TDSLDA Today and the Road Ahead

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✓ In 2006 we promised to implement SLDA/TDSLDA with no symmetry restrictions as an accurate alternative to QRPA for all nuclei (A>16). Here we are now:

✓ we developed: the extension of DFT to superfluid systems: (A)SLDA
✓ " the extension of SLDA to time-dependent phenomena: TDSLDA
✓ " the appropriate accurate numerics for both SLDA and TDSLDA
✓ we implemented SLDA/TDSLDA on leadership class supercomputers with massive parallelization, fast I/O, checkpoint/restart, extensive use of the latest advanced visualization techniques for the analysis of results and their presentation
(the nuclear code is 1,000-2,000 more complex than any existing TDHF code)
✓ we have used cca 70M+ CPU hours on Jaguar PF in 2010 and 5M+ CPU hours on Hopper in 2011
✓ we established a very accurate relation between *ab initio* QMC results and the energy density functional for the unitary Fermi gas, which was amply confirmed by experiments
✓ we demonstrated the ability to calculate: collective spectra of open shell nuclei, nucleon scattering and capture/knockout, nuclear fission, a limited (so far) number of nuclear reactions
✓ we revealed a number of new qualitative physics phenomena:

- superfluid flow at supercritical phenomena
- Higgs-Anderson modes, shock waves, dark solitons/domain walls
- generation of vortices, vortex rings and their real-time dynamics
- the first simulation of the vortex crossing and reconnection and the incipient phases of quantum turbulence in a fermionic superfluid

Capabilities of the SLDA/TDSLDA suite of codes:

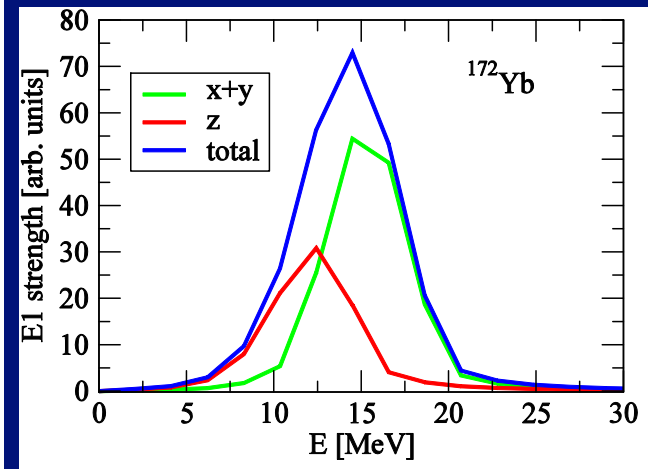
(extensively documented in: J. Phys.: Conf. Ser. 125, 012064 (2008),
Joule DOE metric report for FY 2010, SOM of Science, 332,1288 (2011))

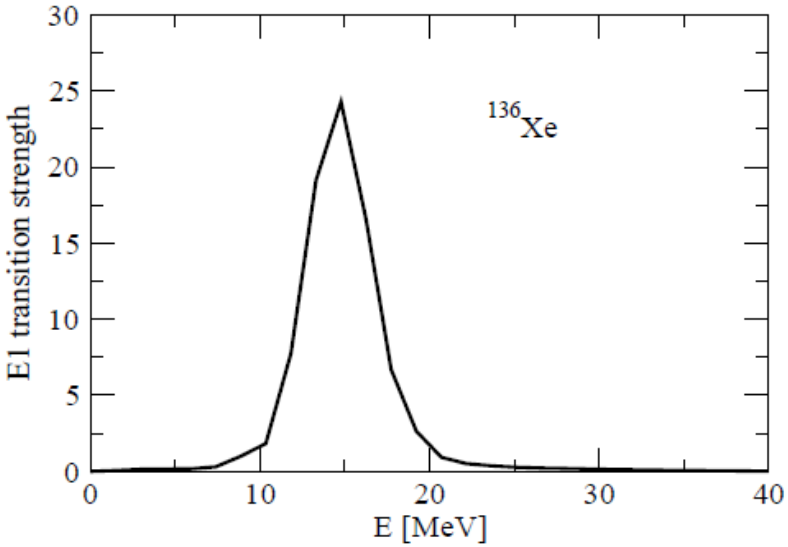
- ✓ full 3D simulations with no symmetry restrictions
- ✓ number of coupled nonlinear PDEs for ^{238}U = 546,512
- ✓ describe both closed-shell and open-shell systems of arbitrary shapes
- ✓ correct description of all spurious modes (translation, rotation, gauge invariance)
- ✓ wave functions are accurately represented on a 3D spatial lattice
- ✓ (for ^{238}U $40^2 \times 64 = 60^2 \times 80$ fm^3 for a lattice constant 1.25 fm)
- ✓ 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
- ✓ full diagonalization of Hermitian matrices 409,600x409,600 on JaguarPF (for ^{238}U)
- ✓ performance:

Static: ins/wall-time = 1.37e19/18,393= 7.46e14, flops/wall-time=9.42e16/18,393= 5.12e13
PEs = 217,800

TD: ins/wall-time = 7.11e17/2,031= 3.50e14, flops/wall-time= 1.89e16/2,031= 0.93e13
PEs = 136,628

