Nuclear Fission Dynamics 2019

2019.10.31 @ YITP

Theoretical study on Z=120 super-heavy element synthesis with time-dependent mean-field models

S. Ebata, S.Chiba, F. Ivanyuk, V. Litnevsky

Tokyo Institute of Technology

Key words:
Super-heavy element,
Fusion, TDMF calculation

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Charge polarization of fission products deduced from the microscopic calculation

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[1]Nuclear Data Section, IAEA

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Fusion, Fission, Charge Polarization
MF calculation

Contents

1, Fission : Charge polarization of fission products

2, Fusion : Super-heavy element synthesis w/ Z=120

Physical quantities demands on
Nuclear physics, Nuclear engineering, Nuclear astrophysics, etc.
(Nuclear dynamics, Fission fragments, EoS, etc.)

Mean-field calculation based on the energy density functional theory

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Charge polarization of fission products deduced from the microscopic calculation

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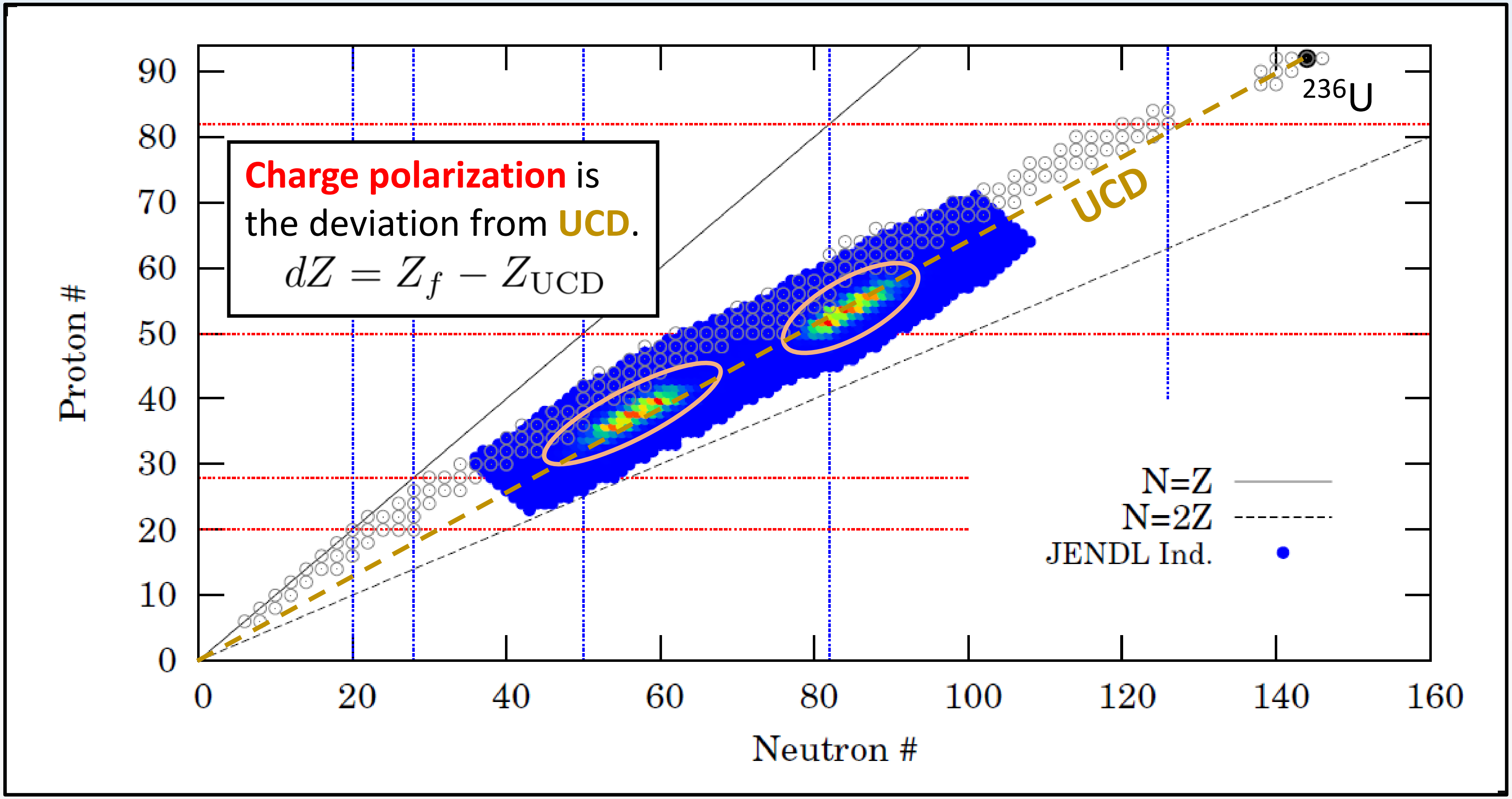
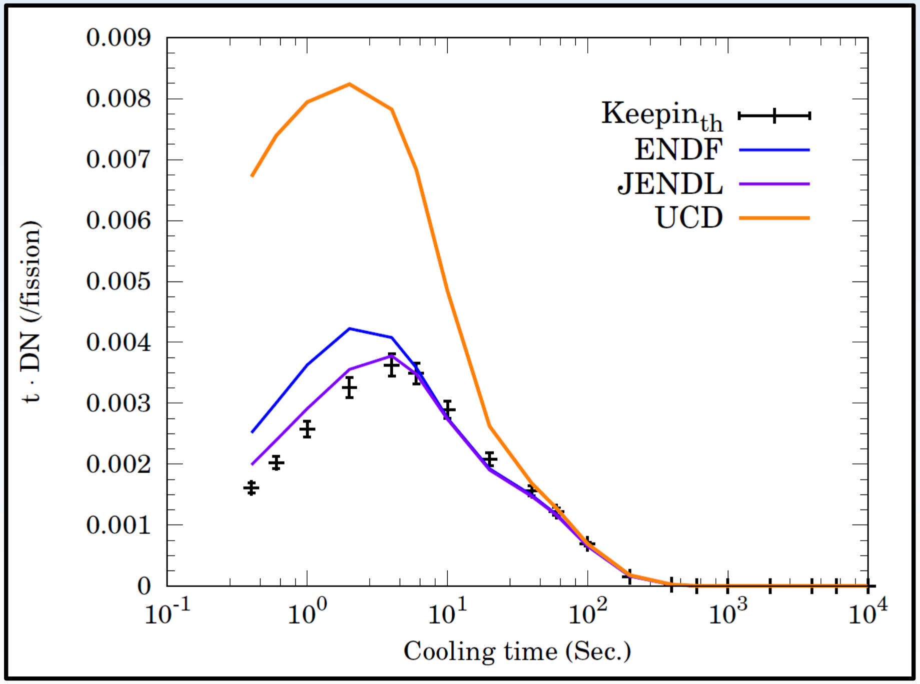
Background: Charge polarization of fission products (FPs)

Charge distribution of FPs (e.g. $^{235}U(n_{th},f)$) & UCD(Unchanged Charge Distribution) assumption



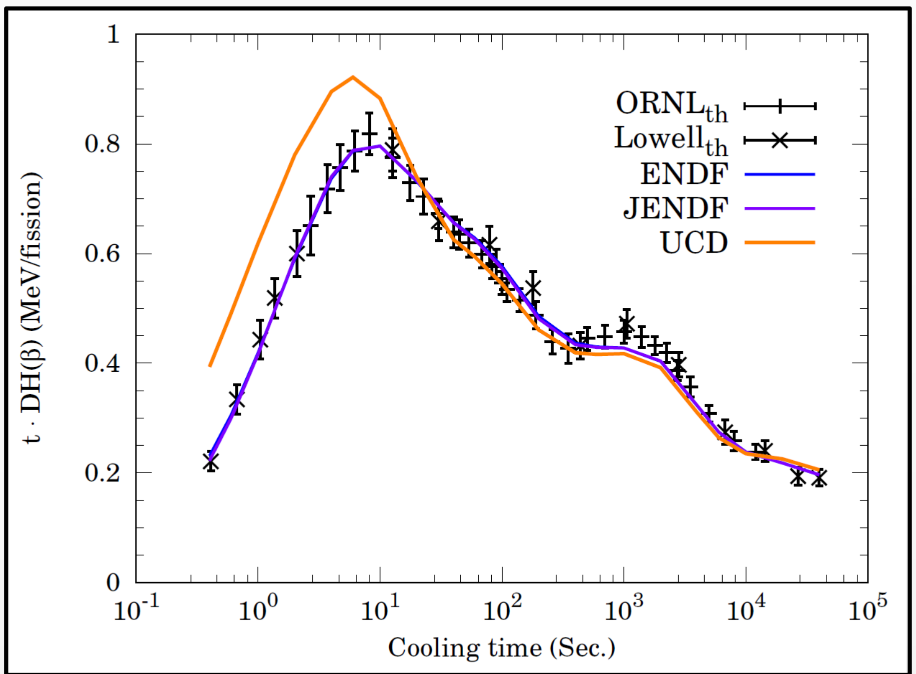
- ✓ The charge distribution is important to simulate yields from FPs.
- ➢ Although the typical amplitude of the charge polarization (CP) is from about 0.5 to 1.0, it results in the several times of yields (delayed neutron, decay heat, etc.).

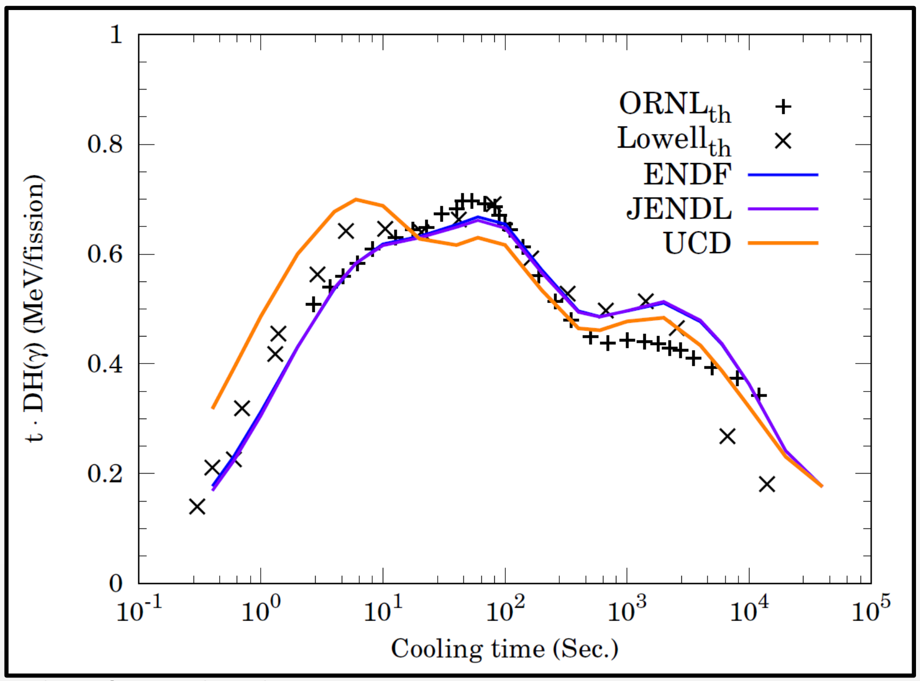
Cal. w/ UCD assumption vs. Exp. data (Delayed Neutron & Decay heats)



The peak positions in decay-heat time-evolution are shifted.

The delayed neutron yield is several times overestimated.
It indicates a danger phase in nuclear reactor operation.





Background: Charge polarization (CP) of FPs

How to prepare the CP in the nuclear engineering? → Using the library: **Wahl's systematics**

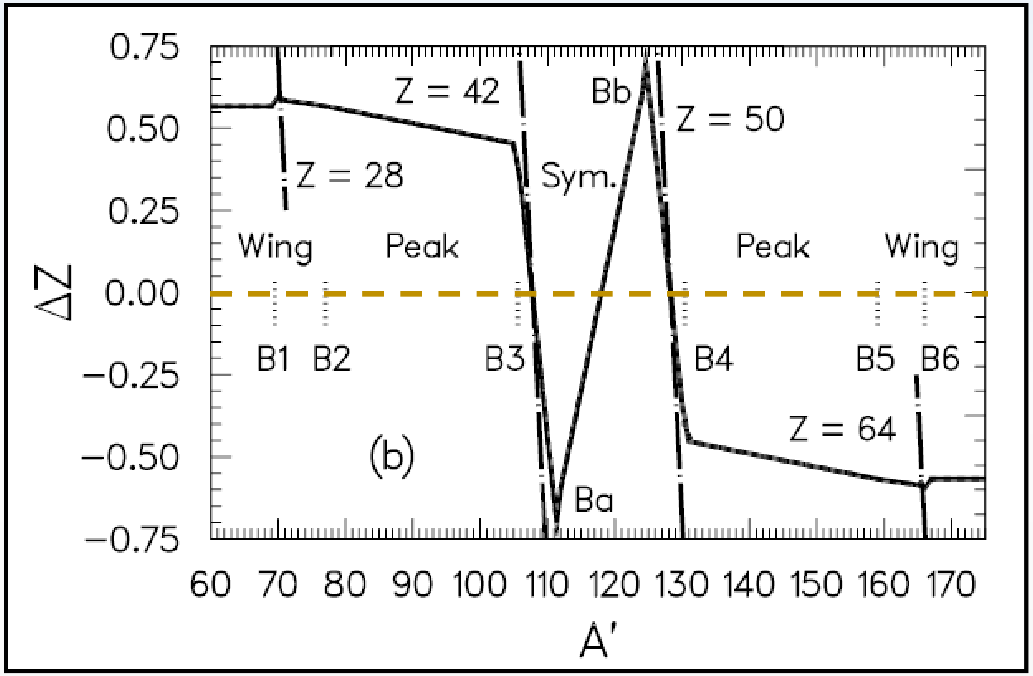
The CP in Wahl's systematics is evaluated to reproduce the measurements (mass yields, and fractional independent yields etc.).

Wahl's systematics: 12 reaction systems are related to the nuclear reactor physics.

