Microscopic Theory of Nuclear Fission

VECC Colloquium
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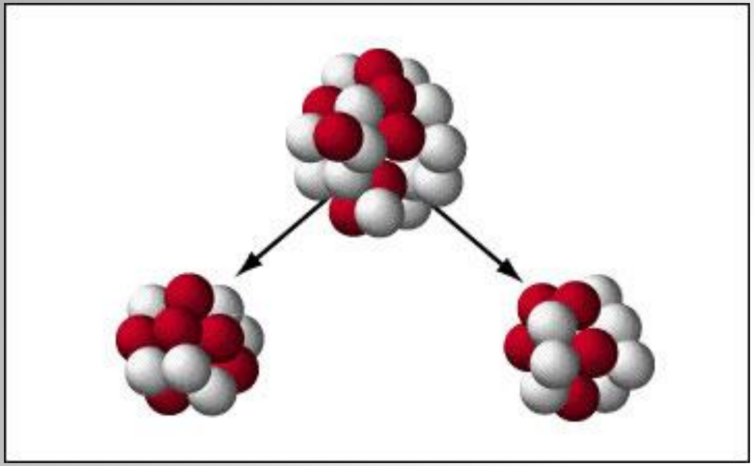
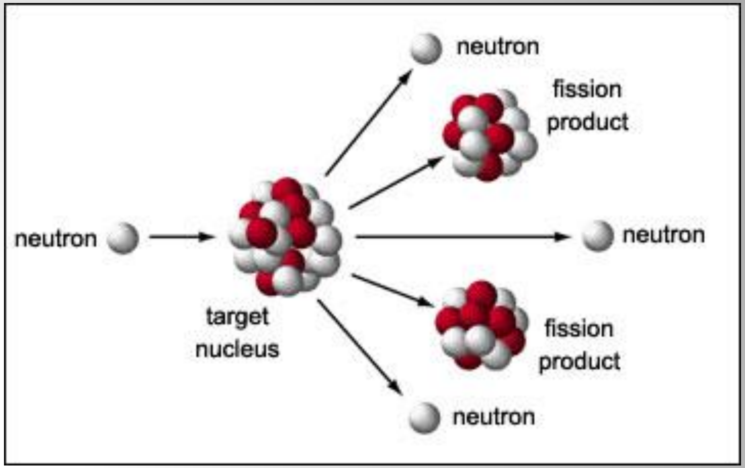
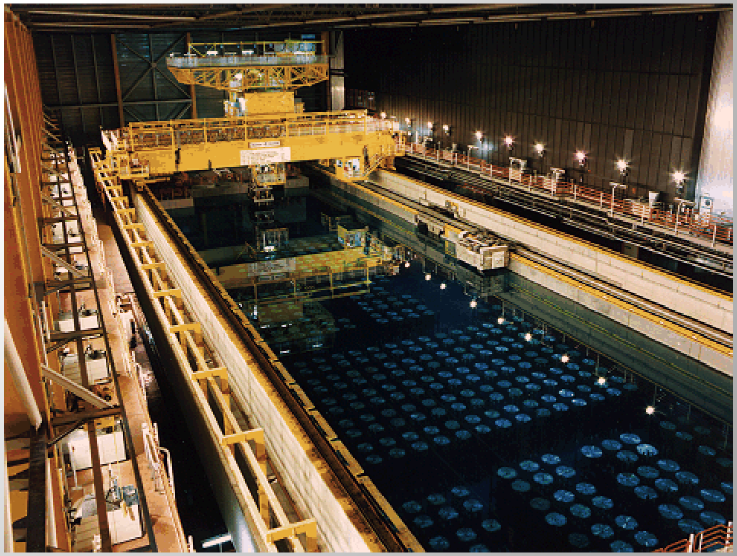
First, Some Definitions

Spontaneous fission



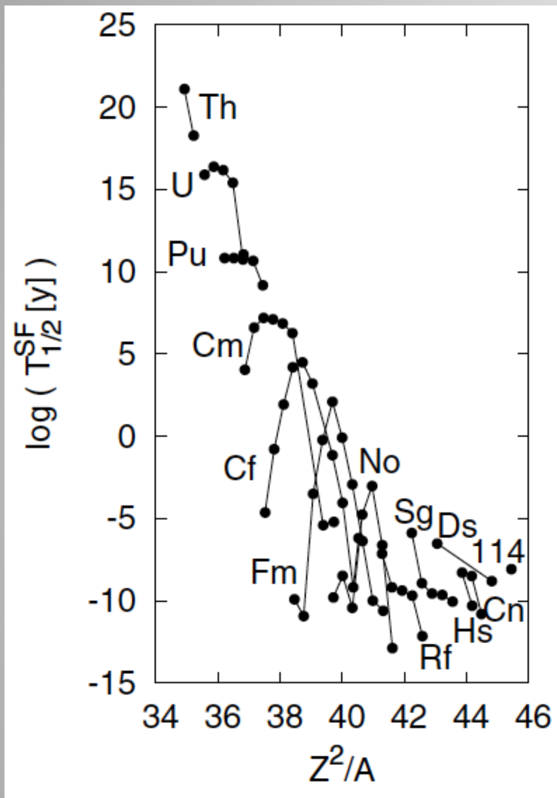
Induced fission





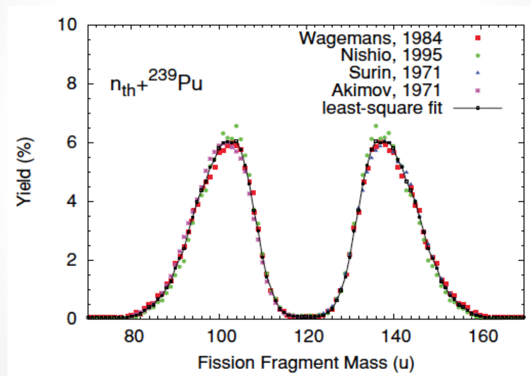
- Half-life: from 10^{21} years (^{232}Th) to …0.25 ms (^{250}No) covering more than 30 orders of magnitude!
- Applications of induced fission in energy production… and other things

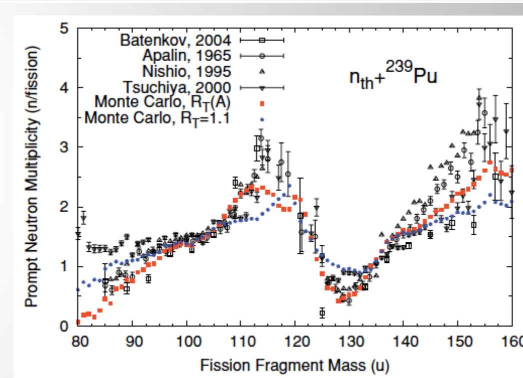
What Should Theorists Look At?

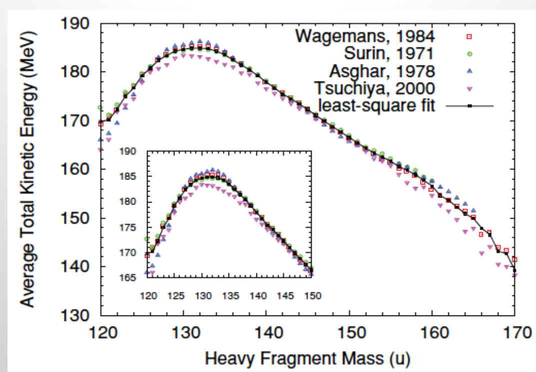


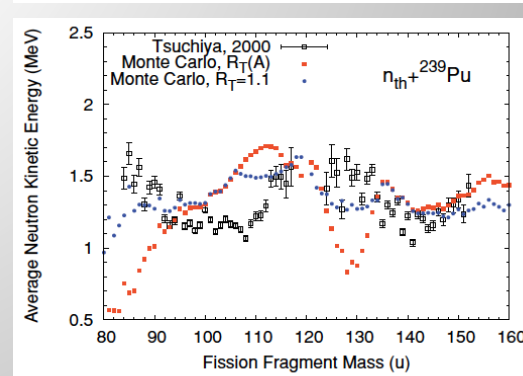
Krappe & Pomorski, *Theory of Nuclear Fission*, Springer-Verlag 2012

Spontaneous fission	Induced fission
Half-lives	▪ Properties of fission fragments • Charge and mass distribution • Total kinetic energy • Excitation energy ▪ Neutron spectrum









Phys. Rev. C **83**, 064612 (2011)

