# *Microscopic Description of Induced Nuclear Fission: Static Aspects*

INT Workshop on Large Amplitude Collective Motion
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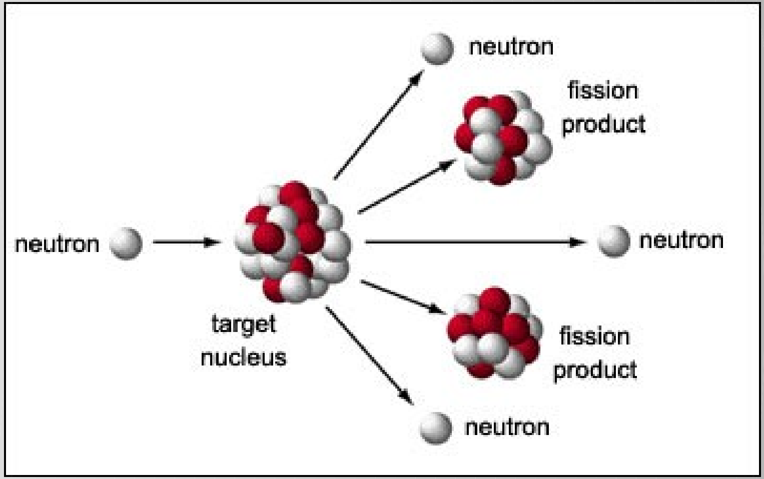
# NNSA Needs

- Predictive model of nuclear fission
  - Use where experimental data is missing
  - High accuracy, high precision, known error bars
- Fission fragment properties
  - Charge and mass of all fragments
  - Coulomb repulsion between the fragments = the total kinetic energy (TKE)
  - Excitation energy (TXE)

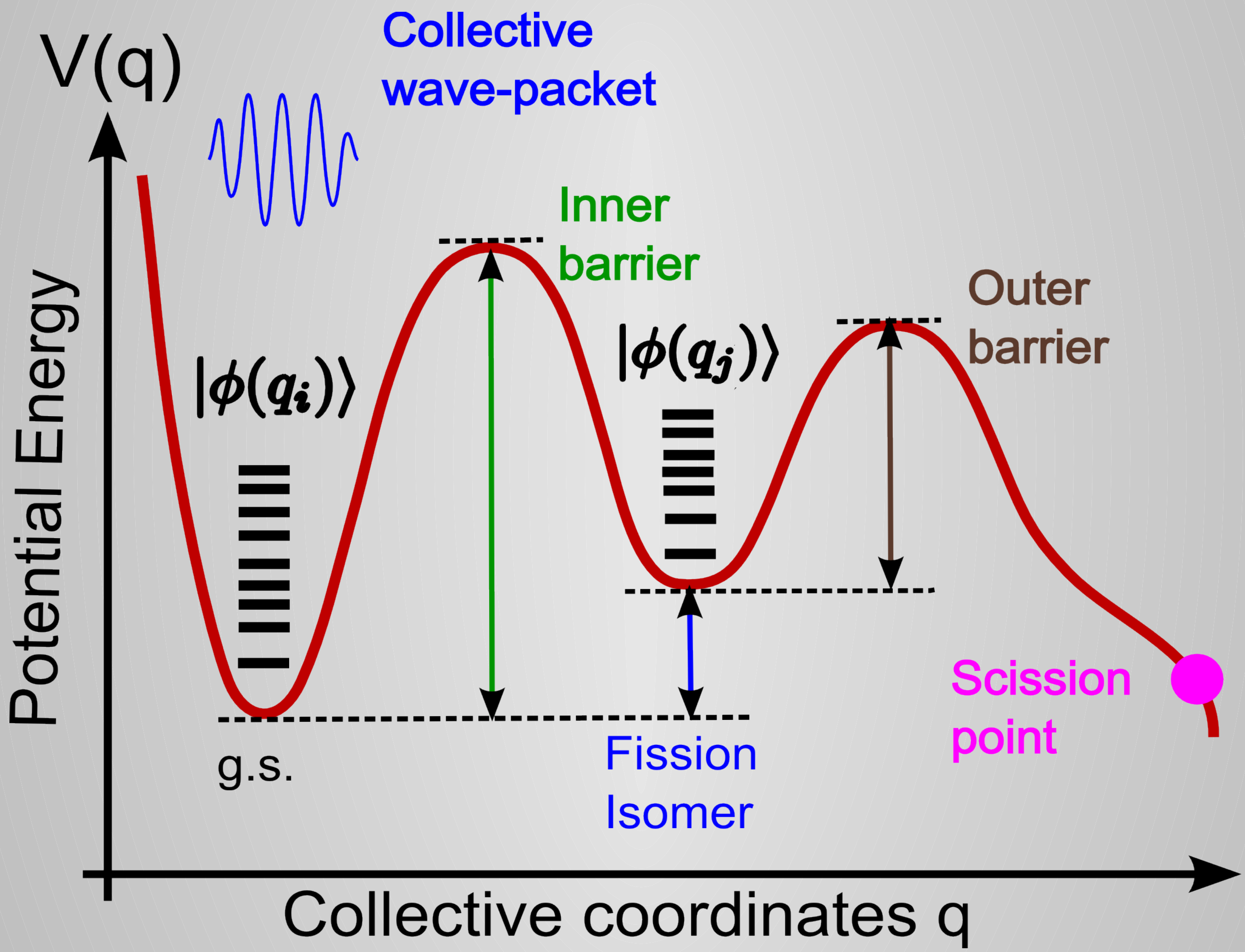



- Fission fragment distributions
- Fission spectrum: pre-, post-scission neutrons, gammas, etc.
- Important constraint: quantitative evolution as function of incident neutron energy

# Theoretical Approach

- Compound nucleus at given excitation energy
  - Separation between intrinsic and collective degrees of freedom
  - Collective variables describe, e.g., nuclear shape
  - Time evolution gives fragment distributions
- Requirements for a predictive theory
  - Use many-body methods of quantum mechanics
  - Build upon best knowledge of nuclear forces
  - Keep number of free parameters to strict minimum
- Nuclear density functional theory
  - Effective nuclear forces between protons and neutrons
  - Various levels of approximations
  - Time-dependent extensions exist
  - Suitable for large-scale applications

