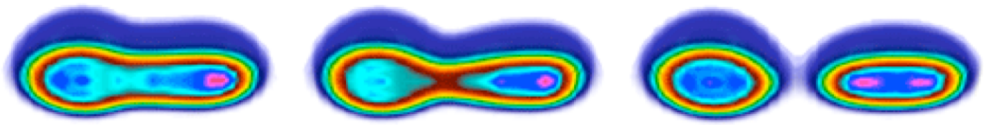
# Real time description of fission



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P. Magierski, N. Schunck, KJ Roche
T. Kawano, P. Talou

# Outline

- Overview of the fission process
- Dynamic models for fission
- Time-dependent density functional theory (TDDFT)
- Fission results from TDDFT
- Overview and outlook

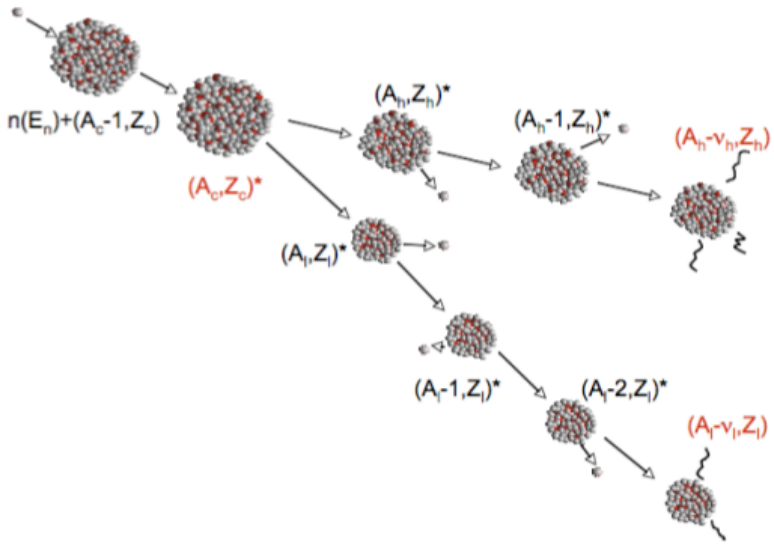
# Goals

- Understand fission from a microscopic model
- Estimate the validity of different approximations used in more phenomenological approaches
- Obtain trends of different observables that cannot be measured

**Not a goal: perfect agreement with experiment at this point**

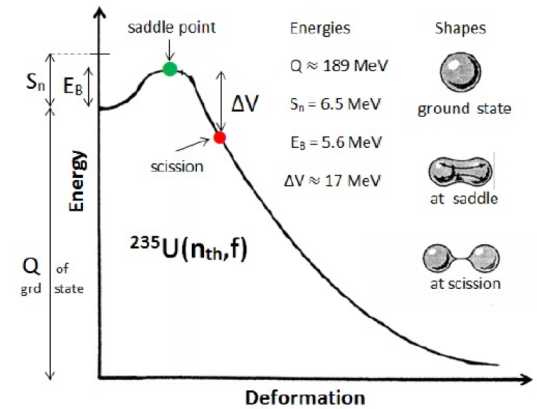
# Fission process

- Discovery: L. Meitner & J.A. O.R. Frisch, Nature **143** (1939) 239
- First theoretical model: N. Bohr & J.A. Wheeler, Phys. Rev 56 (1939) 426




All the information about fission (FF, prompt neutrons and gammas) comes after neutron emission

