Computational Approaches to Whole Process of Nuclear Fission

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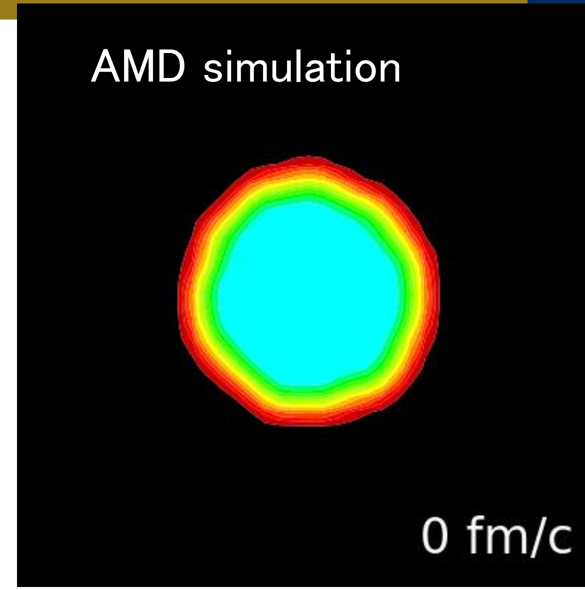
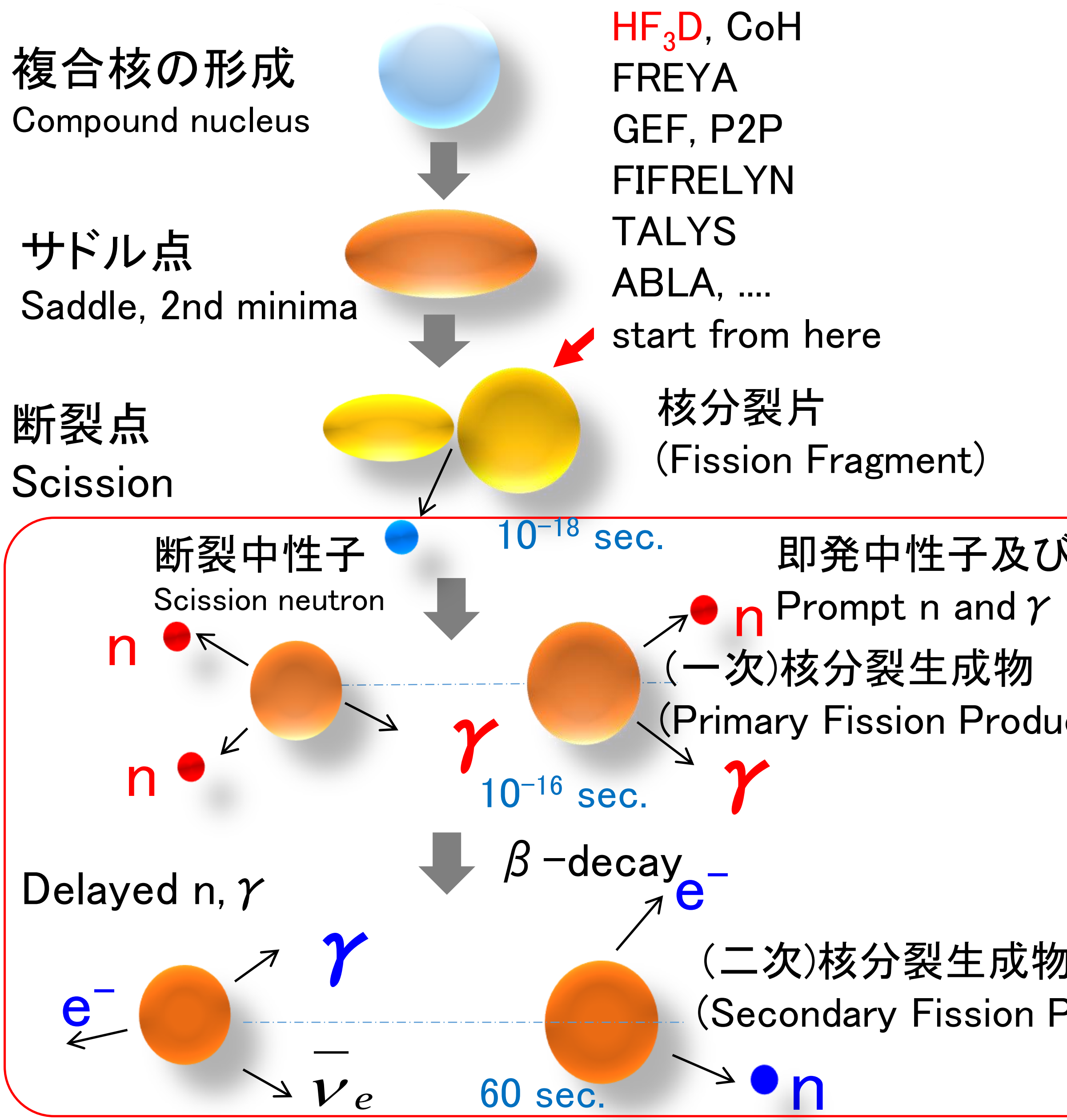
Contents

Background and introduction

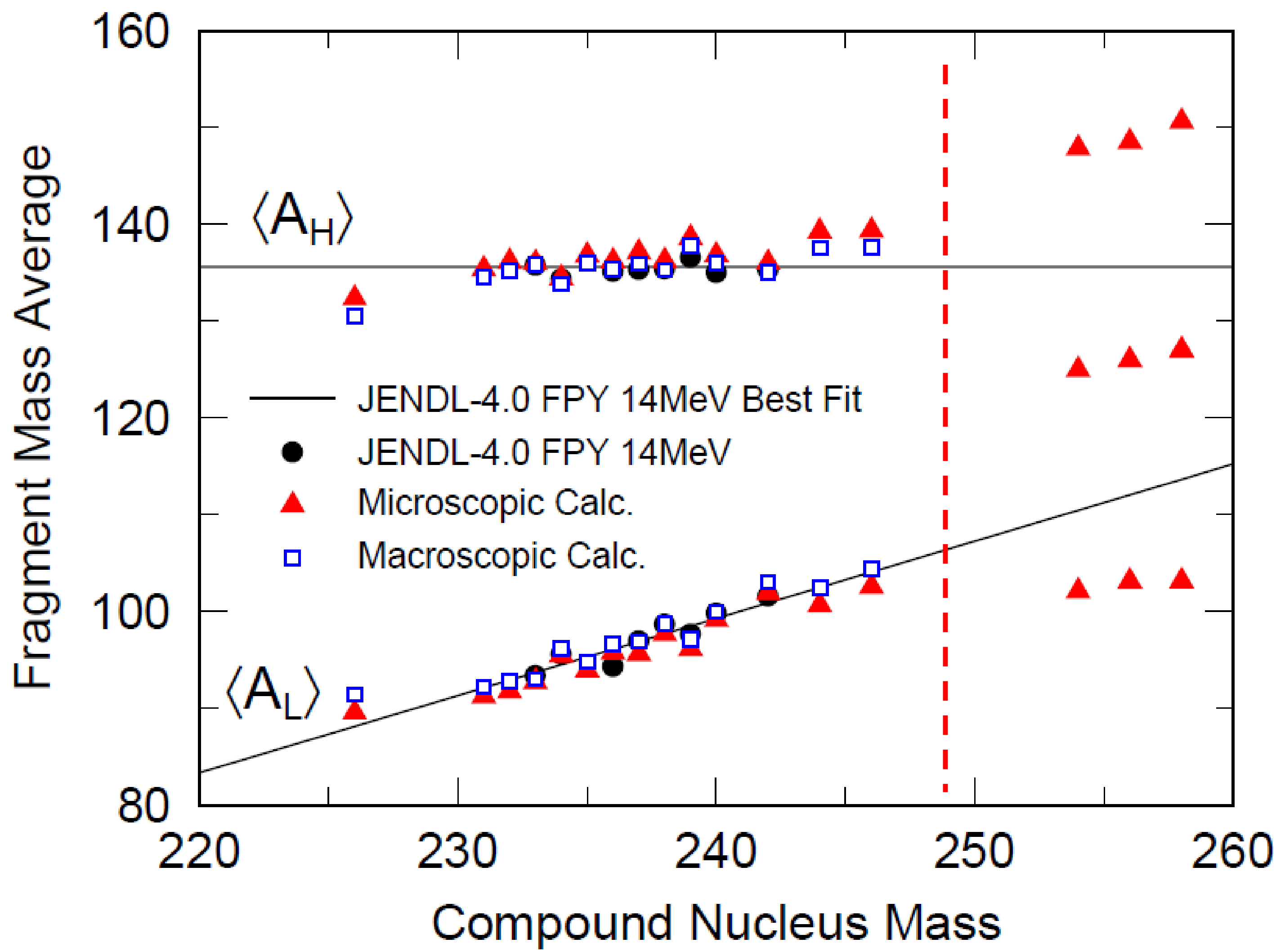
1. Nuclear fission is the key physics process as a base for generation of energy in nuclear technology
2. Therefore, nuclear data related to nuclear fission is most important
3. Nuclear fission is also important in understanding origin of heavy elements in r-process nucleosynthesis, since fission recycling seems to be occurring on NS-NS merger scenario
4. Due to complexity of the process, nuclear fission still offers a field of big challenges for nuclear physics, especially, the process from compound nucleus to scission is still a mysterious process

