Modern approaches to fission

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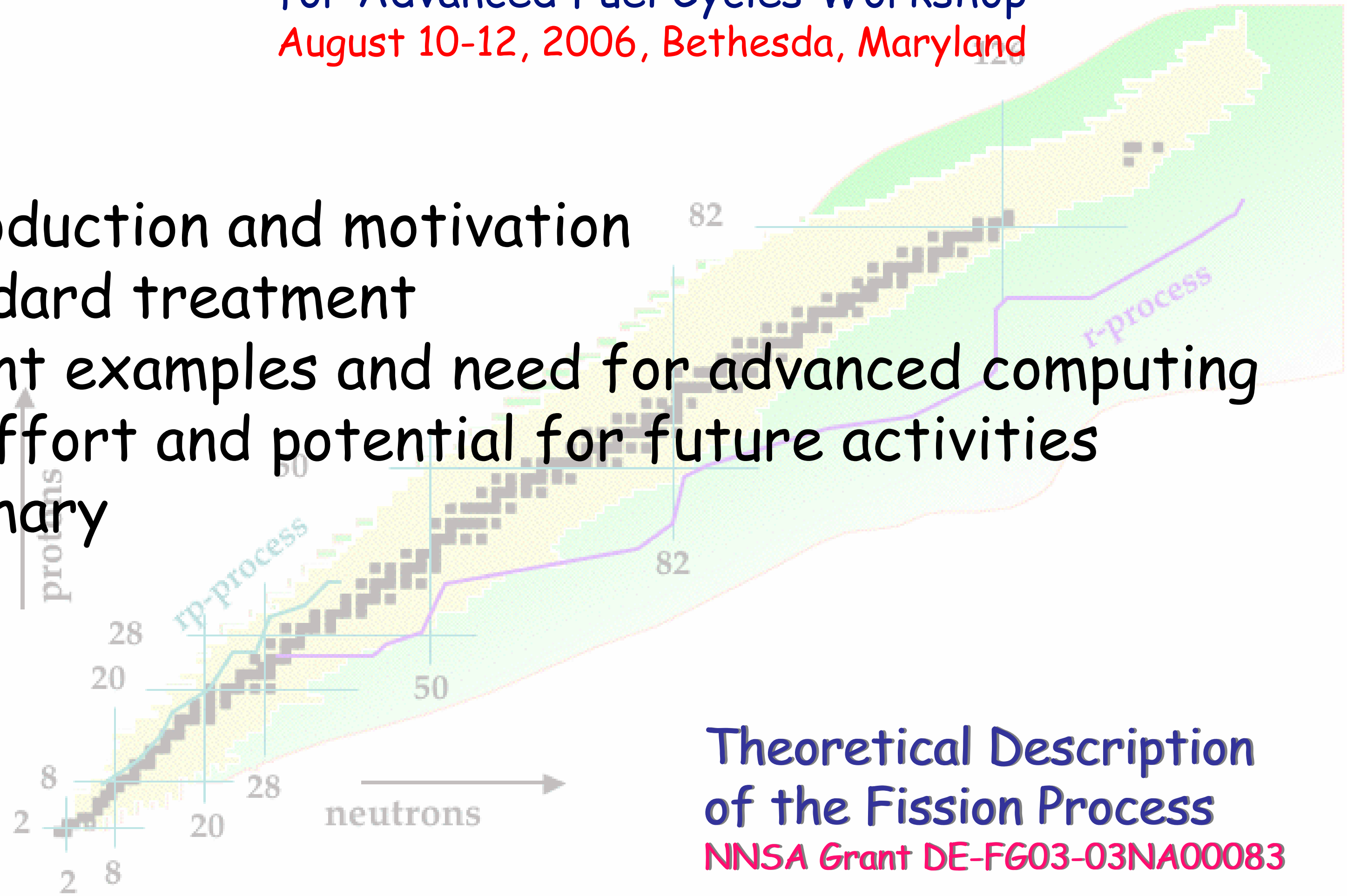
Nuclear Physics and Related Computational Science R&D
for Advanced Fuel Cycles Workshop

August 10-12, 2006, Bethesda, Maryland

- Introduction and motivation
- Standard treatment
- Recent examples and need for advanced computing
- US effort and potential for future activities
- Summary



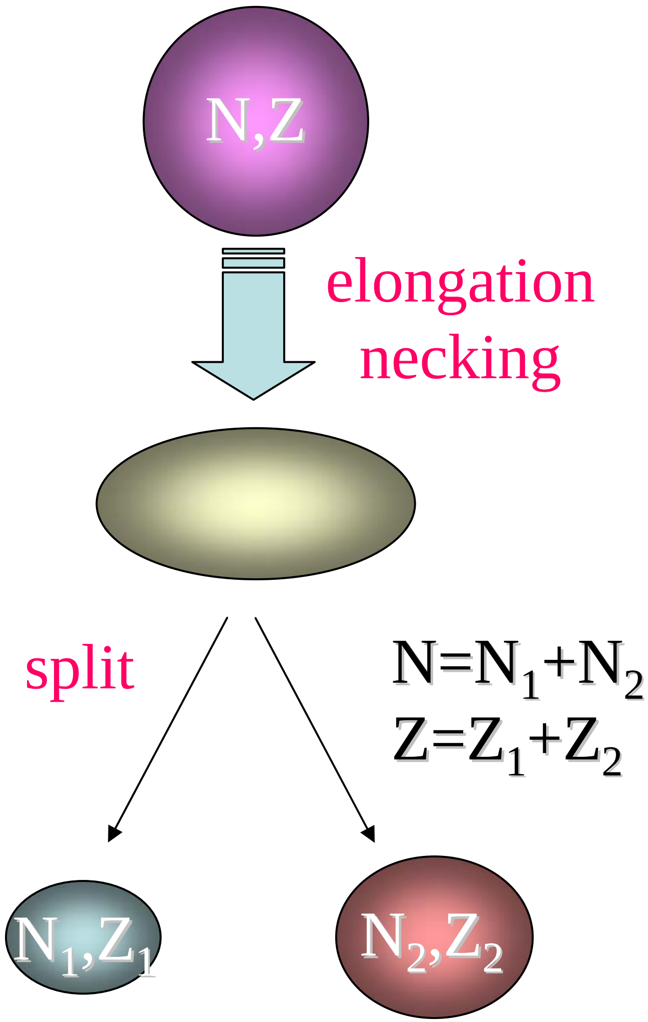
Theoretical Description of the Fission Process

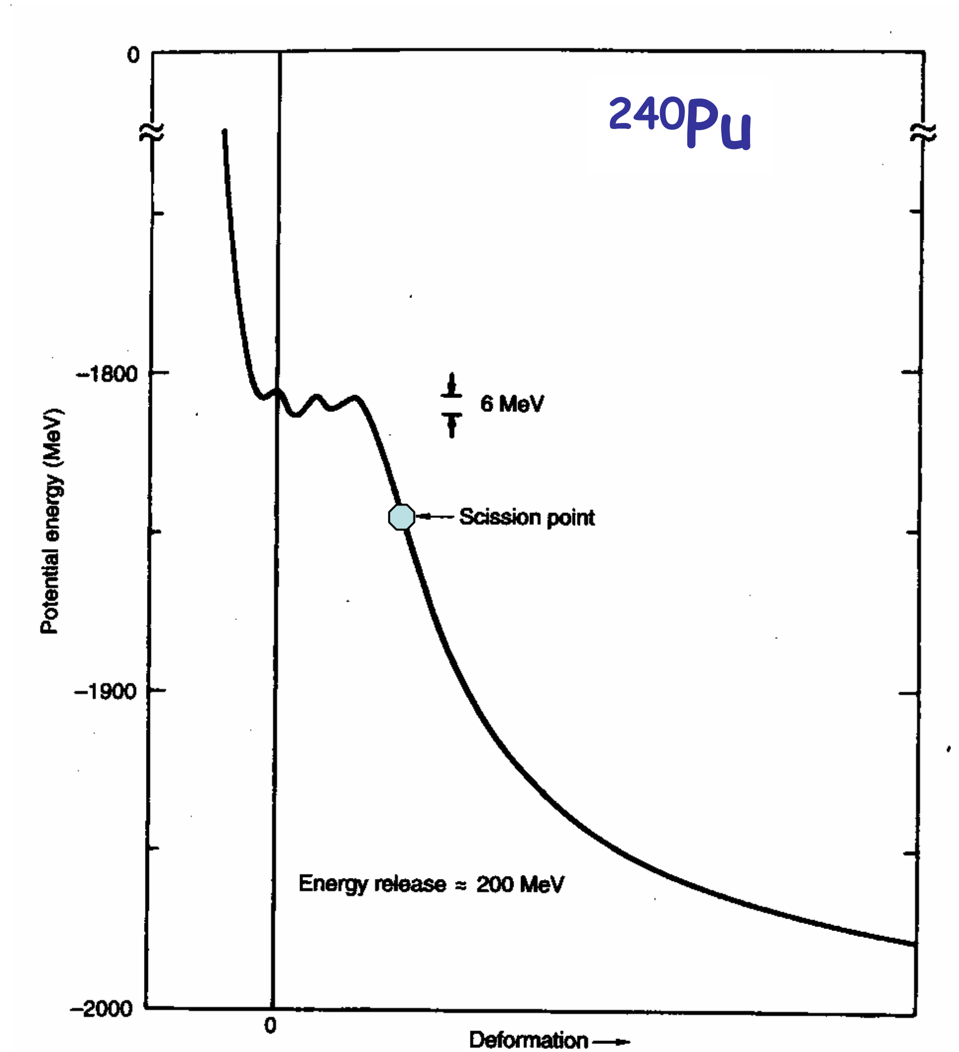
NNSA Grant DE-FG03-03NA00083

http://www.phys.utk.edu/witek/fission/fission.html

Fission

1938 - Hahn & Strassmann
1939 - Meitner & Frisch
1939 - Bohr & Wheeler
1940 - Petrzhak & Flerov

