LARGE-SCALE MOLECULAR DYNAMICS SIMULATIONS OF NUCLEAR PASTA

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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. During this process and between the crust and the core of the left-over neutron star a strong competition between attractive nuclear forces and repulsive electromagnetic interactions takes place. This competition causes matter to rearrange itself into a range of exotic shapes collectively known as nuclear pasta. In our work we use the Indiana University Molecular Dynamics (IUMD) Fortran code to study the shapes and properties of this phase of matter.

MODEL

We assume a minimal model where nuclear matter is made up of point-like neutrons and protons immersed in a degenerate relativistic electron gas and interact via a two-body potential

$$V_{np}(r) = ae^{-r^2/\Lambda} + [b-c]e^{-r^2/2\Lambda},$$
$$V_{nn}(r) = ae^{-r^2/\Lambda} + [b+c]e^{-r^2/2\Lambda},$$
$$V_{pp}(r) = ae^{-r^2/\Lambda} + [b+c]e^{-r^2/2\Lambda} + \frac{\alpha}{r}e^{-r/\lambda}.$$

Here V_{np}, V_{nn} and V_{pp} are the neutron-proton, neutron-neutron and proton-proton interactions. By carefully adjusting the parameters a, b, c, Λ and λ one can reproduce some observables of finite nuclei and bulk properties of nuclear matter [1]. Therefore, by evolving the equations of motion of the system we are able to study the dynamics of matter at high densities and how it transitions from nuclei to nuclear matter [2].

Due to the simplicity of this model we are able to simulate systems orders of magnitude larger and for much longer times than currently possible with more sophisticated calculations.

CODE

Recently the IUMD code has undergone a major reformulation in order to take full advantage of supercomputers that have CPU/GPU compute nodes, such as the BIG RED II supercomputer at Indiana University.

Most of the computational time in our MD simulations is spent calculating the forces acting on each nucleon. While the CPUs build neighbor lists and compute the short-range nuclear forces, the GPUs compute the long-range Coulomb forces on proton pairs. We use MPI to distribute tasks amongst the CPU/GPU compute nodes, and OpenMP in each compute node to distribute threads amongst the CPU cores. GPU calculations are accelerated using CUDA Fortran.

The code scales very efficiently to 512 or more GPU nodes, for large MD simulations.

RESULTS

Configurations of 51 200 nucleon systems evolved for 5×10^6 MD time steps at constant density, $n = 0.050\,\mathrm{fm}^{-3}$, and temperature, $T = 1.0\,\mathrm{MeV}$, for four different proton fractions Y_p.

| $Y_p = 0.10$ | $Y_p = 0.20$ | $Y_p = 0.30$ | $Y_p = 0.40$ |
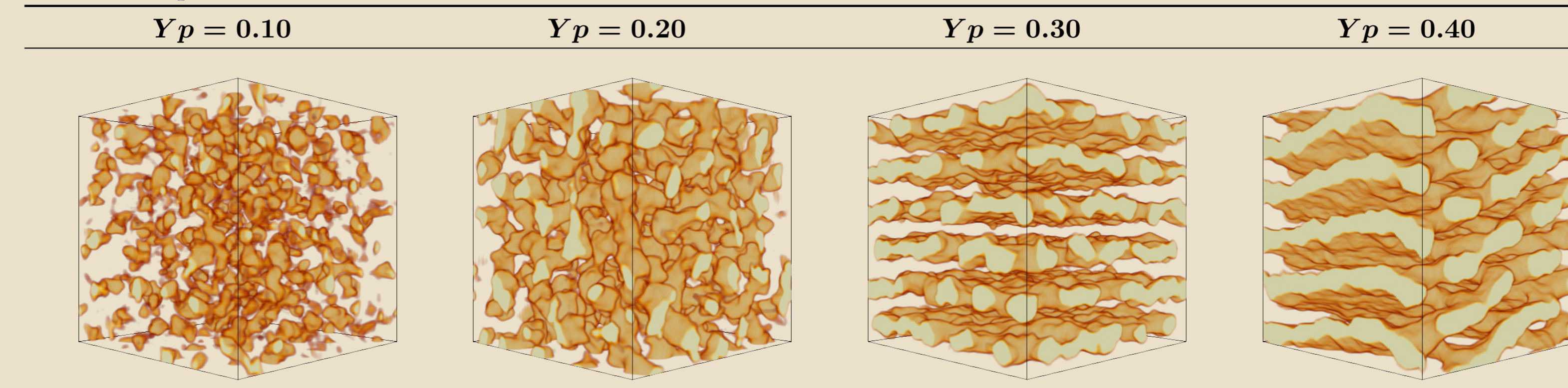
Comparison of 51 200 and 409 600 nucleon systems evolved for 15×10^6 MD time steps at constant density, $n = 0.050\,\mathrm{fm}^{-3}$, and temperature, $T = 1.0\,\mathrm{MeV}$, for a proton fraction of $Y_p = 0.30$.

