Nuclear response functions from Brussels EDF models

***Pepijn Demol**, S. Goriely, W. Ryssens, E. Vancayseele*

MITP Mainz, Many-body theory: nuclear physics meets quantum chemistry

24 Aug - 04 Sept 2026

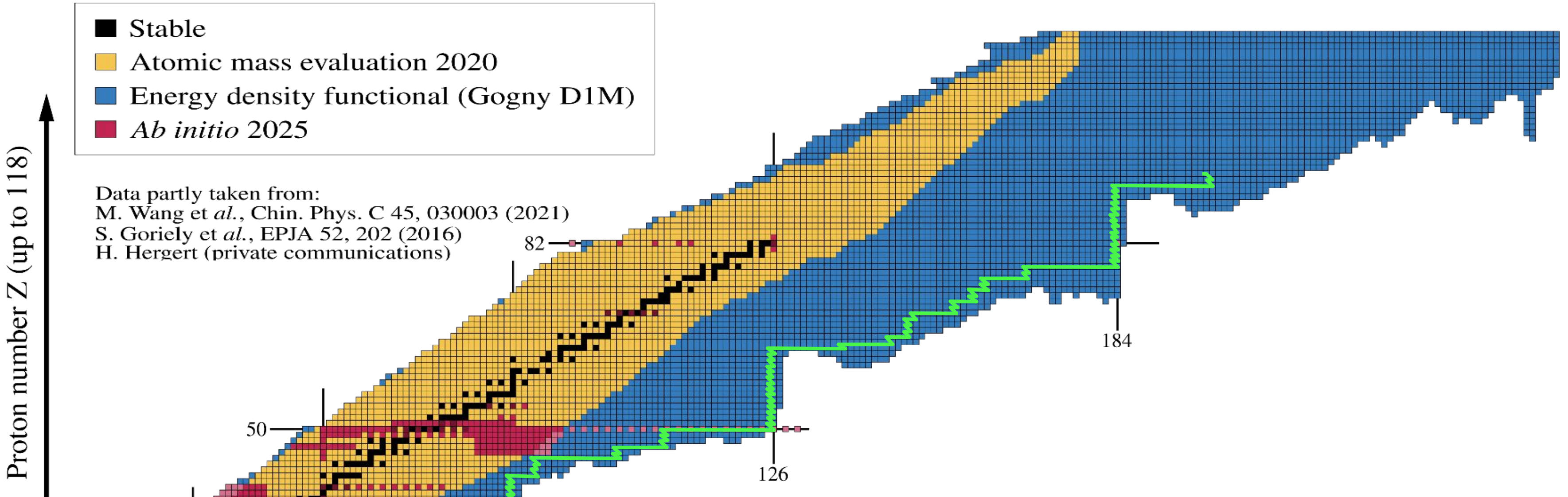
Ab initio

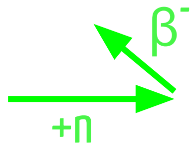
- Bare internucleon interaction from chiral EFT
- Many-body methods capture correlations into $|\Psi_n^A\rangle$

$\longleftrightarrow$

Energy density functional (EDF)

- In medium interaction casted into effective EDF
- Simple mean-field wavefunctions





r-process (~5000 nuclei)
(n,γ), (γ,n), β, βdn, fission

Courtesy of B. Bally

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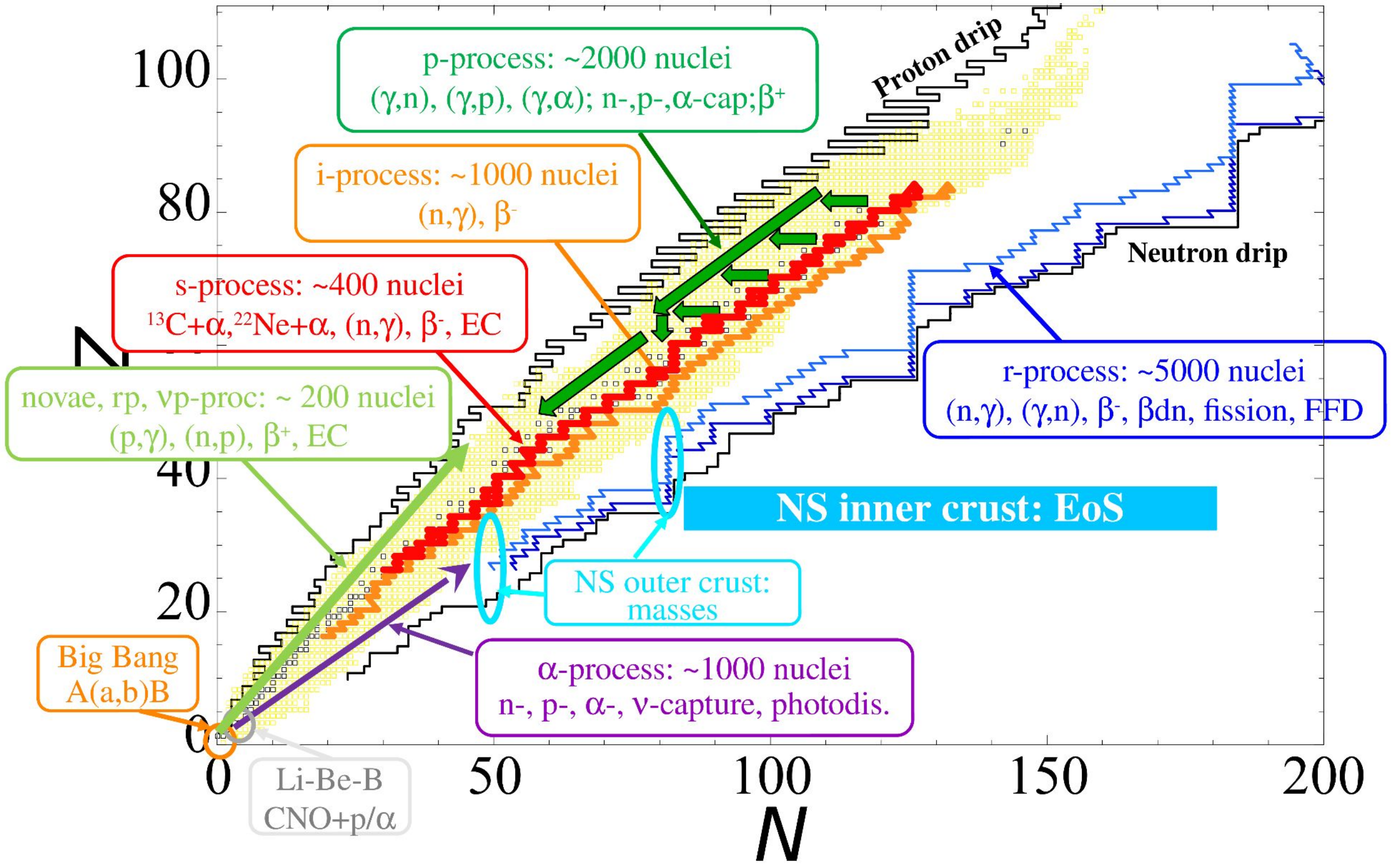
3



Ab initio

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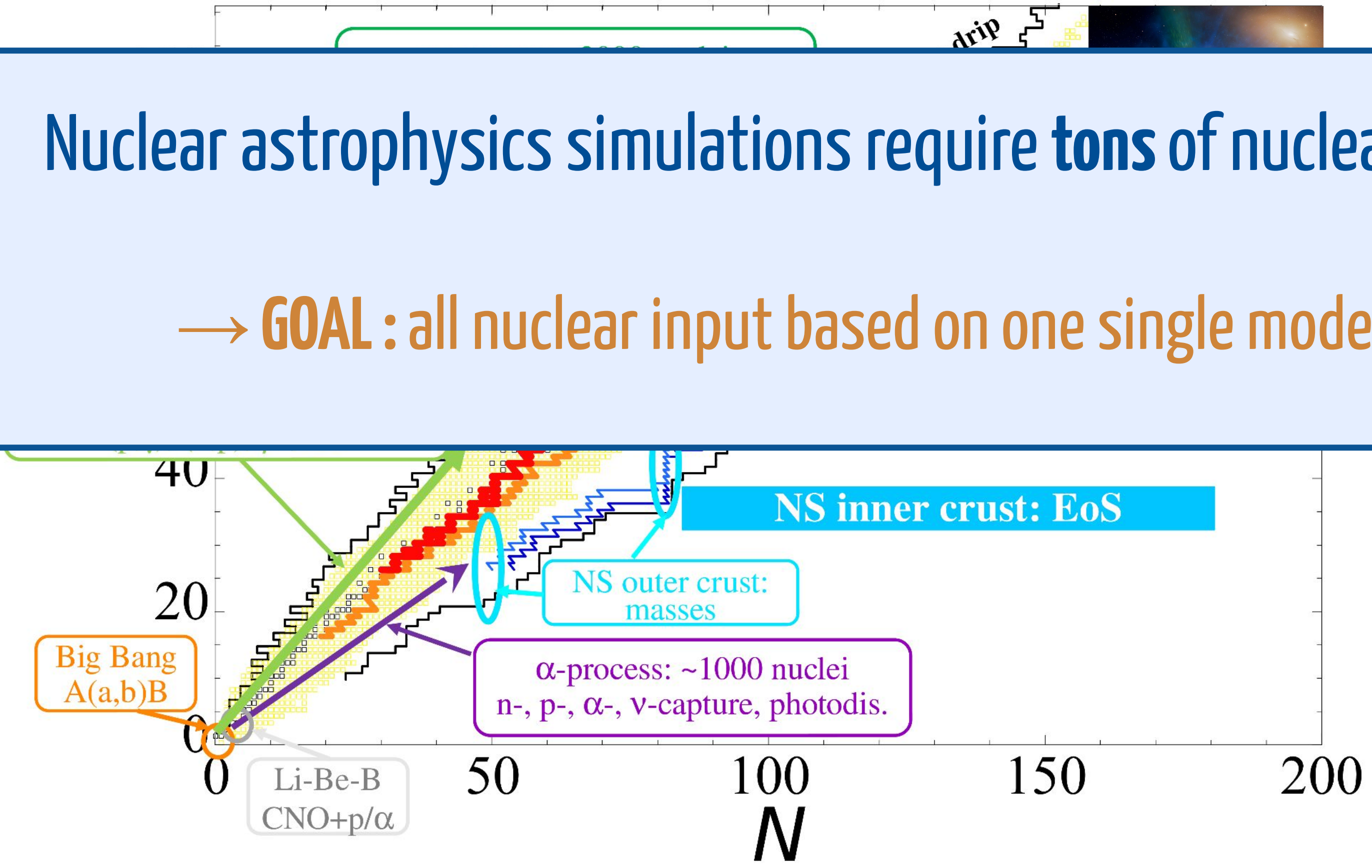
Nuclear astrophysics simulations require **tons** of nuclear data

$\longrightarrow$ **GOAL :** all nuclear input based on one single model



Skyrme energy density functional (EDF) theory

Coupling constants to be fitted to data

$$E_{\text{Skyrme}}[\rho] \sim \int \mathrm{d}^3\mathbf{r}\, [\boxed{C^\rho}\boxed{\rho(\mathbf{r})\rho(\mathbf{r})} + \boxed{C^\tau}\boxed{\tau(\mathbf{r})\rho(\mathbf{r})} + \boxed{C^\gamma}\boxed{\rho(\mathbf{r})^\gamma\rho(\mathbf{r})\rho(\mathbf{r})} + \cdots]$$

Local densities and currents of the wavefunction $\longrightarrow$ Represent on a lattice

$$\min_{\boxed{\rho}} E_{\text{tot}} = \underbrace{\boxed{E_{\text{Skyrme}} + E_{\text{kin}} + E_{\text{Coul}} + E_{\text{pair}} + E_{\text{cm}}^{(1)}}}_{\text{Included in mean-field}} + \underbrace{\boxed{E_{\text{cm}}^{(2)} + E_{\text{rot}} + E_{\text{W}}}}_{\text{Corrections treated semi-variationally}}$$

Set of trial wavefunctions:
Mean-field states = Slater determinant + **symmetry breaking**
$\longrightarrow$ solving the **Hartree-Fock(-Bogoliubov)** problem

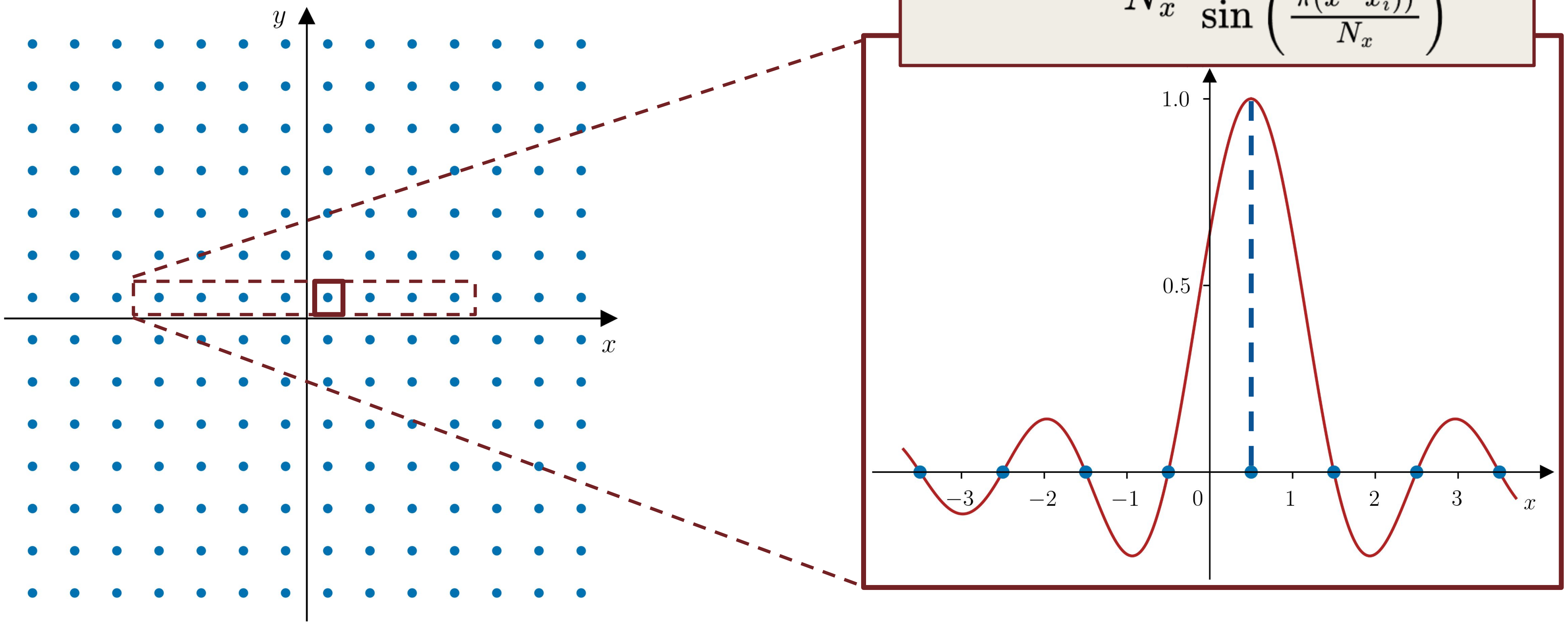
- + Wavefunction with individual nucleons
- + Feasible for 1000s of nuclei (incl. odds)
- + Many observables accessible

- – Unclear how to improve functional form
- – Lack of systematic uncertainty quantification

D. Baye, Phys. Rep. **565**, 1-107 (2015).

3D Lagrange-Fourier mesh

$$f_i(x) = \frac{1}{N_x}\frac{\sin(\pi(x-x_i))}{\sin\left(\frac{\pi(x-x_i))}{N_x}\right)}$$



- Exact quadrature

$$\int dx\,dy\,dz\,f(x,y,z) = \Delta L^3 \sum_i^{N_x}\sum_j^{N_y}\sum_k^{N_z} f(x_i,y_j,z_k)$$

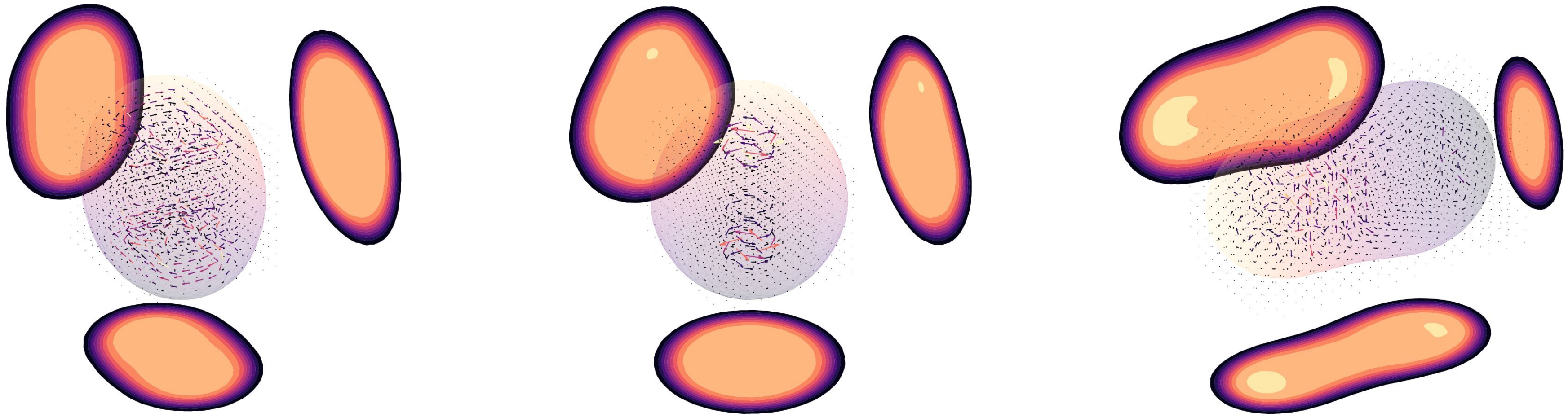
- Accurate derivatives informed over the whole mesh