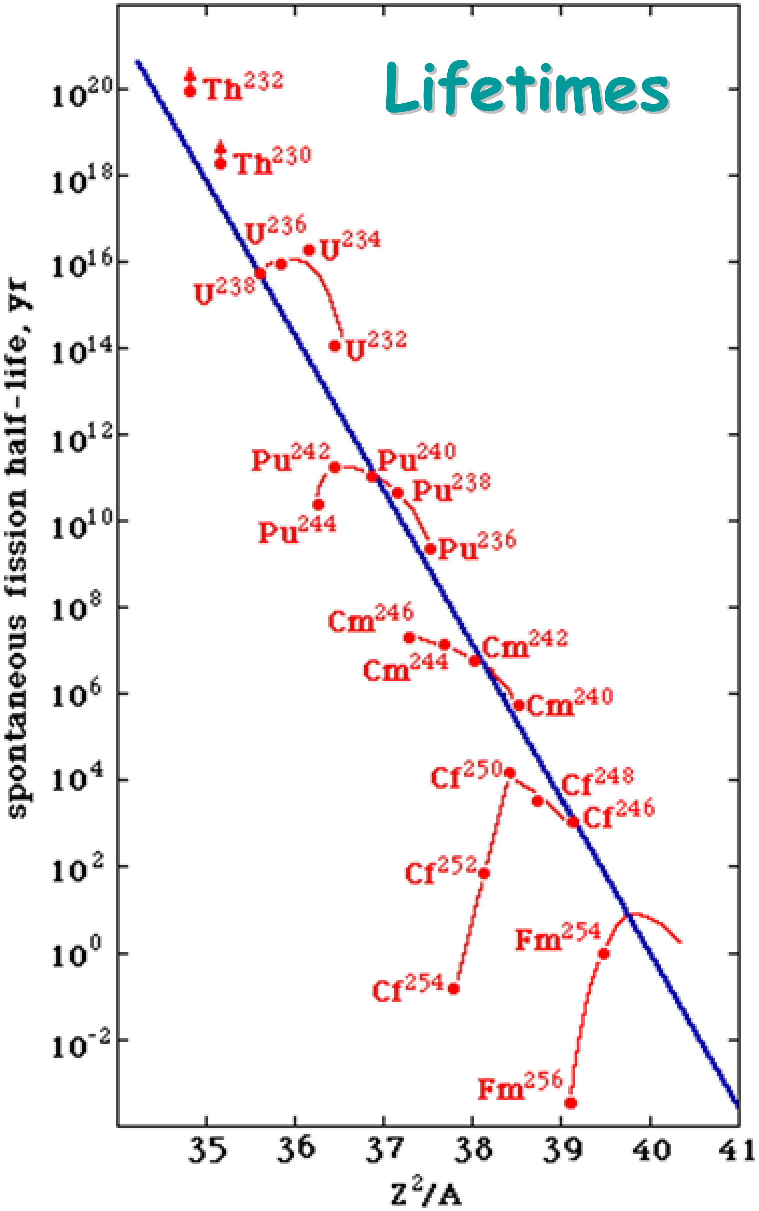




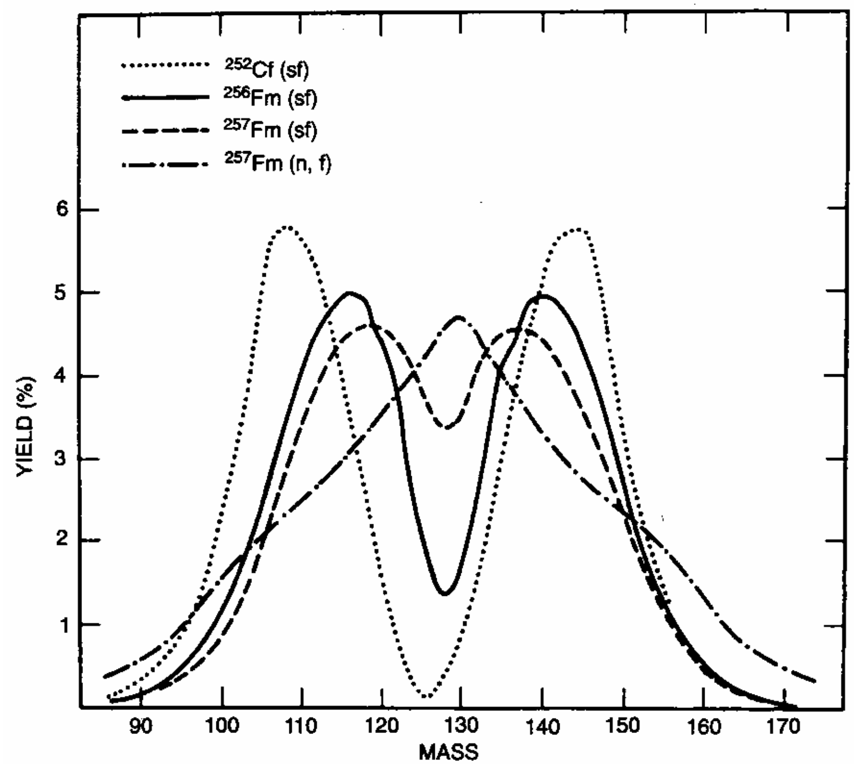
Spontaneous and Induced Fission

n, d, EM...

Lifetimes

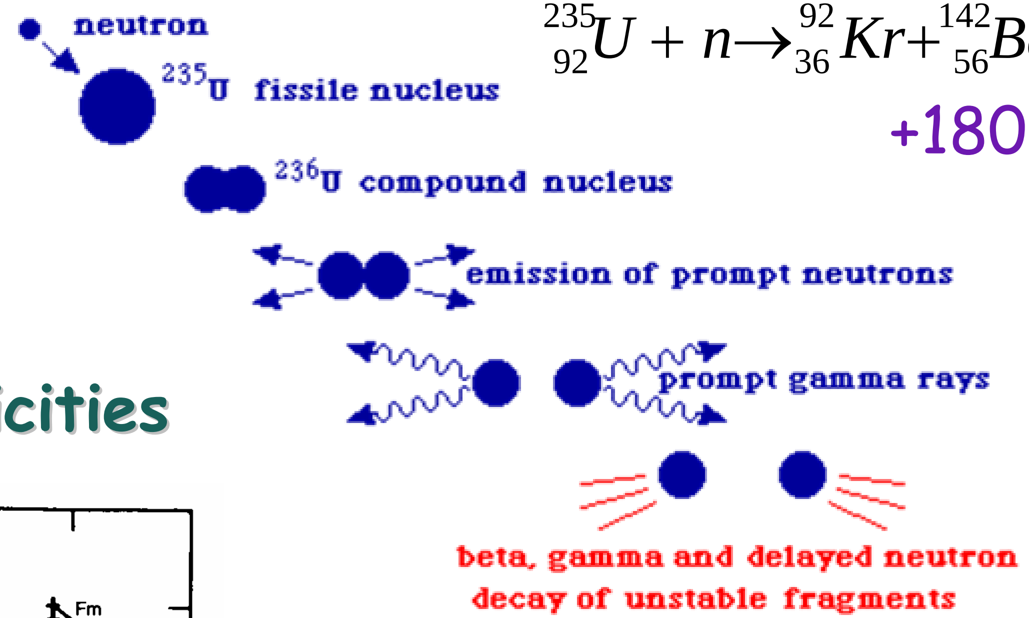


Fragment distributions

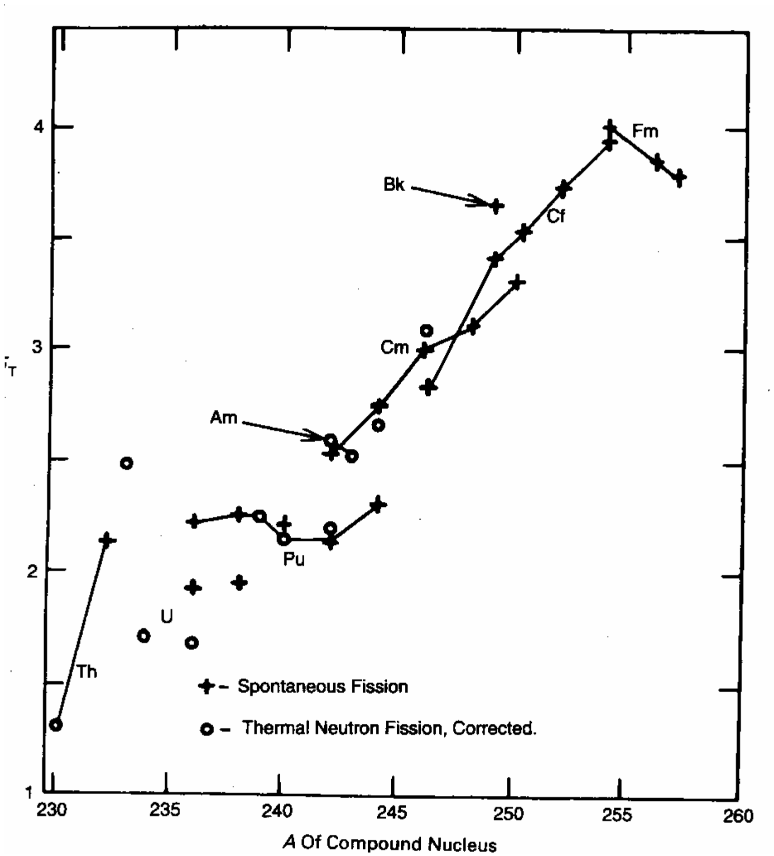


$$^{235}_{92}U + n \rightarrow ^{92}_{36}Kr + ^{142}_{56}Ba + 2n$$

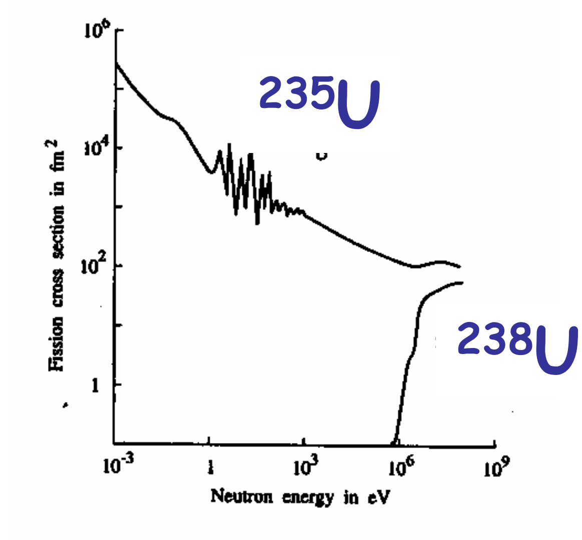
+180 MeV



Neutron multiplicities



Cross sections



Fission and Fusion

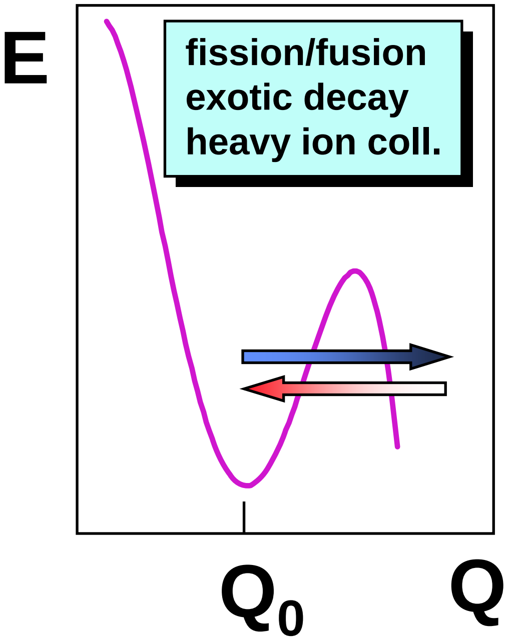
nuclear collective dynamics

Variety of phenomena:

- symmetry breaking and quantum corrections
- LACM: fission, fusion, coexistence
- phase transitional behavior

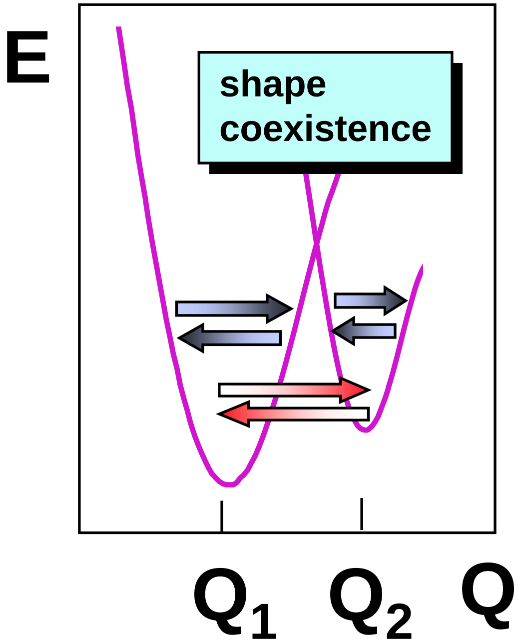
Significant computational resources required:

- Generator Coordinate Method
- Projection techniques
- Imaginary time method (instanton techniques)
- QRPA and related methods
- TDHFB, ATDHF, and related methods



<u>Challenges:</u>

- selection of appropriate degrees of freedom
- treatment of symmetry breaking effects
- coupling to continuum in weakly bound systems
- dynamical corrections; fundamental theoretical problems.
    - rotational, vibrational, translational
    - particle number
    - isospin



Powerful phenomenology exists…

… but no satisfactory microscopic understanding of:

- Barriers
- Fission half-lives
- Fission dynamics
- Cross sections
- …

What is needed?

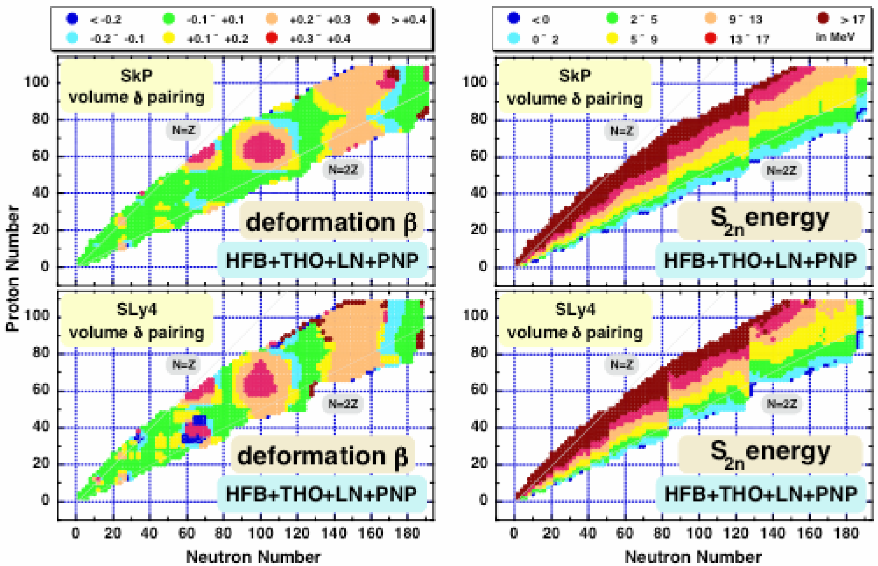
- Effective interaction (UNEDF)
- Microscopic many-body technique

Nuclear DFT

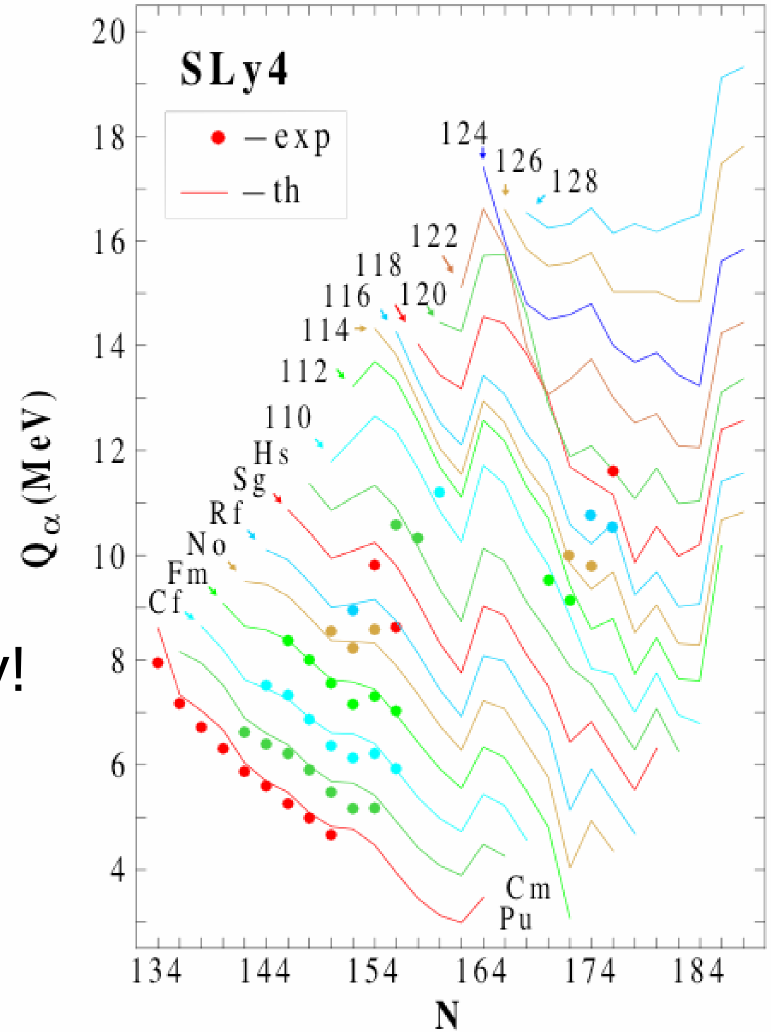
From Qualitative to Quantitative!

Microscopic Mass Table

M.V. Stoitsov et al., nucl-th/0406075
J. Dobaczewski et al., nucl-th/040407



S. Cwiok, P.H. Heenen, W. Nazarewicz
Nature, 433, 705 (2005)



Deformed Mass Table in one day!

- HFB mass formula: Δm~700keV
- Good agreement for mass differences

UNEDF (SCIDAC-2) will address this question!

A comment on time scales…

$$T_{1/2} = \ln 2 \frac{\hbar}{\Gamma}, \qquad \hbar = 6.58 \cdot 10^{-22}\ \mathrm{MeV} \cdot \mathrm{sec}$$

Can one calculate Γ with sufficient accuracy?

$$T_{s.p.} \approx 3 \cdot 10^{-22}\,\mathrm{sec} = 3\,\mathrm{baby}\,\mathrm{sec}.$$

^{238}U: $T_{1/2}$=10^{16} years

^{256}Fm: $T_{1/2}$=3 hours

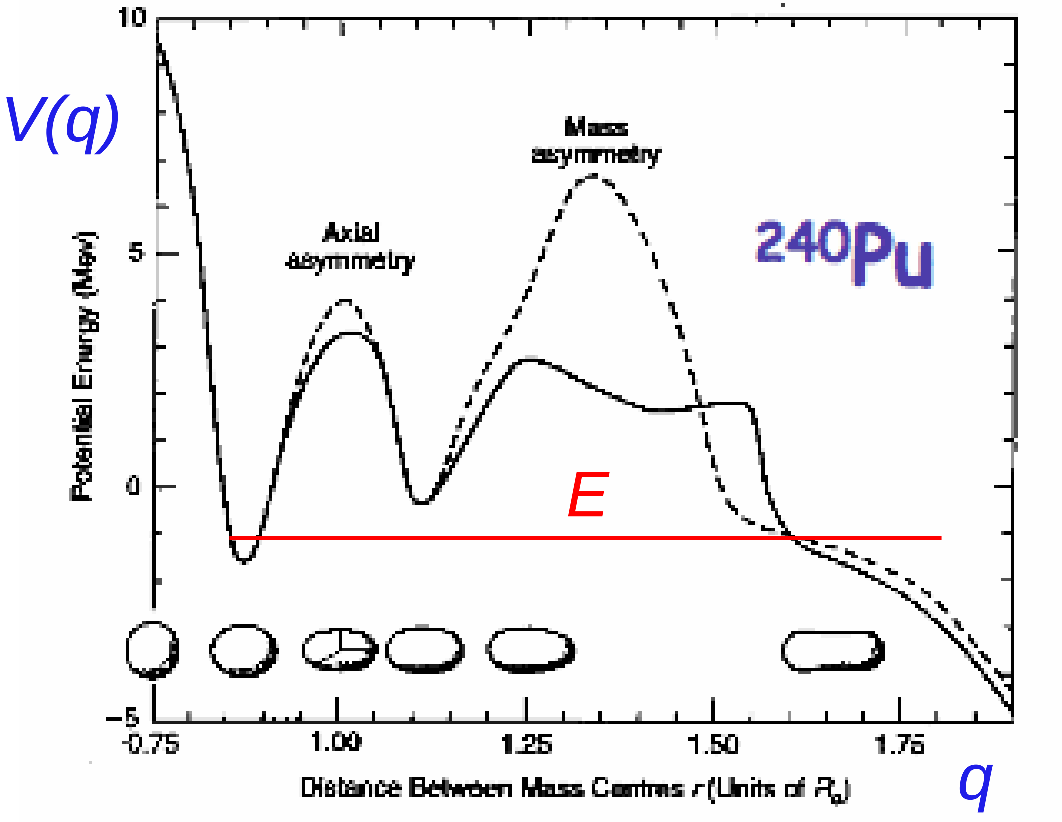
For very narrow resonances, explicit time propagation impossible!

