LA-UR-21-20367

HPC for Fission Modeling in Support of Nuclear Data

Workshop for Applied Nuclear Data Activities (WANDA 2021)

Connecting the humans behind the nuclear data

January 25 - February 3, 2021 virtually via WebEx

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Background

The problem: (induced) fission of heavy nuclei

- Wide range of applications
- Properties of neutrons and gammas emitted in fission depend of the properties of fission fragments, which are not directly accessible in experiments

My work: combination of microscopic and phenomenological approaches with the goal to improve the description of prompt particles emitted in fission:

- Describe the evolution of a fissioning nucleus from the compact form to fully separated fission fragments within a time-dependent density functional theory approach (so called TD-SLDA)
- Extract from microscopic calculations observables/information to be used in phenomenological approaches (e.g., energy sharing, angular momentum distributions)
- The goal is not accuracy necessarily, but trends

Why does it matter for nuclear data:

- consistent evaluation of prompt fission observables

Computational Needs

HPC resources used:

- Small and medium-size clusters for modeling emission of prompt neutrons and gamma rays using the open-source code CGMF (https://github.com/lanl/CGMF)
- Leadership-class machines for microscopic simulations of fission dynamics using the open-source package LISE (https://github.com/lanl/LISE)
  - Large machines required because of the size and complexity of the problem
  - Summit (Titan, JaguarPF) @ ORNL, Sierra (40x40x80*), Lassen @LLNL, Moonlight/Kodiak @ LANL (small calculations), Pizdaint in Switzerland, Tsubame in Japan, NERSC (pre-CUDA implementation)

Do you use ML or AI?

- No, but some of the colleagues in the group are (e.g., constructing emulators for CGMF simulations)
- We will consider as an options once we develop the code to introduce fluctuations and dissipation

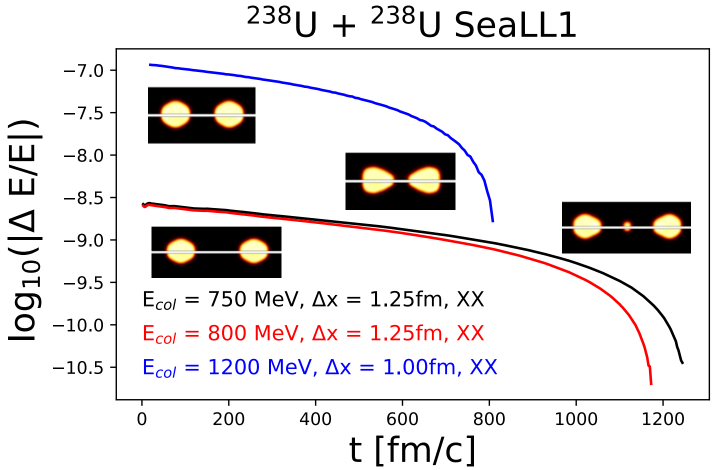
* Our biggest calculation to date

Computational Techniques

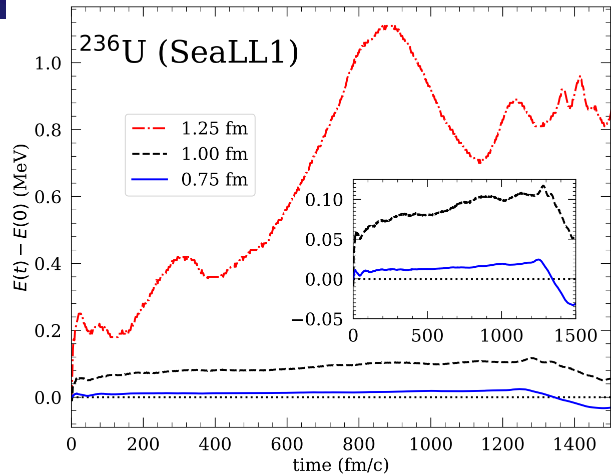
Time evolution of nuclear system in a density functional approach:

- ❑ Initial conditions: obtained by large scale diagonalizations of Complex Hermitian Matrices
  - ❖ Half of eigenvectors necessary
  - ❖ discrete variable representation on a lattice(good description of continuum states)
  - ❖ Iterative method (expensive, replaced by interfacing with less expensive codes)
  - ❖ Largest dimension $4N_xN_yN_z$: 512,000
  - ❖ Algorithm/Software: block-cyclic decomposition/SCALAPACK, FFTW
  - ❖ Runs on CPU architecture, useful to have a GPU accelerated version of the SCALAPACK libraries
  - ❖ Efficient I/O (based on Lustre/MPI libraries)
- ❑ Time evolution:
  - ❖ Adams-Bashforth-Milne alogorithm for integrating in time.
  - ❖ Full representation of each vector (q.p. wavefunction) in the memory, spread over available number of GPUs.
  - ❖ Runs exclusively on GPUs now, although we do have older versions running on CPUs
  - ❖ CUDA libraries (including CUDA FFTW), some FFTW (on CPU)
  - ❖ Non-trivial restarting capabilities (Lustre and MPI libraries)

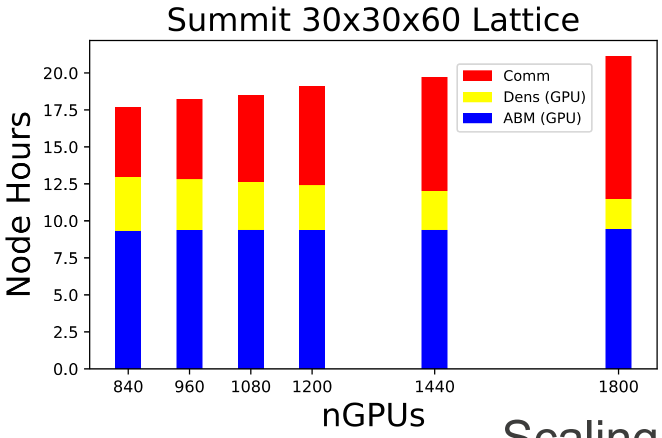
HPC Highlights: stability, accuracy, scaling



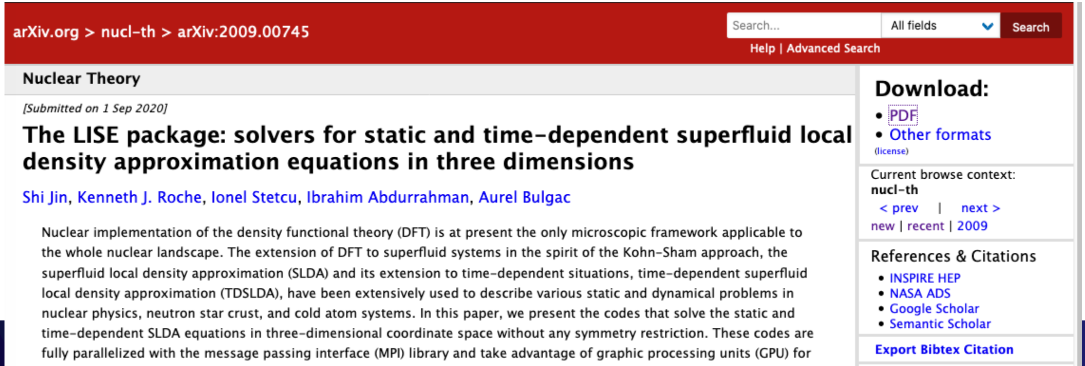
Time-reversal properties



Energy conservation in fission



Scaling



arXiv.org > nucl-th > arXiv:2009.00745

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Nuclear Theory

[Submitted on 1 Sep 2020]

The LISE package: solvers for static and time-dependent superfluid local density approximation equations in three dimensions

