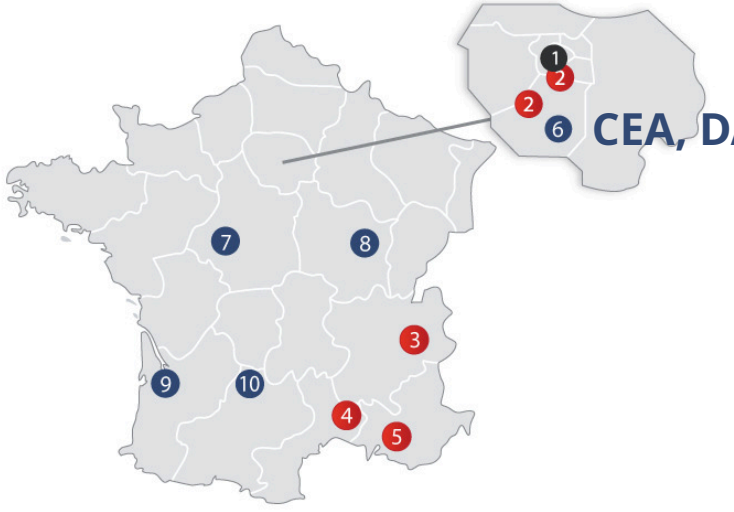
Dynamics of heavy nuclei

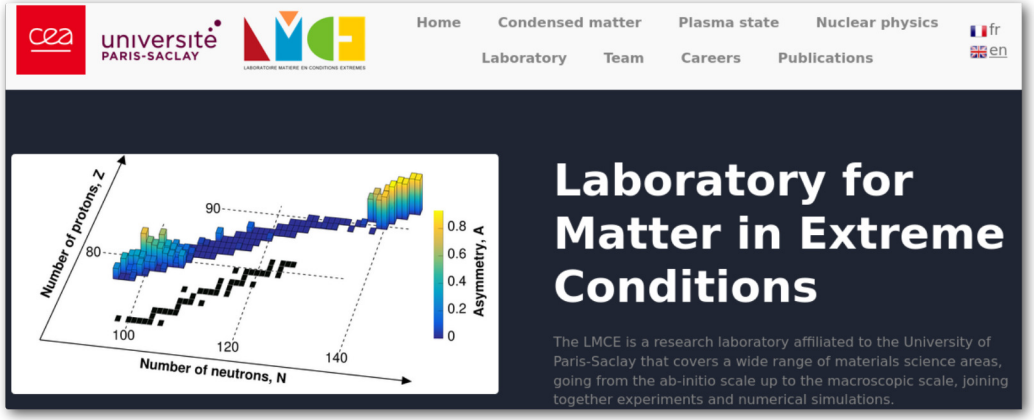
David Regnier[1,2]

1. CEA, DAM, DIF, 91297 Arpajon, France
2. Université Paris-Saclay, CEA, LMCE, 91680 Bruyère-le-Châtel, France

david.regnier@cea.fr

About CEA, DAM, DIF





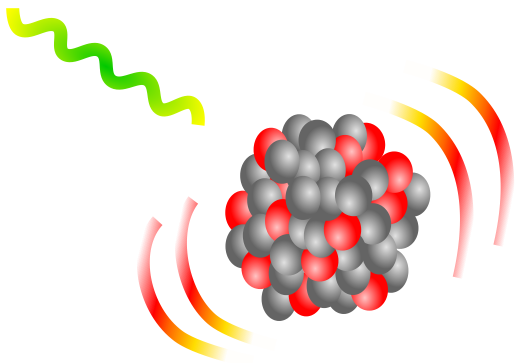
www-lmce.cea.fr

We are always looking for PhD/post-doc candidates: **do not hesitate to contact us !**

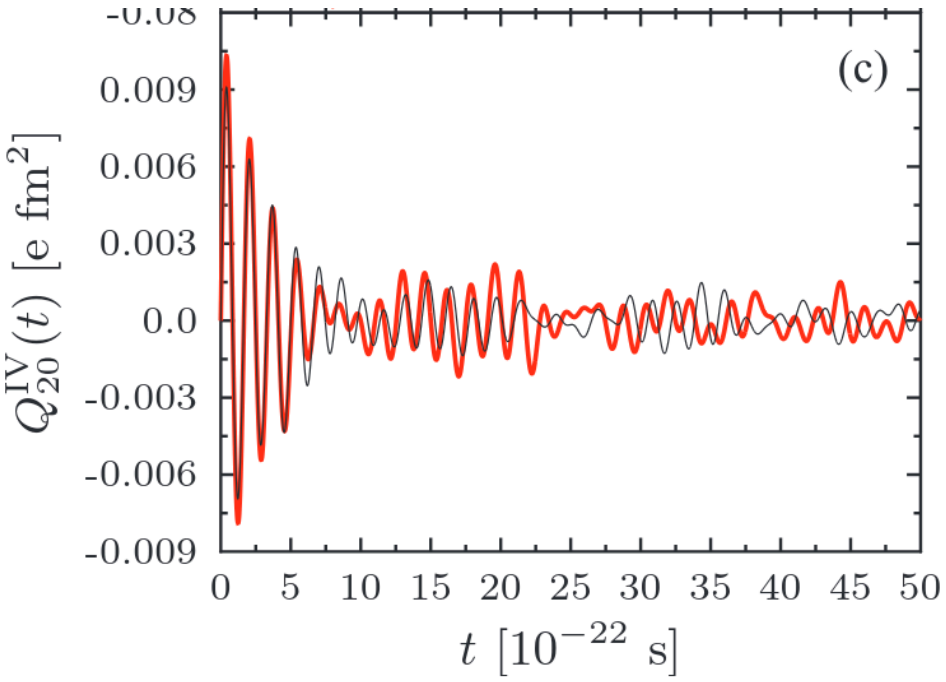
Dynamics of heavy-nuclei ?

Theoretical approaches that explicitly describe the **time evolution** of an atomic nucleus or a nuclear reaction

Non equilibrium initial condition



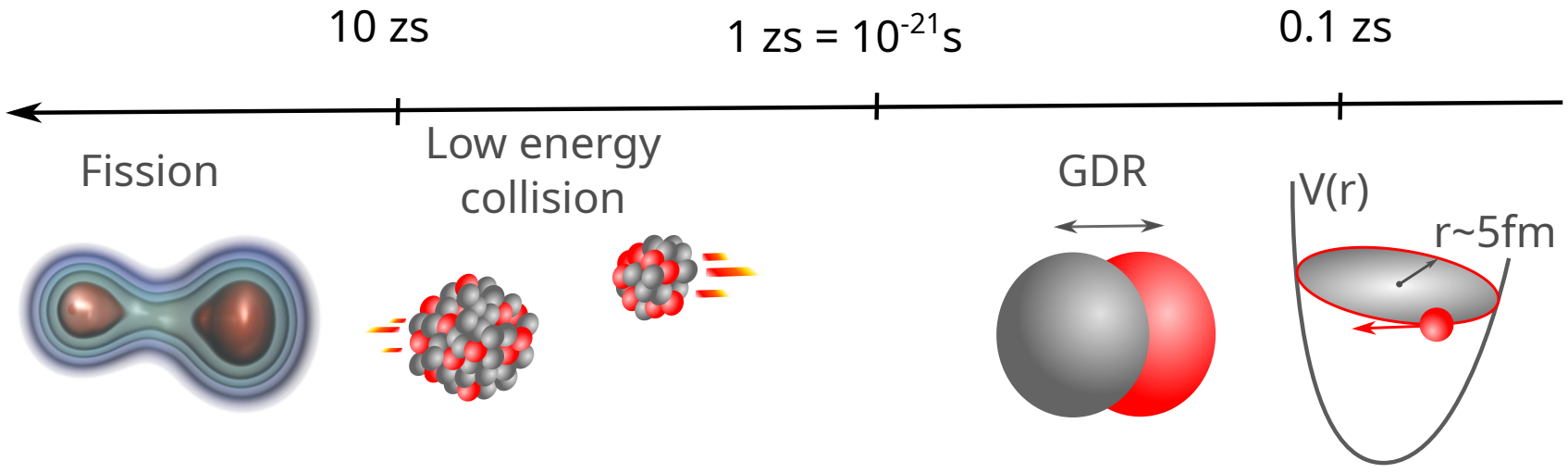
Evolution of observables in time



G. Scamps *et al.*, PRC (2014)

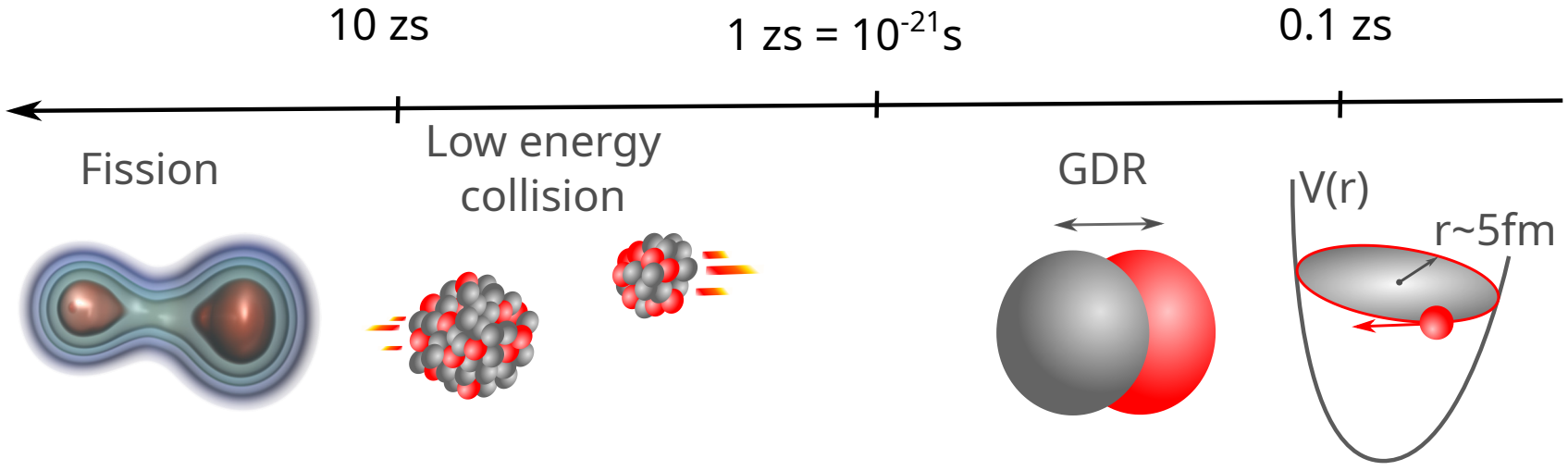
Nuclear time scales

large molecule motion	1 picosecond	10^{-12}s
electronic excitation	1 femtosecond	10^{-15}s
shortest laser pulse	1 attosecond	10^{-18}s
nuclear motion	**1 zeptosecond**	**10^{-21}s** ($\simeq$ 300 fm/c)



Nuclear time scales

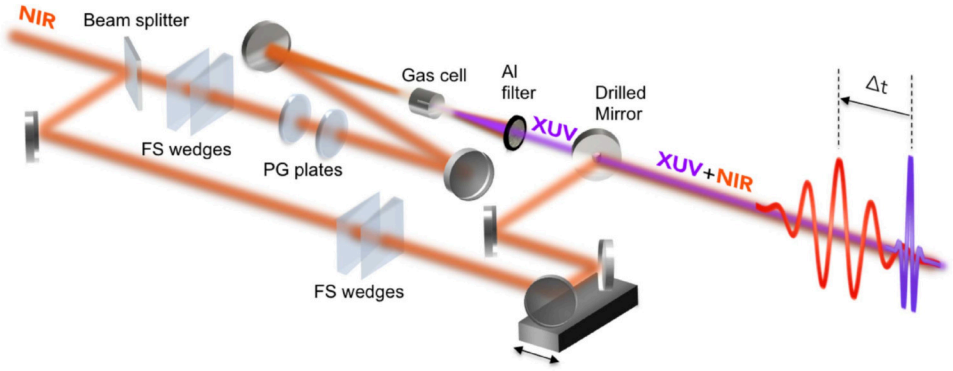
large molecule motion	1 picosecond	10^{-12}s
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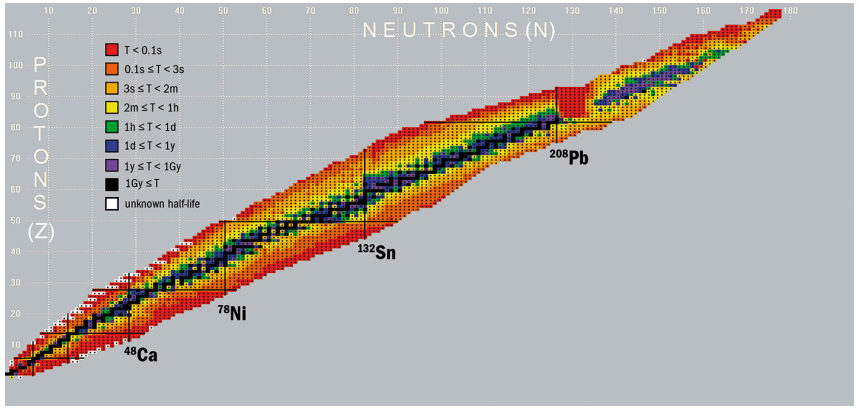
➡️ **No direct observation** of time-dependent observables with our current technology

Why simulating explicitly the dynamics ?

1. To predict how observables evolve in time ?
2. To determine decay lifetimes ?
3. To generate nice animations ?
4. To predict the output of reactions ?
5. To warm up your office during winter ?
6. Because it is easier than static calculations ?



Attosecond lasers, Q. Liu *et al.* J. Opt **20** (2018)



Nuclear half-lives

Static vs time-dependent

Static

$$\hat{H}\psi_n = E_n\psi_n$$

1. Full diagonalization
2. Dynamics for **any** initial condition

$$\psi(t=0) = \sum_n c_n\psi_n$$

$$\psi(t) = \sum_n c_n\psi_n e^{-i\frac{E_n}{\hbar}t}$$

Time-dependent

$$i\hbar\partial_t\psi = \hat{H}\psi$$

1. Numerical integration on time
2. Dynamics for **one** initial condition

$$\psi(1\times dt) \simeq \psi(t=0) - \frac{i}{\hbar}\hat{H}\psi(t=0)$$

$$\psi(2\times dt) \simeq \psi(1\times dt) - \frac{i}{\hbar}\hat{H}\psi(1\times dt)$$

$$\dots$$

Static vs time-dependent

Static

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Cost $\simeq O(\dim^3)$

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$$\dots$$

Cost $\simeq O(N_{\text{inital conditions}} \times N_{\text{steps}} \times \dim^2)$

Static vs time-dependent

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1. Full diagonalization
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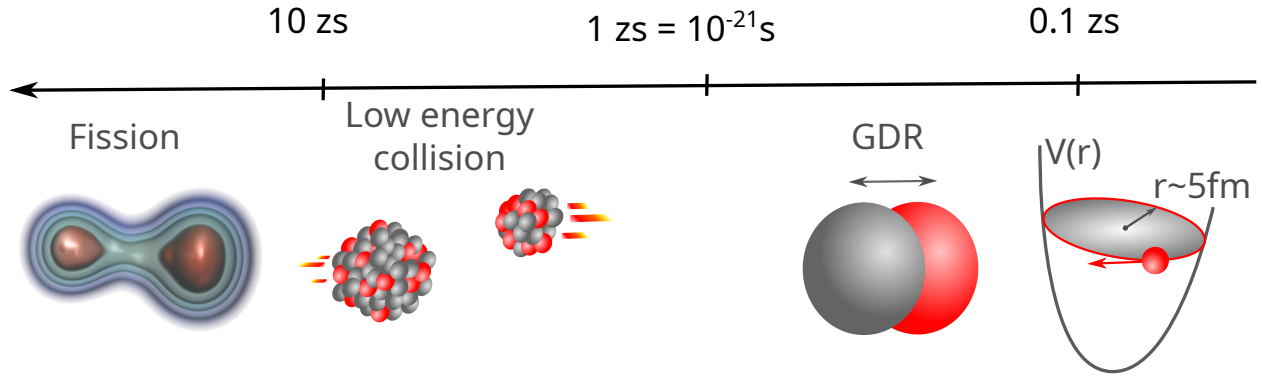
Cost $\simeq O(N_{\text{inital conditions}} \times N_{\text{steps}} \times \dim^2)$

- In practice, **dim >** 10^{200} ($10^{80} \simeq$ atoms in the univers)
- Choose what **converges the fastest**

Which phenomena can we simulate ?

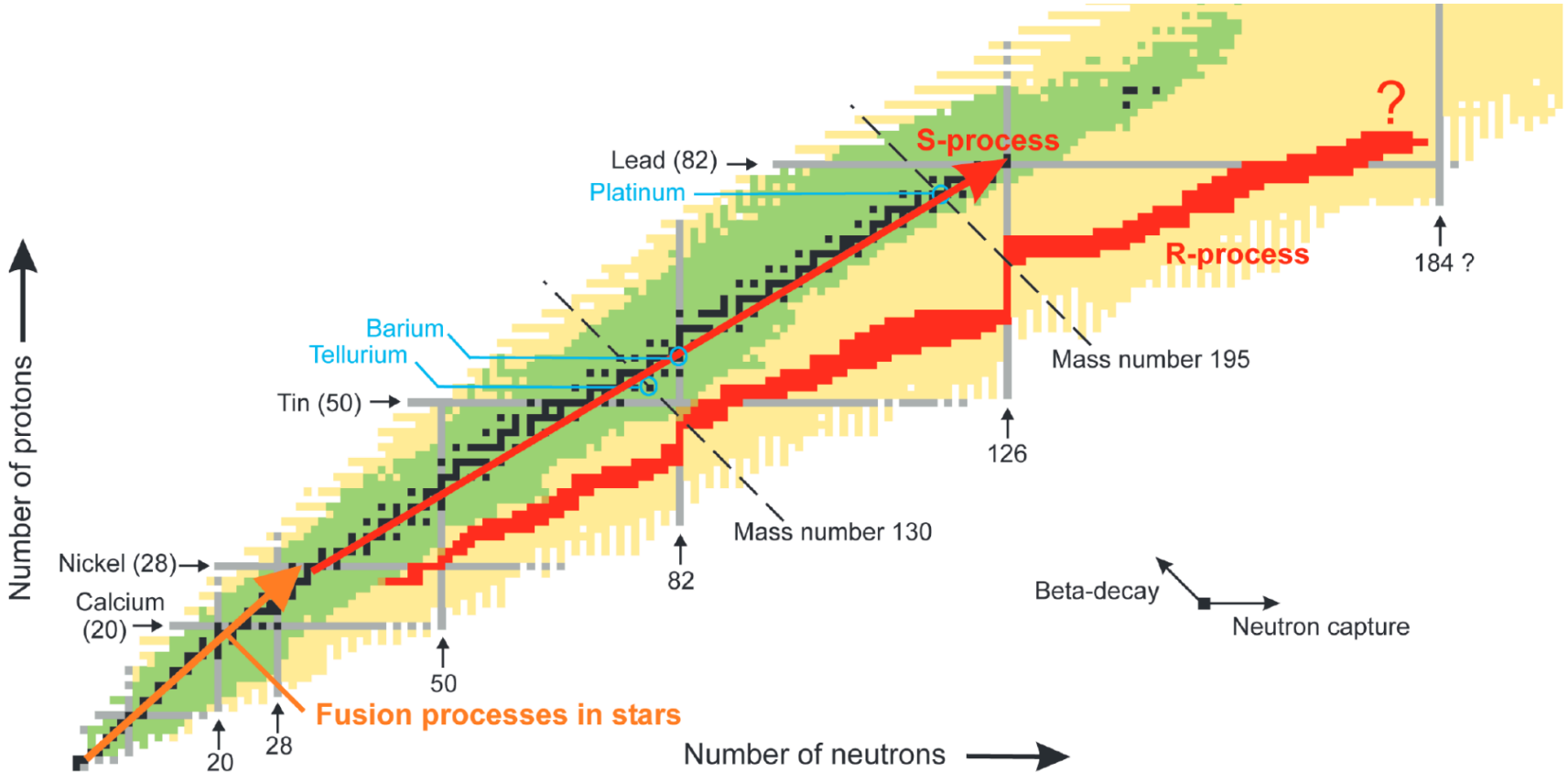
Successful predictions from dynamics in nuclear physics

- **Collective vibrations**:
  - response to a gamma excitation
  - cross section for (n, γ) reactions
- **Fission**:
  - mass and charge yields
  - fragments characteristics
- **Heavy ion collision (low energy)**:
  - fusion barriers
  - nucleon transfer
  - fusion-fission versus quasi-fission



Related fundamental questions

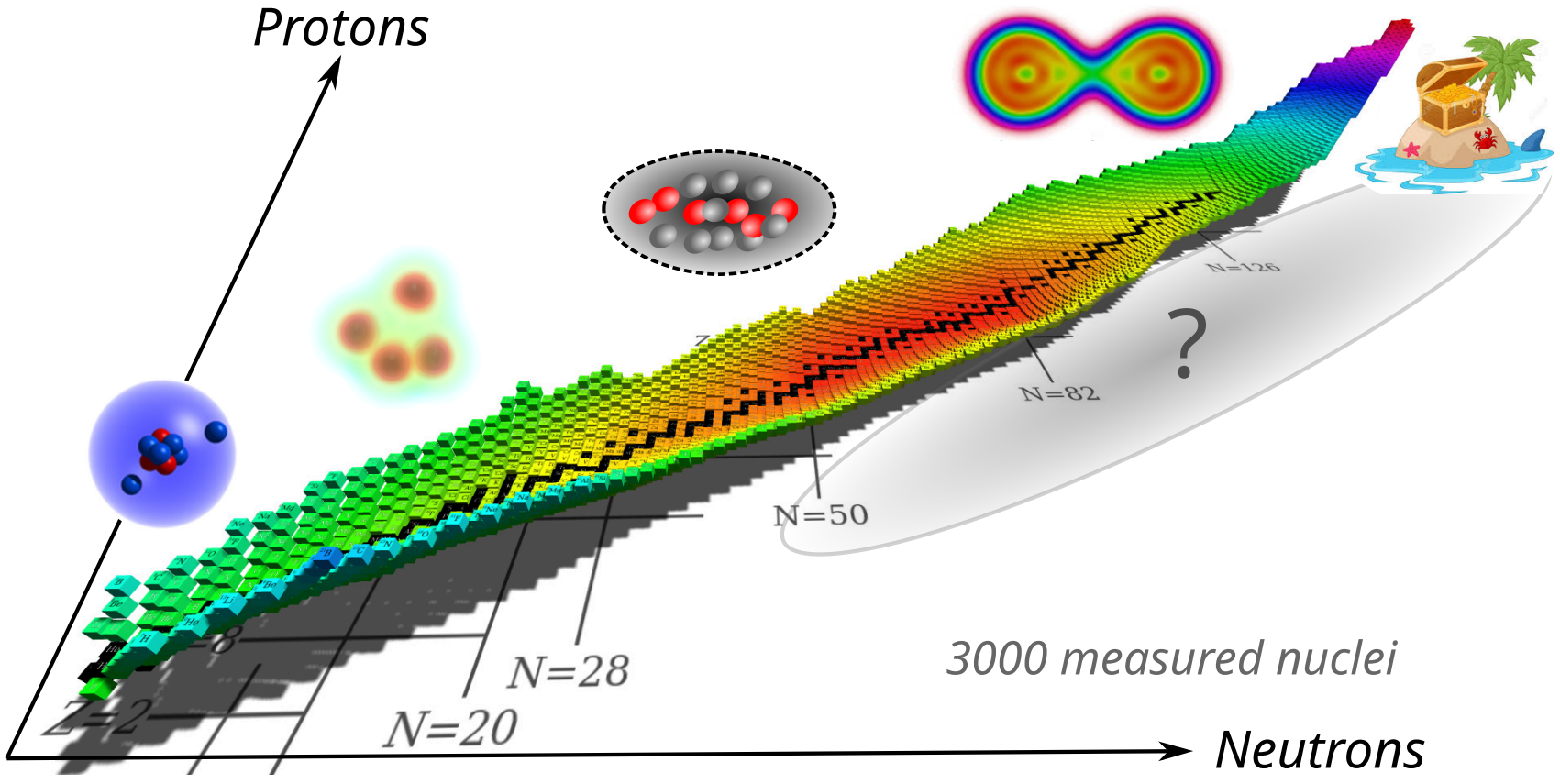
How were the heavy elements synthetized ?