Adiabatic Approaches to Fission

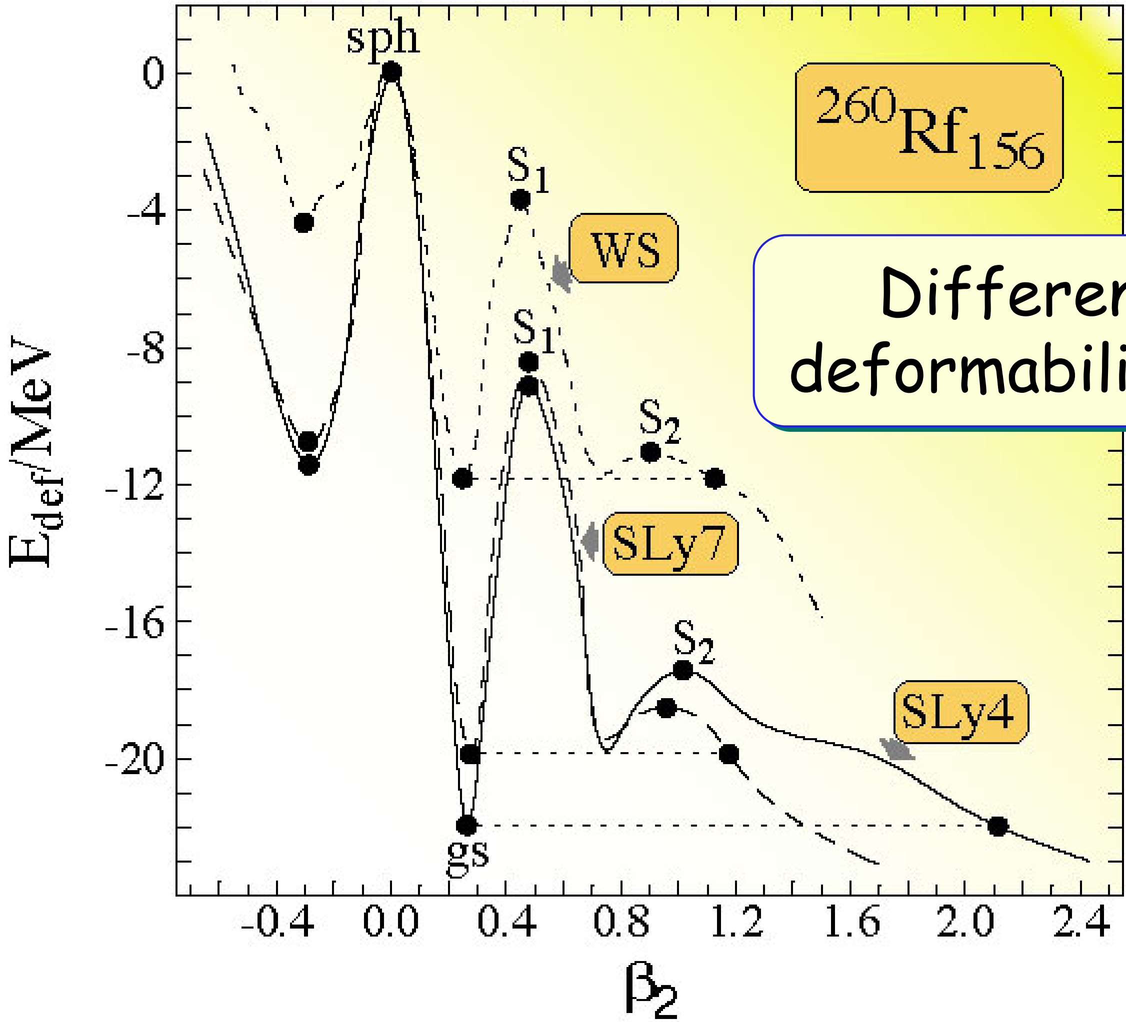
WKB: $$S(L) = \frac{2}{\hbar}\int_L \sqrt{2B(\mathbf{q})[V(\mathbf{q}) - E]}\, dq$$

collective inertia (mass parameter)

multidimensional space of collective parameters



Collective potential V(q)



Different deformabilities!

Universal nuclear energy density functional is yet to be developed

ice of collective
ameters

How to define a barrier?
How to connect valleys?

Dynamical corrections going beyond mean field important

- Center of mass
- Rotational and vibrational (zero-point quantum correction)
- Particle number

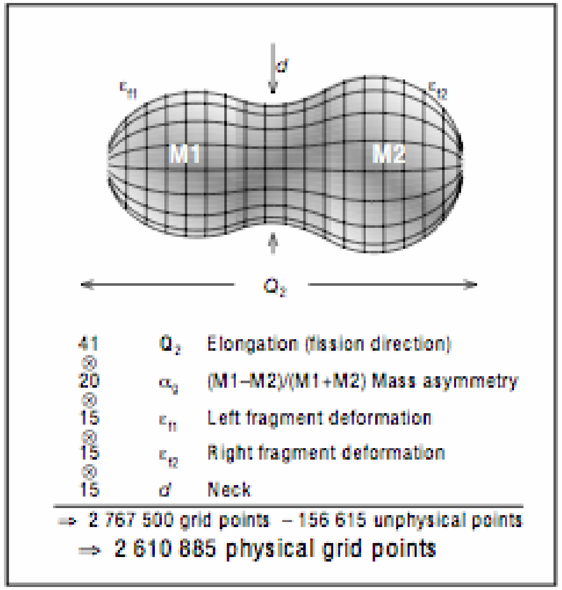
$$V(q) \rightarrow V(q) - (E_{\mathrm{ZPE},\beta} + E_{\mathrm{ZPE,rot}})$$

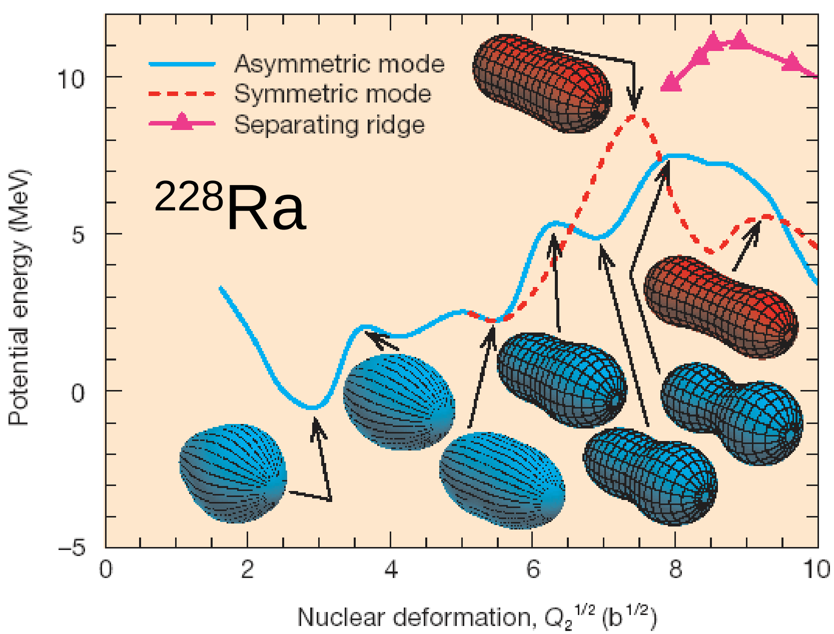
$$\log T_{\mathrm{sf}} = -20.54 + \log\left[1 + \exp\left(2S(L_{\mathrm{min}}\right)\right] - \log\left(2E_{\mathrm{ZPE}}\right)$$

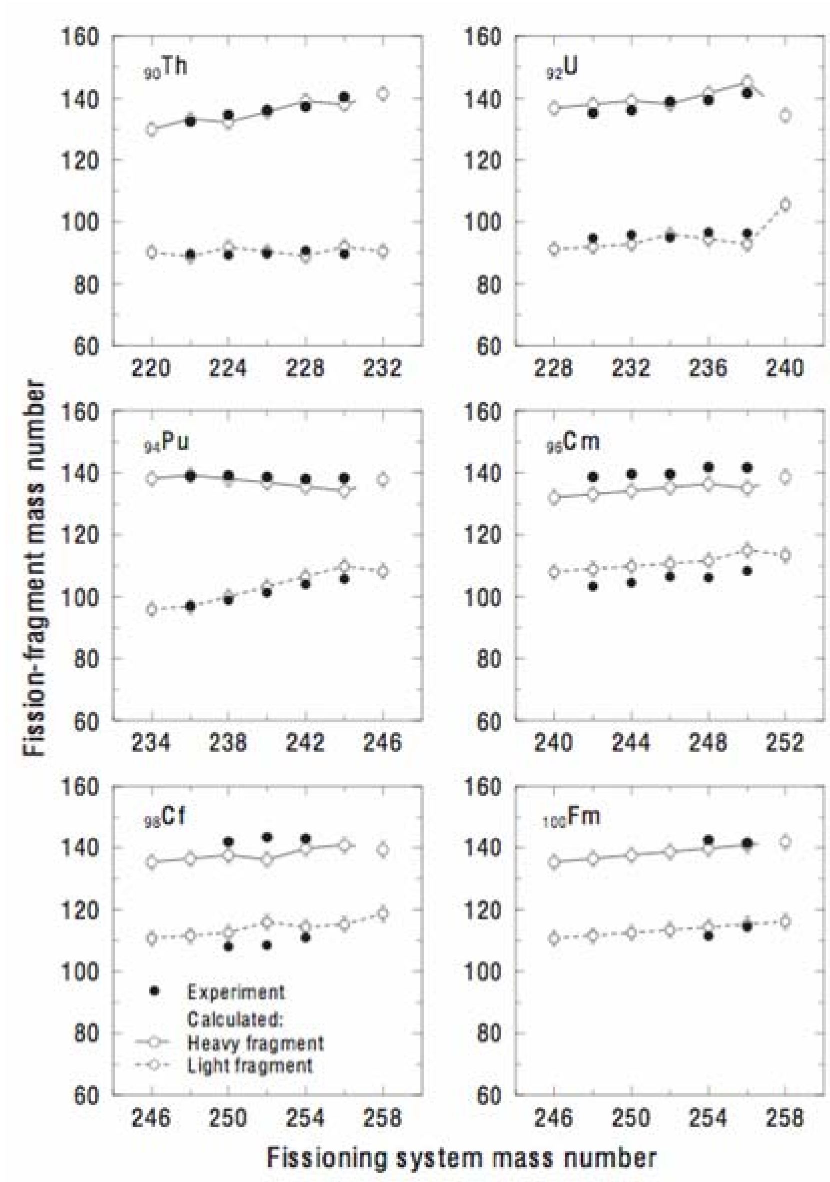
Static description (micro-macro)