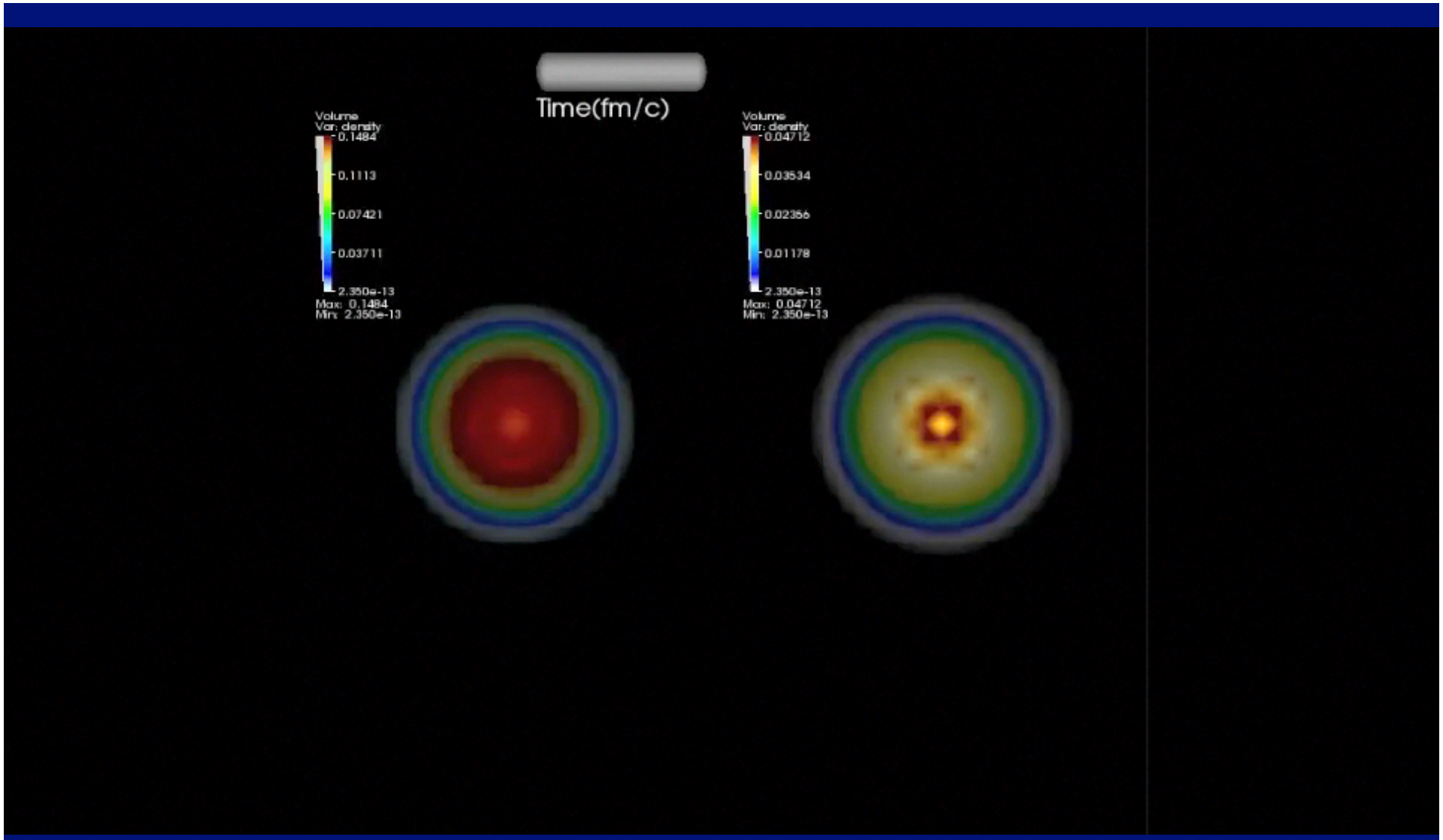
- ✓ excellent weak and strong scaling
- ✓ very fast I/O and checkpoint/restart capabilities
- ✓ nuclear volumes (so far) of the order of (L = 40 to 80 fm)^3, larger volumes possible
- ✓ in such volumes one can describe cca 42,000 neutrons at saturation density
- ✓ capable of simulating up to times of the order of 10^{-18} s (a few million time steps)
- ✓ codes written in Fortran90, with many components in C





