A Predictive Theory for Fission

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Support

This research is supported by the LDRD Office at LANL as part of LDRD-DR project 20120077DR: 'Advancing the Fundamental Understanding of Fission.' This project aims to develop both experimental and theoretical tools allowing significantly improved nuclear data evaluations of fission-fragment properties, particularly as a function of incident neutron energy for induced fission.

Background

45 years of research at LANL calculating nuclear potential energies and dynamical models of fission has matured to the level that we think a quantitatively predictive fission model is feasible. ‘

Background II

The Approach:

Solve Dynamical Equations for the Fissioning Nucleus

1. The relevant degrees of freedom for fission are the nuclear shape.
2. Use the Macroscopic-Microscopic method to calculate the potential energy of the nucleus as a function of its shape.
3. Do Monte-Carlo modeling of the trajectories of fissioning nuclei in a multidimensional space of shape coordinates.

4. Accumulate distributions of dynamical properties of the fragments before neutron evaporation starts.

Background III

Why not a microscopic model?

Self-consistent density functional theory—DFT

1. DFT is still phenomenological, while having the decided advantage of allowing the effective one-body potential to be defined self-consistently.
2. NR HFB models require an arbitrary spin-orbit strength.
3. A competitive global reproduction of nuclear masses, deformations, and ground-state spins has not been accomplished.

4. Nuclear surface properties are wrong (large curvature energy); leads to too high fission barriers for lighter systems.
5. Essentially no novel predictions from this approach (yet).
6. Difficult to calculate. A factor of 10^4–10^5 more computation time than our methods.
7. No way is known to unambiguously determine a fission saddle point.

Background IV

Why we are sanguine about a predictive dynamical model of primary fission-product properties.

1. Predictive success of the Los Alamos global nuclear structure model,
2. Predictive success of the Los Alamos nuclear dynamics model with modified surface dissipation,
3. Predictive success of the semi-dynamical fission model of Randrup and Möller.

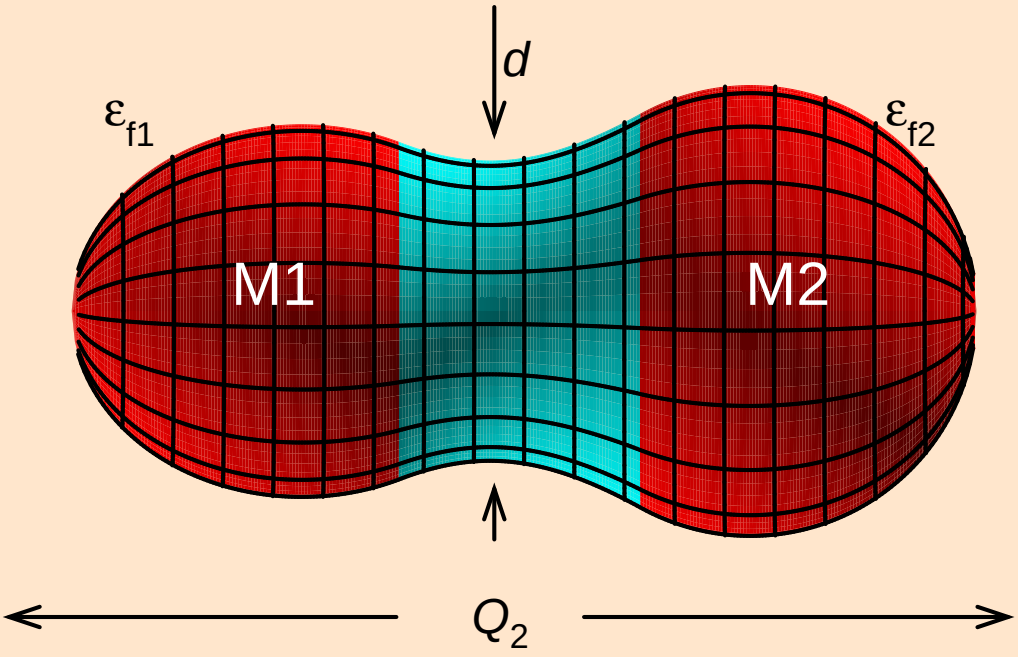
Los Alamos Global Nuclear Structure Model

