Induced fission of ^{240}Pu within a real-time microscopic approach

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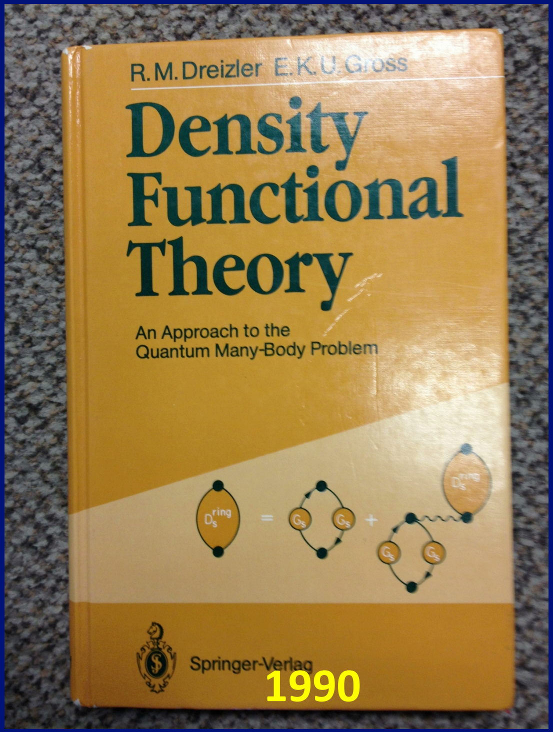
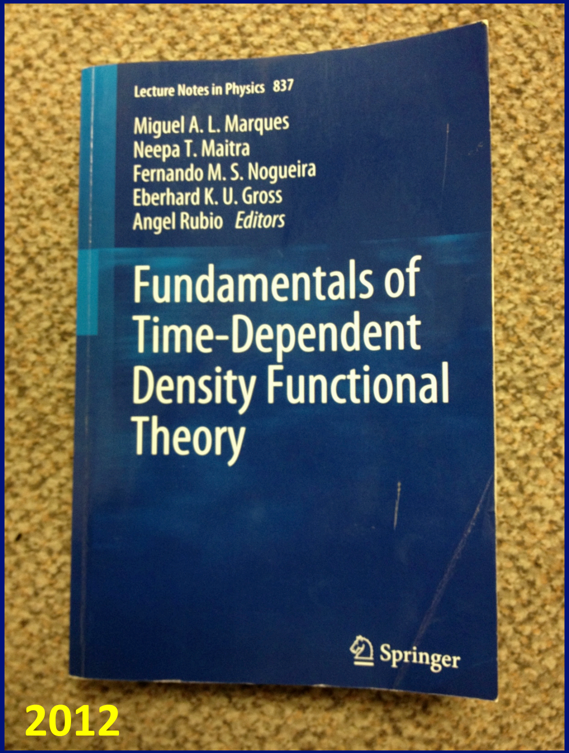
Slides (pptx) with movies will be available for download from
http://www.faculty.washington.edu/bulgac/Pu240/

Main Theoretical Tool





DFT has been developed and used mainly to describe normal (non-superfluid) electron systems – <u>50 years old theory</u>: Kohn and Hohenberg, 1964 and Kohn and Sham, 1965

THEOREM: There exist an universal density functional of particle density.

A new local extension of DFT to superfluid systems and time-dependent phenomena was developed:
Review: A. Bulgac, *Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids*, Ann. Rev. Nucl. Part. Sci. 63, 97 (2013)

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

Time-Dependent Superfluid Local Density Approximation (TDSLDA)

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

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

For time-dependent phenomena one has to add currents.
Galilean invariance determines the dependence on currents.

The ingredients of the SLDA for nuclei

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

$$E_{gs} = \int d^3r \left\{ \varepsilon_N[\rho_n(\vec{r}), \rho_p(\vec{r})] + \varepsilon_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] \right\}$$

$$\begin{cases} \varepsilon_N[\rho_n(\vec{r}), \rho_p(\vec{r})] = \varepsilon_N[\rho_p(\vec{r}), \rho_n(\vec{r})] \\ \varepsilon_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \varepsilon_S[\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})] \end{cases}$$

Isospin symmetry constraints
(Coulomb energy and other relatively small terms not shown here.)

$$\varepsilon_S\left[\rho_n, \rho_p, \nu_p, \nu_n\right] = g(\rho_p, \rho_n)[|\nu_p|^2 + |\nu_n|^2] + f(\rho_p, \rho_n)[|\nu_p|^2 - |\nu_n|^2] \; \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

