Microscopic description of the fission: toward class 3 PESs

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INT-13-3

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Microscopic description of the fission

Two-step approach :

1. Production of microscopic potential energy surfaces (PES)
   - Hartree-Fock-Bogoliubov code using a two-center oscillator basis
   - effective nucleon-nucleon interaction Gogny D1S
   - *N*-dimensional PESs
   - results : statical properties of the fragments
2. Wave packet propagation
   - TDGCM method with GOA
   - initial state : eigenstate of an extrapolated first well
   - microscopic inertia tensor (GCM)
   - results : statistical properties of the fragments

Formalism - HFB2CT

$$\delta\langle\varphi|\hat{H} - \lambda_N\hat{N} - \lambda_Z\hat{Z} - \sum_i \lambda_i\hat{Q}_{i0}|\varphi\rangle = 0$$

Constrained Hartree-Fock-Bogoliubov method:

- D1S Gogny parametrization
- self-consistent mean and pairing fields
- two-center harmonic oscillator basis

Constraints:

- neutron and proton numbers N et Z

$$\begin{aligned}\langle\varphi|\hat{N}|\varphi\rangle &= N\\ \langle\varphi|\hat{Z}|\varphi\rangle &= Z\end{aligned}$$

- q_{10} to avoid spurious center of mass motion
- multipolar moments q_{i0}

$$\langle\varphi|\hat{Q}_{i0}|\varphi\rangle = q_{i0}$$

Formalism - TDGCM + GOA

General GCM state with N different degrees of freedom $\{q_1, \ldots, q_N\}$:

$$|\psi(t)\rangle \equiv \left(\prod_i^N \int dq_i \right) f(q_1, \ldots, q_N, t) |\phi(q_1, \ldots, q_N)\rangle$$

Variational principle:

$$\frac{\partial}{\partial f^*} \int_{t_1}^{t_2} \langle \psi(t)| \left(\hat{H} - i\hbar \frac{\partial}{\partial t} \right) |\psi(t)\rangle = 0$$

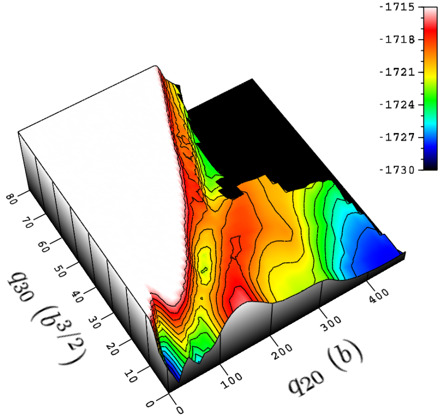
Using the Gaussian Overlap Approximation (GOA), we obtain a Schrödinger-like equation:

$$\hat{H}_{\mathrm{coll}} g(t) = i\hbar \frac{\partial}{\partial t} g(t)$$

with

$$\hat{H}_{\mathrm{coll}} = -\frac{\hbar^2}{2} \sum_{i,j}^N \frac{\partial}{\partial q_i} B^{ij} \frac{\partial}{\partial q_j} + \hat{V}$$