Warming up gently

A Brief History of… Nuclear Fission Theory

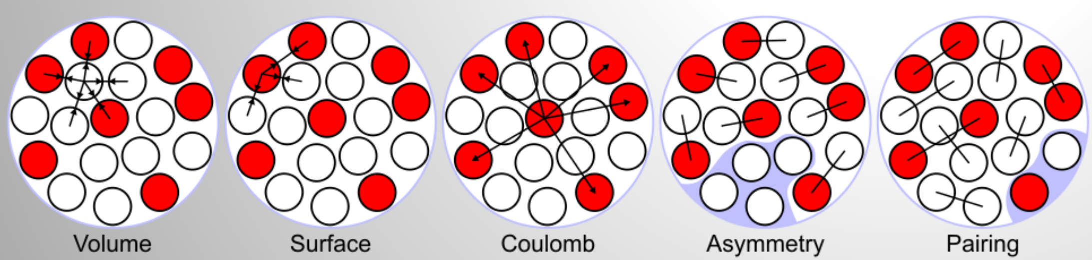
A Brief History of Nuclear Fission Models

The Stone Age (1940ies)

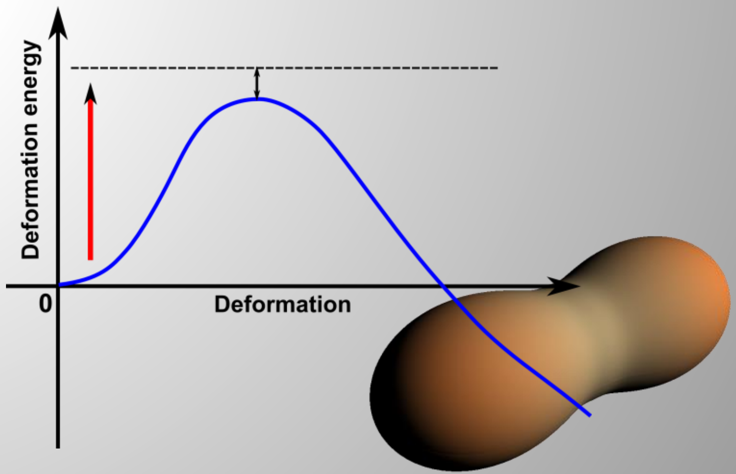
- Nucleus is a charged quantum liquid drop $E_{\mathrm{macro}}(\boldsymbol{q})$ with some deformation parameters $\boldsymbol{q} = (q_1, \ldots, q_n)$
- Mass formula (Bethe-Weiszäcker, 1935) characterized by handful of parameters fitted on atomic masses

$$\frac{E}{A} = a_{\mathrm{vol}} - a_{\mathrm{sur}} b_s(\boldsymbol{q}) A^{2/3} - a_{\mathrm{cou}} b_c(\boldsymbol{q}) Z^2 A^{-1/3} - a_{\mathrm{sym}} \frac{(N-Z)^2}{A}$$

- Incident neutrons bring enough energy to pass the barrier and break the LD



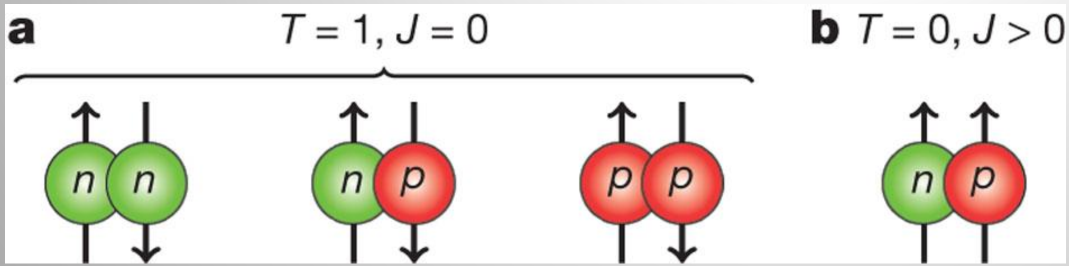
From Wikipedia, "*Semi-Empirical Mass Formula*", http://en.wikipedia.org/wiki/Semi-empirical_mass_formula



A Brief History of Nuclear Fission Models

The Antiquity (1960ies)

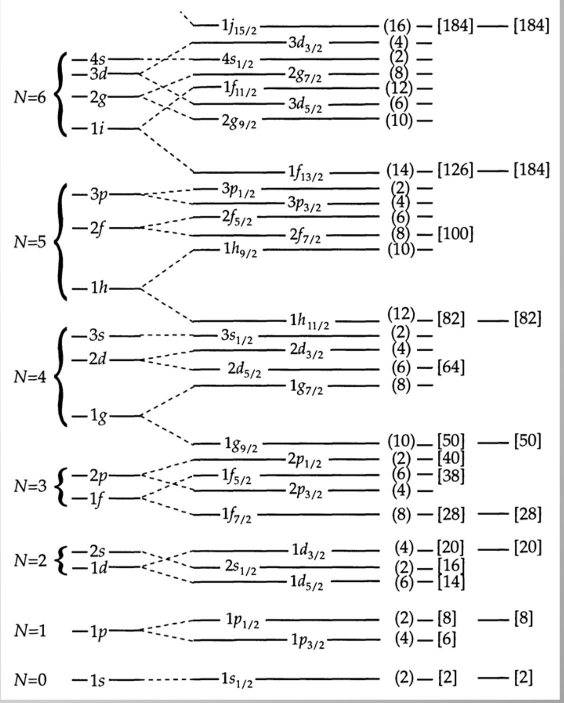
- Recognize the role of individual nucleons: shell correction $\delta E_{\mathrm{shell}}(\boldsymbol{q})$
  - Nuclear Shell Model (1949): nucleons as independent particles in some nuclear potential
  - Quantum mechanics 101 problem: solve Schrödinger equation for some quantum well
  - Shell structure brings a correction to the liquid drop energy
- Recognize the role of residual interactions: pairing correlations bring extra binding and lead to $\delta E_{\mathrm{pair}}(\boldsymbol{q})$



Nature **469**, 68 (2011)

Jensen

Goeppert-Mayer



A Brief History of Nuclear Fission Models

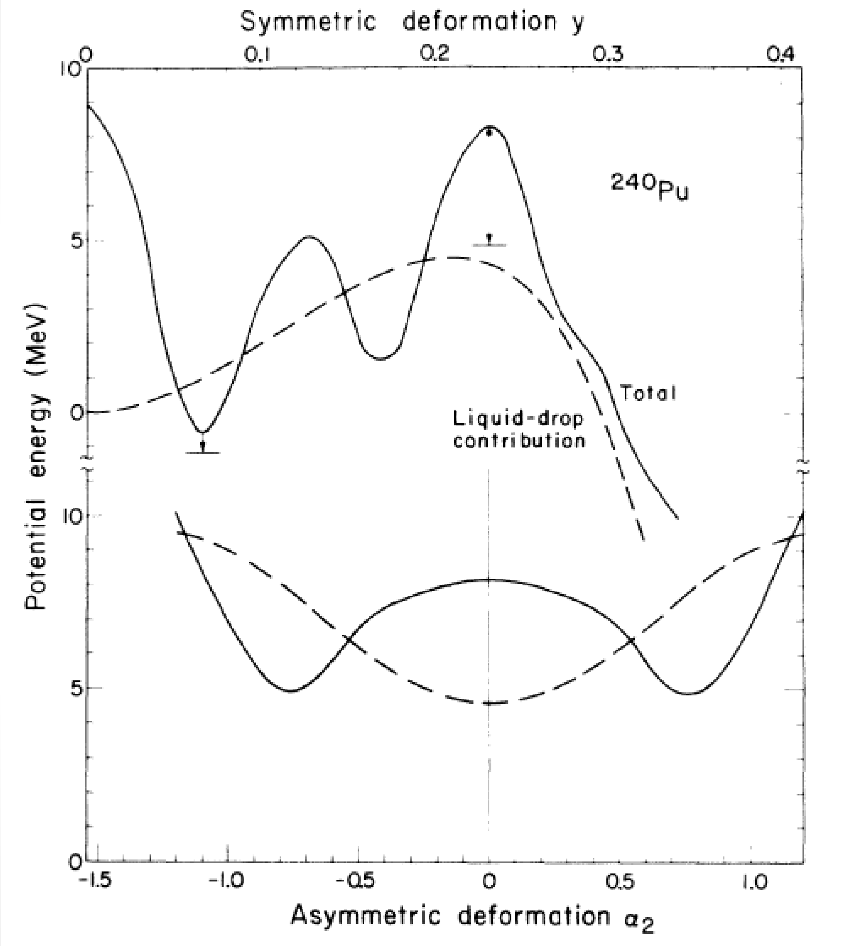
The Antiquity (1960ies)

- Macroscopic-microscopic models

$$E_{\rm nuc}(\boldsymbol{q}) = E_{\rm macro}(\boldsymbol{q}) + \delta E_{\rm shell}(\boldsymbol{q}) + \delta E_{\rm pair}(\boldsymbol{q})$$

- Explains deformed ground-states of nuclei, fission isomers, double-humped fission barriers, variety of fission products, etc.
- Accuracy of the model depends on
  - Fit of free parameters of LD and mean-field (Nilsson, Woods-Saxon)
  - Number of deformations $\boldsymbol{q}$