where $g(\rho_p, \rho_n) = g(\rho_n, \rho_p)$

and $f(\rho_p, \rho_n) = f(\rho_n, \rho_p)$

TDSLDA equations

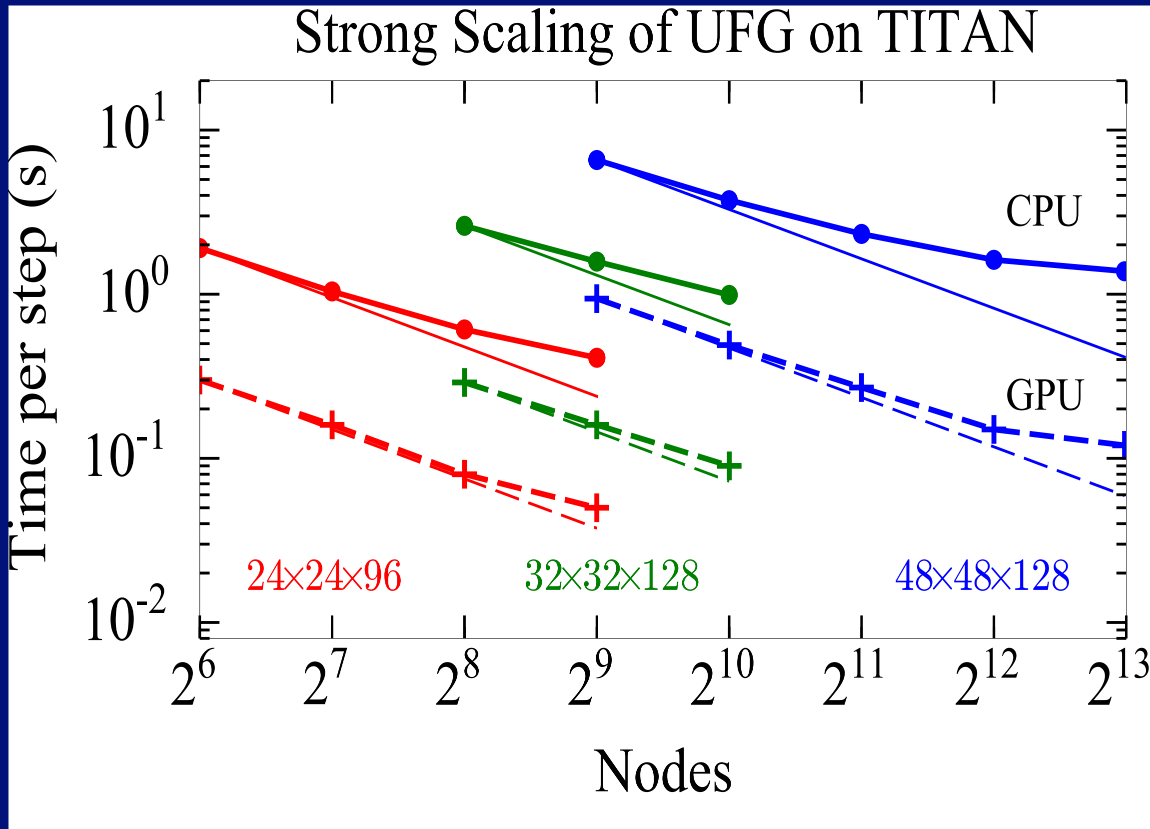
$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t)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

- **The system is placed on a large 3D spatial lattice (adequate representation of continuum)**
- **Derivatives are computed with FFTW (this insures machine accuracy) and is very fast**
- **Fully self-consistent treatment with fundamental symmetries respected (isospin, gauge, Galilean, rotation, translation, parity)**
- **Adams-Bashforth-Milne fifth order predictor-corrector-modifier integrator**
  Effectively a sixth order method
- **No symmetry restrictions**
- ***Number of PDEs is of the order of the number of spatial lattice points – from 10,000s to 1-2,000,000***