Time evolution of fission

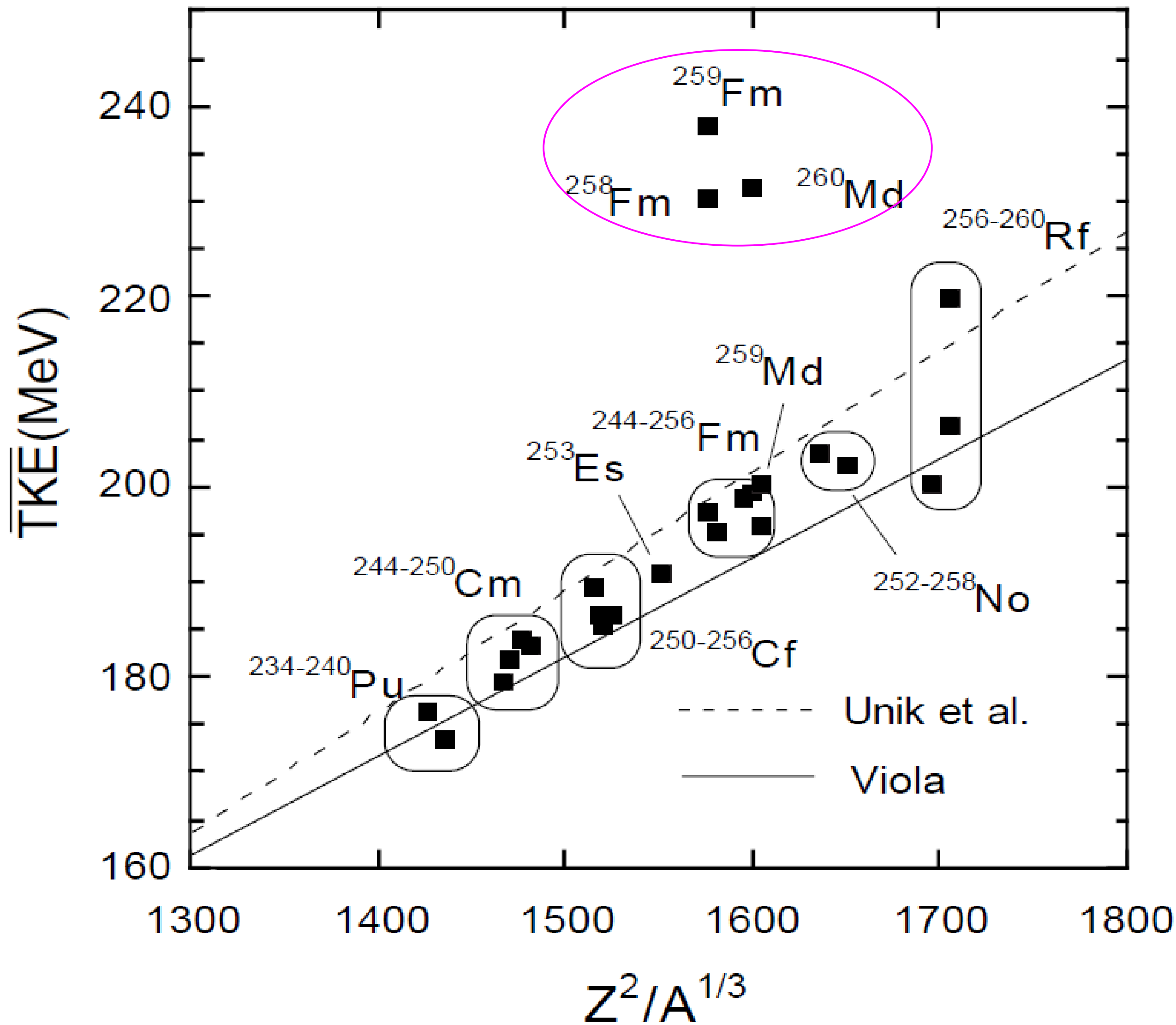




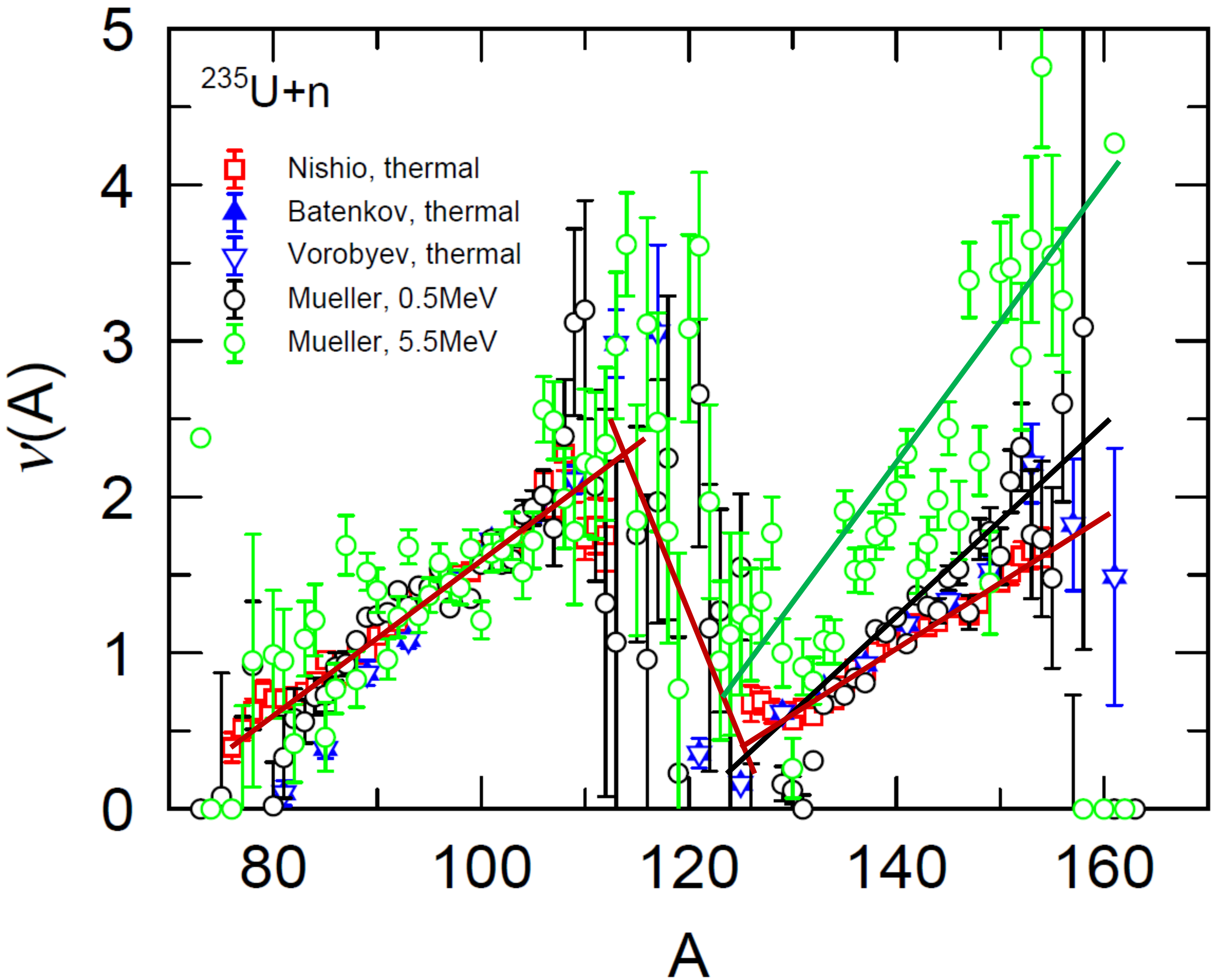
Systematics of average peak position of light (L) and heavy (H) fragments



