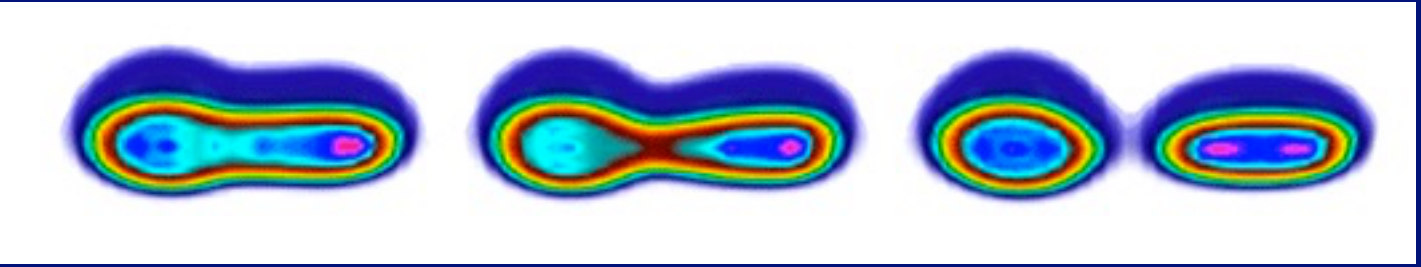
New Results in the Theory of Nuclear Fission



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Ionel Stetcu	**(LANL)**

Several recent developments have radically changed our prospects of attaining a microscopic description of nuclear fission.

- **In THEORY:**

Formulation of a local extension of the Density Functional Theory (DFT), in the spirit of the Local Density Approximation (LDA) formulation of DFT due to Kohn and Sham, to superfluid time-dependent phenomena, the Superfluid Local Density Approximation (SLDA).

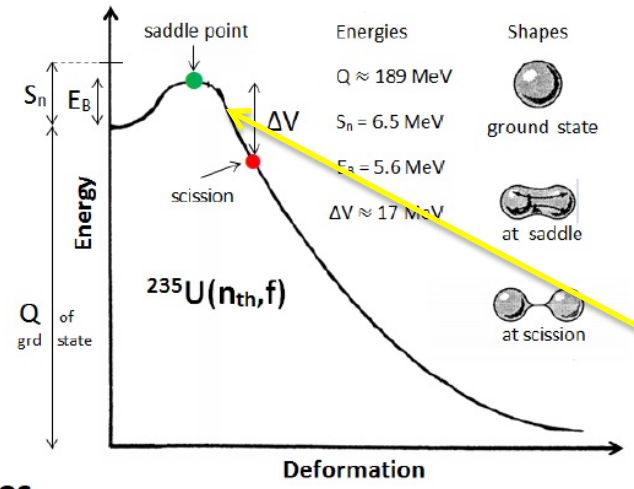
Validation and verification of (TD)SLDA against a large set of theoretical and experimental data for systems of strongly interacting fermions.

- **In HIGH PERFOMANCE COMPUTING:**

Emergence of very powerful computational resources, non-trivial numerical implementation of TDSLDA, advanced capabilities of leadership class computers, in particular tens of thousands of GPUs.

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.

Potential energy versus deformation



The shape of the PES is governed mostly by the competition between the surface and the Coulomb energies.

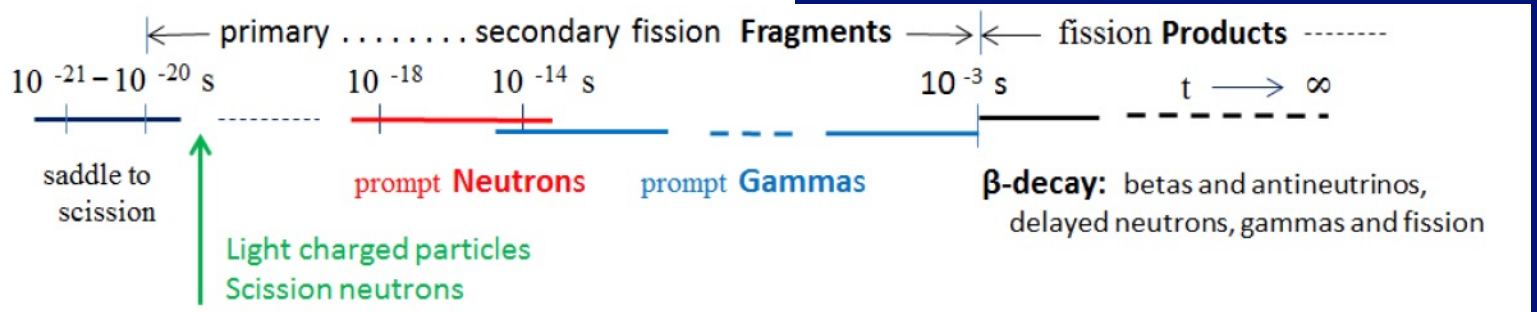
From the outer saddle to the scission the dynamics is relatively fast, likely non-adiabatic and in this region the fission fragments are formed and their properties are defined.

Times

- Time from grd state to saddle in low energy fi — $6 \cdot 10^{-15}$ s
- Time from saddle to scission — ≈ 5 zs
- Neck rupture in — ≈ 0.5 zs
- Acceleration of FF to 90% of final velocity — ≈ 5 *zs*
- Time for relaxation of deformation — ≈ 5 zs
- Evaporation time for 10 MeV n from FF — 10^3 zs

NOTE: 1 zs = 1 zeptosecond = 10^-21 s

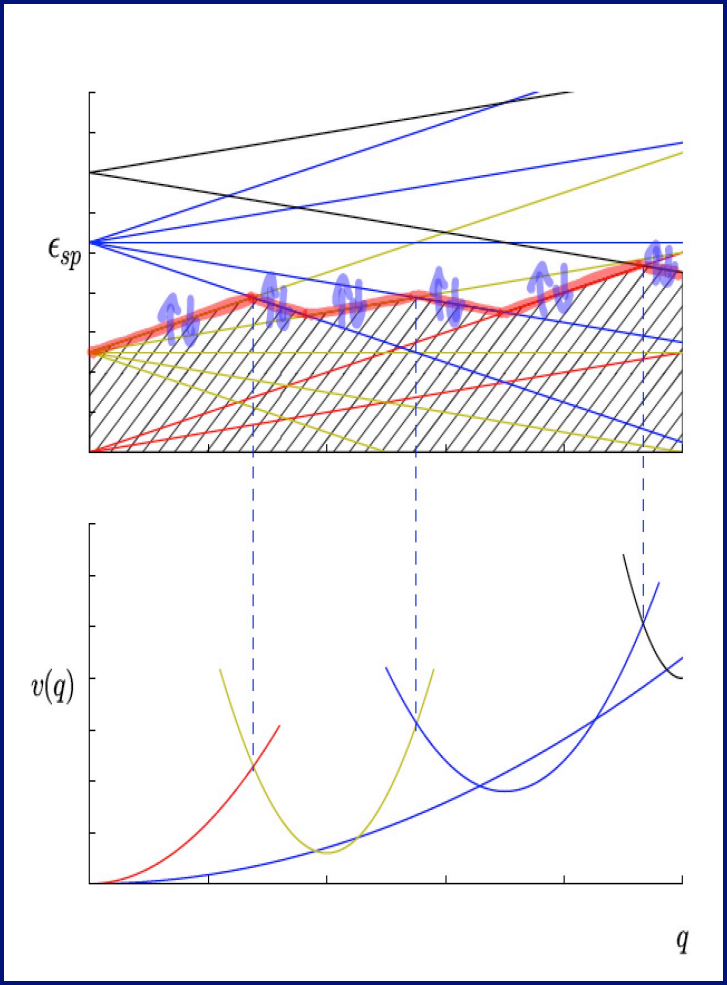
$1\ zs = 10^{-21}\ sec. = 300\ fm/c$



From Lectures given by Gönnenwein at LANL Fiesta School, 2014

Potential energy surface is a bit more complicated than a liquid drop model would suggest!

How nuclei change their shape at a microscopic level?



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)

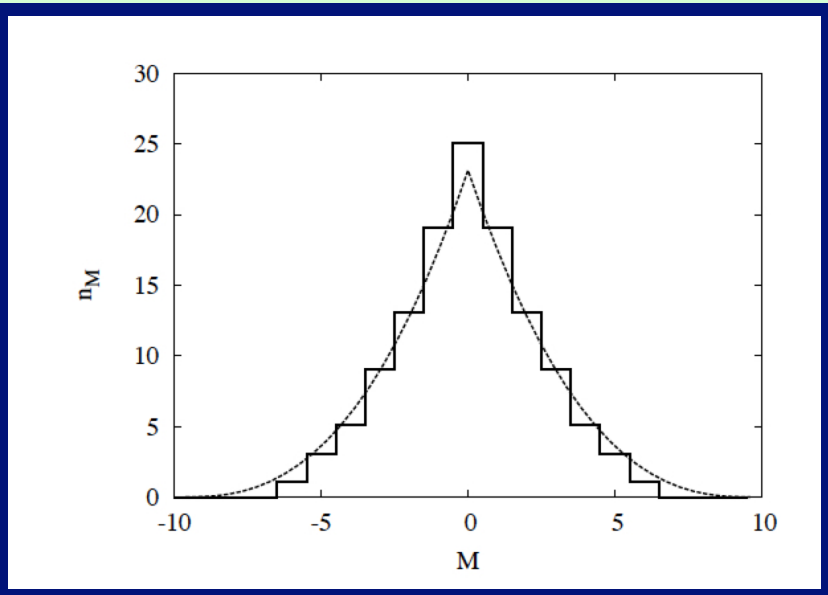
- Each single-particle level is double degenerate (Kramers' degeneracy) and at each level crossing <u>two nucleons must jump simultaneously!</u>

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

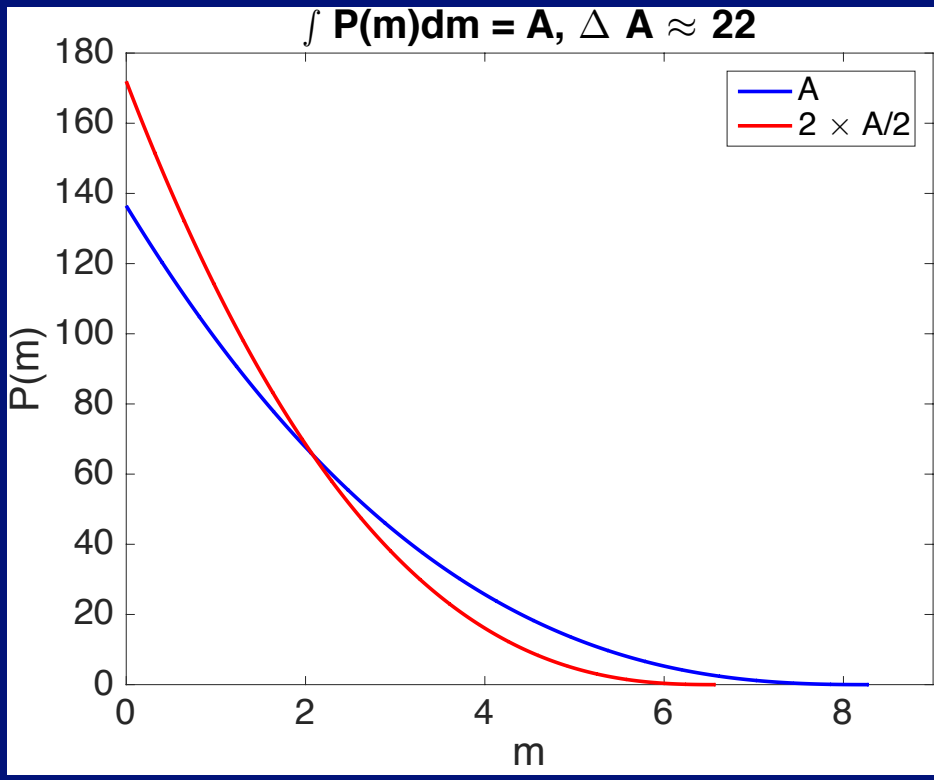
- <u>Pairing interaction/superfluidity is the most effective mechanism at performing shape changes.</u>