Brussels-Skyrme-on-a-Grid: BSkG

Triaxial — β_{20}, β_{22} or β_2, γ

Octupole — β_{20}, β_{30}

Triaxial + octupole — β_{20}, β_{22} **and** β_{30}



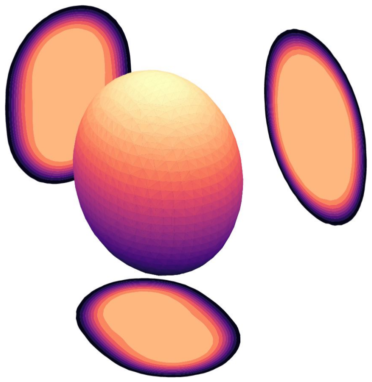
$+\cdots$

- 3D representation agnostic wrt shape
- shape DOF characterized by multipole moments
- Symmetry breaking enlarges variational space
  - + captures collective correlations at modest CPU cost
  - - BUT loss of quantum numbers

Brussels-Skyrme-on-a-Grid: BSkG

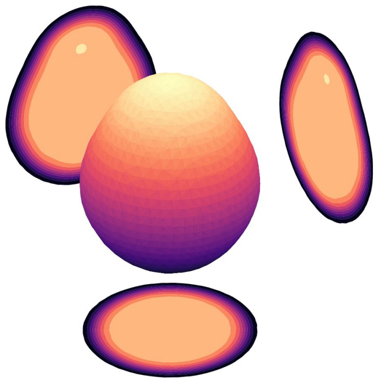
Triaxial

β_{20}, β_{22} or β_2, γ



Octupole

β_{20}, β_{30}



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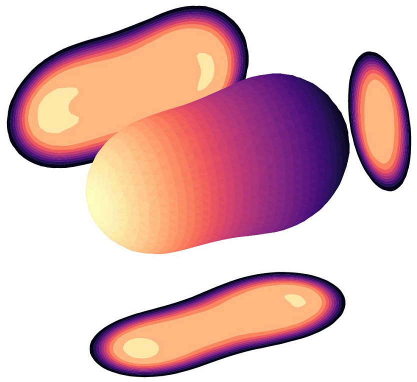

$+ \cdots$

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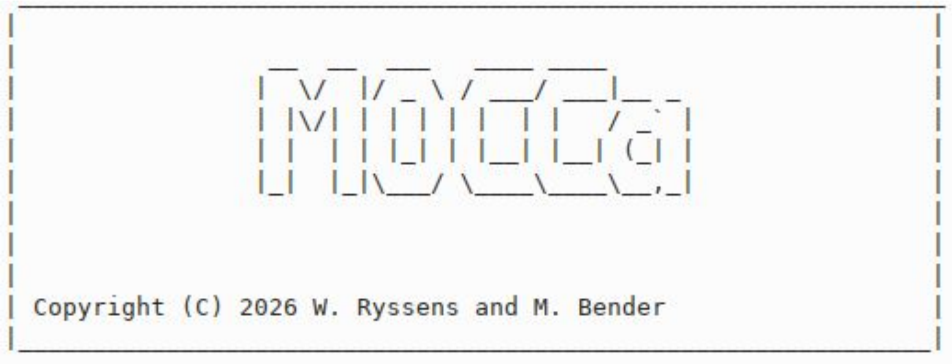
Our solver : MOCCa



v1.0.0 publicly available (APGL v3 license) :

- https://github.com/IAA-ULB/MOCCa
- https://doi.org/10.5281/zenodo.20931651

Typical constrained HFB calculation

Mesh size	$36 \times 36 \times 36$ points	$\times$ ½ or ¼ or ⅛
Mesh spacing	0.8 fm	
Nb of particles	≤ 300	
Nb of HF(B) states	~ 800	$\times$ ½

(Third column: Symmetries)

→ ~ 30 min on 1 cpu (2 Gb of RAM)

Brussels-Skyrme-on-a-Grid: BSkG

Coupling constants (~**25** parameters) fitted to data:

- **2457** masses
- **884** charge radii
- Infinite matter properties

$$E[\rho] = \int d^3\mathbf{r} \left[\boxed{C^\rho}\rho(\mathbf{r})\rho(\mathbf{r}) + \boxed{C^\tau}\tau(\mathbf{r})\rho(\mathbf{r})\right] + E_{\mathrm{rot}}(\boxed{C_r}) + \boxed{\cdots}$$

RMSE (MeV)	FRDM	HFB-14	**BSkG1**	…	**BSkG5**
Masses	0.560	0.729	0.741	…	
Charge radii (fm)	0.038	0.039	0.027	…	
Primary barriers	0.79	0.61	0.87	…	
Secondary barriers	1.35	0.70	0.86	…	
Fission isomers	1.04	0.93	0.45	…	
Max. NS mass ($M_\odot$)			1.8	…	

BSkG1

- \+ Time reversal breaking (blocking)
- \+ Parity breaking (octupole deformation)
- \+ Fit to fission barriers
- \+ Extend Skyrme EDF to four gradients

BSkG5

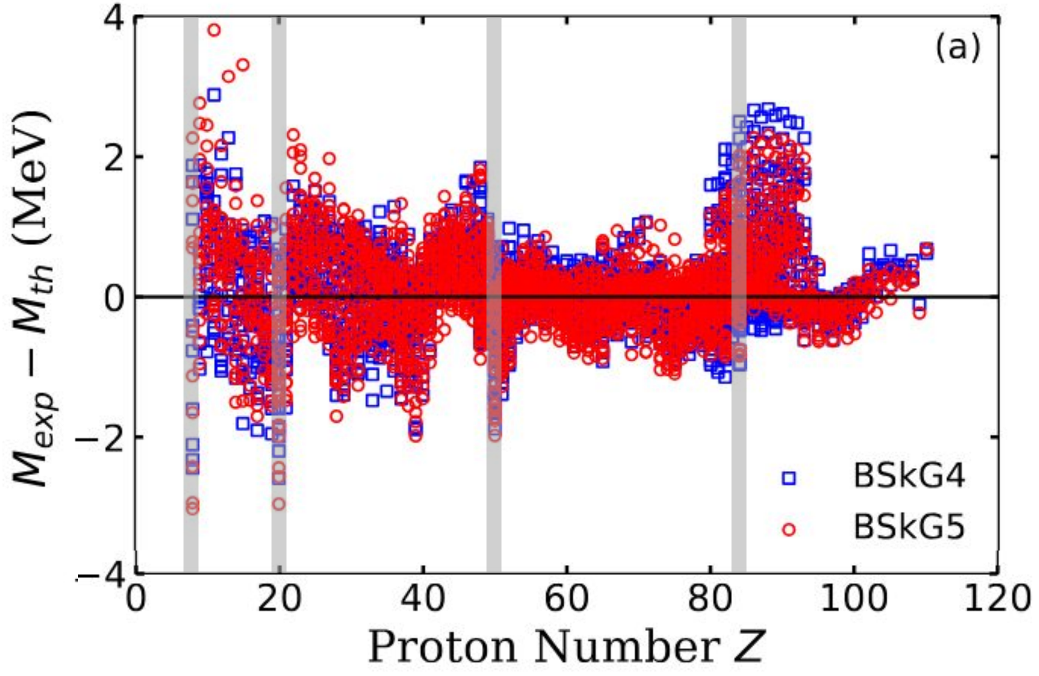
HFB-14: S. Goriely et al., PRC ***75***, 064312 (2007).
FRDM: P. Möller et al., At. Data Nucl. Data Tables, **109-110** (2016).
BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG5: G. Grams et al. arXiv:2601:05968 (2026).

Brussels-Skyrme-on-a-Grid: BSkG

Coupling constants (~**25** paran

$$E[\rho] = \int d^3\mathbf{r} \left[\boxed{C^{\rho}} \rho(\mathbf{r})\rho(\mathbf{r}) + \boxed{C^{\tau}} \tau \right.$$

RMSE (MeV)	FRDM	HFB-14	**BSkG1**	…	**BSkG5**
Masses	0.560	0.729	0.741	…	0.643
Charge radii (fm)	0.038	0.039	0.027	…	0.027
Primary barriers	0.79	0.61	0.87	…	0.43
Secondary barriers	1.35	0.70	0.86	…	0.49
Fission isomers	1.04	0.93	0.45	…	0.59
Max. NS mass ($M_{\odot}$)			1.8	…	2.2



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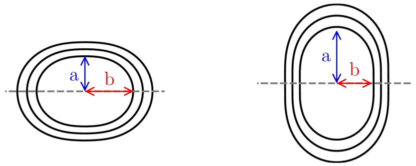
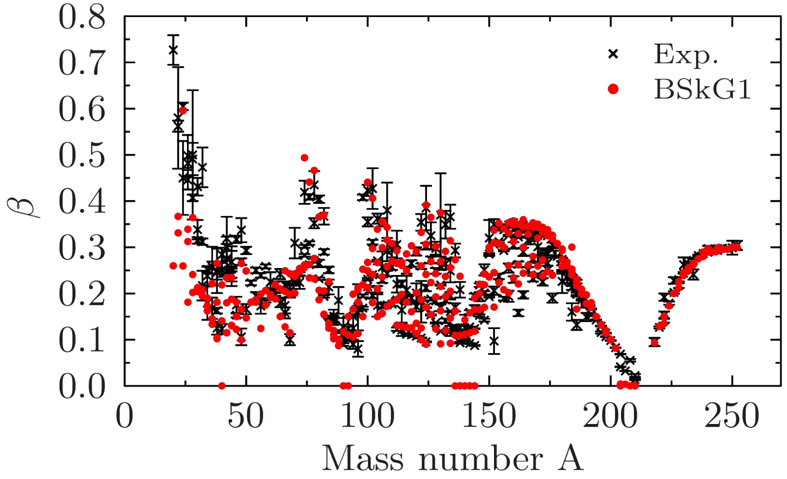
More on shape and charge distributions

"ordinary" quadrupole deformation





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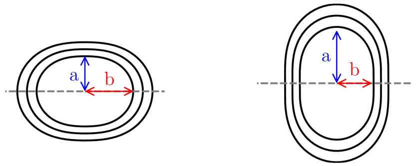
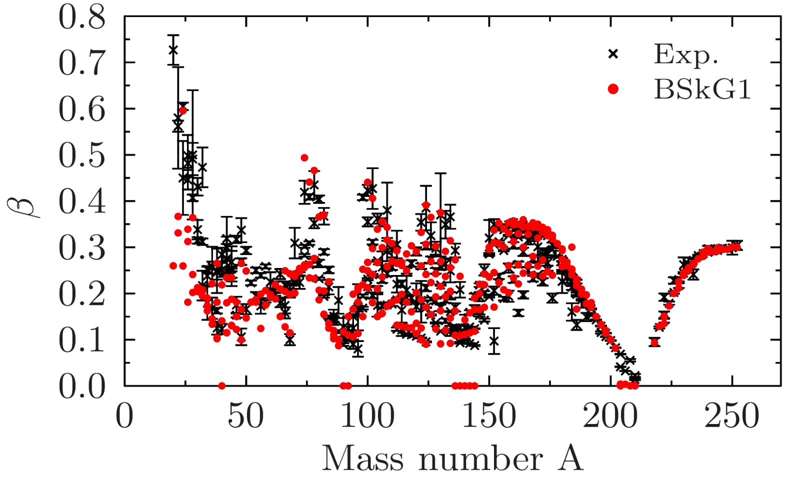
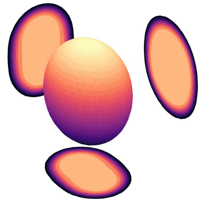
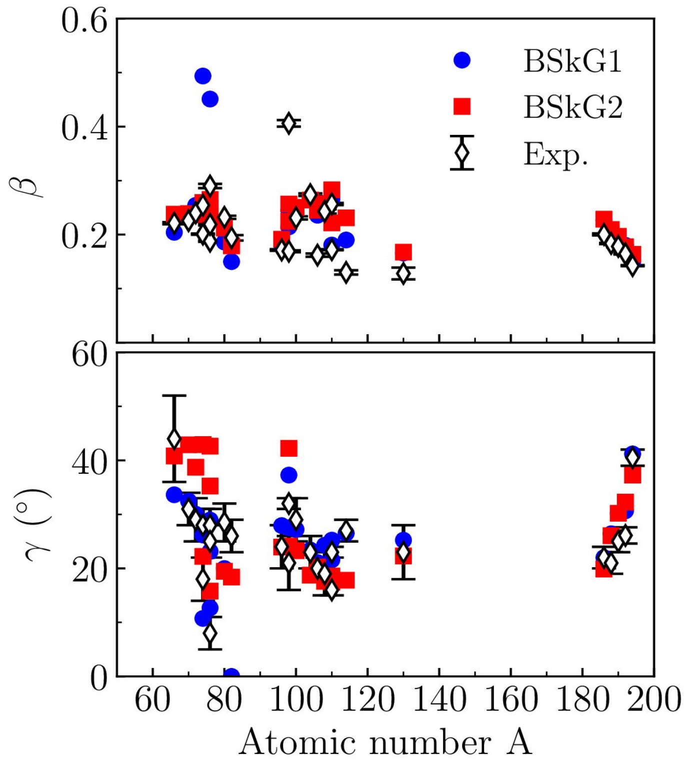




Triaxial deformation





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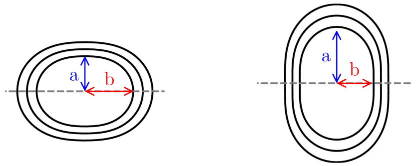

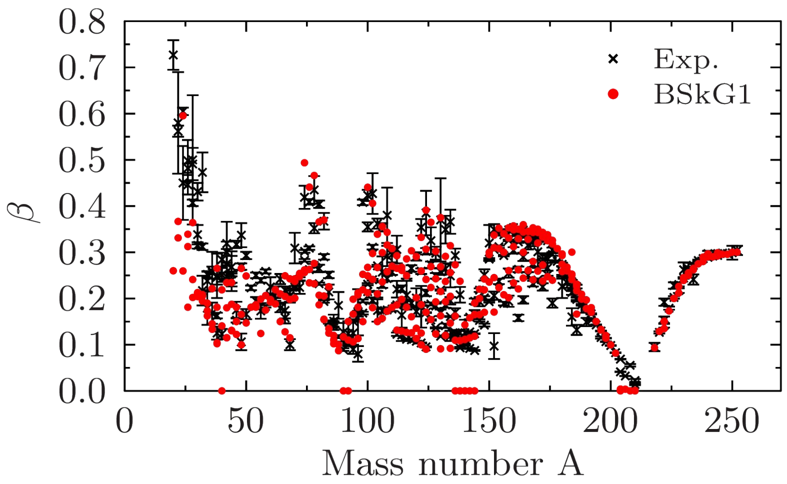

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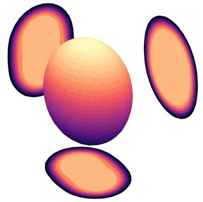
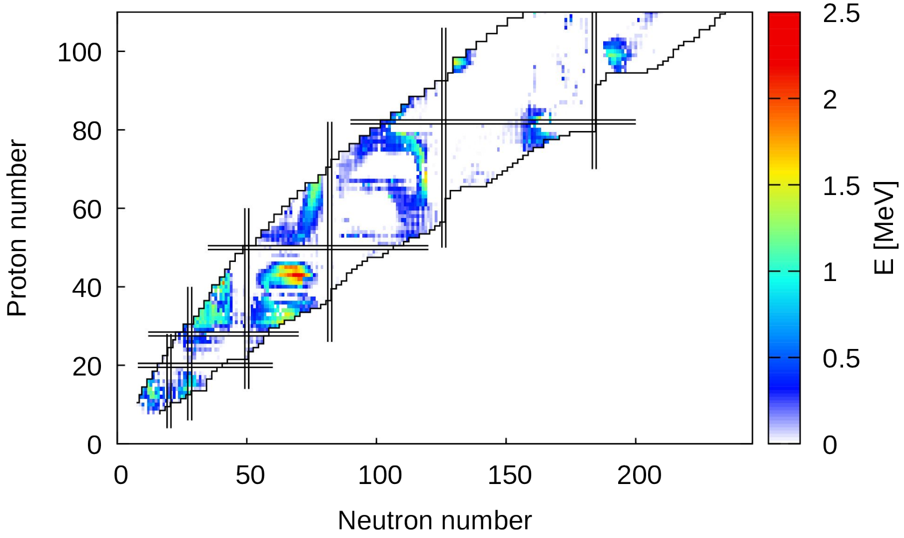