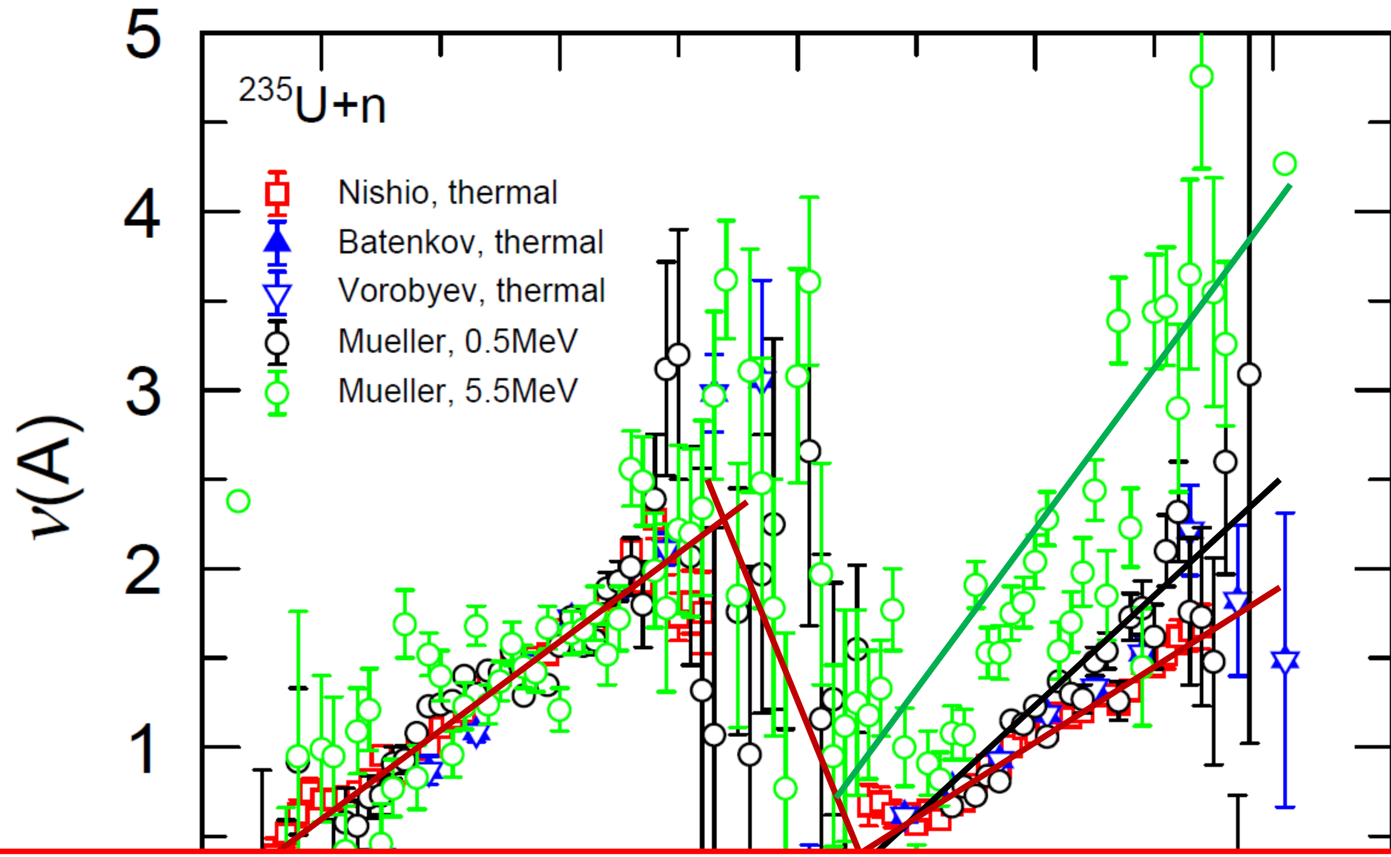
Systematics and anomaly in the average Total Kinetic Energy of Fission Fragments



Multiplicity distributions of prompt neutrons and its dependence on excitation energy



Multiplicity distributions of prompt neutrons and its dependence on excitation energy



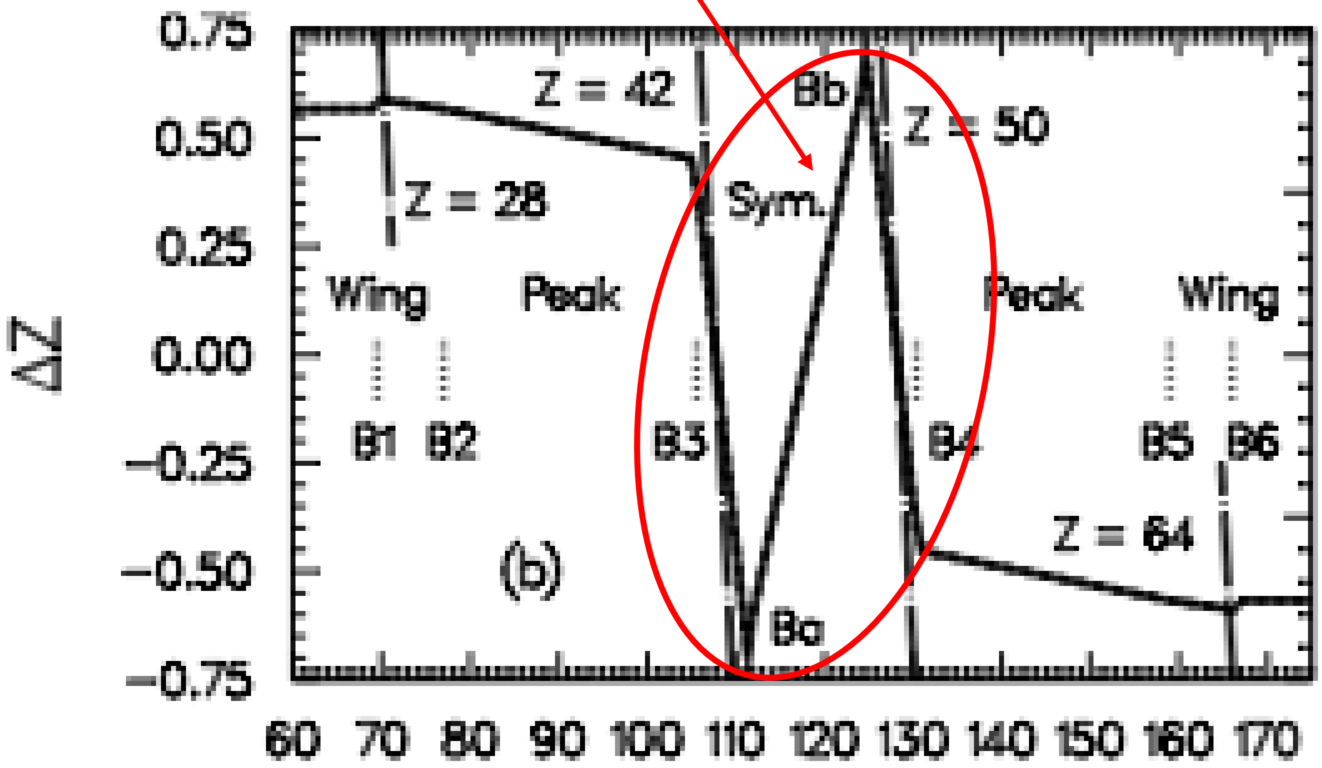
Why does it have saw-tooth structure like this? Why only neutron multiplicity of the heavy fragments increases? Entropy sorting??? Need for interpretation from dynamical theory

Charge polarization and fine structure of FPY by Wahl

$$\Delta Z = Z_{FF}(A_{FF}) - \frac{Z_c}{A_c} A_{FF}$$

Is this behavior real?

Our recent microscopic calculation denies it

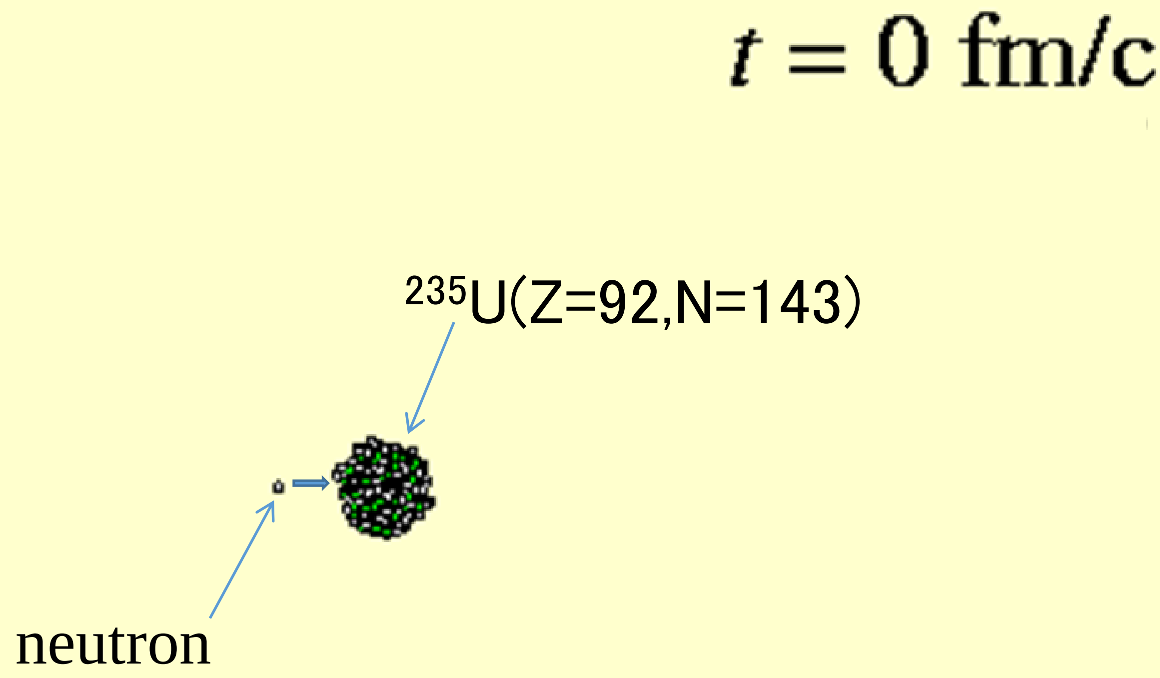


Background and introduction

Tokyo Tech

6. Many observables arise as a result of fission, e.g., fission fragment yield, TKE, population of prompt neutrons and gammas which is followed by a series of β-decay and associated delayed processes, and they must be comprehended in a consistent manner, which is still a formidable task
7. These quantities, either as a single physics quantity or their correlations, have been treated in a phenomenological way in the past
8. We have been treating the process before scission by several theories, such as Langevin model, AMD and TDHF, and their outcomes are connected to statistical decay model HF_3D (presentation by S.Okumura) and Gross theory of β-decay (mostly by T.Yoshida)
9. In this presentation, I concentrate on the process from compound nucleus to the instance of scission, and try to elucidate origin of systematic and anomalous trends in fission observables and their correlations by our 4-dimensional Langevin calculation (a macro-micro approach)