→ Limitation of applicable system.

→ No support of nuclear physics.

CP of $^{235}U(n_{th},f)$ compiled in Wahl's systematics



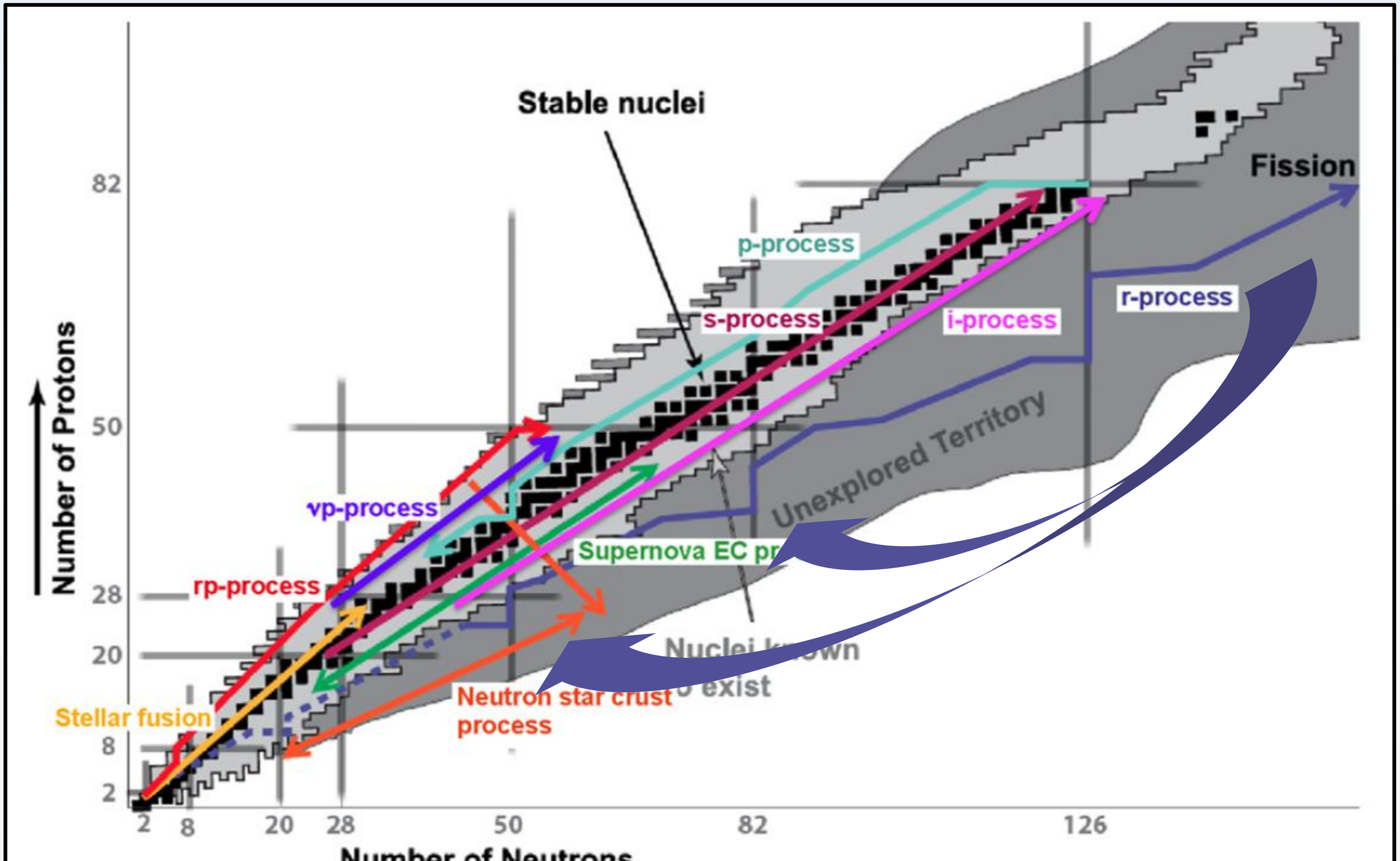
Taken from Arthur C. Wahl, LA-13928, 2002: (Fig.18)

To estimate the delayed neutron yield, charge distribution, and decay heats of FPs from any fissionable nuclei, the microscopic approach is a promising.

Motivation

- The nuclear fission in r-process contributes to the abundance.
- The distribution of fission products is important to decide recycling points.

→ **Charge distribution of fission products from any fissionable nuclei**



Taken from H. Schatz, J. Phys. G 43 (2016) 064001, Fig.1.

Method

Full self-consistent 3D Skyrme HF+BCS
S.E. et al., Phys. Rev. C**82**(2010) 034306.

Interaction (*ph*) : Skyrme (SkM*),

(*pp*, *hh*) : Constant (monopole)

$$\Delta_k(t) = \sum_{l>0} G_{kl}\kappa_l(t) \quad G_{kl} = g f(\epsilon_k^0) f(\epsilon_l^0)$$

$f(\epsilon)$: cutoff function

ϵ_k^0 : s.p. energy at g.s.

3D constrained Skyrme HF+BCS
S.E. and T.Nakatsukasa, Phys. Scr. **92** (2017) 064005.

Adding constraints term to s.p. Hamiltonian,

$$\propto \left(\langle\hat{Q}\rangle - q\right)^2$$

$\hat{Q}$: constraint operator

q : required value

Quadrupole ($l=2, m=0$) &
Octupole ($l=3, m=0$) operators are prepared.

$$\hat{Q}_{l0} = \hat{r}^l \hat{Y}_{l0}$$

(Our) **Definition of Quadrupole & Octupole moment**

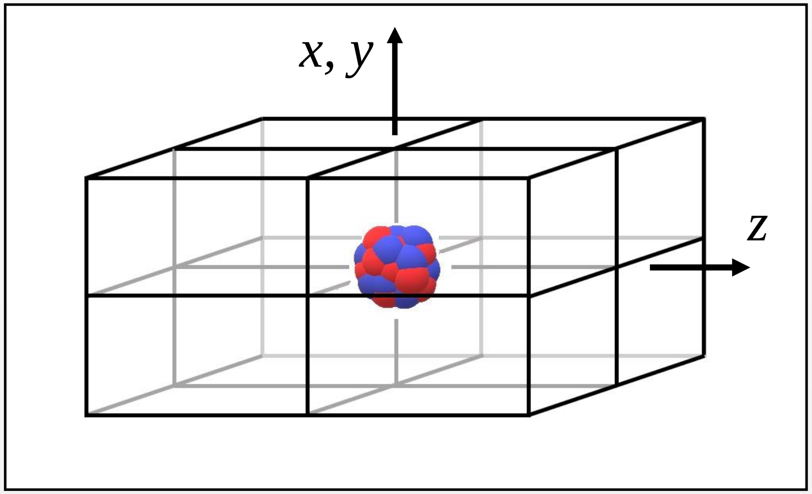
$$Q_{20} = \langle \hat{r}^2 \hat{Y}_{20}\rangle = \sqrt{\frac{5}{16\pi}}\langle 2\hat{z}^2 - \hat{x}^2 - \hat{y}^2\rangle$$

$$Q_{30} = \langle \hat{r}^3 \hat{Y}_{30}\rangle = \sqrt{\frac{7}{16\pi}}\langle 2\hat{z}^3 - 3\hat{x}^2\hat{z} - 3\hat{y}^2\hat{z}\rangle$$

(other) $Q_2 = \langle 2\hat{r}^2 \hat{P}_2\rangle$ By H.Flocard, et al., Nucl. Phys. A**231**(1970)176.

$$Q_2 = \sqrt{\frac{16\pi}{5}} Q_{20} \sim 3.17 Q_{20}$$

Calculation space (3D Cartesian coordinate)



Range of Cal. space:
x, y [-20:20] fm, z [-25:25] or z [-30:30] fm
Mesh size: 1.0 fm

Constraint ranges for Q_{20} & Q_{30}:
Q_{20} [500 : 12,500] fm^2, Q_{30} [0 : 65,000] fm^3 or
Q_{20} [435 : 20,445] fm^2, Q_{30} [0 : 80,000] fm^3

Q_{20} & Q_{30} of ^{236}U g.s.
Q_{20} = 870 fm^2, Q_{30} = 0.00 fm^3

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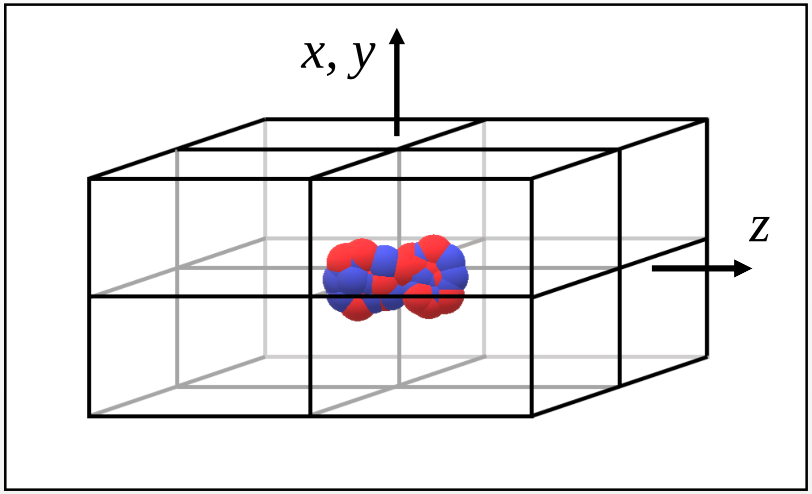

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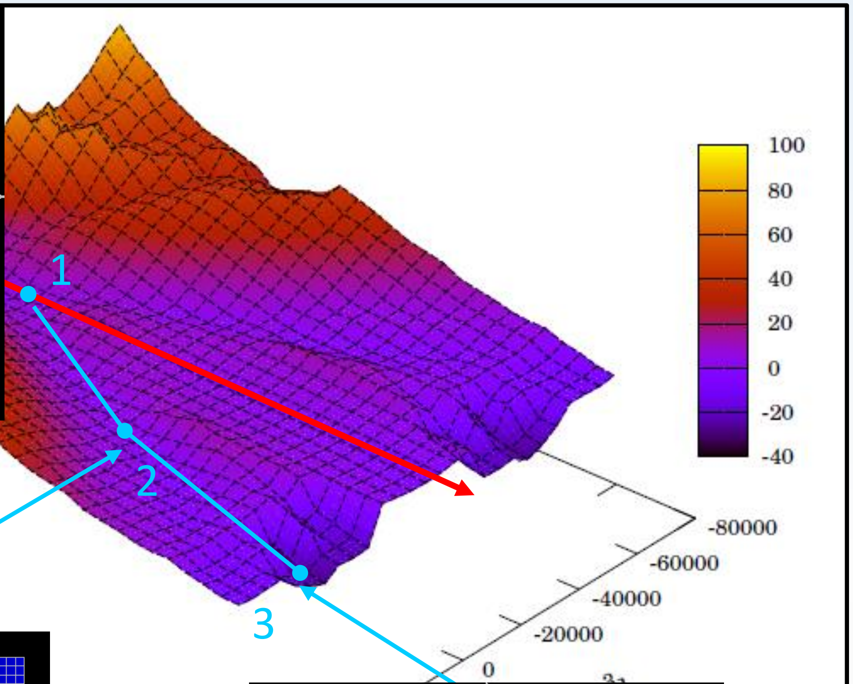
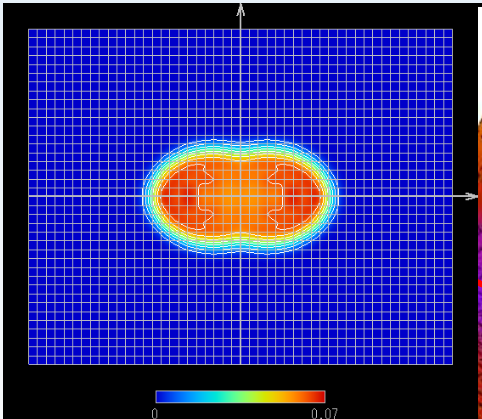
Q_{20} & Q_{30} of ^{236}U g.s.
Q_{20} = 870 fm^2, Q_{30} = 0.00 fm^3

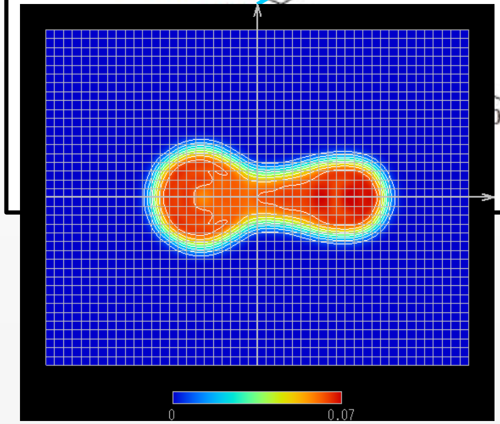
Results: ^{236}U Potential Energy Surface w.r.t Q_{20}, Q_{30}

Potential energy surface (Q_{20}-Q_{30}-dE) w/ SkM*

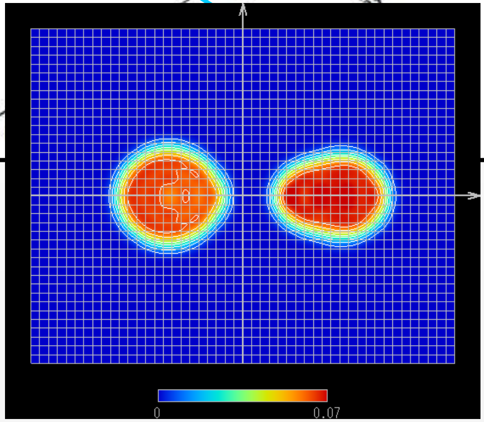




Proton density distribution@1
Q_{20} = 2610 [fm^2], Q_{30} = 0 [fm^3]