Let us consider an axially symmetric nucleus, with Oz the axis of symmetry and evaluate semiclassically the angular momentum distribution

$$P(M)=\int d^3r d^3p\, f(\vec{p},\vec{r})\,\delta\left((\vec{r}\times\vec{p})_z-\hbar M\right)=\frac{A^{2/3}}{p_F r_0}\,g\left(\frac{\hbar M}{p_F r_0 A^{1/3}}\right)$$



Dashed line − semi-classical
Histogram − shell model

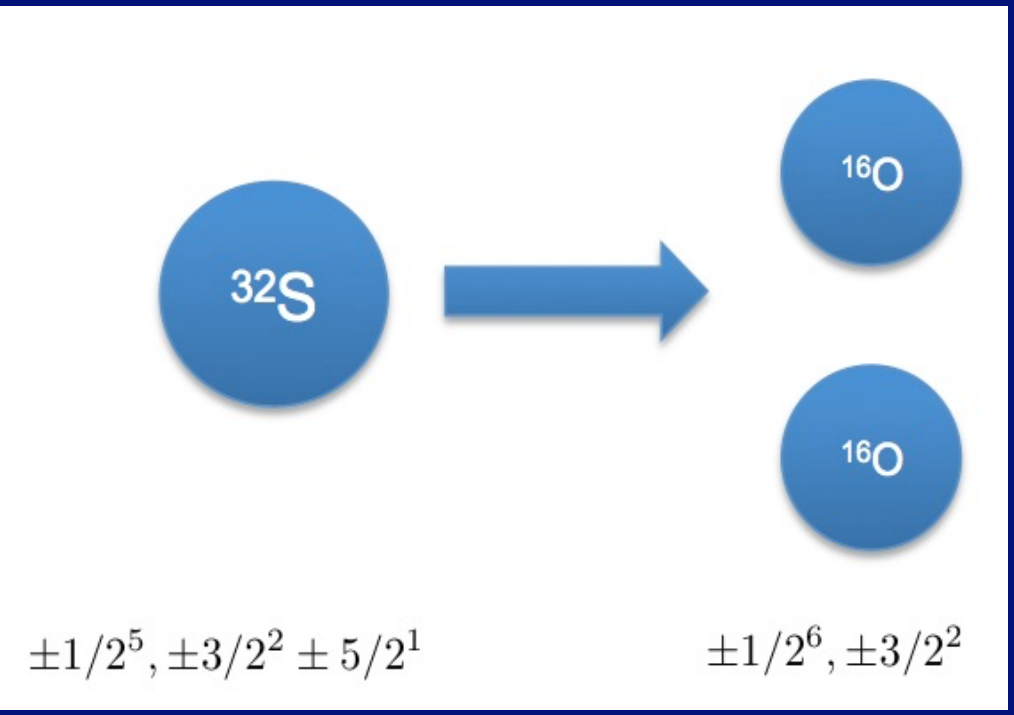


Distribution derived by G.F. Bertsch (2017)

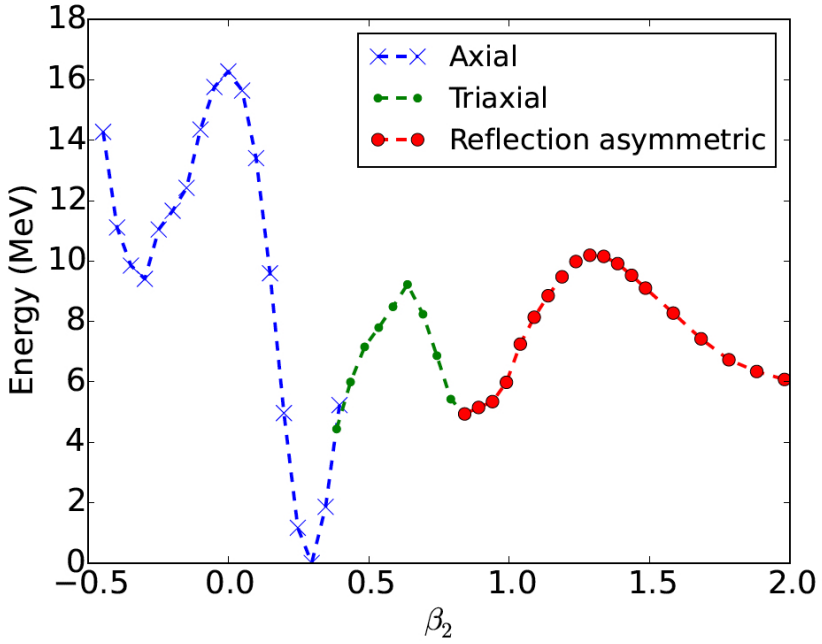
Fission fragments have smaller waists than their "mother" and therefore smaller $|m_{max}|$.

In TDHF or TDHF with frozen occupation probabilities $P(l_z)$ is conserved and single-particle states with $|m_{max}| \approx O(k_F r_0 A^{1/3})$, which should not be occupied in the fission fragments, retain their initial occupation probability.
The initial spherical Fermi momentum distribution acquires an ellipsoidal prolate shape in the final fission fragments.

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



Occupied sp orbitals m-quantum numbers in initial and final configurations



Potential energy curve for ^{240}Pu with SLy4
Ryssens, et al., Phys. Rev C 92, 064318 (2015)

One more problem!

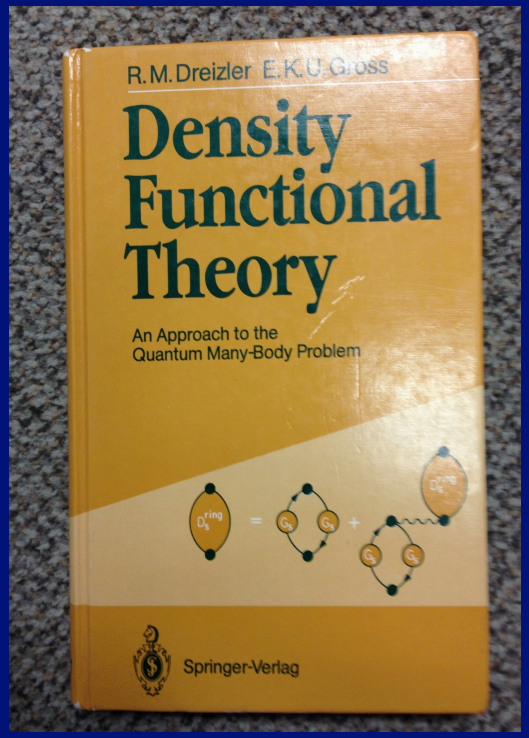
Initial nucleus: 20 positive + 12 negative parity sp orbitals

Final nuclei: 16 positive + 16 negative parity sp orbitals

The Main Theoretical Tool

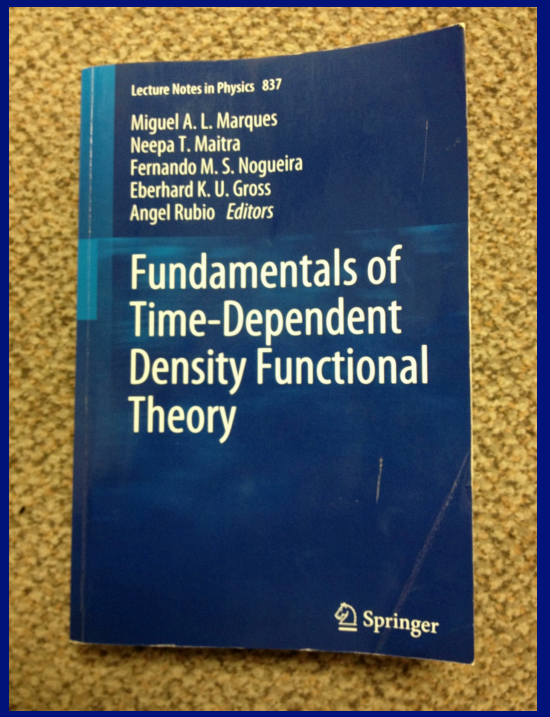
MATHEMATICAL THEOREM:

There exist an universal density functional of particle density.



1990

2012



DFT has been developed and used mainly to describe normal (non-superfluid) electron systems.
DFT provides the framework, the equivalent of the Schrödinger equation. (We might not have the "exact potential" yet)
This theory which is more than 50 years old: DFT - Kohn and Hohenberg, 1964 and LDA - Kohn and Sham, 1965

But not everyone is normal! Hence, 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)

DFT is not a glorified meanfield as some say!

Let us consider the Schrödinger equation for example:

$$H = \sum_{i}^{N} T(i) + \sum_{i<j}^{N} U(ij) + \sum_{i<j<k}^{N} U(ijk) + \ldots + \sum_{i}^{N} V_{ext}(i)$$

$$H\Psi_0(1,2,\ldots N) = E_0\Psi_0(1,2,\ldots N)$$

We know this is the correct framework to describe quantum phenomena, even though we have only an approximate idea about interactions , we do not know the exact NN and NNN potentials and use phenomenology.

$$\Psi_0(1,2,\ldots N) \equiv \Psi_0\left(1,2,\ldots N;\left[n(\vec{r})\right]\right) \Leftrightarrow V_{ext}(\vec{r}) \Leftrightarrow n(\vec{r})$$

$$E\left[n(\vec{r})\right] = \left\langle \Psi_0\left[n(\vec{r})\right] \middle| H \middle| \Psi_0\left[n(\vec{r})\right] \right\rangle$$

We also know that DFT is mathematically equivalent to the Schrödinger equation, even though we cannot always practically show that, and we, as a rule, we do not know the exact functional and use use phenomenology too.

$$E_0 = \min_{n(\vec{r})} \int d^3r \left\{ \frac{\hbar^2}{2m^*(\vec{r})}\tau(\vec{r}) + \varepsilon\left[n(\vec{r})\right] + V_{ext}(\vec{r})n(\vec{r}) \right\}$$

$$n(\vec{r}) = \sum_{i}^{N} \left|\varphi_i(\vec{r})\right|^2, \qquad \tau(\vec{r}) = \sum_{i}^{N} \left|\vec{\nabla}\varphi_i(\vec{r})\right|^2$$

TD Superfluid LDA equations (TDSLDA)

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

- 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 which is effectively a sixth order method
- No symmetry restrictions for the solutions
- *Number of PDEs is of the order of the number of spatial lattice points – from 10,000s to 1-2,000,000*

$$\propto 8\frac{4\pi p_{cut}^3}{3}\left(\frac{L}{2\pi\hbar}\right)^3 \propto N_x N_y N_z$$

- SLDA/TDSLDA (DFT) is formally by construction like meanfield HFB/BdG
- The code was implemented on Jaguar, Titan, Piz Daint, Tsubame3.0, Franklin, Hopper, Edison, Hyak, Athena
- Initially Fortran 90, 95, 2003 …, presently C, CUDA, and obviously MPI, threads, etc.
- Extremely efficient I/O for Check-Point Restart
- For more details (though not latest ones) about the method see INT talk on October 7, 2013:

While in this presentation I have concentrated on a single issue, it is important to summarize that so far TDSLDA has lead to many qualitative new developments:

- **The first microscopic description of structure and creation, and decay of quantized vortices in Fermi superfluid**
- **The first microscopic description of the incipient phases of quantum turbulence in Fermi superfluids predicted in 1954 by Feynman, crossing and recombination of vortices**
- **The correct identification of the creation of domain walls, quantized vortices and vortex rings, their dynamics and decay and of the quantum shock waves in exps.**
- **Described the microscopic structure of quantized vortices in neutron matter**
- **Described microscopically the interaction of quantized vortices with nuclei in neutron star crust**
- **Described microscopically the Coulomb excitation of nuclei with relativistic nuclei**
- **Described induced nuclear fission and revealed unexpected qualitative aspects**
- **Has been applied to collisions of heavy superfluid nuclei and revealed new qualitative phenomena**

The 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.