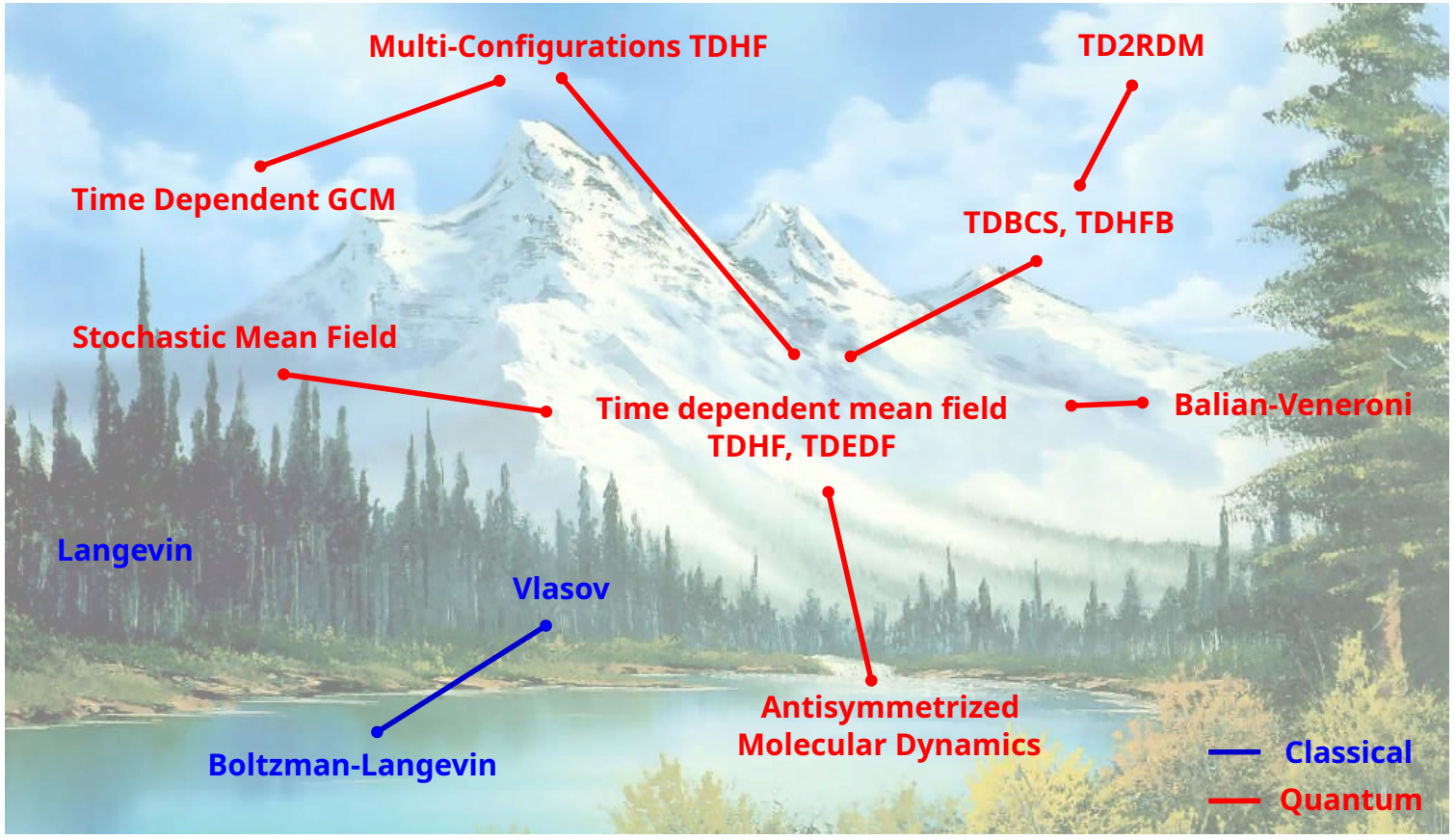
H. Schatz *et al.* Europhysics news 37 (2006)

Related fundamental questions

Is there a superheavy island of stability ?



How to simulate the dynamics ?



Today's focus: methods rooted in the **Energy Density Functional** framework
(cf. M. Bender lecture)

Suggested readings

Reviews

- **Nuclear quantum many-body dynamics (2nd edition)**
  C. Simenel, Eur. Phys. J. A **61** (2025)
- The time-dependent generator coordinate method in nuclear physics
  M. Verriere, D. Regnier, Front. Phys. **8** (2020)
- Time-dependent density-functional description of nuclear dynamics
  T. Nakatsukasa *et al.*, Rev. Mod. Phys, **88** (2016)

Books

- Energy density functional method for atomic nuclei
  N. Schunck *et al.*, IOP (2019)
- The nuclear many-body problem
  P. Ring, P. Schuck, Springer science (2004)
- Quantum theory of finite systems
  J.-P. Blaizot, G. Ripka, MIT Press (1985)

Lectures

- Approches Microscopiques en Physique Nucléaire
  D. Lacroix, Master 2 lecture in english (2010-2012)
- Microscopic approaches for nuclear Many-Body dynamics
  C. Simenel *et al.*, EJC 2007, arXiv:0806.2714v2

Some open-source codes for dynamics

- **Sky3D-1.2**

  Abhishek *et al.*, CPC 301 (2024):

  A reference Skyrme TDHF open source code on CPU
- **LISE**

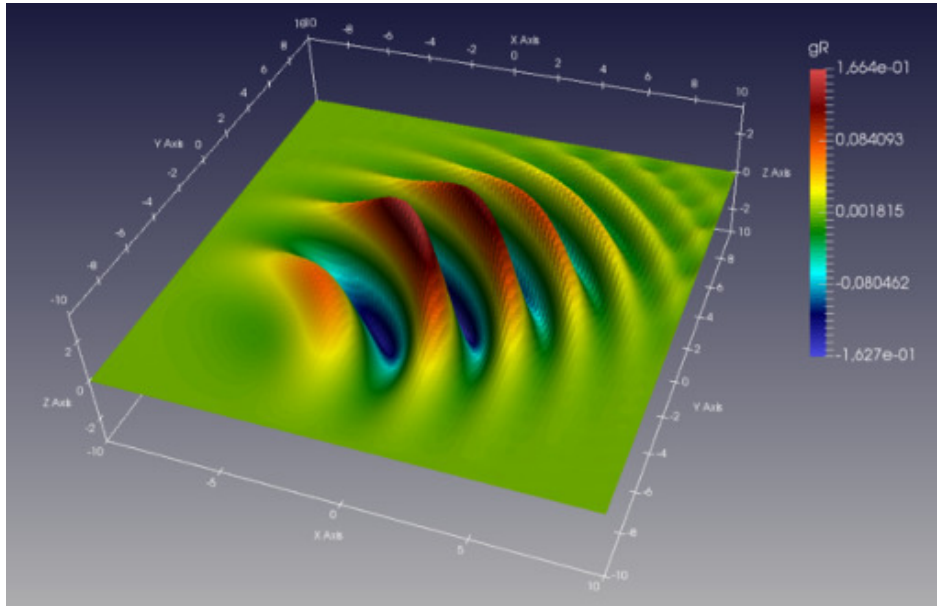
  S. Jin *et al.*, CPC 269 (2020):

  A Skyrme full TDHFB package on GPU
- **FELIX-2.0**

  D. Regnier *et al*, CPC 225 (2018):

  A time-dependent Schrödinger equation solver on CPU

  (designed for fission simulation with TDGCM+GOA)



2D wavefunction propagation with FELIX-2.0

- **ANDy-1.0**

  D. Regnier *et al*, work in progress

  A library for TDHF, TDBCS, et al. on CPU and GPU.

Table of contents

I. Heavy-ion fusion threshold with TDEDF

II. Fission yields with TDGCM

III. State-of-the-art and open challenges

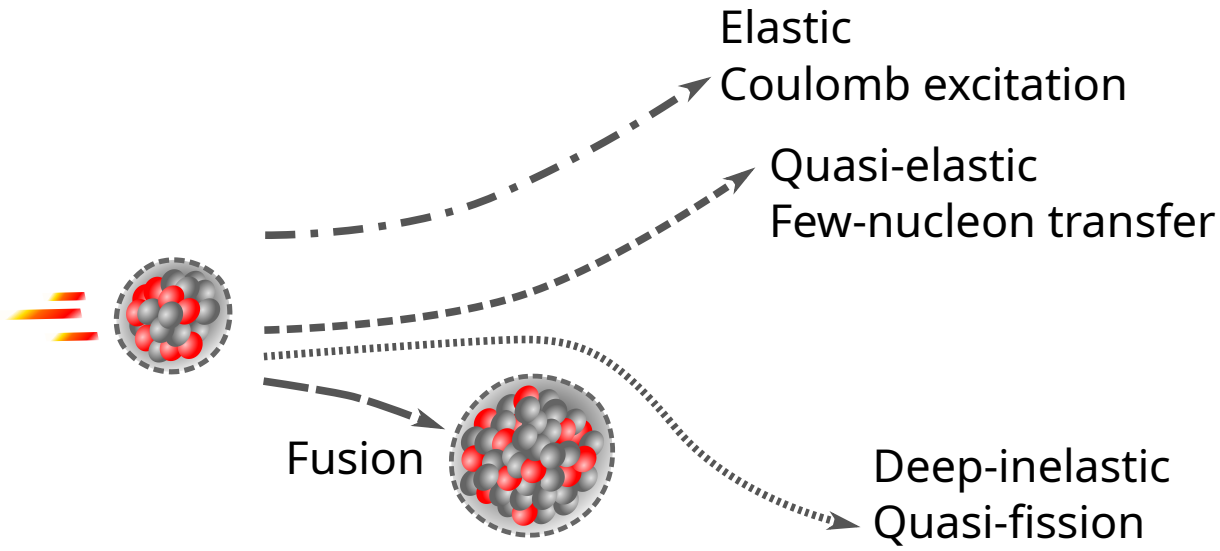
Table of contents

I. **Heavy-ion fusion threshold with TDEDF**

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III. State-of-the-art and open challenges

Low-energy heavy-ion collisions



Focus on **low-energy** heavy-ion collisions

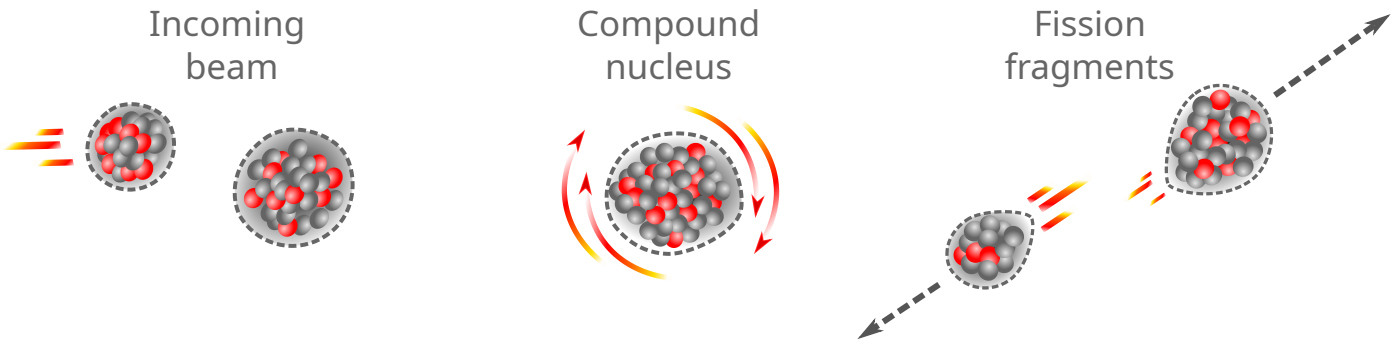
$$E_{\text{Center of mass}} \simeq B_{\text{Coulomb}}$$

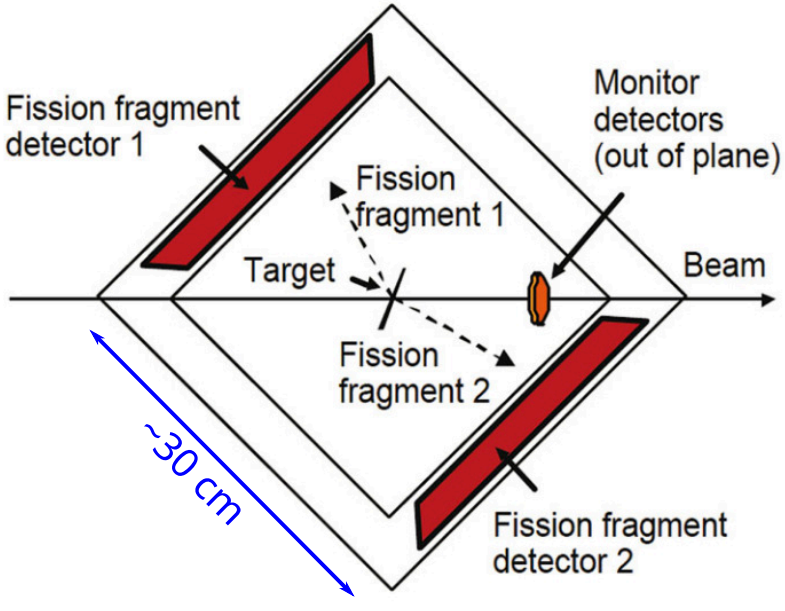
Example: ^{16}O + ^{208}Pb collision

What is the energy required to fusion ?

Experimental clues for fusion

Experimental clues for fusion

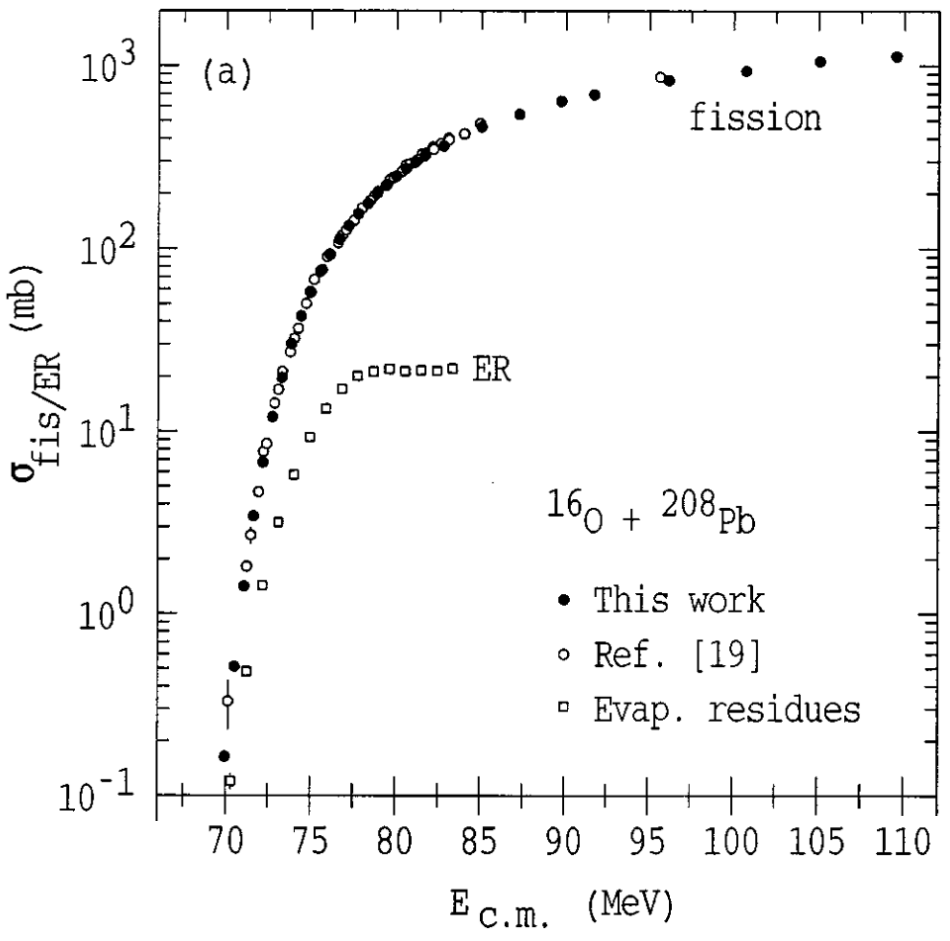




CUBE detector

Adapted from G. Montagnoli *et al.*, Eur. Phys. J. A **59** (2023)

Fusion cross section



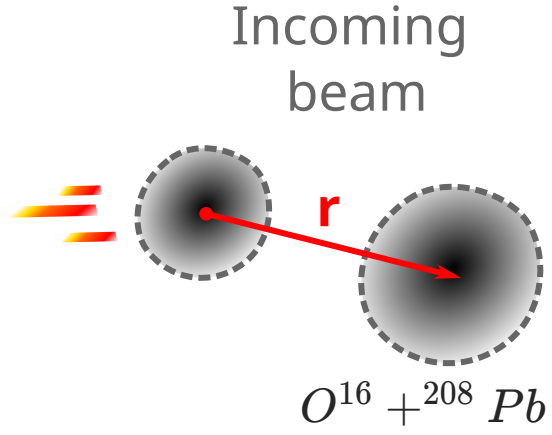
Adapted from C. R. Morton *et al.* Phys. Rev. C **60** (1999)

$$\sigma_{\text{fusion}} = \sigma_{\text{fission}} + \sigma_{\text{evaporation residues}}$$

- A threshold phenomenon (potential barrier)
- Threshold $\simeq$ 75 MeV

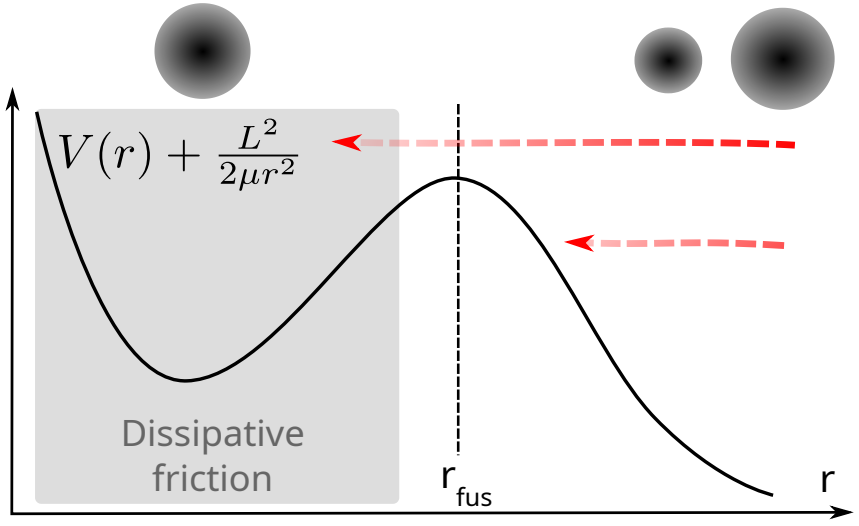
How would you postdict this from a model ?

A two-body picture



Classical Hamiltonian mechanics:

$$H(r,p) = \frac{p^2}{2\mu} + \frac{L^2}{2\mu r^2} + V(r)$$



$$\sigma_{\text{fusion}}(E) = \pi r_{fus}^2 [1 - V(r_{fus})/E]$$

How to determine r_{fus} and $V(r_f)$?

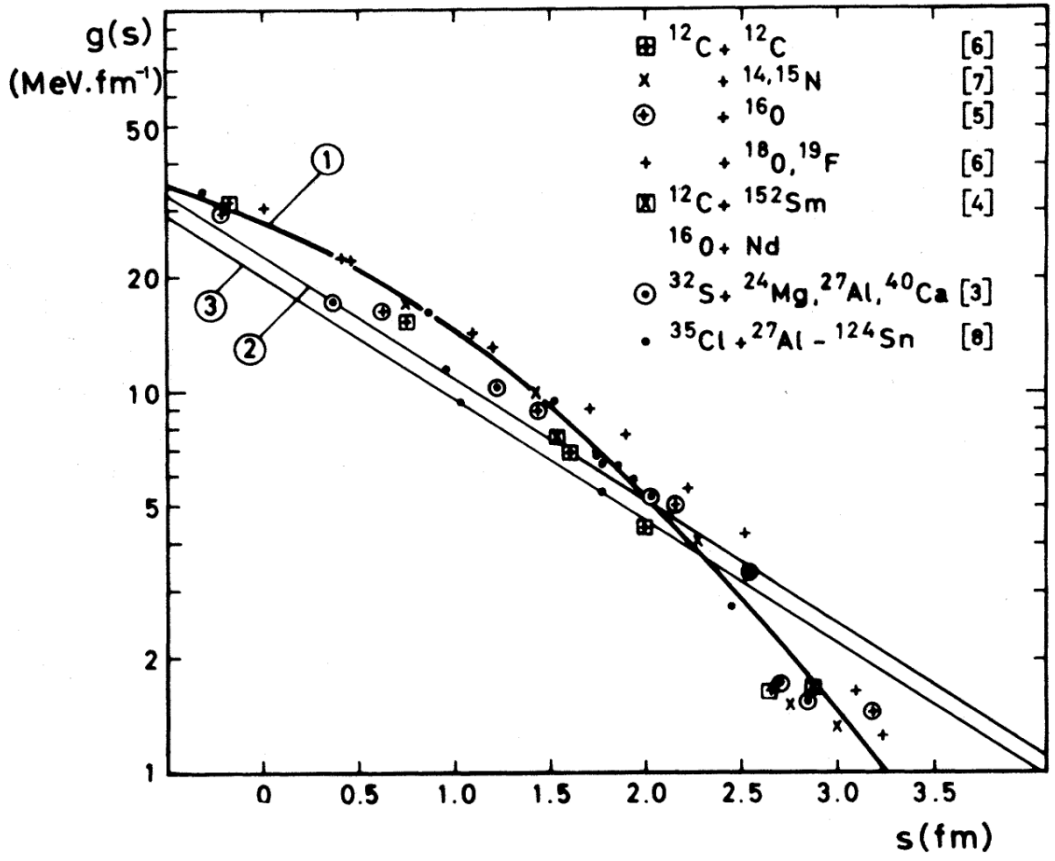
Reducing the number of coordinates:

- All nucleons $(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{224})$
- Removing internal structure $(\boldsymbol{r}_O, \boldsymbol{r}_{Pb})$
- Removing the center of mass $\boldsymbol{r}$
- Assuming a central potential r (1D)

An empirical effective potential

The Bass systematics

Fitting the nucleus independent parts of the effective potential on fusion cross sections

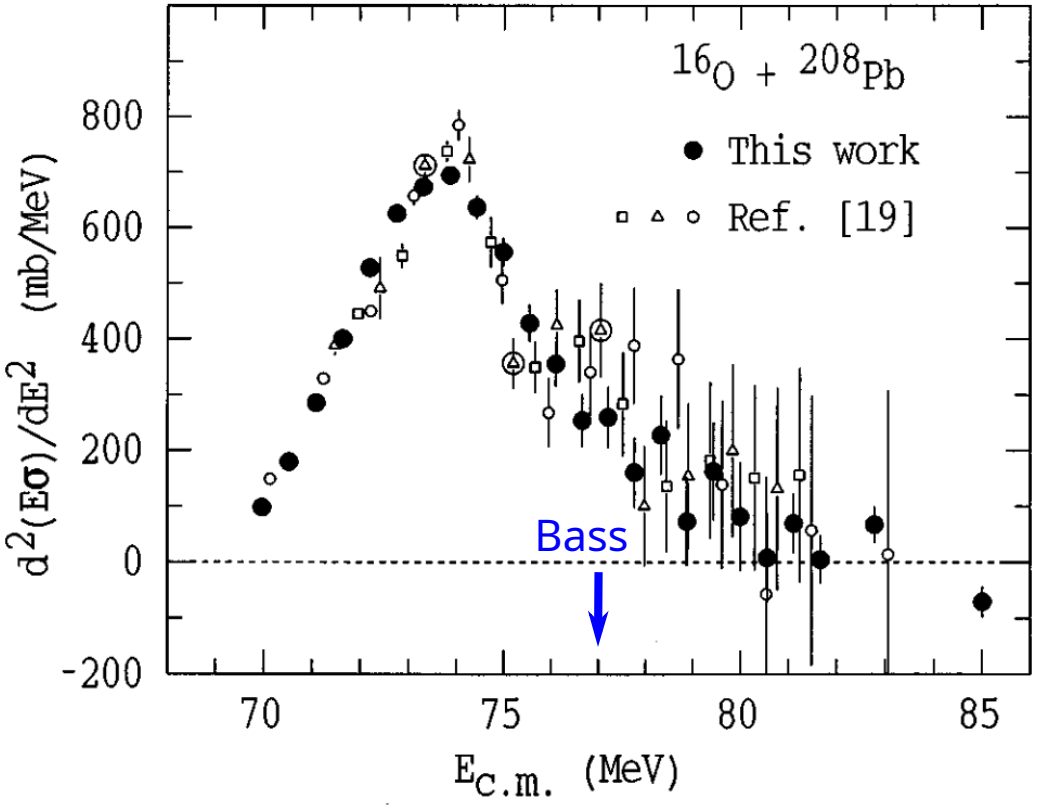


R. Bass Phys. Rev. Lett. 39 (1977)

What does it give for our ^{16}O+^{208}Pb collision ?

