Quantum Dynamics with TDSLDA

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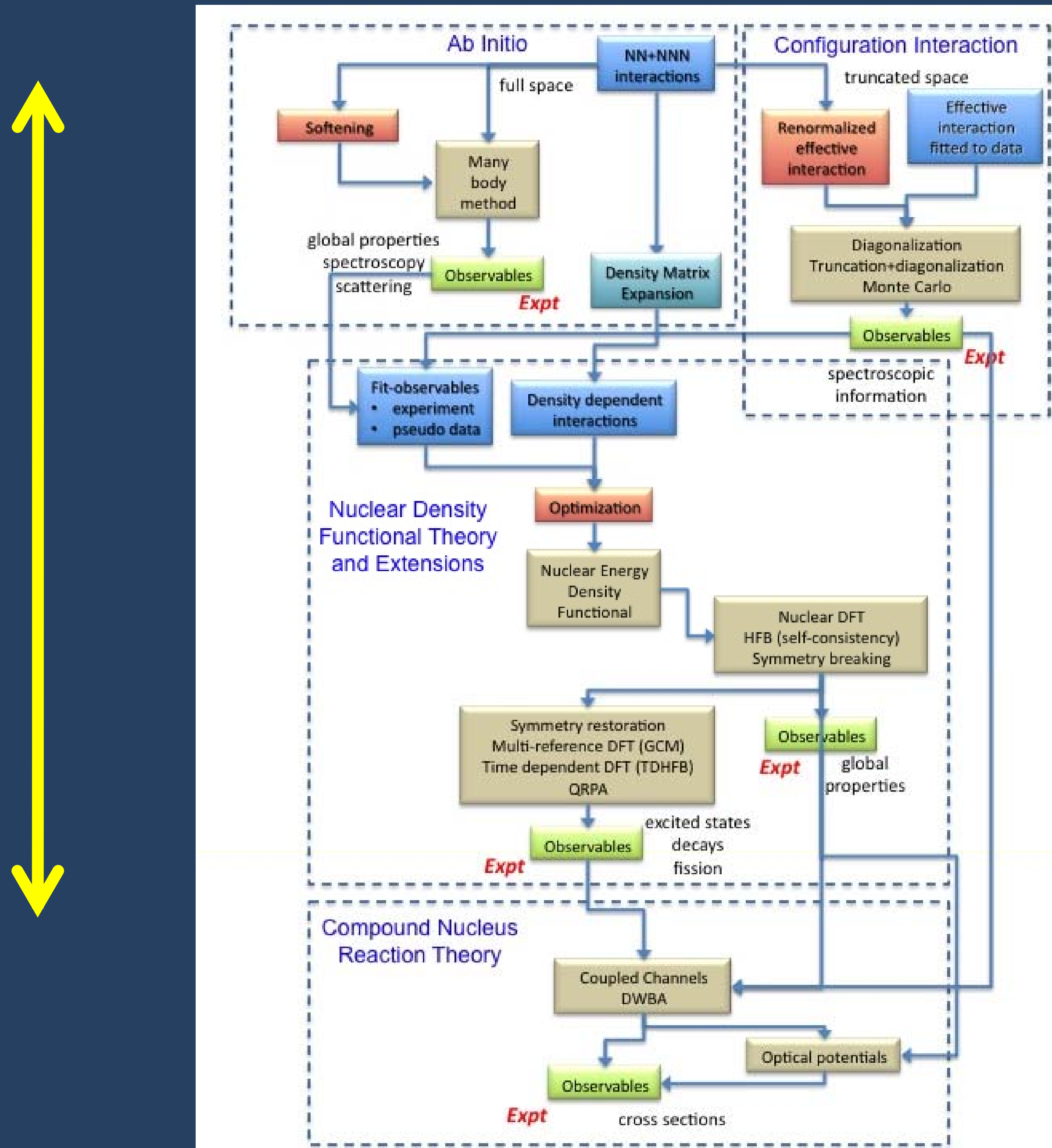

Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Nuclear Density Functional Theory and Extensions
Optimization
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
Observables
Expt
excited states
decays
fission
Compound Nucleus Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections

Year 4 Deliverables

- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - Developed the charge-exchange QRPA code, and use it to study beta decay of nuclei in the r-process.
- **Bulgac, Stetcu, Magierski (UW), Roche (ORNL):**
  - Improve the generation of initial conditions for TD-SLDA, and study dilute fermion systems, and nuclear systems.
- **Horoi, Senkov, Central Michigan Unversity:**
  - Improve the scalability of the CI Moments code, and calculate the nuclear level densities for the heavier nuclei in the rp-process path. **It may require CS help.**
- **Brown, Michigan State University:**
  - Improve the scalability of the CI code NuShellX to hundreds of cores.
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of the new CI code REDSTICK up to 10,000 cores, and use it to investigate ^{12}C, ^{16}O (N_{max}=8) with 3-body interactions **(CS help needed).**

TDSLDA
(equations TDHFB/TDBdG like)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{h}_{\downarrow\uparrow}(\vec{r},t) & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{h}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{h}^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -\hat{h}^*_{\downarrow\uparrow}(\vec{r},t) & -\hat{h}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

- **The system is placed on a 3D spatial lattice**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with Galilean invariance**
- **No symmetry restrictions**
- **Number of quasiparticle wave functions is of the order of the number of spatial lattice points**
- **Initial state is the ground state of the SLDA (formally like HFB/BdG)**
- **The code and implementation on JaguarPf was described in talks by I. Stetcu and K.J. Roche**

I will present five short movies, illustrating the complex time-dependent dynamics in 3D of a unitary Fermi superfluid and of ^{280}Cf excited with various external probes.

In each case we solved on JaguarPf the TDSLDA equations for a 32^3 spatial lattice (approximately 30k to 40k quasiparticle wavefunctions) for about 10k to 100k time steps using from about 30K to approximately 40K PEs

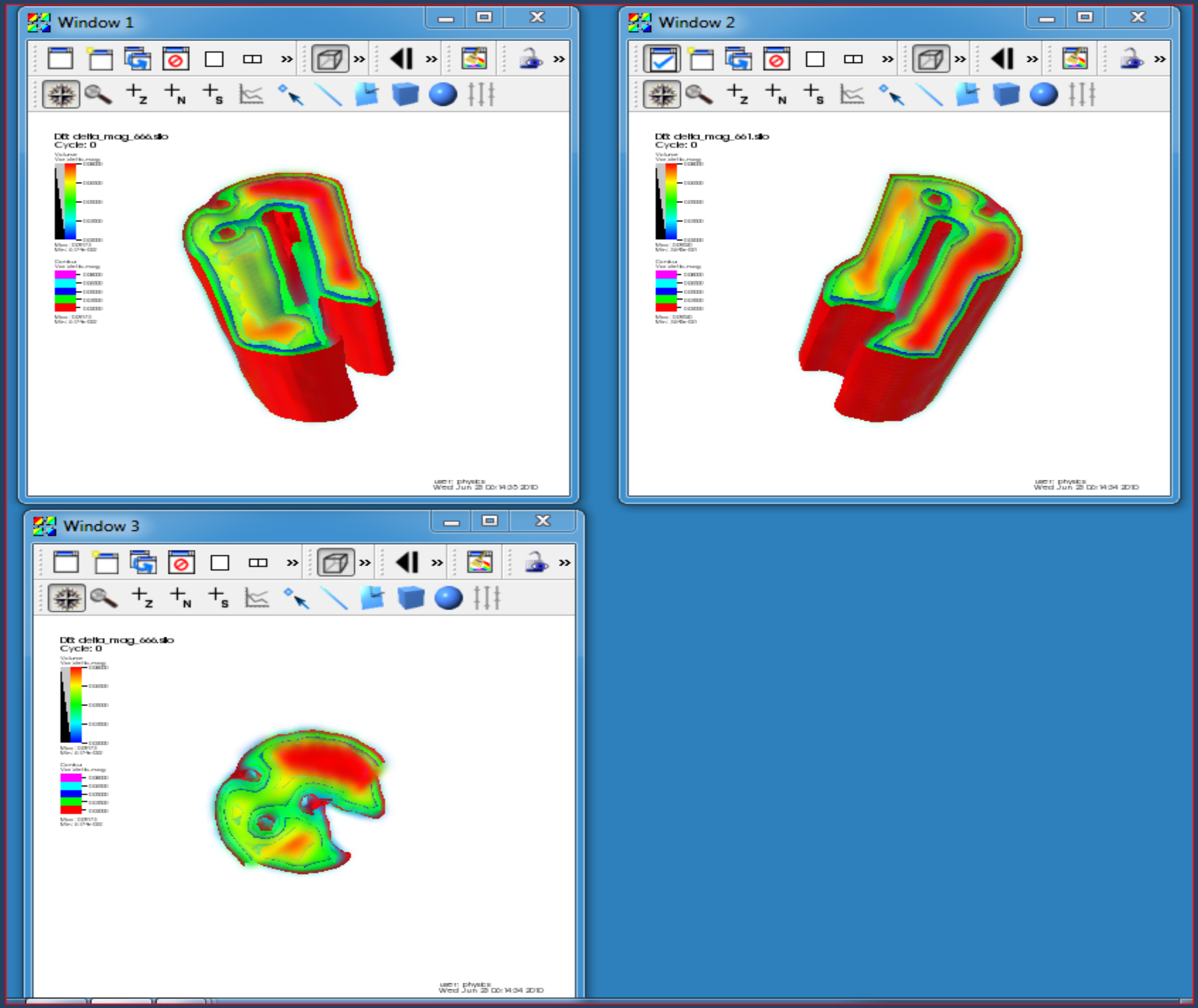
Fully unrestricted calculations!