Rotational correction in ^{24}Mg with BSkG1

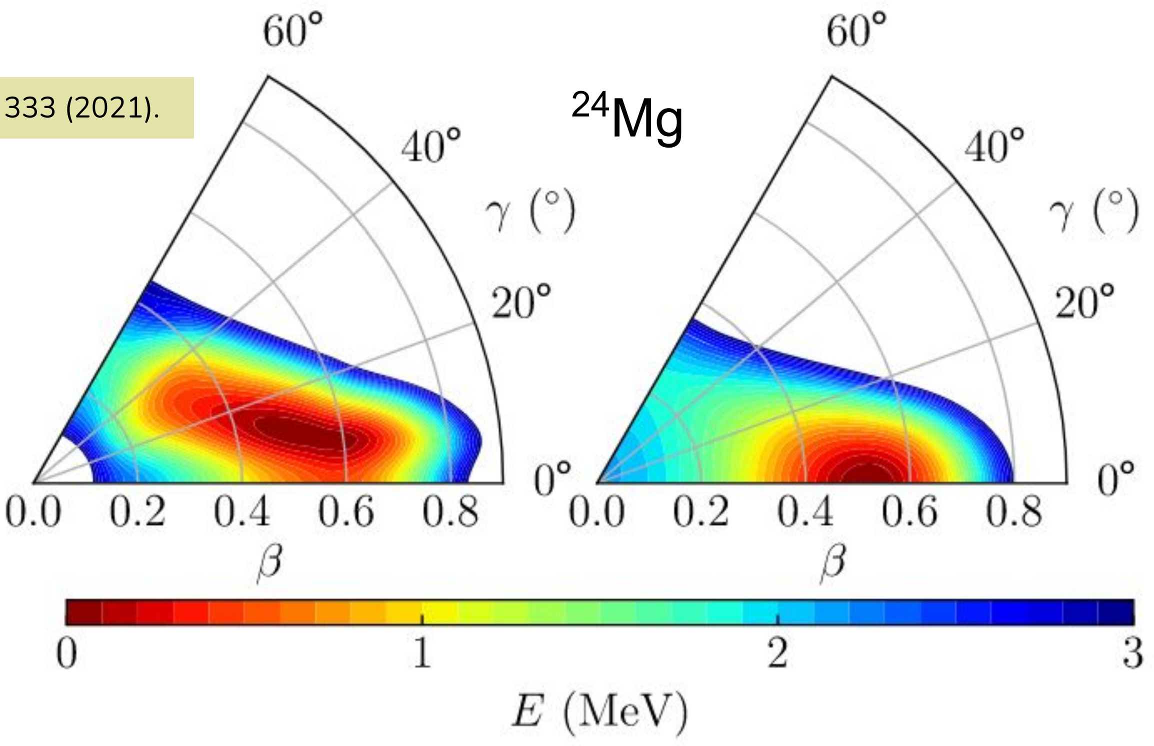
Corrections

$$E_{\text{tot}} = E_{\text{Skyrme}} + E_{\text{kin}} + E_{\text{Coul}} + E_{\text{pair}} + \boxed{E_{\text{corr.}}}$$

✓ INCLUDED

✗ EXCLUDED

G. Scamps et al., EPJA **57**, 333 (2021).

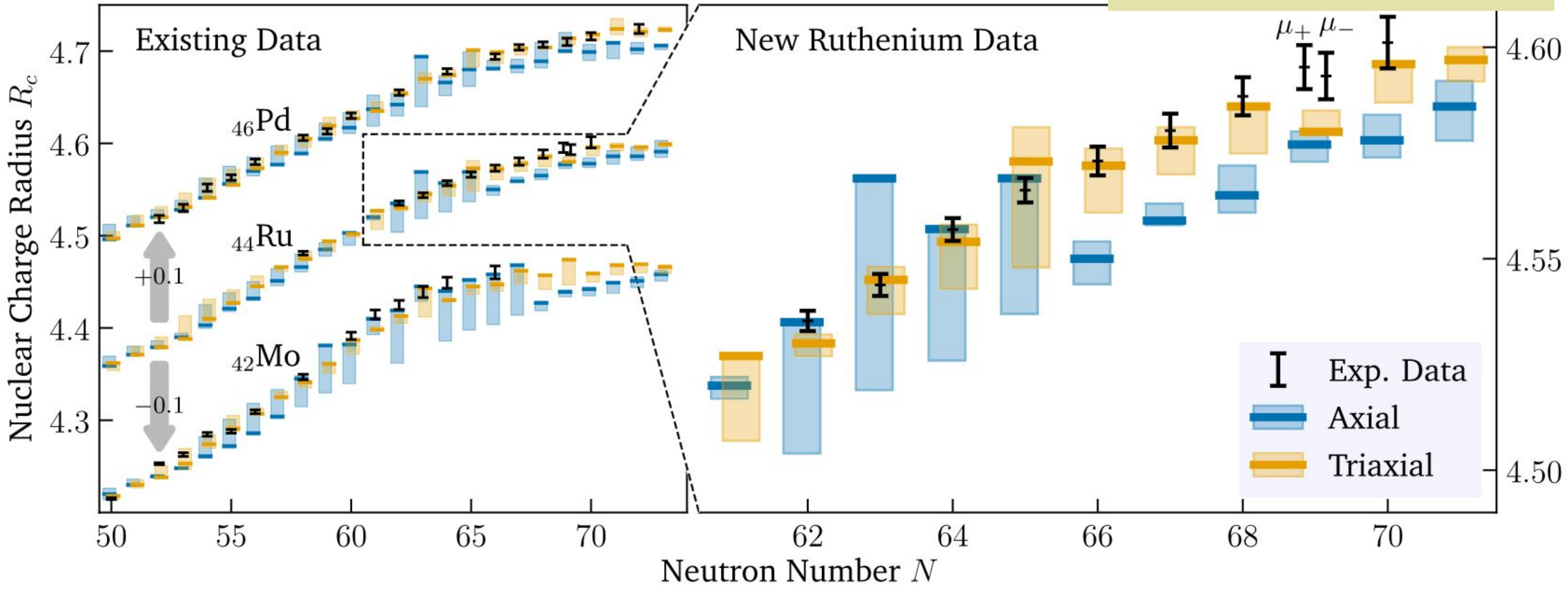


Many nuclei triaxially deformed due to inclusion of rotational correction

Impact of triaxiality on mean-squared charge radii

spread between BSkG[1,2,3,4] as proxy for model uncertainty

B. Maass, *et al.* PRL **135** 202501 (2025)



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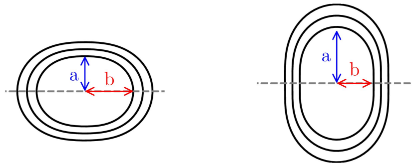
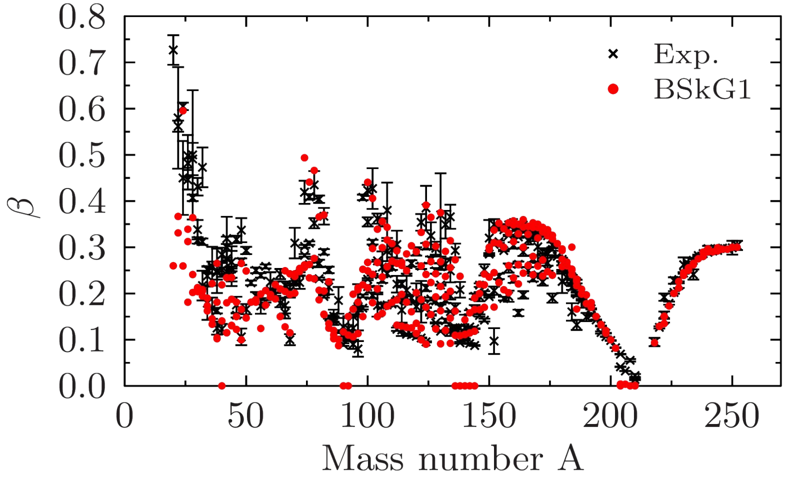
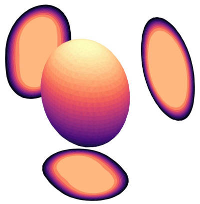
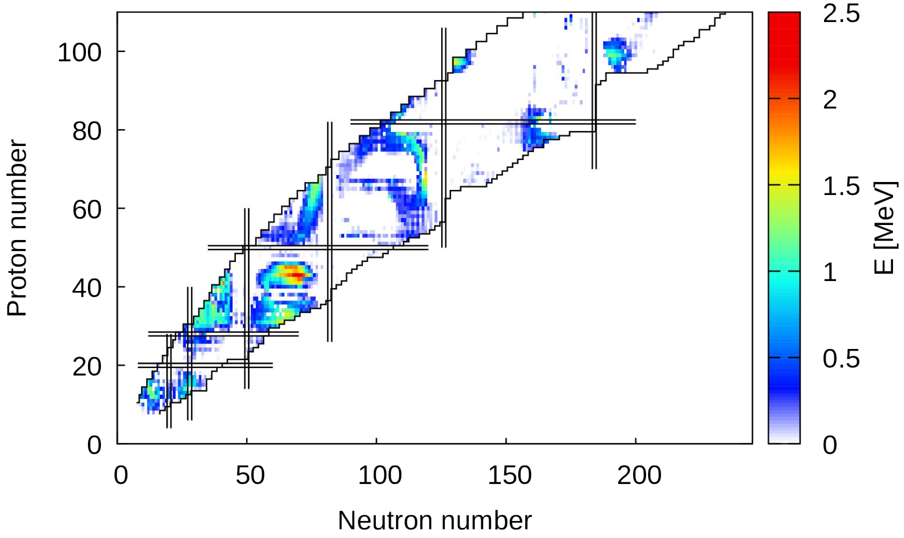
“ordinary” quadrupole deformation



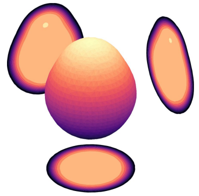


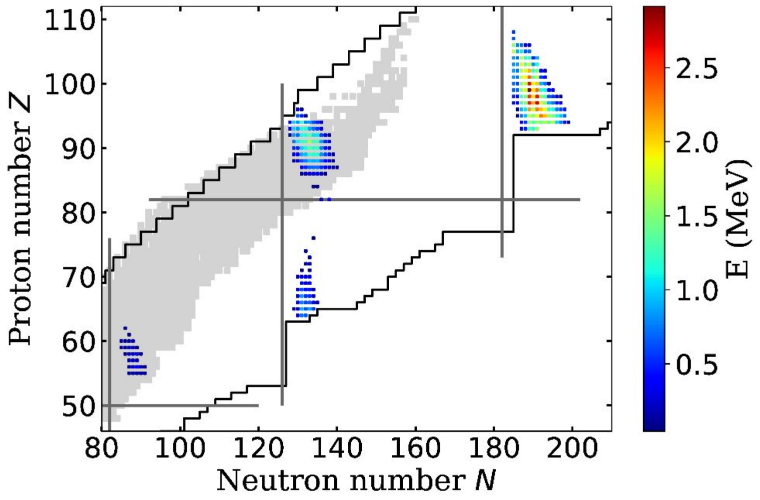
Triaxial deformation





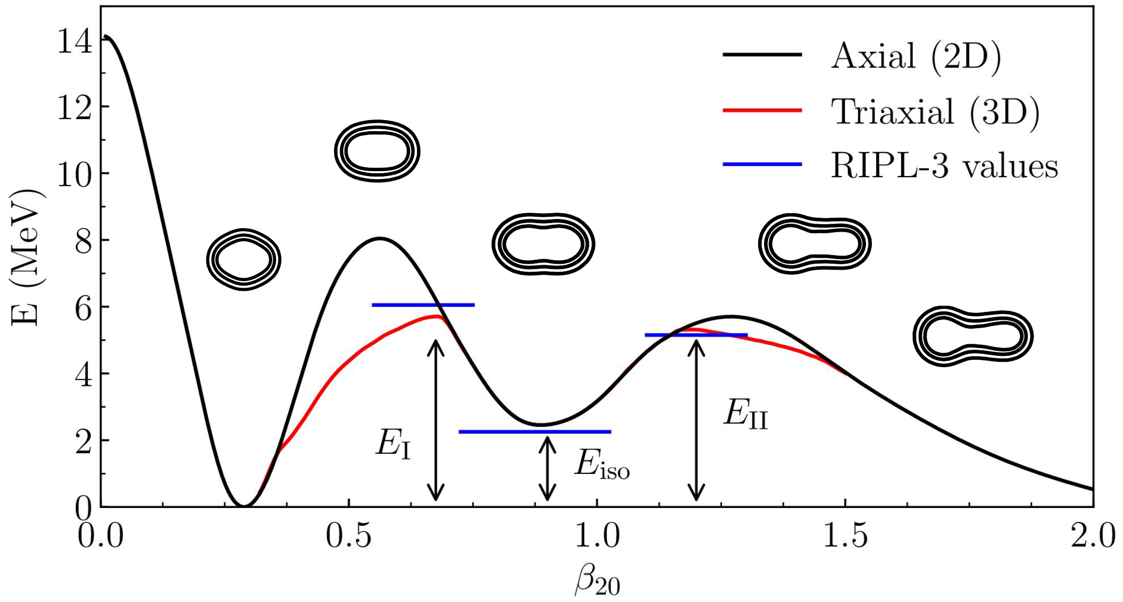
octupole deformation



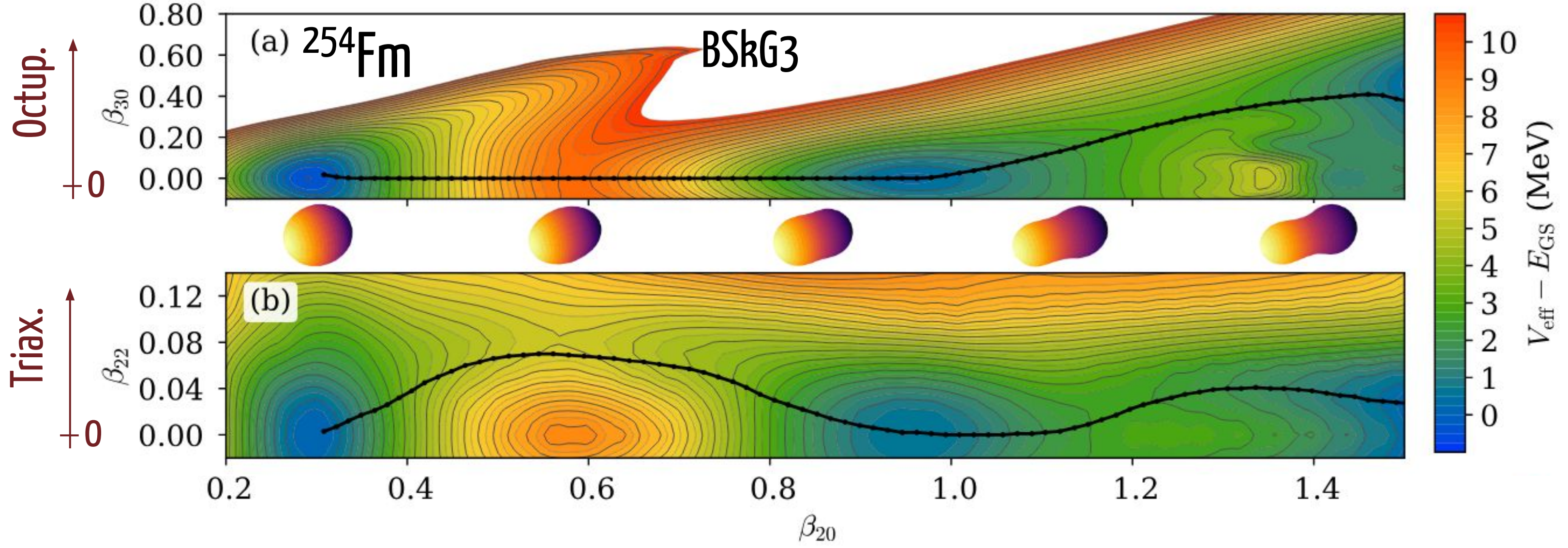


W. Ryssens *et al.*, EPJA **59**, 96 (2023).
E. Flynn *et al.*, PRC **105** (2022).
A. Sánchez-Fernández *et al.*, arXiv:2508.16240
A. Sánchez-Fernández *et al.*, arXiv:2604.25418

