Tokyo Tech

FIESTA2017

Dynamical Microscopic and Macro-Micro Approaches to Nuclear Fission

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- Introduction and Background
- Nuclear fission by Langevin equation : Macr-micro
- Nuclear fission by antisymmetrized molecular dynamics (AMD)
- Nuclear friction by TDHF
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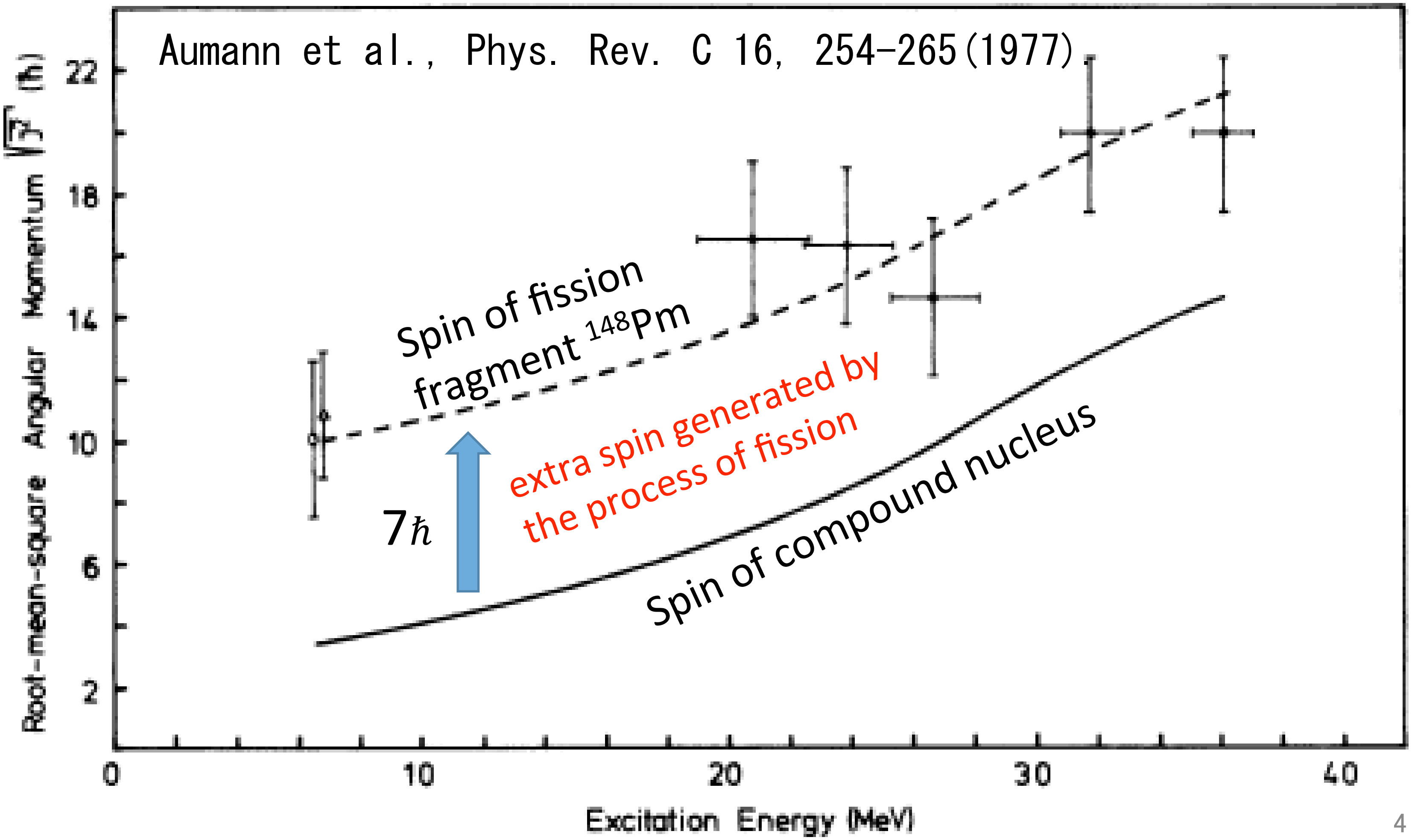
Introduction and Background

- Even though the history of researches in nuclear fission is already more than 70 years-long, many mysteries still exist actually what is going on during the process of nuclear fission, especially before scission
- Due to the difficulties, accuracy of the fission-related nuclear data is still considered not high enough
- To resolve this situation and to understand many different aspects of nuclear fission in a consistent way, we think accurate dynamical treatment of nuclear fission is necessary
- We are making researches in fission by dynamical approaches with Langevin equation, AMD (antisymmetrized molecular dynamics) and TDHF
- Here we explain them briefly

Origin of extra spin that fission fragments have

spin of ^{148}Pm from fission of n+^{235}U system as a function of excitation energy of compound nucleus



Do fission fragments rotate? If so, what is the origin of the rotational motion and how much angular momenta they have ?

Twisting mode in fusion reactions

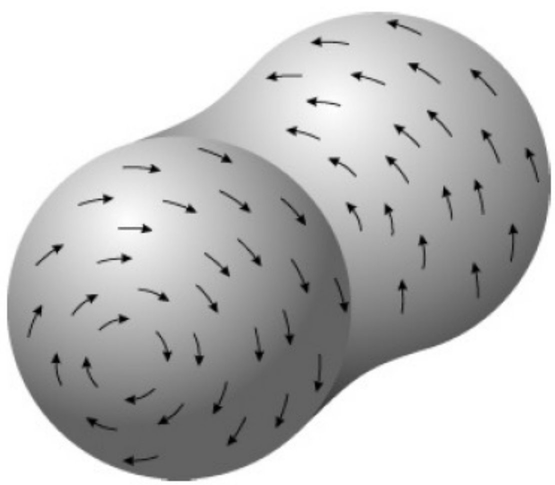
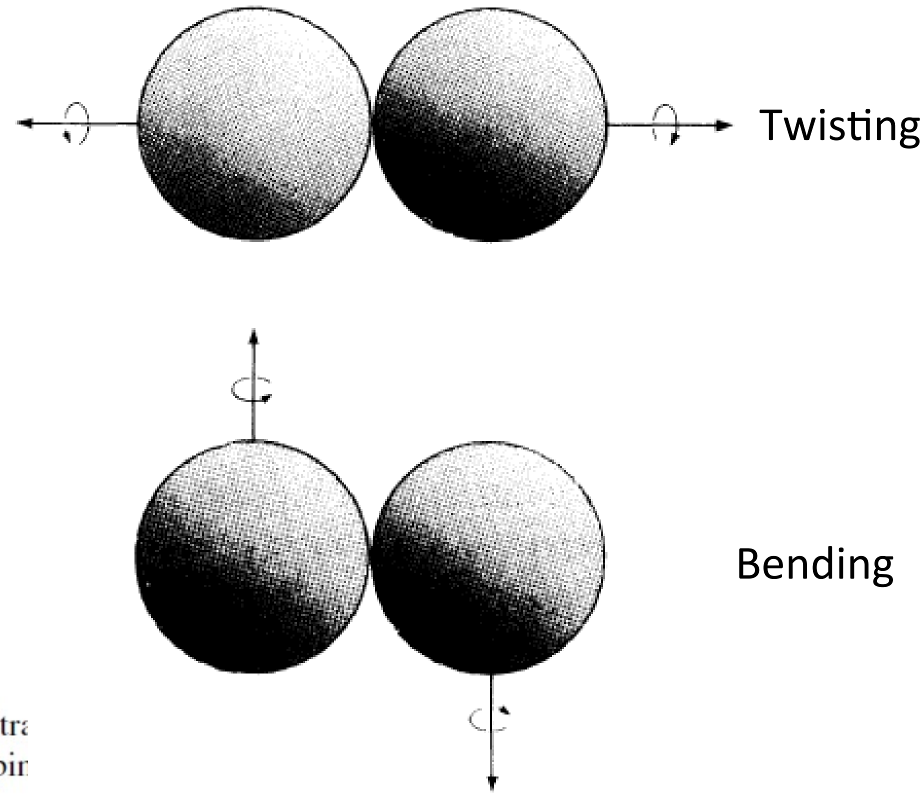


FIG. 3. Artist's view of the spin excitation generated in a centra collision of two ^{16}O nuclei. Closely based on the numerical spir density vectors produced in the calculations.

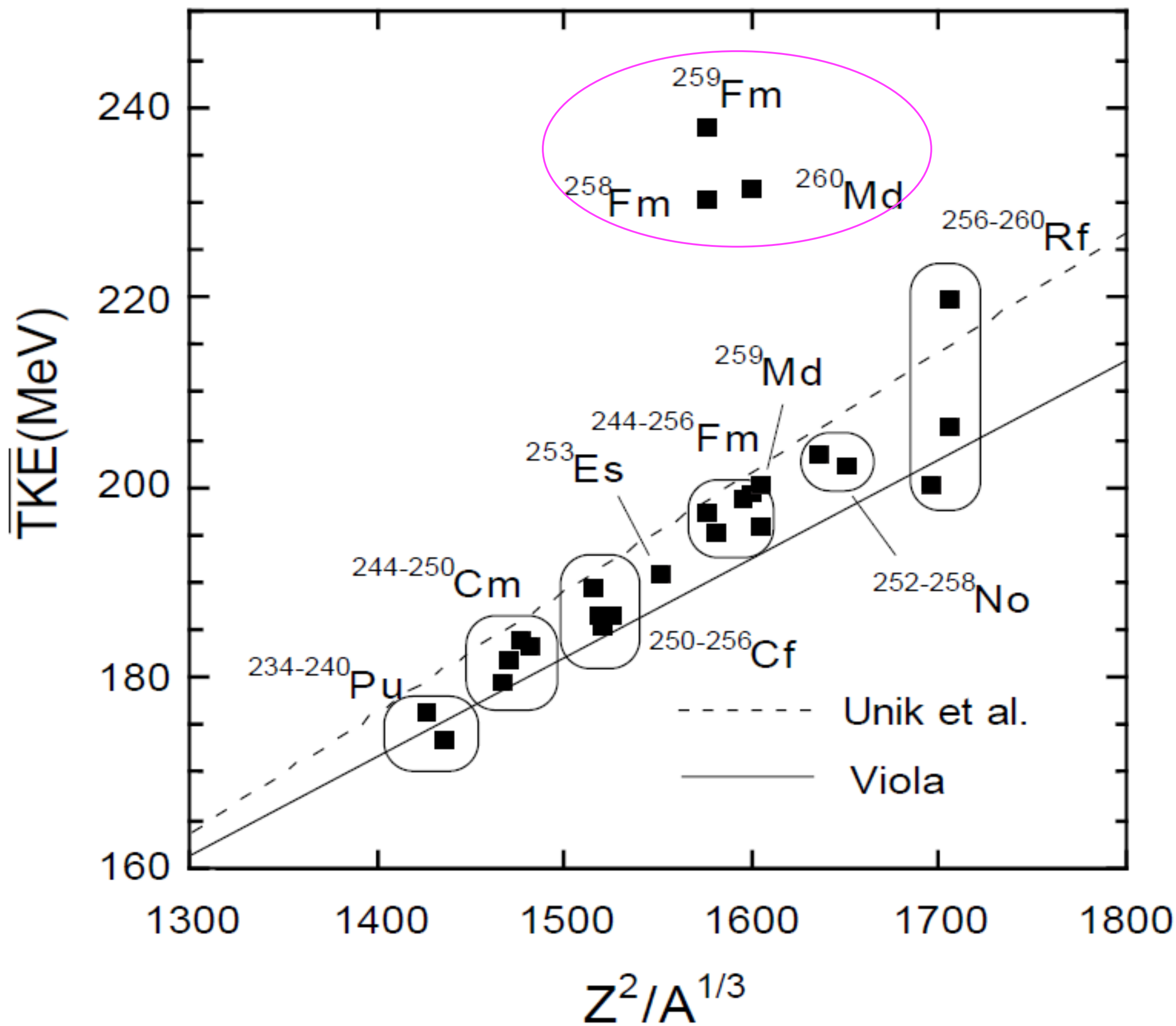
Maruhn et al., Phys. Rev. C 74, 027601(2006).



PRC21, 204(1980)

Twisting & Bending modes in fission

Anomaly in the average Total Kinetic Energy of Fission Fragments



Our approaches (CN to scission)

Macro-micro approach : Langevin model

- PES from macro-micro, transport coefficients from macro or micro + random force
- 3D Langevin with macroscopic transport coefficients (with F.Ivaniuk)
- 3D Langevin with microscopic transport coefficients (by linear response theory)
- 4D Langevin with macroscopic transport coefficients
- 4D Langevin with microscopic transport coefficients
- 5D Langevin -- talk by A. Sierk

Microscopic approaches

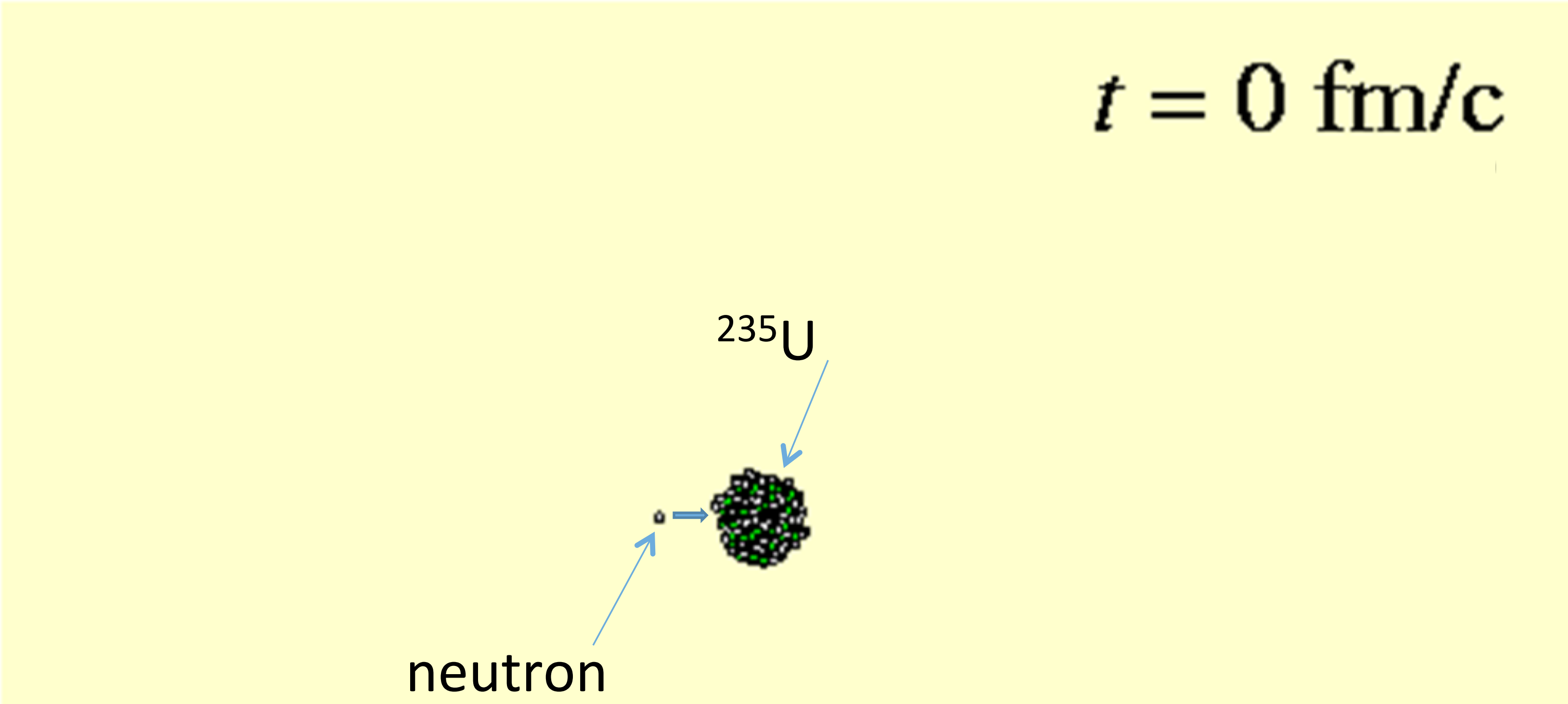
Antisymmetrized Molecular Dynamics (AMD)

- Slater determinant with Gaussian wave packets (coherent state) as basis function
- mean field calculated with SLy4 interaction
- Stochastic nucleon-nucleon collisions to express branching of Slater determinant and deformation of Gaussian wave packet

Time-dependent Hartree Fock (TDHF)

- No restriction on single-particle wave function (3D mesh calculation)
- mean field by SV-Bas interaction
- based on OAK3D and SKY3D (no pairing)
- to obtain nuclear friction coefficient from dynamical model