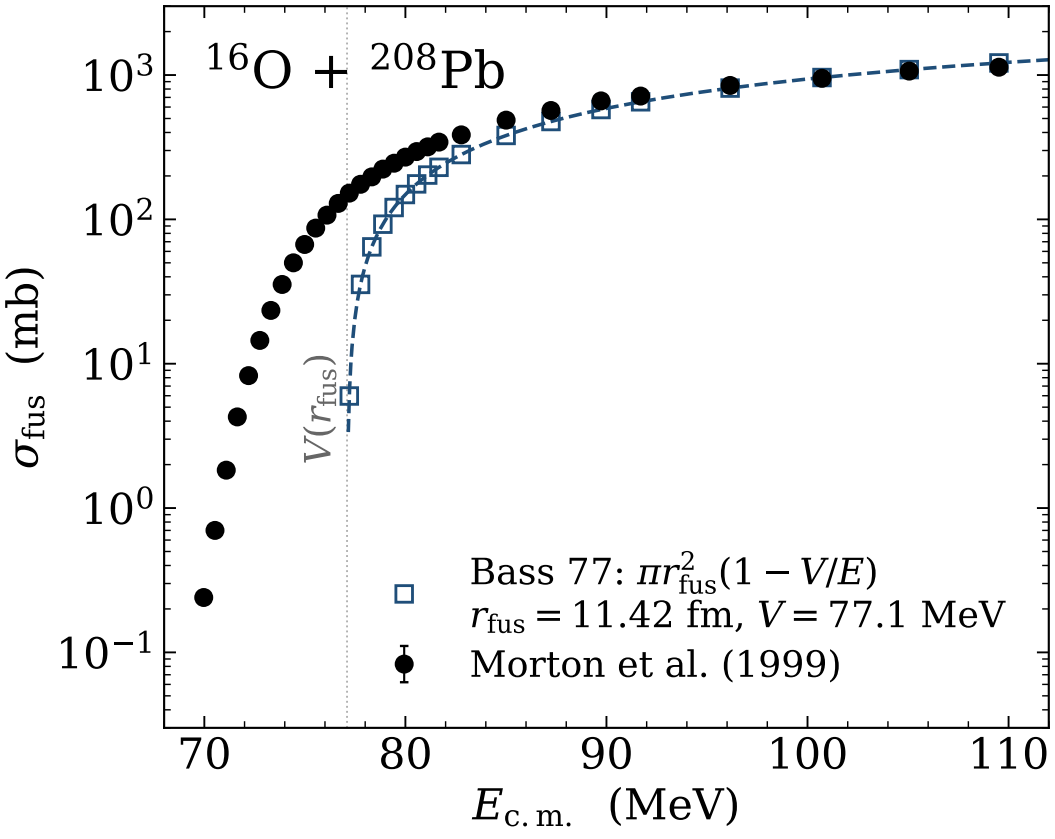
- $r_{fus} = 11.42$
- $V(r_{fus}) = 77.1$ **MeV**

$\frac{\partial^2 E\sigma}{\partial E^2}$ peaks at $V(r_{fus})$
in a simple two-body quantum scattering pb



Distribution of 'fusion barrier'
Adapted from C.R. Morton *et al.* Phys. Rev. C **60** (1999)

What does it give for our ^{16}O+^{208}Pb collision ?



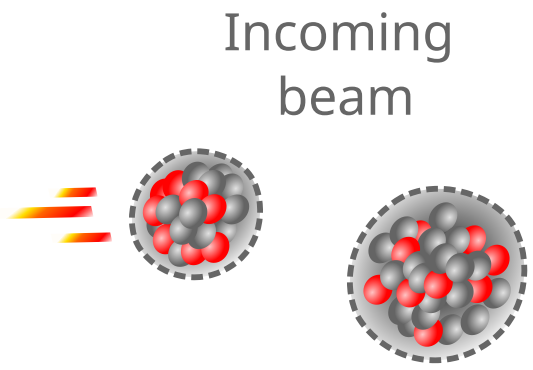
Fusion cross section obtained from a classical 2-body picture

✅ Correct order of magnitude for the fusion threshold

❌ No fusion below the threshold (classical picture)

How to further improve our postdiction ?

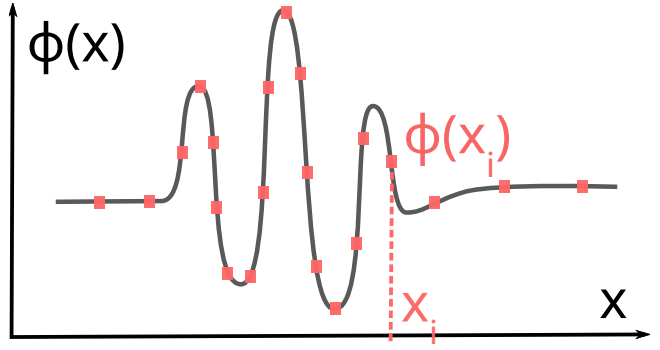
The many-body picture



Exact many-body dynamics

- State
  $|\psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t)\rangle$
- Interactions
  $\hat{H} = \hat{K} + \hat{V}^{(2)} + \hat{V}^{(3)} + \cdots$
- Equation of motion
  $$i\hbar \frac{\partial}{\partial t} |\psi(\boldsymbol{r}_1 \cdots, \boldsymbol{r}_A, t)\rangle = \hat{H} |\psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t)\rangle$$

Discretizing the wavefunction



$$\varphi(x) = \sum_{k}^{K \simeq 40} \varphi(x_k) \times b_k(x)$$

- parameterizing one nucleon wavefunction $\varphi(\boldsymbol{r}_1)$
  $\simeq 40^3$ complex numbers
  $\simeq$ **512 kB**
- parameterizing $\psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t = 0)$
  $\simeq 40^{3\times(16+208)}$ complex numbers
  $\simeq 10^{661}$ **TB** 😱

Time-dependent EDF / Hartree-Fock

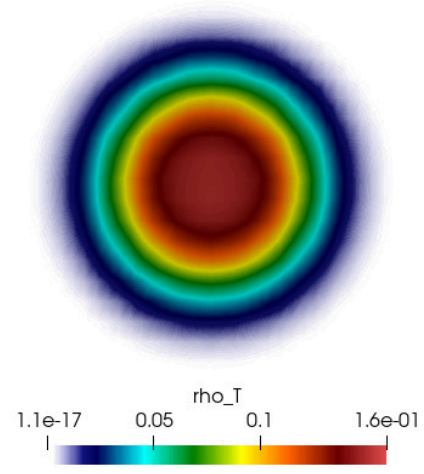
- State: $|\phi_{neutron}(t)\rangle \times |\phi_{proton}(t)\rangle$
  with

$$\phi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N, t) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\boldsymbol{r}_1, t) & \varphi_2(\boldsymbol{r}_1, t) & \cdots & \varphi_N(\boldsymbol{r}_1, t) \\ \varphi_1(\boldsymbol{r}_2, t) & \varphi_2(\boldsymbol{r}_2, t) & \cdots & \varphi_N(\boldsymbol{r}_2, t) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(\boldsymbol{r}_N, t) & \varphi_2(\boldsymbol{r}_N, t) & \cdots & \varphi_N(\boldsymbol{r}_N, t) \end{vmatrix}$$

  and discretized one-body wavefunctions

$$\varphi_i(\boldsymbol{r}, t) = \sum_{k}^{K \simeq 40^3} \varphi_i(\boldsymbol{r}_k, t) \times b_k(\boldsymbol{r})$$

- parameterizing $\phi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t = 0)$
  $\simeq 40^3 \times (16 + 208)$ complex numbers
  $\simeq$ **15 MB** 😄



^{16}O local one-body density $\rho(\boldsymbol{r})$
(probability to measure one nucleon at $\boldsymbol{r}$)

- Interactions:
  $E(\rho, \cdots)$ or $\hat{H}$
- **Which equations of motion ?**

Equations of motion

How do the parameters $\varphi_i(\boldsymbol{r}_k, t)$ of the wavefunction evolve in time ?

Equations of motion

How do the parameters $\varphi_i(\boldsymbol{r}_k, t)$ of the wavefunction evolve in time ?

Time-dependent variational principles

- Variational formulation of the exact Schrödinger equation:

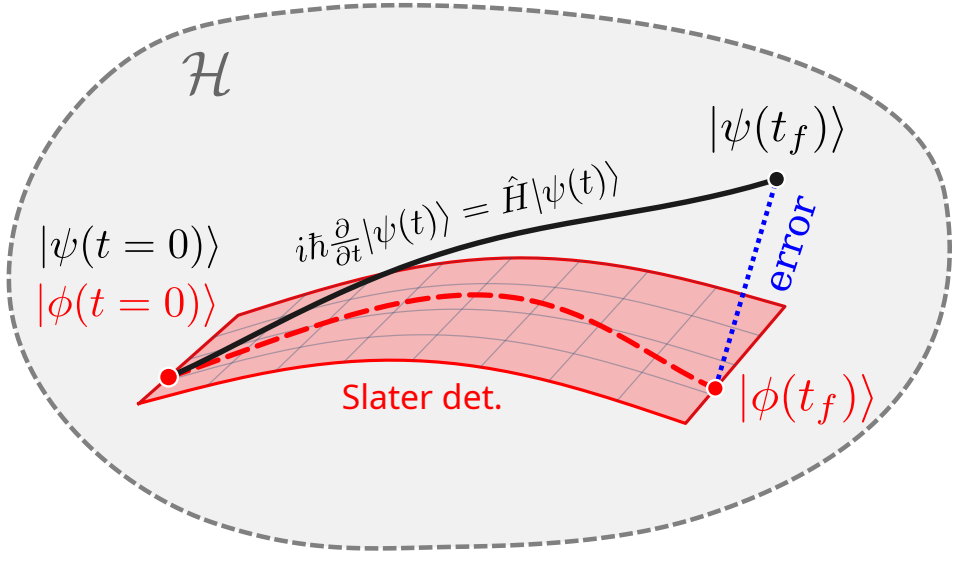
$$\delta_{\mathcal{H}\times\mathbb{R}^+}\left(\int_{t=0}^{t_f} i\hbar\langle\psi(t)|\frac{\partial}{\partial t}\psi(t)\rangle - E(|\psi(t)\rangle)\right) = 0$$

  Look for any $|\psi(t)\rangle$ that makes the action extremum

- Variational approximation:

$$\delta_{\text{Slater det.}}\left(\int_{t=0}^{t_f} i\hbar\langle\phi(t)|\frac{\partial}{\partial t}\phi(t)\rangle - E(|\phi(t)\rangle)\right) = 0$$

  Look for a Slater det. $|\phi(t)\rangle$ that makes the action extremum



Each step in the Slater determinant trajectory **minimizes the approximation error**

Equations of motion

In practice $\delta_{\text{Slater det.}}(\cdots) = 0$ means the set of equations

$$\forall i,k,t: \quad \frac{\partial \mathcal{S}}{\partial \varphi_i^*(\boldsymbol{r}_k,t)} = 0,$$
$$\frac{\partial \mathcal{S}}{\partial \varphi_i(\boldsymbol{r}_k,t)} = 0$$
$$\frac{\partial \mathcal{S}}{\partial \lambda_{ij}(t)} = 0$$
$$\frac{\partial \mathcal{S}}{\partial \lambda_{ij}^*(t)} = 0$$

with the action defined by

$$\mathcal{S} = \left(\int_{t=0}^{t_f} i\hbar \langle \phi(t)| \frac{\partial}{\partial t} \phi(t)\rangle - E(|\phi(t)\rangle) - \lambda_{ij} \langle \varphi_i(t)|\varphi_j(t)\rangle \right).$$

The λ_{ij} are Lagrange parameters to ensure

$$\langle \varphi_i(t)|\varphi_j(t)\rangle = \delta_{ij}.$$

... after some 'straightforward' maths

The usual time-dependent EDF/TDHF equations of motion !

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\varphi_1(\mathbf{r},t)\\ \cdots \\ \varphi_A(\mathbf{r},t)\end{bmatrix} = \begin{bmatrix}\hat{h}[\rho(\boldsymbol{r},t),\cdots]\,\varphi_1(\mathbf{r},t)\\ \cdots \\ \hat{h}[\rho(\boldsymbol{r},t),\cdots]\,\varphi_A(\mathbf{r},t)\end{bmatrix}$$

a system of **A non-linear equations** coupled by $\rho(\boldsymbol{r},t) = \sum_i^A |\varphi_i(\boldsymbol{r},t)|^2$.

... after some 'straightforward' maths

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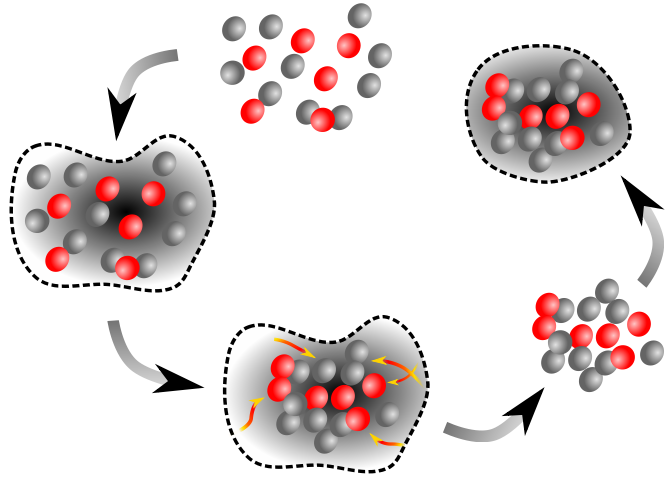
a system of **A non-linear equations** coupled by $\rho(\boldsymbol{r},t) = \sum_i^A |\varphi_i(\boldsymbol{r},t)|^2$.

How to compute the dynamics ?

Given the $\varphi_i(\boldsymbol{r},t)$:

1. Compute densities $\rho(\boldsymbol{r},t)$...
2. Compute $\hat{h}[\rho(\boldsymbol{r},t),\cdots]$
3. $\forall i$ compute

$$\varphi_i(\boldsymbol{r},t+dt) = \varphi_i(\boldsymbol{r},t) + \hat{h}[\rho(\boldsymbol{r},t),\cdots]\varphi_i(\boldsymbol{r},t)$$



Properties of the TDEDF dynamics

The equations of motion conserve

- the norm,
- **the energy** 😌

Ehrenfest theorem for one-body observables

$$\hat{O} = \int_{rr'} O_{rr'} c^\dagger(r) c(r'), \qquad i\hbar \frac{\partial}{\partial t} \langle \hat{O} \rangle = \left\langle [\hat{h}[\rho]; \hat{O}] \right\rangle$$

If $\hat{O}$ commutes with $\hat{h}$, its expectation value is a **constant of the motion**

- Number of particles 😌
- Center of mass momentum

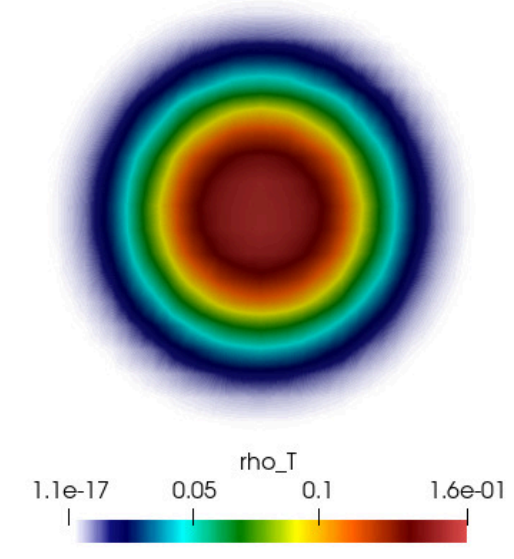
Preservation of self-consistent symmetries

Axiality, parity, ...

Link to static EDF/Hartree-Fock

The mean-field ground state does not evolve

$$|\phi_{GS}(t)\rangle = e^{i\theta(t)} |\phi_{GS}(t=0)\rangle$$



'Movie' of the ^{16}O ground state local one-body density $\rho(\boldsymbol{r}, t)$

Let's simulate a ^{16}O+^{208}Pb collision

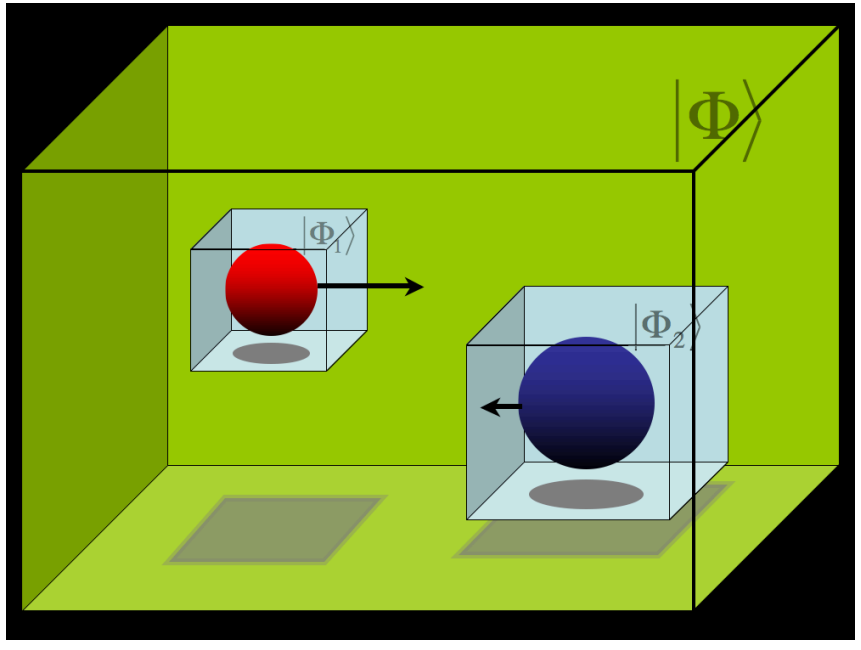
Building the initial state

1. Compute the mean-field ground states of the nuclei
2. Place them in a box
3. Boost their center of mass

$$\forall i \in [1, A_1]: \quad \varphi'_i(\boldsymbol{r}) = e^{i\mathbf{p_1}\cdot\boldsymbol{r}}\varphi_i(\boldsymbol{r})$$
$$\forall i \in [1, A_2]: \quad \varphi'_i(\boldsymbol{r}) = e^{i\mathbf{p_2}\cdot\boldsymbol{r}}\varphi_i(\boldsymbol{r})$$

4. Build the product Slater determinant

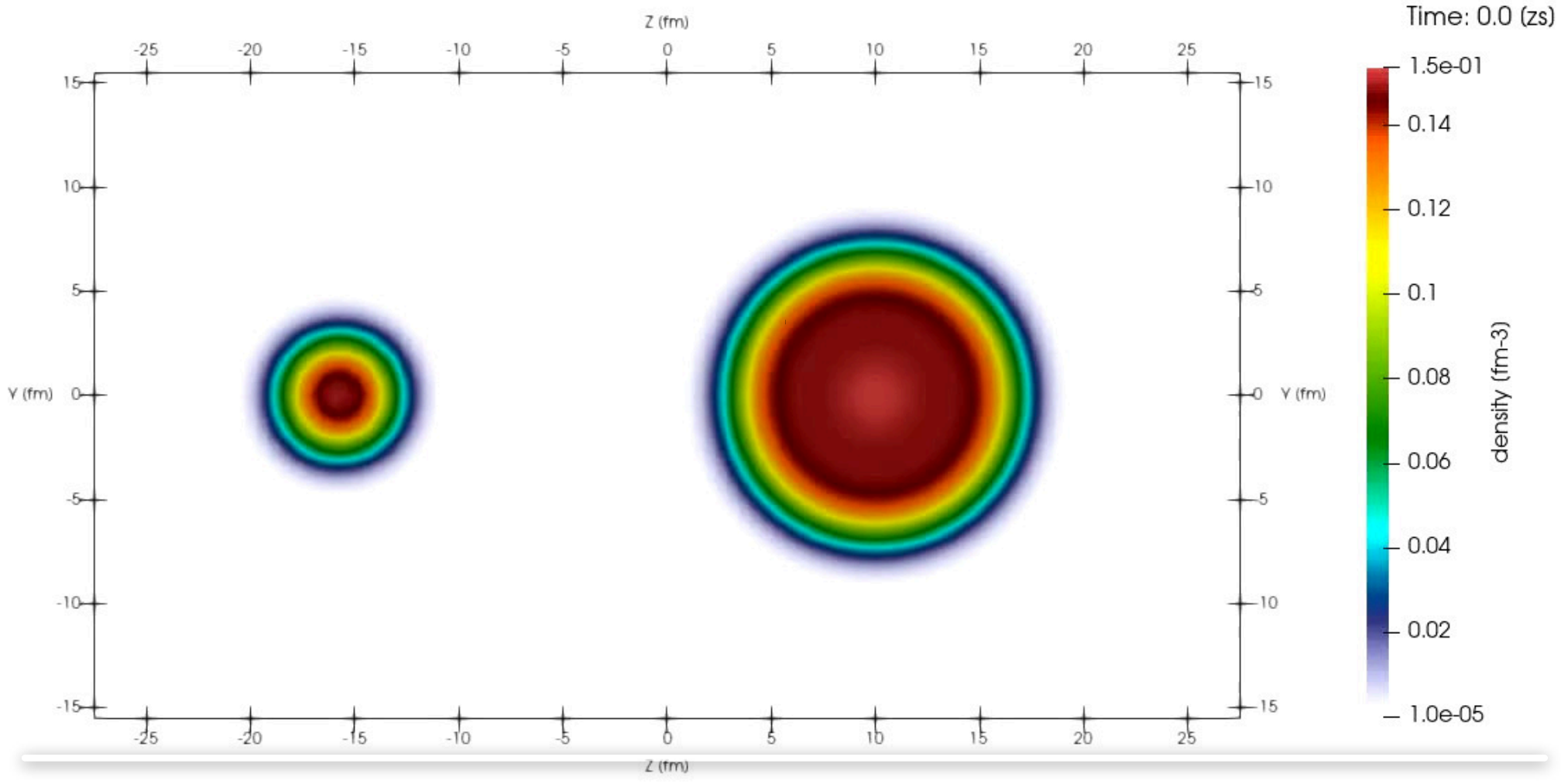
$$\phi_{proton}(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_8, \boldsymbol{r}_9, \cdots, \boldsymbol{r}_{90}) = \frac{1}{\sqrt{(8+82)!}}$$
$$\begin{vmatrix} \varphi_1(\boldsymbol{r}_1) & \cdots & \varphi_8(\boldsymbol{r}_1) & \varphi_9(\boldsymbol{r}_1) & \cdots & \varphi_{90}(\boldsymbol{r}_1) \\ \varphi_1(\boldsymbol{r}_2) & \cdots & \varphi_8(\boldsymbol{r}_2) & \varphi_9(\boldsymbol{r}_2) & \cdots & \varphi_{90}(\boldsymbol{r}_2) \\ \vdots & \cdots & \vdots & \vdots & \ddots & \vdots \\ \varphi_1(\boldsymbol{r}_{90}) & \cdots & \varphi_8(\boldsymbol{r}_{90}) & \varphi_9(\boldsymbol{r}_{90}) & \cdots & \varphi_{90}(\boldsymbol{r}_{90}) \end{vmatrix}$$



