Nuclear Fission: from more phenomenology and adjusted parameters to more fundamental theory and increased predictive power

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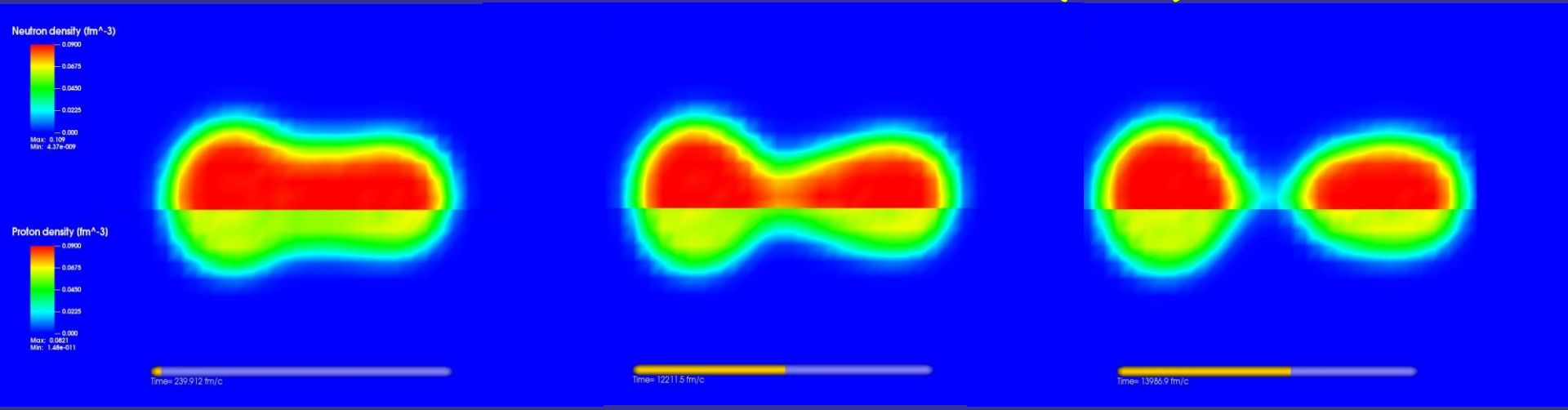


Nuclear fission is unquestionably one of the most challenging quantum many-body problems.

Important for fundamental nuclear theory, origin of elements, applications.

Several recent developments have changed radically our prospects of attaining a microscopic description of fission, almost 80 years after it was experimentally discovered.

(In comparison, superconductivity needed less than 50 years to attain this goal, from 1911 to 1957, despite of the fact that already in 1926 the key ingredient – Schroedinger equation has been formulated)

Why it is so difficult to describe nuclear fission ?

The fundamental equation describing nuclear dynamics is known:

$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$$

However even if we knew nuclear Hamiltonian precisely, the problem of motion of more than 200 strongly interacting nucleons, described in terms of true many-body wave function is computationally intractable.

The wave function of ^{240}Pu depends on 720 coordinates!!!
It has 1.76×10^{72} spin components!!!

Critical new developments

- In THEORY:

Formulation of a local extension of the Density Functional Theory (DFT) to superfluid time-dependent phenomena, the Superfluid Local Density Approximation (SLDA).

Validation and verification of time dependent SLDA (TDSLDA) against a large set of theoretical and experimental data for systems of strongly interacting fermions.

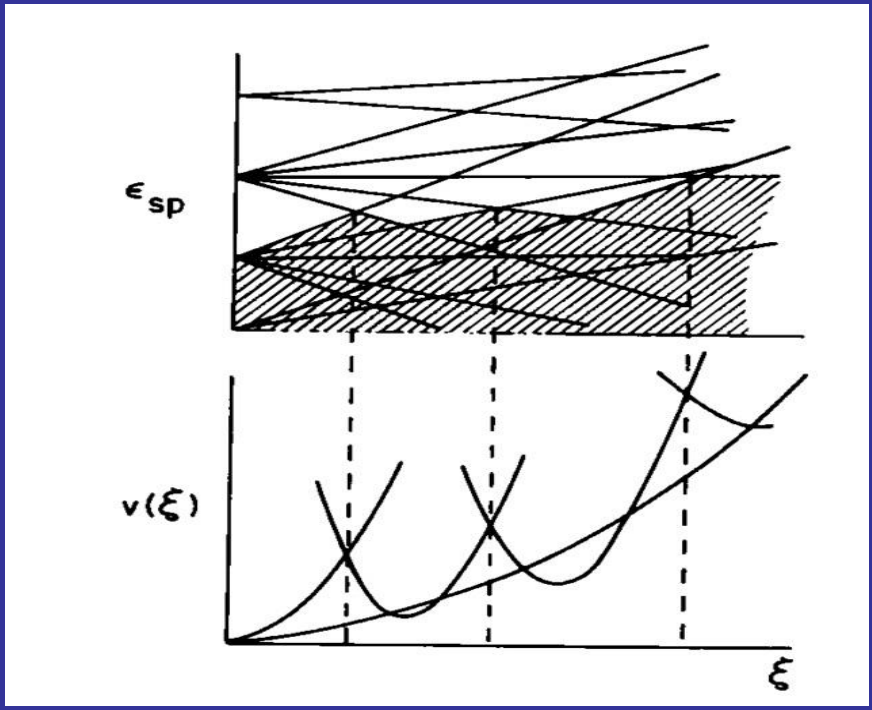
- In HIGH PERFOMANCE COMPUTING:

Emergence of very powerful computational resources, non-trivial numerical implementation of TDSLDA, advanced capabilities of leadership class computers due to hybrid architecture integrating CPUs with Graphics Processing Units (GPU).

SLDA and TDSLDA are problems of extreme computational complexity, requiring the solution of 10,000s … 1,000,000s coupled complex non-linear time-dependent 3D partial differential equations.

Physics of nuclear superfluid dynamics

What is the mechanism of nuclear shape evolution during the fission process?



From Barranco, Bertsch, Broglia, and Vigezzi
Nucl. Phys. A512, 253 (1990)

- While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored
  Hill and Wheeler, PRC, 89, 1102 (1953)
  Bertsch, PLB, 95, 157 (1980)

- Each single-particle level is double degenerate (Kramers' degeneracy) and at each level crossing two nucleons must jump simultaneously!

(m,-m) => (m',-m')
"Cooper pair" => "Cooper pair"

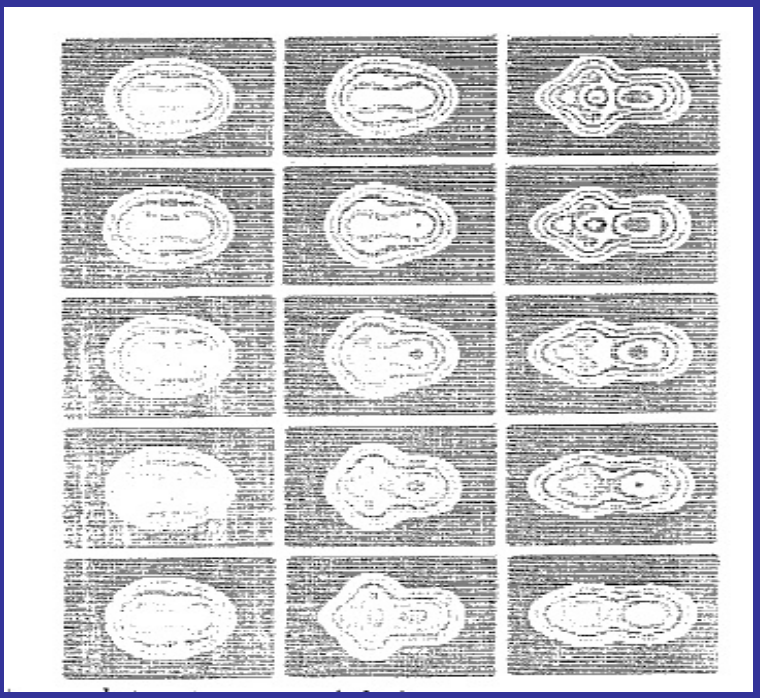
- Pairing interaction/superfluidity is the most effective mechanism at performing shape changes.