The size of the problem we solve here is several orders of magnitude larger than any other similar problem studied by other groups (and we plan to further increase the size significantly).

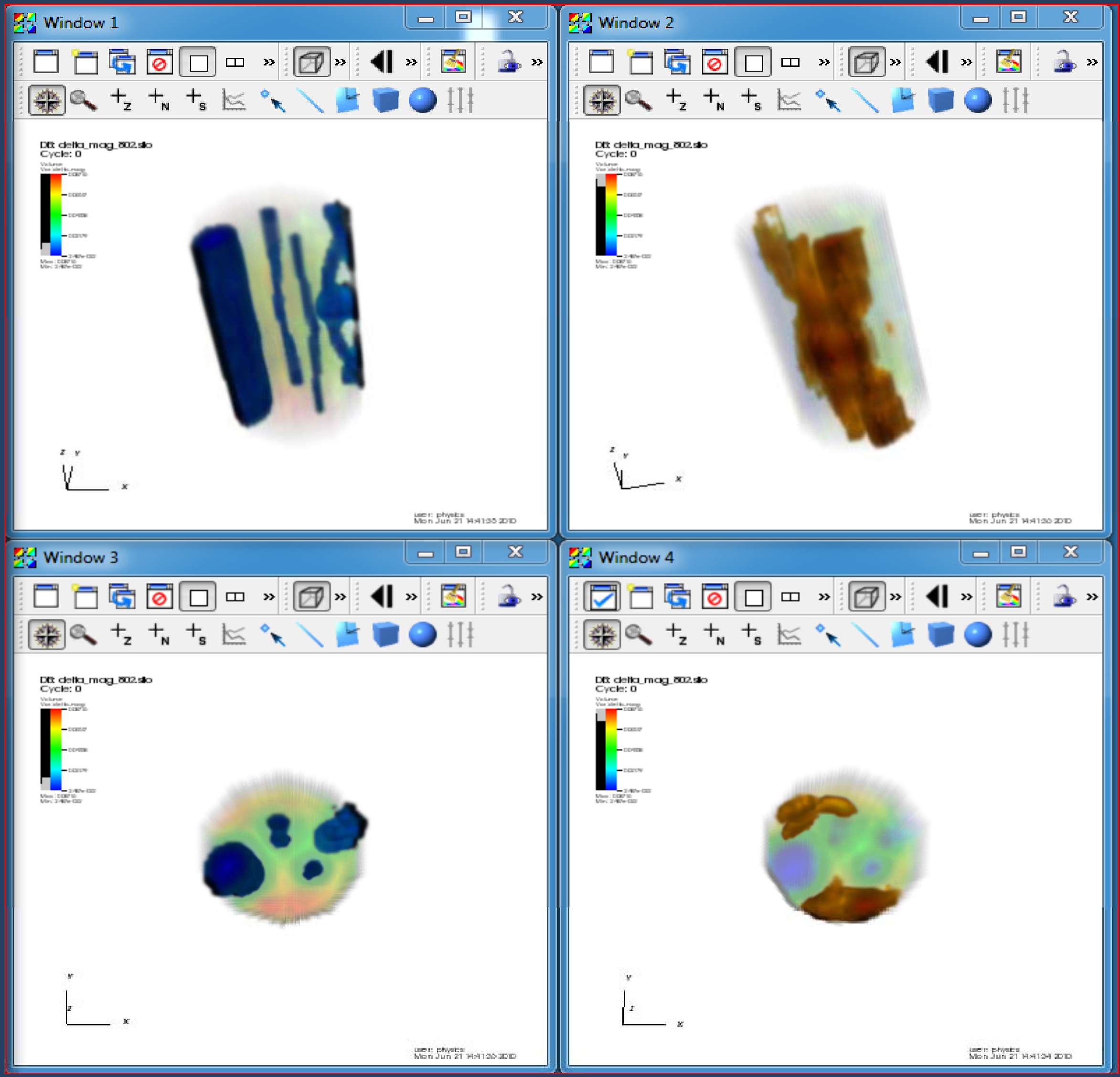