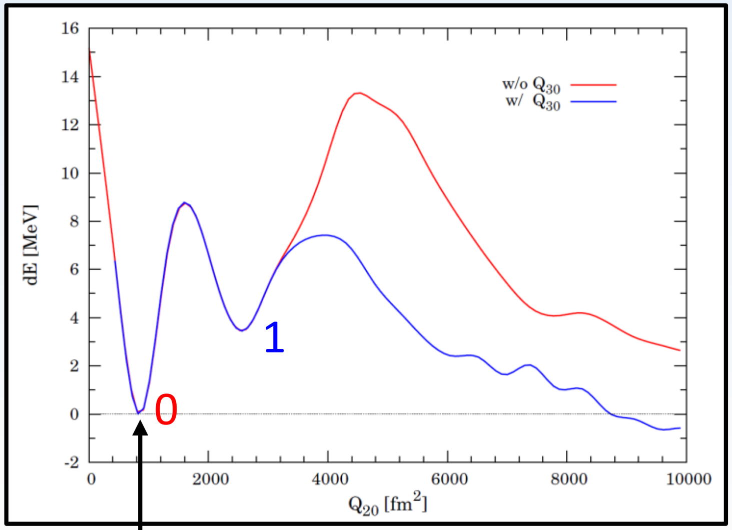


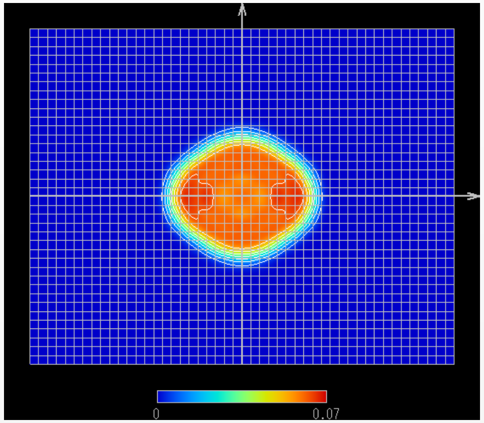
Proton density distribution@2
Q_{20} = 7830 [fm^2], Q_{30} = 30000 [fm^3]



Proton density distribution@3
Q_{20} = 13050 [fm^2], Q_{30} = 40000 [fm^3]

Potential energy surface (Q_{20}-dE)

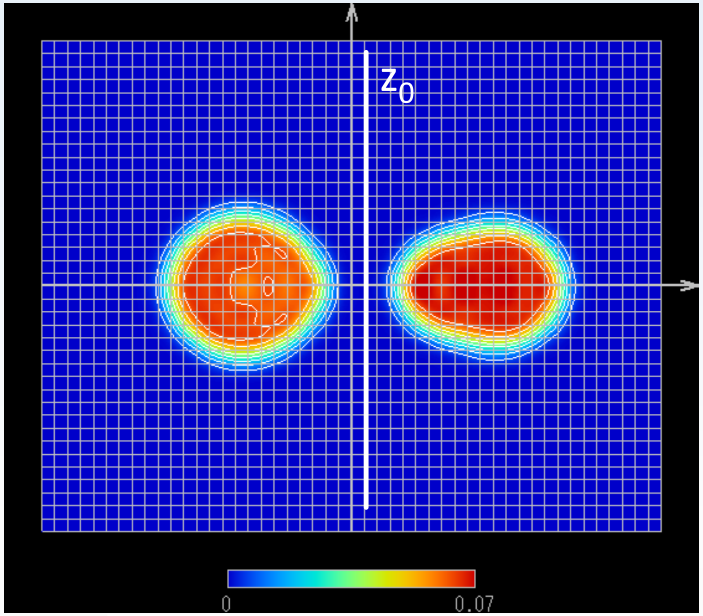




Proton density distribution@0
Q_{20} = 870 [fm^2], Q_{30} = 0 [fm^3]

Results: How to calculate the CP

$$dZ = Z_f - Z_{\mathrm{UCD}}(A_f),\ Z_{\mathrm{UCD}}(A_f) = \frac{92}{236}A_f \sim 0.4A_f$$



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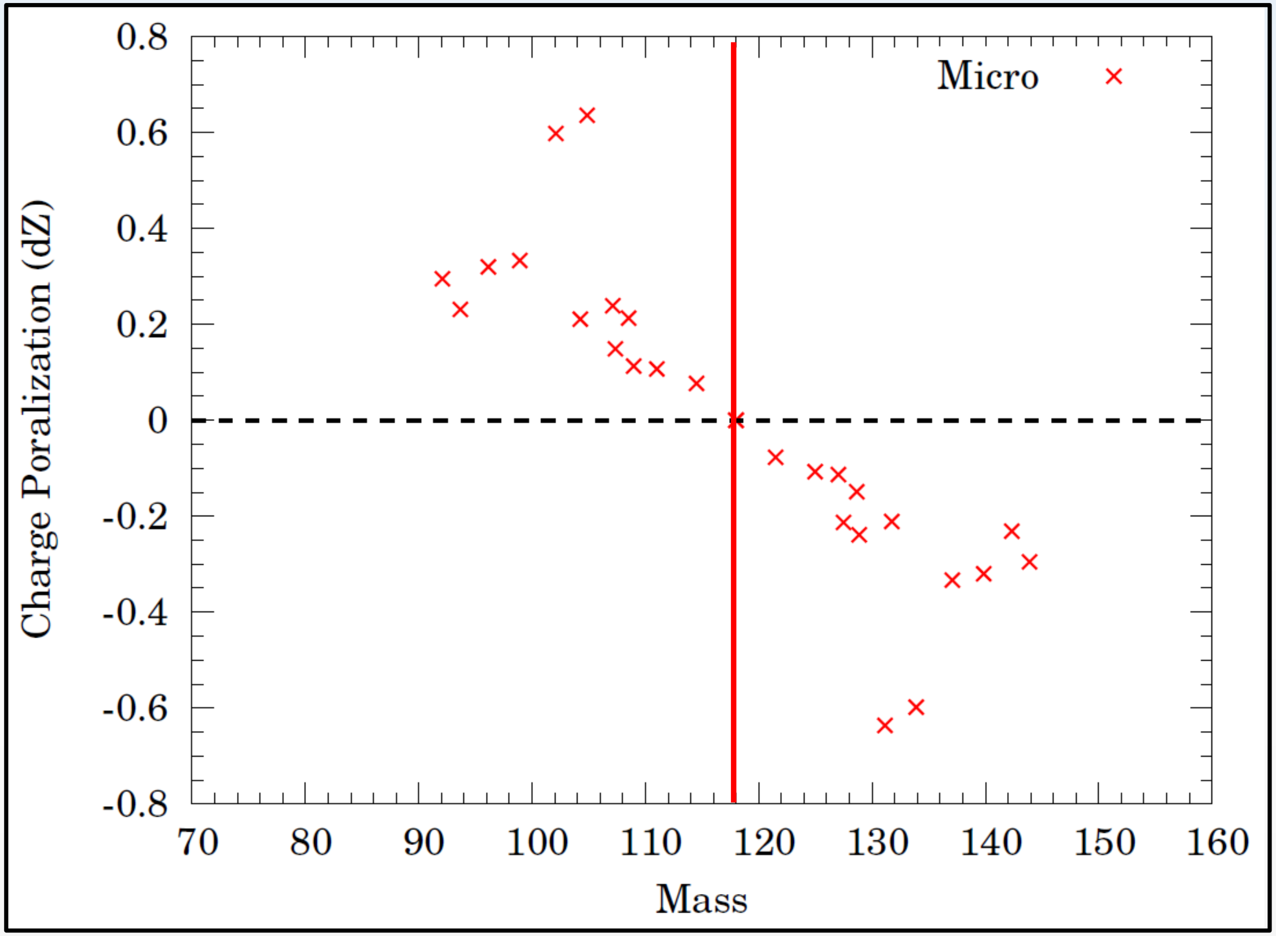


Left and Right regions are defined by the Z_0 at where the neck radius is smallest.

$$N_L^\tau = \int_{-Z}^{z_0} d\boldsymbol{r}\rho_\tau(\boldsymbol{r}) \quad N_R^\tau = \int_{z_0}^{Z} d\boldsymbol{r}\rho_\tau(\boldsymbol{r})$$

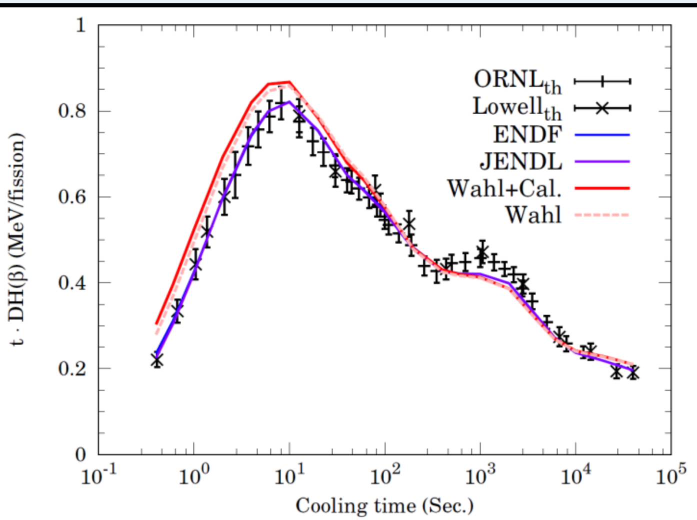
$$\tau = p \text{ or } n$$

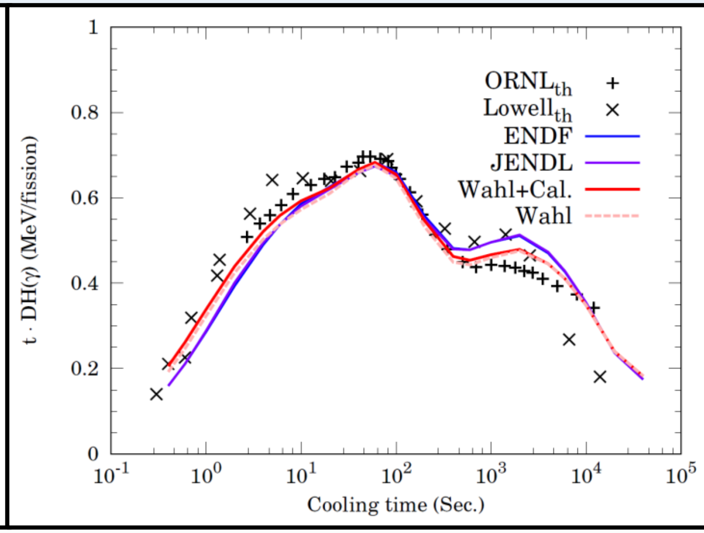
$$A_f^{L(R)} = N_{L(R)}^n + N_{L(R)}^p$$

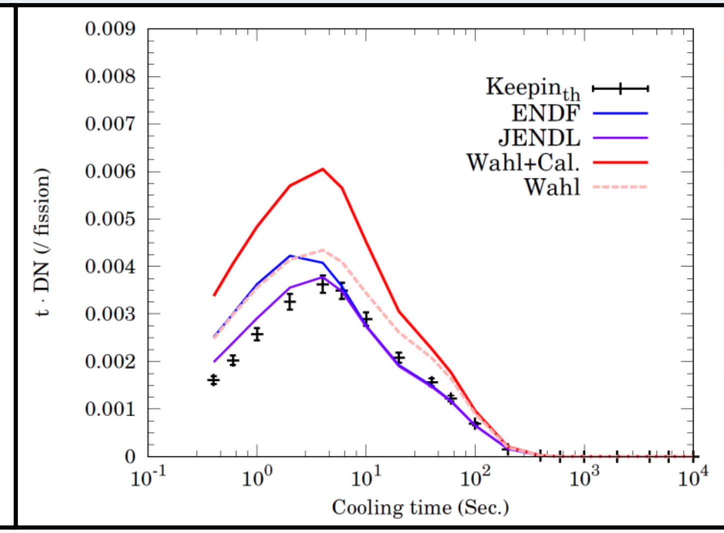
- ✓ The charge polarization appears in the mean-field Cal.
- ✓ The peaks around A=130 have Z=50.0,51.7, N=78.98, 81.78 which indicates the shell effects.

Results: Decay heats, Delayed neutron yields through the Hauser-Feshbach Cal.