$$\propto 4\left(\frac{2p_cL}{2\pi\hbar}\right)^3 = 4N_xN_yN_z$$

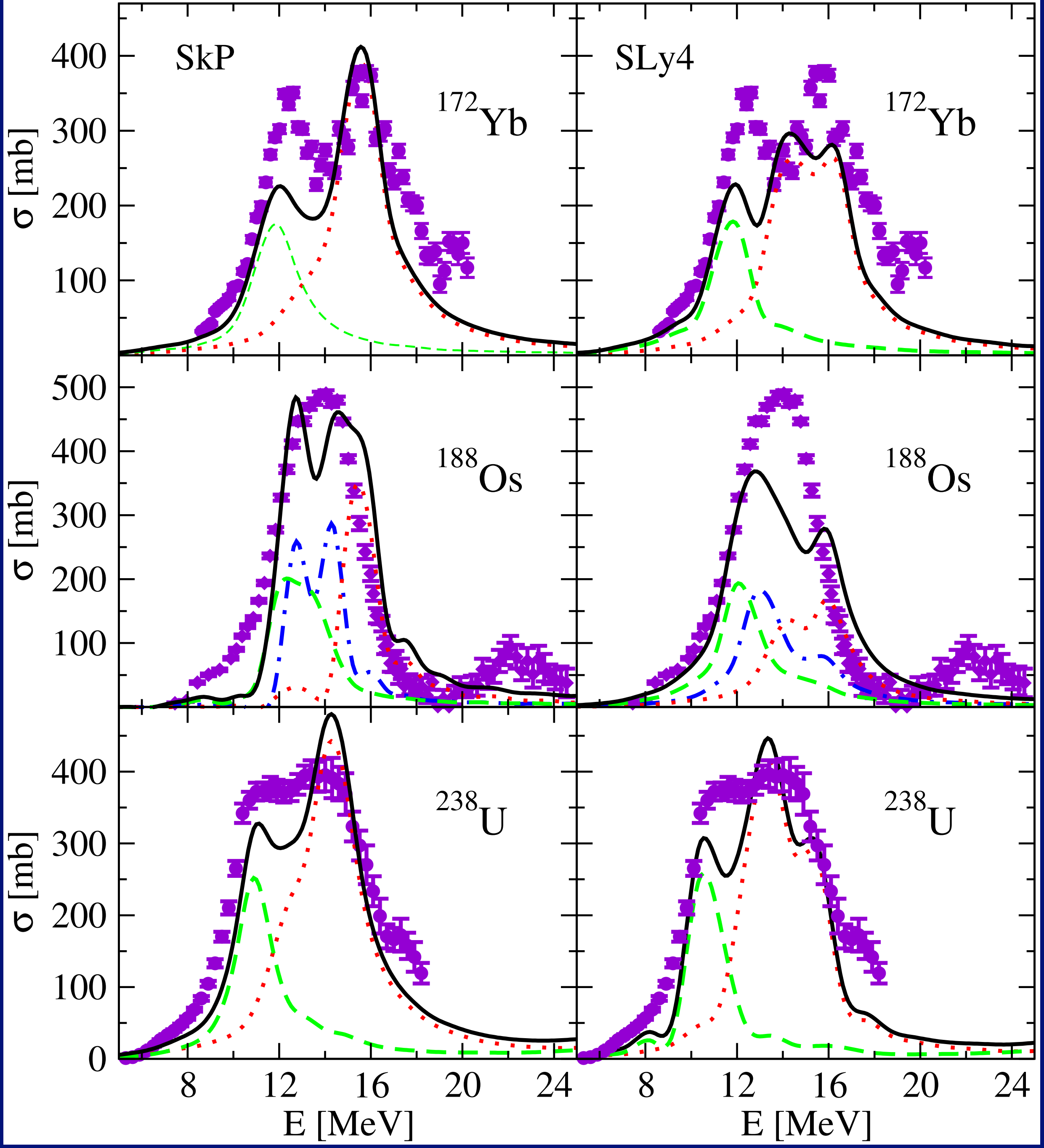
- **SLDA/TDSLDA (DFT) is formally by construction like meanfield HFB/BdG**
- **The code was implemented on Jaguar, Titan, Franklin, Hopper, Edison, Hyak, Athena**
- **Initially Fortran 90, 95, 2003 …, presently C, CUDA, and obviously MPI, threads, etc.**
- **For more details abou the method see INT talk on October 7, 2013:**

http://faculty.washington.edu/bulgac/talks.html#most_recent (pdf and pptx version with movies)



$N_xN_yN_z$	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

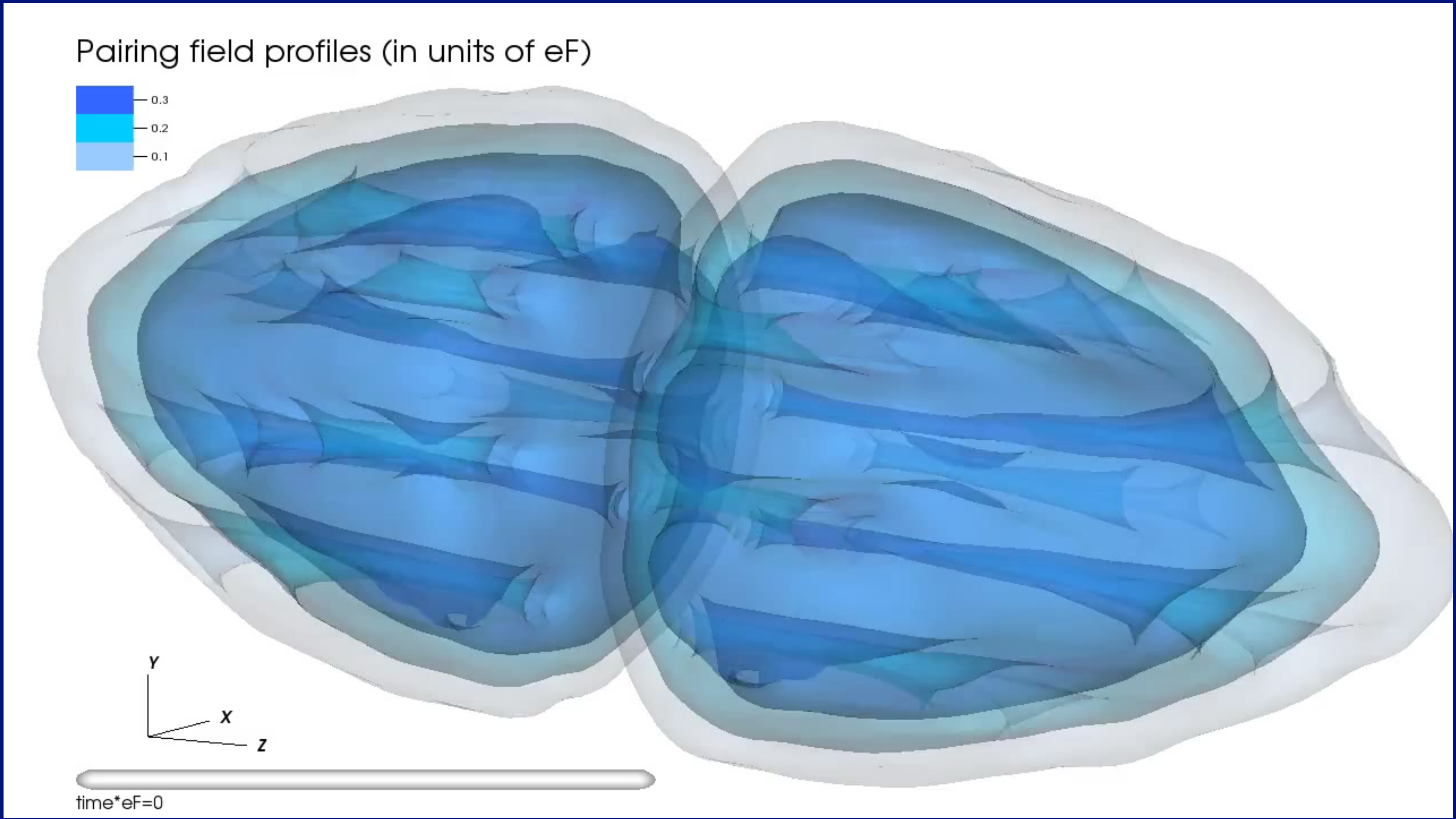
Over 1 million time-dependent 3D nonlinear complex coupled PDEs