The movies will be eventually posted at

http://www.phys.washington.edu/groups/qmbnt/index.html

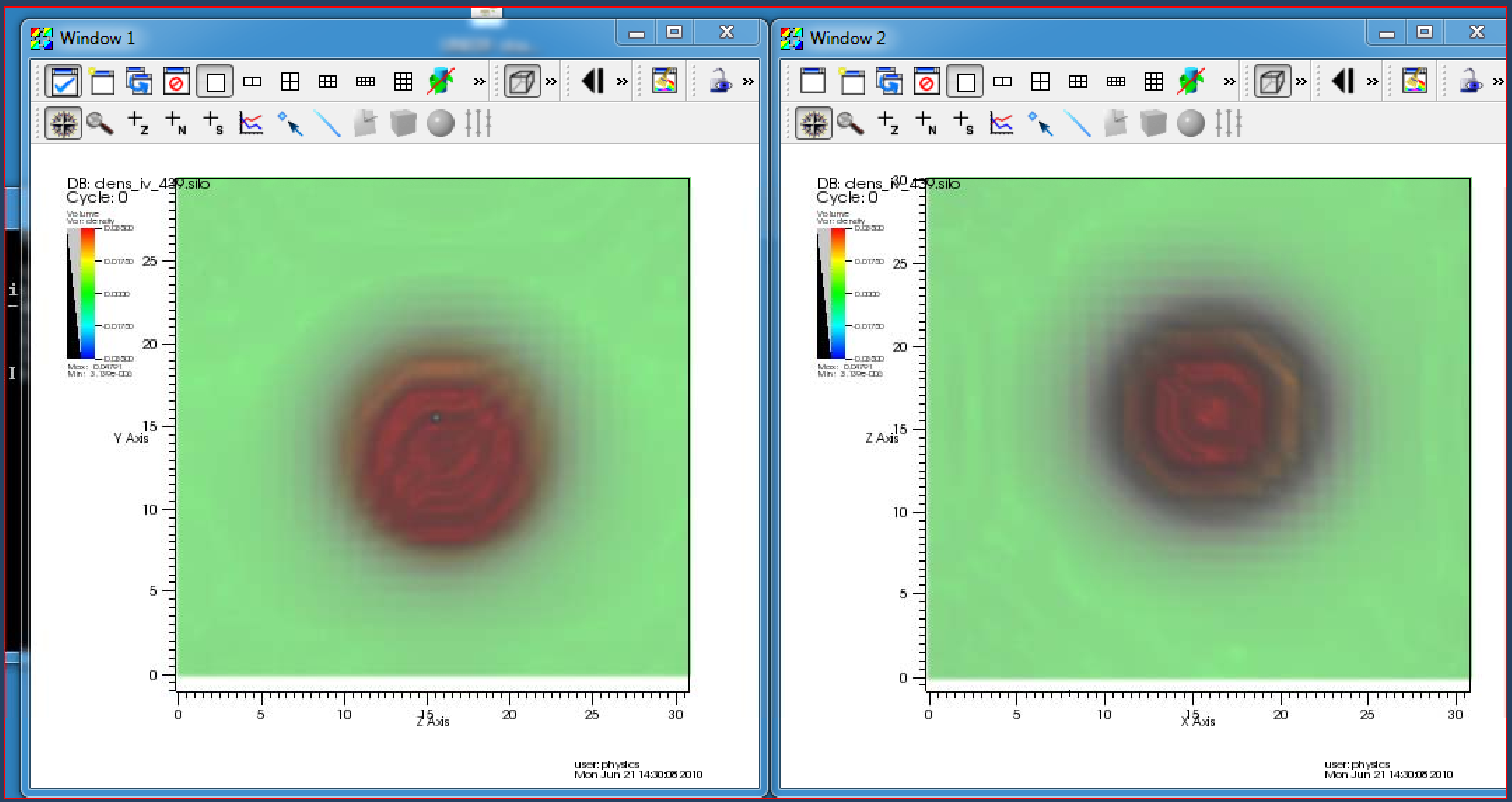
Stirring of a unitary superfluid and generation of complex vortical motion by a rod and ball rotating in a cylindrical container