**Potential energy versus deformation**



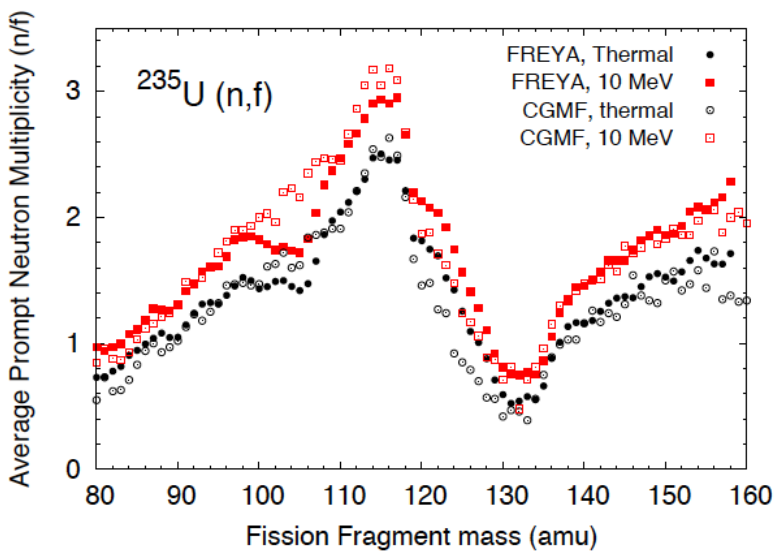

**Times**

- 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

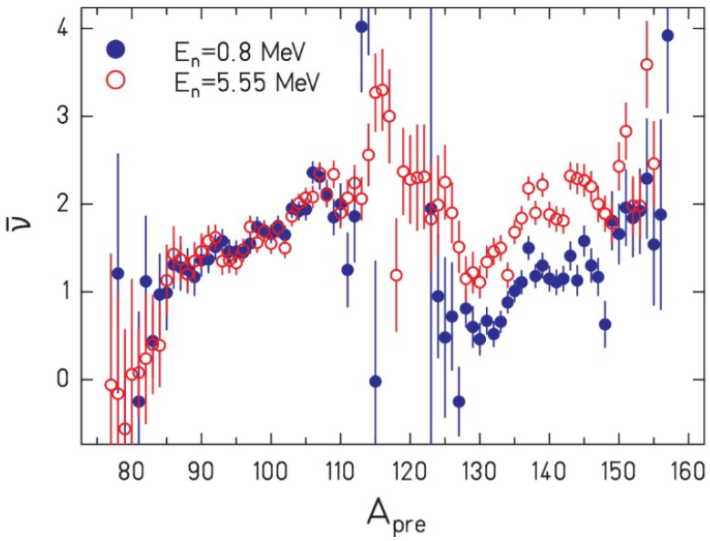
NOTE: 1 zs = 1 zeptosecond = 10^-21 s

Goennenwein, talk at FIESTA 2014

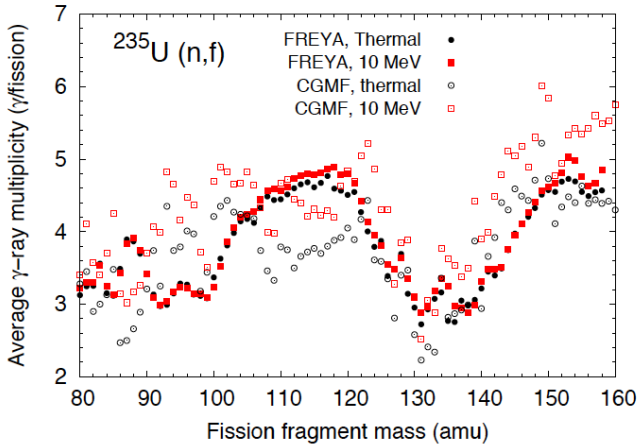
# Model and experiment: excitation energy dependence




Navqi et. al., PRC 34 (1986) 218



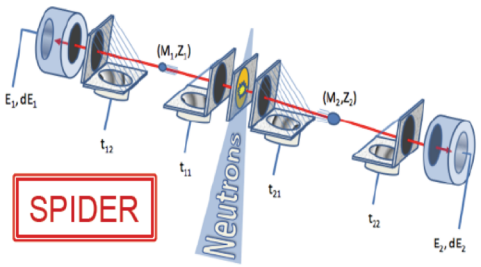

Excitation energy sharing between fragments varies with excitation energy in the fissioning system




- No much experimental information
- Directly connected with the average spin in the FF
- No direct connection with the excitation energy