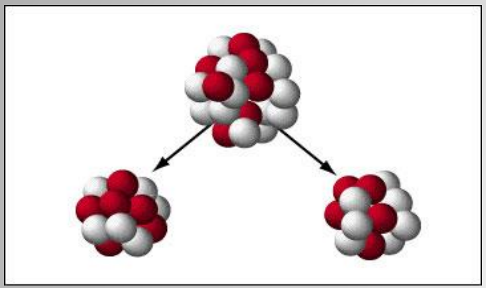
High excitation energies in induced fission also requires nuclear temperature



Phys. Rev. C **5**, 1050 (1972)

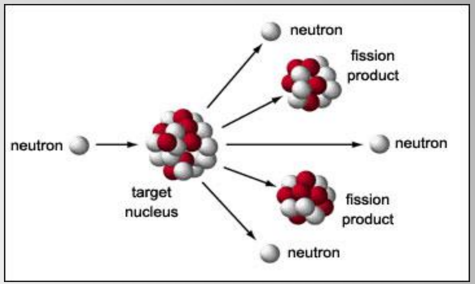
Schematic Model of Fission

Spontaneous

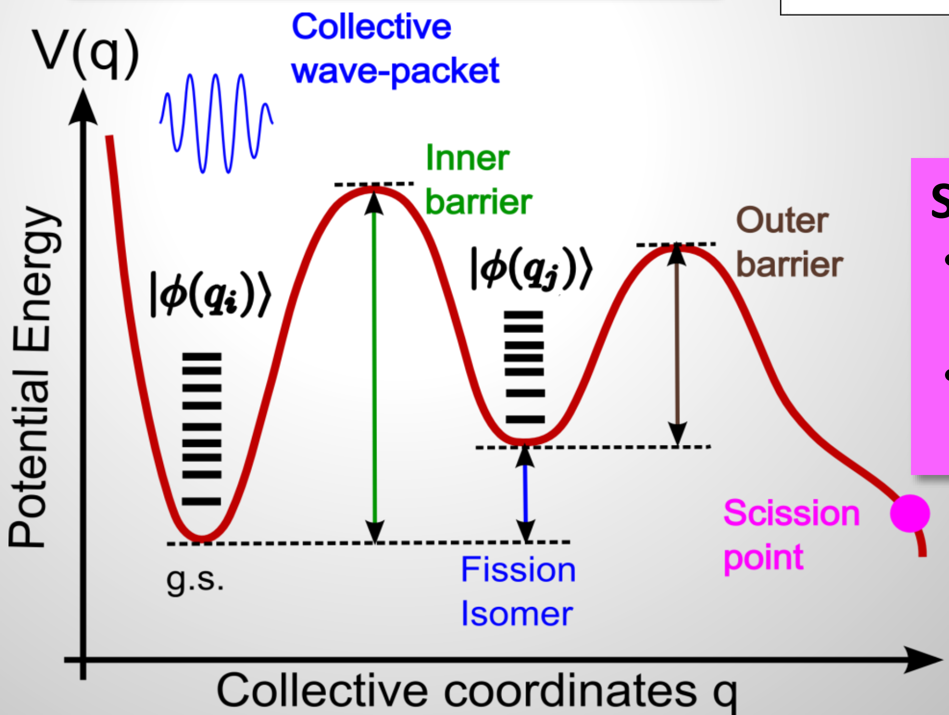


Dynamics
- Semi-classical
- Quantum-mechanical with same Hamiltonian used for static

Induced



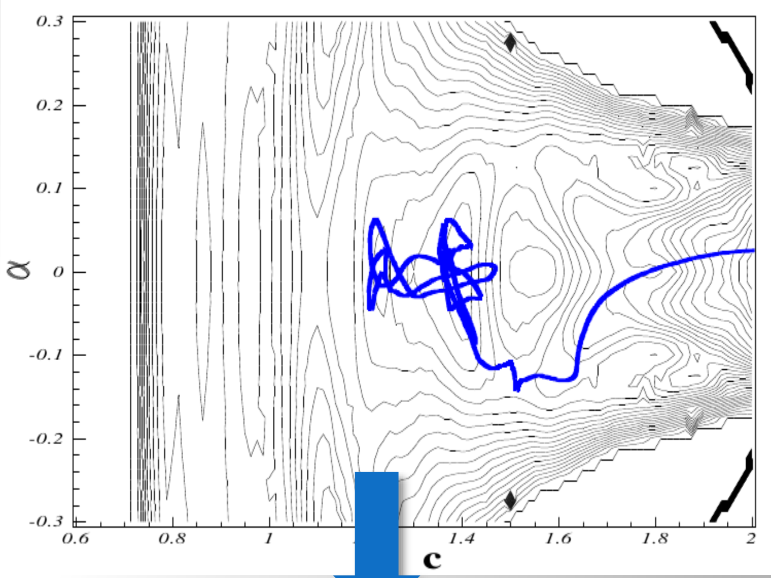
Potential energy surface (PES)
- Phenomenological: parameterized
- Microscopic: derived from (effective) nuclear forces



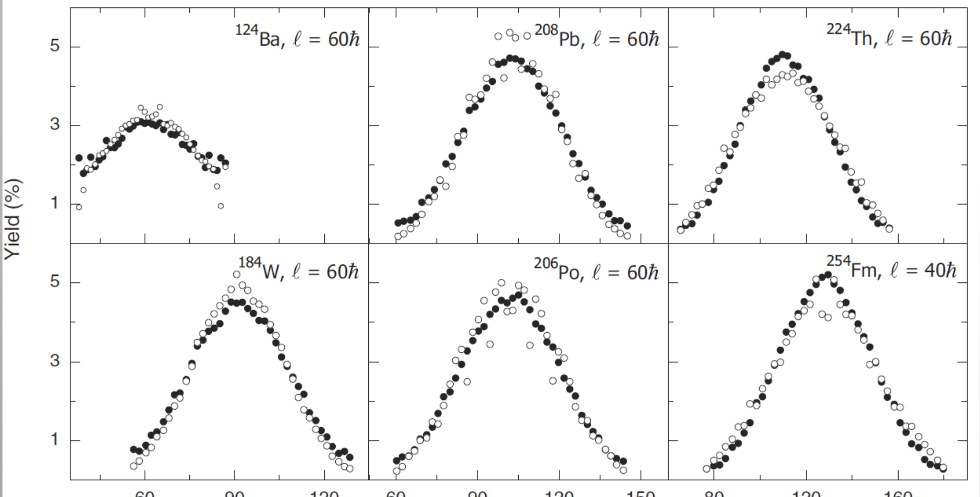
Scission
- Arbitrary criterion
- From quantum mechanics

A Brief History of Nuclear Fission Models
The Classic Age (1980ies)

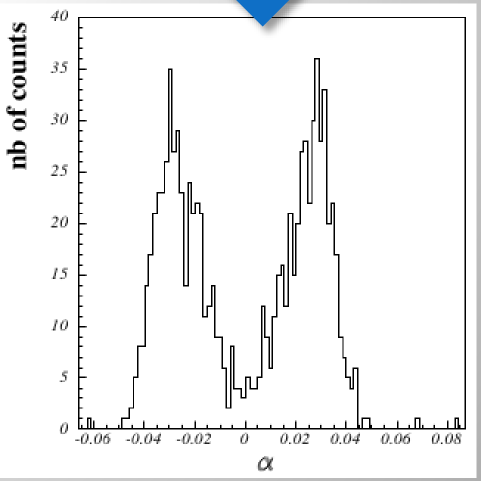
Acta Phys. Polon. B **34** (2003)



- Dynamics of induced fission treated by semi-classical methods
  - Langevin diffusion equations (India, Russia, France)
  - Brownian motion model, flooding algorithms, etc. (LANL/LBNL)
- Charge and mass distributions



Phys. Rev. C **84**, 044610 (2011)