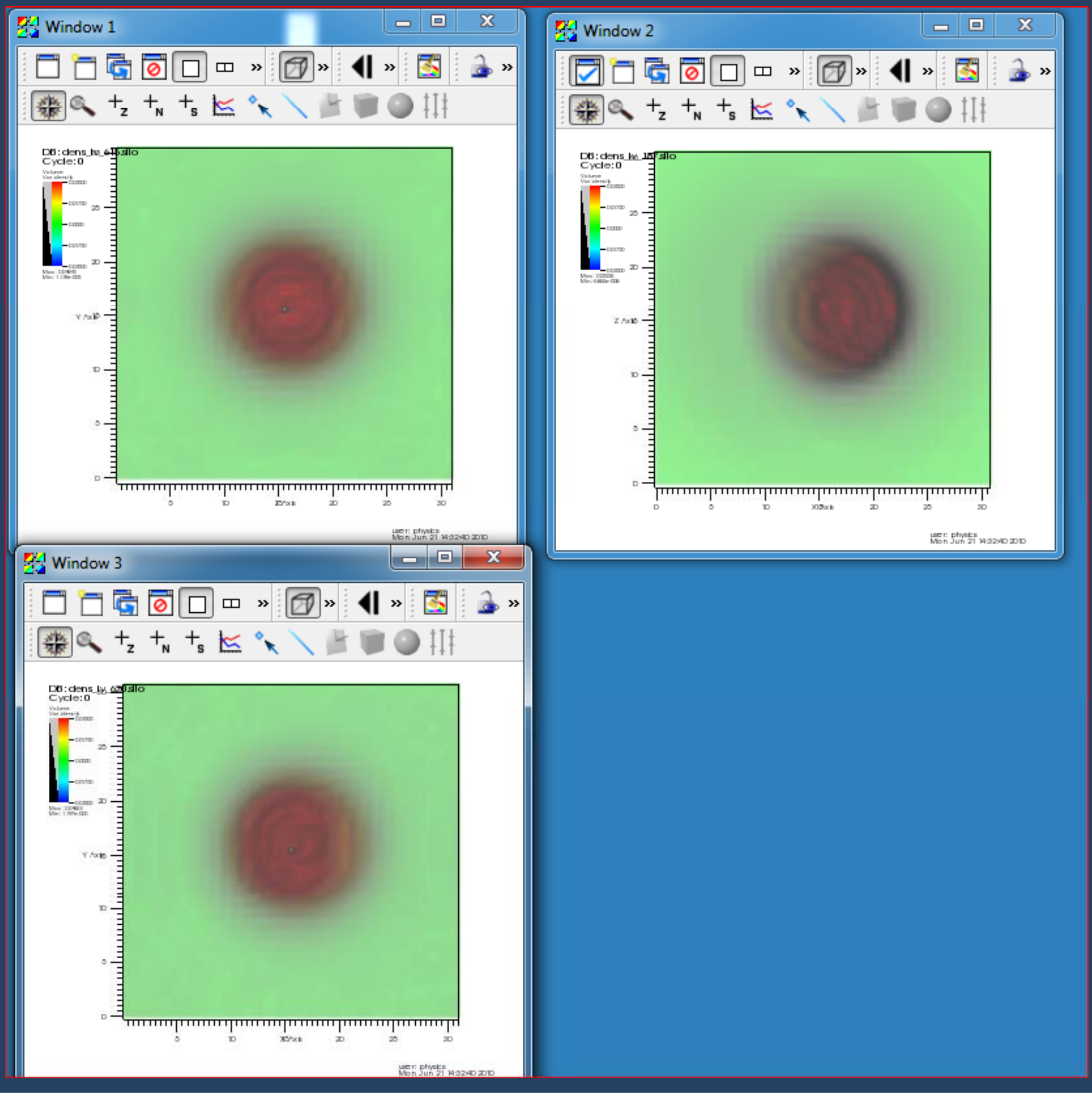
Stirring of a unitary superfluid and generation of complex vortical motion by a rod and ball rotating in a cylindrical container



