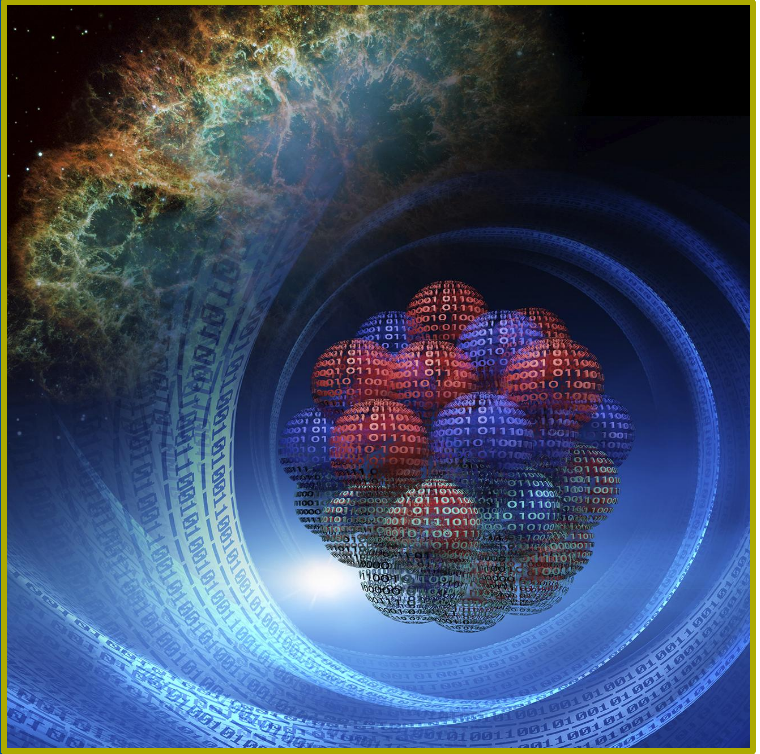
WOUTER RYSSENS



Andy Sproles, ORNL

Nuclear structure at scale

from ground states to fission

ULB-Kansai University Workshop

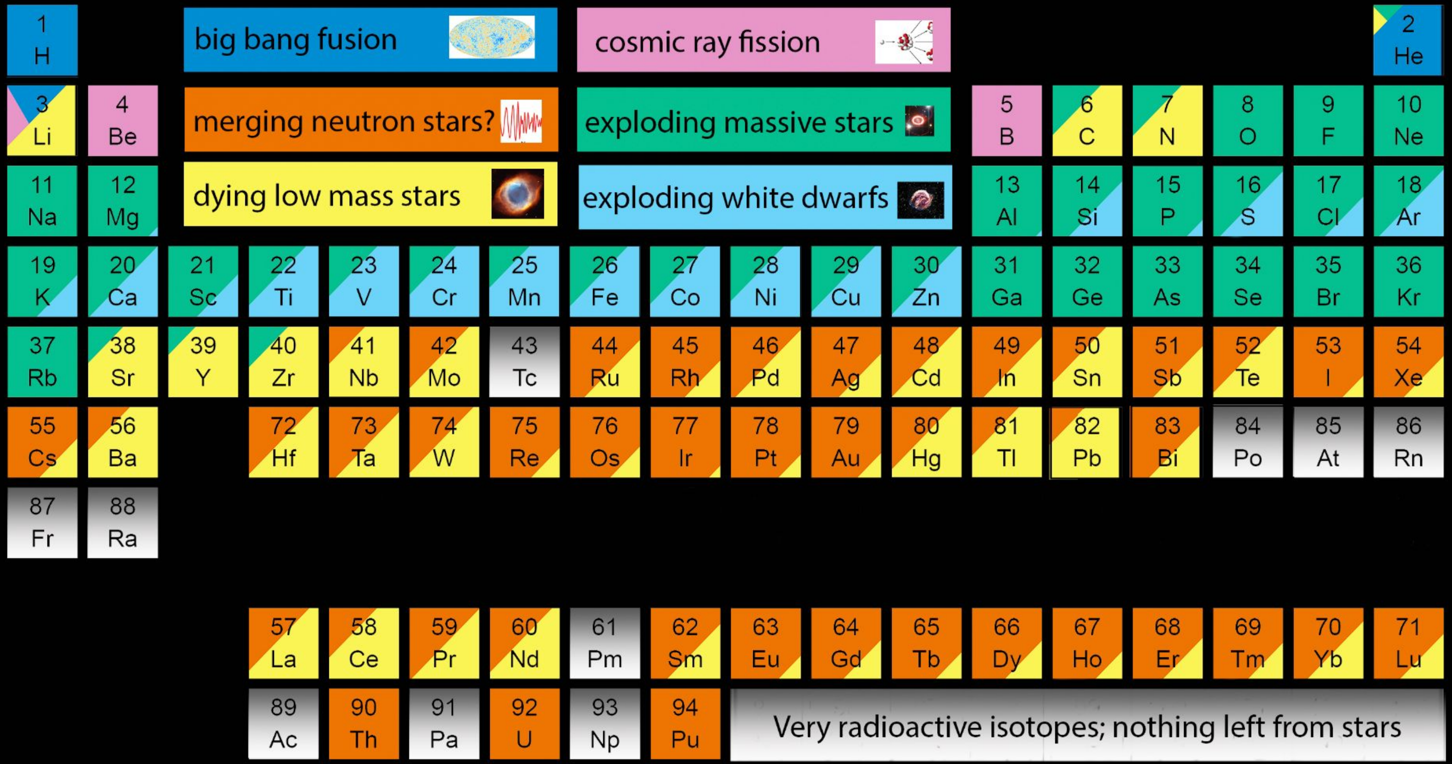
February 28th 2025

wryssens.com

wryssens@ulb.be

ULB

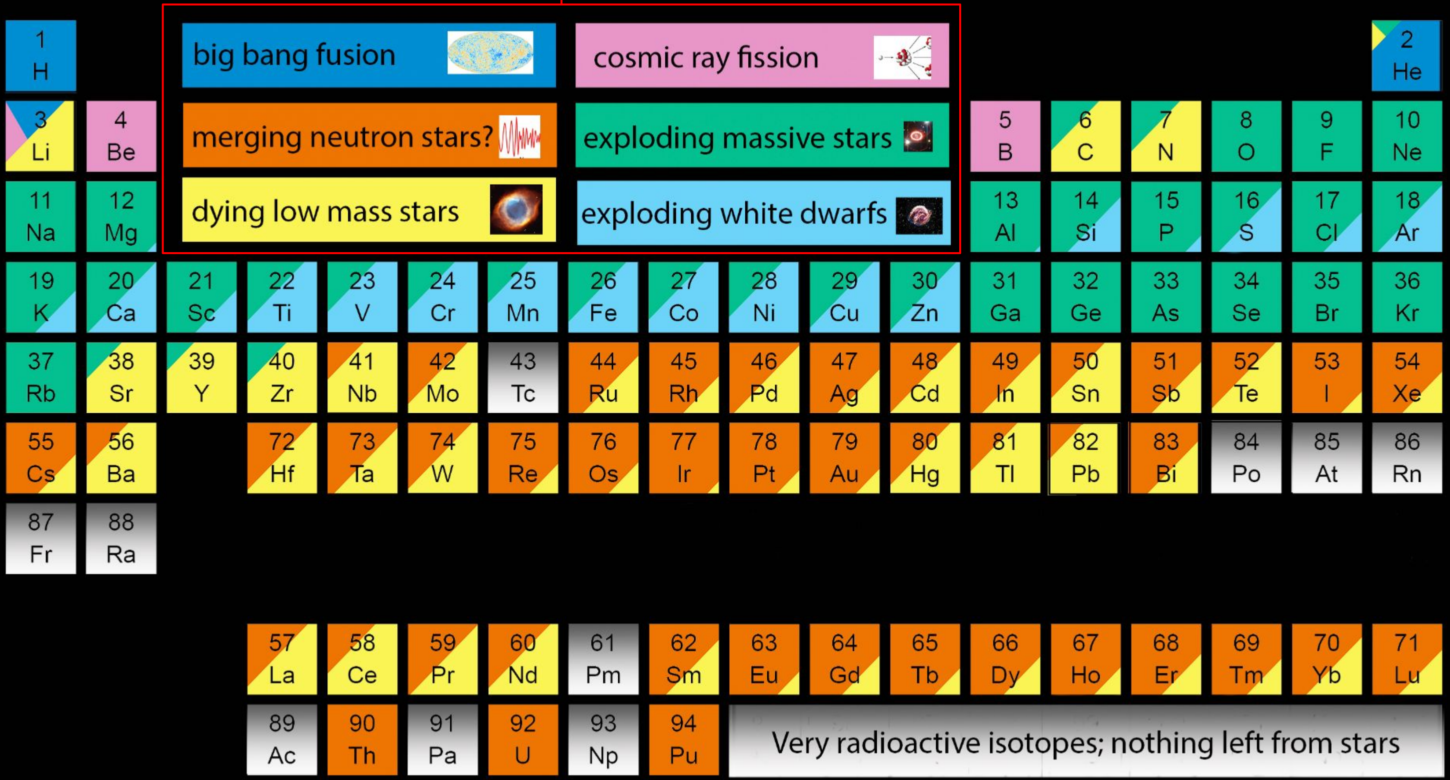
fnrs LA LIBERTÉ DE CHERCHER



Graphic created by Jennifer Johnson
http://www.astronomy.ohio-state.edu/~jaj/nucleo/

Astronomical Image Credits:
ESA/NASA/AASNova

Tentative assignments!