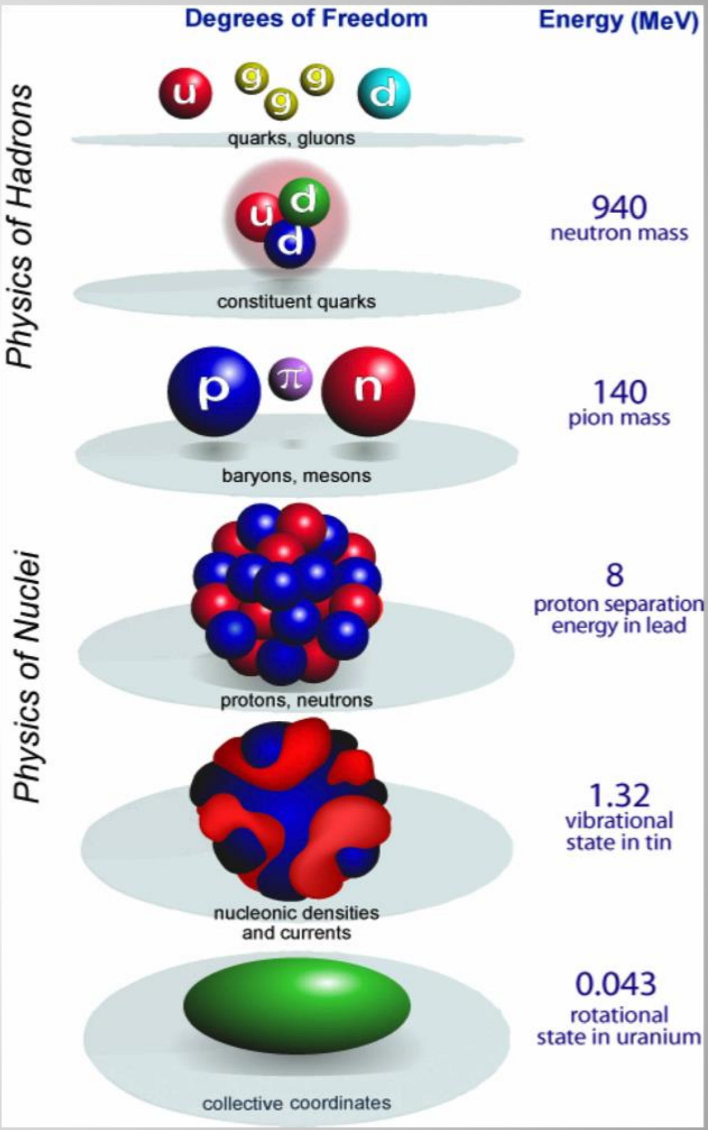


Setting the stage

From Macroscopic-Microscopic Models to a Fully Microscopic Theory of Fission

Of Scales in Nuclear Physics

- Nuclear physics ranges from quarks and gluons (QCD, scale >GeV) to collective states in nuclei (low-energy nuclear structure, scale > keV)
- Of the importance of identifying the right degrees of freedom
- A predictive theory can not ignore the interactions among nucleons
- What’s wrong with macroscopic-microscopic models?
  - Liquid drop: no internal degree of freedom
  - Shell effects: only one-body theory (independent particles with ad hoc quantum well)



Nuclear Density Functional Theory

- Basic assumption: all observables depend only on the density of nucleons (and the pairing tensor)

$$E = \int d^3\boldsymbol{r}\, \mathcal{H}[\rho(\boldsymbol{r})]$$

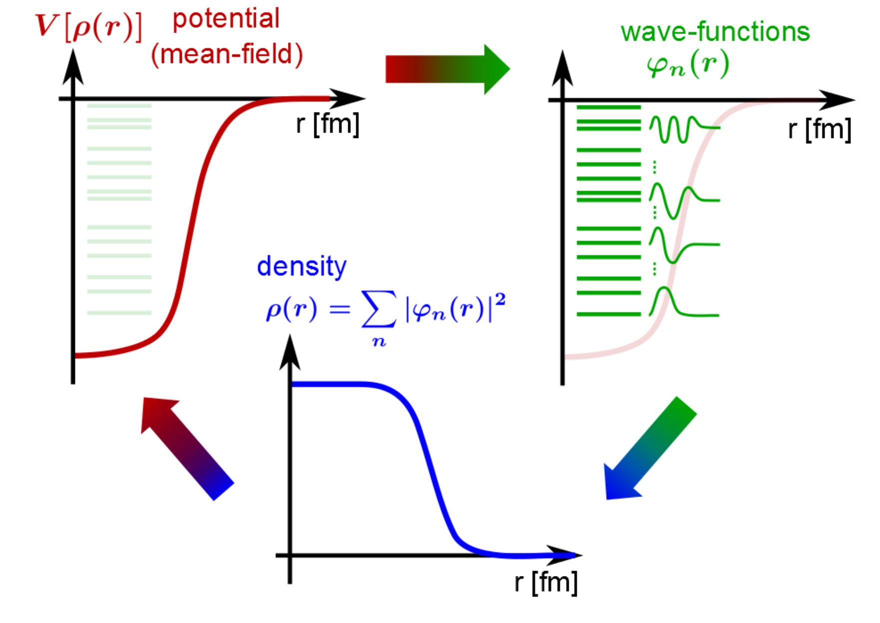
- Use of the variational principle: find the actual density (and pairing tensor) by requesting that the energy be minimal
- Allow the density (and the pairing tensor) to break symmetries (translational, rotational invariance, particle number, etc.)
  - Introduce deformation degrees of freedom, $\rho(\boldsymbol{r}) \rightarrow \rho(\boldsymbol{r}; q_1, \ldots, q_n)$
  - Provides consistent framework to build potential energy surface, compute collective mass, do the dynamics, etc.

- *Nuclear DFT is a reformulation of the nuclear self-consistent mean-field theory*
- *Formal issues actively researched: restoration of broken symmetries, configuration mixing, connections with the theory of nuclear forces, etc.*

Solving the DFT Equations

- Non-linear differential equations = Schrödinger equation where the potential $V(\boldsymbol{r})$ depends on the solutions $\varphi_n(\boldsymbol{r})$
- Common technique: Expand solutions on a basis (linear algebra problem)
  - Deal with ~2000 x 2000 matrices
  - Iterate until nothing changes, requires 100 – 10000 iterations

The self-consistent DFT loop



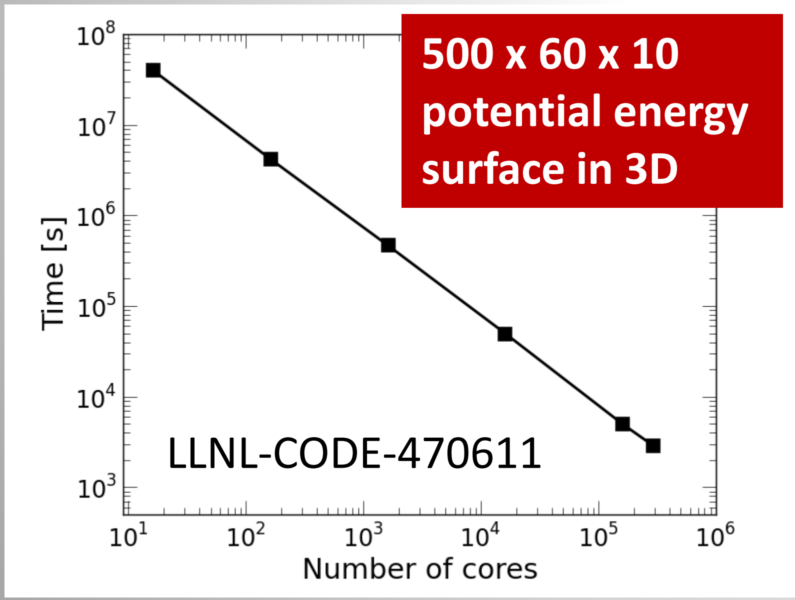
Self-consistent mean-field theory

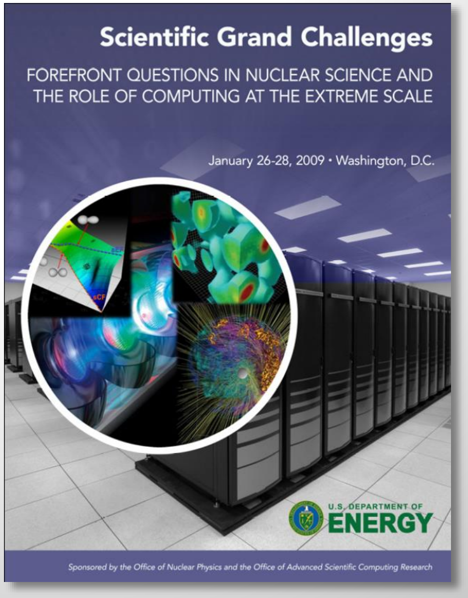
	Spherical symmetry (1D)	Axial symmetry (2D)	Symmetry unrestricted (3D)
r-space	< 1 min, 1 thread	5 hours, 100 cores	-
HO basis	< 1 min, 1 thread	1 min, 6-8 threads	6 hours, 1 core, 6-8 threads

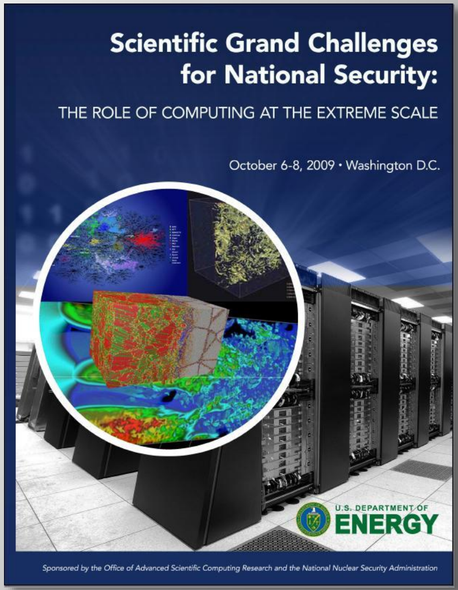
Computational Nuclear Structure

- Nuclear fission is a very large-scale computational problem
  - Size of collective space is > 500 x 100 x 100 x 100 x 40 = 5×10^8 (without including temperature or spin)
  - Each point takes between 1 minute (axial, near ground-state) and 2 days (triaxial, near scission)
  - Need for highly optimized DFT solvers scaling to 1M+ cores
- SciDAC collaborations help develop, optimize and scale nuclear simulations codes