Möller et al., Nature 409, 785 (2001)

- 5D landscapes
- Bimodal fission
- “Flooding” algorithm
- Saddle points
- Outer barrier and scission shapes







Collective inertia B(q) and ZPE

$$S(L) = \frac{2}{\hbar} \int_L \sqrt{2B(\mathbf{q})[V(\mathbf{q}) - E]}\, dq$$

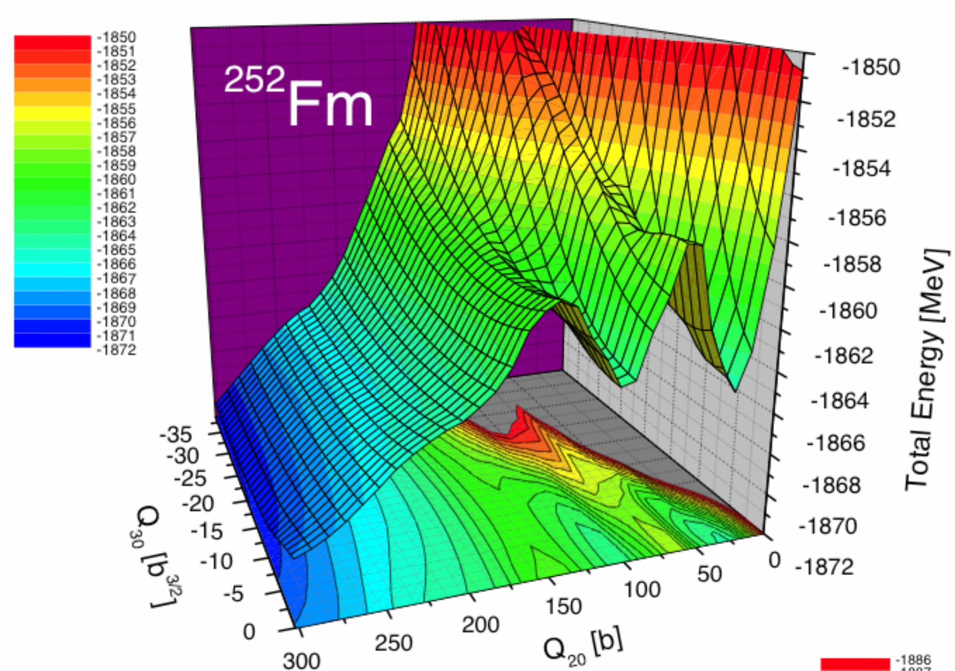
The action has to be minimized by, e.g., the dynamic programming method. It consists of calculating actions along short segments between adjacent, regularly spaced hyperplanes, perpendicular to the q-direction [A. Baran et al., Nucl. Phys. A361, 83 (1981)]

Various prescriptions for collective inertia and ZPE exist:

GOA of the GCM Ring and P. Schuck, The Nuclear Many-Body Problem, 1980

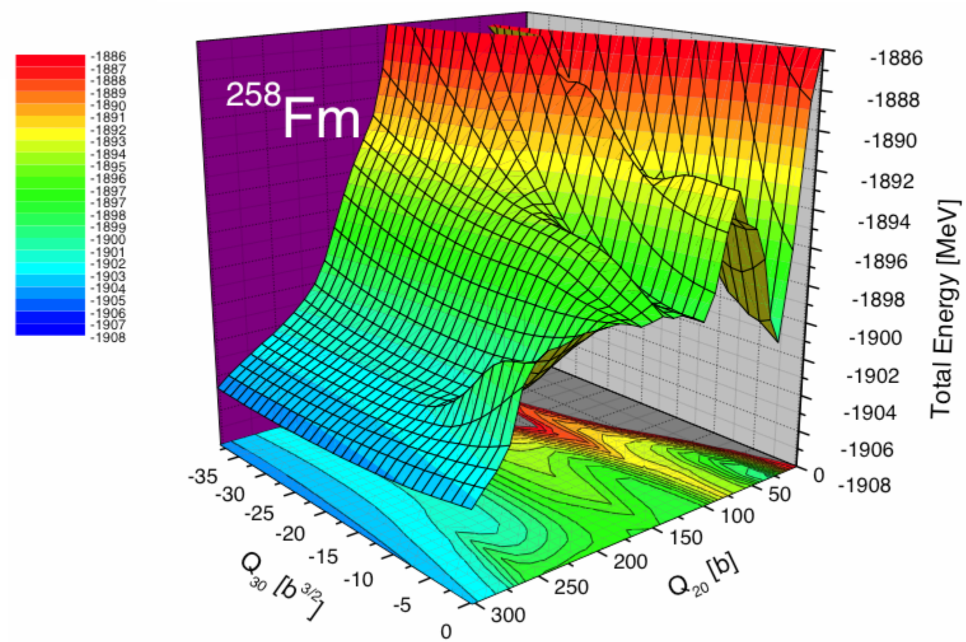
ATDHF+Cranking Giannoni and Quentin, Phys. Rev. C21, 2060 (1980);
Warda et al., Phys. Rev. C66, 014310 (2002)
Goutte et al., Phys. Rev. C71, 024316 (2005)

Self-consistent Static Fission Paths Calculations



A. Staszczak, J. Dobaczewski
W. Nazarewicz, in preparation

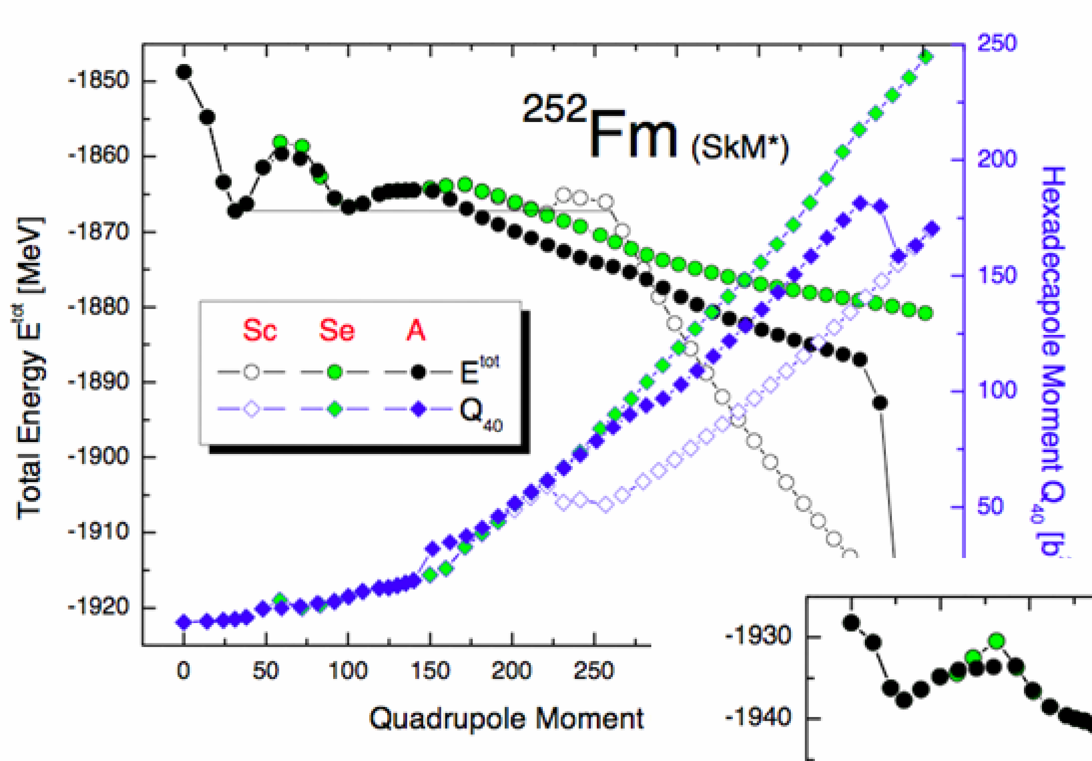
See also L. Bonneau,
Phys. Rev. C74, 014301 (2006)



See also:

A. Warda et al., Phys. Rev. C66, 014310 (2002)
and IJMP E13, 169 (2004) **Gogny**

A. Staszczak et al., IJMP E14, 395 (2005) **Skyrme**



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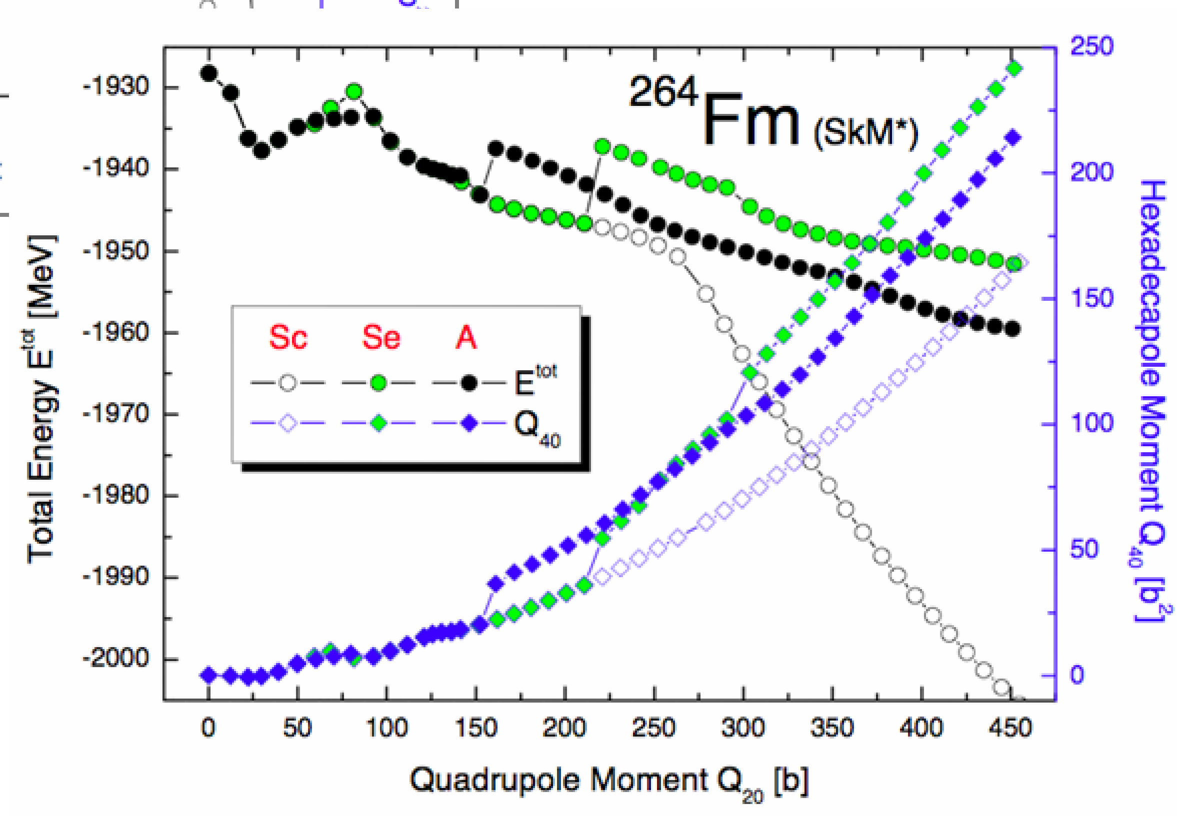
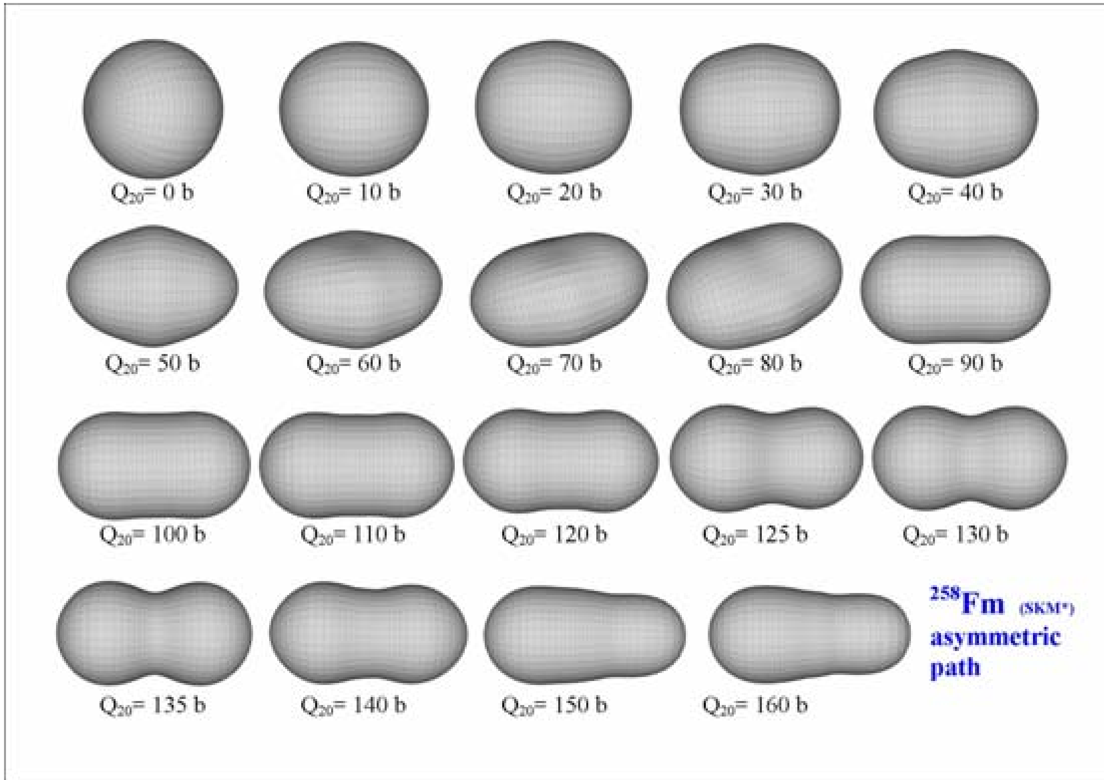
W. Nazarewicz, in preparation





A. Staszczak, J. Dobaczewski
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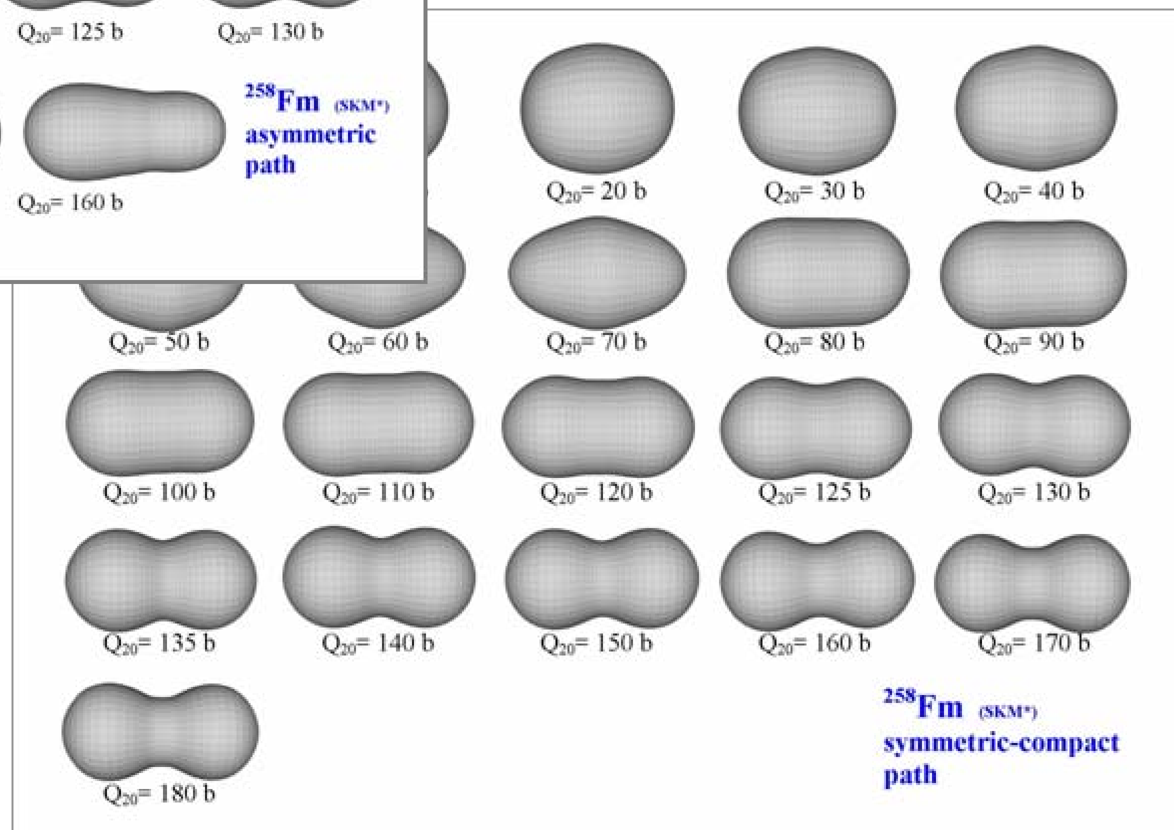
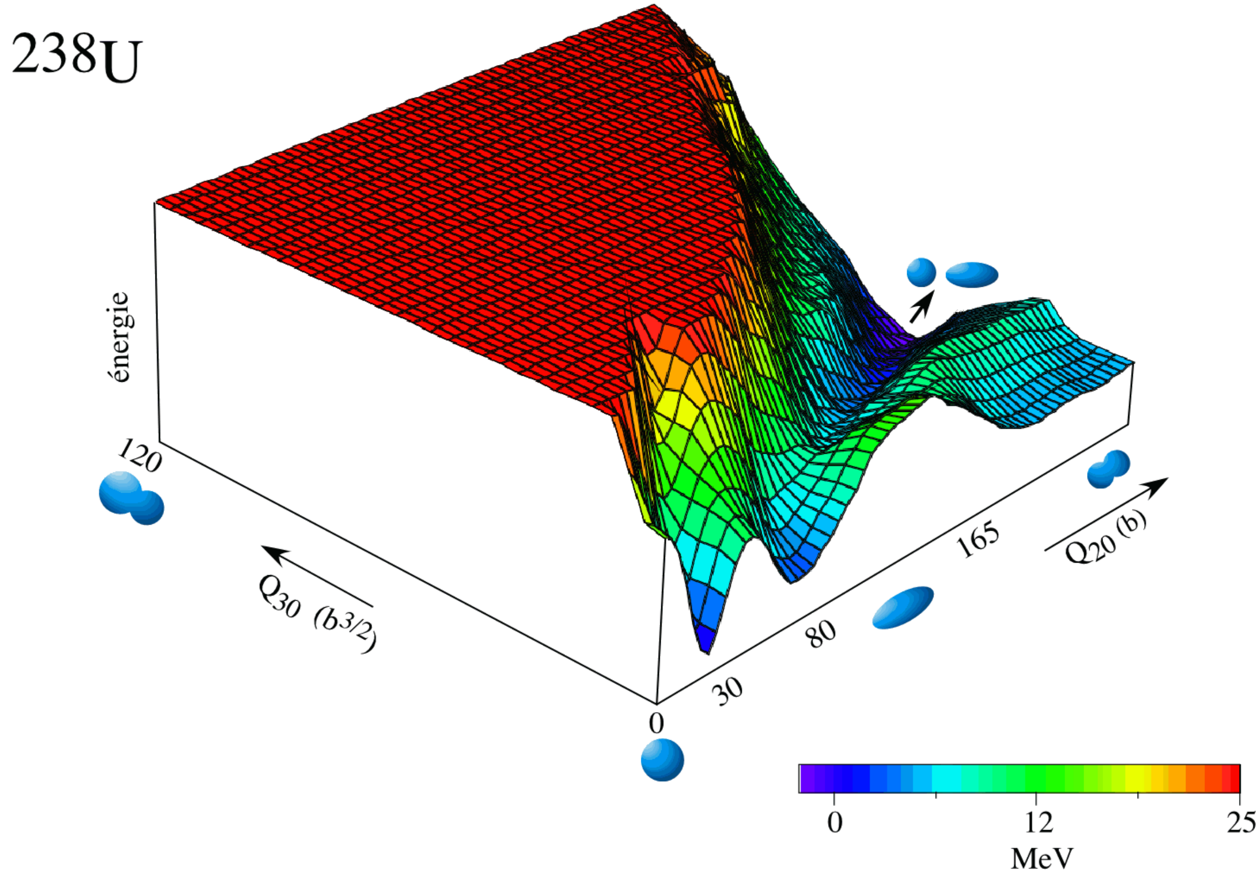