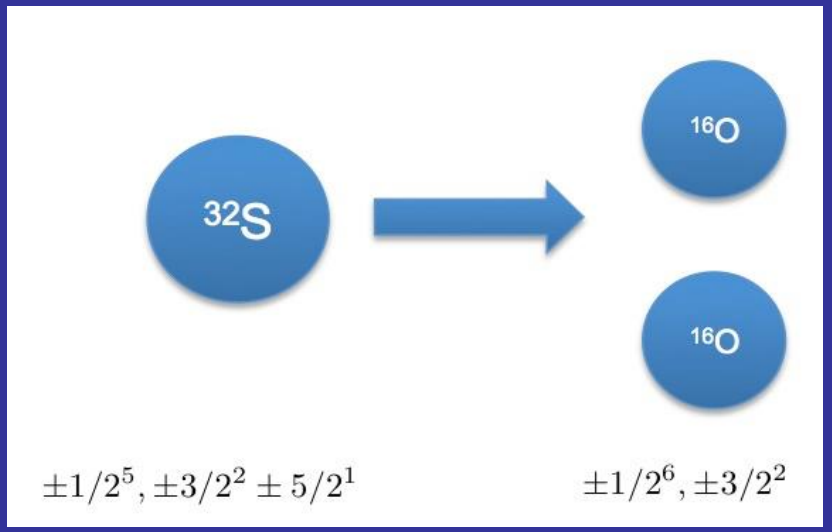
However, in TDHF calcs. starting from the axial nuclear configuration the initial spherical Fermi momentum distribution acquires an ellipsoidal prolate shape in the final fission fragments leading to extremely excited states.

Bertsch and Bulgac, Phys. Rev. Lett. 79, 3539 (1997)

A different mechanism for nuclear shape evolution was advocated by

J.W. Negele, Nucl. Phys. A 502, 371c-386c (1989)
Microscopic theory of fission dynamics





Occupied single-particle orbitals m-quantum numbers in initial and final configurations

One more problem!
Initial nucleus: 20 positive + 12 negative parity s.p. orbitals
Final nuclei: 16 positive + 16 negative parity s.p. orbitals

- Can the adoption of a TDHF + TDBCS approach to fission help restore the sphericity of the Fermi sphere in the fission fragments?

- A little bit.

  - In TDHF the nucleus is allowed to acquire in principle any shape, but whether dynamically that is realized is not a foregone conclusion.

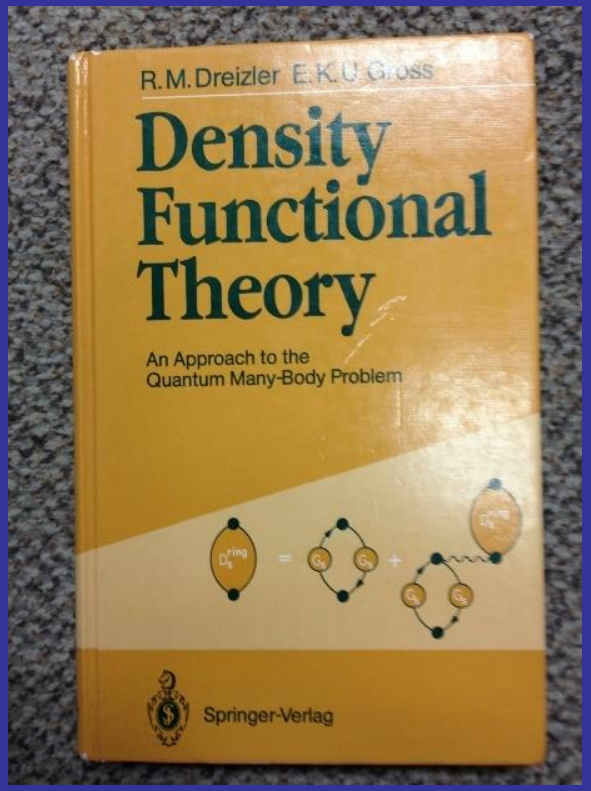
  - By adding TDBCS to TDHF one adds one "complex" collective degree of freedom to the many shape degrees of freedom: a spatially constant throughout the entire space complex time-dependent pairing field $\Delta(t)$. Thus TDHF+TDBCS amounts to adding practically only one additional collective degree of freedom.

  - Practice shows that nuclei cannot always fission within TDHF + TDBCS. This is likely related to the fact that the initial spherical Fermi surface cannot evolve into two spherical Fermi surfaces in the fission fragments within TDHF + TDBCS.

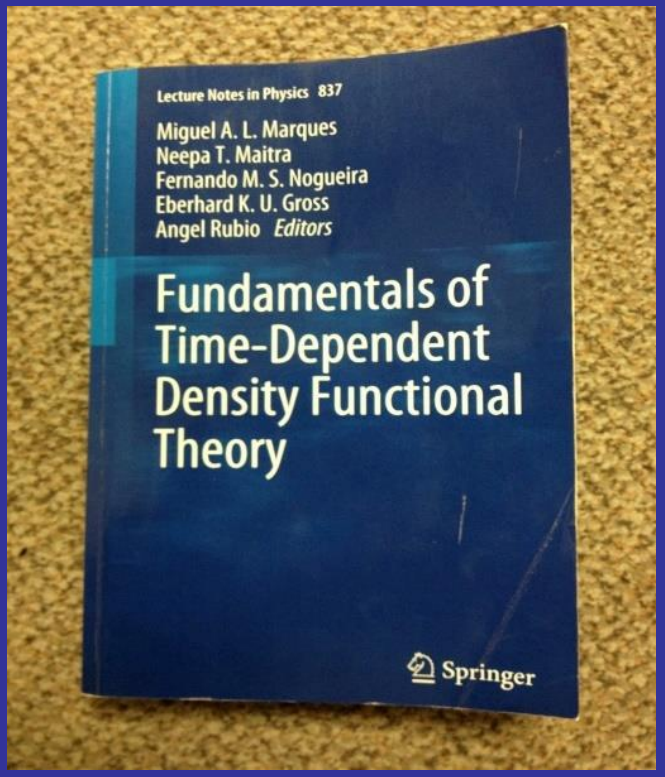
  - Continuity equation is violated in a TDHF + TDBCS approach.

Main Theoretical Tool

THEOREM (Hohenberg & Kohn): There exist an universal density functional of particle density.



1990



2012

Runge Gross mapping

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle, \quad \left|\psi_0\right\rangle = \left|\psi(t_0)\right\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\left.\begin{array}{l}\rho(\vec{r},t)\\ \left|\psi(t_0)\right\rangle\end{array}\right\} \leftrightarrow e^{i\alpha(t)}\left|\psi(t)\right\rangle$$

Up to an arbitrary function α(t)

and consequently the functional exists:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1}\left\langle\psi[\rho]\right|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\left|\psi[\rho]\right\rangle dt$$

E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

Kohn-Sham approach

Suppose we are given the density of an interacting system.
There exists a unique noninteracting system with the same density.

