Large-Scale Simulations of Nuclear Pasta via Advanced Computing

I. Sagert[1], D.K. Berry[1] , M.E. Caplan[1] , G.I. Fann[2], C.J. Horowitz[1], S. Postnikov[1], A. S. Schneider[3]
[1]Nuclear Theory Center, Indiana University, Bloomington, Indiana, USA
[2]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA
[3]TAPIR, California Institute of Technology, Pasadena, California, USA

INDIANA UNIVERSITY

NUCLEI Nuclear Computational Low-Energy Initiative

Introduction

We perform classical *Molecular Dynamcis* (MD) and *quantum Hartree-Fock* (HF) simulations of *nuclear pasta phases*. These are exotic shapes of nuclear matter that are expected to exist in the interior of neutron stars. Their transport and elastic properties can impact neutron star observables such as their thermal evolution, magnetic field, oscillations and rotation. Furthermore, pasta phases can be produced during the death of massive stars in core-collapse supernovae and in the ejecta of binary neutron star mergers. Both are discussed as sites for nucleosynthesis. With that, the presence of pasta phases and their neutrino opacities can impact the formation of heavy elements.

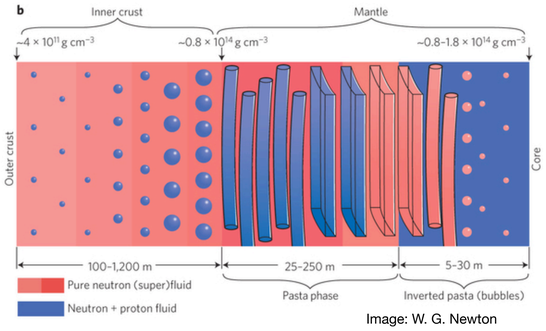


Image: W. G. Newton

A challenge in numerical studies of nuclear pasta is the requirement to maximize the simulation volume and number of nucleons in order to minimize finite size effects. The *Indiana University Molecular Dynamics* (IUMD) code uses a simple approach to implement nuclear forces between neutrons and protons. This, together with its ability to take advantage of CPU/GPU architectures of supercomputers enables studies of large pasta structures, their transport and elastic properties.

However, IUMD's simple model of the nuclear force does not include quantum mechanical features which are important for a correct description of nuclear matter. To include these effects, we are developing a quantum HF code for nuclear pasta. HF simulations are computationally much more demanding than Molecular Dynamics and to efficiently solve the corresponding equations on modern supercomputing environments we apply the numerical framework *MADNESS*.

Indiana University Molecular Dynamics

IUMD solves the equations of motion of neutrons and protons in a simulation volume with periodic boundaries. Nucleons are treated as point-particles that interact via simple two-body potentials:

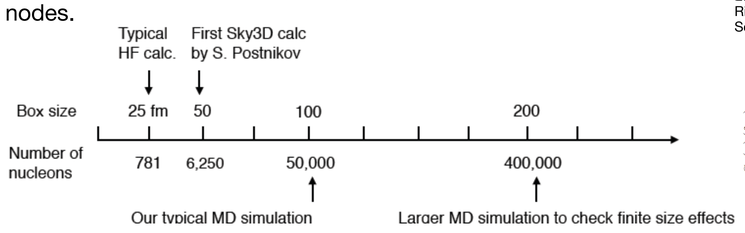
$$V_{nq}(r_{ij}) = a\exp^{-r_{ij}^2/\Lambda} + [b \pm c]\exp^{-r_{ij}^2/2\Lambda},\ q = \begin{matrix} n \\ p \end{matrix}$$

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

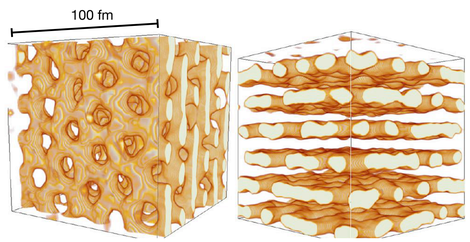
The parameters a, b, c and Λ are fitted to reproduce nuclear matter properties and binding energies of nuclei (1).