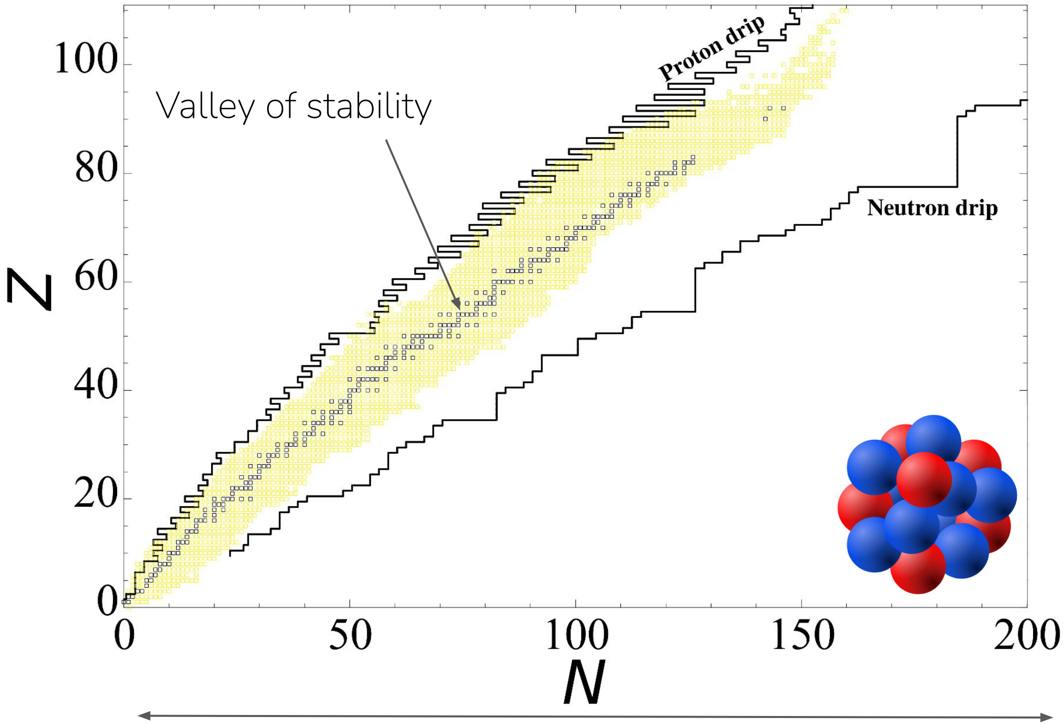


Graphic created by Jennifer Johnson
http://www.astronomy.ohio-state.edu/~jaj/nucleo/

Astronomical Image Credits:
ESA/NASA/AASNova

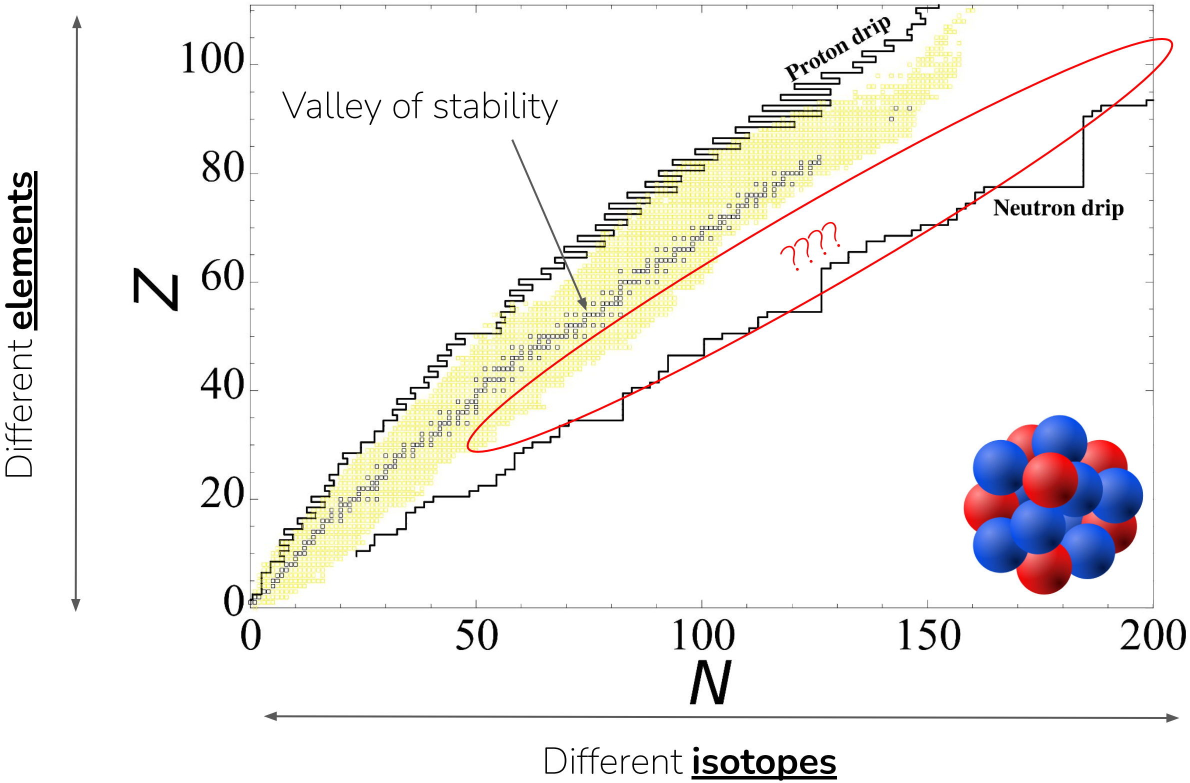
The nuclear chart...