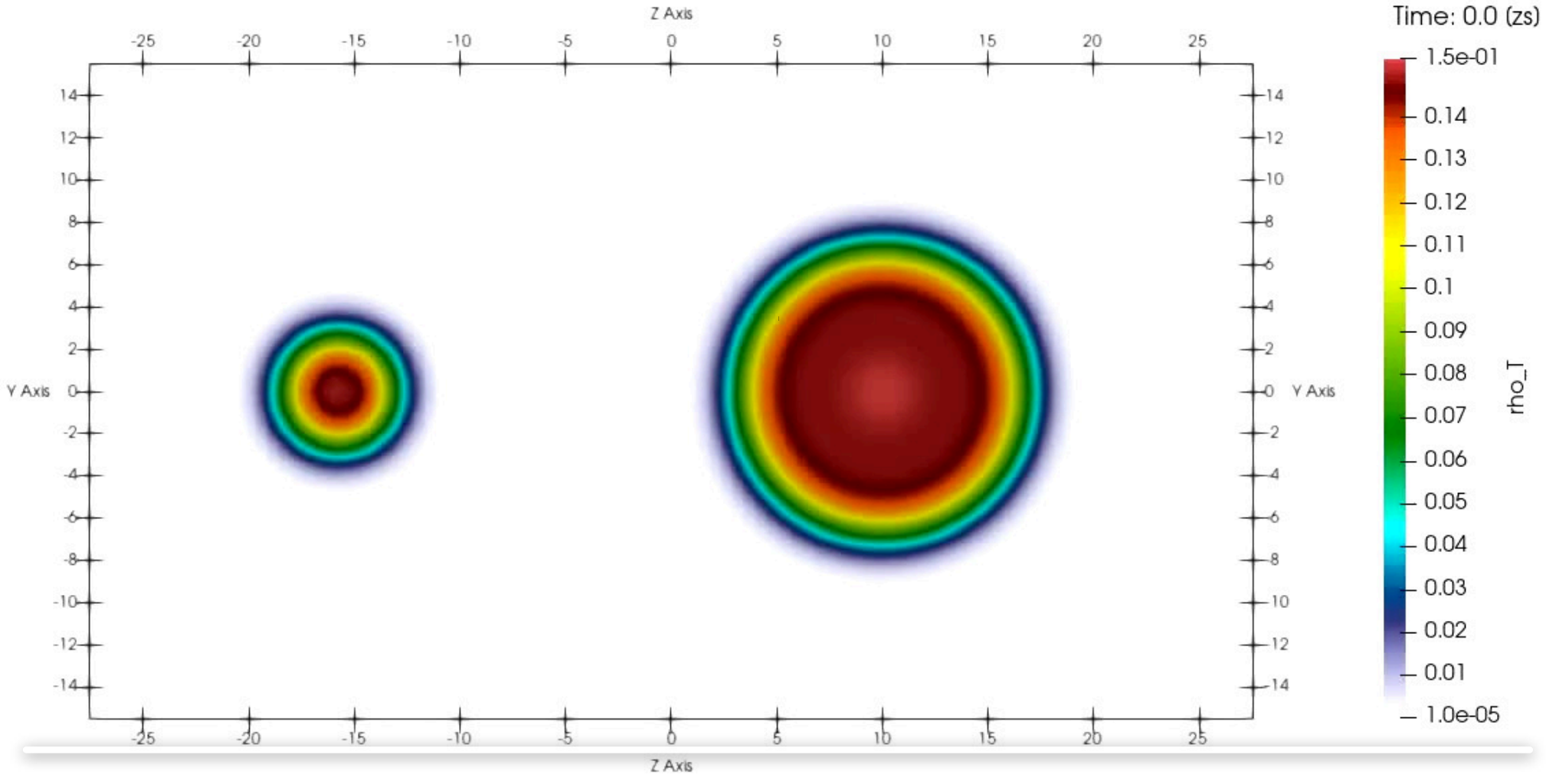
C. Simenel *et al.*. arXiv:0806.2714v2 (2009)

What impact parameter ?

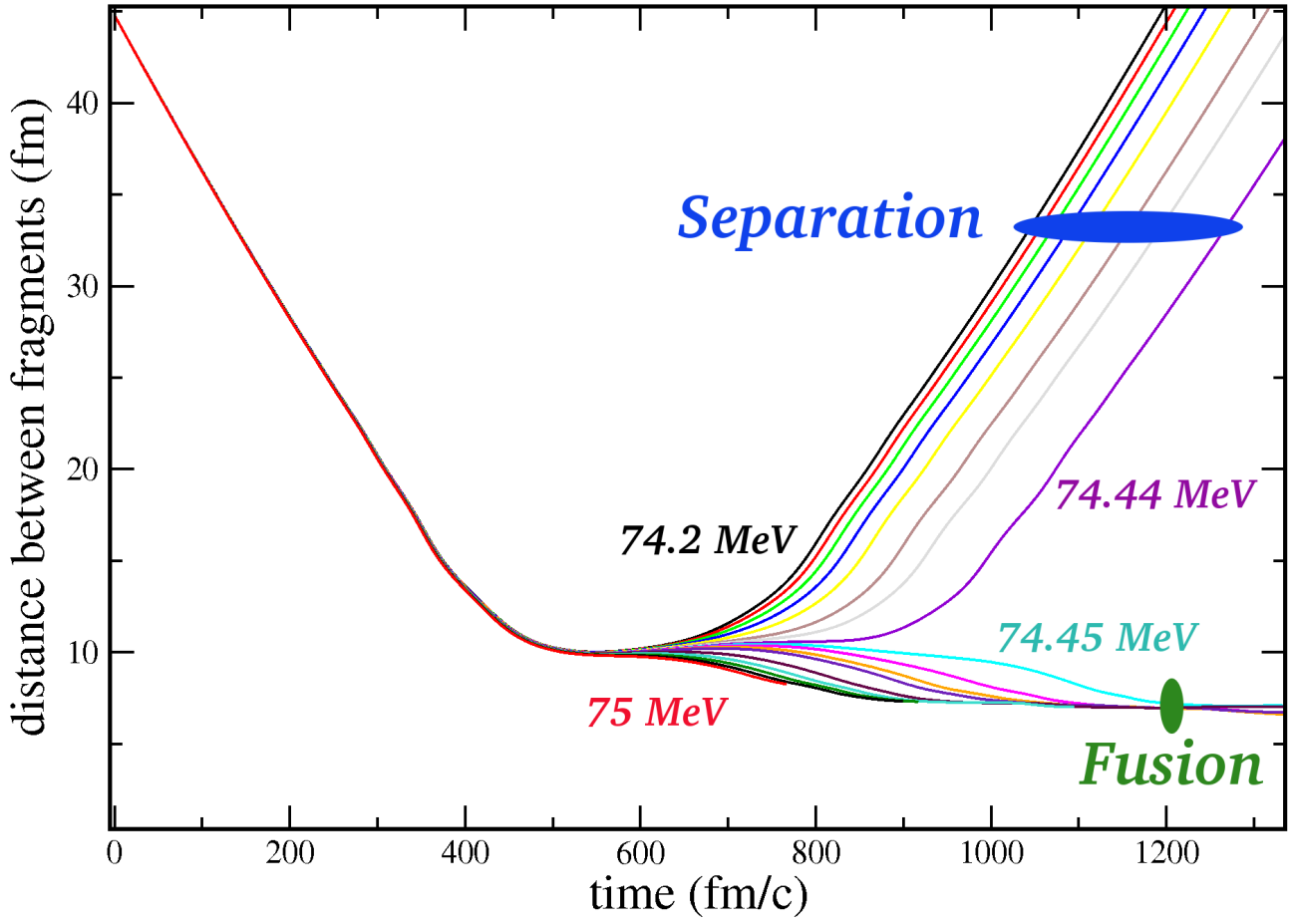
Head-on collision simulation below barrier



Head-on collision simulation above barrier



Determination of the 'fusion barrier'



C. Simenel, Eur. Phys. J. A. 61 (2025)

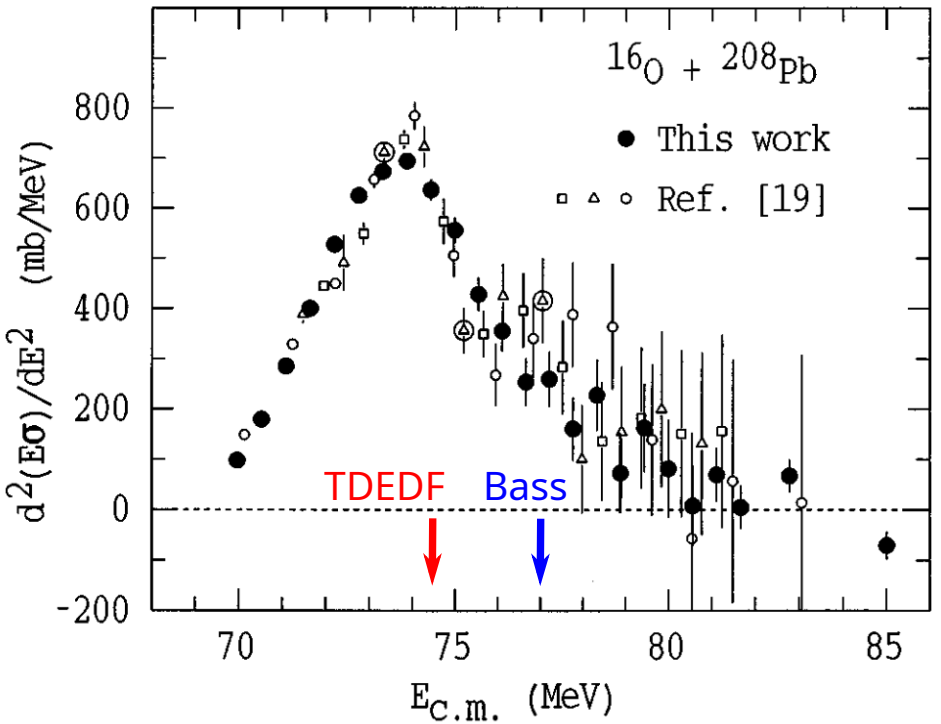
Wrapping up what we achieved...

We

- Started from an EDF
  (mostly fitted on **masses and radii**)
- Approximated the many-body dynamics
- Implemented the equations of motion
- Simulated collisions from various initial conditions
- Estimated the minimal energy to fusion !



Minimal energy to fusion 74.44 **MeV**



Distribution of 'fusion barrier'
Adapted from C.R. Morton *et al.* Phys. Rev. C **60** (1999)

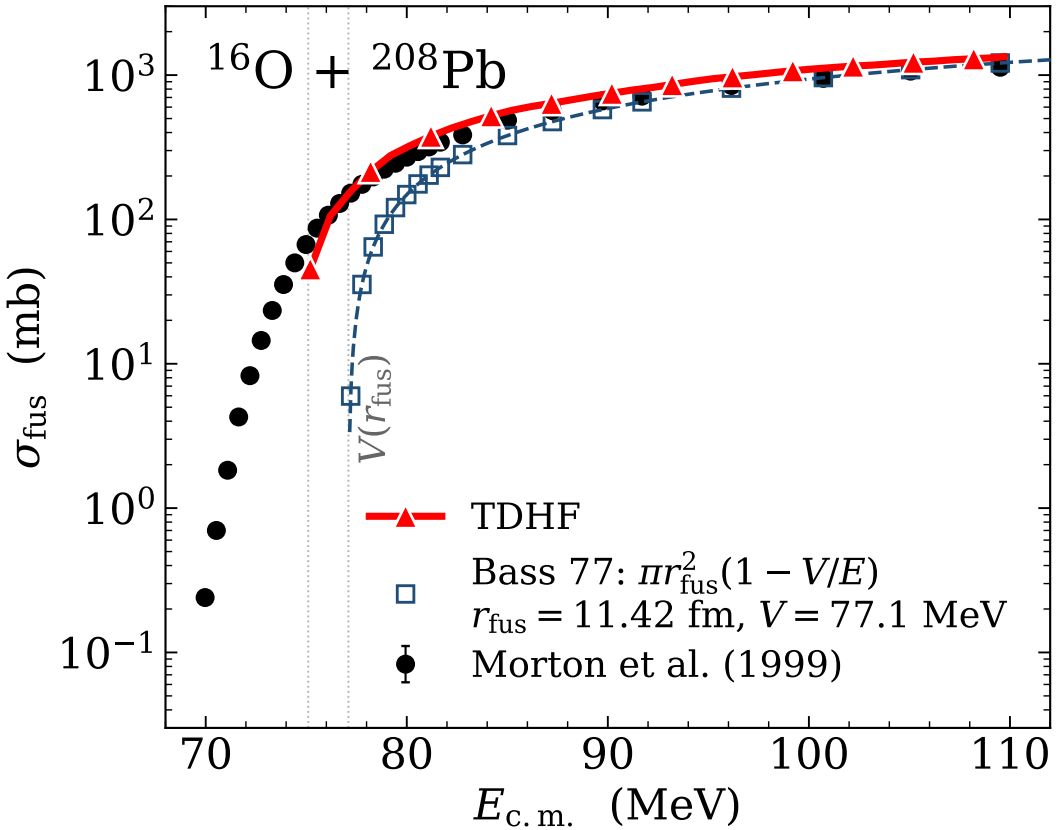
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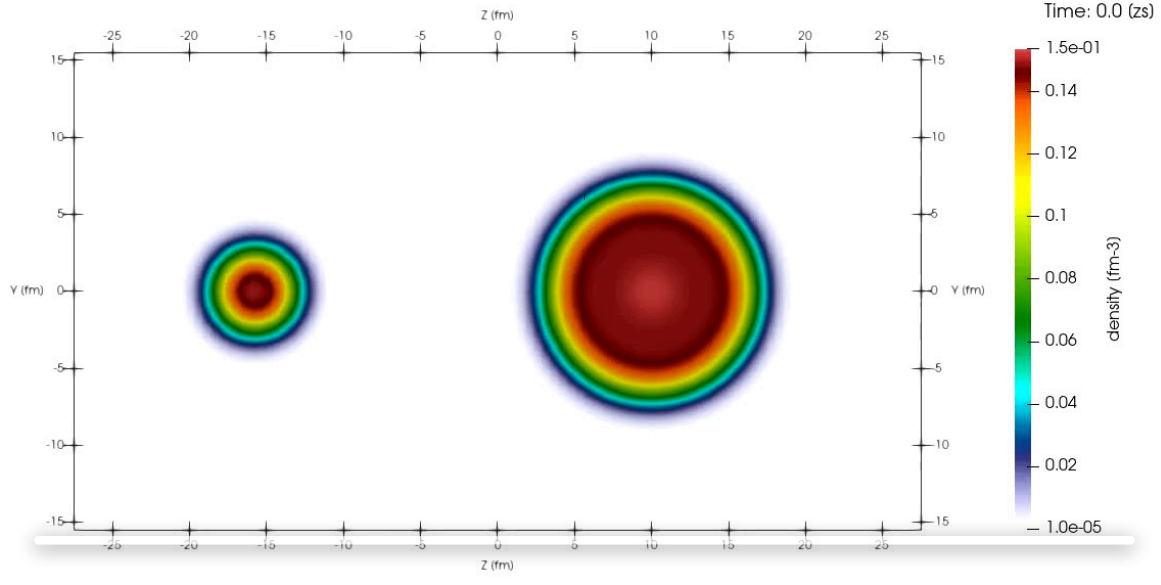
Estimated fusion cross section

Why TDEDF differs from Bass ?

Why TDEDF differs from Bass ?

1. **Coulomb excitation** of the low lying states of ^{208}Pb
   - First 3^- state
2. **Transfer reaction** just below the fusion threshold
   - $^{16}O +^{208} Pb \rightarrow^{14} C +^{210} Po$
   - change of $Z_1 Z_2 \implies$ change of Coulomb barrier

C. Simenel, Eur. Phys. J. A. 61 (2025)



At any time, we can count

- the number of particles on the left hand side
- the excitation energy in ^{208}Pb

Summary on time-dependent EDF

Pros

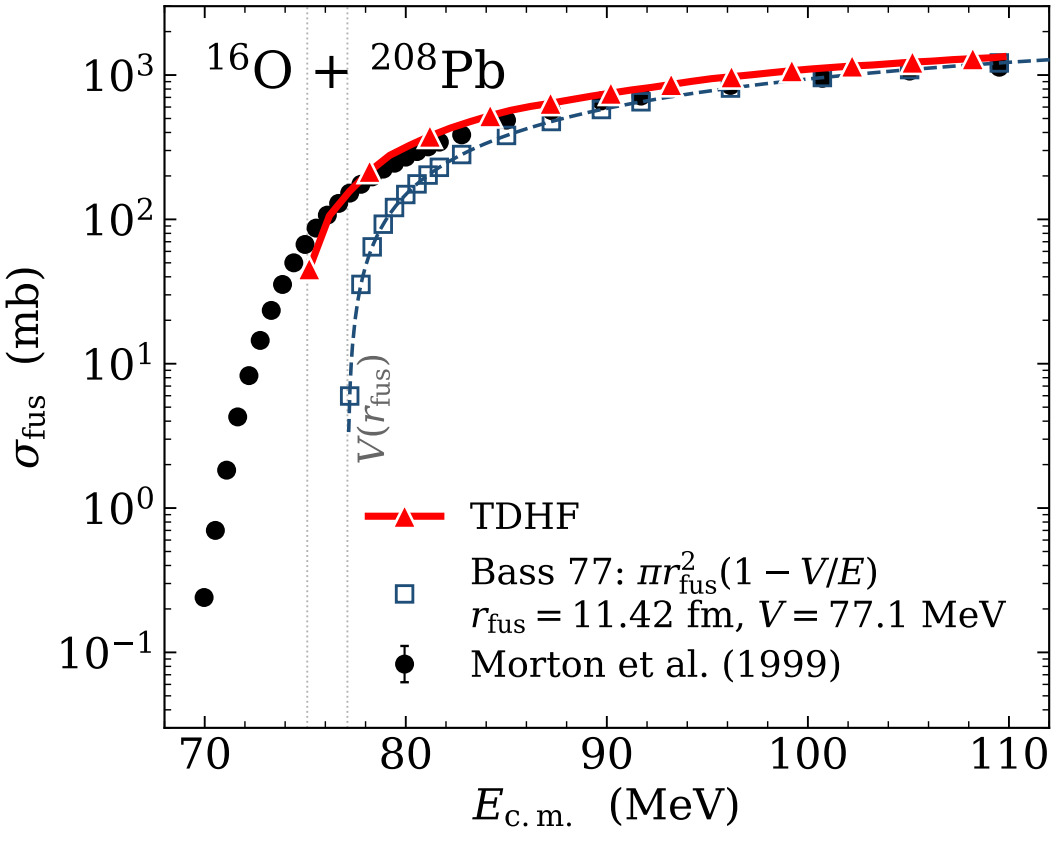
- A time-dependent variational approximation
- All the degrees of freedom
- **Systematic prediction** of fussion thresholds

  K. Sekizawa, Front. in Phys., Mini Review (2019)
- Predictions of transfer reactions
- Nice movies...

You can do these calculations !

Limitations

- Not able to predict the cross section
- No fusion probability below the threshold
- It evolves the center of mass coordinate



Estimated fusion cross section

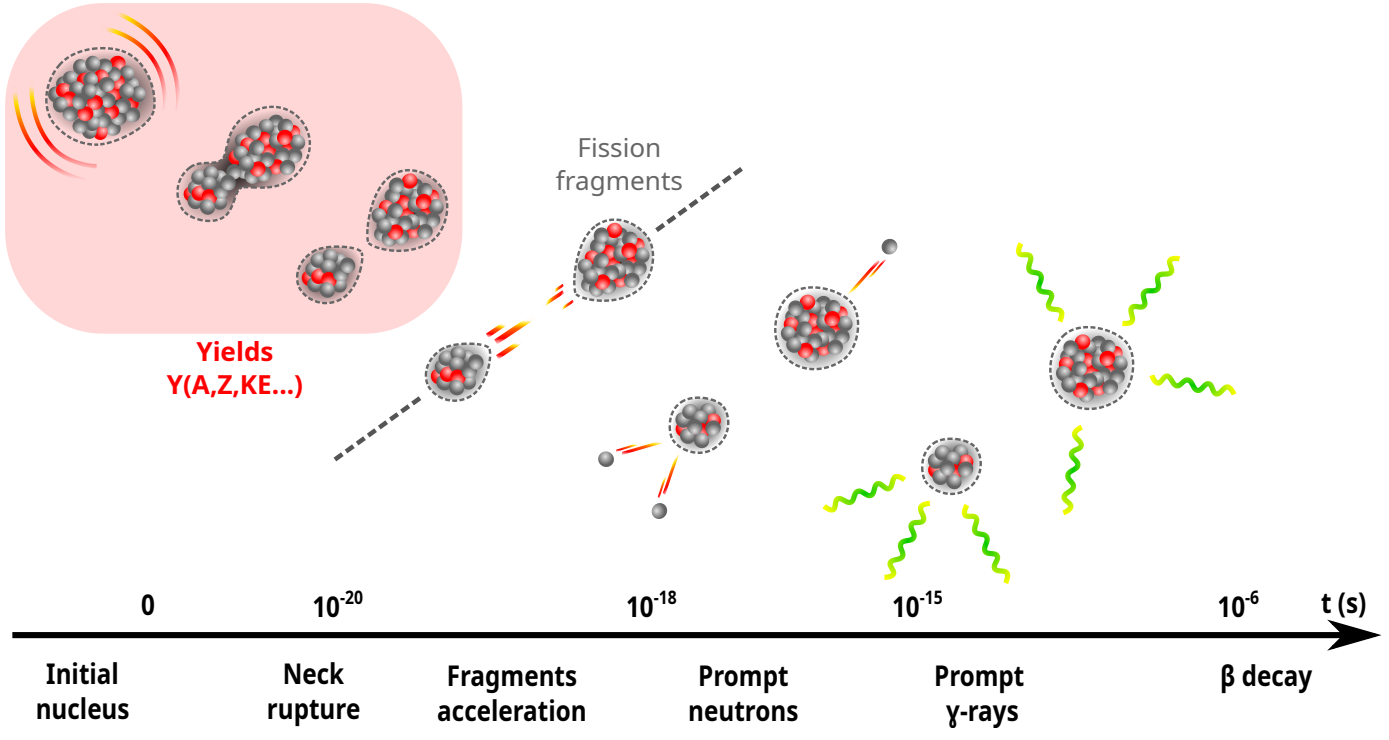
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I. Heavy-ion fusion threshold with TDEDF

II. **Fission yields with TDGCM**

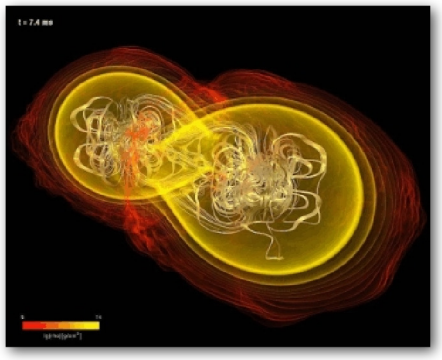
III. State-of-the-art and open challenges

