HPC for Fission Modeling in Support of Nuclear Data

Workshop for Applied Nuclear Data Activities (WANDA 2021)

Connecting the humans behind the nuclear data

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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 on 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)
  o Large machines required because of the size and complexity of the problem
  o 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 $4N_x N_y N_z$: 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 algorithm 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

$^{238}\text{U} + ^{238}\text{U}$ SeaLL1

$E_{\text{Col}} = 750$ MeV, $\Delta x = 1.25\text{fm}$, XX
$E_{\text{Col}} = 800$ MeV, $\Delta x = 1.25\text{fm}$, XX
$E_{\text{Col}} = 1200$ MeV, $\Delta x = 1.00\text{fm}$, XX

Time-reversal properties

Energy conservation in fission

Summit 30x30x60 Lattice

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References & Citations
- INSPIRE HEP
- NASA ADS
- Google Scholar
- Semantic Scholar

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Results

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


Trends with excitation energy

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:

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