Symmetry breaking on the scale of the nuclear chart

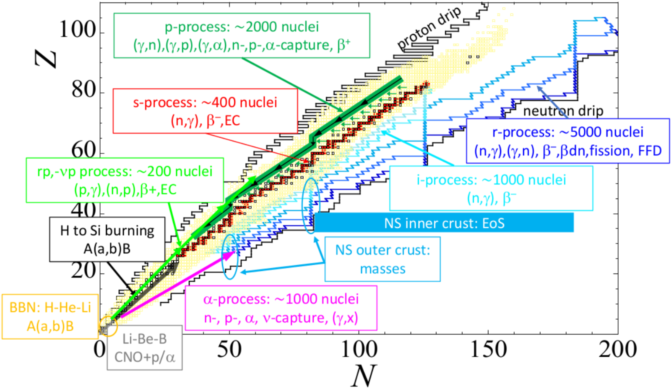
W. Ryssens, G. Scamps, M. Bender, & S. Goriely

3rd of December 2021

Table of contents

Table of contents

Nuclear data for astrophysics



M. Arnould & S. Goriely, Prog. Part. Nuc. Phys. **112**, 103766 (2020).

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^{\rho}\, \rho(\vec{r})\rho(\vec{r}) + C^{\tau}\, \rho(\vec{r})\, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\rm HFB}$

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^\rho \, \rho(\vec{r})\rho(\vec{r}) + C^\tau \, \rho(\vec{r}) \, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\rm HFB}$

+ microscopic method
+ feasible for 1000s of nuclei

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^\rho \, \rho(\vec{r})\rho(\vec{r}) + C^\tau \, \rho(\vec{r}) \, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\mathrm{HFB}}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^{\rho}\, \rho(\vec{r})\rho(\vec{r}) + C^{\tau}\, \rho(\vec{r})\, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\mathrm{HFB}}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

"Astro" models

- Study **global** masses
- More parameters $(22/25)$
- **Simplified** calculations

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^\rho \, \rho(\vec{r})\rho(\vec{r}) + C^\tau \, \rho(\vec{r}) \, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\mathrm{HFB}}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

"Astro" models

- Study **global** masses
- ! Fitted on **2408** masses
- More parameters $(22/25)$
- **Simplified** calculations

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^\rho \, \rho(\vec{r})\rho(\vec{r}) + C^\tau \, \rho(\vec{r})\, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\rm HFB}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

→ $\sigma_{\rm rms}(M) \sim$ **2-10** MeV

"Astro" models

- Study **global** masses
- ! Fitted on **2408** masses
- More parameters $(22/25)$
- **Simplified** calculations

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^{\rho}\, \rho(\vec{r})\rho(\vec{r}) + C^{\tau}\, \rho(\vec{r})\, \tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\mathrm{HFB}}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

→ $\sigma_{\mathrm{rms}}(M) \sim$ **2-10** MeV

"Astro" models

- Study **global** masses
- ! Fitted on **2408** masses
- More parameters $(22/25)$
- **Simplified** calculations

→ $\sigma_{\mathrm{rms}}(M) \sim$ **0.6** MeV

Energy density functionals (EDFs)

$$E \sim \int d^3r \left[C^{\rho} \rho(\vec{r})\rho(\vec{r}) + C^{\tau} \rho(\vec{r})\,\tau(\vec{r}) + \ldots\ldots \right]$$

- Pheno. form and fit of C's
- Simple $|\Psi\rangle = |0\rangle_{\mathrm{HFB}}$

+ microscopic method
+ feasible for 1000s of nuclei

"Structure" models

- Study observables **locally**
- Fitted on $\lesssim 10$ nuclei
- Typically ~ 15 parameters
- **Advanced** calculations

$\rightarrow$ $\sigma_{\mathrm{rms}}(M) \sim$ **2-10** MeV

"Astro" models

- Study **global** masses
- ! Fitted on **2408** masses
- More parameters $(22/25)$
- **Simplified** calculations

$\rightarrow$ $\sigma_{\mathrm{rms}}(M) \sim$ **0.6** MeV

We are bringing the "structure" to the "astro" scale!

Table of contents

Some history of Brussels Skyrme models

Year		$N_{\rm nuc}$
1977	First Skyrme HF+BCS mass table (spherical)	142

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492
2000-2001	**MSk1-7**: HF+BCS including deformed nuclei	1719

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492
2000-2001	**MSk1-7**: HF+BCS including deformed nuclei	1719
2002	**BSk1**: BCS $\rightarrow$ HFB	1754

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492
2000-2001	**MSk1-7**: HF+BCS including deformed nuclei	1719
2002	**BSk1**: BCS $\rightarrow$ HFB	1754
2003	**BSk7**: Realistic effective mass	2135
2006	**BSk13**: Improved pairing and NLD	2149
2007	**BSk14**: (partial) refit on fission barriers	2149
2009	**BSk17**: below 0.6 MeV rms on the masses	2149
2009	**BSk18**: Stiff EOS through ext. Skyrme form	2149
2013	**BSk27**: lowest rms ever (0.512 MeV)	2353
2016	**BSk32**: best reproduction of INM	2353

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492
2000-2001	**MSk1-7**: HF+BCS including deformed nuclei	1719
2002	**BSk1**: BCS $\to$ HFB	1754
2003	**BSk7**: Realistic effective mass	2135
2006	**BSk13**: Improved pairing and NLD	2149
2007	**BSk14**: (partial) refit on fission barriers	2149
2009	**BSk17**: below 0.6 MeV rms on the masses	2149
2009	**BSk18**: Stiff EOS through ext. Skyrme form	2149
2013	**BSk27**: lowest rms ever (0.512 MeV)	2353
2016	**BSk32**: best reproduction of INM	2353
2021	**Birth of the BSkG**	2408

Some history of Brussels Skyrme models

Year		N_{nuc}
1977	First Skyrme HF+BCS mass table (spherical)	142
1985-1995	**ETFSI1/2**: Ext. Thomas-Fermi + Strutinsky $\int$	1492
2000-2001	**MSk1-7**: HF+BCS including deformed nuclei	1719
2002	**BSk1**: BCS $\rightarrow$ HFB	1754
2003	**BSk7**: Realistic effective mass	2135
2006	**BSk13**: Improved pairing and NLD	2149
2007	**BSk14**: (partial) refit on fission barriers	2149
2009	**BSk17**: below 0.6 MeV rms on the masses	2149
2009	**BSk18**: Stiff EOS through ext. Skyrme form	2149
2013	**BSk27**: lowest rms ever (0.512 MeV)	2353
2016	**BSk32**: best reproduction of INM	2353
2021	**Birth of the BSkG**	2408

Also Gogny (**D1M**, 2009)and relativistic EDFs (**DD-MEB1/2**, 2016)!