The simulations are mainly performed on *BigRedII* - the supercomputer at Indiana University (recently also granted time on TITAN at the OLCF). Here, IUMD takes advantage of the CPU/GPU node architecture: short range nuclear forces are computed on CPUs while GPUs compute the long-range Coulomb forces (2)

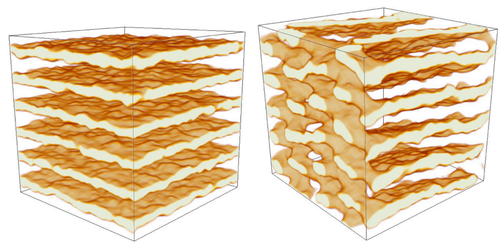
Typical simulations contain ~5×10^4 nucleons and are run on 32 nodes for about 24h and 10^7 simulation time-steps. The largest configuration is currently running with ca. 3M nucleons on 256 nodes.

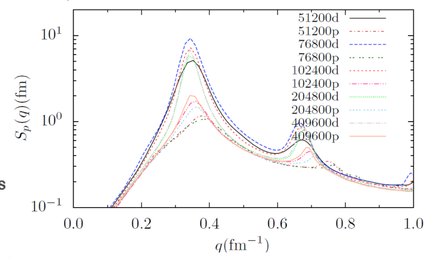


The large-scale nature of the simulations allows to eliminate finite-size effects, find novel pasta structures (2,3) and study the transport and structural properties of different pasta configurations (3,4).



A novel pasta structure found with the IUMD code, the so-called *nuclear waffle phase* - slabs of nuclear matter with periodic holes. The simulation was performed with 51200 nucleons at a proton fraction of 0.3 and temperature of 1 MeV. (Image: Andre Da Silva Schneider)


Left: The normal lasagna phase - periodic slabs of nuclear matter. Right: The lasagna phase with defects (4). (Image: Andre Da Silva Schneider)



Proton structure factor (related to the cross-section of electron scattering) of pasta for different nucleon numbers. The larger S_0 for configurations with defects (marked "d") imply decreased thermal and electrical conductivities (4). (Image: Andre Da Silva Schneider)

Multi-resolution ADaptive Numerical Environment for Scientific Simulations

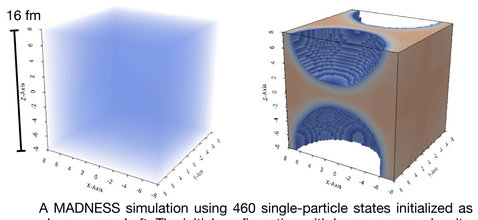
MADNESS is a numerical framework to efficiently solve multi-D integral and partial differential equation problems on modern supercomputers. Its main feature is the representation of functions and operators via **multi-wavelets** at a **user-given precision** (*for more details, see poster of G. Fann*) (5,6,7). We apply MADNESS to perform self-consistent studies of nuclear pasta phases by solving the Lippmann-Schwinger equations

$$\left(-\frac{\hbar^2}{2m}\Delta + \hat{V}_{\rm total}(\vec{r})\right)\psi_q(\vec{r}) = E\psi_q(\vec{r})$$