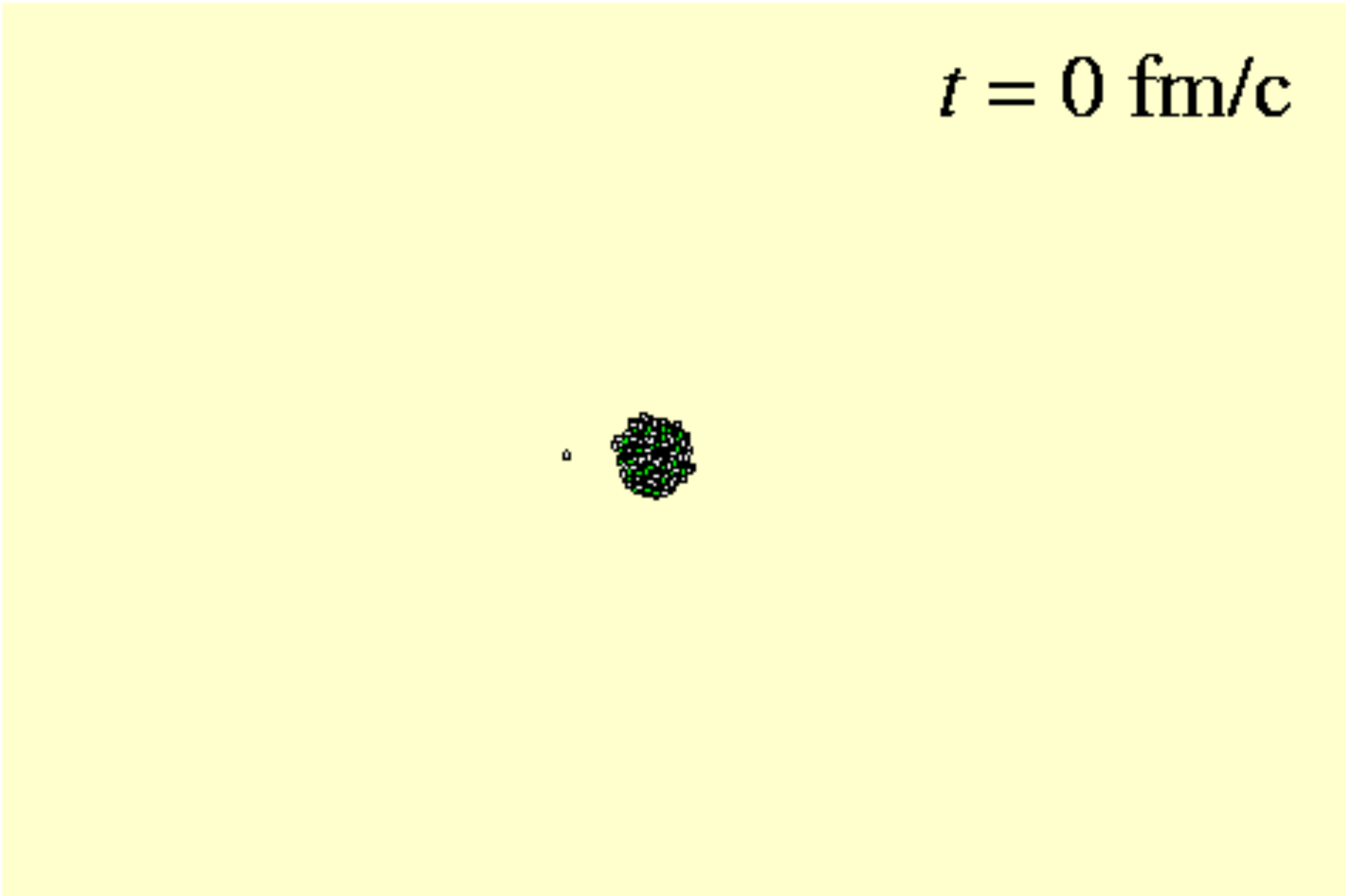
Simulation of nuclear fission (^{235}U + 140 MeV n) by JQMD



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)

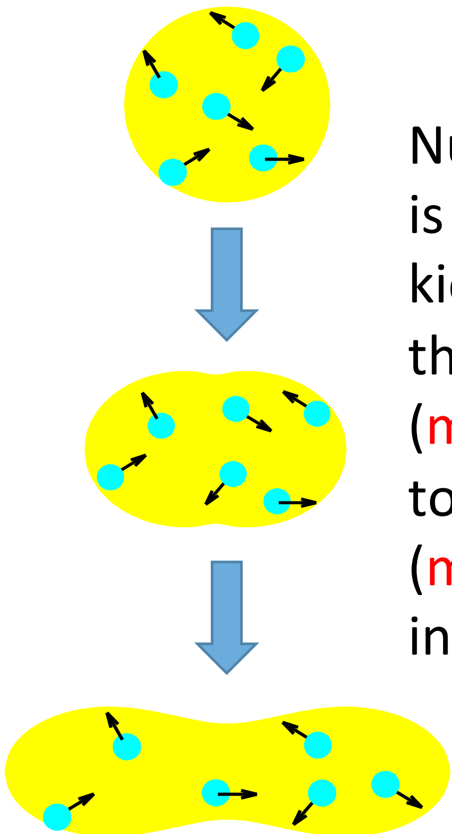
QMD simulation of nuclear fission (^{235}U + 140 MeV n)



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

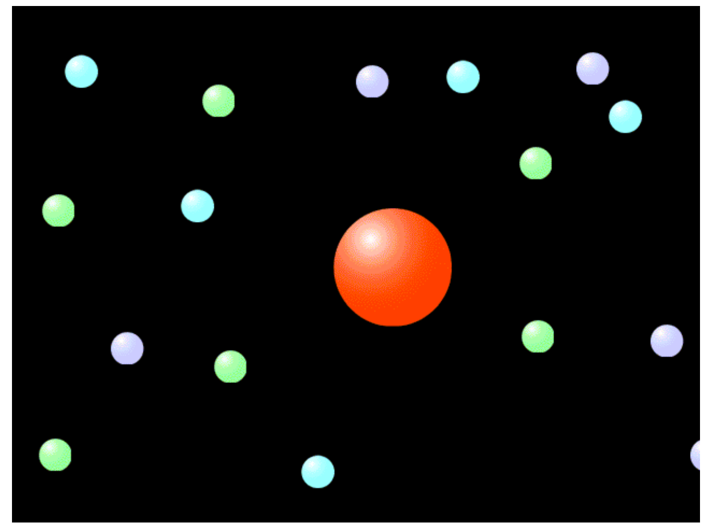
K.Niita, T. Maruyama, Y. Nara, S. Chiba and A. Iwamoto, JAERI-Data/Code 99-042(1999)

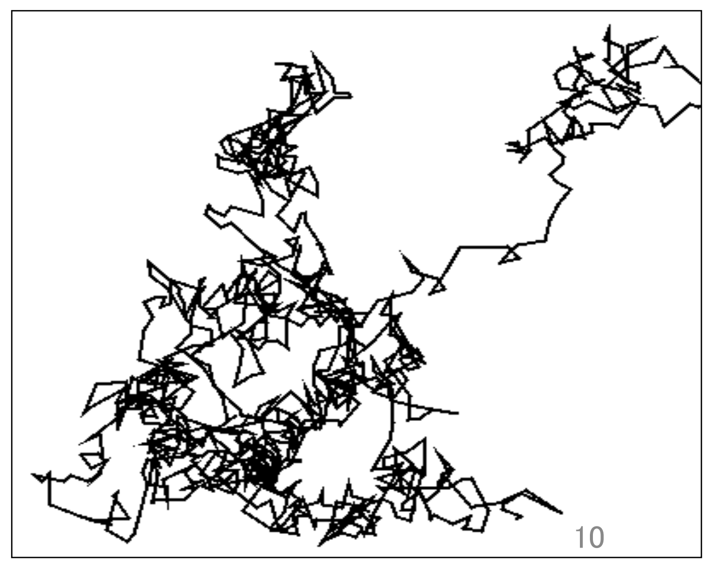
Nuclear fission by Langevin equation



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**

Langevin Equations for nuclear fission

$$\frac{dq_i}{dt} = \left(m^{-1}\right)_{ij} p_j$$

Friction force

Random

$$\frac{dp_i}{dt} = -\frac{\partial V}{\partial q_i} - \frac{1}{2}\frac{\partial}{\partial q_i}\left(m^{-1}\right)_{jk} p_j p_k - \gamma_{ij}\left(m^{-1}\right)_{jk} p_k + g_{ij} R_j(t)$$

q_i : deformation coordinates (nuclear shape) in two-center shell-model parametrization $\{q\}_{3D} = \{ZZ_0, \delta_1 = \delta_2, \alpha\}$ $\{q\}_{4D} = \{ZZ_0, \delta_1, \delta_2, \alpha\}$

p_i : momentum conjugate to q_i

m_{ij} : mass tensor : Hydrodynamical mass (Werner-Wheeler)

γ_{ij} : friction tensor : Wall and Window formula (one-body dissipation)

Macroscopic transport coefficients

or from Linear Response Theory (microscopic)

Random force : $\langle R_i(t)\rangle = 0,\ \langle R_i(t_1)R_j(t_2)\rangle = 2\delta_{ij}\delta(t_1 - t_2)$ White noise

$\sum_k g_{ik} g_{jk} = T\gamma_{ij}$ Einstein relation

Intrinsic energy and Temperature : $E_{\text{int}} = E^* - \frac{1}{2}\left(m^{-1}\right)_{ij} p_i p_j - V(q) = aT^2$

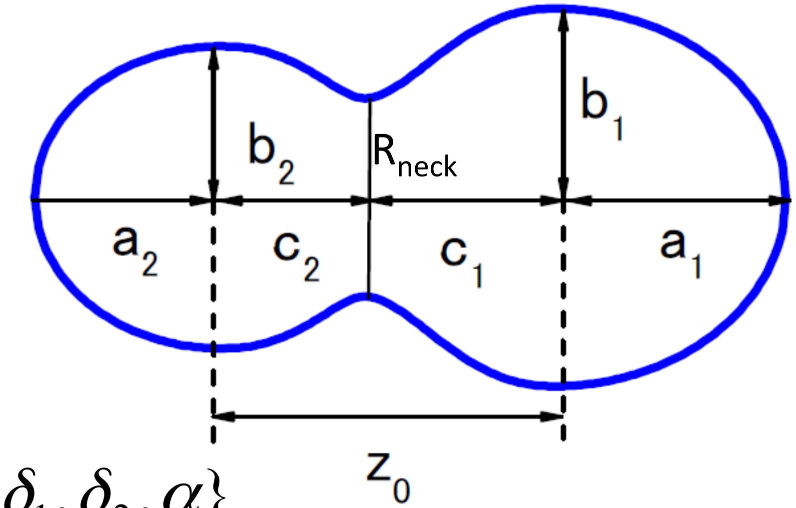
E_{int} : intrinsic energy, E^* : excitation energy, T : temperature

$\mathrm{V}(q)$: potential at deformation q : $V(q) = V_{LDM}(q) + V_{sh}(q)$

$V_{sh}(q)$: Strutinsky shell correction energy

a : level density paramter

Shape parametrization



Two-center oscillator model

(Maruhn and Greiner, Z. Phys. 251(1972) 431)

Collective coordinates (4 dynamical variables)

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

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

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

- $\delta_i = \dfrac{3(a_i - b_i)}{2a_i + b_i}, \; i = 1,2$ Deformation of fragments at outer tips

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

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

  A_1 : mass of the right fragment

  A_2 : mass of the left fragment

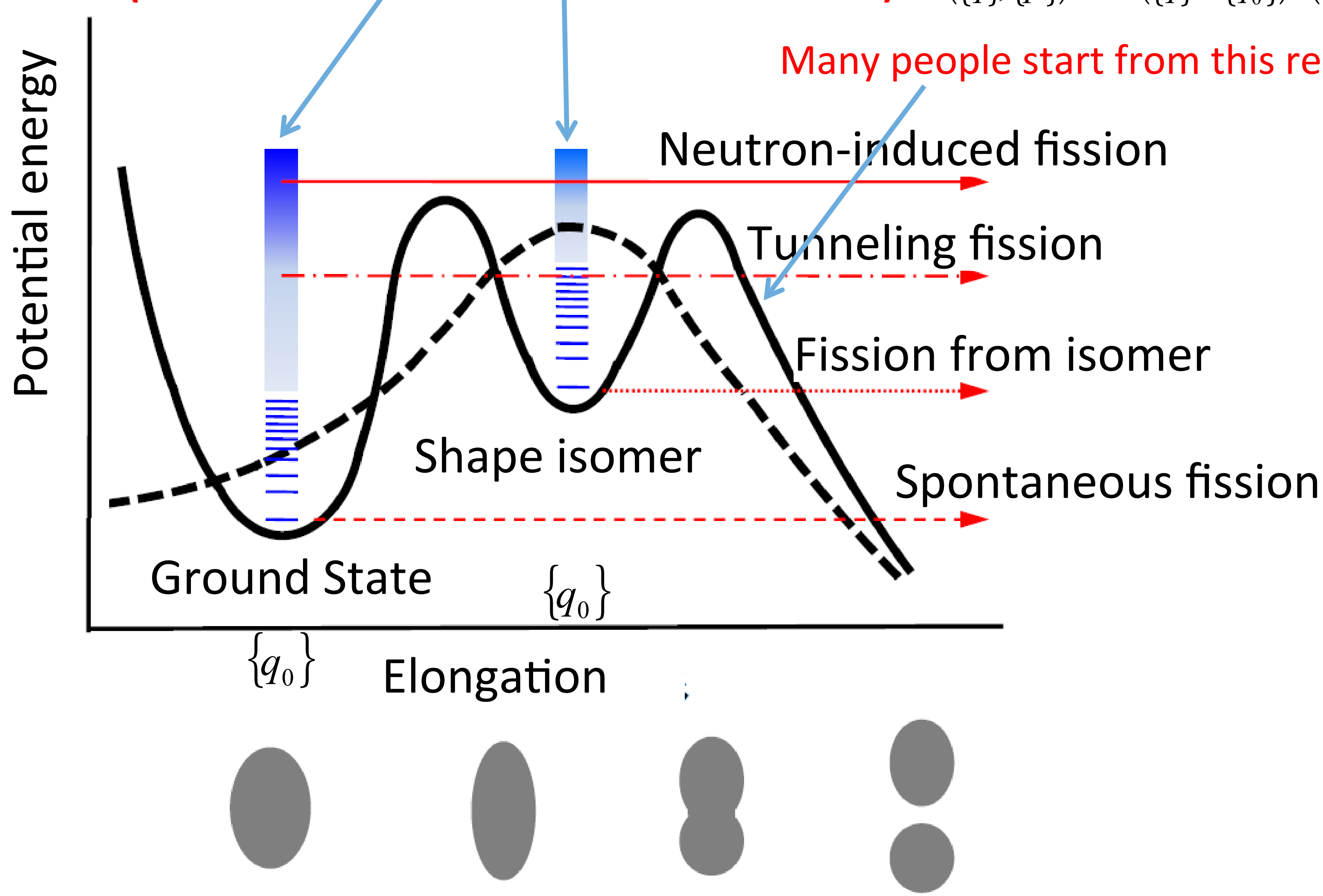
- $\varepsilon = 0.35$ neck parameter : fixed

Note that neck radius depends on all the 5 parameters

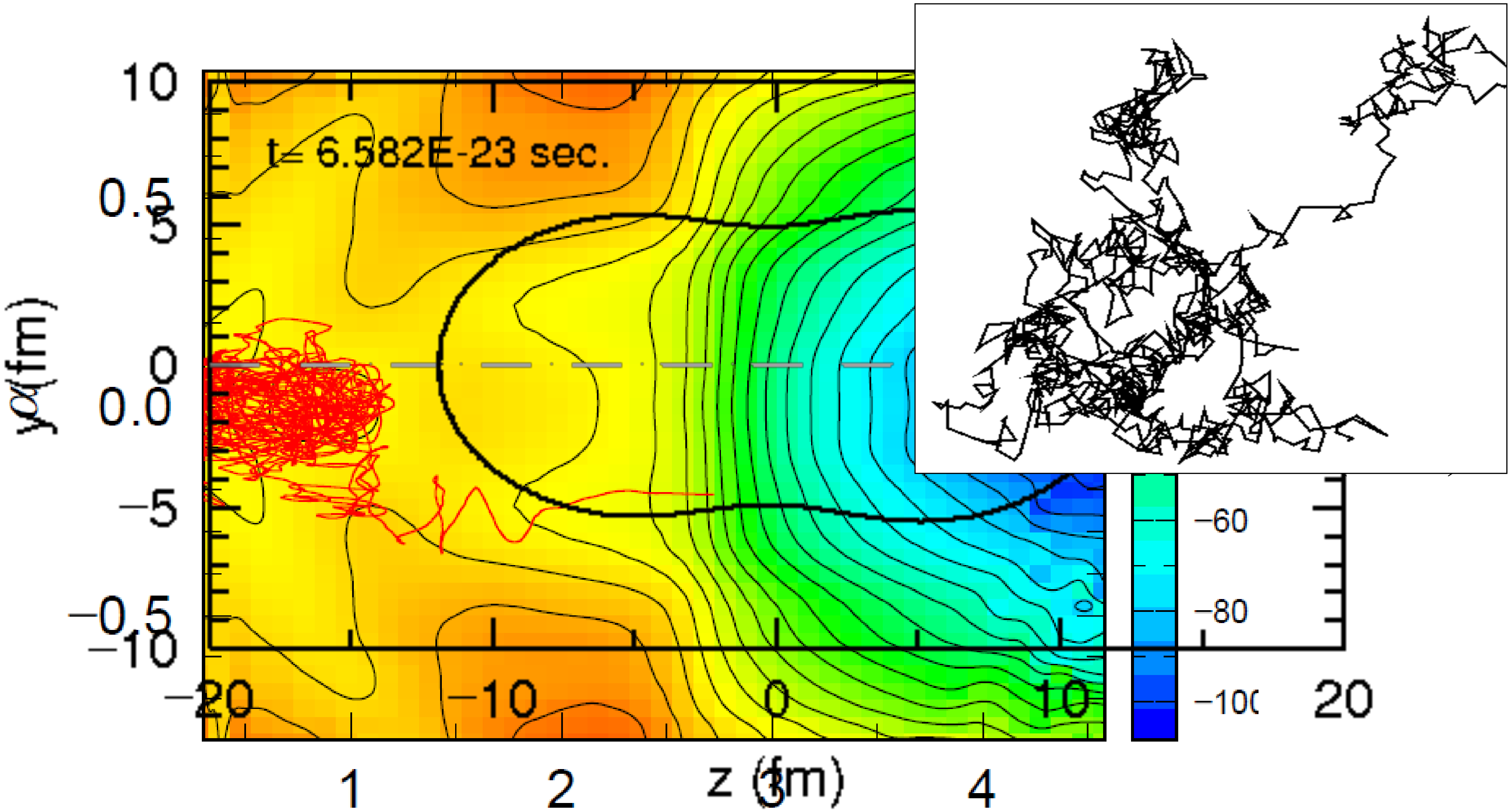
Initial condition of Langevin calculation

We start from here or here with **zero initial momenta**
(there is no distribution in the initial state) $P(\{q\},\{p\}) = \delta(\{q\}-\{q_0\})\delta(\{p\})$

