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 time-dependent 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

Progress / Accomplishments FY10

  - 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