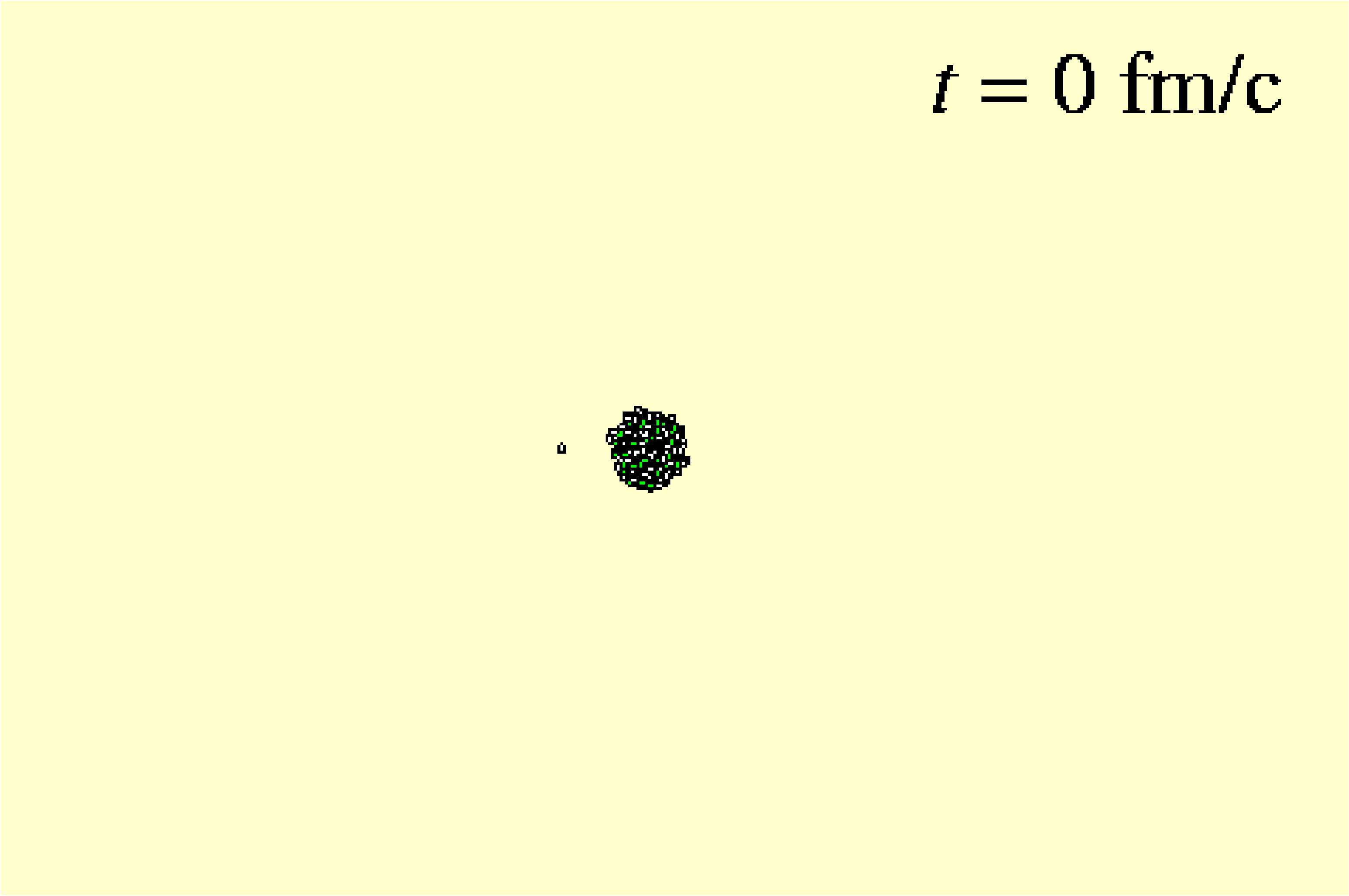
Simulation of nuclear fission (^{235}U + 140 MeV n) by JQMD



JQMD : JAERI Quantum Molecular Dynamics
= a semiclassical molecular dynamics for nuclear reactions (mean field + NN collision)

K.Niita, T. Maruyama, Y. Nara, S. Chiba and A. Iwamoto, JAERI-Data/Code 99-042(1999)

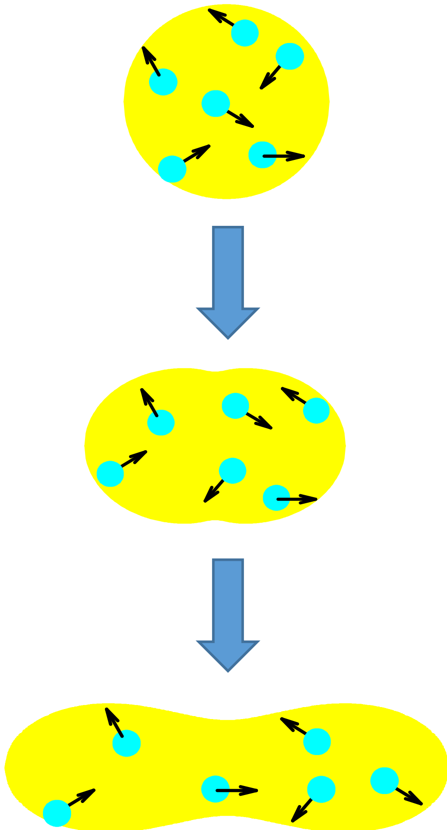
Simulation of nuclear fission (^{235}U + 140 MeV n) by JQMD



Time evolution of ^{235}U + 140 MeV n reaction by JQMD

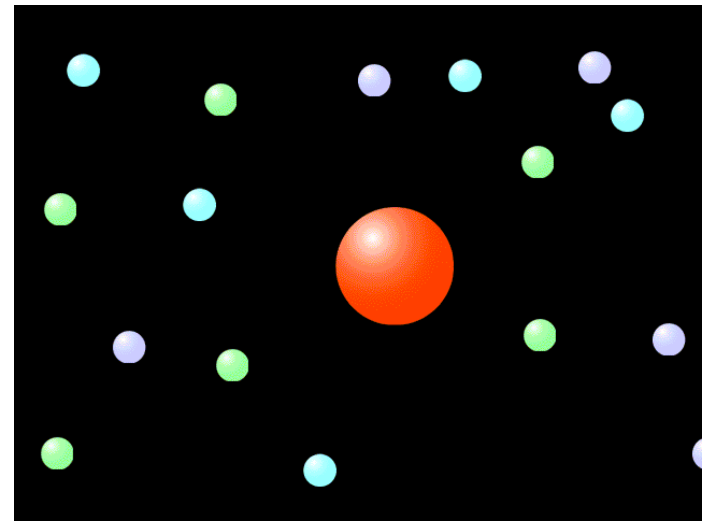
K.Niita, T. Maruyama, Y. Nara, S. Chiba and A. Iwamoto, JAERI-Data/Code 99-042(1999)

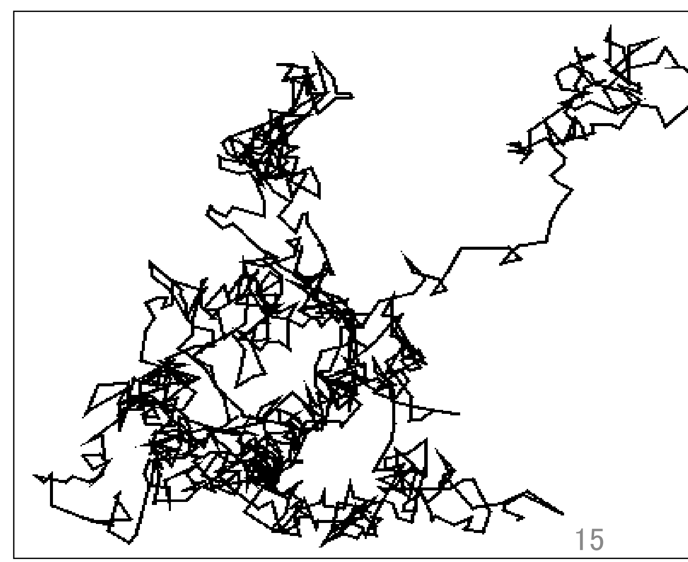
Nuclear fission by Langevin equation



Nuclear shape evolution is driven by random kicks by nucleons in thermal equilibrium (microscopic d.o.f.) given to the nuclear surface (macroscopic d.o.f) from inside the surface

Browning motion





These 2 different d.o.f have different time scales:

- **nucleon motion : 1 to 10 fm/c**
- **shape motion : ～>10,000fm/c**

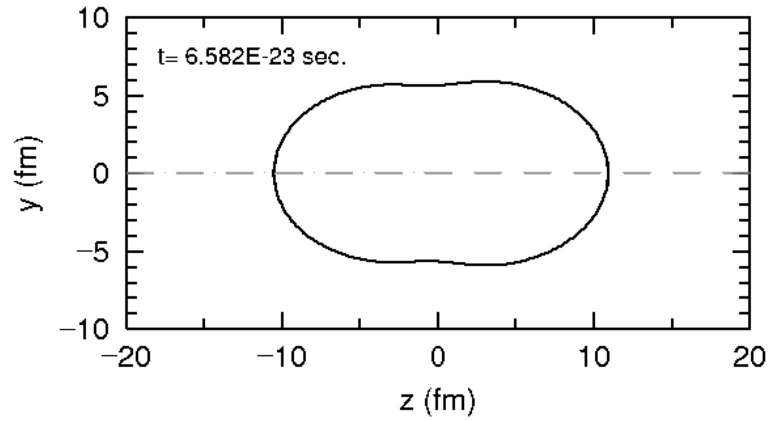
4D Langevin model of fission

C.Ishizuka et al., PRC 96, 064616 (2017).