# Posing the problem



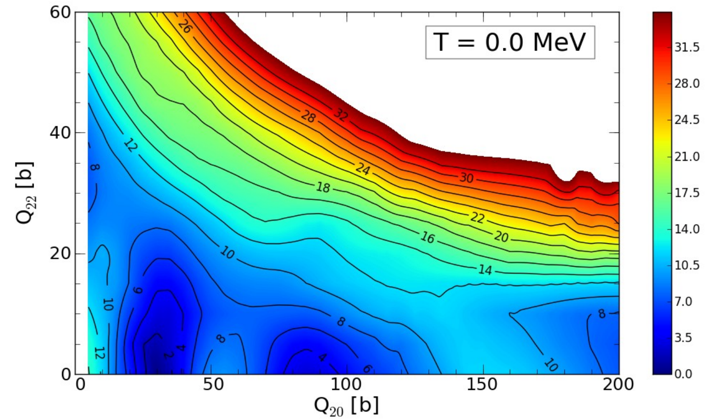
# Some Details

- Basic Ingredients of nuclear DFT
  - An effective interaction / energy functional: Skyrme, Gogny
    - Form of the functional guided by theory of nuclear forces
    - Challenge of determining unknown parameters
  - Identification of suitable collective variables
    - Number of collective variables drives the scale of the computational challenge
    - Optimal set of collective variables may change
  - Need to introduce a scission point
  - Account for excitation energy
    - Low-energy: Intrinsic-collective couplings
    - High-energy: Finite-temperature description
- Fast and/or powerful DFT solvers
  - Take advantage of leadership class computers
  - Computational nuclear structure

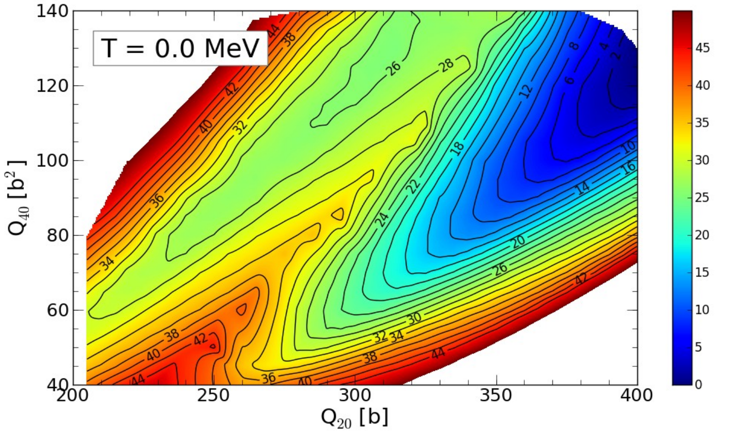
# Highlight 1
## Potential Energy Surfaces

# Managing the Scale

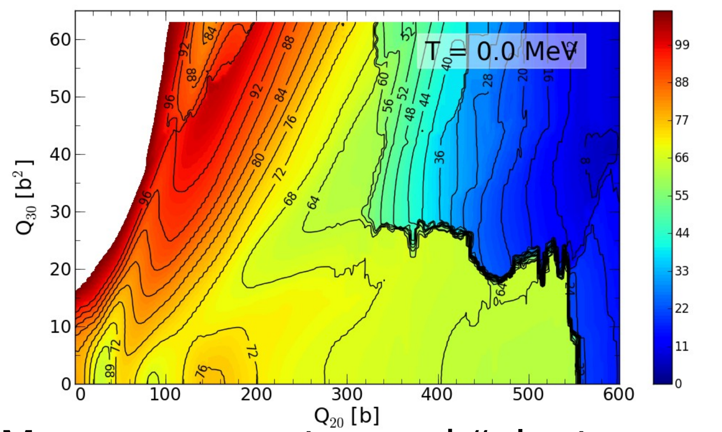
- Testbench: $^{239}$Pu(n,f)
- Relevant collective variables: $q_{20}$, $q_{22}$, $q_{30}$, $q_{40}$
  - Triaxiality near ground-state and first barrier
  - Octupole and hexadecapole beyond first barrier




