Time dependent superfluid DFT for large amplitude nuclear collective motion and nuclear reactions

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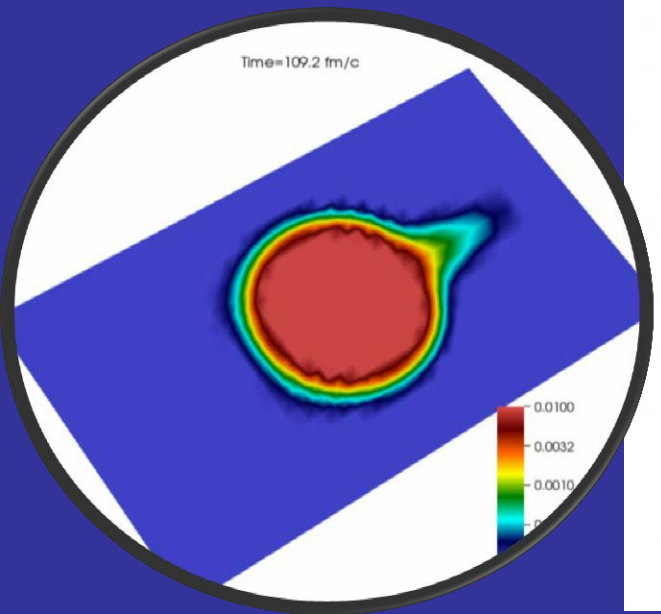

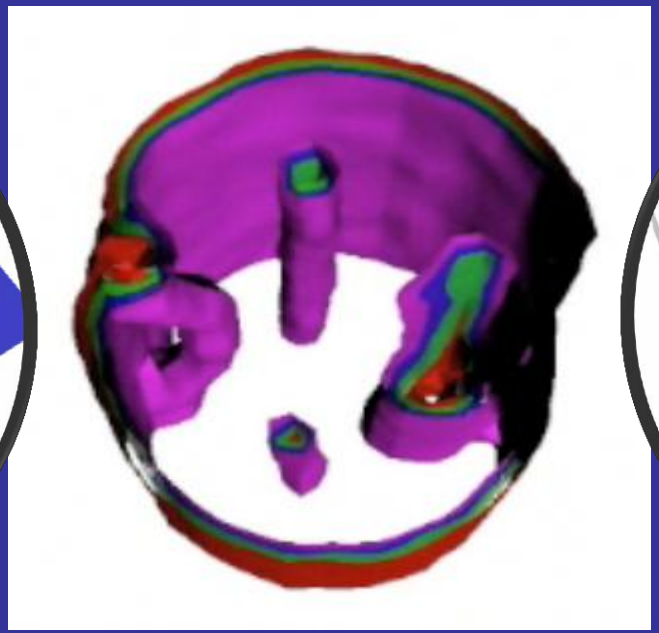

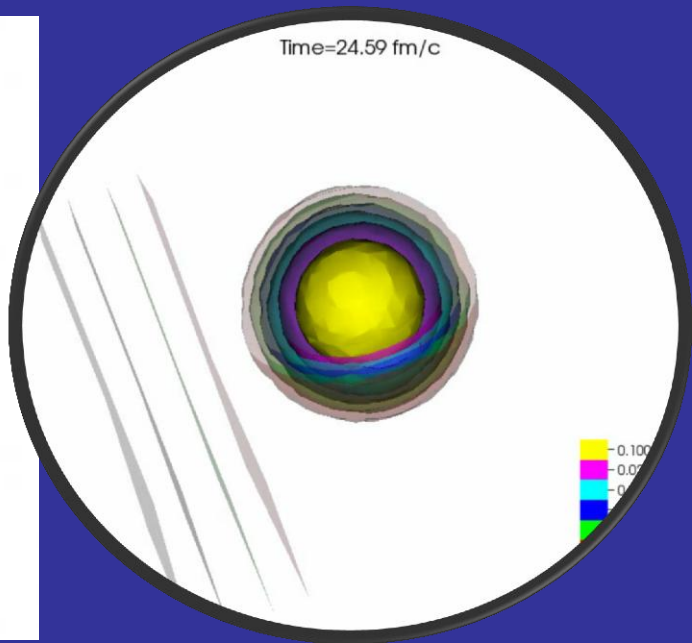

The project is oriented towards the description of strongly correlated, superfluid Fermi systems far from equilibrium in the framework of Density Functional Theory

- Applications: atomic nuclei, neutron star crust and quantum atomic gases
- The numerical codes are fully parallelized and optimized for the efficient use on the most powerful computers available (e.g. JaguarPF, ORNL)

Collaborators:

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Description of the tools:

- SLDA – static superfluid local density approximation
- TDSLDA – time dependent superfluid local density approximation

Both codes are formulated on the 3D lattice without any symmetry restrictions.