Interacting system

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = (\hat{T}+\hat{V}(t)+\hat{W})\left|\psi(t)\right\rangle$$

Noninteracting system

$$i\hbar\frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = (\hat{T}+\hat{V}_{KS}(t))\left|\varphi(t)\right\rangle$$

$$\rho(\vec{r},t) = \left\langle\psi(t)\right|\hat{\rho}(\vec{r})\left|\psi(t)\right\rangle = \left\langle\varphi(t)\right|\hat{\rho}(\vec{r})\left|\varphi(t)\right\rangle$$

Hence the DFT approach is essentially exact.

A new local extension of DFT to superfluid systems (SLDA) and time-dependent phenomena (TDSLDA) was developed.

Reviews: A. Bulgac, *Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids*, Ann. Rev. Nucl. Part. Sci. 63, 97 (2013);
P. Magierski, *Nuclear Reactions and Superfluid Time Dependent Density Functional Theory*,
in "Progress of time-dependent nuclear reaction theory" (Betham Science Publishers 2016)

SLDA for unitary Fermi gas

SLDA – Superfluid Local Density Approximation

SLDA energy density functional at unitarity

$$\varepsilon(\vec{r}) = \left[\alpha\frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

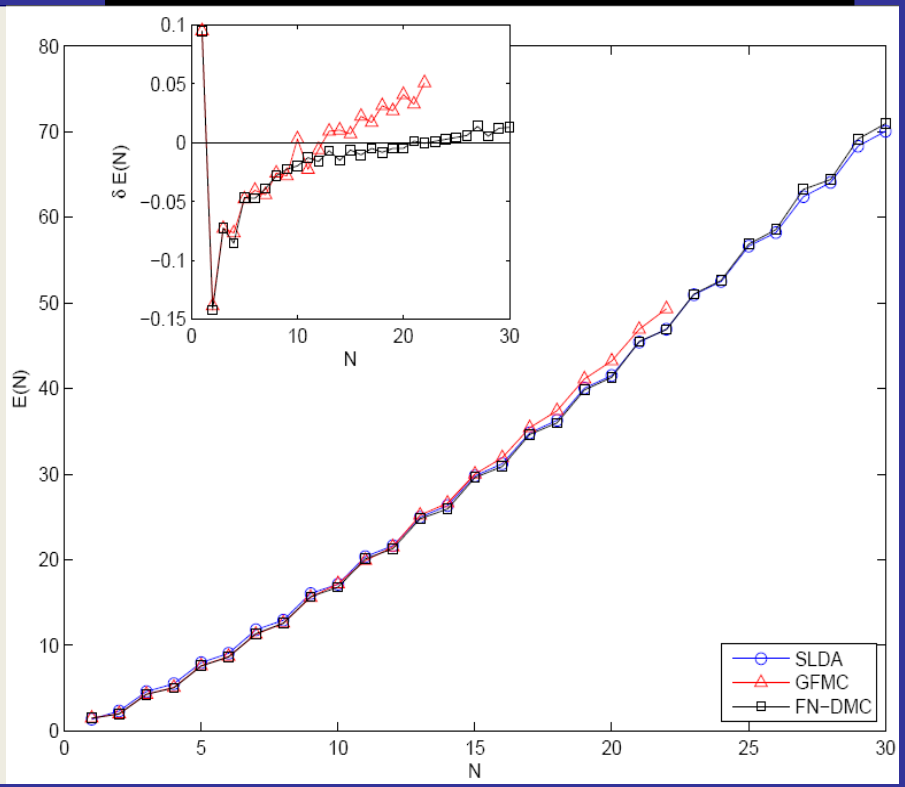
$$n(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\mathrm{v}_\mathrm{k}(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\vec{\nabla}\mathrm{v}_\mathrm{k}(\vec{r})\right|^2,$$

$$\nu_c(\vec{r}) = \sum_{0<E<E_c}\mathrm{u}_\mathrm{k}(\vec{r})\mathrm{v}_\mathrm{k}^*(\vec{r})$$

$$U(\vec{r}) = \beta\frac{(3\pi^2)^{2/3}n^{2/3}(\vec{r})}{2} - \frac{\left|\Delta(\vec{r})\right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r})$$

$$\Delta(\vec{r}) = -g_{eff}(\vec{r})\nu_c(\vec{r})$$

Fermions at unitarity in a harmonic trap
Total energies E(N)



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)
FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)
PRA 76, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

Normal State				Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)	(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(3,1)	6.6 ± 0.01	6.687	1.3%	(1,1)	2.002 ± 0	2.302	15%
(4,1)	8.93 ± 0.01	8.962	0.36%	(2,2)	5.051 ± 0.009	5.405	7%
(5,1)	12.1 ± 0.1	12.22	0.97%	(3,3)	8.639 ± 0.03	8.939	3.5%
(5,2)	13.3 ± 0.1	13.54	1.8%	(4,4)	12.573 ± 0.03	12.63	0.48%
(6,1)	15.8 ± 0.1	15.65	0.93%	(5,5)	16.806 ± 0.04	16.19	3.7%
(7,2)	19.9 ± 0.1	20.11	1.1%	(6,6)	21.278 ± 0.05	21.13	0.69%
(7,3)	20.8 ± 0.1	21.23	2.1%	(7,7)	25.923 ± 0.05	25.31	2.4%
(7,4)	21.9 ± 0.1	22.42	2.4%	(8,8)	30.876 ± 0.06	30.49	1.2%
(8,1)	22.5 ± 0.1	22.53	0.14%	(9,9)	35.971 ± 0.07	34.87	3.1%
(9,1)	25.9 ± 0.1	25.97	0.27%	(10,10)	41.302 ± 0.08	40.54	1.8%
(9,2)	26.6 ± 0.1	26.73	0.5%	(11,11)	46.889 ± 0.09	45	4%
(9,3)	27.2 ± 0.1	27.55	1.3%	(12,12)	52.624 ± 0.2	51.23	2.7%
(9,5)	30 ± 0.1	30.77	2.6%	(13,13)	58.545 ± 0.18	56.25	3.9%
(10,1)	29.4 ± 0.1	29.41	0.034%	(14,14)	64.388 ± 0.31	62.52	2.9%
(10,2)	29.9 ± 0.1	30.05	0.52%	(15,15)	70.927 ± 0.3	68.72	3.1%
(10,6)	35 ± 0.1	35.93	2.7%	(1,0)	1.5 ± 0.0	1.5	0%
(20,1)	73.78 ± 0.01	73.83	0.061%	(2,1)	4.281 ± 0.004	4.417	3.2%
(20,4)	73.79 ± 0.01	74.01	0.3%	(3,2)	7.61 ± 0.01	7.602	0.1%
(20,10)	81.7 ± 0.1	82.57	1.1%	(4,3)	11.362 ± 0.02	11.31	0.49%
(20,20)	109.7 ± 0.1	113.8	3.7%	(7,6)	24.787 ± 0.09	24.04	3%
(35,4)	154 ± 0.1	154.1	0.078%	(11,10)	45.474 ± 0.15	43.98	3.3%
(35,10)	158.2 ± 0.1	158.6	0.27%	(15,14)	69.126 ± 0.31	62.55	9.5%
(35,20)	178.6 ± 0.1	180.4	1%				

A. Bulgac, M.M. Forbes, P. Magierski, *in* BCS-BEC crossover and the Unitary Fermi gas „Lecture Notes in Physics" v.836, p. 305, ed. W. Zwerger (2012)

