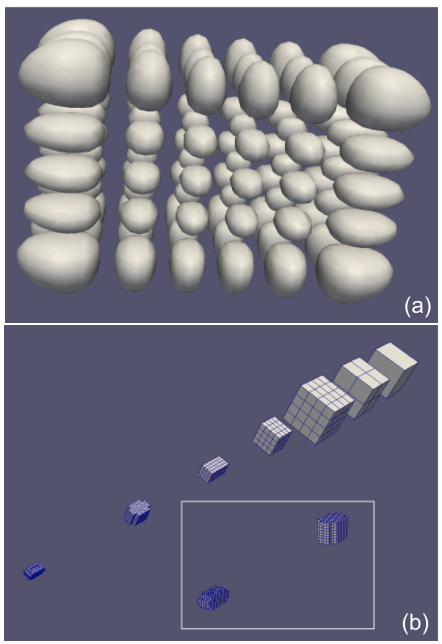
MADNESS-HFB: adaptive multi-resolution 3D DFT solver

Objectives

- Complex many-body systems, such as fissioning nuclei, cold Fermi gases, and pasta phases in neutron star crust, are all characterized by large sizes and complex topologies.
- To describe such systems, we introduce an adaptive pseudospectral method for solving self-consistent equations of nuclear density functional theory (DFT) in three dimensions. The numerical method is based on the multi-resolution and harmonic analysis techniques with a multi-wavelet basis.

Impact

- Enables rigorous predictive modeling in complex physical systems.
- The application of state-of-the-art parallel programming techniques include sophisticated object-oriented templates which parse the high-level code into distributed parallel tasks with a multi-thread task queue scheduler for each multi-core node.
- Provides benchmark for future model developments.



Pedagogical illustration of adaptive representations in MADNESS-HFB. (a) The modulus squared of the single-neutron wave function corresponding to the single-particle energy of −5.214 MeV obtained in MADNESS-HF calculations for ^{110}Mo, and (b) the corresponding spectral refinement structure.

Accomplishments

- The new adaptive multi-resolution solver MADNESS-HFB is benchmarked against a two-dimensional coordinate-space solver based on the B-spline technique and a three-dimensional solver based on the harmonic-oscillator basis expansion.
- The algorithm is variational and is capable of solving coupled complex-geometric systems of equations adaptively, with functional and boundary constraints, in a finite spatial domain of very large size, limited by existing parallel computer memory.
- This paper has been chosen by the Editors of Physical Review C as *Editors Suggestion.*

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