SLDA generates initial conditions for TDSLDA.

Formalism for Time Dependent Phenomena

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only one-body properties are considered.

A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)
V. Peuckert, J. Phys. C 11, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)

http://www.tddft.org

$$E(t) = \int d^3r \; \left[\; \varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \vec{j}(\vec{r},t)) + V_{ext}(\vec{r},t) n(\vec{r},t) + \ldots \right]$$

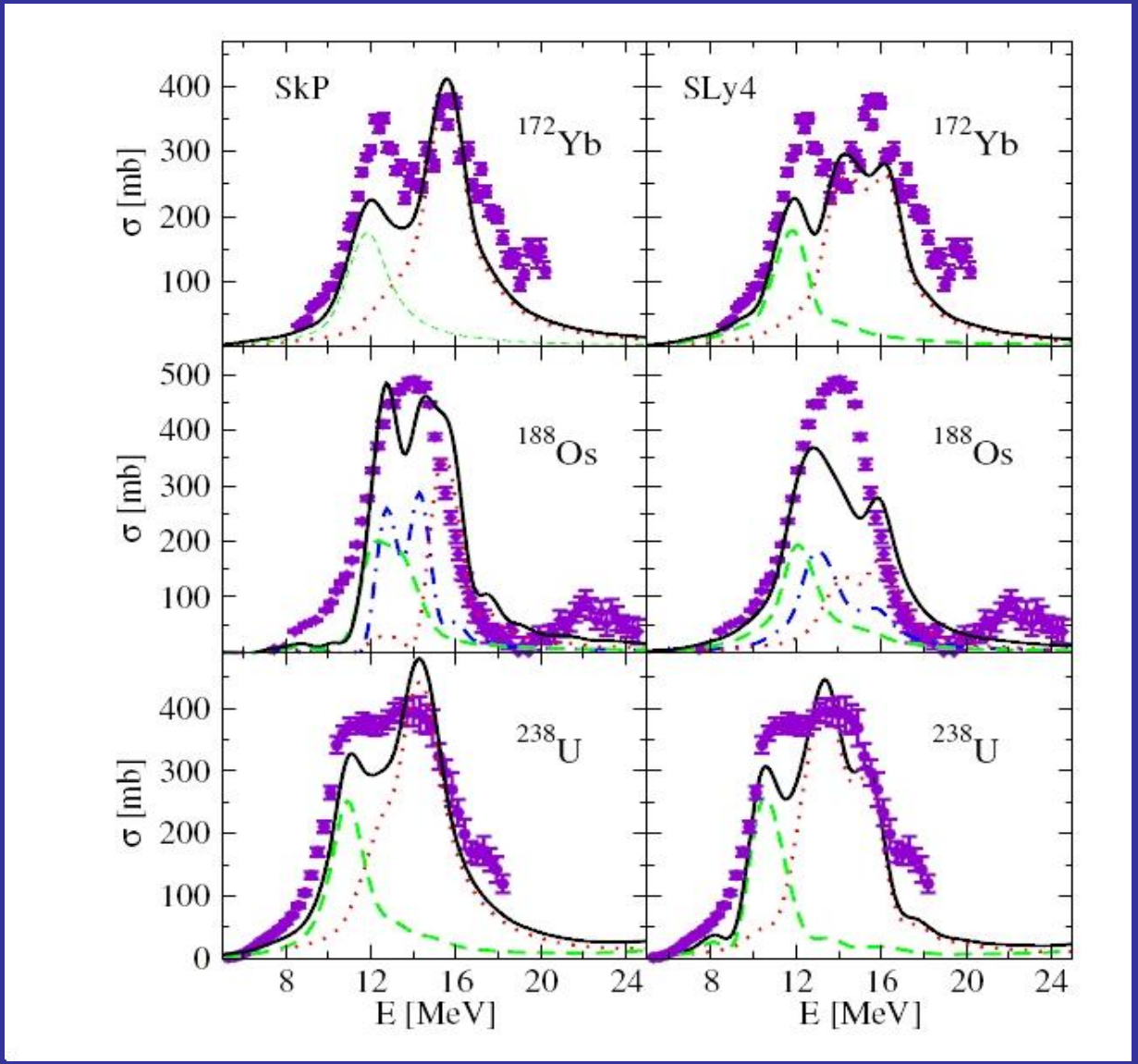
$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{u}_i(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_i(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)] \mathrm{u}_i(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v}_i(\vec{r},t)}{\partial t} \end{cases}$$