Shi Jin, Kenneth J. Roche, Ionel Stetcu, Ibrahim Abdurrahman, Aurel Bulgac

Nuclear implementation of the density functional theory (DFT) is at present the only microscopic framework applicable to the whole nuclear landscape. The extension of DFT to superfluid systems in the spirit of the Kohn-Sham approach, the superfluid local density approximation (SLDA) and its extension to time-dependent situations, time-dependent superfluid local density approximation (TDSLDA), have been extensively used to describe various static and dynamical problems in nuclear physics, neutron star crust, and cold atom systems. In this paper, we present the codes that solve the static and time-dependent SLDA equations in three-dimensional coordinate space without any symmetry restriction. These codes are fully parallelized with the message passing interface (MPI) library and take advantage of graphic processing units (GPU) for

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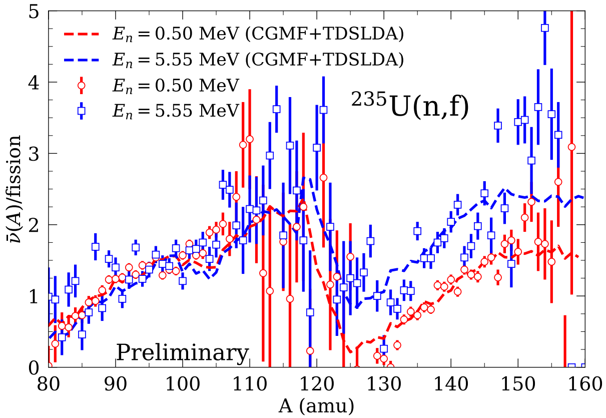
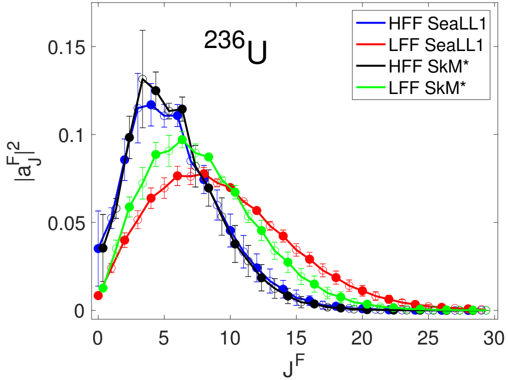
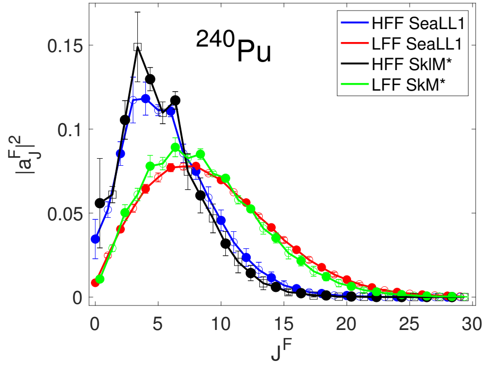


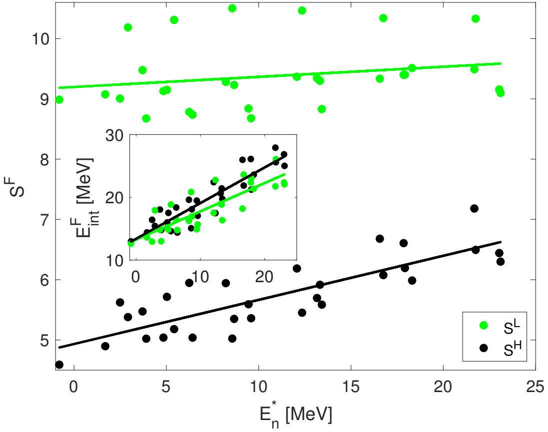
- Energy sharing parameterized from DFT calculations
- Parameterization used in CGMF calculations

A. Bulgac, S. Jin, and I. Stetcu, Frontiers in Physics **8**, 62 (2020).

Trends with excitation energy







- Angular momentum from microscopic calculations
- Correlations between FF angular momenta

A. Bulgac, et. al., arXiv:2012.13442 (2020)

Outlook

What remains to be done?

- A lot! There is a long road ahead of us: energy dependence, fluctuations/dissipation for describing distributions

Benefits for nuclear data:

- Possibility to provide more realistic input to phenomenological simulations, with more reliable extrapolations
- In general, we seek to provide a better understanding of the fission process