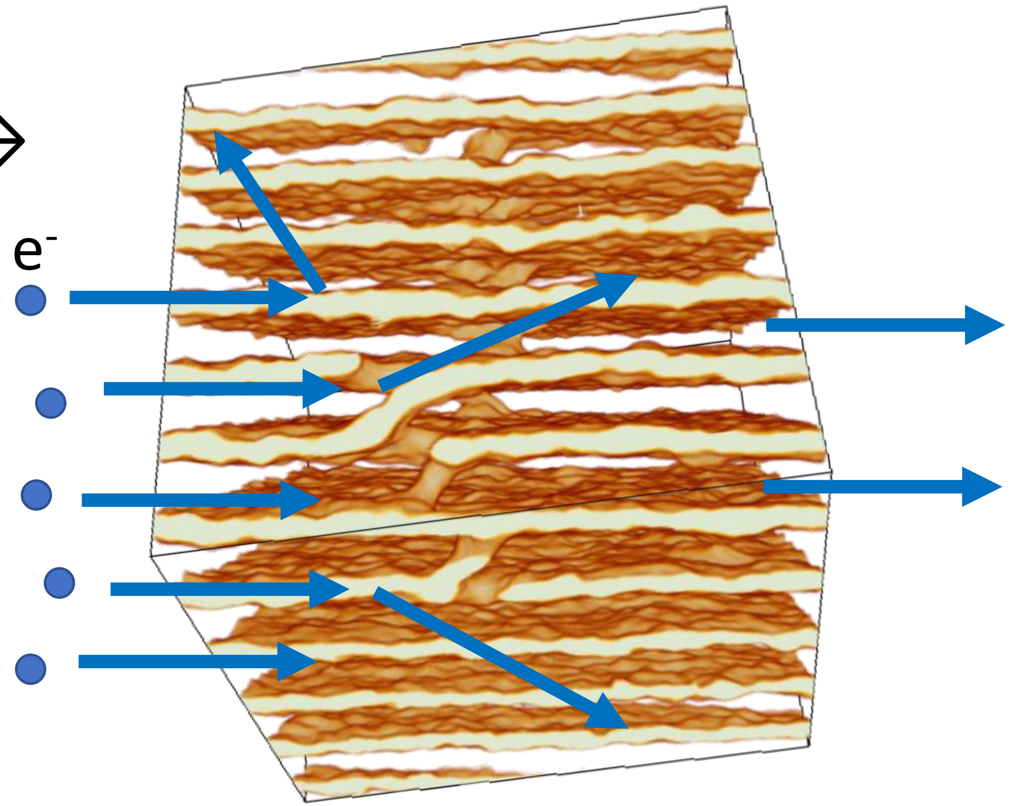
# Pasta Defects

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




← Perfect

Defects →




Pons et al, Nature Physics 9, 431–434 (2013)

# Lepton Scattering

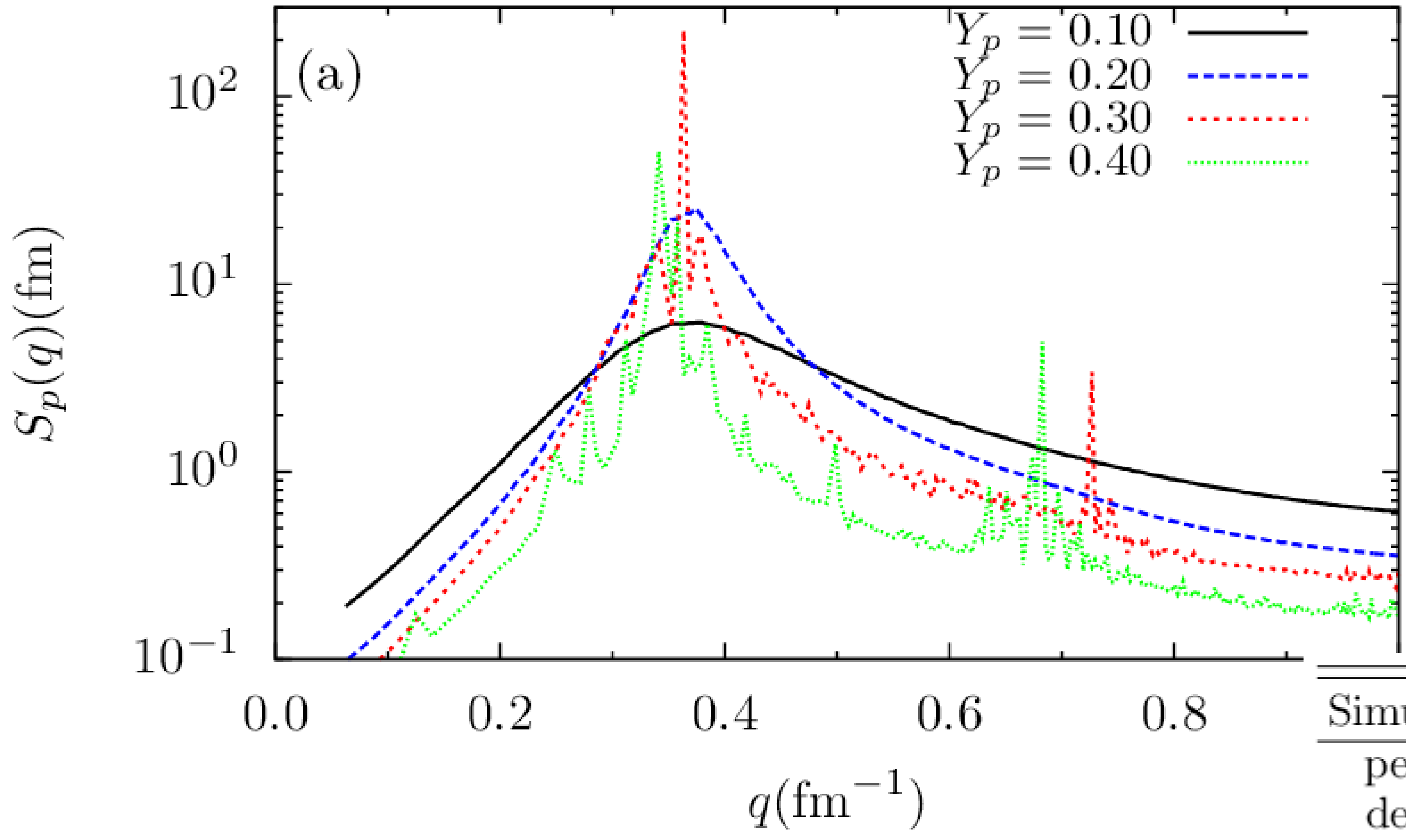
- Lepton scattering from pasta influences a variety of transport coefficients:
- Shear viscosity: $$\eta = \frac{\pi v_F^2 n_e}{20\alpha^2 \Lambda_{\rm ep}^\eta},$$
- Electrical conductivity: $$\sigma = \frac{v_F^2 k_F}{4\pi\alpha\Lambda_{\rm ep}^\sigma}$$ $$\Lambda_{\rm ep}^\eta = \int_0^{2k_F} \frac{dq}{q\epsilon^2(q)} \left(1 - \frac{q^2}{4k_F^2}\right)\left(1 - \frac{v_F^2 q^2}{4k_F^2}\right) S_p(q)$$
- Thermal conductivity: $$\kappa = \frac{\pi v_F^2 k_F k_B^2 T}{12\alpha^2 \Lambda_{\rm ep}^\kappa}.$$ $$\Lambda_{\rm ep}^\kappa = \Lambda_{\rm ep}^\sigma = \int_0^{2k_F} \frac{dq}{q\epsilon^2(q)} \left(1 - \frac{v_F^2 q^2}{4k_F^2}\right) S_p(q).$$