Many people start from this region

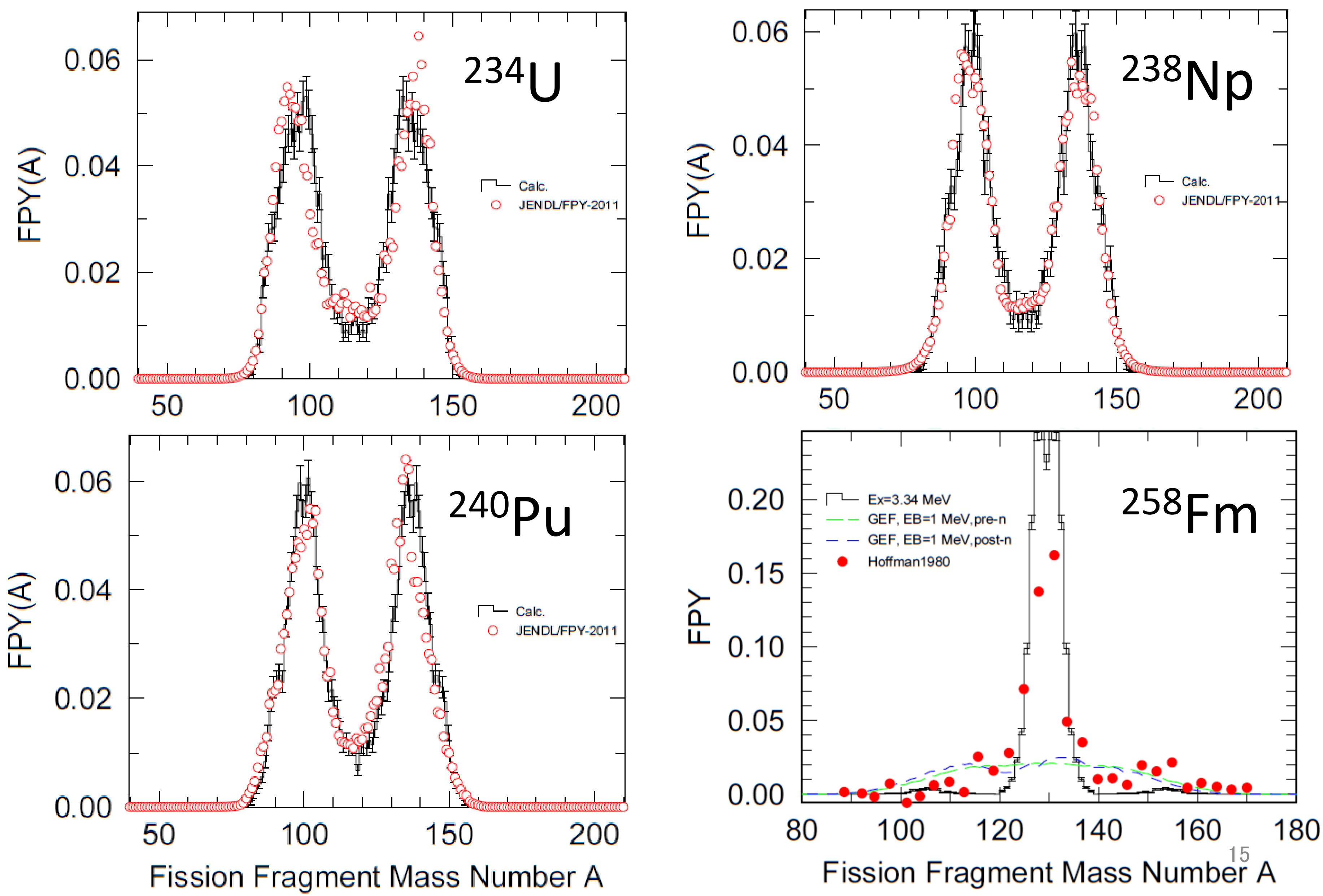


Example of 4D Langevin trajectories (^{236}U)

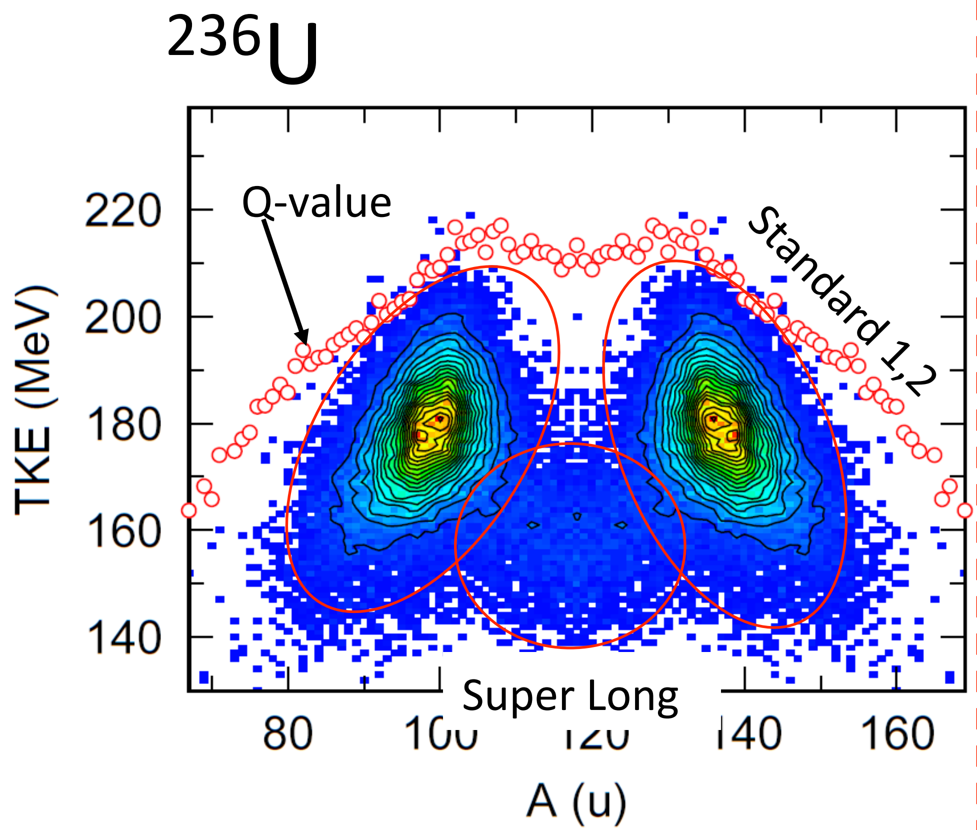


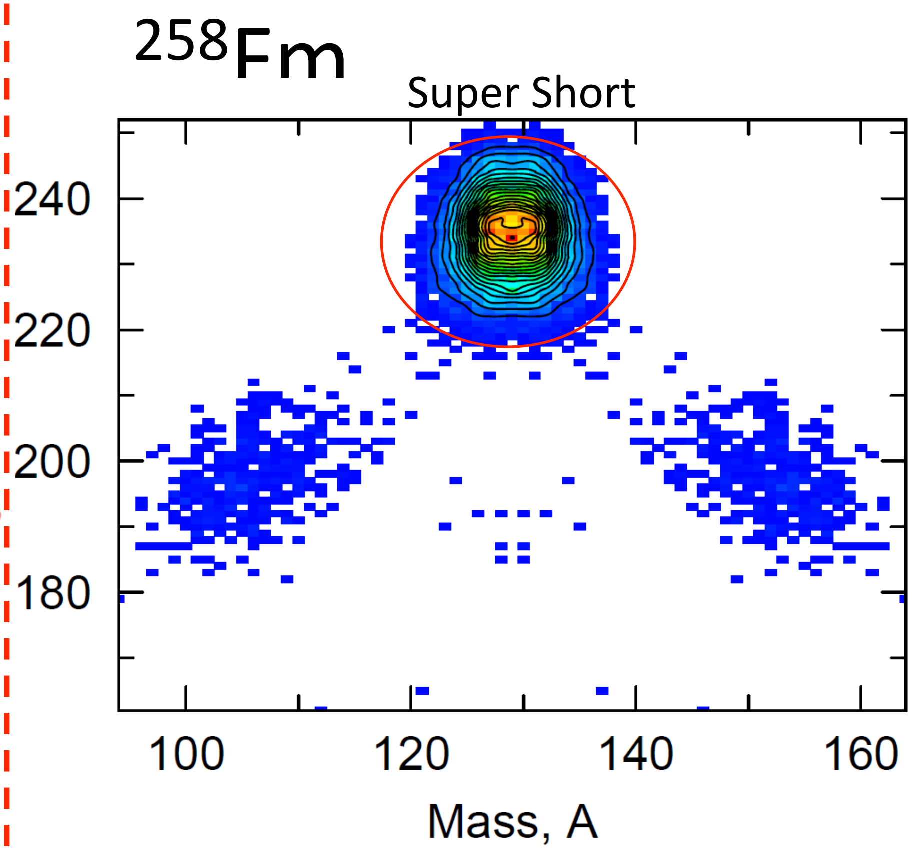
$$ZZ_0 = \frac{z_0}{R}$$

Mass Distribution of Fission Fragments at Ex=20MeV

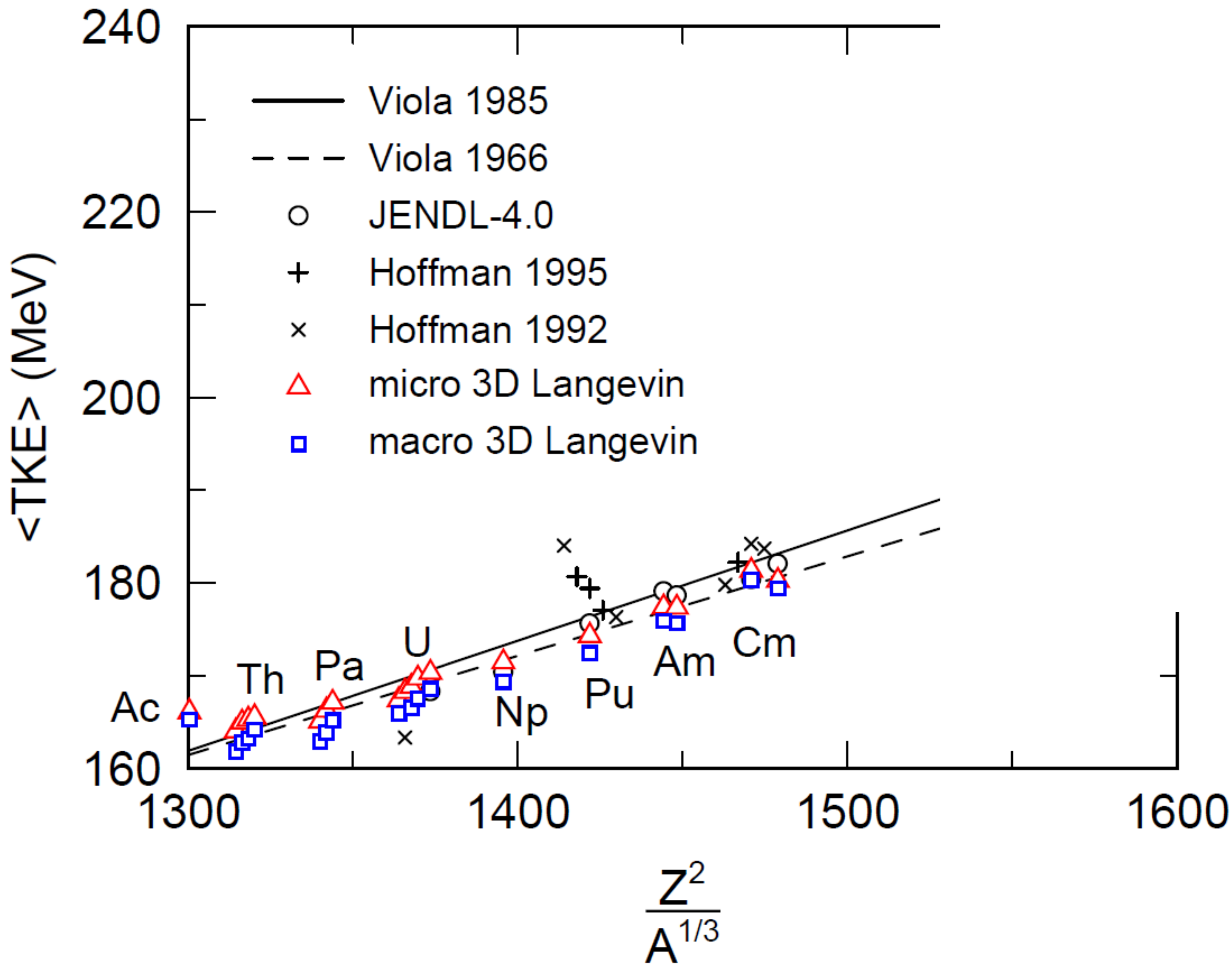


Distributions of TKE (total kinetic energy of fission fragments)