TDSLDA equations:

Local density approximation

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

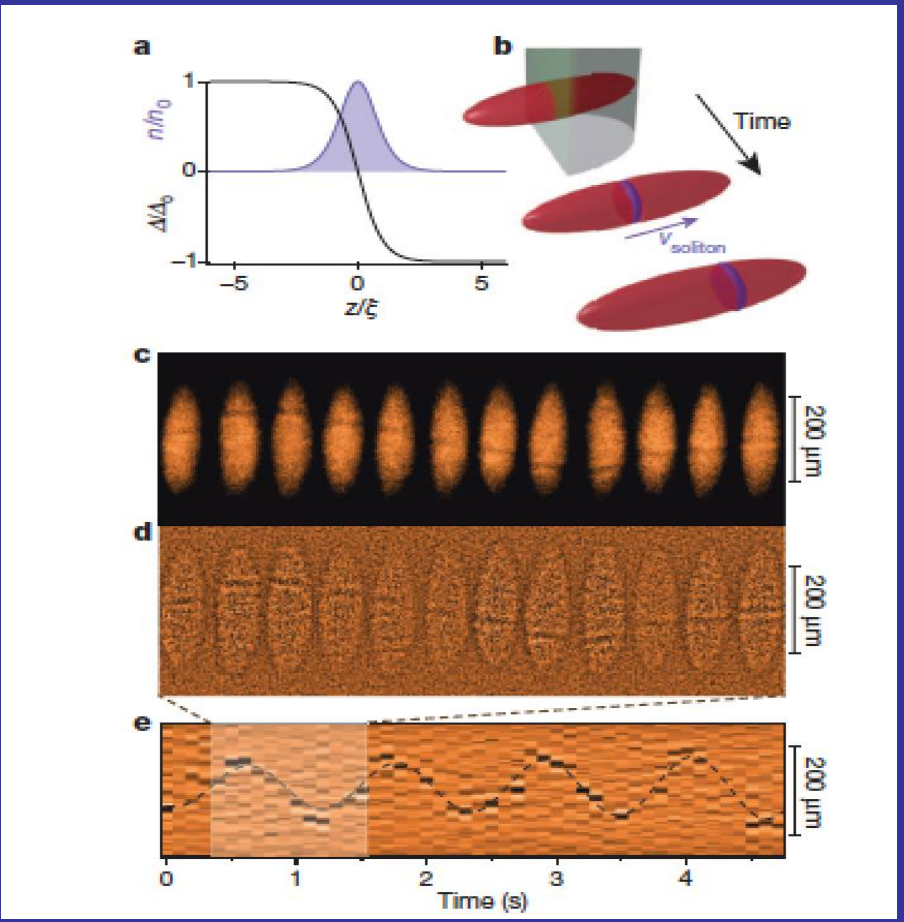
Density functional contains normal densities, anomalous density (pairing) and currents:

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

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions**
- **Number of PDEs is of the order of the number of spatial lattice points**

The main advantage of TDSLDA over TDHF (+TDBCS) is related to the fact that in TDSLDA the pairing correlations are described as a true complex field which has its own modes of excitations, which include spatial variations of both amplitude and phase. Therefore in TDSLDA description the evolution of nucleon Cooper pairs is treated consistently with other one-body degrees of freedom.

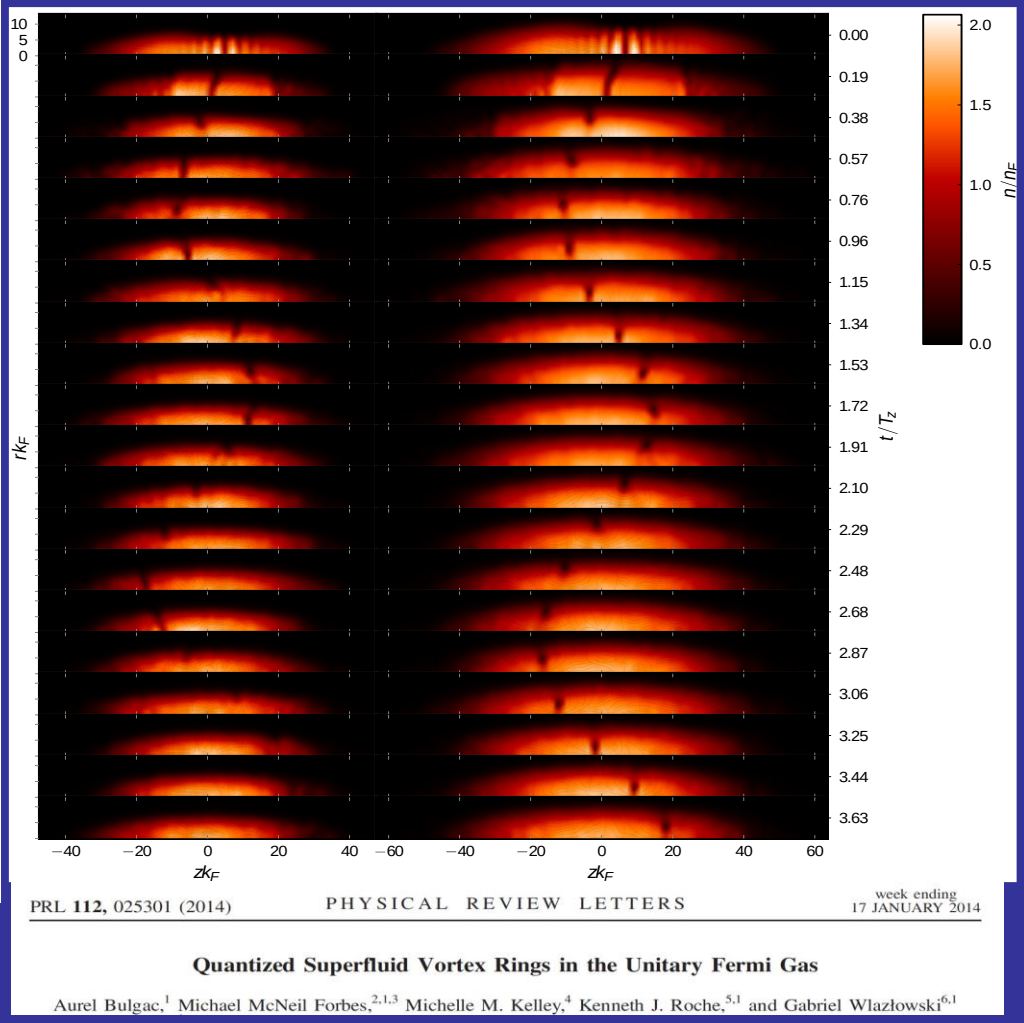
A great example on how TDSLDA help clarify a great puzzle and give a correct interpretation to an experimental result. The "heavy soliton" proved to be a vortex ring.