Elongation and triaxiality

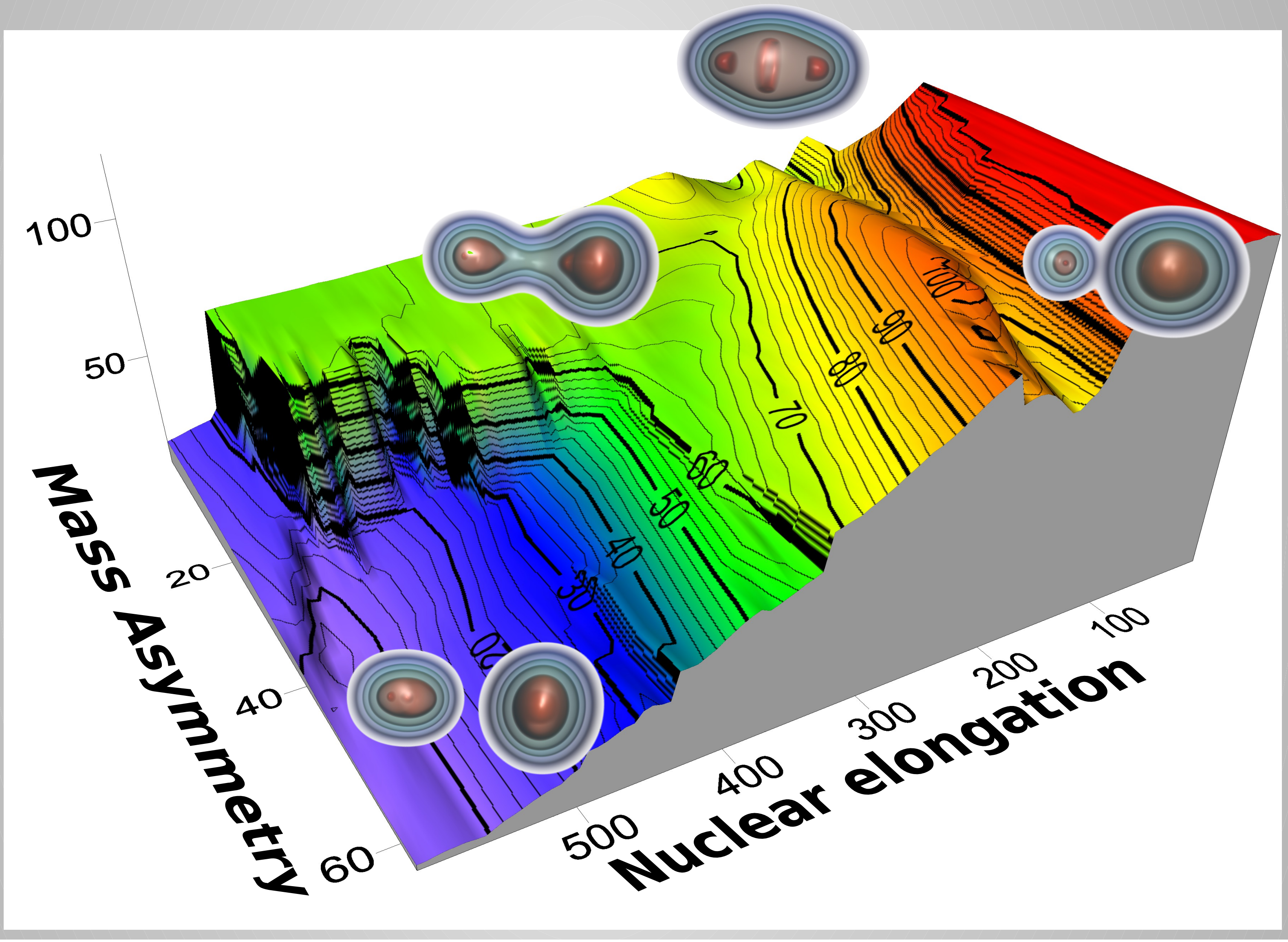



Fission and fusion valleys

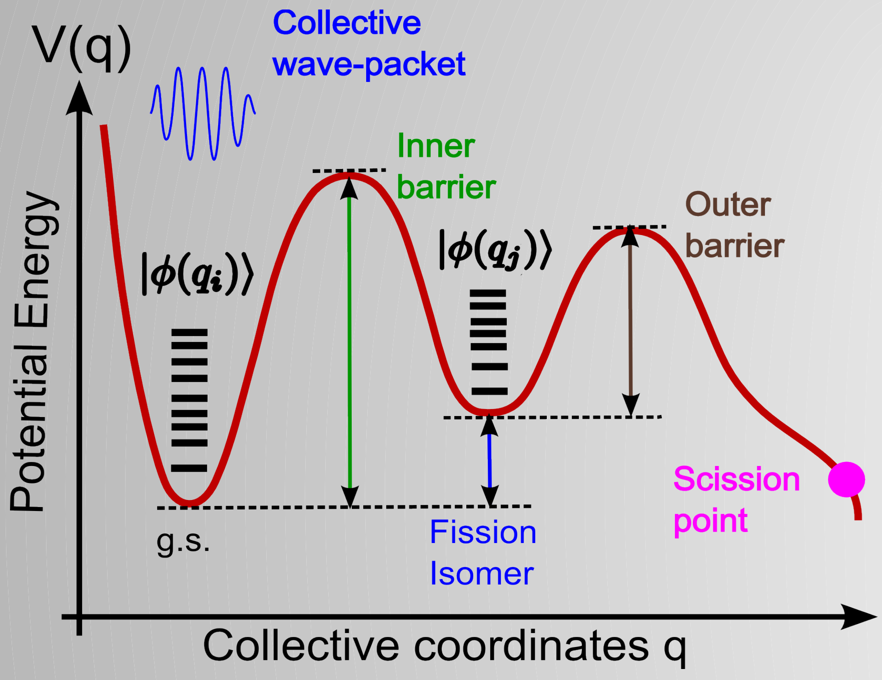


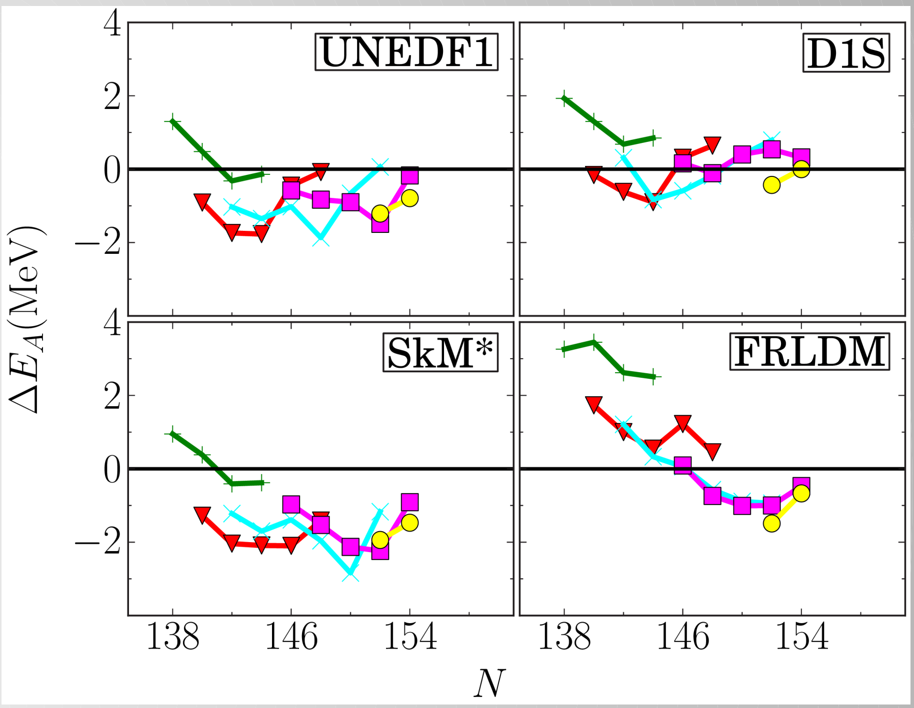

Mass asymmetry and “cluster radioactivity”

