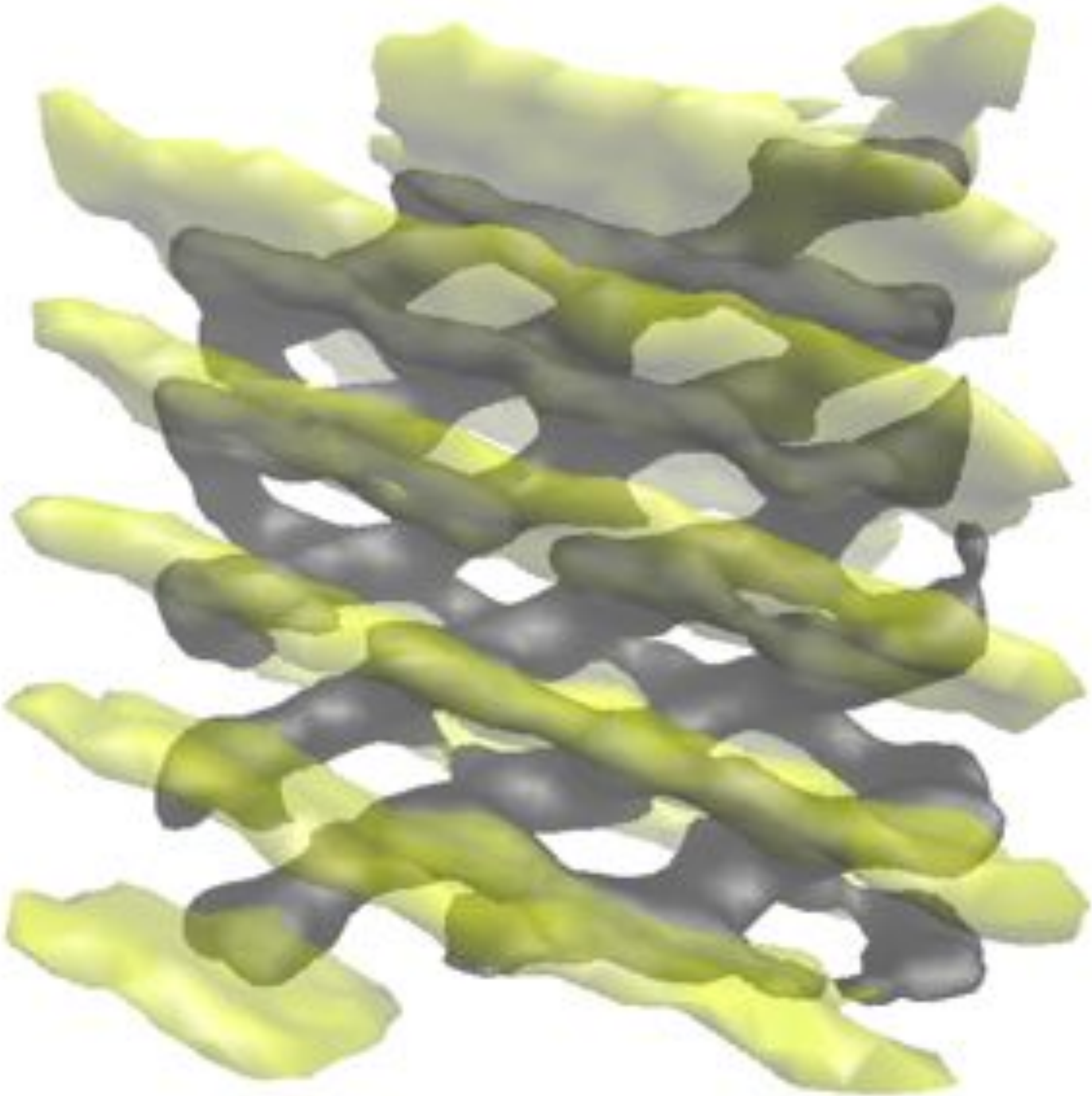
Defects in Nuclear Pasta



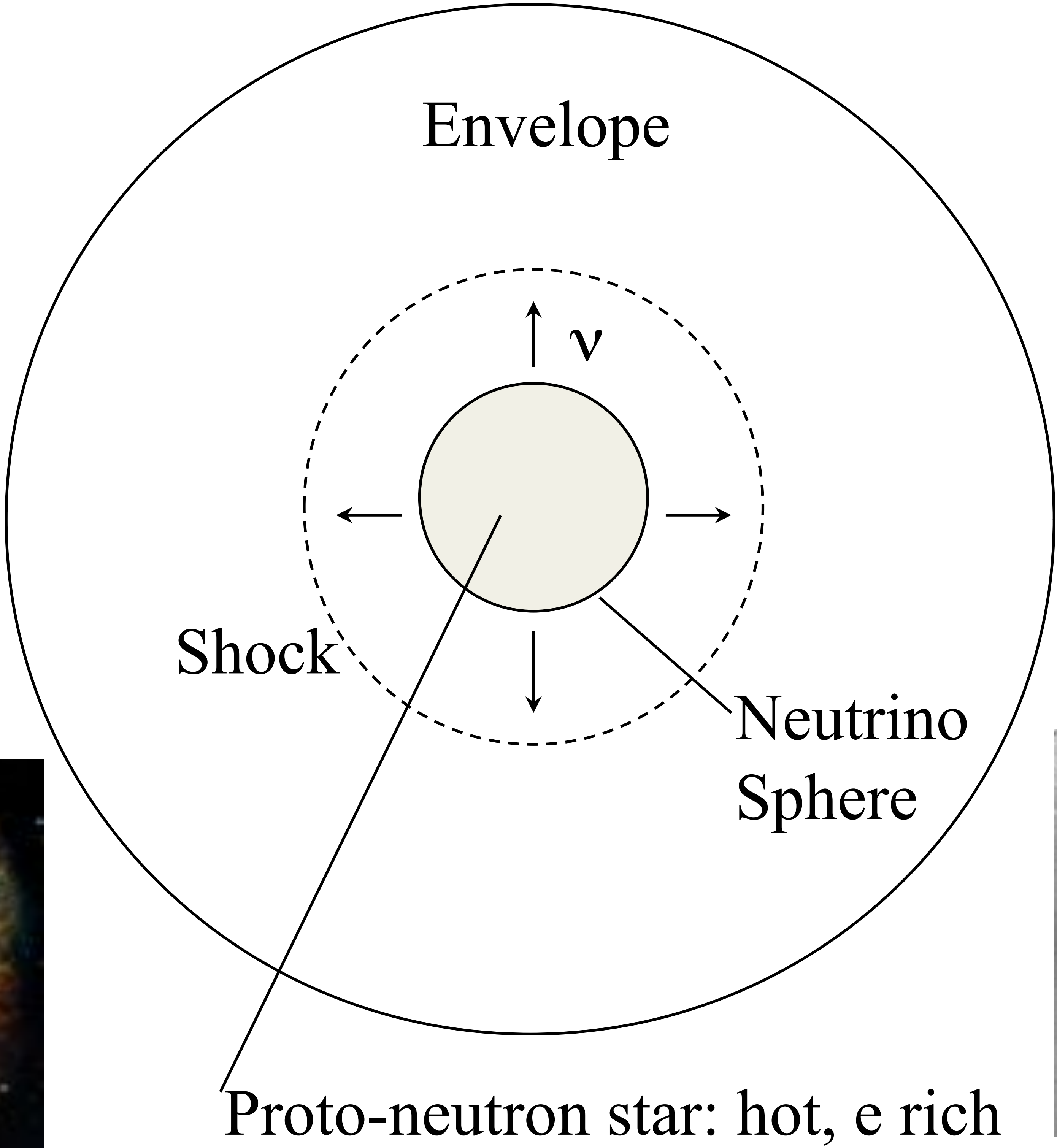
C. J. Horowitz, Indiana University
Computational Challenges … , Stockholm, Sep. 2014

Nuclear Pasta

- Nuclear matter, at somewhat below ρ_0, forms complex shapes because of competition between short range nuclear attraction and long range Coulomb repulsion —> "Coulomb frustration".
- Gravitational collapse during SN increases density: nuclei -> nuclear pasta -> uniform nuclear matter -> neutron star.
- Nuclear pasta expected in neutron stars at base of crust about 1 km below surface at ~1/3ρ_0.
- During NS merger tidal excitation decreases density: uniform nuclear matter -> nuclear pasta -> nuclei + n -> r-process.
- **Quantum density functional** calculations. [Sergey Postnikov, Irina Sagert]
- **Semiclassical molecular dynamics model**: $v(r)=a\, e^{-r^2/\Lambda} + b_{ij}\, e^{-r^2/2\Lambda} + e_i e_j\, e^{-r/\lambda}/r$ Parameters of short range interaction fit to binding E and density of nuclear matter. [Andre Schneider]

NS Born in Core Collapse Supernovae

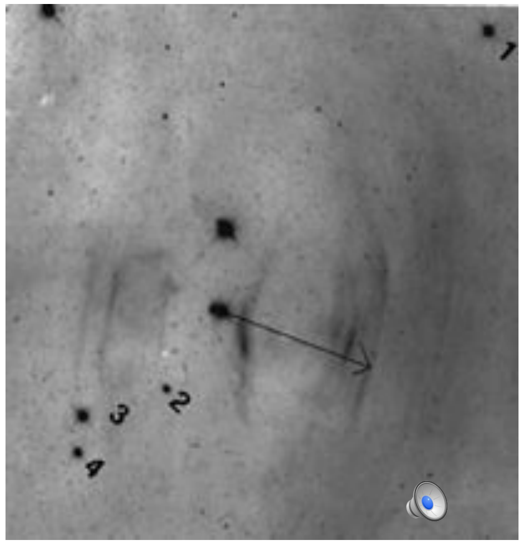
Core of massive star collapses to form proto-neutron star. νs form neutron star energizes shock that ejects outer 90% of star.