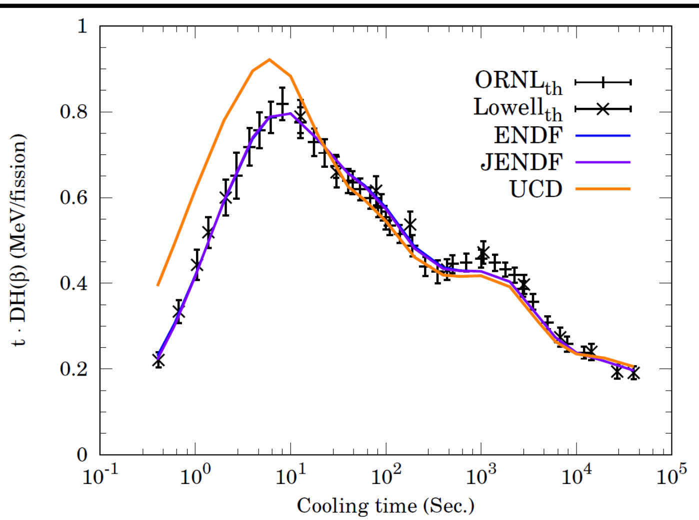
w/ MF results

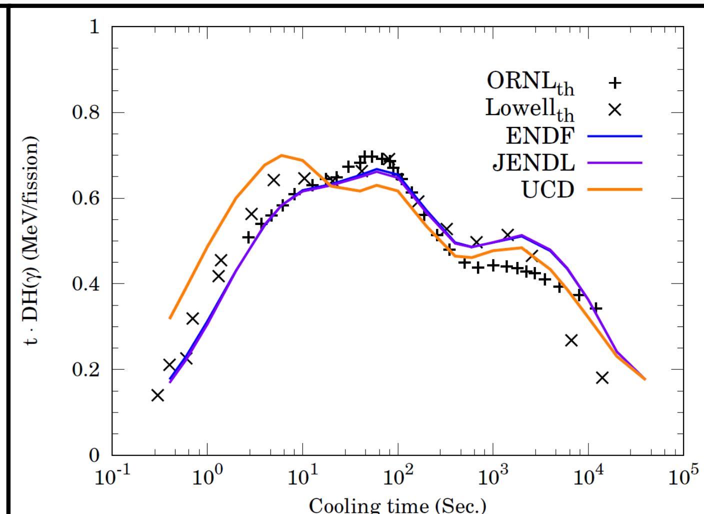


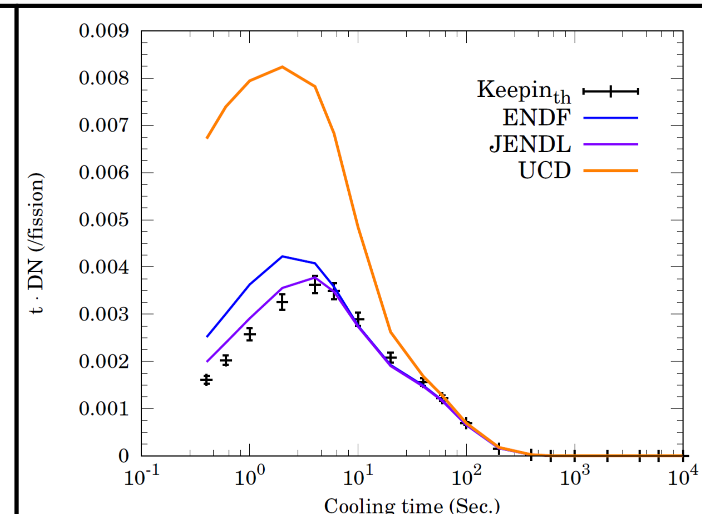




w/ UCD







Summary (Fission : Charge polarization of fission products)

- ✓ We investigate the potential energy surface of ^{236}U, (^{240}Pu, ^{250}Cf) w.r.t Q_{20} and Q_{30} using the constraint 3D Skyrme HF+BCS w/ SkM*.
  - ✓ The nucleon density distributions at the scissions are investigated and, the charge distribution is estimated.
- ✓ The CP is appeared in MF Cal., which indicates the nuclear shell effects.

  ^{236}U: The behavior around the symmetry fission is different from it in Wahl's systematics, although its amplitude is comparable with.
  The yields (delayed neutron, decay heats) through the statistic model using the CP, are not so bad.

Future work

- ➢ Apply to more neutron-rich nuclei(e.g. ^{276}U (N=184))
  - ➢ Number projection
    - ➢ Energy, Neutron number, Pairing functional, Interaction dependence

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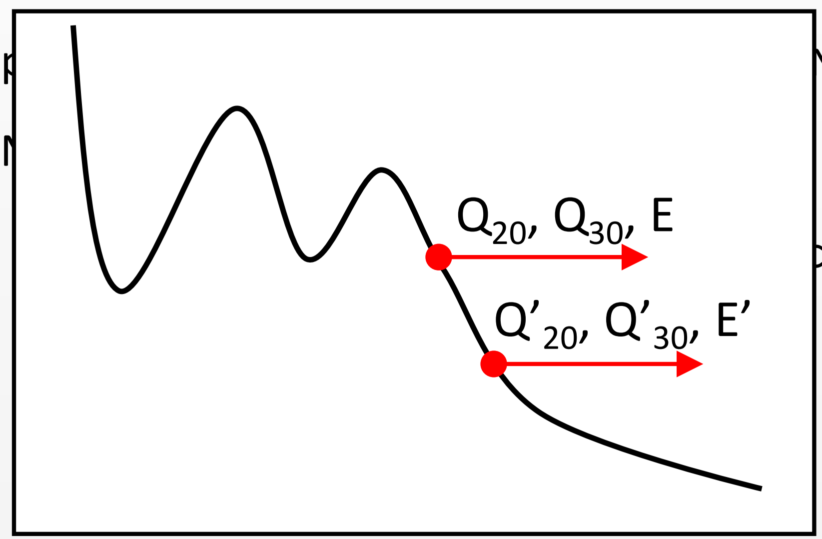
Future work

- App N=184))
  - N

ctional, Interaction dependence



Time-dependent model Cal. with several initial states at the outer barrier configurations.

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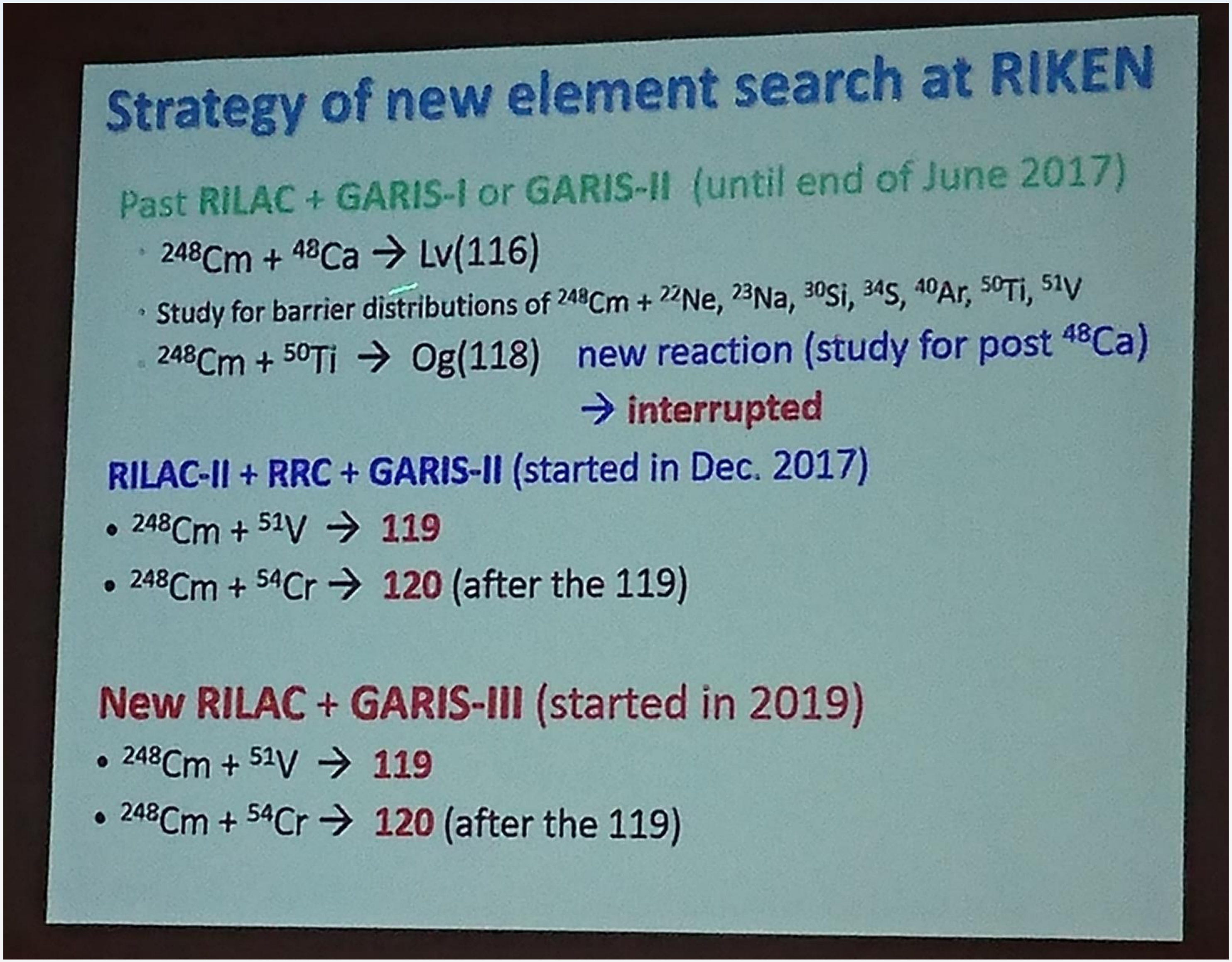
Introduction

30th Nov. 2016

RIKEN http://www.nishina.riken.jp/113

Beyond Nh (Og)!!

Z=120 SHE formation: RIKEN project

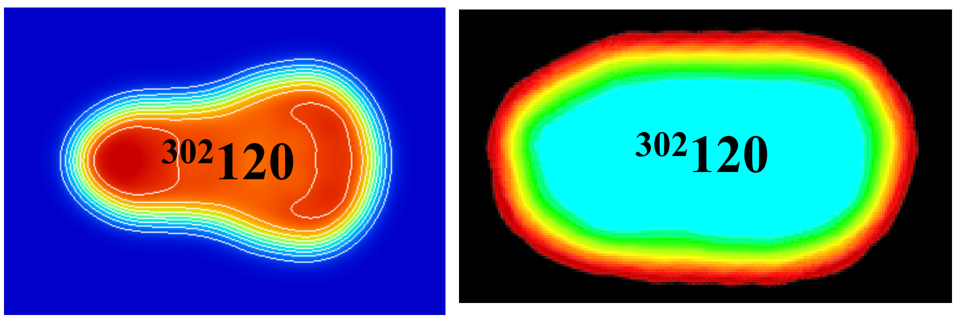


Taken from S. Chiba presentation

Motivation

- To simulate a synthesis process of the super-heavy element and to deduce the synthesis probability P_{SHE} using theoretical methods.
- In order to construct the hybrid model including suitable methods to describe the processes on **touching**, **fusion**, **compound formation** and **evaporation**, to simulate the synthesis process.

Touching process P_{touch}

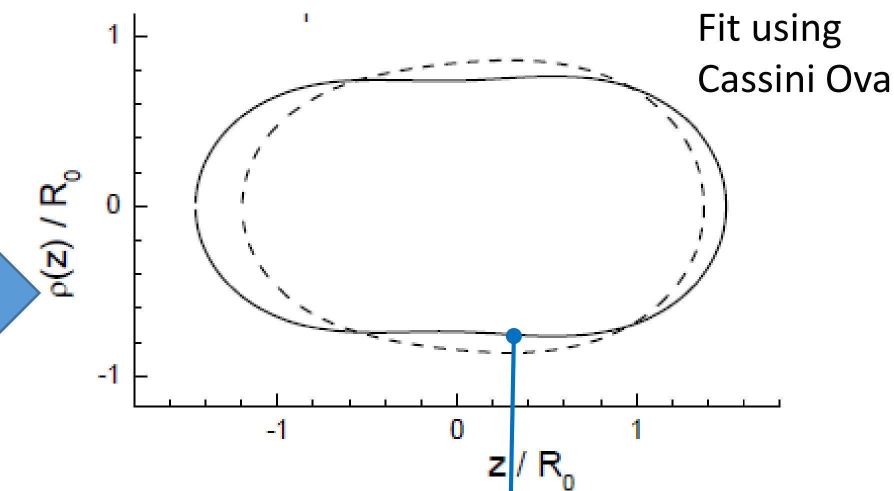


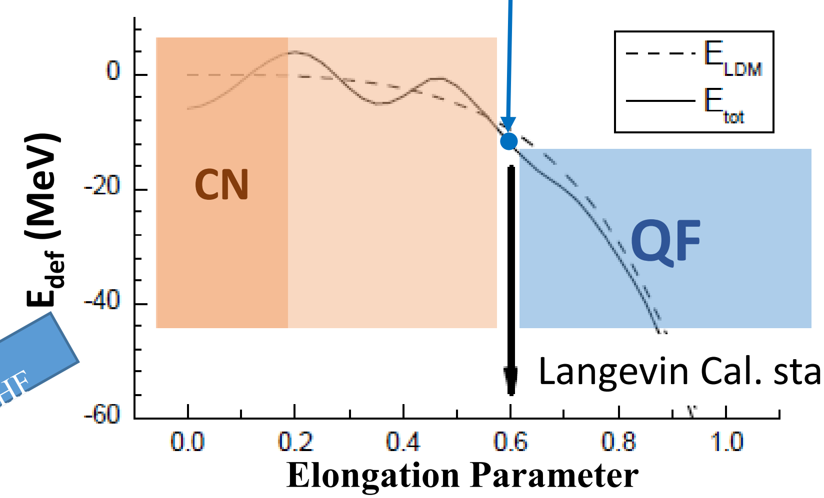
Cb-TDHFB, AMD

Shape profile

Compound & Quasi-fission P_{CNF}

3D or 4D Langevin w/ neutron evaporation





P CHF

Hauser-Feshbach decay P_{survive}

$$P_{\mathrm{survive}} = \frac{\displaystyle\sum_{D=\{n,\gamma\}:l,j} \int_0^{E_{D\max}} \rho(E^* - S_D - E_D, J^\pi) T^J_{D,l,j}(E_D) dE_D}{\displaystyle\sum_{D'=\{\cdots\}:l,j} \int_0^{E_{D'\max}} \rho(E^* - S_{D'} - E_{D'}, J^\pi) T^J_{D',l,j}(E_{D'}) dE_{D'}}$$

Decay mode: $D' = \{n, p, t, {}^3\mathrm{He}, \alpha, \gamma, F\}$

HFBTHO + BeoH
spin & parity

Synthesis probability: $P_{\mathrm{SHE}} = P_{\mathrm{touch}} \cdot P_{\mathrm{survive}} \cdot P_{\mathrm{CNF}}$

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- To simulate a synthesis process of the super-heavy element and to deduce the synthesis probability P_{SHE} using theoretical methods.
- In order to construct the hybrid model including suitable methods to describe the processes on **touching**, **fusion**, **compound formation** and **evaporation**, to simulate the synthesis process.

  - Physical quantities on **the touching process** described a microscopic method.
  - We apply the time-dependent mean-field theory to ^{248}Cm+^{54}Cr, and acquire experience on the super-heavy element (Z=120) synthesis.

Purpose of this work

We show the calculations of ^{248}Cm+^{54}Cr fusion reaction using
the **canonical-basis time-dependent Hartree-Fock-Bogoliubov** (**Cb-TDHFB**) theory,
to check the **nucleon densities** and **energy balance** on the dynamics,
for more accurate simulation, this is one of benchmark calculation.