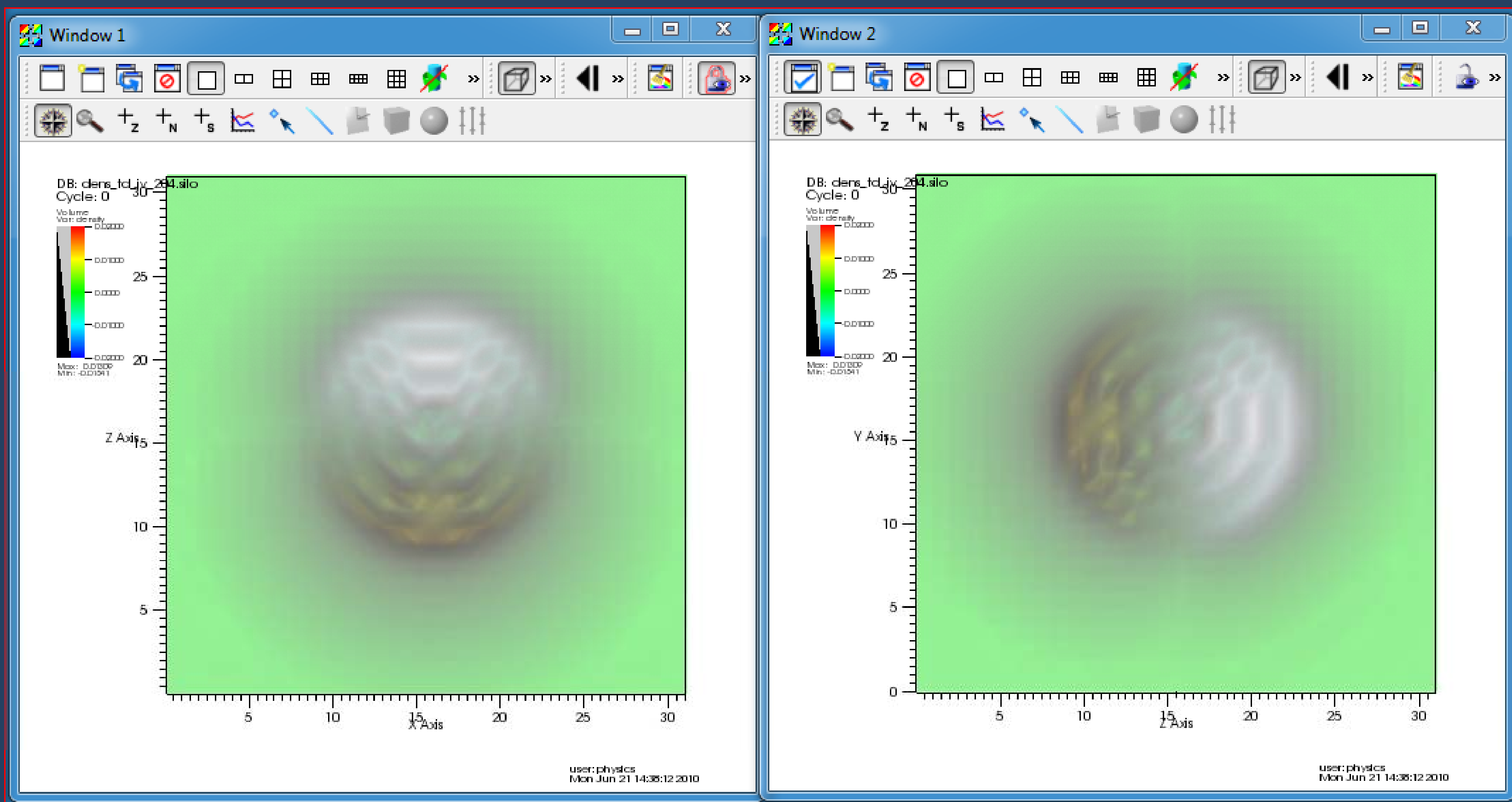
Excitation of an isovector dipole mode in ^{280}Cf by a passing relativistic heavy ion



