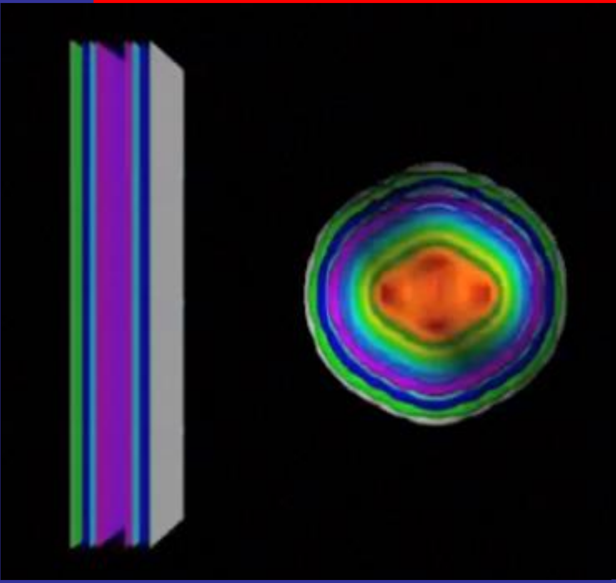
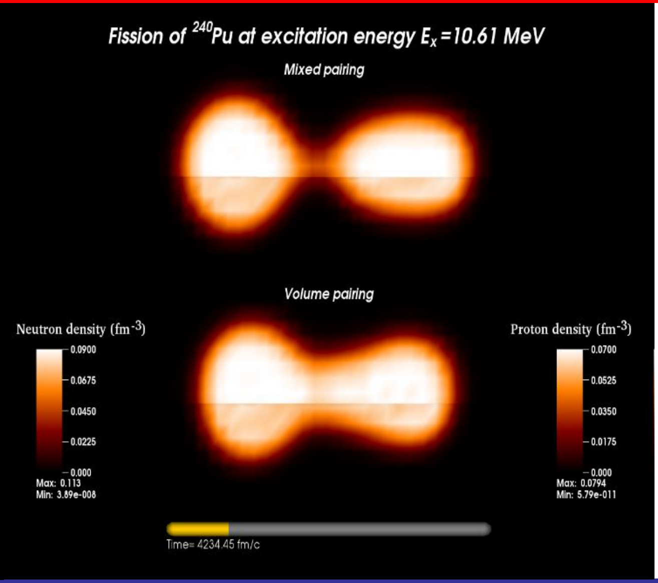
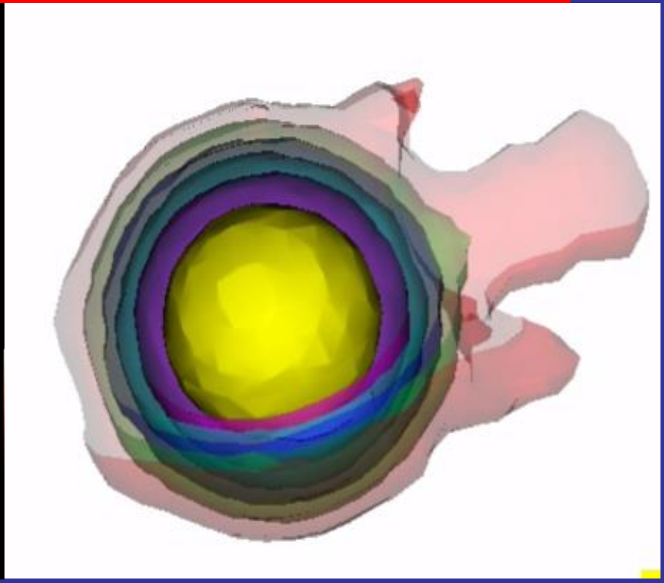
Nuclear Fission and Fusion Reactions within Superfluid TDDFT







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Applications to nuclei, neutron stars and cold atomic gases:
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GOAL:

Description of nuclear dynamics far from equilibrium within the framework of Time Dependent Density Functional Theory (TDDFT).

Why DFT?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system and in particular such phenomena as:

- **Nuclear large amplitude collective motion (induced fission)**
- **Coulomb excitation with realtivistic heavy ions**
- **Excitation of nuclei with gamma rays and neutrons**
- **Nuclear reactions, fusion between colliding heavy ions**
- **Nuclear dynamics in the neutron star crust, dynamics of vortices and their pinning mechanism.**
- **And plenty of phenomena in superfluid clouds of atomic gases: atomic clouds collisions, vortex reconnections, quantum turbulence, domain wall solitons , etc.**

Runge Gross mapping

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

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

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

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.

However as always there is a price to pay:

- **Kohn-Sham potential in principle depends on the past (memory). Very little is known about the memory term and usually it is disregarded (adiabatic TDDFT).**
- **Only one body observables can be reliably evaluated within standard DFT.**

Formalism for Time Dependent Phenomena: TDSLDA

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:

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

- **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**

Current capabilities of the code:

- **volumes of the order of (L = 80^3) capable of simulating time evolution of 42000 neutrons at saturation density (possible application: neutron stars)**
- **capable of simulating up to times of the order of 10^{-19} s (a few million time steps)**
- **CPU vs GPU on Titan ≈ 15 speed-up (likely an additional factor of 4 possible)**

Eg. for 137062 two component wave functions:

CPU version (4096 nodes x 16 PEs) - 27.90 sec for 10 time steps

GPU version (4096 PEs + 4096GPU) - 1.84 sec for 10 time step

Single particle potential (Skyrme):

$$h(\mathbf{r}) = -\vec{\nabla}\cdot\Big(B(\mathbf{r}) + \vec{\sigma}\cdot\vec{C}(\mathbf{r})\Big)\vec{\nabla} + U(\mathbf{r}) + \frac{1}{2i}\Big[\vec{W}(\mathbf{r})\cdot(\vec{\nabla}\times\vec{\sigma}) + \vec{\nabla}\cdot(\vec{\sigma}\times\vec{W}(\mathbf{r}))\Big]$$
$$+\vec{U}_\sigma(\mathbf{r})\cdot\vec{\sigma} + \frac{1}{i}\Big(\vec{\nabla}\cdot\vec{U}_\Delta(\mathbf{r}) + \vec{U}_\Delta(\mathbf{r})\cdot\vec{\nabla}\Big)$$

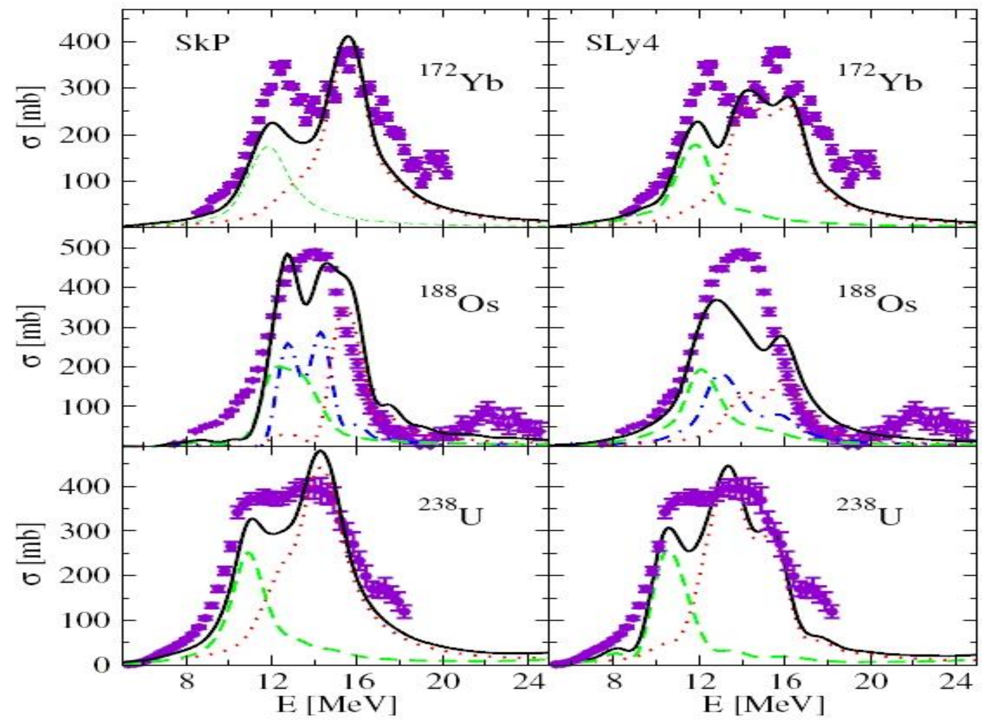
where

$$\begin{aligned}
B(\mathbf{r}) &= \frac{\hbar^2}{2m} + C^\tau\rho \\
\vec{C}(\mathbf{r}) &= C^{sT}\vec{s} \\
U(\mathbf{r}) &= 2C^\rho\rho + 2C^{\Delta\rho}\nabla^2\rho + C^\tau\tau + C^{\nabla J}\vec{\nabla}\cdot\vec{J} + C^\gamma(\gamma+2)\rho^{\gamma+1} \\
\vec{W}(\mathbf{r}) &= -C^{\nabla J}\vec{\nabla}\rho \\
\vec{U}_\sigma(\mathbf{r}) &= 2C^s\vec{s} + 2C^{\Delta s}\nabla^2\vec{s} + C^{sT}\vec{T} + C^{\nabla J}\vec{\nabla}\times\vec{j} \\
\vec{U}_\Delta(\mathbf{r}) &= C^j\vec{j} + \frac{1}{2}C^{\nabla j}\vec{\nabla}\times\vec{s}
\end{aligned}$$

and pairing potential:

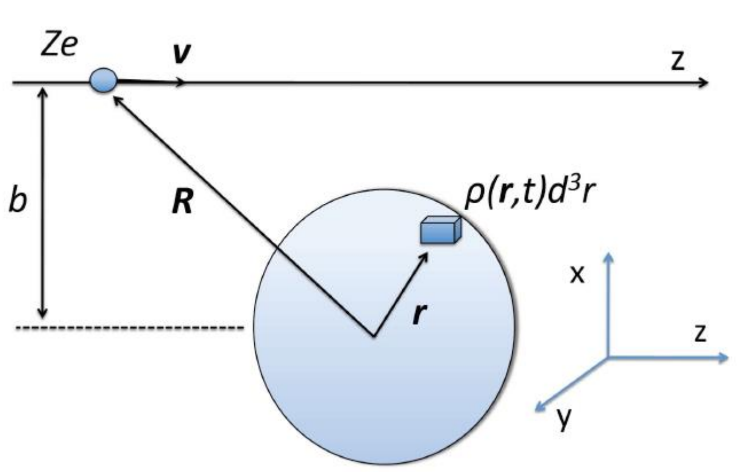
$$\Delta(\mathbf{r},t) = -g_{eff}(\mathbf{r})\chi(\mathbf{r},t)$$