Selected capabilities of the SLDA/TDSLDA codes:

- ✓ full 3D simulations with no symmetry restrictions
- ✓ number of evolved quasiparticle wave functions is of the order of the lattice size
- ✓ wave functions are represented on a 3D spatial lattice (for 238U: 50x50x60)
- ✓ number of coupled nonlinear PDEs for ^{238}U = 546,512
- ✓ describe both closed-shell and open-shell systems of arbitrary shapes
- ✓ correct description of all spurious modes (translation, rotation, etc.)
- ✓ high numerical accuracy for spatial derivatives using FFTW
- ✓ for TD high-accuracy and numerically stable 5th order predictor-corrector-modifier algorithm with only 2 evaluations of the rhs per time step and with no matrix operations
- ✓ excellent weak and strong scaling
- ✓ very fast I/O capabilities
- ✓ nuclear volumes (so far) of the order of (L = 40 to 80 fm)^3, larger volumes possible
- ✓ in such volumes one can describe about 42,000 neutrons at saturation density
- ✓ capable of simulating up to times of the order of 10^{-19} s (a few million time steps)
- ✓ codes were initially written in Fortran90 and have been recently rewritten in C

Nuclear dynamics from time dependent density functional theory - first applications

Photoabsorption cross section for heavy, deformed nuclei.



I.Stetcu, A.Bulgac, P. Magierski, K.J. Roche, Phys. Rev. C84 051309 (2011)

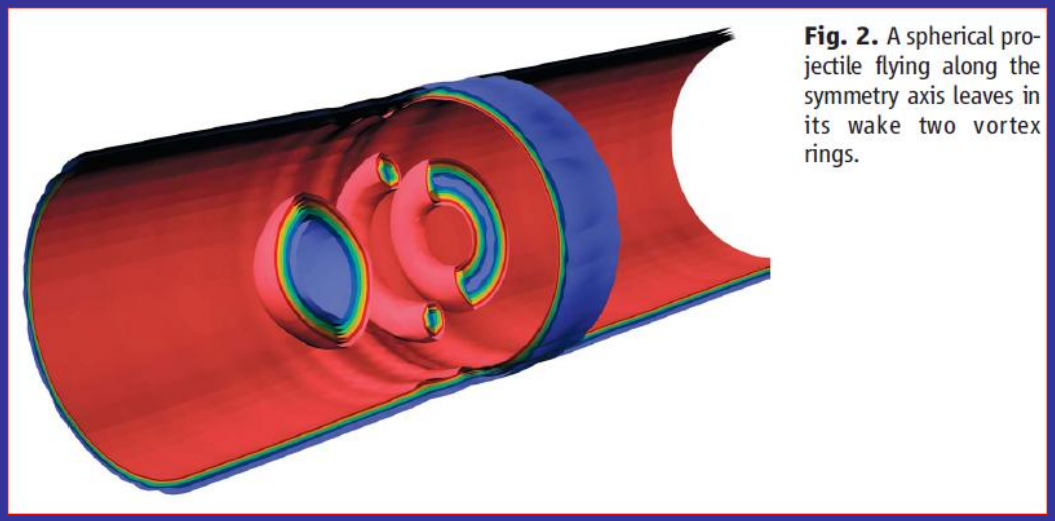


Fig. 2. A spherical projectile flying along the symmetry axis leaves in its wake two vortex rings.