Nix and Möller ∼1970–2013

1. Parametrize the nuclear shape (5–8 parameters),
2. Calculate the macroscopic energy,
3. Calculate the microscopic correction energy,
4. Find the compact shape with a local minimum in the energy (ground-state mass and shape),
5. Vary parameters of the macroscopic energy model to minimize deviations from experimental masses,

6. Möller-Nix nuclear mass model; 2012 version has rms theory error of 0.559 MeV for 2183 masses from AME 2003; predicts 154 masses from AME 2012 with rms error 0.569 MeV,
7. Comparable reproduction of fission-barrier properties,
8. Predicts deformations of ground states, shape isomers, and saddle points.

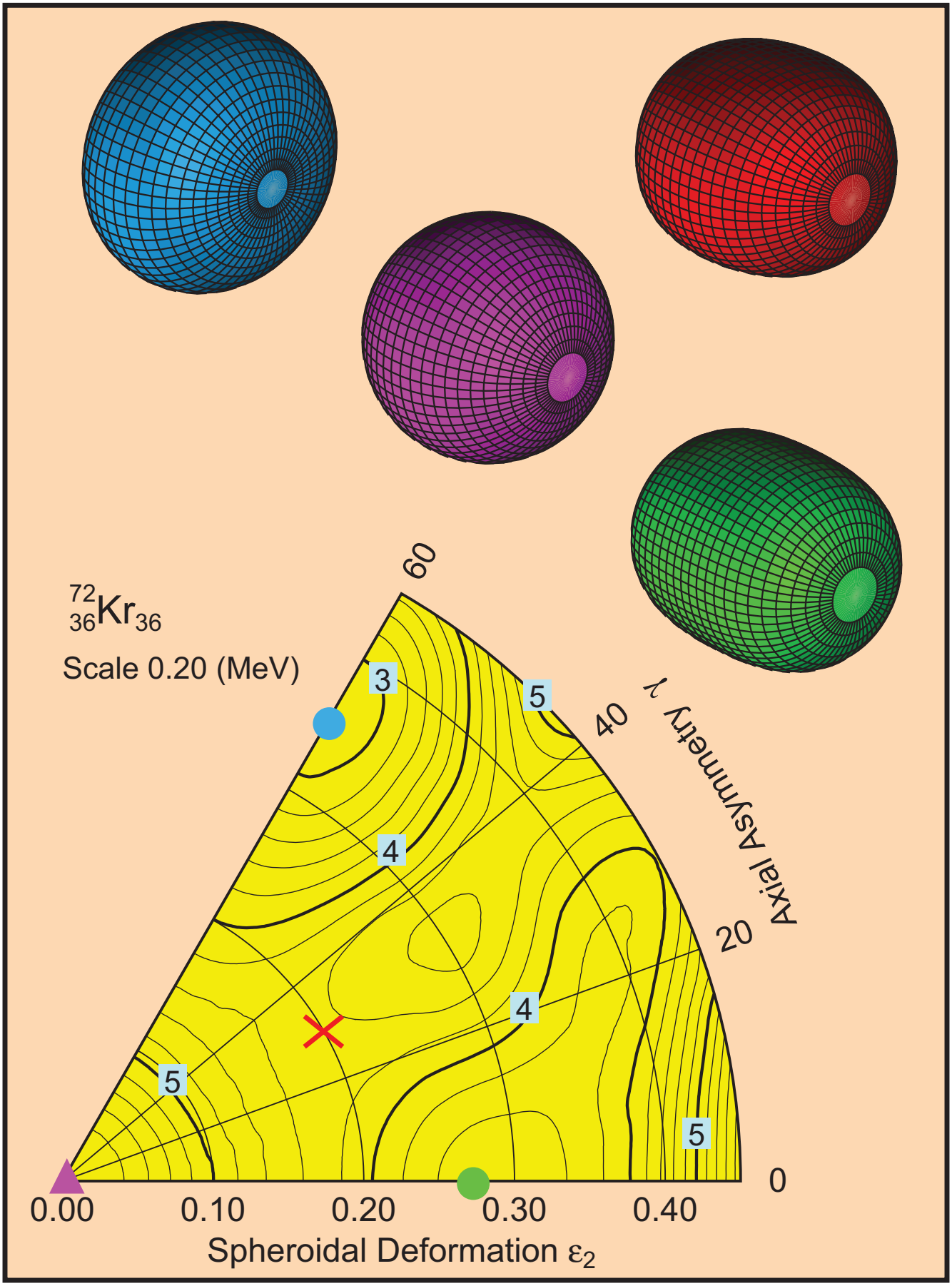
Five Essential Fission Shape Coordinates