July 5, 1054

Crab nebula

Crab Pulsar

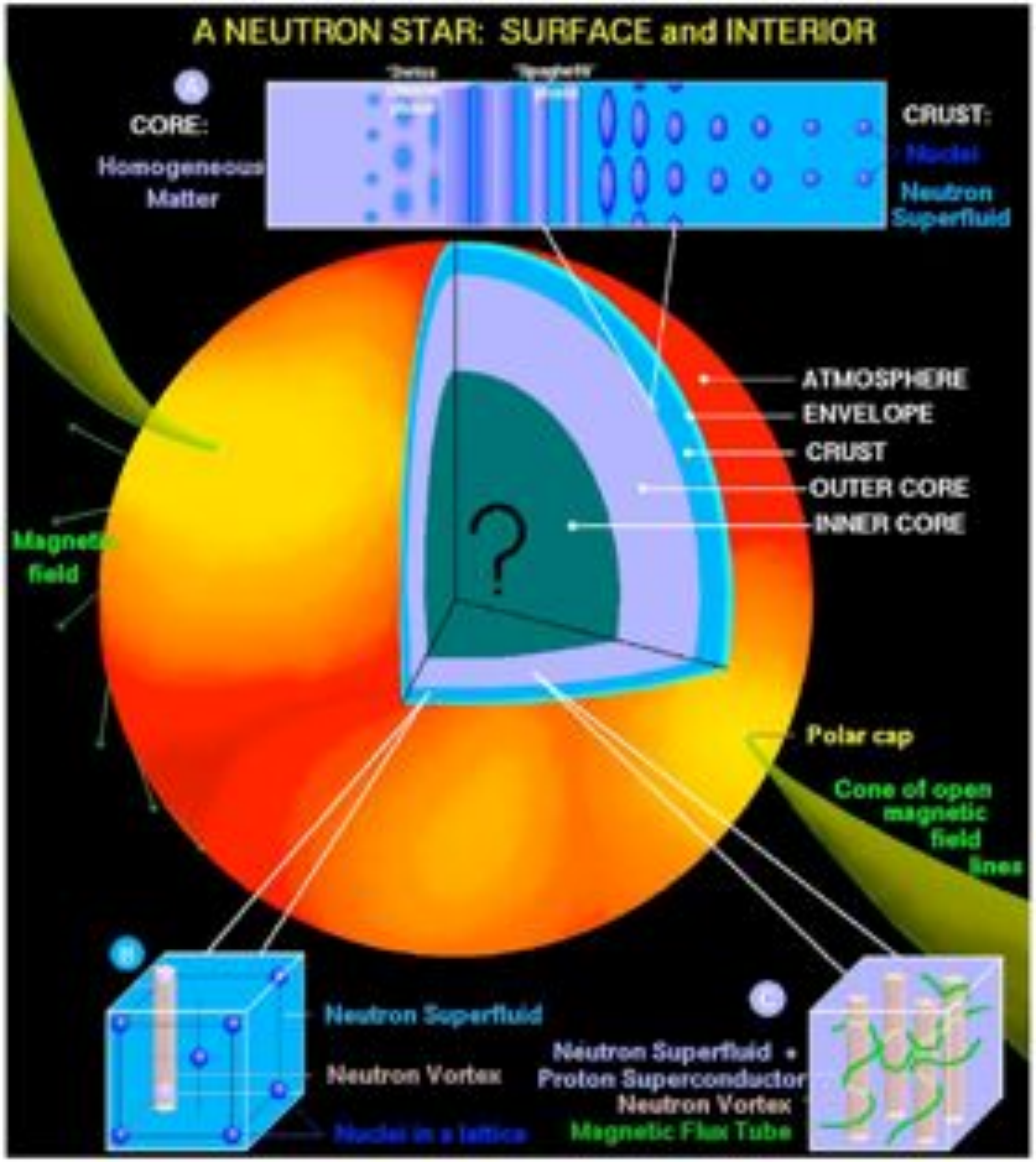


Hubble ST

Audio: Jordal Bank

Neutron stars

- Mass ~1.4 M_{sun}, Radius ~10 km
- Solid crust ~ 1km thick over liquid (outer) core of neutron rich matter.
- Possible exotic phase in center: de-confined quark matter, strange matter, meson condensates, color superconductor...
- Structure determined by Equation of State (pressure vs density) of n rich matter.
- Hyperons could reduce p at high densities but not too much or collapse to black hole. Repulsive three body forces could limit hyperon effects.
- Figure: **Dany Page,** UNAM

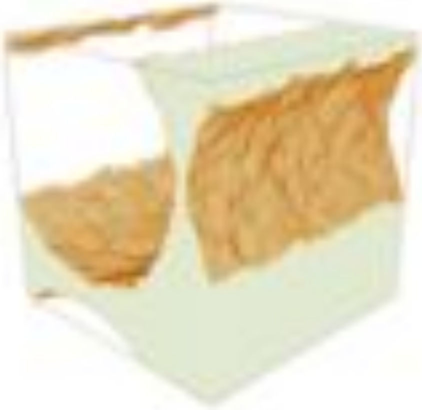
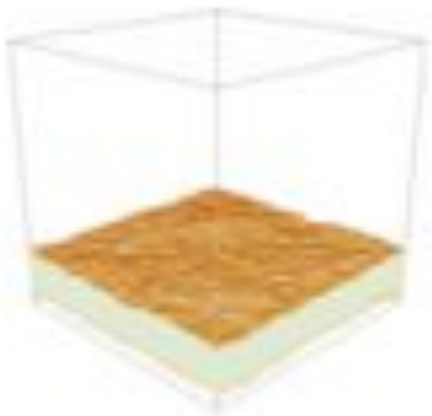


$v(r) = a\, e^{-r^2/\Lambda} + b_{ij}\, e^{-r^2/2\Lambda} + e_i e_j\, e^{-r/\lambda}/r$

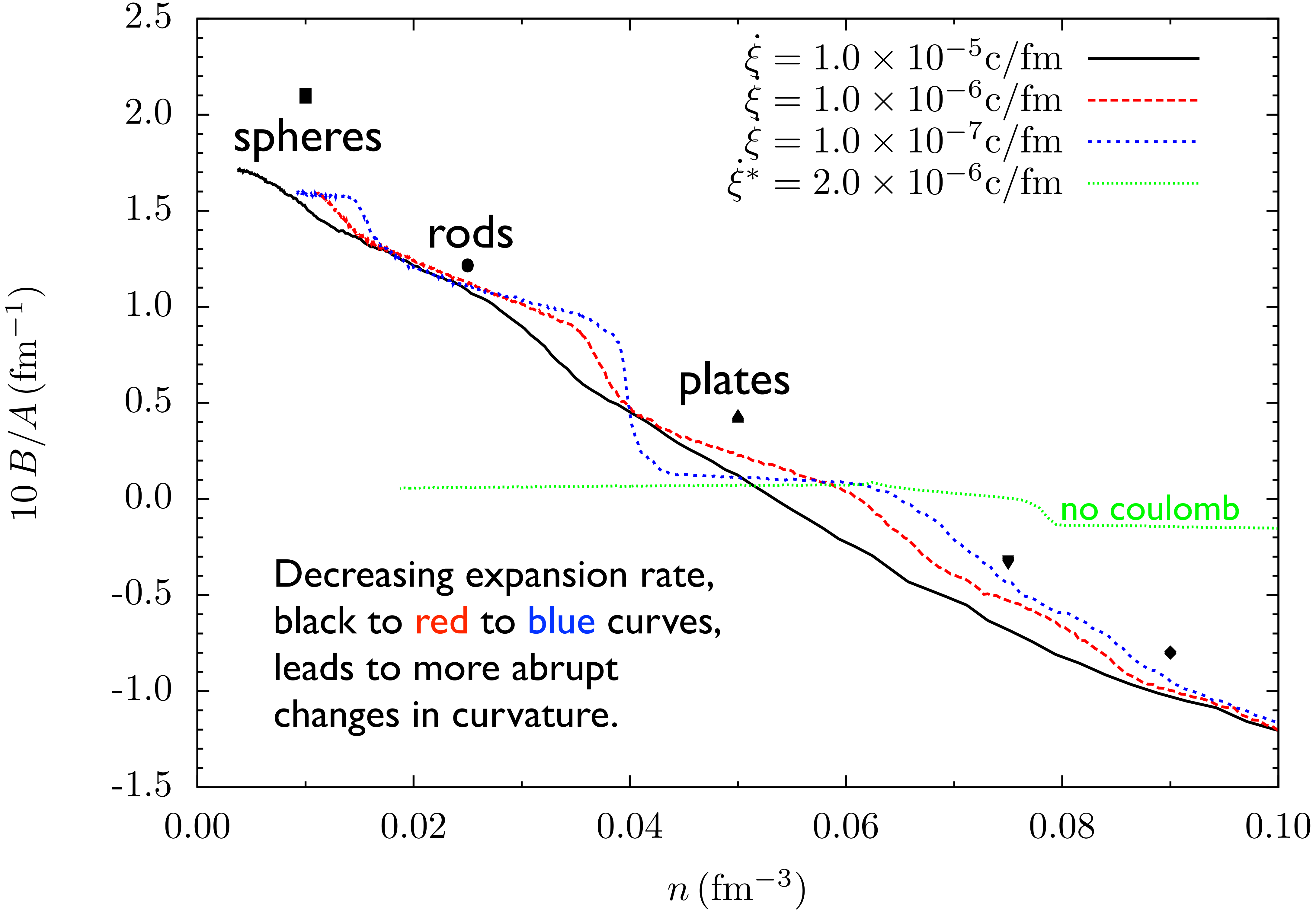
51200
nucleons,
Y_p=0.4,
T=1 MeV,
λ=10 fm,
ξ=2x10^{-8}
c/fm,
L_0=80 fm

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

Andre Schneider

$n\,(\text{fm})^{-3}$	$\dot{\xi} = 1.0 \times 10^{-6}\,\text{c/fm}$ No Coulomb	Constant Density	$\dot{\xi} = 1.0 \times 10^{-5}\,\text{c/fm}$	$\dot{\xi} = 1.0 \times 10^{-7}\,\text{c/fm}$
0.090				
0.050				
0.025				
0.010				

