INSTITUTE for NUCLEAR THEORY

Dense Nuclear Matter Equation of State from Heavy-Ion Collisions

INT WORKSHOP INT-22-84W

December 5, 2022 - December 9, 2022

Classification of nuclear pastas by the alpha shapes method

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University of Texas at El Paso

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Comp. Res. Div., Lawrence Berkeley Laboratory

INSTITUTE for NUCLEAR THEORY

Dense Nuclear Matter Equation of State from Heavy-Ion Collisions

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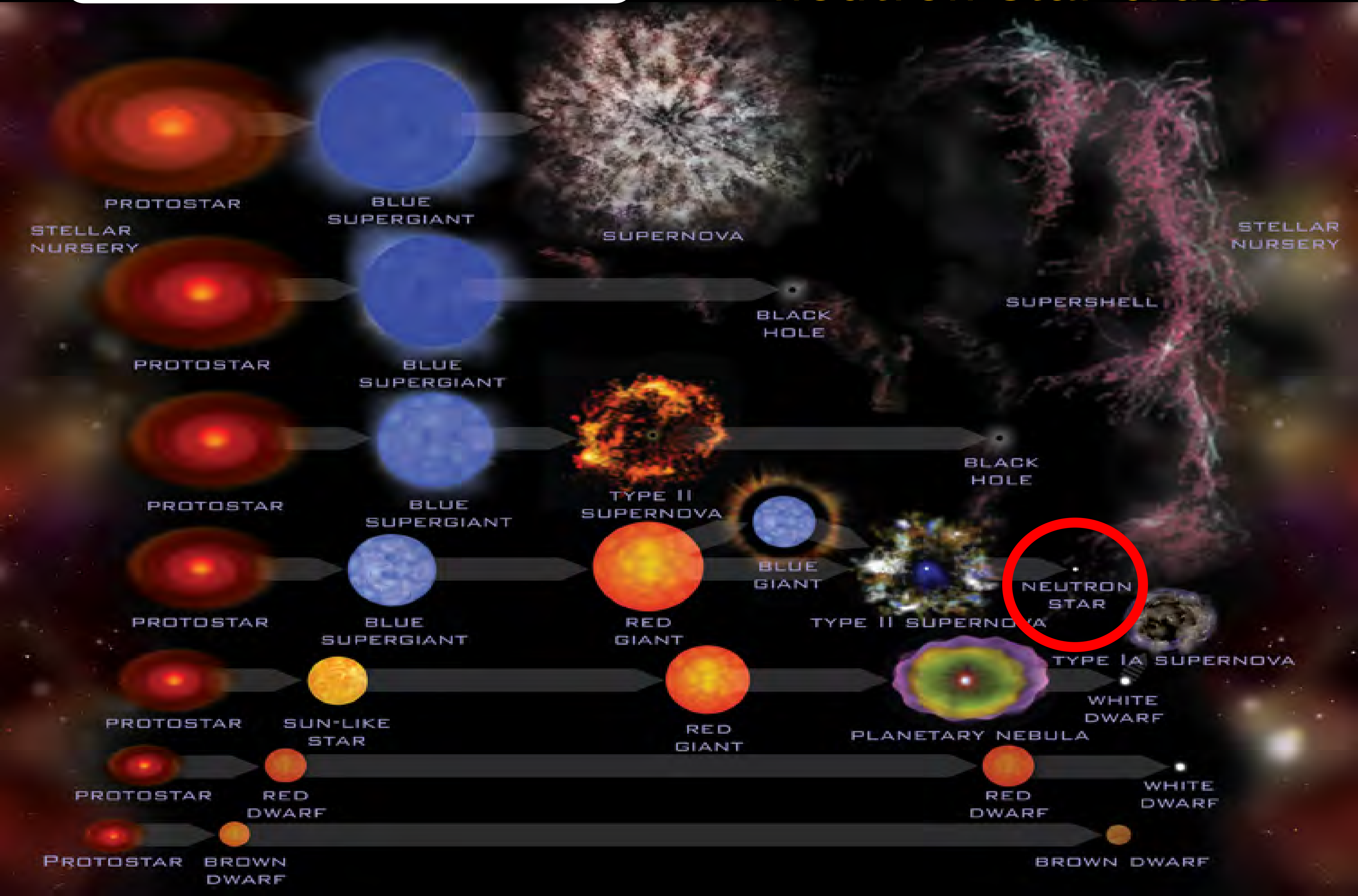
The present calculation helps to determine the EOS applicable to neutron star calculations and different types of heavy-ion collision simulations.

Outline

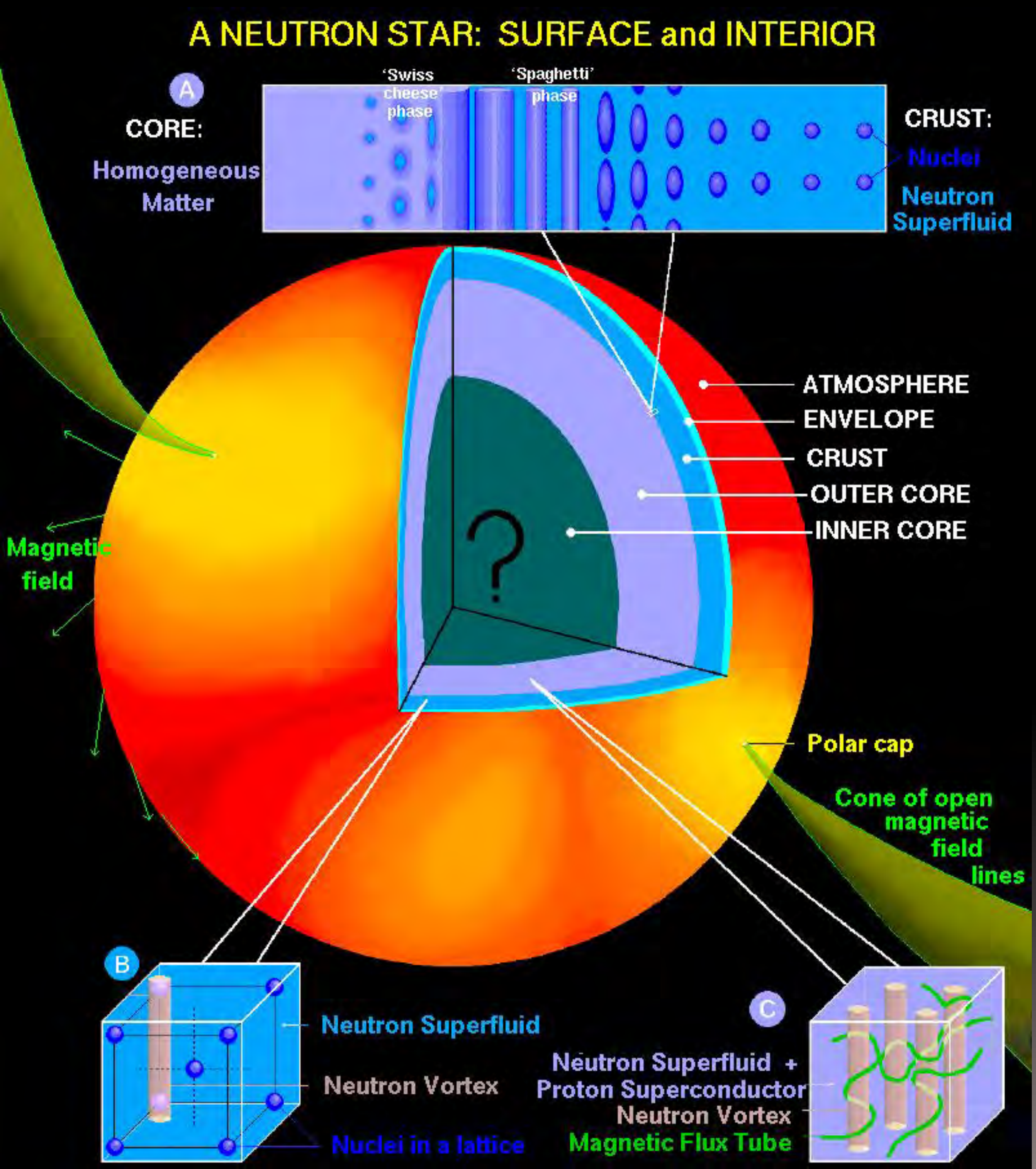
- MOTIVATION
- CLASSICAL MOLECULAR DYNAMICS
- CHARACTERIZATION OF THE PASTA
- RESULTS
- CONCLUSIONS

MOTIVATION

Study the structure of neutron star crusts

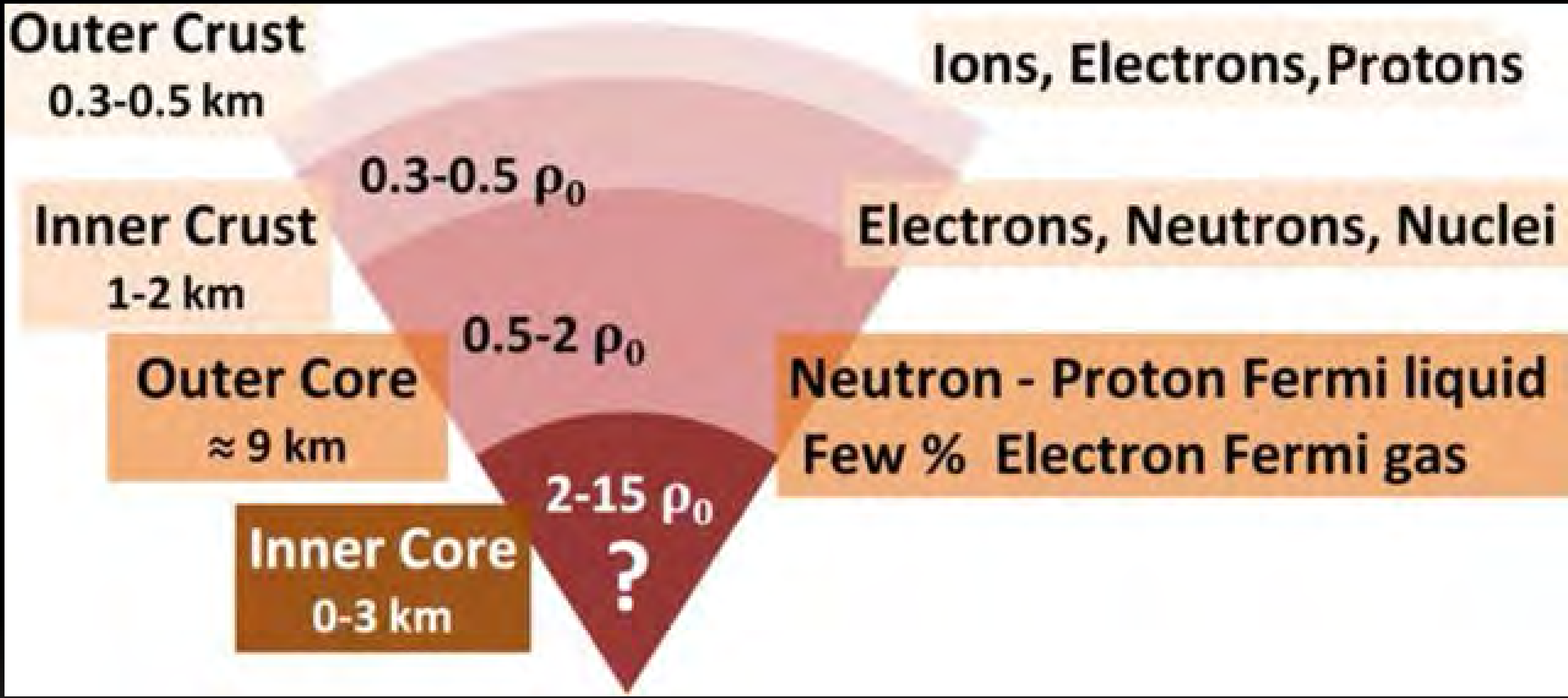


MOTIVATION



What is the composition of the crust?

MOTIVATION



Use molecular dynamics
to study neutron star crust

MOTIVATION

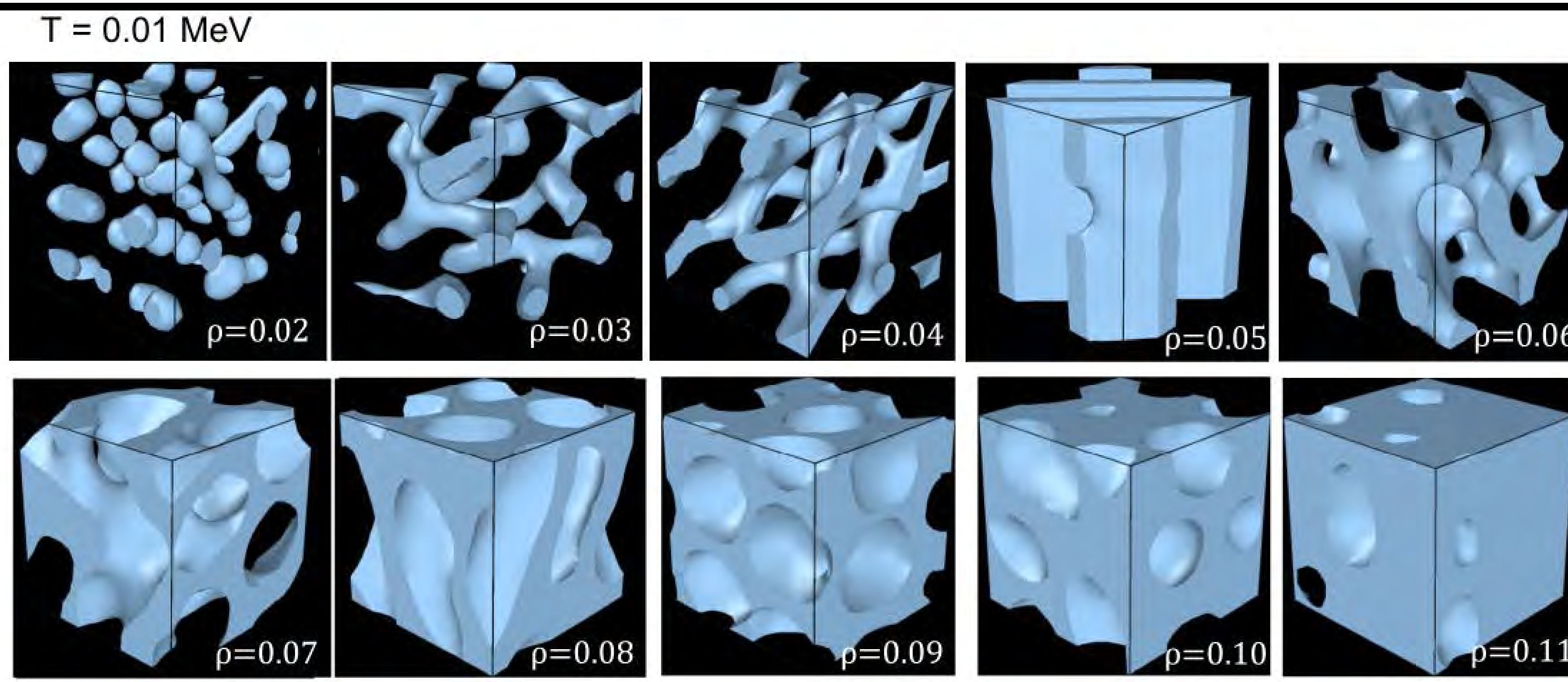
Known: Neutron star matter composed of Protons, neutrons and electrons

Expected: Structure of neutron star crust is "Pasta"

Relevant questions:

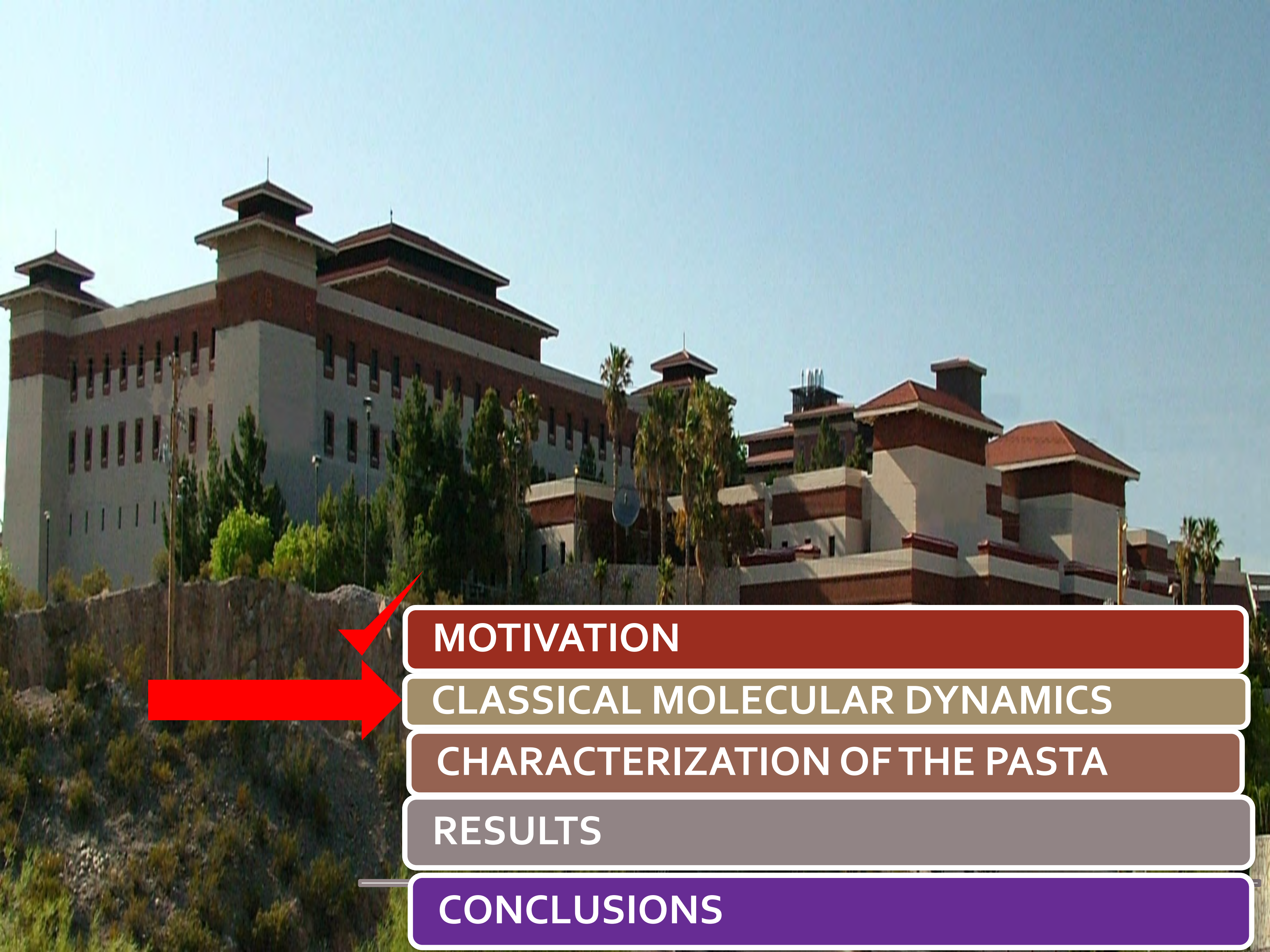
- Does the structure of the pasta evolves as ρ, T and isospin asymmetry vary?
- Are there phase transitions in NSM?