# A Closer Look



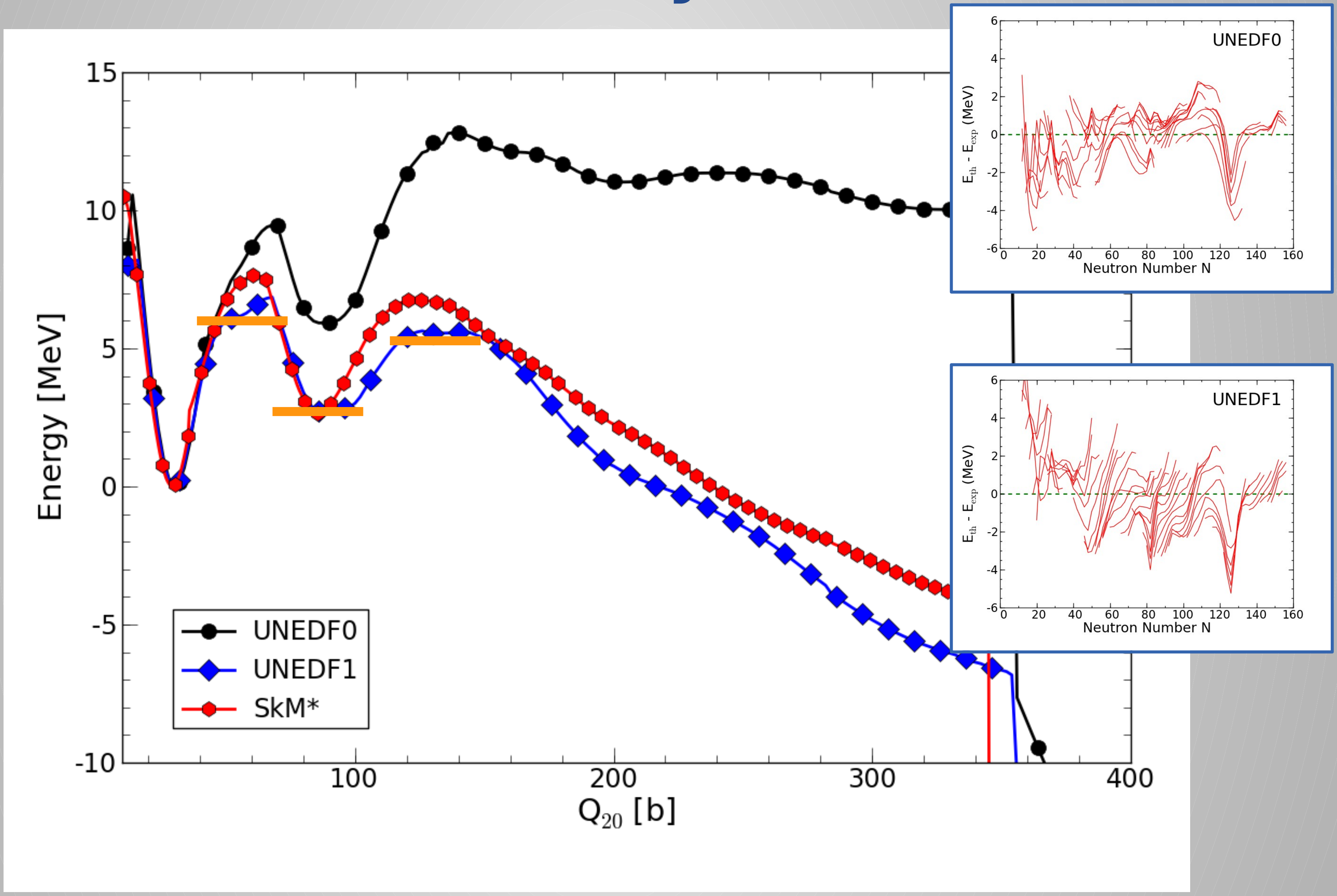
# Fission Barriers



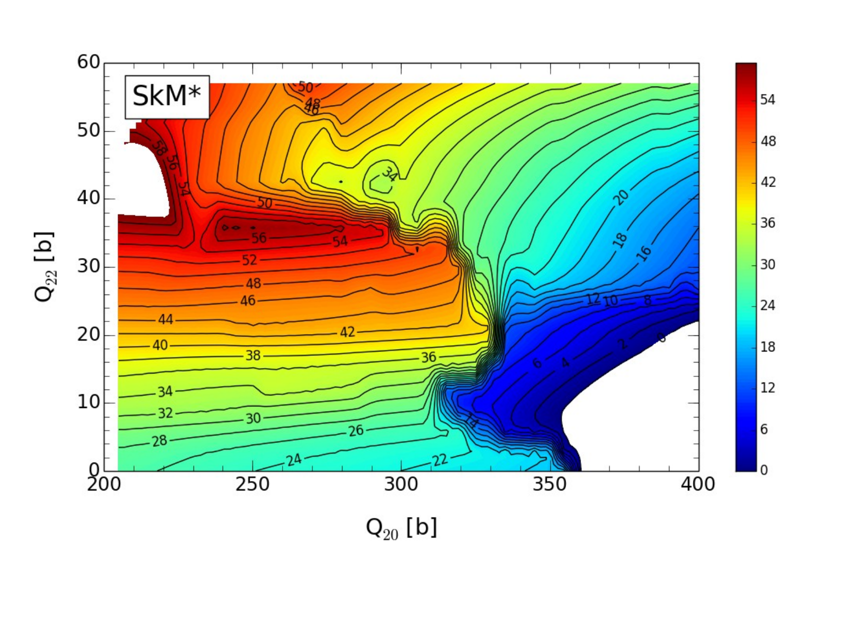



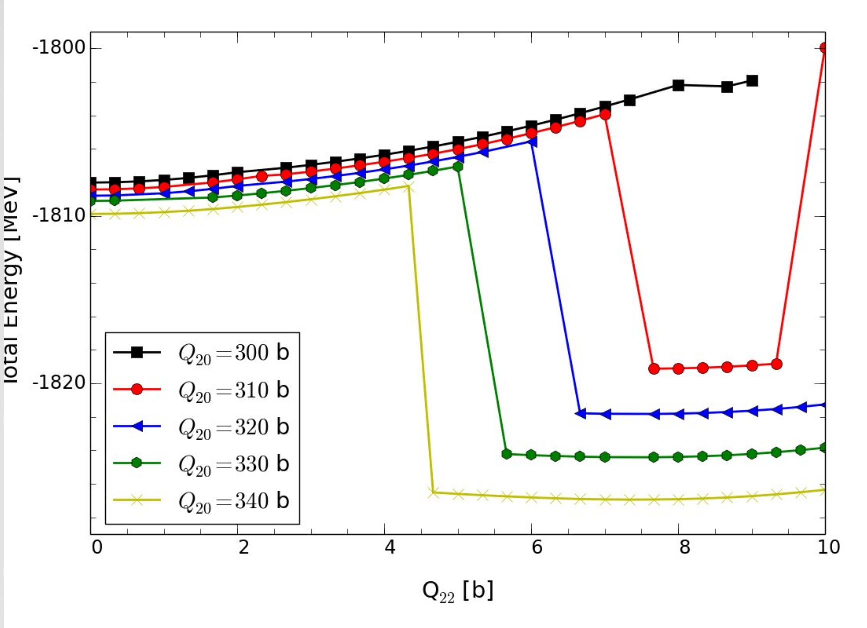

- Calculations: J. McDonnell
- DFT methods better than semi-empirical models
- Small errors on fission barriers = orders of magnitude in lifetimes