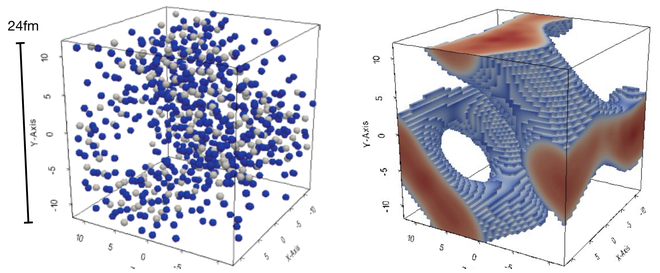
$$\longrightarrow \psi_q^n(\vec{r}) = \int G_{\rm BSH}(\vec{r},\vec{s})\left(\hat{V}_{\rm total}\,(\vec{s})\,\psi_q^{n-1}(\vec{s})\right)d\vec{s},\quad G_{\rm BSH}(\vec{r},\vec{s}) = \frac{e^{-k\,|\vec{r}-\vec{s}|}}{4\pi|\vec{r}-\vec{s}|},\quad k = \sqrt{-\frac{2mE}{\hbar^2}}$$

$$\hat{V}_{\rm total} = V_q - \nabla\cdot(b_1\rho - b_1'\rho_q)\,\nabla + i\vec{W}_q\cdot(\vec{\sigma}\times\nabla)\,(+V_C + V_{ex}),\quad q = n/p$$

for each single-particle state. The complex nuclear potential and the representation of nucleons by wave-functions makes HF simulations computationally every expensive. The maximal number of states is therefore currently limited to several thousand. The initial wave-functions can be set up as plane waves or Gaussians folded around nucleon coordinates of a converged IUMD configuration. The latter can speed up the convergence and test effects of a complex nuclear potential on the pasta structures:



A MADNESS simulation using 460 single-particle states initialized as plane waves. Left: The initial configuration with homogeneous density. Right: The converged pasta configuration in the bubble phase. (image: I.S.)



Simulation using 700 single-particle states, initialized as Gaussians folded around nucleon coordinates (marked by spheres, finite sphere size for visualization only) from a converged IUMD simulation in the so-called waffle phase (left). Right: The converged configuration (8). (image: I.S)

Our first MADNESS pasta simulations run on BigRedII at Indiana University and EOS at the OLCF (8). Typical simulations have several hundred nucleons and run for several days on about 20-40 CPU nodes. After first proof-of-principle studies our goal is to optimize the code to explore larger pasta structures with more nucleons.

Acknowledgements

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Summary

We are studying nuclear pasta phases via advanced numerical simulations. Using a simple model for the nuclear potential and applying both, CPU and GPU nodes of modern supercomputers, the Indiana University Molecular Dynamics code is able to perform large-scale pasta simulations with minimal finite size effects. To compare the results to self-consistent quantum-mechanical methods, we are developing a Hartree-Fock code using the MADNESS framework. The latter allows the efficient solution of Hartree-Fock equations on supercomputers and is an ideal tool to perform large-scale pasta simulations with sophisticated nuclear potentials.

References

(1) C.J. Horowitz, M.A. Pérez-García, J. Carriere, D.K. Berry and J. Piekarewicz, Phys. Rev. C 69 065806 (2004)
(2) A.S. Schneider, D.K. Berry, C.M. Briggs, M.E. Caplan, C.J. Horowitz, Phy. Rev. C 90 055805 (2014)
(3) C.J. Horowitz, D.K. Berry, C.M. Briggs, M.E. Caplan, A. Cumming, A.S. Schneider, Phys. Rev. Lett. 114 031102 (2015)
(4) A.S. Schneider, M.E. Caplan, D.K. Berry, C.J. Horowitz, manuscript in preparation
(5) R.J. Harrison, G. Beylkin, F.A. Bischoff, J.A. Calvin, G.I. Fann et al., arXiv:1507.01888 (2015)
(6) G. I. Fann, J. Pei, R.J. Harrison, J. Jia, J. Hill, M. Ou, W. Nazarewicz, W. A. Shelton, N. Schnuck, JPG, Phys. Conf. Ser. 180 012080 (2004)
(7) J.C. Pei, G.I. Fann, R.J. Harrison, W. Nazarewicz, Y. Shi, S. Thornton, Phys. Rev. C 90 024317 (2014)
(8) I.S., G.I. Fann, F. Fattoyev, S. Postnikov. C.J. Horowitz, manuscript in preparation