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING





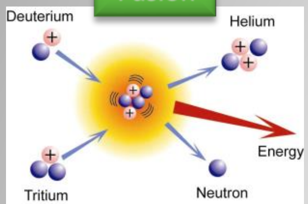


The SciDAC 3 NUCLEI Collaboration

SciDAC Scientific Discovery through Advanced Computing

NUclear Computational Low-Energy Initiative

Fusion



TJNAF

NIF

Validated Nuclear Interactions

Chiral EFT
Ab-initio

Optimization
Model validation
Uncertainty Quantification

LENP facilities

FRIB

SciDAC Scientific Discovery through Advanced Computing

www.computingnuclei.org

Neutron drops

Structure and Reactions: Light and Medium Nuclei

Structure and Reactions: Heavy Nuclei

EOS

Correlations

Stellar burning

Ab-initio
RGM
CI

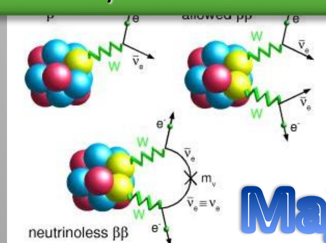
Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification

DFT
TDDFT

Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis

Oak Ridge National Laboratory
Argonne National Laboratory
Los Alamos National Laboratory
Berkeley Lab
The Ohio State University
The University of North Carolina at Chapel Hill
University of Washington
Michigan State University
Iowa State University
The University of Tennessee
CMU Central Michigan University

Neutrinos and Fundamental Symmetries

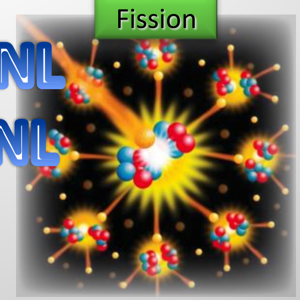


SNS

Majorana

Neutron Stars

Fission

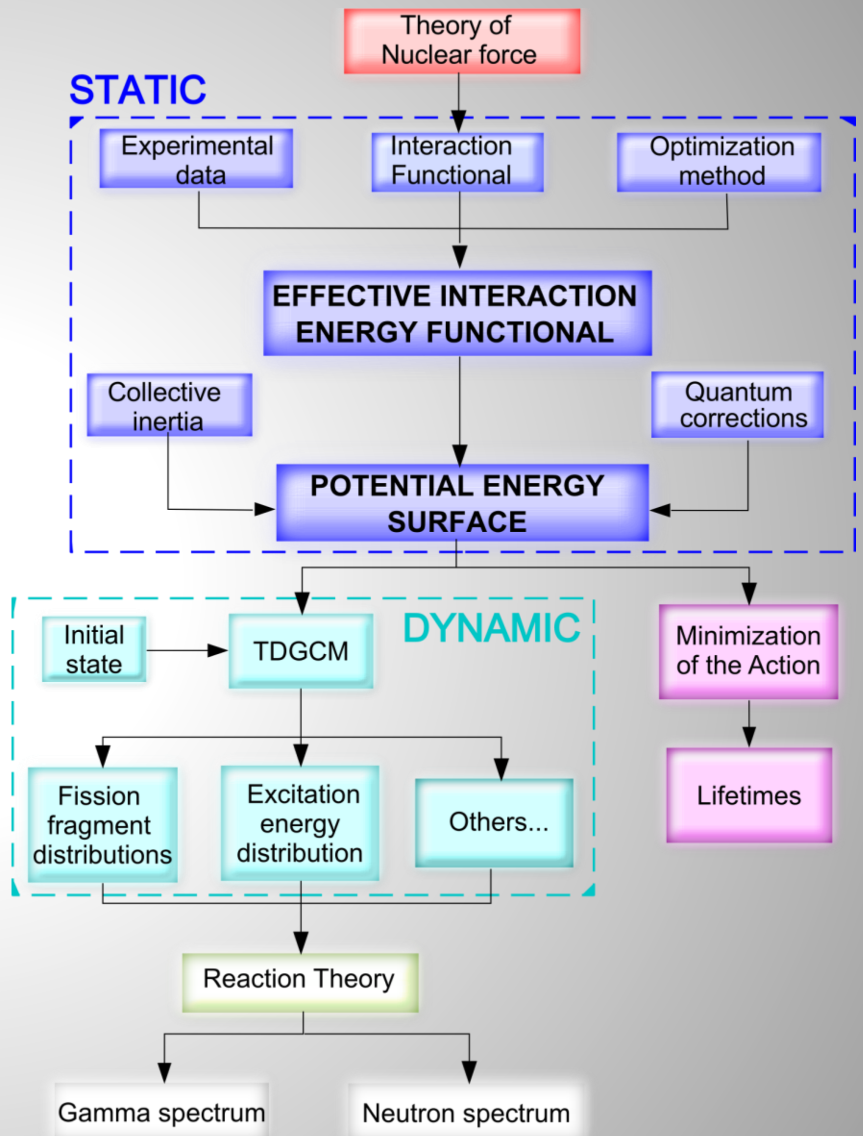


LANL

LLNL

The Big Picture

- Requirements for a microscopic theory of fission
  - Uses the right degree of freedom: for low-energy nuclear structure and reactions, nucleons (as point-like particles) in interaction
  - Quantum mechanics always rules
  - Predictive power comes from internal consistency and rigorous connections to underlying theory of the nuclear force
- Nobody said it's going to be easy…
  - Nuclear forces come with high uncertainties
  - Computational problem is formidable

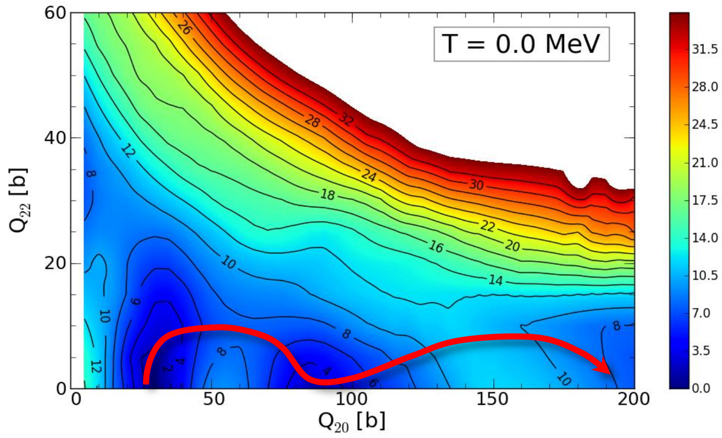


Into the heart of matter

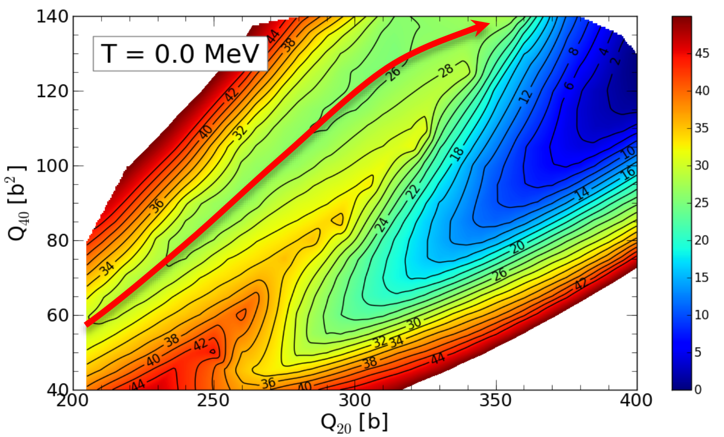
Spontaneous and Induced Fission at High Excitation Energies