BSkG = Brussels Skyrme on a Grid

	Old		New	
	BSk27	BSk32	BSkG1	BSkG2
Parameters	24	33	22	25
$\sigma(M)$ [MeV]	0.512	0.529		
$\sigma(S_n)$ [MeV]	0.425	0.489		
$\sigma(Q_\beta)$ [MeV]	0.516	0.601		
$\sigma(R_c)$ [fm]	0.028	0.027		
Skyrme form	Standard	Extended		
Micr. Pairing	No	Yes		
EOS n-matter	Soft	Stiff		
Deformation	Axial	Axial		
Representation	Oscillator 2D	Oscillator 2D		
Odd nuclei	Equal Filling	Equal Filling		
Status	Published	Published		

BSk27: S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302 (2013).
BSk32: S. Goriely, N. Chamel and J. M. Pearson, PRC **93**, 034337 (2016).
BSkG1: G. S. et al., arXiv:2011.07904 [nucl-th].

BSkG = Brussels Skyrme on a Grid

	Old		New	
	BSk27	BSk32	BSkG1	BSkG2
Parameters	24	33	22	25
$\sigma(M)$ [MeV]	0.512	0.529		
$\sigma(S_n)$ [MeV]	0.425	0.489		
$\sigma(Q_\beta)$ [MeV]	0.516	0.601		
$\sigma(R_c)$ [fm]	0.028	0.027		
Skyrme form	Standard	Extended	Standard	
Micr. Pairing	No	Yes	No	
EOS n-matter	Soft	Stiff	Soft	
Deformation	Axial	Axial	Triaxial	
Representation	Oscillator 2D	Oscillator 2D	$\vec{r}$-space 3D	
Odd nuclei	Equal Filling	Equal Filling	Equal Filling	
Status	Published	Published	Accepted	

BSk27: S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302 (2013).
BSk32: S. Goriely, N. Chamel and J. M. Pearson, PRC **93**, 034337 (2016).
BSkG1: G. S. et al., arXiv:2011.07904 [nucl-th].

BSkG = Brussels Skyrme on a Grid

	Old		New	
	BSk27	BSk32	BSkG1	BSkG2
Parameters	24	33	22	25
$\sigma(M)$ [MeV]	0.512	0.529		
$\sigma(S_n)$ [MeV]	0.425	0.489		
$\sigma(Q_\beta)$ [MeV]	0.516	0.601		
$\sigma(R_c)$ [fm]	0.028	0.027		
Skyrme form	Standard	Extended	Standard	Standard
Micr. Pairing	No	Yes	No	No
EOS n-matter	Soft	Stiff	Soft	Soft
Deformation	Axial	Axial	Triaxial	Triaxial
Representation	Oscillator	Oscillator	$\vec{r}$-space	$\vec{r}$-space
	2D	2D	3D	3D
Odd nuclei	Equal Filling	Equal Filling	Equal Filling	T-break
Status	Published	Published	Accepted	Preliminary!

BSk27: S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302 (2013).
BSk32: S. Goriely, N. Chamel and J. M. Pearson, PRC **93**, 034337 (2016).
BSkG1: G. S. et al., arXiv:2011.07904 [nucl-th].

BSkG = Brussels Skyrme on a Grid

	Old		**New**	
	BSk27	BSk32	BSkG1	BSkG2
Parameters	24	33	22	25
$\sigma(M)$ [MeV]	0.512	0.529	0.741	0.678
$\sigma(S_n)$ [MeV]	0.425	0.489	0.466	0.500
$\sigma(Q_\beta)$ [MeV]	0.516	0.601	0.645	0.619
$\sigma(R_c)$ [fm]	0.028	0.027	0.0267	0.0274
Skyrme form	Standard	Extended	Standard	Standard
Micr. Pairing	No	Yes	No	No
EOS n-matter	Soft	Stiff	Soft	Soft
Deformation	Axial	Axial	Triaxial	Triaxial
Representation	Oscillator 2D	Oscillator 2D	$\vec{r}$-space 3D	$\vec{r}$-space 3D
Odd nuclei	Equal Filling	Equal Filling	Equal Filling	T-break
Status	Published	Published	Accepted	Preliminary!

BSk27: S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302 (2013).
BSk32: S. Goriely, N. Chamel and J. M. Pearson, PRC **93**, 034337 (2016).
BSkG1: G. S. et al., arXiv:2011.07904 [nucl-th].

BSkG1 & 2

$$E_{\rm tot} = E_{\rm HFB} + E_{\rm collective} \,,$$

BSkG1 & 2

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

BSkG1 & 2

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}}\,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

BSkG1 & 2

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

BSkG1 & 2

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} ,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

Variational!

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

BSkG1 & 2

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

Variational!

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

Semi-variational!

BSkG1 & 2

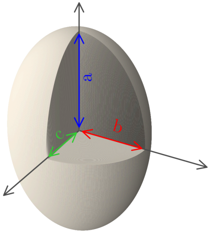
$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \, ,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

Variational!

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

Semi-variational!



Two DOF: (β_{20}, β_{22}) or (β, γ)

BSkG1 & 2

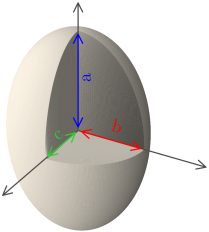
$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

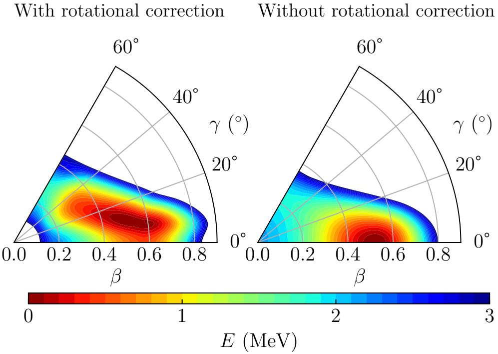
Variational!

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG2]

Semi-variational!



Two DOF: (β_{20}, β_{22}) or (β, γ)



BSkG1 vs. BSkG2

BSkG2 = BSkG1 + time-odd terms + vibrational correction

BSkG1 vs. BSkG2

BSkG2 = BSkG1 + time-odd terms + vibrational correction

$$\mathcal{E}_{\rm t-odd}(\vec{r}) = C_t^{ss}\,\mathbf{s}_t(\vec{r})\cdot\mathbf{s}_t(\vec{r}) + C_t^{ss\rho^\gamma}\,\rho_0^\gamma(\vec{r})\,\mathbf{s}_t(\vec{r})\cdot\mathbf{s}_t(\vec{r}) + C_t^{jj}\,\mathbf{j}_t(\vec{r})\cdot\mathbf{j}_t(\vec{r}) + C_t^{j\nabla s}\,\mathbf{j}_t(\vec{r})\cdot\nabla\times\mathbf{s}_t(\vec{r})\,.$$

- Many different approaches exist
- “Simplest” possible form
- No extra parameters
- No sΔs for stability
- Never before included in a fit
- Blocking calculations with polarisation!