Linear response regime:
GDR of deformed nuclei



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

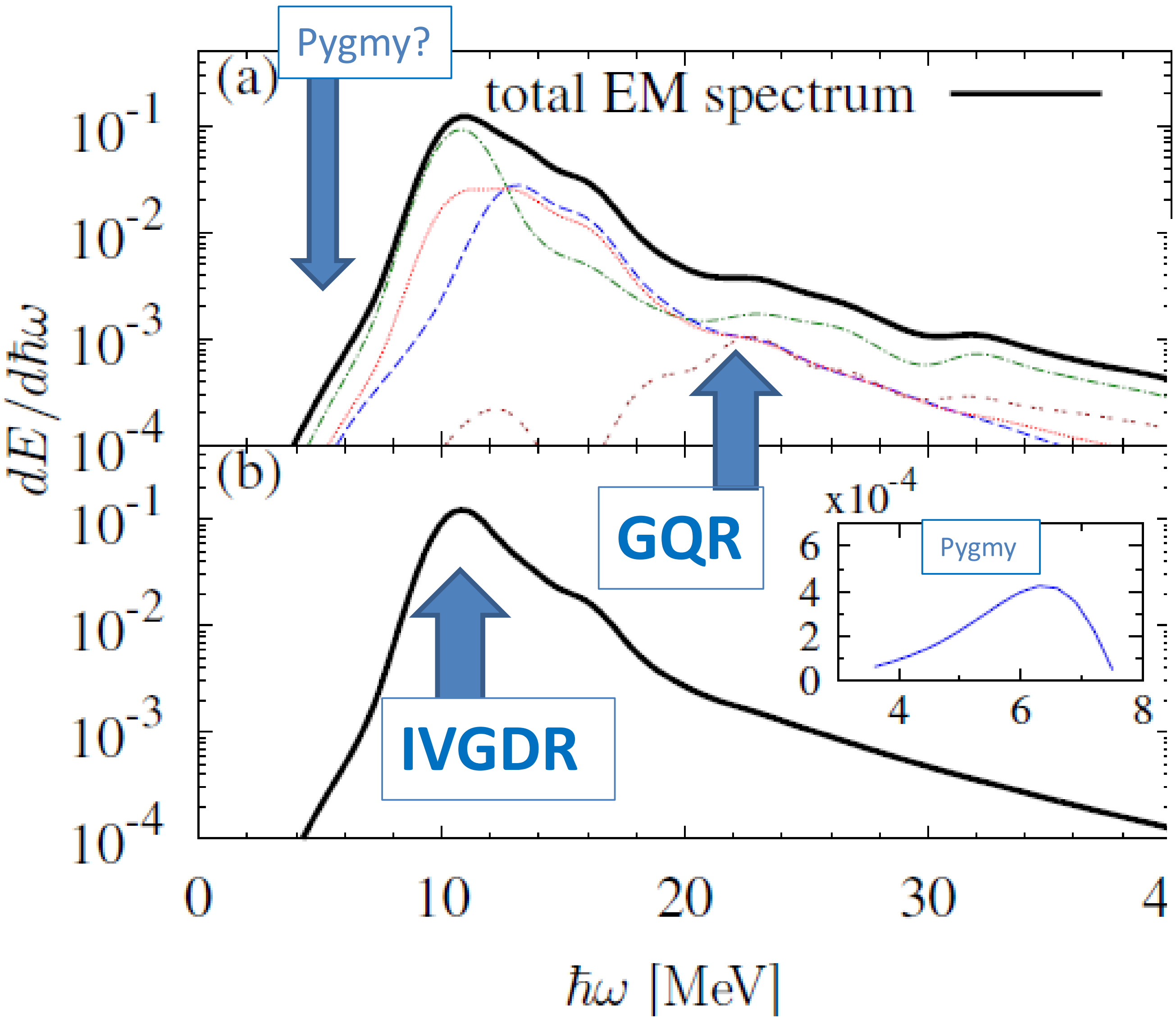
Beyond linear regime:
Relativistic Coulomb excitation

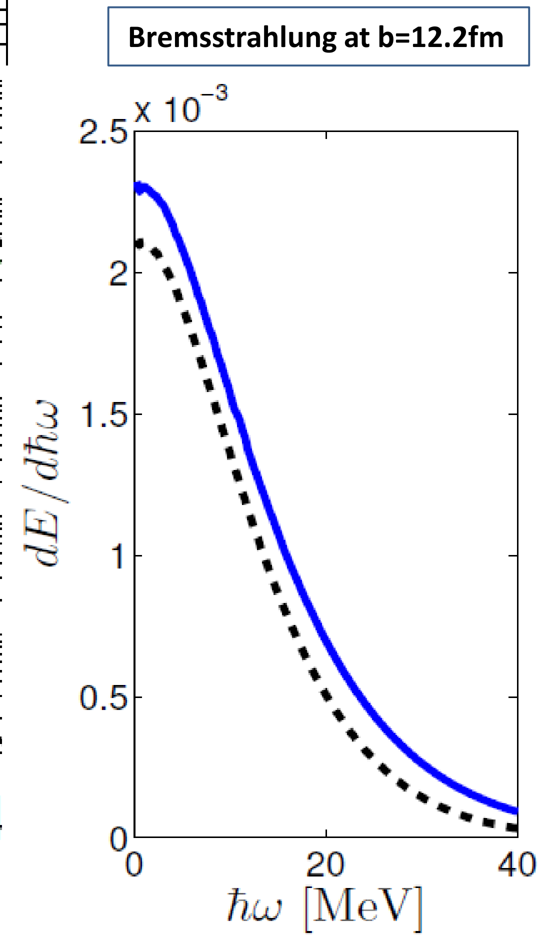


$$\hbar\omega \approx \hbar/\tau_{coll} = \frac{\gamma v}{b} \approx 12 MeV \quad ; \quad \gamma = \frac{1}{\sqrt{1-\left(v/c\right)^2}}$$