Heavy solitons in a fermionic superfluid

Tarik Yefsah[1], Ariel T. Sommer[1], Mark J. H. Ku[1], Lawrence W. Cheuk[1], Wenjie Ji[1], Waseem S. Bakr[1] & Martin W. Zwierlein[1]

Nature, 429, 426-430 (2013)



PRL 112, 025301 (2014) PHYSICAL REVIEW LETTERS week ending 17 JANUARY 2014

Quantized Superfluid Vortex Rings in the Unitary Fermi Gas

Aurel Bulgac,[1] Michael McNeil Forbes,[2,1,3] Michelle M. Kelley,[4] Kenneth J. Roche,[5,1] and Gabriel Wlazłowski[6,1]

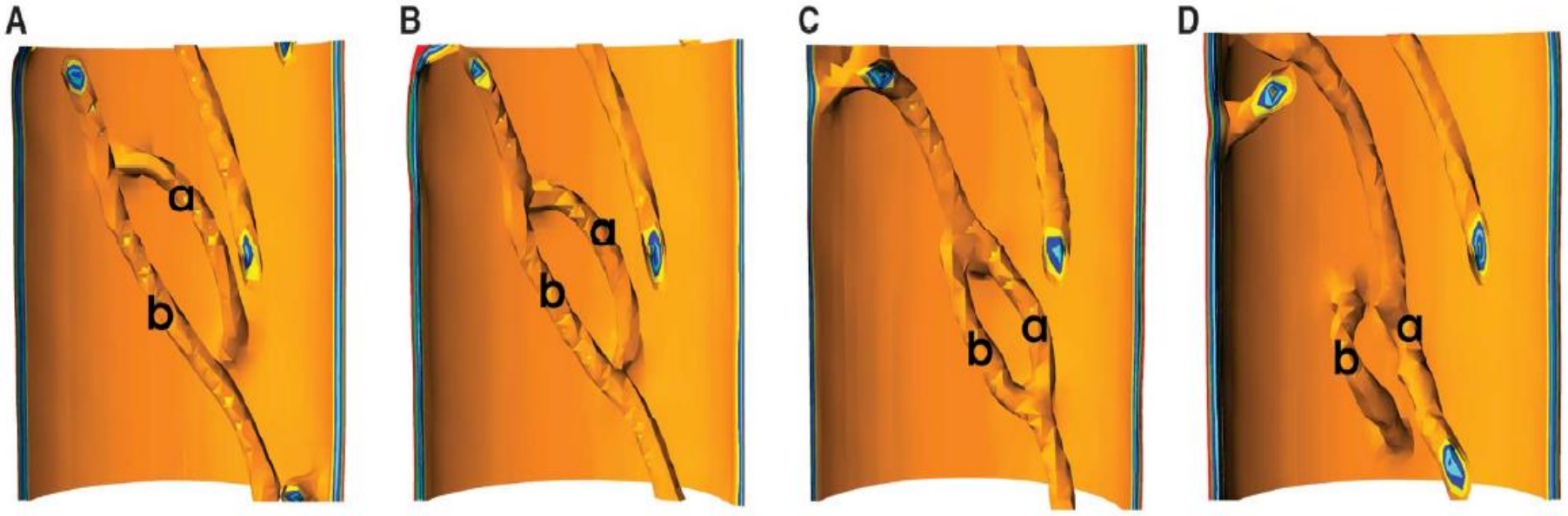
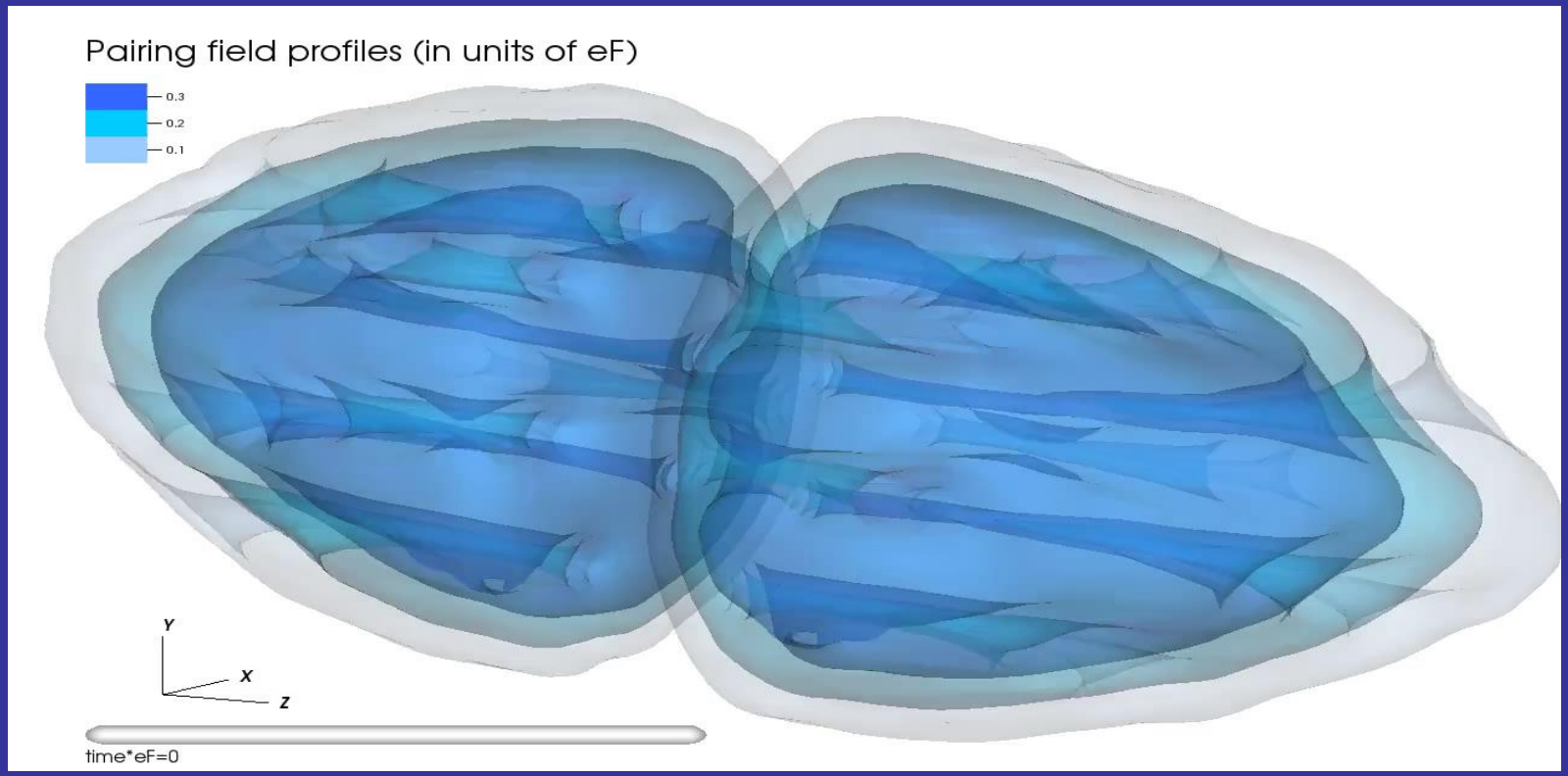


Fig. 3. (**A** to **D**) Two vortex lines approach each other, connect at two points, form a ring and exchange between them a portion of the vortex line, and subsequently separate. Segment (a), which initially belonged to the vortex line attached to the wall, is transferred to the long vortex line (b)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

TDSLDA can describe vortex reconnections as well as the energy transfer between collective and single particle degrees of freedom (which is a problem for simplified treatments based e.g. on Gross-Pitaevskii equation)