Examples of pastas



Nuclear pastas formed at the final temperature 0.01 MeV

- Nuclear pastas found gnocchi, spaghetti, lasagna, anti-spaghetti and anti-gnocchi.



- MOTIVATION
- CLASSICAL MOLECULAR DYNAMICS
- CHARACTERIZATION OF THE PASTA
- RESULTS
- CONCLUSIONS

CLASSICAL MOLECULAR DYNAMICS

PHYSICAL REVIEW C VOLUME 52, NUMBER 6 DECEMBER 1995
Fluctuations in n
A. Aranda,[1] C. O. Dors
[1]Department of Physics, University
[2]Departamento de Física, Universid

Brazilian Journal of Physics, vol. 34, no. 3A, September, 2004
The Transition Temperature of the Nuclear Caloric Curve
A. Barrañón[1], J. Escamilla Roa[2], and J. A. López[2]

Revista Mexicana de Física **38**, *Suplemento 2 (1992) 95-101*
Nuclear Spinodal Decomposition
JORGE ALBERTO LÓPEZ
University of Texas at El Paso

Volume 219, number 2,3 PHYSICS LETTERS B 16 March 1989
NUCLEAR SPINODAL DECOMPOSITION ☆
Jorge A. LÓPEZ
Lawrence Berkeley Laboratory,
Georg LÜBECK [1]
The Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

APH N.S., Heavy Ion Physics **11** (2000)
Power Law in Nuclear Fragmentation
C.O. Dorso,[1] J.A. López[2] and R. Medellín

REVISTA MEXICANA DE FÍSICA 45 SUPLEMENTO 2, 110–115 OCTUBRE 1999
LATINO: A semi-classical model to study nuclear fragmentation
A. Barrañón A. Chernomoretz and C.O. Dorso J.A. López and J. Morales

PHYSICAL REVIEW C, VOLUME 64, 044605
Obtaining the caloric curve from collisions
A. Chernomoretz,[1] C. O. Dorso,[1] and J. A. López[2]

PHYSICAL REVIEW C 69, 014601 (2004)
Entropy in the nuclear caloric curve
A. Barrañón,[1] J. Escamilla Roa,[2] and J. A. López[2]

Nuclear Physics A 791 (2007) 222–231
NUCLEAR PHYSICS A
Time dependence of isotopic temperatures
Armando Barrañón [a], Claudio O. Dorso [b], Jorge A. López

APH N.S., Heavy Ion Physics 17/1 (2003)
The Critical Exponent of Nuclear Fragmentation
A. Barrañón,[1] R. Cárdenas,[2] C.O. Dorso[3] and J.A. López[2]

AMERICAN INSTITUTE OF PHYSICS
AIP CONFERENCE PROCEEDINGS ■ VOLUME 884
Thermal symmetry in isoscaling
C. R. Escudero*, J. A. López* and C. O. Dorso†

PHYSICAL REVIEW C 73, 044601 (2006)
Dynamical aspects of isoscaling
C. O. Dorso,[1] C. R. Escudero,[2] M. Ison,[1] and J. A. López[2]

- Inter
- Uses p
- Prope
- Does not use "test particles"
- Does not use gaussian density distributions
- Produces fr
- Deexcites fragments
- Uses a unique set of p

But . . . is classic and not quantum

- Potential
- Solve equation of motion (Verlet)
- Recognize clusters (MSE)
- Track evolutions in space-time

PANDHARIPANDE (NEW MEDIUM) POTENTIAL

- Reproduce experimental cross-sections in n-n collisions

$$V_{np}(r) = \frac{V_r}{r}{}^{-\mu_r r} - \frac{V_r}{r_c}{}^{-\mu_r r_c} - \frac{V_a}{r}{}^{-\mu_a r} + \frac{V_a}{r_c}{}^{-\mu_r r_c}$$

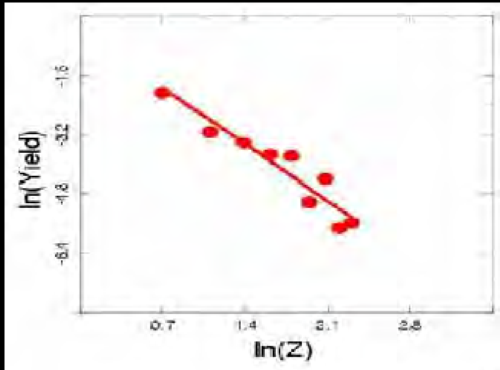
$$V_{nn}(r) = \frac{V_0}{r}{}^{-\mu_0 r} - \frac{V_0}{r_c}{}^{-\mu_0 r_c}$$

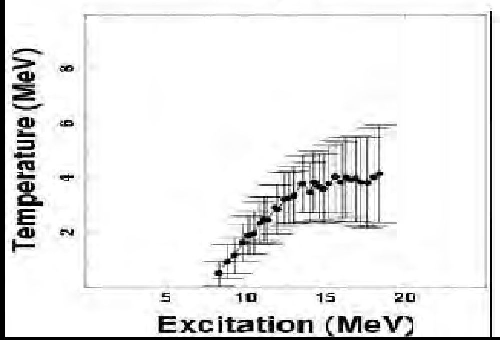
Parameter	Pandharipande	New Medium	Units
V_r	3088.118	3097.0	MeV
V_a	2666.647	2696.0	MeV
V_0	373.118	379.5	MeV
μ_r	1.7468	1.648	fm^{-1}
μ_a	1.6000	1.528	fm^{-1}
μ_0	1.5000	1.628	fm^{-1}
r_c	5.4	5.4/20	fm

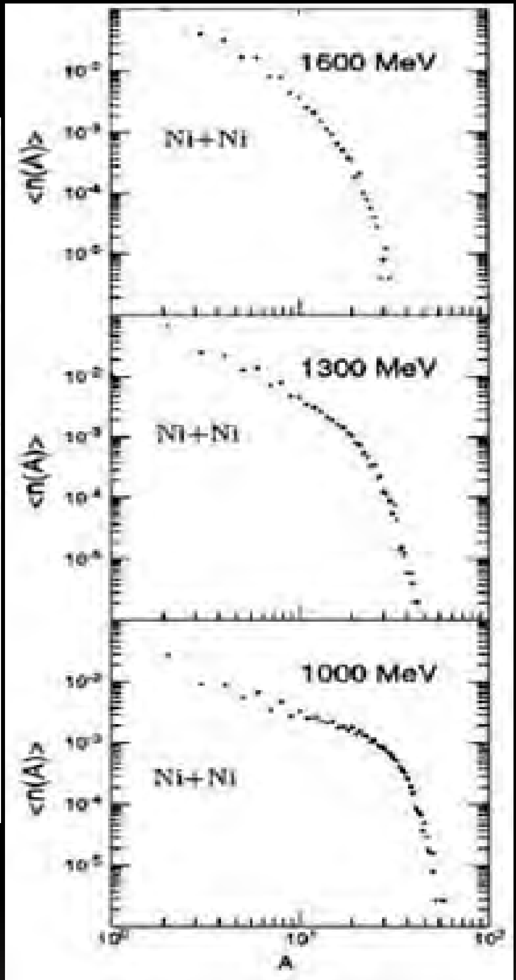
CLASSICAL MOLECULAR DYNAMICS

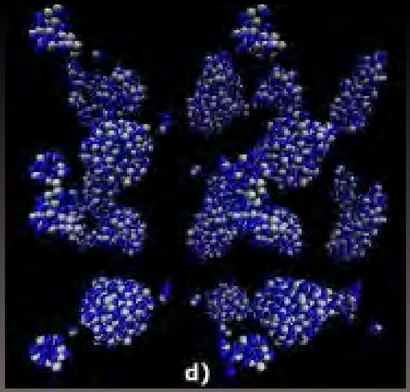
CMD can determine

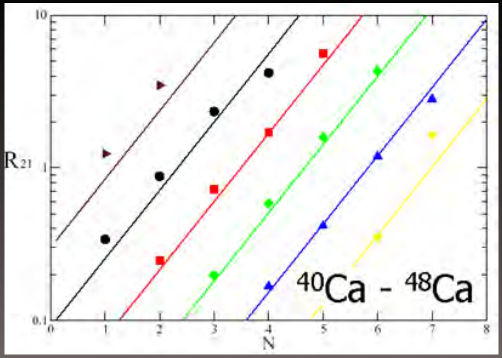
- Mass distributions
- Critical phenomena
- Caloric curves
- Isoscaling
- Nuclear pasta

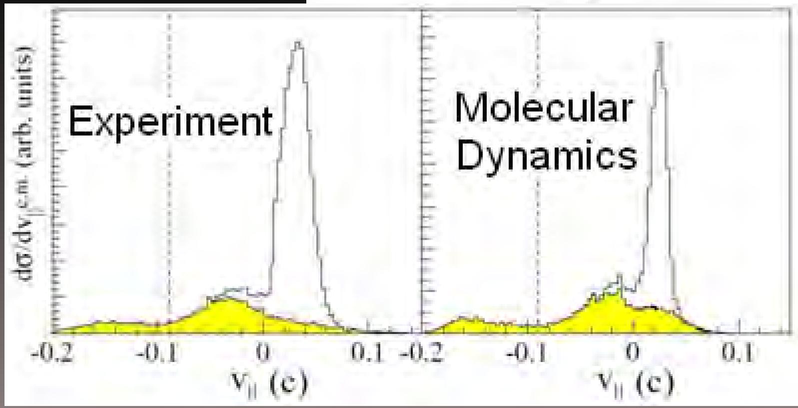






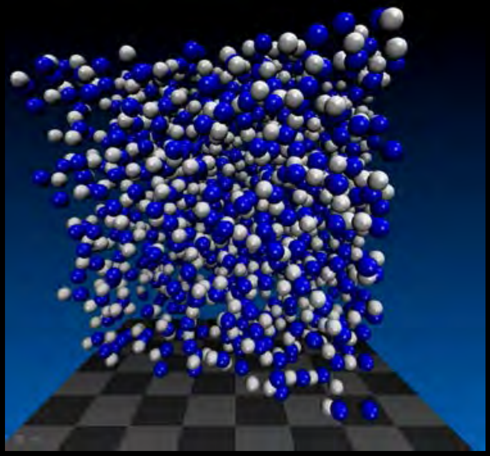






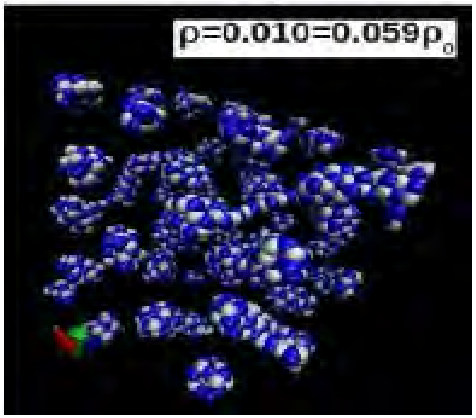
Procedure to study infinite nuclear matter

- Create an infinite system
  - Select density ρ
  - Select temperature
  - Select isospin content
- Equilibrate
- Measure
  - Binding energy E(ρ,T)
  - Pressure p(ρ,T)
  - Compressibility K(ρ,T)
- Obtain equation of state
- Obtain phase diagram
- Obtain structure at various ρ, T, isospin content

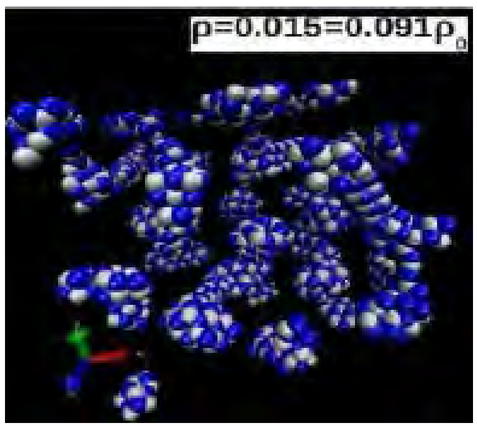


Pasta !

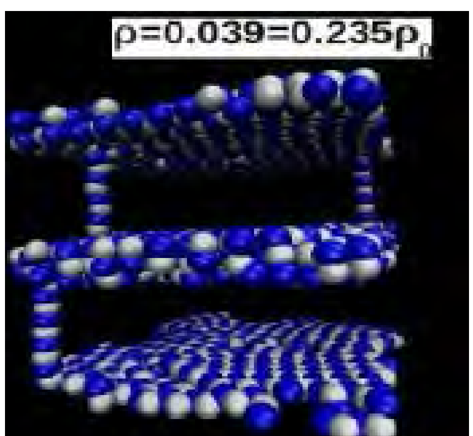
Gnocchi



Spaghetti

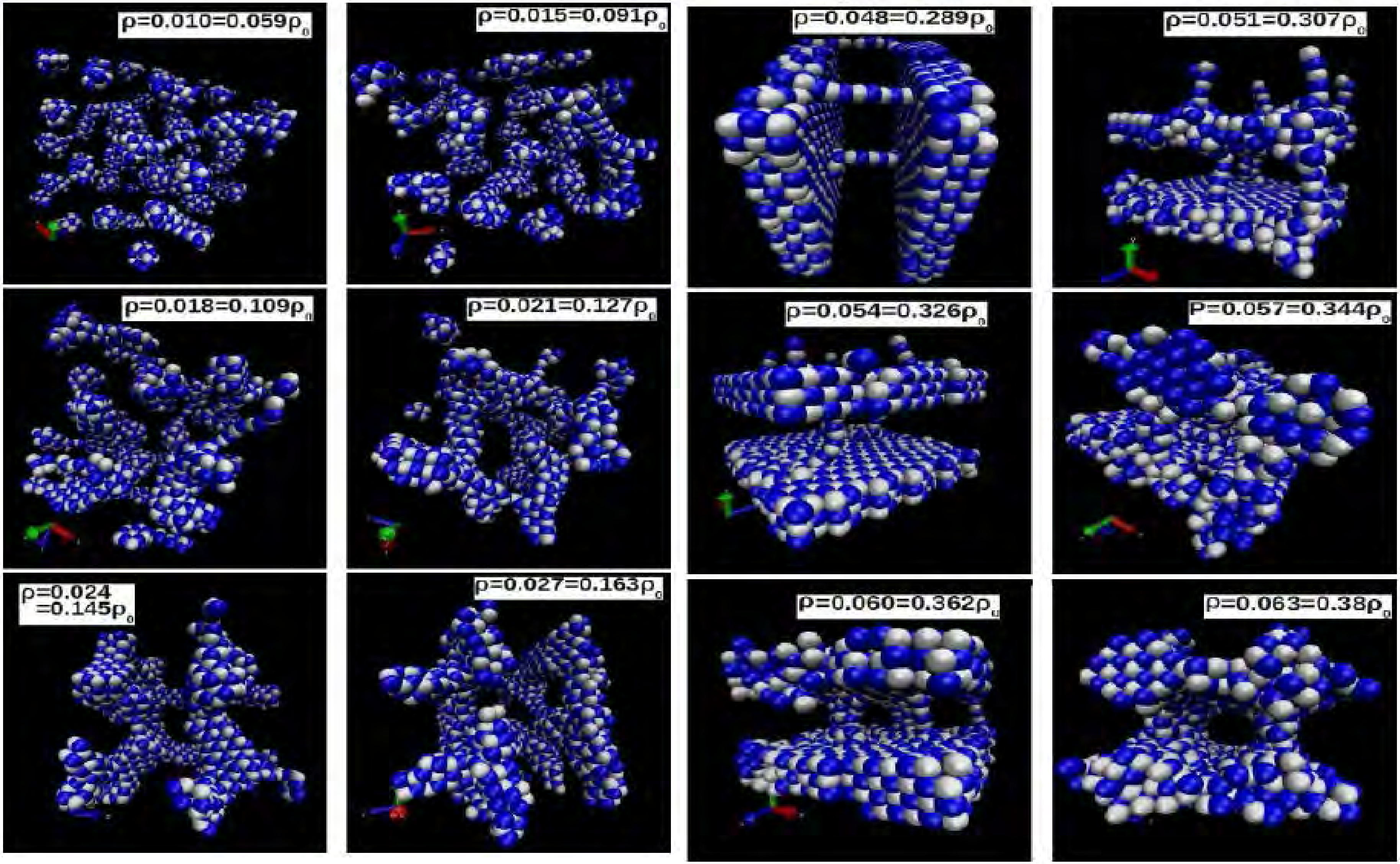


Lasagna



CLASSICAL MOLECULAR DYNAMICS

“Pasta” shapes



X=0.5, T=0.1 MeV

Review Article | Published: 25 November 2020

Springer Link

Properties of nuclear pastas

Jorge A. López, Claudio O. Dorso & Guillermo Frank

Frontiers of Physics **16**, Article number: 24301 (2021)