I. Stetcu, C. Bertulani, A. Bulgac, P. Magierski, K.J. Roche Phys. Rev. Lett. 114, 012701 (2015)

Electromagnetic radiation due to the internal nuclear motion

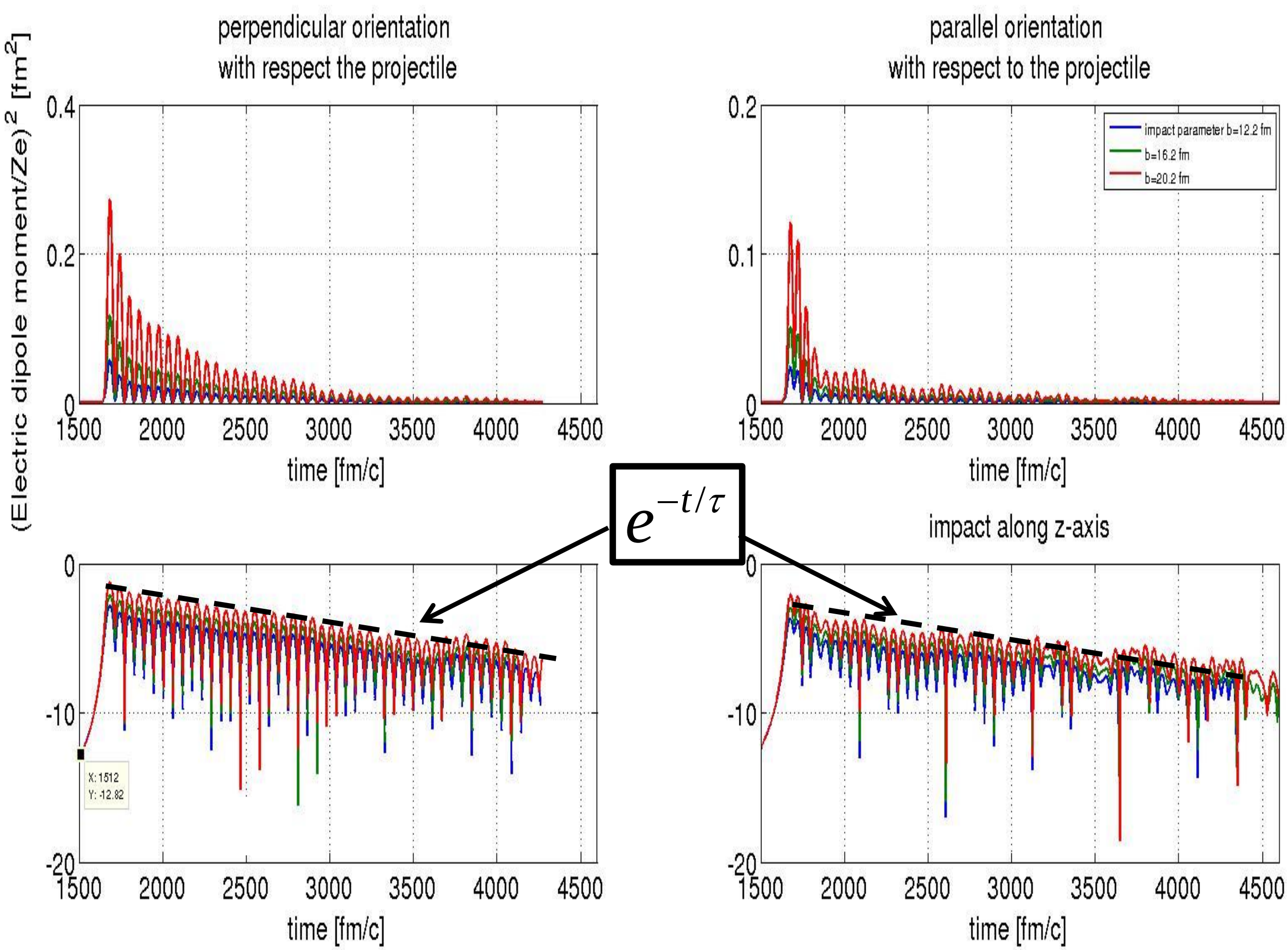




I. Stetcu, C. Bertulani, A. Bulgac, P. Magierski, K.J. Roche
Phys. Rev. Lett. 114, 012701 (2015)

One body dissipation can be fully accounted for in this formalism

Damping of GDR (excited ion coulex reaction) due to one-body dissipation mechanism:



$$E_{coll}(t) \propto e^{-t/\tau}; \quad \tau \approx 500\ fm/c \Rightarrow \Gamma_{\downarrow} \approx 0.4MeV$$

$$E_{coll}(t) \propto \left[D_{\max}(t)\right]^2$$

Description of the fission process within TDSLDA

Time scale for nuclear processes that can be described within TDSLDA: 10^(-19) sec.