Impact of triaxiality on fission barriers

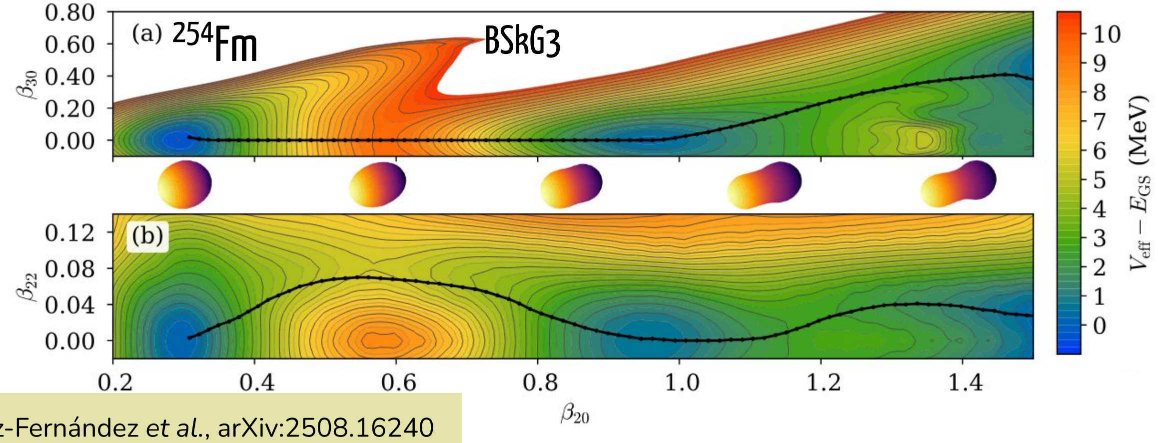


- Inner-barriers are triaxial
- Outer-barriers are triaxial + octupole deformed



Applications which will not be discussed

Fission



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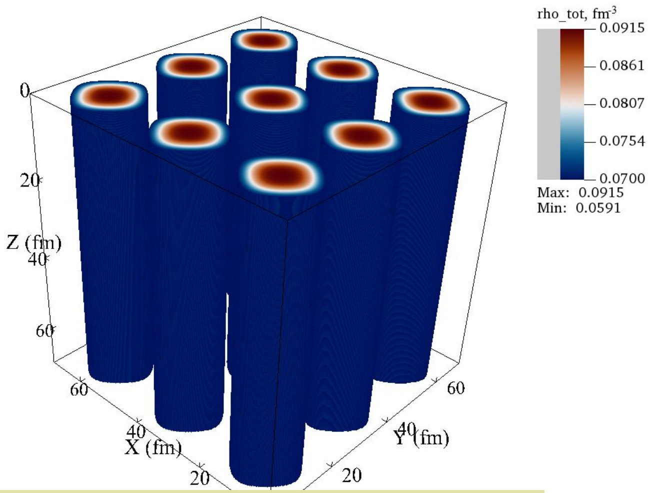
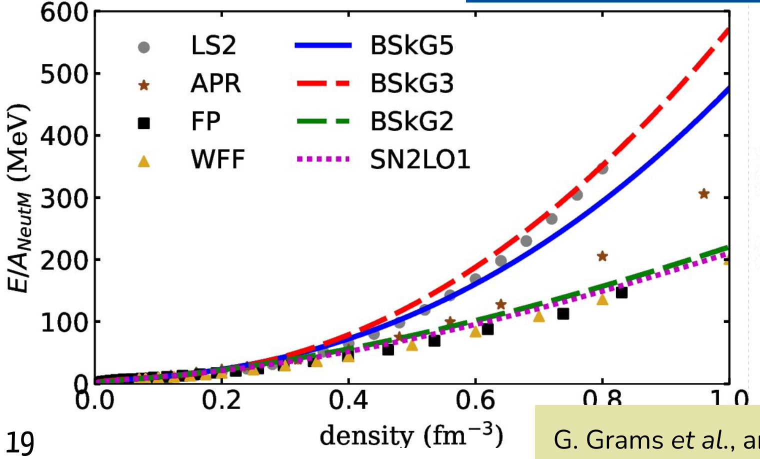
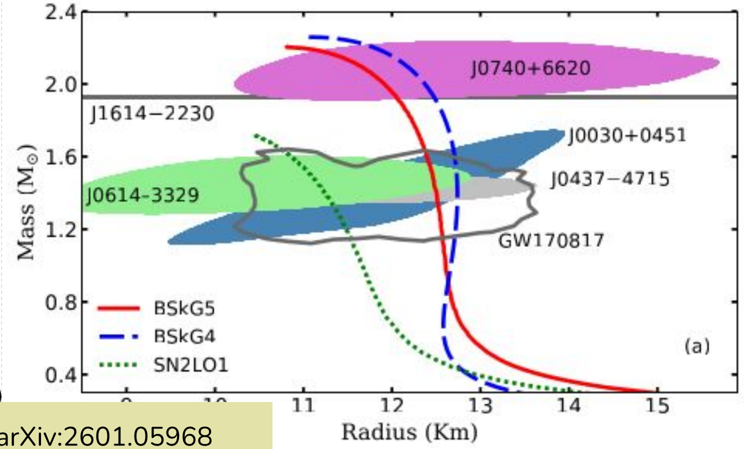
Nuclear Pasta



N. Shchechilin, PhD thesis, ULB, Brussels (2026)

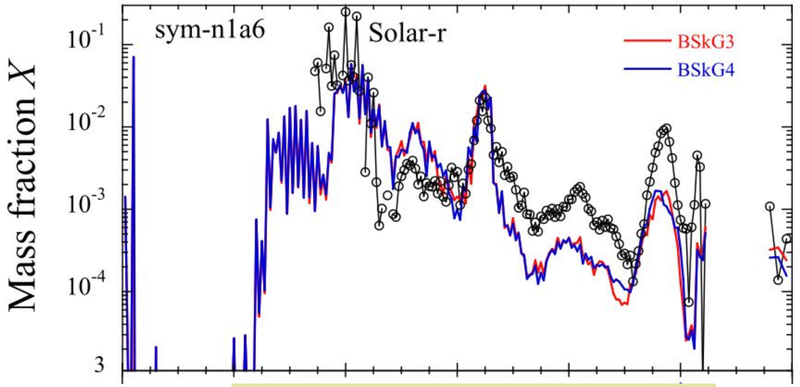
Neutron star Equation of State (EoS)





G. Grams *et al.*, arXiv:2601.05968

r-process simulations



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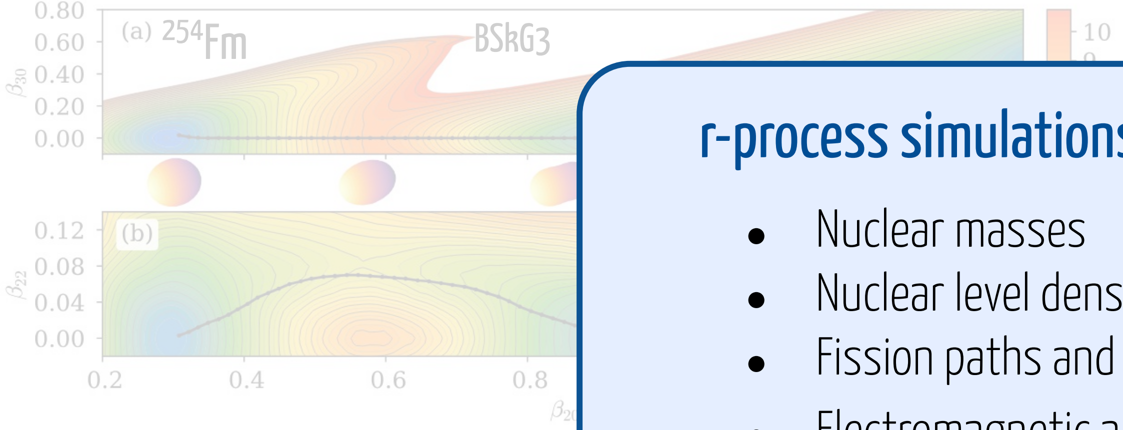

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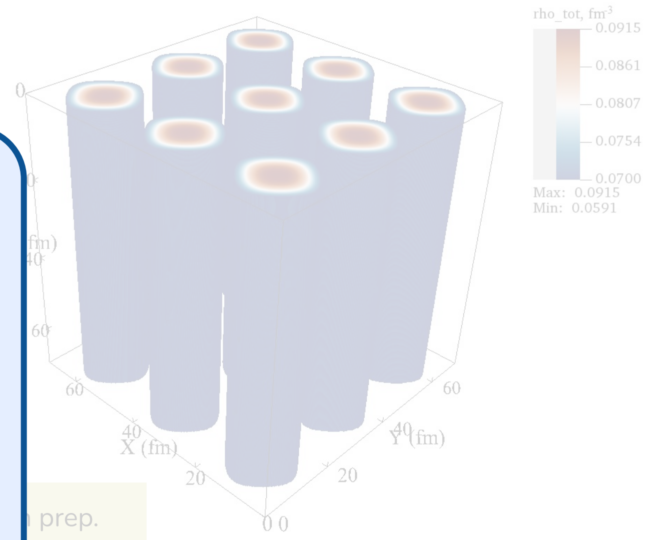
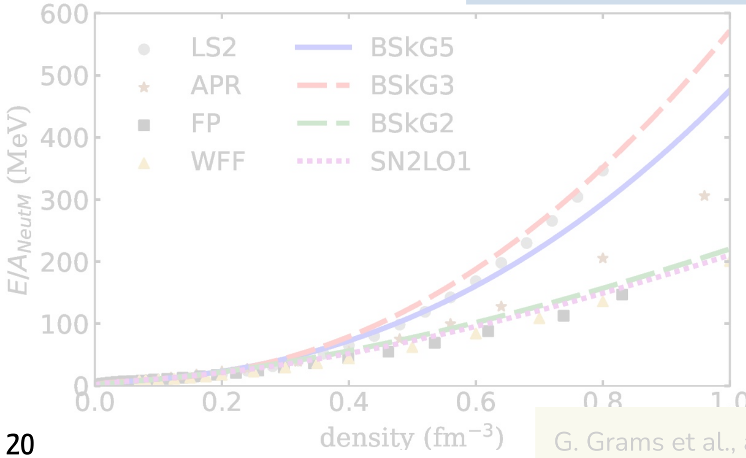


r-process simulations require a lot of data

- Nuclear masses
- Nuclear level densities
- Fission paths and fragment yields
- Electromagnetic and weak strength functions

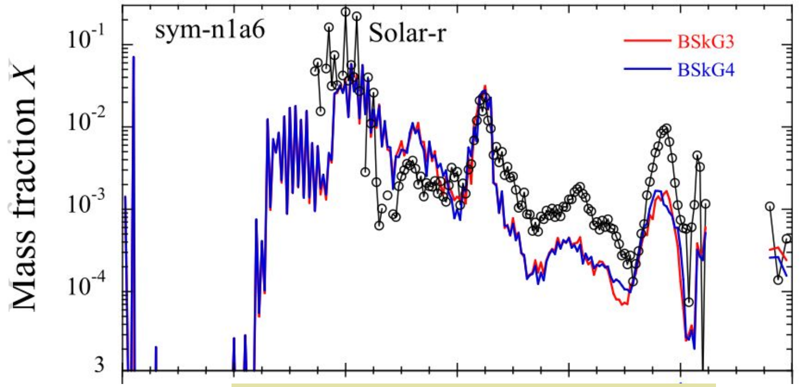
for ALL nuclei

Neutro[n]
Equation of State (EoS)



G. Grams et al., arXiv2601.05968

r-process simulations



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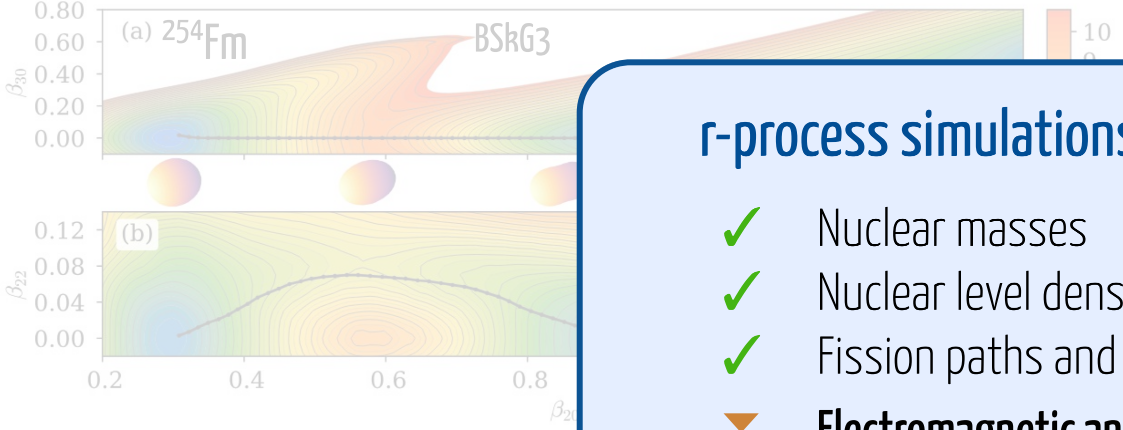
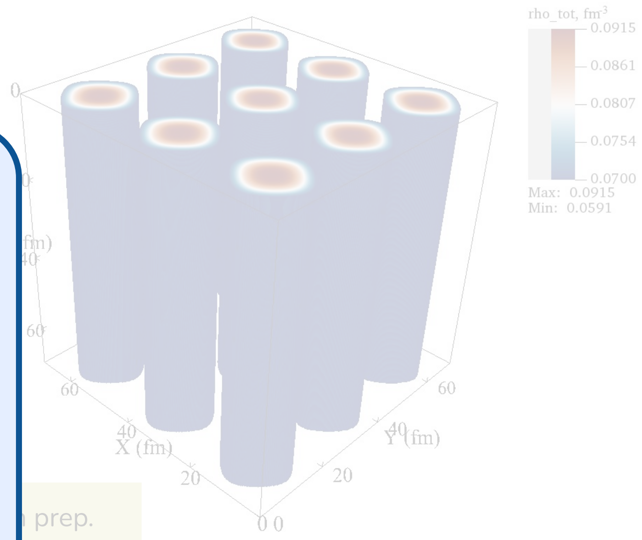


Nuclear Pasta



r-process simulations require a lot of data

- ✓ Nuclear masses
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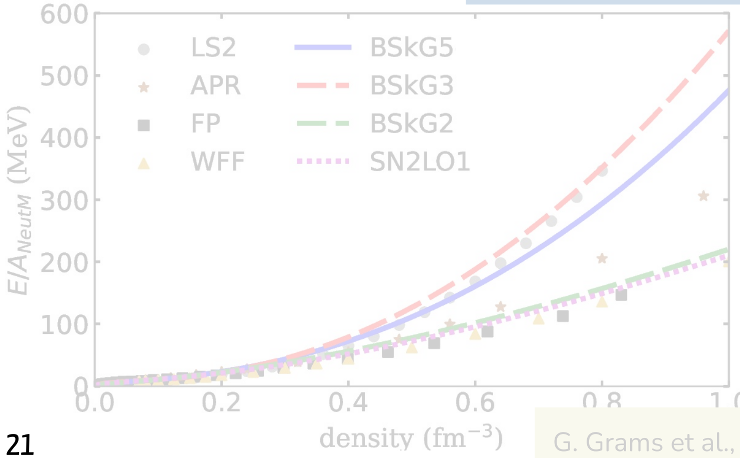
- ✓ Fission paths and fragment yields
- ⧗ **Electromagnetic and weak strength functions**

for ALL nuclei

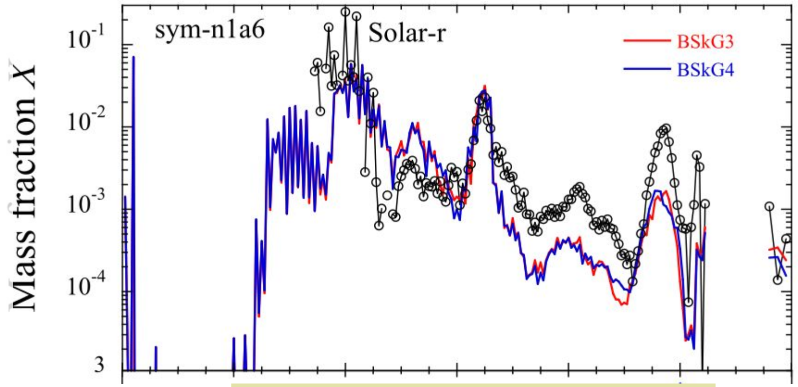
prep.

Neutro
Equation of State (EoS)



G. Grams et al., arXiv2601.05968

r-process simulations



G. Grams et al., arXiv2601.05968

Nuclear linear response

1) Solve mean-field problem for ground-state density ρ_0

2) Add a harmonic external perturbation $F(\omega)$, e.g. E0, E1, ..., M1, M2, ...

$$E[\rho] \rightarrow E[\underbrace{\boxed{\rho_0}}_{\text{Static mean-field solution}}] + \frac{\partial E[\rho]}{\partial \rho} \cdot \underbrace{\boxed{\delta\rho(\omega)}}_{\text{Harmonic oscillations around } \rho_0} + F(\omega)$$

3) Quantify response through **strength function** $S(\omega, F) = \sum\!\!\!\!\!\!\int_n |\langle \Psi_n | F | \Psi_0 \rangle|^2 \delta(\omega - E_n)$

$$= \frac{-1}{\pi} \operatorname{Im} \operatorname{Tr}(F\, \delta\rho(\omega))$$

Nuclear linear response

$$E[\rho] \to E[\boxed{\rho_0}] + \frac{\partial E[\rho]}{\partial \rho} \cdot \boxed{\delta\rho(\omega)} + F(\omega)$$

Static mean-field solution

Harmonic oscillations around ρ_0
$\longrightarrow$ in terms of **1-particle 1-hole excitations**

Solving linear response in 1p1h space boils down to solving

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \boxed{\begin{pmatrix} X \\ Y \end{pmatrix}} = -\cancel{\begin{pmatrix} F^{ph} \\ F^{hp} \end{pmatrix}}$$

Random phase approximation (RPA)
$\longrightarrow$ Casida eq. in quantum chemistry

where $$A_{aibj}, B_{aibj} \sim \frac{\delta^2 E[\rho]}{\delta \rho_{ai} \rho_{bj}}$$

Very big matrices !