Abstract

In this review we study the nuclear pastas as they are expected to be formed in neutron star crusts. We start with a study of the pastas formed in nuclear matter (composed of protons and neutrons), we follow with the role of the electron gas on the formation of pastas, and we then investigate the pastas in neutron star matter (nuclear matter embedded in an electron gas).

symmetry

Symmetry Energy and the Pauli Exclusion Principle

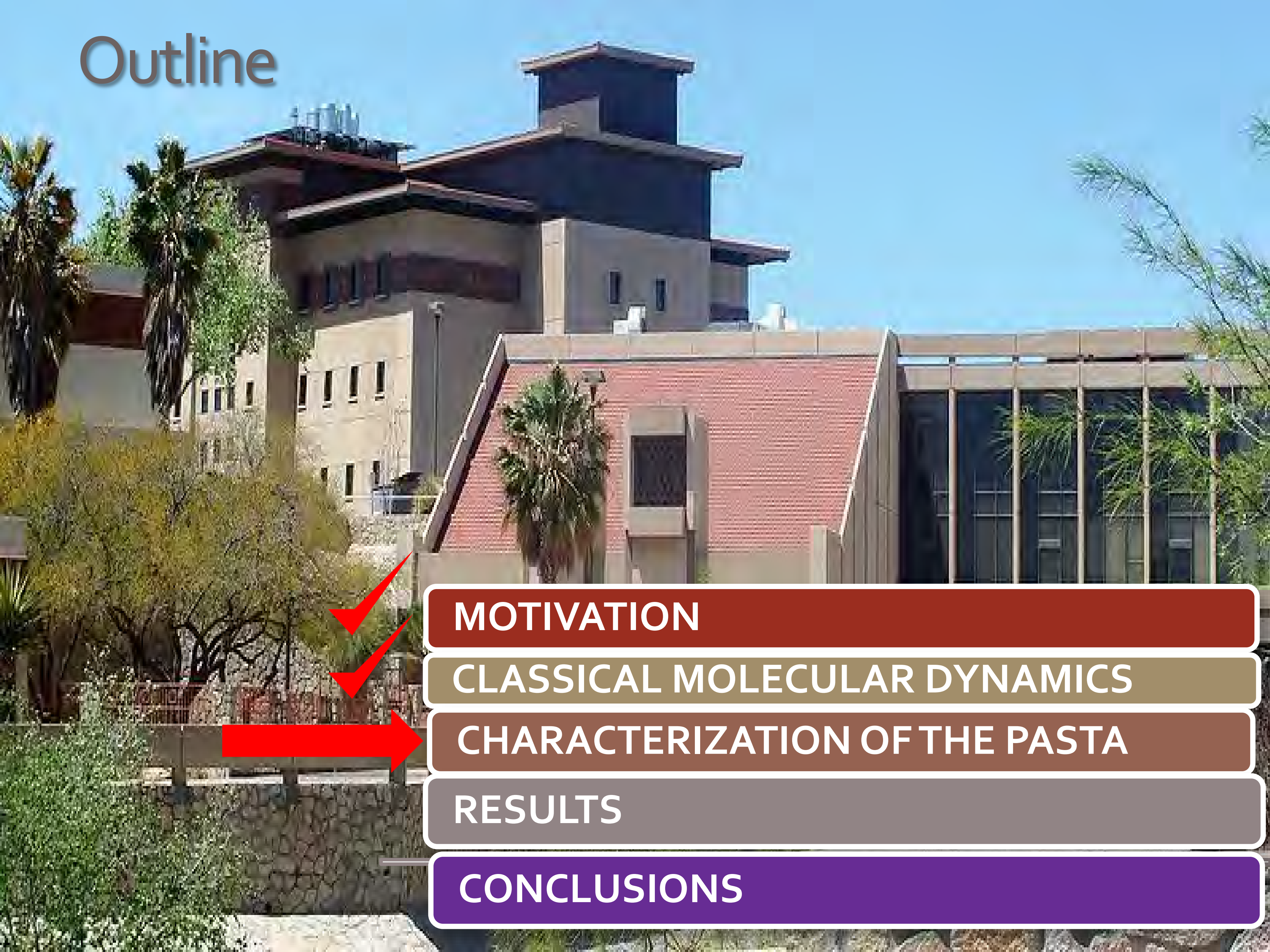
by Claudio O. Dorso [1,†], Guillermo Frank [2,†] and Jorge A. López [3,*,†]

Symmetry **2021**, *13*(11), 2116; https://doi.org/10.3390/sym13112116

Abstract

In this article we present a classical potential that respects the Pauli exclusion principle and can be used to describe nucleon-nucleon interactions at intermediate energies. The potential depends on the relative momentum of the colliding nucleons and reduces interactions at low momentum transfer mimicking the Pauli exclusion principle. We use the potential with Metropolis Monte Carlo methods and study the formation of finite nuclei and infinite systems. We find good agreement in terms of the binding energies, radii, and internal nucleon distribution of finite nuclei, and the binding energy in nuclear matter and neutron star matter, as well as the formation of nuclear pastas, and the symmetry energy of neutron star matter.

Outline



- MOTIVATION
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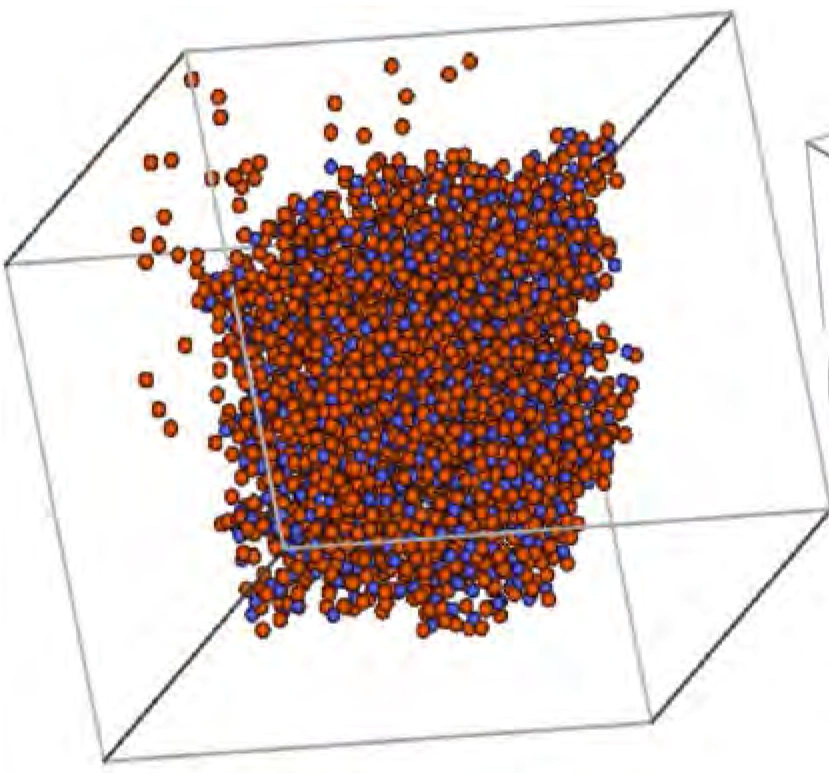
- RESULTS
- CONCLUSIONS

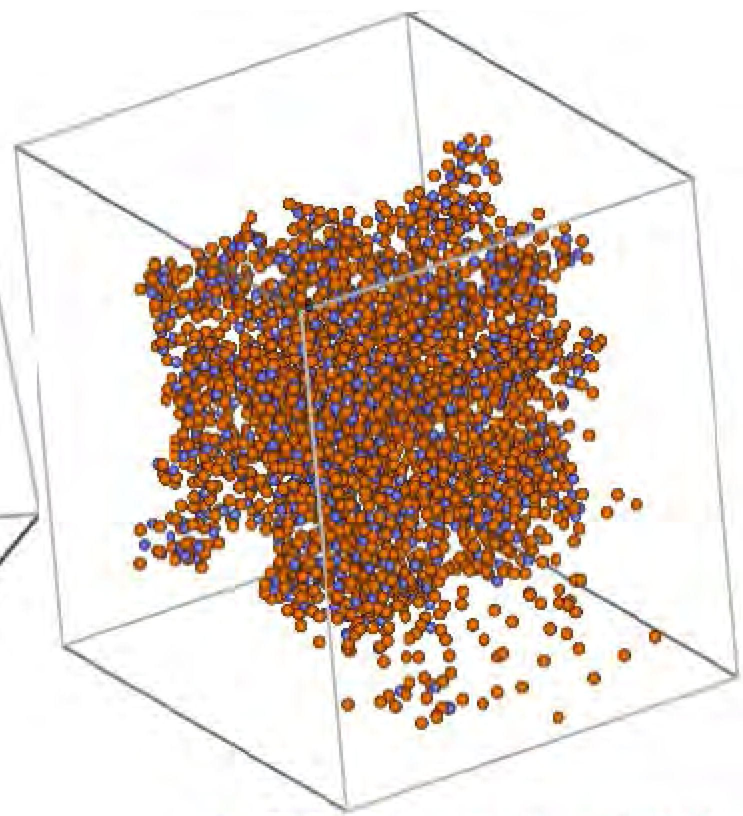
CHARACTERIZATION OF THE PASTA

Example:

These two structures look alike, are they equal?

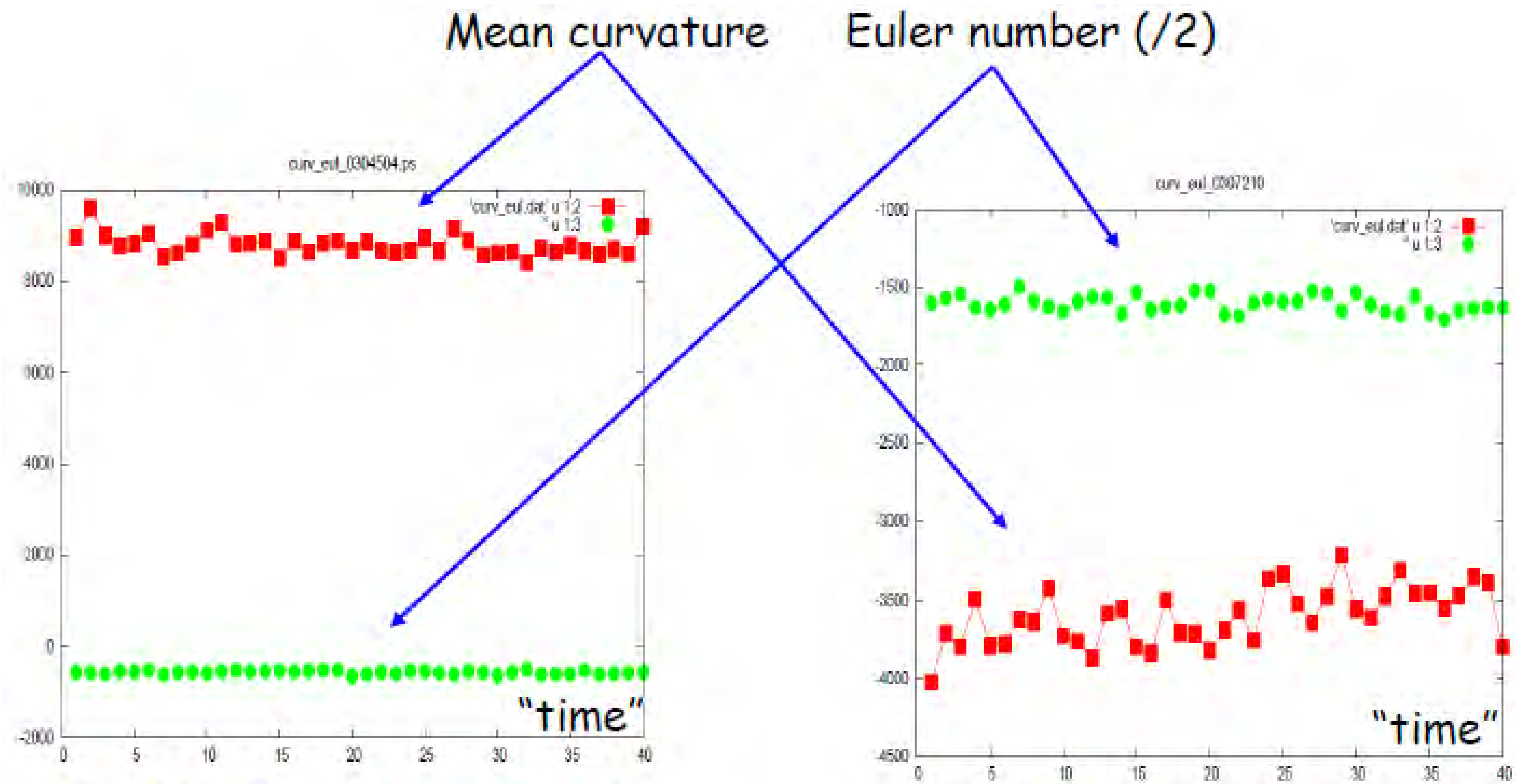


$\rho = 0.72\ \rho_0$ X=0.3 T=1.0



$\rho = 0.45\ \rho_0$ X=0.3 T=0.4

No, they have different Euler numbers and curvatures

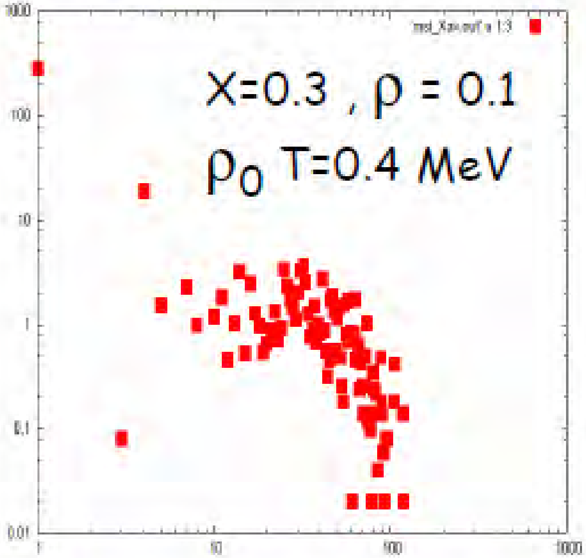


$\rho = 0.45\ \rho_0$ X=0.3 T=0.4

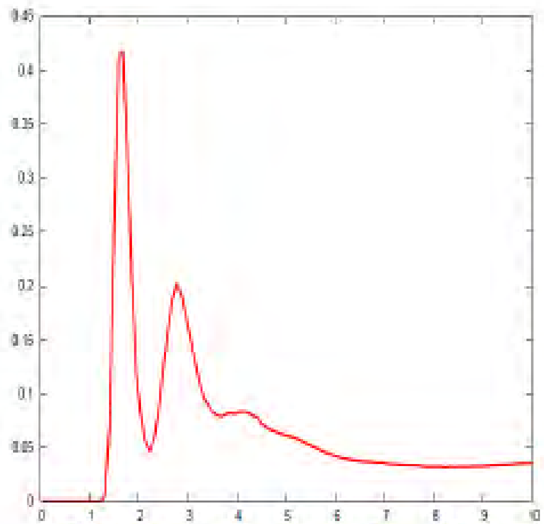
$\rho = 0.72\ \rho_0$ X=0.3 T=1.0

How to characterize the pasta

Study:

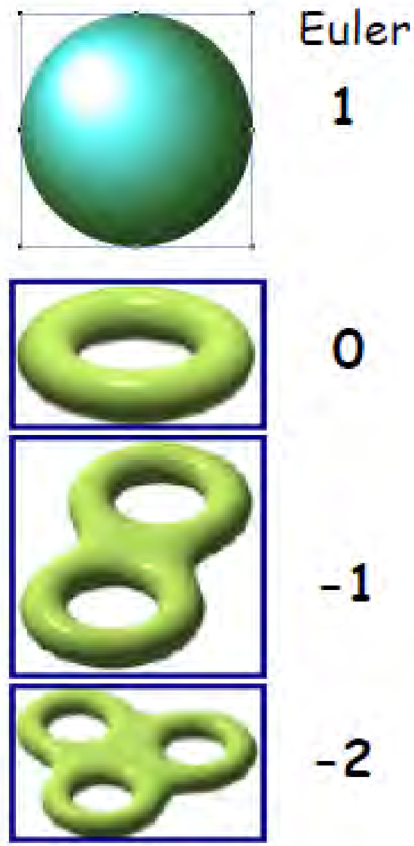


Fragments and their mass distribution



Pair correlation function

Topology



Minkowski functionals

Lindemann coefficient

Lindemann coefficient

The Lindemann coefficient [36] provides an estimation of the root mean square displacement of the particles respect to their equilibrium position in a crystal state, and it serves as an indicator of the phase where the particles are in, as well as of transitions from one phase to another. Formally,

$$\Delta_L = \frac{1}{a}\sqrt{\sum_{i=1}^{N}\left\langle \frac{\Delta r_i^2}{N} \right\rangle}$$

where $\Delta r_i^2 = (r_i - \langle r_i \rangle)^2$, N is the number of particles, and a is the crystal lattice constant; for the nuclear case we use the volume per particle to set the length scale through $a = (V/N)^{1/3}$.