| $N = 51\,200$ | $N = 409\,600$ |
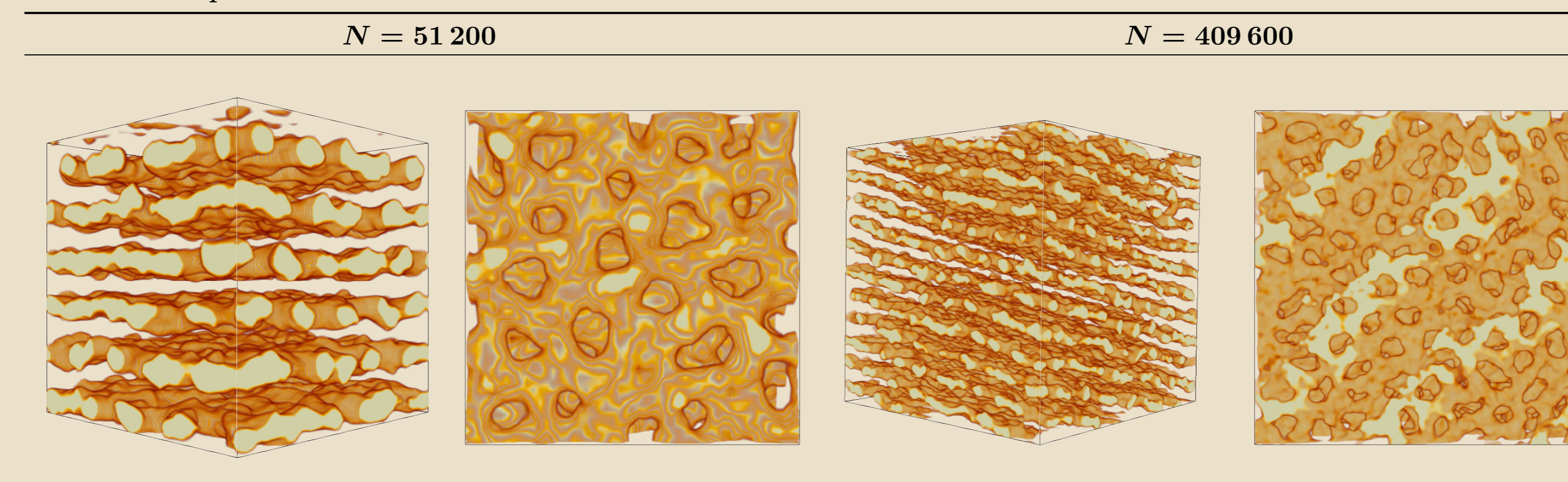
To the right we show our largest simulation yet: 3 276 800 nucleons evolved for 3.5×10^5 MD time steps at constant density, $n = 0.050\,\mathrm{fm}^{-3}$, and temperature, $T = 1.0\,\mathrm{MeV}$, for a