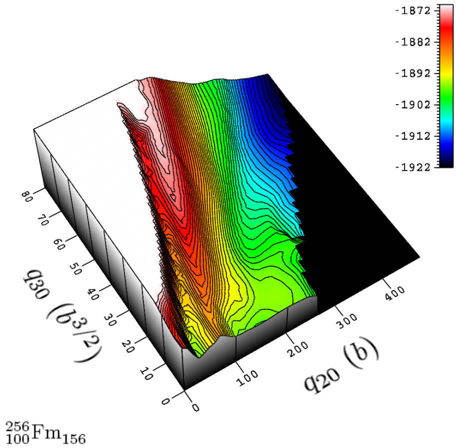
Results - PESs



$^{226}_{90}\mathrm{Th}_{136}$

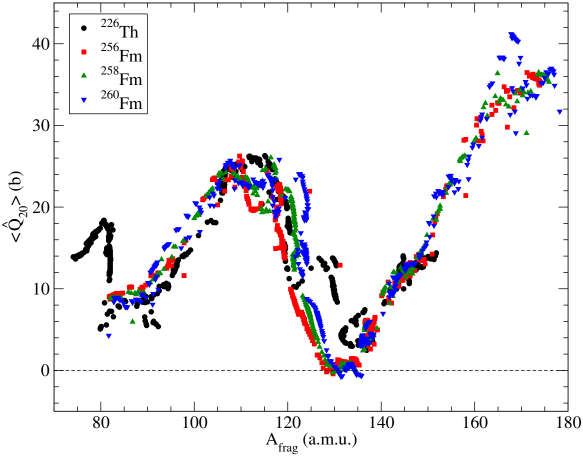
N. Dubray et al., Phys. Rev. C **77**, 014310 (2008).

Results - PESs



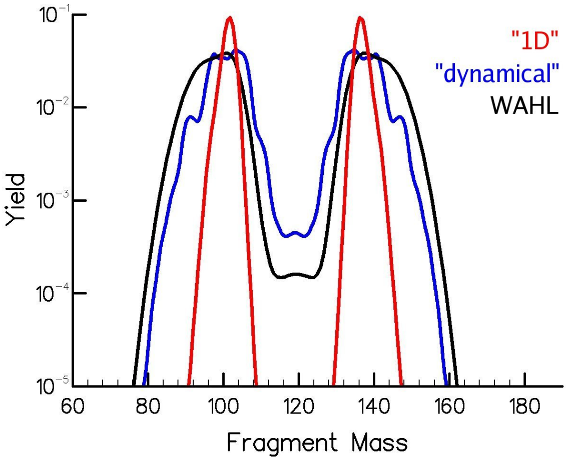
N. Dubray et al., Phys. Rev. C **77**, 014310 (2008).

Results - Fragment deformation $\langle \hat{Q}_{20} \rangle$



N. Dubray et al., Phys. Rev. C **77**, 014310 (2008).

Results - Fragment mass distribution for ^{238}U



H. Goutte et al., Phys. Rev. C **71**, 024316 (2005).

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Problem 1 - Convergence

- Problem: the HFB solver does not converge.
- Consequence: the HFB solution is bad.
- Symptom: the convergence quantity is too high.

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Problem 3 - Discontinuity

- Problem: two solutions close in the constraint deformation subspace are not close in the full deformation space.
- Consequence: a dynamical description using these points is missing a part of the physics (wrong barrier, saddle point, . . .).
- Symptom: none easily visible.

PES classes

Class	Convergence	Minimization	Discontinuity
0	maybe	maybe	maybe
1	OK	maybe	maybe
2	OK	OK	maybe
3	OK	OK	OK

The density-distance operator

We define the density-distance operator

$$D_{\rho\rho'}(|\psi\rangle, |\psi'\rangle) \equiv \int \mathrm{d}\tau^3 |\rho(\vec{r}) - \rho'(\vec{r})|$$

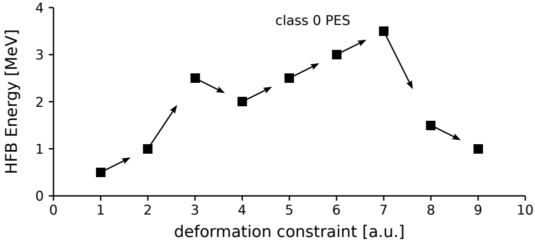
where $\rho(\vec{r})$ and $\rho'(\vec{r})$ are the total local densities of the states $|\psi\rangle$ and $|\psi'\rangle$.