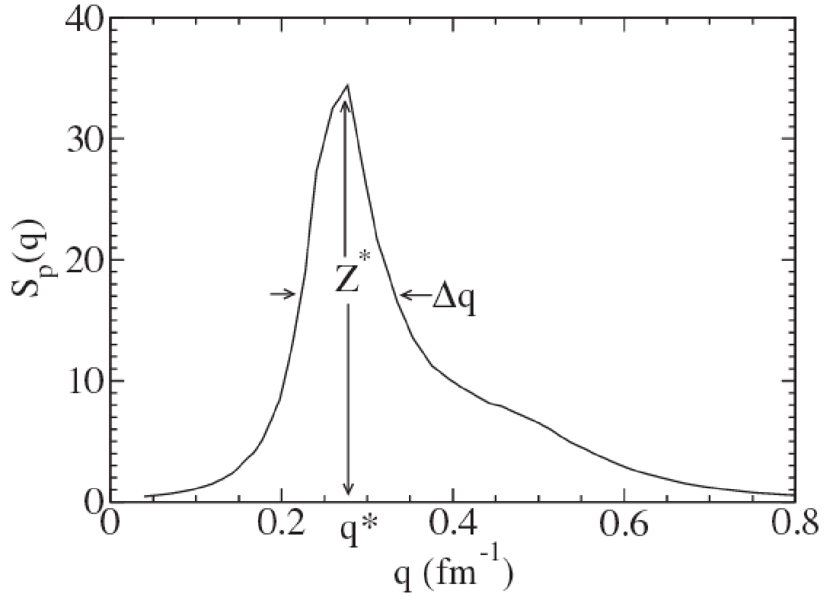
# Lepton Scattering

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

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

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

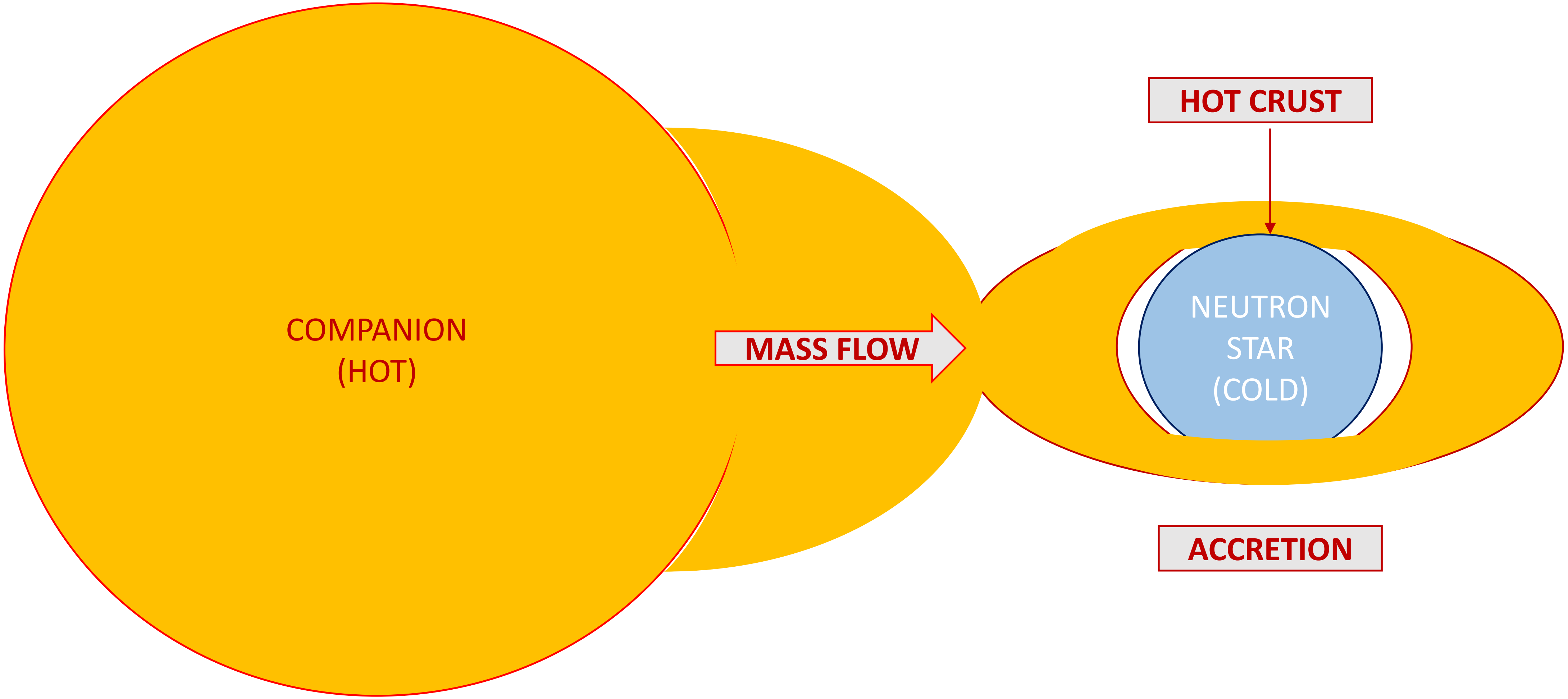


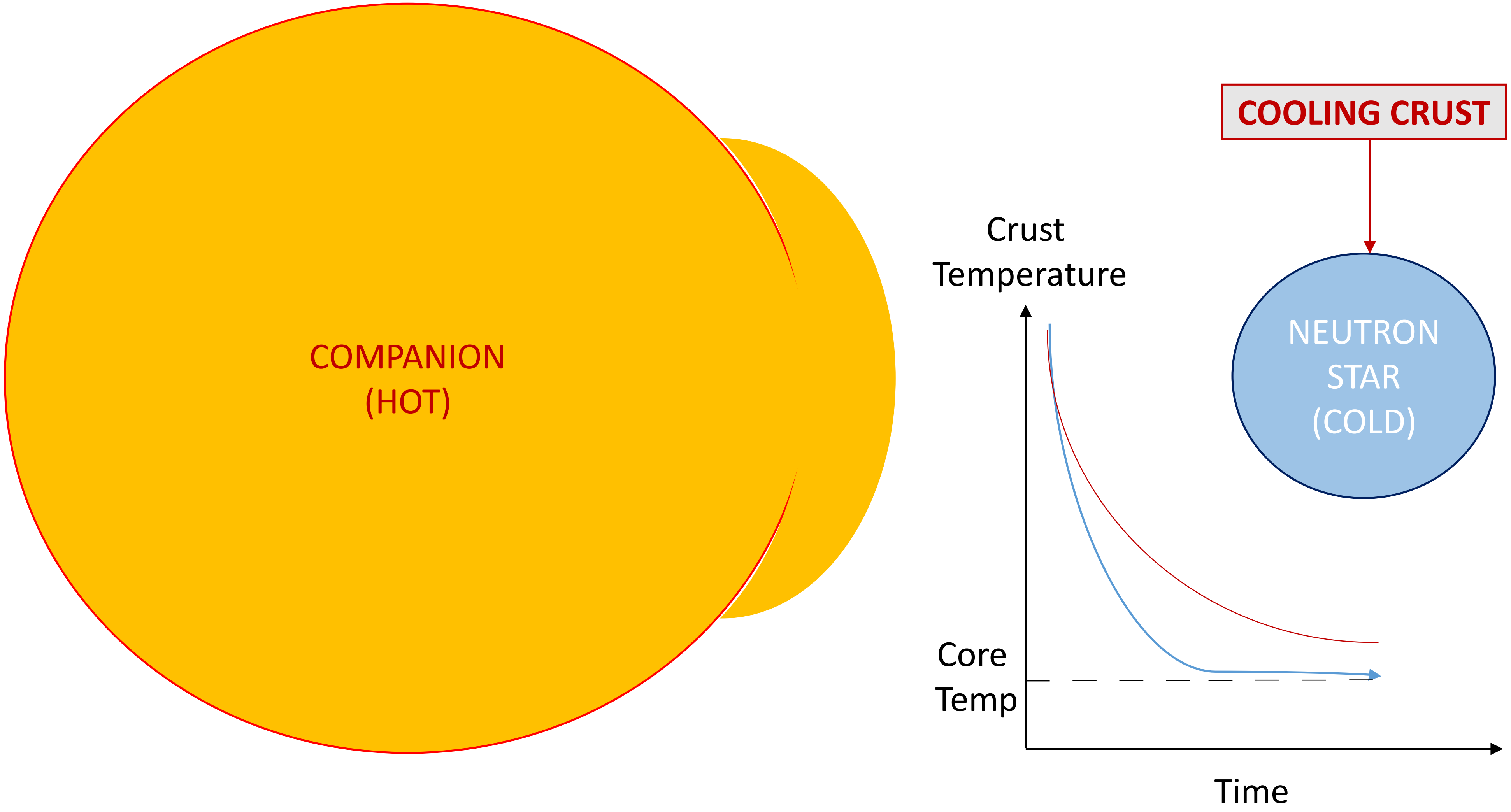

| Simulation | $\bar{\eta}(\mathrm{fm}^{-3})$ | $\bar{\kappa}(10^3 k_B\ \mathrm{MeV/fm})$ | $\bar{Z}^*$ |
|---|---|---|---|
| perfect | 87.7 | 6.66 | 5.5 |
| defects | 55.5 | 4.15 | 50.2 |

# Crust Cooling

# Low Mass X-Ray Binaries



# Low Mass X-Ray Binaries

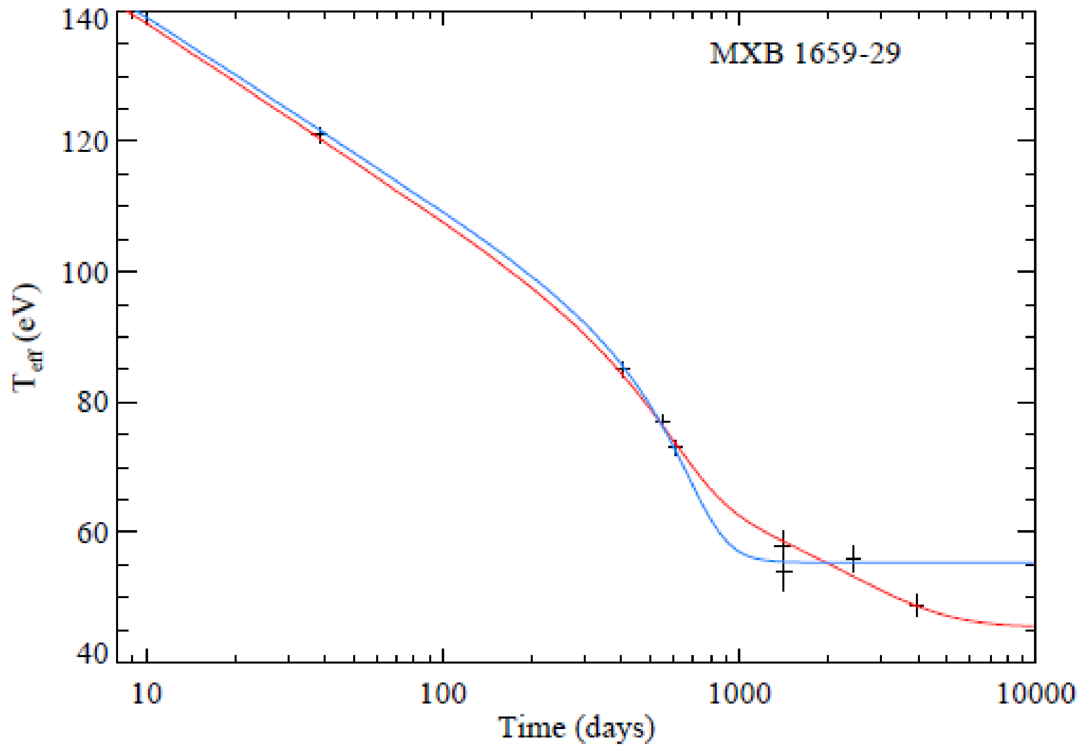


# Observables – Thermal Properties

- Guess an effective impurity parameter for defects and try to fit neutron star cooling curves

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

- Cooling curves: low mass X-ray binary MXB 1659-29
  - Blue: normal isotropic matter
    $Q_{imp} = 3.5$
    $T_c = 3.05 \times 10^7$ K
  - Red: impure pasta layer
    $Q_{imp} = 1.5$ (outer crust)
    $Q_{imp} = 30$ (inner crust)
    $T_c = 2 \times 10^7$ K