BSkG1 vs. BSkG2

BSkG2 = BSkG1 + time-odd terms + vibrational correction

$$\mathcal{E}_{\mathrm{t-odd}}(\vec{r}) = C_t^{ss}\, \mathbf{s}_t(\vec{r}) \cdot \mathbf{s}_t(\vec{r}) + C_t^{ss\rho^\gamma} \rho_0^\gamma(\vec{r})\, \mathbf{s}_t(\vec{r}) \cdot \mathbf{s}_t(\vec{r}) + C_t^{jj}\, \mathbf{j}_t(\vec{r}) \cdot \mathbf{j}_t(\vec{r}) + C_t^{j\nabla s}\, \mathbf{j}_t(\vec{r}) \cdot \nabla \times \mathbf{s}_t(\vec{r})\,.$$

- Many different approaches exist
- "Simplest" possible form
- No extra parameters

- No $\mathrm{s}\Delta\mathrm{s}$ for stability
- Never before included in a fit
- Blocking calculations with polarisation!

$$E_{\mathrm{vib}} = -d \sum_{\mu=x,y,z} B_\mu e^{-l(B_\mu - B_0)^2} \frac{\langle \hat{J}_\mu^2 \rangle}{2\mathcal{I}_\mu}\,,$$

- Three additional parameters
- Refit on 12 even-even RIPL-3 fission barriers

Table of contents

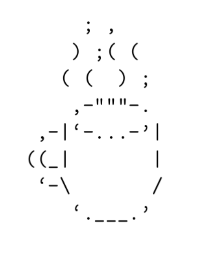
Tools

How do we fit $> \mathbf{20}$ parameters on $\mathbf{2408}$ masses efficiently?

Tools

How do we fit $> \mathbf{20}$ parameters on $\mathbf{2408}$ masses efficiently?

MOCCa



- 3D $\vec{r}$-space solver
- Robust and quick
- Symmetry options

Tools

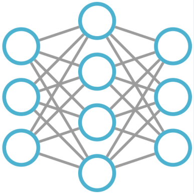
How do we fit $> \mathbf{20}$ parameters on $\mathbf{2408}$ masses efficiently?

MOCCa

```
       ;  ,
      )  ;( (
     (  (   )  ;
        ,-"""-.
    ,-|`-...-'|
   ((_|       |
    `-\       /
       `.___.'
```

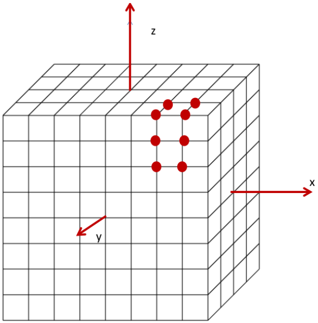
- 3D $\vec{r}$-space solver
- Robust and quick
- Symmetry options

Machine learning



- 100s of Neural Networks
- Keras implementation
- Learning parameter space

MOCCa: speed & accuracy

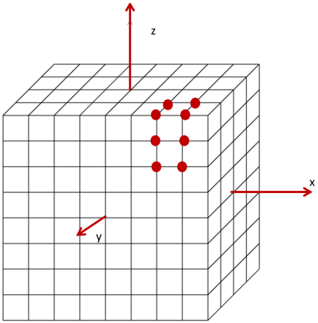


Lagrange mesh for accuracy

- 10s of keV on energies
- 0.01 fm on radii.

D. Baye et al., JPA **19**, 2041-2059 (1986).
W. R. et al. , PRC **92**, 064318 (2015).

MOCCa: speed & accuracy



Lagrange mesh for accuracy

- 10s of keV on energies
- 0.01 fm on radii.

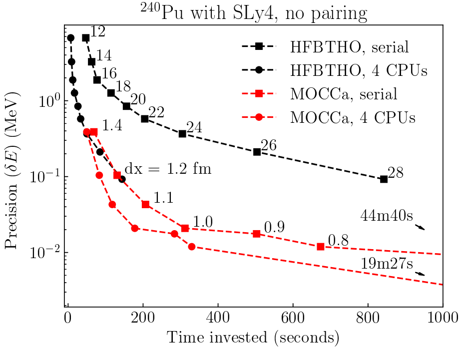
D. Baye et al., JPA **19**, 2041-2059 (1986).
W. R. et al. , PRC **92**, 064318 (2015).

Better algorithms for speed

- factor 10 over EV8
- human-tweaking free

W. R. et al., EPJA 55, 93 (2019).

MOCCa: speed & accuracy



Lagrange mesh for accuracy

- 10s of keV on energies
- 0.01 fm on radii.

D. Baye et al., JPA **19**, 2041-2059 (1986).
W. R. et al. , PRC **92**, 064318 (2015).

Better algorithms for speed

- factor 10 over EV8
- human-tweaking free

W. R. et al., EPJA 55, 93 (2019).

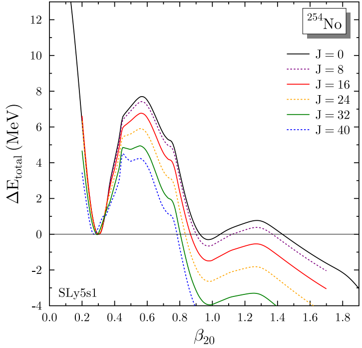
MOCCa: robustness

Algorithms for constraints

- All multipoles, cranking, ...
- Many **simultaneous** constraints
- human-tweaking free

W. Ryssens et al., in preparation.

MOCCa: robustness



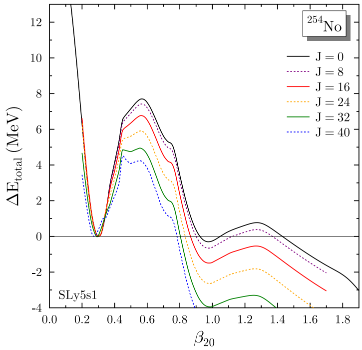
M. Bender and W. Ryssens, in preparation.

Algorithms for constraints

- All multipoles, cranking, . . .
- Many **simultaneous** constraints
- human-tweaking free

W. Ryssens et al., in preparation.

MOCCa: robustness



M. Bender and W. Ryssens, in preparation.

Algorithms for constraints

- All multipoles, cranking, . . .
- Many **simultaneous** constraints
- human-tweaking free

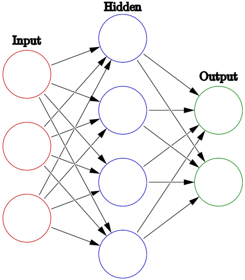
W. Ryssens et al., in preparation.

Blocked HFB $|\Psi\rangle$ with gradient solver

- lowest E **guaranteed**
- 99% convergence rate
- human-tweaking free

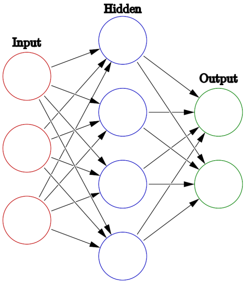
W. Ryssens, in preparation.