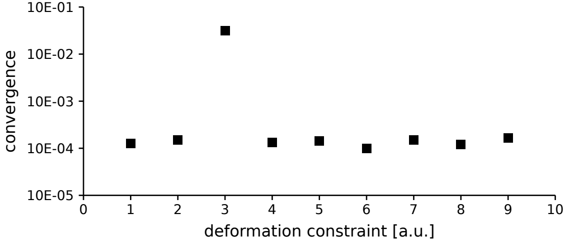
4-lines long algorithm to clean a PES

- all solutions with a too high convergence value are marked as "bad",
- all solutions with a too high maximum density distance value AND with their energy being higher than the corresponding partner's energy are marked as "bad",
- all solutions marked as "bad" are recalculated from the neighboring solution with the lowest energy that has not been used for the same calculation before,
- recalculate the density distances and restart.

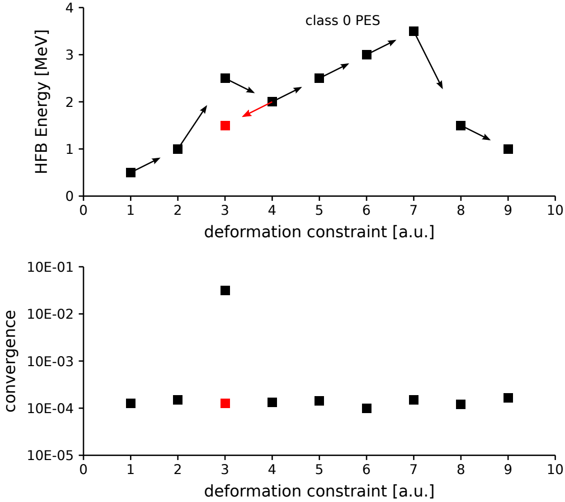
- this algorithm can be used during or after the production of a N-dimensional PES.
- if there is no fatal convergence problem and if all valleys have been discovered, the result is at least a class 2 PES.

Example of a PES cleaning





Example of a PES cleaning



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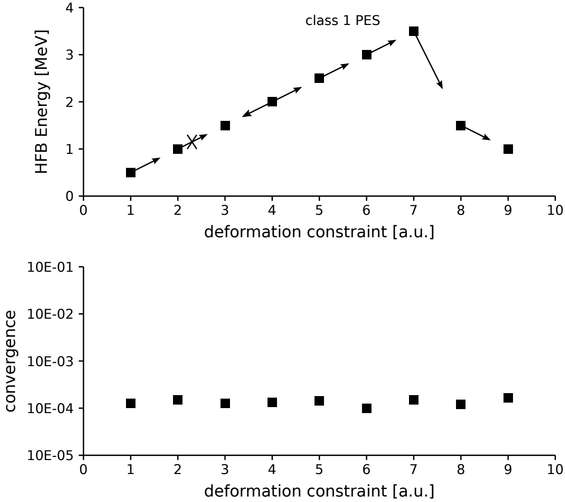

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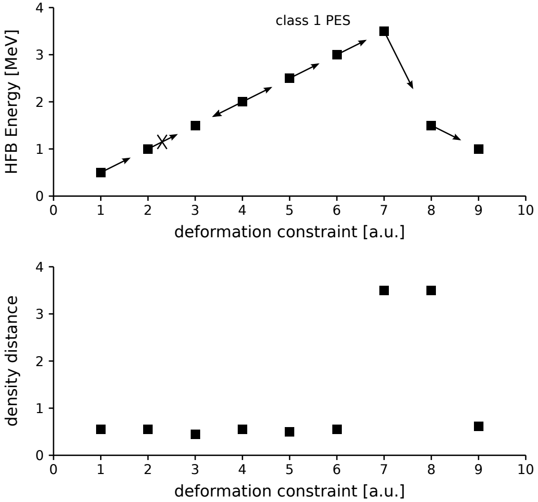