New experimental results presented at FIESTA2017

# Fission observables goals

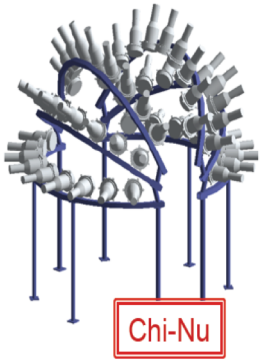



**Fission fragment distributions of:**

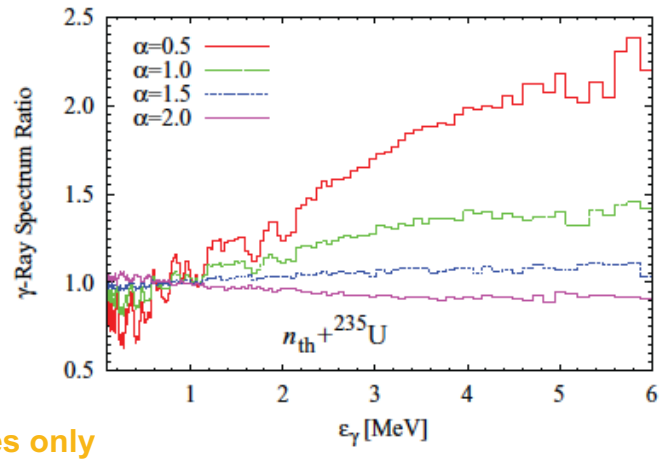
- ❑ mass
- ❑ charge
- ❑ TKE

Direct comparison with experiment (where available)

- ❑ angular momentum distribution
- ❑ sharing of excitation energy




Input into CGMF and comparison with prompt neutron and gamma-ray emission data



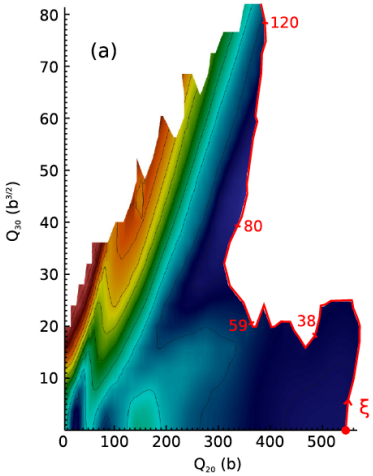

**At the moment: averages of one-body observables only (extensions possible)**

# Fission models

- Scission point model
  - Static model, based on a the structure of the energy surface
  - Y(A)
  - Low computational cost

- Macro-micro + Langevin
  - Based on a random walk on the energy surface
  - Classical dynamics, analog to classical model of diffusion
  - Collective Coordinate → Generalized coordinate → Conjugate momenta
  - Adiabatic approximation → ``cold'' FFs
  - Y(A, TKE)
  - Low computational cost

$$|\Psi(t)\rangle = \int d\mathbf{q}\, f(\mathbf{q},t)|\Phi(\mathbf{q})\rangle$$




- DFT + TDGCM
  - Based on DFT
  - Adiabatic approximation
  - Y(A, TKE)
  - Moderate-high computational cost

- TD-SLDA
  - Based on a time-dependent formulation of the superfluid-local-density approximation
  - Y(A, TKE, $E^*_L$, $E^*_H$, $J_L$, $J_H$)

# Density functional theory

For any Hamiltonian

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

There is an **exact** one to one correspondence between the many-body wave function, the external field and the density. The ground-state energy of the system can be obtained by minimizing a **universal** EDF

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

The DFT we use is phenomenological and **local**

$$\rho(\vec{r}) = \sum_n^A |\phi_n(\vec{r})|^2$$

$$\left( -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r}) + V_{ext}(\vec{r}) \right) \phi_n(\vec{r}) = \epsilon_n \phi_n(\vec{r})$$

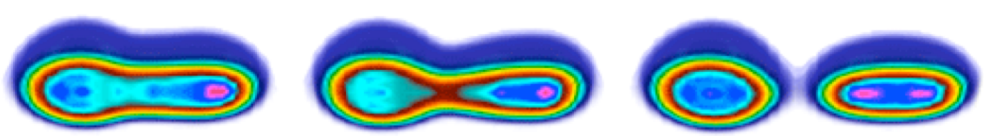
$$\tau(\vec{r}) = \sum_n^A |\nabla\phi_n(\vec{r})|^2$$