Neural networks



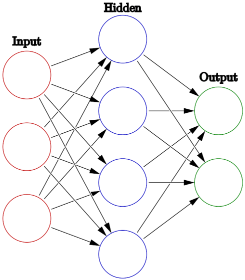
- Many interconnected nodes
- Turing complete (in theory)

Neural networks



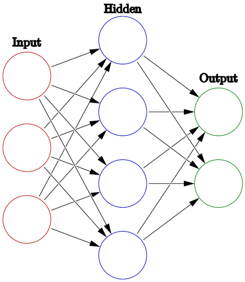
- Many interconnected nodes
- Turing complete (in theory)
- Training is hard
  - HUGE number of weights
  - Overfitting is dangerous
  - Depends on initialisation
  - Need clever input

Neural networks



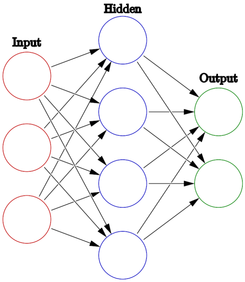
- Many interconnected nodes
- Turing complete (in theory)
- Training is hard
  - HUGE number of weights
  - Overfitting is dangerous
  - Depends on initialisation
  - Need clever input
- Once trained, useage is **trivial**

Neural networks



- Many interconnected nodes
- Turing complete (in theory)
- Training is hard
    - HUGE number of weights
    - Overfitting is dangerous
    - Depends on initialisation
    - Need clever input
- Once trained, useage is **trivial**
- Extrapolation is dangerous

Neural networks



- Many interconnected nodes
- Turing complete (in theory)
- Training is hard
  - HUGE number of weights
  - Overfitting is dangerous
  - Depends on initialisation
  - Need clever input
- Once trained, useage is **trivial**
- Extrapolation is dangerous

AI in nuclear physics

R. Lasseri et al., PRL 124, 162502 (2020).
N. Schunck et al., EPJA 51, 169 (2015).
N. Schunck et al., J. Phys. G 47 , 10 (2020).
Z. M. Niu and H.Z. Liang, PLB 778 , 48 (2018).
L. Neufcourt et al., PRC 98, 034318 (2018).
E. Yüksel et al., IJMP E30, 2150017 (2021).
Z. Gao et al., arXiV 2105.02445 (2021).
. . . [many more]. . .

Replacing MOCCa by a neural network

Input

- N, Z
- model params

```
      ;  ,
    )  ;(  (
   (  (   )  ;
    ,_"""_.
 ,-|`-...-'|
((_|       |
 `-\       /
    `.___.'
```

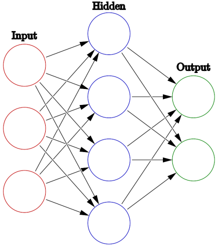
Output

- Energy
- Charge radius
- Deformation
- . . .

Replacing MOCCa by a neural network

Input

- N, Z
- model params
- $A^{2/3}, (N-Z)^2/A, \ldots$
- magic numbers



Output

- Energy
- Charge radius
- Deformation
- ...

- **4** hidden layers
- 128/64/32/16 neurons
- **12289** parameters
- necessarily biased

Replacing MOCCa by 300 neural networks

Input

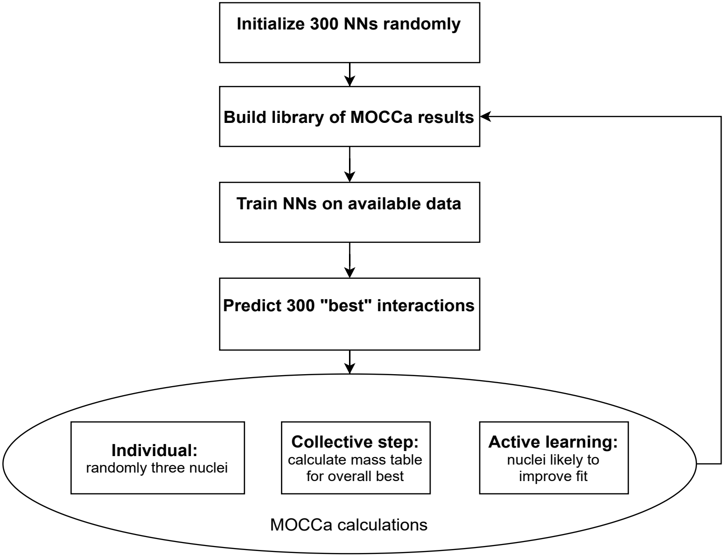
- N, Z
- model params
- $A^{2/3}, (N-Z)^2/A, \ldots$
- magic numbers

Output

- Energy
- Charge radius
- Deformation
- ...

- **4** hidden layers
- 128/64/32/16 neurons
- **12289** parameters
- Power in numbers

Fitting algorithm



Fitting algorithm

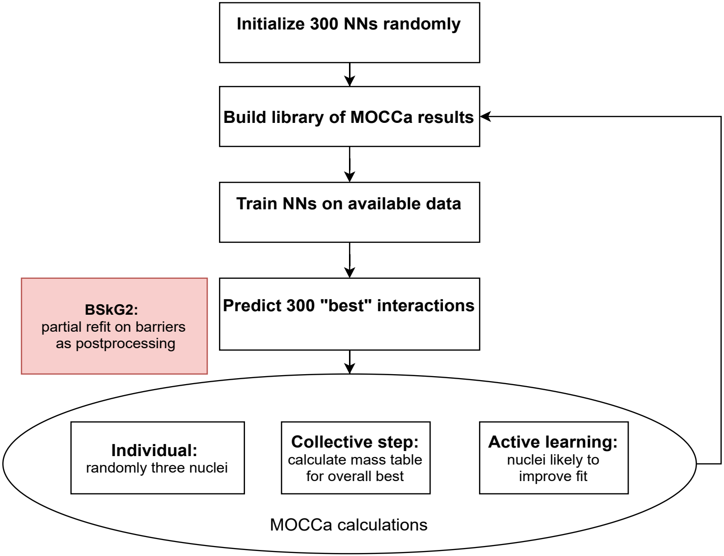


Table of contents

Clarification

All results shown were obtained with a **full** MOCCa calculation.

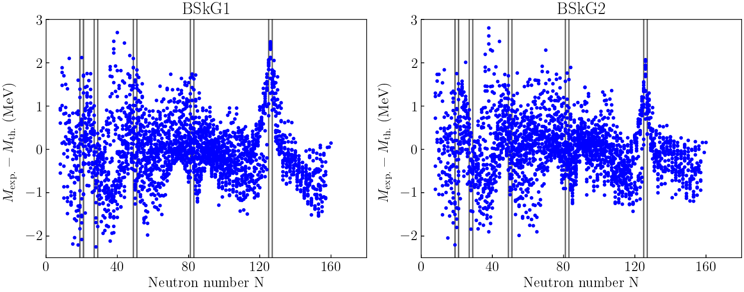
Clarification

All results shown were obtained with a **full** MOCCa calculation.
None of the results shown have been extra/interpolated with machine learning.

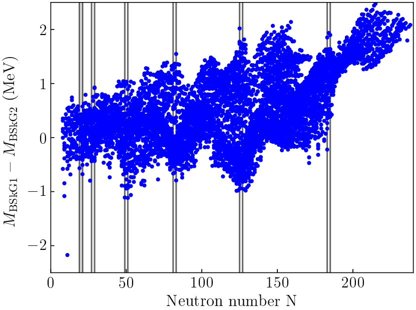
Clarification

All results shown were obtained with a **full** MOCCa calculation.
None of the results shown have been extra/interpolated with machine learning.
Machine learning is **only** used to perform the interaction fitting.