EDF : SLy4 and currently SeaLL1 and SkM*mod

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: currently 60×30^2 fm^3

Momentum cutoff: $p_c = \frac{\hbar\pi}{\Delta x} \approx 500$ MeV$\cdot$fm in each Cartesian direction, cubic momentum spa

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: $= 0.03$ fm/c

Number of time steps: $\approx$ up to 120,000, approximately 2.5 time-steps per sec.

Number of PDEs: $\approx 2(\text{for n and p})\times 2\times N_x N_y N_z(\text{for } E_n > 0) = 442{,}368$

Number of DoF $= (4N_xN_yN_z)^2 = (4\times 24^2\times 48)^2 \approx 1.2\times 10^{10}$ or approximately 0.2 TB

Number of GPUs: $\approx$ 1,728+2 (balance between speed and cost) thus 256 PDEs per GPU

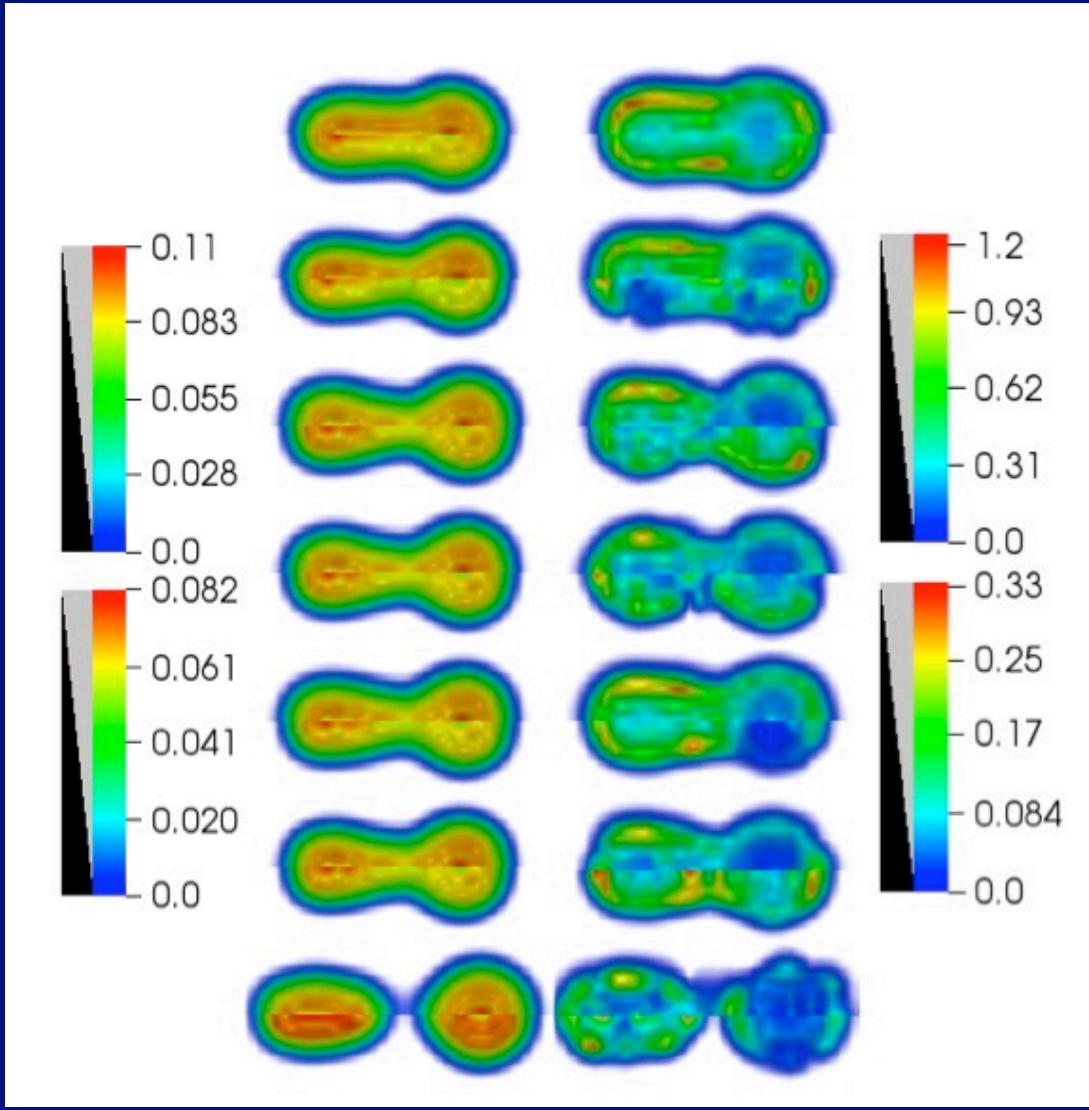
Wall time: $\approx$ 4-12 hours

OLCF Titan - Cray XK7

ETH - Piz Daint

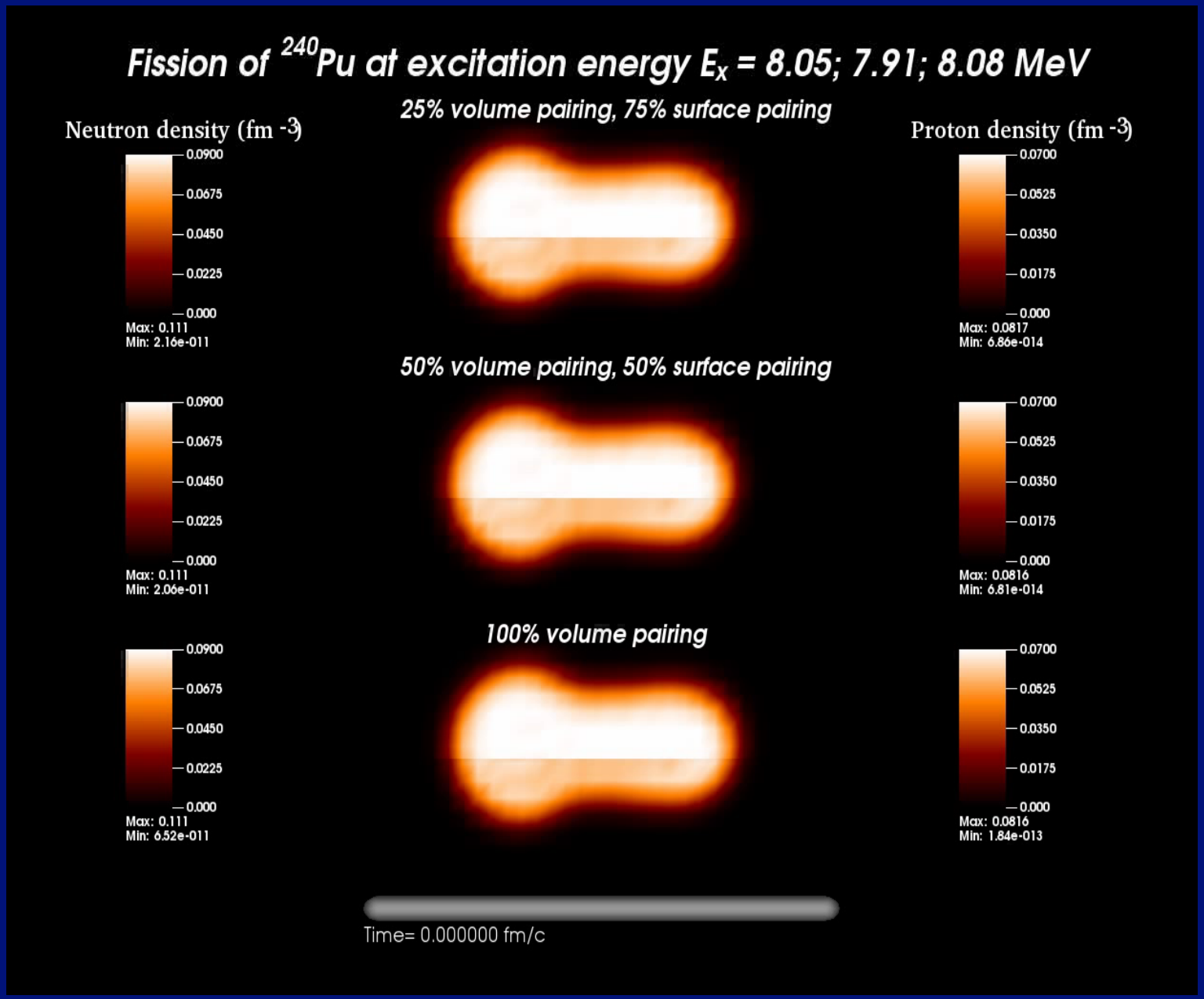
Induced Fission of ^{240}Pu

Induced fission of ^{240}Pu

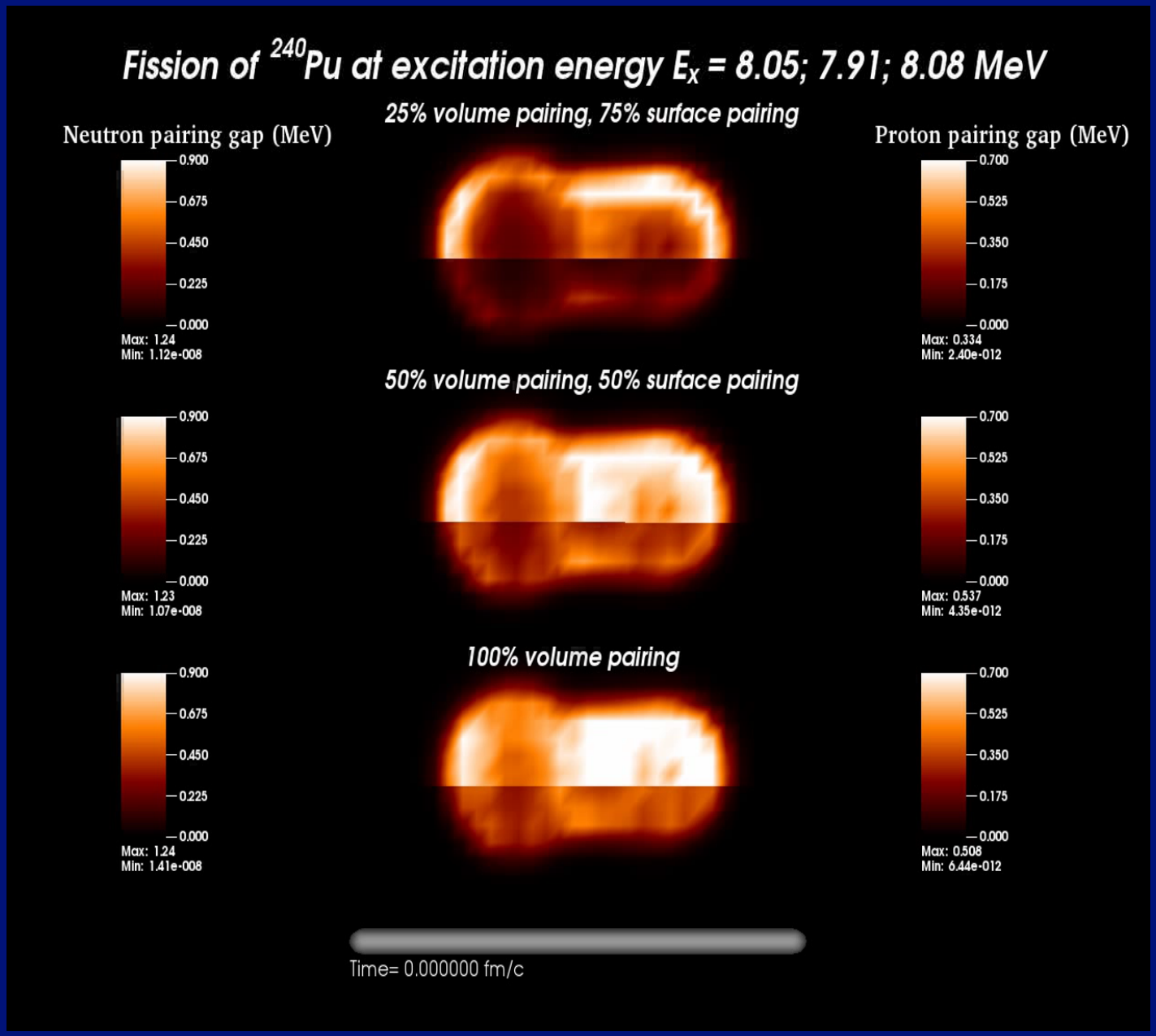


Neutron/proton densities (left and top/bottom)
Neutron/proton pairing gaps (right and top/bottom)

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