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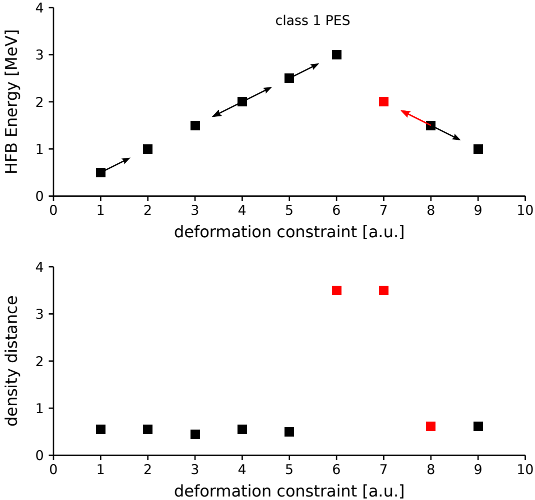

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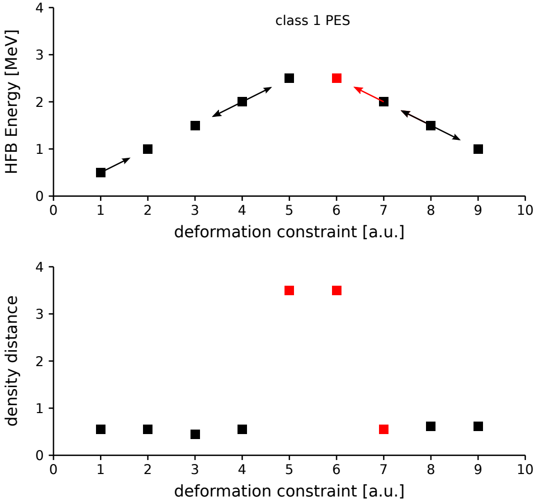

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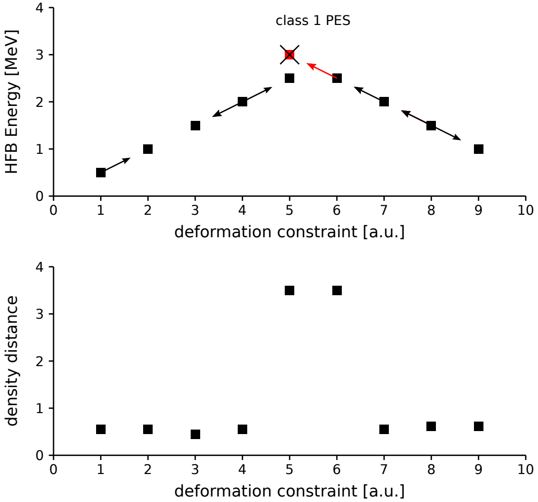

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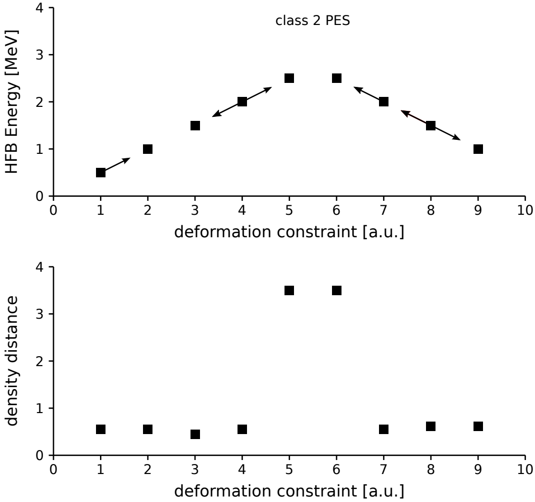

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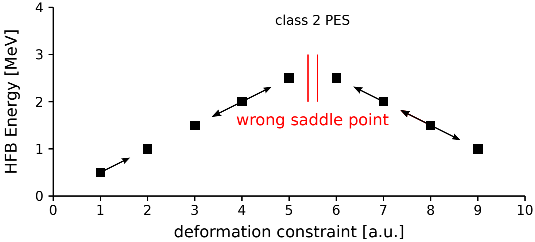
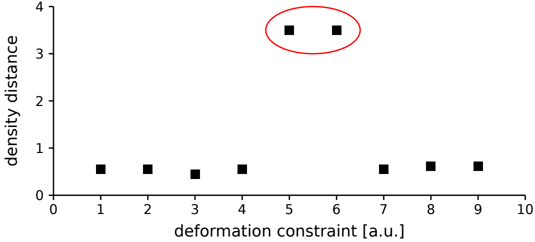