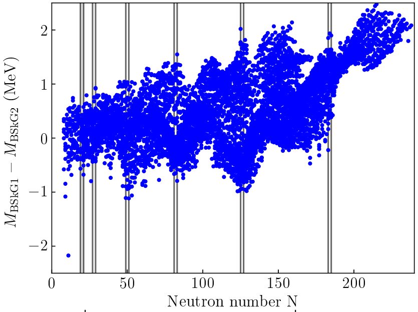
Masses


BSkG1
BSkG2
$M_{\mathrm{exp.}} - M_{\mathrm{th.}}$ (MeV)
Neutron number N
3
2
1
0
−1
−2
0
40
80
120
160

Masses

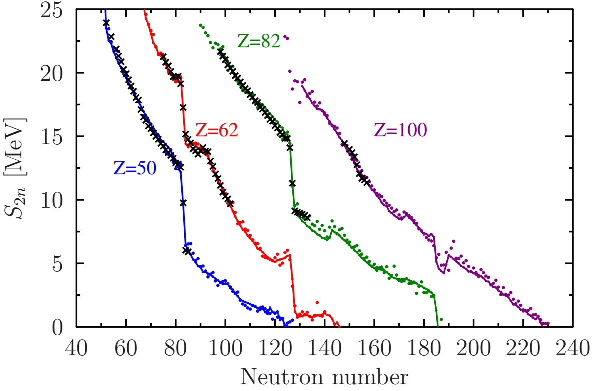

$M_{\mathrm{BSkG1}} - M_{\mathrm{BSkG2}}$ (MeV)
Neutron number N
2
1
0
−1
−2
0
50
100
150
200

Masses

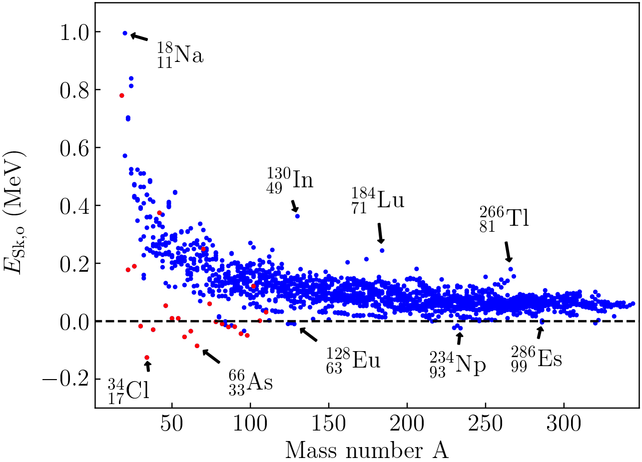


	Old		New	
	BSk27	BSk32	BSkG1	BSkG2
Parameters	24	33	22	25
$\sigma(M)$ [MeV]	0.512	0.529	0.741	0.678
$\sigma(S_n)$ [MeV]	0.425	0.489	0.466	0.500
$\sigma(Q_\beta)$ [MeV]	0.516	0.601	0.645	0.619
$\sigma(R_c)$ [fm]	0.028	0.027	0.027	0.027

Accuracy: S_{2n}

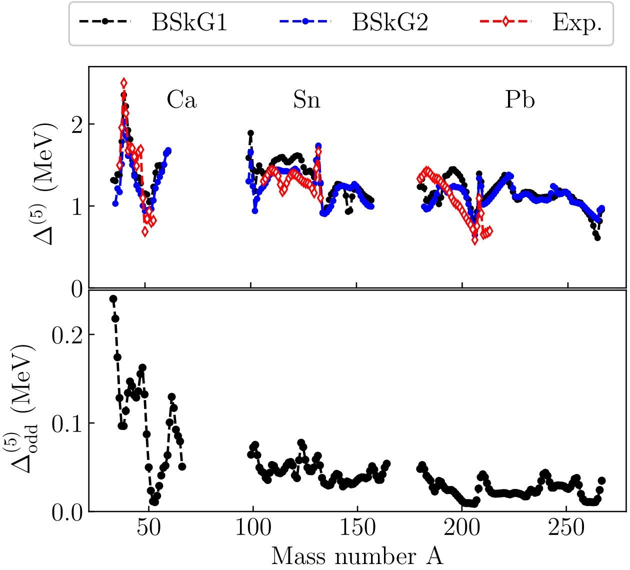


Time-odd energies

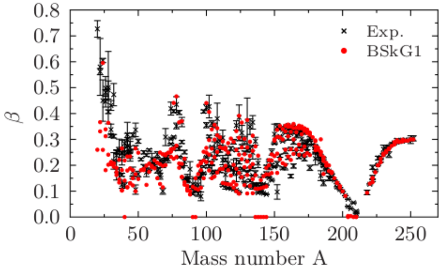


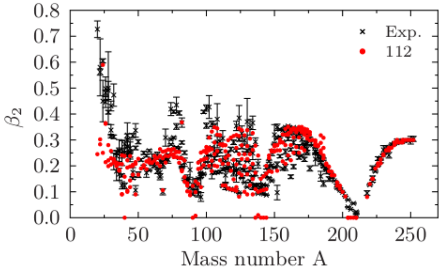
- Virtually all time-odd energies are positive ($\neq$ standard!)
- For $N = Z$ the effect can be negative
- Particularly large effects just outside shell closures

Mass differences

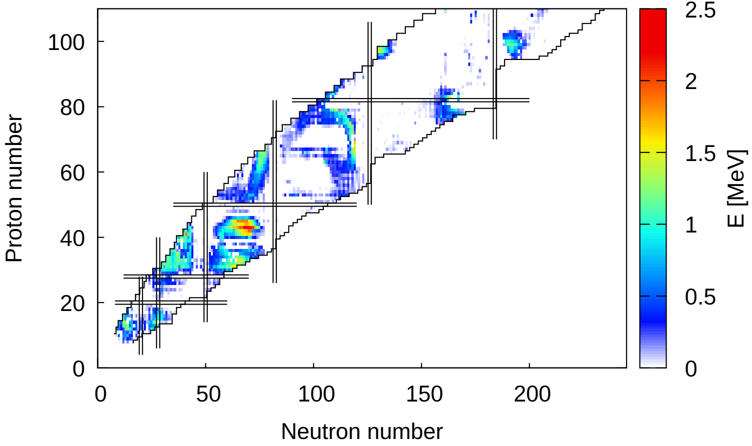


Deformations

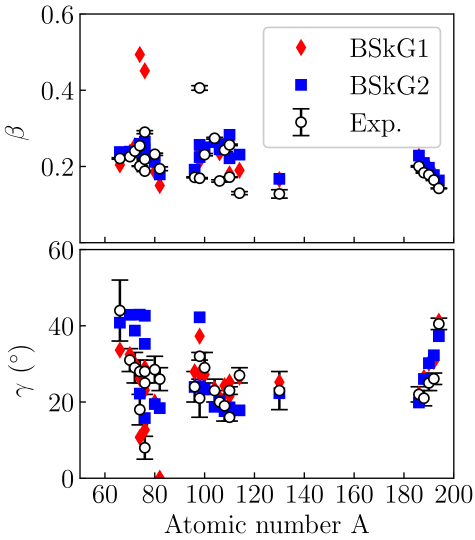




Triaxiality: where?