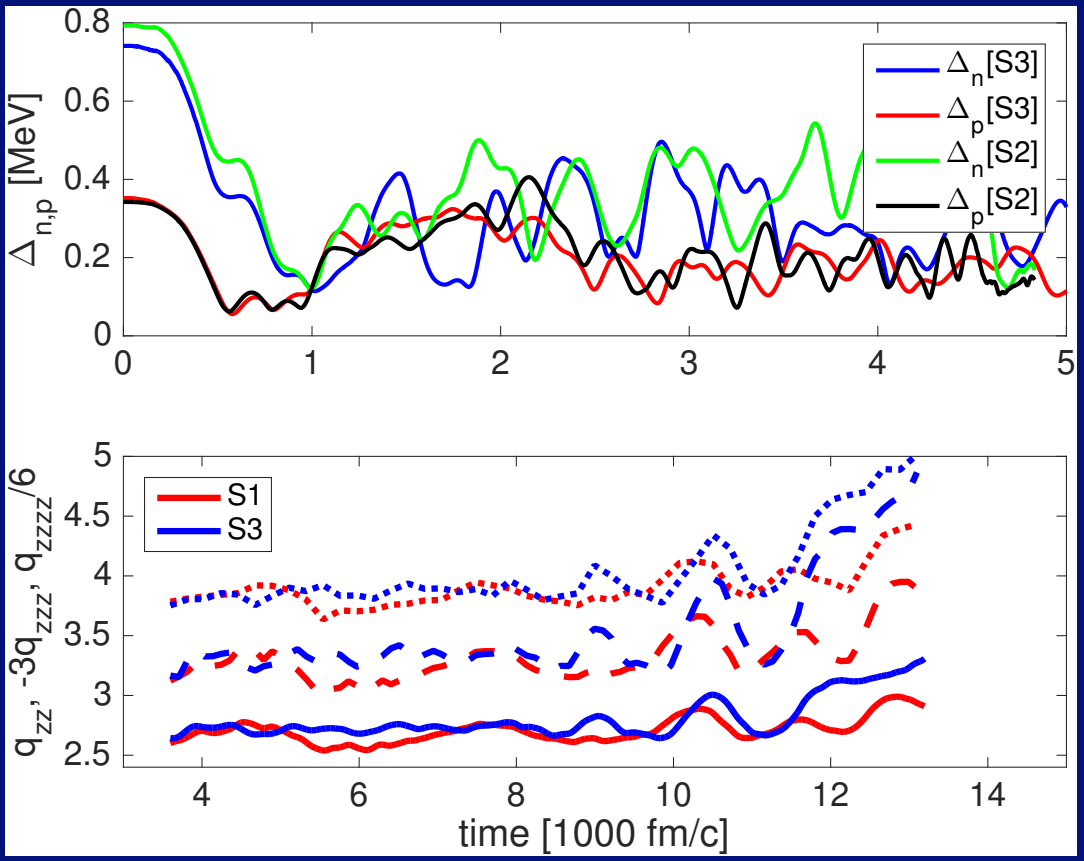
1 zs = 10^{-21} sec. = 300 fm/c



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

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.

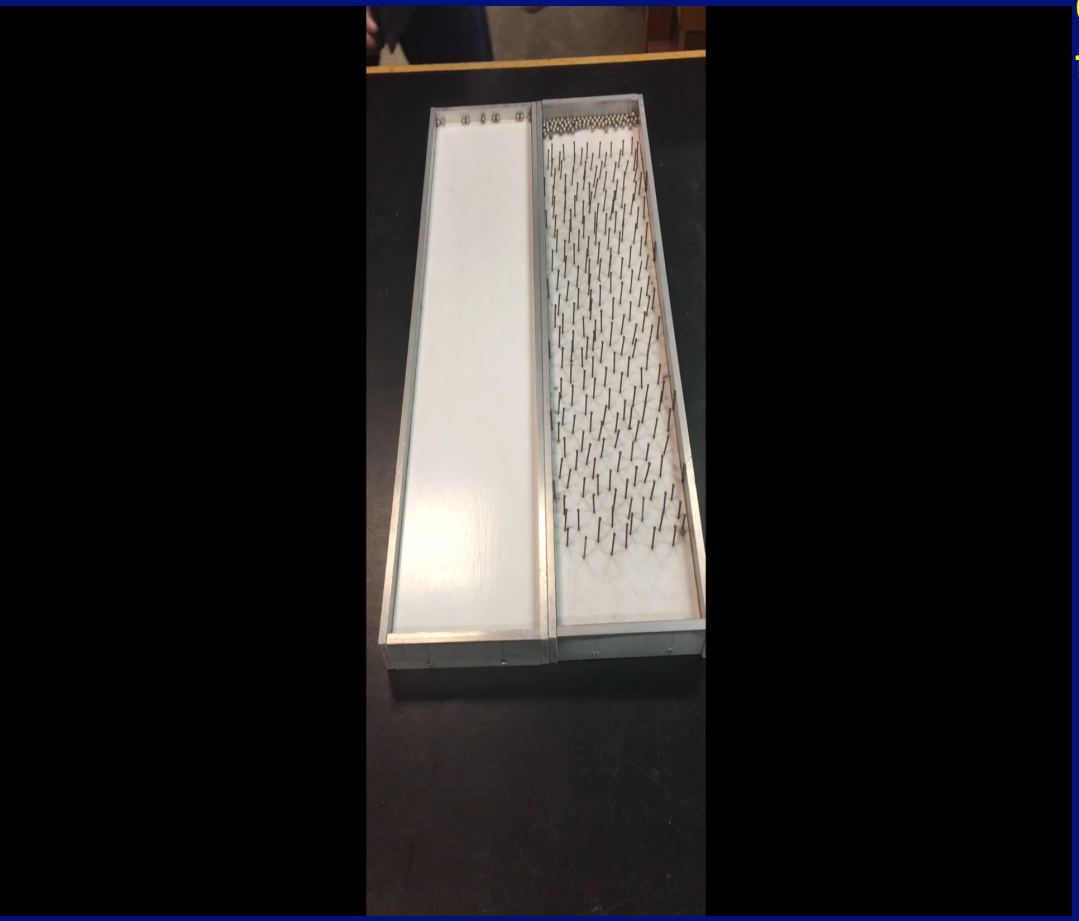
S no.	η	E^*	E_n	q_{zz}	q_{zzz}	t_{SS}	TKE^{syst}	TKE	A_L^{syst}	A_L	N_L^{syst}	N_L	Z_L^{syst}	Z_L	E^*_H	E^*_L	ν_H	ν_L
$S1$	0.75	8.05	1.52	1.78	−0.742	14 419	177.27	182	100.55	104.0	61.10	62.8	39.45	41.2	5.26	17.78	0	1.9
$S2$	0.5	7.91	1.38	1.78	−0.737	4360	177.32	183	100.56	106.3	60.78	64.0	39.78	42.3	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.

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



One cause: all collective degrees of freedom present.

2D classical analog model of the Drude model for electron conduction in metals.

On the left side there is no "ion lattice" present, only electrons in an "uniform electric field."

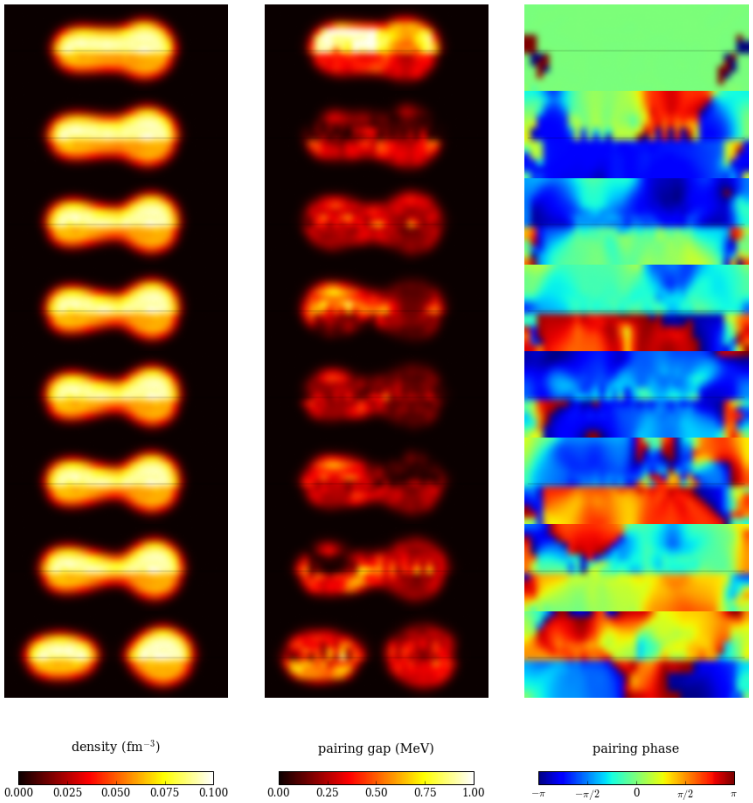
On the right side the electrons, again in the presence of an "uniform electric field," collide elastically with the "ions."

Another reason:
fluctuating pairing field.