Method Time-dependent density functional theory

Cb-TDHFB S.E. et al., Phys. Rev. C**82**(2010) 034306, S.E. and T.Nakatsukasa, JPS Conf. Proc. **6**, 020056 (2015)

Interaction (*ph*) : Skyrme (SkM* w/o Center of Mass correction),

(*pp*, *hh*) : delta-function $V^{\tau}(\boldsymbol{r}_1,\sigma_1;\boldsymbol{r}_2,\sigma_2) = V^{\tau}_{pair}\frac{1-\hat{\sigma}_1\cdot\hat{\sigma}_2}{4}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$ $\Delta_l(t) = -\sum_{k>0}\kappa_k(t)V_{l\bar{l}k\bar{k}}(t)$

Cb-TDHFB equations

$$i\hbar\frac{\partial}{\partial t}|\phi_k(t)\rangle = \big(h(t)-\eta_k(t)\big)|\phi_k(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}\rho_k(t) = \kappa_k(t)\Delta^*_k(t) - \Delta_k(t)\kappa^*_k(t)$$

$$i\hbar\frac{\partial}{\partial t}\kappa_k(t) = \big(\eta_k(t)+\eta_{\bar{k}}(t)\big)\kappa_k(t) + \Delta_k(t)(2\rho_k(t)-1)$$

Properties of Cb-TDHFB

$$d/dt\langle\phi_k(t)|\phi_{k'}(t)\rangle = 0$$

$$d/dt\langle\hat{N}\rangle = 0,\ d/dtE_{\mathrm{Total}} = 0$$

In the limit of Δ=0 ➡ **TDHF**

In the static limit, ➡ **HF+BCS**

$$\eta_k(t) \equiv \langle\phi_k(t)|h(t)|\phi_k(t)\rangle + i\hbar\left\langle\frac{\partial\phi_k}{\partial t}\middle|\phi_k\right\rangle$$

Subjective reaction system: ^{248}Cm+^{54}Cr → ^{302}120 E_{in} = 300, 310, 320, 330, 340 [MeV]

Pairing strength V_{pair} for target and projectile
are defined to reproduce the Δ^{ν}, Δ^{π} deduced by 3-points formula.
Averaged pairing strength of nuclei is used in the Cb-TDHFB calculation.

e.g. $\Delta^{\nu}_3(N,Z) \equiv \frac{1}{2}(B(N-1,Z)+B(N+1,Z)-2B(N,Z))$

Method Procedure for the reaction calculation

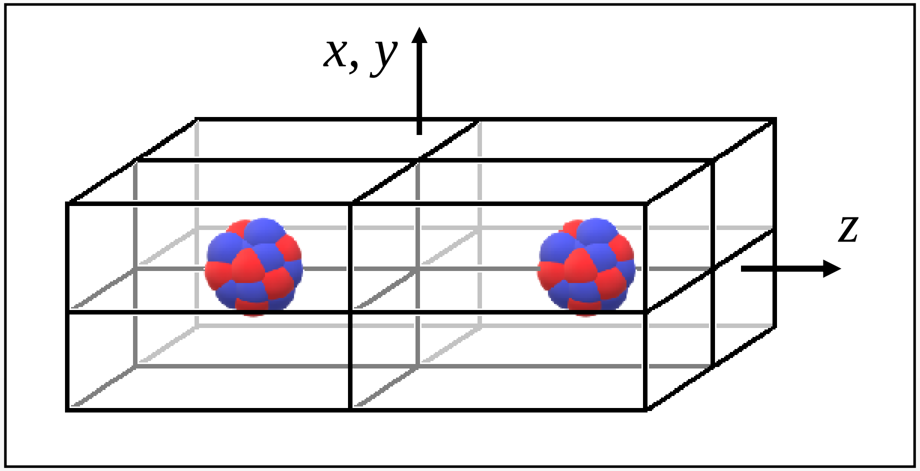
1, Calculate the ground states of ^{248}Cm, ^{54}Cr using 3D Skyrme HF+BCS self-consistently.

2, Set the ^{248}Cm, ^{54}Cr on the points with the distance working Coulomb force dominantly.

3, Boost them with an energy E_{in} considering the incidence from the infinite-point.

4, Calculate the nuclear dynamics with Cb-TDHFB.

Calculation space (3D Cartesian coordinate)



Rectangular box of 30 fm × 30 fm × 60 fm, discretized in the square mesh of $\Delta x = \Delta y = \Delta z = 1.0$ fm

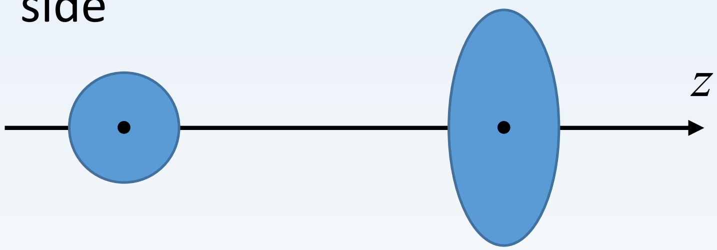
Calculate the head-on collision (*b=0*).

Results (Coulomb barrier height: Frozen Density Approximation)

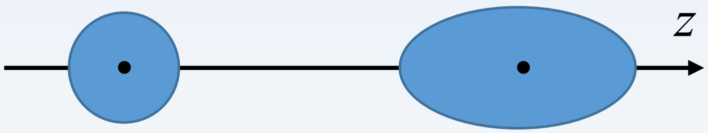
^{248}Cm has quadrupole deformed shape

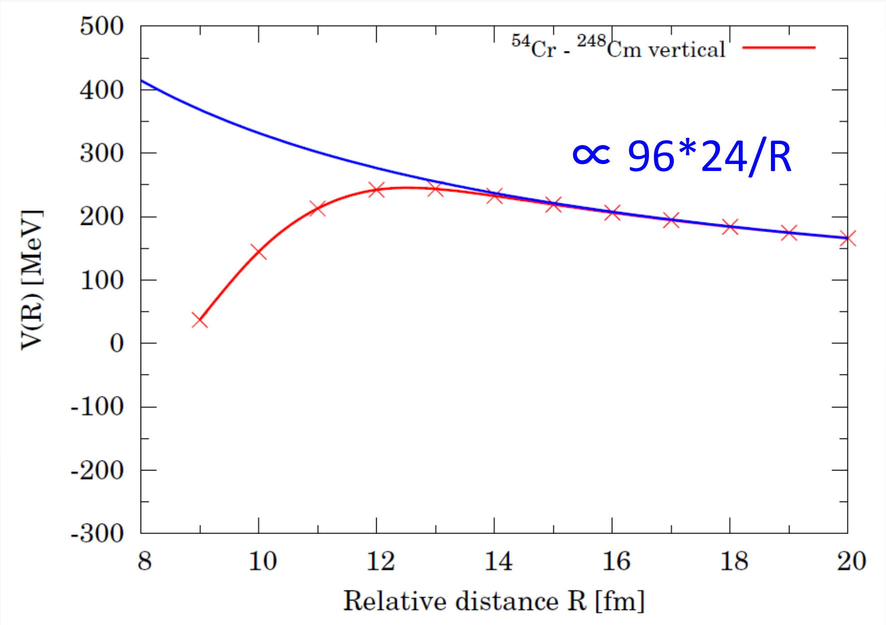
→ The Coulomb barrier heights are different depending on the reaction direction.

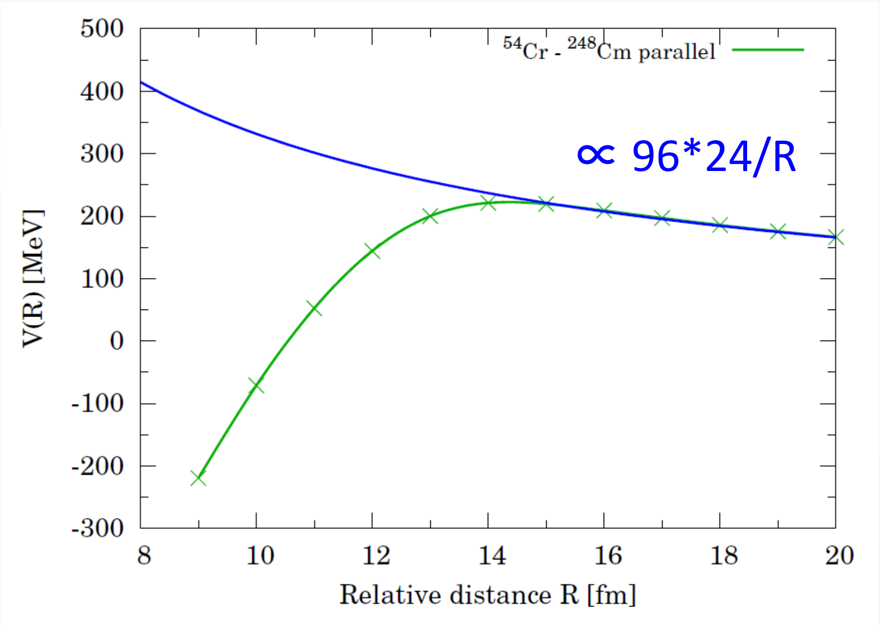
side



tip



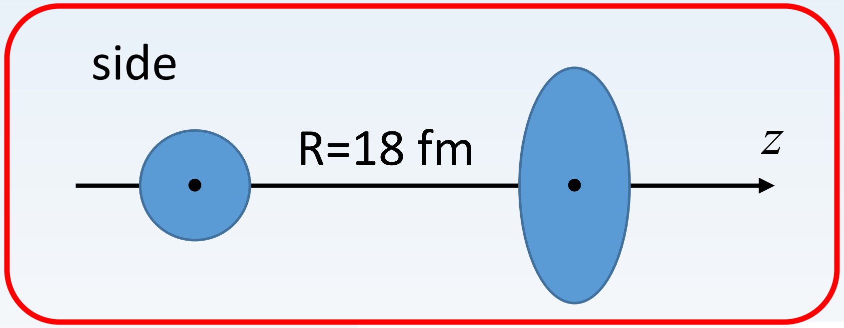


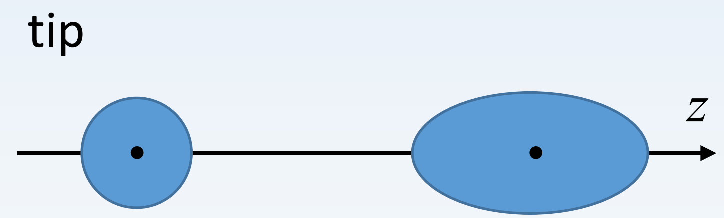


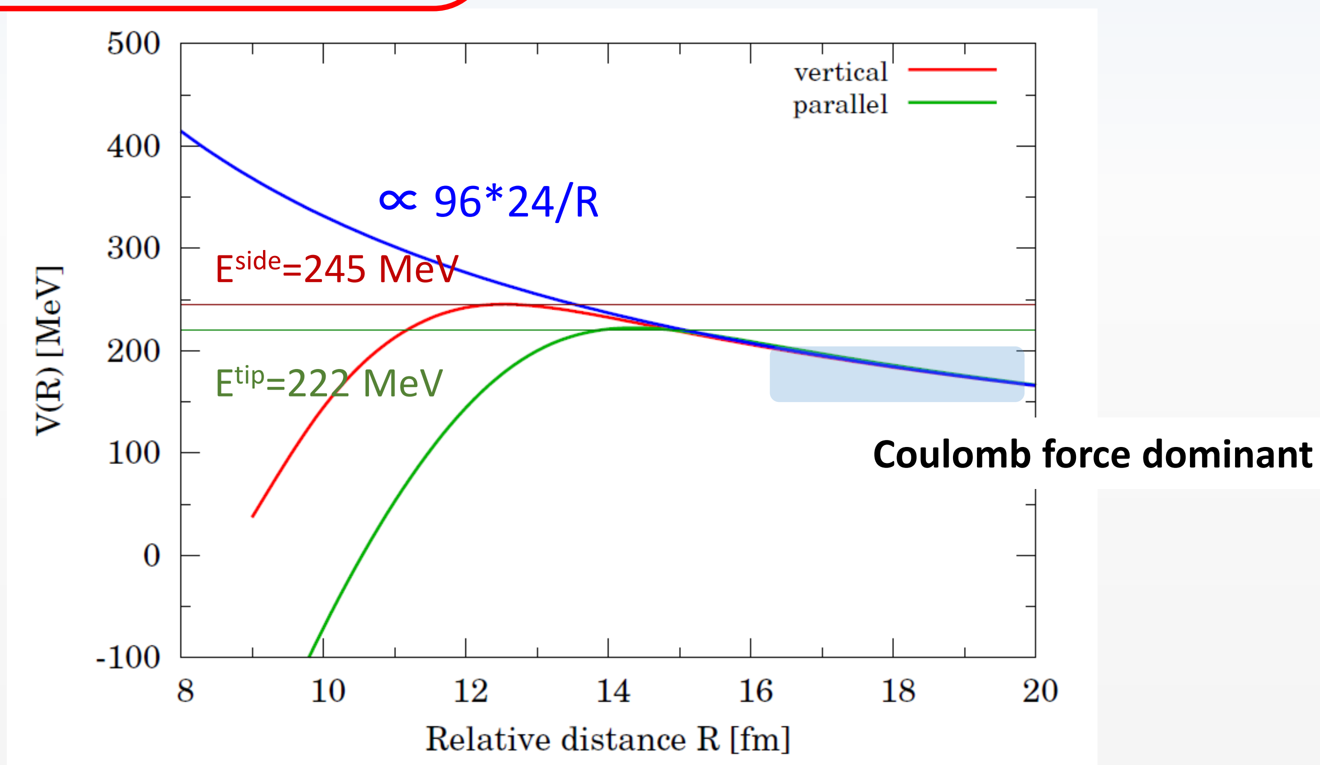
Results (Coulomb barrier height: Frozen Density Approximation)

^{248}Cm has quadrupole deformed shape

→ The Coulomb barrier heights are different depending on the reaction direction.