Finite amplitude method (FAM) = matrix-free RPA solver

$\longrightarrow$ see T. Nakatsukasa's talk

Nuclear linear response

Solving linear response in 1p1h space boils down to solving

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \begin{pmatrix} X \\ Y \end{pmatrix} = - \begin{pmatrix} F^{ph} \\ F^{hp} \end{pmatrix}$$

where $$A_{aibj}, B_{aibj} \sim \frac{\delta^2 E[\rho]}{\delta\rho_{ai}\rho_{bj}}$$

Finite amplitude method (FAM) = matrix-free RPA solver

$\longrightarrow$ see T. Nakatsukasa's talk

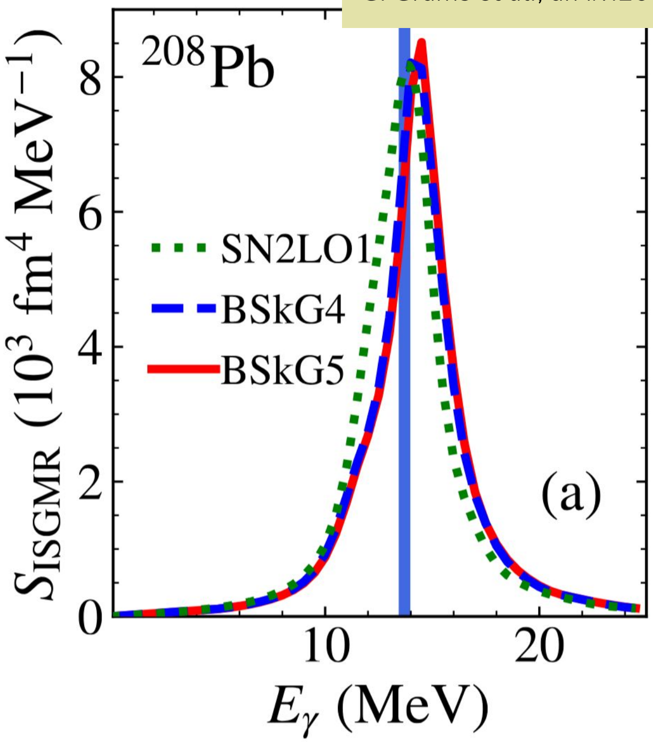
$$\begin{pmatrix} \delta h^{ph}(X,Y) \\ \delta h^{hp}(X,Y) \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = - \begin{pmatrix} F^{ph} \\ F^{hp} \end{pmatrix}$$

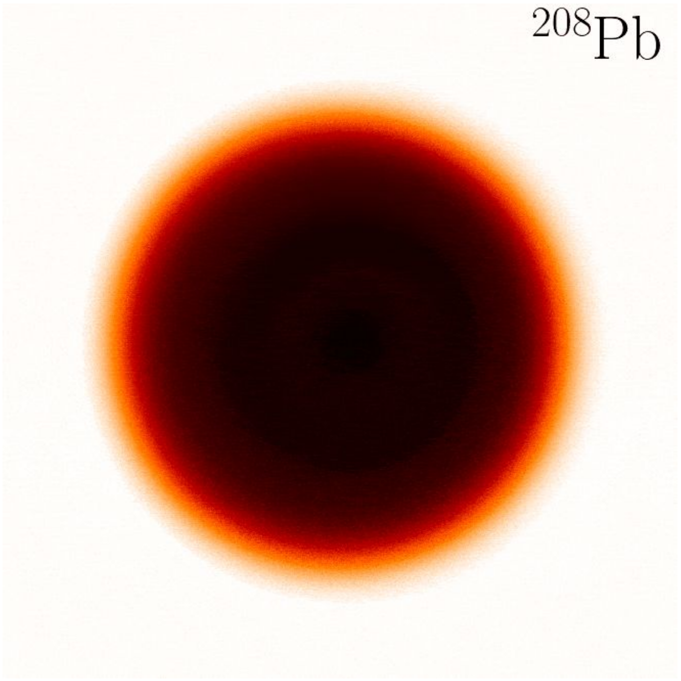
Perturbed single-particle Hamiltonian evaluated at mean-field cost*

Adding complex smearing $\omega \to \omega + i\gamma$ replaces delta peaks by Lorentzians

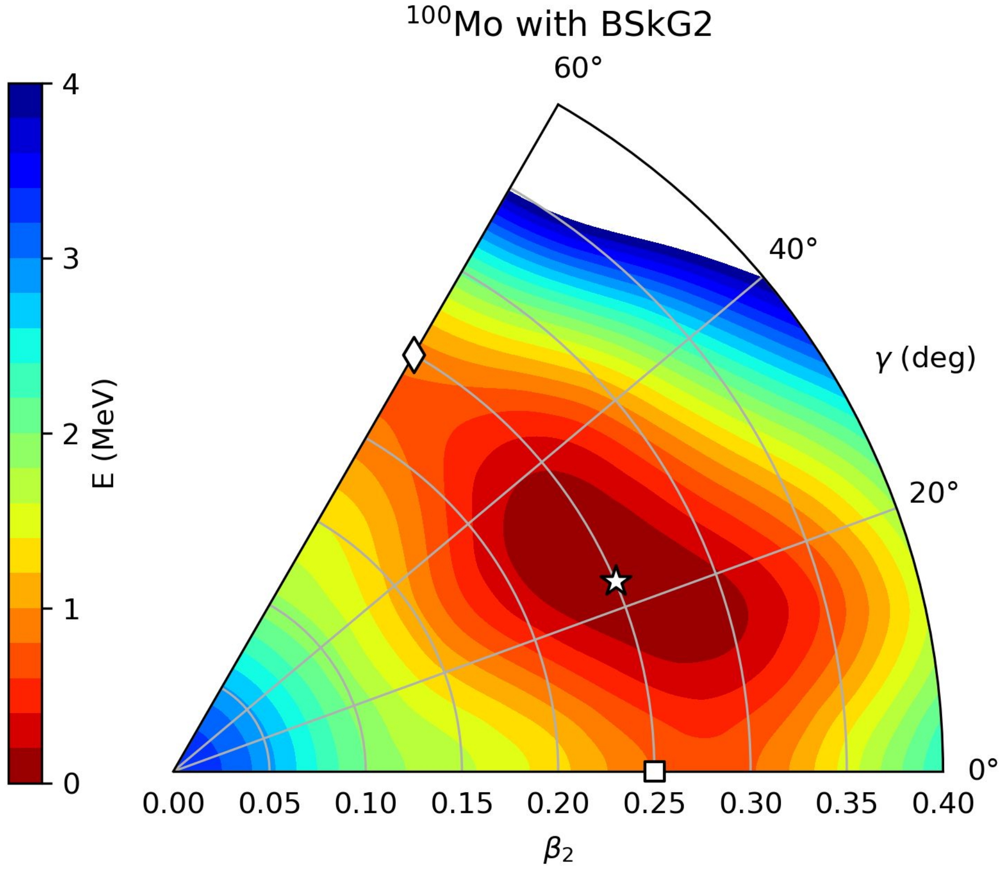
Giant monopole resonance of ^{208}Pb with BSkG5

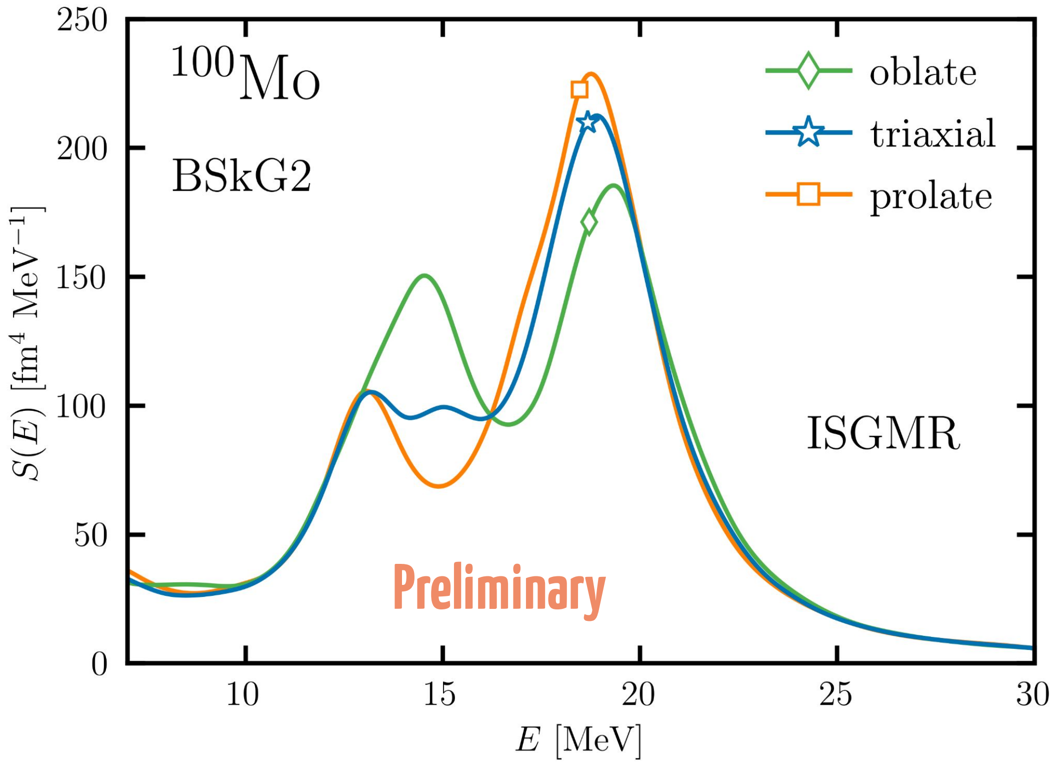
G. Grams *et al.*, arXiv:2601.05968





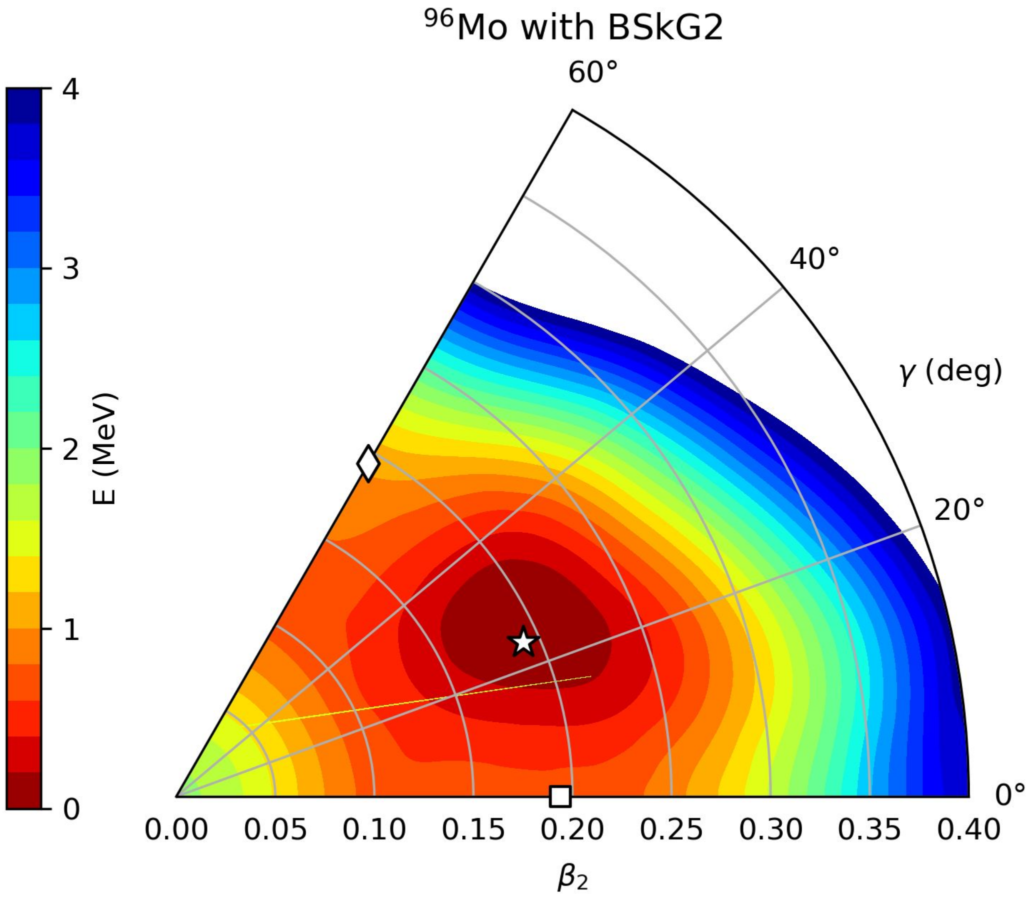
Impact of triaxiality on isoscalar giant monopole resonance (ISGMR)

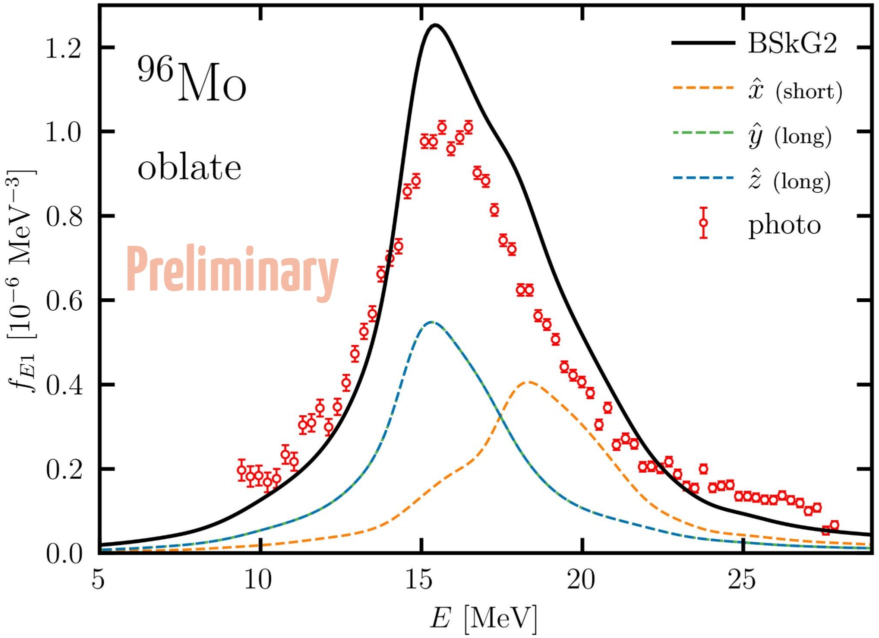




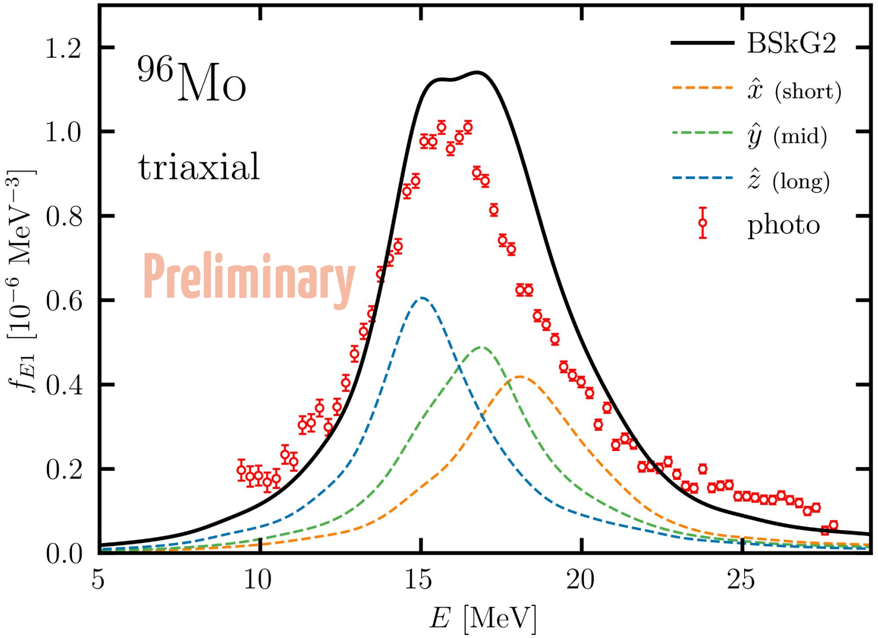
Appearance of a third peak, in accordance with Washiyama et al PRC 109 (2024)

Impact of triaxiality on isovector giant dipole resonance (IVGDR)

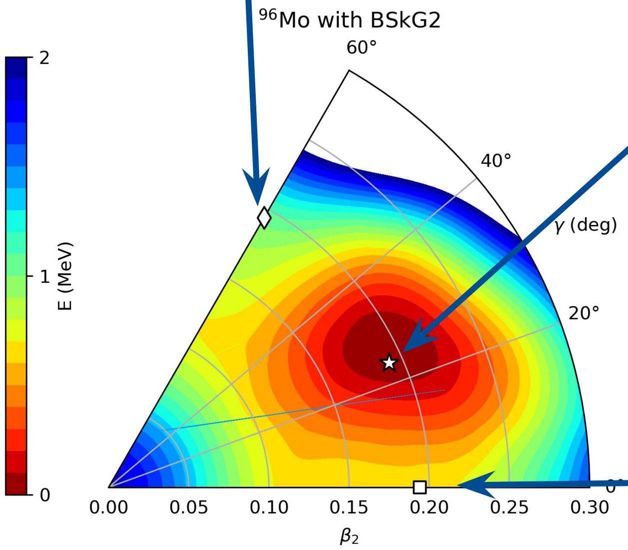




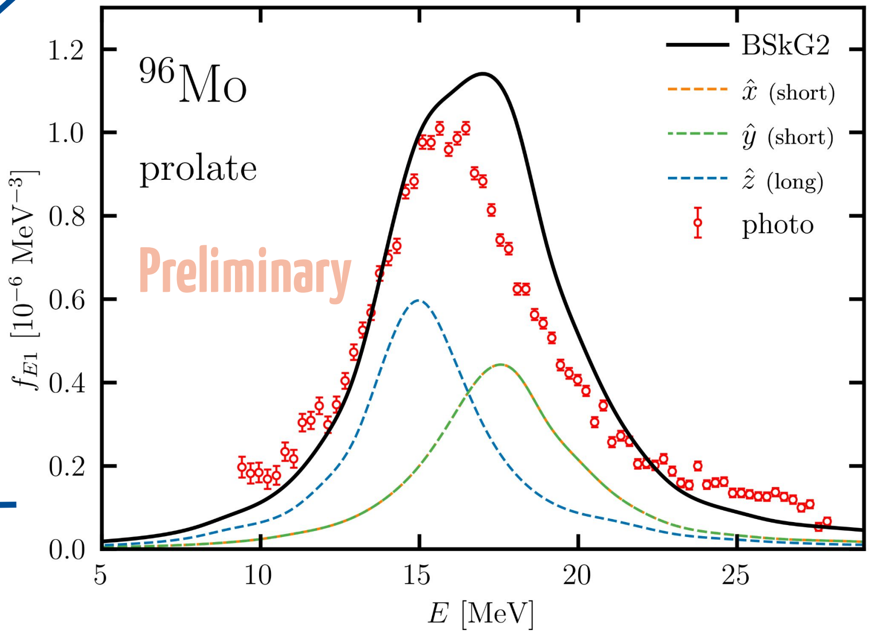
^{96}Mo
oblate
Preliminary
BSkG2
$\hat{x}$ (short)
$\hat{y}$ (long)
$\hat{z}$ (long)
photo
f_{E1} [10^{-6} MeV^{-3}]
E [MeV]