Important remark

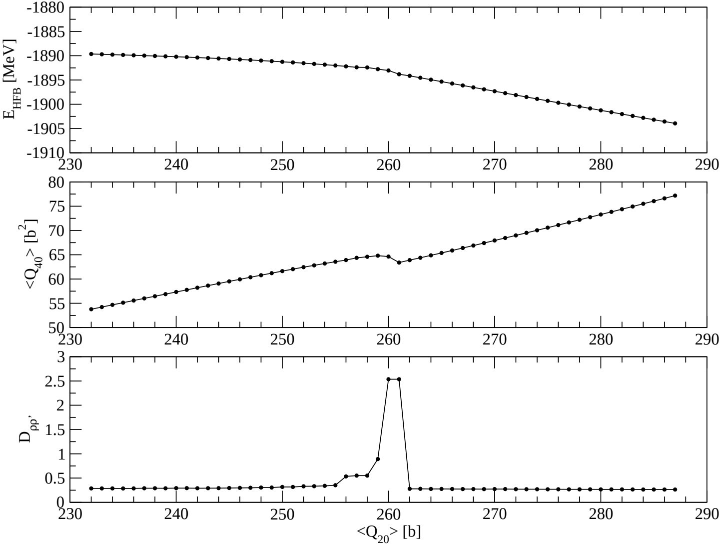
We call a good point a solution that does not change when taking a bigger deformation subspace with the same symmetries.

If there has been no fatal convergence problem and if all valleys have been discovered,

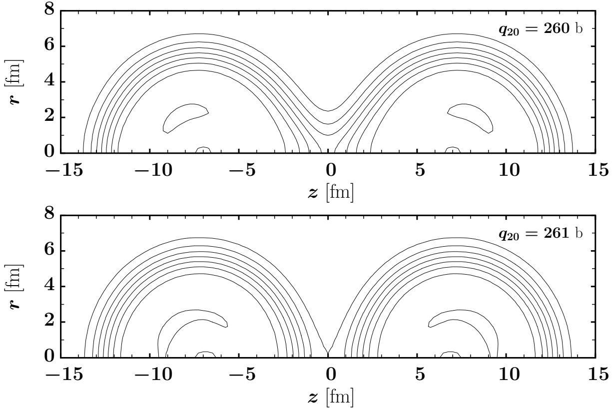
- a class 2 PES can have wrong or missing saddle points,
- a class 3 PES has only good points (minima, saddle points, etc. . .).

N. Dubray and D. Regnier, Comp. Phys. Comm. **183**, 2035 (2012).

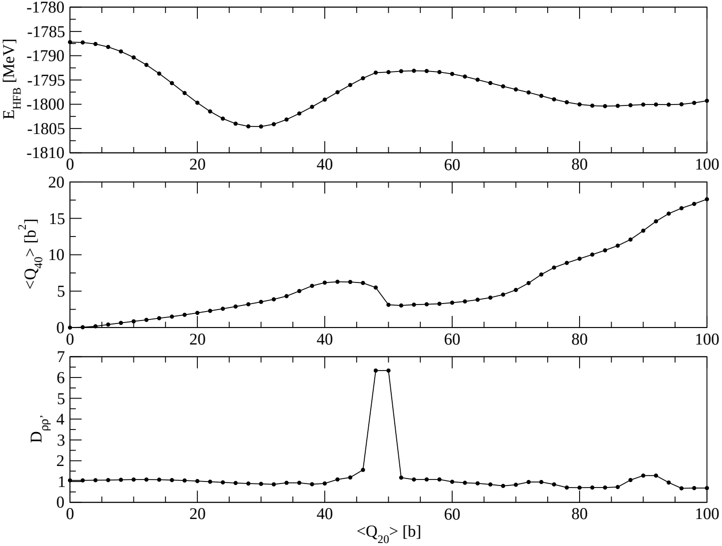
Symmetric "scission" of ^{256}Fm - class 2



