"MADNESS for SciDAC UNEDF"

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ASCR- Applied Mathematics Highlight

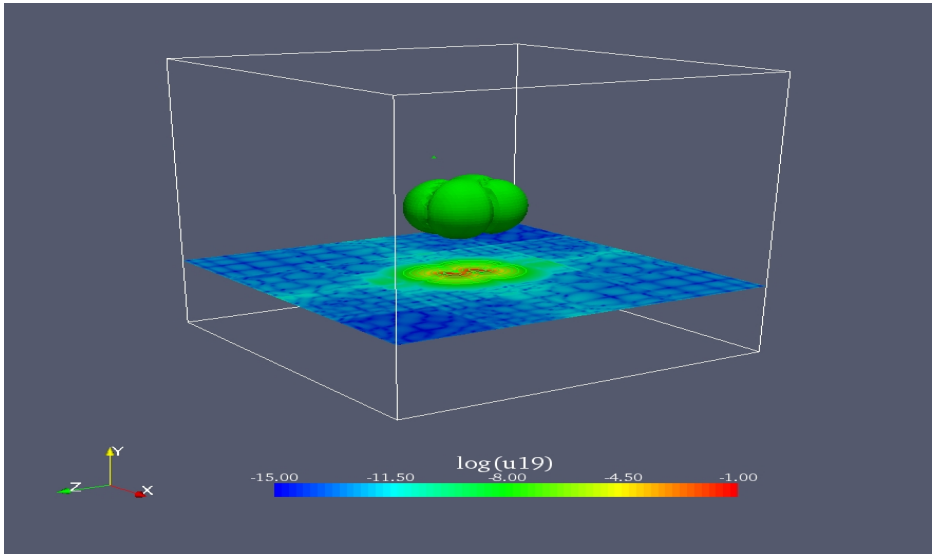
Objectives

- Develop mathematical foundations and calculus for solving the systems of integro-differential equations of the density functional theory (DFT) with multiple adaptive pseudo-spectral representations of functions and operators in 3-D
- Scalable solution to symmetry-free nuclear DFT models with arbitrary finite precision

Impact

- Provides research community with a scalable 3-D adaptive pseudo-spectral method for advanced nuclear structure simulations
- Enables computations of many-body systems with unusual geometries as encountered in fission, fusion, and the crust of neutron stars
- Each wave-function or quasi-particle wave-function and operator has its own adaptive structure for accurate representation and computation

Example of a quasi-particle wavefunction



Progress and Accomplishments 2010

- Benchmark and comparisons of 3-D multiwavelets, 2-D splines and 3-D harmonic oscillator bases
- Calculations of superfluid condensates in elongated traps
- "Fast Multiresolution Methods for Density Functional Theory in Nuclear Physics," G. I. Fann, J. Pei, R. J. Harrison, J. Jia, J. Hill, M. Ou, W. Nazarewicz, W. A. Shelton, and N. Schunck, Journal of Physics: Conference Series 180, 012080 (2009)
- "Multiple Multiresolution Representation of Functions and Calculus for Fast Computation," G. Fann, R. Harrison, J. Jia, J. Hill and D. Galindo, Proc. of SciDAC Conf. 2010