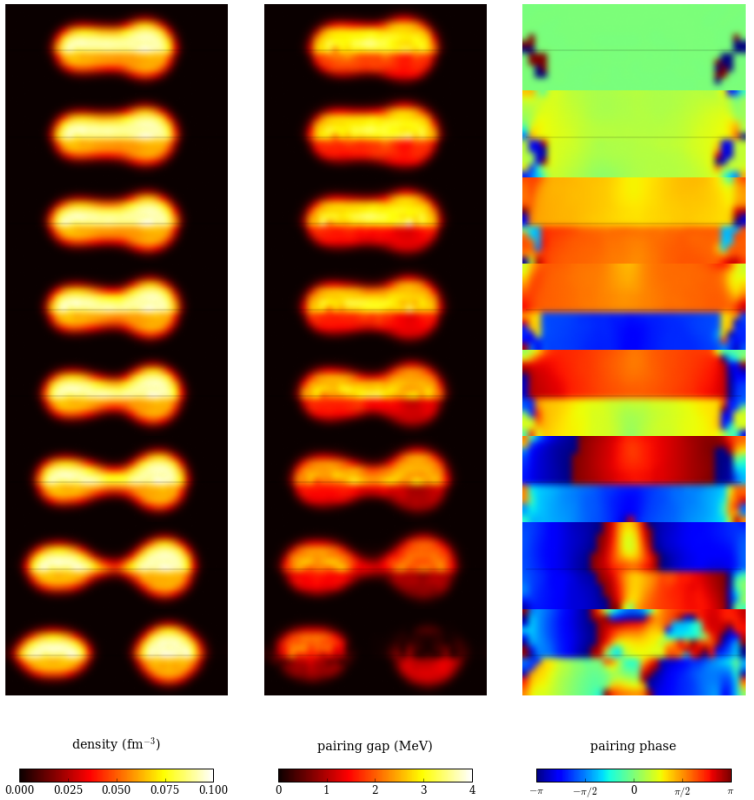
Note that kinetic energy is not dissipated and in both cases and the "electrons" arrive at the bottom with the same speed but at different times!

How important pairing is?

^{240}Pu fission in the normal pairing gap



^{240}Pu fission in a larger pairing gap



Normal pairing strength
Saddle-to-scission 14,000 fm/c

Enhanced pairing strength
Saddle-to-scission 1,400 fm/c !!!

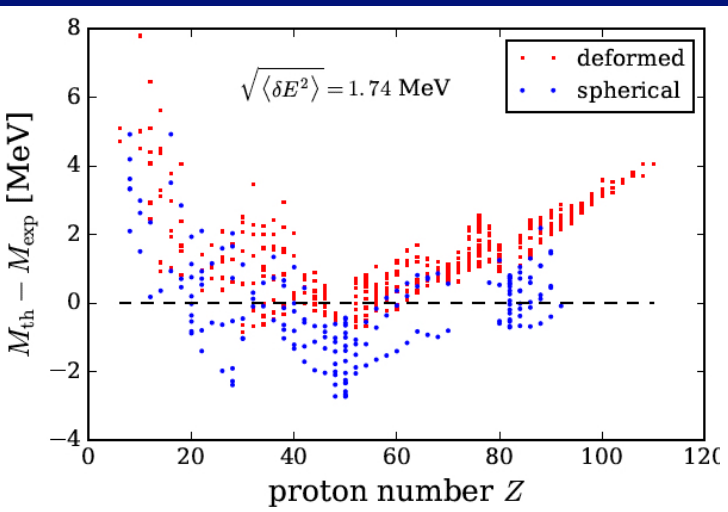
SeaLL1 - a qualitatively new nuclear energy density functional (not fully optimized yet).

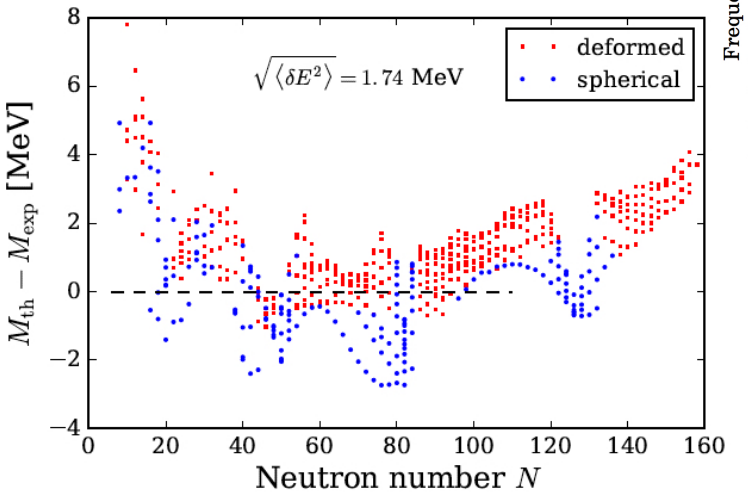
- Number of parameters = 7 (as compared to 14 or more in typical nuclear DFT approaches)

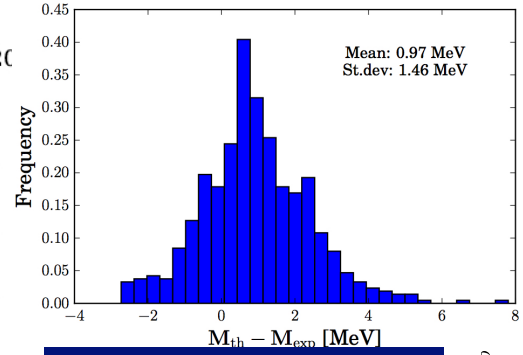
  2 (isoscalar: $\rho_0, E/A$) + 2 (isovector: S, L) + 1 (surface tension) + 1 (spin-orbit) + 1 (pairing)

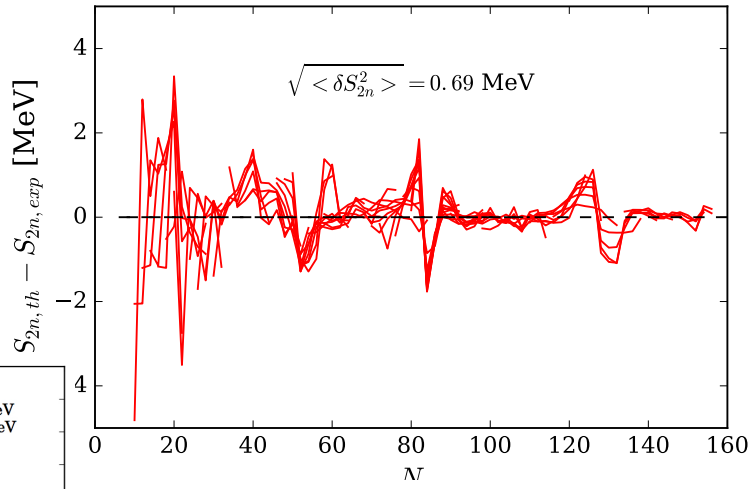
- For 606 even-even nuclei from AME2012 Mean energy error: 0.97 MeV.

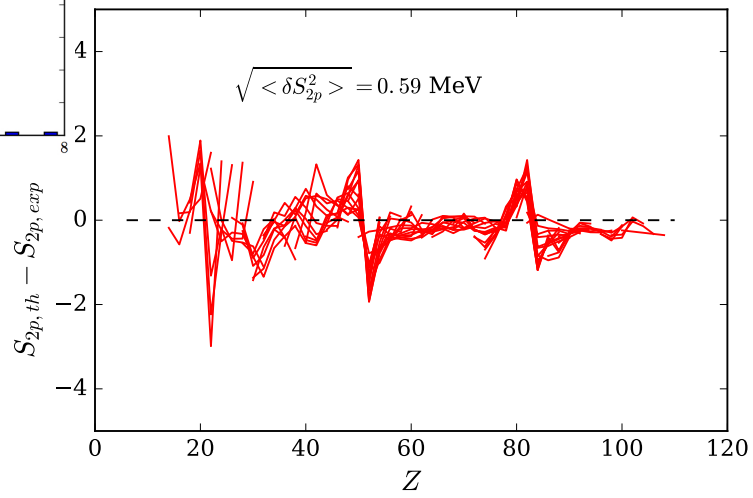
  Standard deviation: 1.46 MeV.