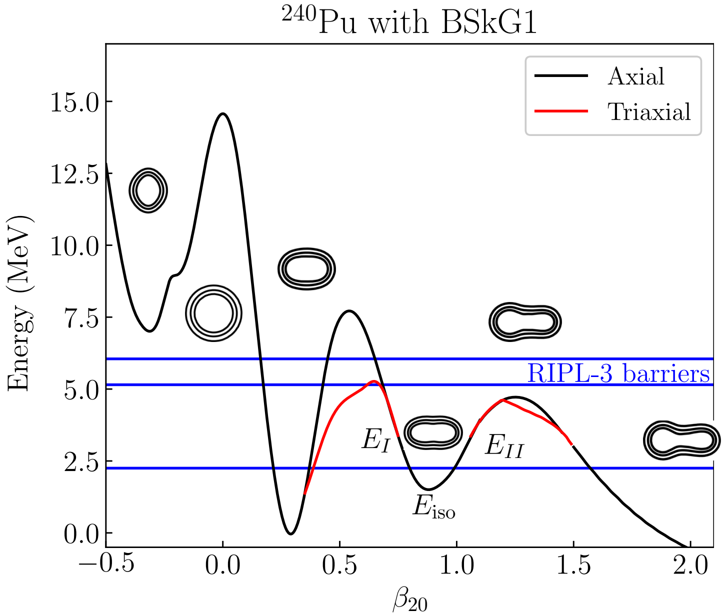
Triaxiality: comparison to experiment



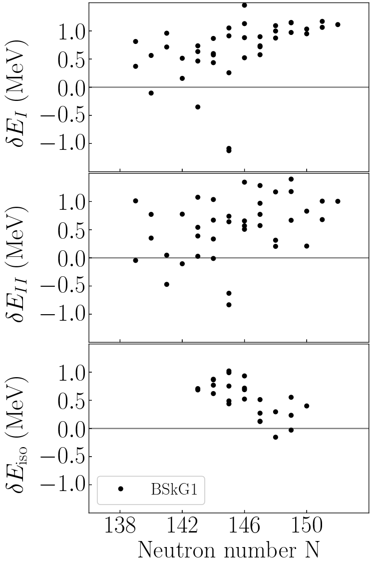
Exp. data from COULEX extracted by M. Zielińska

M. Rocchini et al., PRC **103**, 014311 (2021).
M. Sugawara et al., EPJA, **16**, 409 (2003).
A. D. Ayangeakaa et al., PLB **754**, 254 (2016).
Y. Toh et al. , EPJA **9**, 353 (2000).
A. D. Ayangeaka et al., PRL **123**, 102501 (2019).
E. Clément et al., PRC **75**, 054313 (2007).
A. E. Kavka et al., NPA **593**, 177 (1995).
E. Clément et al., PRC **94**, 054326 (2016).
M. Zielińska, Ph.D. thesis, Warsaw U., (2005).
M. Zielińska et al., NPA **712**, 3 (2002).
K. Wrzosek-Lipska et al., PRC **86**, 064305 (2012).
J. Srebrny et al., NPA **766**, 25 (2006).
K. Wrzosek-Lipska et al., APB **51**, 789 (2020).
C. Fahlander et al., NPA **485**, 327 (1988).
L. E. Svensson et al., NPA **584**, 547 (1995).
L. Morrison et al., PRC **102**, 054304 (2020).
C. Y. Wu et al., NPA **607**, 178 (1996).

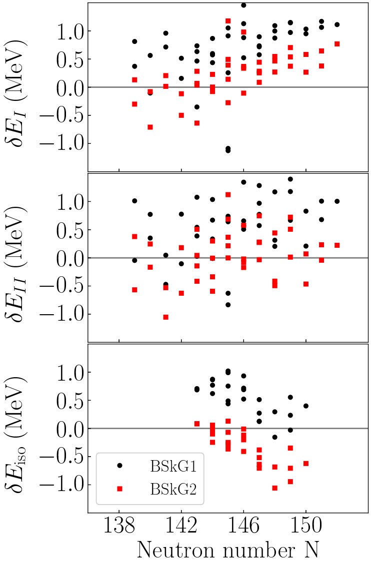
Triaxiality: fission



BSkG2: improved fission barriers above $Z > 90$



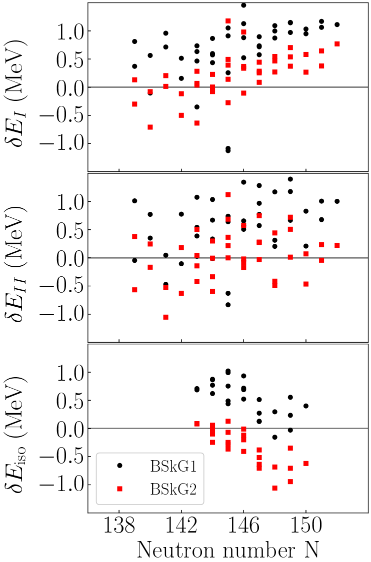
BSkG2: improved fission barriers above $Z > 90$



(MeV)	BSkG1	BSkG2
$\sigma(M)$	0.741	0.668
$\sigma(E_I)$	0.853	**0.447**
$\sigma(E_{II})$	0.792	**0.450**
$\sigma(E_{\text{iso}})$	0.620	**0.465**
	HFB-14	FR(L)DM
$\sigma(M)$	0.729	0.560
$\sigma(E_I)$	0.591	0.763
$\sigma(E_{II})$	0.717	n.a.
$\sigma(E_{\text{iso}})$	0.730	n.a.

HFB-14 from S. Goriely *et al.*, PRC **75**, 064312 (2007).
FRLDM from P. Möller *et al.*, PRC **79**, 064304 (2009).

BSkG2: improved fission barriers above $Z > 90$

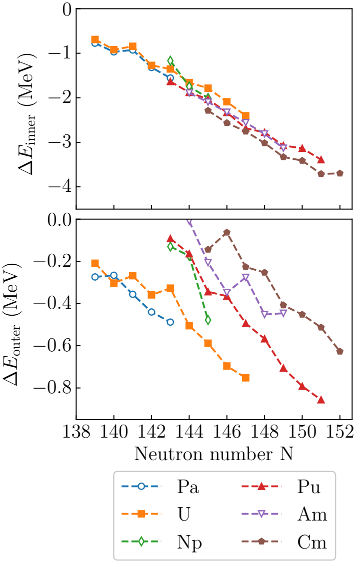


Refitting with **axial** barriers requires **sacrificing** either masses or barriers!

(MeV)	BSkG1	BSkG2
$\sigma(M)$	0.741	0.668
$\sigma(E_I)$	0.853	**0.447**
$\sigma(E_{II})$	0.792	**0.450**
$\sigma(E_{\mathrm{iso}})$	0.620	**0.465**
	HFB-14	FR(L)DM
$\sigma(M)$	0.729	0.560
$\sigma(E_I)$	0.591	0.763
$\sigma(E_{II})$	0.717	n.a.
$\sigma(E_{\mathrm{iso}})$	0.730	n.a.

HFB-14 from S. Goriely *et al.*, PRC **75**, 064312 (2007).
FRLDM from P. Möller *et al.*, PRC **79**, 064304 (2009).