For superfluid systems, we use a local pairing field $\Delta(\vec{r}) = -g(r)\,\nu^*(\vec{r})$ and the equations are formally equivalent to HFB/BdG

# Time-dependent density functional theory implementation for local functionals

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

- Lattice implementation on a 3D special lattice (continuum well represented)
- Fully self consistent
- No symmetry restrictions
- Requires somewhat large computational resources:
  - Adams-Bashforth-Milne fifth order predictor-corrector-modifier
  - FFTW for derivatives
  - Number of equations solved ~ number of lattice points (from thousands to 1-2 million)

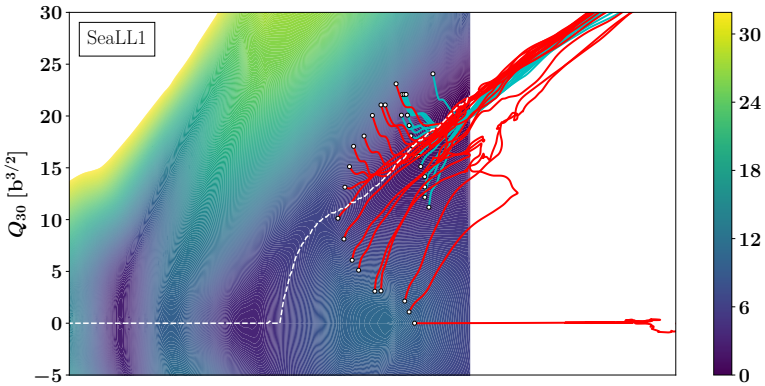


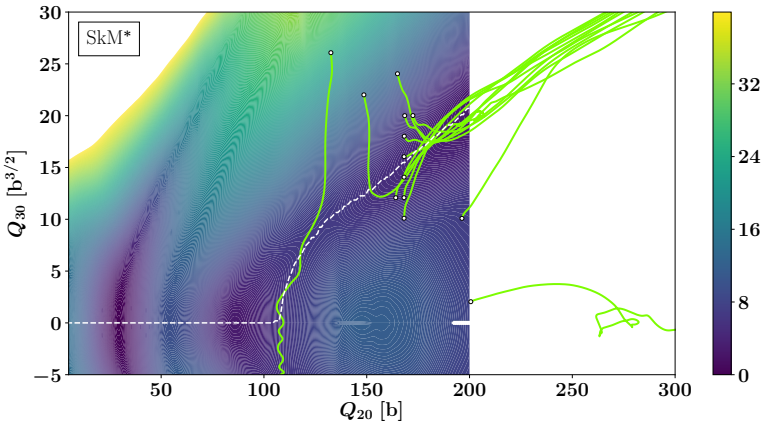
| Code | CUs | Computer | PDEs | Lattice | Cost (sec.) |
|---|---|---|---|---|---|
| Sky3D [63] | 128 | Titan | 1,024 | $18^2 \times 30$ | $3.86 \times 10^{-6}$ |
| U&S [64] | 16 | Linux cluster | 714 | $40^2 \times 70$ | $8.72 \times 10^{-5}$ |
| TDSLDA | 514 | Titan | 442,368 | $24^2 \times 48$ | $4.35 \times 10^{-8}$ |
| TDSLDA | 256 | Piz Daint | 442,368 | $24^2 \times 48$ | $1.26 \times 10^{-8}$ |
| TDSLDA | 240 | Summit | 442,368 | $24^2 \times 48$ | $1.05 \times 10^{-8}$ |
| TDSLDA-simp | 2 | Titan | 684 | $20^2 \times 60$ | $7.55 \times 10^{-8}$ |