# Full Fission Pathways



# Triaxiality at Scission



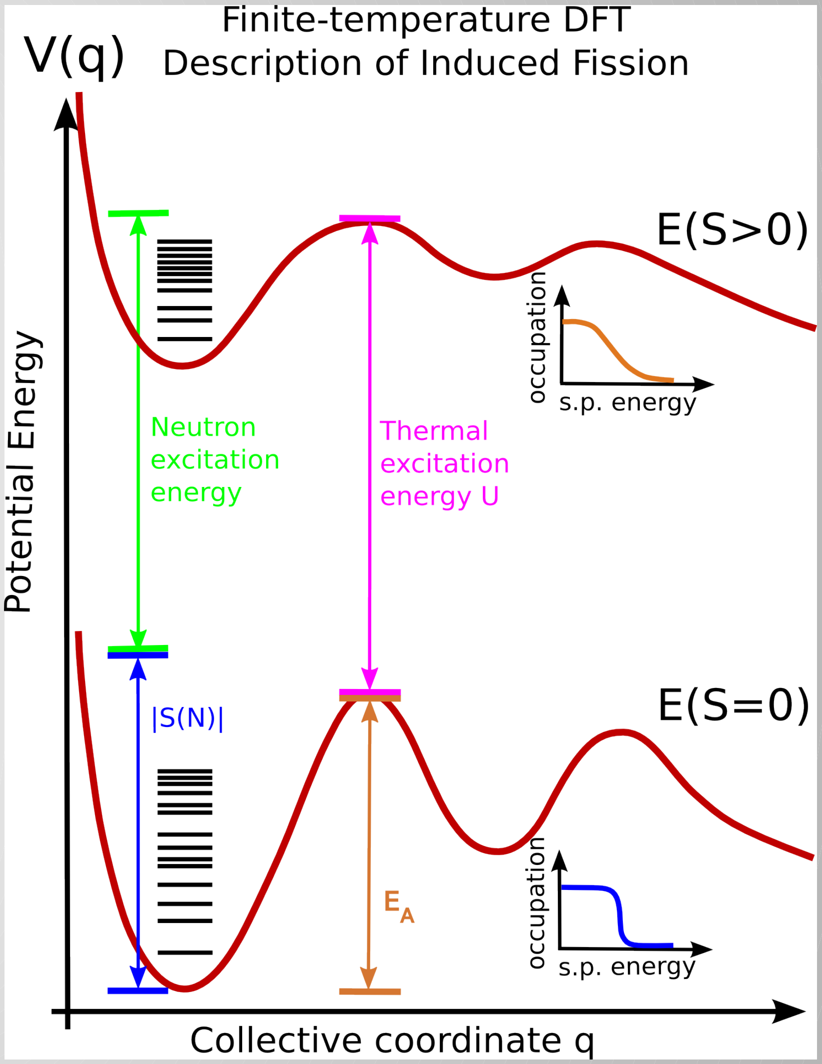

- Local PES in the ($q_{20}$,$q_{22}$) plane around least-energy fission path
- Shallow axial valley:
  - Distributions of fission fragments will be different
  - Dissipation of energy in "transverse" modes

# Highlight 2

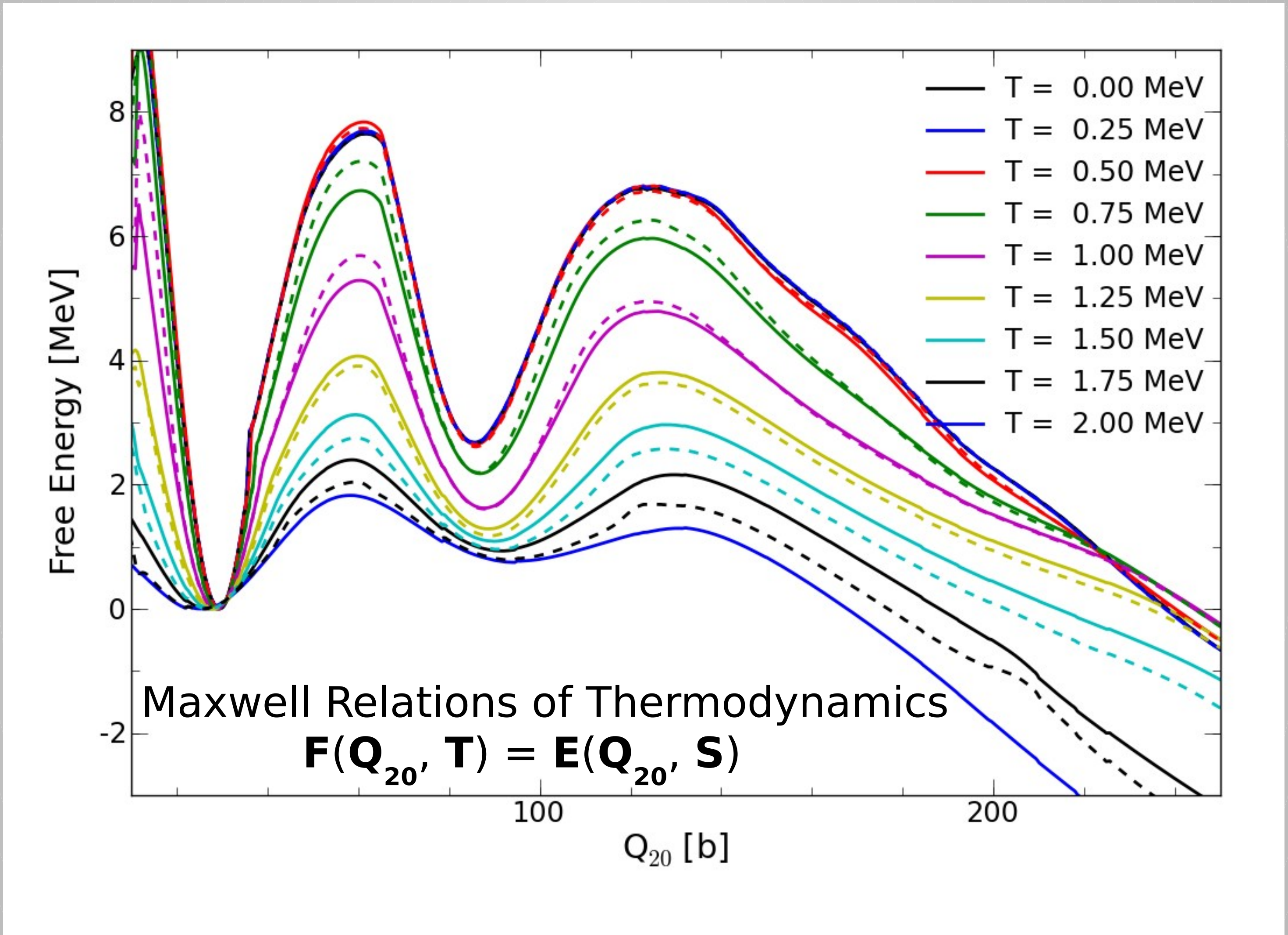
## Validation of Nuclear Density Functional Theory at Finite Temperature