Isovector dipole strength computed in TDSLDA with SLy4

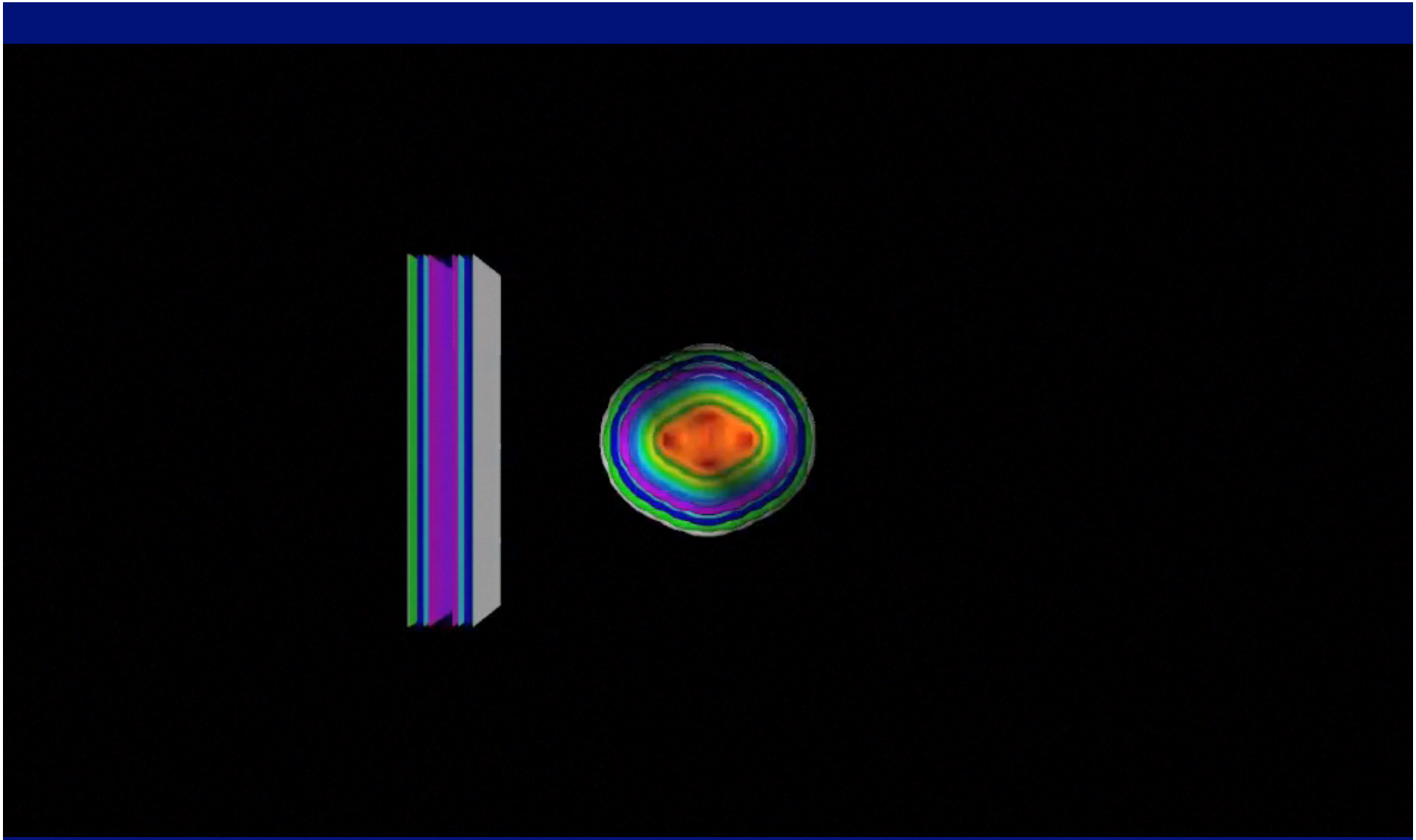
I. Stetcu *et al.*



Coulomb excitation of GDR with a relativistic heavy-ion computed in TDSLDA

Movie

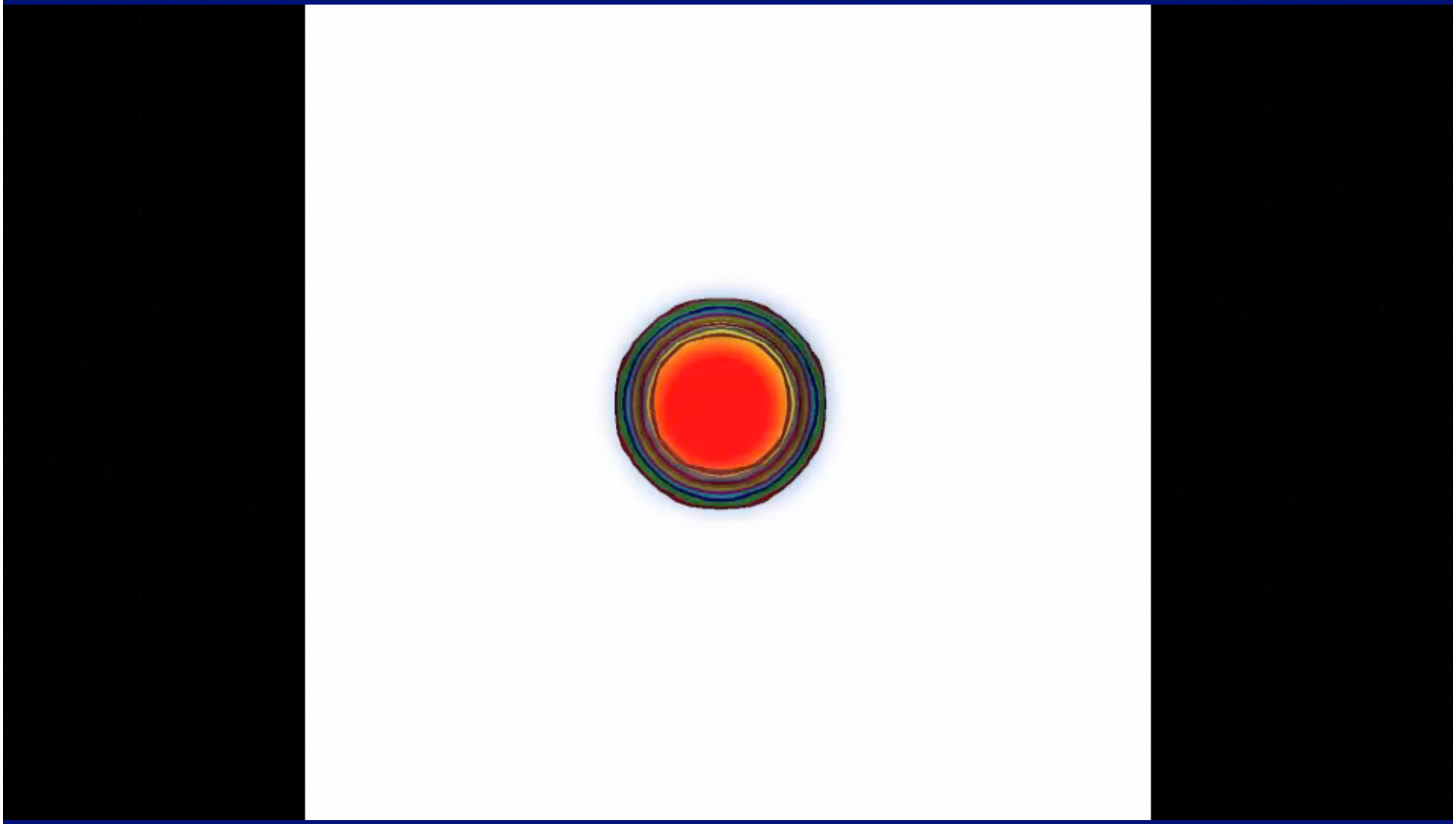
I. Stetcu *et al.*



Neutron scattering of ^{238}U computed in TDSLDA

I. Stetcu *et al.*

Movie



Real-time induced fission of ^{280}Cf computed in TDSLDA

I. Stetcu *et al.*

Movie

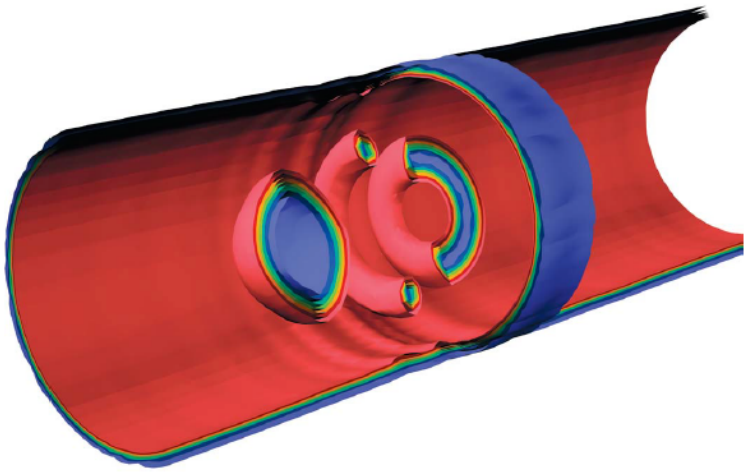


Fig. 2. A spherical projectile flying along the symmetry axis leaves in its wake two vortex rings.