Kolmogorov statistic

Kolmogorov statistic

The Kolmogorov statistic measures the difference between a sampled (cumulative) distribution F_n and a theoretical distribution F. The statistic, as defined by Kolmogorov [37], applies to univariate distributions (1D) as follows

$$D_N = \sup_{\{x\}} |F_n(x) - F(x)|$$

where "sup" means the supremum value of the argument along the x domain, and N is the total number of samples. This definition is proven to represent univocally the greatest absolute discrepancy between both distributions.

In the nuclear case, the Kolmogorov 3D (that is, the Franceschini's version) quantifies the discrepancy in the nucleons positions compared to the homogeneous case.

Tools

Euler characteristic

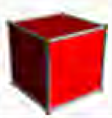
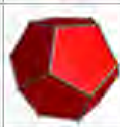
In 3D Convex Polyhedra

The **Euler characteristic** $\chi = V - E + F = 2$

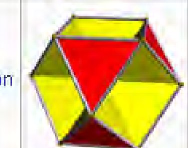
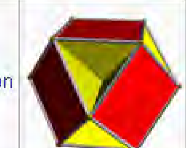
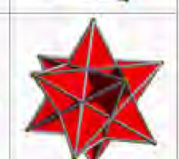
V numbers of vertices (corners)

E numbers of edges

F numbers of faces

Name	Image	Vertices V	Edges E	Faces F	Euler characteristic: $V - E + F$
Tetrahedron		4	6	4	**2**
Hexahedron or cube		8	12	6	**2**
Octahedron		6	12	8	**2**
Dodecahedron		20	30	12	**2**
Icosahedron		12	30	20	**2**

In 3D non-convex polyhedra χ can have any value, and thus can be used to characterize the shape

Name	Image	Vertices V	Edges E	Faces F	Euler characteristic: $V - E + F$
Tetrahemihexahedron		6	12	7	**1**
Octahemioctahedron		12	24	12	**0**
Cubohemioctahedron		12	24	10	−2
Great icosahedron		12	30	20	2

How to use the Euler number with the "pasta"

Early efforts: Watanabe et al.

Phase diagram of nuclear "pasta" and its uncertainties in supernova cores

Hidetaka Sonoda[a,b], Gentaro Watanabe[c,d,b], Katsuhiko Sato[a,e,f], Kenji Yasuoka[g] and Toshikazu Ebisuzaki[b]

We examine the model dependence of the phase diagram of inhomogeneous nulcear matter in supernova cores using the quantum molecular dynamics (QMD). Inhomogeneous matter includes crystallized matter with nonspherical nuclei – "pasta" phases – and the liquid-gas phase separating nuclear matter. Major differences between the phase diagrams of the QMD models can be explained by the energy of pure neutron matter at low densities and the saturation density of asymmetric nuclear matter. We show the density dependence of the symmetry energy is also useful to understand uncertainties of the phase diagram. We point out that, for typical nuclear models, the mass fraction of the pasta phases in the later stage of the collapsing cores is higher than 10–20 %.

(Dated: March 12, 2010)

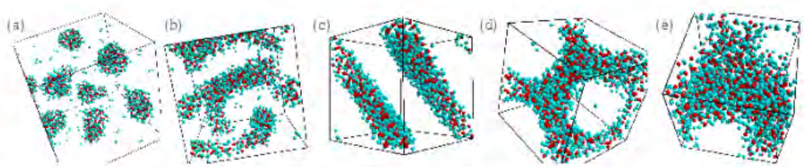


FIG. 2: (Color online) Nucleon distribution of the pasta phases at zero temperature for QMD model 2. Simulations are performed with 2048 nucleons at a proton fraction $x_p = 0.3$. Each red (blue) particle corresponds to a proton (neutron). Each picture shows the pasta phase with (a) spherical nuclei ($0.1\rho_0 = 0.0168\,\mathrm{fm}^{-3}$), (b) cylindrical nuclei ($0.2\rho_0 = 0.0336\,\mathrm{fm}^{-3}$), (c) slablike nuclei ($0.393\rho_0 = 0.0660\,\mathrm{fm}^{-3}$), (d) cylindrical holes ($0.49\rho_0 = 0.0823\,\mathrm{fm}^{-3}$), and (e) spherical holes ($0.575\rho_0 = 0.0966\,\mathrm{fm}^{-3}$). Box sizes are (a) 49.58 fm, (b) 39.35 fm, (c) 31.42 fm, (d) 29.19 fm, and (e) 27.67 fm.

mean curvature $\langle H \rangle$
Euler characteristic χ

$$\begin{cases} \langle H\rangle > 0 \text{ and } \chi/V > 0 & \text{for spherical nuclei (SP)} \\ \langle H\rangle > 0 \text{ and } \chi/V = 0 & \text{for cylindrical nuclei (C)} \\ \langle H\rangle = 0 \text{ and } \chi/V = 0 & \text{for slablike nuclei (S)} \\ \langle H\rangle < 0 \text{ and } \chi/V = 0 & \text{for cylindrical holes (CH)} \\ \langle H\rangle < 0 \text{ and } \chi/V > 0 & \text{for spherical holes (SH).} \end{cases}$$

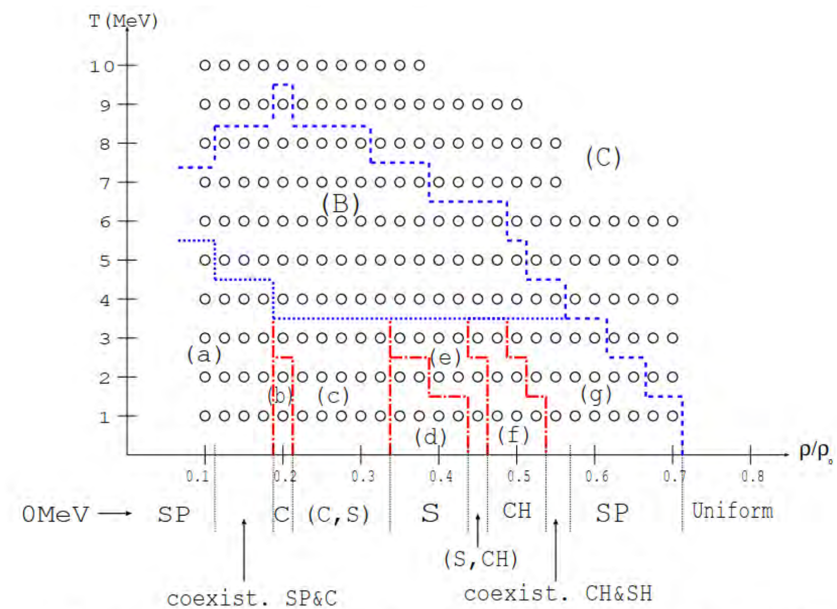


FIG. 5: (Color online) Phase diagram of nuclear matter of $x_p = 0.3$ at subnucear densities by QMD model 2 plotted in the ρ–T plane. The horizontal axis is normalized in unit of the nuclear saturation density. The dashed lines correspond to phase separation lines. The dotted lines show the boundary above which nuclear surface cannot be identified. The dash-dotted lines show boundaries between different phases. Abbreviations are the same as described in the caption to Fig. 1. The meanings of regions (a)–(g), (B), and (C) are explained in the text. Simulations have been carried out at the points denoted by circles.

CHARACTERIZATION OF THE PASTA

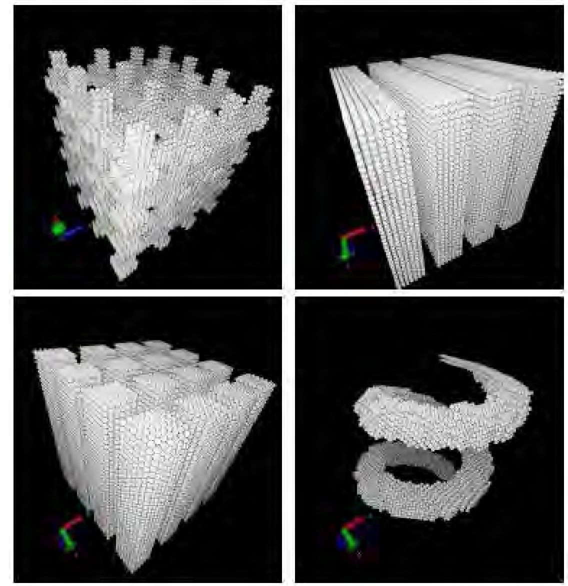
Pasta can be characterized with topology

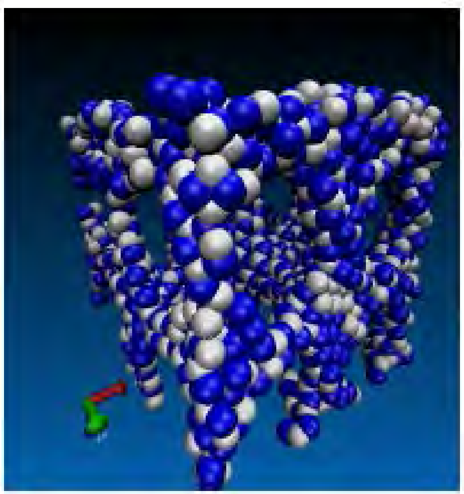
PHYSICAL REVIEW C
nuclear physics

Topological characterization of neutron star crusts

Phys. Rev. C **86**, 055805 – Published 29 November 2012

C. O. Dorso, P. A. Giménez Molinelli, and J. A. López





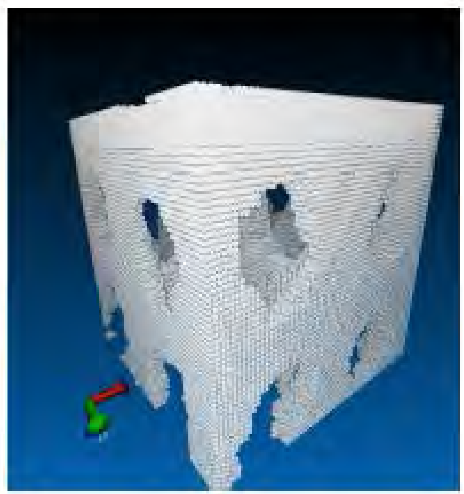
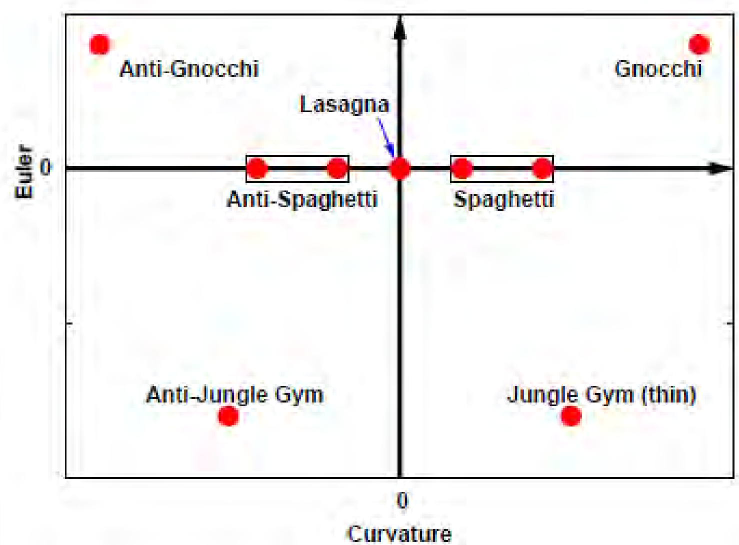


TABLE I: Classification Curvature - Euler

	Curvature < 0	Curvature ~ 0	Curvature > 0
Euler > 0	Anti-Gnocchi		Gnocchi
Euler ~ 0	Anti-Spaghetti	Lasagna	Spaghetti
Euler < 0	Anti-Jungle Gym		Jungle Gym



CHARACTERIZATION OF THE PASTA

Physics
spotlighting exceptional research

Synopsis: Italian Delicacies Served Up in a Neutron Star Crust

C. O. Dorso *et al.*, Phys. Rev. C (2012)

Topological characterization of neutron star crusts
C. O. Dorso, P. A. Giménez Molinelli, and J. A. López
Phys. Rev. C **86**, 055805 (2012)
Published November 29, 2012

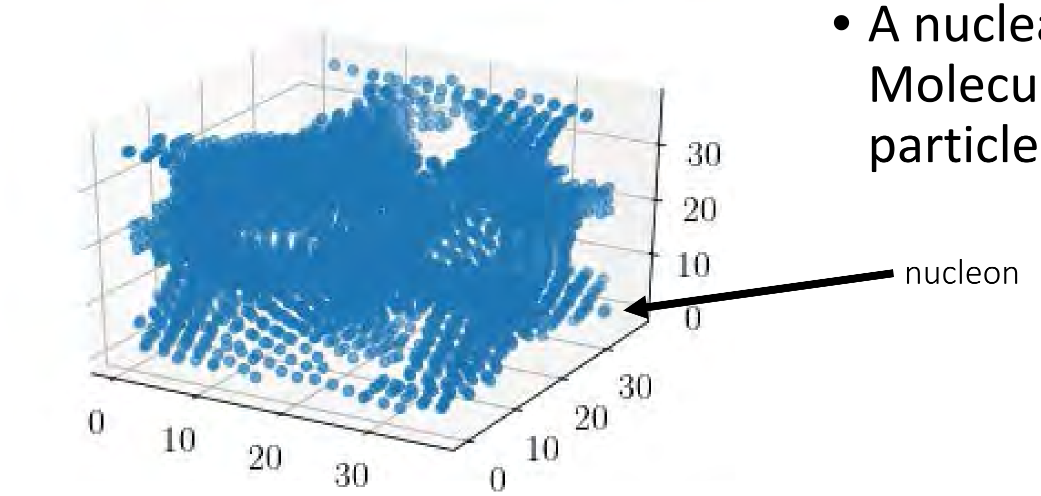
The matter in the outermost layer, or "crust," of a neutron star (the remnant of a supernova) is believed to host a variety of phases in which dense regions of nucleons are filled with voids of lower density. The presence of the phases, euphemistically referred to as "nuclear pasta" because of their resemblance to the shapes of lasagna, gnocchi, and spaghetti, may affect the emission of neutrinos, the primary mechanism by which the neutron star cools. In *Physical Review C*, Claudio Dorso of the University of Buenos Aires, Argentina, and colleagues report that a set of topological and geometric descriptors can accurately identify each pasta phase predicted by dynamical simulations, a labeling scheme that could be used to directly map the shape of a pasta phase to its effect on neutrino emission and neutron star cooling.

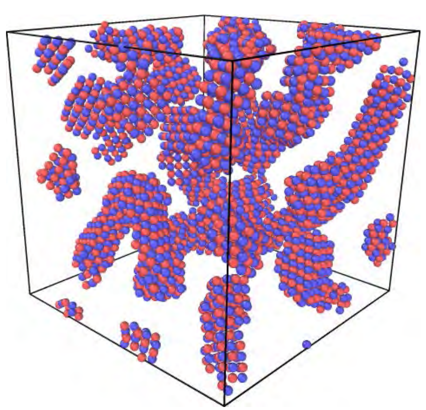
Dorso *et al.* classify a particular pasta phase by defining its volume, area, mean curvature, and its Euler characteristic—a number that represents the phase's topology. Although pasta phases have long been studied theoretically, the authors' calculations are some of the first to use a classical molecular dynamics model that is consistent with low- to medium-energy nuclear reactions. Moreover, they make no initial assumptions about the phase structure, which should help clarify the balance of forces and parameters that lead to the formation of each phase. – *Joseph Kapusta*

Alpha Shapes Method

How do you go from a set of points to a 3D structure?

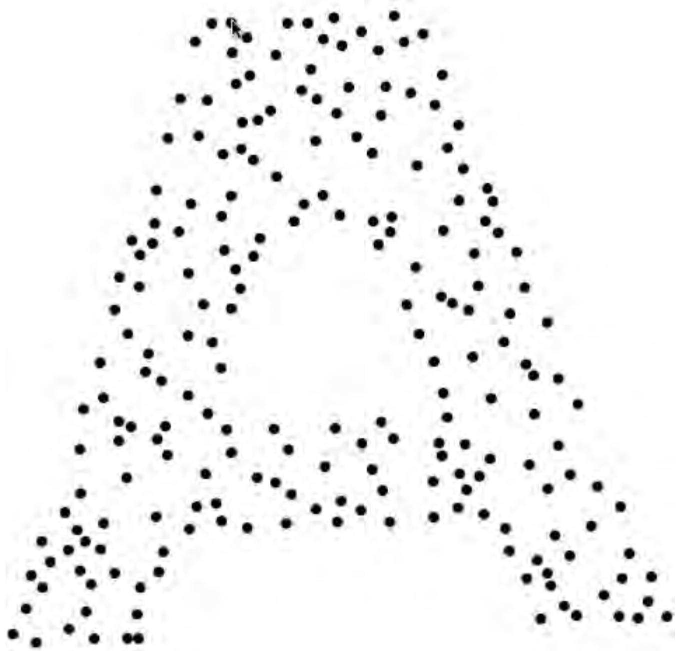
- A nuclear structure generated by Molecular dynamics calculates the particles' positions for specific parameters.