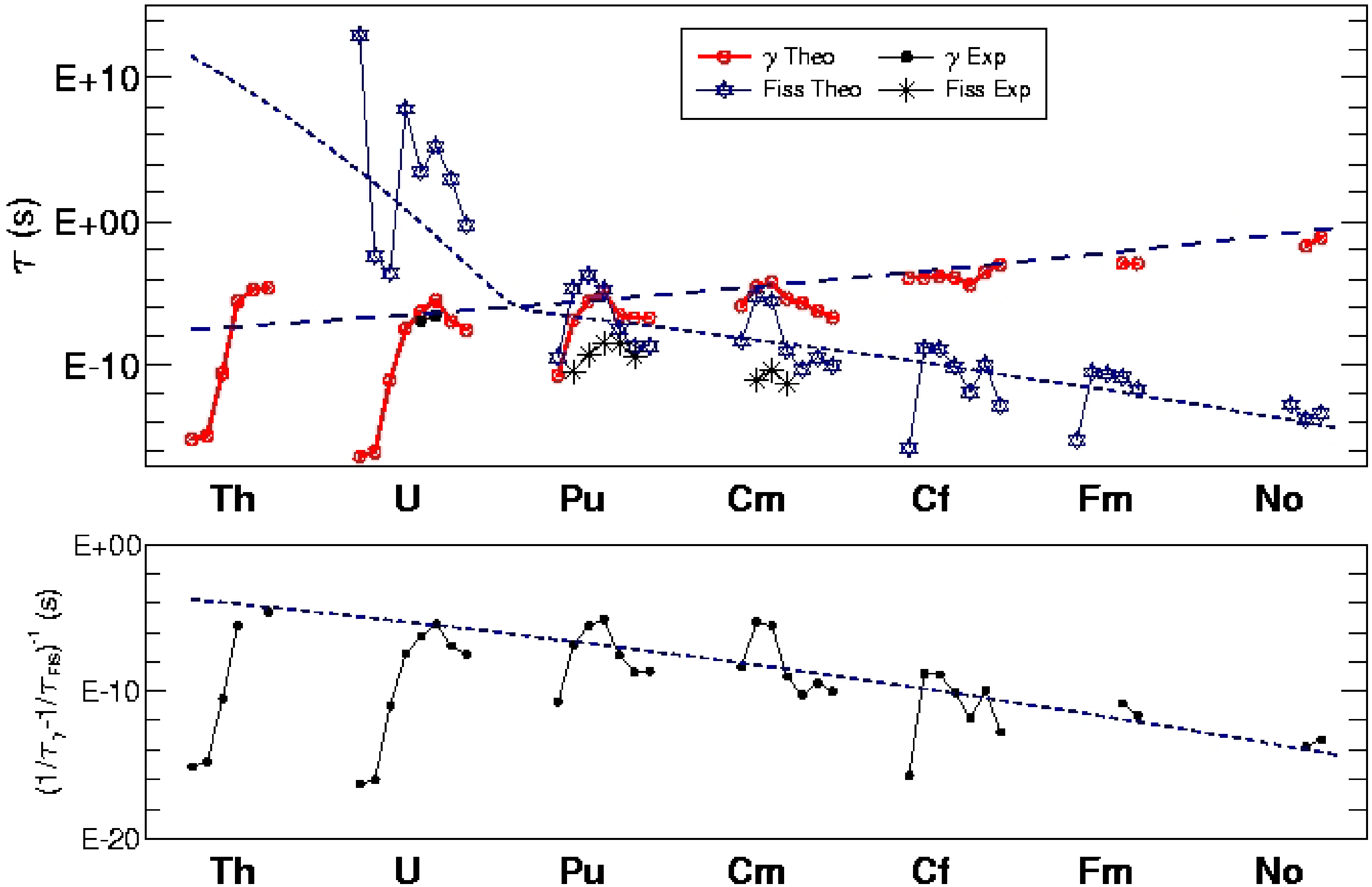


Calculation of the flux along the scission line
→ Fission yields

HFB + Gogny D1S

H. Goutte, P. Casoli, J.-F. Berger Nucl. Phys. A734, 217 (2004)

Lifetimes

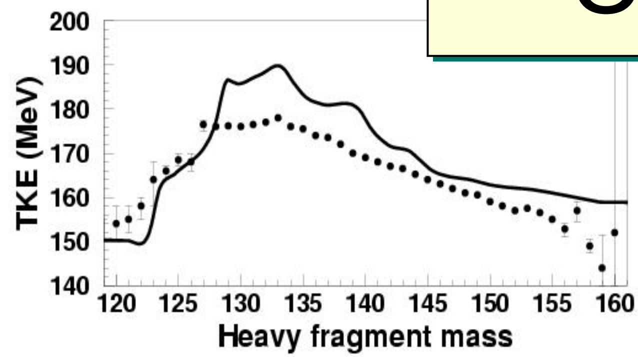


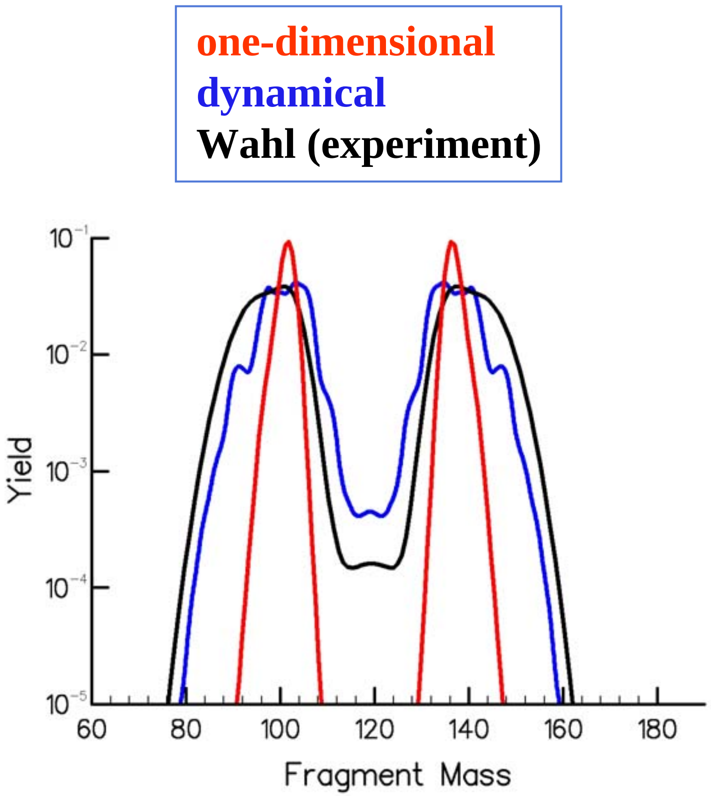
HFB + Gogny D1S

M. Girod, J. Libert, J.P. Delaroche and H. Goutte to be published

Kinetic Energy and Mass Distributions
in HFB+TDGCM(GOA)

^{238}U





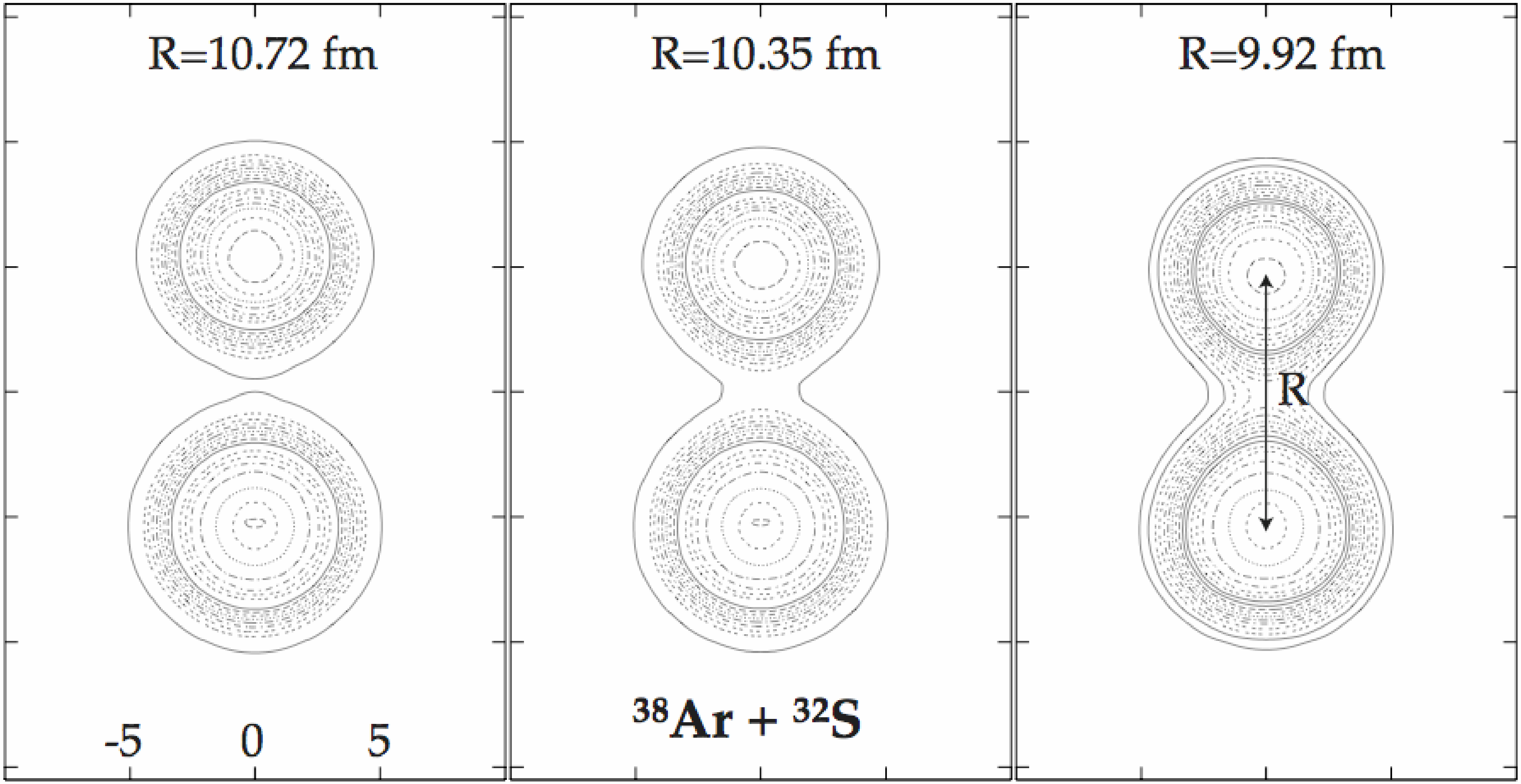
- Time-dependent microscopic collective Schroedinger equation
- Two collective degrees of freedom
- TKE and mass distributions reproduced
- Dynamical effects are responsible for the large widths of the mass distributions
- No free parameters

