Molecular Dynamics of Nuclear Pasta Formation

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Abstract

In a fraction of a second a supernovae transforms the core of a massive star, with 10^{55} separate nuclei, into a single large nucleus, a neutron star. Between the crust and the core of a neutron star competition between attractive nuclear and repulsive electromagnetic interactions causes nuclear matter to rearrange itself into exotic shapes such as sheets, cylinders, etc. These shapes are collectively known as nuclear pasta. We use molecular dynamics (MD) simulations to study the phase transitions between different pasta shapes as density decreases from nuclear saturation density to less than a tenth of saturation density. We, then, use topological quantities known as Minkowski functionals to characterize the pasta shapes and study the equilibration of the system.

Model

High density matter is modeled as a collection of protons and neutrons immersed in a degenerate electron gas. Nucleons are assumed to interact via a two-body potential:

$$v_{ij} = a e^{-\frac{r_{ij}^2}{\Lambda}} + [b + c\tau_z(i)\tau_z(j)]\, e^{-\frac{r_{ij}^2}{2\Lambda}} + \frac{\alpha}{r_{ij}} e^{-\frac{r_{ij}}{\lambda}} \tau_p(i)\tau_p(j).$$

Parameters a, b, c and Λ were chosen to reproduce some bulk properties of nuclear matter and binding energy of selected nuclei [1] while the Coulomb screening length was set to $\lambda = 10\,\mathrm{fm}$. Knowing the inter-particle potential allows us to calculate the force on each nucleon and evolve the system using Newton's laws.

Simulations

We simulated 51 200 nucleons with a proton fraction of $Y_p = 0.40$ and temperature $T = 1\,\mathrm{MeV}$ in a cubic box with periodic boundary conditions. While some runs were performed with a fixed simulation volume (constant density runs) others had their simulation volume increased at a constant rate (expansion runs). For the expansion runs the side l of the box changed according to

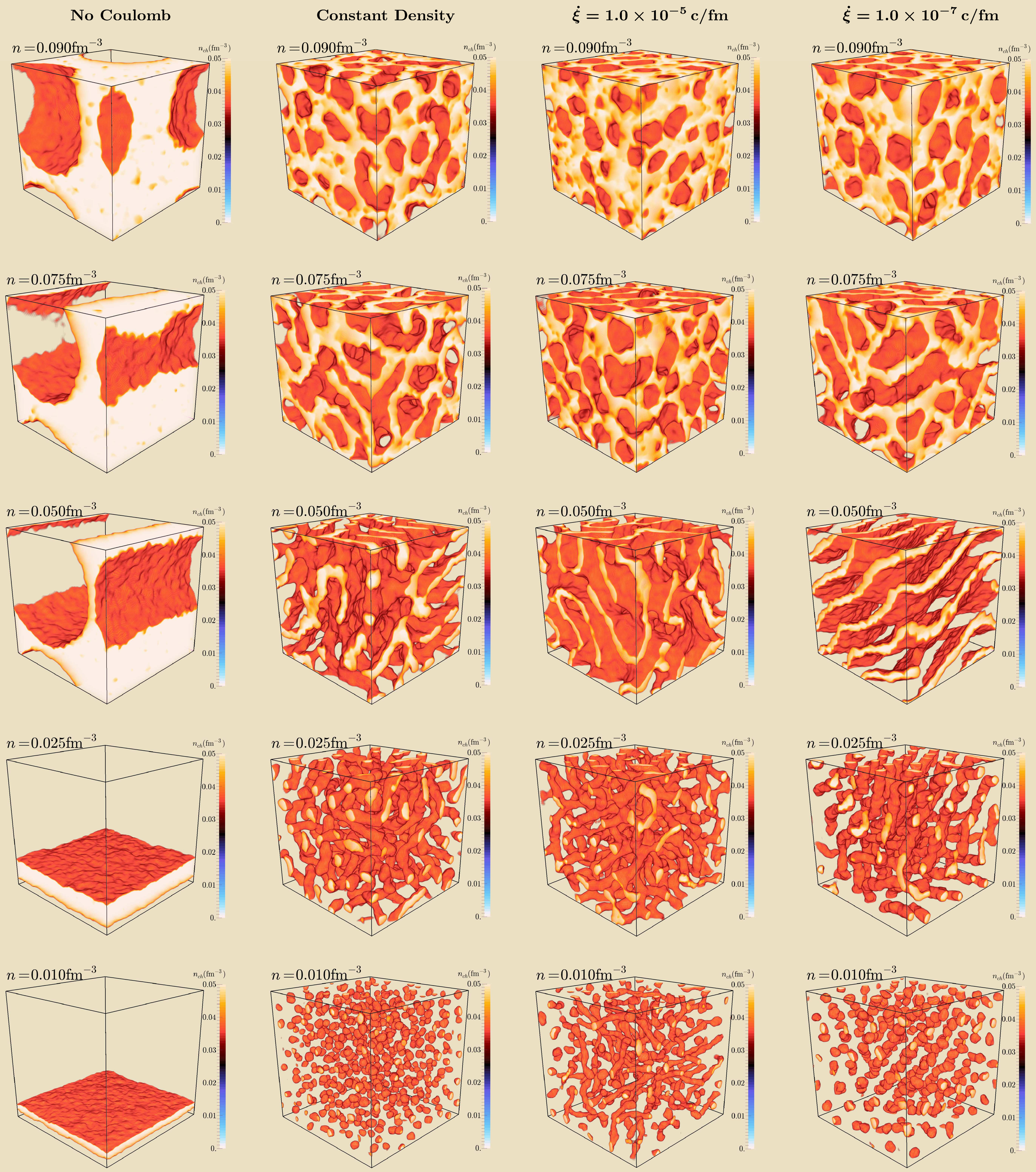
$$l(t) = l_0(1 + \dot{\xi}t)$$

where $l_0 = 80\,\mathrm{fm}$ is the initial size of the box and $\dot{\xi}$ the stretching rate. Our simulations were performed on the Kraken [2] and BigRed supercomputers.