Simulating the fission dynamics

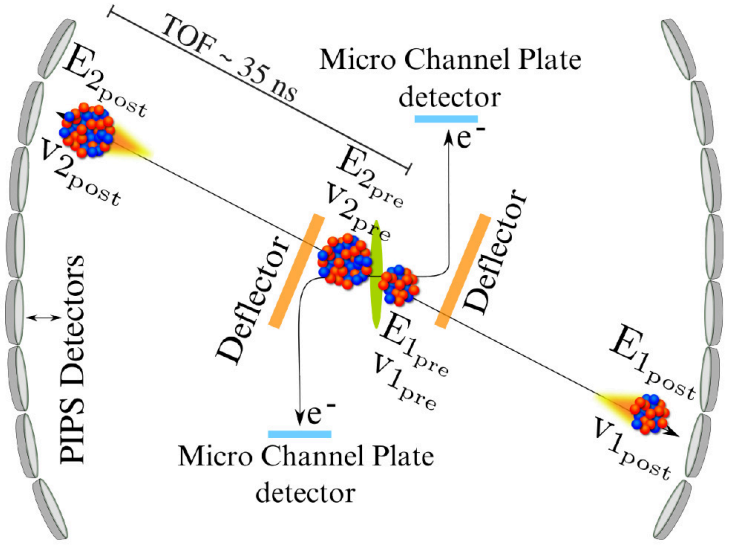






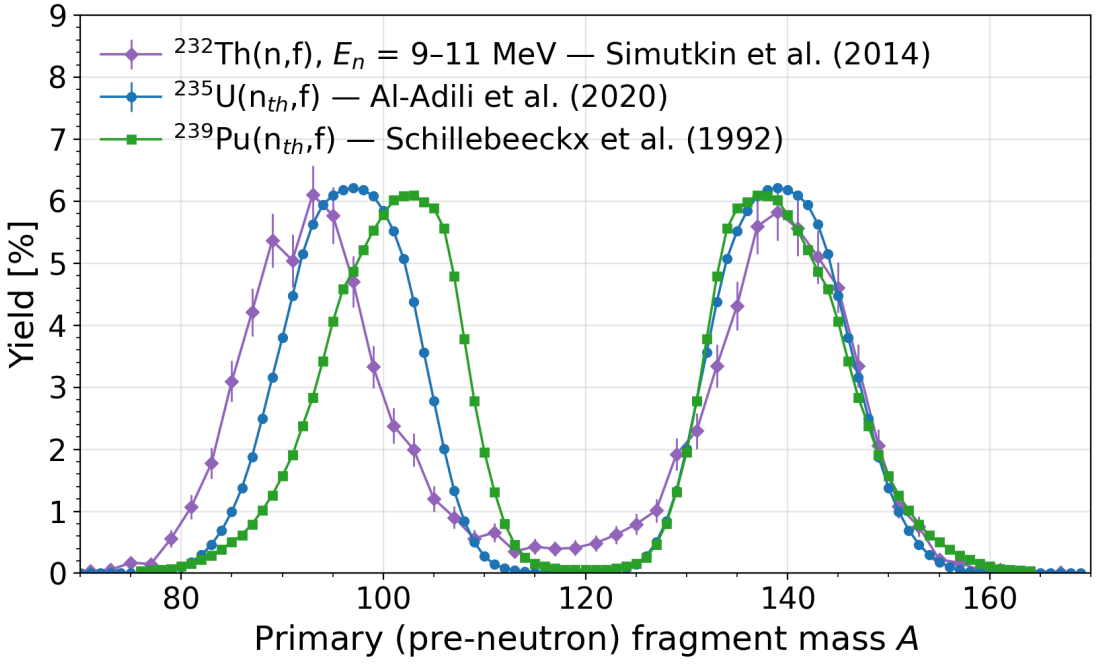


Fission yields of actinides



The VERDI detector

A. M. Gomez *et al.* EPJ Web of Conf. (2025)

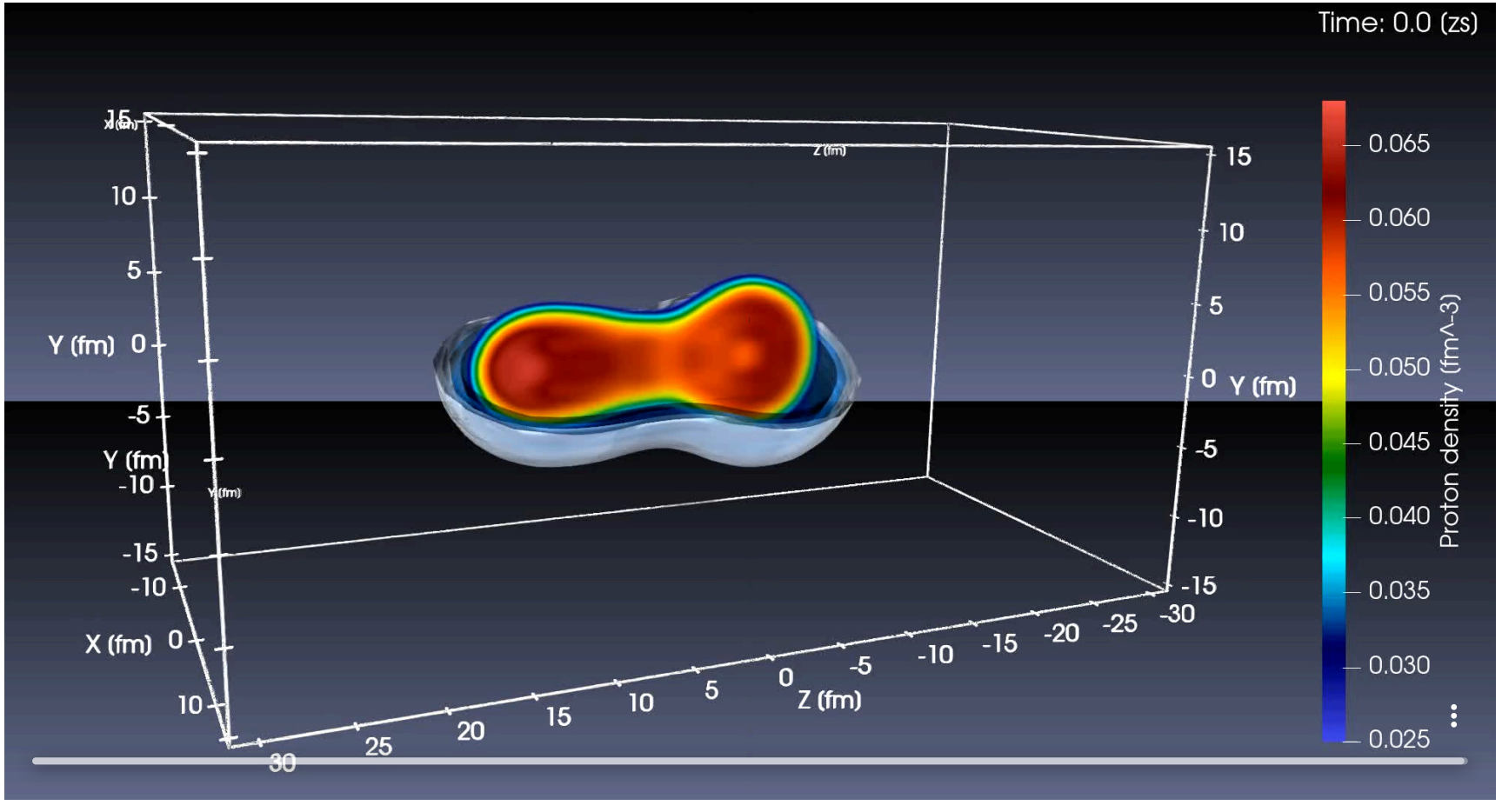


Experimental primary fission mass yields

- Large width of the mass distribution
- Stability of the heavy peak

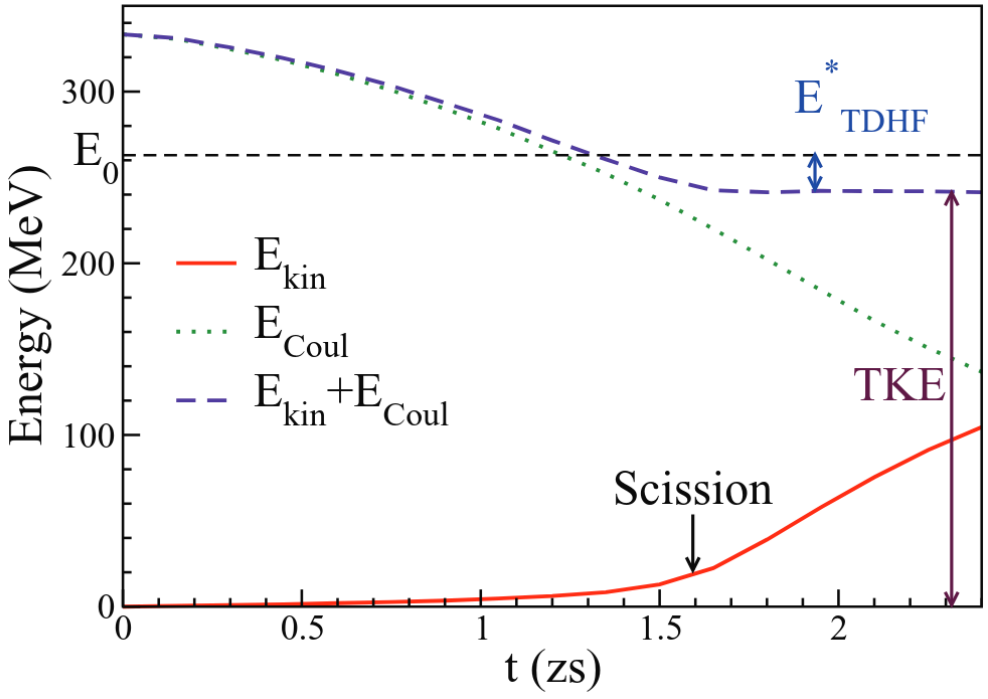
How could we predict fission mass yields ?

Fission with time-dependent EDF



TDEDF (with pairing) simulation of fission of ^{240}Pu

Comparison to experimental data



Energy balance

C. Simenel PRC 89 (2014)

Total kinetic energy

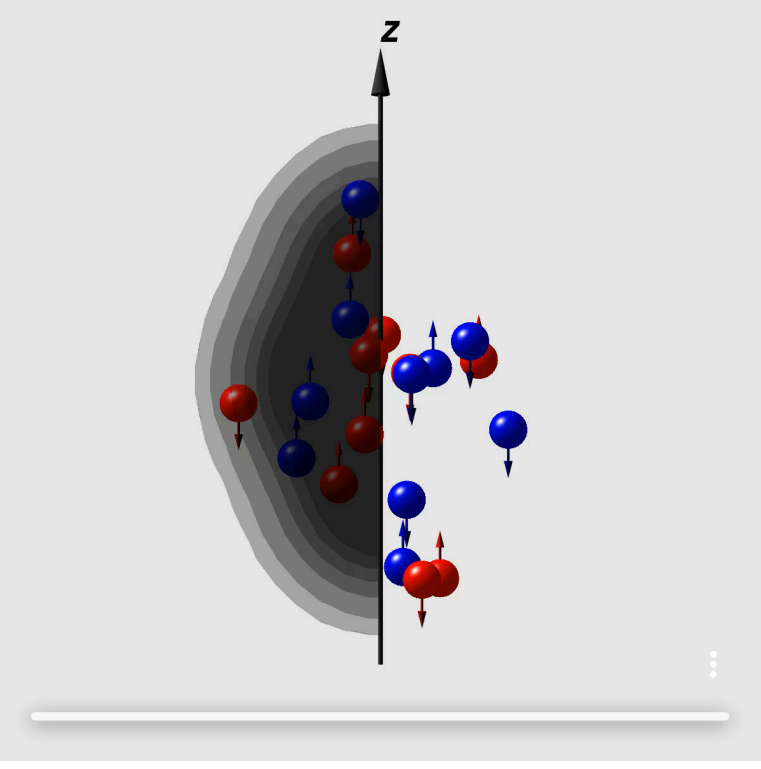
^{240}Pu fission events with a A=135 fragment

Ref.	TKE [MeV]
Wagemans (1984) [4]	183.92
Geltenborg (1986) [5]	184.29
Nishio (1995) [6]	184.83
Tsuchiya (2000) [7]	181.55

TDEDF predicts **184.9 MeV** 😄

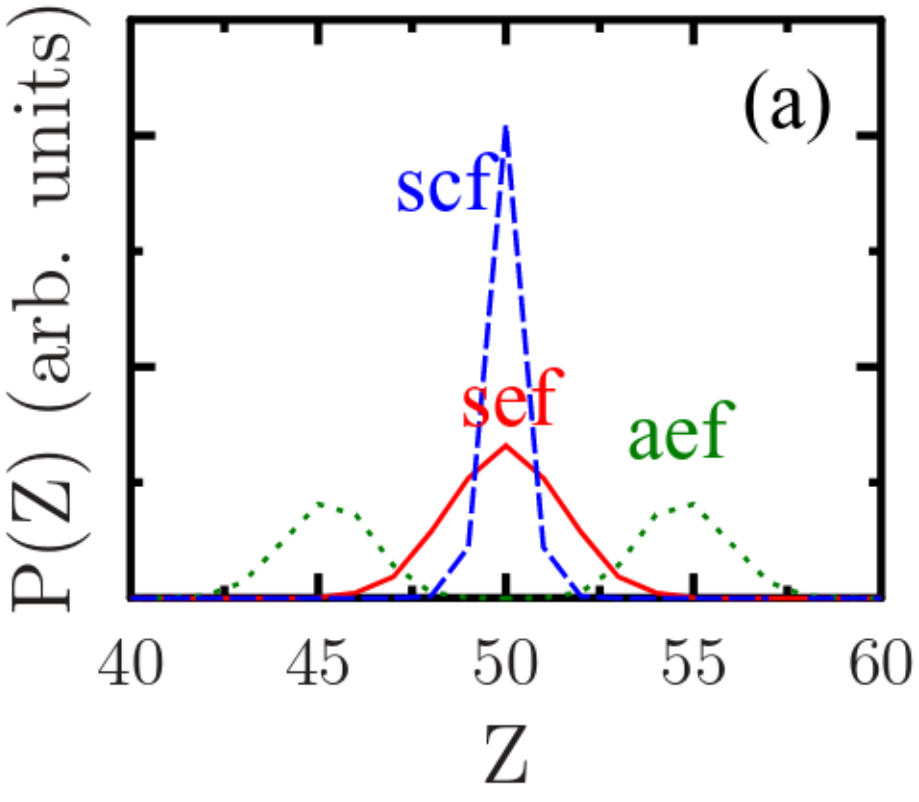
Yes but what about the yields ?

Counting the particles in the fragments



Distribution of the nucleons in a ^{20}Ne mean-field ground state

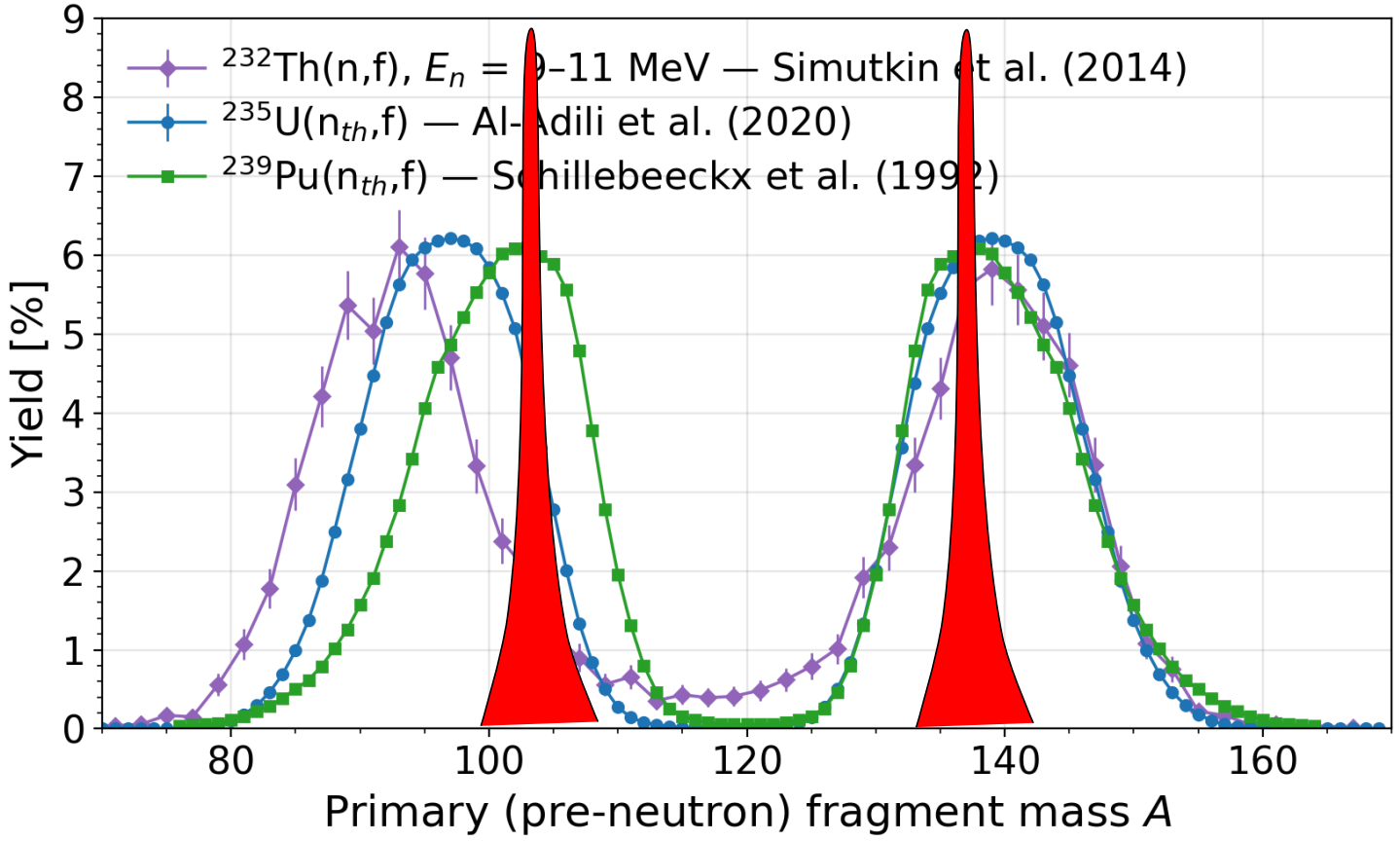
$$p(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A) = |\phi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_2)|^2$$



Charges in one fragment after 3 TDEDF simulations

G. Scamps *et al.*, PRC **92** (2015)

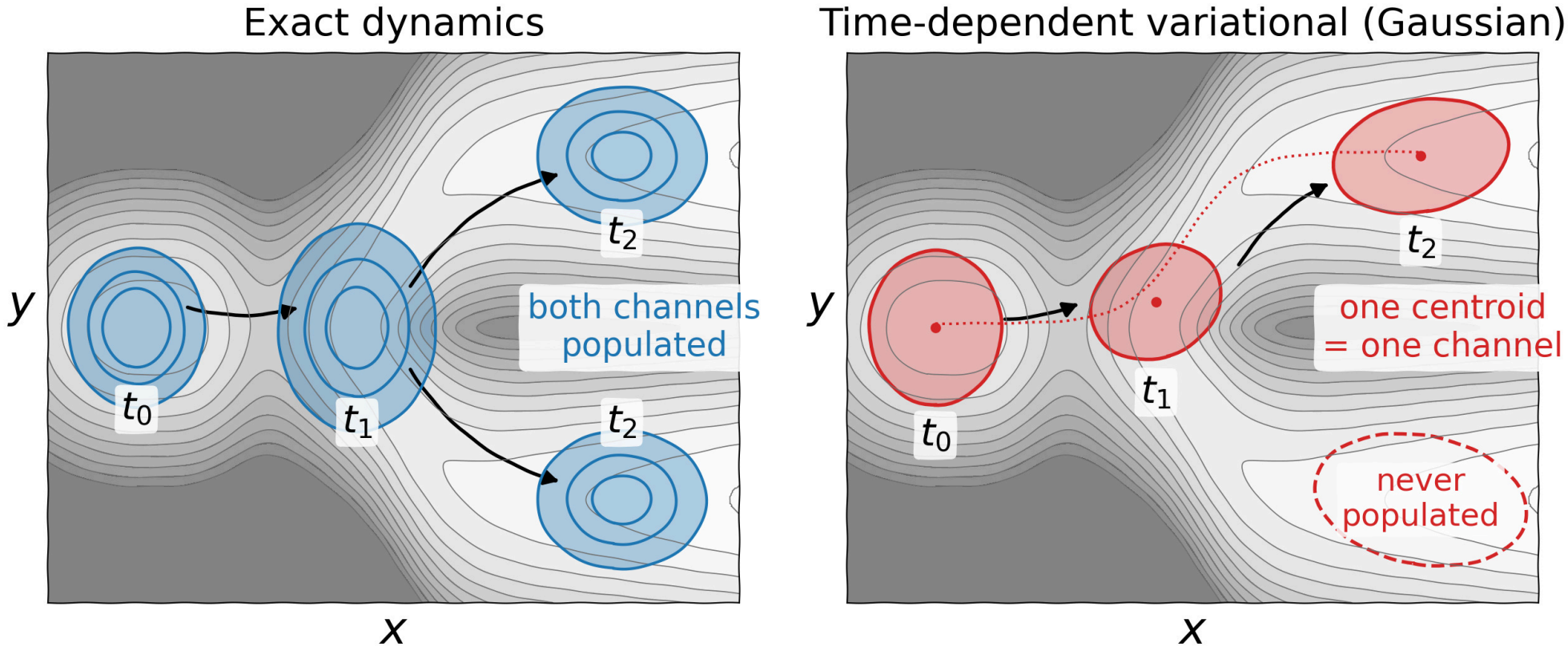
Typical results from TDEDF



Way too sharp...

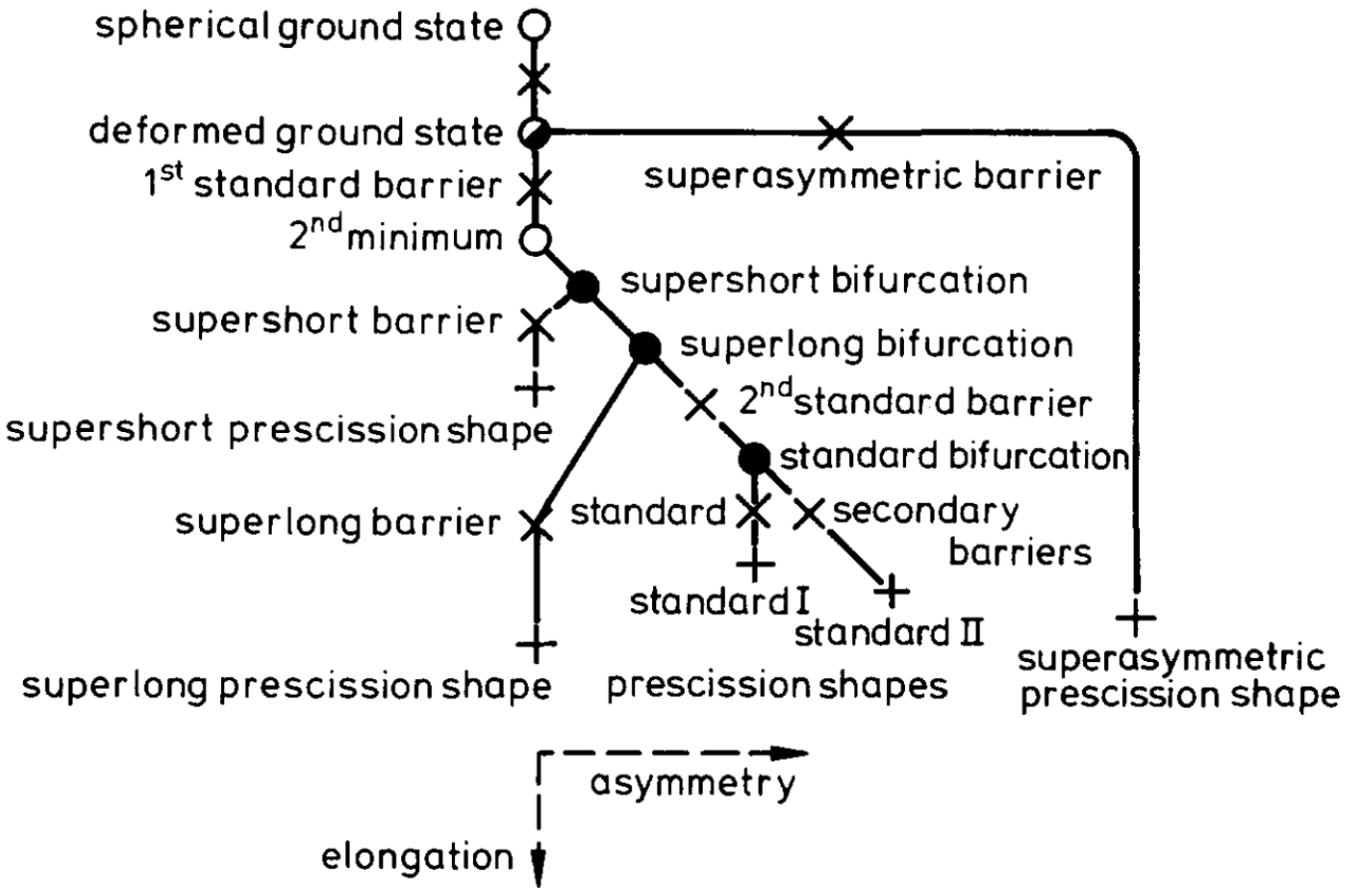
Why does TDEDF fail for the yields ?