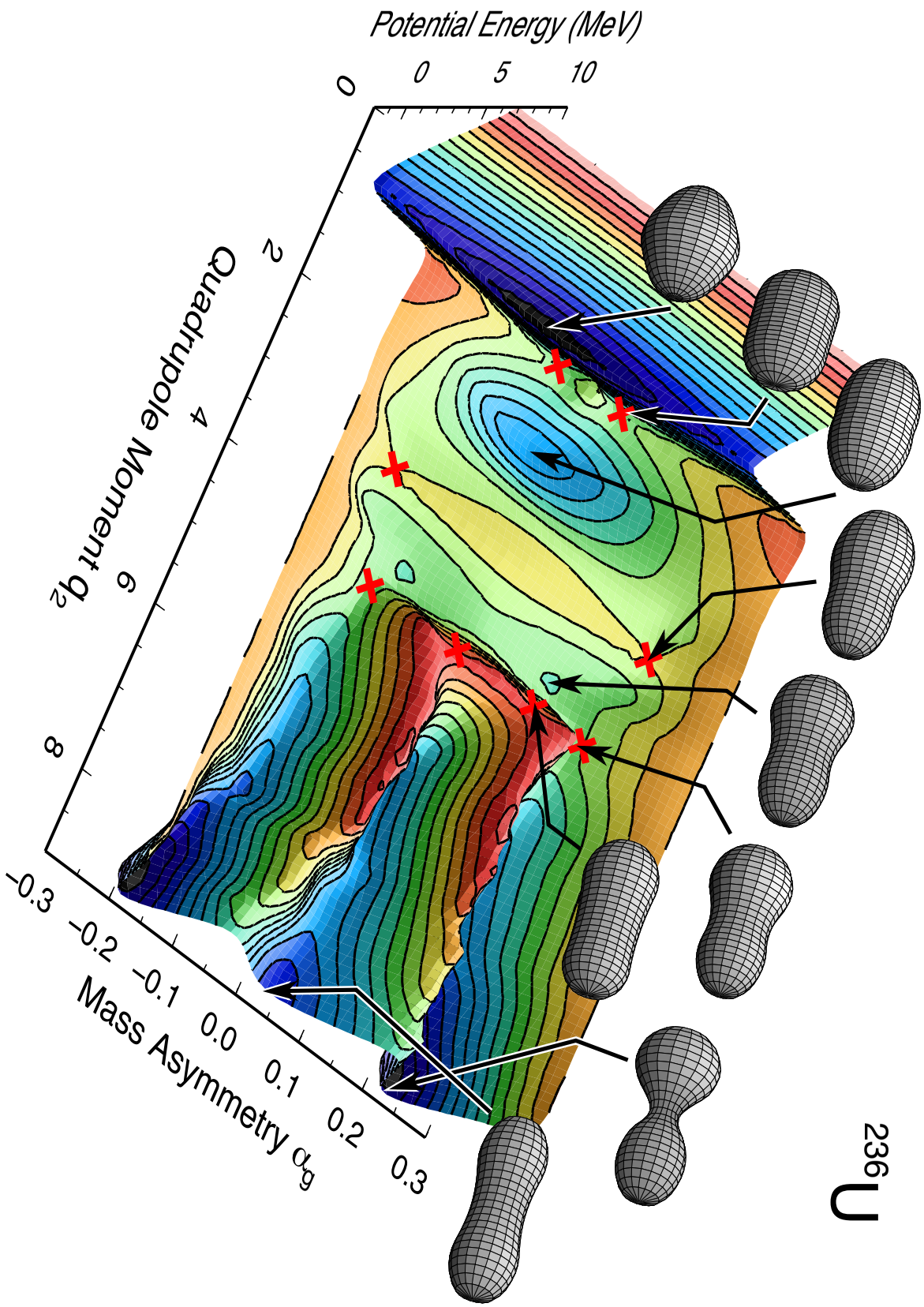


45	Q_2 ~	Elongation (fission direction)
⊗		
35	α_g ~	(M1-M2)/(M1+M2) Mass asymmetry
⊗		
15	ε_{f1} ~	Left fragment deformation
⊗		
15	ε_{f2} ~	Right fragment deformation
⊗		
15	d ~	Neck