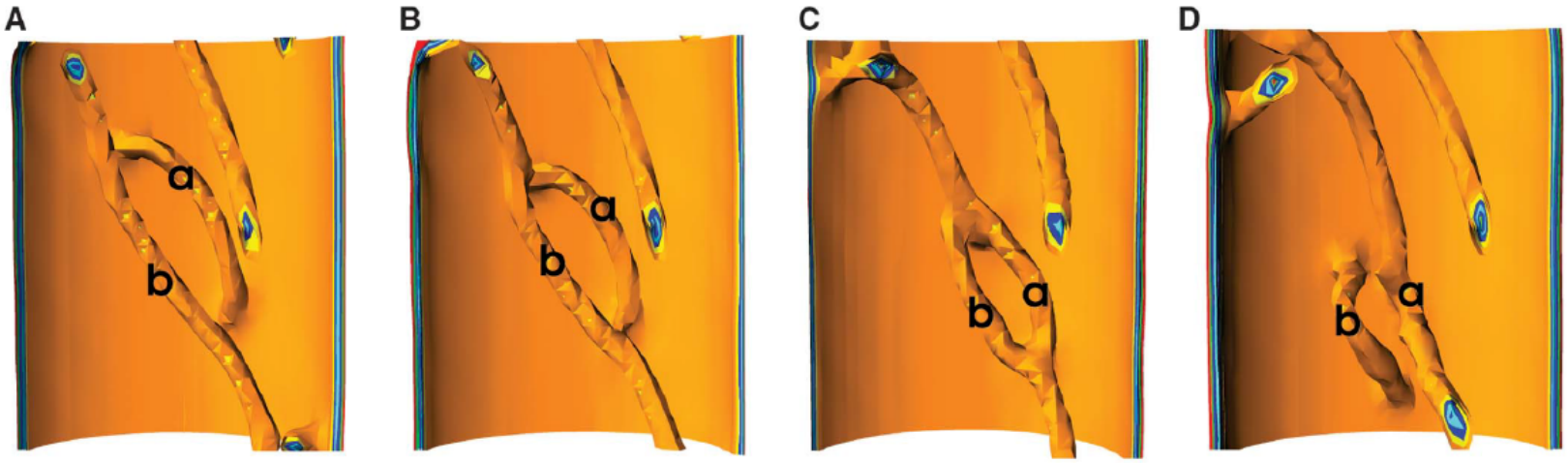
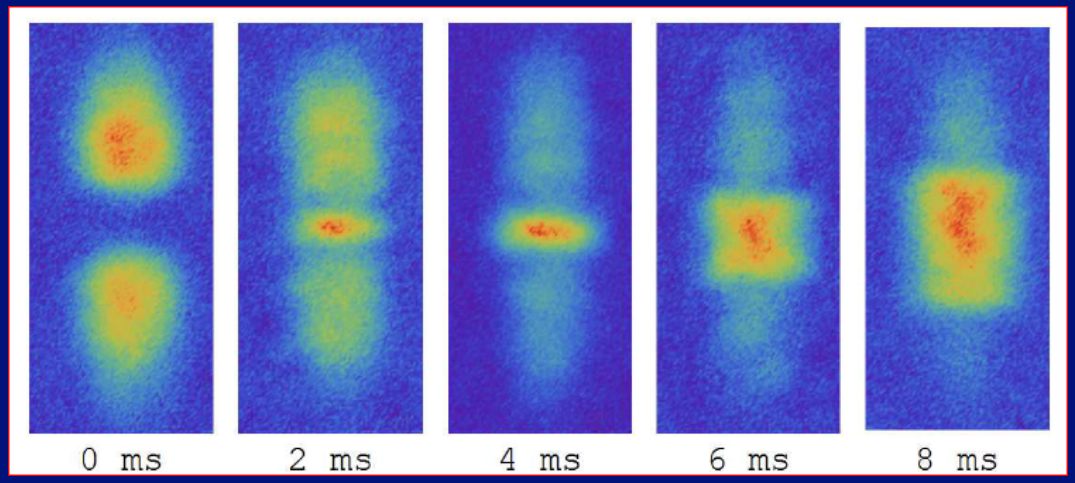
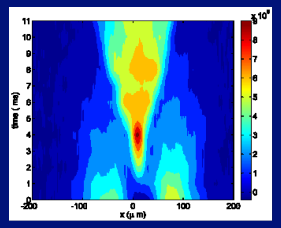


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b)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

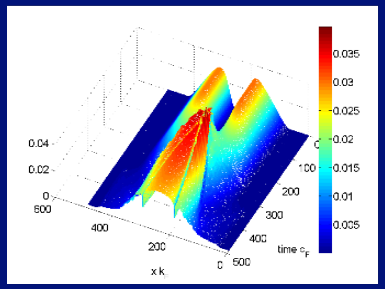
A. Bulgac, Y.-L. Luo, P. Magierski, K.J. Roche, Y. Yu
Science, 332, 1288 (2011)





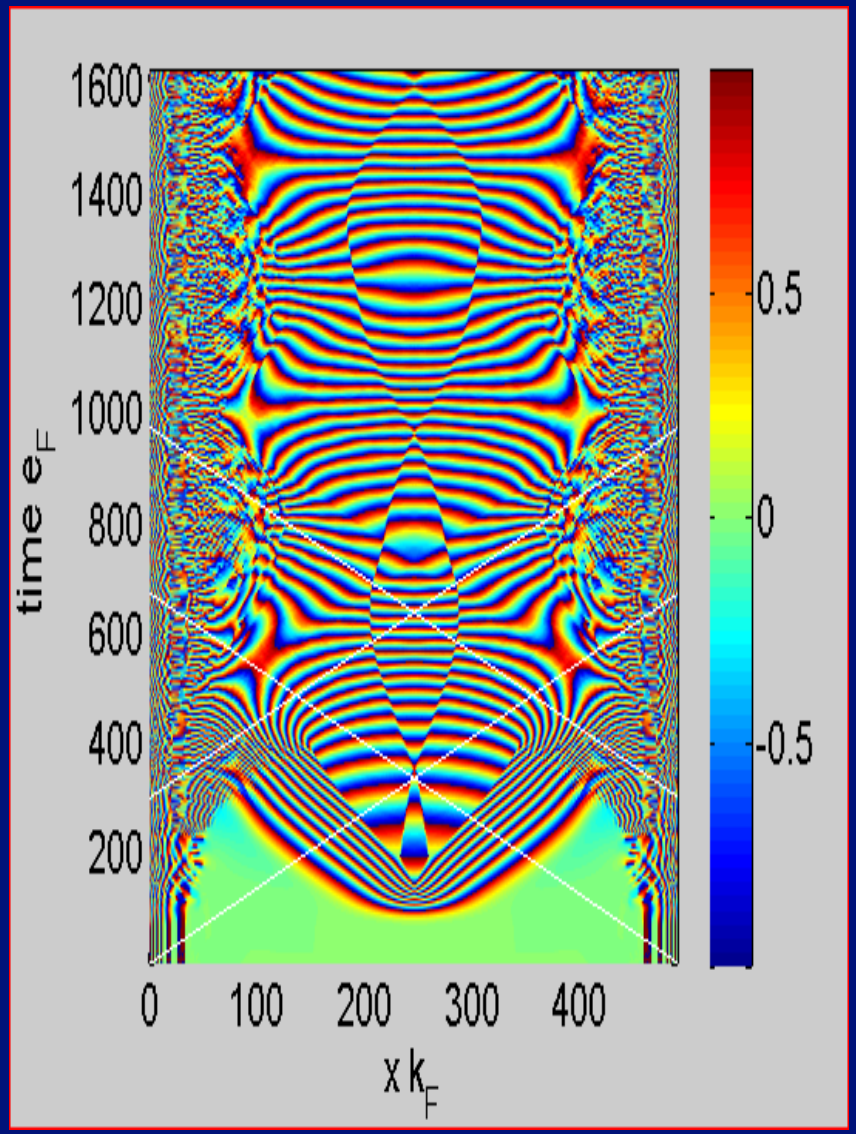
Observation of shock waves in a strongly interacting Fermi gas