Giant Dipole Resonance deformed and superfluid nuclei

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

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



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)

Wlazłowski et al, Phys. Rev. Lett. 112, 025301 (2014), Phys. Rev. A 91, 031602(R) (2015)

EDF : SLy4

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

Simulation box: $40 \times 22.5^2\ \text{fm}^3$

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

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

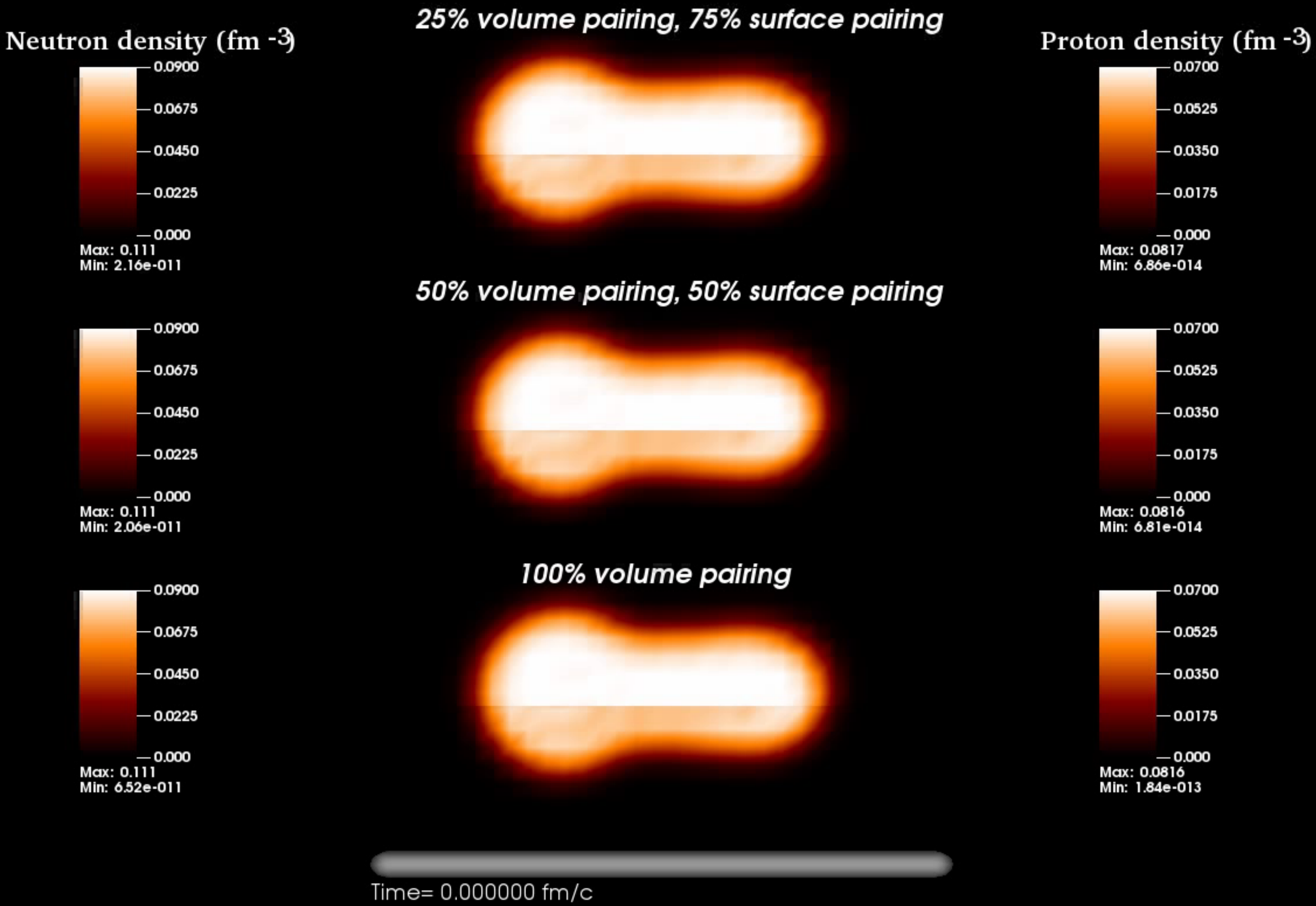
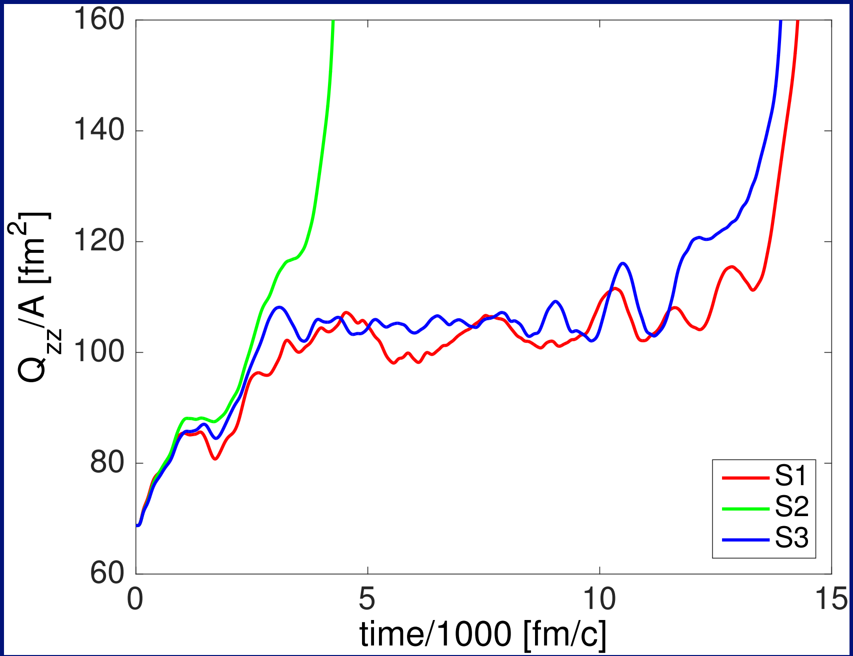