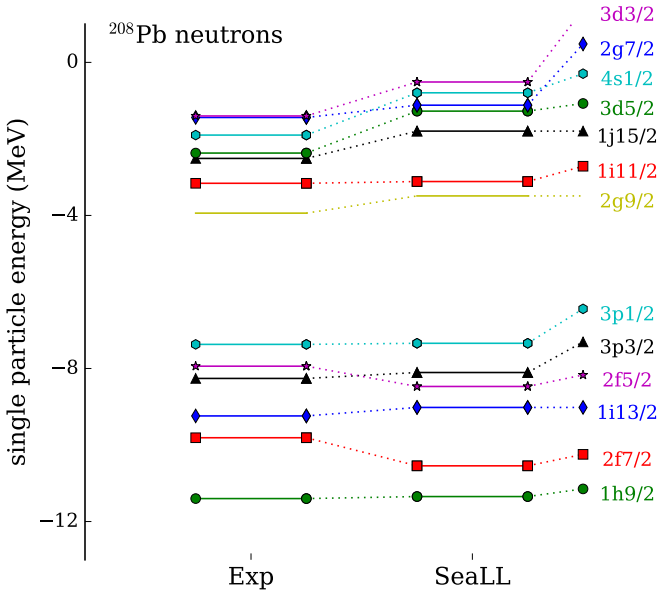


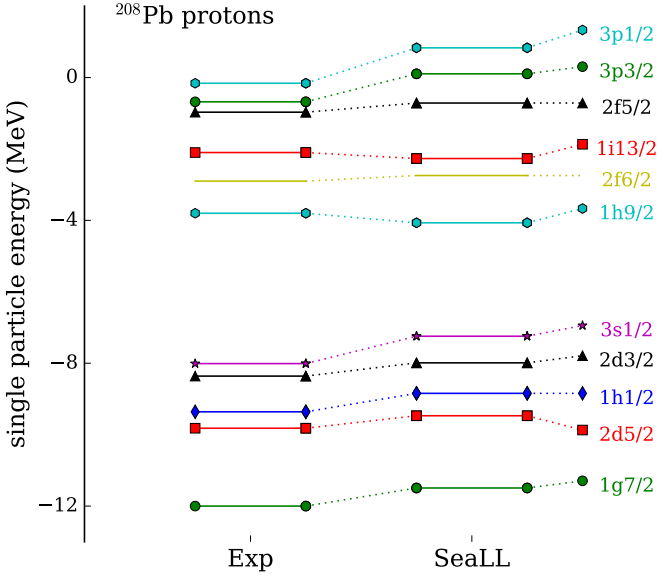


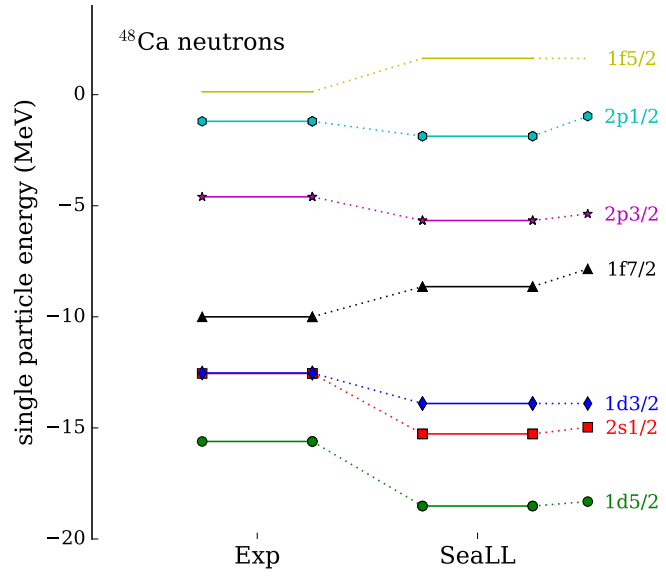


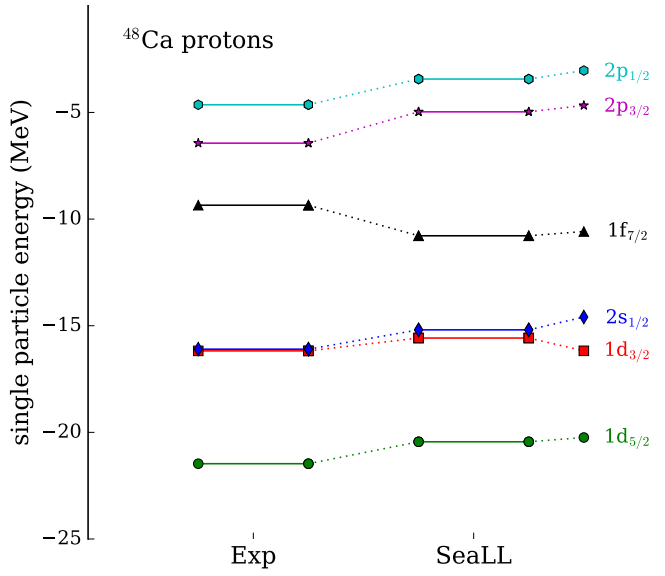


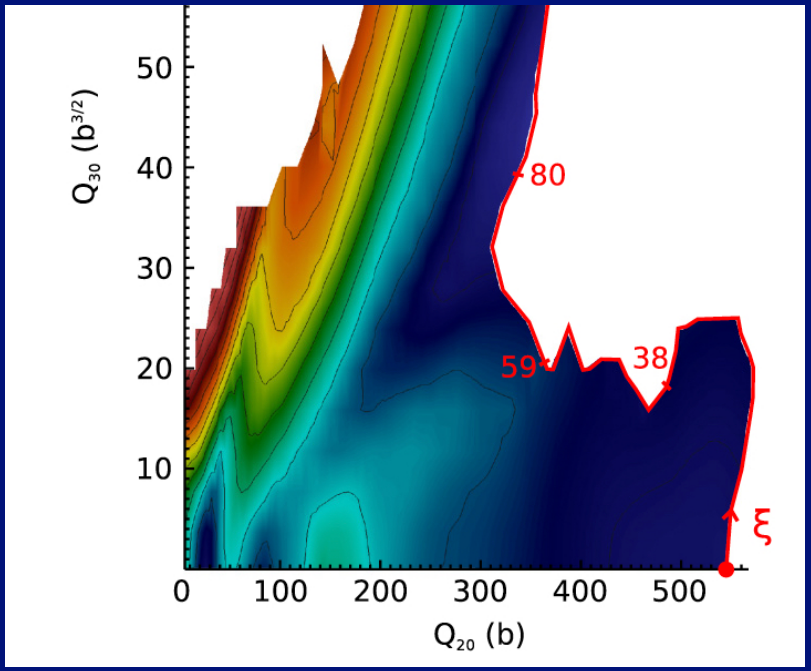



^{208}Pb neutrons
single particle energy (MeV)
0
−4
−8
−12
Exp
SeaLL
3d3/2
2g7/2
4s1/2
3d5/2
1j15/2
1i11/2
2g9/2
3p1/2
3p3/2
2f5/2
1i13/2
2f7/2
1h9/2


^{208}Pb protons
single particle energy (MeV)
0
−4
−8
−12
Exp
SeaLL
3p1/2
3p3/2
2f5/2
1i13/2
2f6/2
1h9/2
3s1/2
2d3/2
1h1/2
2d5/2
1g7/2

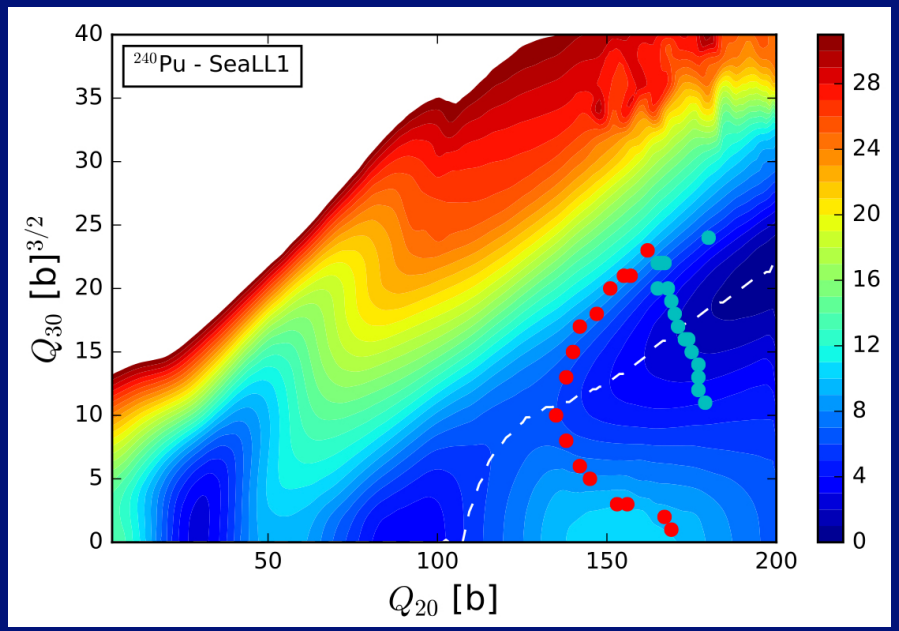

^{48}Ca neutrons
single particle energy (MeV)
0
−5
−10
−15
−20
Exp
SeaLL
1f5/2
2p1/2
2p3/2
1f7/2
1d3/2
2s1/2
1d5/2

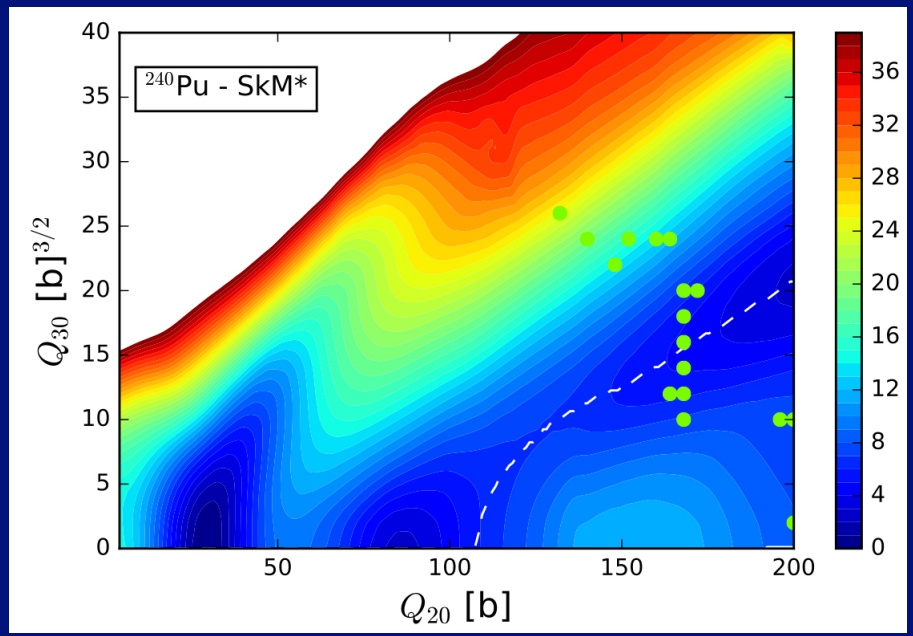

^{48}Ca protons
single particle energy (MeV)
−5
−10
−15
−20
−25
Exp
SeaLL
2p$_{1/2}$
2p$_{3/2}$
1f$_{7/2}$
2s$_{1/2}$
1d$_{3/2}$
1d$_{5/2}$



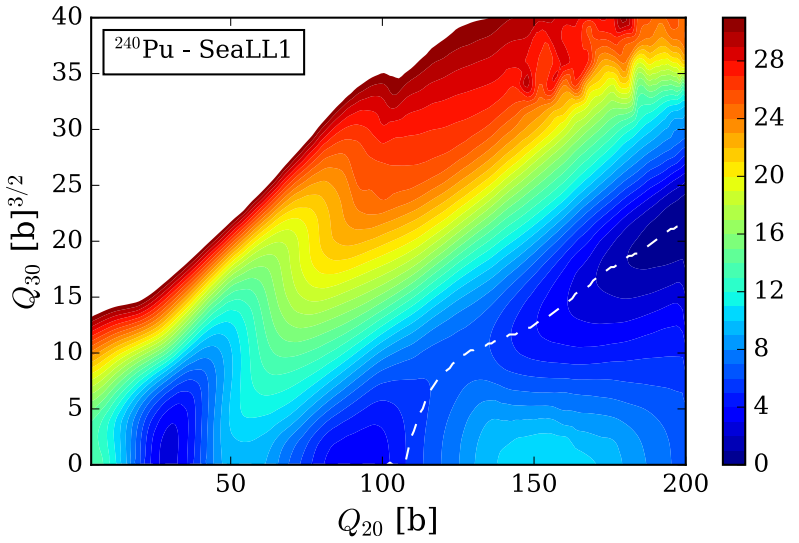
The red line corresponds to Q_N=4 nucleons in the "neck"

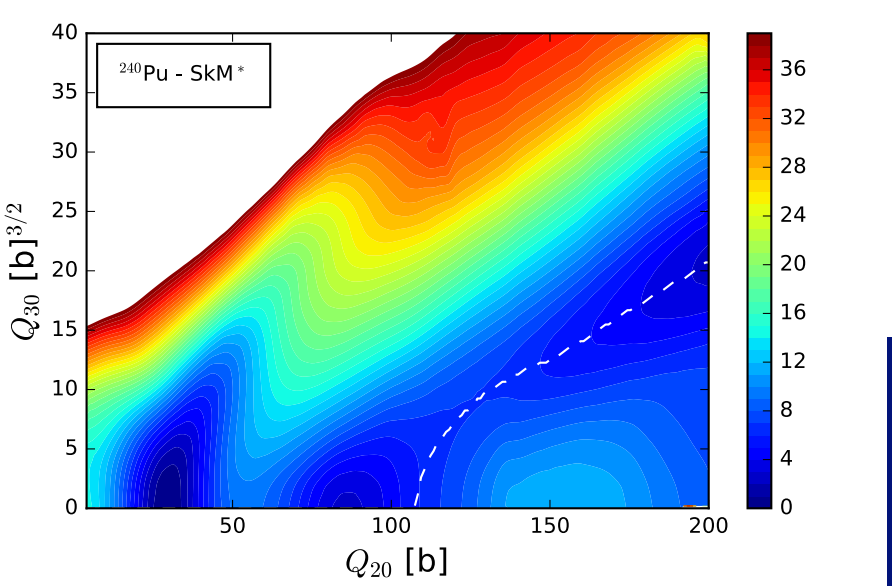
PES obtained with SkM* in
Regnier, Dubray, Schunck, and Verrière
Phys. Rev. C 93, 054611 (2016)