Average curvature of pasta shapes

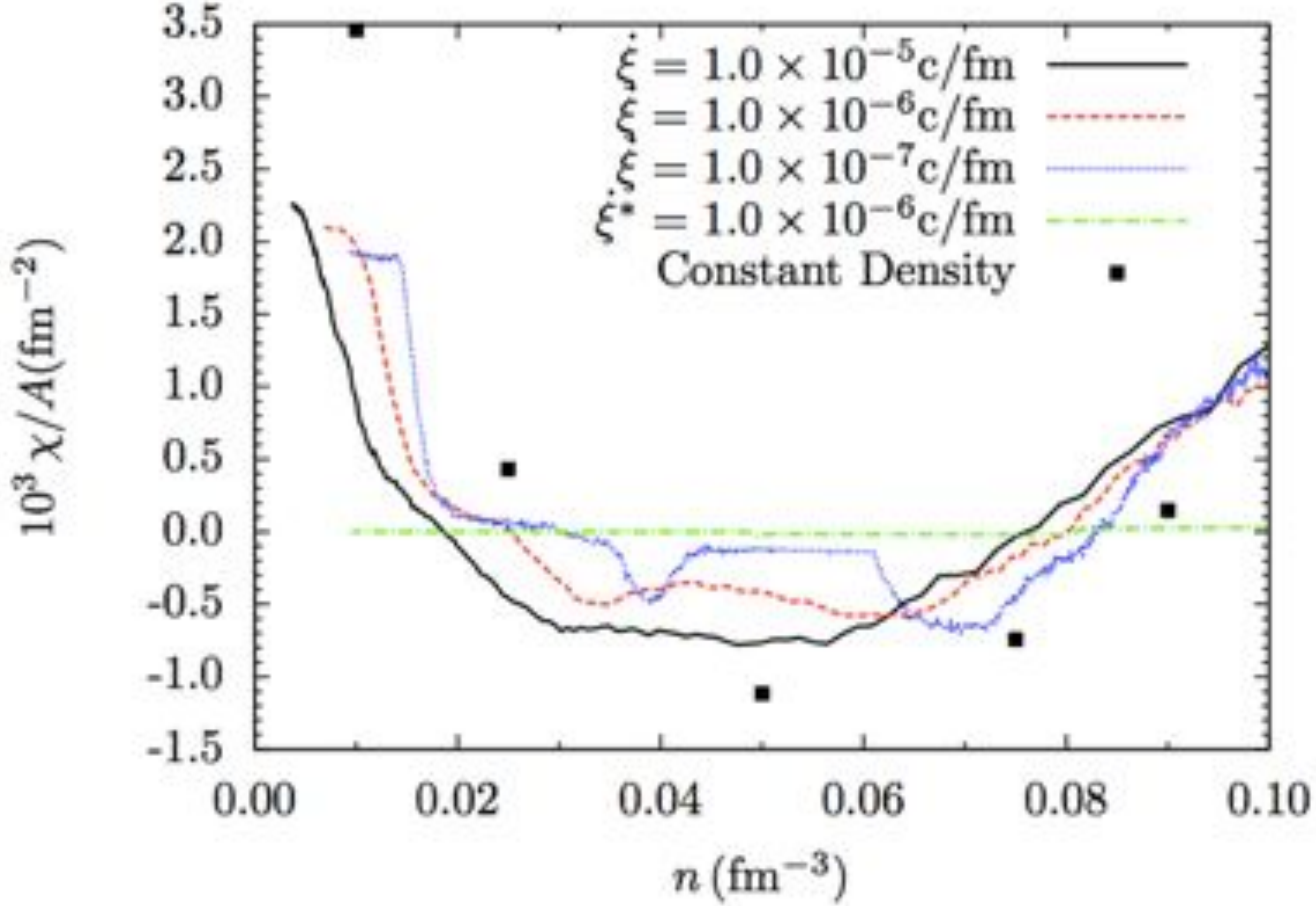


Decreasing expansion rate, black to red to blue curves, leads to more abrupt changes in curvature.

- Average curvature vs density. Abrupt transitions for slow expansion suggest series of first order phase transitions.

Minkowski functionals to characterize shapes

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

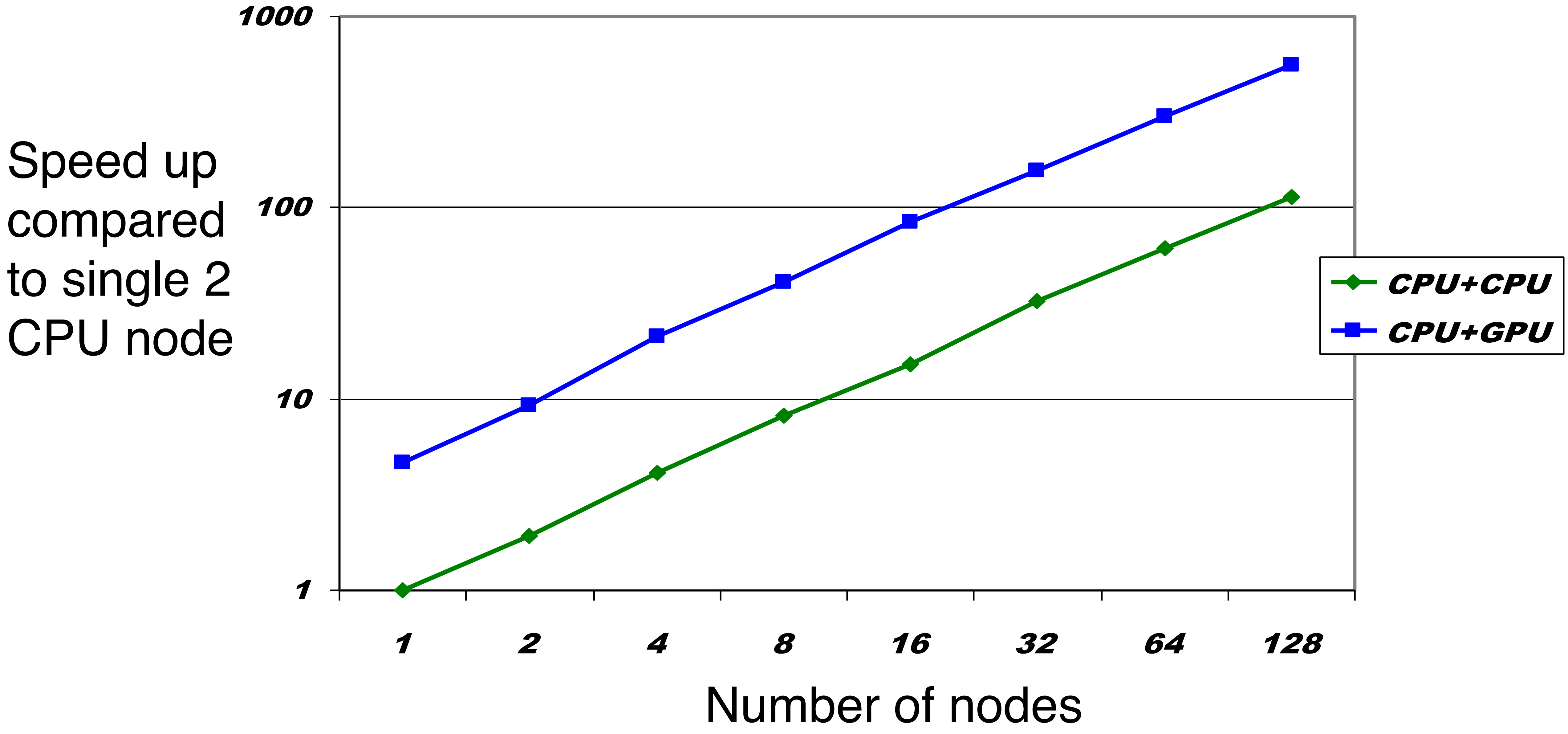


MD code IUMD

- Use GPUs for calculation of long range screened coulomb interactions. [Fast multipole expansions could improve code for very large systems (but complicated to scale to many GPUs?)]
- Short range nuclear interaction calculated on CPUs with nearest neighbor lists (or localized cubes).
- MPI+OpenMP+CUDA for GPU accelerated multiple nodes. GPUs do coulomb and CPUs do nuclear force concurrently.

Don Berry

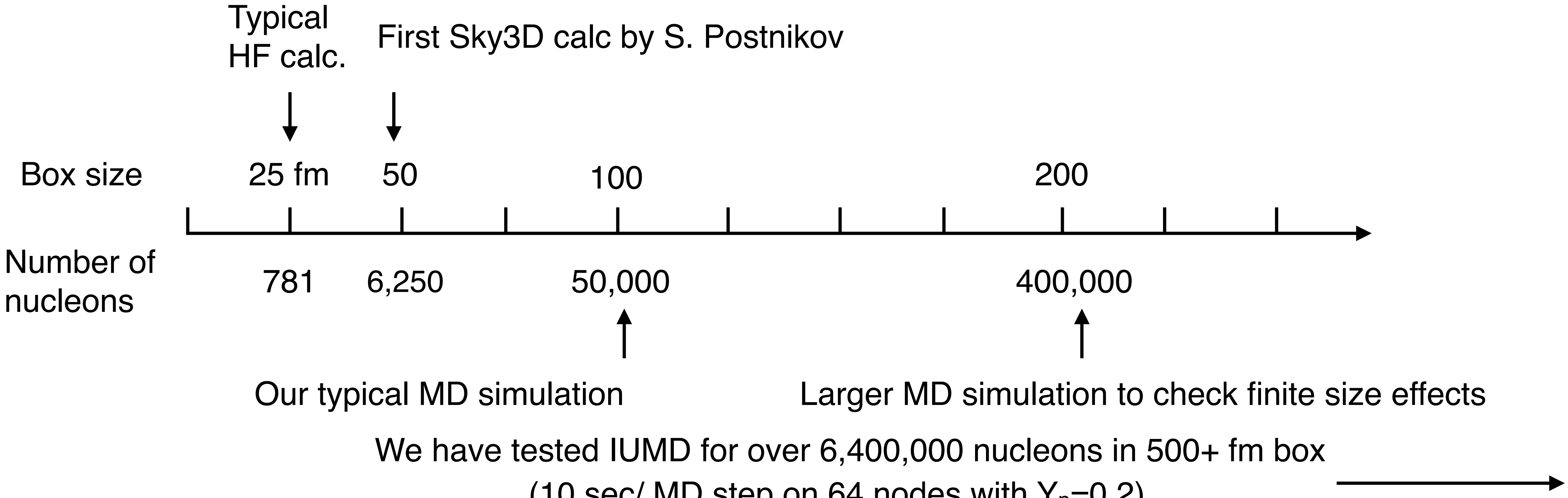
Scaling on Big Red II a Cray XE6/XK7



- Speed up compared to performance on a single 2 CPU node (with 32 cores) for pasta simulation with 409,600 particles.
- Each GPU node (with 16 core CPU+GPU) has about 5 times performance of a 2 CPU node.