Why does TDEDF fail for the yields ?



Schematic of a 2D quantum evolution

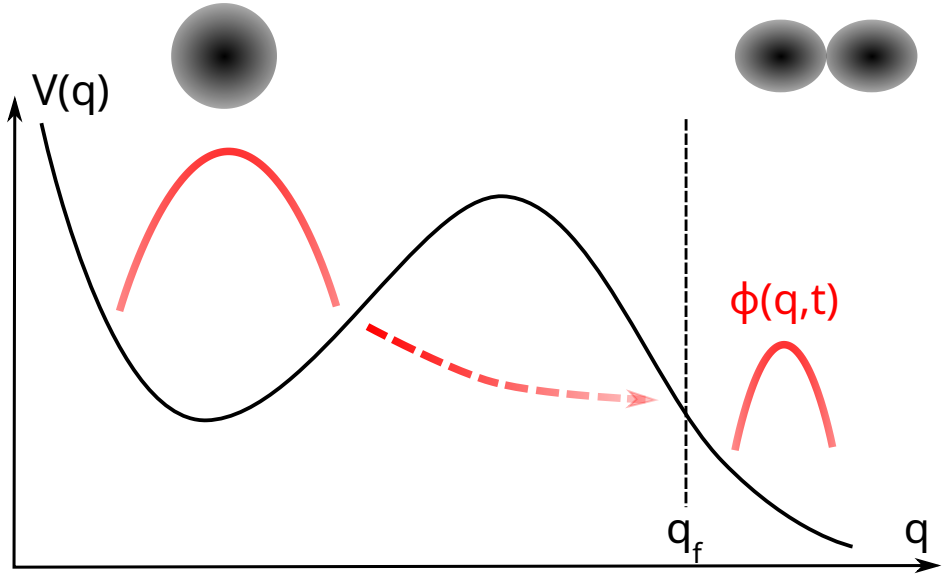
Fission modes



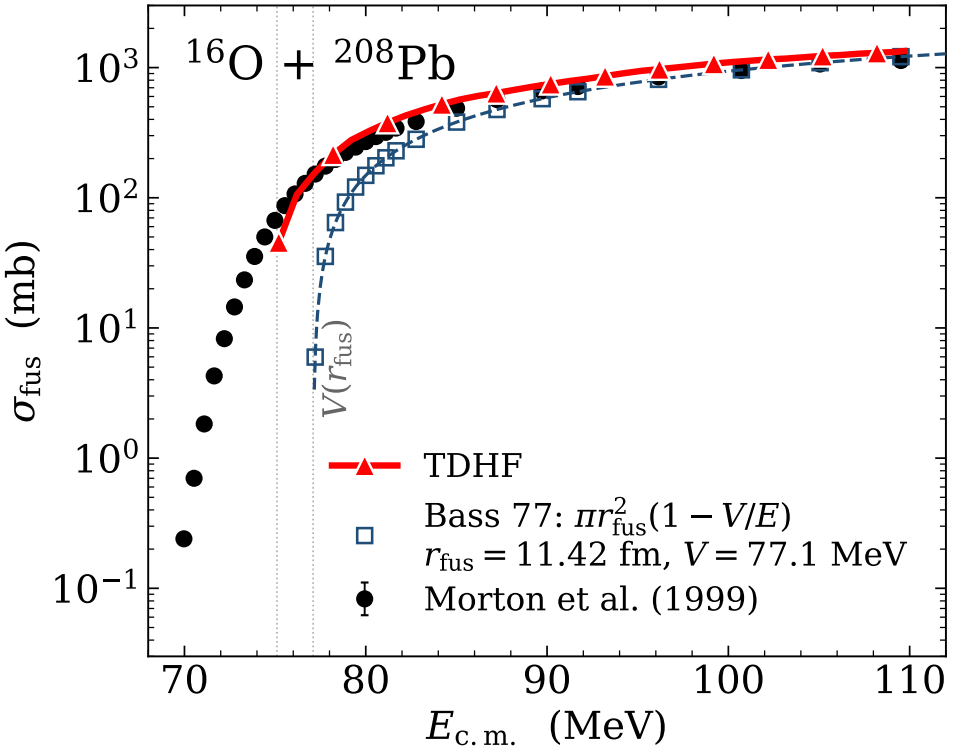
The 'tree of nuclear fission'
U. Brosa *et al.* Phys. Rep. 197 (1990)

- Exact dynamics populates all modes
- **TDEDF chooses one**

Side comment on quantum tunneling...



- After tunneling the wavefunction is **bi-modale**
- Cannot be described by a Gaussian approximation



Estimated fusion cross section

TDEDF poorly describes tunneling

How to predict multi-modal dynamics ?

How to predict multi-modal dynamics ?

TDGCM = Time-Dependent Generator Coordinate Method

Main idea

- We would like to describe at the same time



How to predict multi-modal dynamics ?

TDGCM = Time-Dependent Generator Coordinate Method

Main idea

- We would like to describe at the same time



- Let's work with the superposition

$$|\psi(t)\rangle = f_1(t)\Big|\quad\Big\rangle + f_2(t)\Big|\quad\Big\rangle$$

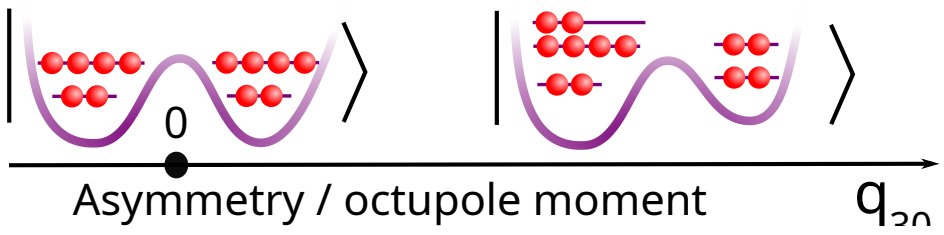
The wavefunction will be able to populate the two modes/channels

Time-dependent generator coordinate method

- State:

$$|\psi(t)\rangle = \int_{\boldsymbol{q}} f(\boldsymbol{q},t)|\phi(\boldsymbol{q})\rangle d\boldsymbol{q}$$

  - $\boldsymbol{q}$ are called **collective coordinates**
  - The function $\boldsymbol{q} \rightarrow |\phi(\boldsymbol{q})\rangle$ is the **reaction path**.



- Interaction:
  $\hat{H}$ or $E(|\psi\rangle)$

Method

1. Build a reaction path
2. Compute the evolution of the $f(\boldsymbol{q}_k,t)$

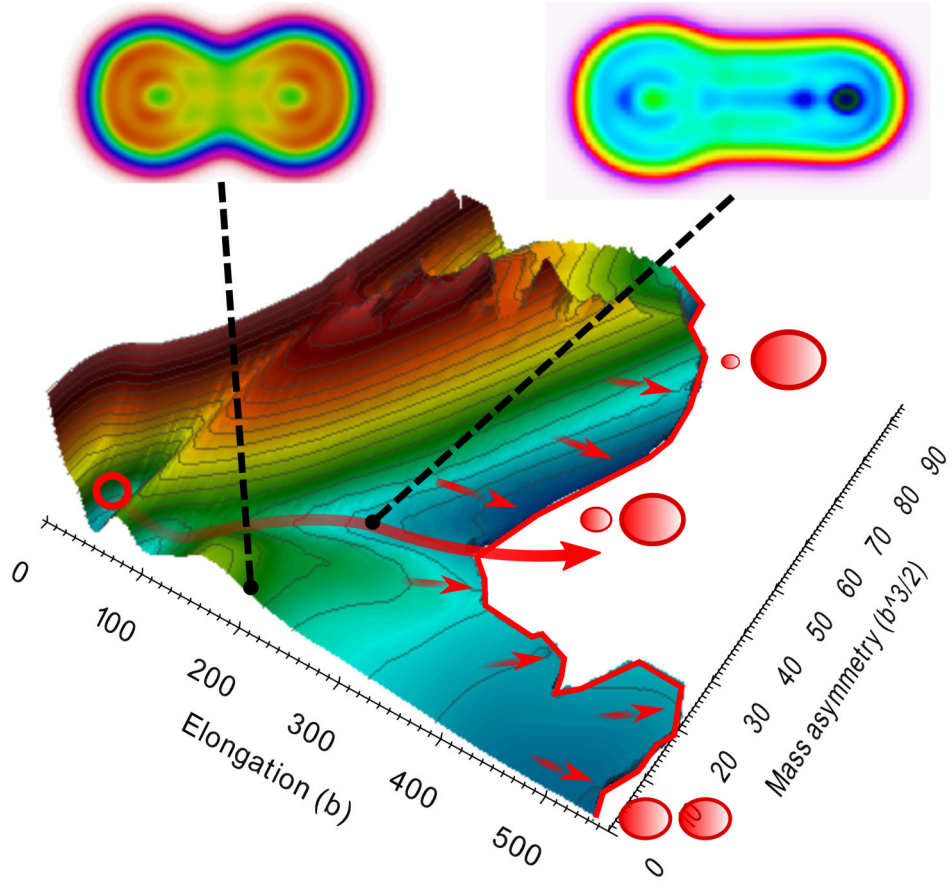
- Discretization

$$f(\boldsymbol{q},t) = \sum_{k=1}^{K\simeq 5.10^3} f(\boldsymbol{q}_k,t) \times b_k(\boldsymbol{q})$$

- parameterizing $\psi(\boldsymbol{r}_1 \cdots \boldsymbol{r}_A, t=0)$
  $\simeq 5.10^3 \times 2.10^6$ complex numbers
  $\simeq 100$ **GB**

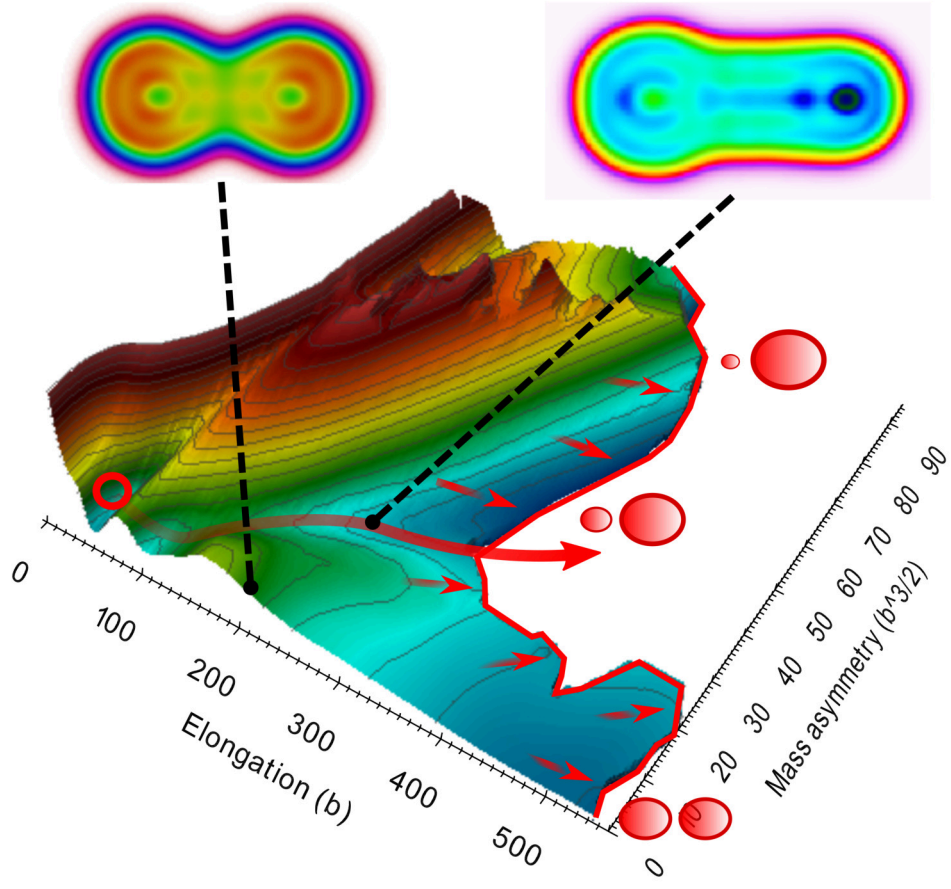
Reaction path for a n + ^{239}Pu fission

1. Collective variables:
   - elongation q_{20} [b],
   - mass asymmetry q_{30} [b$^{3/2}$]
2. $\forall(q_{20}, q_{30})$ compute the Boboliubov vacuum $|\phi(q_{20}, q_{30})\rangle$ that
   - verifies $\langle\hat{Q}_{20}\rangle = q_{20}$,
   - verifies $\langle\hat{Q}_{30}\rangle = q_{30}$,
   - minimizes the energy.



Reaction path for a n + ^{239}Pu fission

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   - minimizes the energy.



The physicist **chooses** the channels that can be explored

Equation of motion for the weights

How do the parameters $f(\boldsymbol{q}_k, t)$ of the wavefunction evolve in time ?

Equation of motion for the weights

How do the parameters $f(\boldsymbol{q}_k, t)$ of the wavefunction evolve in time ?

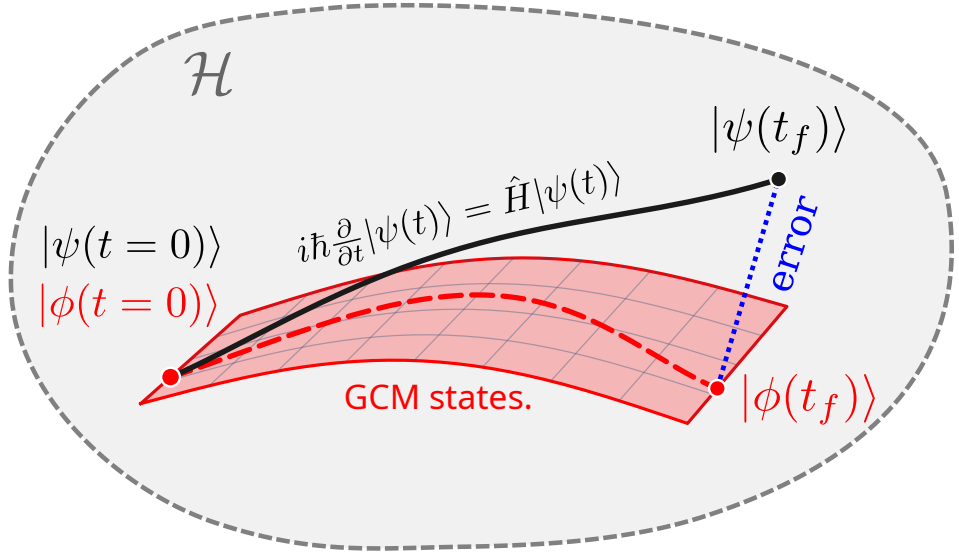
Time-dependent variational principles

- Variational approximation:

$$\delta_{\text{GCM states}} \left(\int_{t=0}^{t_f} i\hbar \langle \phi(t) | \frac{\partial}{\partial t} \phi(t) \rangle - E(|\phi(t)\rangle) \right) = 0$$

Look for the $f(\boldsymbol{q}_k, t)$ that make the action extremum

$$\forall \boldsymbol{q} : \quad i\hbar \int_{q'} \mathcal{N}_{qq'} \frac{\partial f(\boldsymbol{q}', t)}{\partial t} = \int_{q'} \mathcal{H}_{qq'} f(\boldsymbol{q}', t)$$



with

$$\mathcal{N}_{qq'} = \langle \phi(\boldsymbol{q}) | \phi(\boldsymbol{q}') \rangle$$

$$\mathcal{H}_{qq'} = \langle \phi(\boldsymbol{q}) | \hat{H} | \phi(\boldsymbol{q}') \rangle$$

Simpler equations of motion for the weights

Without additional approximation

We do the change of variable

- $g(\boldsymbol{q},t) = \mathcal{N}^{1/2}\, f(\boldsymbol{q},t)$
- $\mathcal{H}^{coll} = \mathcal{N}^{-1/2}\, \mathcal{H}\, \mathcal{N}^{-1/2}$

$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \mathcal{H}^{coll} g(\boldsymbol{q},t)$$

A few dimensional Schrödinger equation !

Observables can be computed as

$$\langle \hat{O} \rangle = \int_{\boldsymbol{q}\boldsymbol{q}'} g^*(\boldsymbol{q},t)\, \mathcal{O}^{coll}(\boldsymbol{q},\boldsymbol{q}') g(\boldsymbol{q}',t)$$

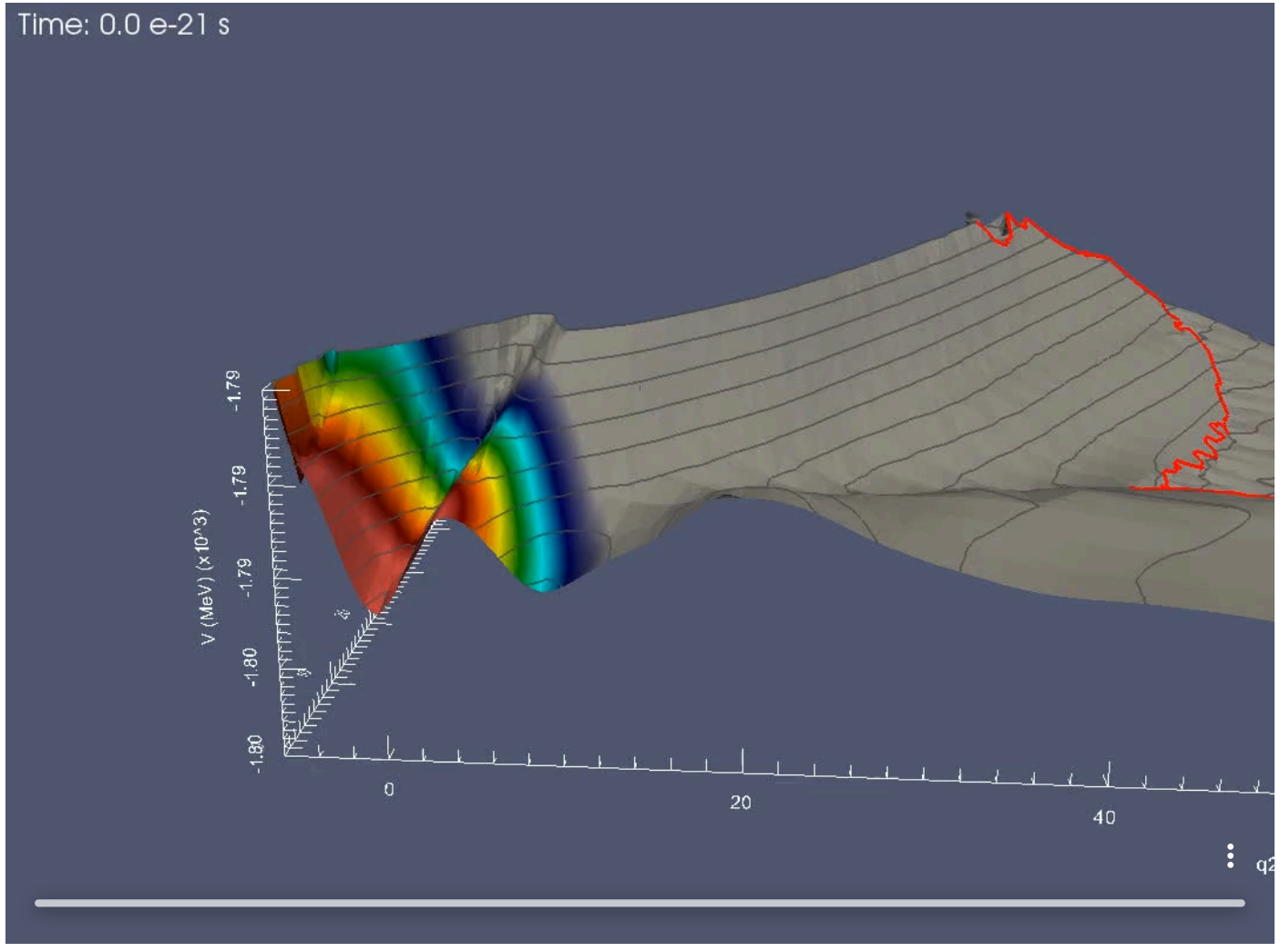
With additional approximation

- Gaussian Overlap Approximation
- Symmetric Moment Expansion

$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \left[-\frac{\hbar^2}{2} \nabla \frac{1}{M(\boldsymbol{q})} \nabla + V(\boldsymbol{q}) \right] g(\boldsymbol{q},t)$$

A local Schrödinger equation !