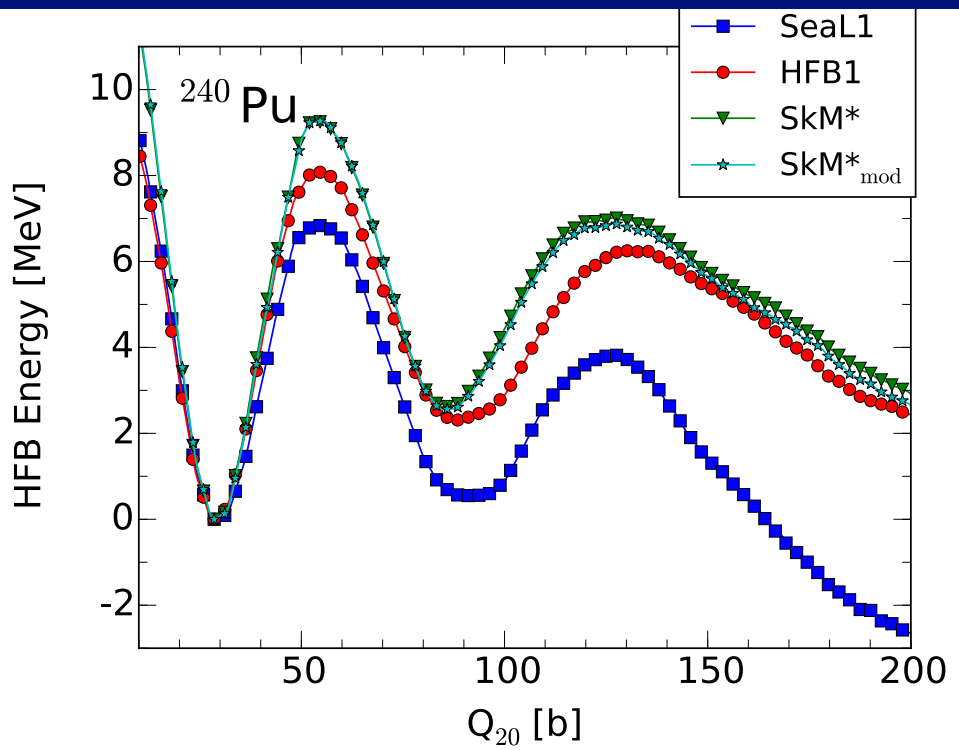




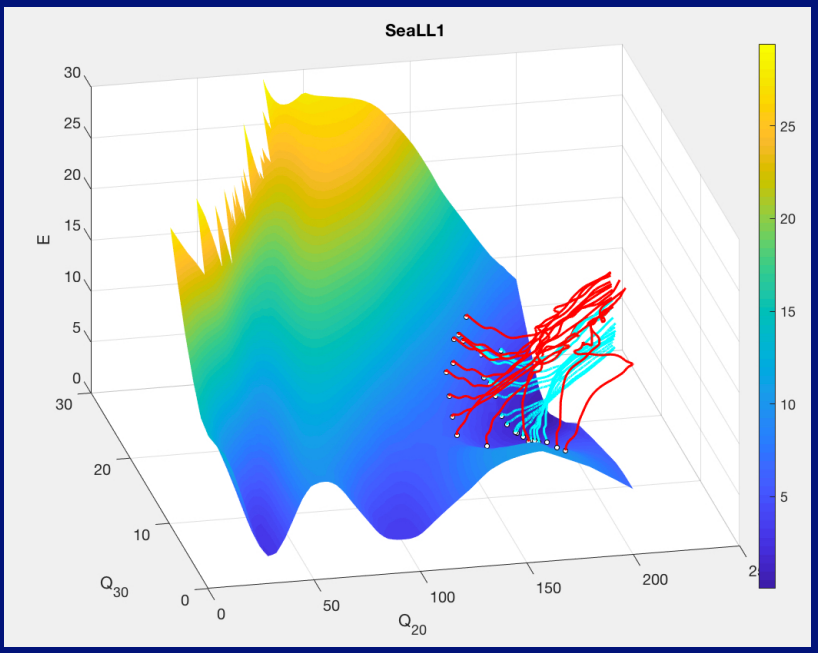
The following slides contain unpublished results which are still preliminary!

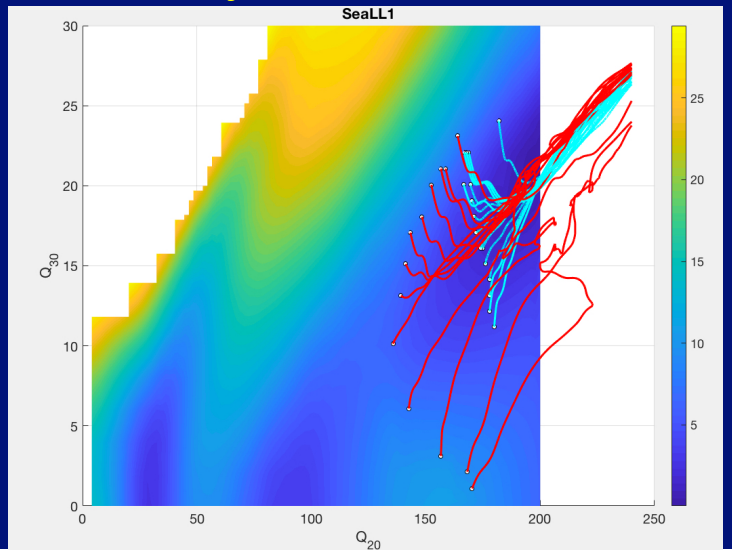

^{240}Pu - SeaLL1
Q_{30} [b]$^{3/2}$
Q_{20} [b]

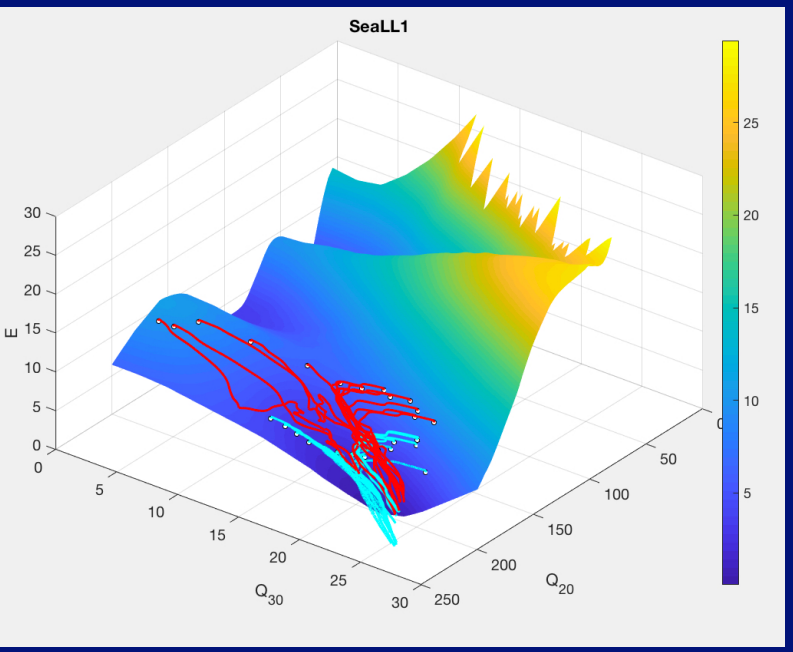

^{240}Pu - SkM*
Q_{30} [b]$^{3/2}$
Q_{20} [b]


SeaL1
HFB1
SkM*
SkM*$_{mod}$
^{240}Pu
HFB Energy [MeV]
Q_{20} [b]

^{240}Pu potential energy surface $E(Q_{20},Q_{30})$ together with fission trajectories in case of SeaLL1







E_{init} =-1813.9±1.1 MeV

N_H = 82.9±0.4, Z_H = 52.9±0.2, T_H = 1.15±0.08 MeV, Q_{20} = 2.58 ± 0.61b

N_L = 63.3±0.5, Z_L = 41.5±0.3, T_L = 1.19±0.12 MeV, Q_{20} = 17.09 ± 1.09b

TKE = 178.0±2.3 MeV

TXE = 33.5±5.1 MeV, E^*_H=19.5±3.8 MeV, E^*_L=14.0±1.9 MeV

TKE+TXE = 211.5±3.3 MeV

$$E^* = \frac{A}{10} T^2$$

E_{init} =-1808.0±2.4 MeV

N_H = 83.5±0.4, Z_H = 53.2±0.4, T_H = 1.11±0.08 MeV, Q_{20} = 2.59 ± 0.47b

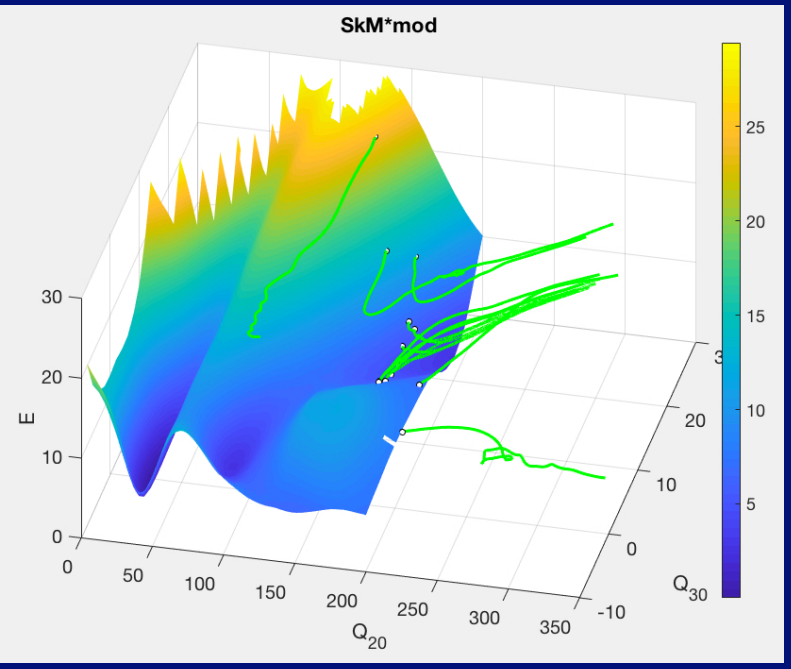
N_L = 62.8±0.5, Z_L = 41.1±0.4, T_L = 1.39±0.07 MeV, Q_{20} = 15.65 ± 0.91b

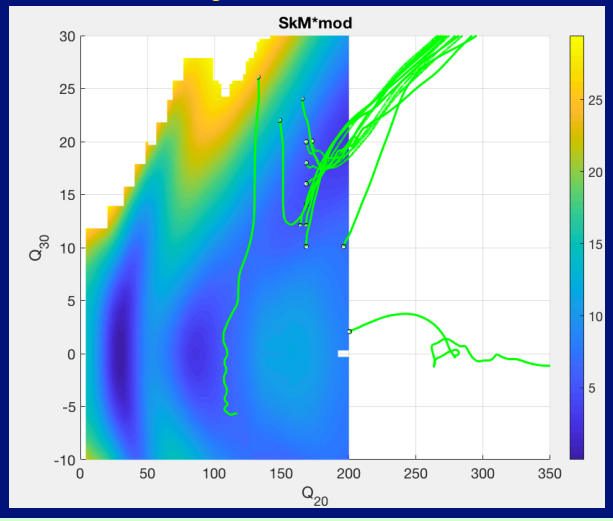
TKE = 177.8±2.8 MeV

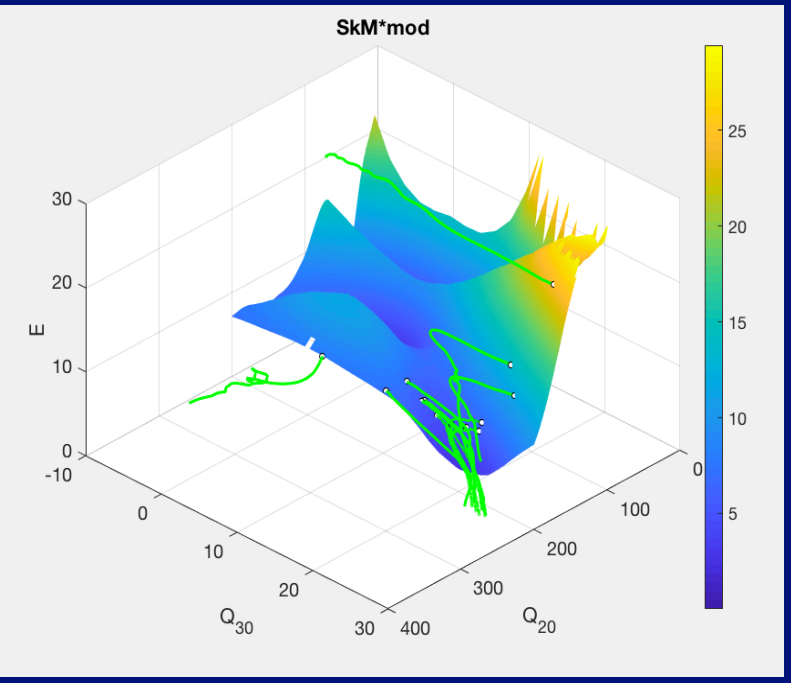
TXE = 37.1±2.7 MeV, E^*_H=17.0±2.4 MeV, E^*_L=20.1±2.0 MeV