Simulation Size

- Use computational advances to simulate larger systems, for longer times, and or calculate more complicated observables.
- At typical pasta density $\rho=0.05\ \mathrm{fm}^{-3}$ $(1/3\rho_0)$



Typical HF calc.

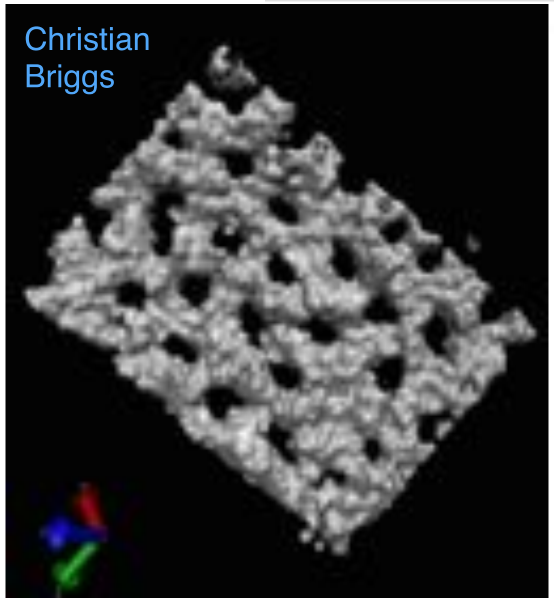
First Sky3D calc by S. Postnikov

Our typical MD simulation

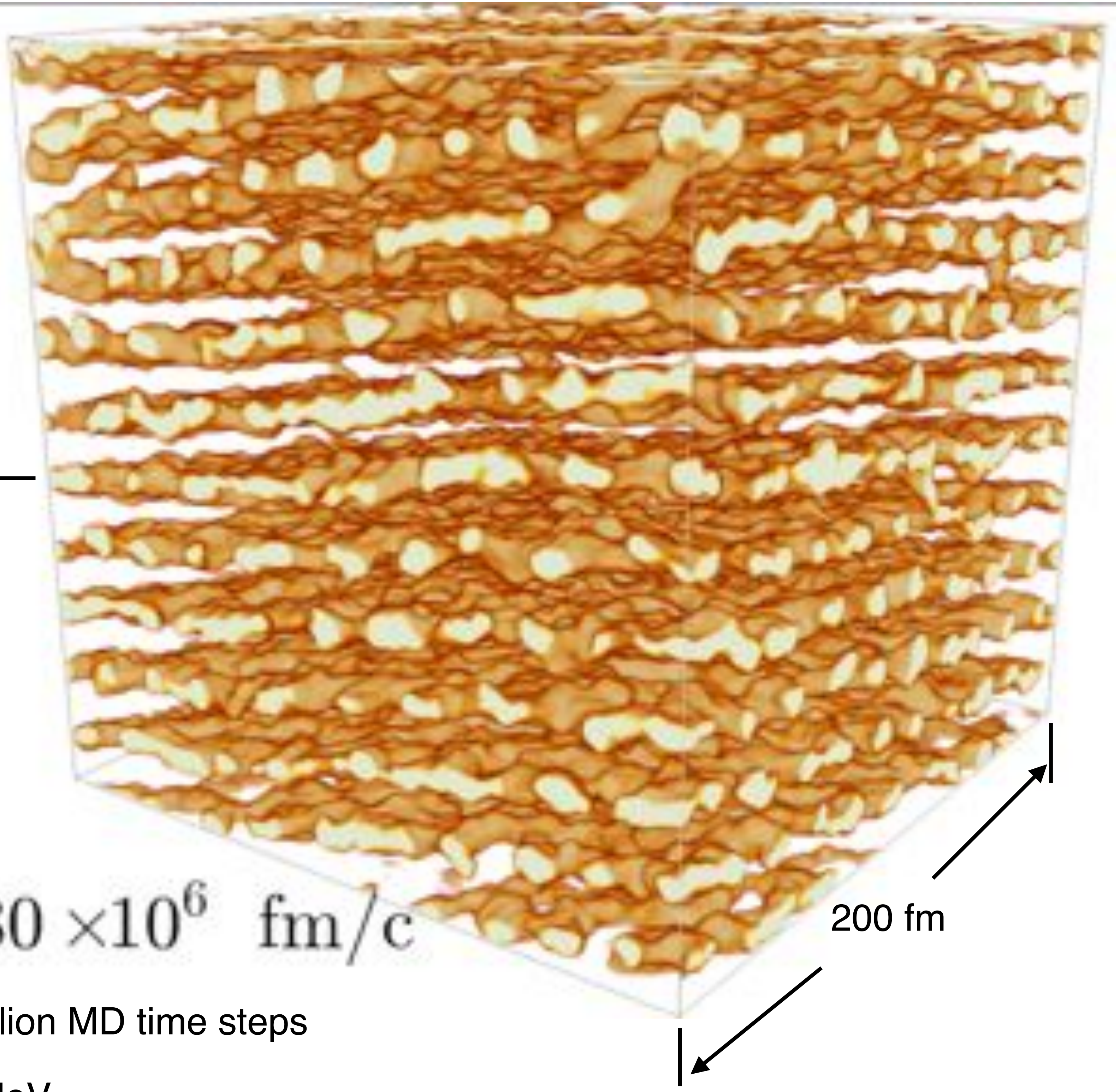
Larger MD simulation to check finite size effects

We have tested IUMD for over 6,400,000 nucleons in 500+ fm box (10 sec/ MD step on 64 nodes with Y_p=0.2)

Pasta configuration with 409,600 nucleons



Waffle configuration each 2D plane has a lattice of holes



$t = 29.80 \times 10^6$ fm/c

Run for 15 million MD time steps

Y_p=0.3, T=1 MeV

Nuclear Waffles

Some different pasta configurations that depend on density (how much below saturation density of n_0=0.16 fm^{-3}) and proton fraction (ratio of coulomb/ surface E).