Different **elements**

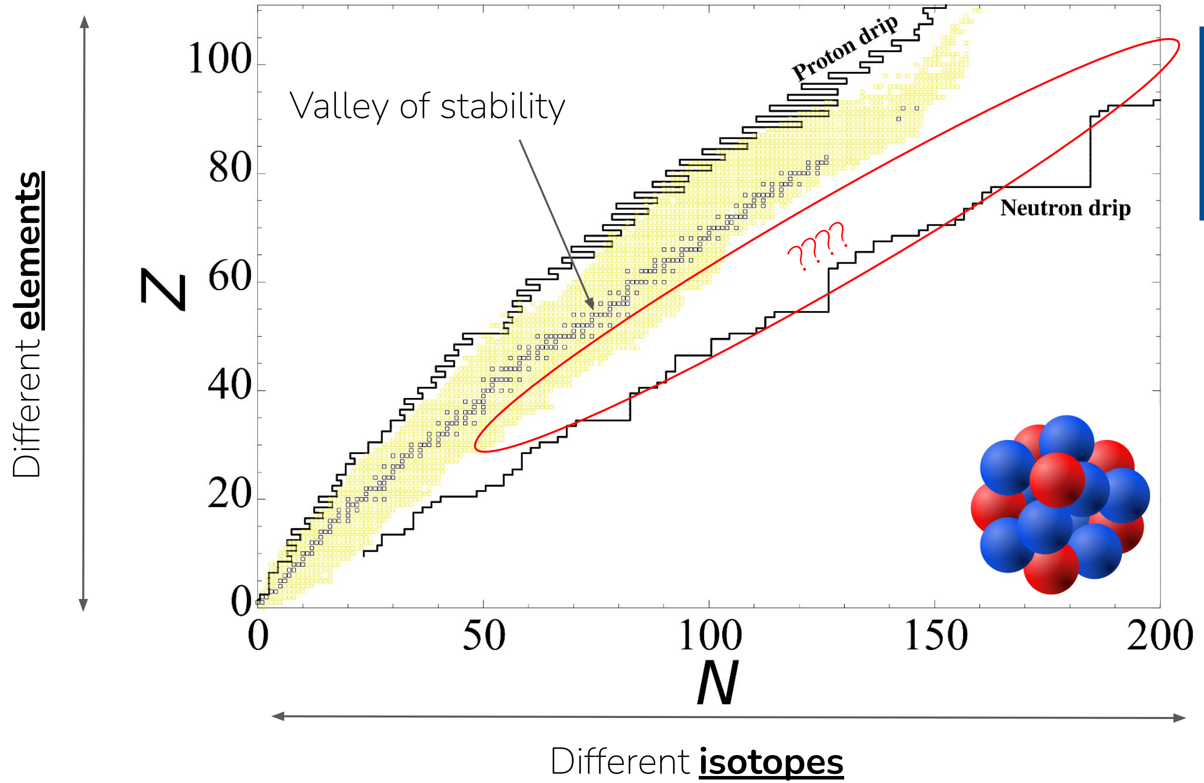


Different **isotopes**

The nuclear chart…



The nuclear chart…

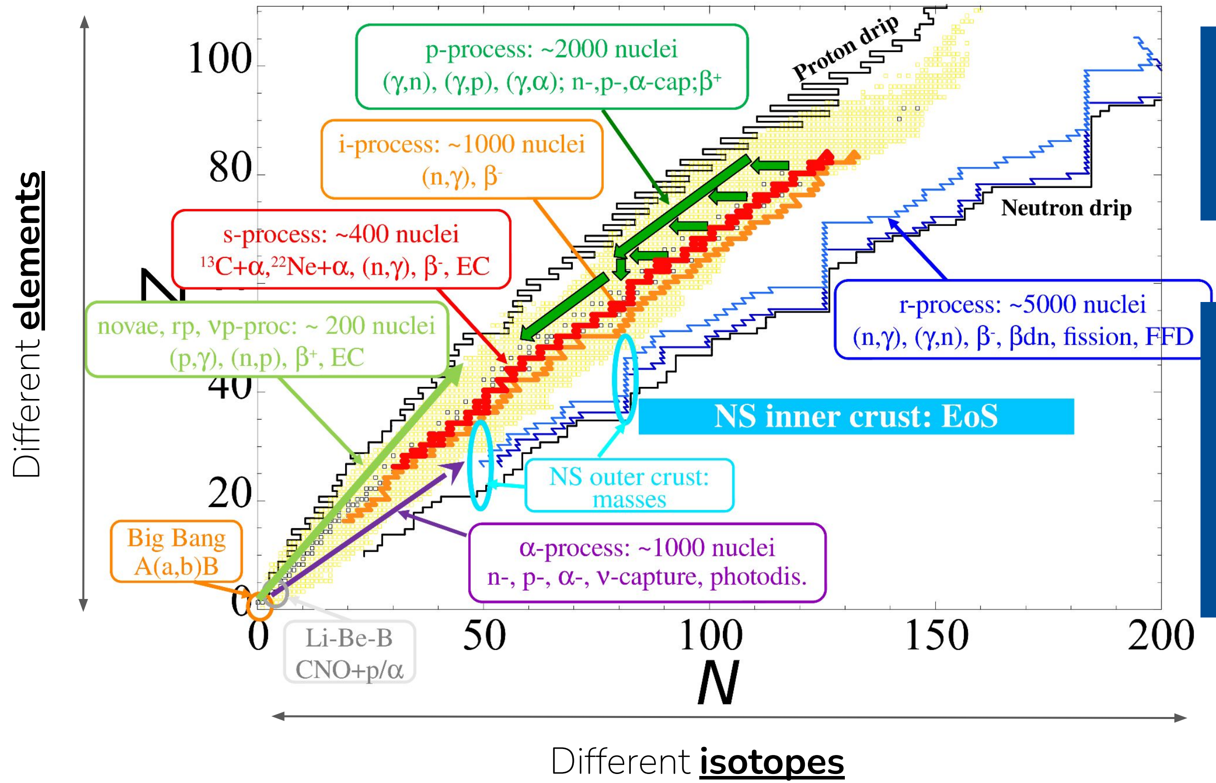


Transmutation

1. neutron capture
2. β+ and β- decay
3. different types of fission

and many others…

The nuclear chart and the processes traversing it



Transmutation

1. neutron capture
2. β+ and β- decay
3. different types of fission

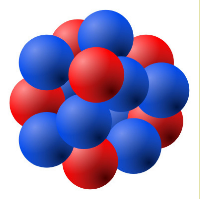
and many others…

Need for theory!

1. many astrophysical processes
   - r-process, s-process, …
   - neutron star structure
2. operating in different conditions
   - temperature, density, …
3. properties of 1000s of nuclei
   - masses, sizes, …
   - reaction rates

The Belgian landscape

Nuclear physics

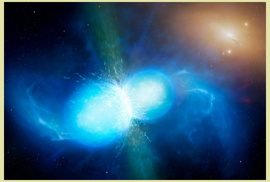


KU LEUVEN
ULB

Masses, reaction and decay rates

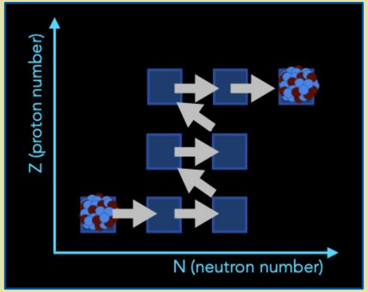
Neutron star properties

Hydrodynamic simulations



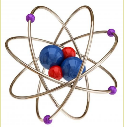
Temperature, densities, ...

Reaction networks



ULB

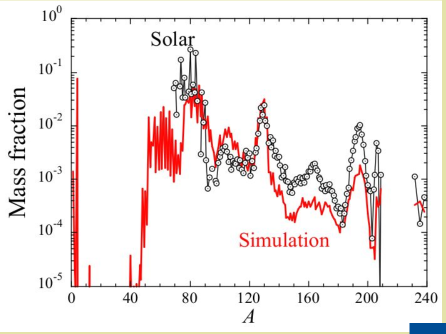
Atomic Theory



ULB
UMONS

Opacities

Observables!



ULB

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

$$E \sim \int d^3r \Big[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \ldots \Big]$$

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

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

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

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

Energy

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

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

Energy

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

Local densities and currents of a wavefunction

This is an attractive strategy...

- **simple** wavefunctions but **individual** nucleons
- rooted in many-body theory
- many observables accessible
- Feasible for ~**7000** nuclei

Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

Energy

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

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

Local densities and currents of a wavefunction

This is an attractive strategy...

- **simple** wavefunctions but **individual** nucleons
- rooted in many-body theory
- many observables accessible
- Feasible for ~**7000** nuclei

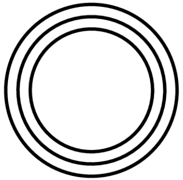
... but how to make it predictive?

We attempt to maximise

- the physics included in the model
- the experimental data in the fit
- ❗ the observables described **at the same time**