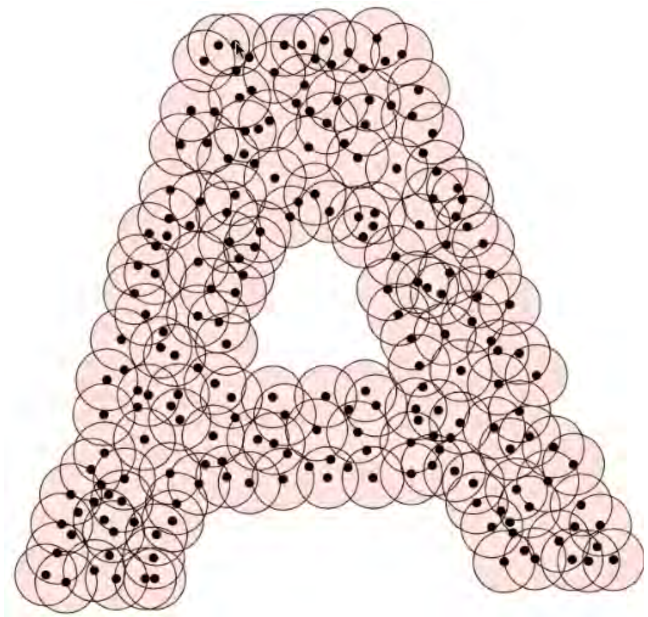




Positions of the neutrons and protons for T = 0.01 MeV, and density 0.02 fm^{-3}

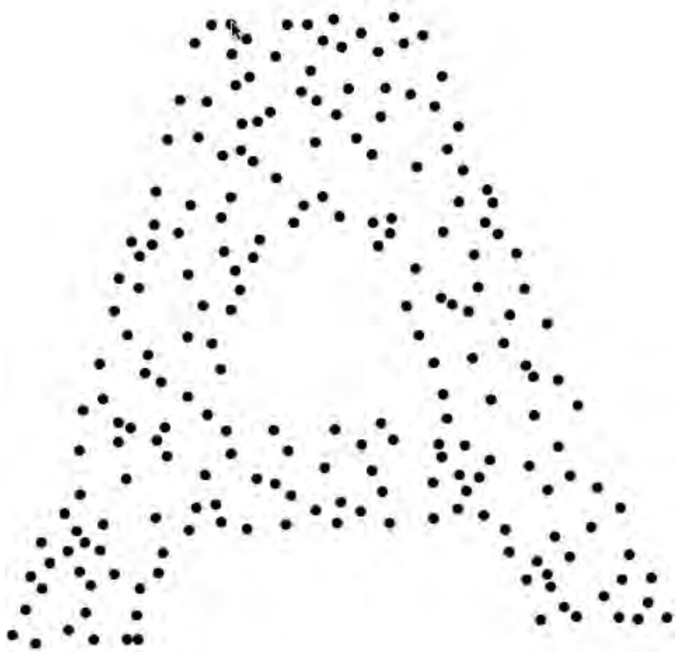
ALPHA SHAPES MODEL: UNION OF BALLS

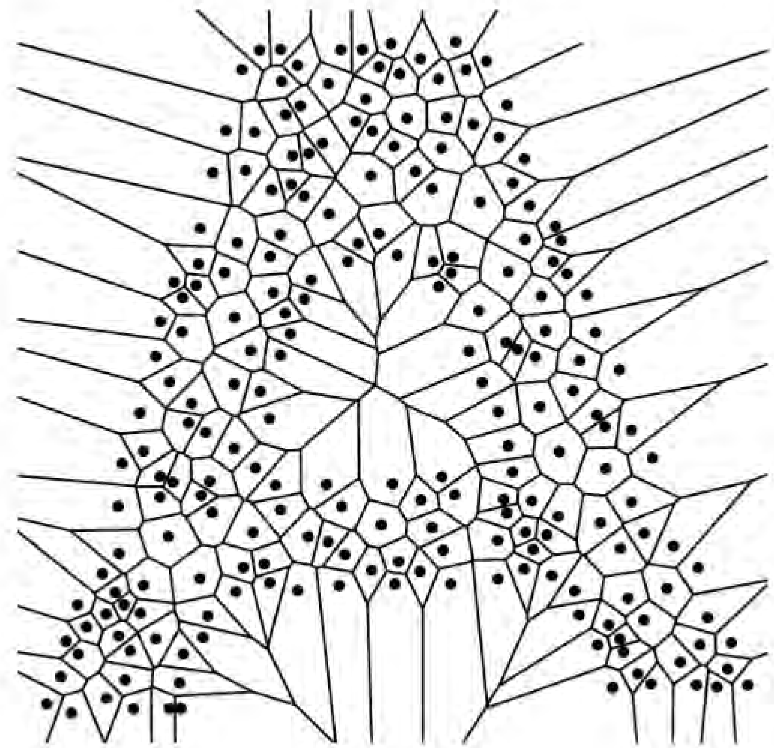




union of balls of radius α: $\bigcup_p \mathrm{B}_\alpha(p)$

Voronoi diagrams

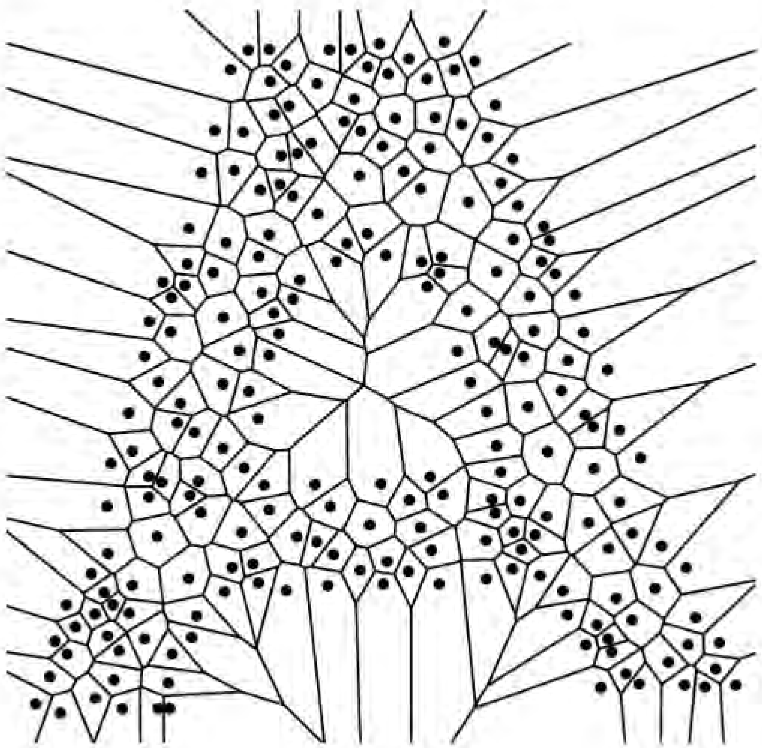


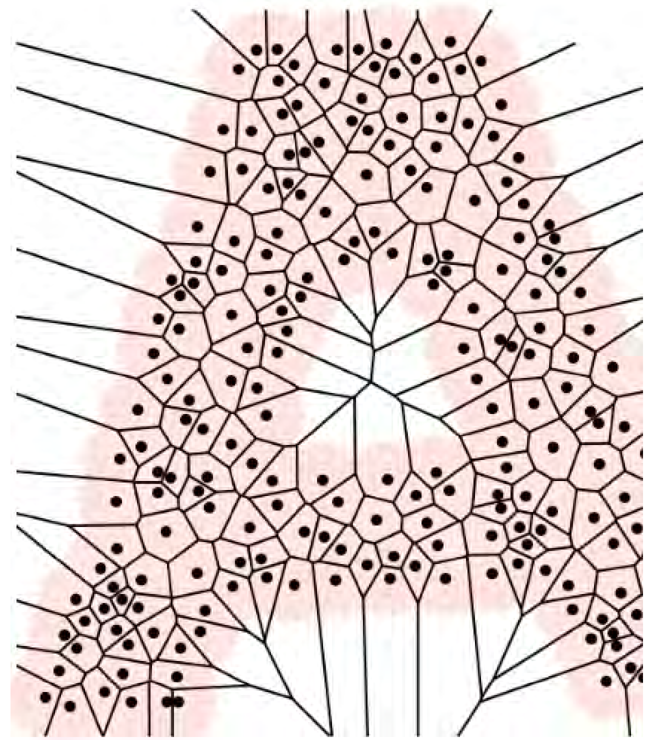


Voronoi diagram:

$$\mathrm{Vor}(p) = \{x \in \mathbb{R}^n \mid \|x - p\| \leq \|x - q\| \ \forall q \in P\}$$

Voronoi diagrams + spheres

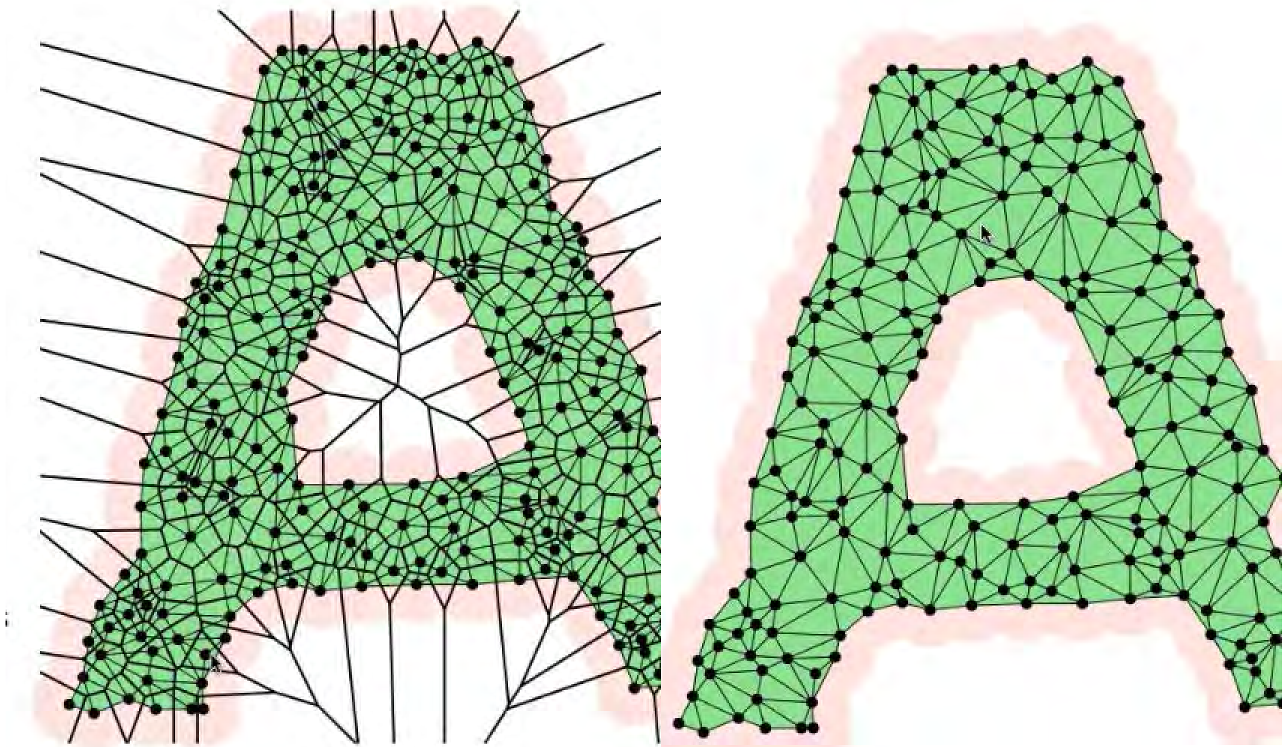




Voronoi diagram:

$$\mathrm{Vor}(p) = \{x \in \mathbb{R}^n \mid \|x - p\| \leq \|x - q\| \ \forall q \in P\}$$

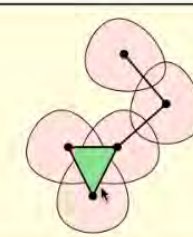
Nerves: Voronoi diagrams + spheres - overlaps



Nerve

$\mathcal{C}$ = collection of sets

$$\operatorname{Nrv}\mathcal{C} = \{\sigma \subseteq \mathcal{C} \mid \cap\sigma \neq \emptyset\}$$

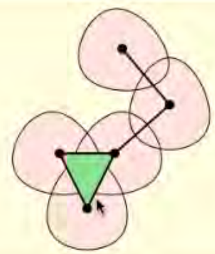


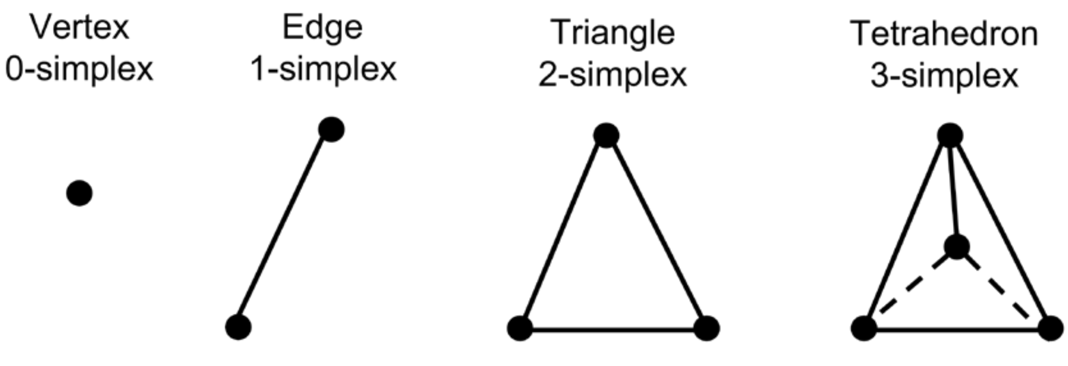
NERVES

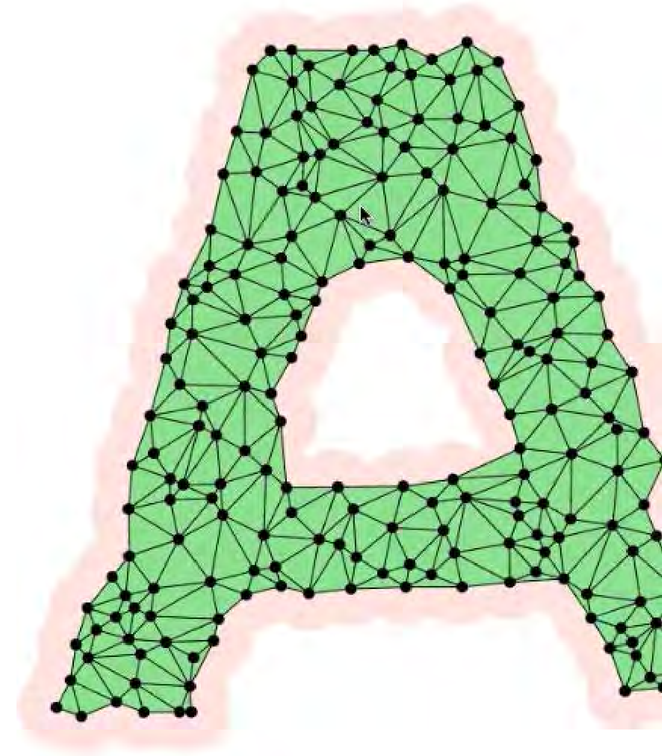
Nerve

$\mathcal{C}$ = collection of sets

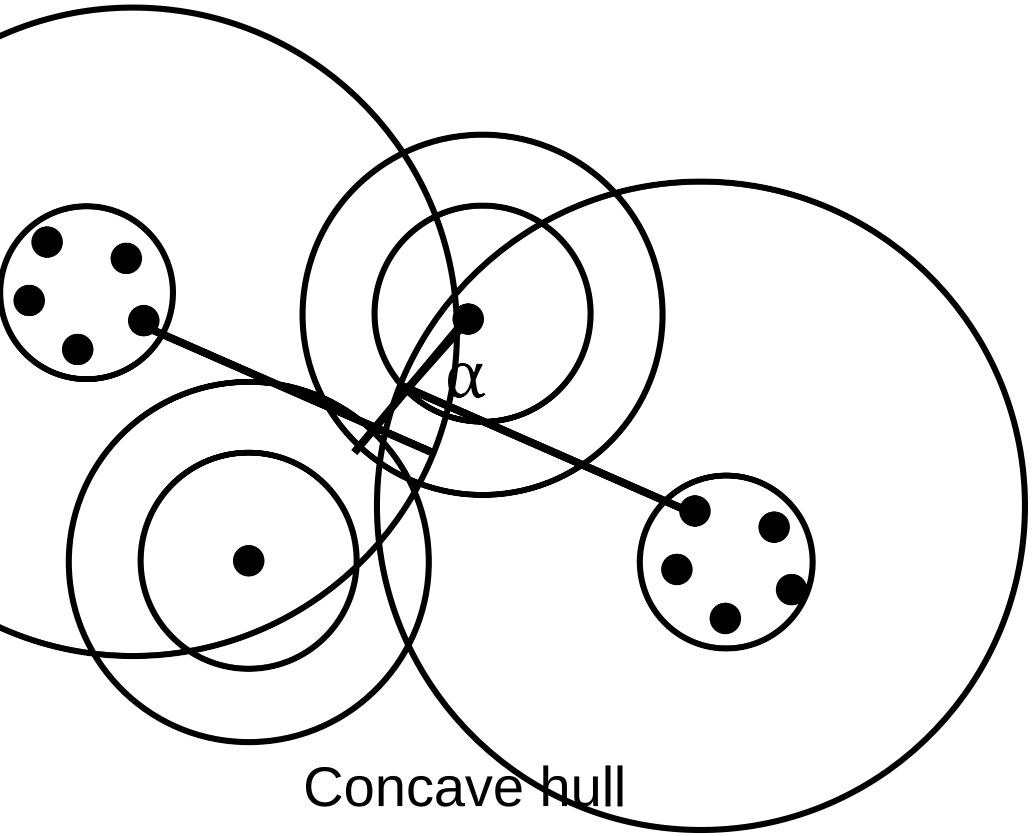
$\mathrm{Nrv}\,\mathcal{C} = \{\sigma \subseteq \mathcal{C} \mid \cap\sigma \neq \emptyset\}$