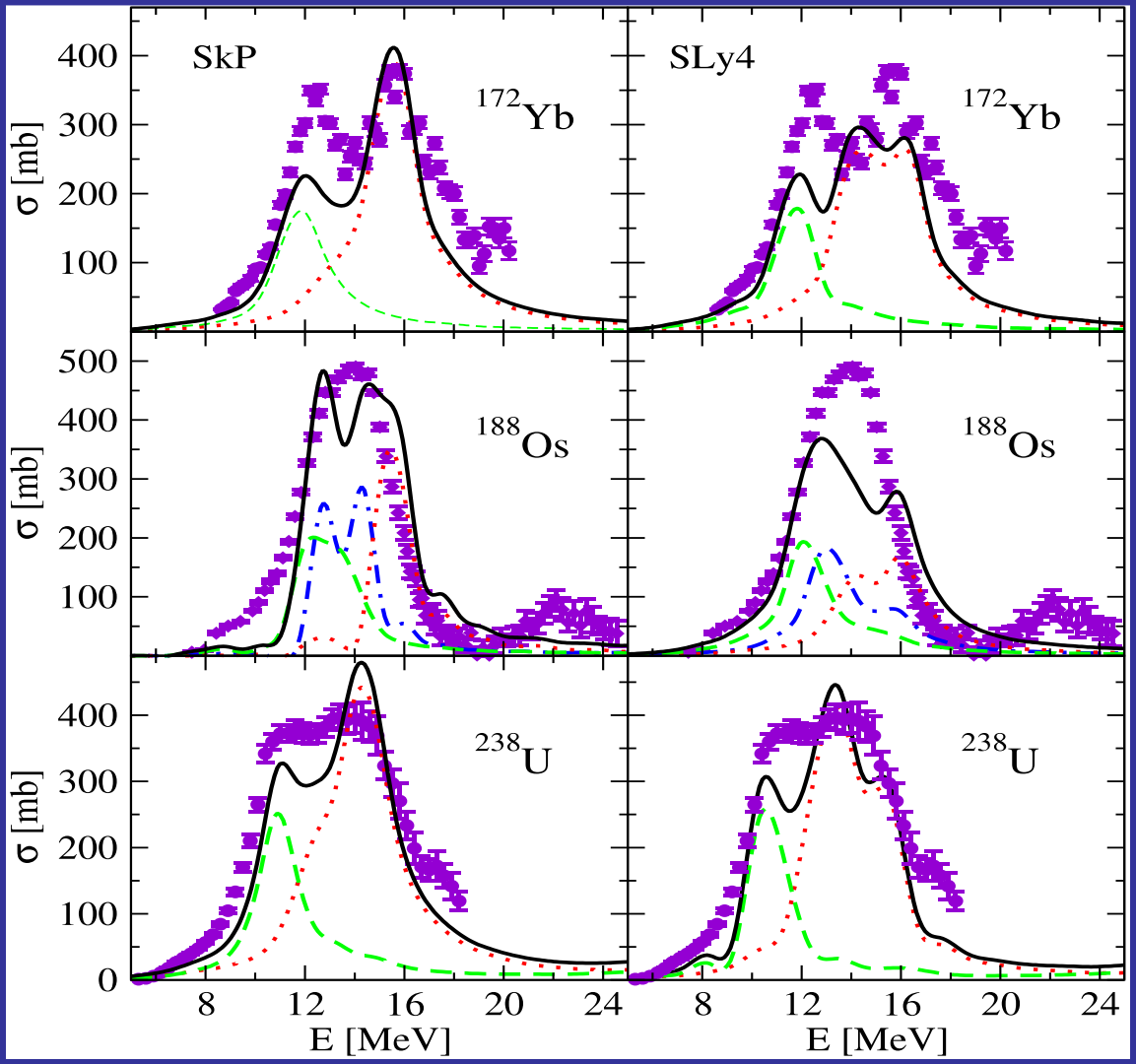
Bulgac, Luo, Magierski, Roche, Yu, *Science* 332, 1288 (2011)

The first ab initio simulation of quantum turbulence in a fermionic superfluid.



Aproximately 1270 fermions on a 48x48x128 spatial lattice, ≈ 260,000 complex PDEs, ≈ 309,000 time-steps, 2048 GPUs on Titan, 27.25 hours of wall time (initial code).

Moreover with TDSLDA we can reproduce the sequence of topological excitations observed experimentally (M.H.J. Ku et al. Phys. Rev. Lett. 113, 065301 (2014)),
see Wlazłowski, et al., Phys. Rev. A91, 031602 (2015)



Giant Dipole Resonance in deformed and superfluid nuclei.

Osmium is triaxial, and both protons and neutrons are superfluid.

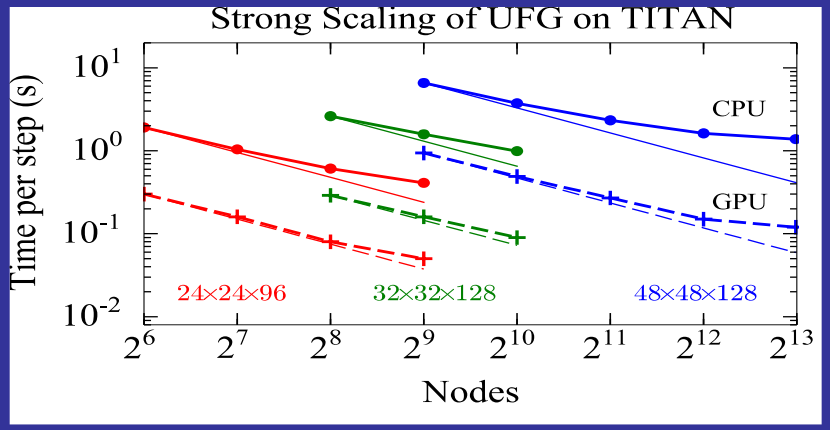
Stetcu, *et al.*, Phys. Rev. C 84, 051309(R) (2011)

Main computational tool

Cray XK7, ranked at peak ≈ 27 Petaflops (Peta – 10^{15})

On Titan there are 18,688 GPUs which provide 24.48 Petaflops !!!
and 299,008 CPUs which provide only 2.94 Petaflops.

A single GPU on Titan performs the same amount of FLOPs as approximately 134 CPUs.



$N_xN_yN_z$	N_{wf}	memory	CPU comp. + comm.	CPU comp.	GPU comp. + comm.	GPU comp.	# of GPUs	speedup
48^3	110592	10 TB	3.9s	2.4s	0.39s	0.023s	6912	10
64^3	262144	56 TB	20s	9.1s	0.80s	0.48s	16384	25

Over 1 million time-dependent 3D nonlinear complex coupled PDEs

EDF : SLy4

Pairing coupling: $g_{\text{eff}}(\vec{r}) = g\left(1-\eta\frac{\rho(\vec{r})}{\rho_0}\right)$, respects isospin symmetry, very accurate

Simulation box: 40×22.5^2 fm^3

Momentum cutoff: $p_c = \frac{\hbar\pi}{\Delta x} = 500$ fm/c, of the same order as in χ-perturbation EFT

Extremely efficient use of FFT to calculate derivatives with machine precision (10^{-15})

Adams-Bashforth-Milne O(Δt^6) time integration method

with only two evaluations of the rhs of the equations per time-step

Time-step: $= 0.119$ fm/c

Number of time steps: $\approx 120{,}000$, approximately 4 time-steps per sec.

Number of PDEs: $\approx 56{,}000$

Number of GPUs: $\approx 1{,}750$, approximately 32 PDEs per GPU

Wall time: $\approx$ 550 minutes

OLCF Titan - Cray XK7

Induced Fission of ^{240}Pu

- No need to introduce and to guess the number and character of collective variables. The number of excited shape degrees of freedom is large and it increases during the evolution. This makes treatments like GCM, based on a fix number of collective coordinates quite doubtful.