^{96}Mo
triaxial
Preliminary
BSkG2
$\hat{x}$ (short)
$\hat{y}$ (mid)
$\hat{z}$ (long)
photo
f_{E1} [10^{-6} MeV^{-3}]
E [MeV]



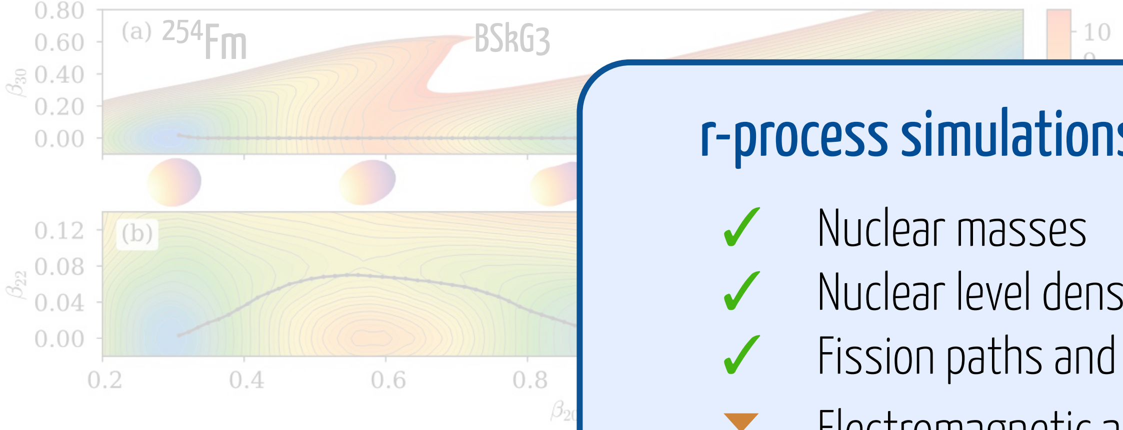
^{96}Mo with BSkG2
60°
40°
20°
0°
γ (deg)
E (MeV)
β_2



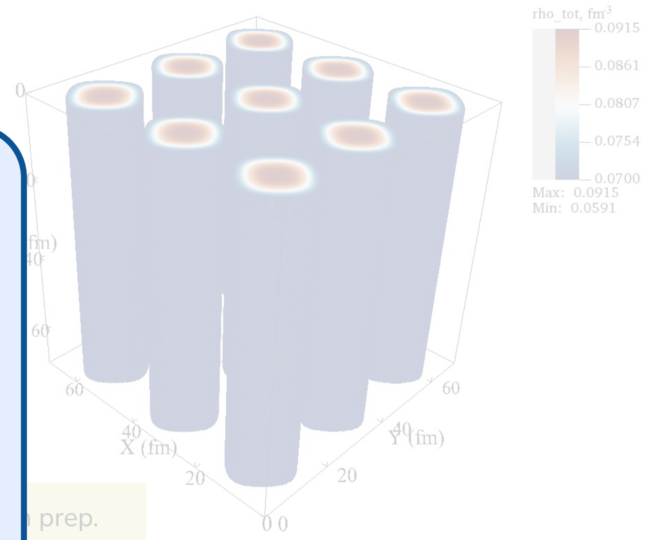
^{96}Mo
prolate
Preliminary
BSkG2
$\hat{x}$ (short)
$\hat{y}$ (short)
$\hat{z}$ (long)
photo
f_{E1} [10^{-6} MeV^{-3}]
E [MeV]

Applications which will not be discussed

Fission



Nuclear Pasta

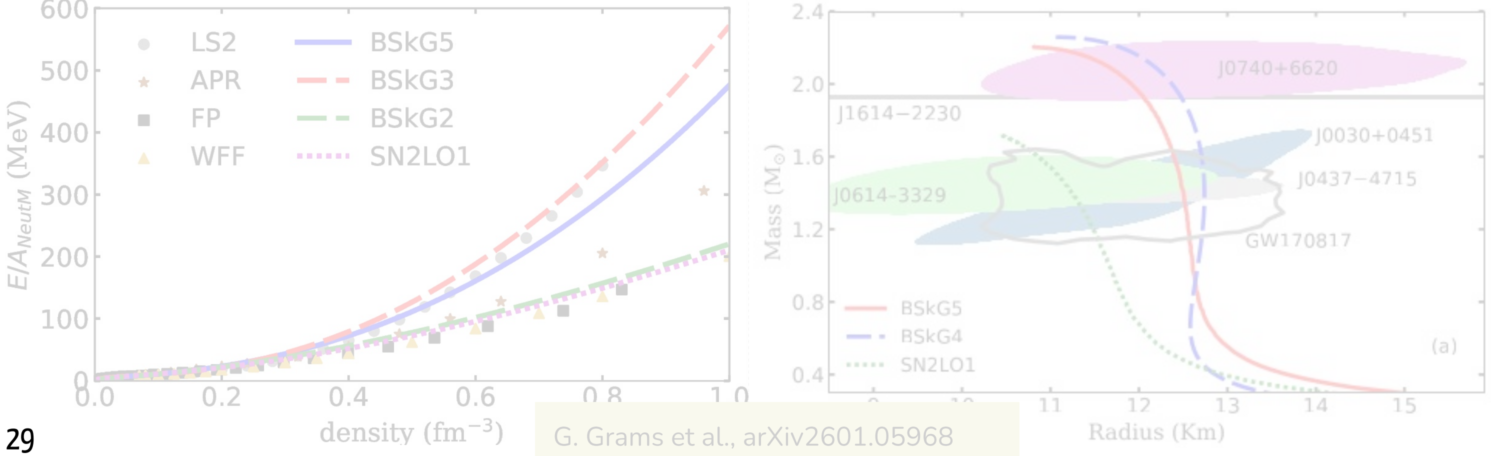


r-process simulations require **a lot** of data

- ✓ Nuclear masses
- ✓ Nuclear level densities
- ✓ Fission paths and fragment yields
- ⧗ Electromagnetic and weak strength functions

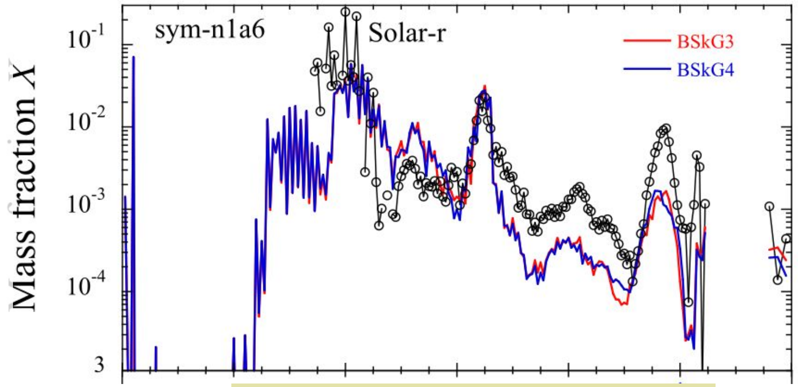
for ALL nuclei

Neutron Star Equation of State (EoS)



G. Grams et al., arXiv2601.05968

r-process simulations



G. Grams et al., arXiv2601.05968

Emulating FAM via reduced order modelling (ROM)

Work of master's student **Emma Vancayseele**

- Solve FAM for a handful of sample frequencies

$\longrightarrow$ snapshot basis : $\left\{ \left(X(\omega_i)\; Y(\omega_i) \right)^T \mid i = 1, \ldots, N_s \right\}$

- Approximate any other frequency in snapshot basis

$$\left(X(\omega)\; Y(\omega) \right)^T \approx \sum_{i=1}^{N_s} \alpha_i \left(X(\omega_i)\; Y(\omega_i) \right)^T$$

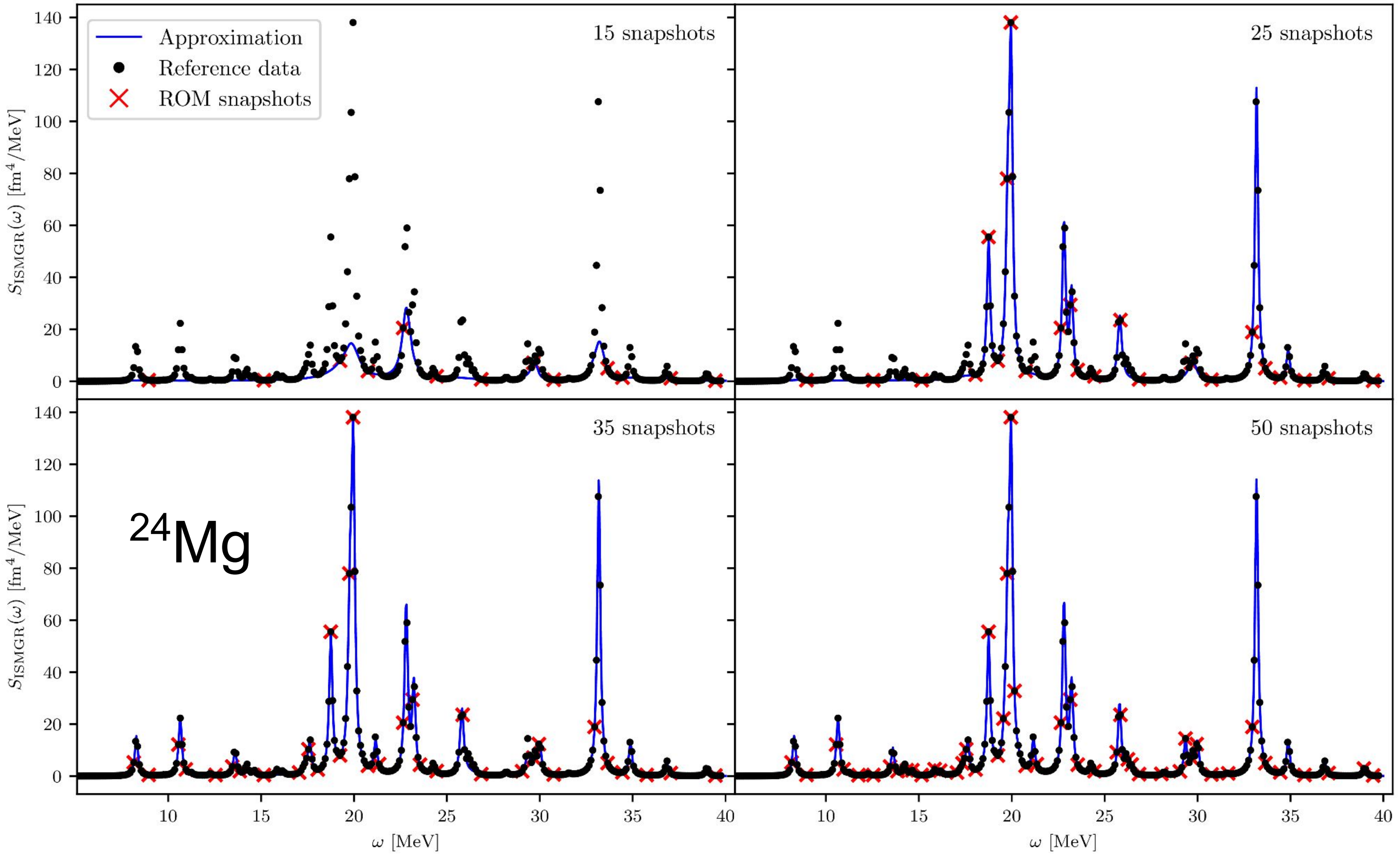
- Coefficients obtained by solving subspace projected FAM equation

$\longrightarrow$ **Petrov Galerkin** least-squares projection

Minimize cost function (residual): $r(\omega) = \begin{pmatrix} \delta h^{ph}(\tilde{X}, \tilde{Y}) \\ \delta h^{hp}(\tilde{X}, \tilde{Y}) \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} + \begin{pmatrix} F^{ph} \\ F^{hp} \end{pmatrix}$

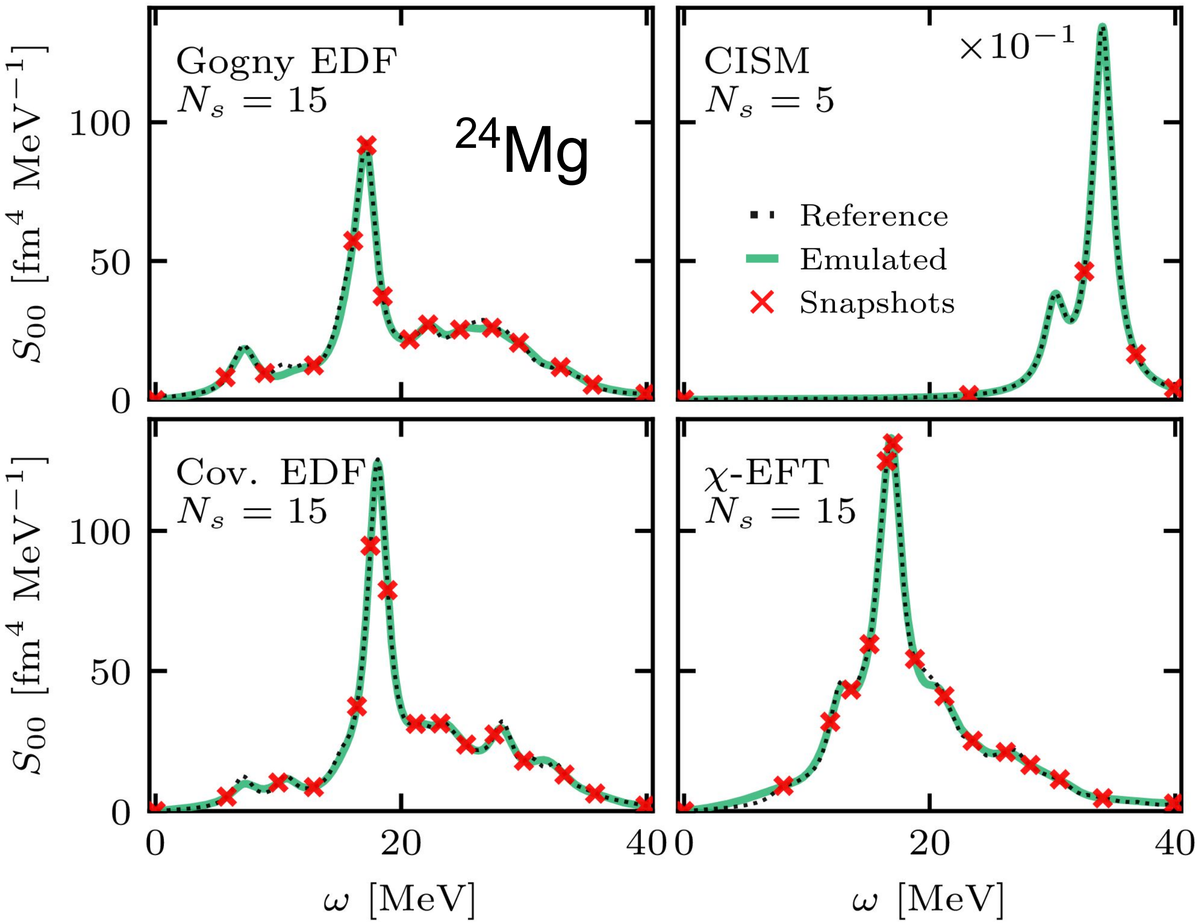
$\longrightarrow$ FAM reduced to trivial linear problem of dimension $N_s \times N_s$

Emulating FAM via reduced order modelling



Emulating FAM via reduced order modelling

Isoscalar monopole strength of ^{24}Mg



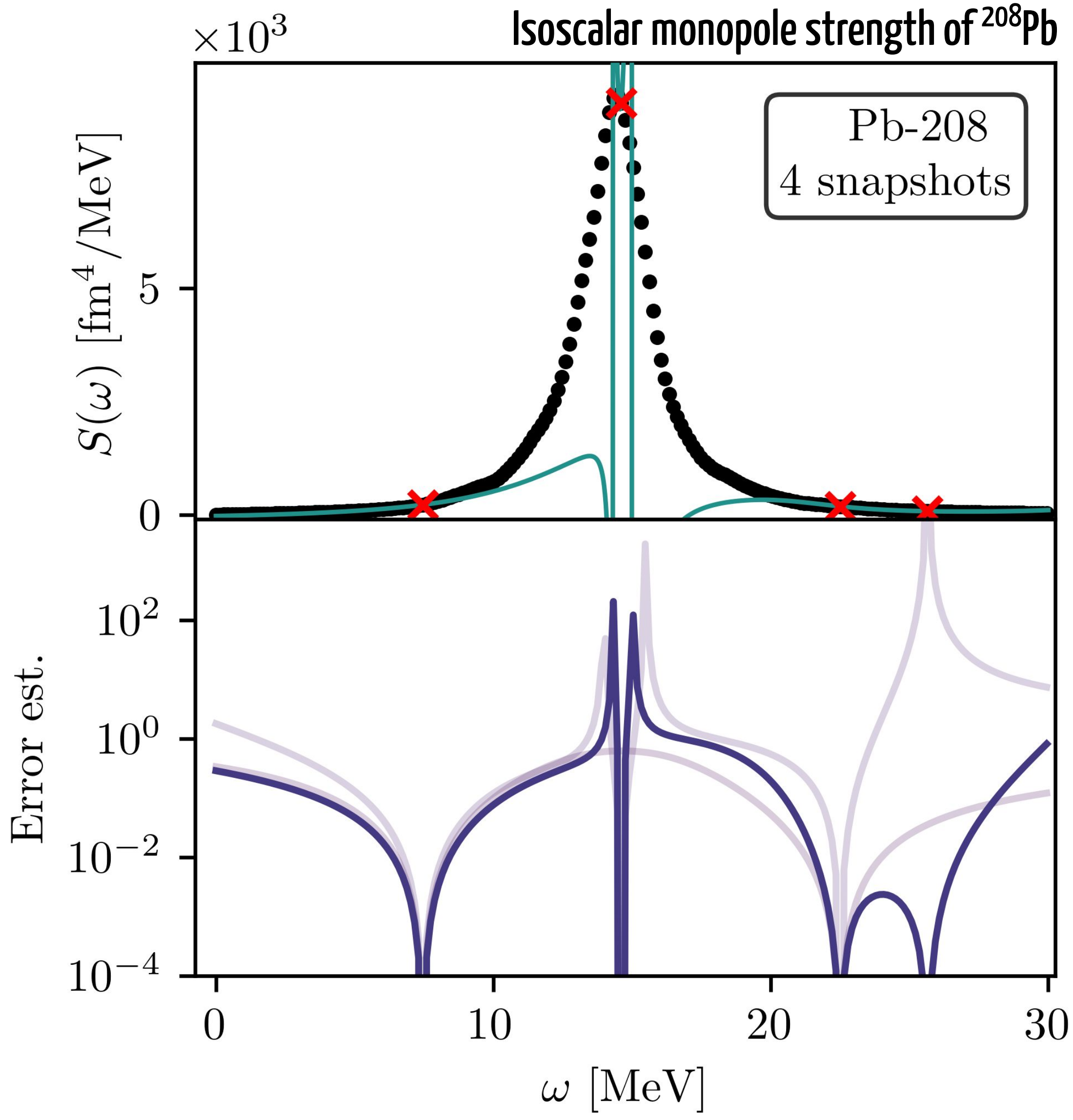
Universally applicable: ab initio, EDF, shell model

Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

→ Greedy sampling based on cost function $r(\omega)$

Isoscalar monopole strength of ^{208}Pb

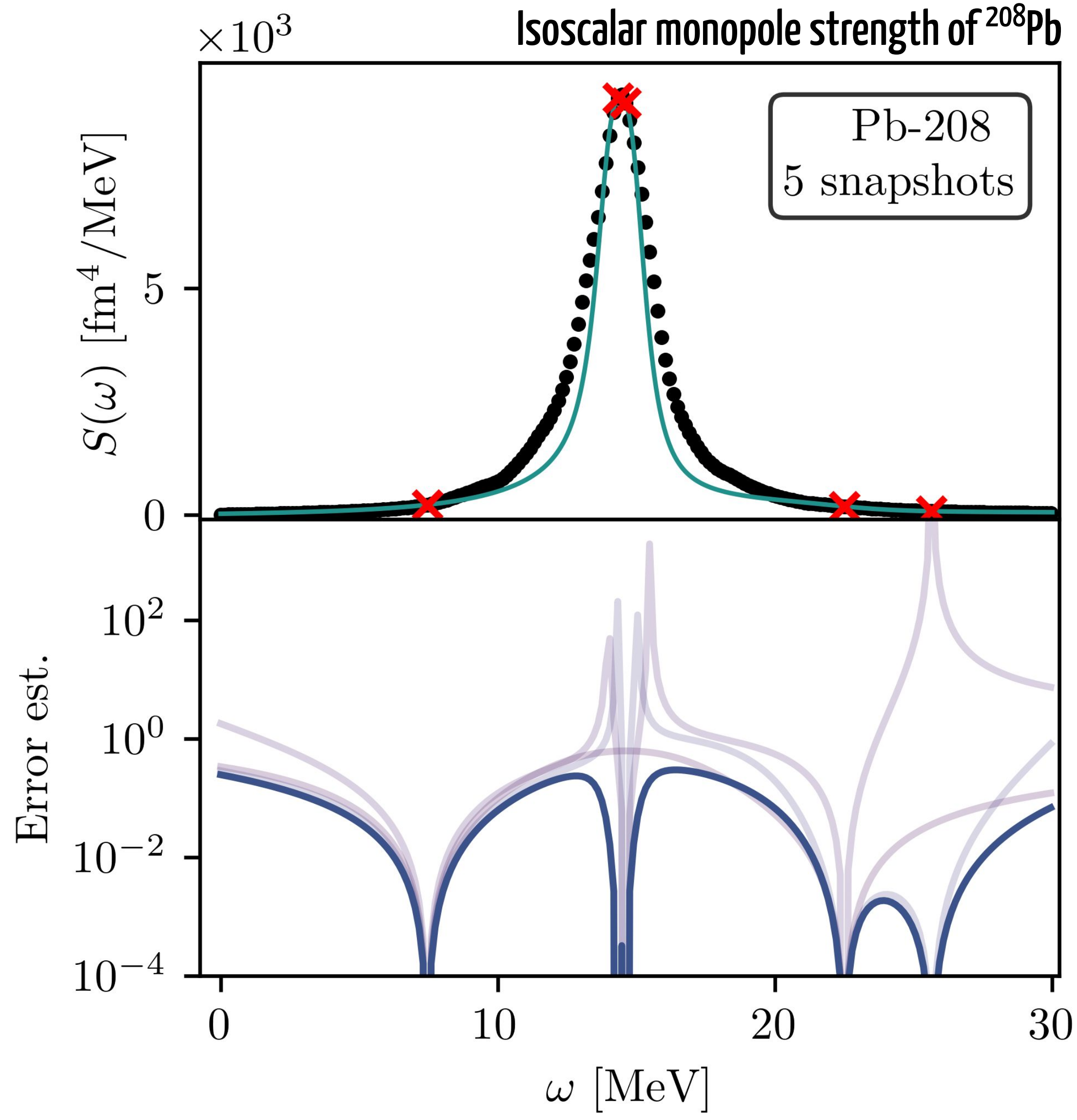


Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

$\longrightarrow$ Greedy sampling based on cost function $r(\omega)$

Isoscalar monopole strength of ^{208}Pb

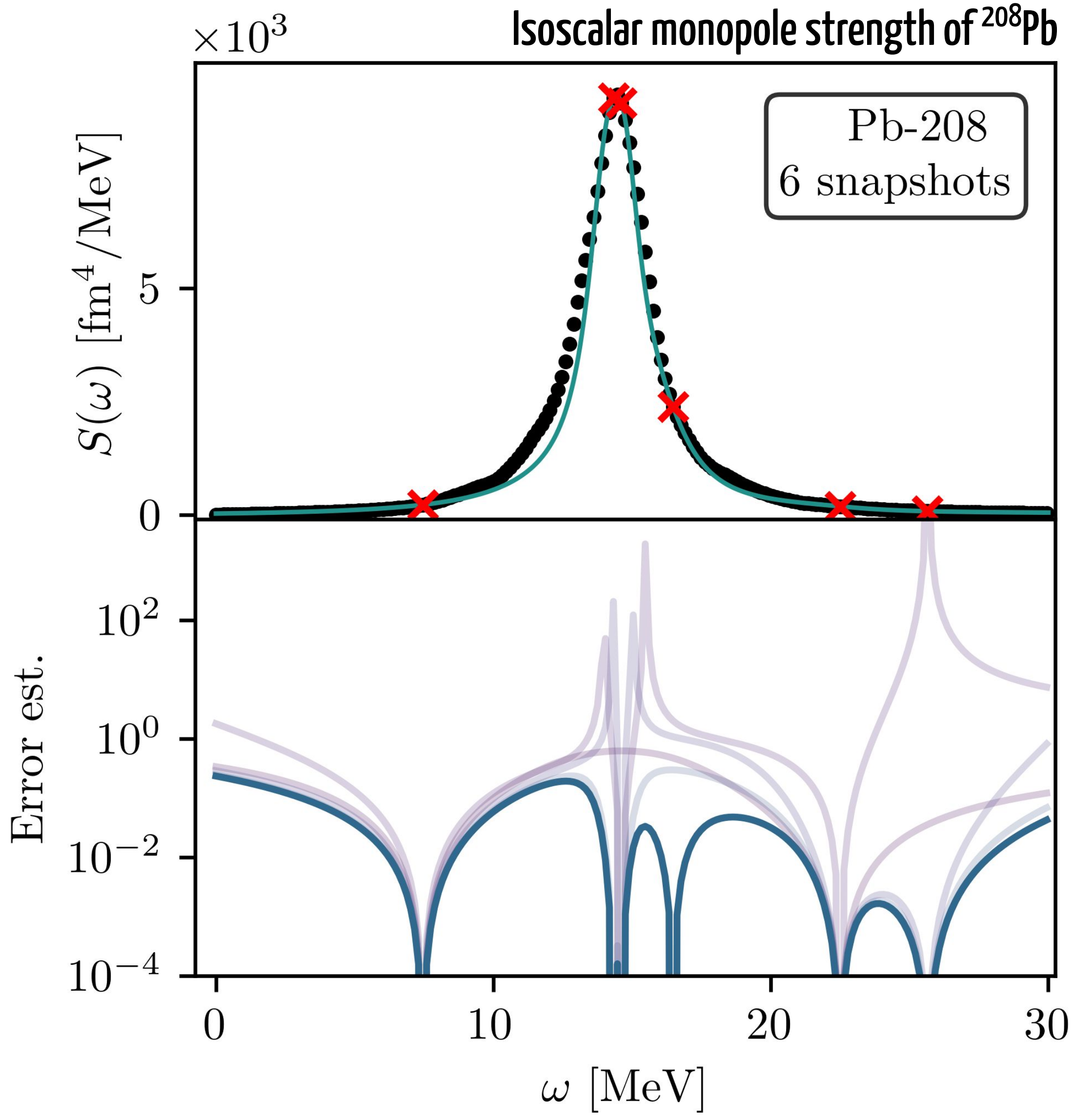


Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

$\longrightarrow$ Greedy sampling based on cost function $r(\omega)$

Isoscalar monopole strength of ^{208}Pb



Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

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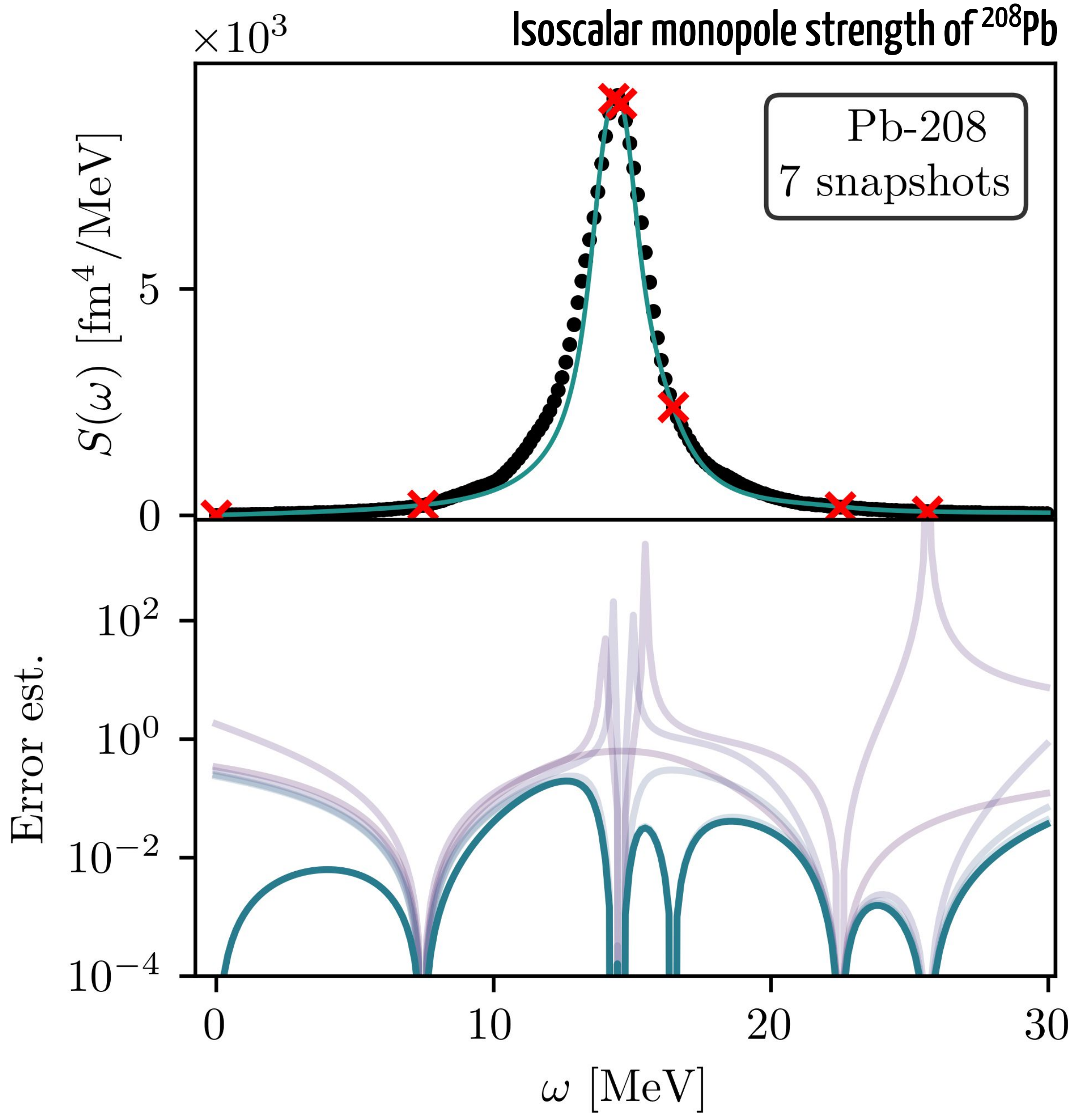

Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

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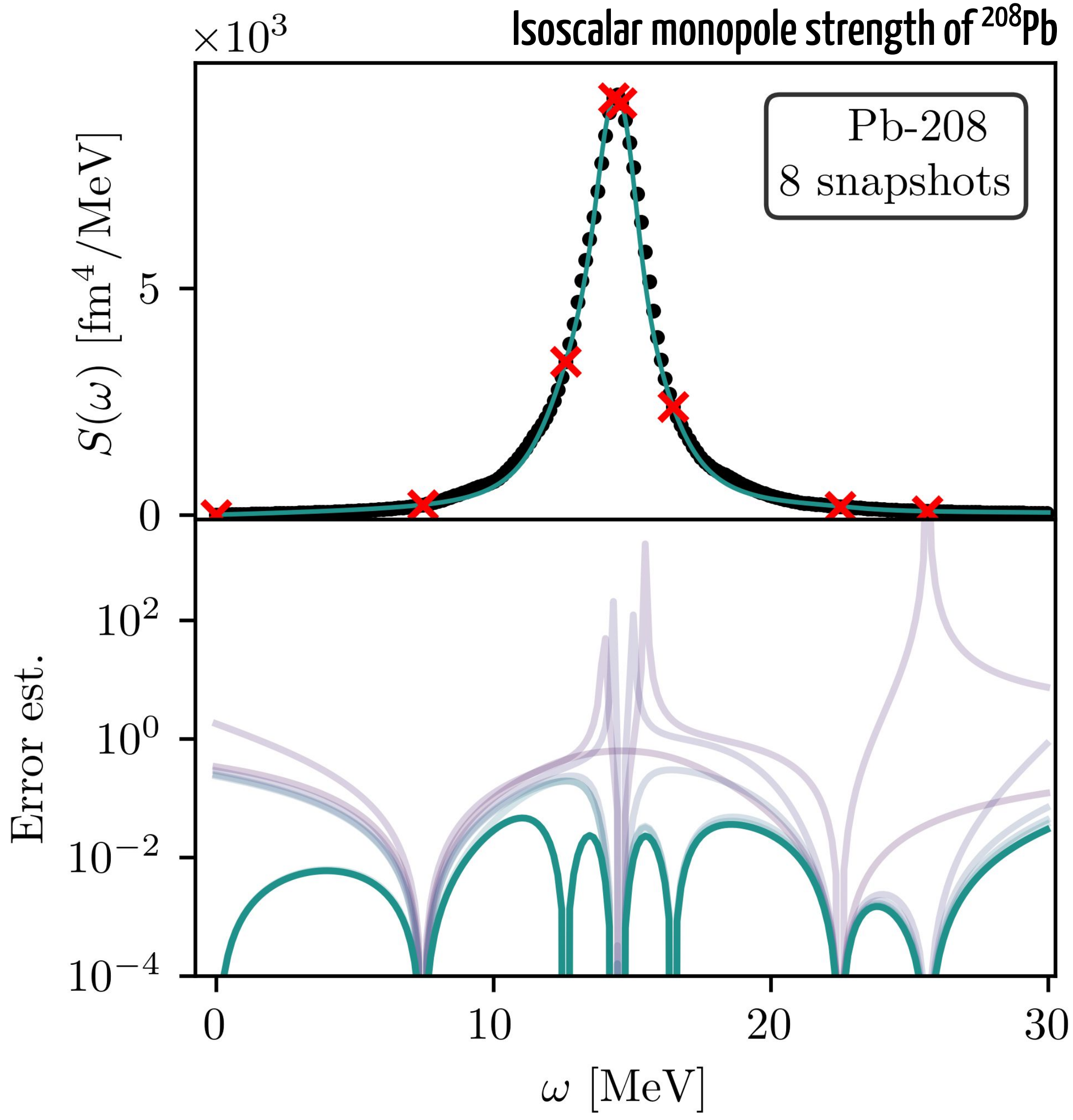
Isoscalar monopole strength of ^{208}Pb