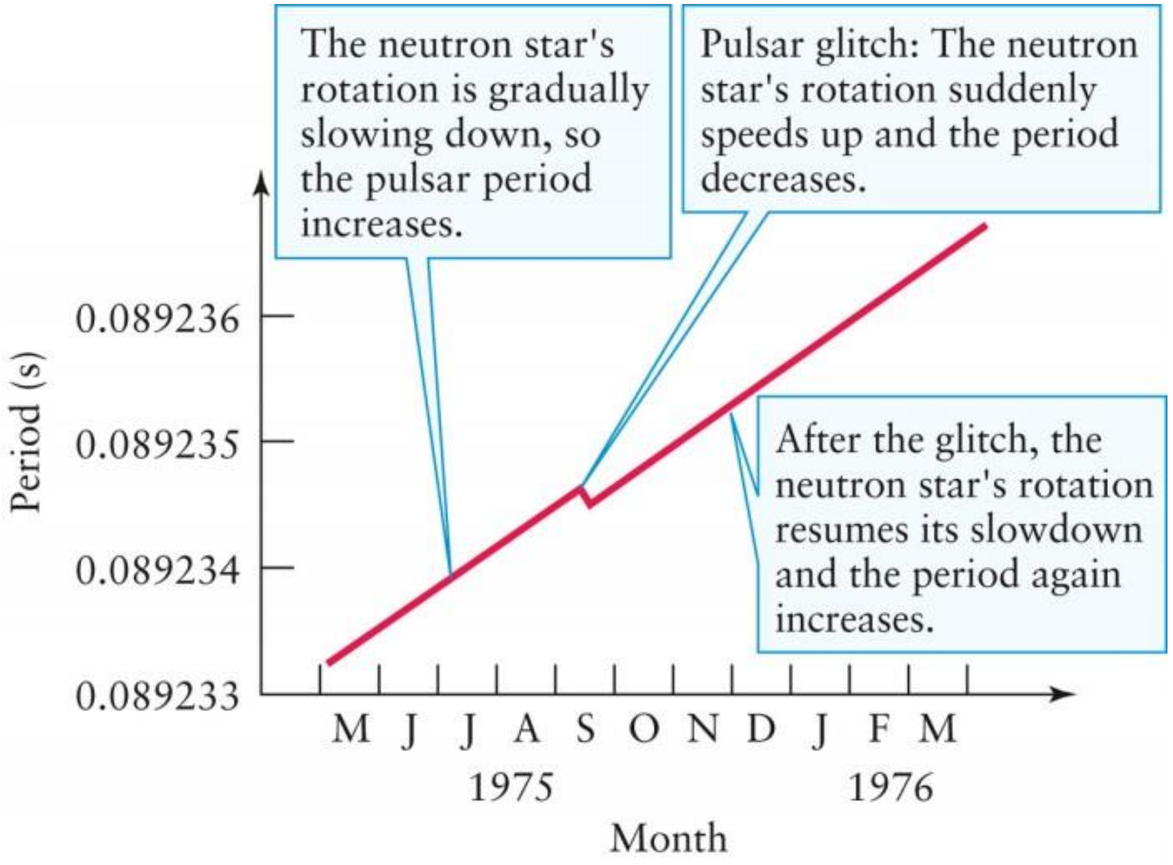



Horowitz et al (2015) PhysRevLett 114, 031102

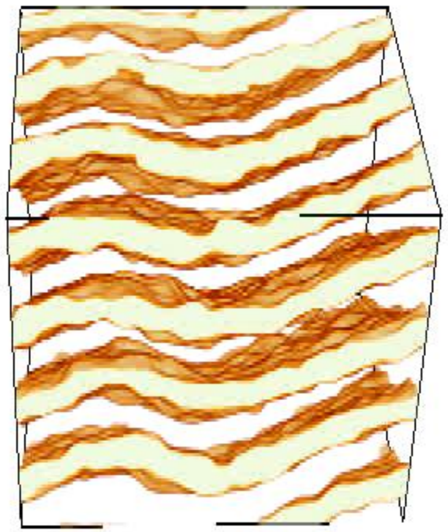
# Crust Breaking

# Pulsar Glitches

- Pulsars slowly *spin down,* their period gets longer
- Occasionally, they ‘glitch’ and start to spin faster
- Is this crust breaking? Is this a *starquake*?
- The breaking strain of the crust determines the frequency and ‘intensity’ of glitches



# Linear Elasticity



$$l_z = 100.80 \text{ fm}$$

$$l_x = l_y = 100.80 \text{ fm}$$

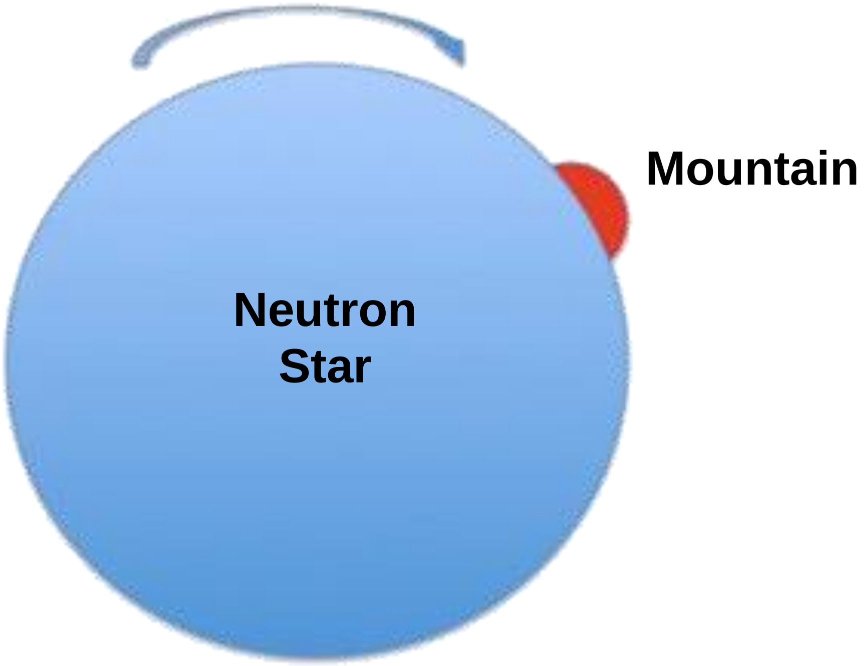
# Gravitational Waves

# Mountains

- What if the surface is lumpy? Are there mountains?
- Dense, fast lump produces ripples in spacetime

- How big can they be? A few centimeters?
- How long do they last?

- The pasta is the densest stuff, therefore, it’s the stiffest. Could pasta support mountains?

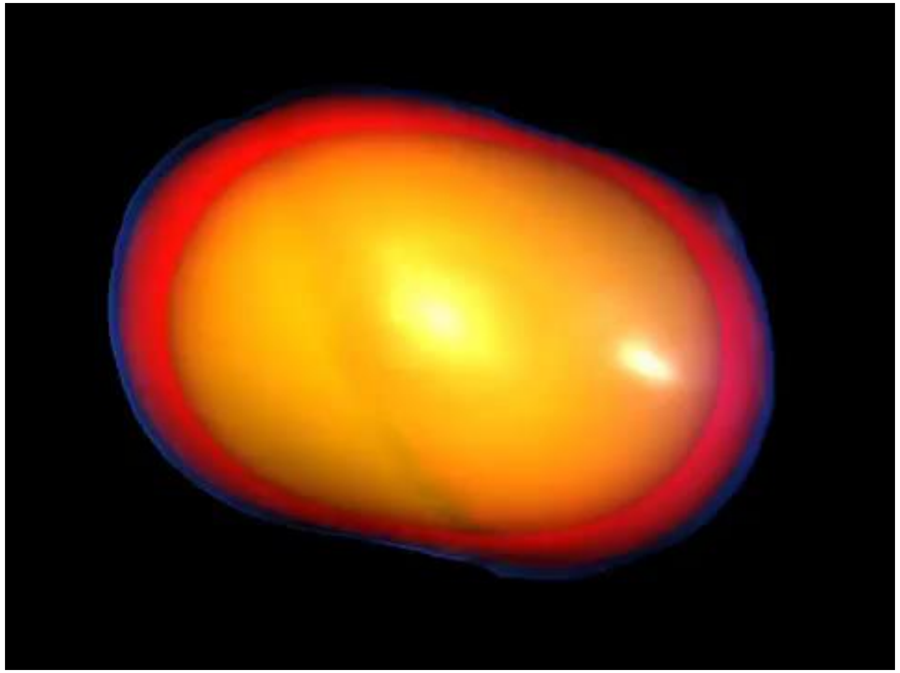


# R-mode instability

- *Rotational*-mode – toroidal oscillation of neutron star that is unstably driven by gravitational wave emission

$$\vec{u} = \left(w_l \hat{r} \times \nabla Y_{ll} + v_{l+1} \nabla Y_{l+1\ l} + u_{l+1} Y_{l+1\ l} \hat{r}\right) e^{i\omega t}$$