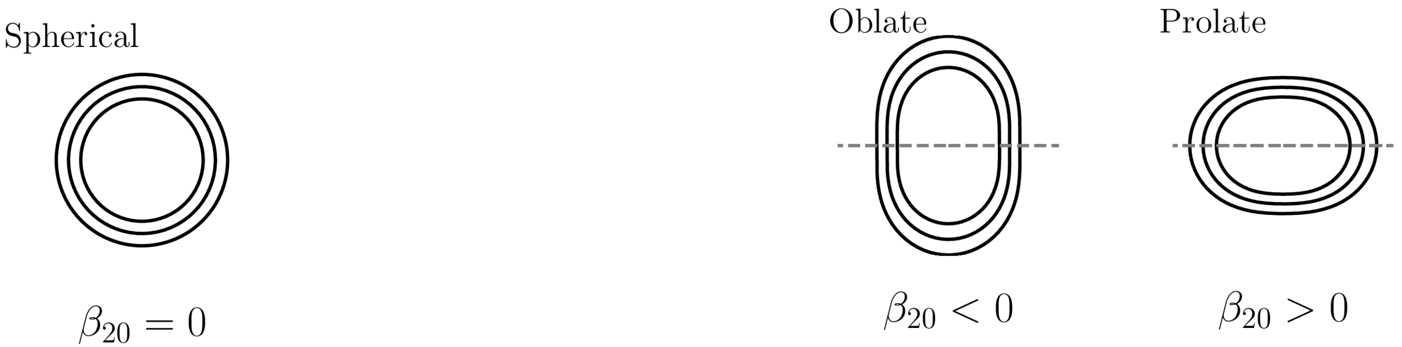
Large-scale models in 1 dimensions

Spherical



$\beta_{20} = 0$

Large-scale models in 1-2 dimensions

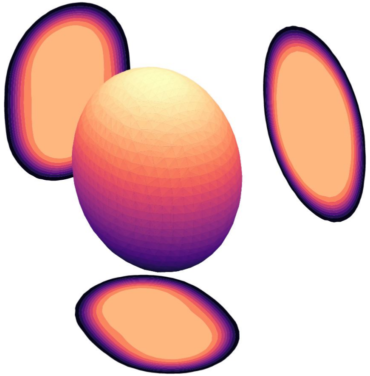


Nuclear deformation

- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

Large-scale models in 1-2-3 dimensions

β_{20}, β_{22} or β_2, γ



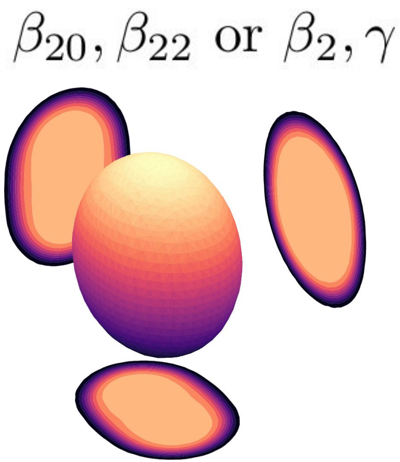
Nuclear deformation

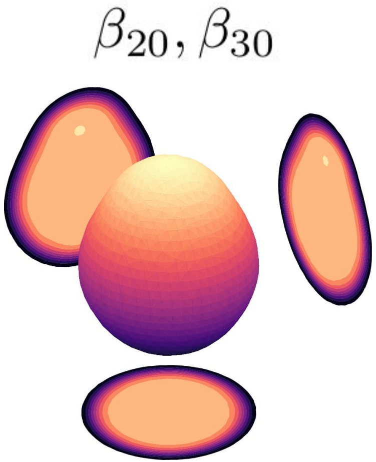
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

Large-scale models in 1-2-**3** dimensions





Nuclear deformation

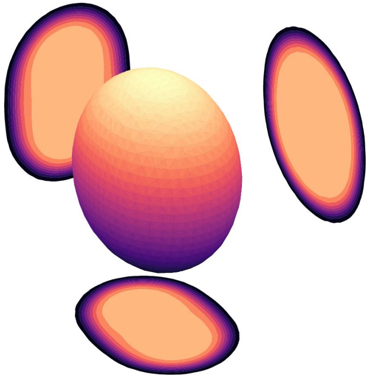
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

More general configurations

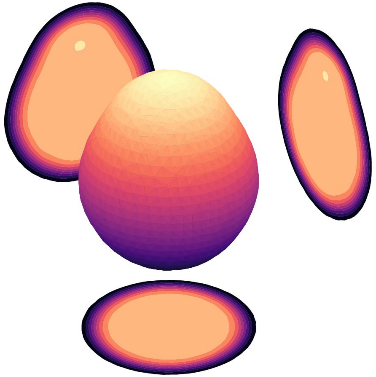
- triaxial shapes
- reflection asymmetry
- elongated shapes

Large-scale models in 1-2-**3** dimensions

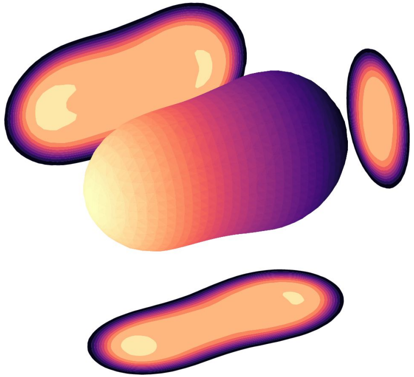
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Nuclear deformation

- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

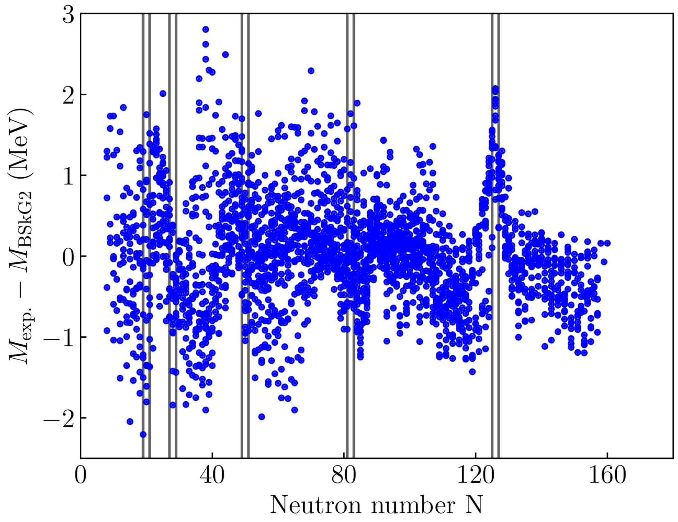
More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

The **B**russels **Sk**yrme on a **G**rid models

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025



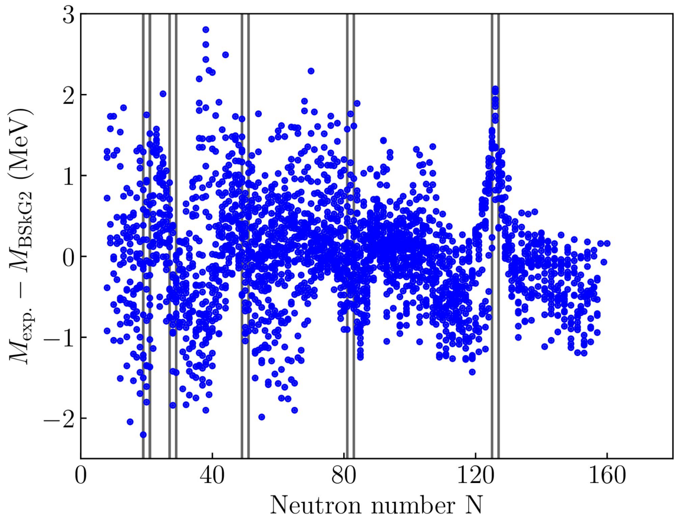
The fit includes

- 2457 masses
- 884 charge radii

The **B**russels **Sk**yrme on a **G**rid models

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
Prim. barriers [MeV]	0.88	0.44	0.33	0.36
Sec. barriers [MeV]	0.87	0.47	0.51	0.53
Fission isomers [MeV]	1.0	0.49	0.34	0.33



The fit includes

- 2457 masses
- 884 charge radii

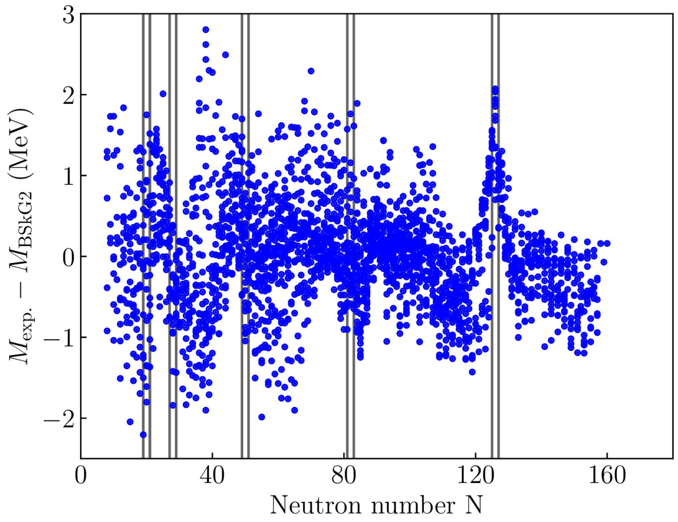
as well as...

- 45 fission barriers
- 28 fission isomer energies

The **B**russels **Sk**yrme on a **G**rid models

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
Prim. barriers [MeV]	0.88	0.44	0.33	0.36
Sec. barriers [MeV]	0.87	0.47	0.51	0.53
Fission isomers [MeV]	1.0	0.49	0.34	0.33
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	2.3



The fit includes

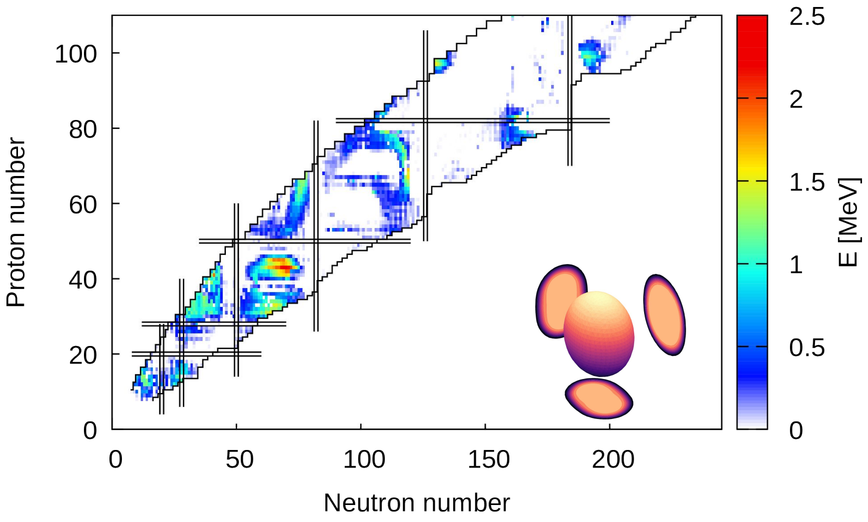
- 2457 masses
- 884 charge radii

as well as...