EDF : SLy4

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

Simulation box: $40 \times 27.5^2 \ \text{fm}^3$

Momentum cutoff: $p_c = \frac{\hbar\pi}{\Delta x} = 500 \ \text{fm/c}$

Time-step: 0.119 fm/c

Number of time steps: $\approx 120{,}000$

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

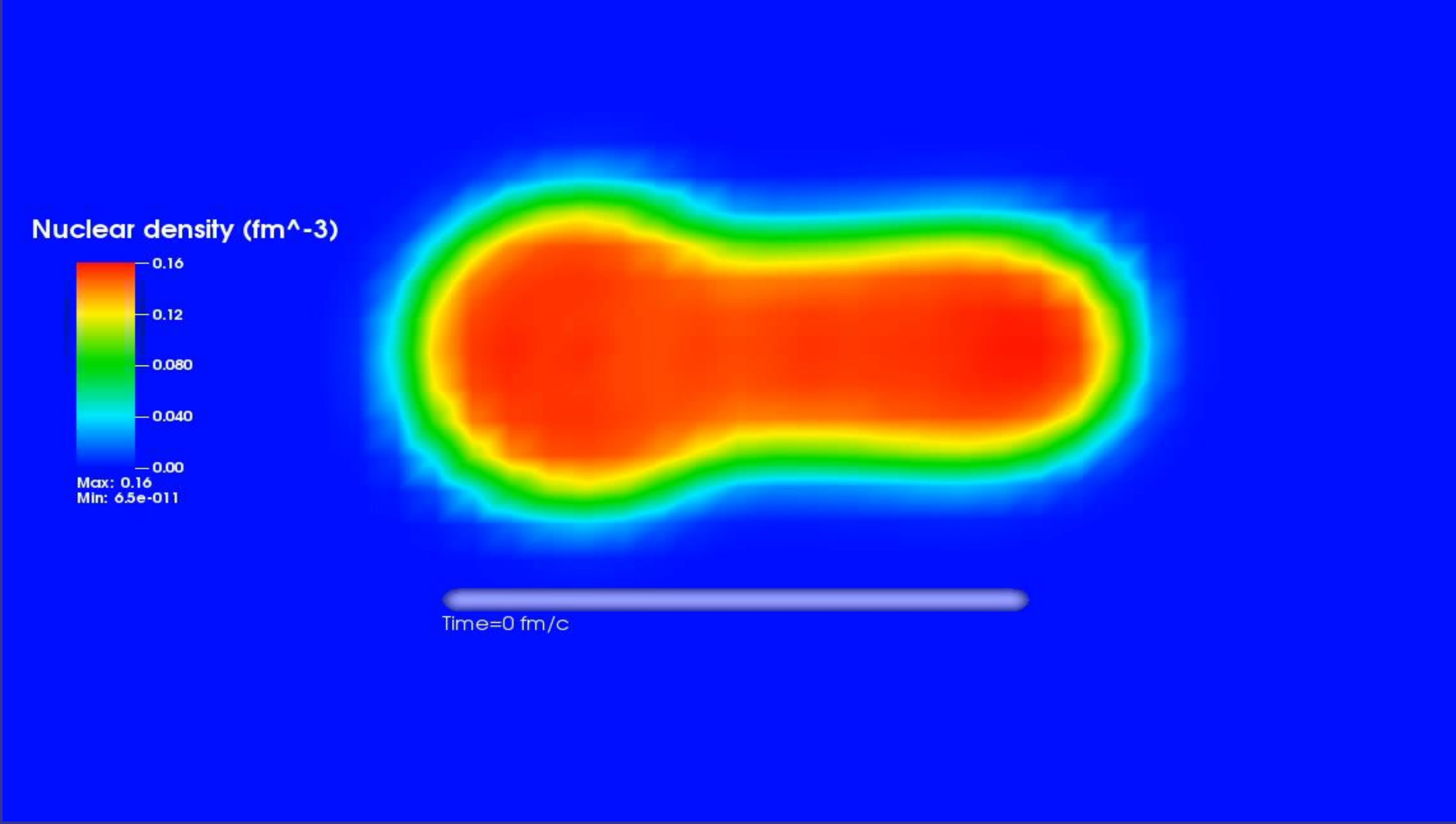