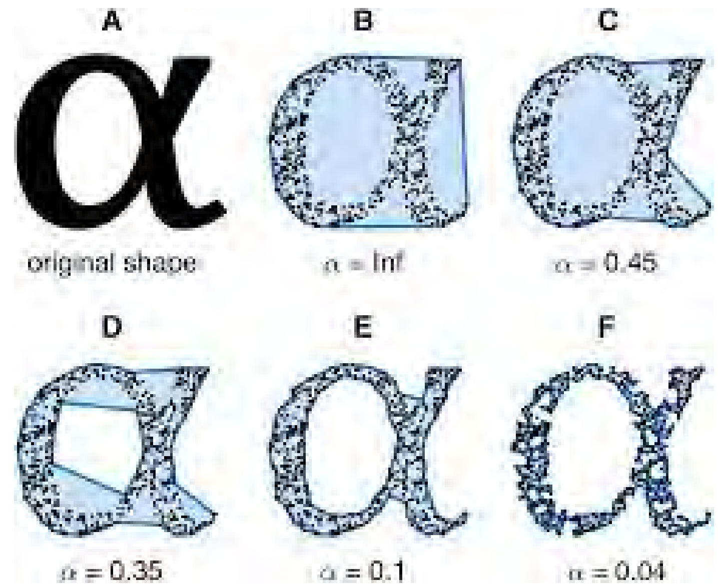


DEPENDENCE ON THE ALPHA RADIUS



Concave hull

Convex hull



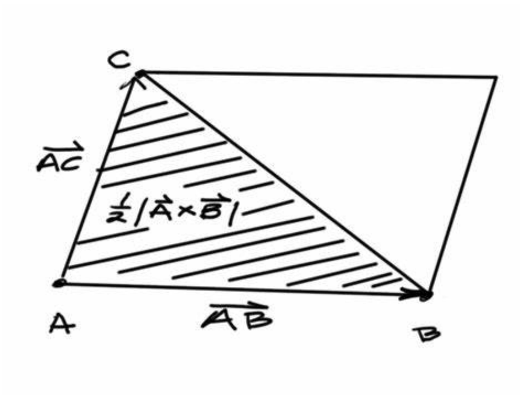
Gardiner, J.D., Behnsen, J. & Brassey, C.A. Alpha shapes: determining 3D shape complexity across morphologically diverse structures. *BMC Evol Biol* **18**, 184 (2018). https://doi.org/10.1186/s12862-018-1305-z

DioDe

- DioDe uses CGAL to generate alpha shapes filtrations in a format Dionysus understands (designed by Dmitriy Morozov).
- Produces simplexes with varying radii from data input.

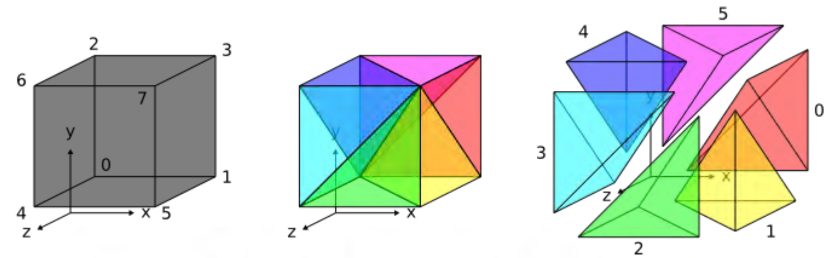
DioDe and Minkowski functionals: Volume and Area

- Area



$$S = \frac{1}{2}||(\vec{B} - \vec{A}) \times (\vec{C} - \vec{A})||$$

- Volume



$$V = \frac{1}{6}[(\vec{B} - \vec{A}) \times (\vec{C} - \vec{A})] \cdot \vec{A}$$

$$= \frac{1}{6}\begin{vmatrix} B_x - A_x & B_y - A_y & B_z - A_z \\ C_x - A_x & C_y - A_y & C_z - A_z \\ A_x & A_y & A_z \end{vmatrix}$$

DioDe and Minkowski functionals: *χ* and *B*

- Euler Characteristic

$$\chi = \sum_{k}^{n} (-1)^k$$

k represents a simplex.

- Curvature

$$cos(\gamma) = \frac{\vec{A} \times \vec{B}}{||\vec{A} \times \vec{B}||}$$

$$cot(\gamma) = \frac{cos(\gamma)}{sin(\gamma)}$$

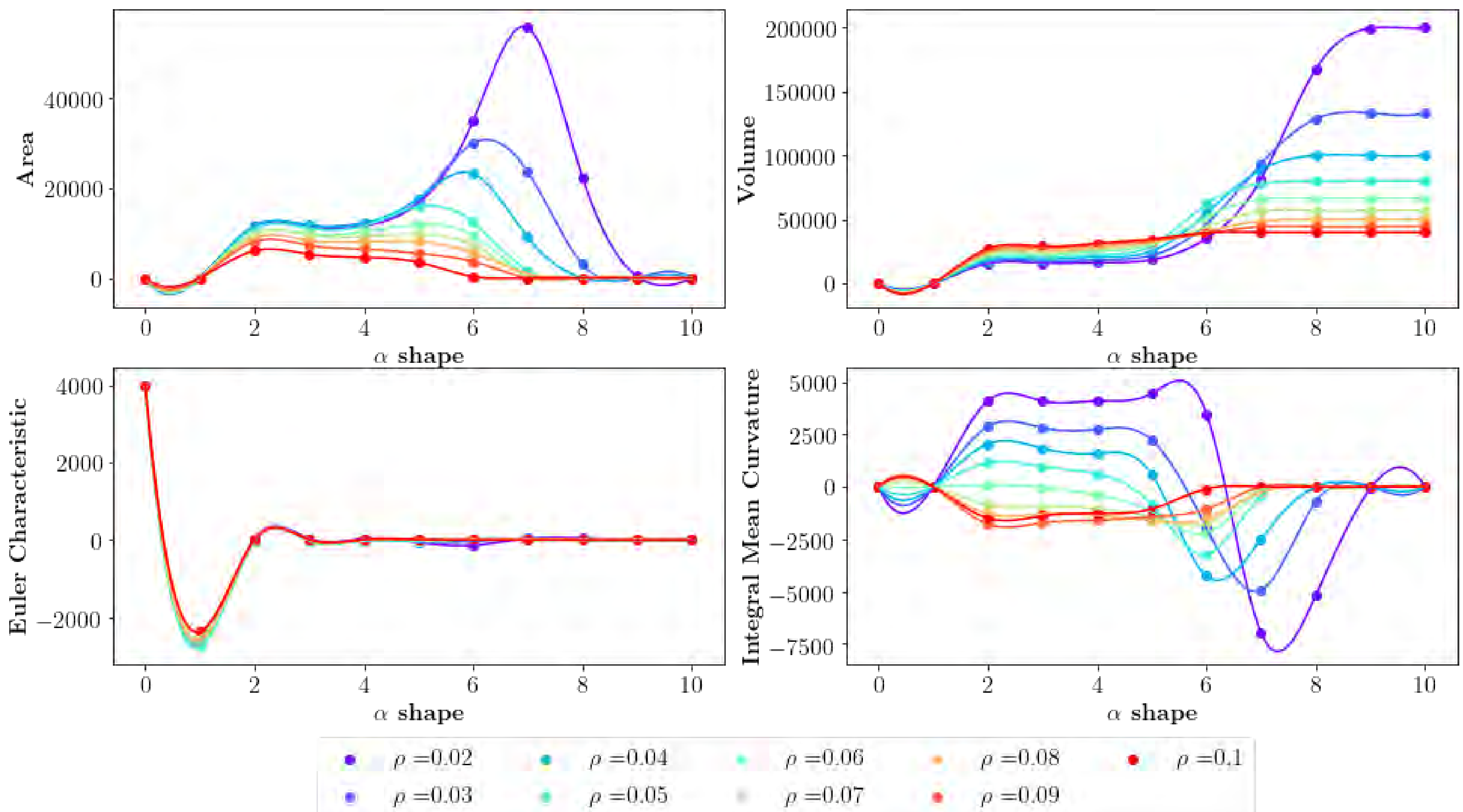
$$curv_A = \frac{\vec{B} - \vec{A}}{2} cot(\gamma)$$

Alpha – shapes model method

- Each structure had to be analyzes with, at least, 40 α radii to find the optimized radii length.
- For each α, the volume, area, Euler, and curvature were calculated.
- A minimum of 160 calculations were performed for each structure.
- In total, there were over 9,120 calculations.

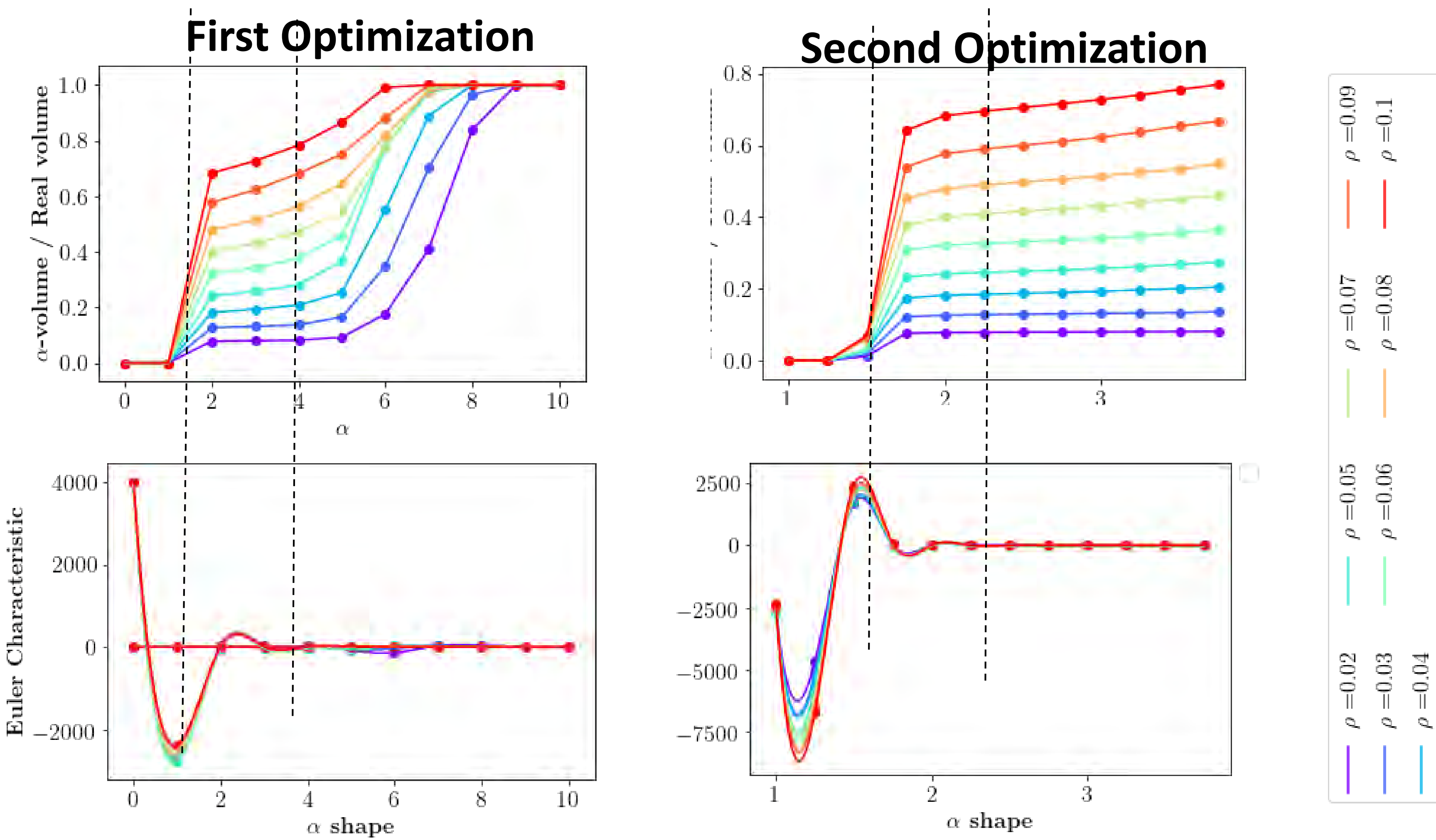
Determining the optimal alpha

Minkowski functionals for T = 1 MeV with 0< α <10,
x = 0.5, and density from 0.04 fm^{-3} to 0.20 fm^{-3}.



CHARACTERIZATION OF THE PASTA

Volume normalization and χ for two optimizations of α



Conclusion: $1.5 < \alpha < 2 \rightarrow \alpha = 1.6$

- MOTIVATION
- CLASSICAL MOLECULAR DYNAMICS
- CHARACTERIZATION OF THE PASTA
- RESULTS
- CONCLUSIONS

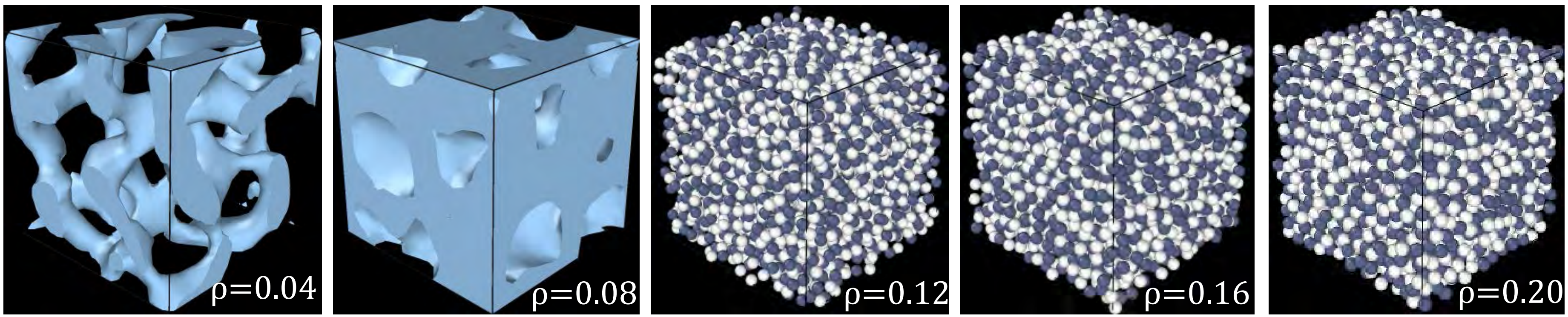
RESULTS

APPLICATION OF THE α-SHAPE METHOD

- Molecular dynamics simulations
  - Use LAMMPS, 4000 nucleons, x = 0.5.
  - Cool down a nuclear matter system from T = 4 MeV to a final temperature between 0.01 MeV to 1 MeV, using 1 million time steps.
  - Densities from 0.02 fm^{-3} to 0.20 fm^{-3}.
- Alpha shapes method
  - Import MD simulations output (x,y,z) file.
  - Calculate simplexes of the final temperature for a specific α.
  - Compute Minkowski functionals: Area, Volume, Euler number, Curvature.
  - Repeat to optimize α radius.
- Results and conclusion
  - Analyze correlations between A,V,C and E
  - Euler *versus* Curvature looks promising.