Evolution of the collective function $|g(\boldsymbol{q}, t)|^2$

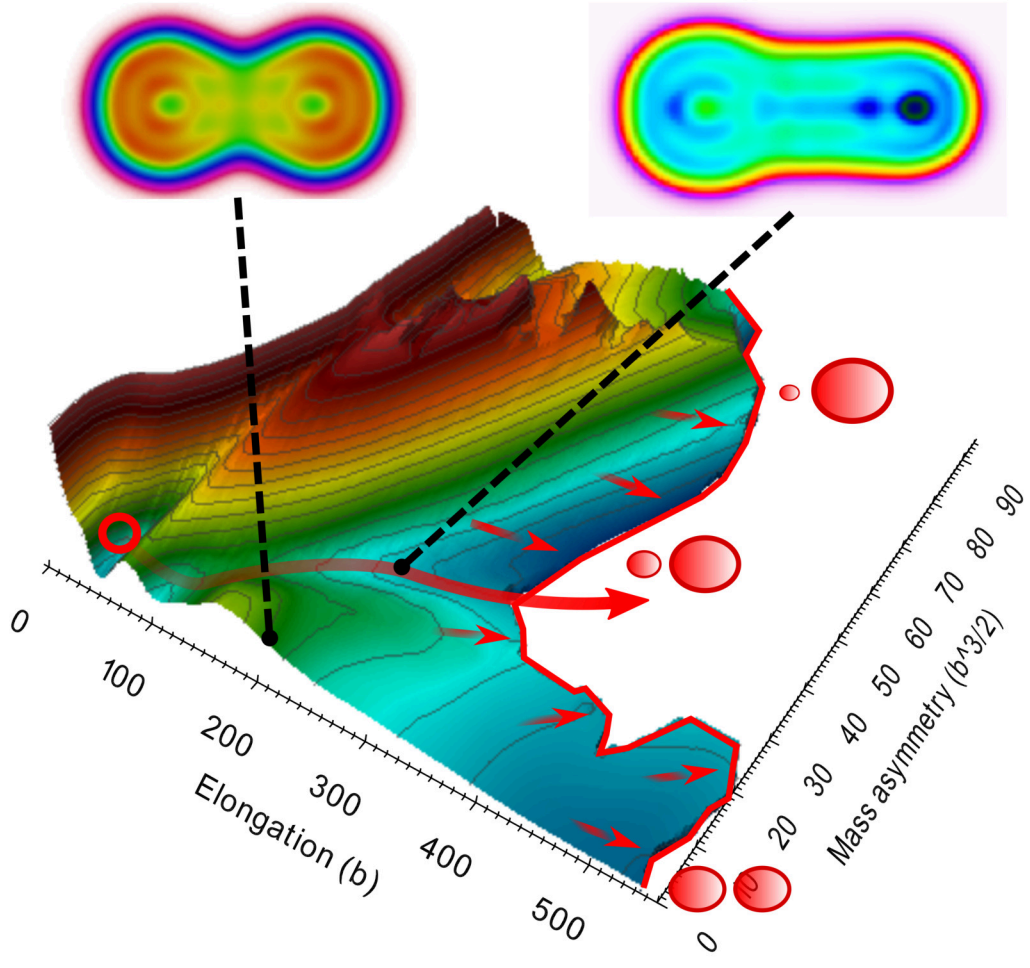


Last step to the fission yields

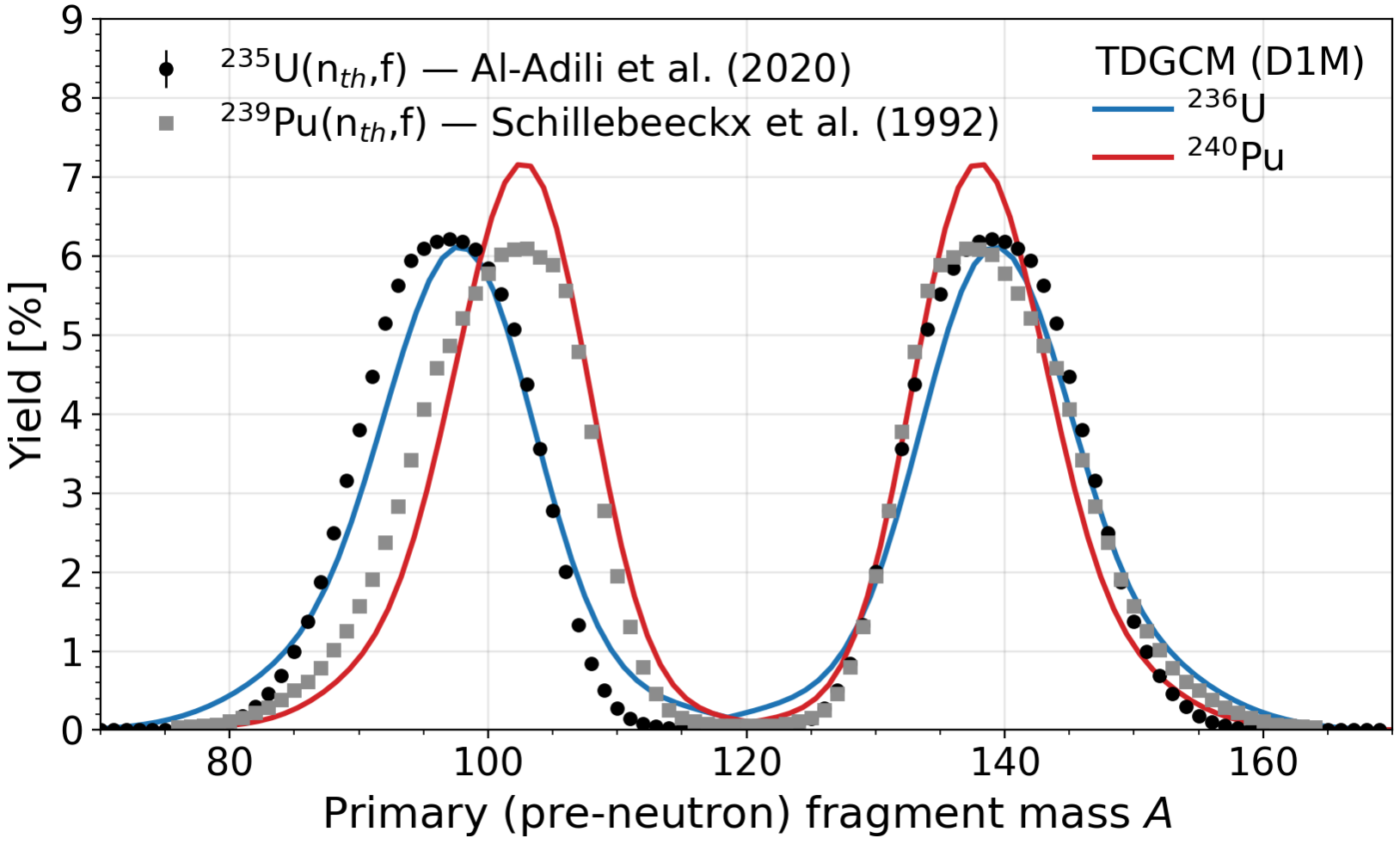
$$P(A_{Heavy}) \simeq \int_{\boldsymbol{q} \in \text{red line}} p(\boldsymbol{q}) \times p(A_{Heavy}|\boldsymbol{q})$$

We estimate $p(A_{Heavy}|\boldsymbol{q})$

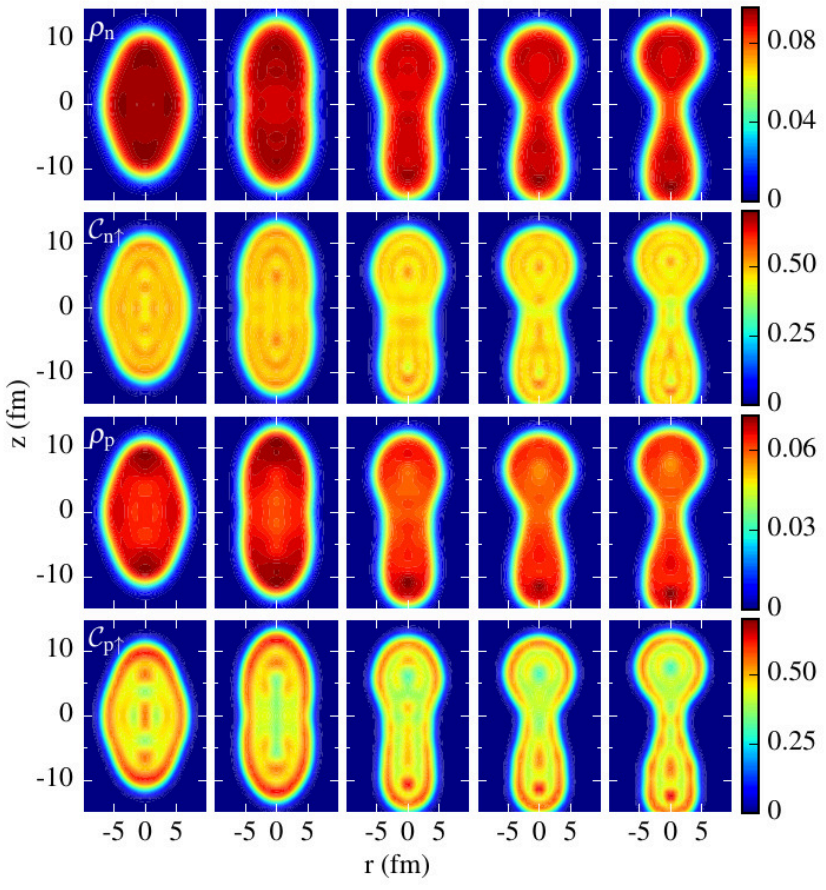
- either by counting fragments particles in $|\phi(\boldsymbol{q})\rangle$
- or with a Gaussian centered on $\langle\phi(\boldsymbol{q})|\hat{A}_H|\phi(\boldsymbol{q})\rangle$



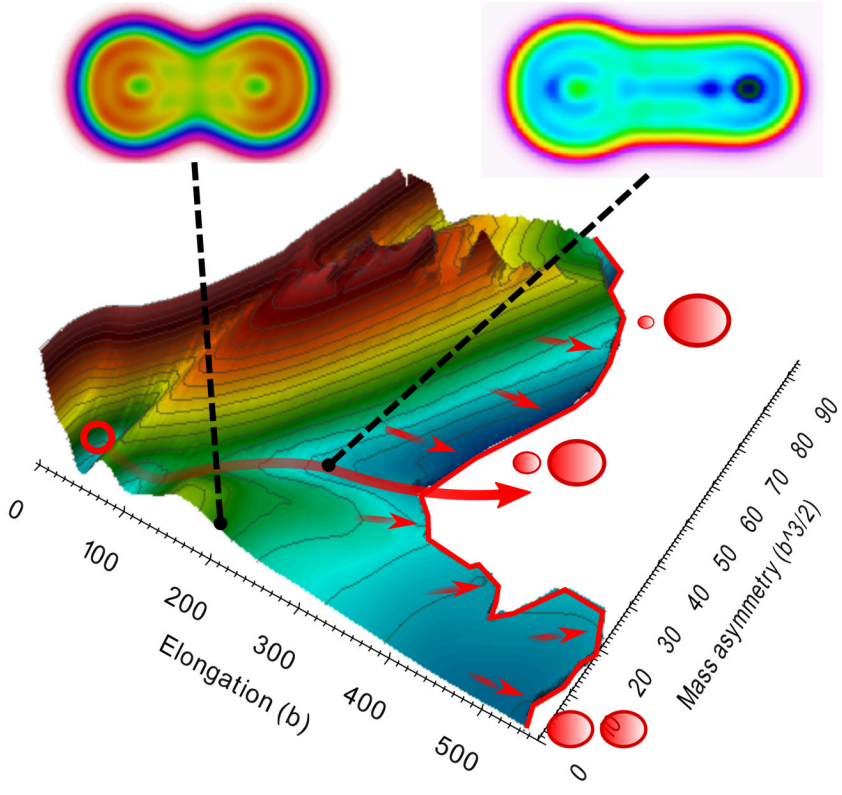
Finally our postdiction !



On the stability of the heavy peak



Densities and correlation functions in constrained HFB states C. L. Zhang *et al.* PRC 94 (2016)



The **structure of the heavy pre-fragment** favors $A_H \simeq 140$ in the asymmetric energy valley

Summary on time-dependent GCM

Pros

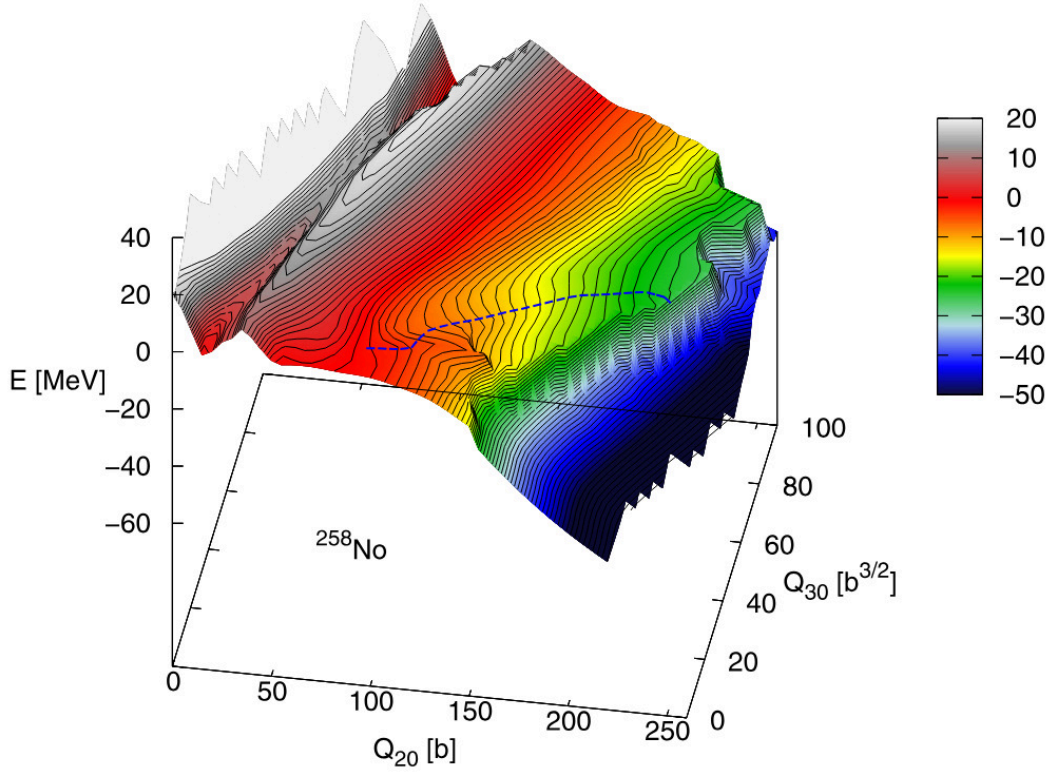
- Enables multi-channels reaction simulation
- Affordable in 2-3 dimensions
- Can 'in principle' do systematics

Could it be used to simulate tunneling ?
(*i.e.* for fission half-lives)

Limitations

(in current applications)

- Reaction paths obtained with **constrained HFB** have a lot issues
  - not the good physics
  - bad mathematical properties
- Some remaining approximations (collective inertia)



M. Han *et al.* PRC 104 (2021)

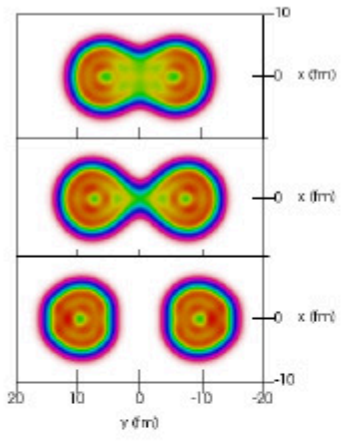
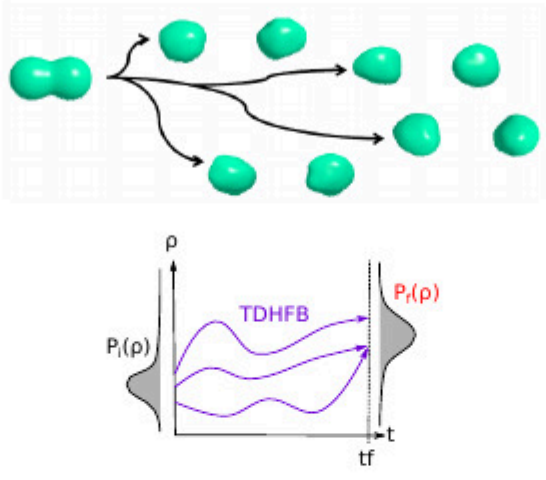
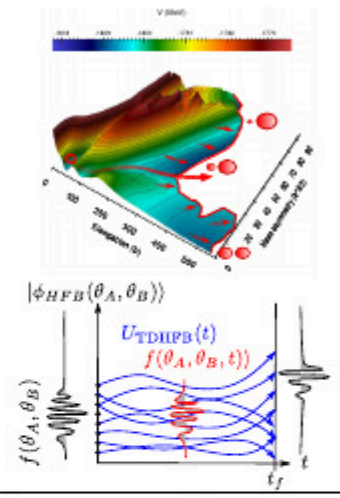
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II. Fission yields with TDGCM

III. **State-of-the-art and open challenges**

2020 status

Single reference	Semi-classical ensemble	Multi-configuration
		
• Diabatic dynamics • Misses collective fluctuations • Breaks symmetries • No collective tunnelling	• More collective fluctuations (standard deviation of 1-body observables) • Low cost, parallel algorithms • Misses quantum interferences	• Quantum fluctuations, probability distribution • Difficulty to get both fluctuations and diabatic motion • High cost, parallel algorithms in some cases • Issue with EDF kernels

2020-2025: a wealth of improvements

On the TDGCM side

- Spin of the fragments

  P. Marevic *et al.* PRC **104** (2021)

  P. Marevic *et al.* arXiv:2506.10777 (2025)
- Odd systems

  N. Schunck *et al.* PRC **107** (2023)
- Symmetry restoration

  P. Marevic *et al.* PRL **125** (2020)
- New methods to build the 'working space'

  W. Lau *et al.* PRC **105** (2022)

  R. Lasseri *et al.* PRC **109** (2024)

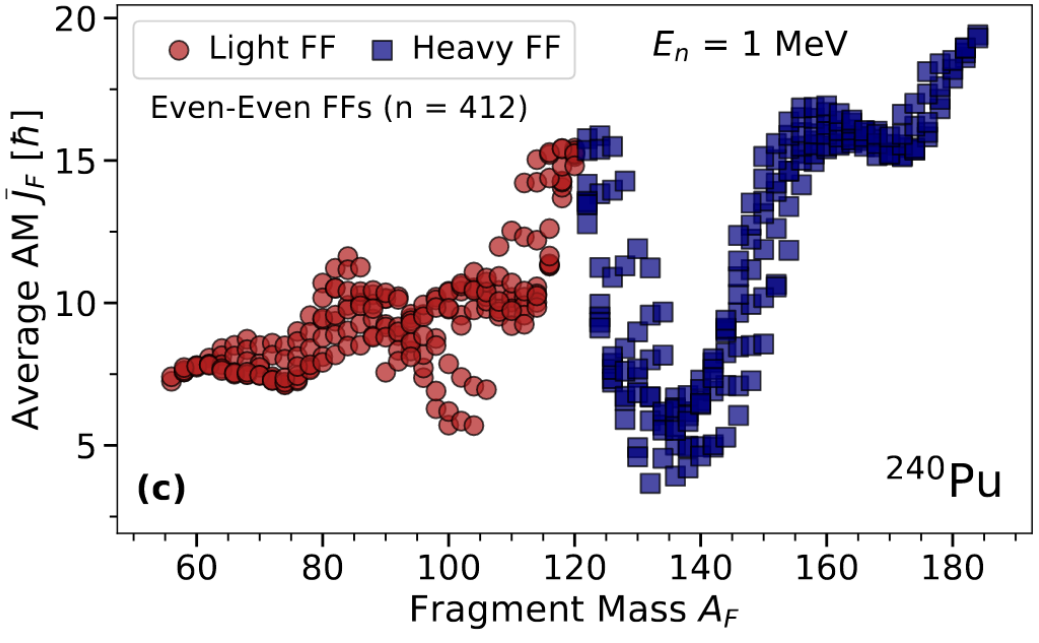
  P. Carpentier *et al.* PRL **133** (2024)

  Z. Li *et al.* PLB **866** (2025)

- 3D-TDGCM

  J. Zhao *et al.* PRC **104** (2021) (pairing strength)

  J. Zhao *et al.* PRC **105** (2022) (temperature)

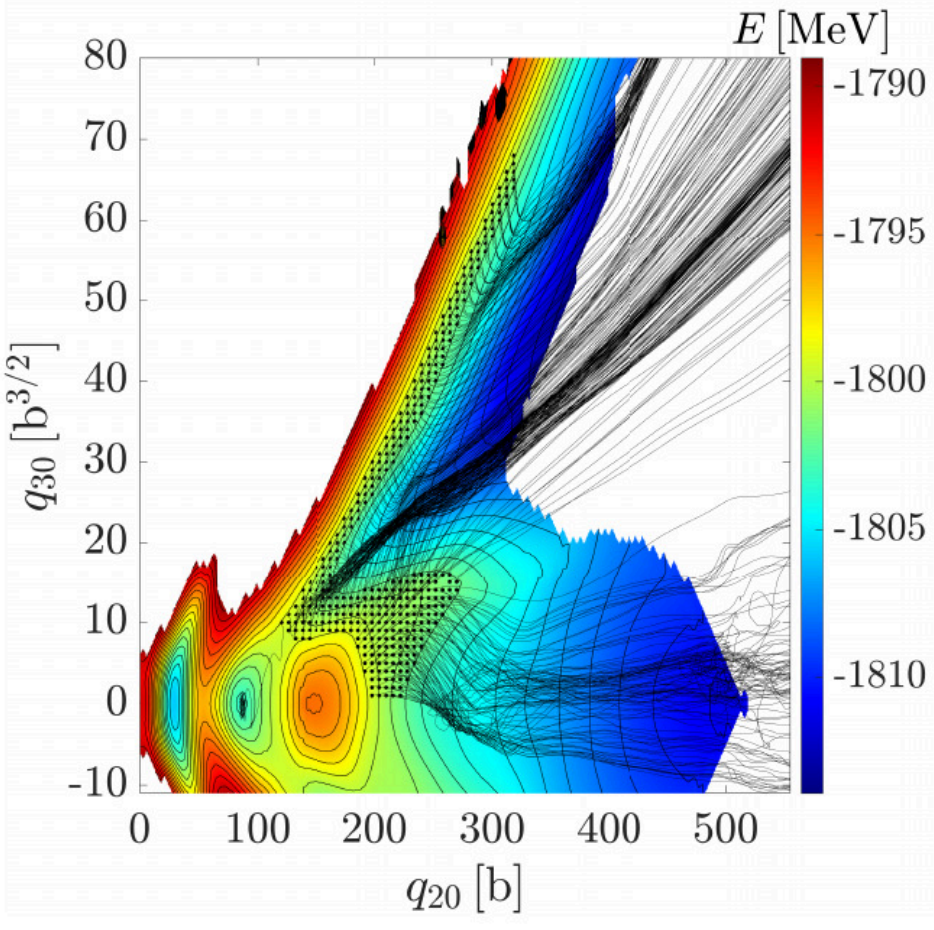


P. Marevic *et al.* arXiv:2506.10777 (2025)

2020-2025: a wealth of improvements

On the TDEDF side

- Spin of the fragments
  - A. Bulgac *et al.* PRL **126** (2021)
  - A. Bulgac *et al.* PRL **128** (2022)
  - G. Scamps *et al.* PRC **106** (2022)
  - A. Bulgac *et al.* PRC **106** (2022)
  - G. Scamps *et al.* PRC **108** (2023)
  - G. Scamps *et al.* PRC **108** (2023)
  - G. Scamps *et al.* PRC **109** (2024)
  - A. Francheteau *et al.* PRL **132** (2024)
- Odd systems
  - A. Bulgac *et al.* PRL **135** (2025)
- Axial TDHFB on a HO basis
  - A. Bjelcic *et al.* arXiv:2510.06701 (2025)
- TDHFB with Gogny on a hybrid basis
  - To be published



A. Bjelcic *et al.* arXiv:2510.06701 (2025)

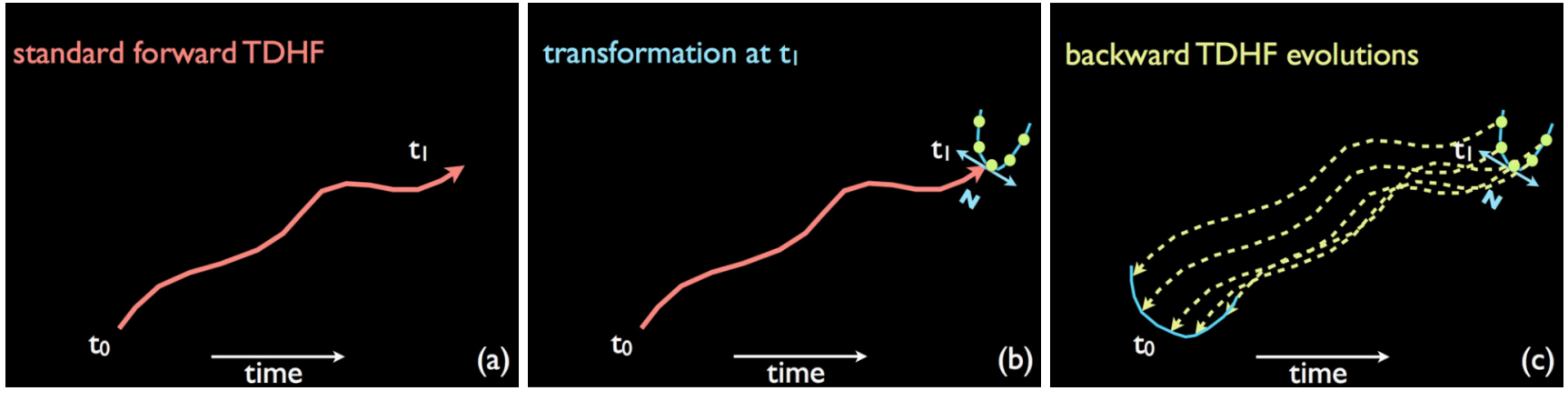
Studies on new methods

How to get both **large quantum fluctuations** (correct yields) and the **kinetic and dissipative aspects** (correct energies) ?