- 45 fission barriers
- 28 fission isomer energies
- a constraint on maximum NS mass

Ground state properties: masses

M. Hukkanen, W.R. et al., PRC **107**, 014306 (2023).
M. Hukkanen, W.R. et al., PRC **108**, 064315 (2023).
M. Hukkanen, W.R. et al., PLB **856**, 138916 (2024).
M. Stryjczyk, W. R. et al., PLB (in press).

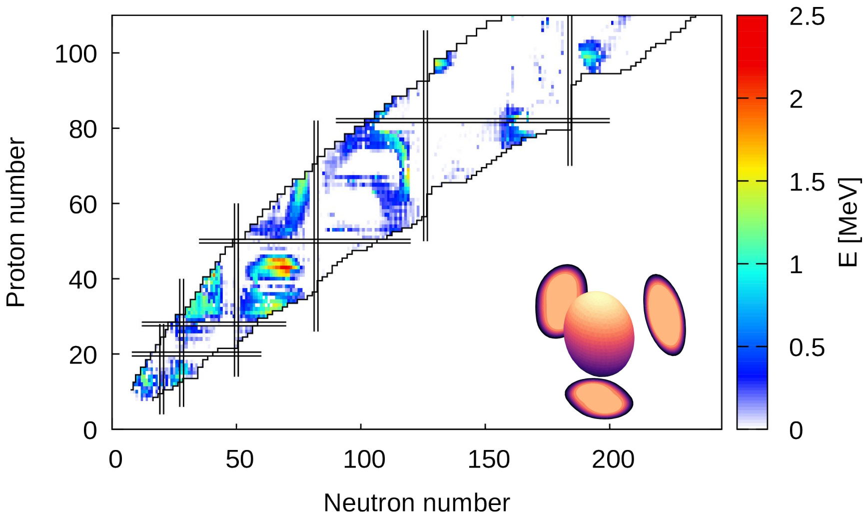


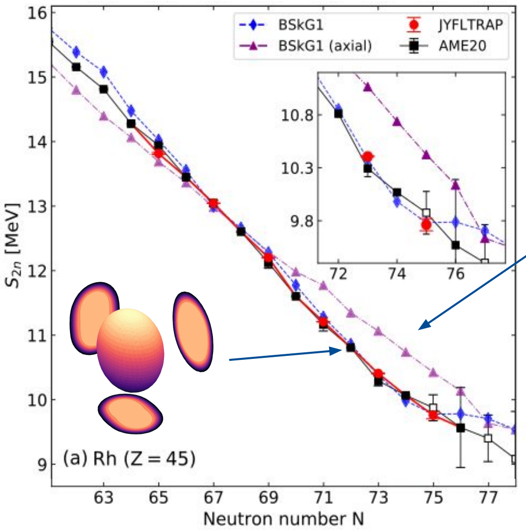
Triaxial deformation is not rare

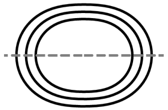
- many nuclei are affected
- effects up to 2.5 MeV near Z~44

Ground state properties: masses

M. Hukkanen, W.R. et al., PRC **107**, 014306 (2023).
M. Hukkanen, W.R. et al., PRC **108**, 064315 (2023).
M. Hukkanen, W.R. et al., PLB **856**, 138916 (2024).
M. Stryjczyk, W. R. et al., PLB (in press).







Triaxial deformation is not rare

- many nuclei are affected
- effects up to 2.5 MeV near Z~44

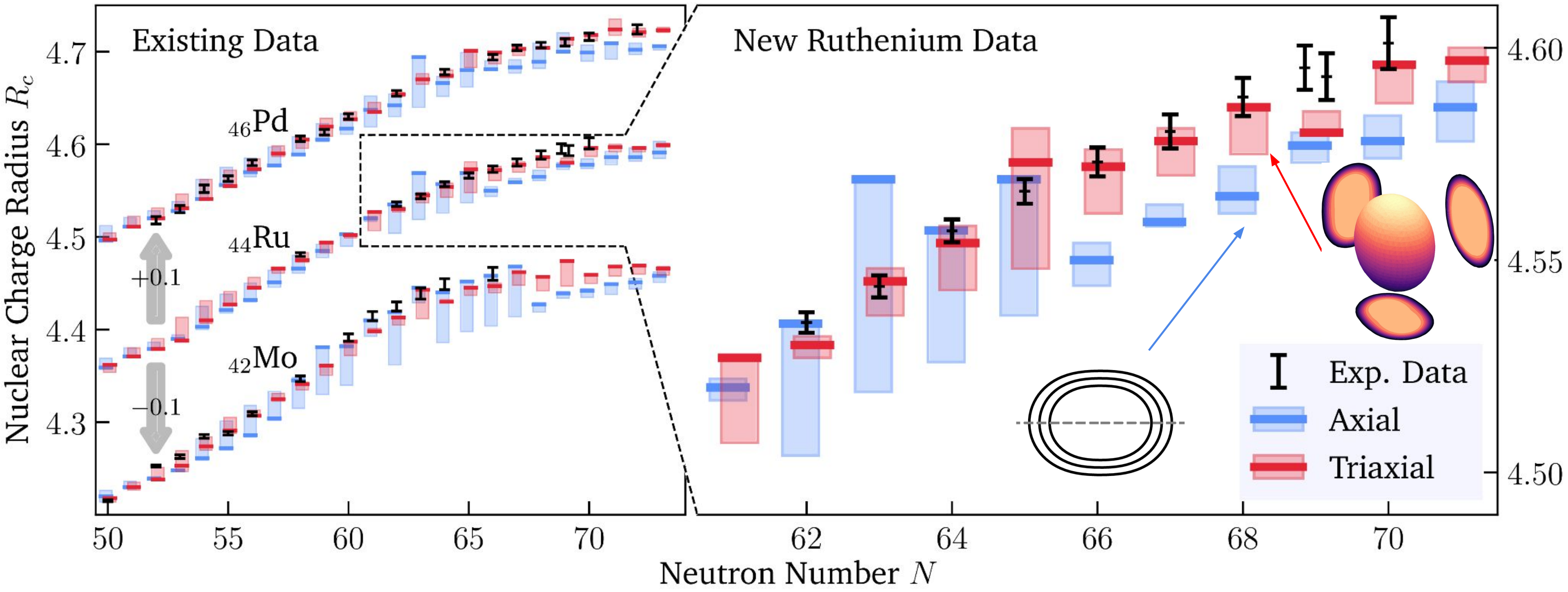
… and imprints on observables!

- spectroscopy
- binding energies
- existence and structure of isomers
- nuclear radii

and many more!

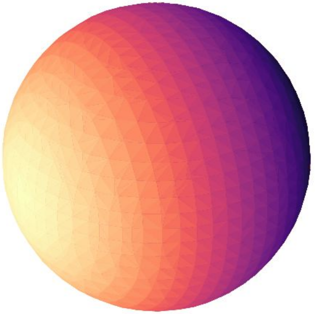
Ground state properties: radii

B. Maaβ, W.R. et al., submitted to PRL



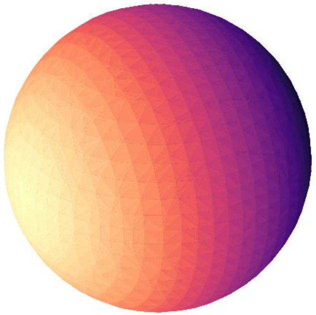
Modelling fission microscopically

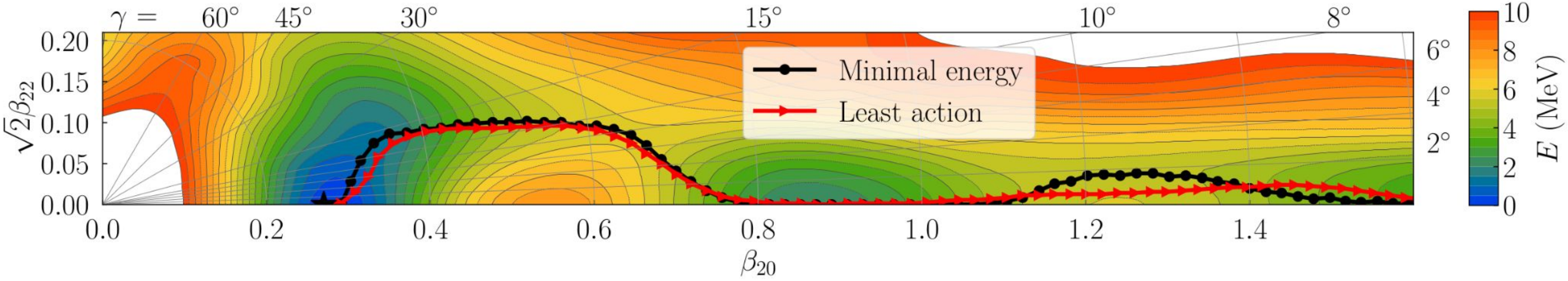
W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.