$$\begin{cases} \dfrac{dq_i}{dt} = \left(m^{-1}\right)_{ij} p_j \\ \dfrac{dp_i}{dt} = -\dfrac{\partial F}{\partial q_i} - \dfrac{1}{2}\dfrac{\partial}{\partial q_i}(m^{-1})_{jk} p_j p_k - \gamma_{ij}(m^{-1})_{jk} p_k + g_{ij} R_j(t) \end{cases}$$

Drift term; Friction term; Wiener term

$\{q_i : i = 1..4\} = \{ZZ_0,\ \alpha,\ \delta_L,\ \delta_R\}$



F : Helmholtz' free energy, $F = E - TS$

q_i : Nuclear shape motion

p_i : Momentum conjugate to q_i

m_{ij} : Inertia tensor

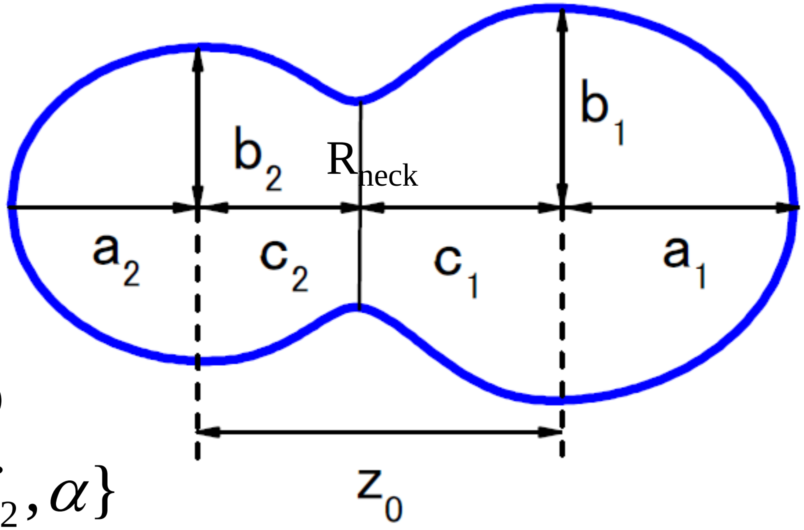
γ_{ij} : friction tensor

$g_{ij} g_{ij} = \gamma_{ij} T$: Fluctuation dissipation theorem (+Einstein relation)

$$T = \sqrt{\frac{E^* - \frac{1}{2} m_{ij} p_i p_j - E_{rot}}{a}}$$

E^* : Total excitation energy of the system

Shape parametrization



Two-center model
(Maruhn and Greiner, Z. Phys. 251(1972) 431)

Collective coordinates (3 or 4 dynamical variables)

$$\{q\}_{3D} = \{ZZ_0, \delta, \alpha\} \qquad \{q\}_{4D} = \{ZZ_0, \delta_1, \delta_2, \alpha\}$$

- $ZZ_0 = \dfrac{z_0}{R}$ Elongation

  R : Radius of compound nucleus $= 1.2 A_{CN}^{1/3}$

- $\delta_i = \dfrac{3(a_i - b_i)}{2a_i + b_i}$ Deformation of fragments

  3D : $\delta_1 = \delta_2 = \delta$ 4D : δ_1, δ_2 are independent

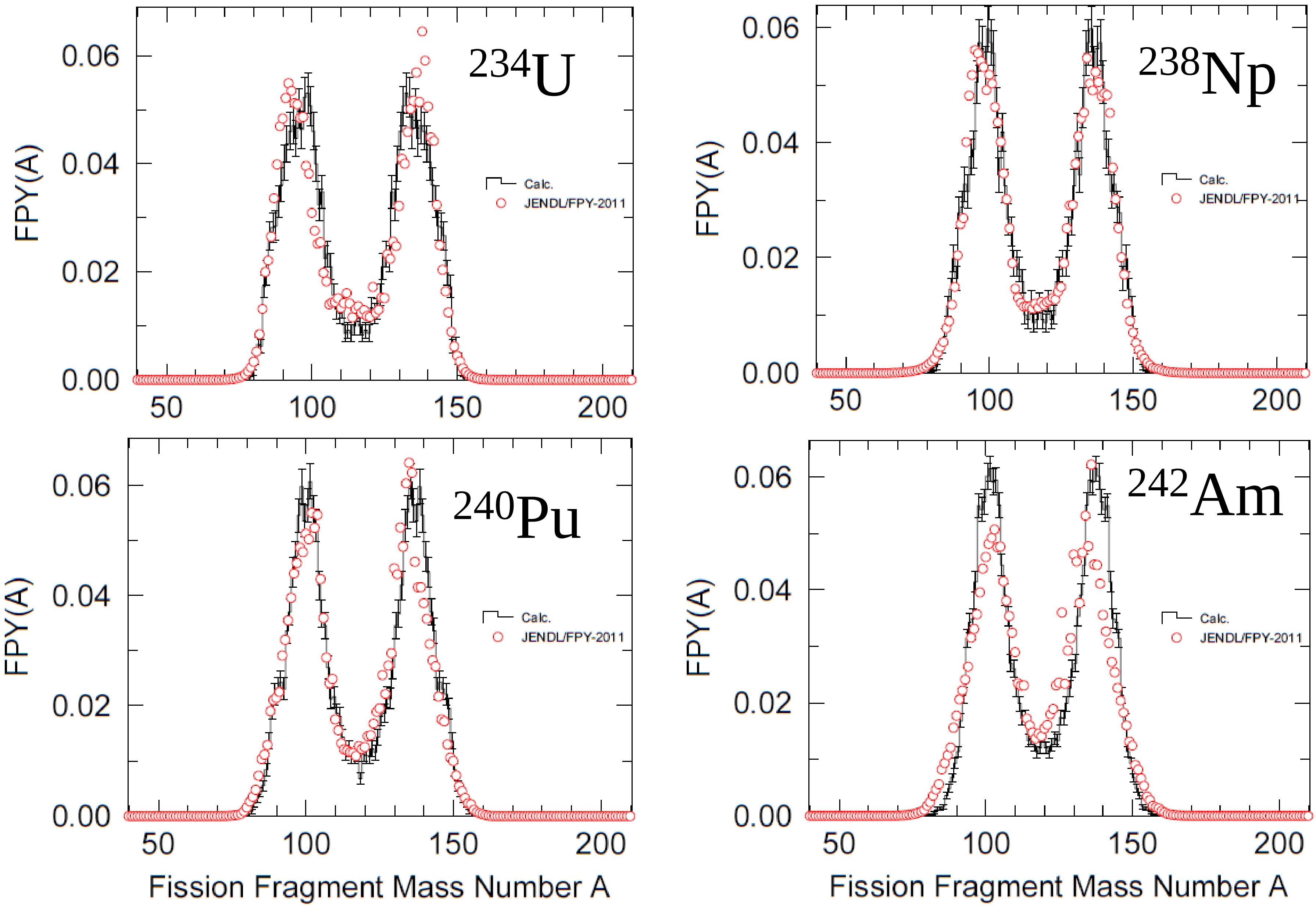
- $\alpha = \dfrac{A_1 - A_2}{A_1 + A_2}$ Mass asymmetry