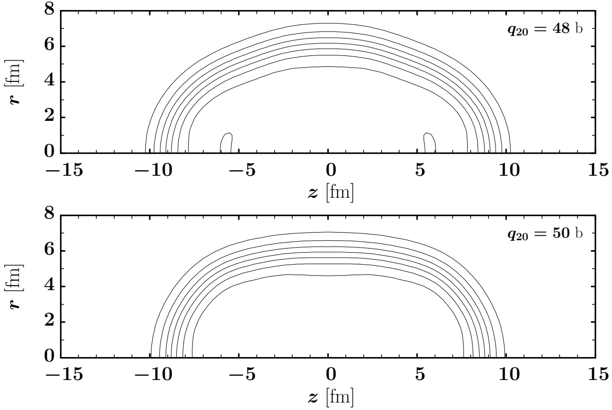
Symmetric "scission" of ^{256}Fm - densities



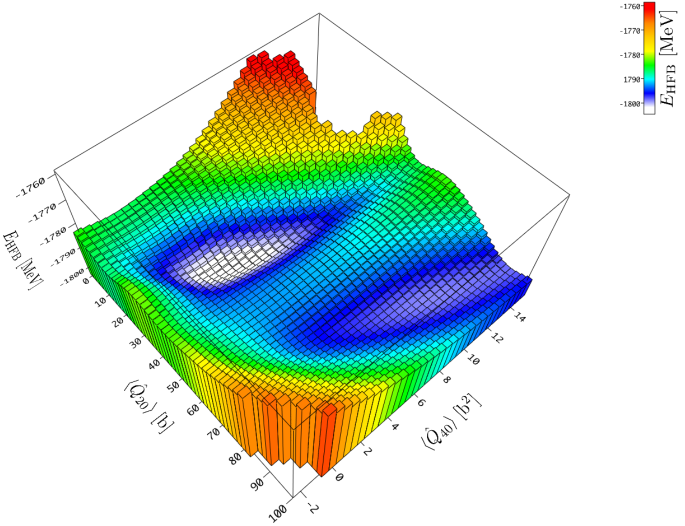
Symmetric barrier of ^{240}Pu - class 2



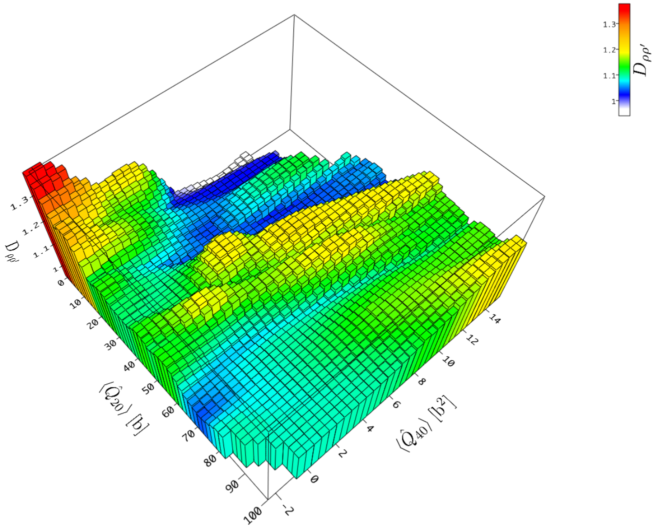
Symmetric barrier of ^{240}Pu - densities