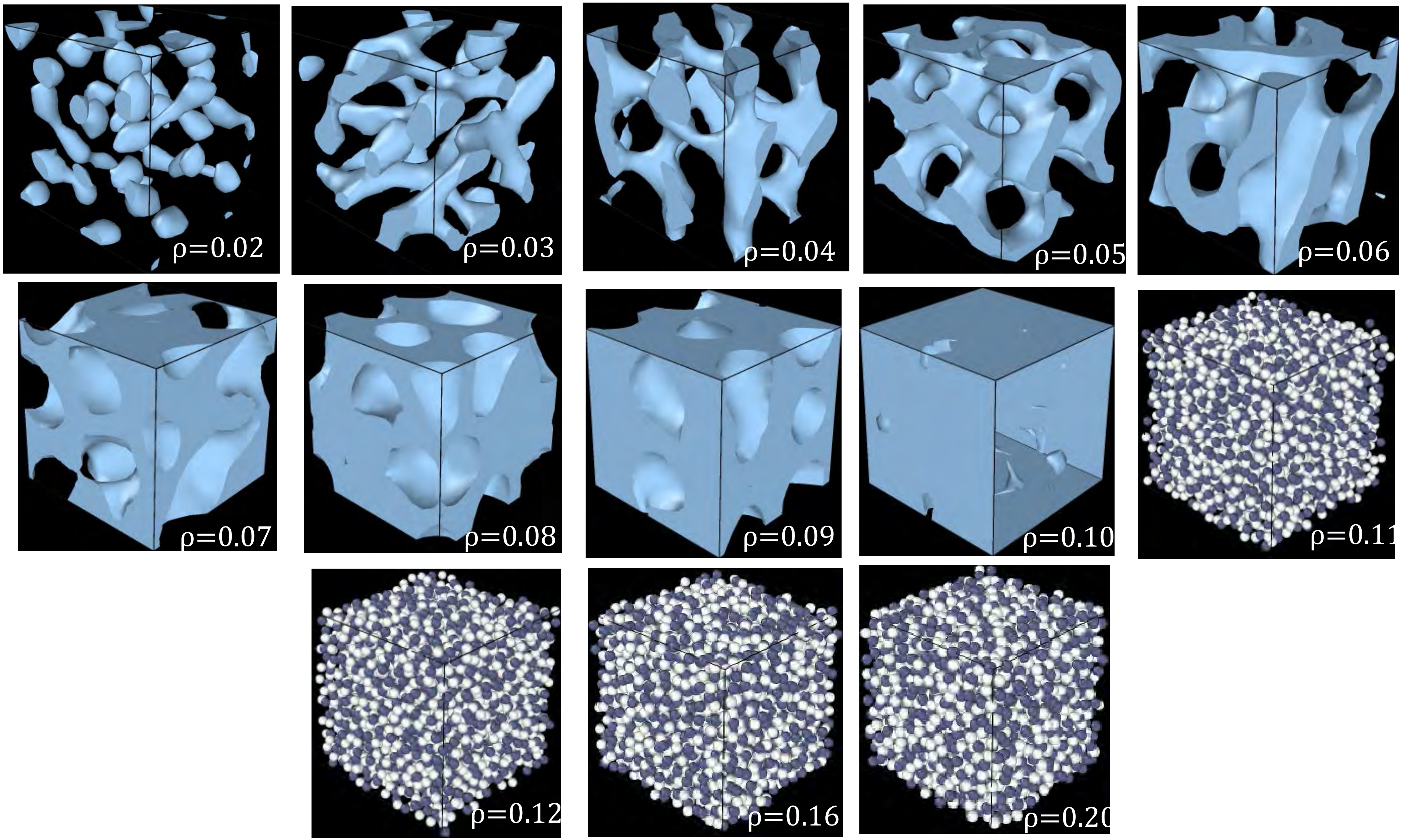
RESULTS

T = 1 MeV



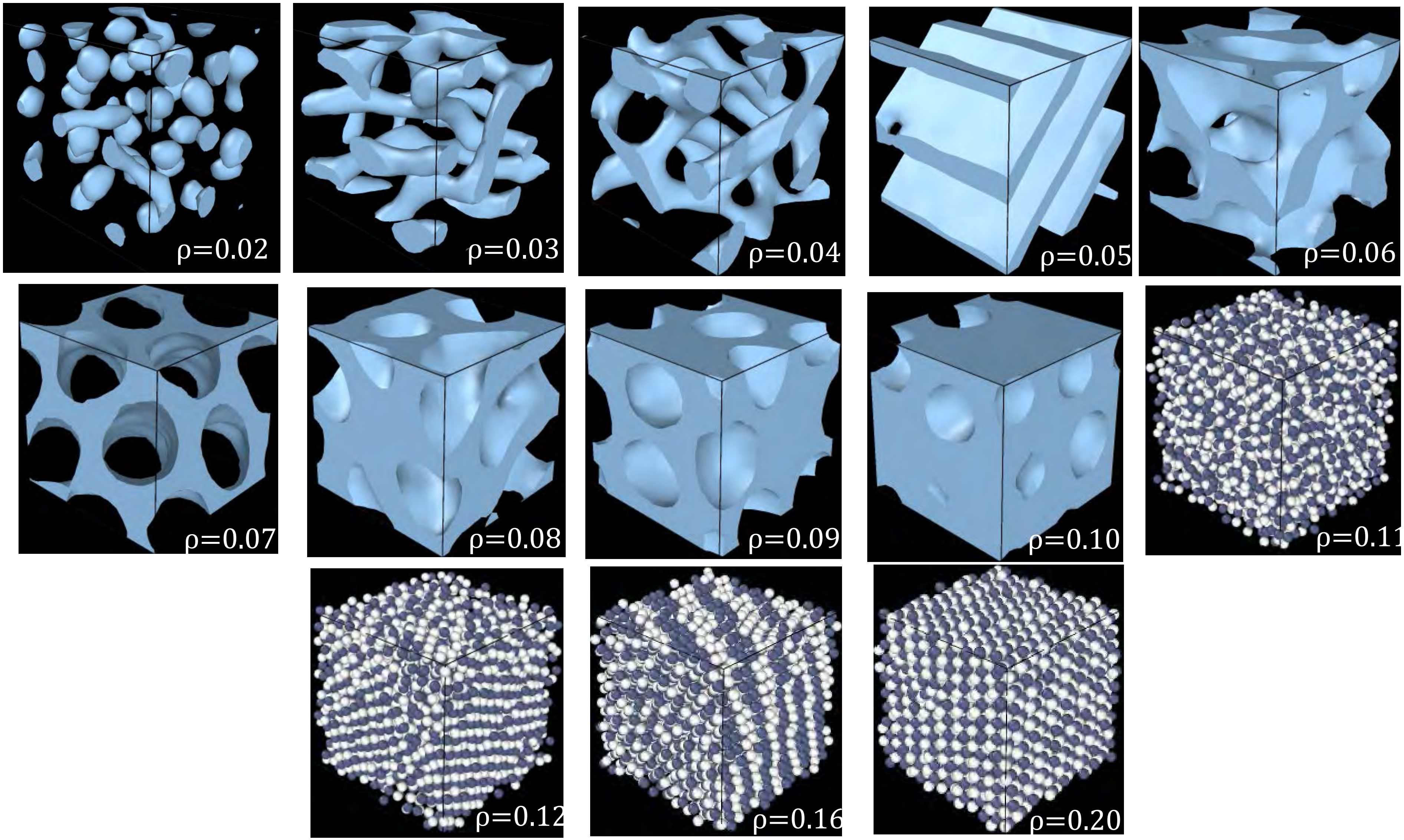
RESULTS

T = 0.75 MeV



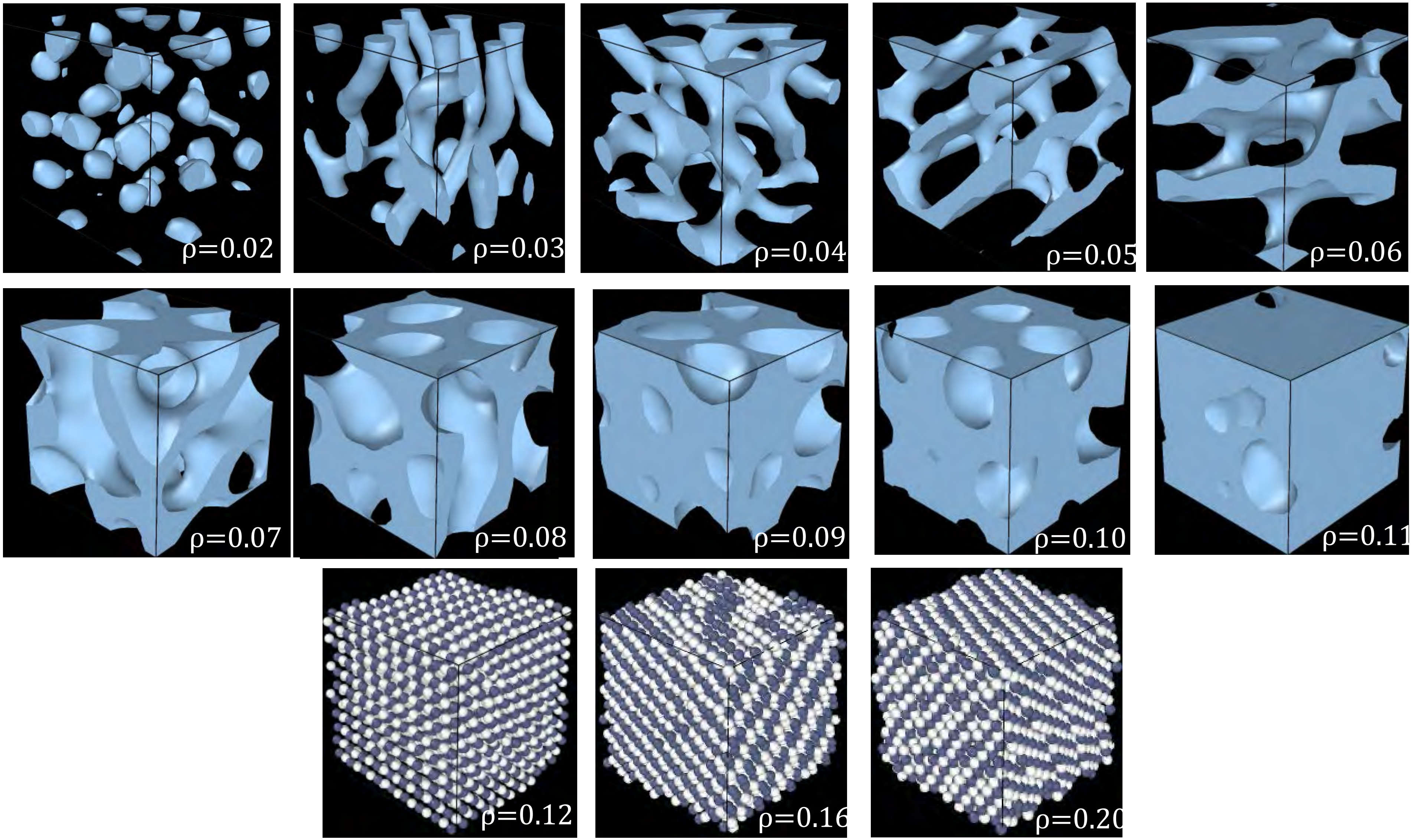
RESULTS

T = 0.50 MeV



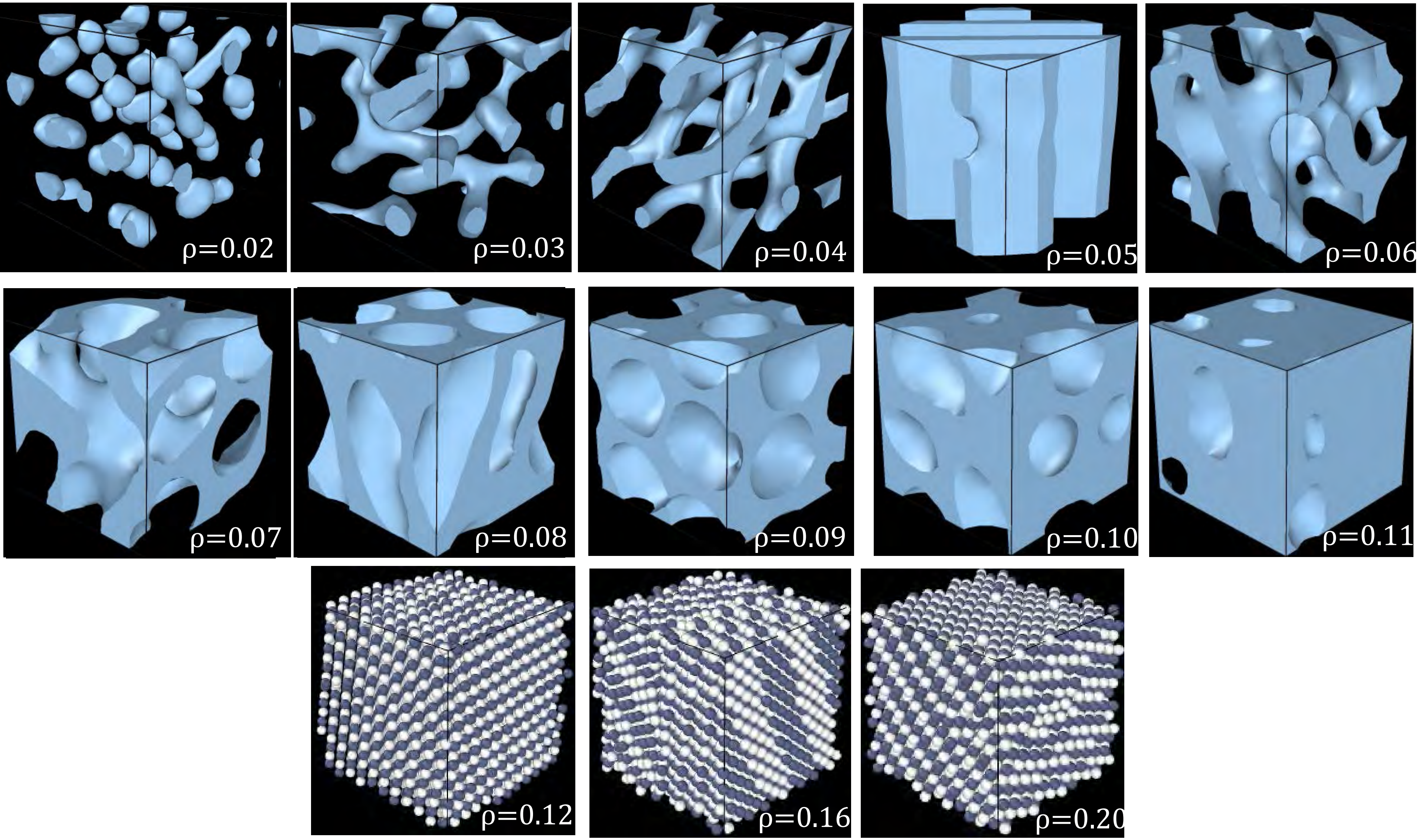
RESULTS

T = 0.25 MeV



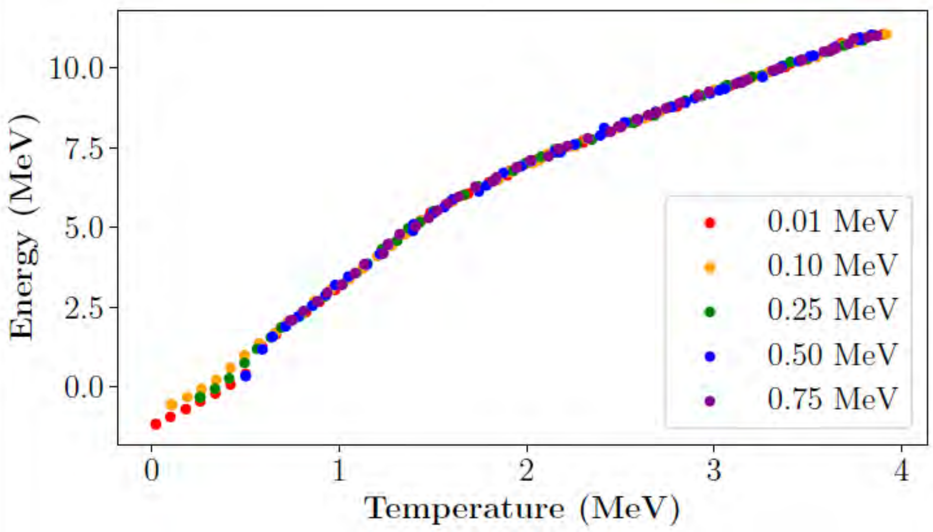
RESULTS

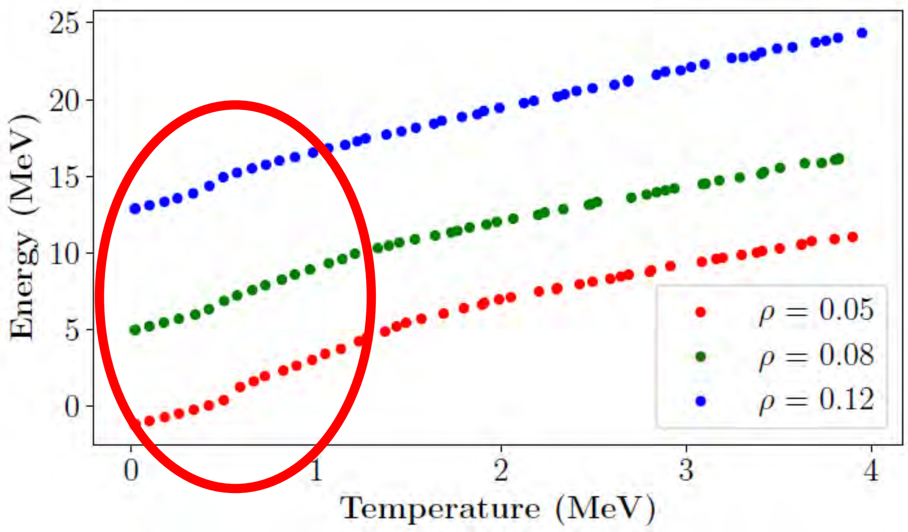
T = 0.01 MeV, x = 0.5



RESULTS

PROPERTIES OF THE COOLING PROCESS





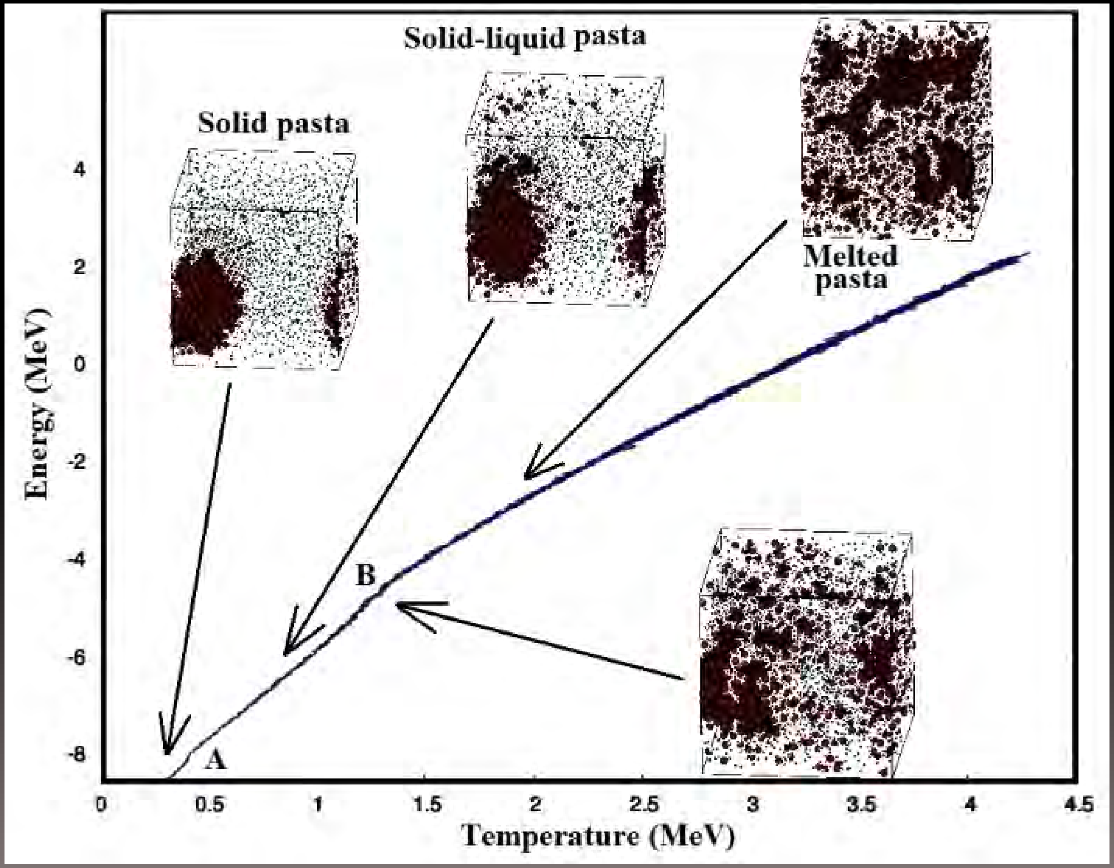
Caloric curve, E vs T, for cooling of systems

- The left figure is for ρ = 0.05 fm^{-3} with the final temperatures of 0.01 to 0.75 MeV.
- The right figure computes three densities with a final temperature of 0.01 MeV

RESULTS

Phase transitions within the pasta

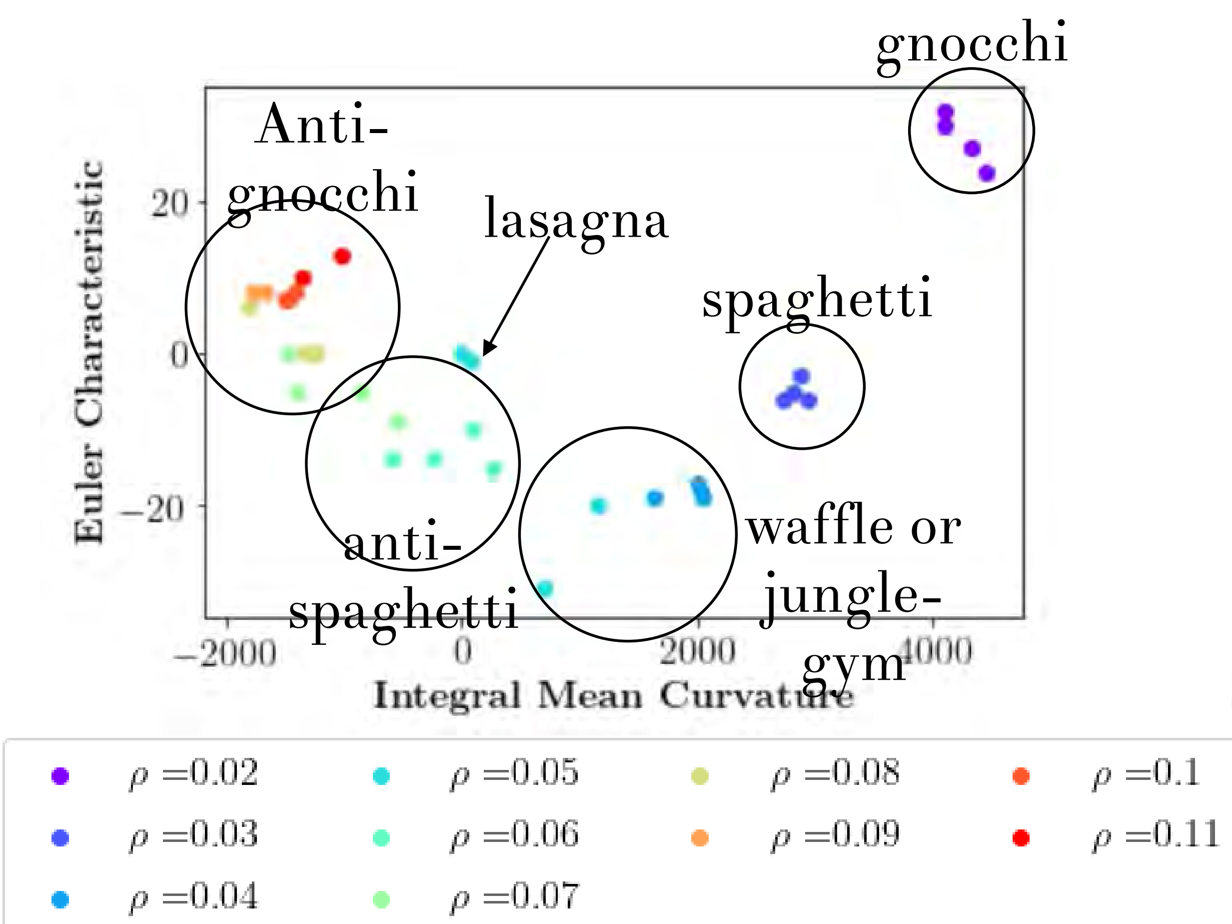
Solid Pasta ⟷ Solid-Liquid Pasta ⟷ Liquid Pasta



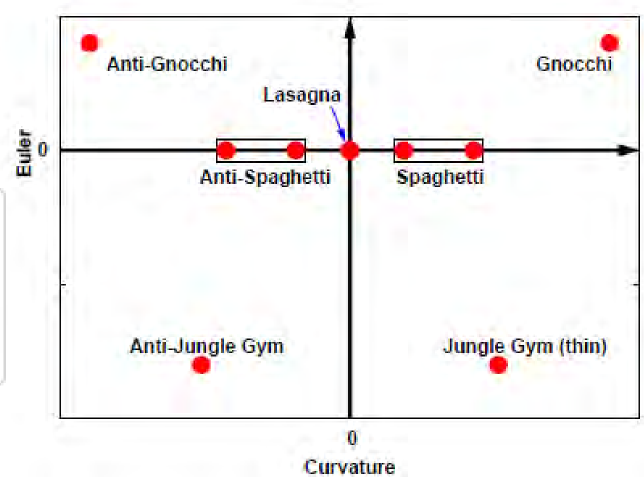
MOLECULAR DYNAMICS RESULTS

- In total, 57 nuclear matter simulations were produced.
- Each structure had between 1 million and 8 million time steps to reach final equilibrium position.
- Run on the supercomputer Cori of the National Energy Research Scientific Computing Center (NERSC).

Euler – Curvature



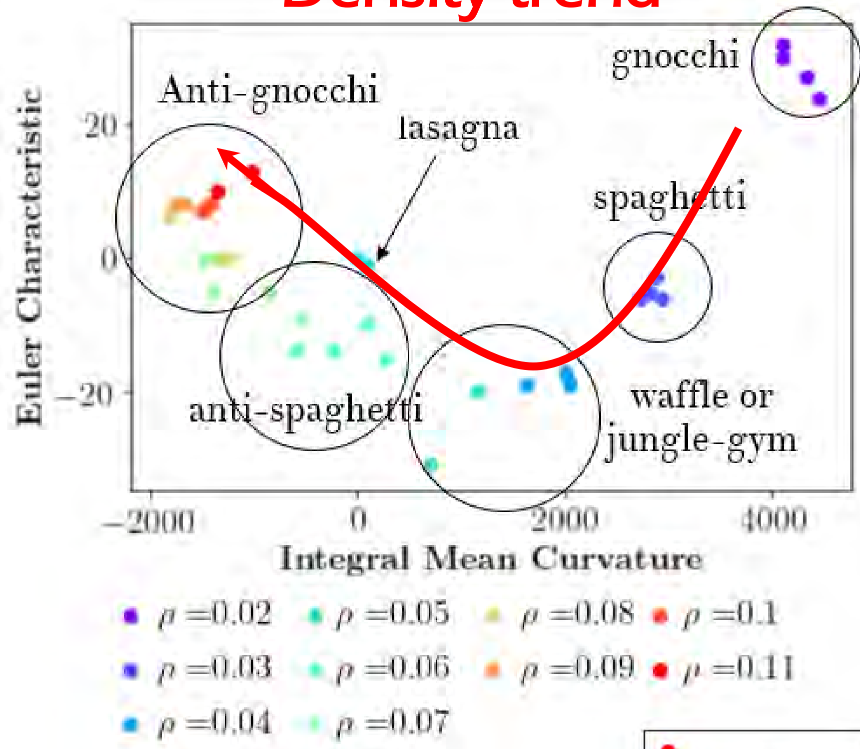
- Each structure has a unique alpha.