- No need to evaluate the rather ill-defined potential energy surface. *Not clear how to choose the collective coordinates, how to choose the constraints, how to choose their number, and whether to require the nucleus to be cold or not.*

- No need to determine the rather ill-defined inertia tensor. *Several prescriptions are used in literature.*

- There is no need to invoke (or not) adiabaticity, since as a matter of fact the dynamical evolution is not close to equilibrium, at either zero or at a finite temperature. The evolution is truly a non-equilibrium one.

- One-body dissipation, the window and wall dissipation mechanisms are automatically incorporated into the theoretical framework.

- No modeling (except for the energy density functional, which so far is tested in completely unrelated conditions and which has a relative accuracy of $\approx 10^{-3}$).

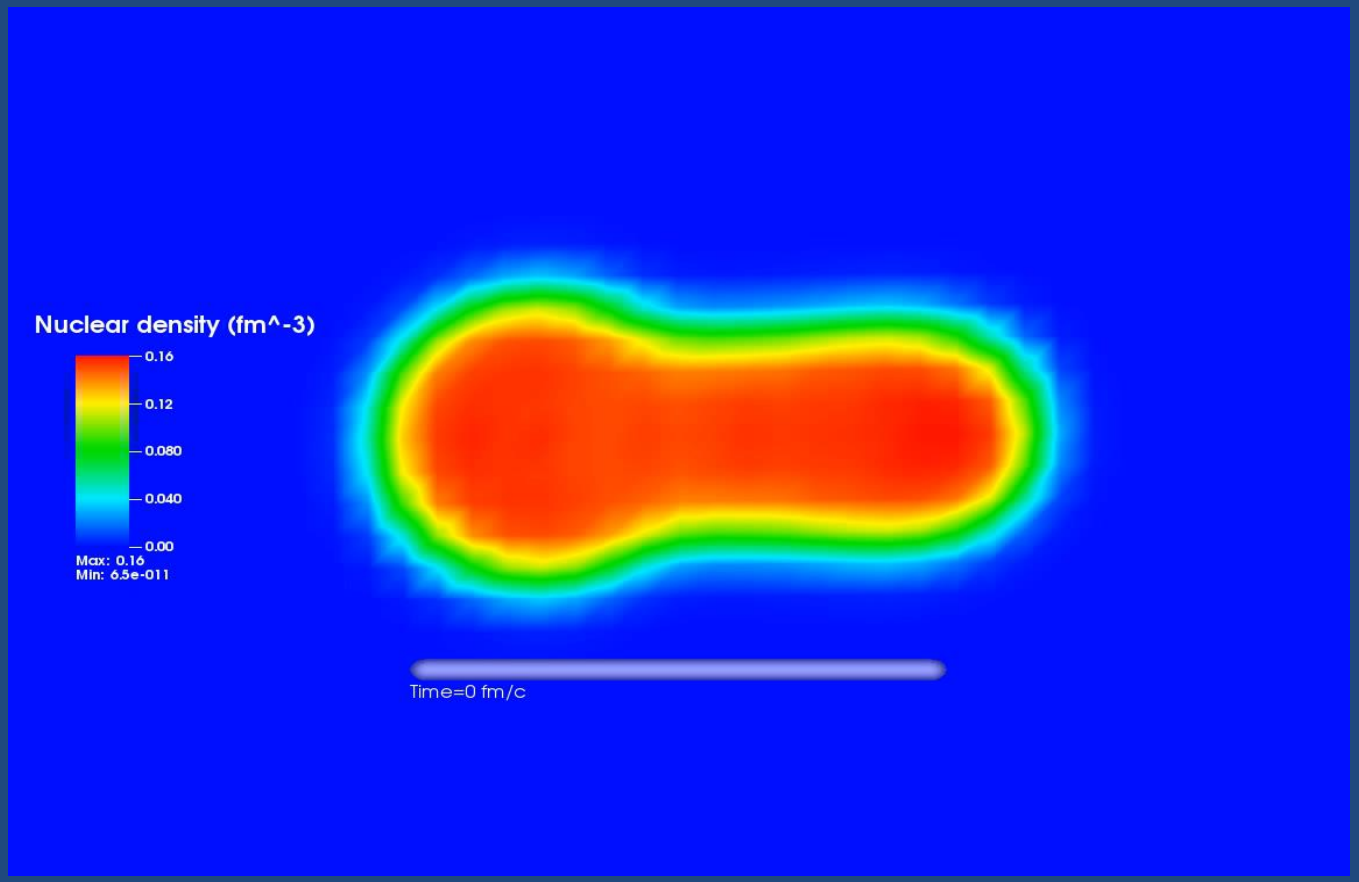
- All shapes are allowed and the nucleus chooses dynamically the path in the shape space, the forces acting on nucleons are determined by the nucleon distributions and velocities, and the nuclear system naturally and smoothly evolves into separated fission fragments.

- There is no need to introduce such unnatural quantum mechanical concepts as "rupture" and there is no worry about how to define the scission configuration.

- One can extract difficult to gain otherwise information: angular momentum distribution and excitation energies of the fission fragments, ...

Complexity of fission dynamics

Initial configuration of ^{240}Pu is prepared beyond the barrier at quadrupole deformation *Q=165b* and excitation energy *E=8.08 MeV*:

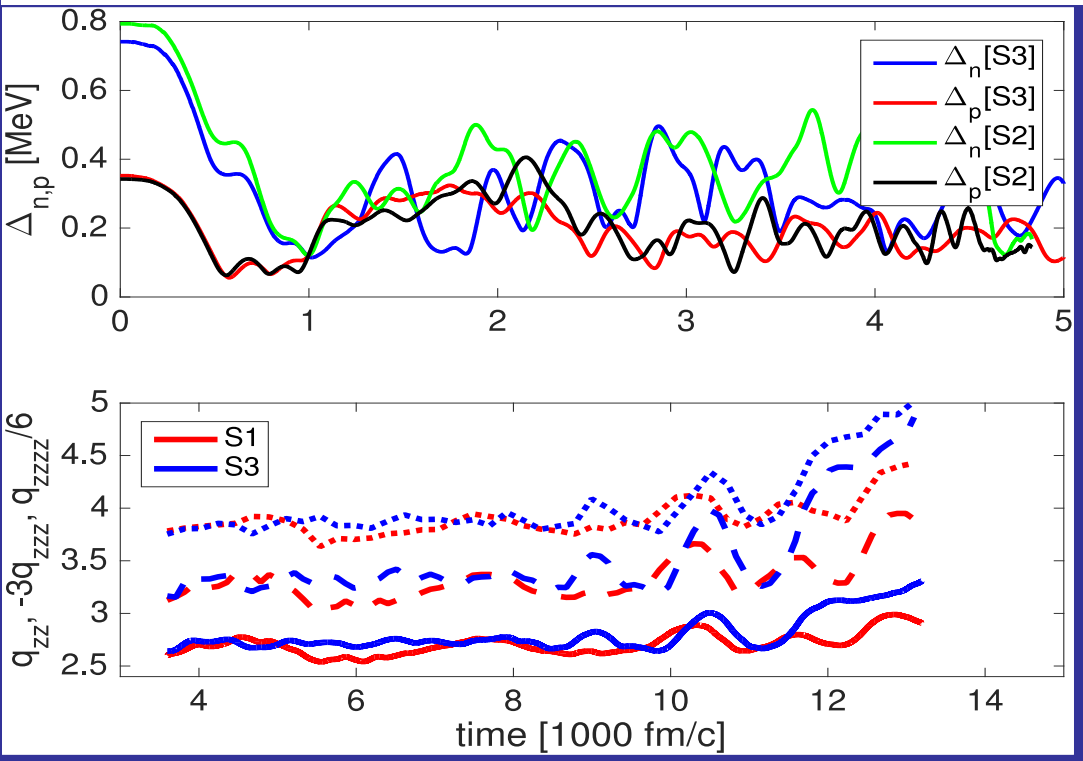


During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.
Interestingly the fragment masses seem to be relatively stiff with respect to changes of the initial conditions.