J. Joseph, J.E. Thomas, M. Kulkarni, and A.G. Abanov PRL 106, 150401 (2011)

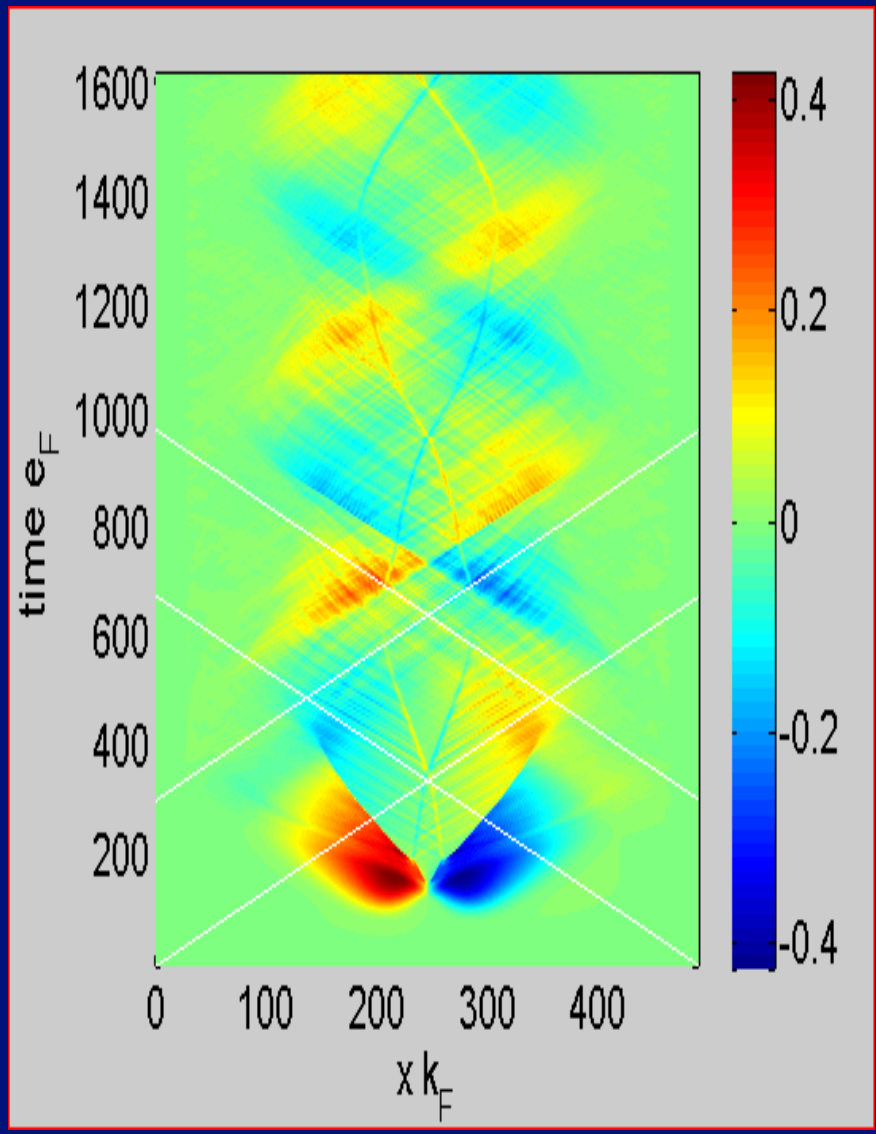


Number density of two colliding cold Fermi gases in TDSLDA

Dark solitons/domain walls and shock waves in the collision of two UFG clouds



Phase of the pairing gap normalized to



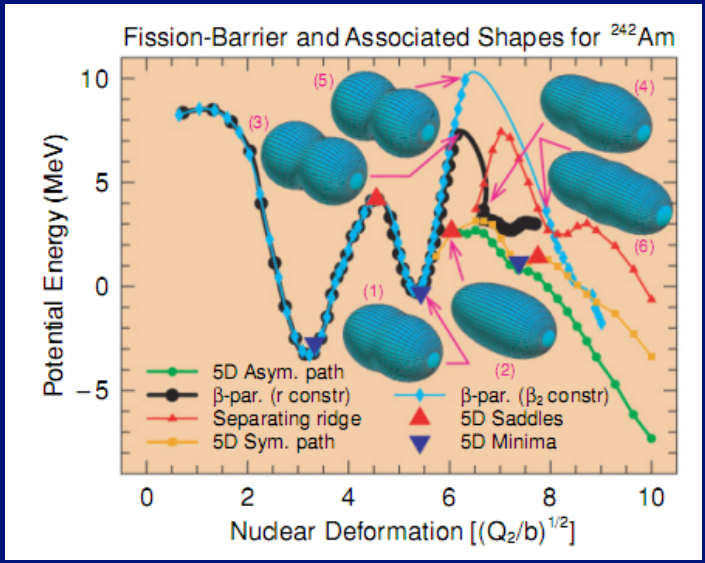
Local velocity normalized to Fermi velocity

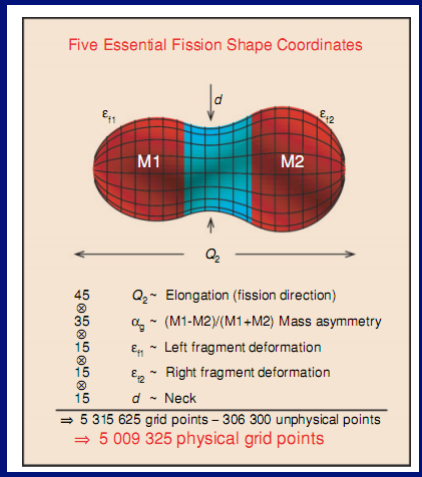
Why we need exascale and the extension of the TDSLDA to the Stochastic TDSLDA?