  A_1 : mass of the right fragment

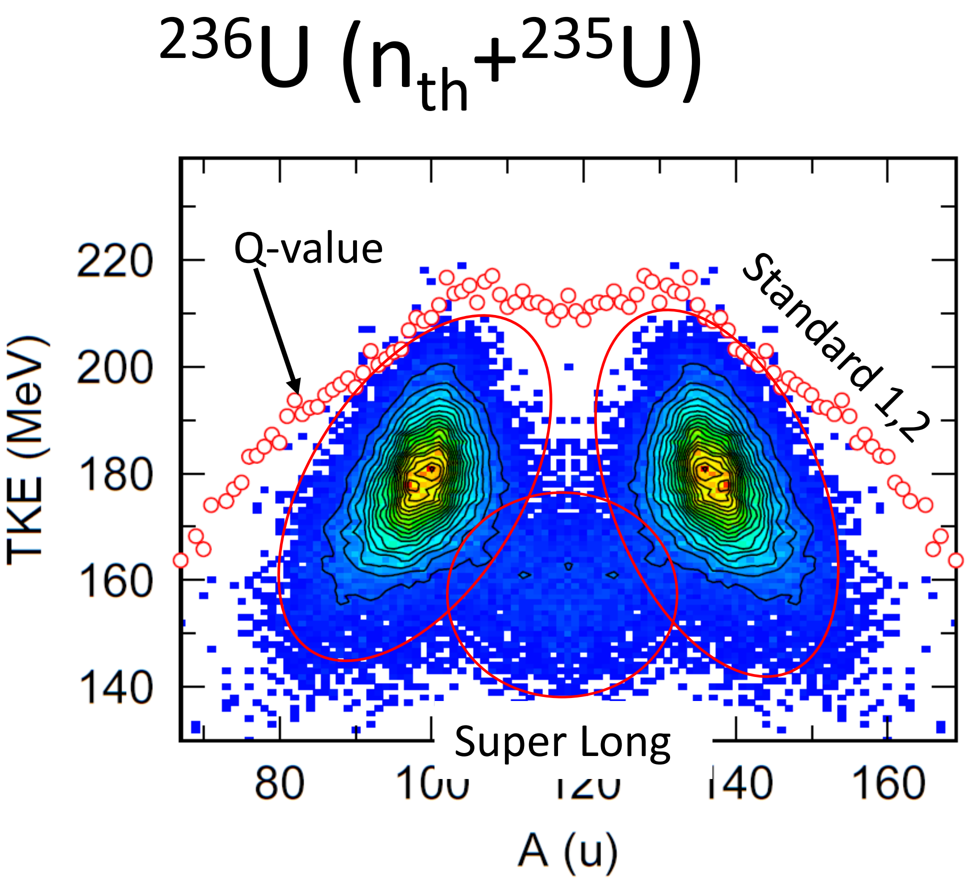
  A_2 : mass of the left fragment

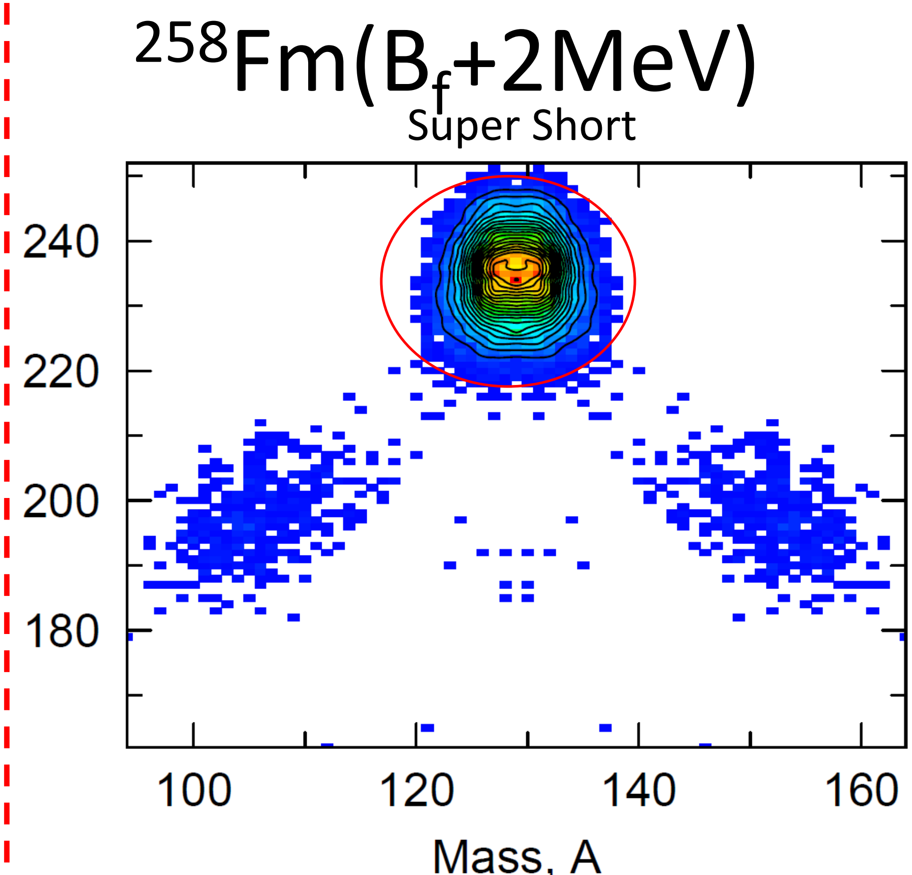
- $\varepsilon = 0.35$ neck parameter : fixed
- volume conservation condition is applied

Predictions for mass distributions (Ex=20MeV)