Vortex reconnections

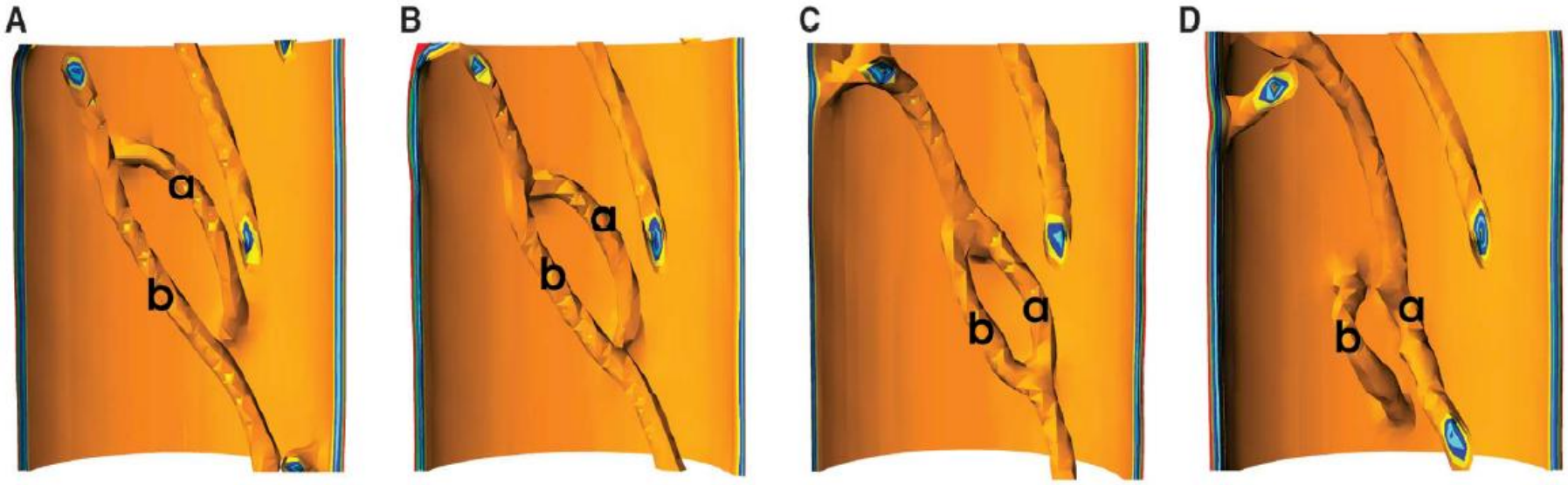


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b) after reconnection and vice versa.

Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

Plans for the next few years:

- Improve performance and numerical accuracy of the codes, study alternative numerical methods, improve the treatment of the absorbing boundary conditions, extend calculations to larger nuclear simulation volumes and longer times)
- Perform real-time calculations of excitation of nuclear reaction with neutrons and excitation of nuclei with gamma rays
- Simulate the excitation of single, double and triple GDR with relativistic heavy ions
- Simulate the induced nuclear fission with relativistic heavy ions
- Simulate the dynamics of vortices in neutron star crust and attempt to finally elucidate the pinning mechanism of vortices and their role in starquakes
- Study the dissipation in spontaneous fission by simulating the real-time dynamics of a fissioning nucleus from the scission point onward
- Extend/apply TDSLDA approach to nuclear reactions
- Stochastic extension of TDSLDA to account for a full dissipation and identification of various reaction channels.

Advantages:

- **We do not need to determine any collective coordinates, potential energy surfaces, inertia tensor, non-abelian gauge fields, etc. as the system will find naturally the right collective manifold**
- **We should be able to follow in real time a real experimental situation, such as induced fission or fusion**
- **This kind of simulations will answer in particular real needs of national security/nuclear forensics**
- **New theoretical techniques however would allow us to address new types of theoretical questions, in particular we would be able to study, with quantifiable theoretical errors, very fast non-equilibrium processes in strongly interacting many-fermion systems**

All this is naturally not limited to nuclear physics alone, this is a general approach to solve a large class of many-body problems numerically exactly, with quantifying errors, within the next decade …