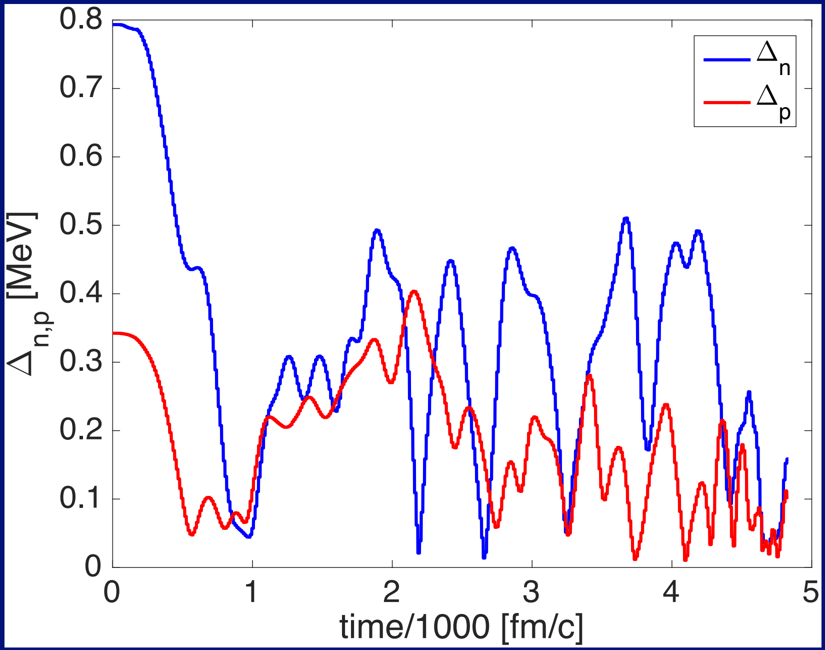
TABLE I: The simulation number, the pairing parameter η, see Eq. (1), the excitation energy (E^*) of the mother ${}^{240}_{94}\mathrm{Pu}_{136}$ and of the daughter nuclei ($E^*_{H,L}$), the equivalent neutron incident energy (E_n), the starting initial quadrupole moment, the "saddle-to-scission" time, 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