Nuclear LACM and fission studies using a GCM type of many-body wave function:

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}(q_1,\ldots,q_n)\Psi_{\text{Slater det.}}(x_1,\ldots,x_A,\{q_1,\ldots,q_n\})$$

P. Moller and collaborators need more than 5,000,000 shapes in a five dimensional space.



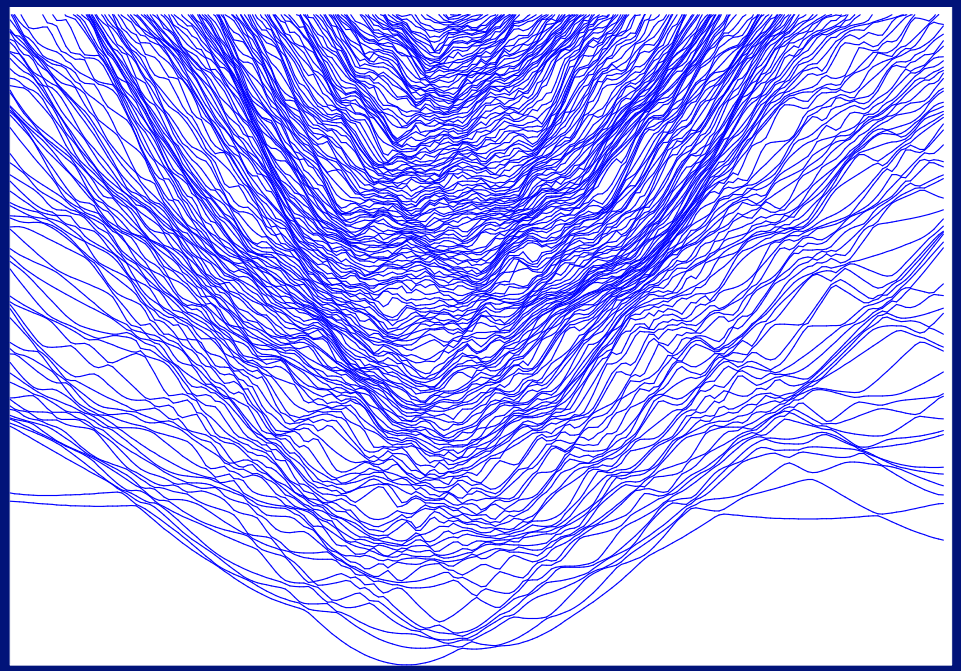


P.Moller *et al.* Phys. Rev. C 79, 064304 (2009)

Why this is inadequate? (just a few reasons)

- **Many more collective degrees of freedom needed, theoretical accuracy hard to quantify**
- **Only one potential energy surface, while many are needed**
- **Inertia tensor difficult to calculate, ambiguous prescriptions**
- **Adiabaticity is definitely violated, unclear how to describe dissipation within LACM**
- **Theory becomes impractical (even at exascale) for many collective degrees of freedom**

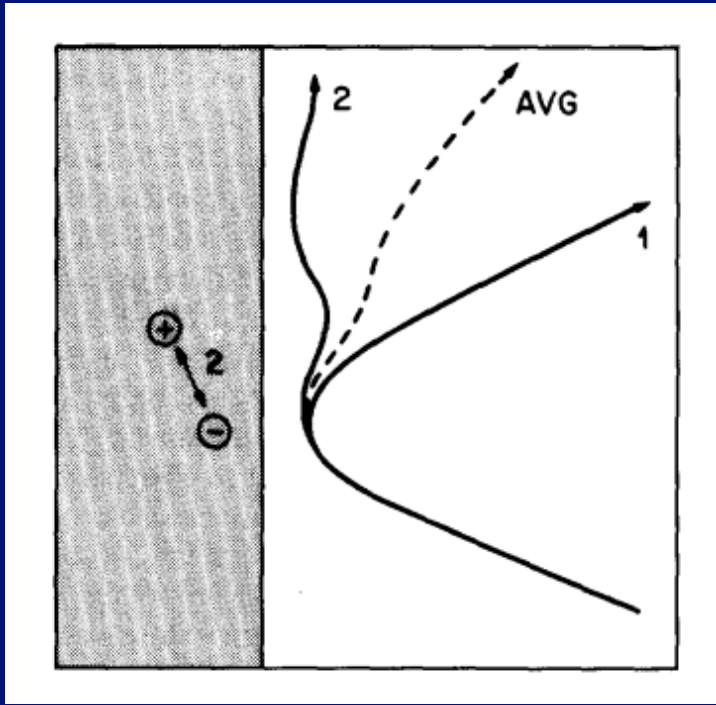
We need to consider the generic situation with multiple potential energy surfaces.