# Dealing with Excitation Energy

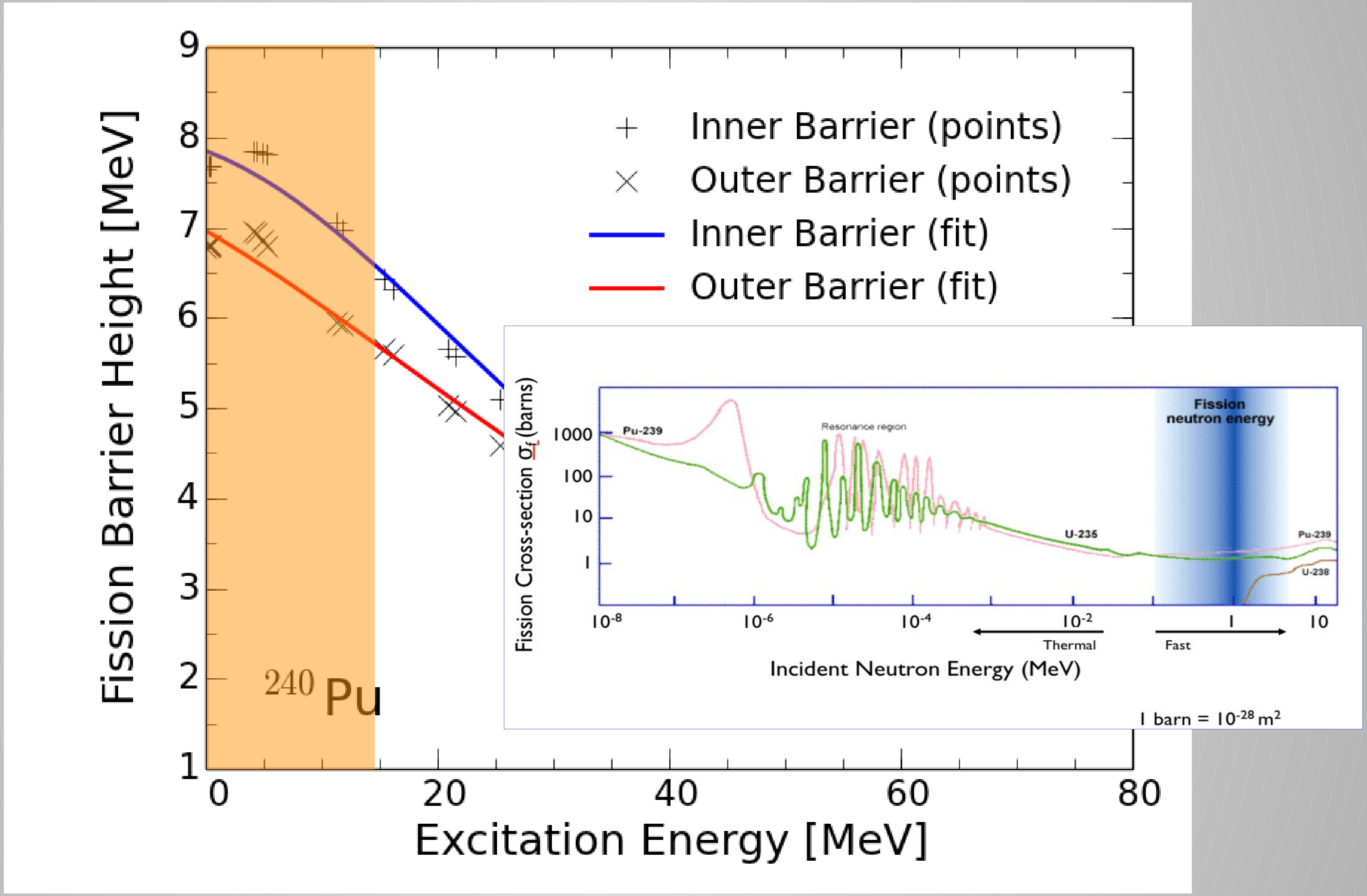
- Question: how to describe highly-excited compound nucleus?
- Potential energy surfaces from finite-temperature DFT calculations
  - System in thermal equilibrium
  - Ground-state is statistical superposition of pure quantum mechanical states
- Attention: at given $0 < T \lesssim 2.5$ MeV (or $0 < E^* \lesssim 100$ MeV excitation energy), ***there is still a barrier!***
  - Temperature must be such that the system remains fissile
  - There is not a single good recipe here



# Potential Energy Surface at T>0



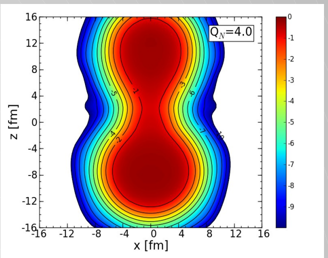
# Evolution of Fission Barriers

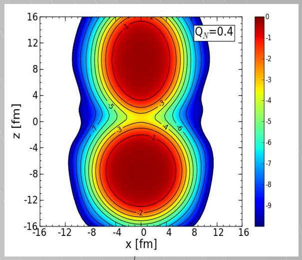


# Highlight 3

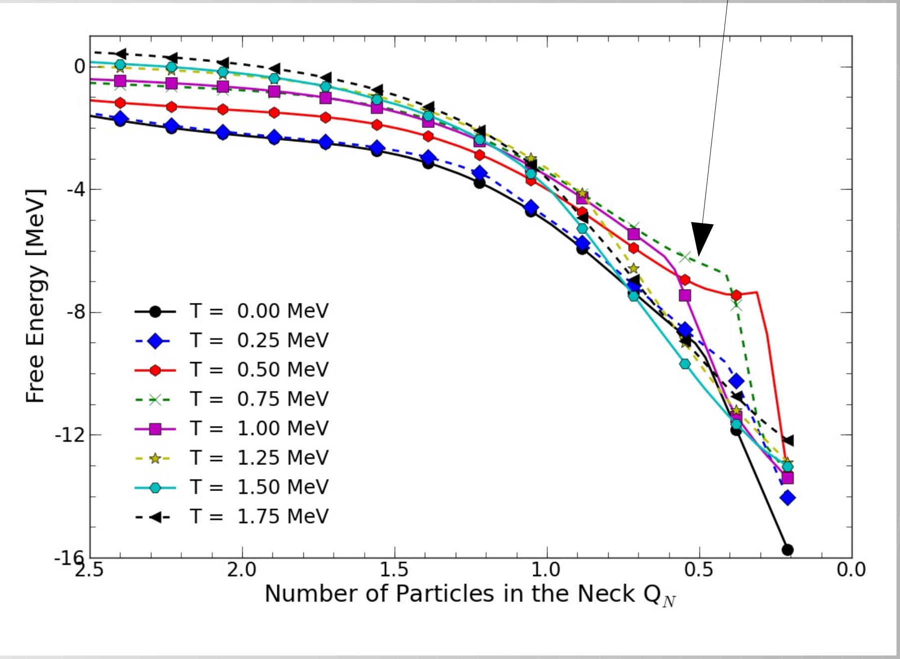
## Fission Fragment Properties at Finite Temperature