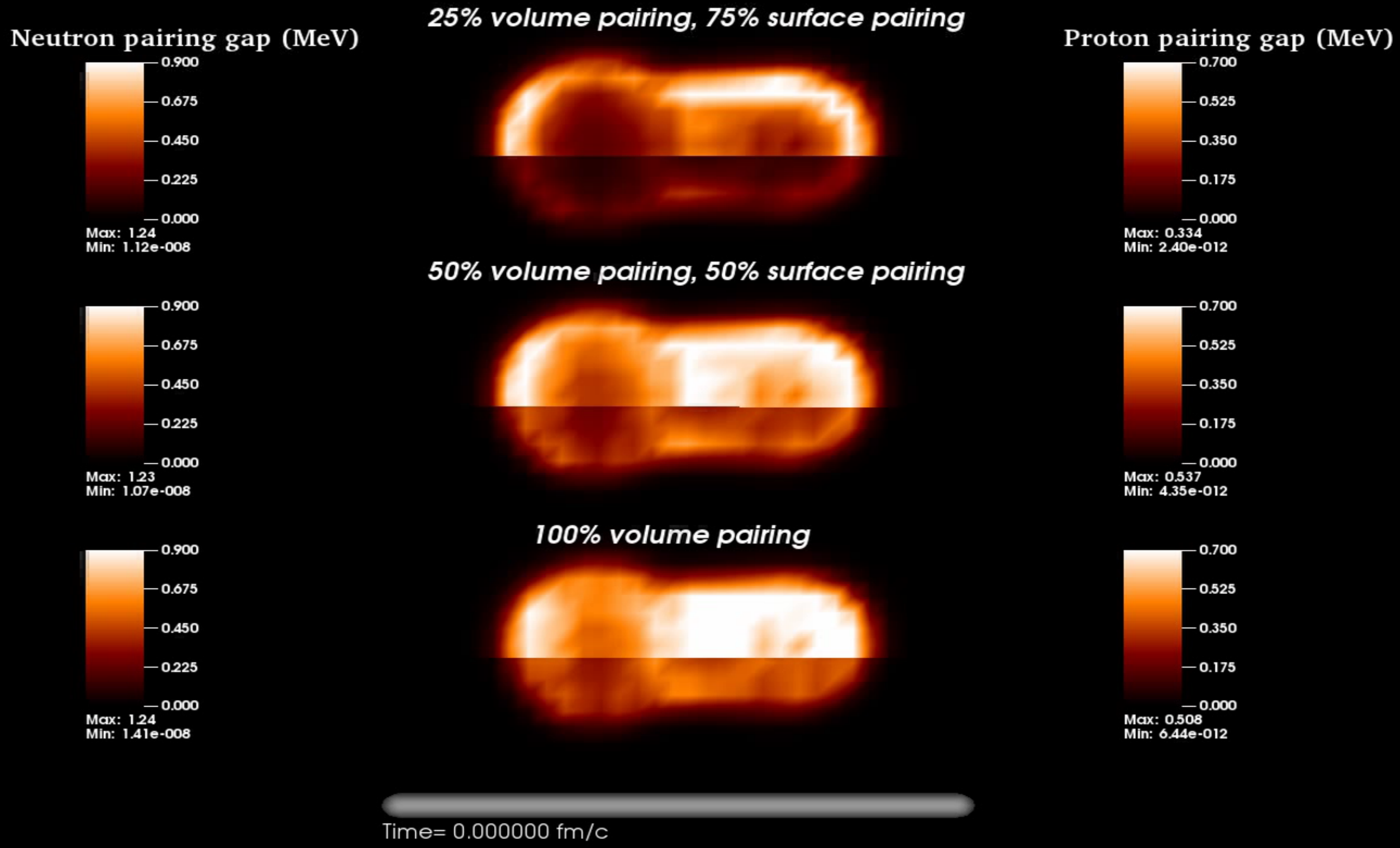
$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