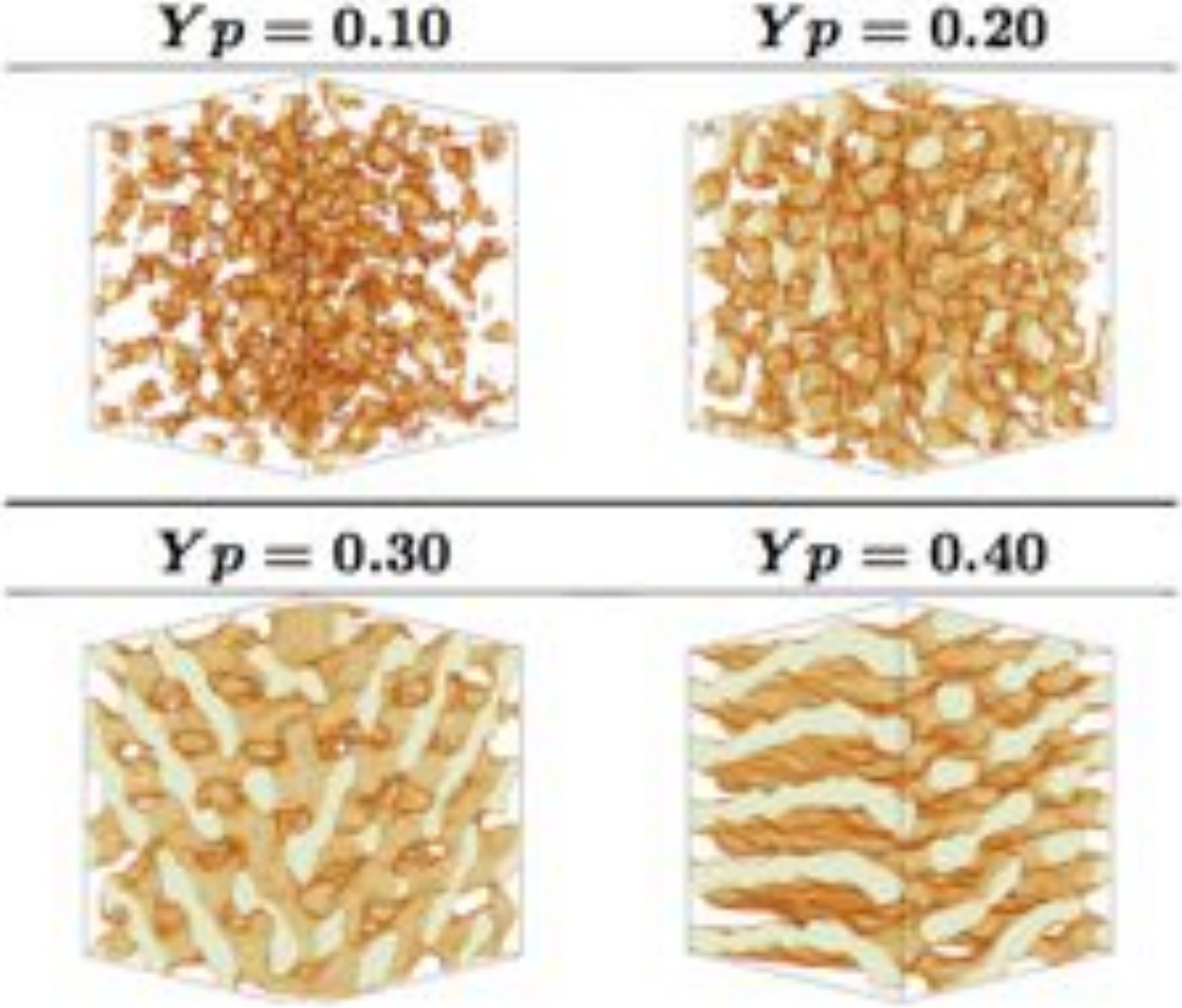
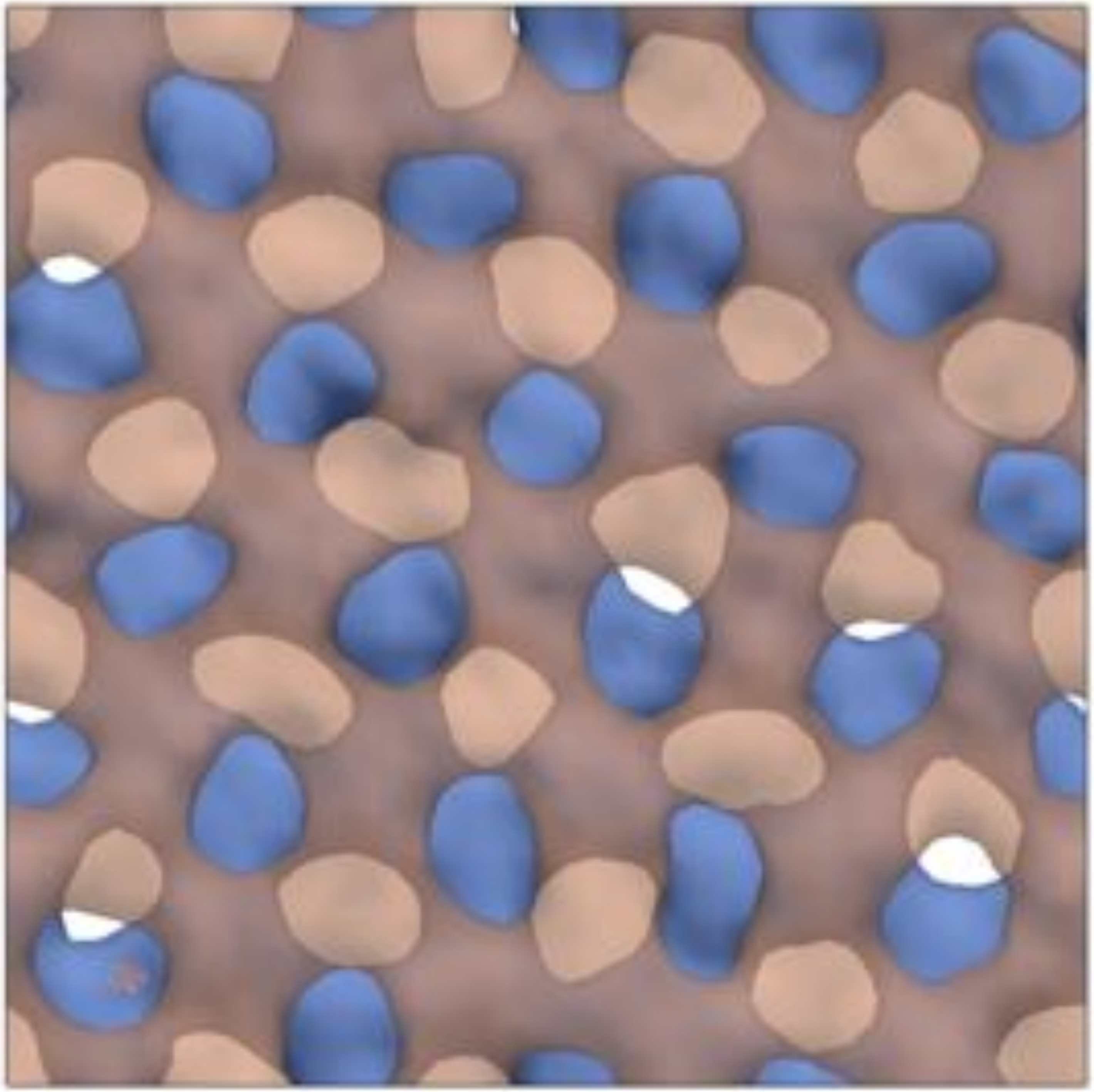
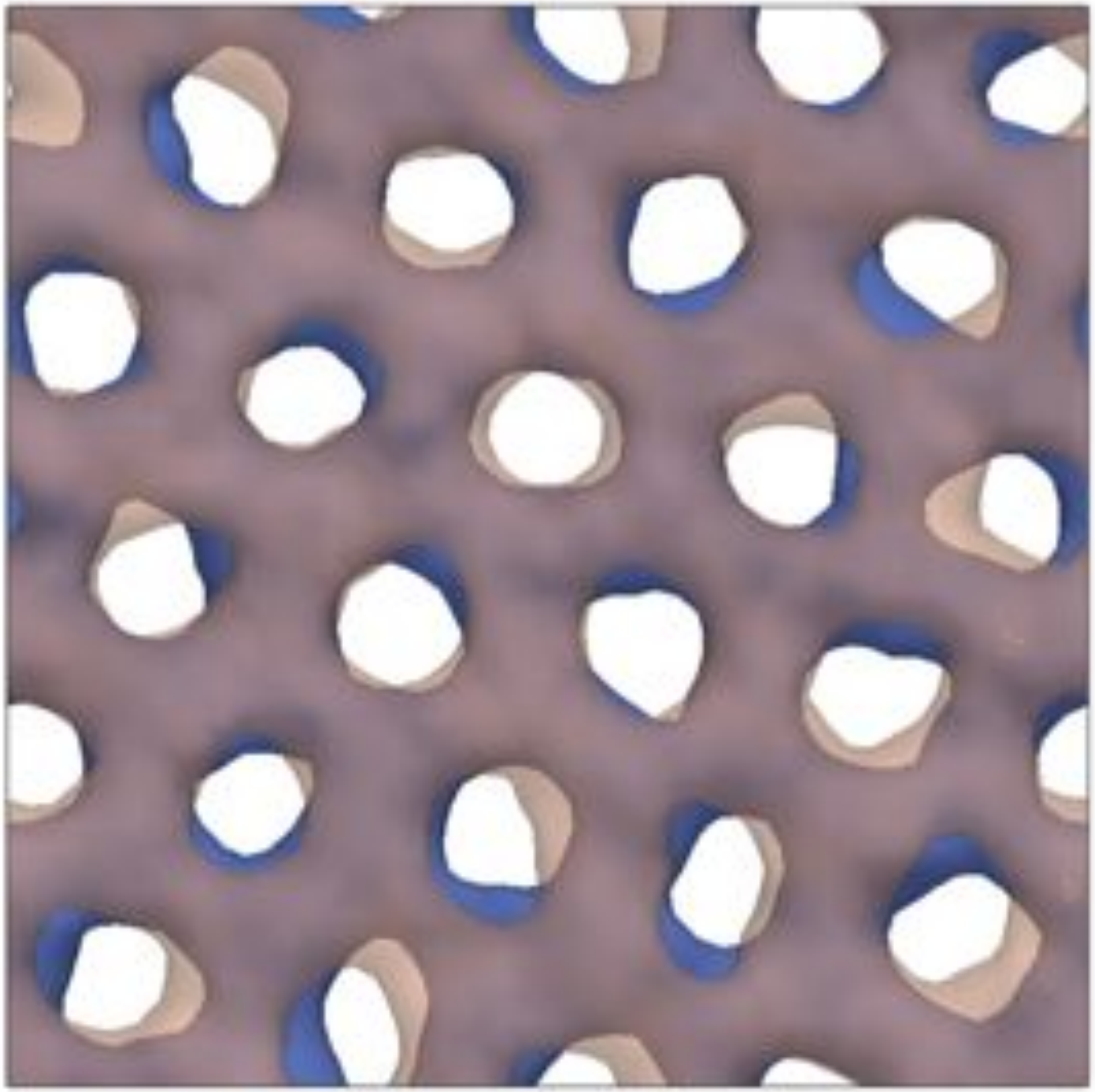


FIG. 1: (Color online) Charge density isosurfaces of runs with proton fractions $Y_p = 0.10, 0.20, 0.30$ and 0.40 after 10^7 fm/c evolution time. The golden surfaces represent isosurfaces of charge density with $n_{ch} = 0.03\,\mathrm{fm}^{-3}$ while the cream color shows regions such that $n_{ch} > 0.03\,\mathrm{fm}^{-3}$.

Plot of one waffle and its nearest neighbor (system cooled to 0.5 MeV)

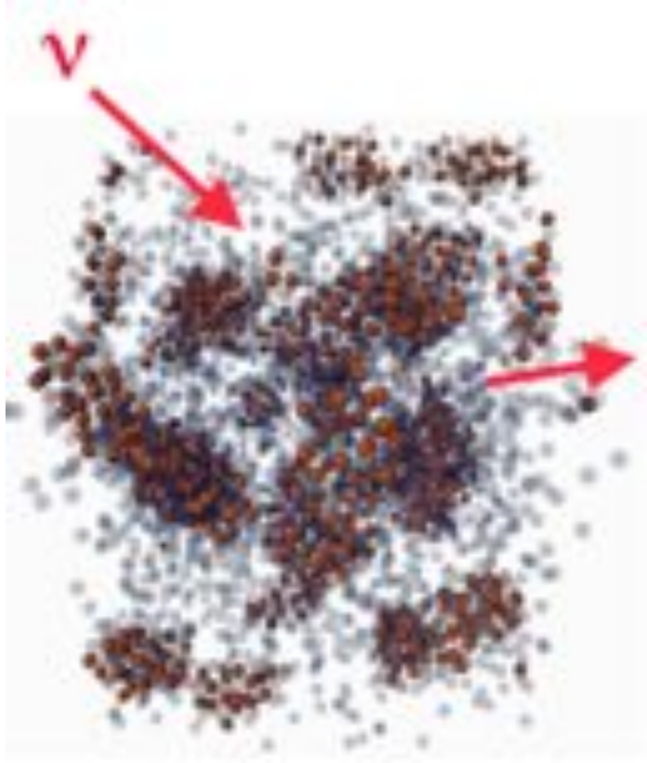


Plot of a Waffle and its next nearest neighbor



How to smell the pasta?