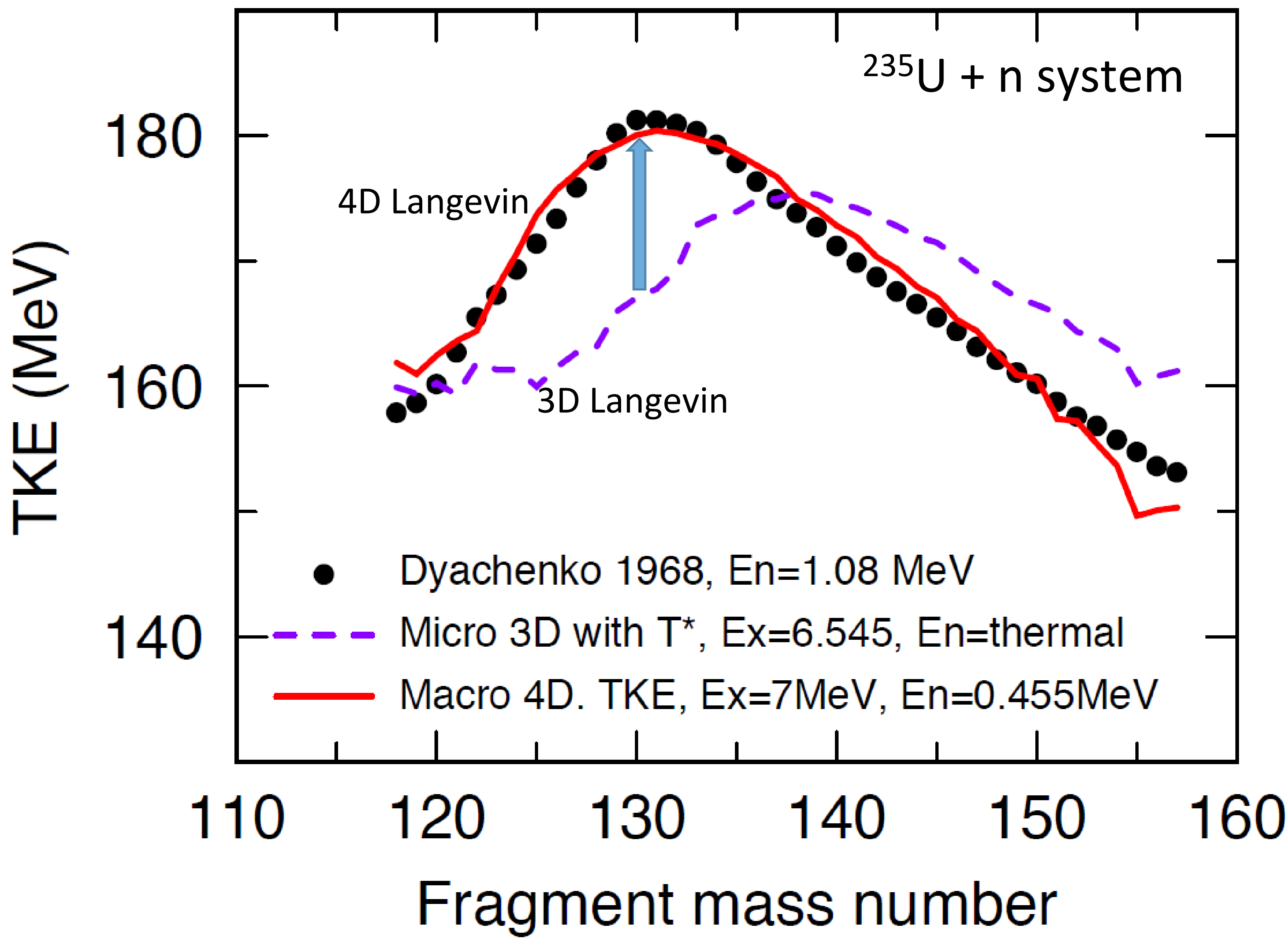




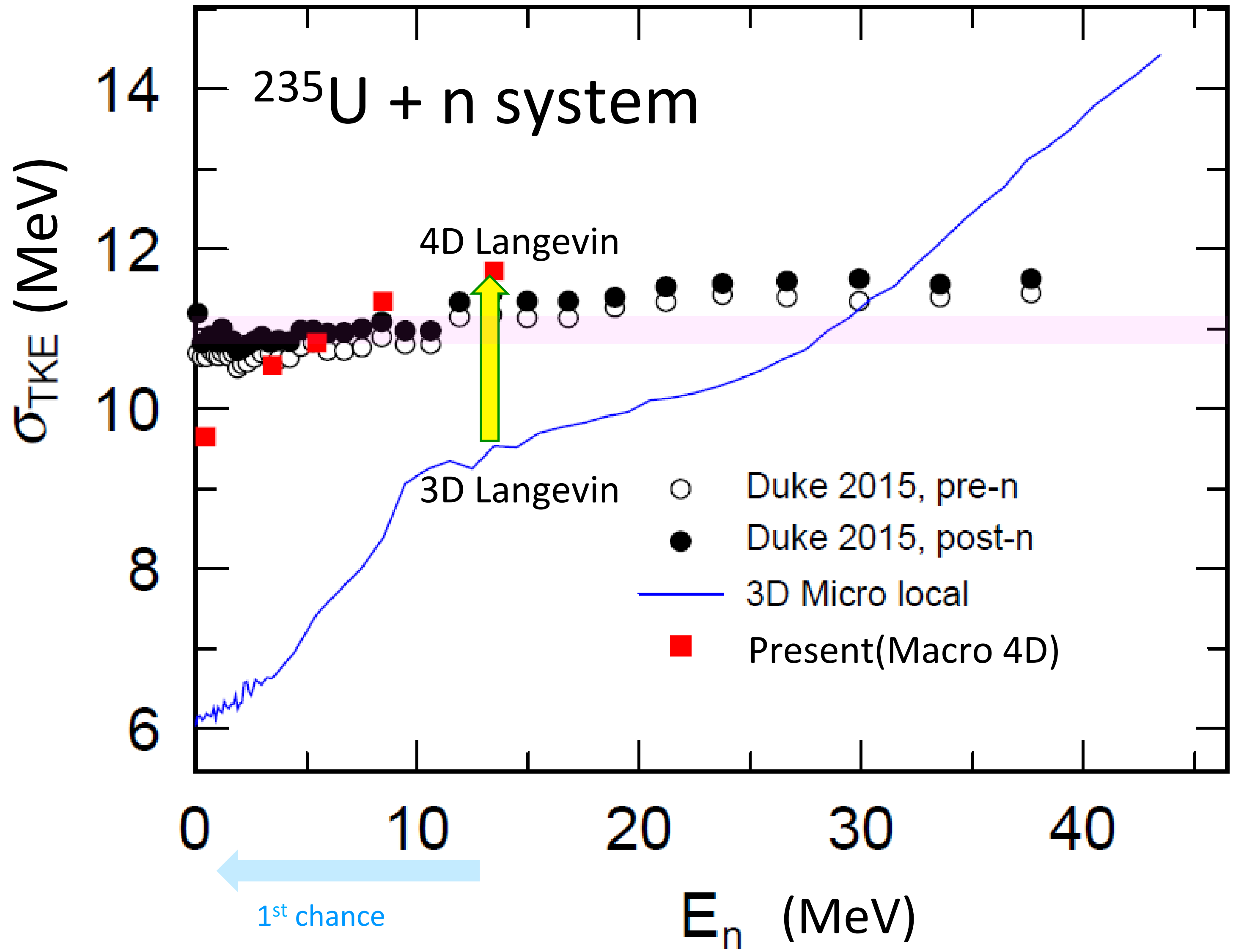
Systematics of <TKE> by 3D Langevin



Extension to 4D Langevin $\{q\}_{4D} = \{ZZ_0, \delta_1, \delta_2, \alpha\}$



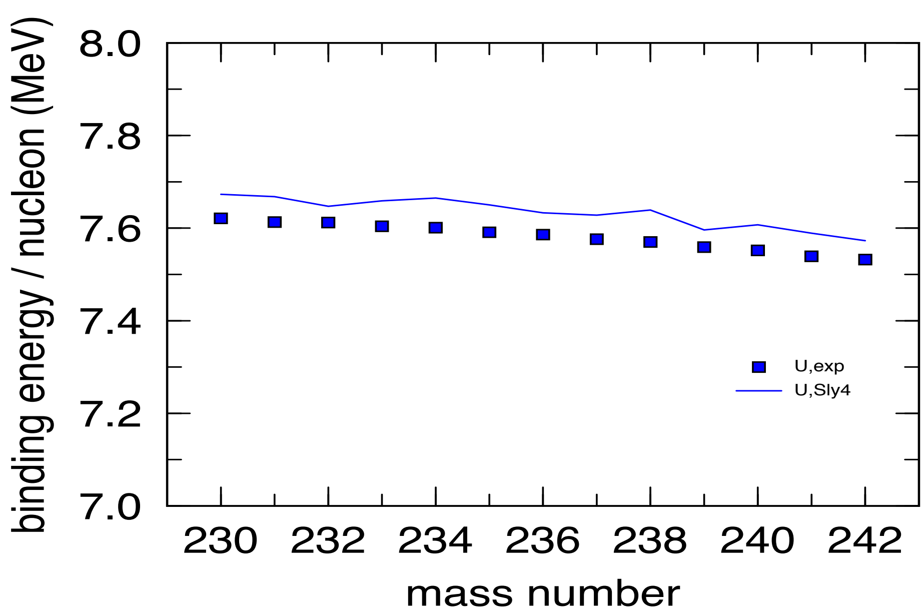
σ_{TKE} by 4D Langevin



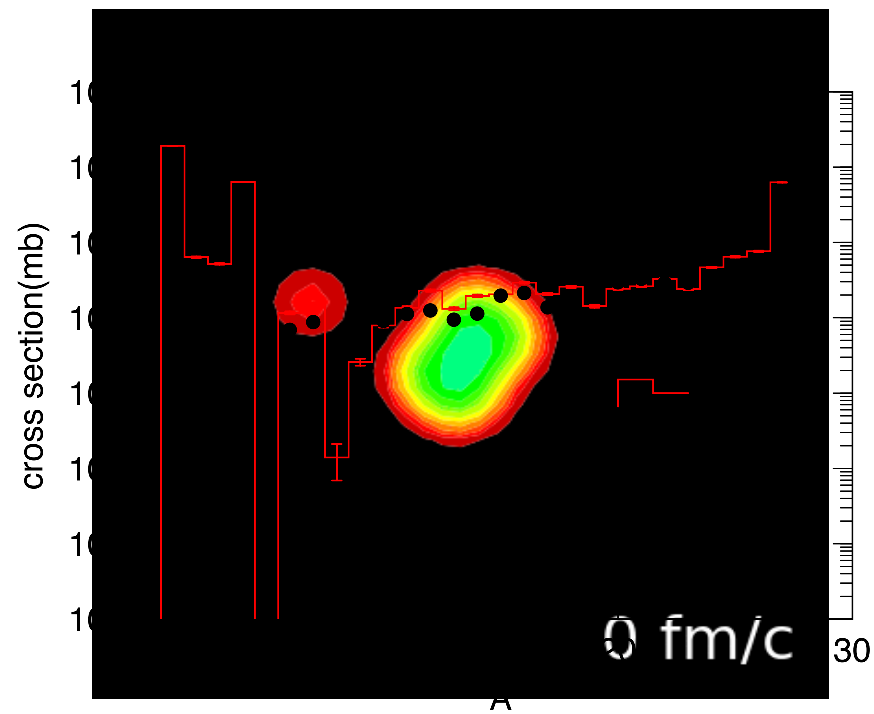
Nuclear fission by Antisymmetrized Molecular Dynamics: AMD

- Even though the Langevin-model description gives satisfactory results in many aspects of nuclear fission, it has only 3 to 4 degrees-of-freedom to express nuclear shape. It should be better to have ways to describe the nuclear fission by microscopic theories having d.o.f. of all the nucleons
- AMD is a very successful microscopic model of nuclear reactions and structures (A. Ono et al, Prog. Theor. Phys.,87(5),(1992), 1185-1206)

BE/A for U isotopes



180 MeV p+^{27}Al



AMD-1 : Basic formulation

Single-particle wave function : Gaussian coherent state

$$\langle \boldsymbol{r}|\phi_{Z_i}\rangle = (2\nu/\pi)^{3/4}\exp[-\nu(\boldsymbol{r}-\boldsymbol{Z}_i/\sqrt{\nu})^2]\chi_{\alpha_i}$$

$$\boldsymbol{Z}_i = \sqrt{\nu}\,\boldsymbol{r}_i + i/2\hbar\sqrt{\nu}\,\boldsymbol{p}_i$$

$$\chi_{\alpha_i} = p\uparrow, p\downarrow, n\uparrow, n\downarrow$$

Total wave function

$$|\Phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_A)\rangle = 1/\sqrt{A!}\ \det[\varphi_i(\boldsymbol{r}_j)]$$

$$\delta\int_{t_1}^{t_2} dt\, \Phi\, i\hbar\, d/dt - H\, \Phi\ /\Phi\Phi\ =$$

Time-dependent variational principle:

$$i\hbar\sum_{j\tau} C_{i\sigma,j\tau}\,\dot{Z}_{j\tau} = \partial\mathcal{H}/\partial Z_{i\sigma}^{*}$$

Equation of motion of the mean field:

$$C_{i\sigma,j\tau} = \partial^2/\partial Z_{i\sigma}^{*}\,\partial Z_{j\tau}\ \log\langle\Phi|\Phi\rangle$$

where $\mathcal{H} = \langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle$

AMD-2 : NN interactions

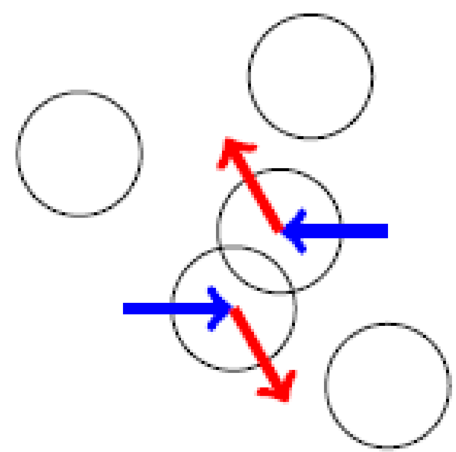
- Effective N-N interaction (origin of nuclear mean-field)

$$v_{ij} = t_0 (1+x_0 P_\sigma)\delta(\boldsymbol{r}) + 1/2\, t_1 (1+x_1 P_\sigma)[\delta(\boldsymbol{r})\boldsymbol{k}^2 + \boldsymbol{r}\delta(\boldsymbol{r})] + t_2 (1+x_2 P_\sigma)\boldsymbol{k}\cdot\delta(\boldsymbol{r})\boldsymbol{k} + t_3 (1+x_3 P_\sigma)[\rho(\boldsymbol{r}_i)]^\alpha \delta(\boldsymbol{r})$$

where $\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$ $\quad \mathbf{k} = \frac{1}{2\hbar}\left(\mathbf{p}_i - \mathbf{p}_j\right)$ $\quad B_{ij} = \langle \varphi_i | \varphi_j \rangle$

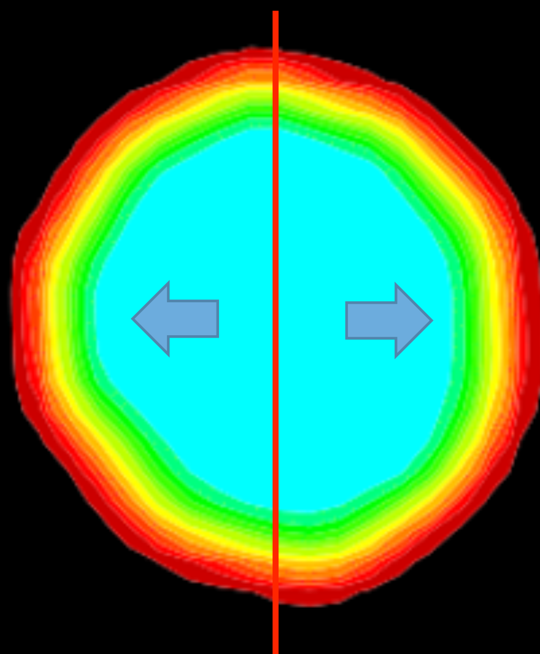
$$\rho(\mathbf{r}) = \left(\frac{2\nu}{\pi}\right)^{3/2} \sum_{i=1}^{A}\sum_{j=1}^{A} e^{-2\nu\left(\mathbf{r}-\mathbf{R}_{ij}\right)^2} B_{ij} B_{ji}^{-1} \qquad \mathbf{R}_{ij} = \frac{1}{2\sqrt{\nu}}\left(\mathbf{Z}_i^* + \mathbf{Z}_j\right)$$

- Stochastic NN collision as a part of residual interaction (A test particles from Wigner function) mimics random force in Langevin theory
  - ✓In-medium NN cross section
  - ✓Pauli Blocking after the collision
  - ✓branching and deformation of wave functions--> tunneling, distribution



Initial state of ^{236}U ($^{235}U + n$)

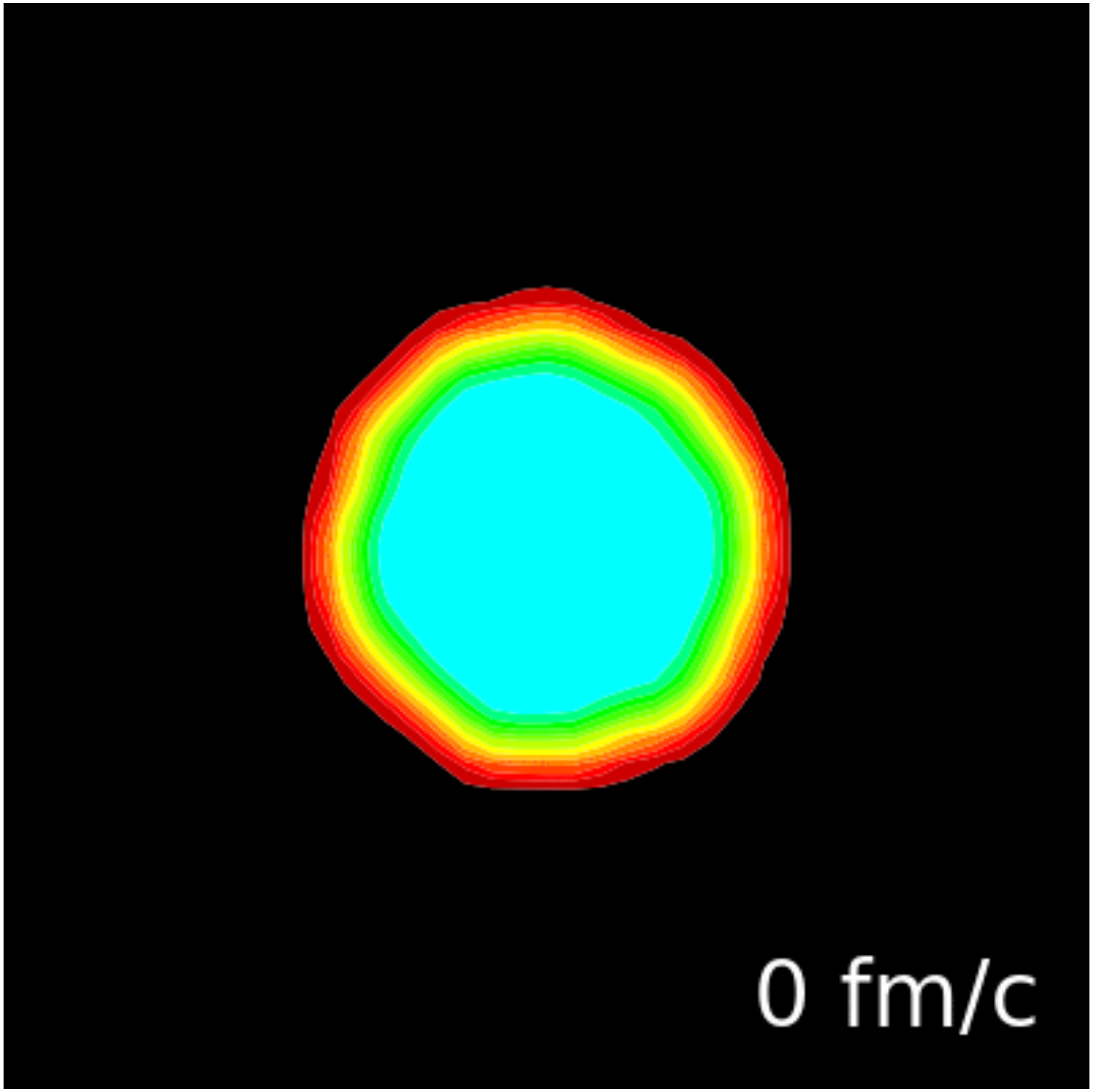
As a first step to simulation of nuclear fission by AMD, here we simply give a boost momentum to each nucleon, to the opposite directions for nucleons staying at the left region and right region



$E^{+} \sim 1.3$MeV/u

0 fm/c

Time evolution by AMD, ^{236}U ($^{235}U + n$)

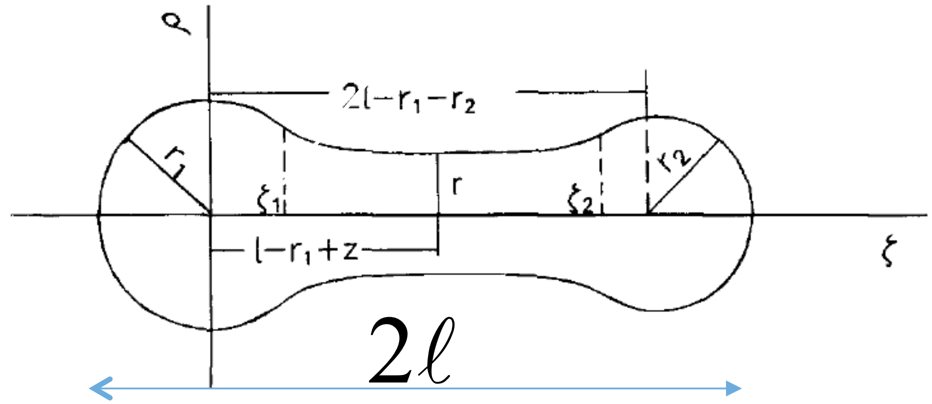


Examination of phenomenological assumptions

- Brosa's random neck rupture condition due to hydrodynamical Rayleigh instability

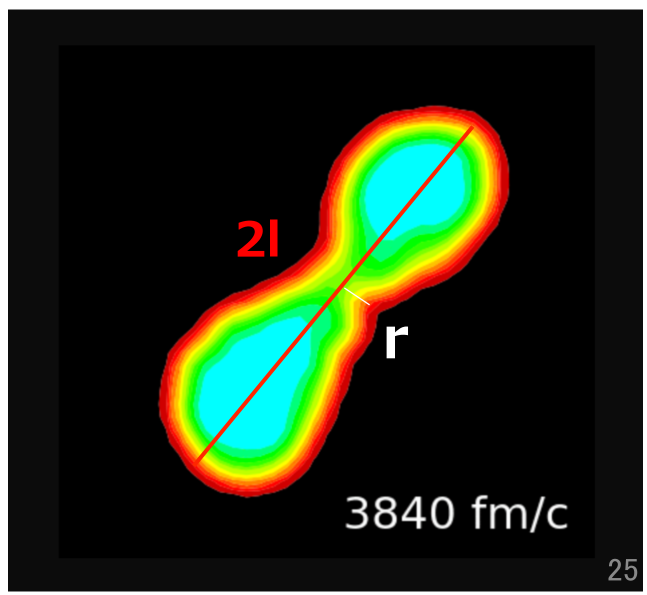
$2l = 11r$
$l = 5.5r$

Brosa, Grossmann & Müller, Phys.Rep.197, 167(1990)