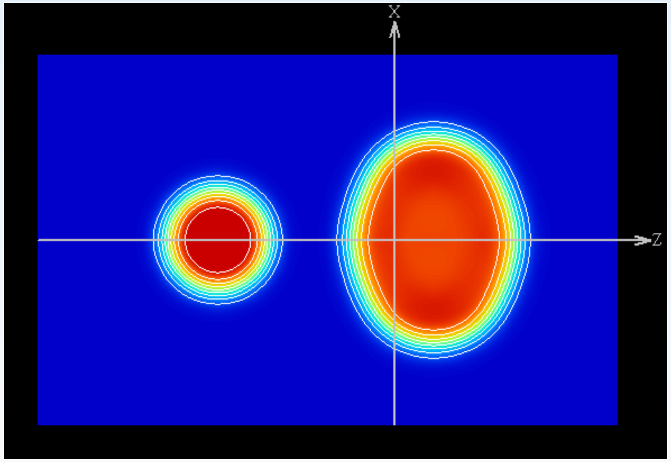




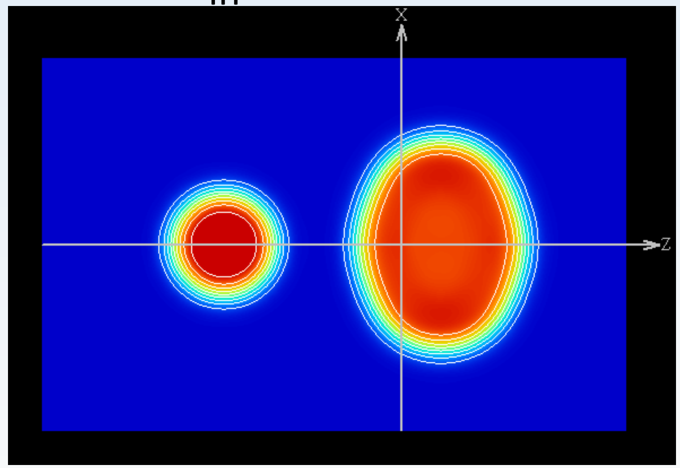


Results (TD Cal. : Nucleon density distribution)

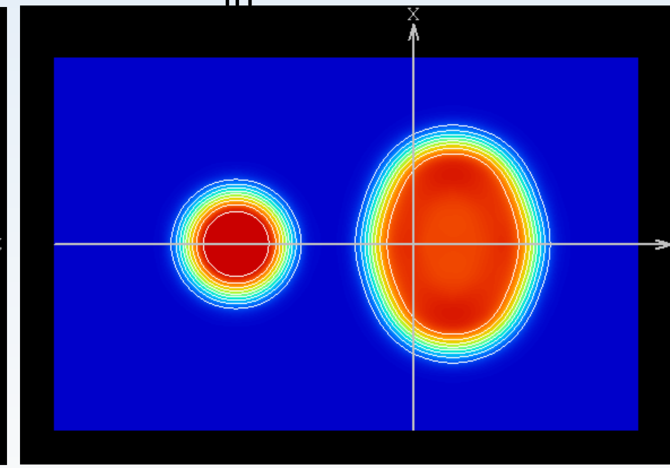
E_{in}=300 MeV



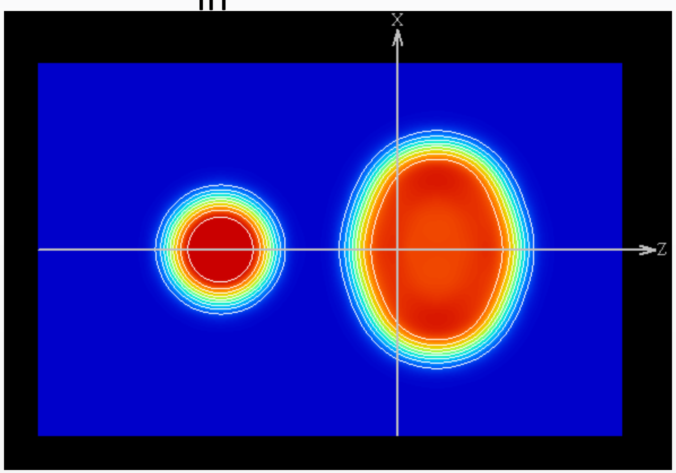
E_{in}=310 MeV



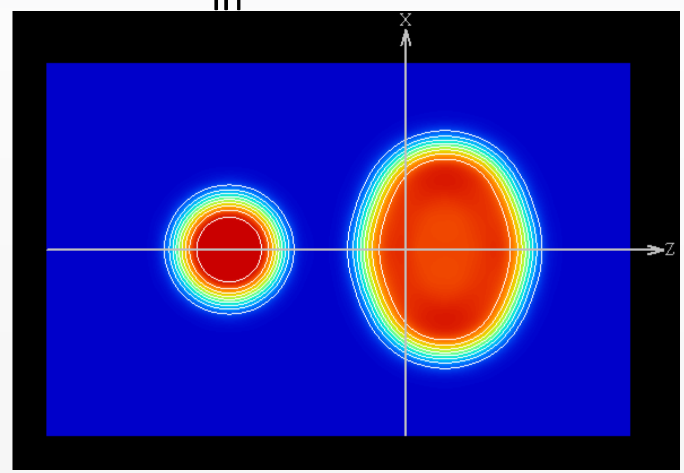
E_{in}=320 MeV



E_{in}=330 MeV

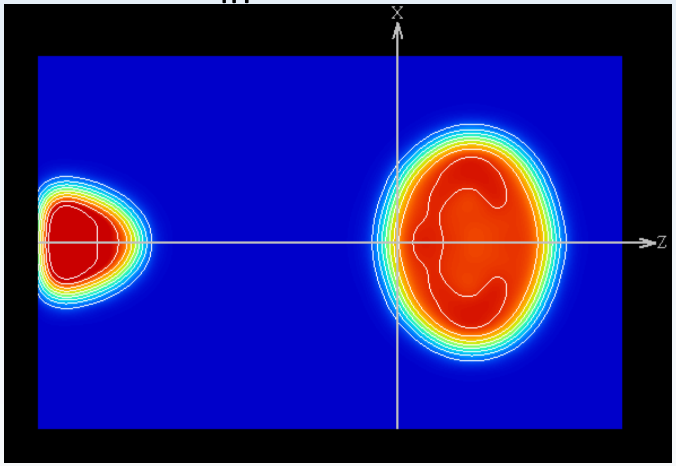


E_{in}=340 MeV

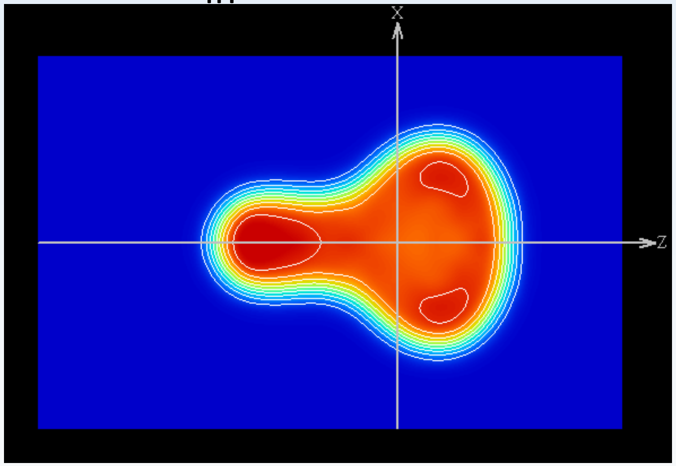


Results (TD Cal. : Nucleon density distribution @ Time#100 ~ 1000 fm/c ~ 30 x10^{-22}s)

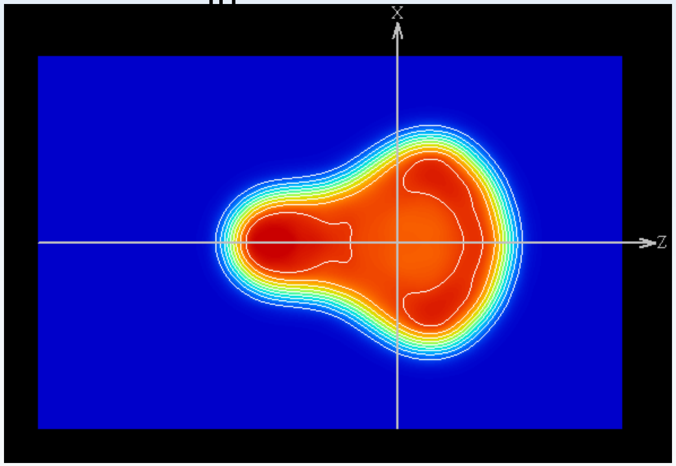
E_{in}=300 MeV



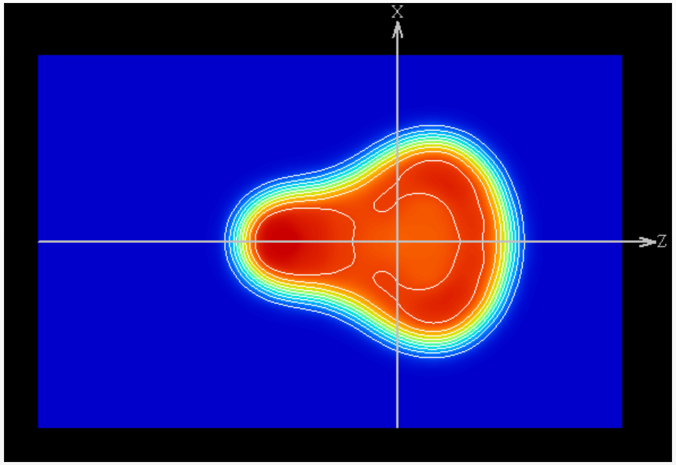
E_{in}=310 MeV



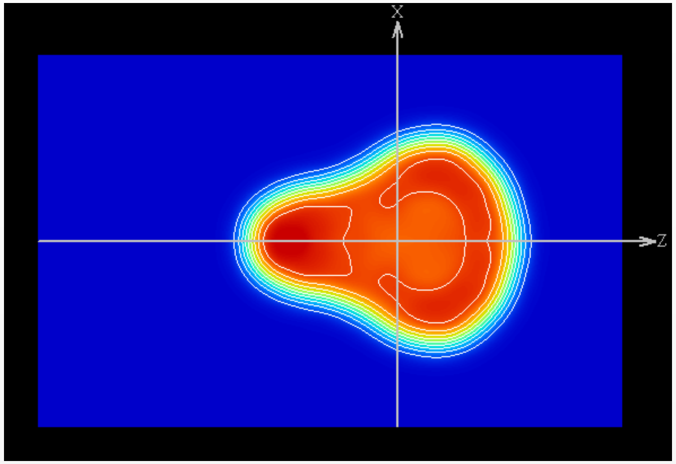
E_{in}=320 MeV



E_{in}=330 MeV

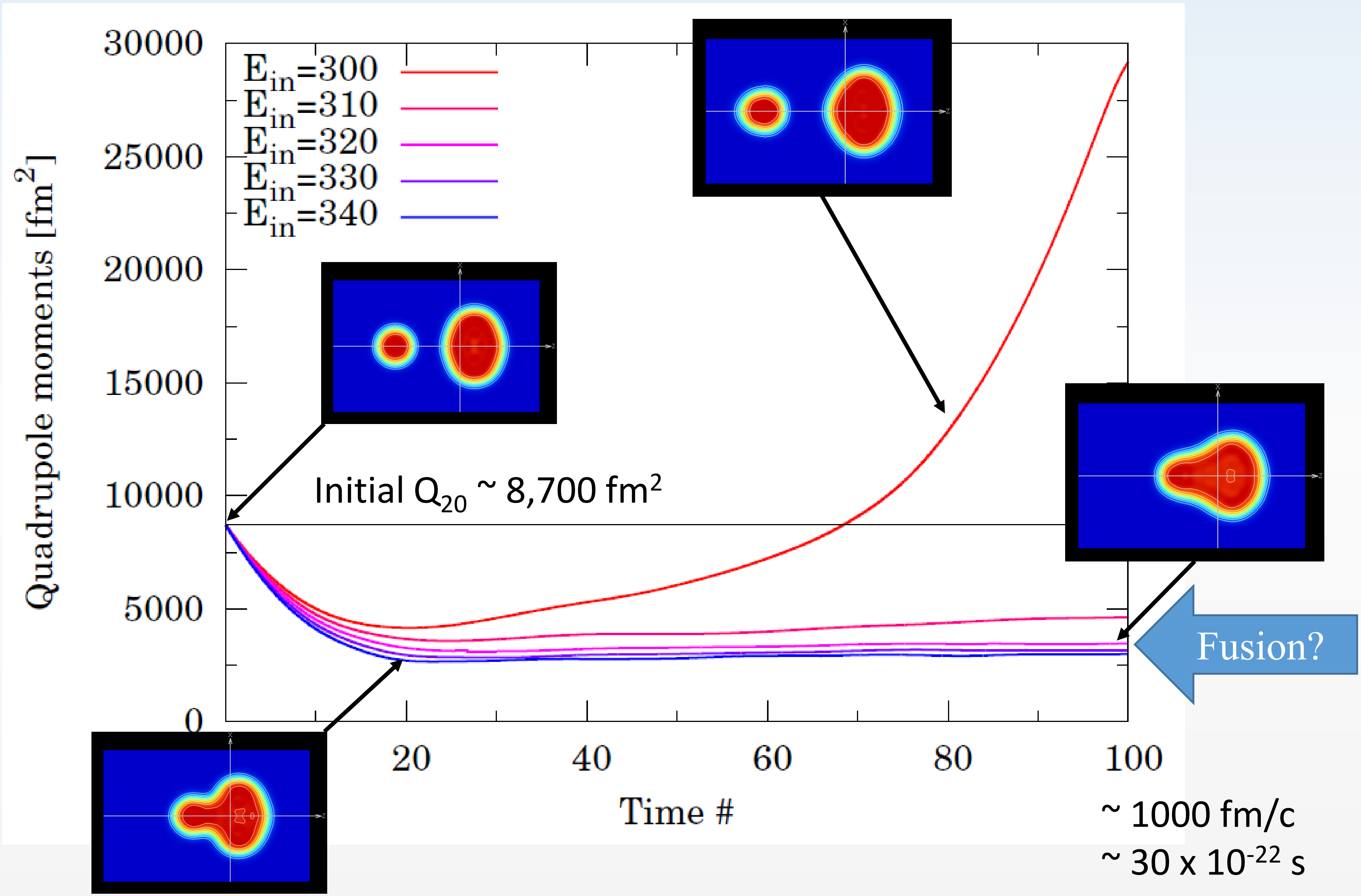


E_{in}=340 MeV



✓ For the fusion, (at least) E_{in} = 310 MeV is necessary. (Coulomb barrier E^{side}=245MeV)