Number of GPUs: ≈ 1750

Wall time: $\approx$ 550 minutes

OLCF Titan - Cray XK7

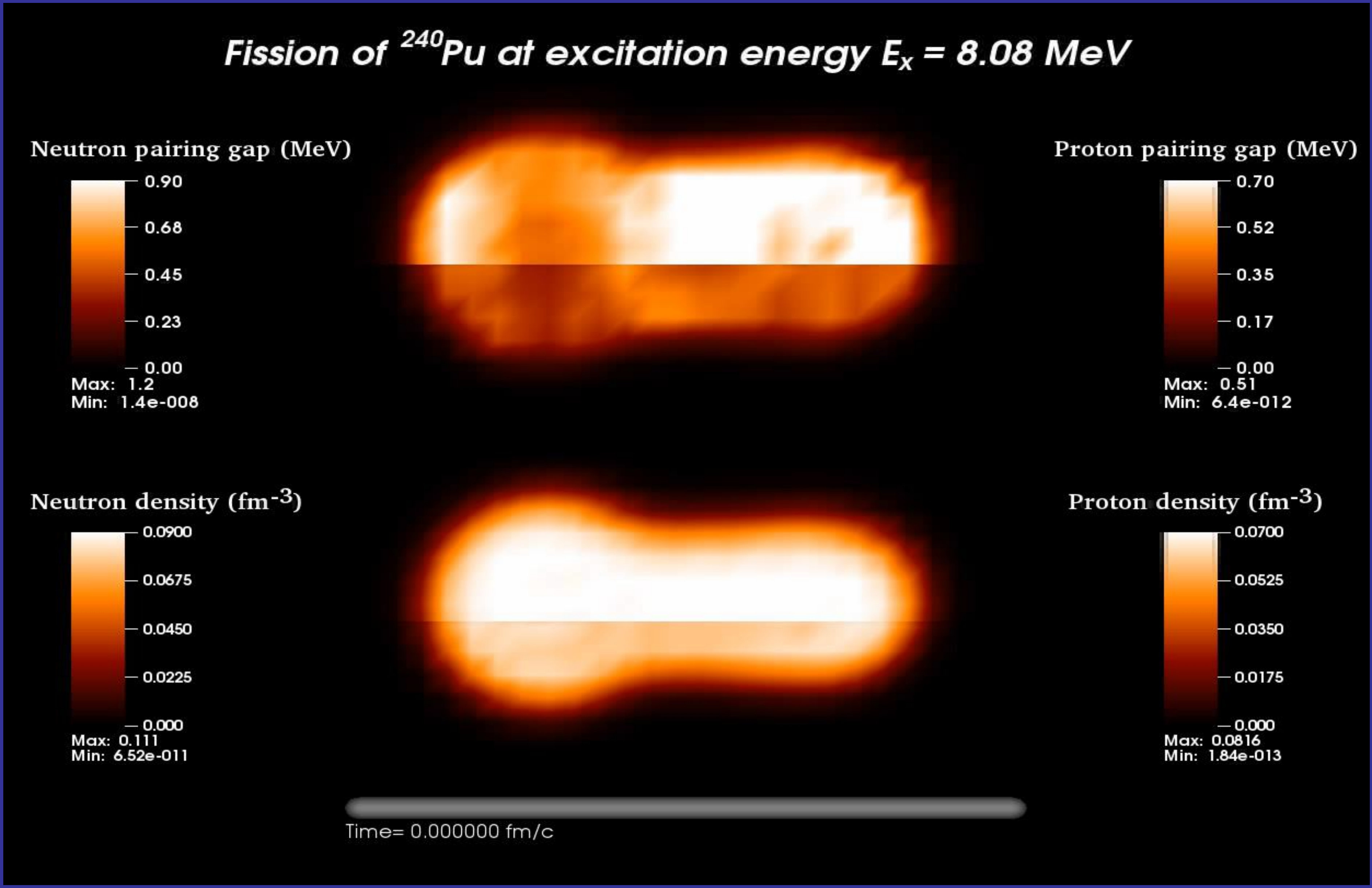
Complexity of fission dynamics

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

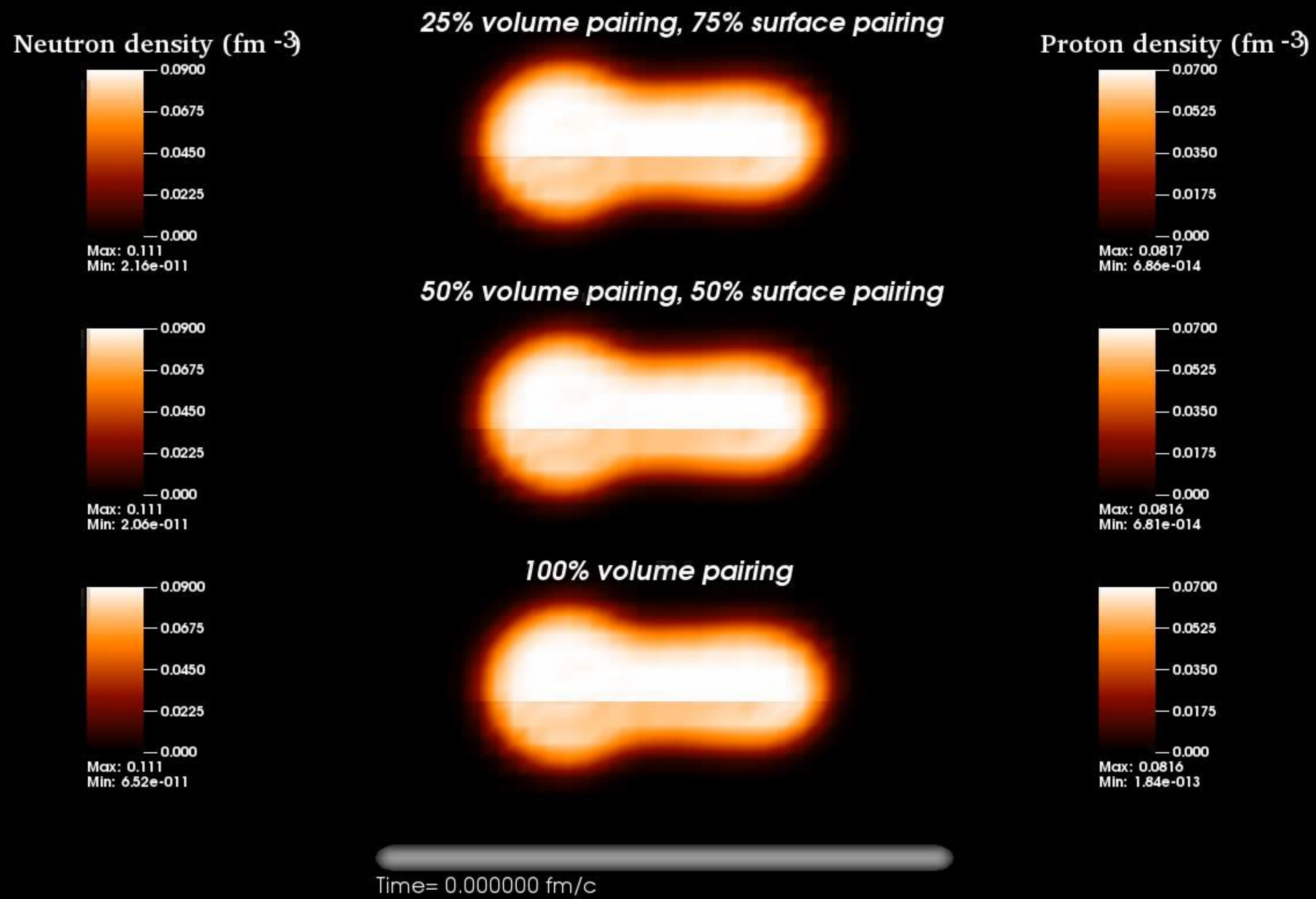


During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.