⇒ 5 315 625 grid points – 306 300 unphysical points

⇒ 5 009 325 physical grid points

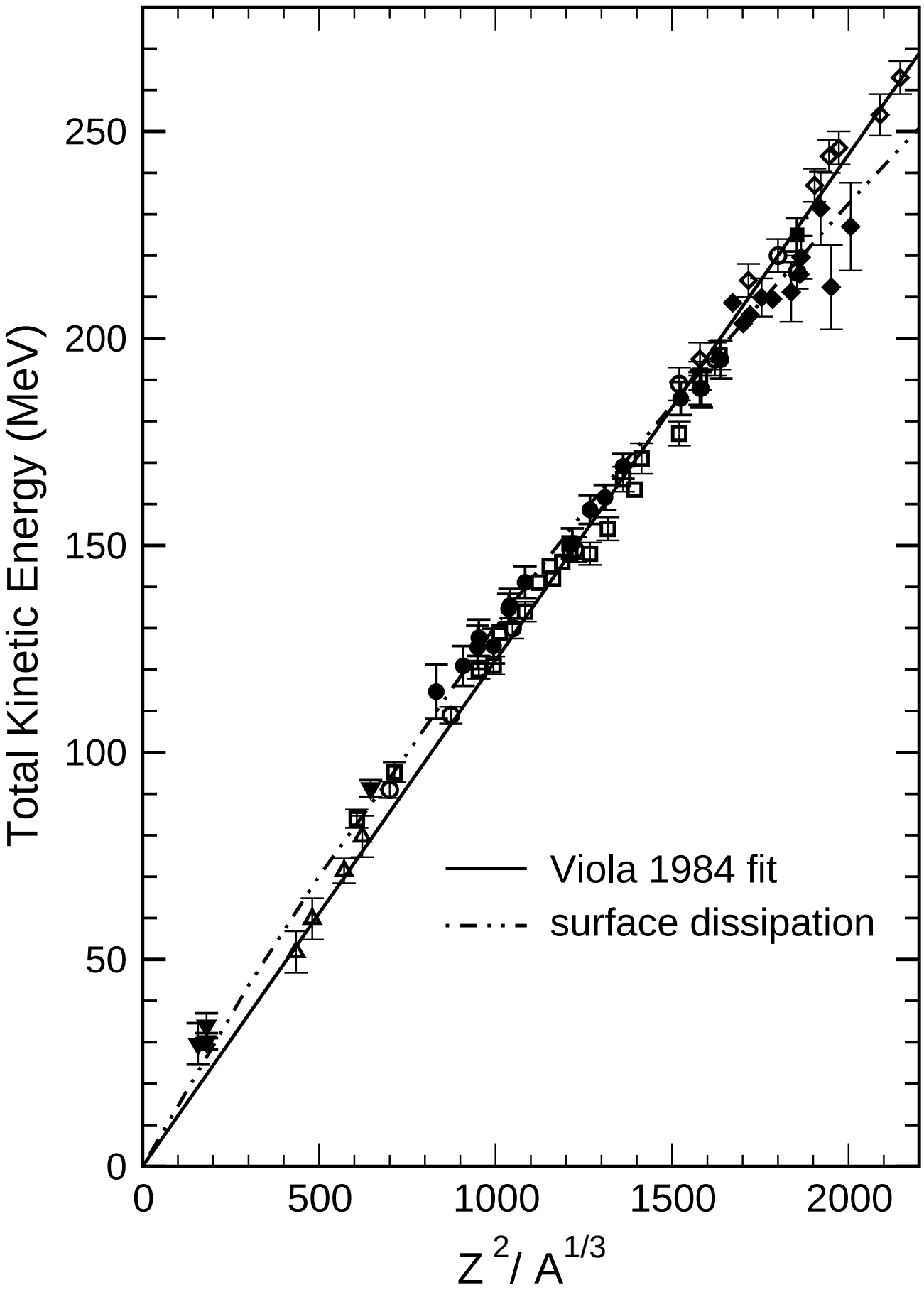

$^{72}_{36}Kr_{36}$
Scale 0.20 (MeV)
60
40
20
0
Axial Asymmetry γ
3
5
4
4
5
5
0.00
0.10
0.20
0.30
0.40
Spheroidal Deformation ε2


Potential Energy (MeV)
0
5
10
Quadrupole Moment q_2
0
2
4
6
8
Mass Asymmetry α_g
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
^{236}U

Mean Dissipative Dynamical Trajectories

1. Potential energy vs. shape from macroscopic part of LAGNS model,
2. Define an inertia tensor for dynamical shape changes,