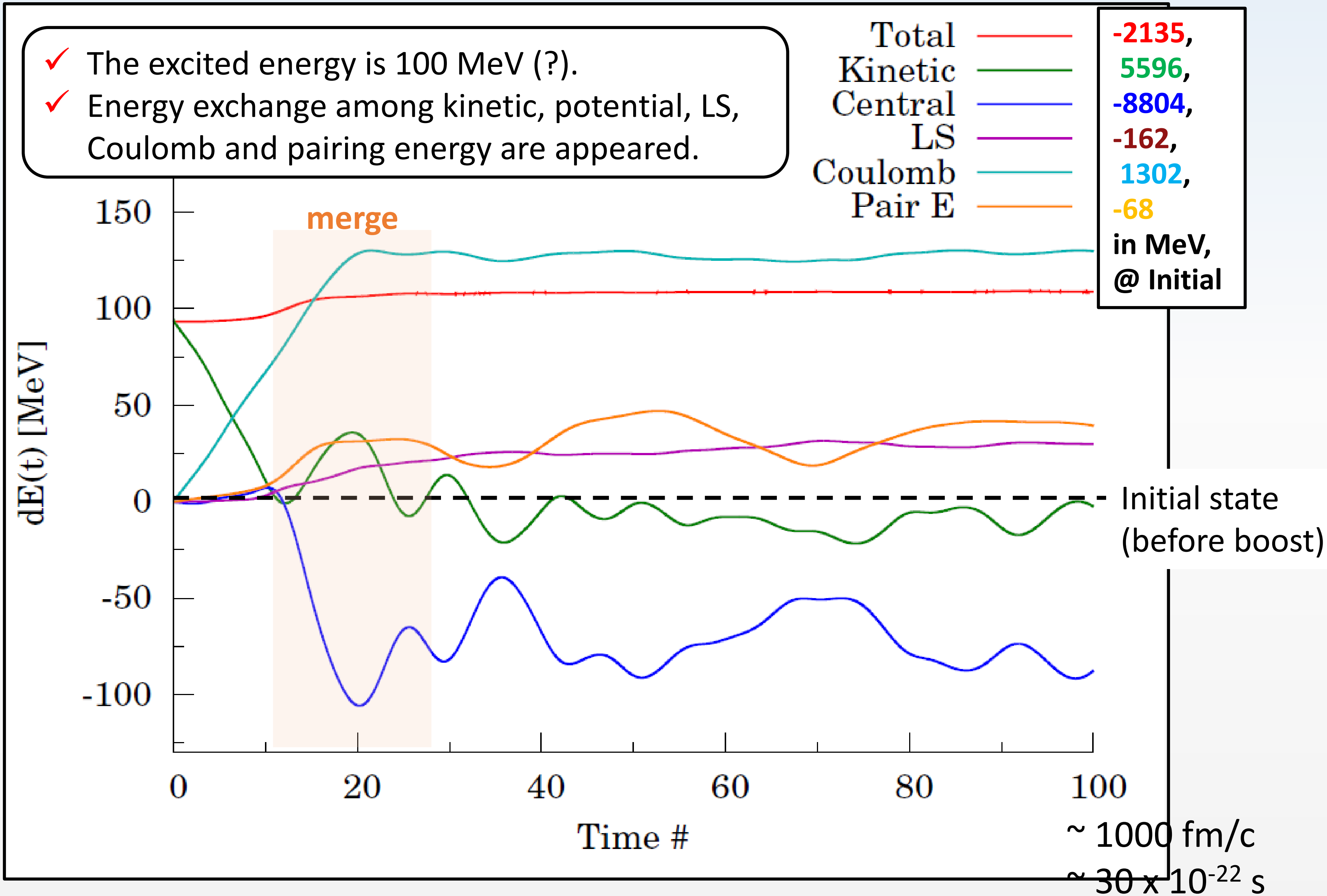
Results (TD Cal. : Quadrupole momentum)



Results (TD Cal. : Energy balance on E_{in}=340MeV reaction)

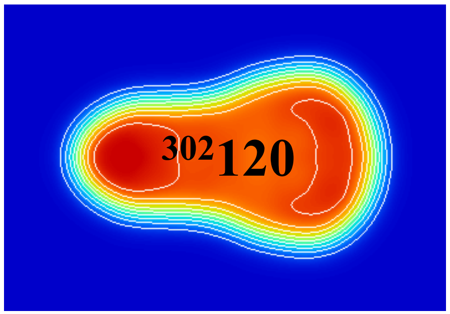
Time-dependence of energy change from initial state $dE_\mu(t) = E_\mu(t) - E_\mu(0^-)$

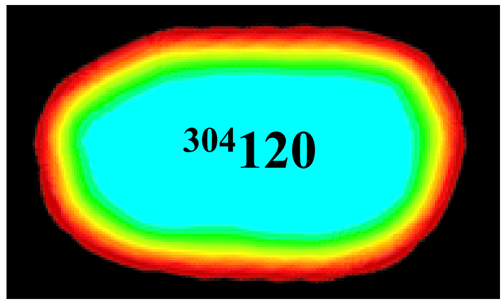
$\mu = \{\mathrm{Total, Kinetic, Central, LS, Coulomb, Pairing}\}$



Again …

Touching process $P_{\rm touch}$



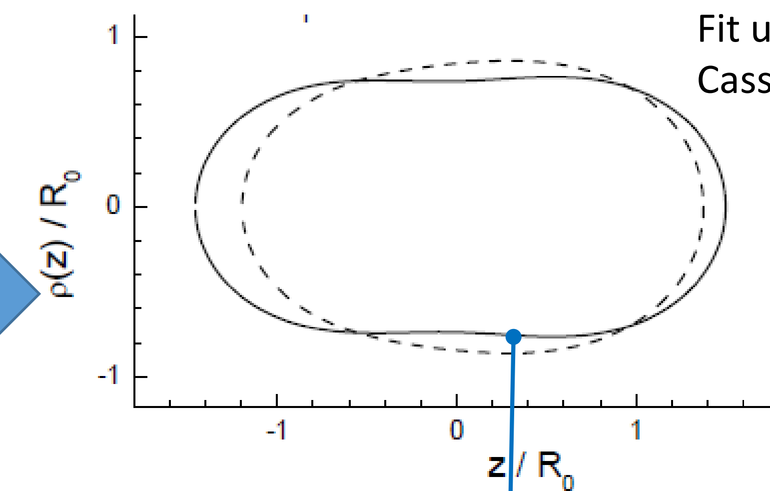


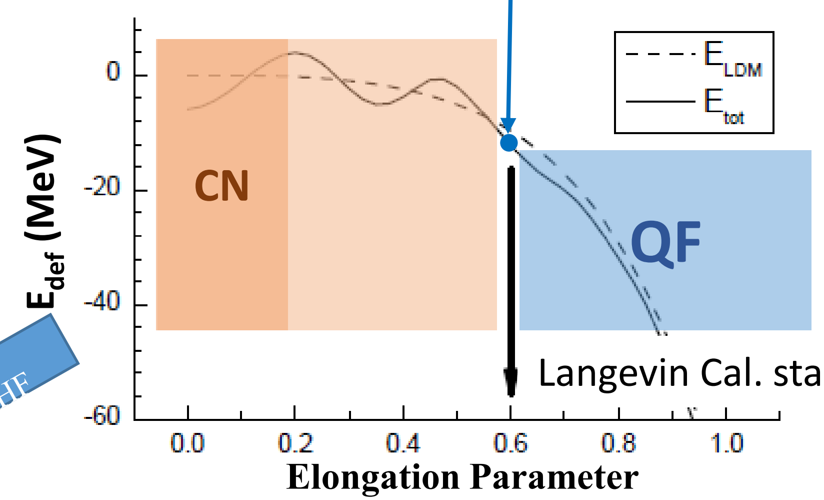
Cb-TDHFB, AMD

Shape profile

Compound & Quasi-fission $P_{\rm CNF}$

3D or 4D Langevin w/ neutron evaporation





Hauser-Feshbach decay $P_{\rm survive}$

$$P_{\rm survive} = \frac{\displaystyle\sum_{D=\{n,\gamma\}:l,j} \int_0^{E_{D\max}} \rho(E^* - S_D - E_D, J^\pi) T^J_{D,l,j}(E_D)\, dE_D}{\displaystyle\sum_{D'=\{\cdots\}:l,j} \int_0^{E_{D'\max}} \rho(E^* - S_{D'} - E_{D'}, J^\pi) T^J_{D',l,j}(E_{D'})\, dE_{D'}}$$

Decay mode: $D' = \{n, p, t, {}^3\mathrm{He}, \alpha, \gamma, F\}$

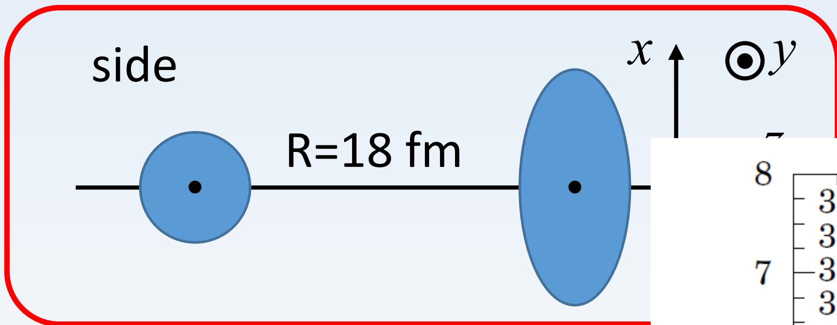
HFBTHO + BeoH
spin & parity

$P_{\rm CHF}$

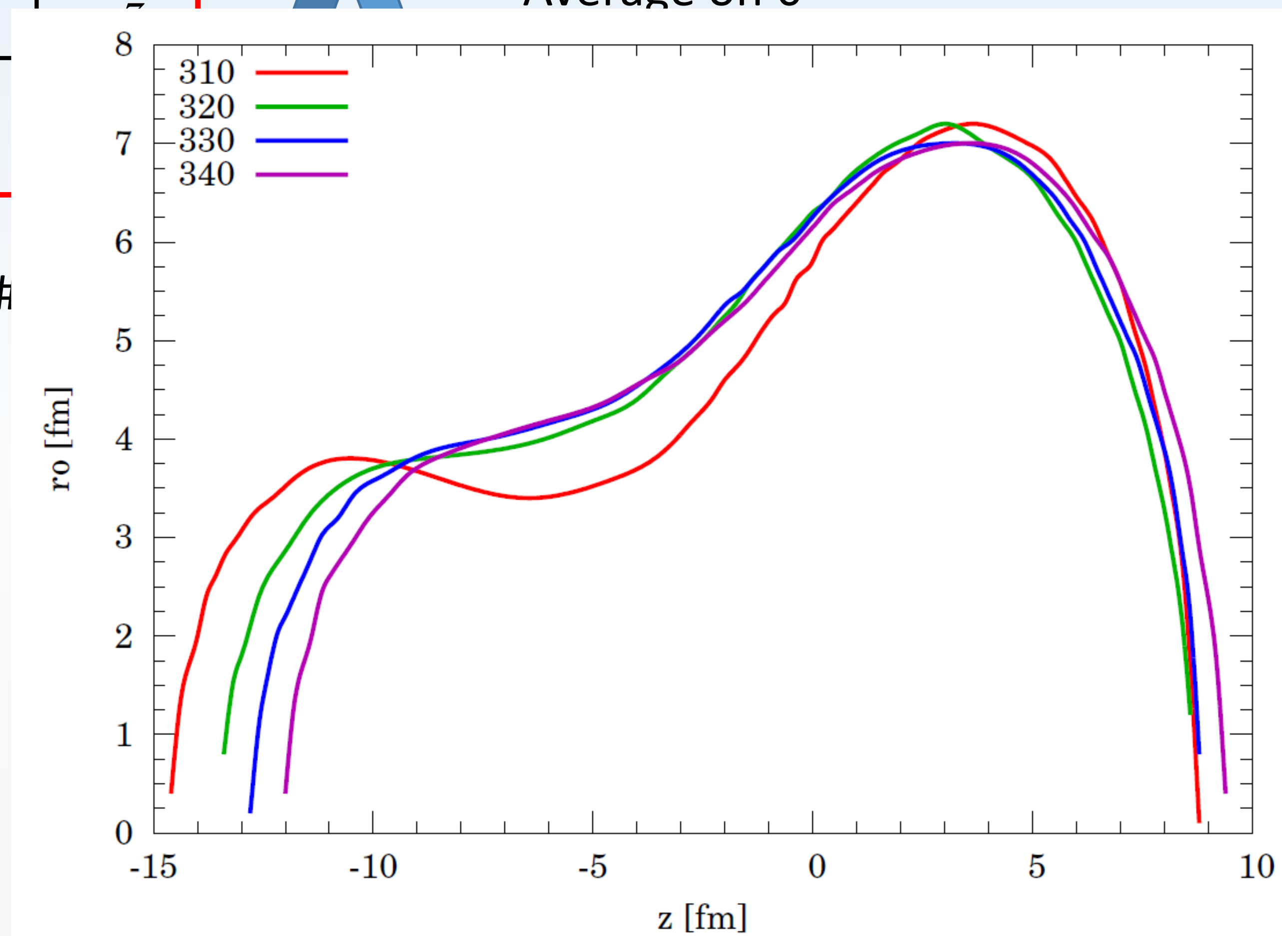
Synthesis probability: $P_{\rm SHE} = P_{\rm touch} \cdot P_{\rm survive} \cdot P_{\rm CNF}$

Results (Shape profile → Cassini Oval fitting)

Shape profile → Cassini Oval fitting → Langevin Cal. → Hauser-Feshbach Cal.