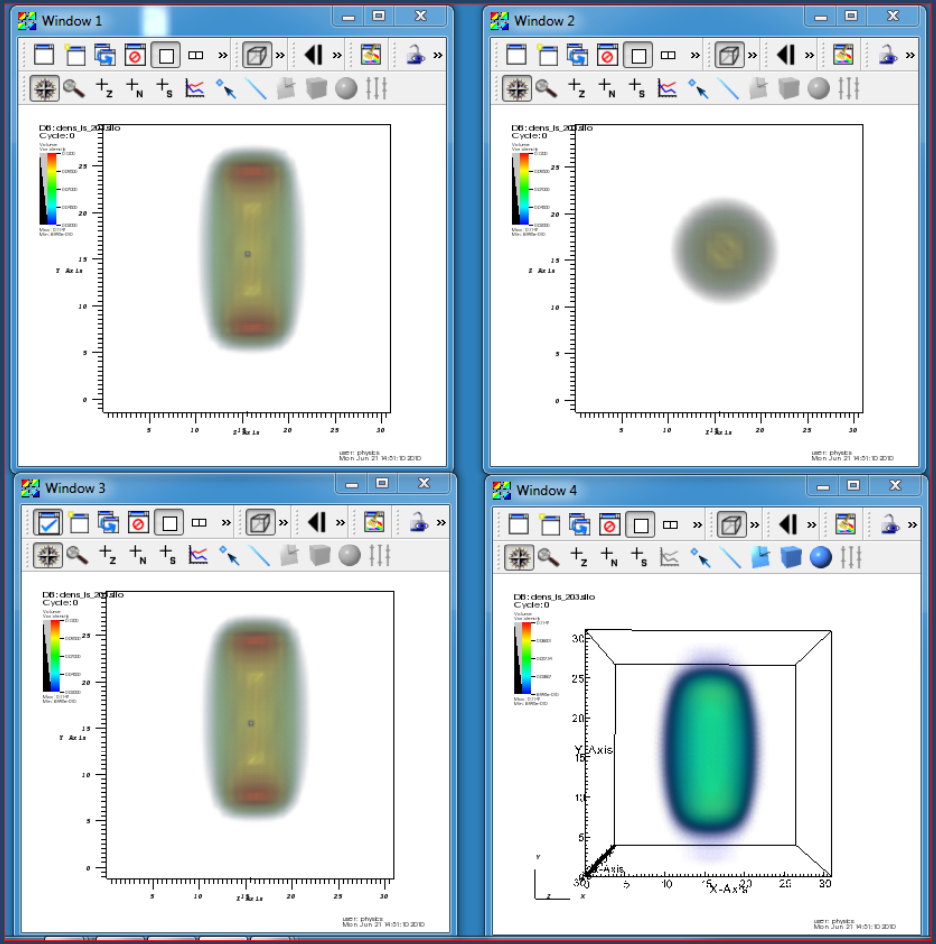
Excitation of an isovector dipole mode in ^{280}Cf by "two" passing relativistic heavy ions



Excitation of an isovector dipole mode in ^{280}Cf by a quasi-adiabatic time-dependent external isovector dipole field, which is switched off suddenly



Excitation of an isoscalar quadrupole mode in ^{280}Cf by a quais-adiabatic time-dependent external isoscalar quadrupole field + a smaller isovector dipole field, which are switched off very rapidly and followed by its subsequent induced fission



Summary

• *Created a set of accurate and efficient tools for the petaflop regime*

Successfully implementated on leadership class computers (Franklin, JaguarPF)

• Currently capable of treating nuclear volumes as large as 50^3 fm^3 , for up to 10,000-20,000 fermions , and for times up to a fraction of an attosecond fully self-consistently and with no symmetry restrictions and under the action of complex spatio-temporal external probes

• Capable of treating similarly large systems of cold atoms

• The suites of codes can handle systems and phenomena ranging from:

ground states properties
excited states in the linear response regime,
large amplitude collective motion,
response to various electromagnetic and nuclear probes,
up to various types of nuclear reactions (including induced fission)

• In the remaining time we plan to optimize and increase the performance of all codes. Great challenges: analysis and presentation

• There is a clear path towards exascale applications and implementation of the Stochastic TD(A)SLDA

Hyak (UW MRI-NSF funded and UW - part of UW eScience) is online
a 140 nodes x 8 = 1320 PEs and 48 Gb per node.
This is a dedicated development machine for the NPLQCD multi-baryon effort
led by M.J. Savage and for the Stoch-TDSLDA