Emulating FAM via reduced order modelling

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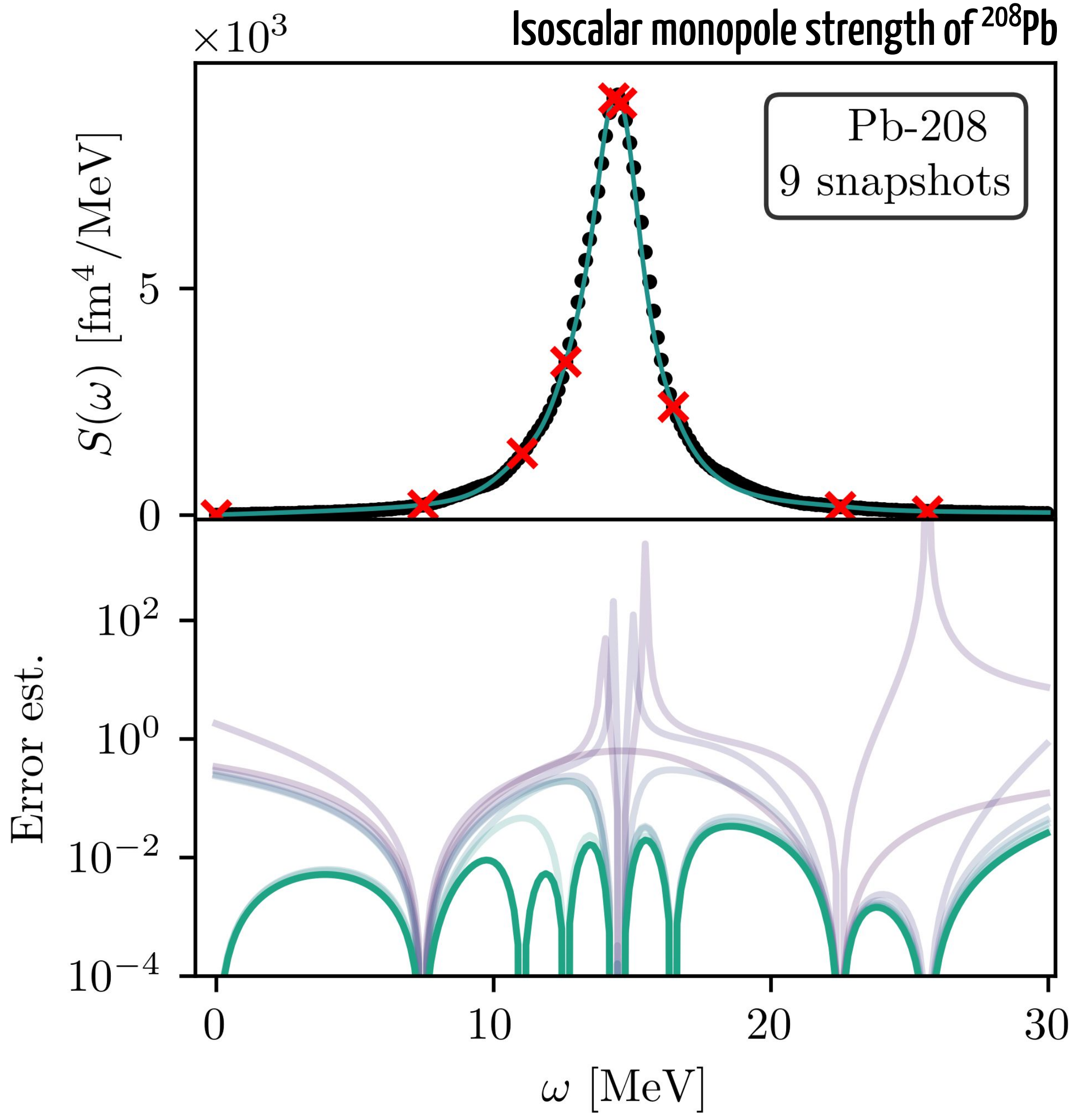
Isoscalar monopole strength of ^{208}Pb



Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

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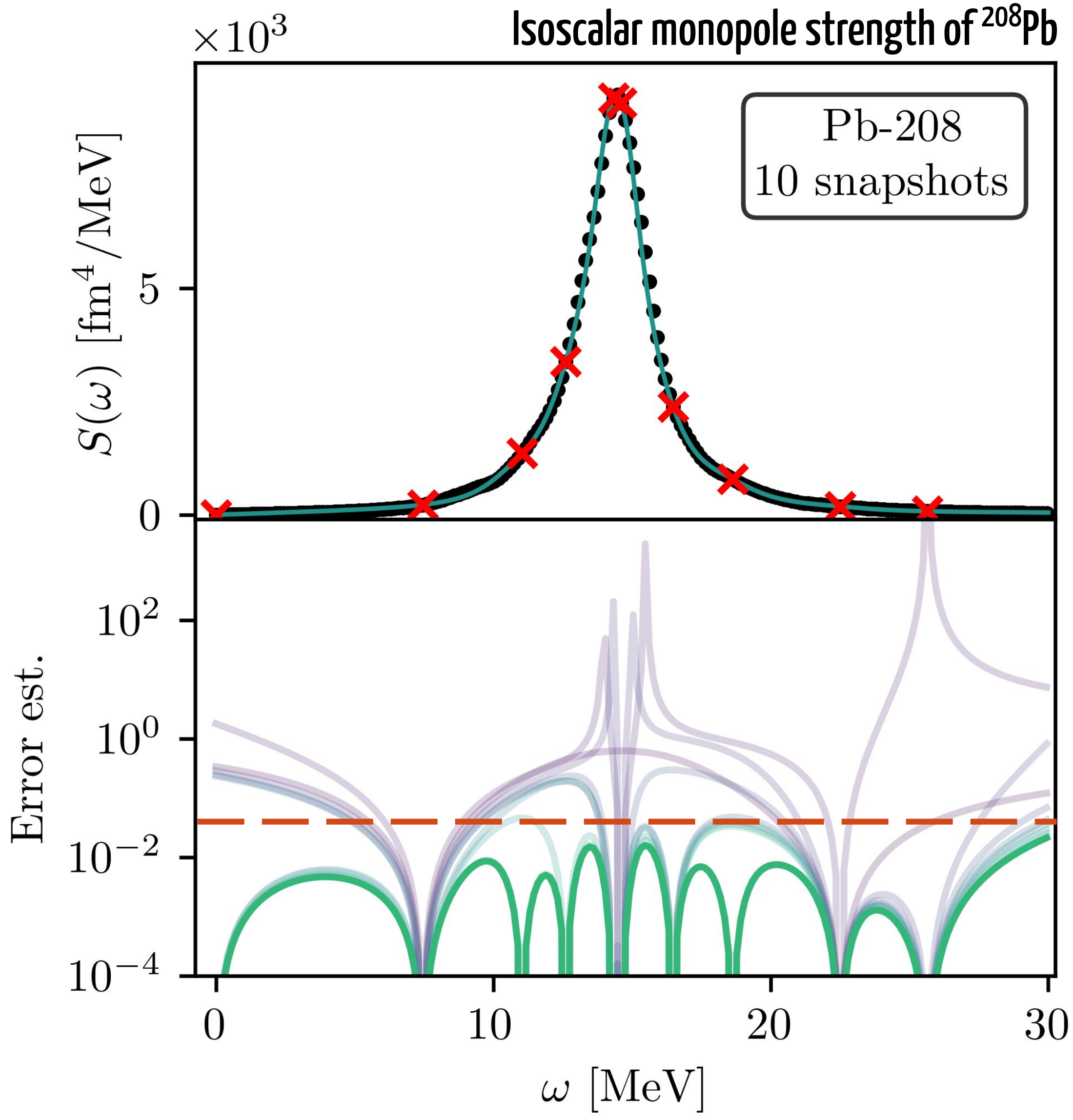
Isoscalar monopole strength of ^{208}Pb



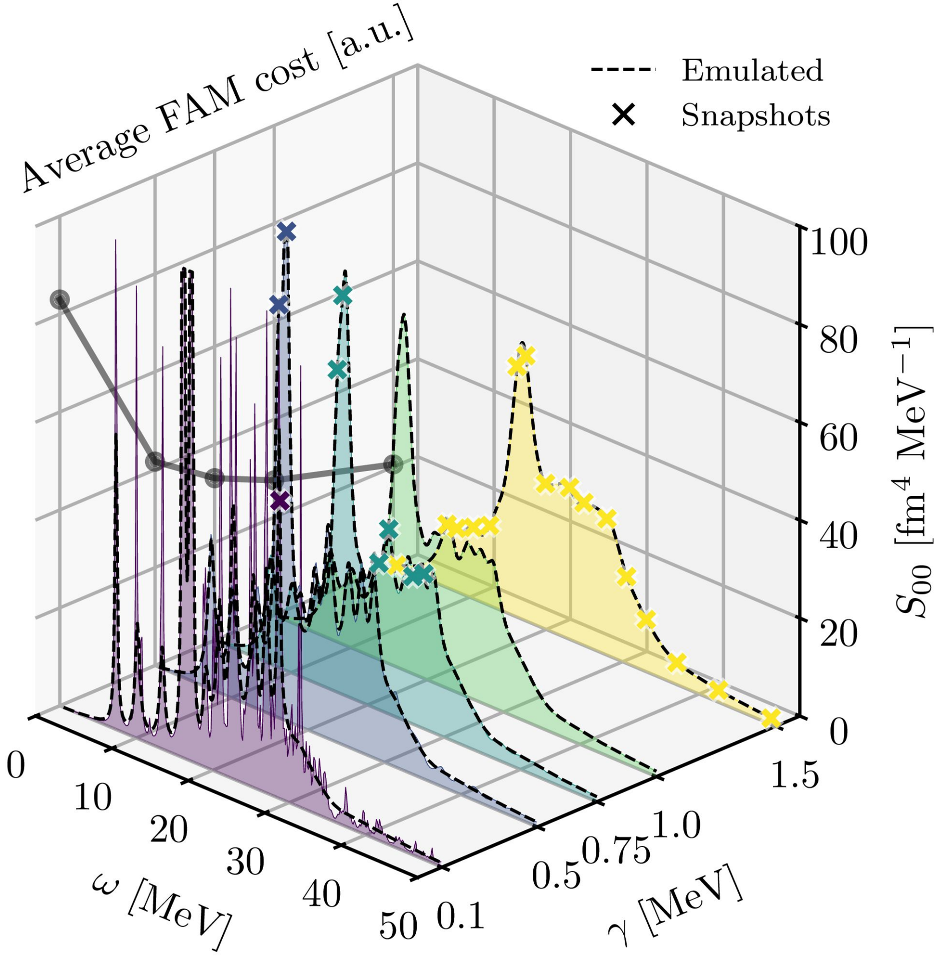
Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

$\longrightarrow$ Greedy sampling based on cost function $r(\omega)$

Can we reduce computational cost even further ?

$\longrightarrow$ Leverage cheaper FAM for larger complex γ smearing



Emulating FAM via reduced order modelling

How can we efficiently select snapshot?

→ Greedy sampling based on cost function $r(\omega)$

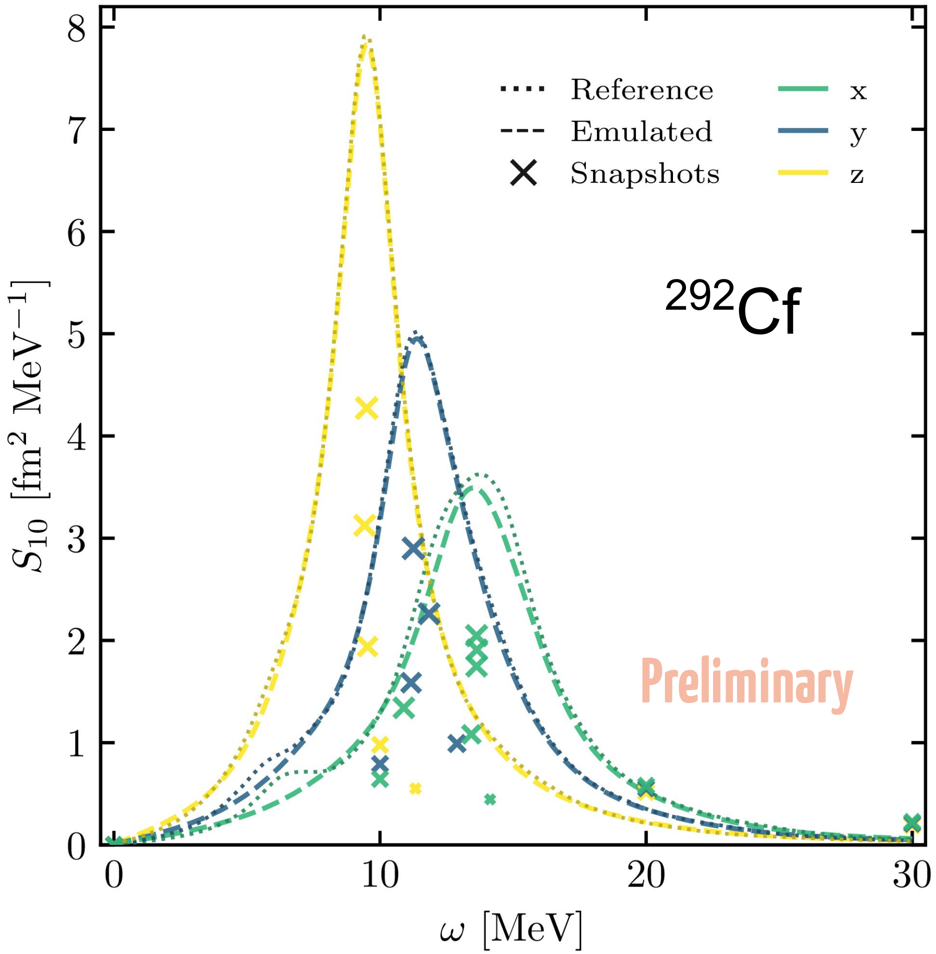
Can we reduce computational cost even further ?

→ Leverage cheaper FAM for larger complex γ

smearing

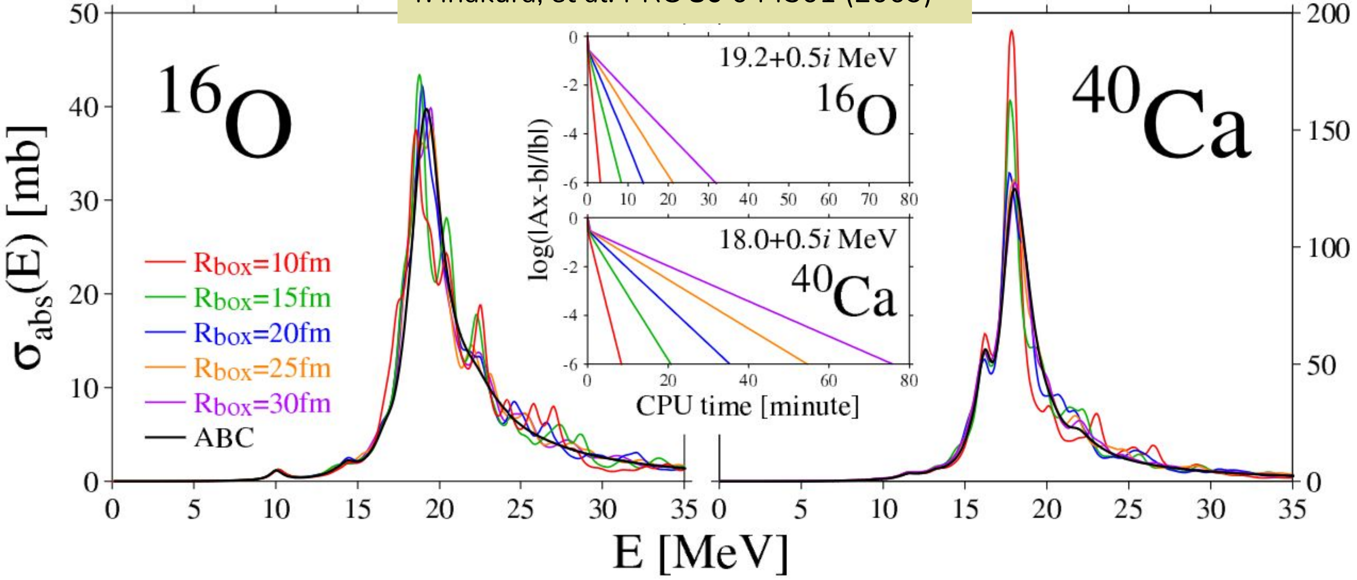
Method	# snap.	# iter.	speed-up
Full spectrum	151	4992	1.0
(a) Interpolation	35	1161	4.3
(b) Equidistant ROM	18	590	8.5
(c) Greedy 1D ROM	9	271	18.4
(d) Greedy 2D ROM	8	104	48.0

Isovector dipole strength of triaxial ^{292}Cf



Remaining challenges : convergence wrt box size

T. Inakura, *et al.* PRC **80** 044301 (2009)



PROBLEM : Spurious oscillations at high energies

REASONS : Outgoing spherical waves not well represented on the mesh.

SOLUTION : Absorbing boundary conditions

Thanks to **Wouter Ryssens** for several slides

Conclusion

BSkG provides **large-scale**, **microscopic** model of nuclear structure

- **Large-scale** : **thousands** of nuclei and **many observable**
- **Microscopic** : simple wave functions yet complex **symmetry breaking** (triaxial, octupole, time-reversal)
- with accurate bulk predictions of **masses, radii, fission properties**
- Recently extended to **photo strength functions**

Triaxiality leaves its fingerprints on **many** nuclear observables : radii, fission barriers, NLDs, PSFs

Outlook: synergy with *ab initio* ?

Can **BSkG** models be **improved by** constraining on carefully chosen ***ab initio*** **pseudo-data** of exotic nuclei?

Thanks to all my collaborators

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