BSkG2: improved fission barriers above $Z > 90$

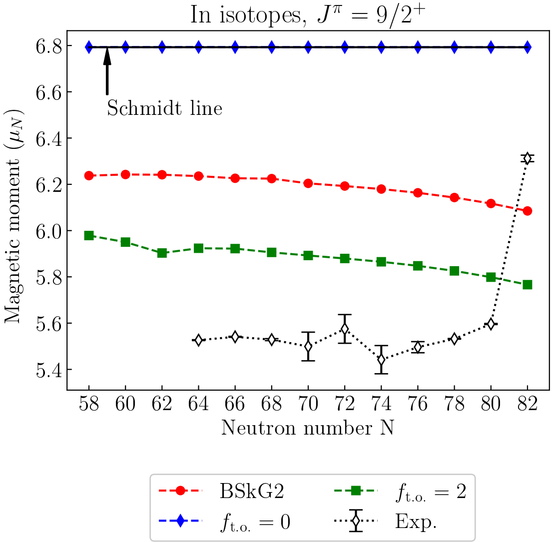


Refitting with **axial** barriers requires **sacrificing** either masses or barriers!

(MeV)	BSkG1	BSkG2
$\sigma(M)$	0.741	0.668
$\sigma(E_I)$	0.853	**0.447**
$\sigma(E_{II})$	0.792	**0.450**
$\sigma(E_{\mathrm{iso}})$	0.620	**0.465**
	HFB-14	FR(L)DM
$\sigma(M)$	0.729	0.560
$\sigma(E_I)$	0.591	0.763
$\sigma(E_{II})$	0.717	n.a.
$\sigma(E_{\mathrm{iso}})$	0.730	n.a.

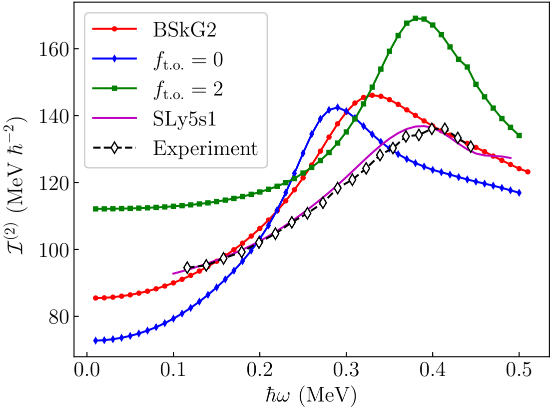
HFB-14 from S. Goriely *et al.*, PRC **75**, 064312 (2007).
FRLDM from P. Möller *et al.*, PRC **79**, 064304 (2009).

Magnetic moments



Exp. data from A. Vernon et al., under review at Nature. DOI:10.21203/rs.3.rs-611360/v1

Superdeformed rotational band in ^{194}Hg



Exp. data from B. Singh, Nuclear Data Sheets 97, 241 (2002).

Conclusions

We are bringing nuclear-state-of-the-art to large-scale modelling.

Conclusions

We are bringing nuclear-state-of-the-art to large-scale modelling.

Tools

- MOCCa is fast, accurate, robust and versatile
- Machine learning brings MOCCa to the scale of the nuclear chart

Models

- BSkG1: first global model with triaxial deformation
  - competitive on $\sigma(M)$
  - excellent reproduction of COULEX data on triaxial deformation

Conclusions

We are bringing nuclear-state-of-the-art to large-scale modelling.

Tools

- MOCCa is fast, accurate, robust and versatile
- Machine learning brings MOCCa to the scale of the nuclear chart

Models

- BSkG1: first global model with triaxial deformation
  - competitive on $\sigma(M)$
  - excellent reproduction of COULEX data on triaxial deformation
- BSkG2: first global model with time-odd terms
  - competitive on $\sigma(M)$
  - among the best for actinide fission barriers
  - Analysis ongoing: new observables accessible

Outlook

Theory questions

- How to improve collective corrections? Linear response?
- Can we finetune the time-odd sector? Should we?
- Can we build continuous fission barriers for odd nuclei?
- Can we use MOCCa for nuclear pasta calculations?
- Can we gain another factor 10 in CPU time through algorithms?

Outlook

Theory questions

- How to improve collective corrections? Linear response?
- Can we finetune the time-odd sector? Should we?
- Can we build continuous fission barriers for odd nuclei?
- Can we use MOCCa for nuclear pasta calculations?
- Can we gain another factor 10 in CPU time through algorithms?

Model construction

- Extend the fission model
  - Calculate thousands of nuclei with MLNN help
  - including fission yields with scission point model (SPY by J.-F. Lemaître)
  - and half-life calculation with collective inertias
- Develop associated level density model
- BSkG4-5-. . . will be extended Skyrme forms
  - $t_4 \& t_5$ terms for stable INM and stiff EOS
  - N2LO generalized Skyrme functionals for spectroscopy
  - MOCCa has code-generation for complicated EDFs!

Thanks!

Thanks for. . .

. . . the **help**:

BSkG1/2		MOCCa	
• S. Goriely	ULB	• P.-H. Heenen	ULB
• G. Scamps	ULB	• M. Bender	IP2I
• J.-F. Lemaître	CEA	• B. Bally	UAM

Thanks!

Thanks for. . .

. . . the **help**:

BSkG1/2		MOCCa	
• S. Goriely	ULB	• P.-H. Heenen	ULB
• G. Scamps	ULB	• M. Bender	IP2I
• J.-F. Lemaître	CEA	• B. Bally	UAM

. . . the **CPU time**:

- CÉCI network, Belgium
- The Zenobe cluster

Thanks!

Thanks for…

…the **help**:

BSkG1/2

- S. Goriely — ULB
- G. Scamps — ULB
- J.-F. Lemaître — CEA

MOCCa

- P.-H. Heenen — ULB
- M. Bender — IP2I
- B. Bally — UAM

…the **CPU time**:

- CÉCI network, Belgium
- The Zenobe cluster

…the **support**:

ULB

fnrs
LA LIBERTÉ DE CHERCHER

Thanks!

Thanks for. . .

. . . the **help**:

BSkG1/2

- S. Goriely — ULB
- G. Scamps — ULB
- J.-F. Lemaître — CEA

MOCCa

- P.-H. Heenen — ULB
- M. Bender — IP2I
- B. Bally — UAM

. . . the **CPU time**:

- CÉCI network, Belgium
- The Zenobe cluster

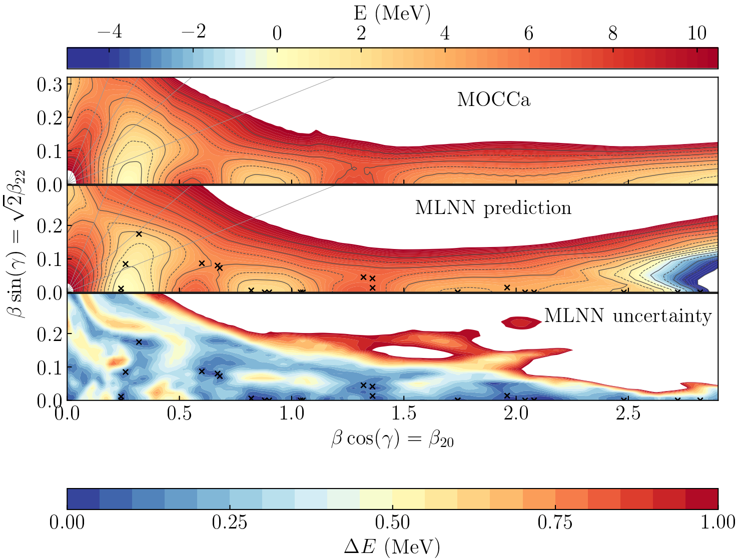
. . . the **support**:

ULB

fnrs LA LIBERTÉ DE CHERCHER

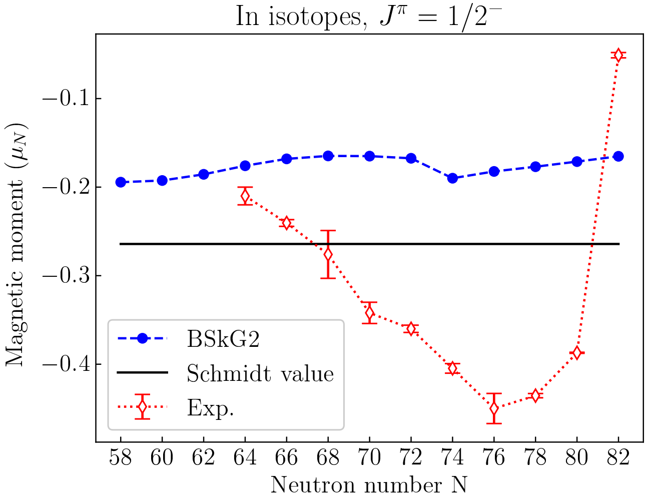
. . . your **attention**!

A taste of things to come

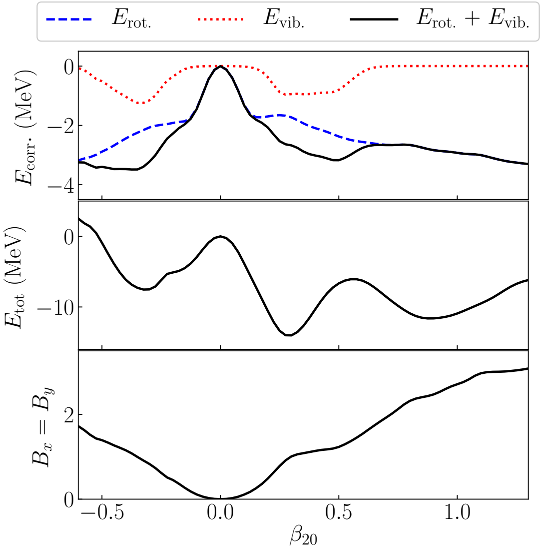


Bonus!

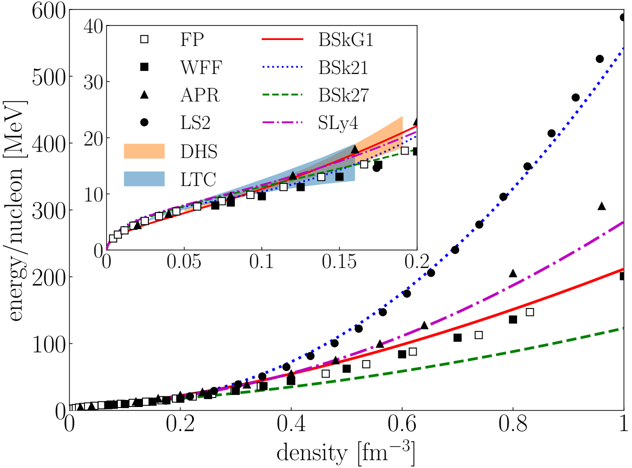
More In isotopes



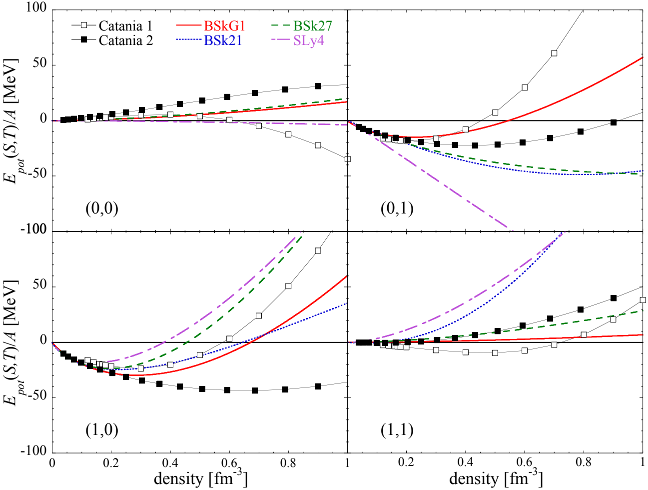
Example of the collective correction: ^{240}Pu



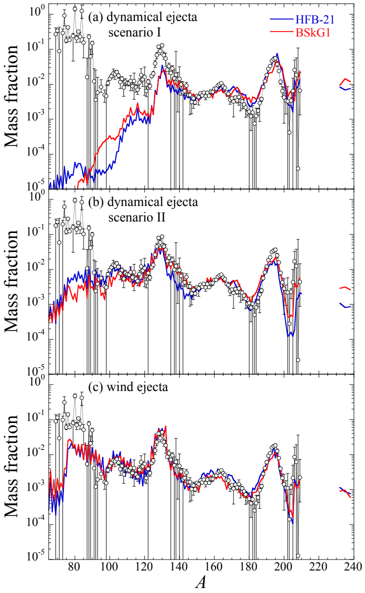
Neutron matter



Symmetric matter

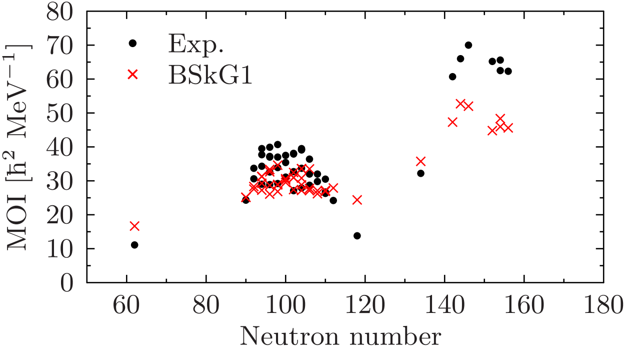


R-process

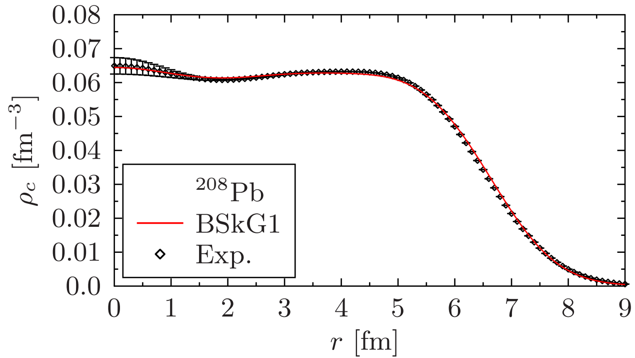


(a) dynamical ejecta
scenario I
HFB-21
BSkG1
(b) dynamical ejecta
scenario II
(c) wind ejecta
Mass fraction
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
80
100
120
140
160
180
200
220
240
A

Moment of inertias



Charge density



Charge radii