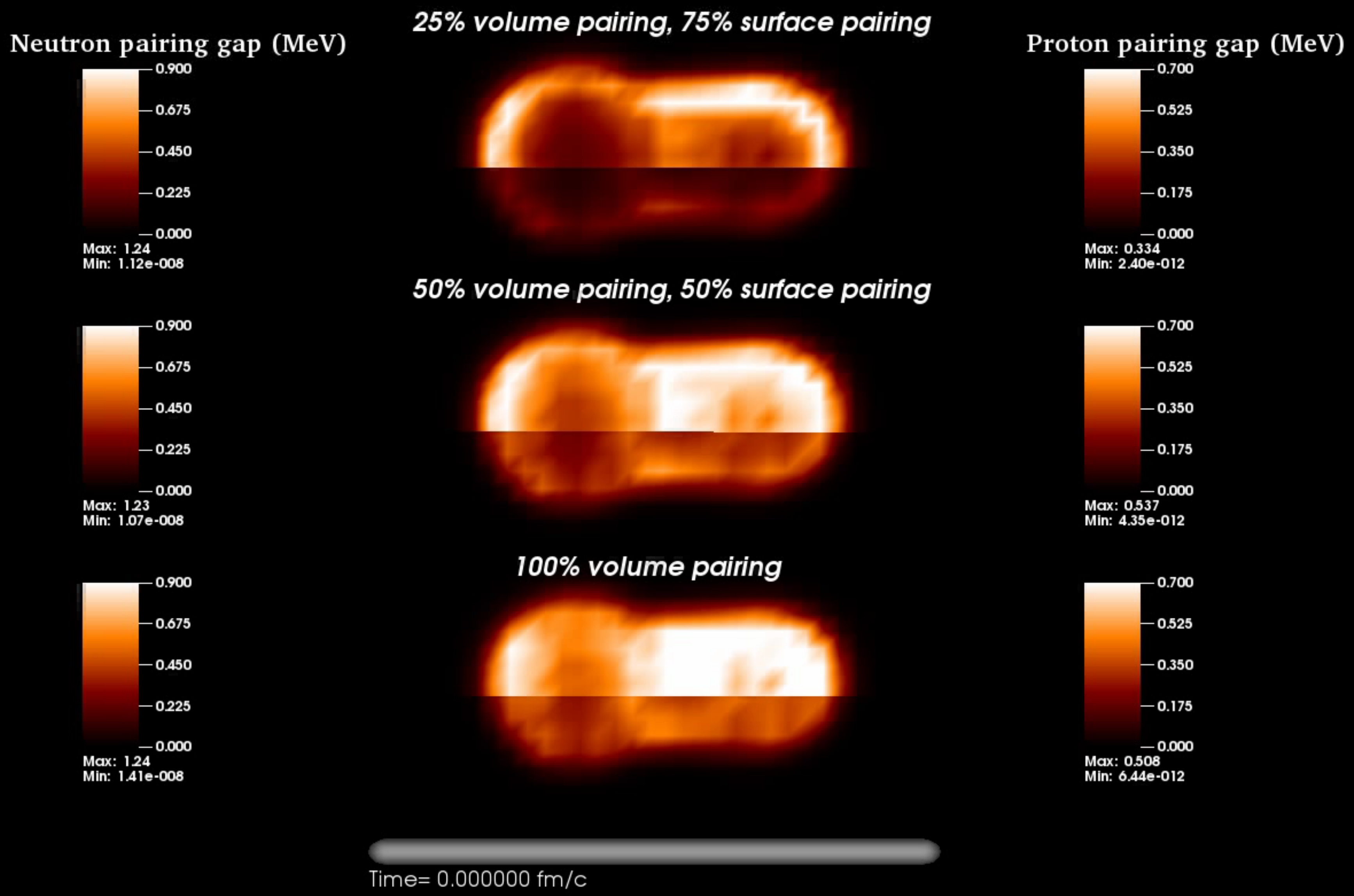




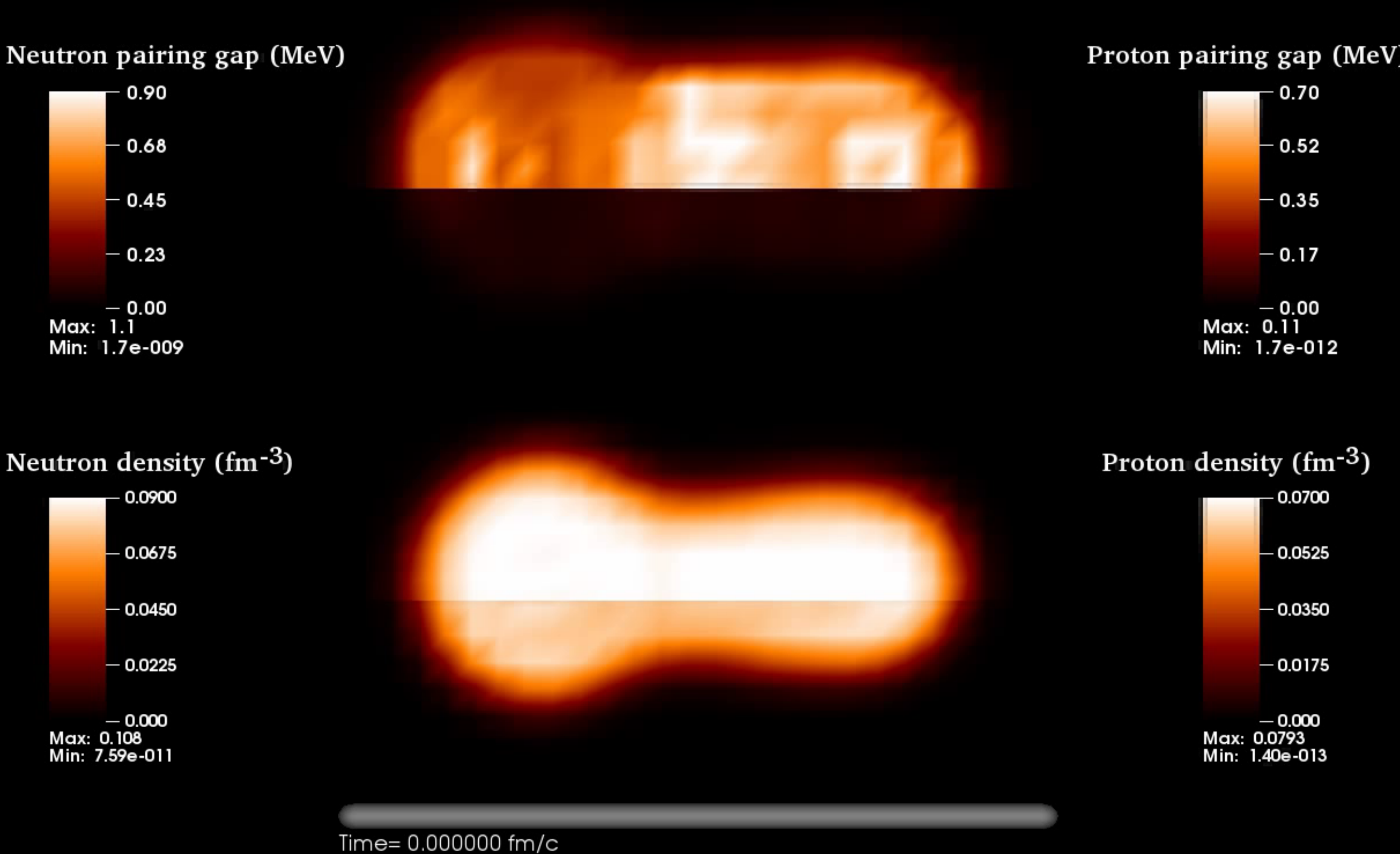
Fission of ^{240}Pu at excitation energy E_x = 8.05; 7.91; 8.08 MeV