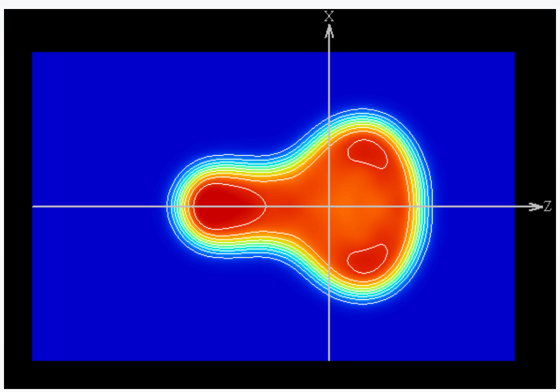


Average on θ

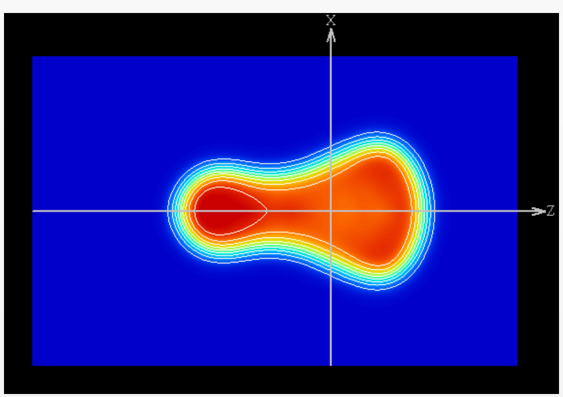


Nucleon density E_{in}=310 MeV @ T#

zx-plane



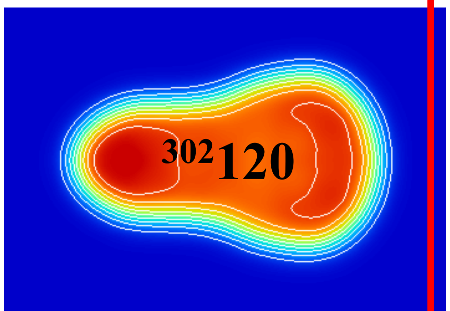
zy-plane

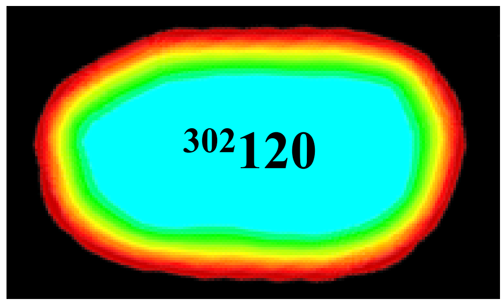


Unfortunately,
the fitting has not done yet. . .

Again …

Touching process P_{touch}



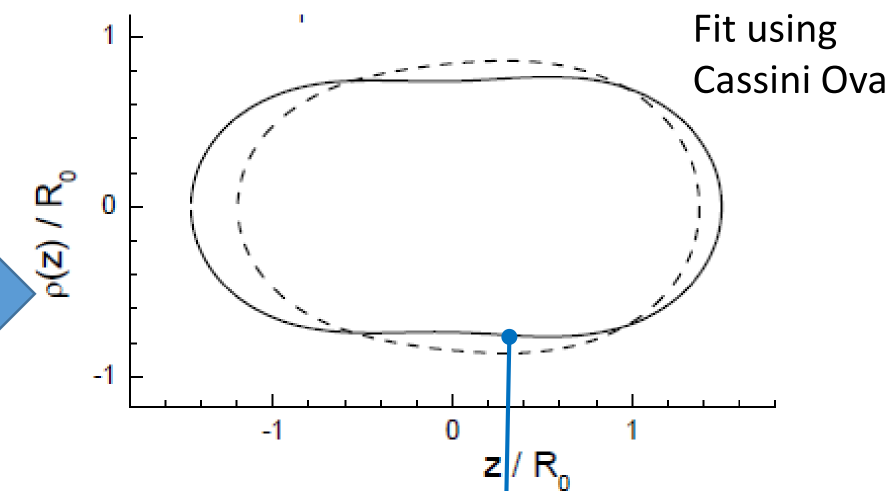


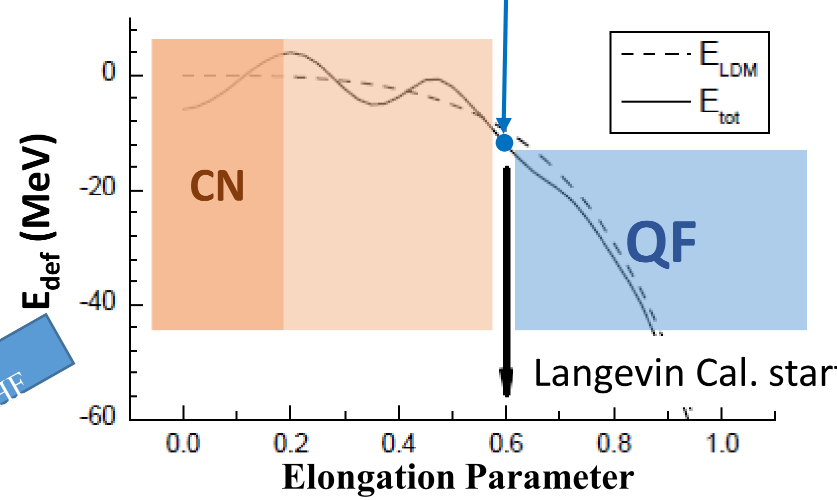
Cb-TDHFB, AMD

Shape profile

Compound & Quasi-fission P_{CNF}

3D or 4D Langevin w/ neutron evaporation





Hauser-Feshbach decay P_{survive}

$$P_{\text{survive}} = \frac{\displaystyle\sum_{D=\{n,\gamma\}:l,j} \int_0^{E_{D\max}} \rho(E^* - S_D - E_D, J^\pi) T^J_{D,l,j}(E_D)\, dE_D}{\displaystyle\sum_{D'=\{\cdots\}:l,j} \int_0^{E_{D'\max}} \rho(E^* - S_{D'} - E_{D'}, J^\pi) T^J_{D',l,j}(E_{D'})\, dE_{D'}}$$

Decay mode: $D' = \{n, p, t, {}^3\text{He}, \alpha, \gamma, F\}$

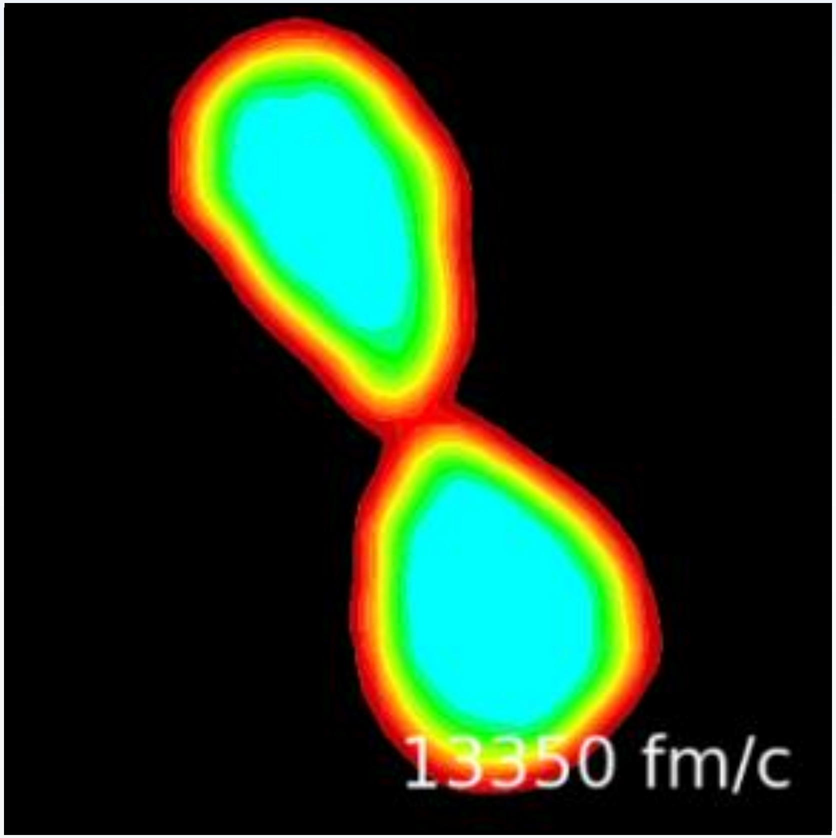
HFBTHO + BeoH
spin & parity

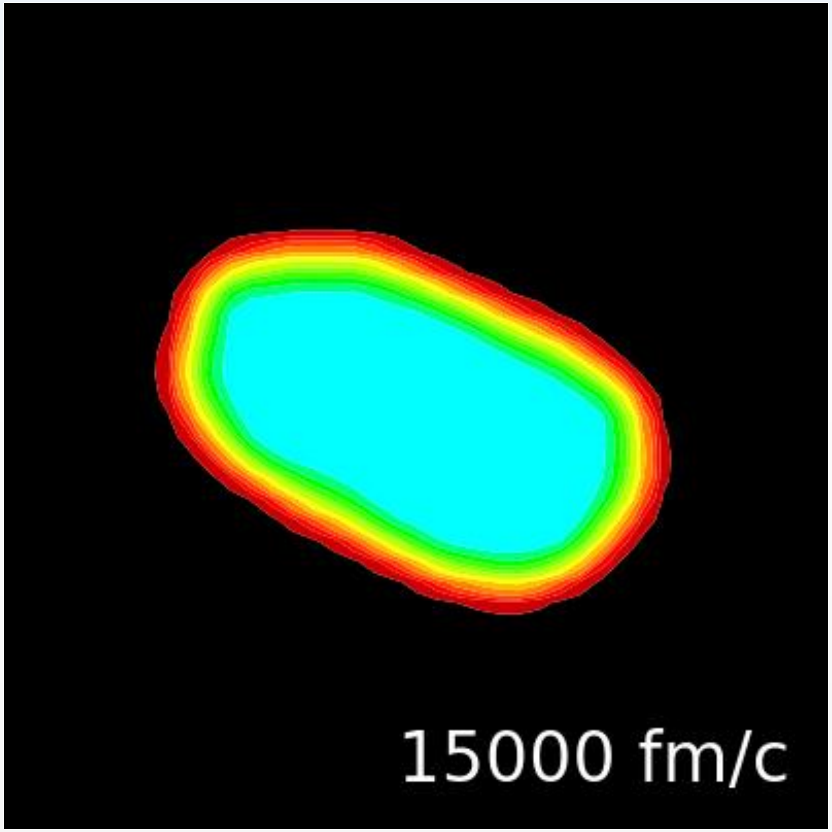
P_{CHF}

Synthesis probability: $P_{\text{SHE}} = P_{\text{touch}} \cdot P_{\text{survive}} \cdot P_{\text{CNF}}$

Touching process (b=0) by AMD

$^{54}Cr\ (324MeV) + ^{248}Cm \rightarrow ^{302}120$





The fates of these 2 events are different due to stochasticity brought by the NN collision : TDHF is a deterministic theory

Taken from S. Chiba presentation

Results from AMD+Langevin＋HF

Initial $U^*=50$	0n	1n	2n	3n	4n
Residue	$^{302}120$	$^{301}120$	$^{300}120$	$^{299}120$	$^{298}120$
<U*> (MeV)	50	39.7	32.3	23.6	17.1
① P_{CNF}	7.54×10^{-4}	7.87×10^{-5}	3.41×10^{-5}	2.33×10^{-6}	5.79×10^{-9}
② P_{surv}	1.87×10^{-8}	1.30×10^{-7}	1.18×10^{-6}	9.71×10^{-6}	1.70×10^{-5}
$P_{CNF}\times P_{surv}$ ①×②	1.41×10^{-11}	1.02×10^{-11}	4.02×10^{-11}	2.26×10^{-11}	9.84×10^{-14}

Summary (Fusion : Super-heavy element synthesis w/ Z=120)

- ✓ We calculate the head-on reaction ^{248}Cm+^{54}Cr → ^{302}120 using Cb-TDHFB, with $E_{in} = 300, 310, 320, 330, 340$ MeV.
  - ✓ The Coulomb barriers of ^{248}Cm+^{54}Cr are evaluated 245 (side) and 222 (tip) MeV on the reaction direction using Frozen density approximation.
  - ✓ Over 60 MeV from Coulomb barrier is necessary for the fusion.
    - ✓ We describe the energy balance on the fusion reaction using Cb-TDHFB.

Future work

- ➢ To distinguish Quasi-fission and Fusion, more long-time calculation is necessary.
  - ➢ Optimization of the calculation space and Revision of algorithm to time-evolution
- ➢ Large-scale calculation for P_{touch} w.r.t the impact parameter, nuclear rotation
- ➢ For pairing correlation : strength, functional form, phase between target and projectile

Summary

For Fission:

- ✓ We employ the constraint MF model to estimate the charge polarization of FPs.
- ✓ The charge polarization of FPs appears in the microscopic calculation,
- ✓ and is evaluated through the Hauser-Feshbach calculation.

For Fusion:

- ✓ We employ the Cb-TDHFB to simulate the fusion reaction for the super-heavy element synthesis: $^{54}Cr+^{248}Cm \rightarrow {}^{302}120$ with E_{in} = 300, 310, 320, 330, 340 MeV.
- ✓ And AMD Cal. also are performed to simulate the synthesis reaction.
  From the AMD results, the survival probabilities are estimated.

Thank you!