

Inhomogeneous dense matter simulations with three-dimensional coordinate space meshes

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I. SCIENTIFIC ISSUE

Our understanding of atomic nuclei is key to several applications: energy, medicine, and non-proliferation are but three entries on a long list. There are also questions of fundamental curiosity: the inner workings of the nuclei themselves, how they behave in extreme circumstances, what role they play in astrophysical phenomena, and even how the observed abundances were produced [1, 2]. Simulations are the only way to answer this need but are difficult for several reasons; progress in these areas of physics will only be possible through sustained investment in technical innovation aimed at efficiently leveraging available computational and human resources both.

Nuclear energy density functionals (EDFs) are the only advanced microscopic tool that today has any hope of addressing all these questions. Such models treat nuclei in terms of their constituent nucleons yet still manage the description of the structure and reactions of even the heaviest nuclei. The fundamental degrees of freedom for all EDF approaches are the single-particle wavefunctions (spwfs), and their numerical representation is the most defining feature of a simulation tool. We aim to unite computational scientists who perform EDF-based simulations of different realizations of nuclear matter on three-dimensional (3D) coordinate grids. The main advantage of such representations is their flexibility: the spwfs are constrained only by the size of the simulation volume. This means that 3D meshes can represent arbitrary nuclear shapes with constant accuracy [3], which stands in stark contrast with approaches that expand the spwfs in the eigenstates of a simple Hamiltonian or impose a restrictive amount of symmetries.

The generality of 3D coordinate techniques is particularly important to dynamical processes. When nuclei fission, collide or get perturbed by their environment, they evolve into complicated and asymmetric configurations that are hard to capture using any other type of representation. Yet 3D meshes are also relevant to static calculations. For one, the freedom in terms of shape allows calculations targeting nuclear ground states to leverage the power of spontaneous symmetry breaking. Second, static treatments of fission also necessarily probe extremely elongated nuclear shapes. Third, the extreme densities in the outer layers of neutron stars are expected to force the nuclear matter into (periodically repeating) crystalline arrangements often referred to as "nuclear pasta" [5?]. Coordinate space techniques were first championed in the 1970s by Paul Bonche at CEA [6–8] and have since been used in all of the mentioned contexts. Although 3D mesh representations are computationally demanding and are - perhaps for this reason - not in wide use, several state-of-the-art tools rely on them for either static or dynamic calculations of either finite nuclei or nuclear matter in the context of neutron star crusts [9–13].

Because of the computational demands, individual research groups tend to focus on just one type of simulation and develop only a single tool. Each group faces similar challenges: these range from the modeling of the interaction between nucleons to the stability of numerical evolution algorithms and even the technical difficulties of using the newest HPC infrastructure. Despite these common challenges, advances tend to diffuse slowly throughout the community. Our long-term aim is to establish a small network of developers of 3D tools to sustainably accelerate progress; our working group consists of members of four research groups and covers the same number of tools to tackle static and dynamic calculations of both isolated nuclei and nuclear matter.

One key short-term goal is establishing interoperability: during this workshop, we will define a common standard for information exchange and implement it within all our tools. This will result in groups being able to use data generated by others as starting points for the computation: the workflow of dynamic simulations will benefit enormously, as initial conditions can be generated in a more general and more efficient way by dedicated static tools. Another item of discussion will be the EDF parameterizations: the continuous improvement of the latter is powered by tools performing static mean-field level calculations. Hence both dynamical and beyond-mean-field calculations often stick to decades-old EDF parameterizations because of the latter's simplicity. If we hope to construct a truly general model that is capable of simultaneously describing static and dynamic properties with high accuracy, then this situation has to change. Another predefined topic we already foresee is the use of GPUs: although the nature of 3D meshes lends itself well to extreme parallelism, the practical use of such infrastructure requires significant investment from developers. Finally, setting up standards for the data exchange will allow for detailed cross-checks between codes. Such a step was essential to solid-state physics [14, 15], where the results of different codes, even if authors claimed that they are using the same functional, depended more strongly on implementation than commonly thought. Only collaborative work and detailed cross-checks allowed that community to get satisfactory convergence between several toolkits. This workshop aims to trigger this process for nuclear EDF solvers relying on 3D meshes.

We believe that a gathering of developers is timely for two reasons. First, a wealth of new data and modeling studies point to the need for 3D simulations of isolated nuclei and nuclear matter: many open questions remain with regards to fission processes [16], accelerator complexes across the world aim to synthesize ever-more short-lived nuclei with exotic shapes and observations of the thermal evolution and glitches of neutron stars become more numerous and precise [17]. Remarkably, all of our tools are relevant to unravel the mysteries of nucleosynthesis in binary neutron star mergers, a process only recently confirmed through multimessenger astronomy [18]. A second reason is practical: the EU along with the CEA are strongly investing in new GPU based HPC machines that offer unparalleled opportunities for European computational physicists but that will require development effort to leverage.

II. GOALS OF THE PROJECT

We will gather a small core of scientists: *developers* of simulation tools for atomic nuclei and nuclear matter on three-dimensional coordinate space meshes. Our main goal is to identify common challenges and build communal resources to tackle them; from open physics questions to the technical advances needed to address them as well as practical developments of benefit to the community at large. Two specific goals are: (i) establish and implement a common standard to achieve interoperability between existing tools and (ii) cross-validate all tools in simple systems. On a larger timescale, we hope to forge a small but responsive and integrated community to accelerate progress.

III. SHORT-TERM VISITORS

We foresee staying at the ESNT as a working group twice. A first session at the ESNT (26/05/2025 - 28/05/2025) will serve as a discussion ground to identify the most important working points. After sufficient time for each working group member to lay the groundwork, a second session at the ESNT (27/10/2025 - 29/10/2025) will benchmark and test implementations and discuss issues encountered or improvements developed. One specific outcome will be developing a common standard for information exchange and cross-validation. We will prepare a design document and decide on test cases during the first session; the final implementation in all tools and the matching of test cases will be validated in the second session.

The members of the working group are:

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IV. LIST OF SPEAKERS

- *W. Ryssens*: ULB (Brussels), wouter.ryssens@ulb.be.
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Monday 26 - 05	Tuesday 27 - 05	Wednesday 28 - 05
09h00 Start	09h00 Start	09h00 Start
09h05 Words of welcome	09h10 Discussion/Implementation	09h00 Discussion/Implementation
09h30 Discussion/Implementation		
11h00 Coffee break	11h00 Open lecture	11h00 Coffee break
	12h30 Lunch	
13h00 Lunch		13h00 Lunch
14h00 Discussion/implementation	13h30 Discussion/implementation	14h Closing remarks
17h00 End	17h00 End	15h30 End

V. PROGRAM OF SESSION I: 26/50 - 28/05

Our main goal is to open up the possibility for in-depth technical discussions between our (small) number of participants and collaborate on (joint) implementations and test cases. This is why the majority of the program is described as "Discussion/Implementation"; nevertheless, we foresee a few anchoring points:

1. a moment of introduction on Monday morning of the different participants that includes a clear outline of the more practical goals of the meeting: (i) the collective design and specification of a data exchange format between the existing 3D coordinates codes and (ii) the enumeration of a set of validation tests.
2. an open lecture on the techniques of coordinate space representation at 11am on Tuesday. Entitled "Coordinate space simulations with nuclear EDFs", the talk will review the use of coordinate space techniques for energy density functional applications; particular attention will be paid to the breadth of physics that can be tackled with such techniques but also to the open challenges facing practitioners.
3. closing remarks on Wednesday afternoon with a clear-cut list of implementations/tests to be performed by the participants before session II of this workshop.

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