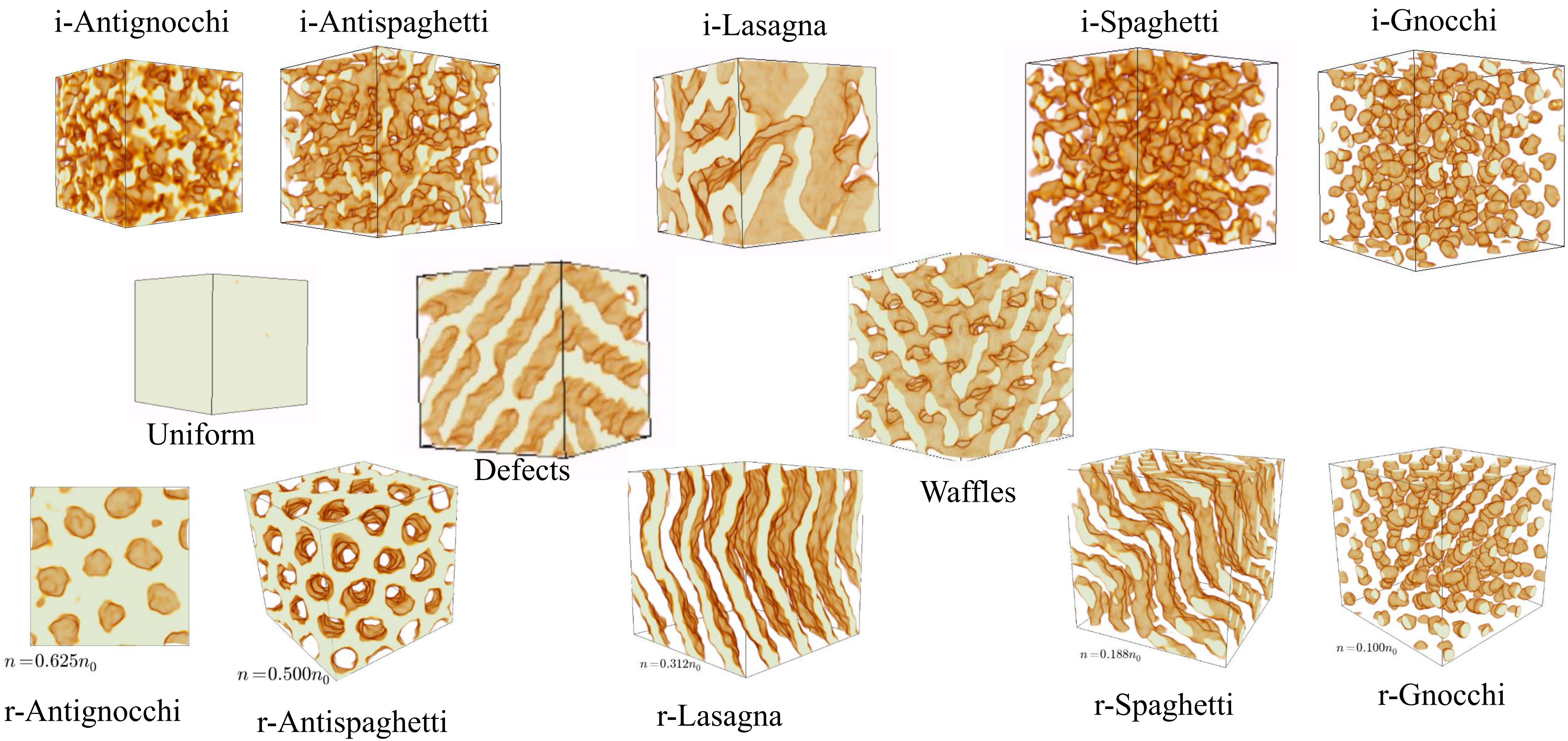
- Primarily the *l=m=2* mode
- Solution: Is the damping from the crust enough to stabilize the star?



Source: LSU_Astrophysics

# Phase Diagrams

# Phases


i-Antignocchi
i-Antispaghetti
i-Lasagna
i-Spaghetti
i-Gnocchi
Uniform
Defects
Waffles
$n = 0.625n_0$
$n = 0.500n_0$
$n = 0.312n_0$
$n = 0.188n_0$
$n = 0.100n_0$
r-Antignocchi
r-Antispaghetti
r-Lasagna
r-Spaghetti
r-Gnocchi

# "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 |

0

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

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

- 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 |
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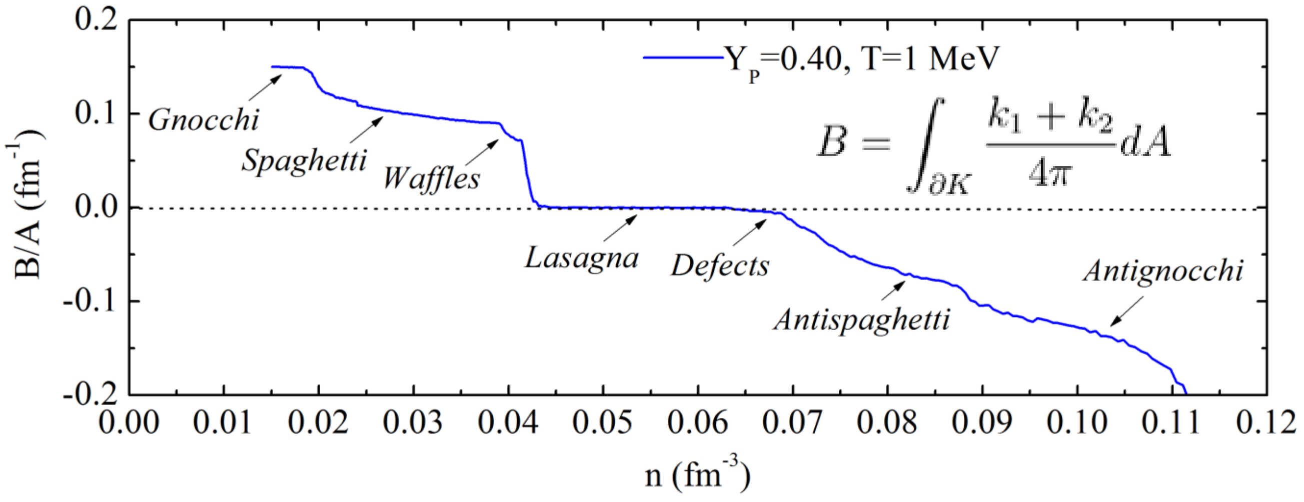
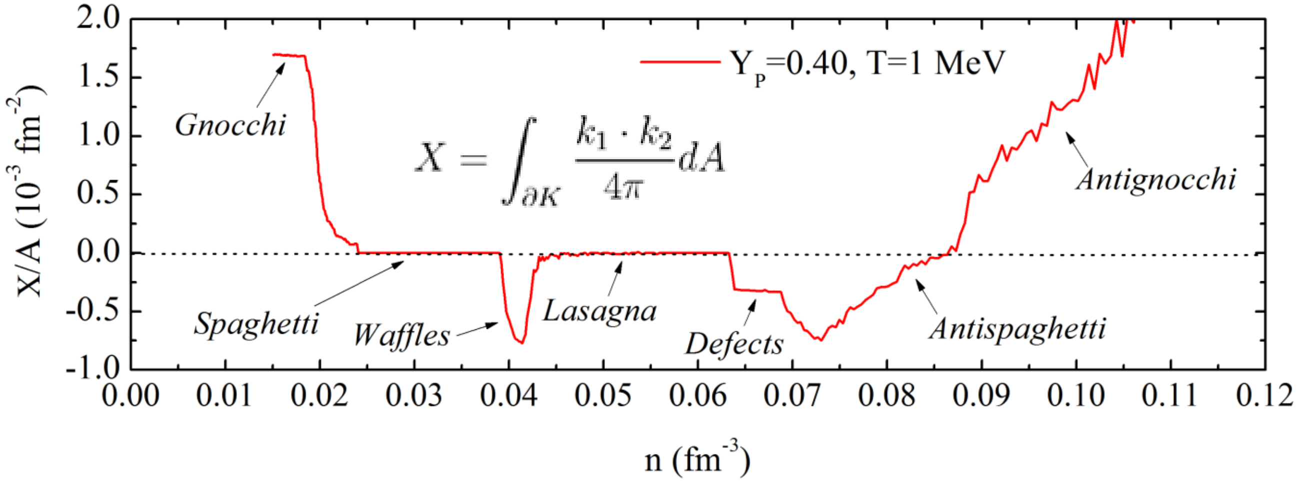
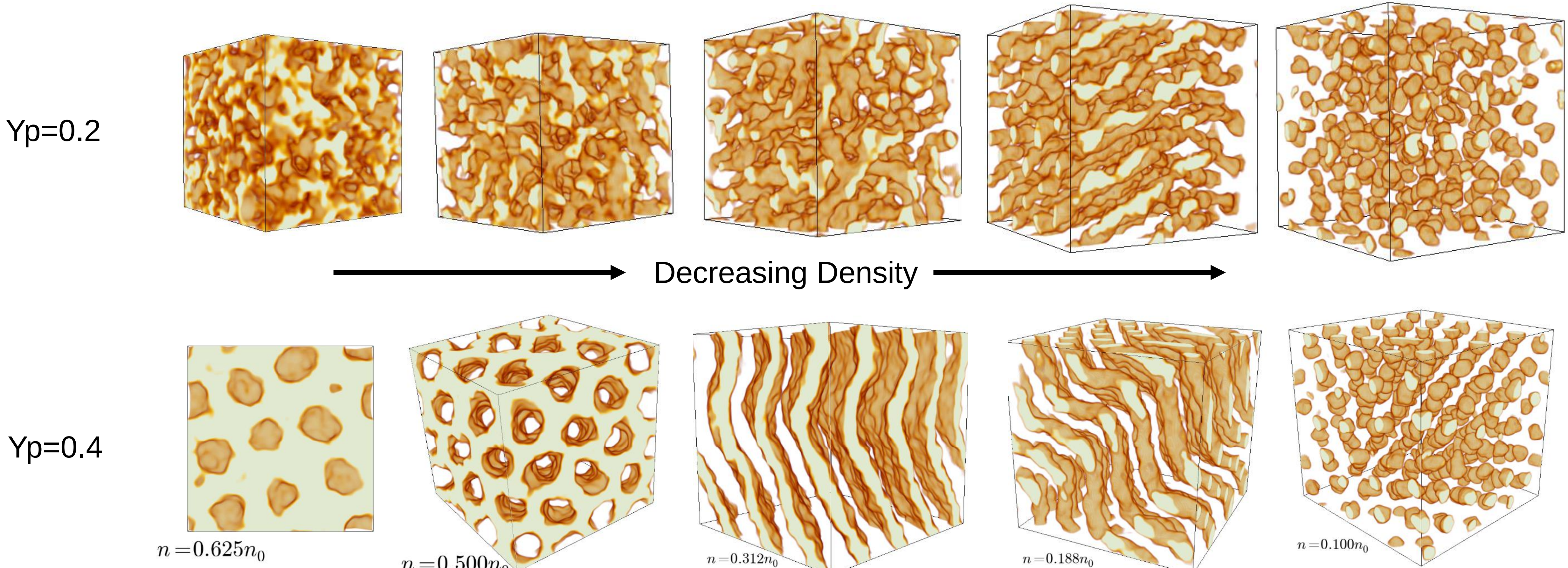
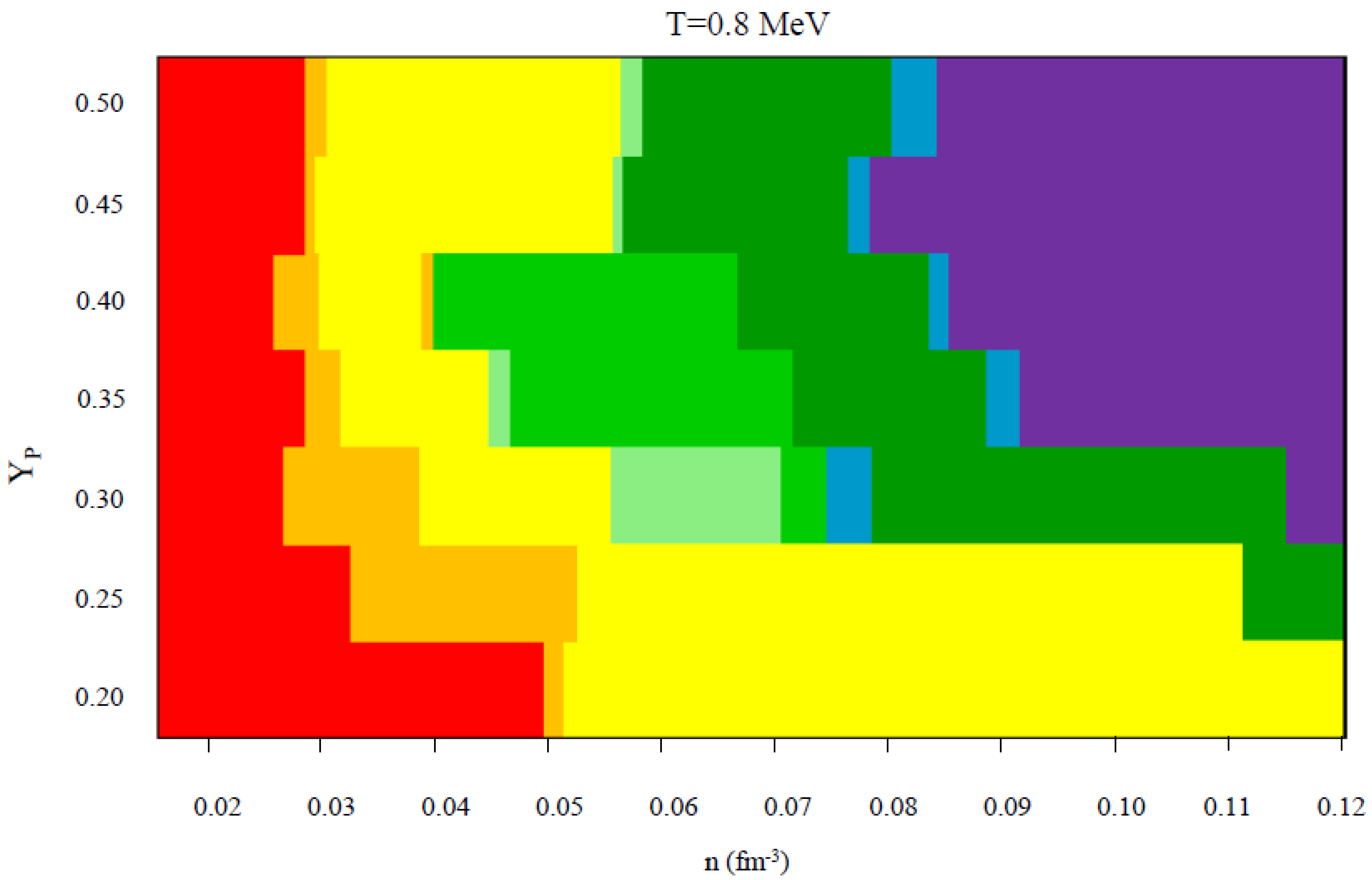