Modelling fission microscopically

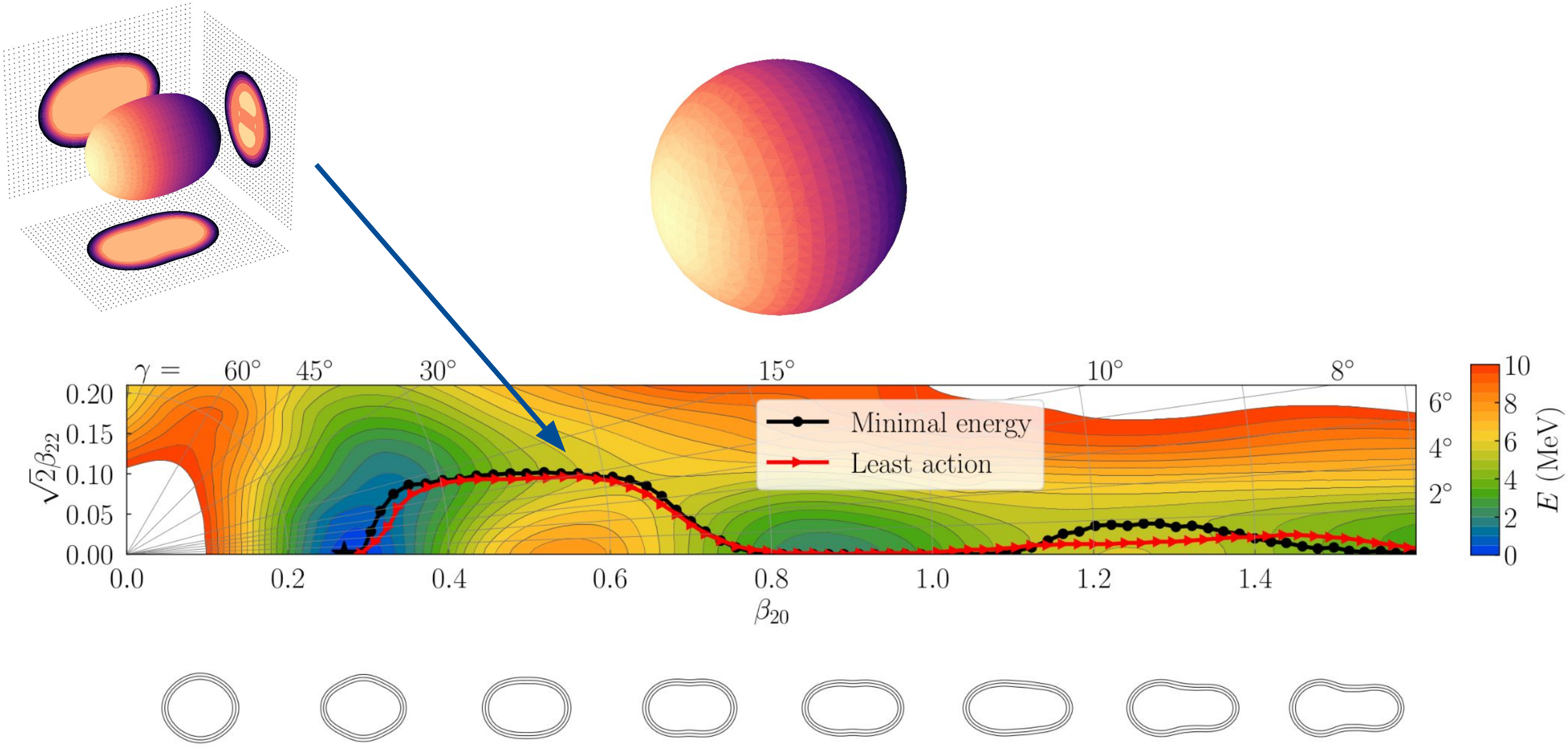
W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.