3. Define a dissipation tensor giving the damping of shape motion into internal excitations (heat),
4. Calculate dynamical trajectories of the fission process,
5. Leads to average fragment TKE, average fragment excitation energy after separation,

6. TKE for symmetric fission reproduced with chi-squared per point = 3.6 with NO fitting.


Total Kinetic Energy (MeV)
0
50
100
150
200
250
0
500
1000
1500
2000
Z 2 / A 1/3
Viola 1984 fit
surface dissipation

Stochastic Dynamics

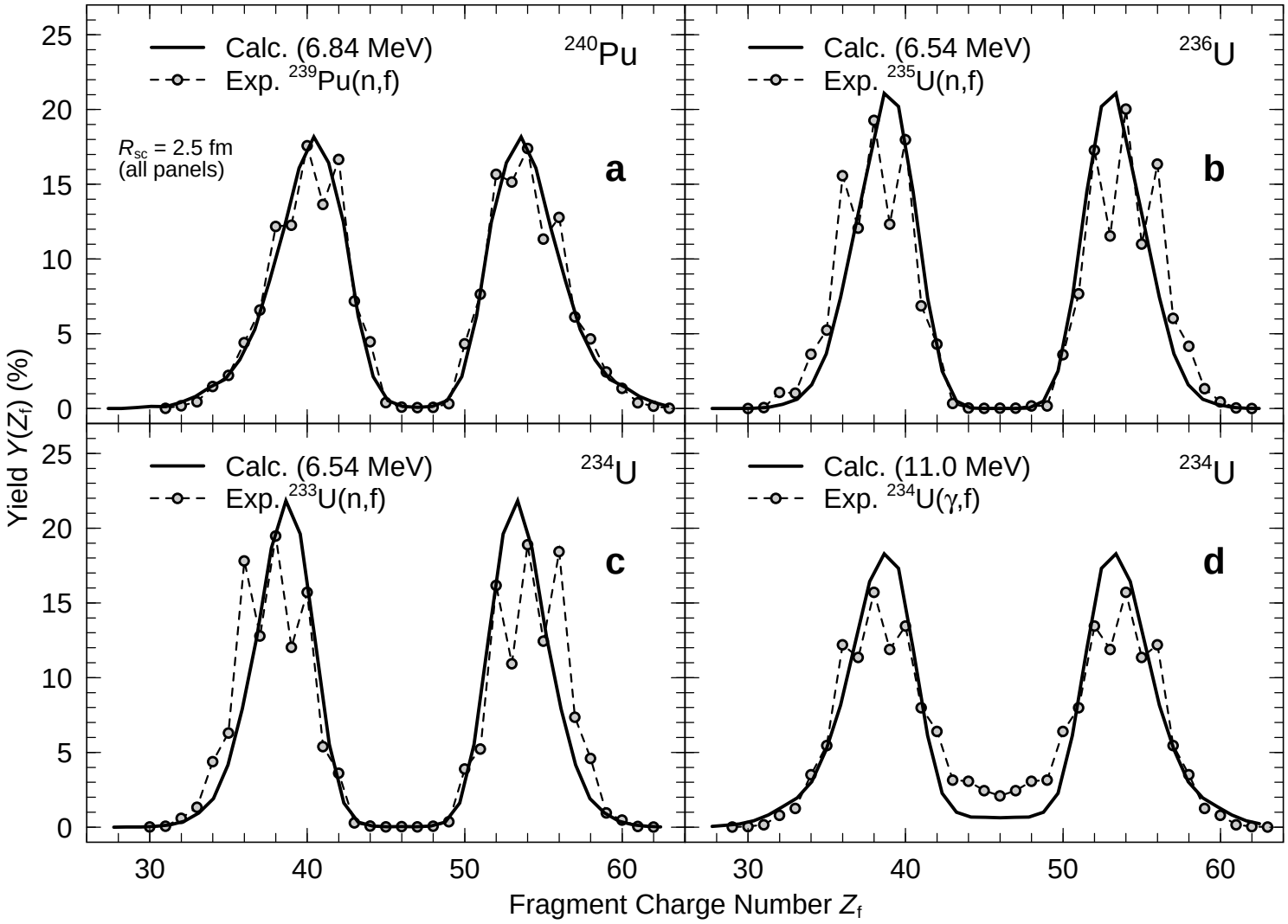
Something is missing.