Mass-TKE correlation and its decomposition

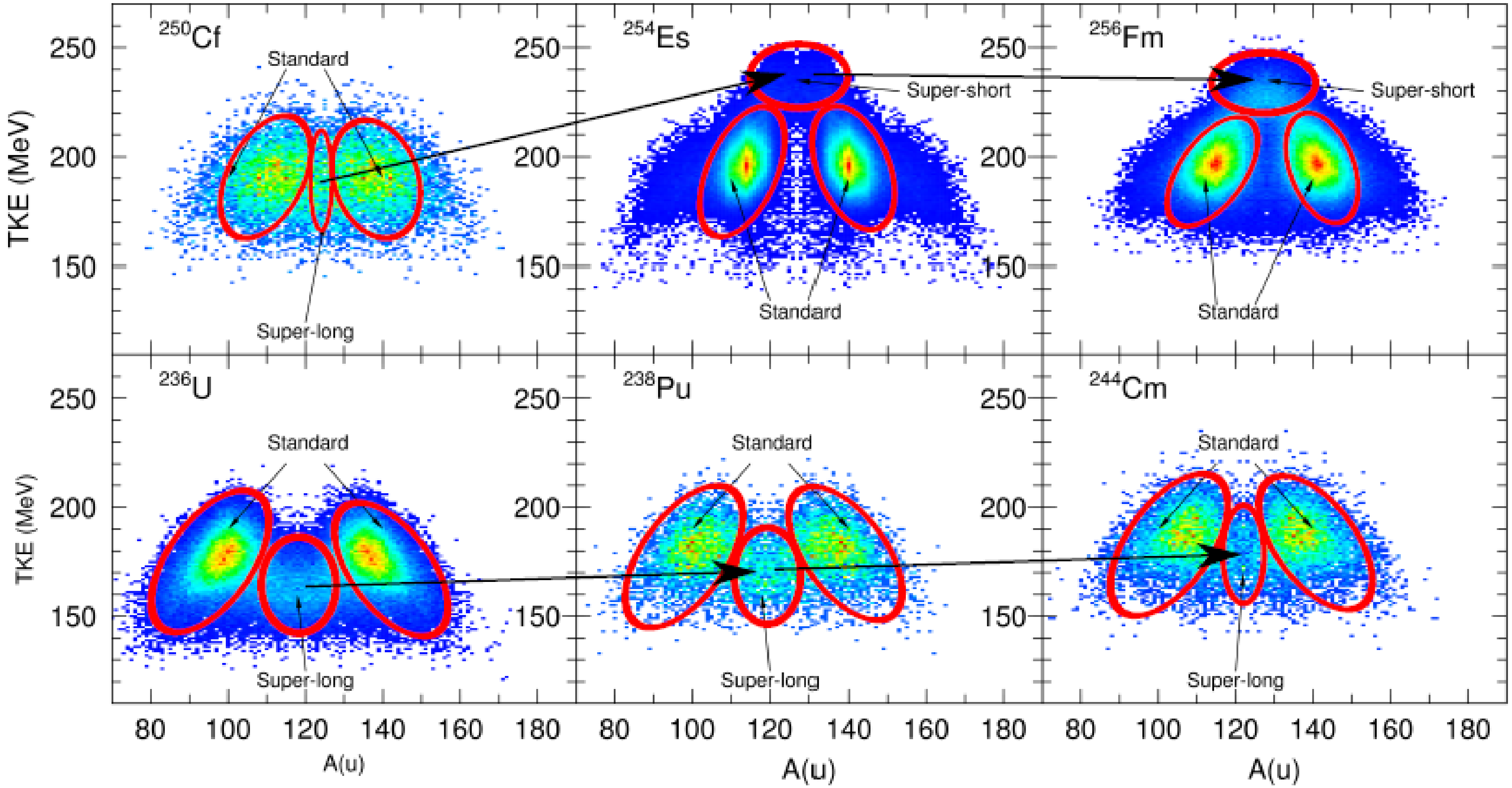




Systematics in Mass-TKE correlations

U236 to Fm256

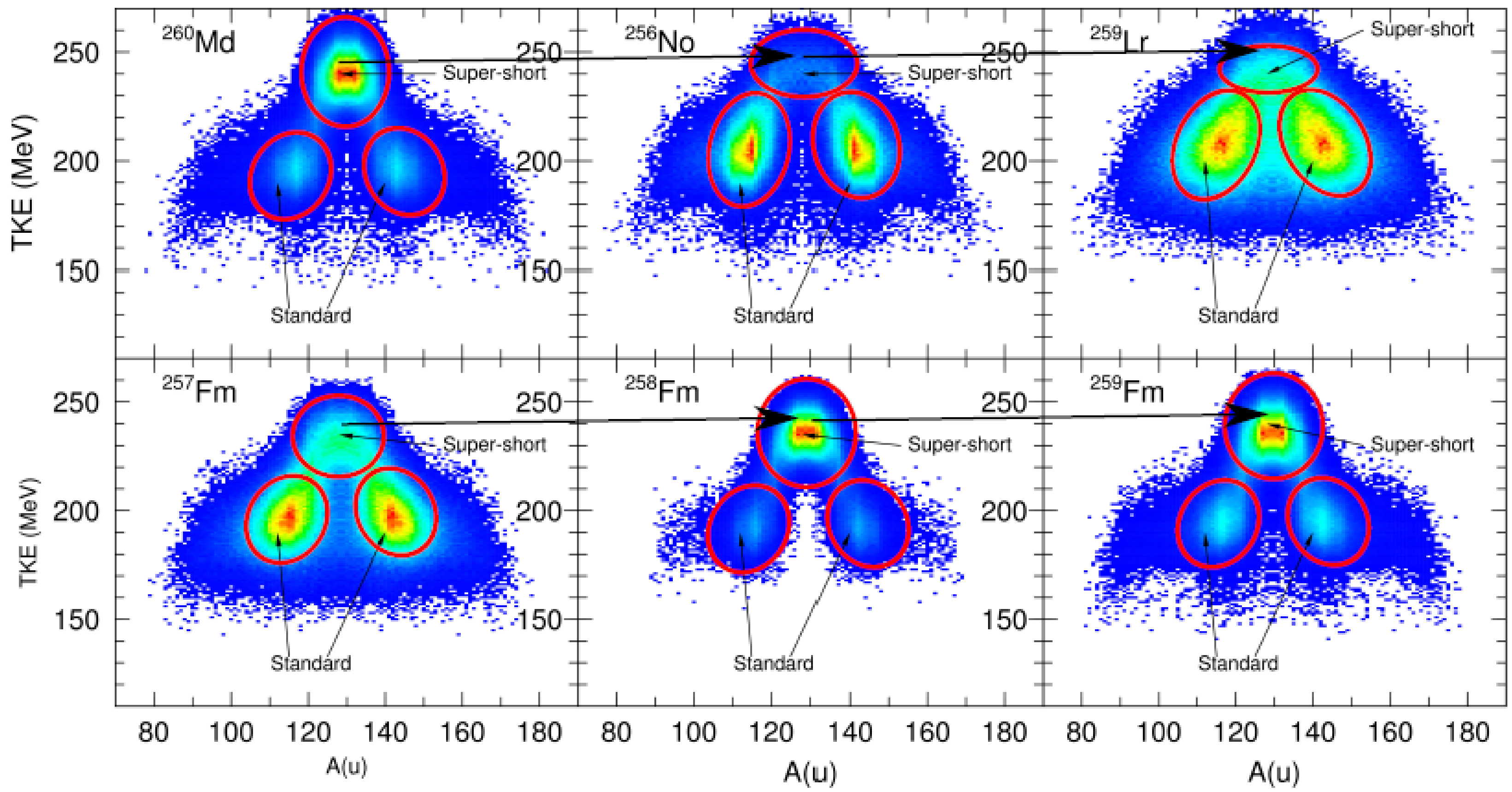
Neck parameter, $\epsilon = 0.35$



Systematics in Mass-TKE correlations

From Fm257 to Lr259

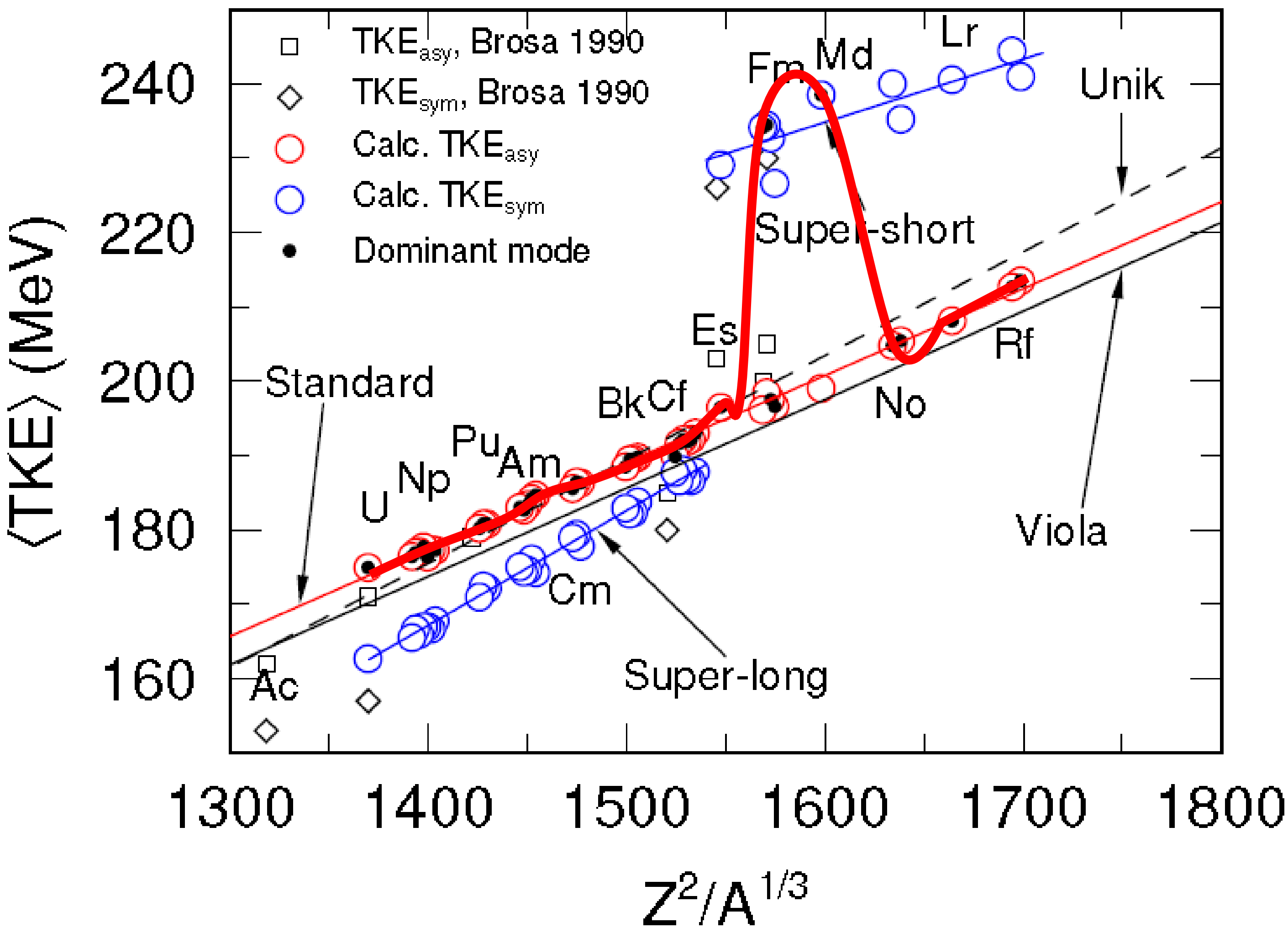
Neck parameter, $\epsilon = 0.35$



Results of mass-TKE correlations

TKE Systematics: fission mode components

(ε=0.35)



Estimation of excitation energy of fragments :
important input to subsequent statistical-decay calculation

1. Estimation from TKE (Langevin) and Q-value

$$TXE = EX(A_L) + EX(A_H) = Q - TKE_{\text{Langevin}}$$

$$EX(A_{FF}) = a(A_{FF})T(A_{FF})^2 + \text{correction}(A_{FF})$$

$$\frac{T_L}{T_H} \approx 1.3,\ or\ f(A_{FF})$$

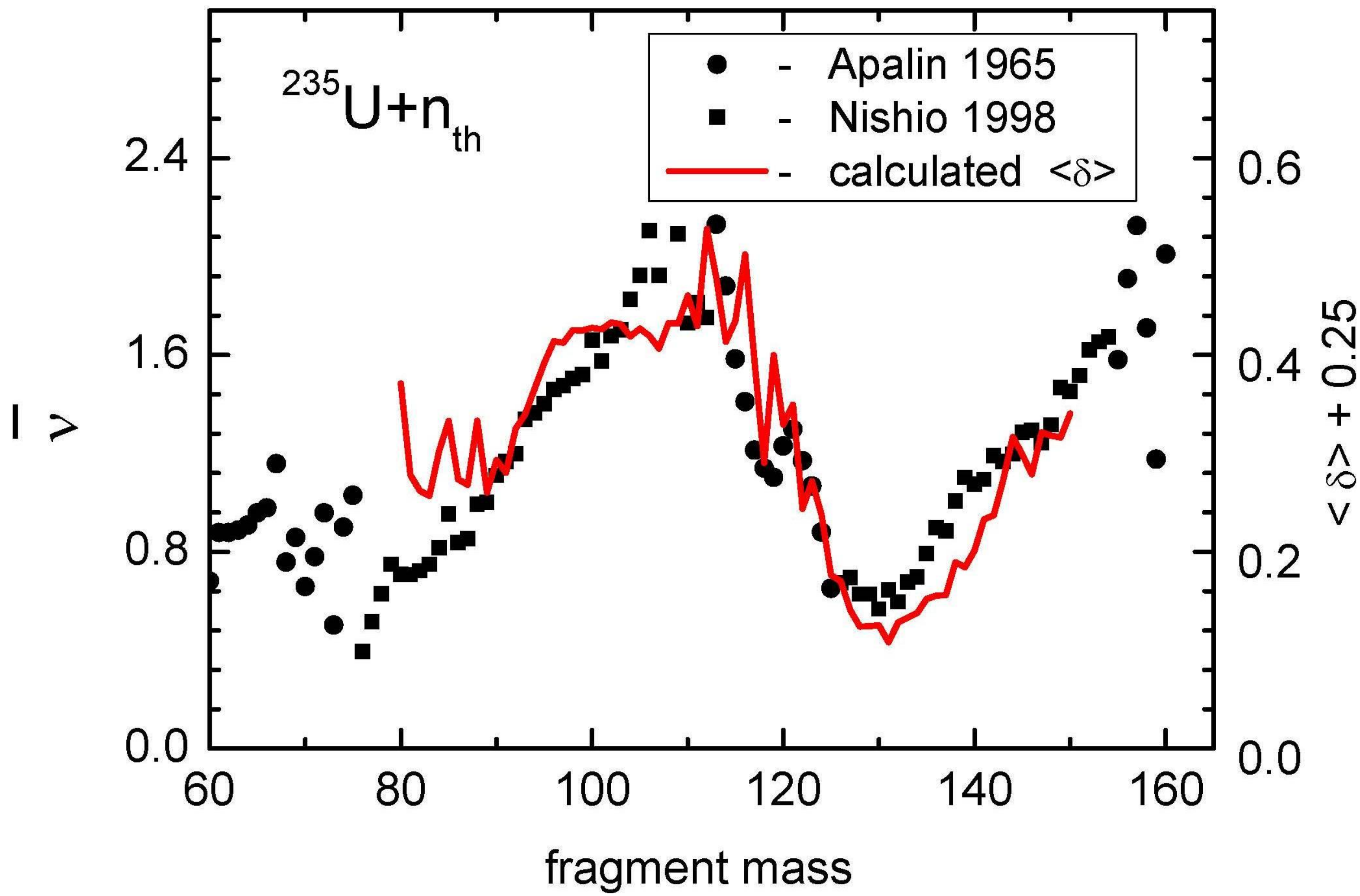
2. Direct estimation from Langevin result

$$EX(A_{FF}) = E_{def}(A_{FF}) + E_{vib}(A_{FF}) + a(A_{FF})T^2_{Langevin} + E_{rot}$$