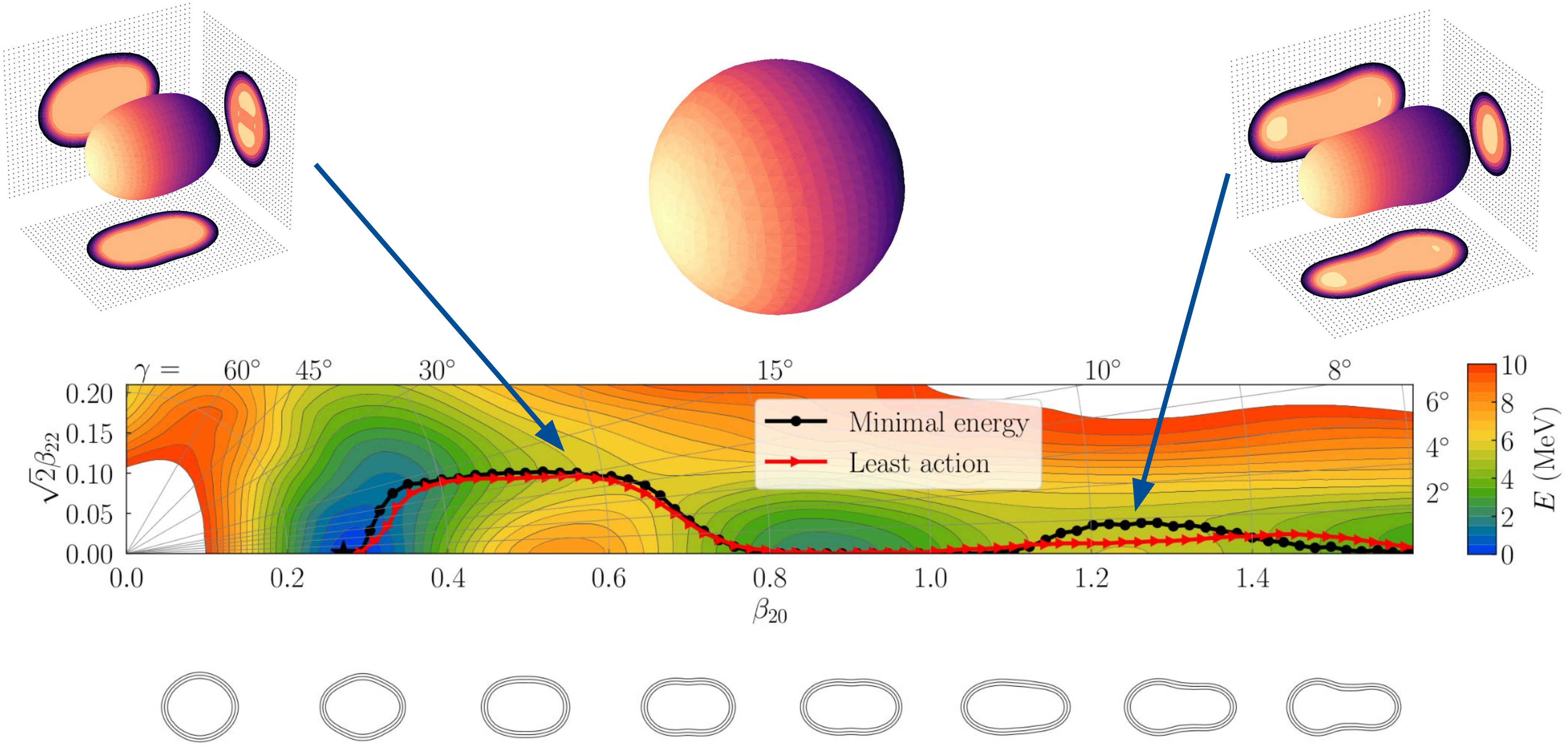
Modelling fission microscopically

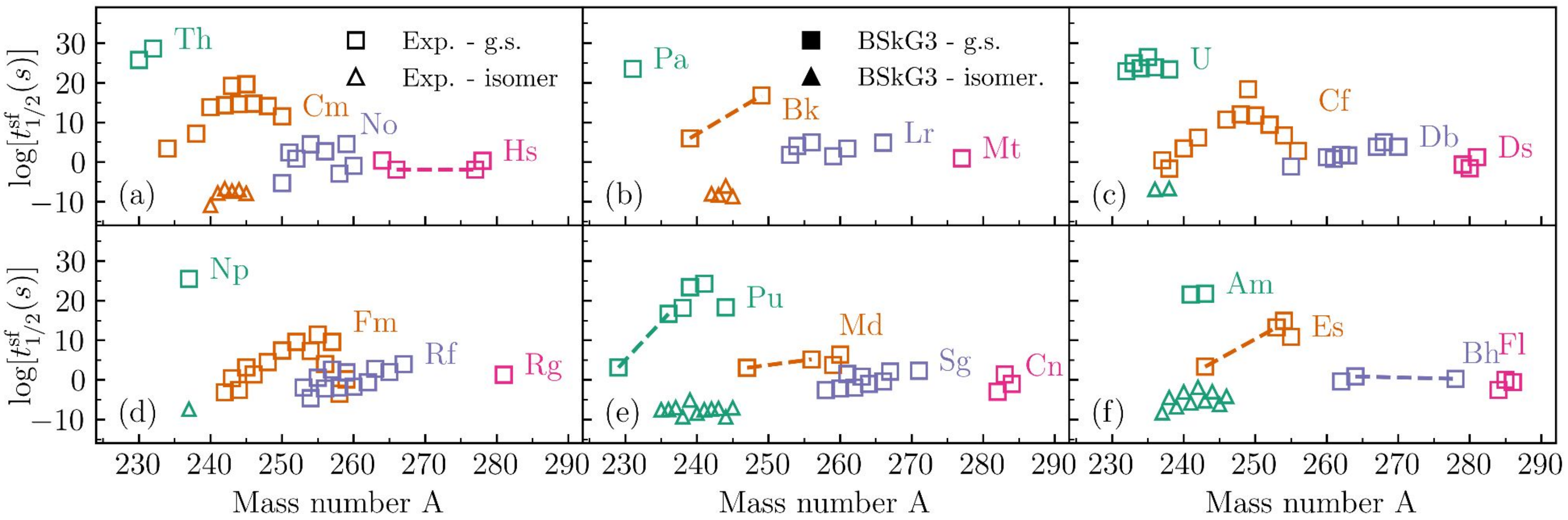
W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.



Modelling fission microscopically

W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.



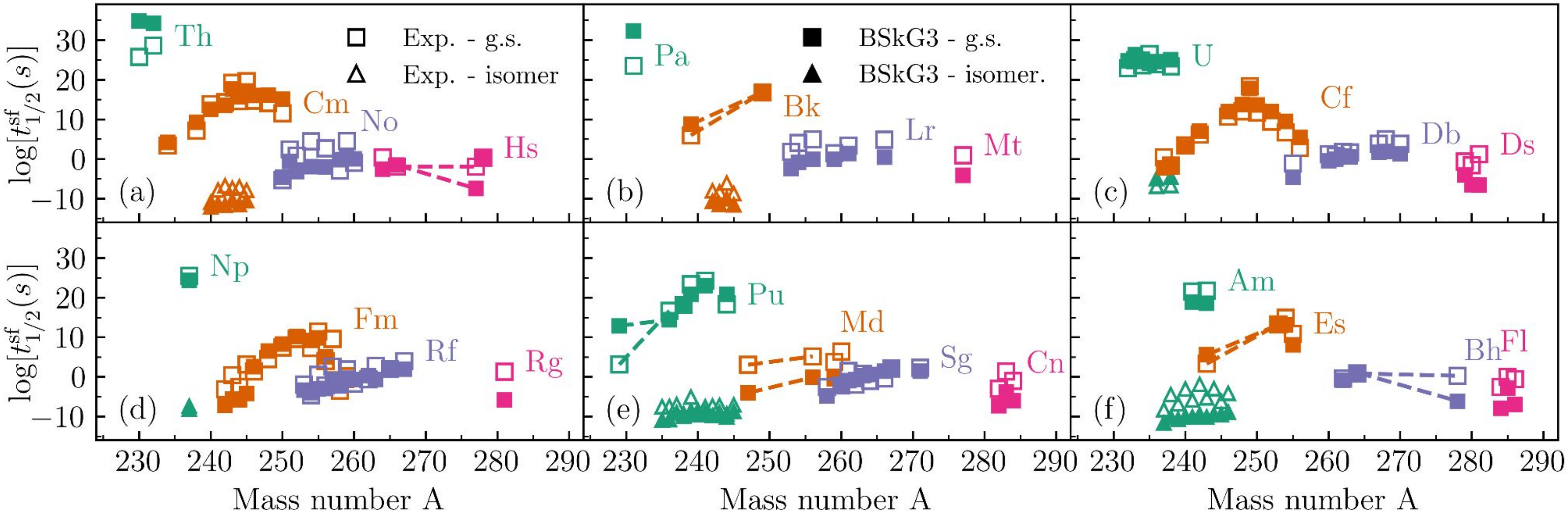


Spontaneous fission half-lives

Experimental data:

- 124 ground state half-lives
- 34 half-lives of isomeric states

... that span > **40** orders of magnitude!



Spontaneous fission half-lives

Experimental data:

- 124 ground state half-lives
- 34 half-lives of isomeric states

… that span **> 40** orders of magnitude!

… at scale from microscopic models!

- unprecedented scale and accuracy
  ~ 4 orders of magnitude
- … without adjustable parameters!

A. Sánchez-Fernández et al., in prep.

Computing brought us this far ...

MOCCa

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

Density functional theory with MOCCa

- nonlinear optimisation problem
- algorithms for speed and robustness
- open-source later this year

Computing brought us this far ...

MOCCa

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

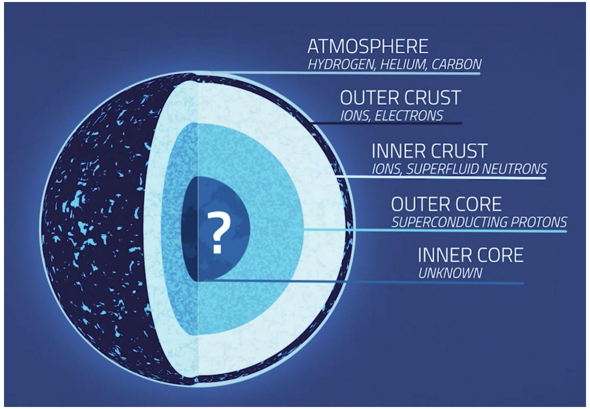
Density functional theory with MOCCa

- nonlinear optimisation problem
- algorithms for speed and robustness
- open-source later this year

Raw computing power

- CÉCI & VSC: academic support in Belgium
- TIER-1 resources by Cenaero
  - Lucia - ranked 388th - our development workhorse
- TIER-0 resources by EuroHPC
  - MN 5 - ranked 11th - large scale fission
  - LUMI - ranked 8th - ???

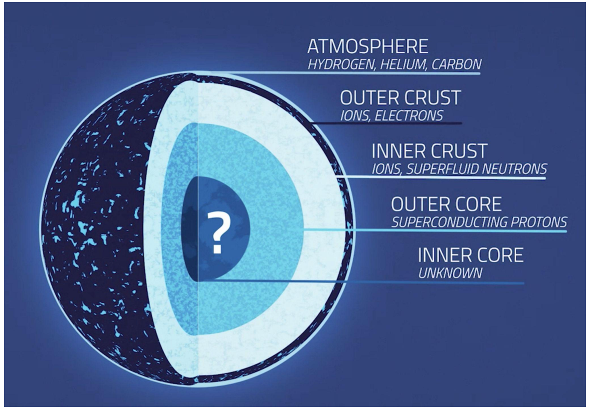
… and it is just the beginning!

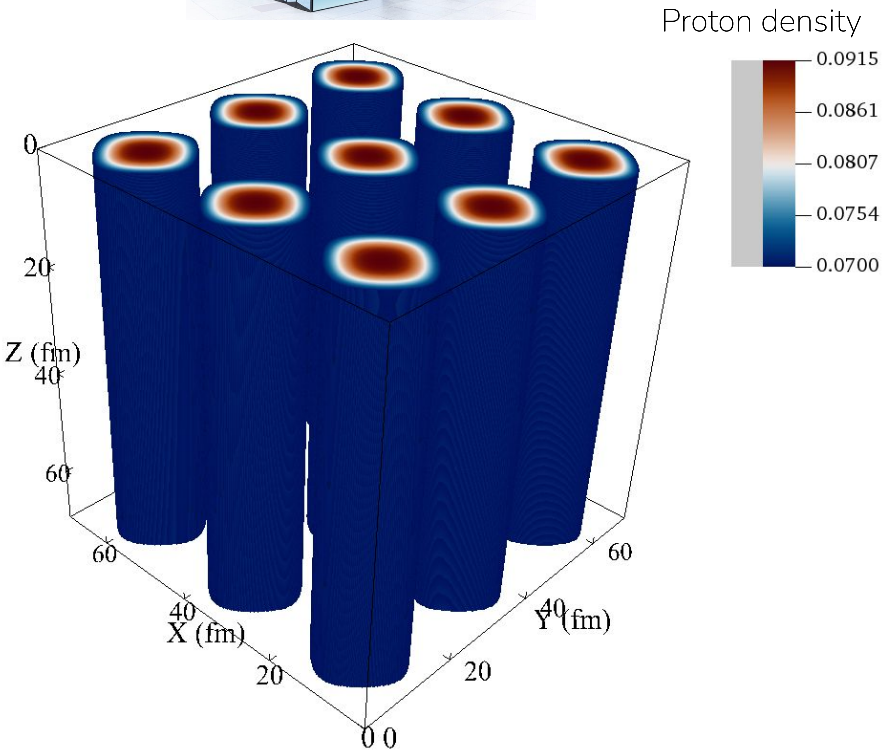


Nuclear pasta

- crystalline structures in NS crusts spaghetti, lasagna, buccatini, swiss cheese, …
- QM treatment with NS-appropriate EDFs
- simulating ~$\mathbf{10^6}$ particles in large volumes

… and it is just the beginning!