# General applications of TD-DFT

- Description of structure, creation and decay of quatized vortices in Fermi superfluids
- Microscopic description of incipient phases of quantum turbulencce in Fermi superfluids, crossing and recombination of vortices
- Creation of domain walls, quantized vortices and vortex rings, their dynamics and decay; quantum shock waves
- Microscopic description of quantized votices in neutron matter
- Interaction of quantized vortices with nuclei in neutron star crust
- Coulomb excitation of nuclei
- **Nuclear fission**
- Collisions of heavy nuclei

# Fission fragments from TDSLDA for $^{240}$Pu*



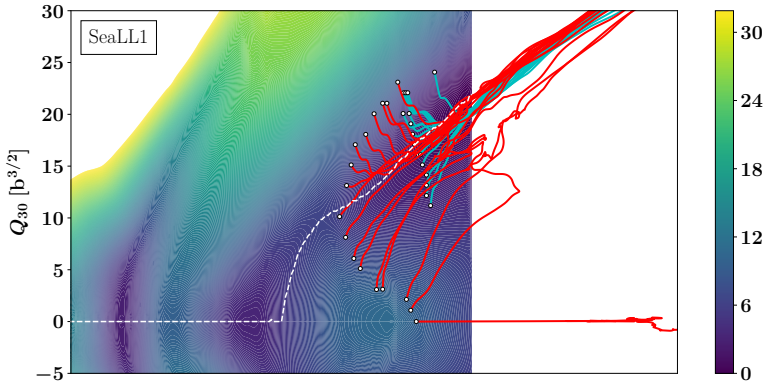

| NEDF | $E^*_{\rm ini}$ | TKE | $N_{\rm H}$ | $Z_{\rm H}$ | $N_{\rm L}$ | $Z_{\rm L}$ | $E^*_{\rm H}$ | $E^*_{\rm L}$ | TXE | TKE+TXE | $\tau_{s\to s}$ (fm/c) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| SeaLL1-1asy | 7.9(1.7) | 177.8(3.1) | 83.4(0.4) | 53.2(0.4) | 62.9(0.5) | 41.1(0.4) | 17.1(3.0) | 20.3(2.0) | 37.4(3.1) | 215.2(2.5) | 2317(781) |
| SeaLL1-2asy | 2.6(1.8) | 178.0(2.3) | 82.9(0.4) | 52.9(0.2) | 63.3(0.5) | 41.5(0.3) | 19.5(3.8) | 14.0(1.9) | 33.5(5.1) | 211.5(3.3) | 1460(176) |
| SeaLL1-sy | 9.2 | 147.1 | 77.5 | 48.9 | 68.8 | 45.4 | 45.2 | 29.0 | 74.2 | 221.3 | 10103 |
| SkM*-asy | 8.2(3.0) | 174.5(2.5) | 84.1(0.9) | 53.0(0.5) | 61.8(0.9) | 40.9(0.5) | 16.6(3.1) | 14.9(2.3) | 31.5(3.8) | 206.0(2.4) | 1214(448) |
| SkM*-sy | 9.6 | 149.0 | 73.4 | 47.2 | 72.6 | 46.7 | 29.4 | 28.5 | 57.9 | 206.9 | 3673 |