- A clockwise trend is found for the density, from smaller to greater.
- Non-pastas are expected at the origin (and lasagnas).



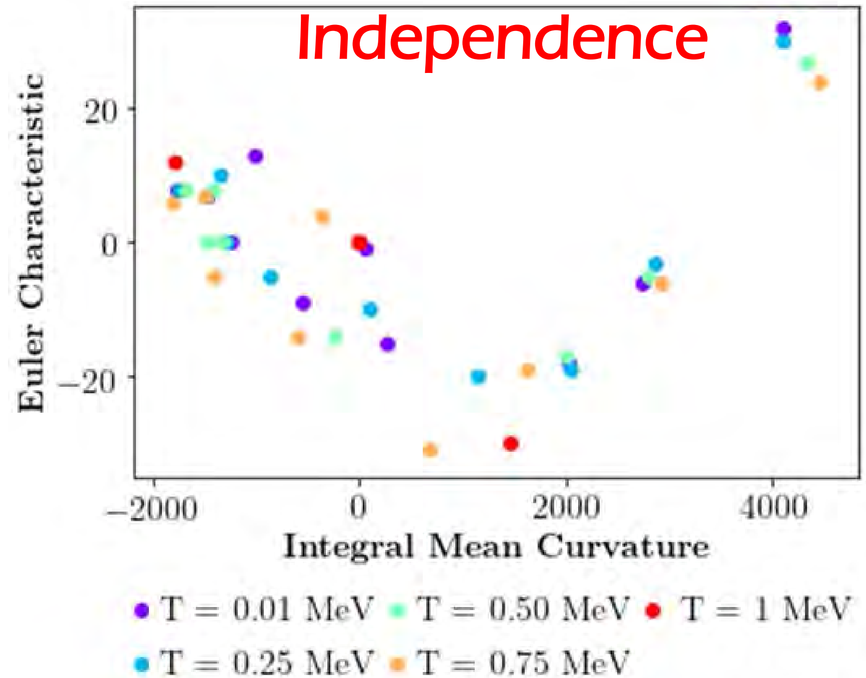
RESULTS

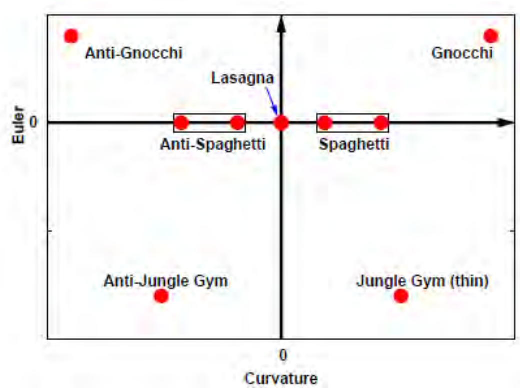
Euler – Curvature

Density trend



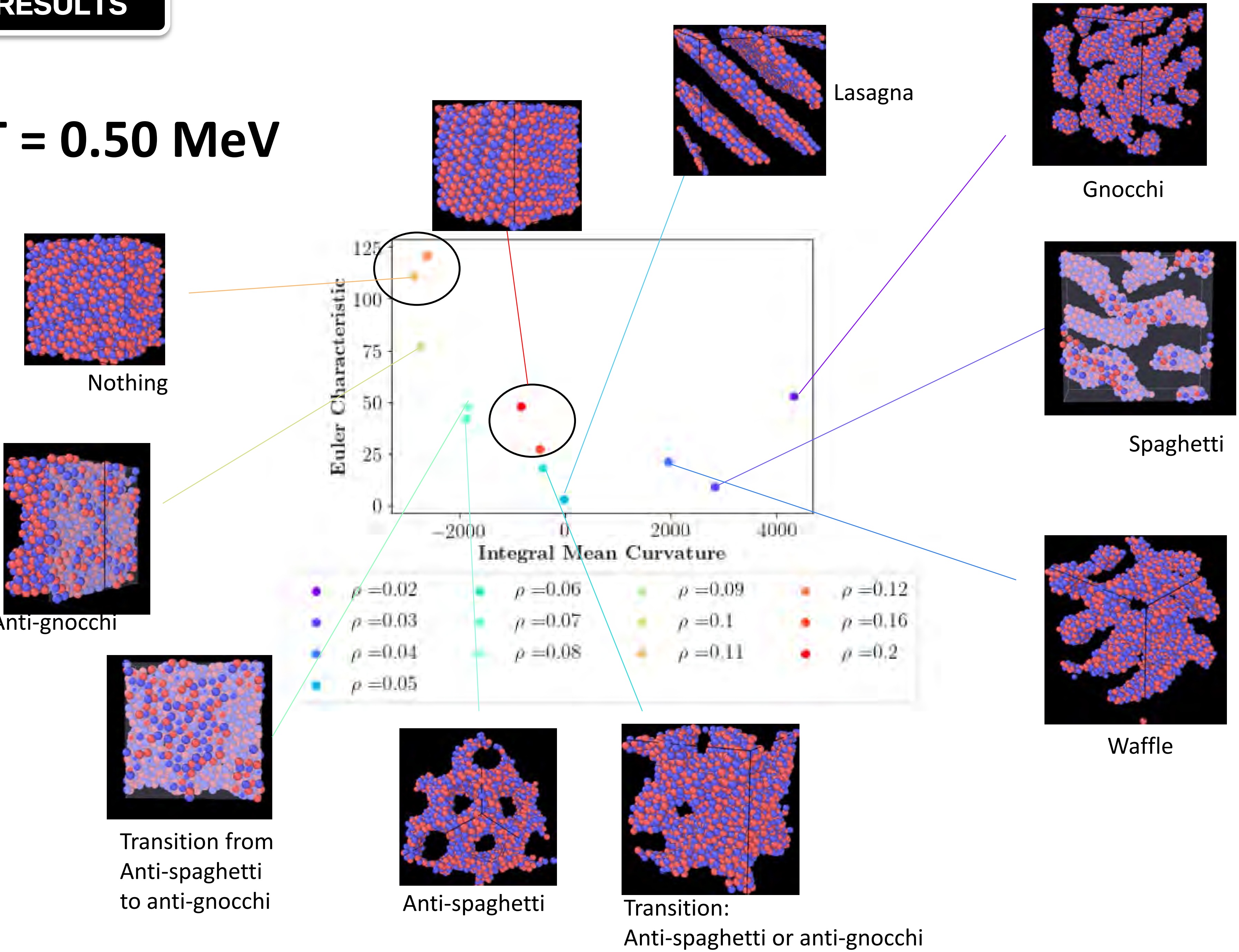
Temperature Independence





RESULTS

T = 0.50 MeV



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CONCLUSIONS

- Pasta structures are formed at low temperatures and subcritical densities
- Topology helps to study shapes of pasta

CONCLUSIONS

- The pasta structures were created using molecular dynamics (LAMMPS).
- The alpha-shapes method was used to construct the 3D structures.

CONCLUSIONS

- The Minkowski functionals were calculated out of the structures.
- Pasta structures can be identified by their values of Euler characteristic and curvature.

- There is a relationship between the pasta structures and their density in the Euler - curvature plane.
- The relationship follows a clockwise trend in the E-C plane as the density increases.
- The trend is independent of temperature.

Thanks !

Current work:

- *Momentum-dependent potentials*
- *Introduction of Pauli exclusion principle*
- Collisions!