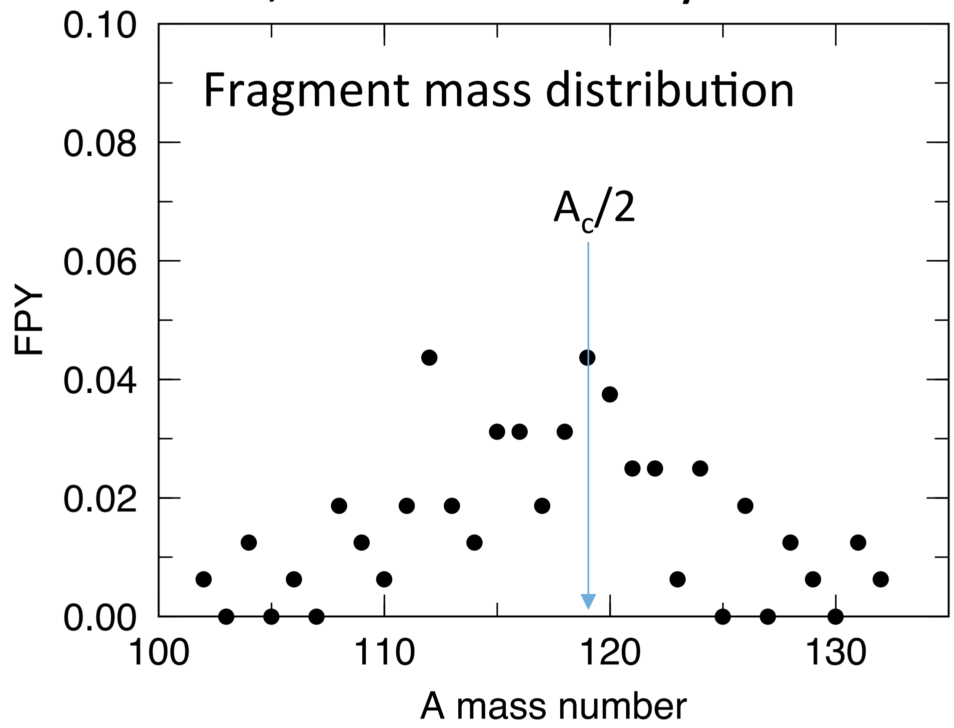
AMD : $l \sim 5r$

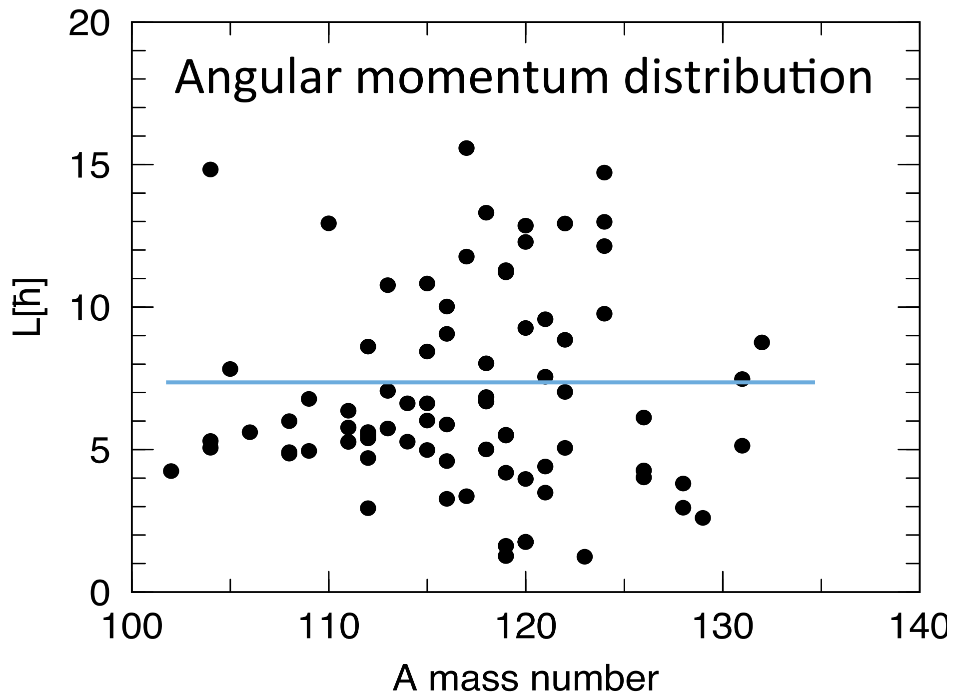
This verifies that Brosa's estimation of neck rupture condition is sensible



Results : FPY (left) and rotational angular momenta (left)

^{236}U, boost fission by AMD

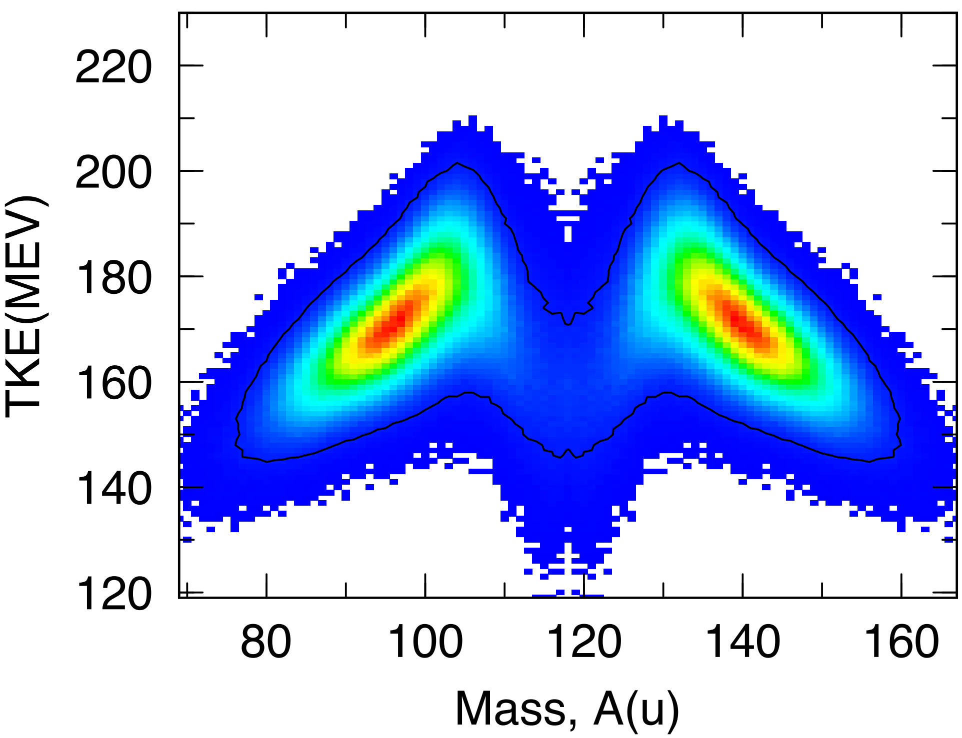


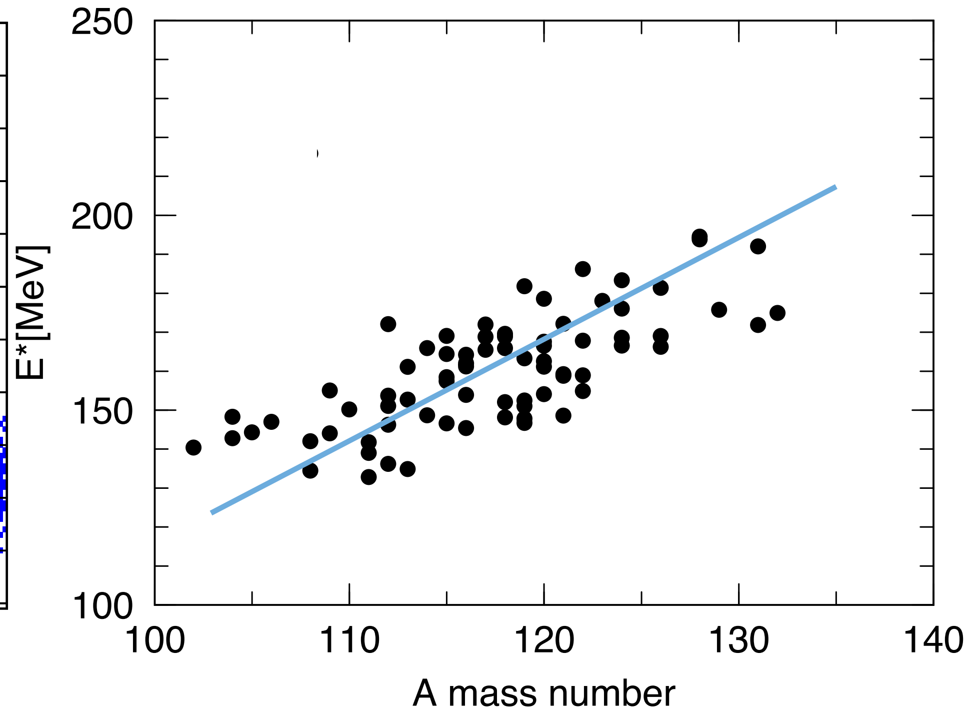


- Due to our specific way of boost, the mass distribution corresponds to symmetric fission, which is categorized as super-long mode in Brosa's terminology (low TKE component)
- Each fragment has, on the average 5 to 10$\hbar$ (on the average around 7$\hbar$) of rotational angular momentum, which is enough to account for the origin of extra spins of fission fragments as explained in the introduction

Results : Mass-TKE correlation (left) and excitation energy of each fragment (left)

exp : ^{236}U at excitation energy of 12 MeV





- Our result, which corresponds to the symmetric components, has the same TKE values deduced from experiment. This is in some sense quite satisfactory as well as surprising if we consider the difference of excitation energy of the data (20MeV) and our calculation (300 MeV).
- This model has a capability to deduce excitation energy of each fragment, which is not the case in Langevin-type approaches. The results E*～A denotes equi temperature Fermi-gas scheme

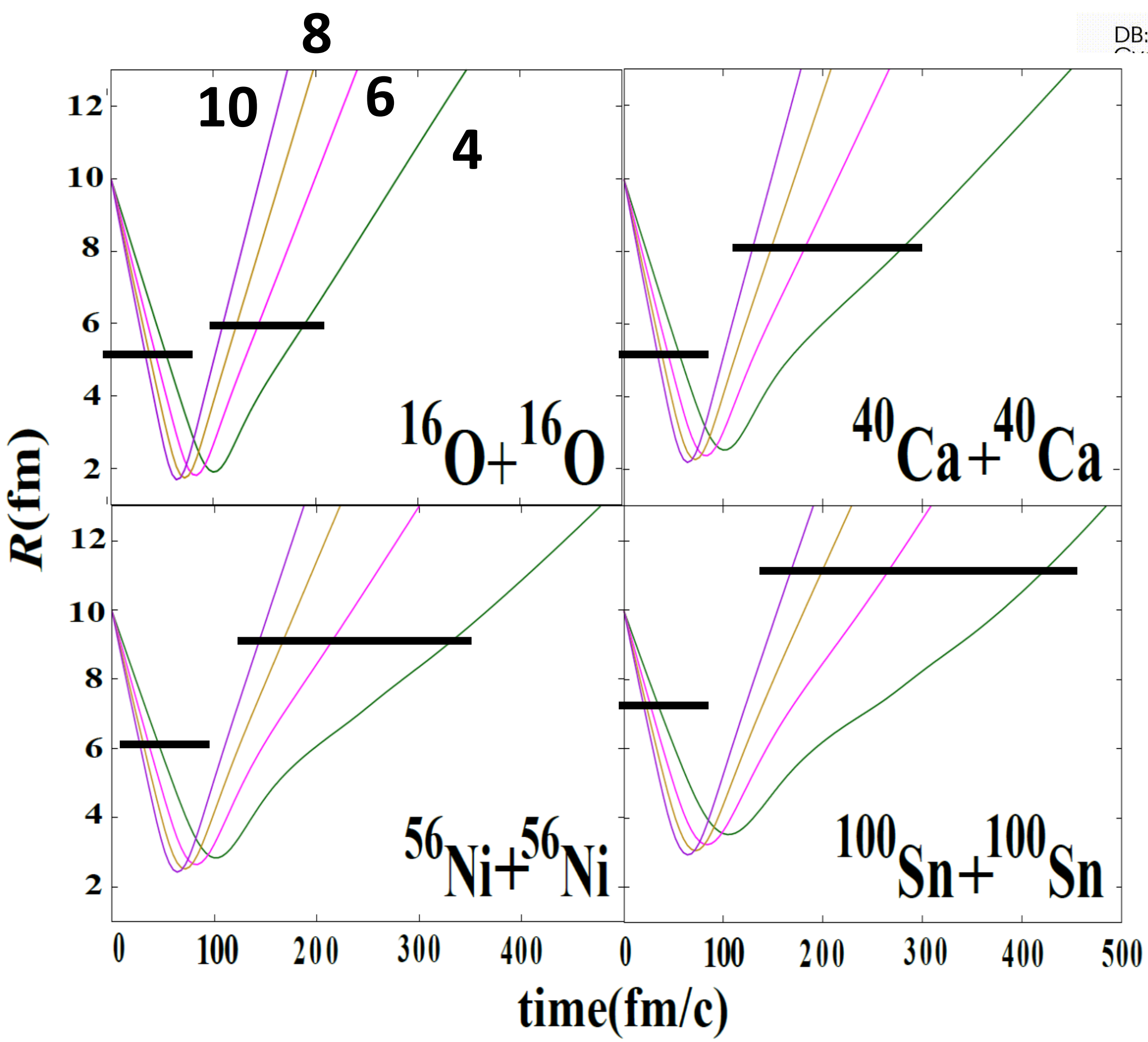
Results from AMD calculation for ^{236}U (^{235}U + n)

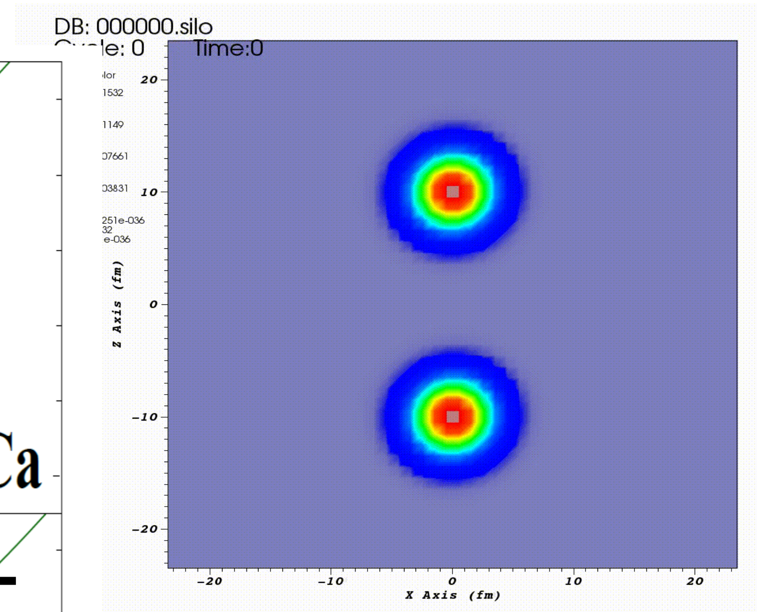
1. There seems to be no oscillation in the elongation direction at all even though the fact that the way we gave the initial condition is expected to result in strong oscillation. However, there do exist surface oscillation
2. This result is in contradiction to Langevin theory predictions, but in accord with TDHF and QMD results
3. We notice that neck is thicker than we expected, and particle exchange through the neck region seems to be quite important, which may result in rotation of fragments
4. Nuclear shape is quite complicated during fission, which is out of reach if we use only 3, 4 or 5 shape parameters (such as used in Langevin description). In this respect, description of nuclear fission by microscop s is recognized to be very important

skip
TDHF
Summary

Nuclear friction by TDHF

$i\hbar \frac{d}{dt}\varphi_i = h_i \varphi_i$ → $\rho(\boldsymbol{r})=\sum_i^N |\varphi_i|^2$ → $R=|\int \boldsymbol{r}\rho(\boldsymbol{r})d\boldsymbol{r}|$





- We calculate the relative distance of fragment centers
- From its time evolution, we derive average friction coefficient as explained in the next slide