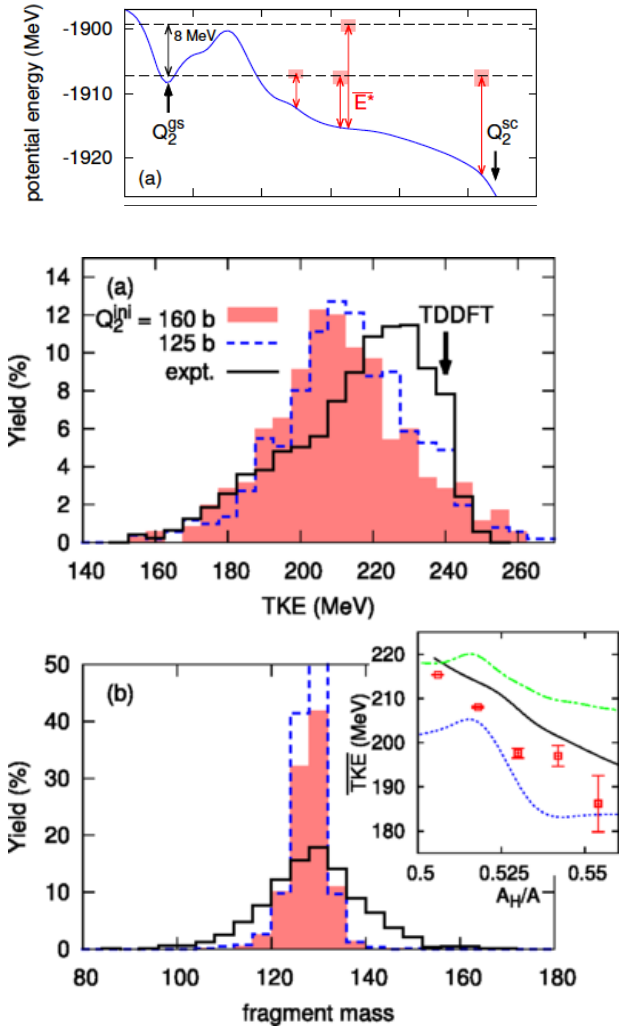
- Large number of initial conditions, but small dispersion (focusing effect)
- Different energy sharing mechanism for neutron-induced and spontaneous fission (mass yields significantly different)

Bulgac et. al., arXiv:1806.00694 (2018)

# Comparison with TDHF+BCS

$^{240}$Pu

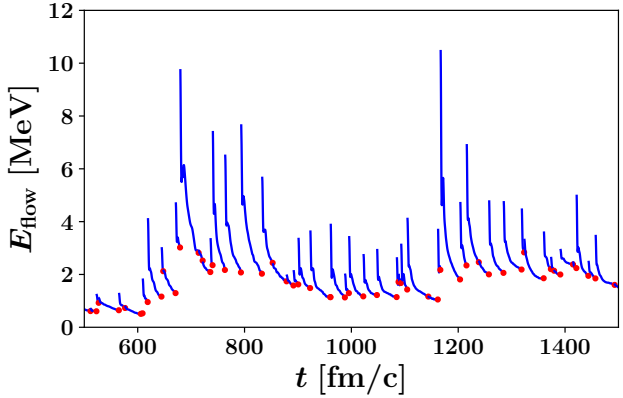


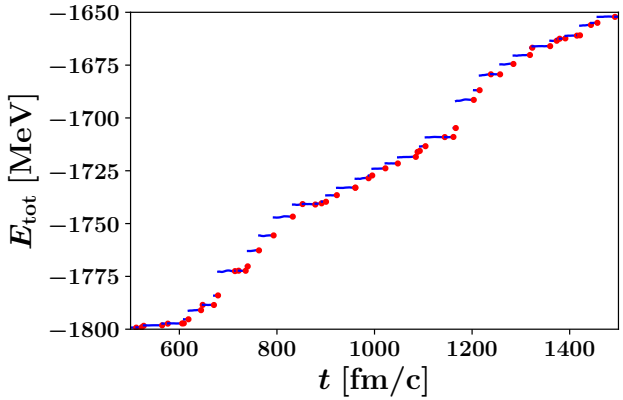



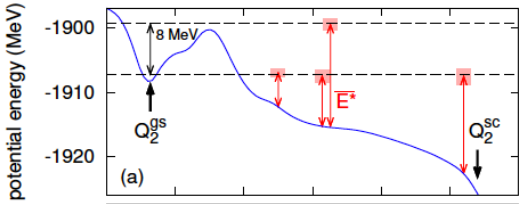

- Our calculation does not support the large width of the mass distribution due to initial conditions