The Fluctuation-Dissipation Theorem implies that along with damping, a stochastic force acts on a system.

The semi-dynamical model of Randrup and Möller (2011):

Start near the saddle point and randomly evolve over the potential-energy surface with thermal weighting.

- Time has a direction, but not a magnitude,
- Predict mass distributions,
- No information about energies of fragments.


Calc. (6.84 MeV)
Exp. 239Pu(n,f)
240Pu
Rsc = 2.5 fm
(all panels)
a
Calc. (6.54 MeV)
Exp. 235U(n,f)
236U
b
Calc. (6.54 MeV)
Exp. 233U(n,f)
234U
c
Calc. (11.0 MeV)
Exp. 234U(γ,f)
234U
d
Yield Y(Zf) (%)
Fragment Charge Number Zf
0
5
10
15
20
25
30
40
50
60

Full Dynamical Model

Solve multi-dimensional Langevin dynamical equations:

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} = \frac{\partial (T+V)}{\partial p_j} = \frac{\partial (\frac{1}{2} M^{-1}_{ik} p_i p_k)}{\partial p_j}$$

$$\frac{dp}{dt} = -\frac{\partial V}{\partial q} + \frac{1}{2}\frac{\partial M}{\partial q}\dot{q}\dot{q} - \eta\dot{q} + \sqrt{\frac{2\eta T}{\Delta t}}\Theta(t),$$

where Θ is a normally distributed random number with variance 1.0.