# Phase Diagrams

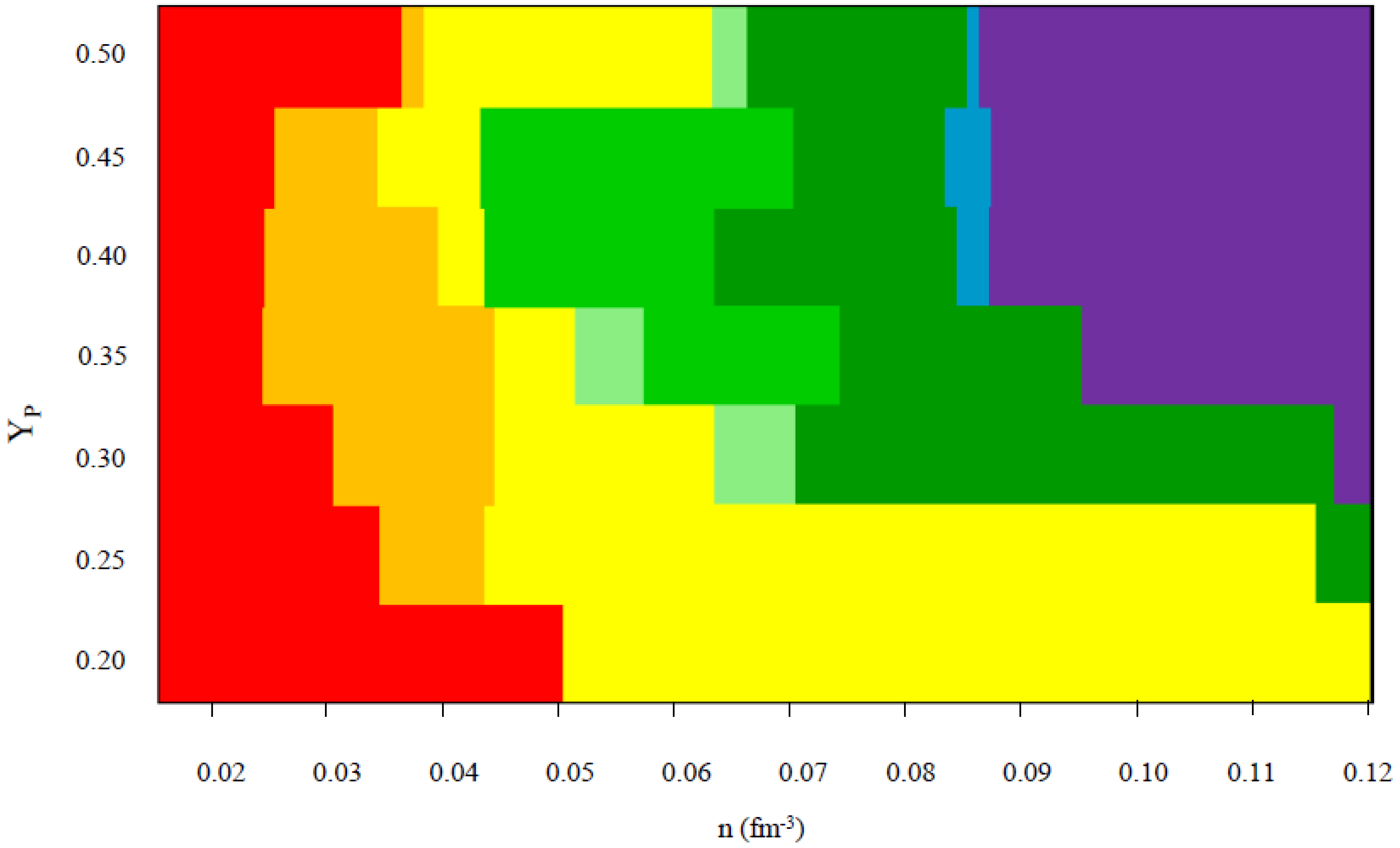
- Simulate pasta with constant temperature and proton fraction
- Observe phase transitions as a function of density