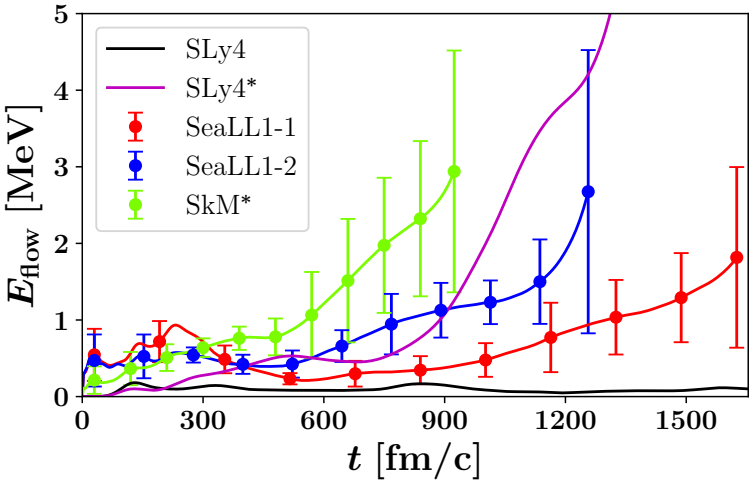
Tanimura et. al, PRL **188**, 152501 (2017)

# Strong one-body dissipation




$$E_{flow} = \int d^3r \frac{|\vec{p}(\vec{r},t)|^2}{2M_n n(\vec{r},t)}$$

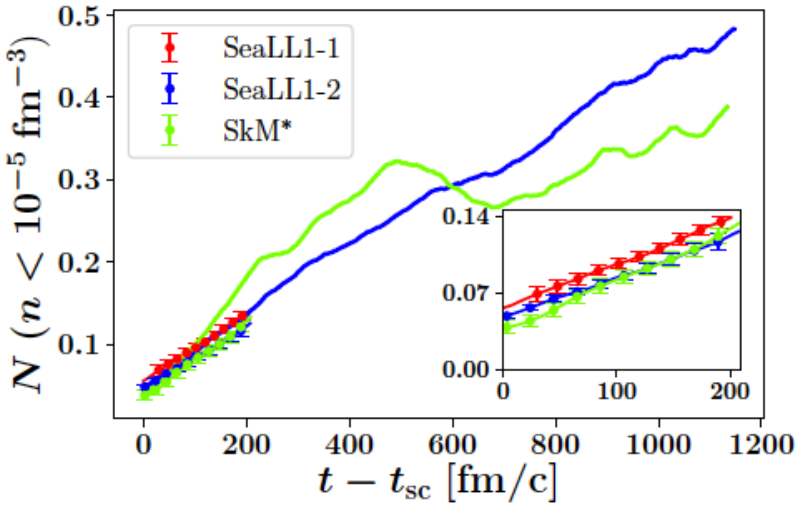
- Saddle-to-scission: viscous fluid, with the trajectory following predominantly the steepest descent => microscopic justification of the overdamped Brownian motion approach (Moller and Randrup)
- Langevin dynamics should be driven by force given by the gradient of the free energy:

$$F_Q = -\nabla \left(E_{int} - TS(Q,T)\right)$$

(generalization of the work by Ward et. al., PRC 95, 024618 (2017))

# Evidence for neutron emission during scission/acceleration

$^{240}$Pu




Robust independence of the initial conditions and nuclear energy density functional used