Managing the Scale

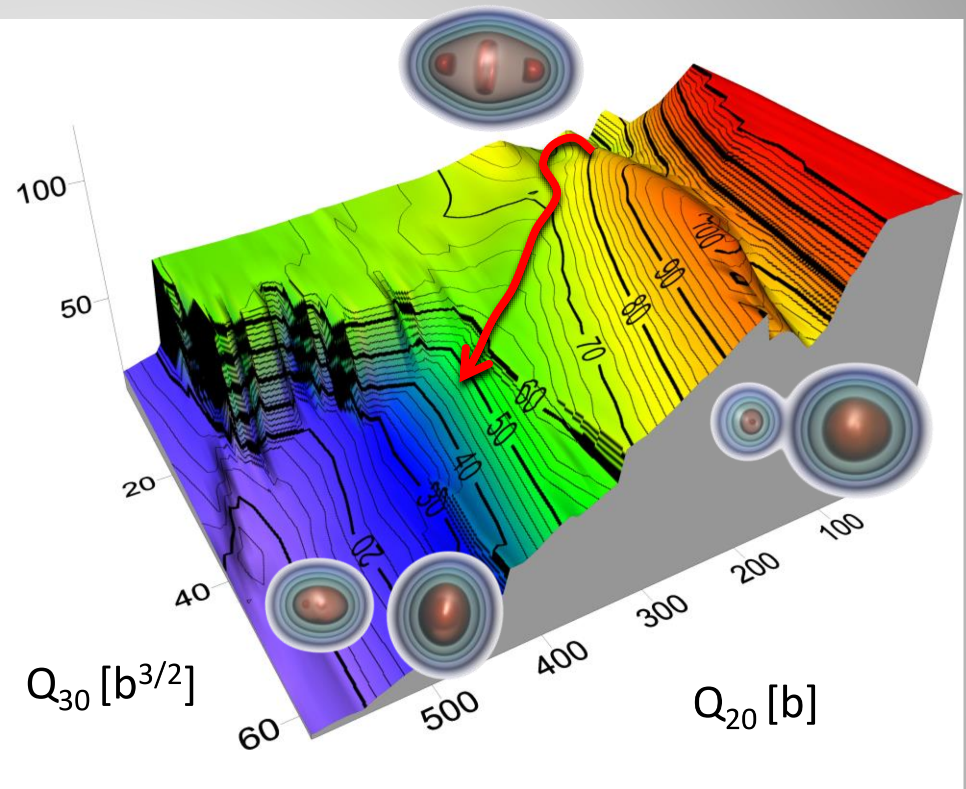
Phys. Rev. C **90**, 054305 (2014)



Elongation and triaxiality



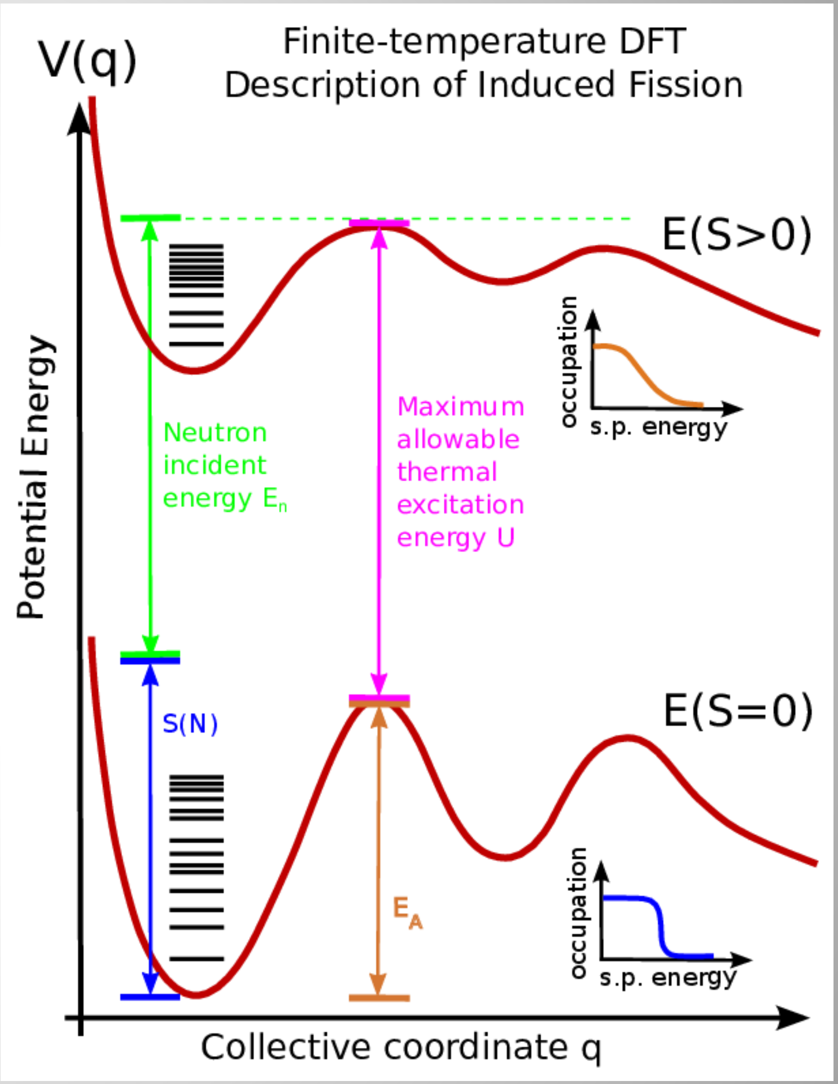
Fission and fusion valleys



Example of a potential energy surface in 4 dimensions: elongation (q_{20}), triaxiality (q_{22}), mass asymmetry (q_{30}) and thickness of the neck (q_{40})

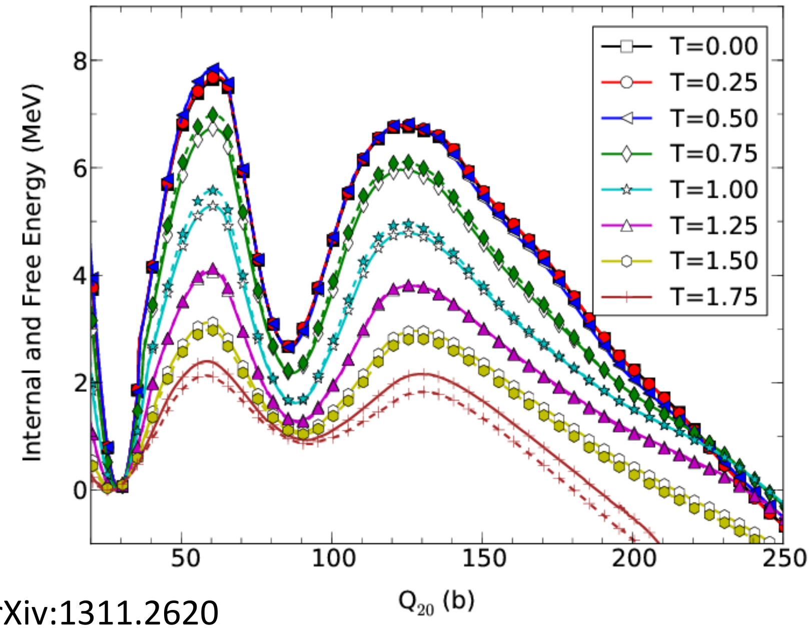
Dealing with Excitation Energy

- Potential energy surfaces from finite-temperature DFT calculations
  - System in thermal equilibrium
  - Ground-state is statistical superposition of pure quantum mechanical states
  - Well-known theory, first large-scale implementations in past 5 years
- Scenario for induced fission
  - Potential energy surfaces at finite temperature define intrinsically excited states
  - Nuclear wave-packet formed from these excited states at energy E_{coll}
  - Time-evolution gives distributions

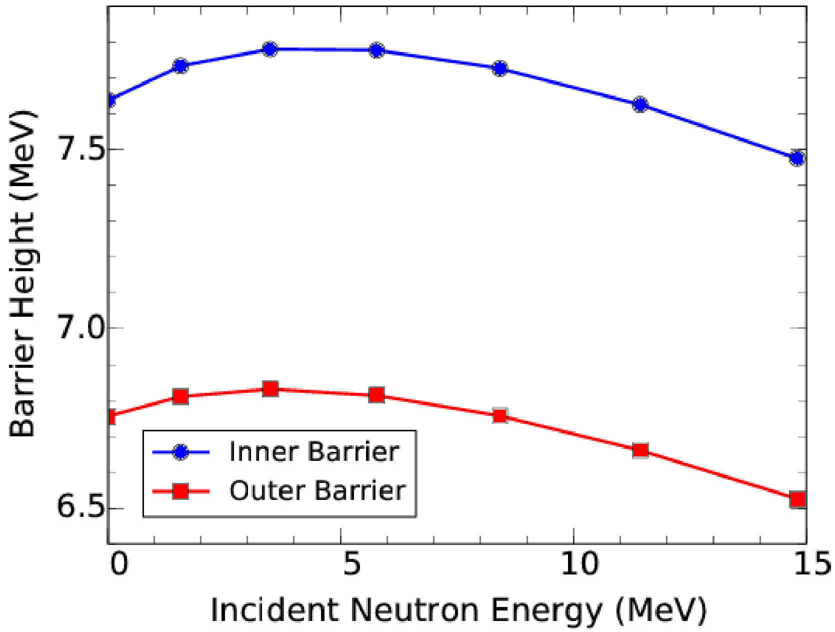


Evolution of Potential Energy Surfaces

- Generic features
  - Small temperatures: anti-pairing and shell restoration effects
  - Larger temperatures: shell effects disappear (more like a liquid drop)
- Range of energy for incident neutron relevant for most applications is 0 – 14 MeV