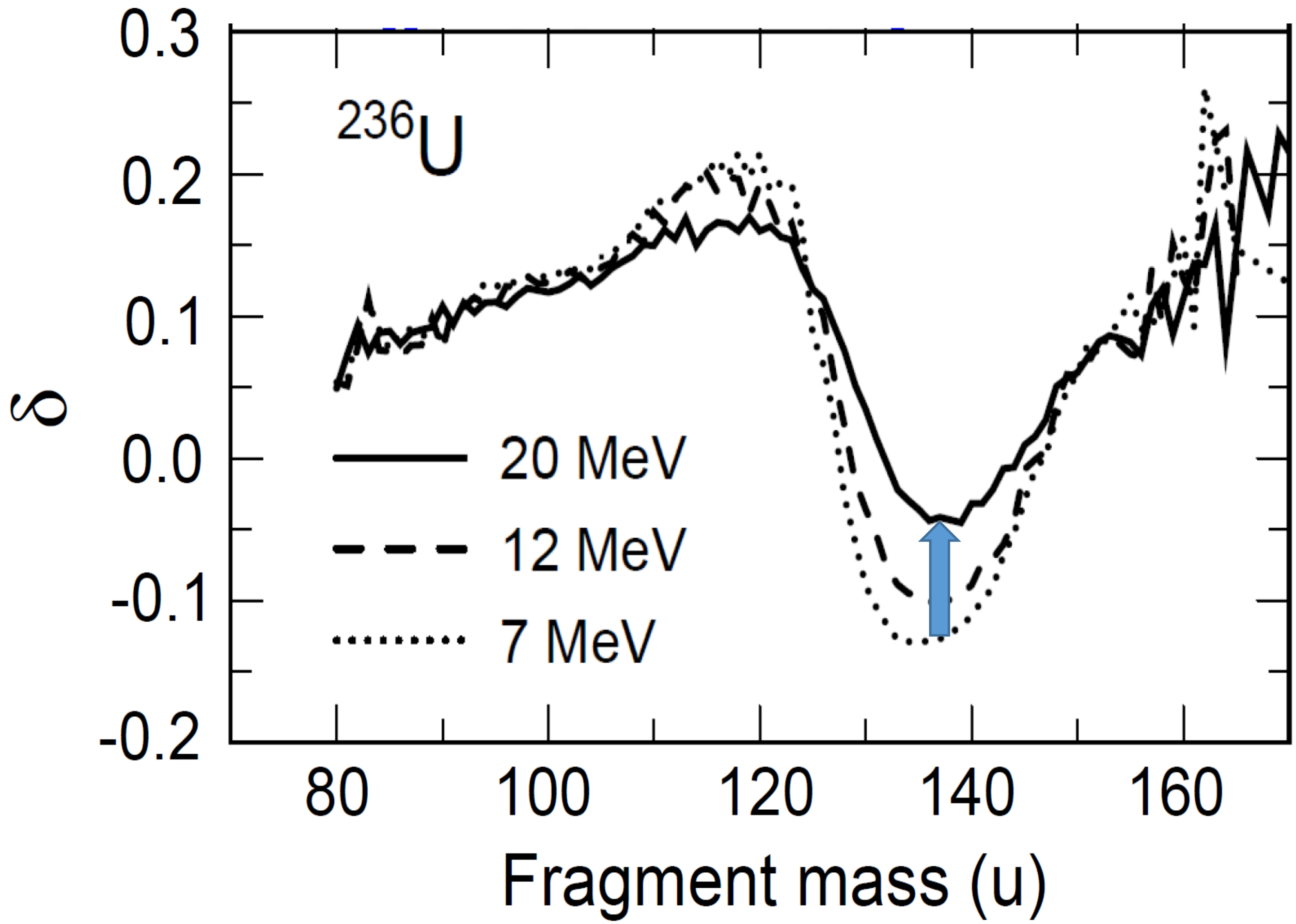
$$= f(\delta(A_{FF})) \qquad = K.E.\text{of}\ \delta(A_{FF}) \qquad = \text{Intrinsic Energy} \qquad ??$$

→presentation by Shin Okumura

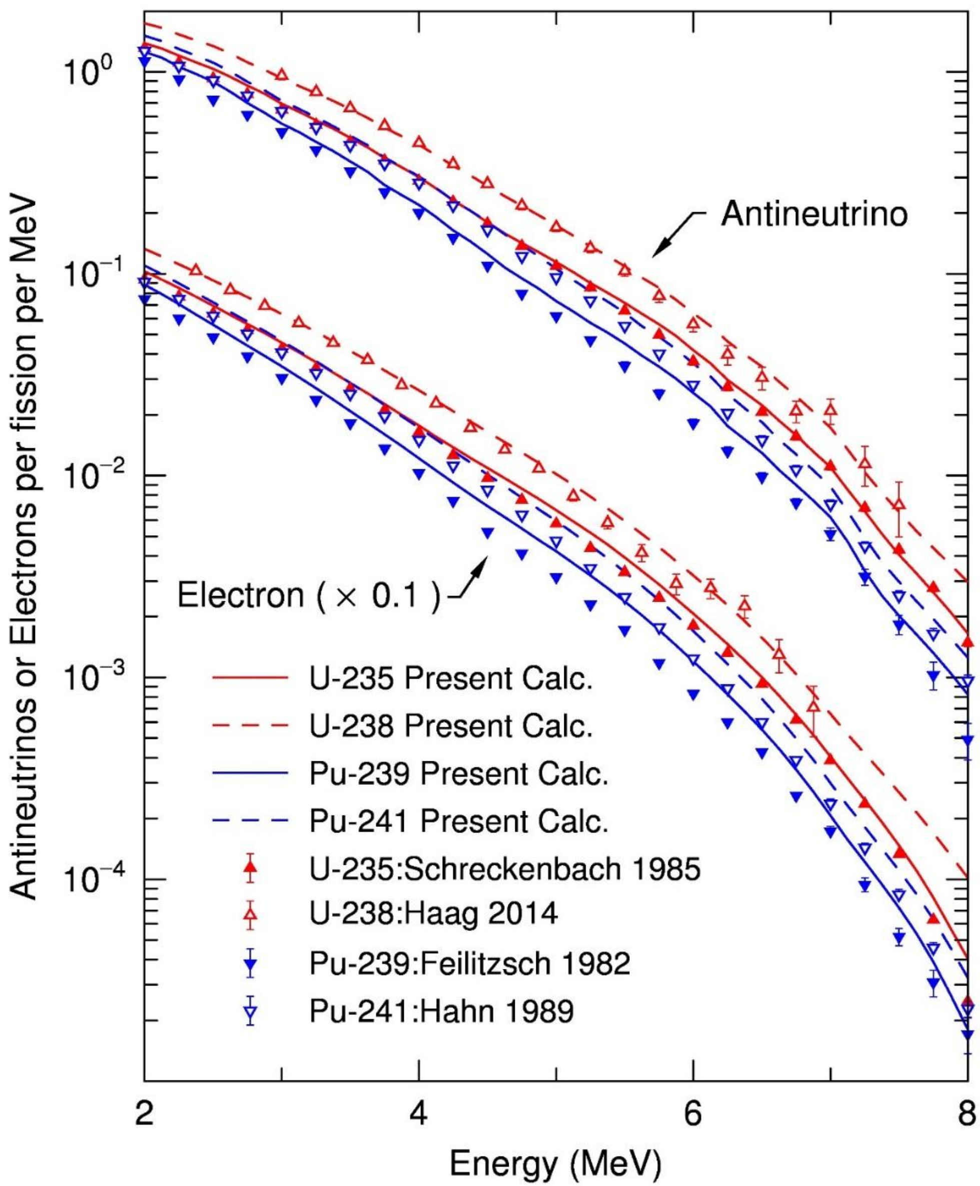
Clear correlation of fragment deformation and saw-tooth structure of prompt neutron multiplicity



Correlation of energy dependence of fragment deformation and saw-tooth structure of prompt neutron multiplicity



Reactor Antineutrino Energy Spectra; Comparison Between the Current Prediction Basis (ILL) and Gross Theory Calculation



Decay heat

Delayed neutrons

T.Yoshida et al, PRC (in press)

Concluding remarks

- We are constructing a computational framework to cover the whole process of fission, starting from compound nucleus, scission, prompt particle emission and β −decay.
- I covered the first part of the fission process, namely, from the compound nucleus to saddle to scission, based on our 4D Langevin approach, which gives the initial conditions to following statistical decay calculations
- The 4D Langevin can explain nicely a systematical and anomalous trends in mass distribution, TKE and their correlation
- Our approach can give reasonable distribution for deformation of fragments, from which we can estimate excitation energy of fission fragments, although the process is still under development
- A microscopic approach to charge polarization is on going (tbs)
- Connection to SHE studies is promising
- Successive statistical decay will be a subject of S. Okumura's talk

Wonder2018, Oct. 2018

Thank you very much