Bulgac, Magierski, Roche, and Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

TABLE I. The simulation number, the pairing parameter η, the excitation energy (E^*) of $^{240}_{94}Pu_{146}$ and of the fission fragments [$E^*_{H,L} = E_{H,L}(t_{SS}) - E_{gs}(N_{H,L}, Z_{H,L})$], the equivalent neutron incident energy (E_n), the scaled initial mass moments $q_{20}(0)$ and $q_{30}(0)$, the "saddle-to-scission" time t_{SS}, TKE evaluated as in Ref. [71], TKE, atomic (A_L^{syst}), neutron (N_L^{syst}), and proton (Z_L^{syst}) extracted from data [72] using Wahl's charge systematics [73] and the corresponding numbers obtained in simulations, and the number of postscission neutrons for the heavy and light fragments ($\nu_{H,L}$), estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8,74,75]. Units are in MeV, fm^2, fm^3, fm/c as appropriate.

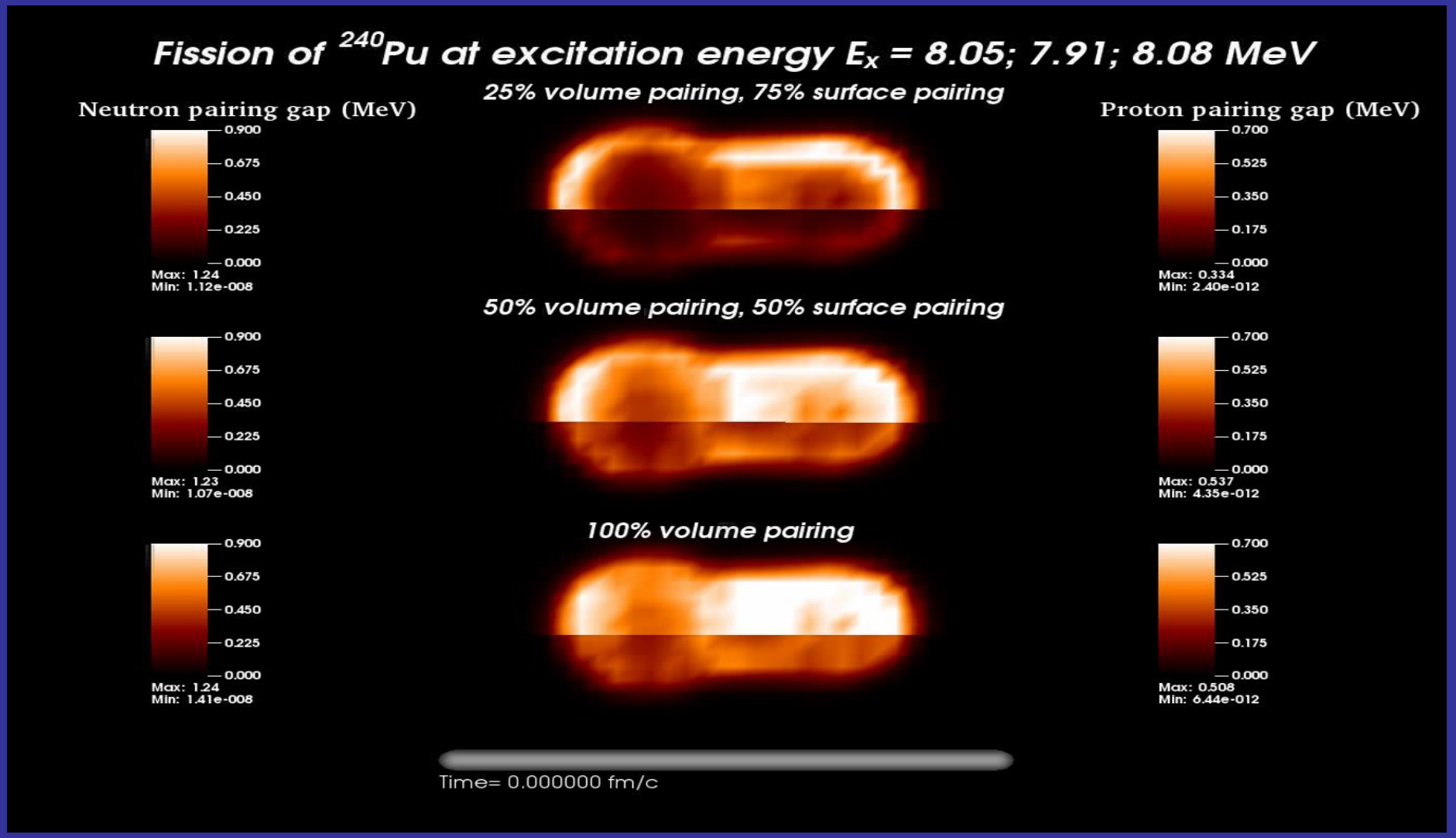
S no.	η	E^*	E_n	q_{zz}	q_{zzz}	t_{SS}	TKE^{syst}	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L	E_H^*	E_L^*	ν_H	ν_L
$S1$	0.75	8.05	1.52	1.78	−0.742	14 419	177.27	182	100.55	104.0	61.10	62.8	39.45	41.2	5.26	17.78	0	1.9
$S2$	0.5	7.91	1.38	1.78	−0.737	4360	177.32	183	100.56	106.3	60.78	64.0	39.78	42.3	9.94	11.57	1	1
$S3$	0	8.08	1.55	1.78	−0.737	14 010	177.26	180	100.55	105.5	60.69	63.6	39.81	41.9	3.35	29.73	0	2.9
$S4$	0	6.17	−0.36	2.05	−0.956	12 751	177.92	181		103.9		62.6		41.3	7.85	9.59	1	1



Evolution of the average magnitude of the pairing fields.

Hexadecapole (dashed), octupole (dotted), and quadrupole (solid) mass moments.

Bulgac, Magierski, Roche, and Stetcu, Phys. Rev. Lett. 116, 122504 (2016)



1 zs = 10^{-21} sec. = 300 fm/c

The most surprising finding was that the saddle-to-scission time was significantly longer than expected from any previous treatments.

Why?

The likeliest cause is the presence in TDSLDA of all possible collective degrees of freedom and that alone, even in the absence of dissipative effects can result in longer saddle-to-scission times.

The fluctuating pairing field might also cause this behavior.

Summary

- TDSLDA will offer insights into nuclear processes and quantities which are either not easy or impossible to obtain in the laboratory:

fission fragments excitation energies and angular momenta distributions, element formation in astrophysical environments, other nuclear reactions …

- TDSLDA offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena, and in new regions of the collective degrees of freedom.

- The quality of the agreement with experimental observations is surprisingly good, especially taking into account the fact that we made no effort to reproduce any measured data.

- TDSLDA predicts long saddle-to-scission time scales and the systems behaves superficially as a very viscous one, while at the same time the collective motion is not overdamped. There is no thermalization and the "temperatures" of the fission fragments are not equal.

- It is straightforward to implement the Balian and Vénéroni recipe to compute two-body observables: fission fragments mass, charge, angular momenta, excitation energy widths, …