Observables sensitive to pasta shapes

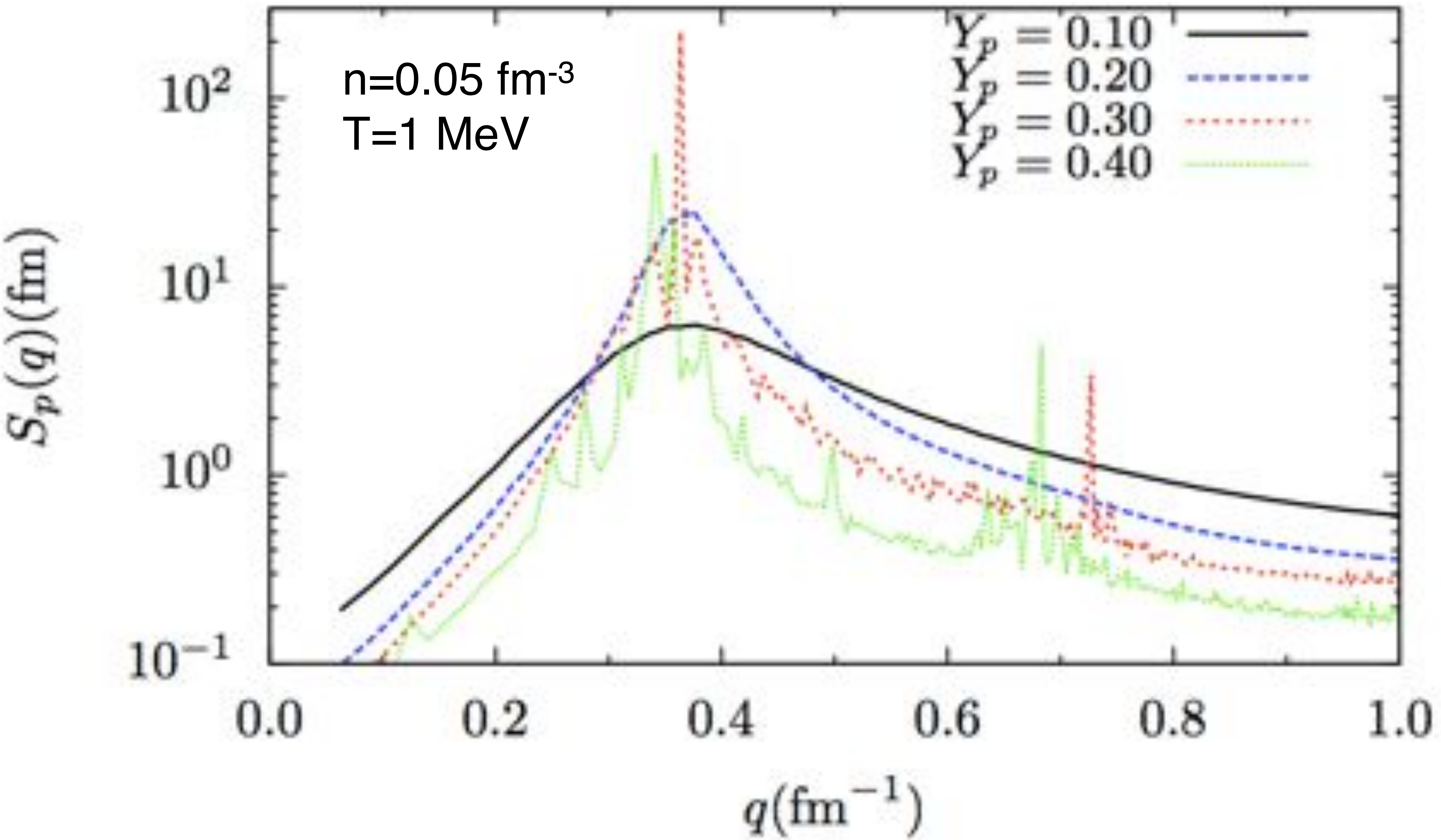


- Coherent ***ν***-pasta scattering gives ***ν*** **opacity** for supernova simulations. Depends on static structure factor $S_n(q)=<\rho_n(q)^*\rho_n(q)>$ or dynamical response function $S_n(q,w)$ [Classical MD -> dynamical response]
- Coherent electron-pasta scattering gives **shear viscosity**, **thermal conductivity**, and **electrical conductivity** of pasta in NS crusts.
- Hysteresis in pasta shapes with density changes gives **bulk viscosity**. Could be important for damping of neutron star r-mode oscillations.
- Response to small deformations of simulation volume gives **shear modulus** -- determines neutron star oscillation frequencies.
- Response to large deformations gives **breaking strain**. Pasta strength important for star quakes (crust breaking), magnetar giant flares, and mountain heights. Deform simulation volume and look at stress vs strain.

Static structure factor

$$S_a(\boldsymbol{q}) = \langle \rho_a^*(\boldsymbol{q}) \rho_a(\boldsymbol{q}) \rangle - \langle \rho_a^*(\boldsymbol{q}) \rangle \langle \rho_a(\boldsymbol{q}) \rangle.$$

$$\rho_a(\boldsymbol{q}) = \frac{1}{\sqrt{N_a}} \sum_{i=1}^{N_a} e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}$$



Disordered Pasta

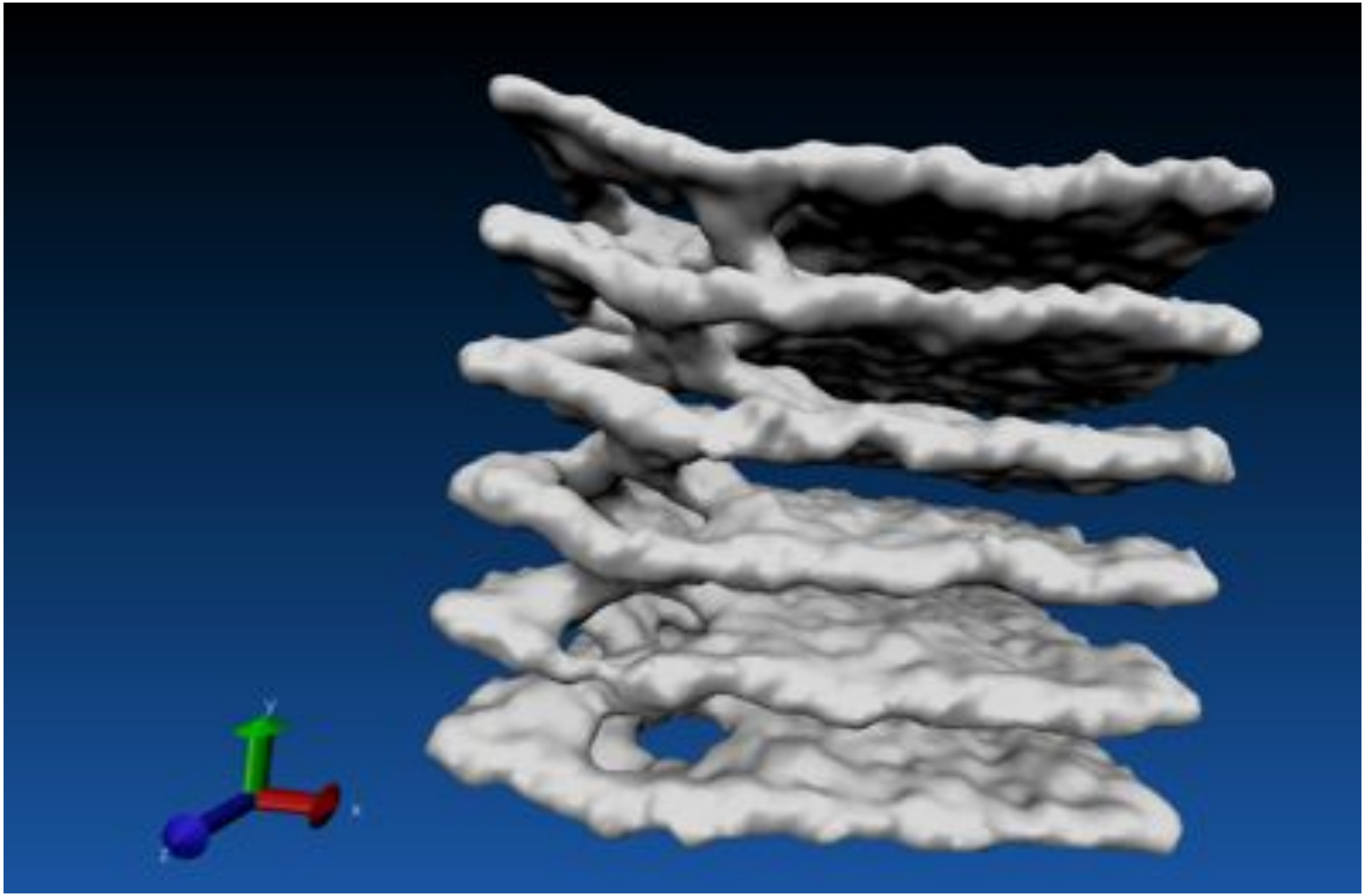
- Jose Pons *et al* speculate [Nature Physics, **9**, 431 (2013)] that an “impure” pasta layer with a low electrical conductivity leads to magnetic field decay (in of order a million years) in neutron stars. This could explain why no X-ray pulsars are observed with rotation periods longer than 20 sec.
- They assumed a crystal lattice of some average charge with random **impurities** of different charges and required a significant spread in charges to produce enough election-pasta scattering for a low conductivity.
- Note this likely also decreases the thermal conductivity which should be observable in X-ray light curves of crust cooling.
- How to describe the amount of disorder in pasta, and could it be large enough to give low electrical and thermal conductivities?

Pasta Defects

- How to describe pasta imperfections?
  - Impurities—unlikely because nucleons may be free to flow and equal out composition.
  - Topological defects— could be very long lived excitations that increase electron-pasta scattering.
  - Grain boundaries between different pasta phases and or orientations.
- Need pasta molding over larger length scales to find elementary excitations and there impact on transport.