Pairing dynamics



Fission of ^{240}Pu at excitation energy E_x = 8.05; 7.91; 8.08 MeV



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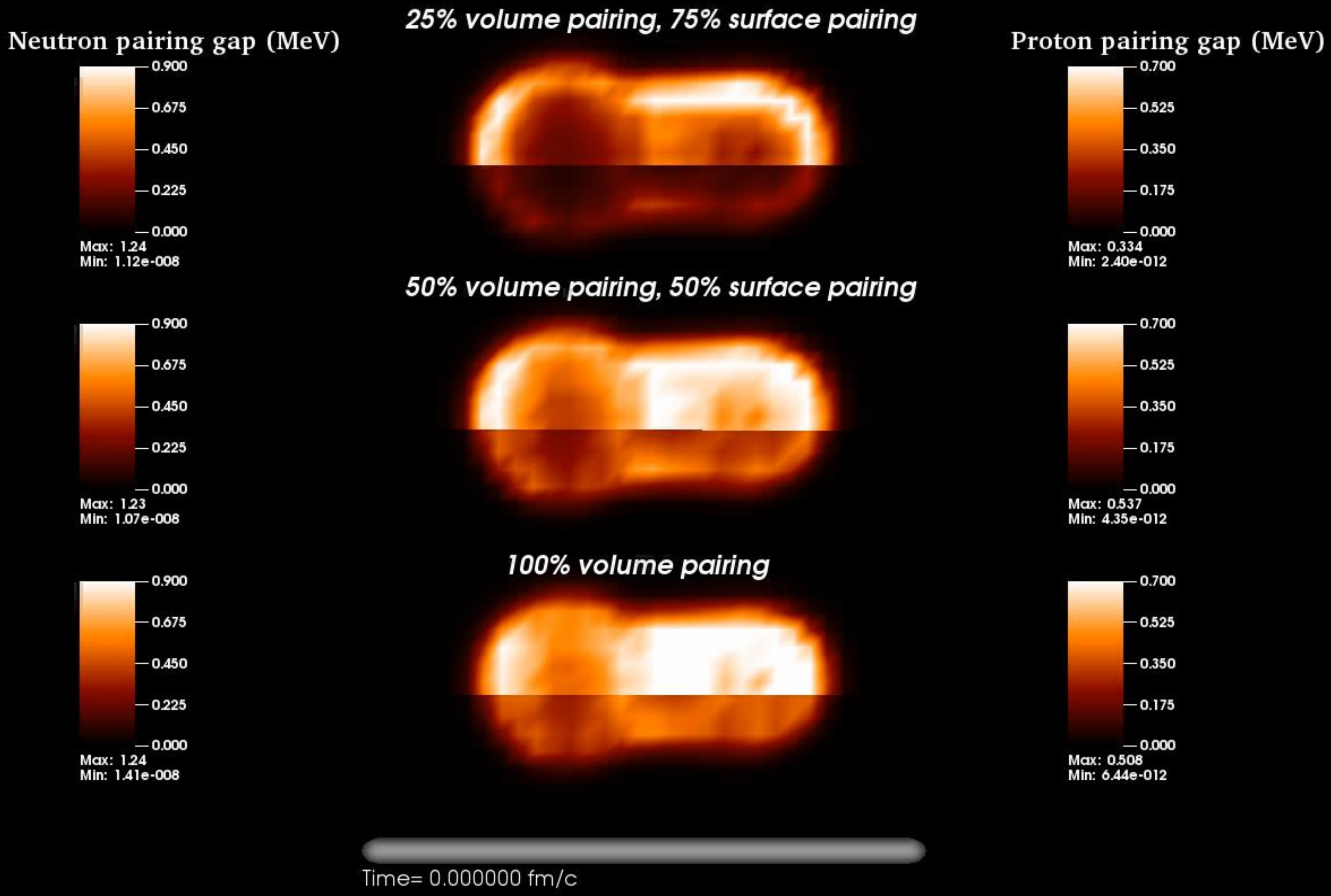