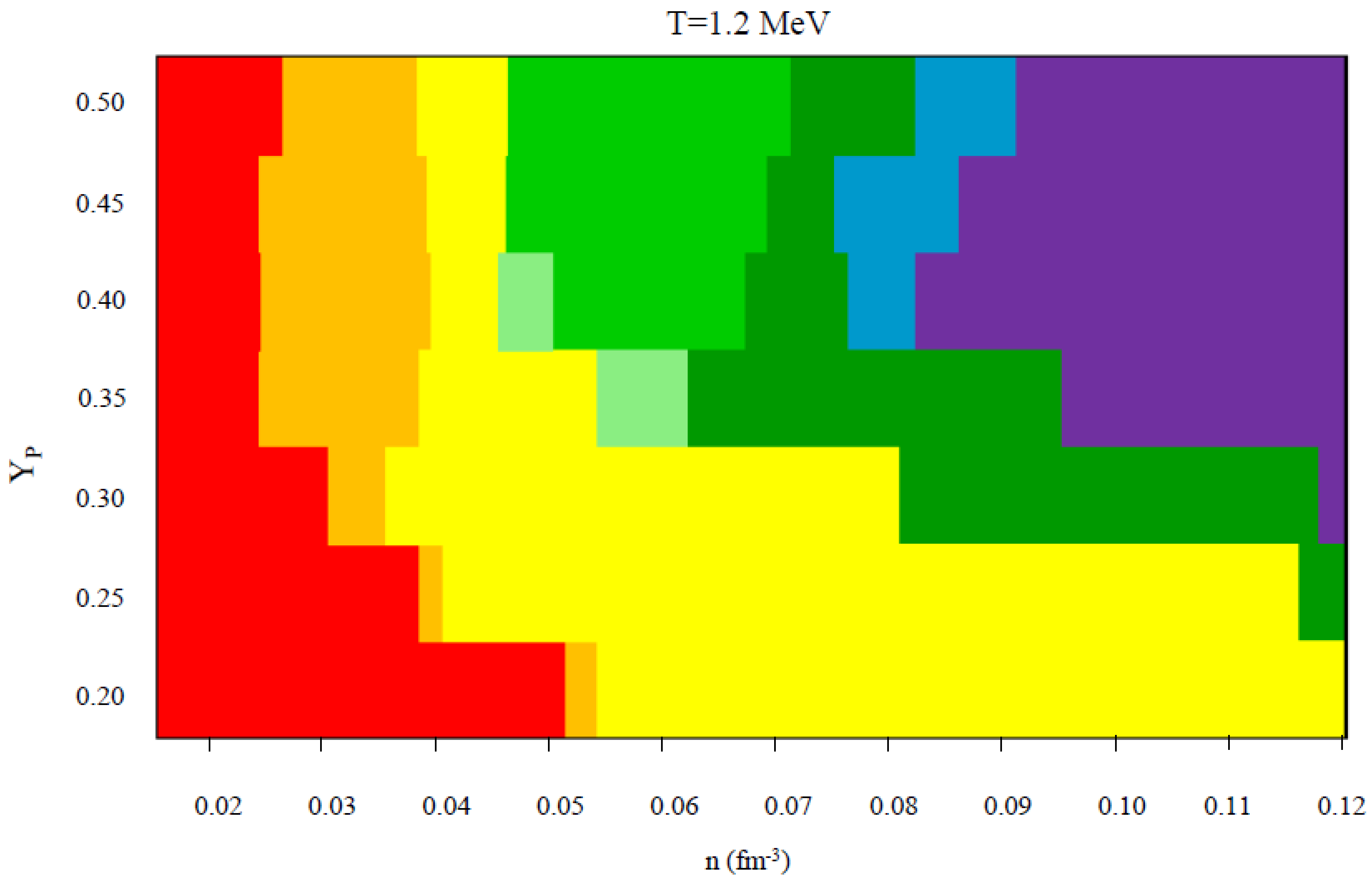



| | $B < 0$ | $B \sim 0$ | $B > 0$ |
|---|---|---|---|
| $\chi > 0$ | sph b | | sph |
| $\chi \sim 0$ | rod-1 b | slab | rod-1 |
| $\chi < 0$ | rod-2 b | rod-3 | rod-2 |

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 |



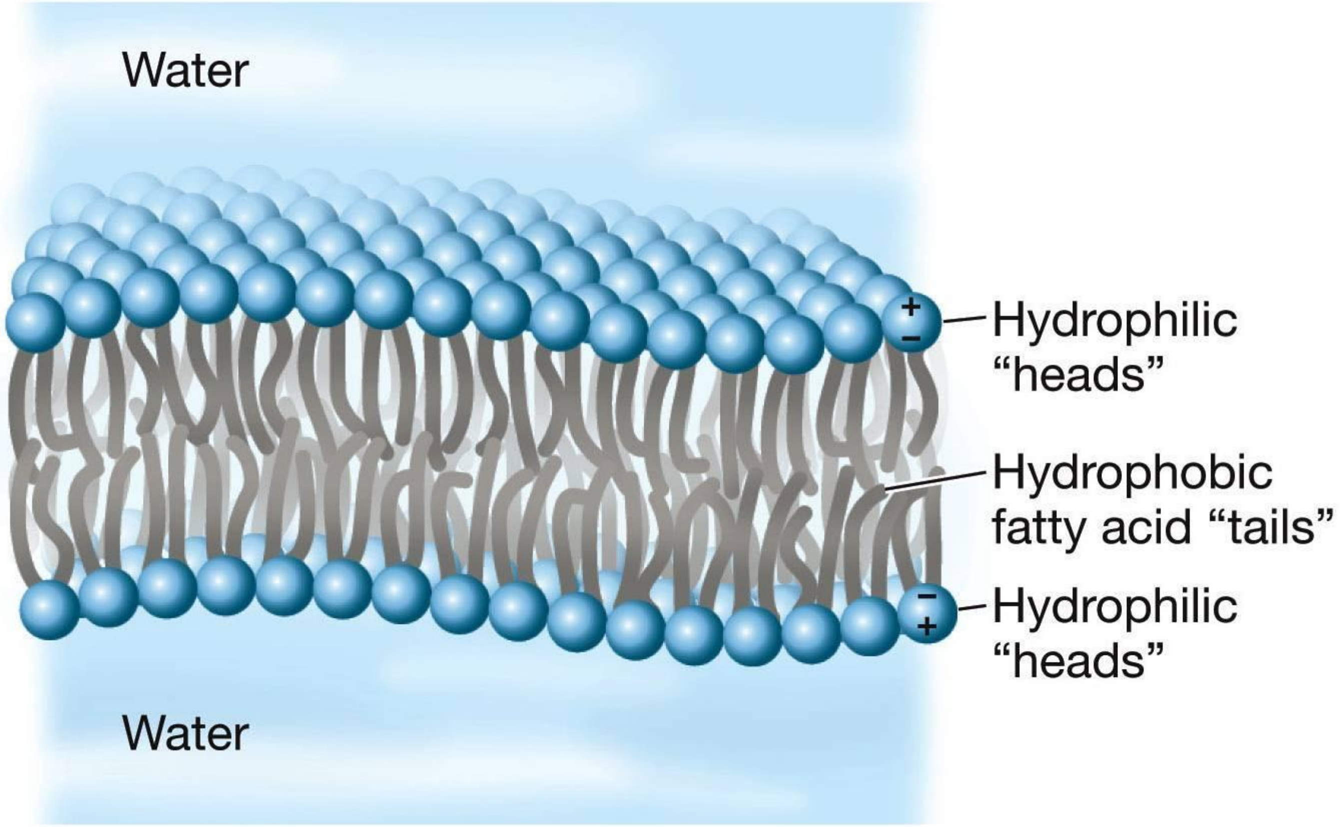

| | $B < 0$ | $B \sim 0$ | $B > 0$ |
|---|---|---|---|
| $\chi > 0$ | sph b | | sph |
| $\chi \sim 0$ | rod-1 b | slab | rod-1 |
| $\chi < 0$ | rod-2 b | rod-3 | rod-2 |

# Soft Matter

# Self Assembly

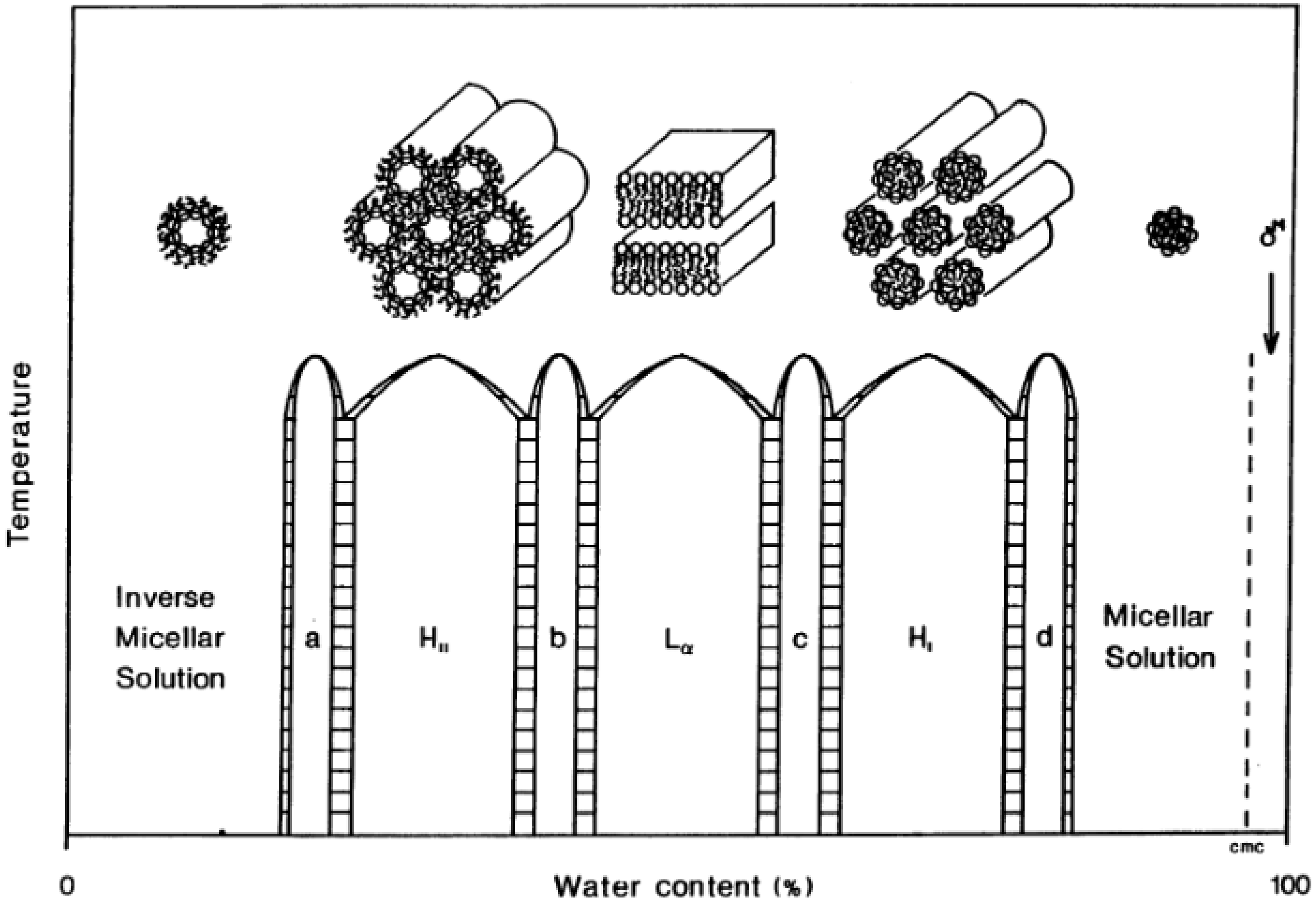
- Well studied in phospholipids: hydrophilic heads and hydrophobic tails self assemble in an aqueous solution

(B) Phospholipid bilayer




LIFE 8e, Figure 3.20 (Part 2)