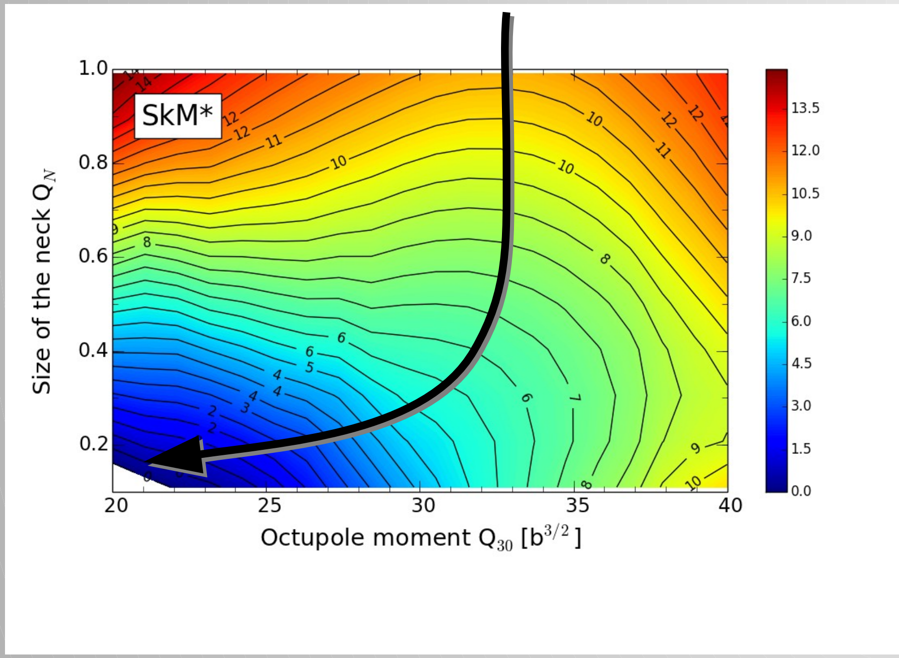
# Approaching Scission



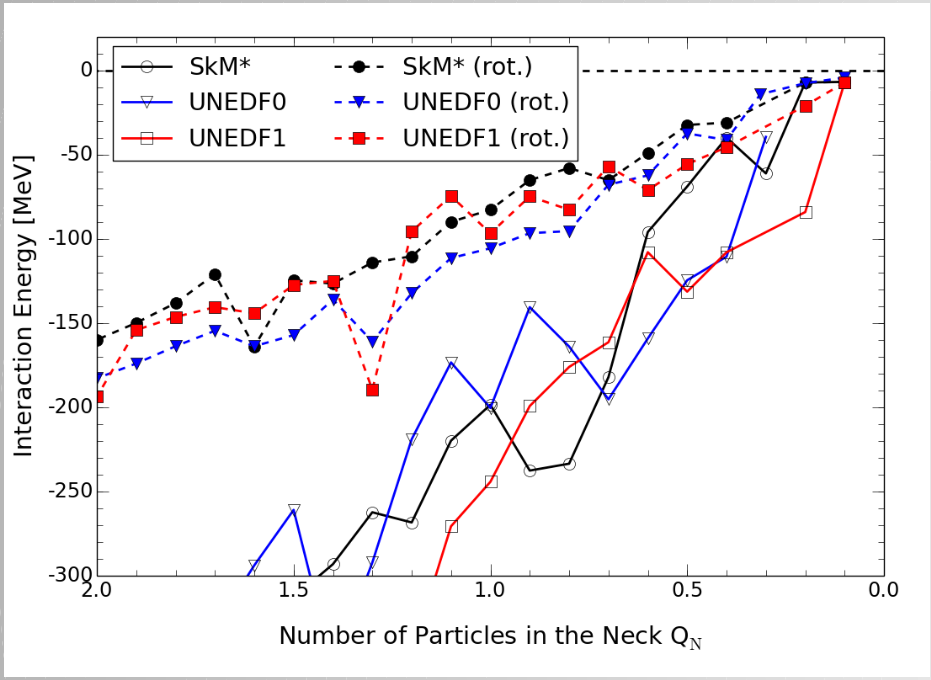

- Discontinuities: poor man's way to define scission
- Need to introduce another collective variable: $Q_N$
- Discontinuities => smooth pathway to scission

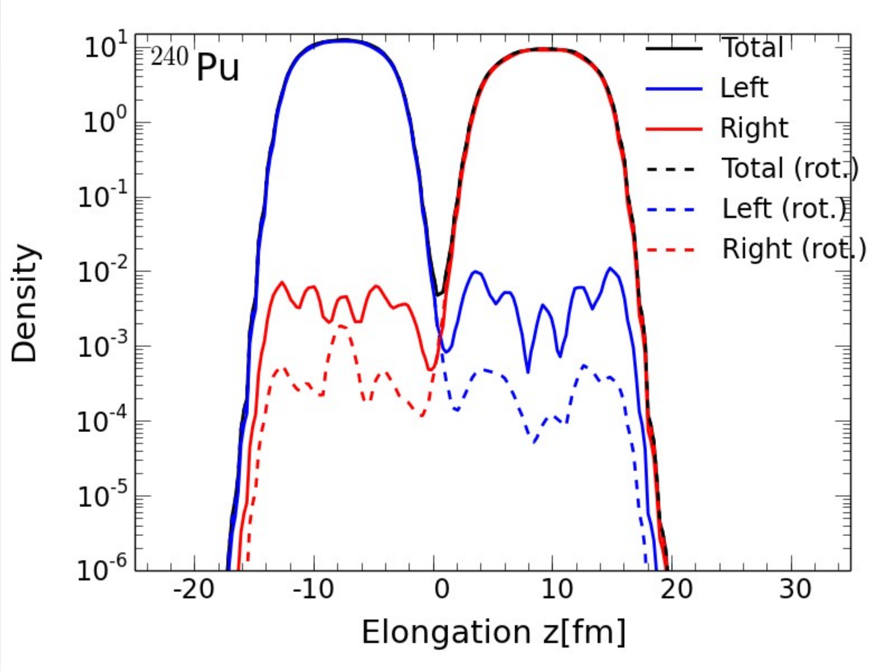



- Impact of $Q_N$ of the order of 10 MeV on prescission energy
- Where is scission?

# Fragment Interaction Energy (T=0)



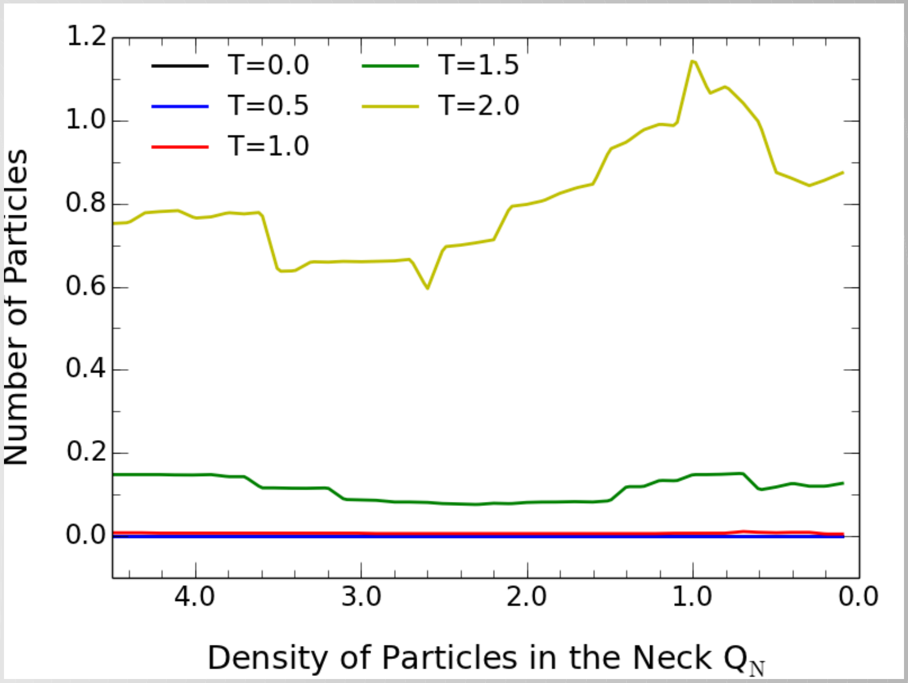

- After scission: independent fragments with nuclear interaction energy equal to 0: use as criterion for scission
- Disentangle the two fragments by unitary transformation of individual quasi-particles
- Does the method work at finite temperature?