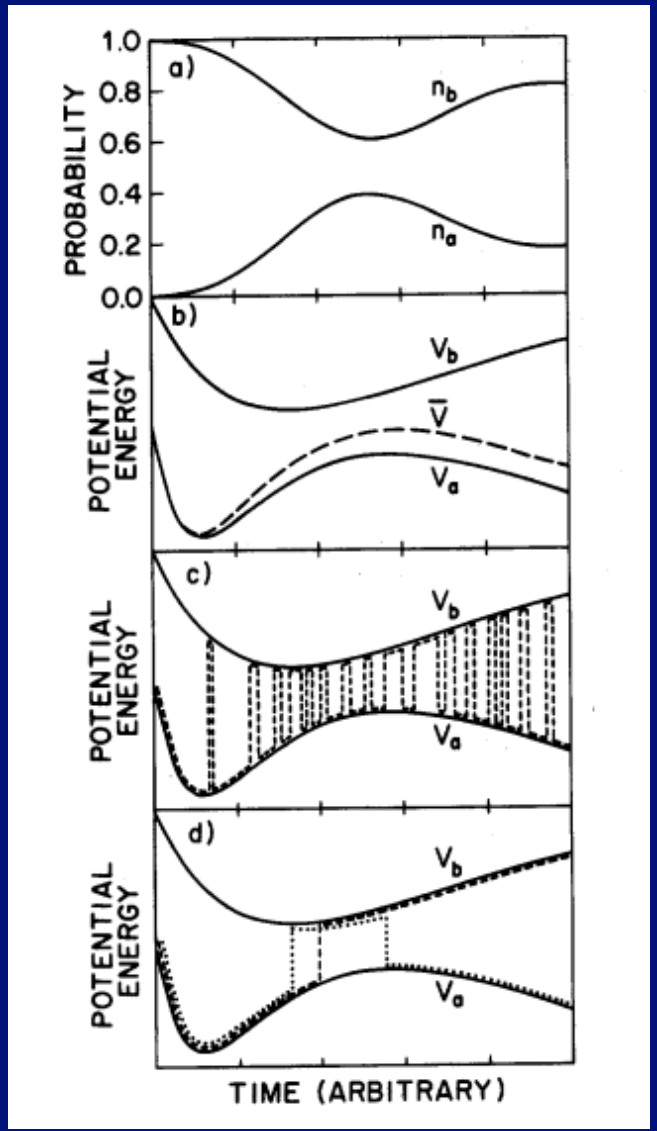
Energy

Deformation

John C. Tully suggested the following recipe for condensed matter and chemistry applications
J. Chem. Phys. 93, 1061 (1990)



$$\psi(\vec{r},\vec{R},t) = \sum_i c_i(\vec{R},t)\varphi_i\left(\vec{r}\,\middle|\,\vec{R}\right)$$



Evolution operator of an interacting many-body system

(after a Trotter expansion and a Hubbard-Stratonovich transformation)

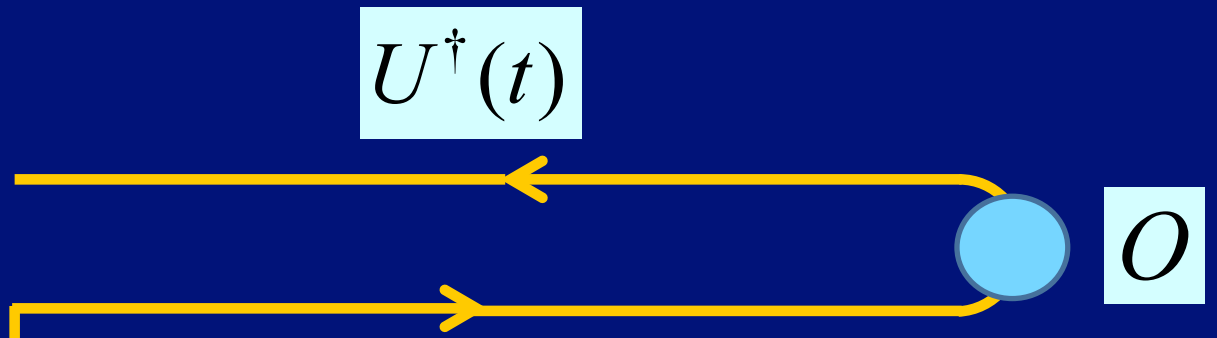
$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i\frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha_a^\dagger \alpha_b \right]$$

This representation is not unique, the one-body evolution operator is arbitrary!!!
Kerman, Levit, and Troudet, Ann. Phys. 148, 443 (1983)

This looks much worse that the infamous fermion sign problem!!!

What we need is a bit more complicated, to simulate dynamics along the Keldysh-Schwinger complex time-ordered contour



$$\rho_0 = \frac{\exp(-\beta H_0)}{Z}$$

Initial state preparation (equilibrium at finite T)

$$U(t) = T_t \exp\left[-i\int_0^t dt H(t)\right]$$

$$H(t) = H_0 + V_{ext}(t), \qquad t>0$$

$$i\hbar\frac{\partial\rho(t)}{\partial t} = \left[H(t),\rho(t)\right], \qquad \rho(0)=\rho_0$$

$$O(t) = \mathrm{Tr}\left[O\rho(t)\right] = \mathrm{Tr}\left[\rho_0 U^{\dagger}(t) O U(t)\right]$$

Here is how this can be done and has already been implemented numerically on Hyak-UW (MRI-NSF funded cluster, Intel chips, 1120 cores, 3Gb RAM/core)

We place several fermions on a square lattice

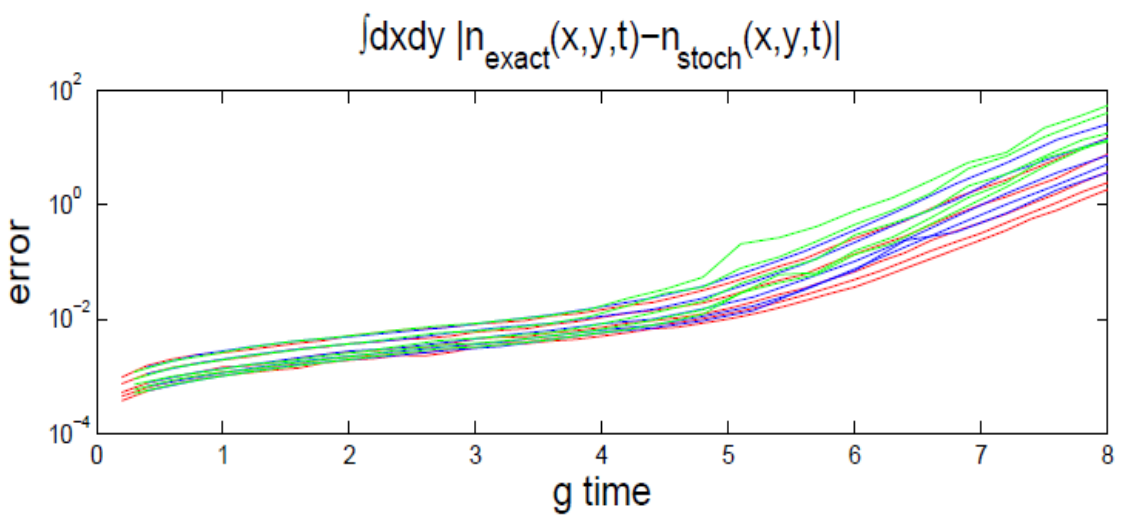
$$H = \sum_{k,\sigma} \frac{\vec{k}^2}{2} \alpha^{\dagger}_{\vec{k},\sigma} \alpha_{\vec{k},\sigma} + g \sum_{\vec{r}} \alpha^{\dagger}_{\vec{r},\uparrow} \alpha^{\dagger}_{\vec{r},\downarrow} \alpha_{\vec{r},\downarrow} \alpha_{\vec{r},\uparrow}$$