# Self Assembly




Seddon, BBA 1031, 1–69 (1990)

*Shape of Nuclei in the Crust of Neutron Star*

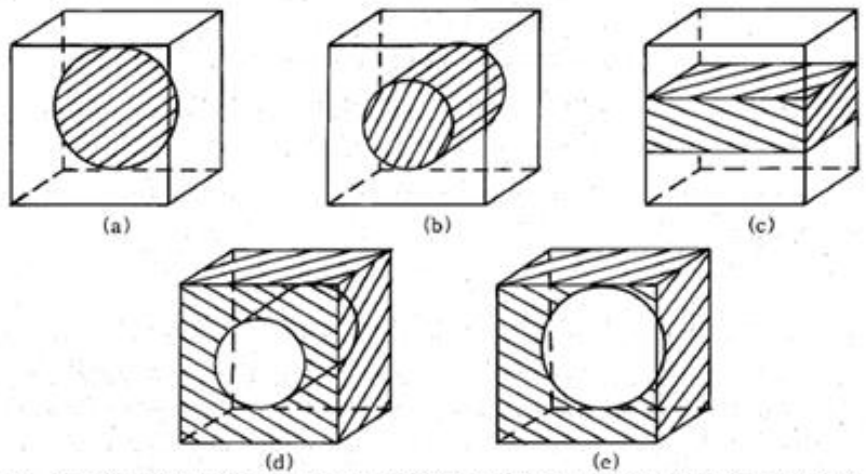
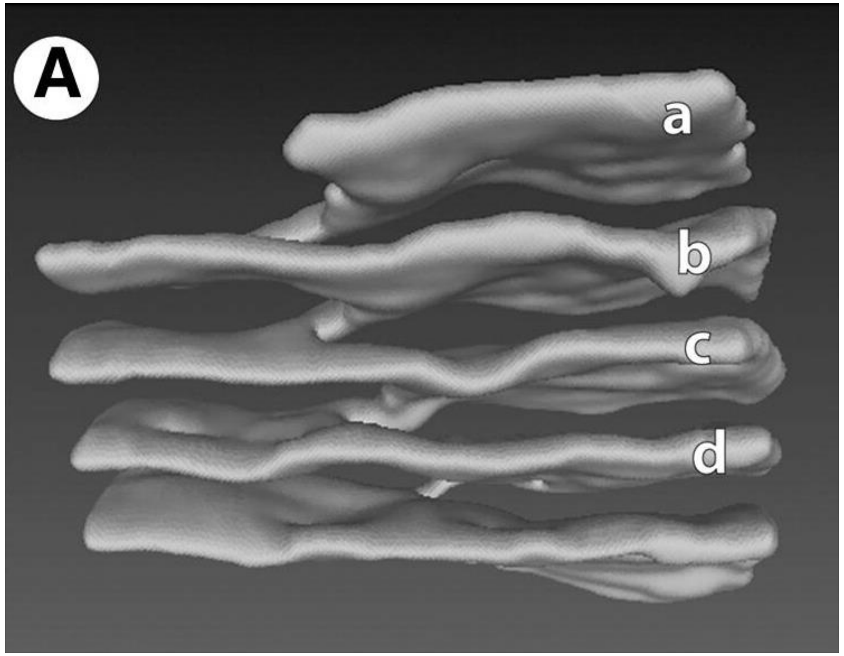


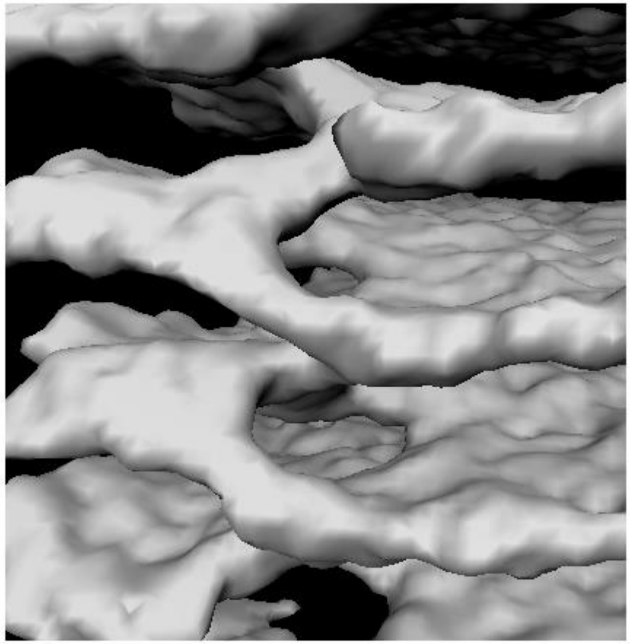

Fig. 1. Candidates for nuclear shapes. Protons are confined in the hatched regions, which we call nuclei. Then the shapes are, (a) sphere, (b) cylinder, (c) board or plank, (d) cylindrical hole and (e) spherical hole. Note that many cells of the same shape and orientation are piled up to form the whole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



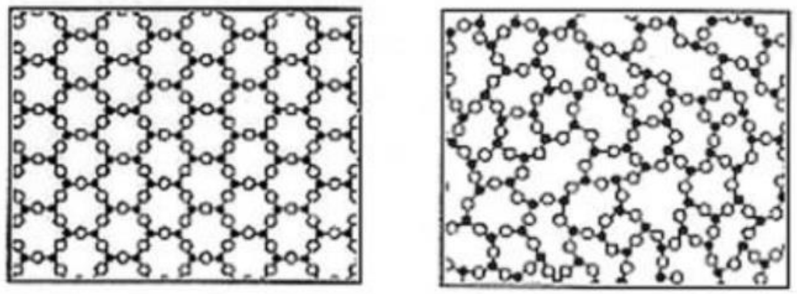
Horowitz et al, PRL.114.031102 (2015)

- Right: Defects in nuclear pasta MD simulations

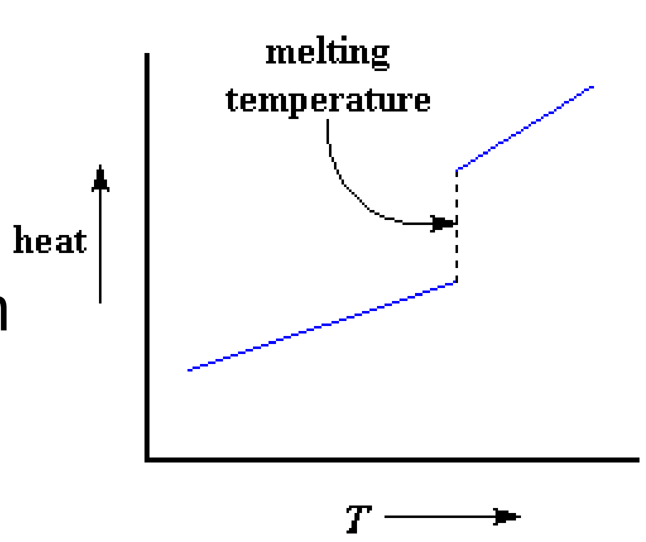
Parking Garage Structures in astrophysics and biophysics (arXiv:1509.00410)

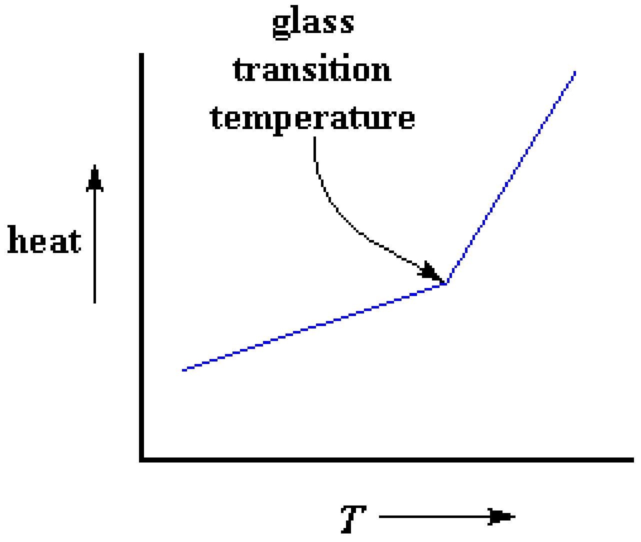
# Glass Transition

- Glass transition – impure substance forms an amorphous solid when quenched
- Solid:
  - Long Range Order
  - Nondiffusive
  - First order phase transition
- Glass:
  - Short range order
  - Low diffusion
  - Second order phase transition