How to obtain friction coefficients

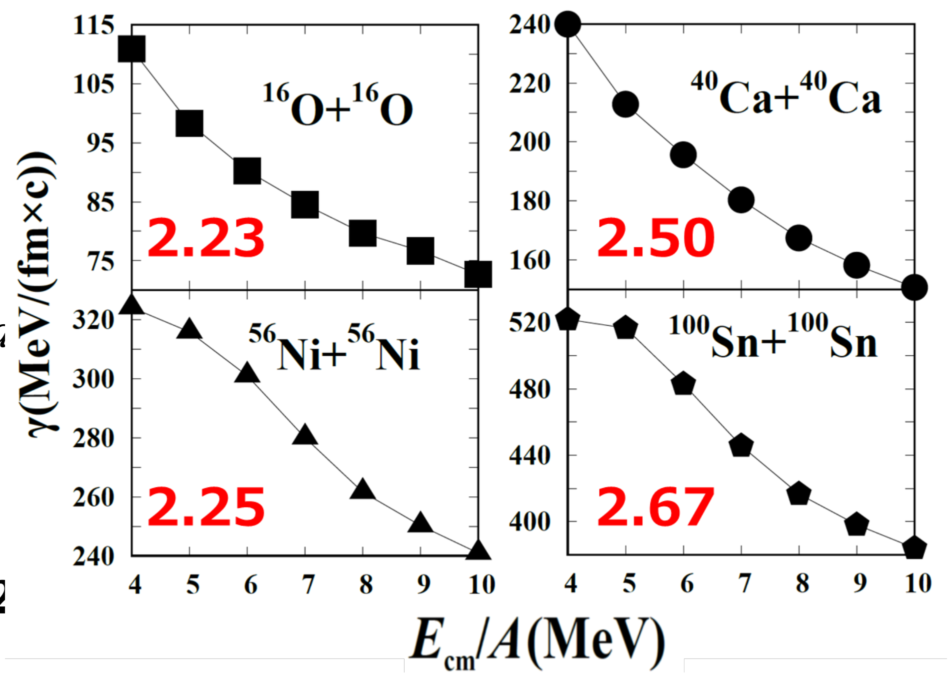
From the macroscopic e.o.m. for the center distance R

$$\mu R + dV/dR + \gamma R = 0$$

We can integrate

$$\int_I^F \mu R \, dR + \int_I^F dV/dR \, dR + \gamma \int_I^F R \, d$$

$$\boldsymbol{\gamma = (1/2\ \mu R_{BF}^{2} + V_{BF}) - (1/2\ \mu R_{AF}^{2}}$$

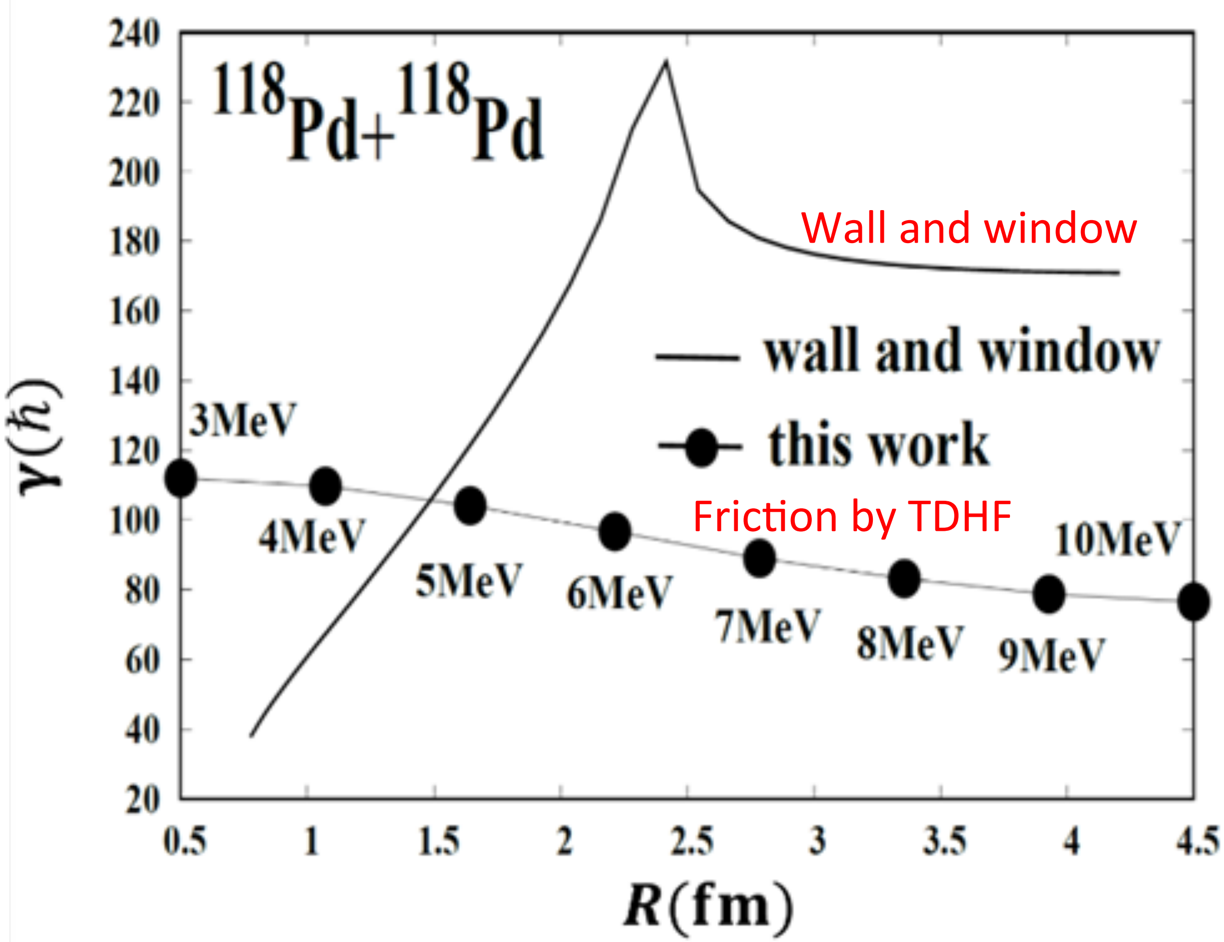


This is the average friction coefficients, which depends on collision energy

Numbers in red characgers inducate γ/A at $E_{cm}/A = 7\mathrm{MeV}$

BF : Before Fusion AF : After Fission

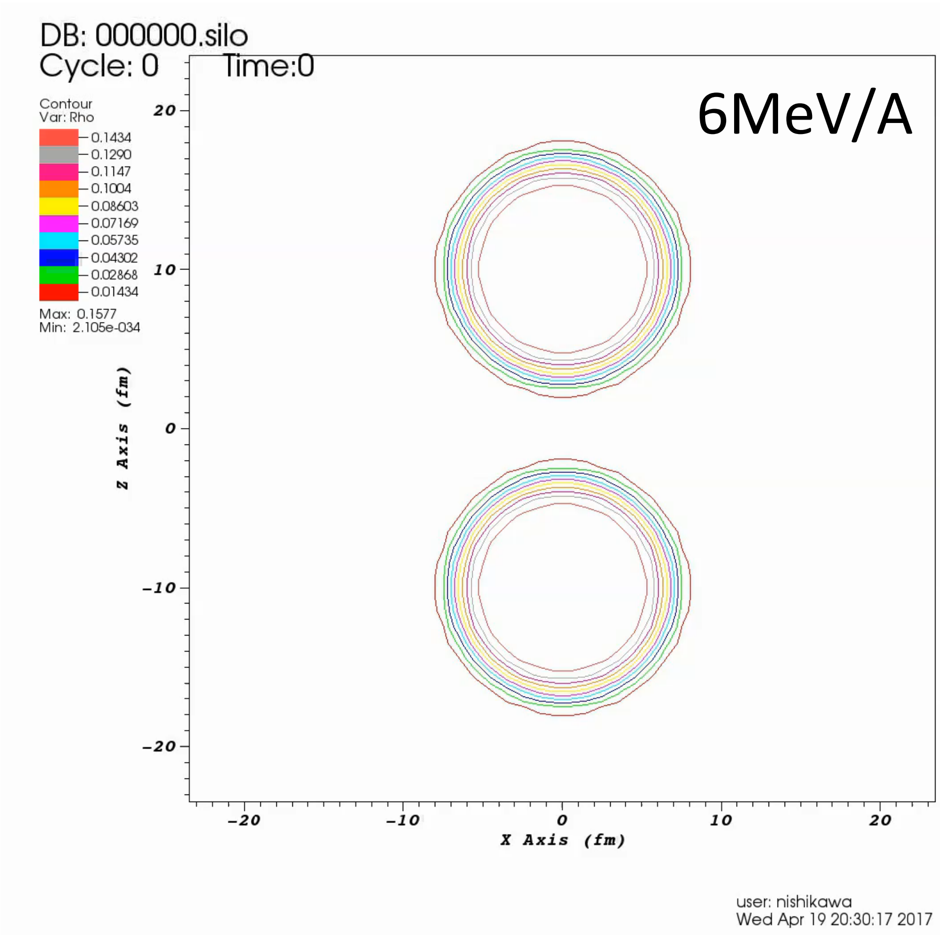
For ^{236}U (=^{118}Pd + ^{118}Pd) system

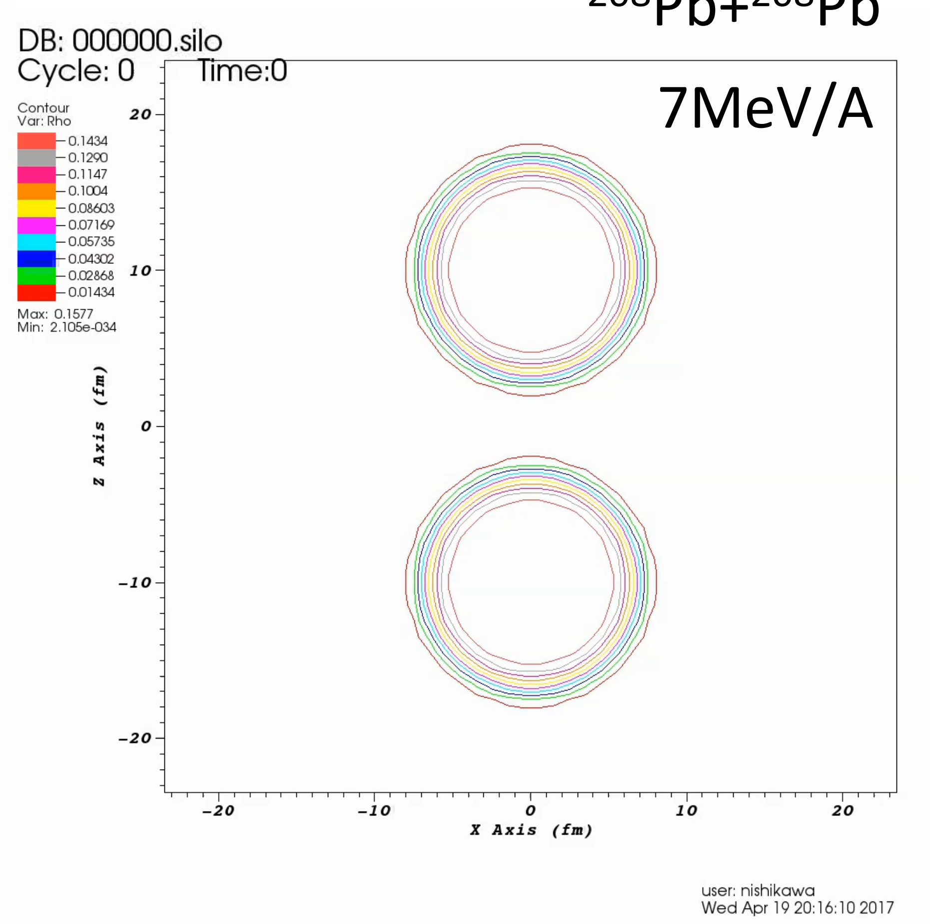


Wall-and-Window friction is a (static and semiclassical) hydrodynamical result, whereas our results are purely dynamical and quantal ones, but they coincide quite well.

Possibility of describing ternary and quarterly fission by TDHF

$^{208}Pb+^{208}Pb$

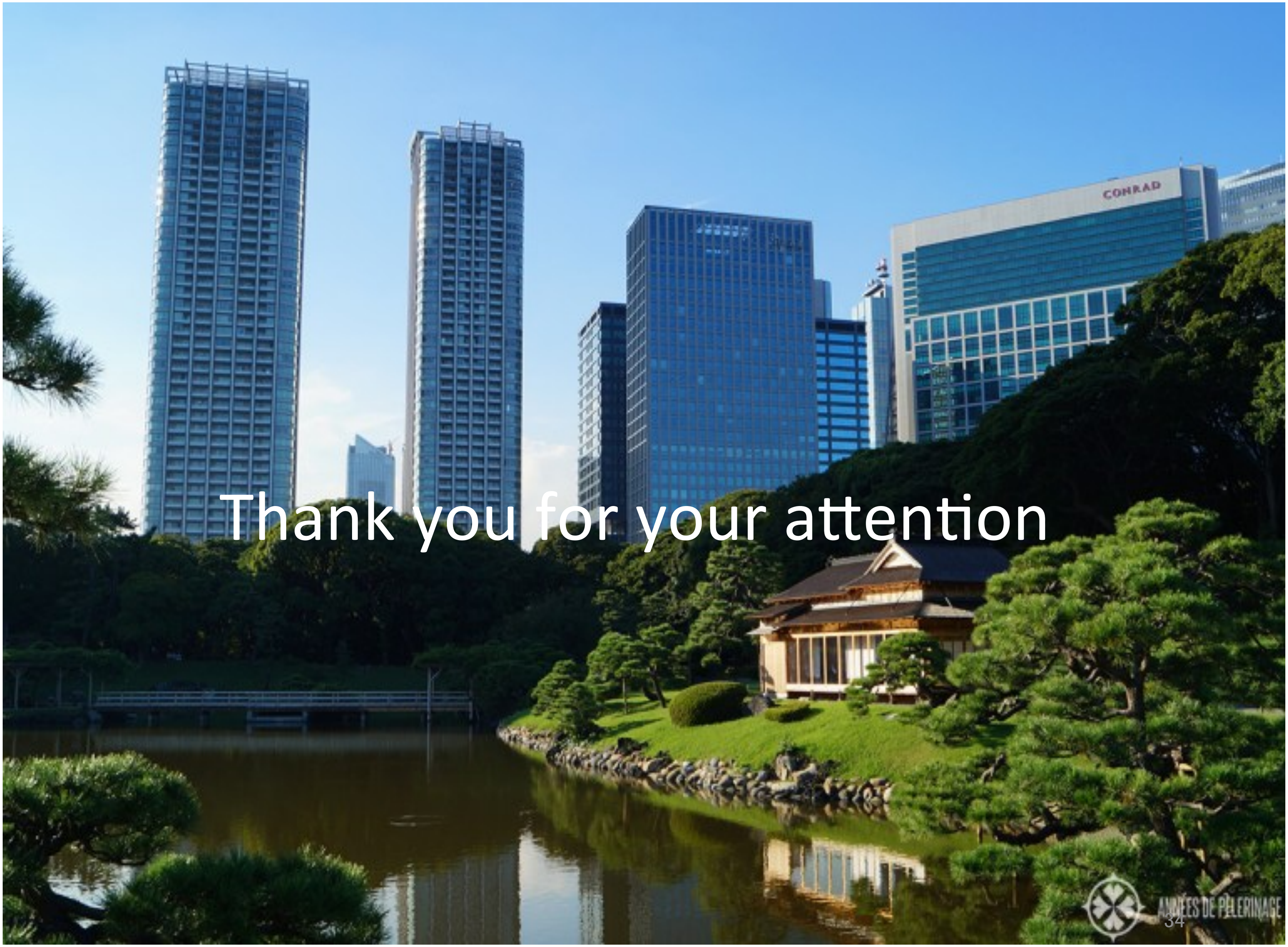




Summary

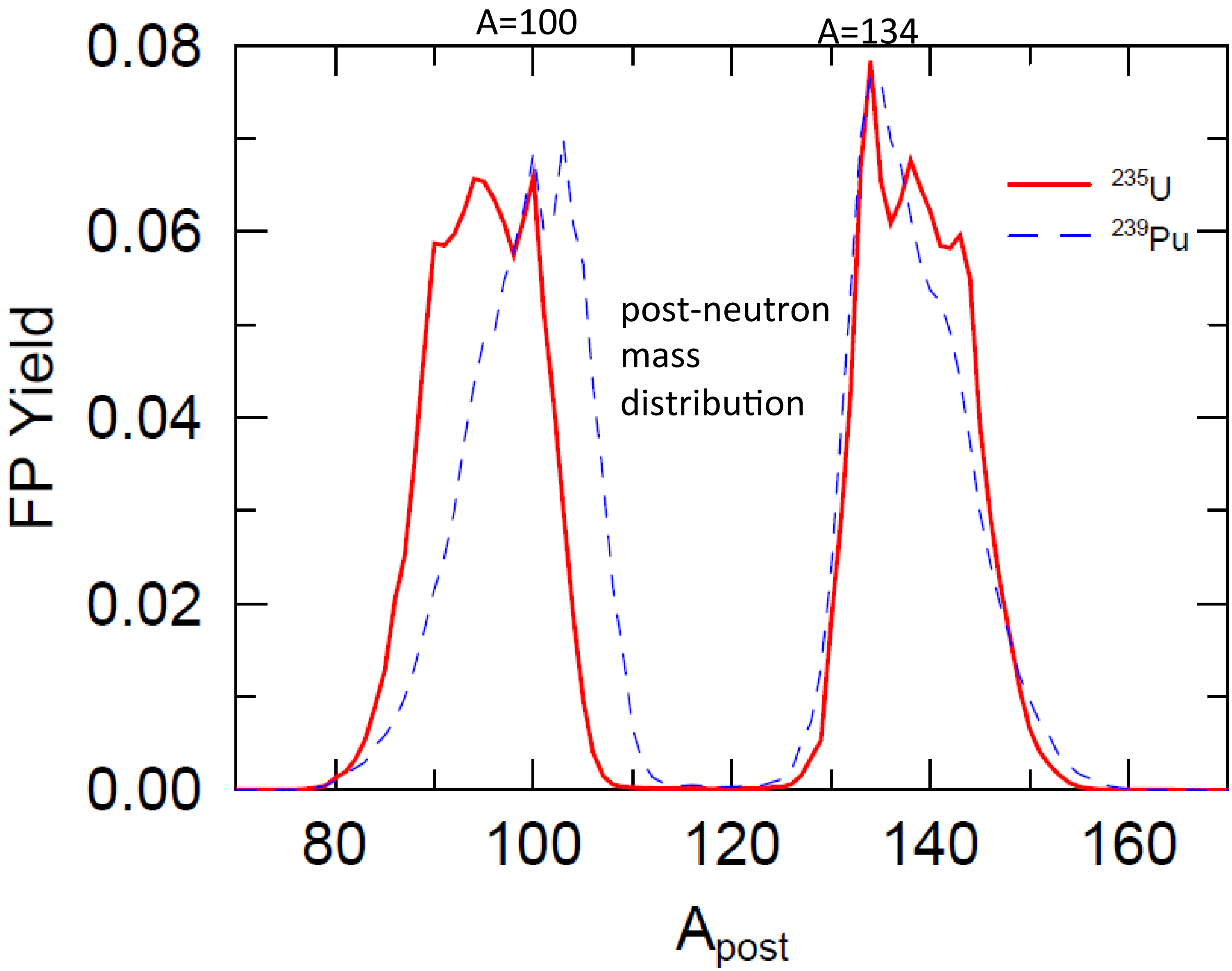
- We have described 3 different dynamical approaches to nuclear fission currently studies at Tokyo Tech:

1. Dynamical description of fission by Langevin equation is explained
   - Calculations are performed for actinides to Fm region with both 3D and 4D versions, macro and micro transport coefficients
   - Mass and TKE distribution of fission fragments are reproduced with a high accuracy, including their systematical trends
   - With this degree of accuracy, this method can be considered to be one of the data production tool
2. Our first attempt to describe nuclear fission by AMD was described
   - Quite promising
   - Rotational angular momentum could be already derived to be finite
   - It can account for the extra spin which fission fragment has at the onset
3. TDHF approach was also described
   - to deduce nuclear friction from quantal dynamical model
   - possibility of describing ternary or quarterly fission

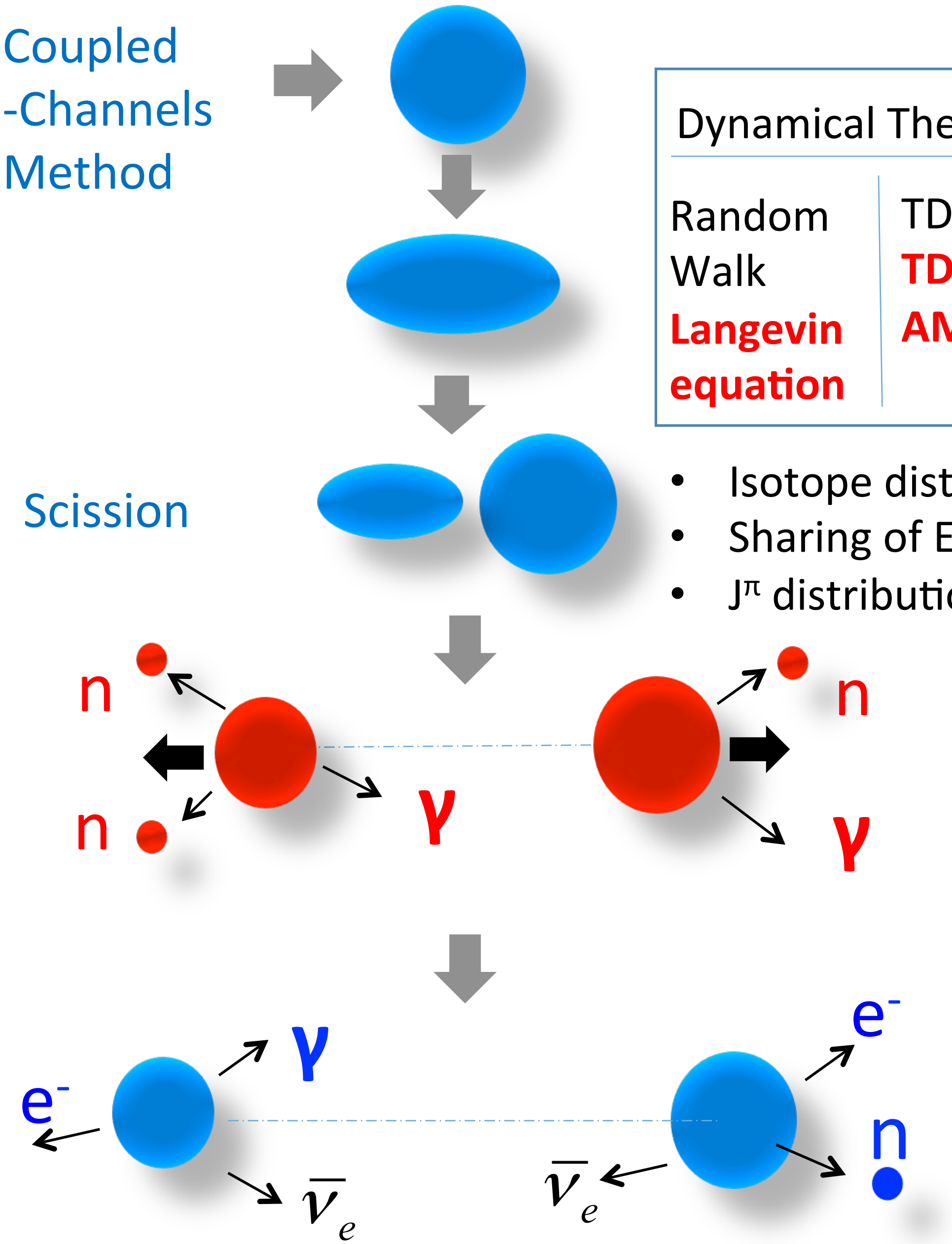


Thank you for your attention

Asymmetric and fine structures of mass distribution of primary fission products from neutron-induced fission



Nuclear Theories which can describe various aspects of fission



Dynamical Theory		Static Theory	Brosa-inspired
Random Walk **Langevin equation**	TDGCM **TDHF** **AMD**	Fong Wilkins CHF **RMF**	Multi-modal analyses

- Isotope distribution
- Sharing of E* between 2 fragments,
- J^{π} distribution

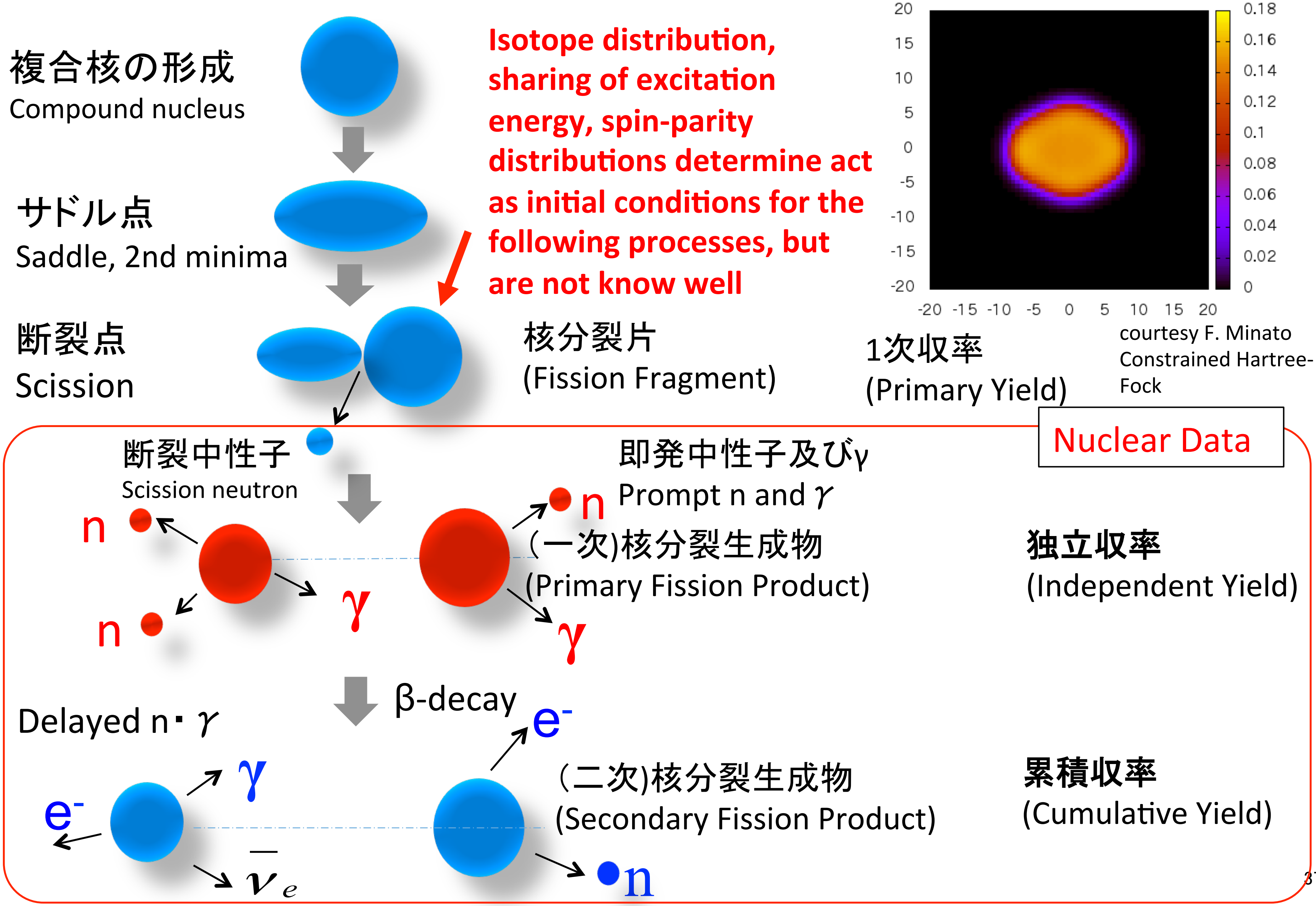
Statistical theory

Weisskopf-Ewing
Madland-Nix (LAM)
Hauser-Feshbach

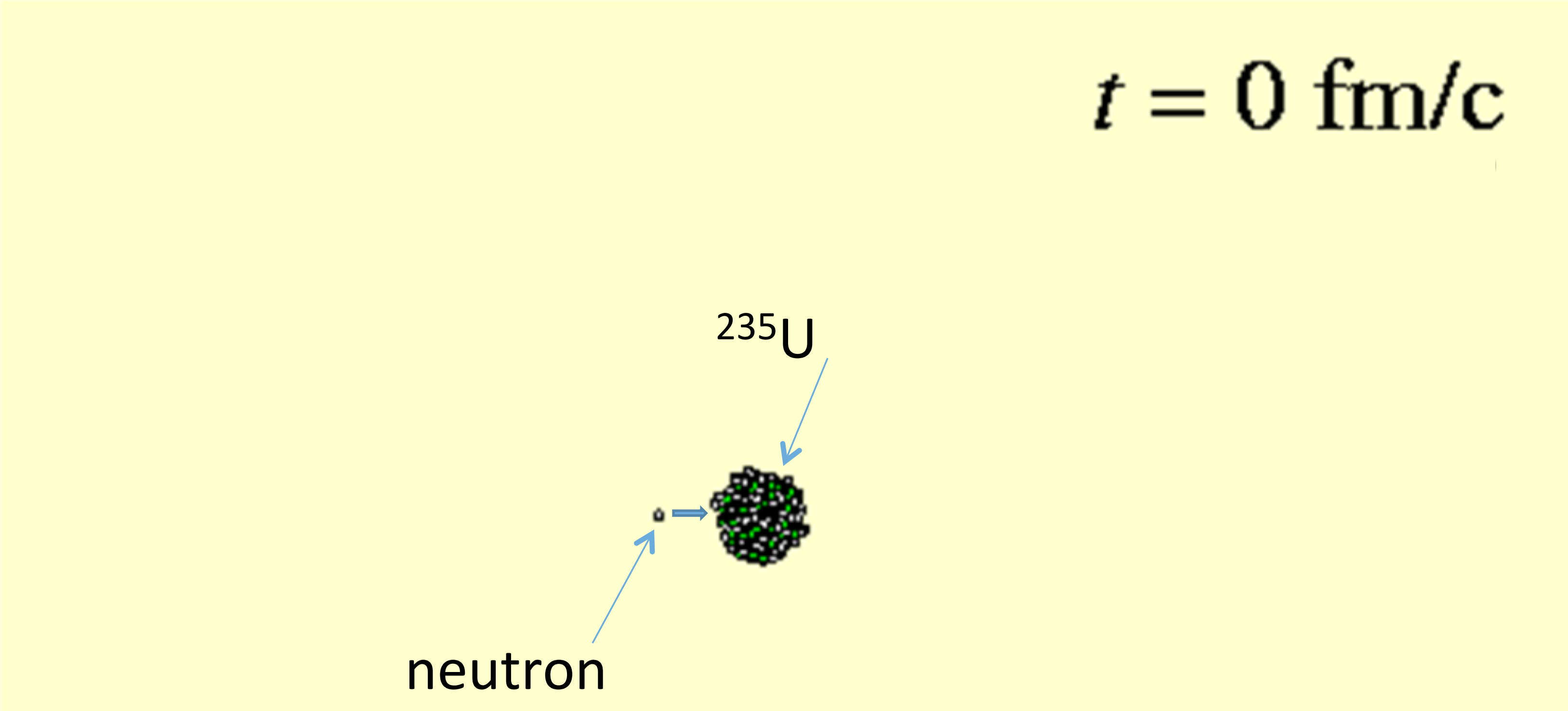
β-decay + statistical theory

β-decay	statistical theory
Gross Theory	Weisskopf-Ewing
QRPA	Hauser-Feshbach
Shell Model	

Time evolution of fission



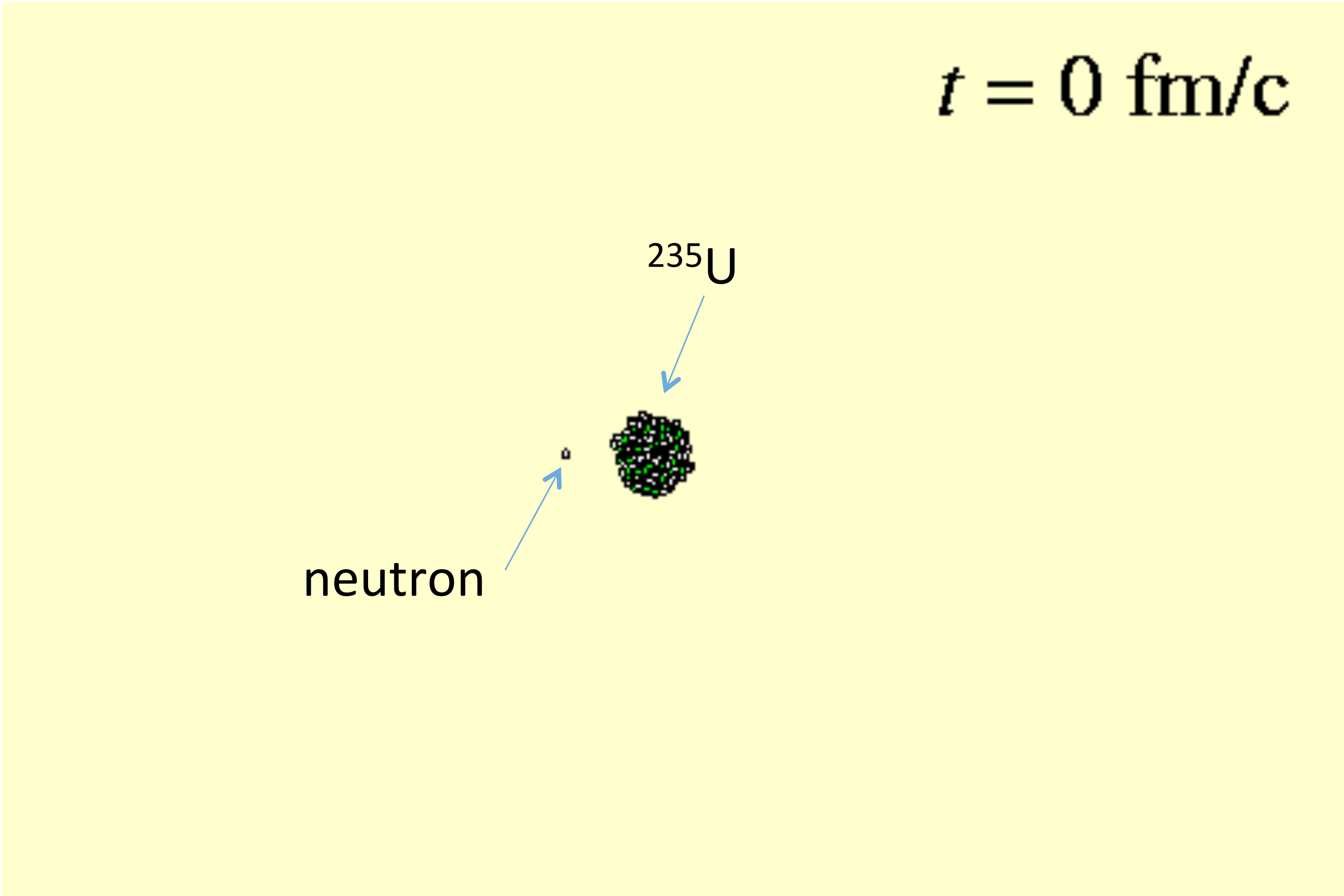
Simulation of nuclear fission (^{235}U + 140 MeV n) by JQMD



JQMD : JAERI Quantum Molecular Dynamics
= a semiclassical molecular dynamics for nuclear reactions