HFB + Gogny D1S + Time-Dependent GOA

H. Goutte, P. Casoli, J.-F. Berger, D. Gogny, Phys. Rev. C71, 024316 (2005)

Related problem: heavy-ion fusion

- nucleus-nucleus potentials
- fusion barriers



J. Skalski, submitted. Coordinate-space Skyrme-Hartree-Fock

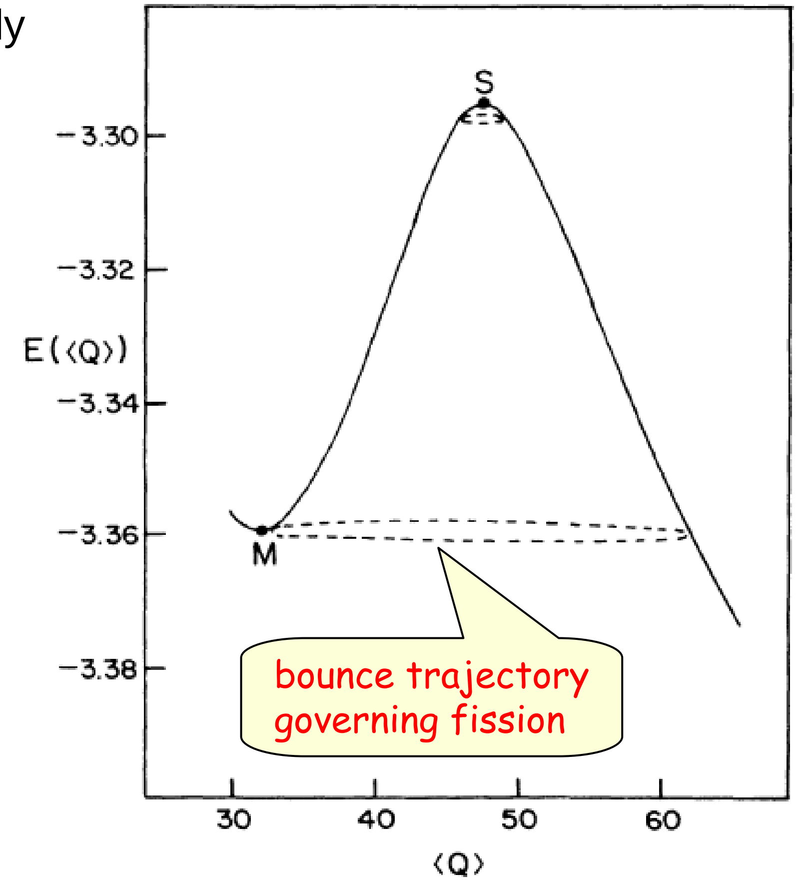
(see also nucl-th/0402033)

Imaginary-time mean-field theory (instanton method)

Levit, Negele, Paltiel, Phys. Rev. C21, 1603 (1980); C22, 1979 (1980)
Puddu and Negele, Phys. Rev. C35, 1007 (1987)
Arve et al., Phys. Rev. C36, 2018 (1987) - simple model
J. Skalski, Phys. Rev. A65, 033626 (2002) - BEC

- Proper quantum treatment of many-body tunneling
- Non adiabatic, properly accounts for level crossings and symmetry breaking effects (collective path strongly influenced by level crossings). HF and ATDHF not adequate

- TDHF equations in an inverted potential
- Evolution in an imaginary time
- The lifetime is expressed by the sum of bounces
- **Difficulty in solving the periodic mean-field equations** (fission bounce equations)
- Important role of pairing correlations (restore adiabaticity)
- Unclear how to restore broken symmetries



For more discussion on non-adiabatic methods, see W. Nazarewicz, Nucl. Phys. **A557**, 489c (1993)

- Quest for the universal interaction/functional

  The major challenge for low-energy nuclear theory

- Many-dimensional problem

  Tunneling of the complex system

  Coupling between collective and single-particle

  Time dependence on different scales

UNEDF (SCIDAC-2)
DOE, NNSA, ASCR

- All intrinsic symmetries broken

  Large elongations, necking, mass asymmetry, triaxiality, time reversal (odd, odd-odd systems),…

- Correlations important

  Pairing makes the LACM more adiabatic. Quantum corrections impact dynamics.

- What happens during the split?

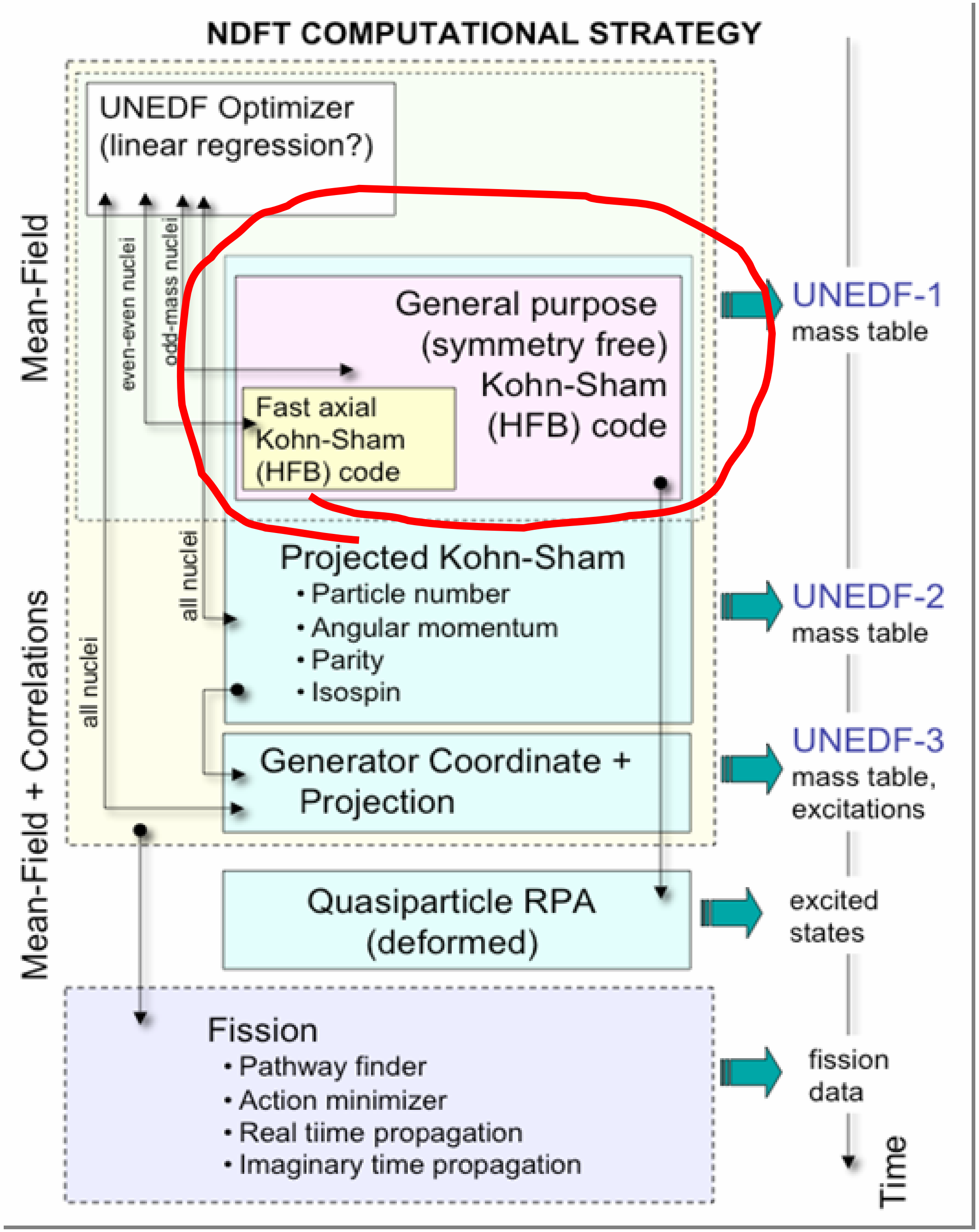
  Center of mass, Wigner energy… (While one knows how to calculate the cm correction to the binding energy for an individual nucleus, ambiguities arise when describing fusion or fission, where, asymptotically, a cm correction should be calculated for each separated fragment.)

What is needed?

Computing (today)
Efficient <u>symmetry-unrestricted</u> HFB (Kohn-Sham) solver
UNEDF fitting: optimization/linear regression, distributed computing
Action minimization in many dimensions, fission pathways
Performance evaluation for existing codes

Computing (tomorrow)
Beyond-mean-field dynamics (GCM, projections)
Real-time evolution for excited states (at and above the barrier)
Imaginary-time evolution at subbarier energies

Theory
Symmetry restoration in DFT
Symmetry-conserving formalism of LACM needs to be developed
Can imaginary-time propagation be replaced by variational approach?


NDFT COMPUTATIONAL STRATEGY
UNEDF Optimizer
(linear regression?)
even-even nuclei
odd-mass nuclei
Mean-Field
General purpose
(symmetry free)
Kohn-Sham
(HFB) code
Fast axial
Kohn-Sham
(HFB) code
UNEDF-1
mass table
all nuclei
Projected Kohn-Sham
• Particle number
• Angular momentum
• Parity
• Isospin
UNEDF-2
mass table
all nuclei
Mean-Field + Correlations
Generator Coordinate +
Projection
UNEDF-3
mass table,
excitations
Quasiparticle RPA
(deformed)
excited
states
Fission
• Pathway finder
• Action minimizer
• Real tiime propagation
• Imaginary time propagation
fission
data
Time

Conclusions

Fission is a fundamental many-body phenomenon that possess the ultimate challenge for theory

Understanding crucial for many areas:

- Nuclear structure and reactions (superheavies)
- Astrophysics (n-rich fission and fusion, neutrino-induced fission)
- Numerous applications (energy, NNSA…)
- …

The light in the end of the tunnel: coupling between **modern microscopic many-body theory** and **high-performance computing**