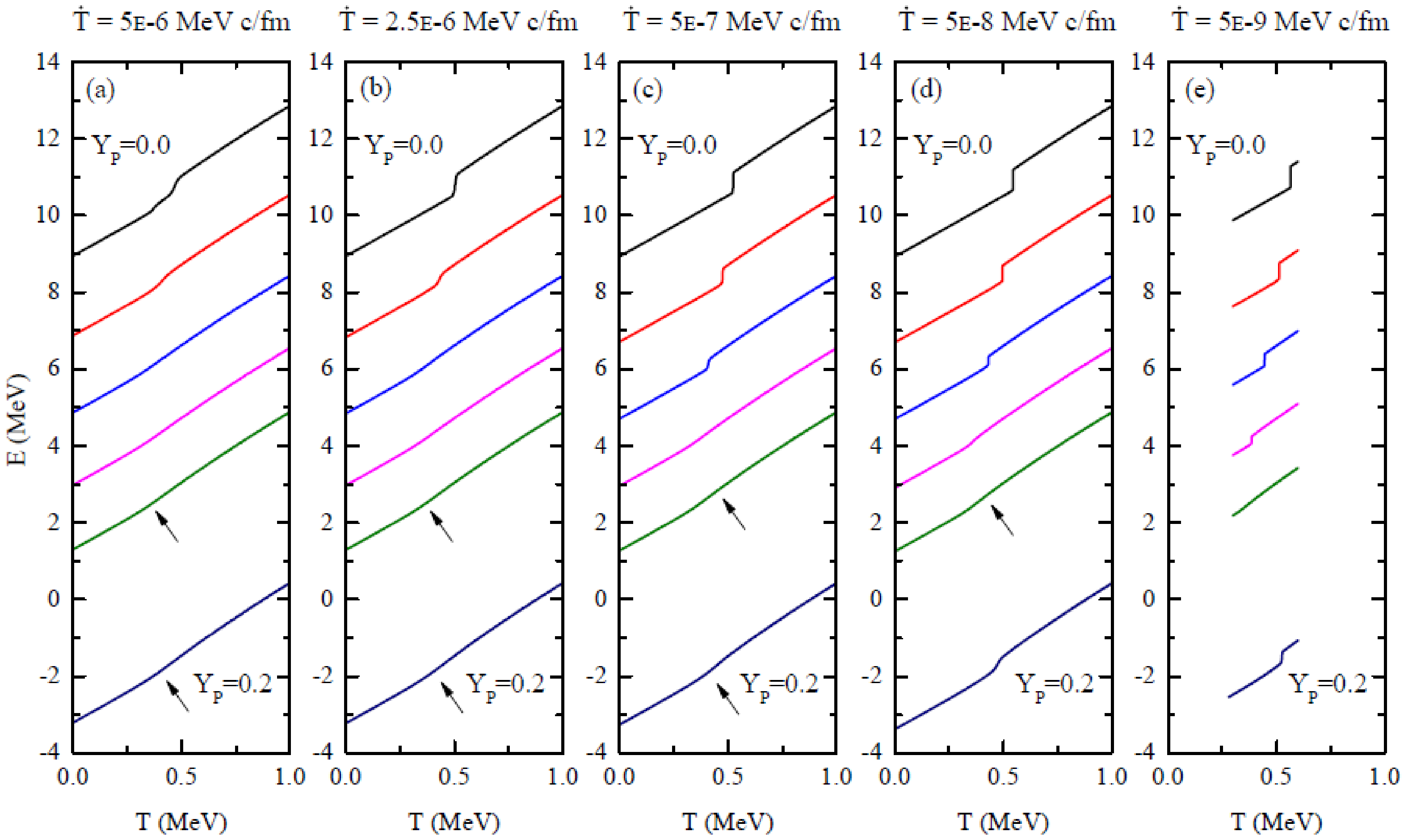
Crystal (e.g. quartz)    Glass (e.g. silica glass)



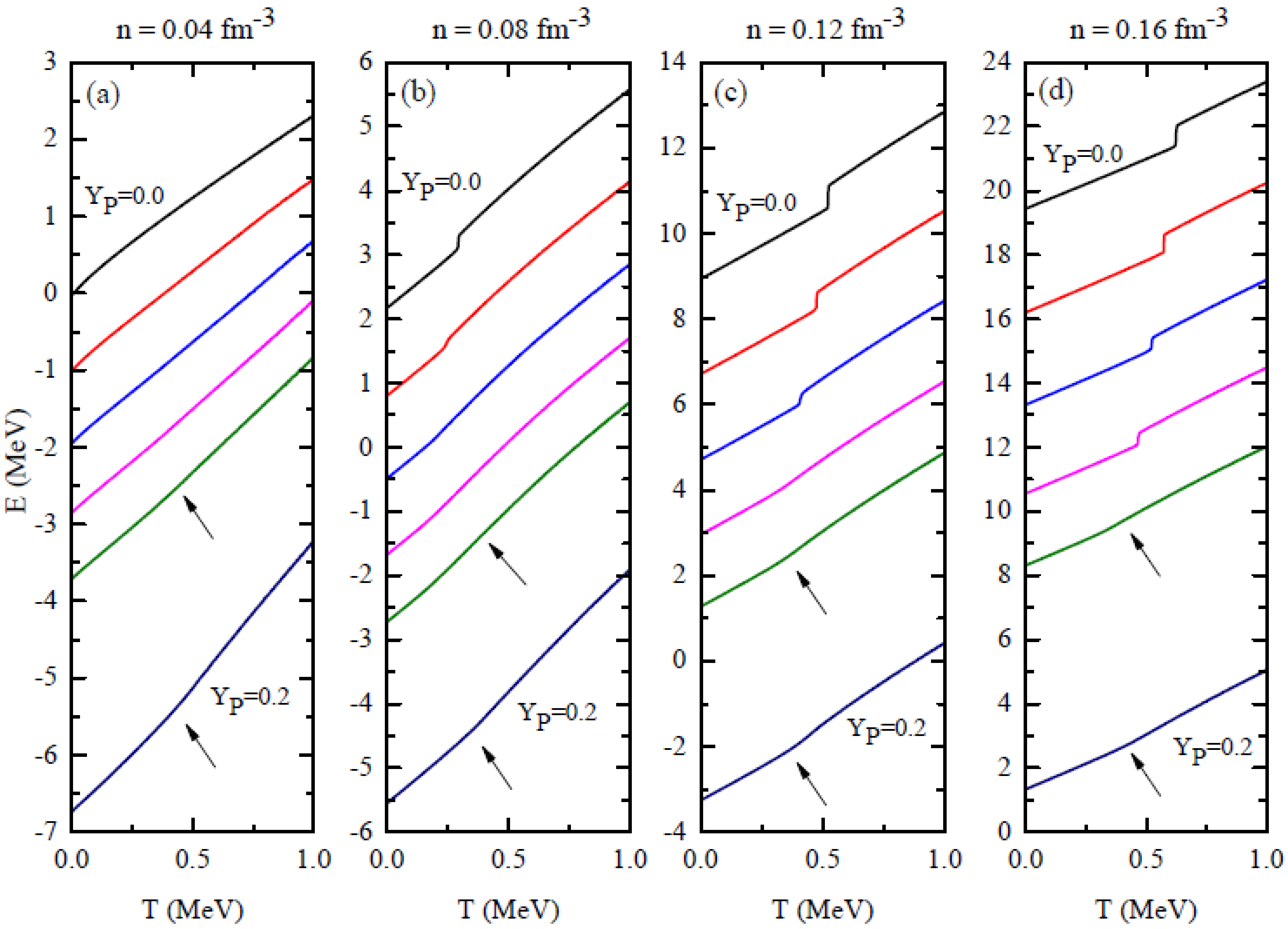



# Quench Rate

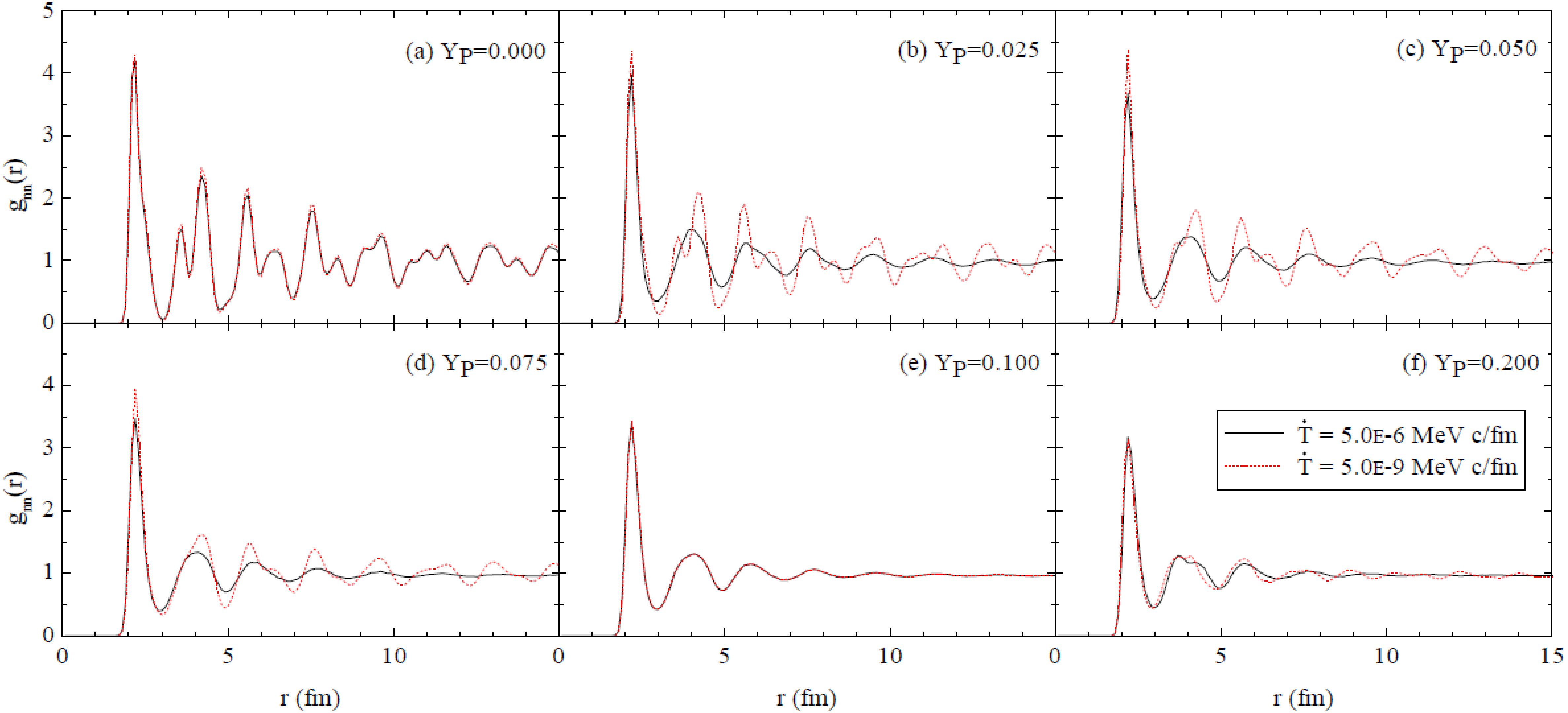
- Cooling quickly and cooling slowly
- Proton fractions: $Y_P = 0.0 – 0.2$
- Density: $n = 0.12\ fm^{-3}$



# Glassy Systems



# Glassy Systems



# Summary

- Neutron stars contain exotic materials which must be studied in order to understand the physical properties and interpret observations of neutron stars
  - Hard astromaterials: Coulomb crystals, such as in the rp-ash
  - Soft astromaterials: Nuclear pasta, at the base of the crust