proton fraction of $Y_p = 0.30$. Note that due to the short simulation time the system did not have time to evolve into a phase of stacked perforated plates as the ones shown above for the same density, temperature and proton fraction.
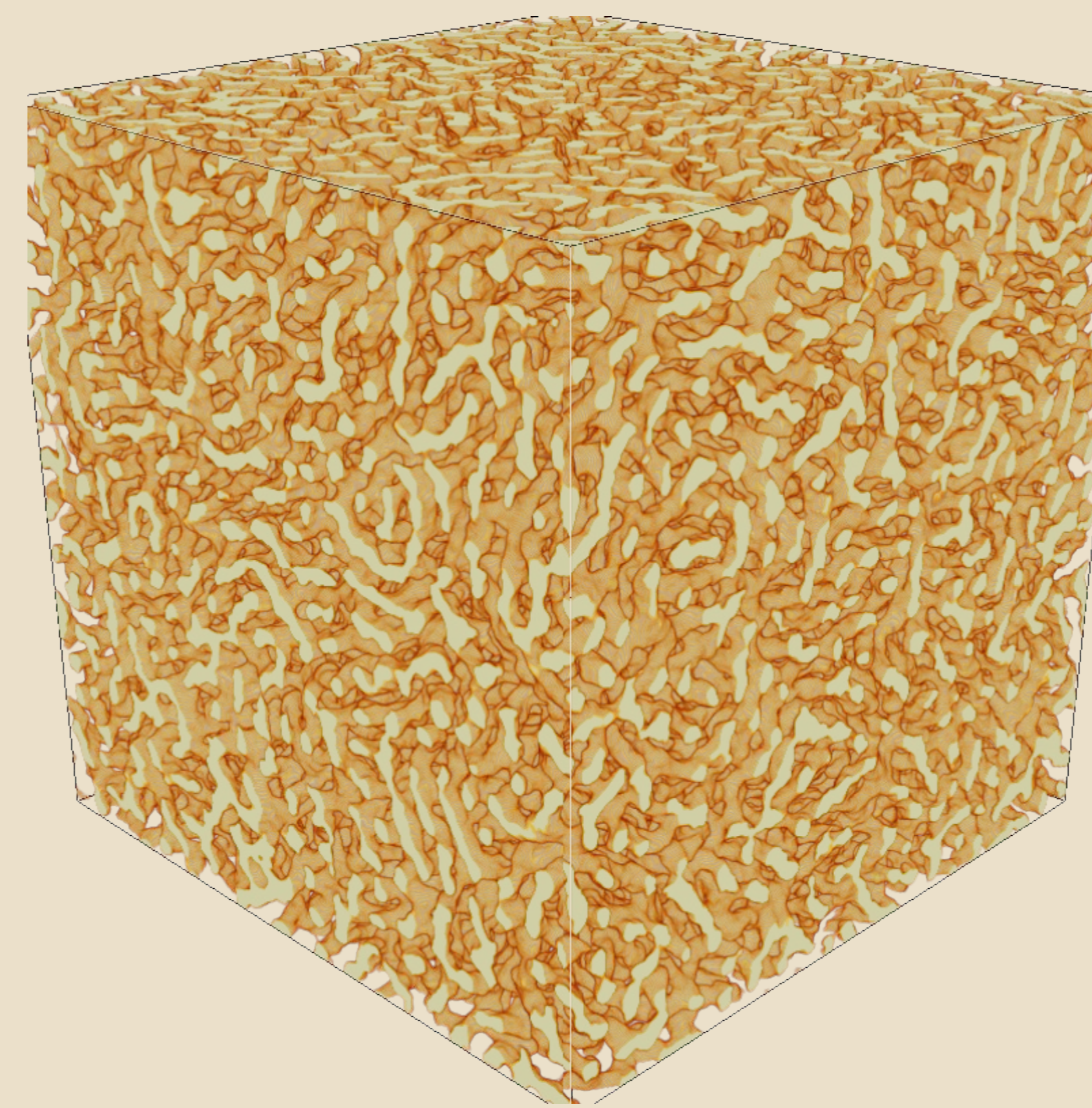