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

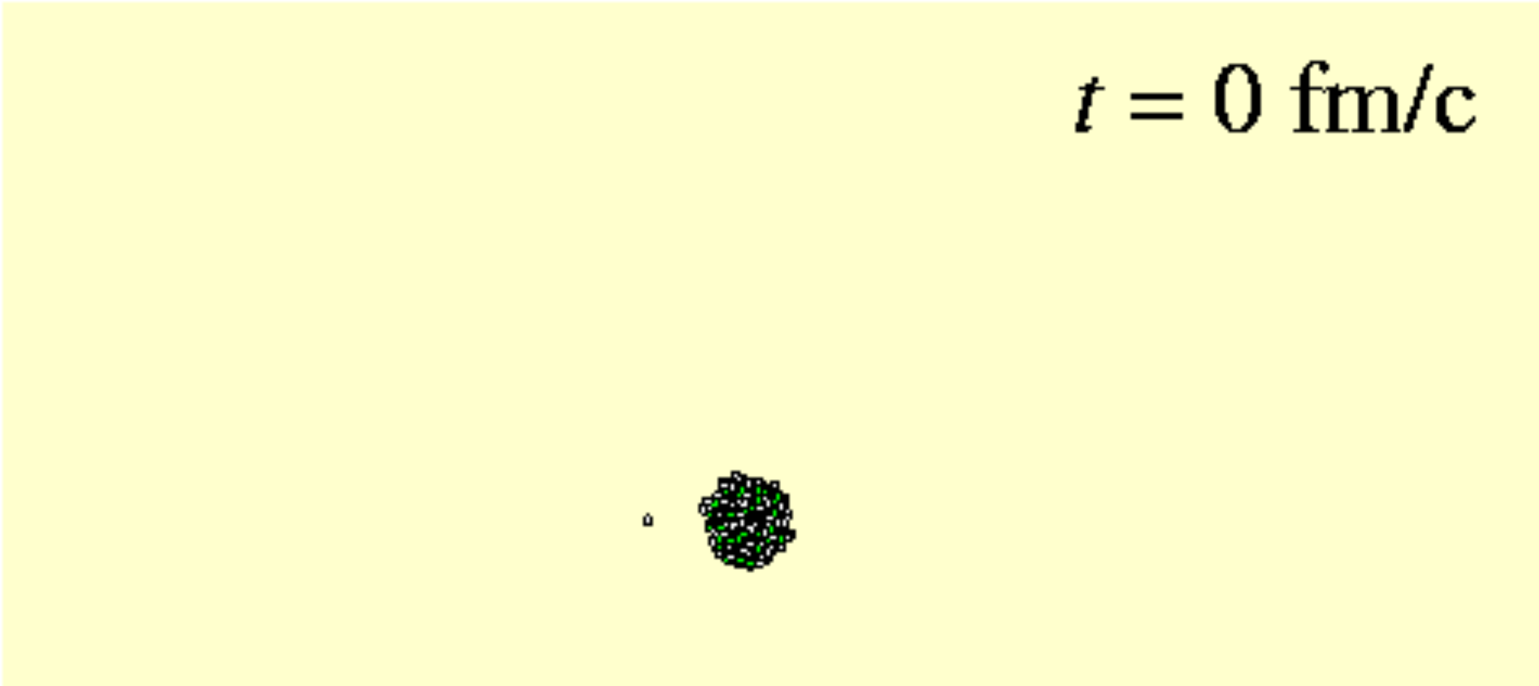
QMD simulation of nuclear fission (^{235}U + 140 MeV n)



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)

QMD simulation of nuclear fission (^{235}U + 140 MeV n)

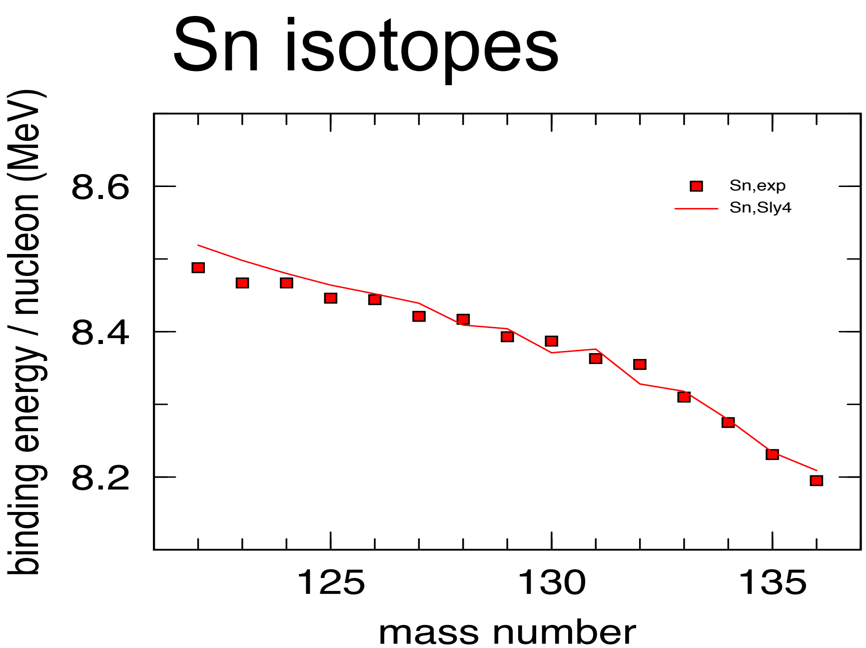


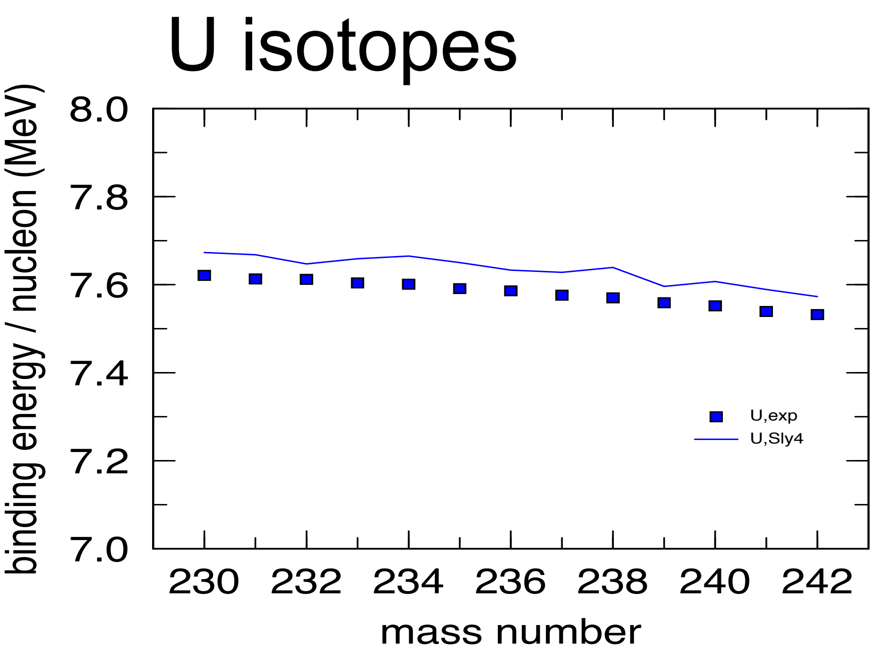
Nuclear elongation seems to evolve monotonically (not oscillatory) in semi-classical molecular dynamics. This is also seen in TDHF calculation by Bulgac et al. (Univ. Washington)
Fission time scale ∼ 10,000fm/c

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

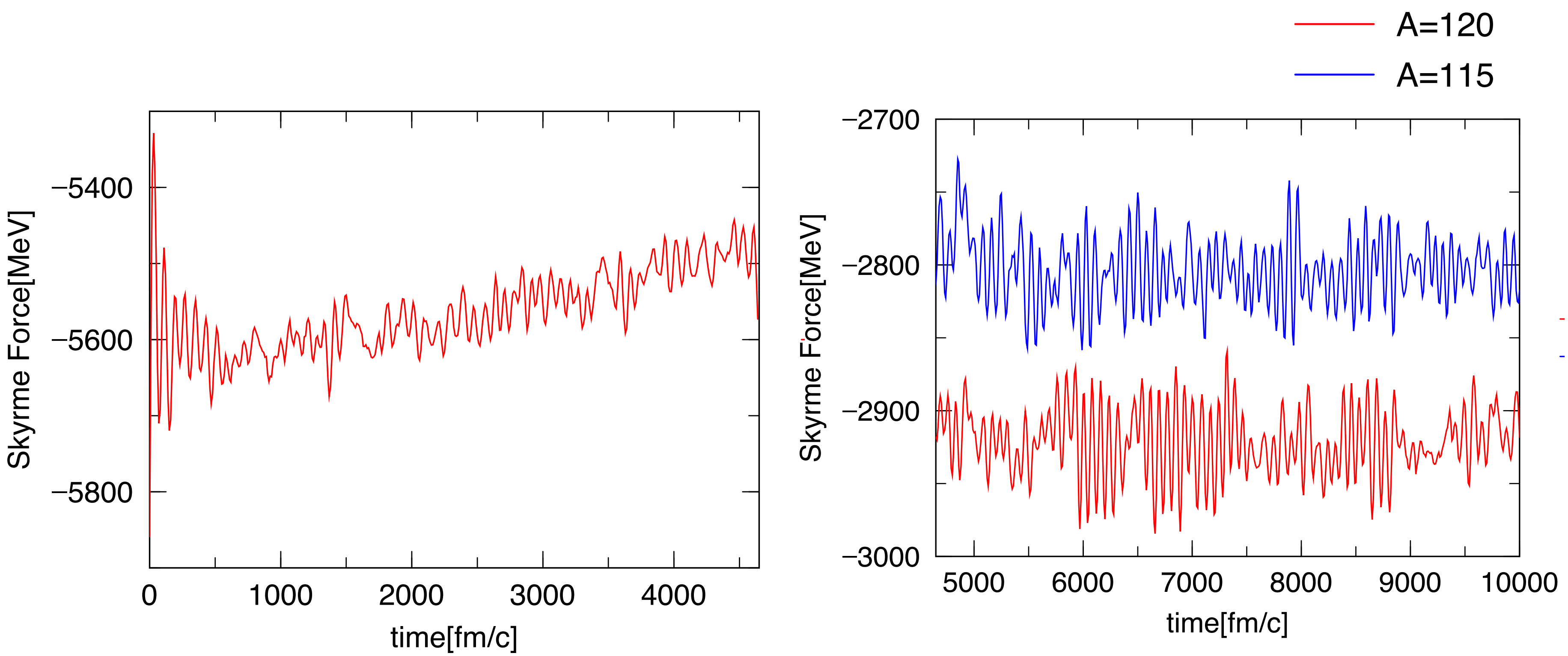
K.Niita, T. Maruyama, Y. Nara, S. Chiba and A. Iwamoto, JAERI-Data/Code 99-042(1999)

Binding energy/A of medium and heavy nuclei by AMD





Time evolution of <V> before (left) and after (right) scission

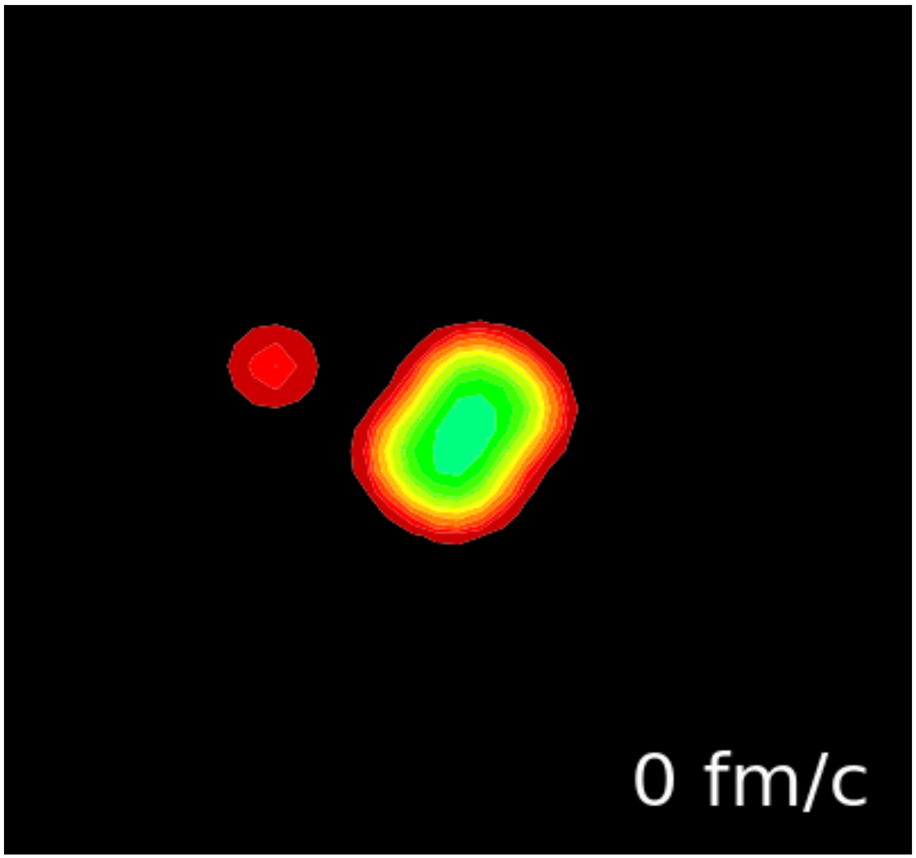


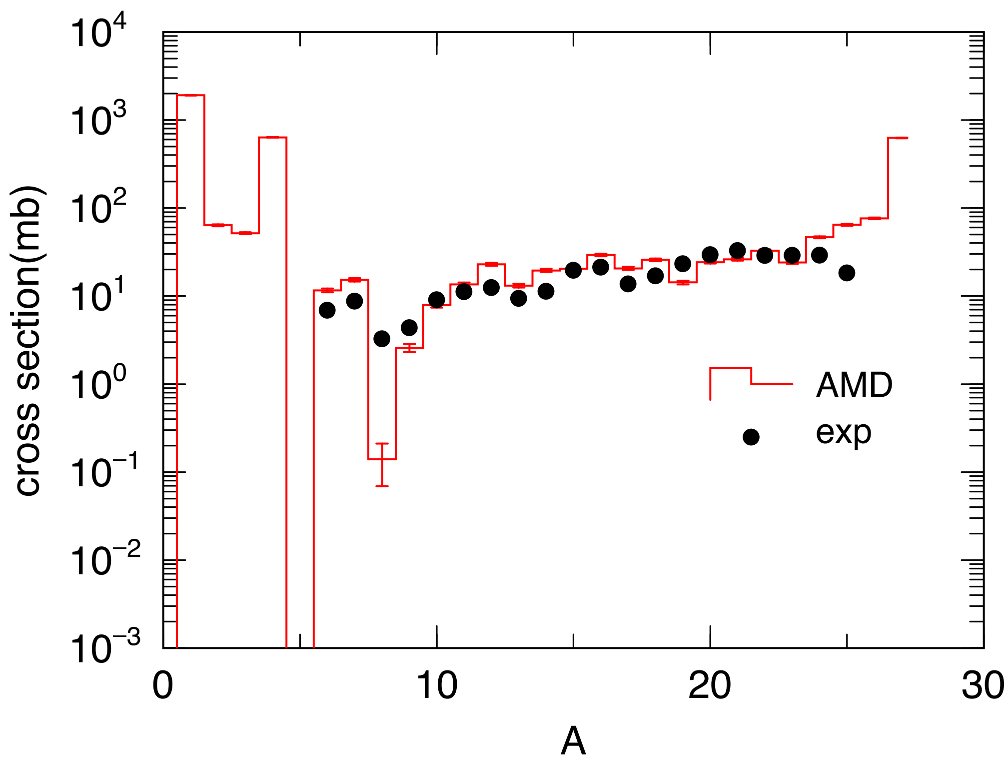
Essence of computational method

- Shape parametrization : Two-center model in 3 and 4 dimensions
- Potential energy -- macroscopic-microscopic method
  - Macroscopic part : Krappe-Nix (double-folded Yukawa model)
  - Microscopic part : two-center shell model or two-center Woods-Saxon model + Strutinsky + BCS
  - Excitation energy dependence of the shell damping : Ignatyuk or Randrup-Moeller prescription
- Transport coefficients
  - Werner-Wheeler method for mass tensor (3D and 4D)
  - Wall-and-Window model for friction tensor (3D and 4D)
  - Linear response theory for microscopic mass and friction tensors (3D only) (Ivaniuk et al., JNST DOI: 10.1080/00223131.2015.1070111)

p(180MeV)+^↾27⇃Al by AMD

impact parameter:**0<b<6**
force:**SLy4**

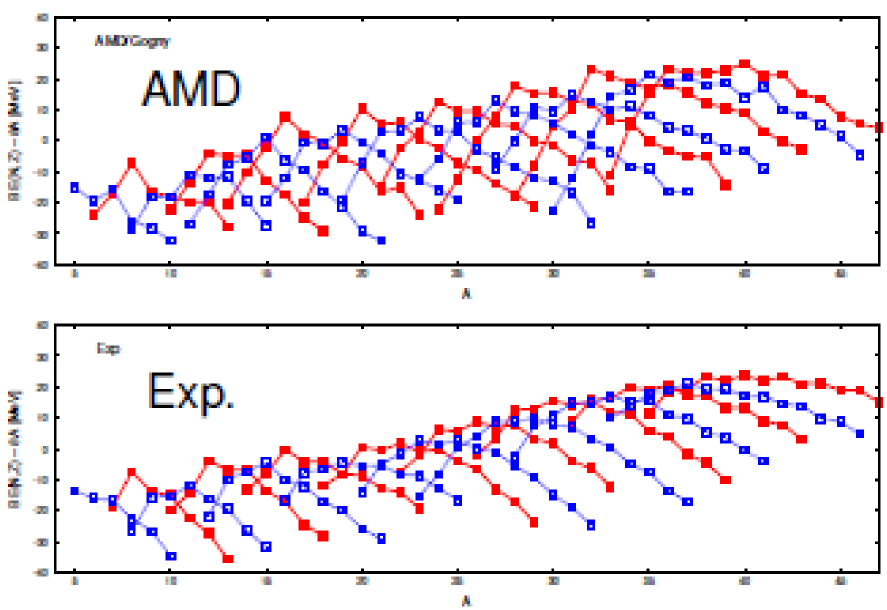




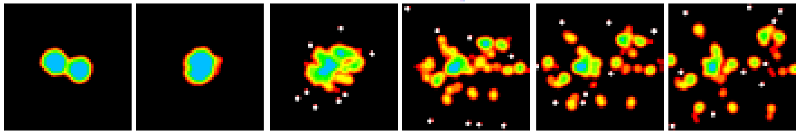
Nuclear fission by Antisymmetrized Molecular Dynamics: AMD

- Even though the Langevin-model description gives satisfactory results in many aspects of nuclear fission, it has only 3 to 4 degrees-of-freedom to express nuclear shape. It should be better to have ways to describe the nuclear fission by microscopic theories having d.o.f. of all the nucleons
- AMD is a very successful microscopic model of nuclear reactions and structures (A. Ono et al, Prog. Theor. Phys.,87(5),(1992), 1185-1206)

Binding Energy$(N, Z) - 8A$ MeV



Xe + Sn at 50 MeV/u, $0 \leq b \leq 4$ fm



Charge distribution