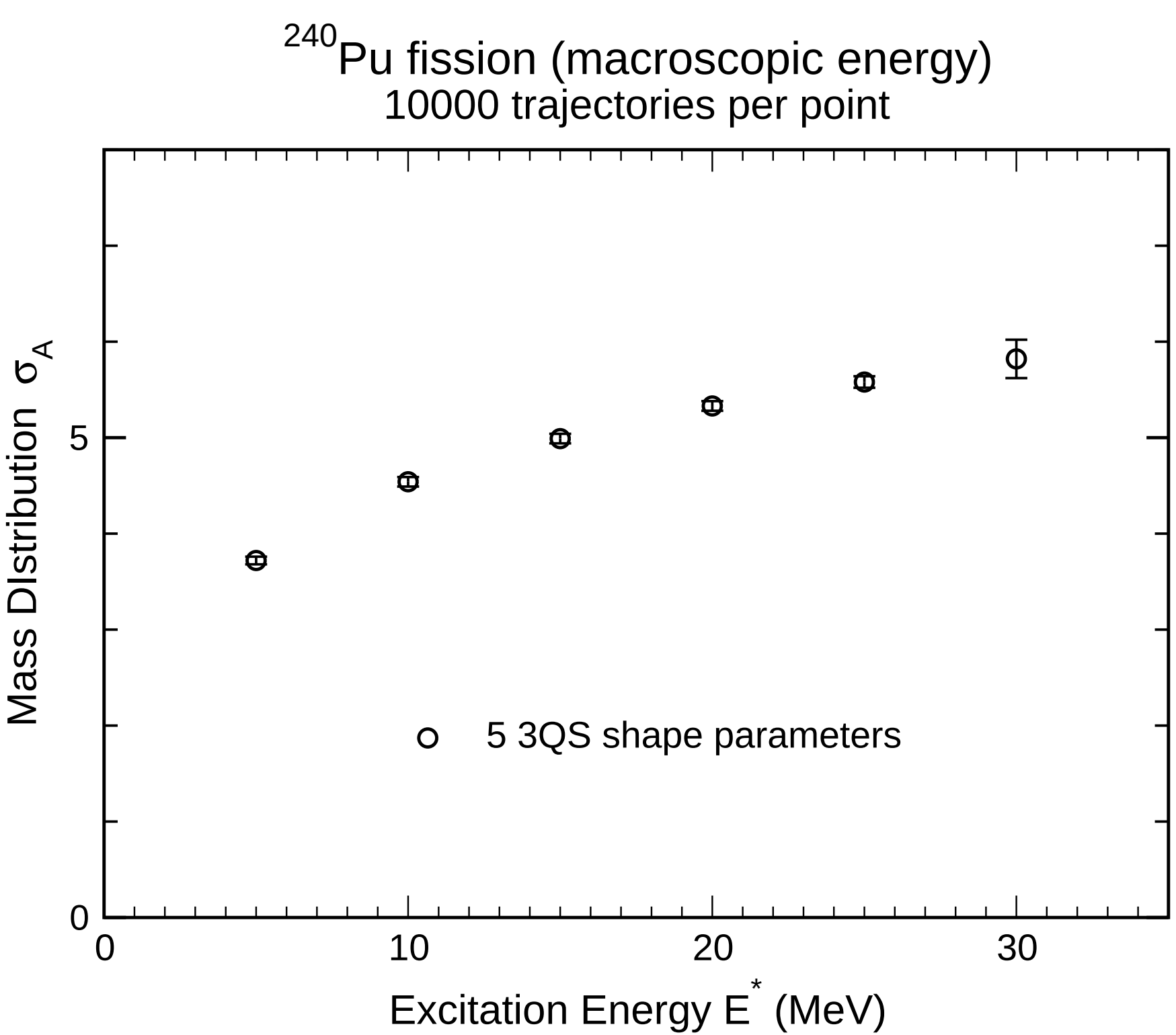
1. Macroscopic-microscopic potential energy from LAGNSM,
2. Irrotational fluid inertia,
3. Surface-plus-Window dissipation,
4. Monte-Carlo solution of dynamical trajectories.