Studies on new methods

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Balian-Veneroni variational principle to predict fluctuations around TDEDF



C. Simenel Eur. Phys. J. A 181 (2025)

- Improving predictions of multi-nucleon transfer reactions

Enlarging the TDEDF variational space

Time dependent Hartree-Fock-Bogoliubov

$$|\psi(t)\rangle = |\phi_{\text{Bogo}}(t)\rangle$$

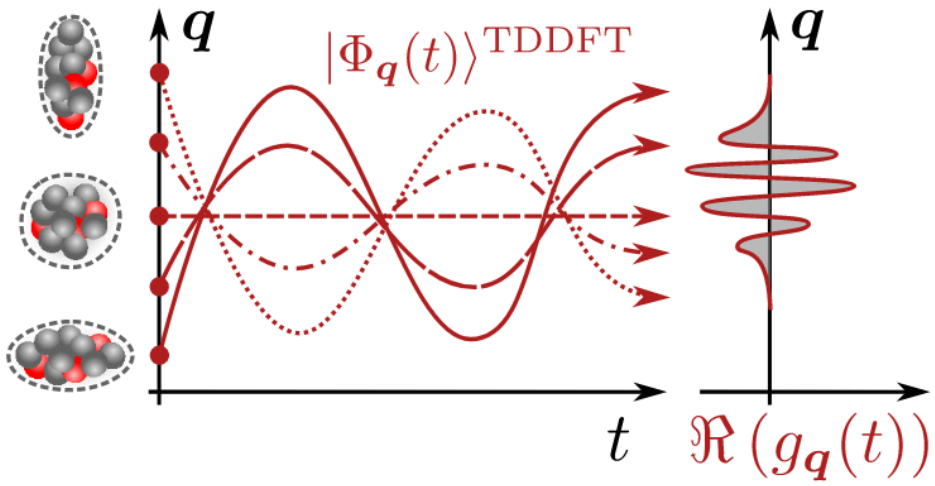
Time dependent GCM

$$|\psi(t)\rangle = \int_{\boldsymbol{q}} f(\boldsymbol{q},t)|\phi_{\text{Bogo}}(\boldsymbol{q})\rangle d\boldsymbol{q}$$

Multi-configurations time-dependent HFB

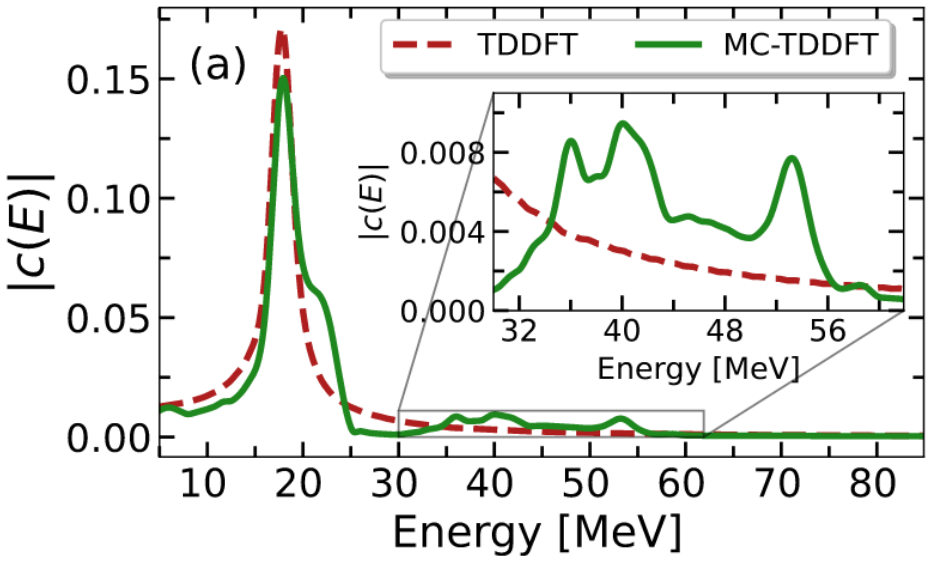
$$|\psi(t)\rangle = \int_{\boldsymbol{q}} f(\boldsymbol{q},t)|\phi_{\text{Bogo}}(\boldsymbol{q},t)\rangle d\boldsymbol{q}$$

- $|\phi_{\text{Bogo}}(\boldsymbol{q},t)\rangle$ from TDHFB
- $f(\boldsymbol{q},t)$ from a variational principle



First applications

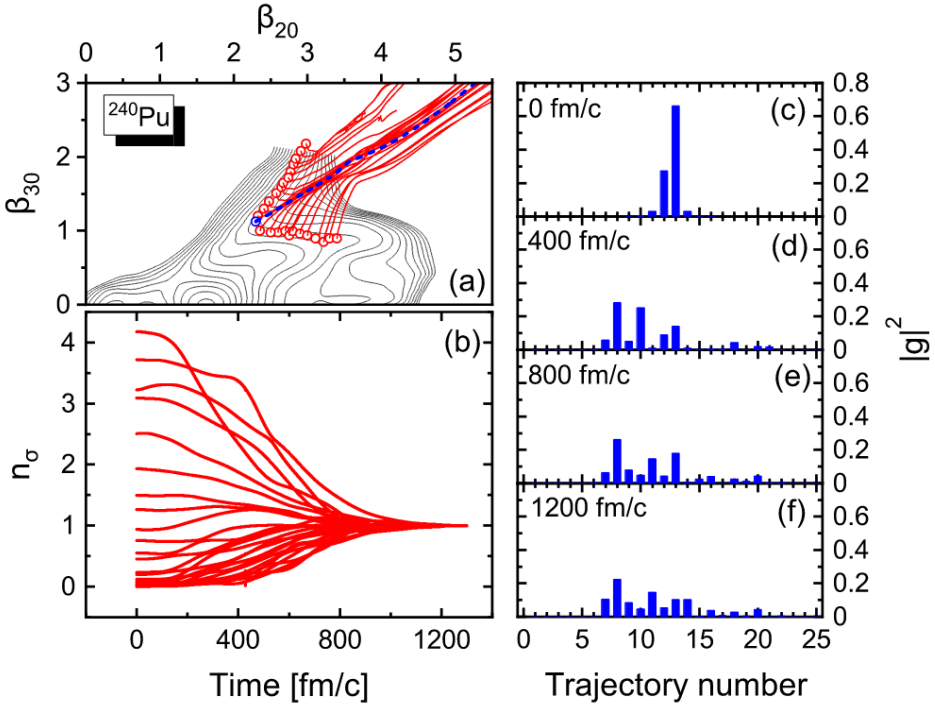
Giant quadrupole resonance of ^{40}Ca



P. Marevic *et al.* PRC **108** (2023)
P. Marevic *et al.* EPJA **60** (2024)

- Mixture of 3 trajectories
- Appearance of **multi-phonons**

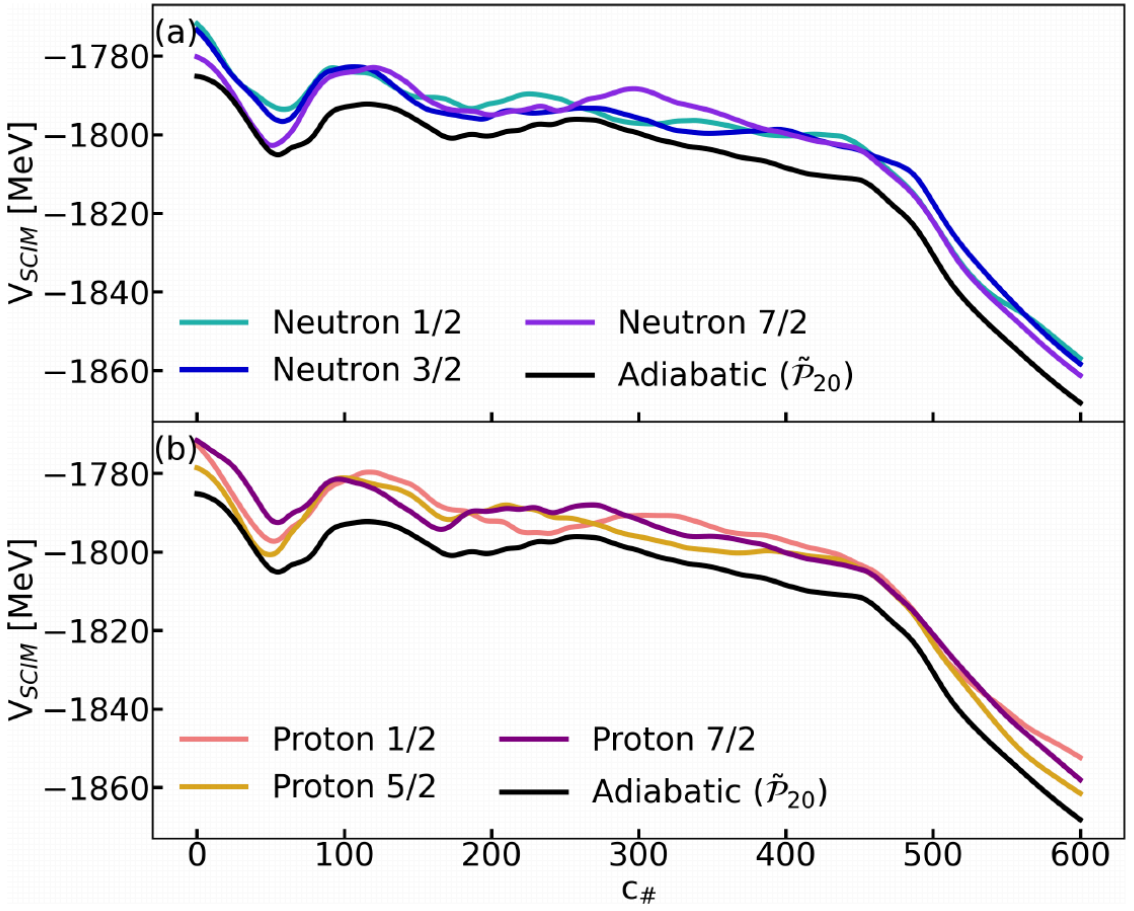
Fission of ^{240}Pu



B. Li *et al.* PRC **111** (2025)

- Mixture of 25 trajectories

Enlarging the TDGCM variational space



P. Carpentier *et al.* arXiv:2608.07137v1 (2026)

Final words

A very interesting moment to work on the 'dynamics' !

We **count on you** to solve this ...

Final words

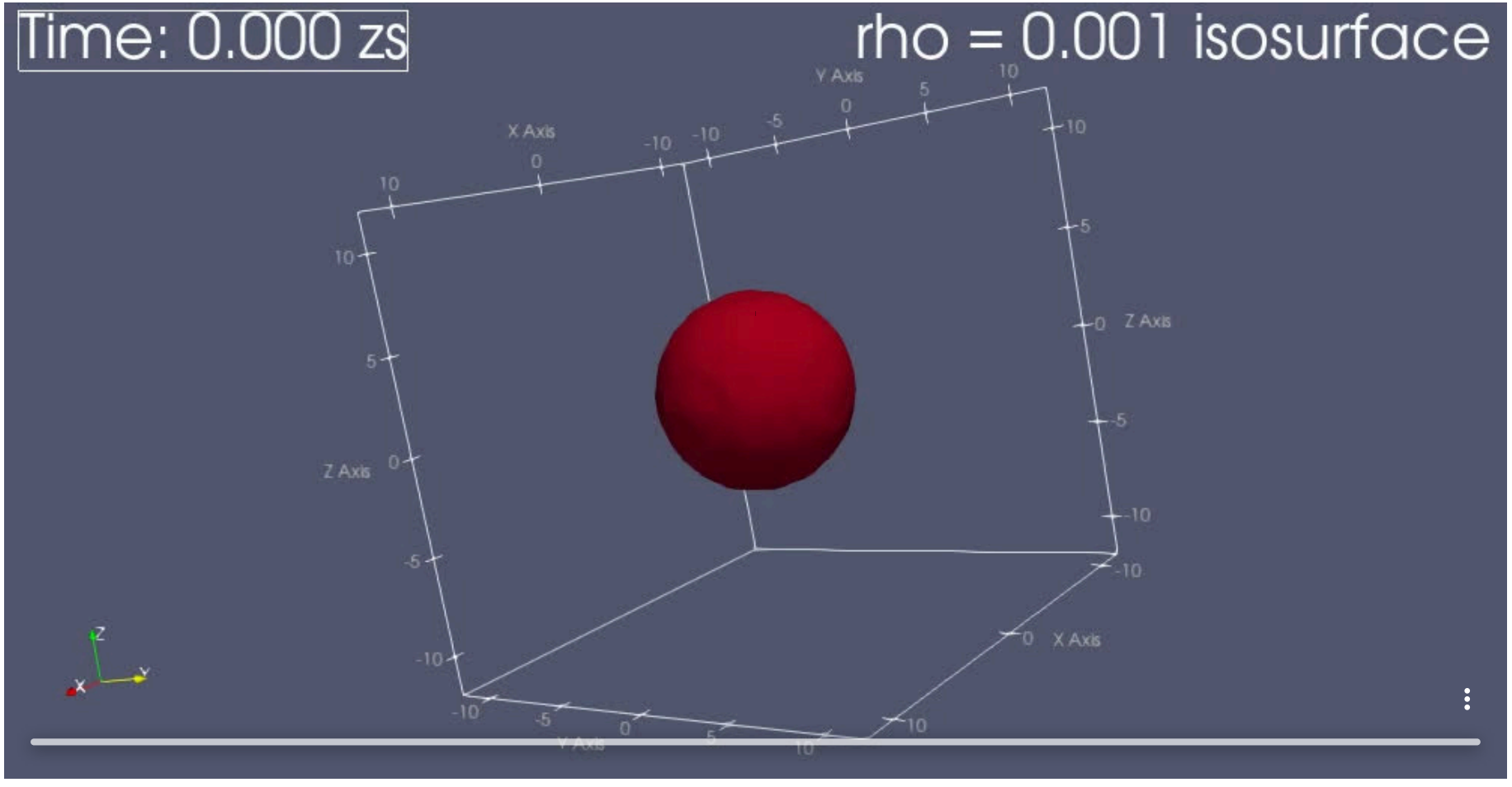
A very interesting moment to work on the 'dynamics' !

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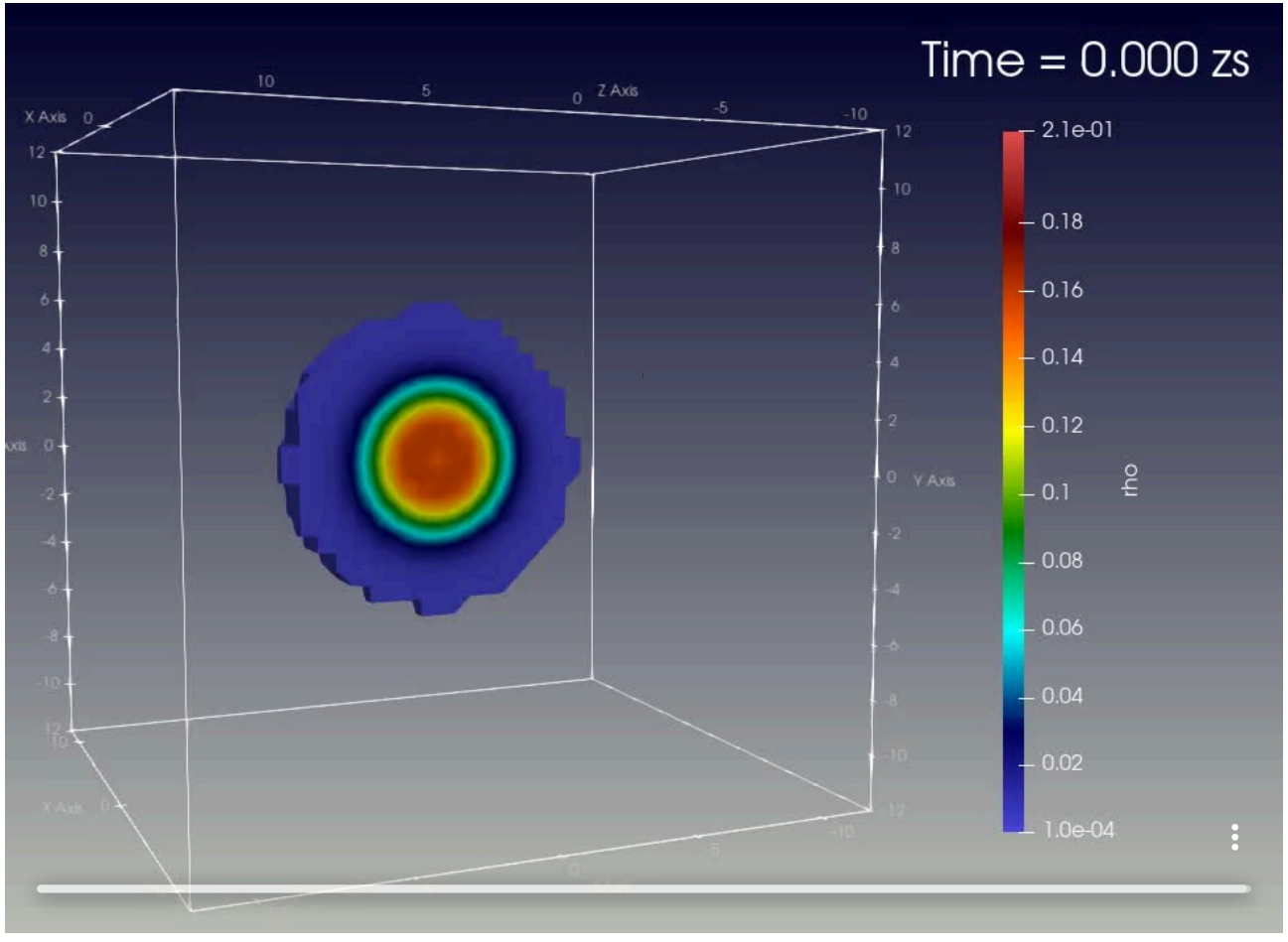
Application to collective vibrations

Quadrupole excitation of ^{16}O



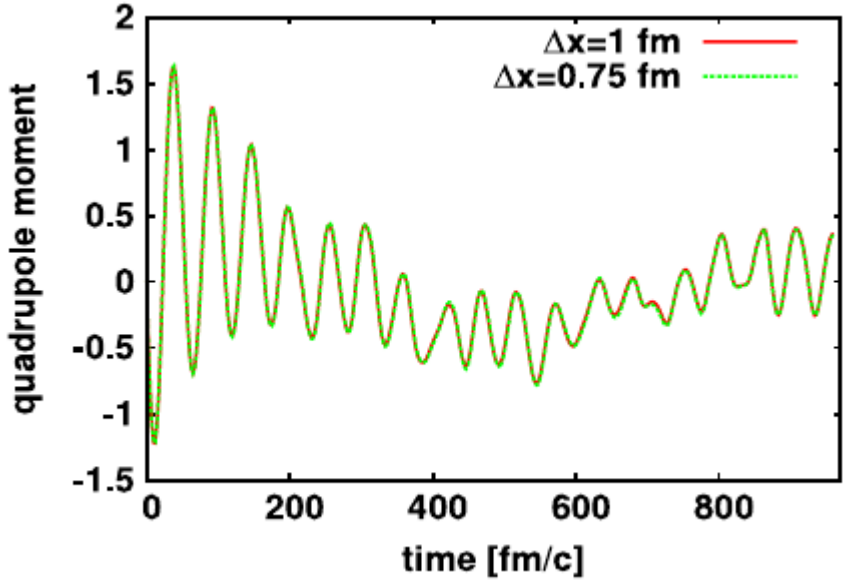
Application to collective vibrations

Monopole excitation of ^{16}O

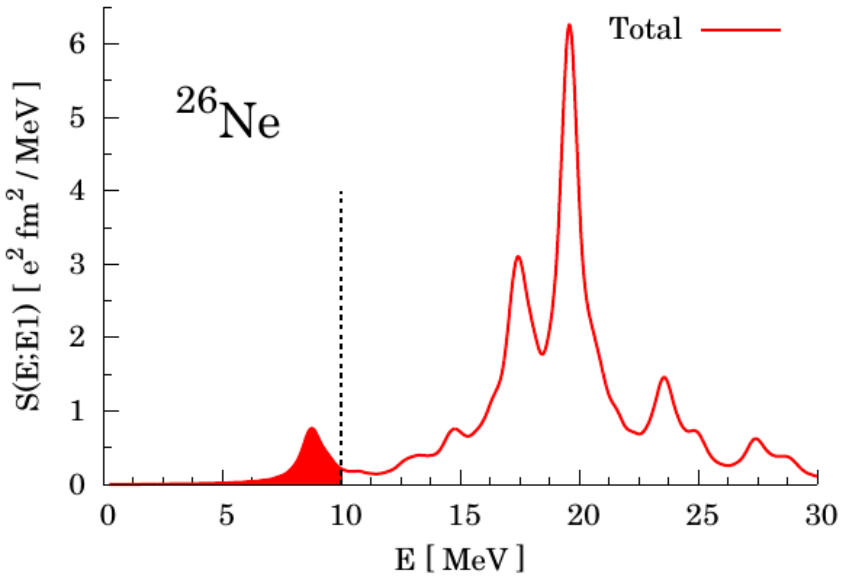


Mean field evolution of multipole moments

Quadrupole moment of ^{16}O from TDHF



Strength function of ^{26}Ne



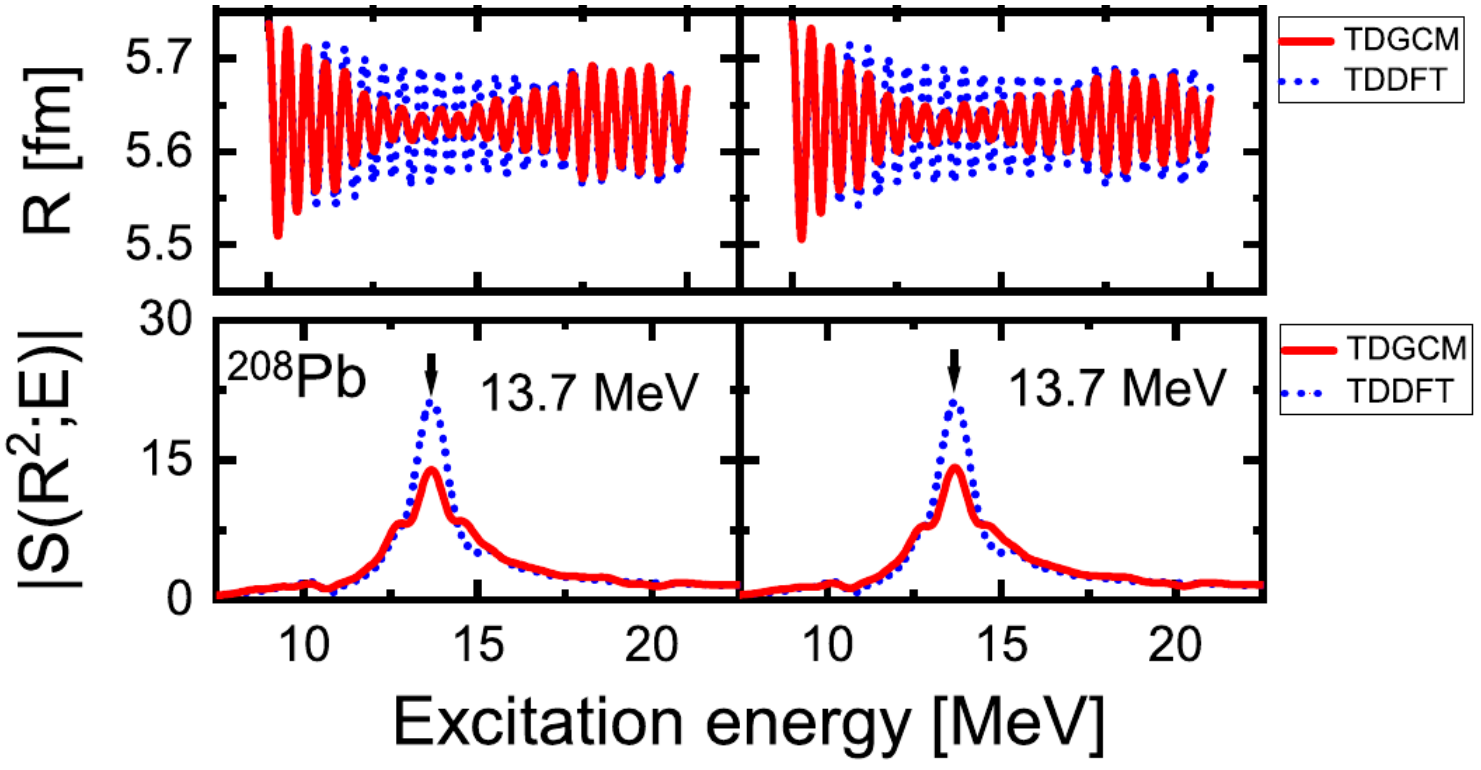
For a given multipol excitation:
The associated strength function is the **Fourier transform** of the time evolution of the expectation value of the multipol observable after the excitation.

Don't forget: 300 fm/c $\simeq$ 1 zs

Need to go beyond TDEDF

Generalized time-dependent generator coordinate method for small and large amplitude collective motion

B. Li, *et al.*, arXiv:2304.13369v1, (**April 26 2023**)



➡️ Time-dependent Hartree-Fock underestimates the **damping** of the oscillation