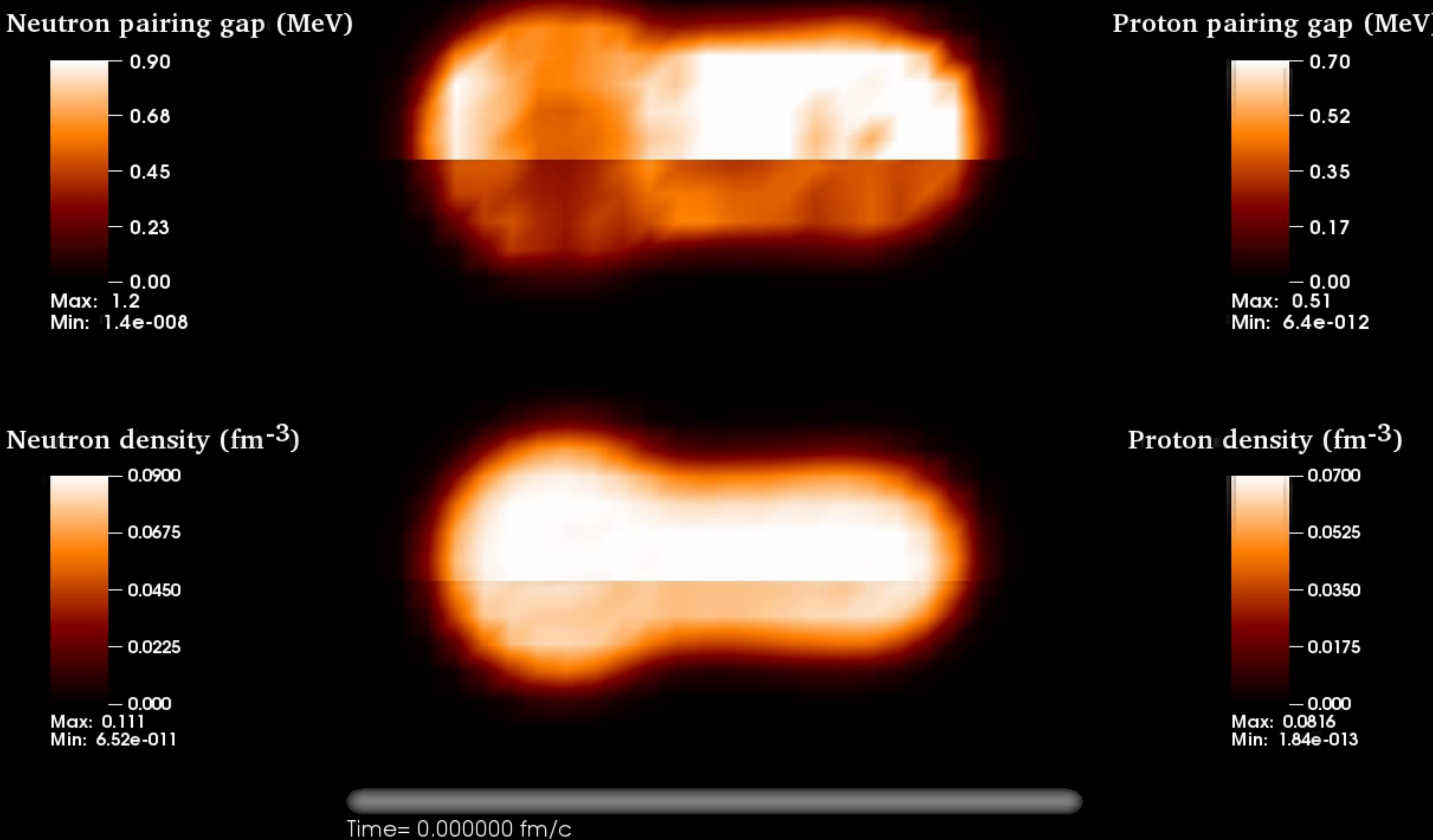
Fission of ^{240}Pu at excitation energy E_x = 8.05; 7.91; 8.08 MeV



Fission of ^{240}Pu at excitation energy $E_X = 6.17$ MeV



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



Papers we have published so far on SLDA and TDSLDA (stars indicate papers with significant nuclear physics content):

Phys. Rev. A 91, 031602(R) (2015)
* Phys. Rev. Lett. 114, 012701 (2015)
Phys. Rev. Lett. 112, 025301 (2014)
* arXiv:1305.6891
* Phys. Rev. Lett. 110, 241102 (2013)
* Phys. Rev. C 87 051301(R) (2013)
* Ann. Rev. Nucl. Part. Phys. 63, 97 (2013)
* Phys. Rev. C 84, 051309(R) (2011)
Phys. Rev. Lett. 108, 150401 (2012)
Science, 332, 1288 (2011)
J. Phys. G: Nucl. Phys. 37, 064006 (2010)
Phys. Rev. Lett. 102, 085302 (2009)
Phys. Rev. Lett. 101, 215301 (2008)
* J.Phys. Conf. Ser. 125, 012064 (2008)
arXiv:1008.3933 chapter 9 in Lect. Notes Phys. vol. 836
Phys. Rev. A 76, 040502(R) (2007)
* Int. J. Mod. Phys. E 13, 147 (2004)
Phys. Rev. Lett. 91, 190404 (2003)
* Phys. Rev. Lett. 90, 222501 (2003)
* Phys. Rev. Lett. 90, 161101 (2003)
* Phys. Rev. C 65,051305(R) (2002)
* Phys. Rev. Lett. 88, 042504 (2002)
Plus a few other chapters in various books.