TKE+TXE = 214.9± 2.4MeV

^{240}Pu potential energy surface $E(Q_{20},Q_{30})$ together with fission trajectories in case of SkM*mod







E_{init} =-1780.5±2.2 MeV

$N_H = 84.1\pm0.9,\ Z_H = 53.0\pm0.5,\ T_H = 1.10\pm0.10$ MeV, $Q_{20} = 3.5\pm0.9$ b

$N_L = 61.8\pm0.9,\ Z_L = 40.9\pm0.5,\ T_L = 1.20\pm0.09$ MeV, $Q_{20} = 11.3\pm1.3$ b

TKE = 174.5±2.5 MeV

TXE = 31.5±3.8 MeV , E^*_H=16.6±3.1 MeV, E^*_L=14.9±2.3 MeV

TKE+TXE = 206.0±2.4MeV

$$E^* = \frac{A}{10}T^2$$

"Symmetric" case

E_{init} =-1780.2 MeV

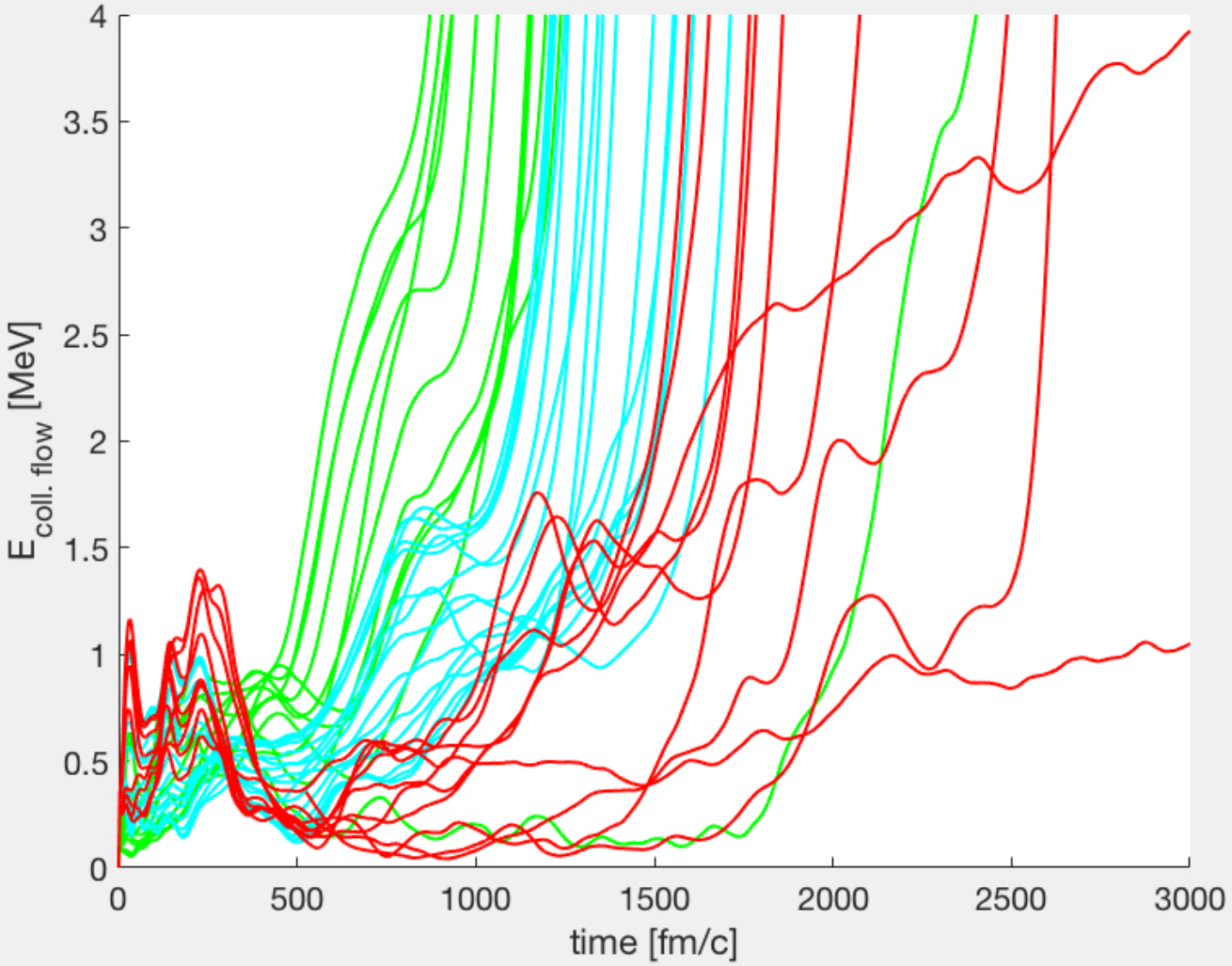
$N_L = 72.6,\ Z_L = 46.7,\ E^*_L = 28.5$MeV

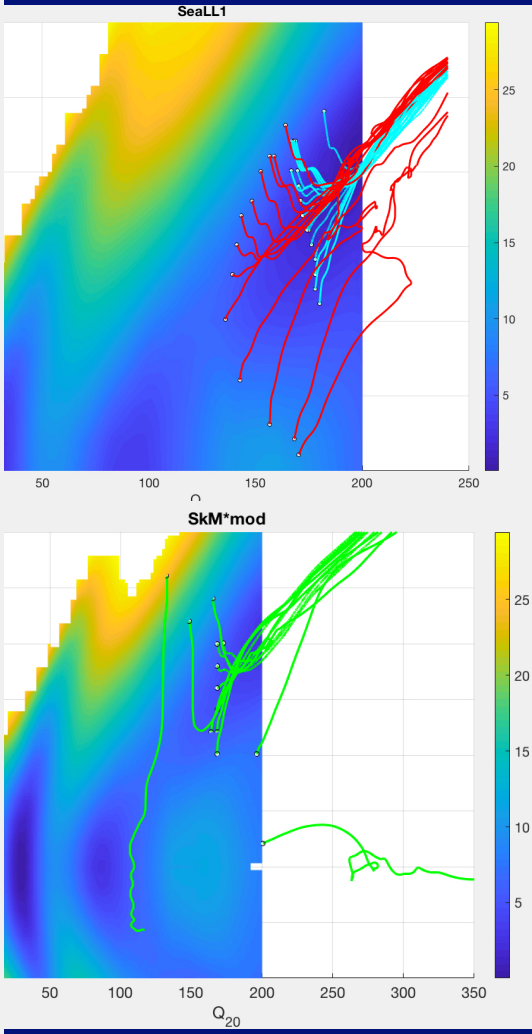
$N_H = 73.4,\ Z_H = 47.2,\ E^*_R = 29.4$MeV

TKE = 149.0 MeV

TXE = 57.9 MeV

TKE+TXE = 206.9 MeV





$$E_{coll.flow} = \int d^3r \frac{\vec{j}^2(\vec{r},t)}{2mn(\vec{r},t)}$$

$$\vec{j}(\vec{r},t) = \frac{i\hbar}{2}\sum_k \mathrm{v}_k^*(\vec{r},t)\vec{\nabla}\mathrm{v}_k(\vec{r},t) - \mathrm{v}_k(\vec{r},t)\vec{\nabla}\mathrm{v}_k^*(\vec{r},t)$$

$$n(\vec{r},t) = \sum_k \left|\mathrm{v}_k(\vec{r},t)\right|^2$$

Effective mass affects the rate at which single-particle levels change with shape

Pairing gaps are basically the same

Smaller effective mass leads to sharper variations of the single-particle levels

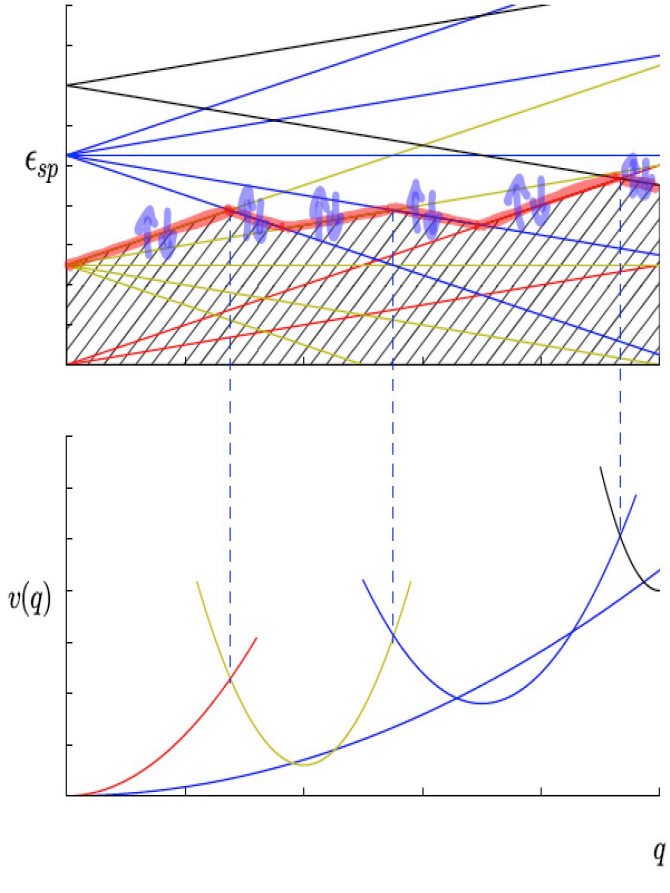
$$P_{LZ}(1 \Rightarrow 2) \propto \exp\left[-\frac{2\pi\Delta^2}{\hbar\dot{q}\dfrac{d(\varepsilon_2(q)-\varepsilon_1(q))}{dq}}\right] = \exp\left[-\#\frac{\Delta^2 m^*}{\dot{q}}\right]$$

$$\frac{d(\varepsilon_2(q)-\varepsilon_1(q))}{dq} \propto \frac{1}{m^*}$$

$m^* = 0.70m$ SLy4

$m^* = 0.79m$ SkM*

$m^* = m$ SeaLL1



Summary

- **While pairing is not the engine driving the fission dynamics, pairing provides the essential lubricant, without which the evolution may arrive quickly to a screeching halt.**

- **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 prior to neutron and γ emission, 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 fission 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. The "temperatures" of the fission fragments are not equal. As W. Mittig pointed recently that this could be the key mechanism to create long lived large nuclear systems with Z≈ 100!**

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