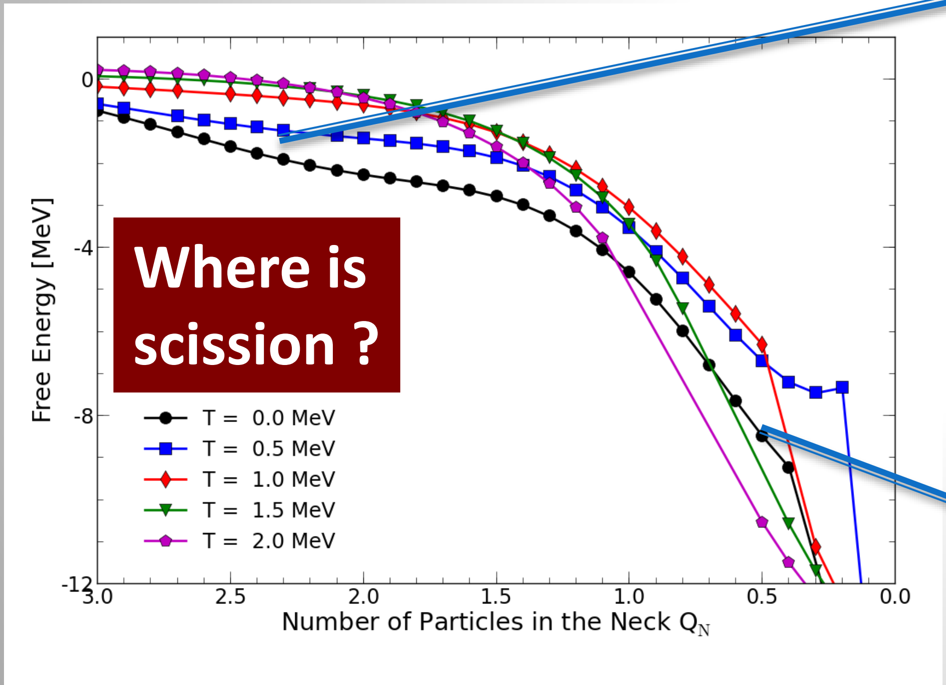


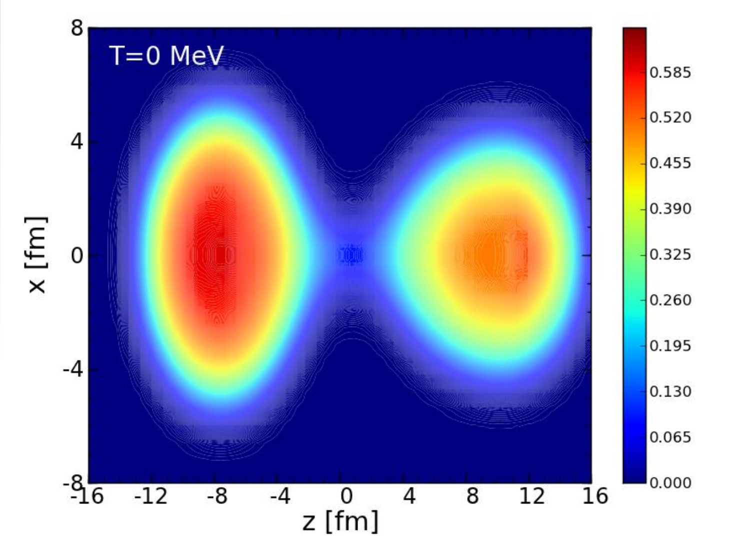
arXiv:1311.2620

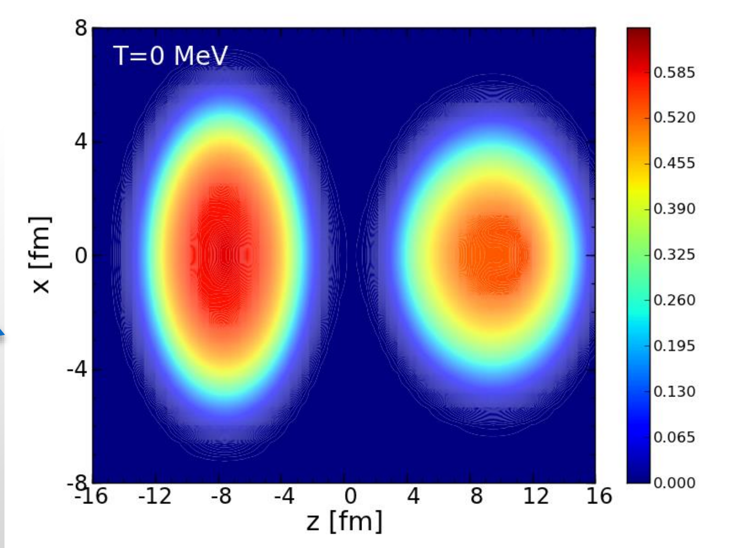


The Elusive Scission Point

- Definition of scission is arbitrary and ambiguous
- Fission fragment properties strongly depend on the scission configurations





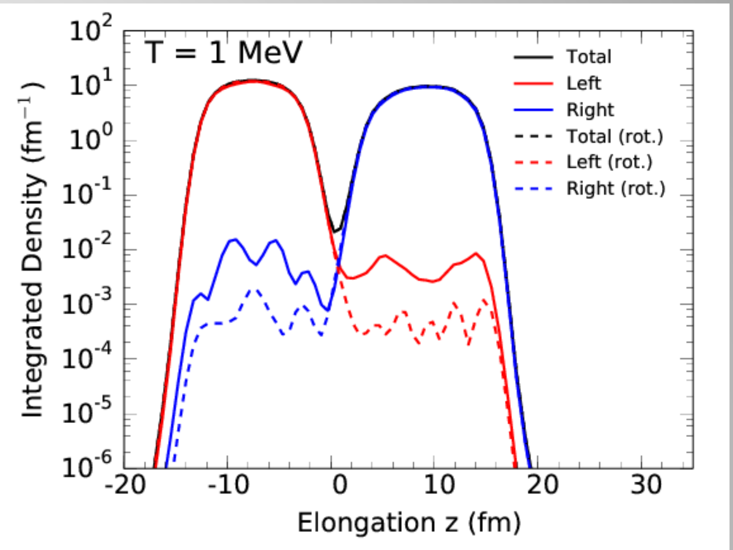


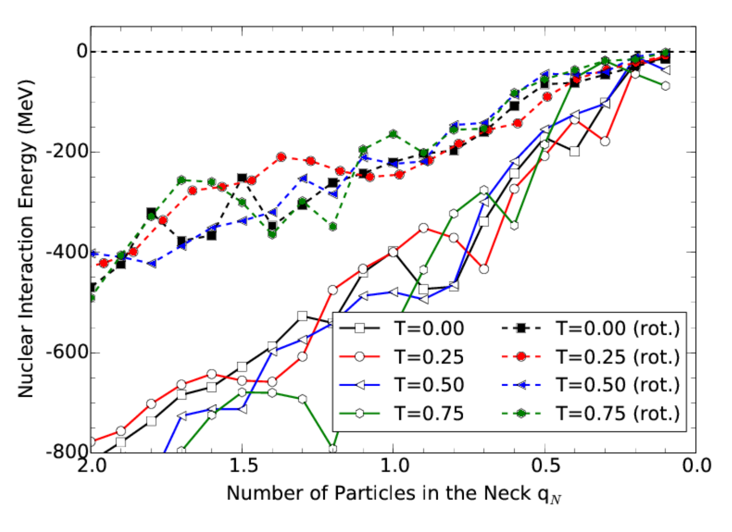
PRC **80**, 054313 (2009), PRL **107**, 132501 (2011), PRC **90**, 054305 (2014)

Fission and Quantum Entanglement

- Quantum identification of fission fragments
  - Tag every nucleon "left" or "right" based on spatial occupation ⇒ defines sets of quasiparticles in each fragment
  - Construct associated ''densities''
- Quantum localization procedure
  - Perform a unitary transformation pairwise to localize the particles:
    - — Doesn't change the energy of the system
    - — Changes fragment properties
- Advantages:
  - Reduce the tail between the fragments
  - Make sure fragments are independent quantum systems