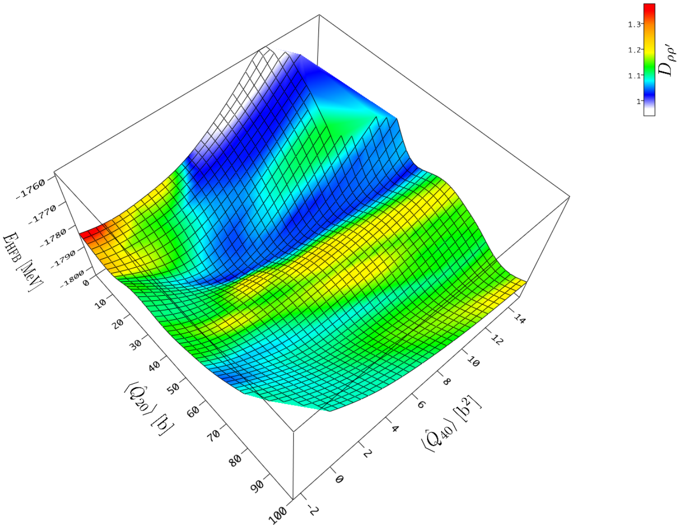
Symmetric barrier of ^{240}Pu - class 3



Symmetric barrier of ^{240}Pu - class 3



Symmetric barrier of ^{240}Pu - class 3



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Class 3 PESs

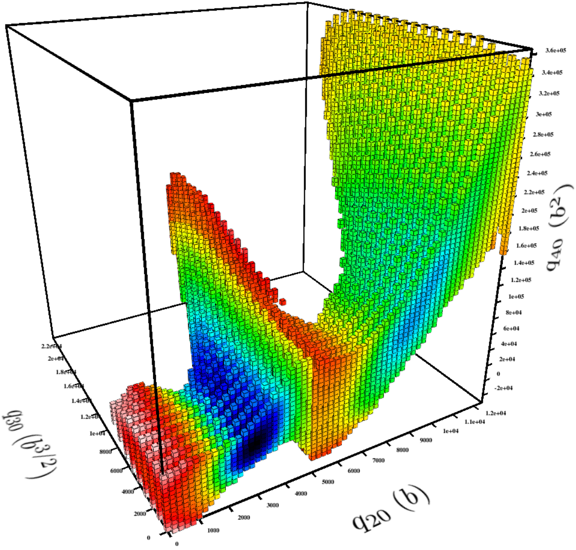
Continuous regular mesh ?

- dimension of a class 3 PES: $N = 1, 2, 3, 4, 5, 6, \ldots$?
- regular mesh + hypercube + $N > 2$ = huge number of points N_p
- dimension of the TDGCM + GOA hamiltonian matrix: N_p^2

Use a sparse mesh !

- no hypercube, focus on the physics in any dimension
- optimal number of points
- solve the TDGCM + GOA equation with FEM

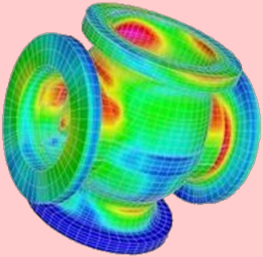
Class 3 PES (q_{20}, q_{30}, q_{40}) for ^{240}Pu

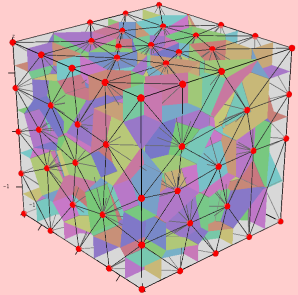


Solving the TDGCM + GOA on a sparse mesh

Generalized Finite Element Method

- *N*-dimensional delaunay triangulation
- piecewise linear function approximation
- very good numerical stability (Runge-Kutta + Jacobi method)
- analytical vertices manipulation (derivation, integration. . .)





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Conclusions

- Publishing class 2 PESs should be the minimum (4-lines !).
- Dynamical considerations are not valid on class 0,1,2 PESs.
- A class 3 N-dimensional PES has the same good saddle points, paths... as any extended $(N + x)$-PES.

Perspectives - fission description

In a near future, we plan to have

- a fully-automatic production of class 3 sparse N-PESs,
- a code to solve the TDGCM + GOA equation on sparse N-PESs with FEM (almost done, cf. video).