# Coupling to the Continuum

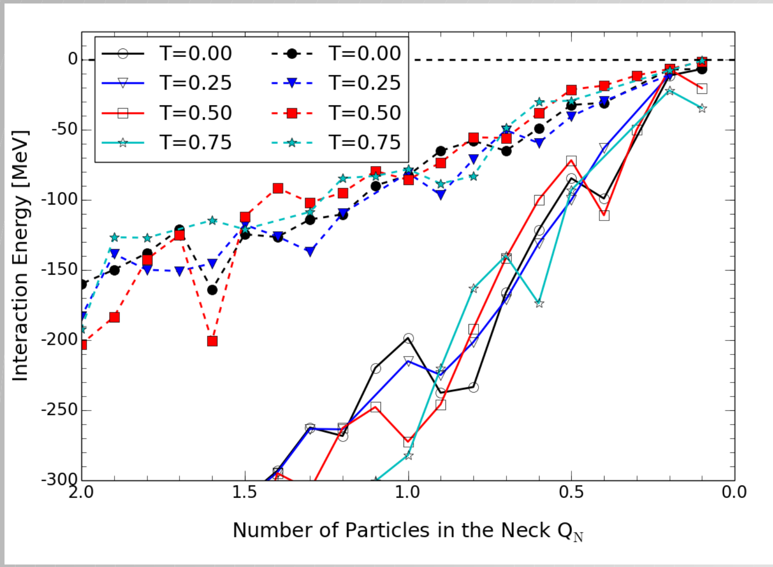
- Contribution to total density comes from localized and delocalized pieces at T>0

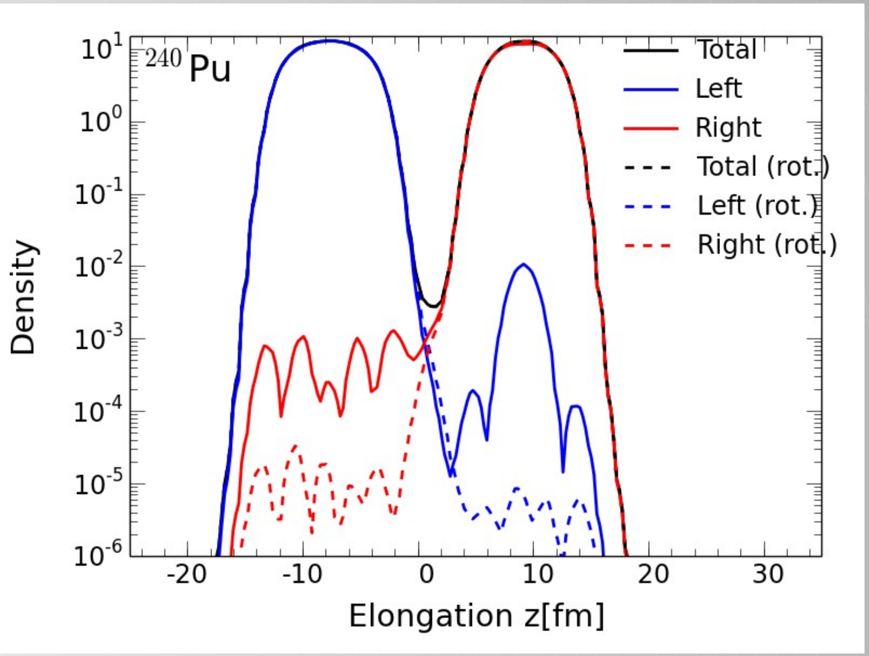
$$\rho = V^*(1-f)V^T + U^* f U^T$$

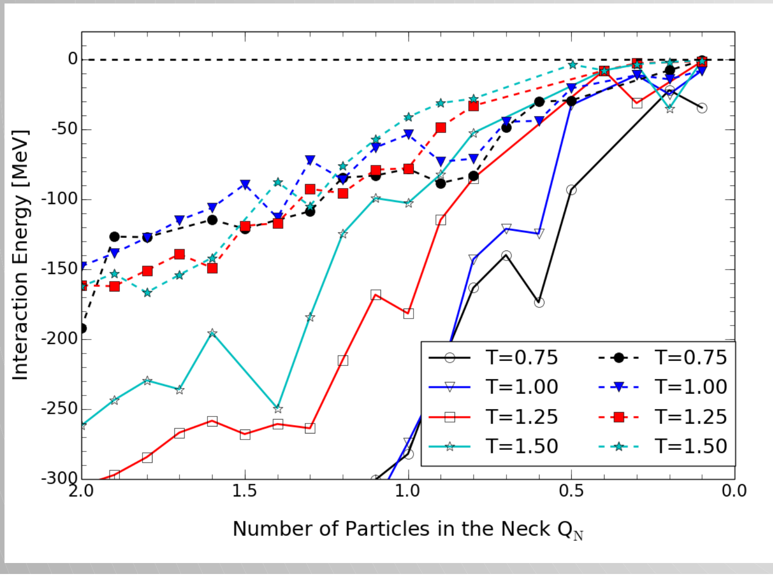
- Can we localize the fragments?
- Delocalized contribution negligible until T≳1.5 MeV (E*~ 40 -50 MeV!)
- Localization should work



# Fragment Interaction Energy (T>0)




- Localization works indeed
- At high temperatures, scission point moves to thicker necks: glass-like behavior

# Conclusions

- Solving nuclear fission with microscopic methods and HPC capabilities
- Recent progress discussed in this talk
  - Mapping five-dimensional collective spaces including triaxiality
  - Assessing the sensitivity on the parametrization of the energy functional
  - Predicting evolution of fission barriers at finite temperature
  - Understanding the impact of finite temperature on fission fragment properties
- Open questions
  - Need better UQ to assess model dependence: model space (HO basis), parametrization of functionals, form of functionals, etc.
  - Dynamics of induced fission: dependence on scission point, on collective inertia
  - Finite-temperature caveats: statistical fluctuations, excitation energy of the fragments, collective mass

# Collaborators

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