Time-Dependent Superfluid Local Density Approximation –TDSLDA A. Bulgac (PI-U. Washington), Y.L. Luo, P. Magierski, K.J. Roche (PI-PNNL), I. Stetcu, Y. Yu

ASCR- SciDAC UNEDF Application Partnership Highlight (www.unedf.org)

Objectives

- Develop a scalable software implementation of the time-dependent density functional theory extended to fermionic superfluid systems
- Apply the code to condensed matter and nuclear phenomena (low-energy excitations and reactions, nuclear fission, neutron stars) for the UNEDF project

Impact

- Scalable, accurate, stable, and fast timedependent software to solve hundreds of thousands of coupled nonlinear 3D PDEs for long time intervals and large spatial simulation volumes
- TDSLDA provides a comprehensive. microscopically consistent approach to address qualitatively new theoretical questions in nuclear and condensed matter physics

- Generation and Dynamics of Quantized Vortices in a Unitary Fermi Superfluid, Bulgac et al, http://arxiv.org/abs/1011.5999
 - Correctly describes superfluid to normal phase dynamics, generation and dynamics of quantized vortices, predicts a qualitatively new phenomenon the superflow at supercritical Landau velocities
- Fast, scalable I/O for TB of data, flexible checkpoint restart capability
- 220,000 cores on JaguarPF, ~65 million CPU hours in 2010 to simulate superfluid and nuclear dynamics



The first microscopic calculation of vortex rings generation (above) and of vortex line recombination (right) in a fermionic superfluid