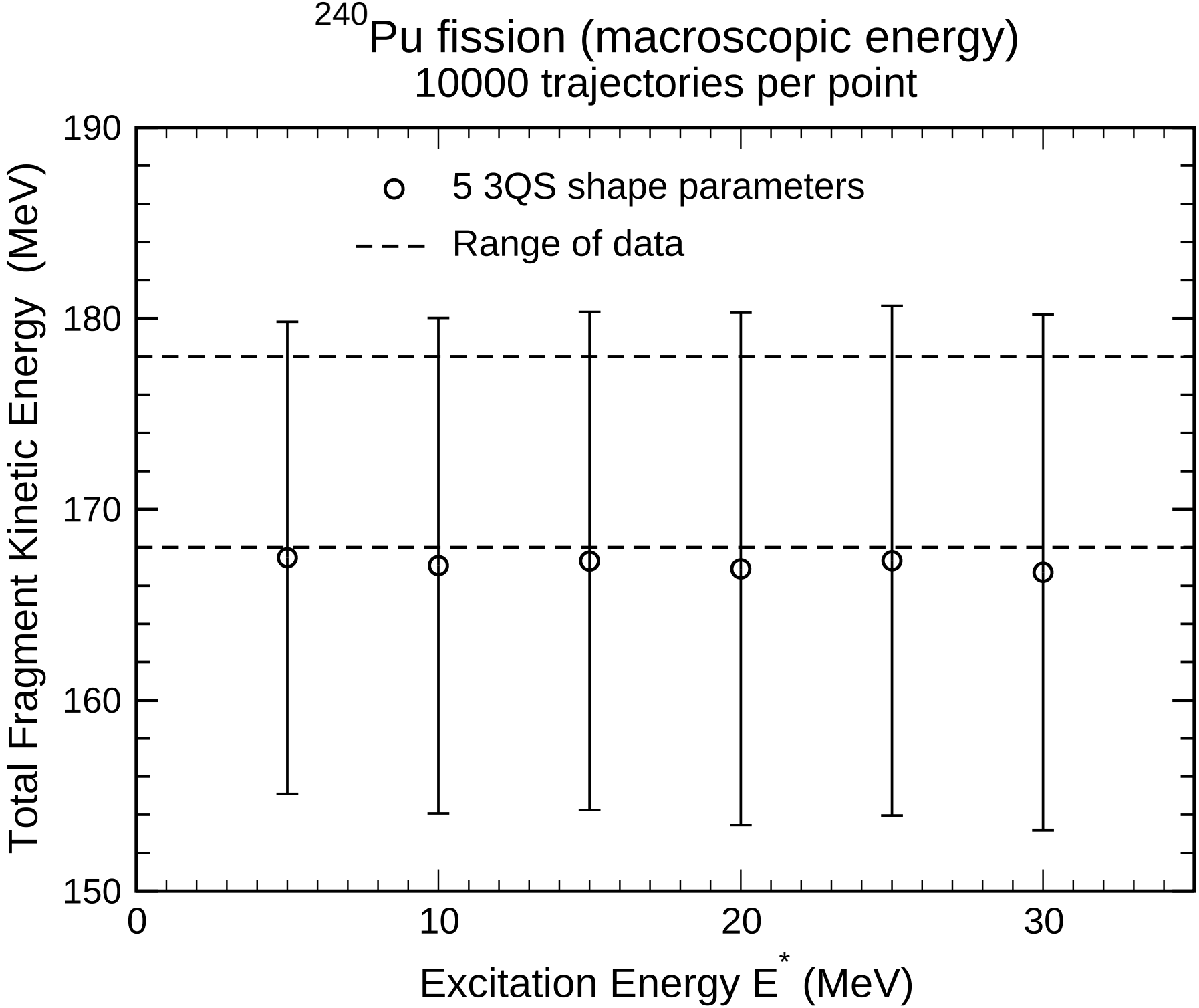
What Comes Out

Dynamical properties of fission fragments calculated as a function of initial E*

1. Fragments' charge and mass (prior to prompt neutrons),
2. Total fragment kinetic energies,
3. Fragment excitation energies—give neutron multiplicities,
4. Distributions and correlations of all these.

Use comparisons to data to inform possible modifications of inertia and dissipation models, level densities.


^{240}Pu fission (macroscopic energy)
10000 trajectories per point
Mass DIstribution σ_A
5
0
0
10
20
30
Excitation Energy E^* (MeV)
5 3QS shape parameters


^{240}Pu fission (macroscopic energy)
10000 trajectories per point
5 3QS shape parameters
Range of data
Total Fragment Kinetic Energy (MeV)
190
180
170
160
150
0
10
20
30
Excitation Energy E* (MeV)

Accomplished so far:

1. Two dynamical Langevin codes for two different parametrizations of the nuclear shape,
2. Defined grid appropriate for dynamics with about 9M points,
3. Calculated macroscopic energy and forces on grid,
4. Calculated microscopic energy on grid,
5. Developed cubic spline algorithim for size 8^5 moving local grid for interpolation of forces,

6. Wrote independent immersion algorithm to locate local minima to check results on new grid.

What remains

I have been unsuccessful so far in debugging a Jacobian routine to convert spline microscopic energy derivatives (grid coordinates) to dynamical coordinates. I am thus resorting to the relatively inefficient expedient of calculating numerical derivatives. This process is about half done. By the time I return from this workshop, I can begin calculating real Z, A, TKE distributions as functions of excitation energy.