# Summary and outlook

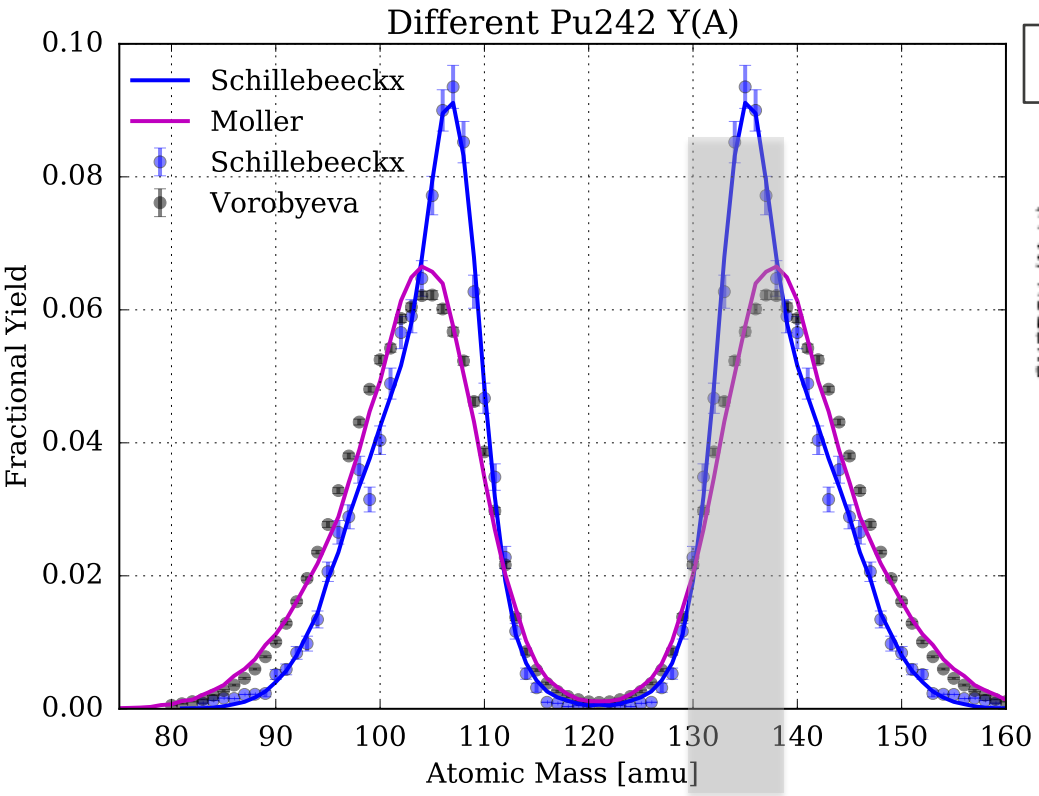
- In nuclear physics, TD-SLDA applied to the description of
  - Linear response: IVGDR
  - LACM: Relativistic Coulomb Excitation of a heavy nucleus and **FISSION**
- Encouragingly accurate description of fission observables (not perfect)
- The spread in initial conditions are not enough to explain the observed widths in mass yields
- Strongly overdamped motion, strong one-body dissipation
- Evidence for emitted neutrons at scission and during the acceleration

- Investigation of other observables (e.g., angular momenta)
- Fluctuations

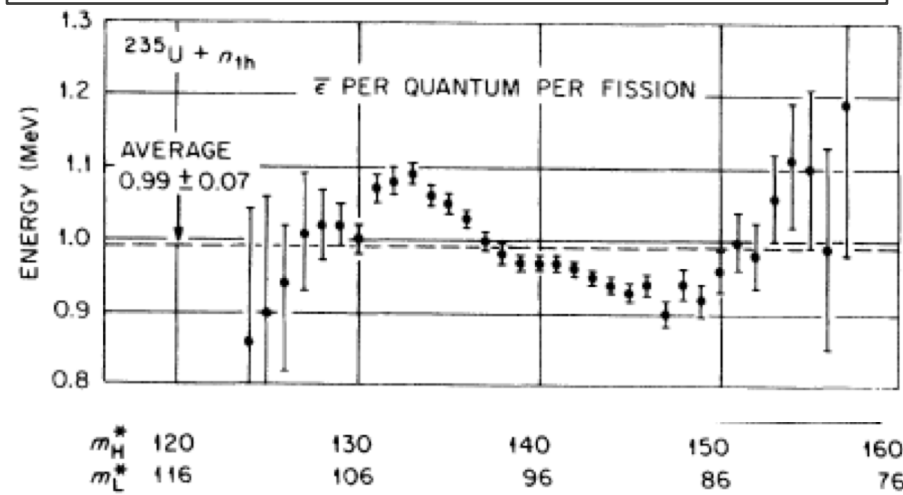
# Additional slides

# Yields in (n,f) vs. (sf)

- Both model (Möller) and data show wider Y(A) in (n,f)
- Y(A) for (sf) are sharply peaked near N=82 closure!




F. Pleasonton *et al.* PRC **6** 1023 (1972)




Avg. $E_\gamma$ increase is a property of products ρ, $J^\pi$, and $U^*$

Courtesy P. Jaffke