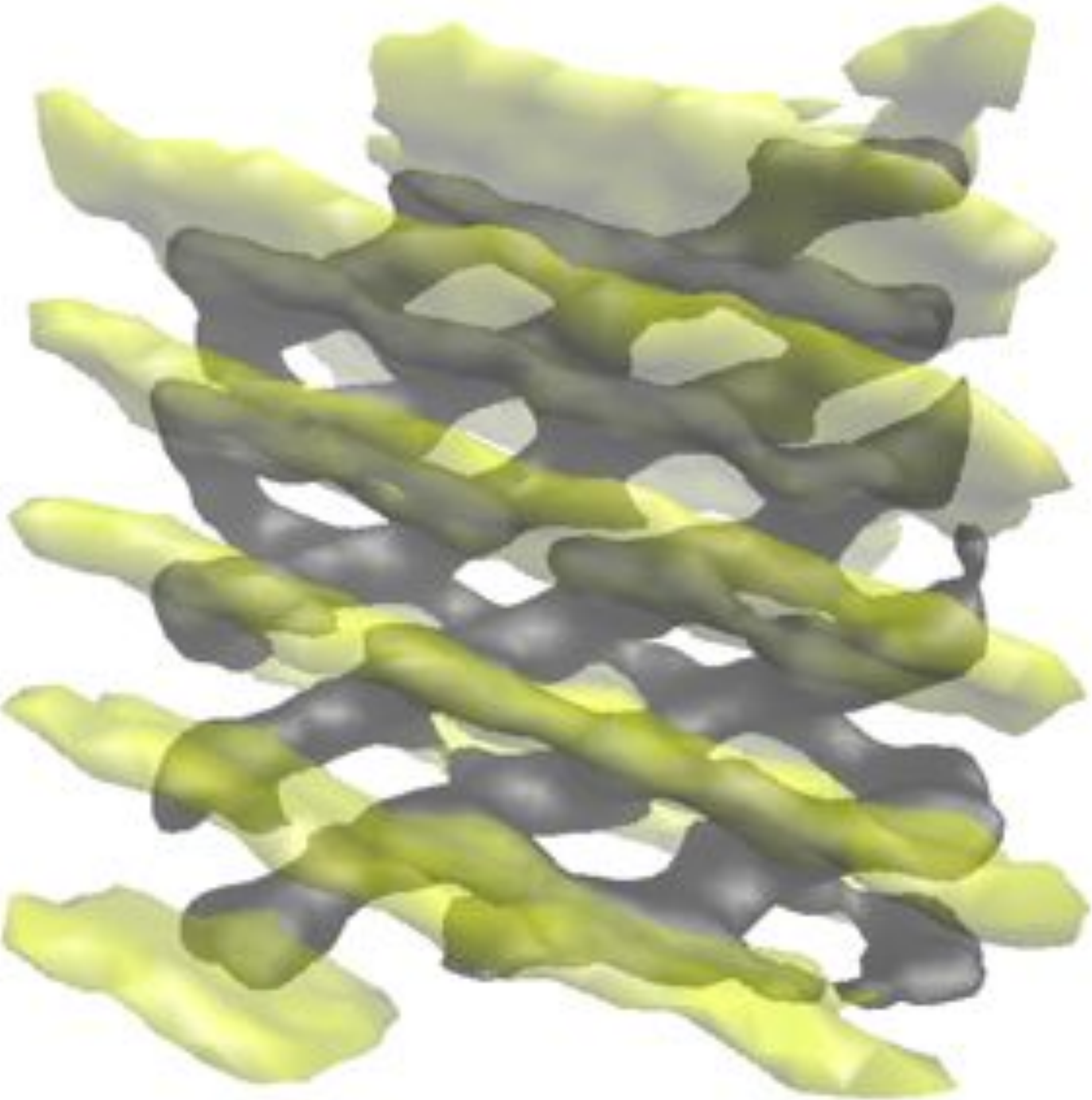
Screw dislocations in nuclear pasta?

Screw defect in Lasagne

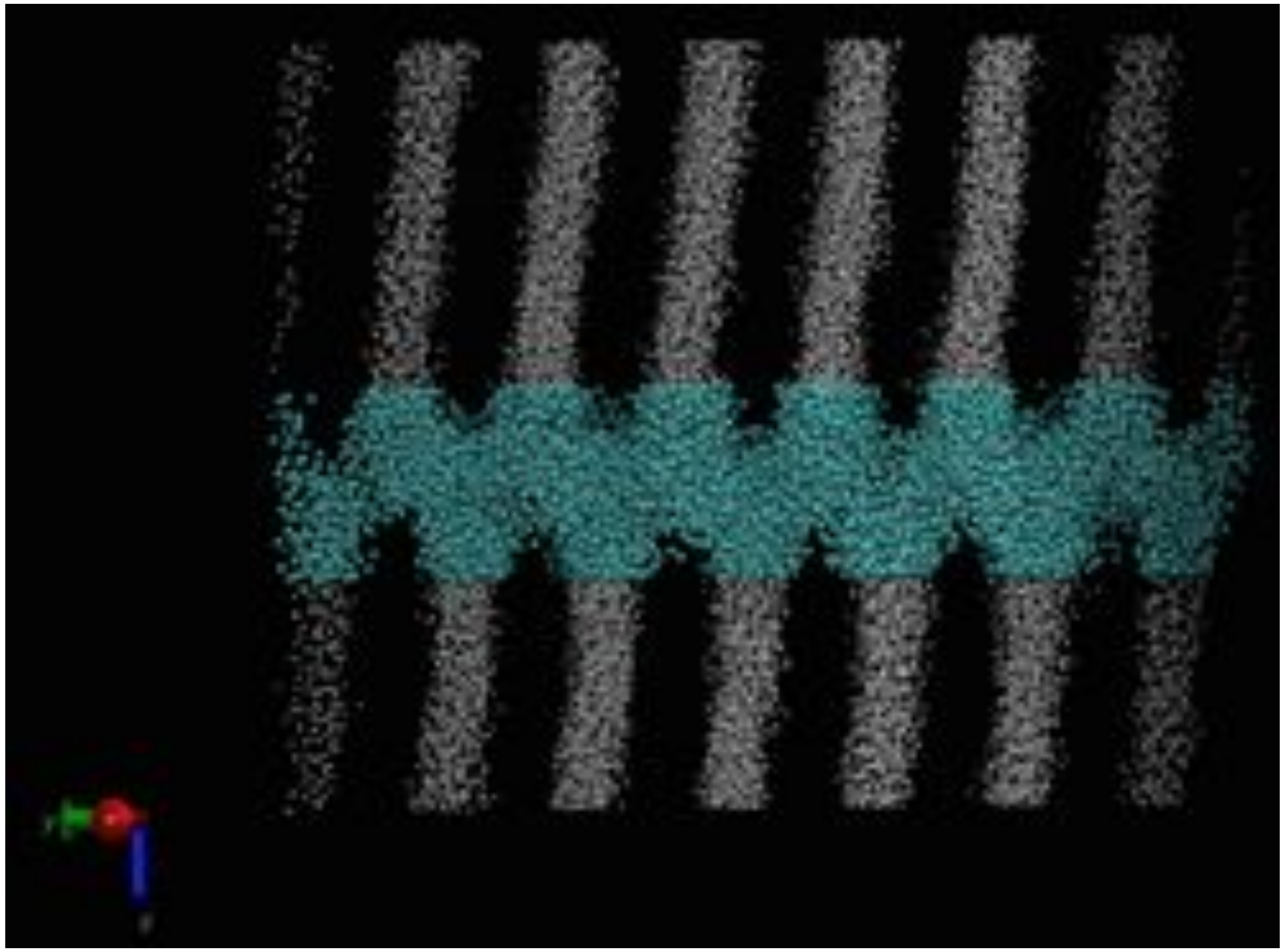


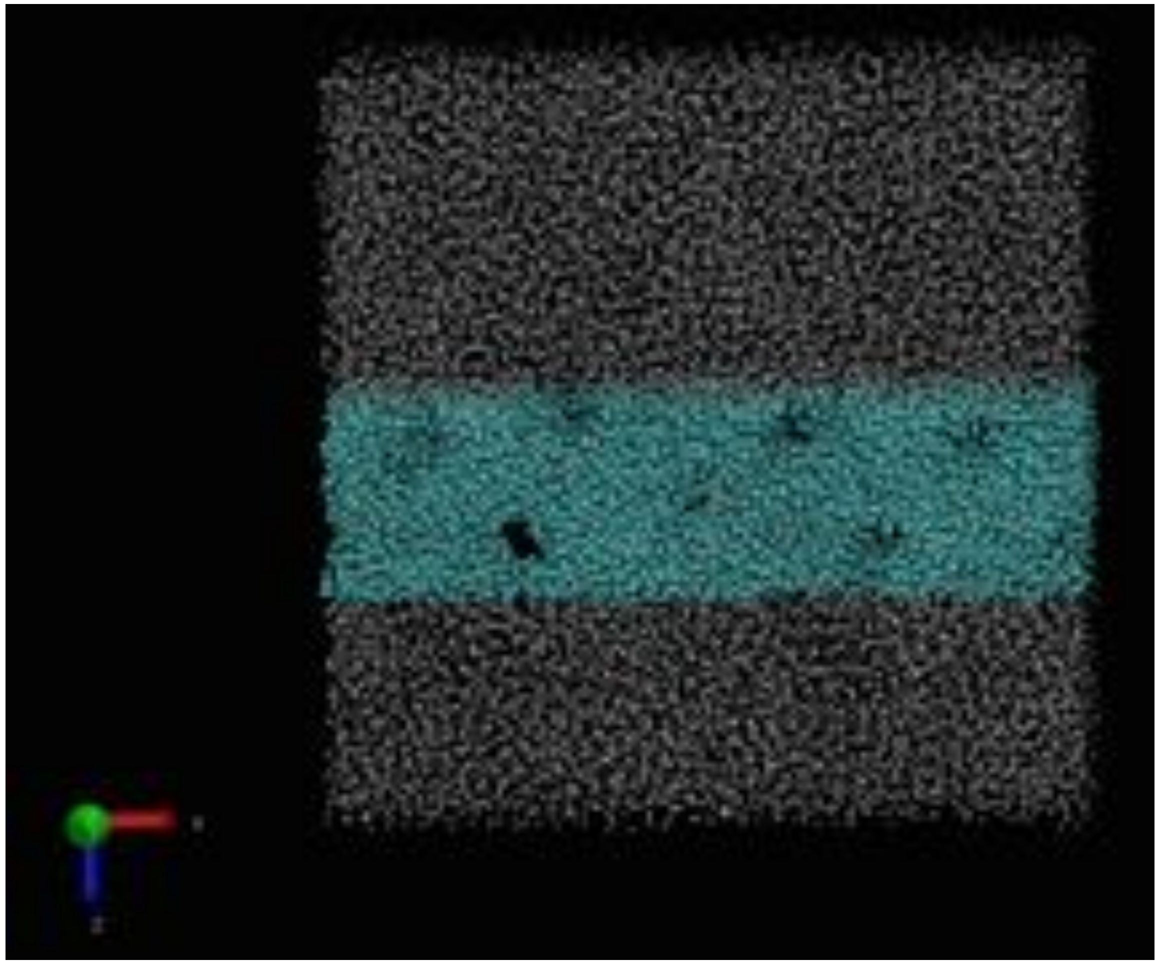
75,000 nucleon configuration (Y_p=0.4, T=1 MeV, ρ=0.05 fm^{-3}) that was started from random positions and quickly formed screw defect. Defect then stable for over 10 million MD time steps.