ACKNOWLEDGMENTS

STRUCTURE FACTORS

One of the important observables that can be calculated from MD simulations is the structure factor $S(q)$ of the pasta shapes. The proton (neutron) structure factors are directly related to the cross section of electron (neutrino) scattering by pasta and determine thermal and electrical conductivity (neutrino opacity).

Below we show the proton structure factors for the four simulations of different proton fractions shown to the left. Note the diffraction peaks on the structure factors of the $Y_p = 0.30$ and $Y_p = 0.40$ simulations characteristic of periodic structures.
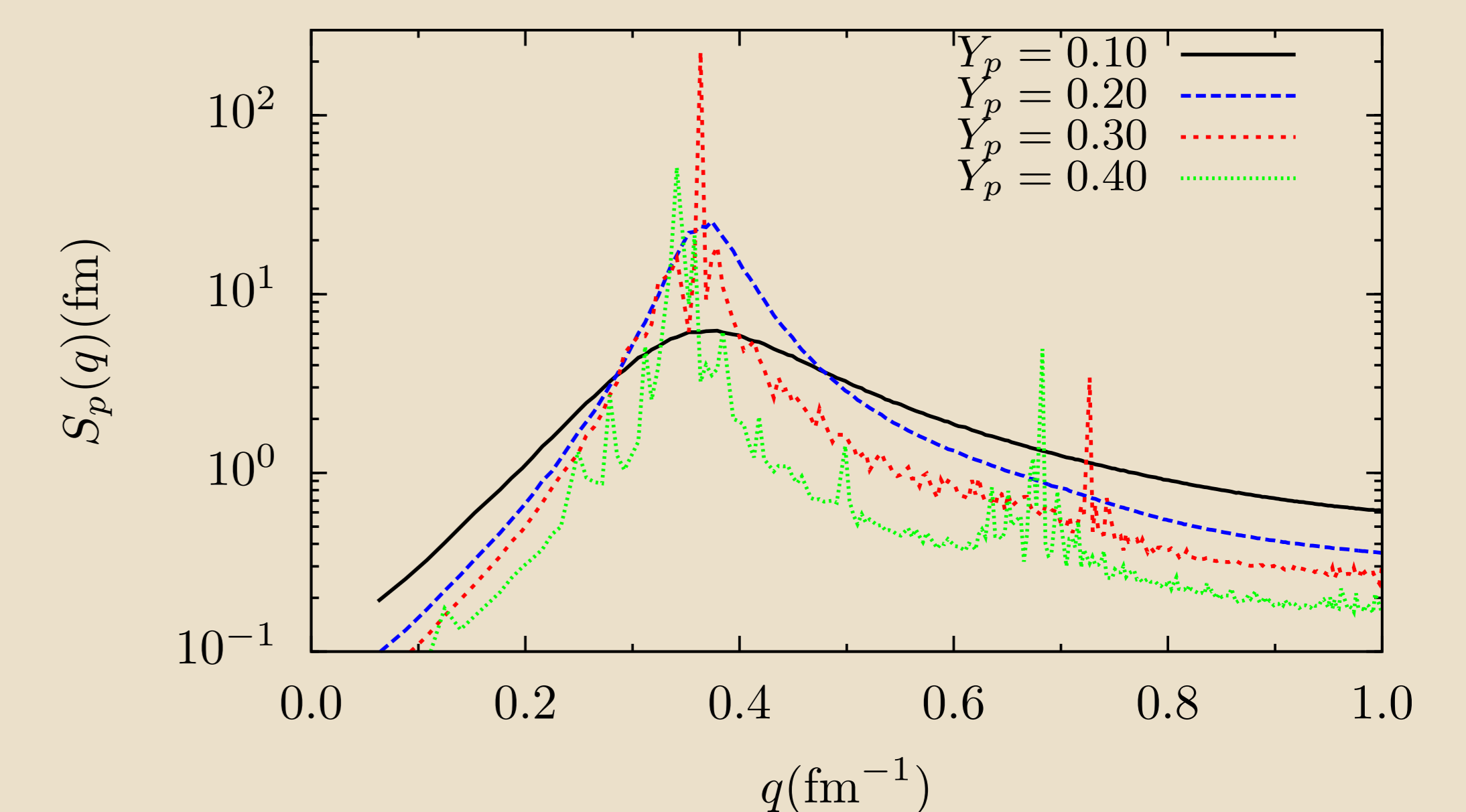
SUMMARY & OUTLOOK

Using a simple model we have developed a Fortran code, IUMD, that can simulate nuclear matter at sub-saturation densities. In the past the code was used to determine the dynamics of phase transitions between pasta phases and their time scale using MD [2]. Recently the code has been optimized to run on supercomputers with CPU/GPU architectures and is currently being used to perform very large simulations, up to 3 million nucleons, and to calculate observables such as the pasta phases structure factors [3], their breaking strain and to study nuclear statistical equilibrium [4].

REFERENCES

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