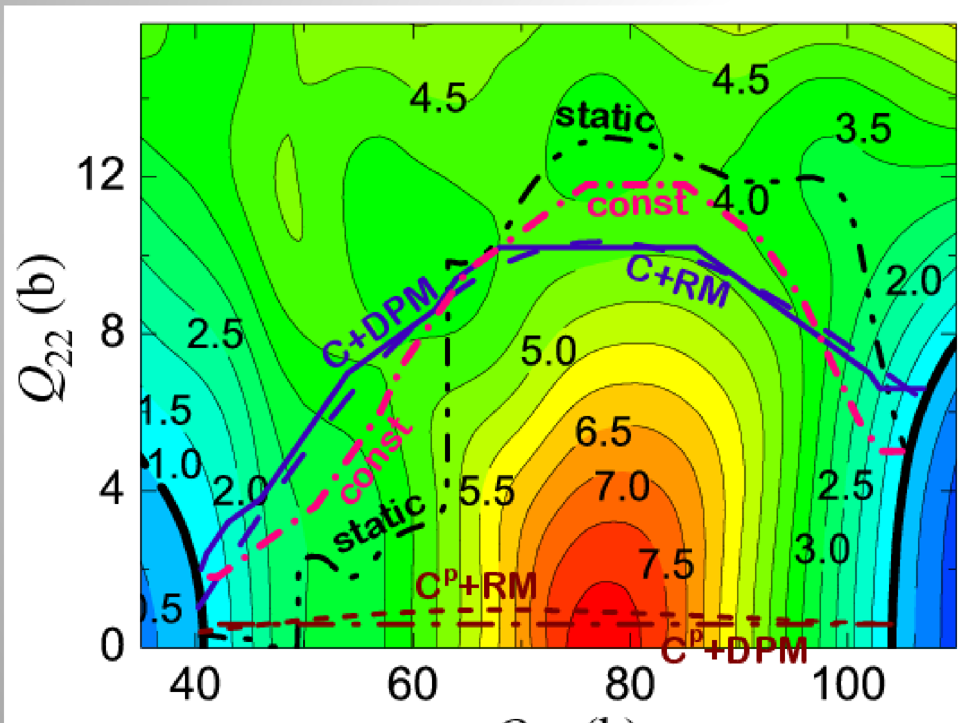
PRL **107**, 132501 (2011), PRC **90**, 054305 (2014), arXiv:1311.2620





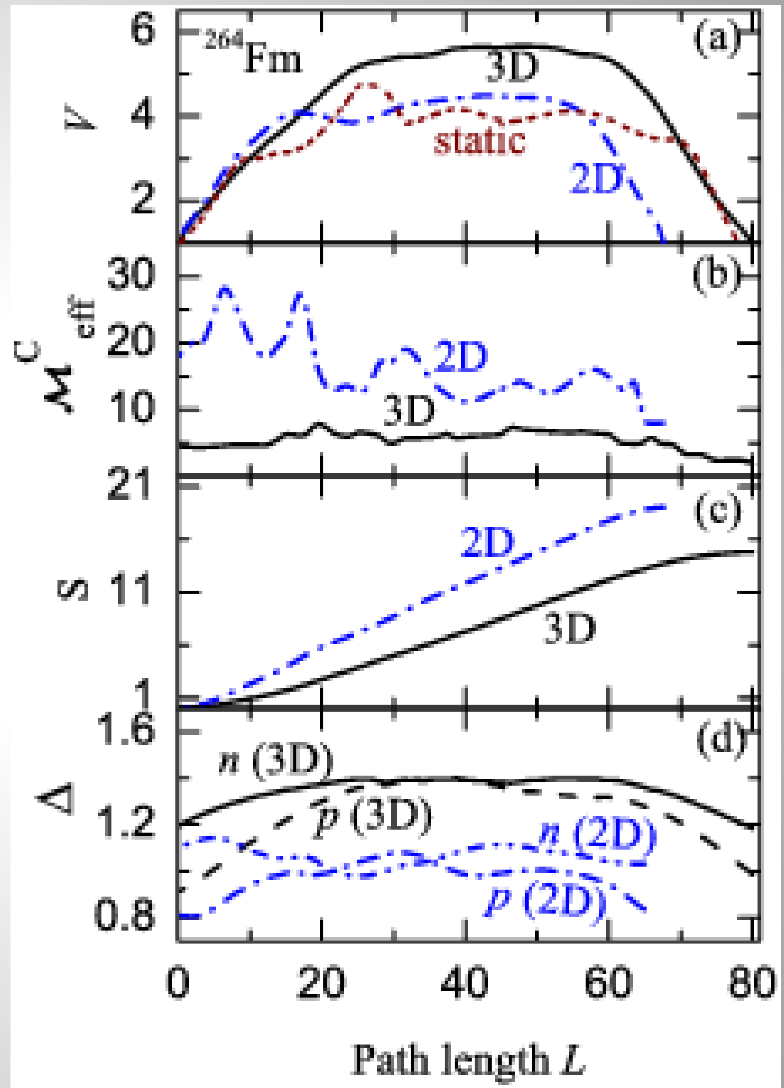
Collective Space

- Importance of the number and type of collective variables
- Popular approximations to compute collective inertia are dangerous!



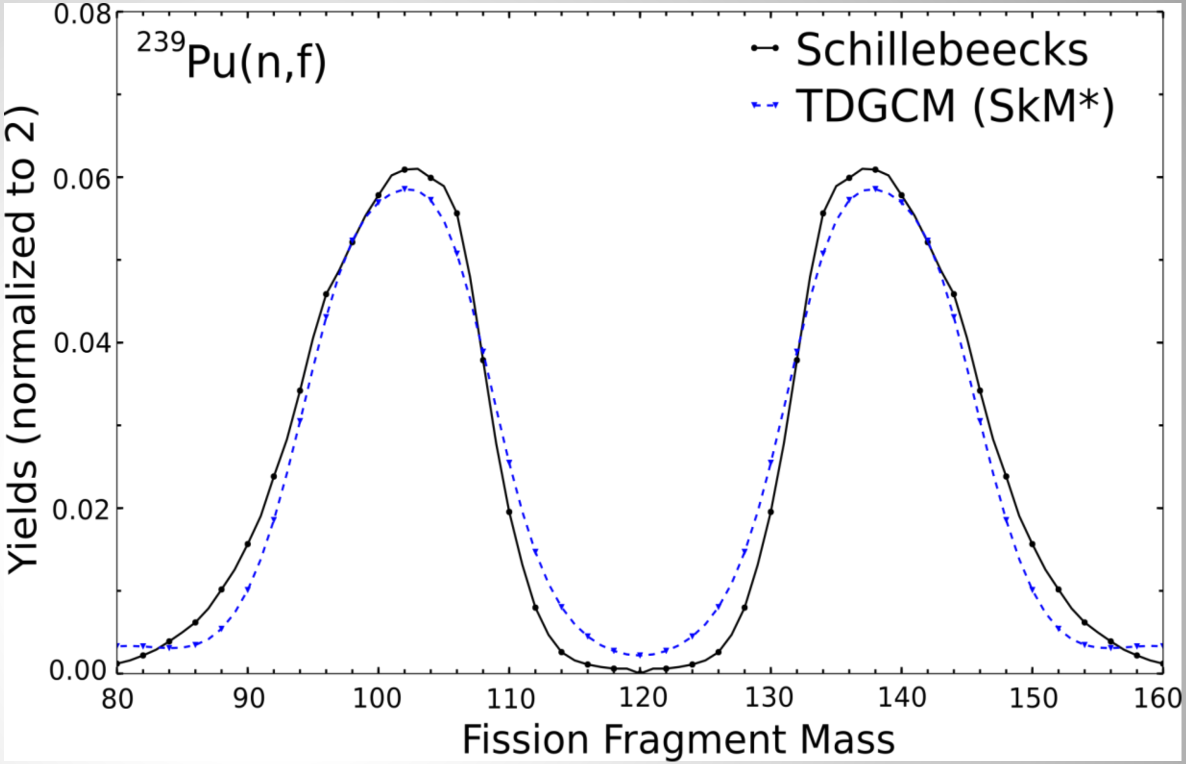
PRC **88**, 064314 (2013)

PRC **90**, 061304(R) (2014)



Fission Fragment Distributions

- Solve dynamics of fission assuming adiabaticity: slow motion in collective space
- Reduce time-dependent Schrödinger equation to diffusion-like equation for the collective amplitude
- Solve using finite element analysis



Fully microscopic calculation of fission fragment distributions in induced fission

Conclusions

Conclusions

- Nuclear fission
  - An 75 year-old problem in nuclear science without an accurate and precise solution yet, in spite of many very practical applications!
  - Microscopic methods based on density functional theory are now applicable and are becoming competitive with more empirical approaches
  - Much progress in last 10 years from
    - better understanding of the physics of fission
    - increased availability and usage of high-performance computing
- Recent progress not discussed here
  - Verification and validation of energy functionals for fission
  - Full study of collective dissipation in 2D dynamics
- Challenges ahead
  - Extending theory of collective inertia at higher excitation energies
  - Realistic studies of fission dynamics in N-dimensions
  - Detailed study of fission fragment properties
    - Charge and mass (requires projection on particle number)
    - Excitation energies and temperature partitioning in the fragments

Collaborators

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