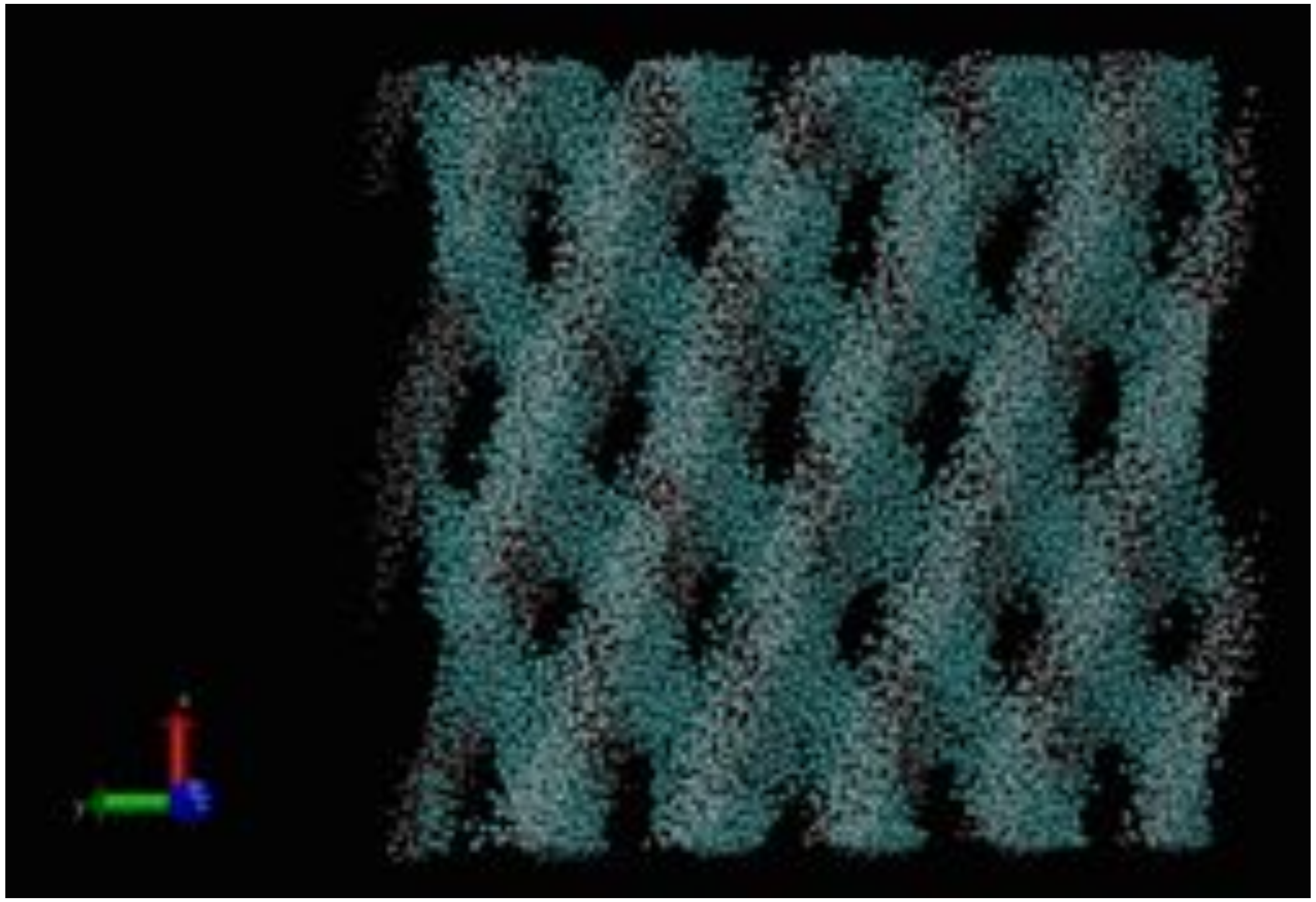
Plane of screw defects



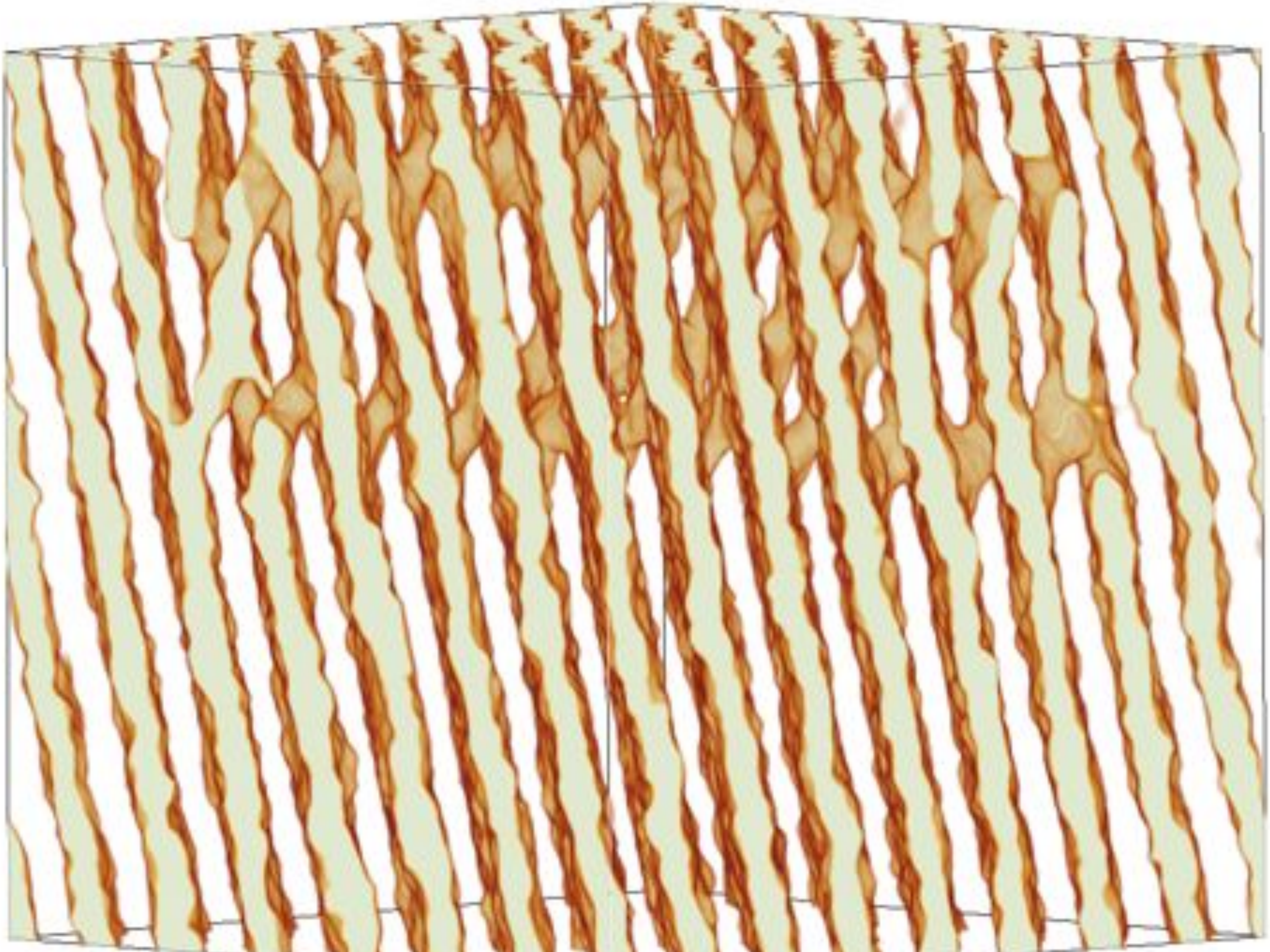
50,000 nucleon configuration of lasagne planes (yellow) with a 2D array of screw defects (gray)







Try and characterize possible nuclear pasta defects. Then calculate effects of defects on electron transport.



Defects in Nuclear Pasta

- Nuclear pasta expected near base of neutron star crust.
- X-ray observations of NS radii probe *liquid* n rich matter.
- Energies of supernova neutrinos and antineutrinos, important for nucleosynthesis, depend on properties of *gaseous* n rich matter.
- Continuous gravitational waves from mountains on NS can probe *solid* n rich matter.

- Collaborators: D. Berry, A. Schneider, M. Caplan, C. Briggs
- Supported in part by DOE grants DE-FG02-87ER40365 (Indiana U.) and DE-SC0008808 (NUCLEI SciDAC).