Results

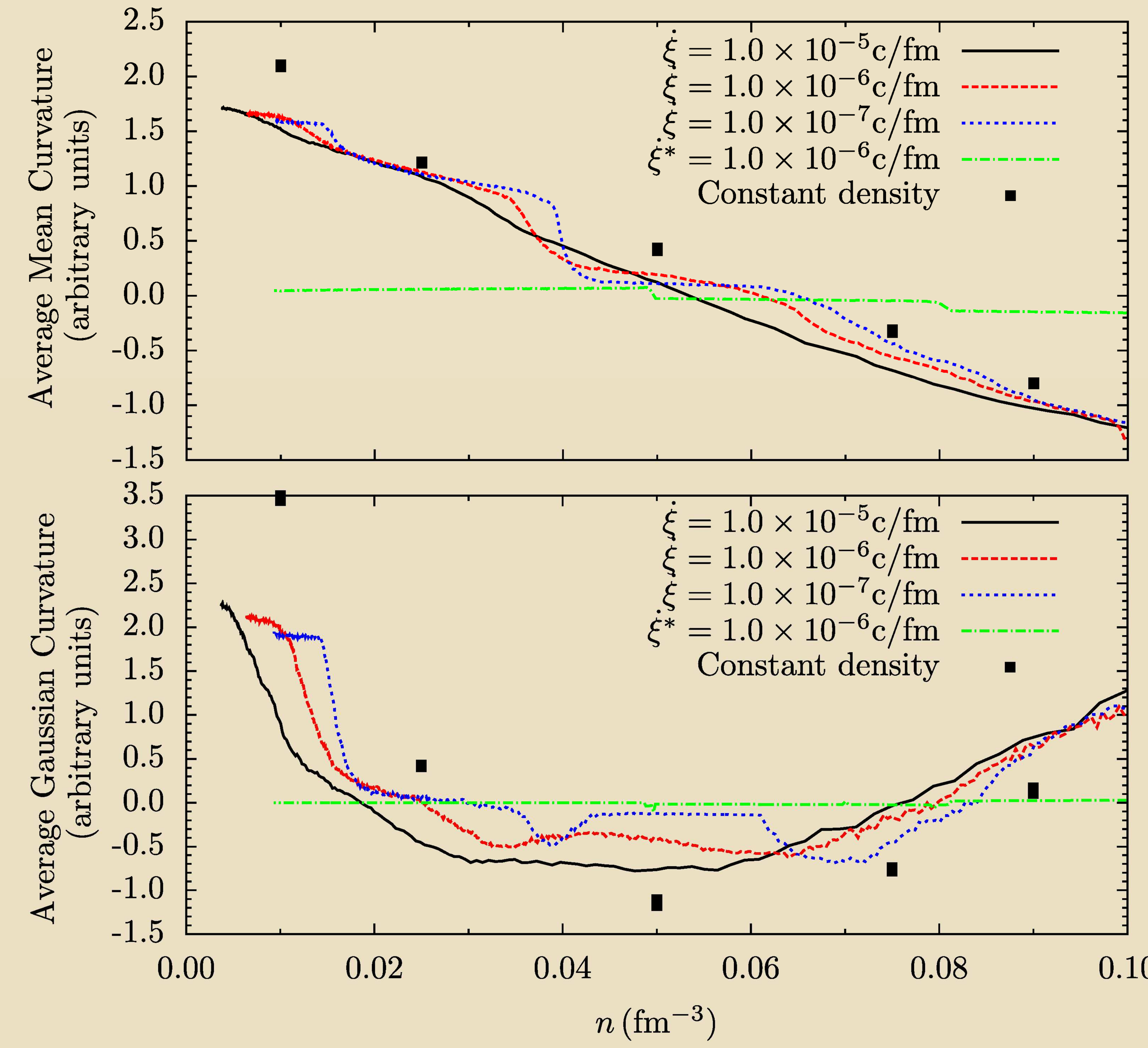
Comparison of pasta shapes obtained for different MD simulations at five different densities.

- **First column**: expansion run with $\dot{\xi} = 1.0 \times 10^{-6}\,\mathrm{c/fm}$ and no Coulomb potential.
- **Second column**: constant density runs evolved for a time of $500\,000\,\mathrm{fm/c}$.
- **Third column**: expansion run with $\dot{\xi} = 1.0 \times 10^{-5}\,\mathrm{c/fm}$.
- **Fourth column**: expansion run with $\dot{\xi} = 1.0 \times 10^{-7}\,\mathrm{c/fm}$.



Curvature

Pasta phases can be characterized by their average mean and average Gaussian curvatures.



Summary & Outlook

The purpose of this work was to study the dynamics of phase transitions between pasta phases and their time scale using MD. In the future we intend to perform larger simulations, simulations with slower expansion rates as well as explore regions of phase space with lower proton fractions and temperatures. Our final goal is to use our simulations to obtain a variety of observables.

References

[1] C.J. Horowitz, M.A. Pérez-García, J. Carriere, D.K. Berry and J. Piekarewicz, Phys. Rev. C **69** 065806 (2004)

[2] National Institute for Computational Sciences, U. Tenn. and Oak Ridge National Laboratory.

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