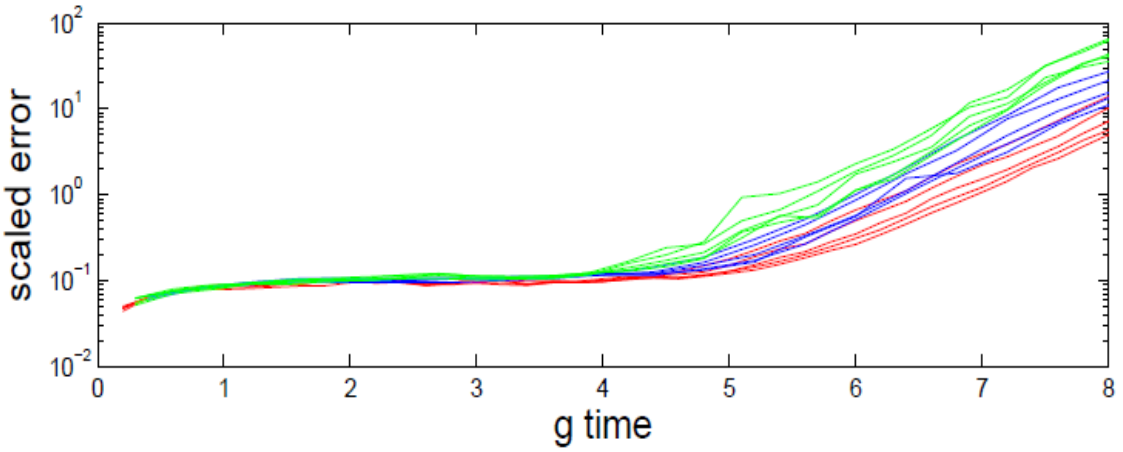
NB The coordinate and momentum creation/anihilation operators are linked by the usual unitary transformations.

We evolve an initial many-fermion wave function using independent real-time path integral representations of the propagators for the bra (backward in time) and ket (forward in time) many-body wave functions:

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i \frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n) \right] \times \exp\left[i \Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd} \sigma_{cd}(n) \right) \alpha^{\dagger}_a \alpha_b \right]$$

We used both discrete and continuous HS transformations, and simulated up to 6 fermions.





Results for two fermions, for g=1 (red), 2 (blue), and 3 (green), and a 16x16 lattice
Sample sizes for the propagator M= 2,500, 5,000, 10,000 and 20,000.
Lower plot shows that error scales as theoretically expected

$$\propto \exp(gt/2)/\sqrt{M}.$$

Theoretical analysis and further numerical simulations show that for N interacting fermions the simulation error behaves as

$$\propto \exp(Ngt/2)/\sqrt{M}.$$

NB The error is independent of:

- the dimensionality of the space
- the spatial volume/size of lattice
- a relatively small number of samples is needed for a decent accuracy

What we could in principle be able to calculate?

- **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 will not need to assume either isentropic, isothermal, … meanfield solutions. Instead the temperature and entropy of the collective subsystem will evolve according to the rules of QM. This will be the most natural framework to describe dissipation in collective nuclear motion.**
- **We should be able to compute directly the mass, charge distributions and the excitation energy, and maybe even quantum number distributions of each fragment**
- **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 … or sooner.

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)
- Systematic calculations of collective states in nuclei across the periodic table (likely new collaboration with K. Nakatsukasa and his colleagues)
- 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 (new collaboration with C. Bertulani, GSI experiment)
- Simulate the induced nuclear fission with relativistic heavy ions (new collaboration with C. Bertulani, GSI experiment)
- Simulate the dynamics of vortices in neutron star crust and attempt to finally elucidate the pinning mechanism of vortices and their role in starquakes (new collaboration with S. Reddy)
- 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
- Further studies of the UFG
- Vigorously pursue the Stochastic extension of TDSLDA and prepare the grounds for doing nuclear physics in the exascale regime (new collaborations envisioned with G.F. Bertsch, M.M. Forbes, S. Moroz, …)

Computational and Computer Science needs:

- Next three years between 100-200 M CPU hours/year
- 3-5 years 1-20 billion CPU hours/year (assuming the 10-100 petascale regime)
- 5-7 and after 20-200 billion CPU hours/year (assuming the exascale regime)
- Likely we will need to perform a large number of calculations in extended precision
- We will vigorously examine the use of GPUs (K.J. Roche + S. Cohen (postdoc))

Quantum Monte Carlo for nuclei on the lattice with EFT interactions and pions (new collaboration with J.E. Drut, M.M. Forbes, S. Moroz, …)

- ***3D lattice techniques were initially introduced and extensively tested (Bulgac, Drut, Magierski) for finite temperature QMC calculations and we simulated successfully systems with up to about 100 fermions***
- ***We have predicted a large number of various observable and their dependence on coupling constant and temperature (EOS, critical temperature, phase transitions, high-momentum distribution, quasi-particle spectrum, pairing gap and the pseudogap phase, etc.) many of which have been accurately confirmed in subsequent experiments***

- **We have already developed parallel codes capable of simulating systems in lattice sizes in principle up to 100^3 (tested so far 20^3 on Hyak)**
- **We plan to simulate even-even nuclei with N=Z up to A=100, as well as neutron matter and symmetric nuclear matter as in these systems the fermion sign problem is expected to be rather benign**
- **In lattices 32^3 and above the numerical accuracy should be at the level of a 2-3 % or lower**
- **and this approach should become competitive with NCSM and CC**
- **Following the approach pioneered by Epelbaum, Krebs, Lee and Meissner, PRL 106, 192501 (2011) we envision to be able to calculate both ground states as well as excited states properties in these nuclei with a much finer and larger spatial lattice**
- **Likely these methods should allow for extension to system with 1 and 2 nucleons above the N=Z even-even core.**