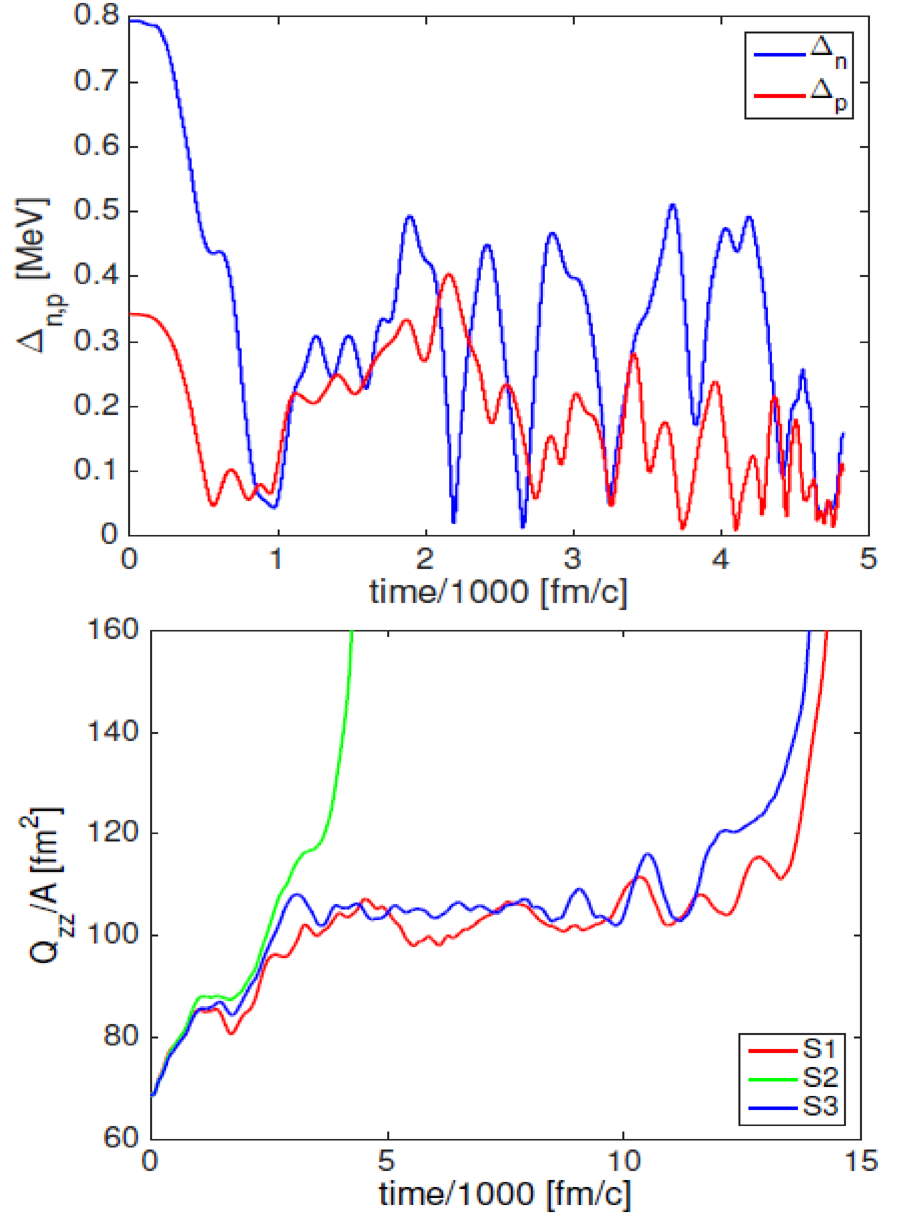

FIG. 2: (Color online) The averaged pairing gaps for neutrons and protons for the case S1 and the $Q_{zz} = 2z^2 - x^2 - y^2$ as a function of time for the cases S1-3, see Table I.

Average pairing gap evolution.

Responsible for the pair excitations:
(m, -m) → (m', -m')
during the evolution

Quadrupole moment along the fission axis.

Note that the oscillations of the Q. moment during the evolution are due to the coupling between collective and intrinsic motions during the fission process.

TABLE I: The simulation number, the pairing parameter η, see Eq. (1), the excitation energy (E^*) of the mother $^{240}_{94}Pu_{136}$ and of the daughter nuclei ($E^*_{H,L}$), the equivalent neutron incident energy (E_n), the starting initial quadrupole moment, the "saddle-to-scission" time, the total kinetic energy (TKE), atomic ($A_{H,L}$), neutron ($N_{H,L}$) and proton ($Z_{H,L}$) numbers of the heavy and light fragments, and the number of neutrons (ν), estimated using a Hauser-Feshbach approach and experimental neutron separation energies [8, 68, 69]. Units are MeV, fm^2 and fm/c where appropriate.

S#	η	E^*	E_n	Q_{zz}	S-S time	TKE	A_H	A_L	N_H	N_L	Z_H	Z_L	E^*_H	E^*_L	ν_H	ν_L
S1	0.75	8.05	1.52	16,500	14,419	182	136.0	104.0	83.2	62.8	52.8	41.2	5.26	17.78	0	1.9
S2	0.5	7.91	1.38	16,500	4,360	183	133.7	106.3	82.0	64.0	51.7	42.3	9.94	11.57	1	1
S3	0	8.08	1.55	16,500	14,010	180	134.5	105.5	82.4	63.6	52.1	41.9	3.35	29.73	0	2.9
S4	0	6.17	-0.36	19,000	12,751	181	136.1	103.9	83.4	62.6	52.7	41.3	7.85	9.59	1	1

$$\text{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

estimated TKEs slightly overestimate the observed values by no more than 3 - 6 MeV.

This is indicative of the fact that in our simulations the system scissions a bit too early.

The evaluated average number of emitted neutrons in this case is close to 3, which is higher than the values we estimate.

Summary

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

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

- *TDSLDA predicts much longer time-scales for fission, even though it takes into account one-body dissipation only (both window and wall mechanisms are present). The nuclear system superficially behaves like an extremely viscous system, but the collective motion at the same time is not overdamped.*

- *Approaches based on an adiabatic approximation seem to be not correct, at least for the description of dynamics beyond the saddle point.*

- *Extension of the present approach to obtain information about two-body observables, such as fission fragment mass, charge, angular momenta, and excitation energies distributions are rather straightforward to implement.*

Collaborators:

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Related studies concerning superfluid dynamics of fermionic systems:

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Janina Grineviciute

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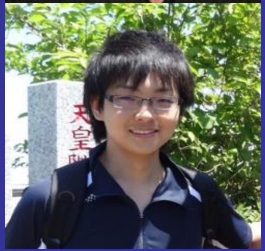

Kazuyuki Sekizawa