Nuclear pasta

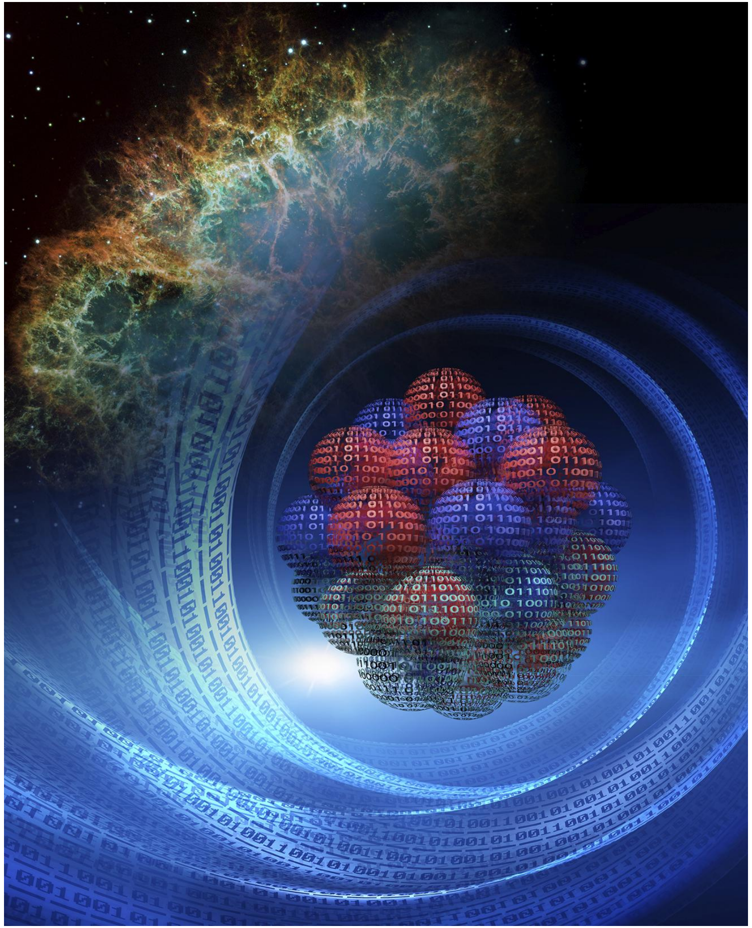
- crystalline structures in NS crusts spaghetti, lasagna, buccatini, …
- QM treatment with NS-appropriate EDFs
- simulating ~$\mathbf{10^6}$ particles in large volumes

N. Shchechilin et al., in preparation

Conclusion

We build **large-scale, microscopic** models for (astro) applications.

Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = rooted in many-body theory



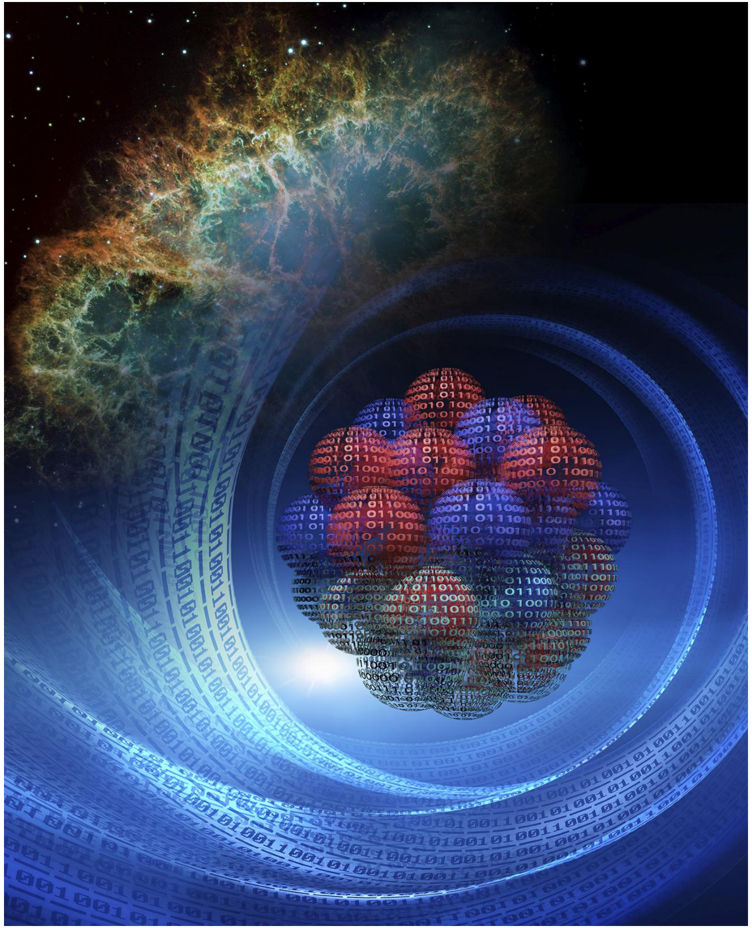
Conclusion

We build **large-scale**, **microscopic** models for (astro) applications.

Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = rooted in many-body theory

The BSkG models

- excellent description of masses and charge radii
- consistent with NS observations
- unmatched for fission properties
- constant exchange with experiment



Conclusion

We build **large-scale**, **microscopic** models for (astro) applications.

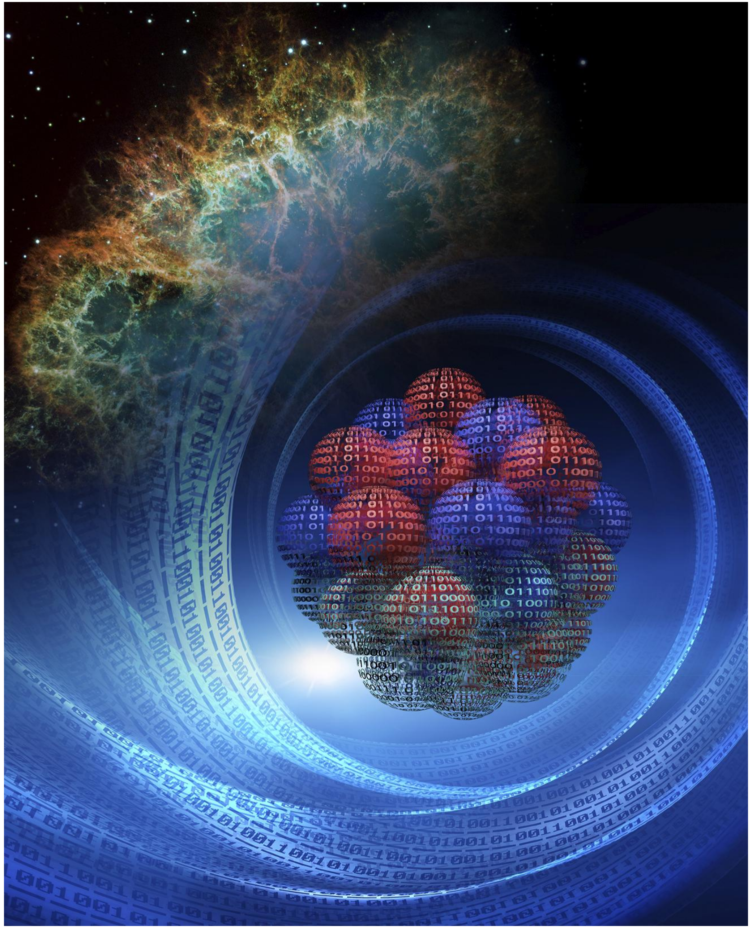
Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = rooted in many-body theory

The BSkG models

- excellent description of masses and charge radii
- consistent with NS observations
- unmatched for fission properties
- constant exchange with experiment

The future is promising:

1. fission properties of ~3000 nuclei
2. BSkG5: more with less
3. nuclear pasta with the BSkGs
4. Electromagnetic transitions and β-decay rates



Conclusion

We build **large-scale**, **microscopic** models for (astro) applications.

Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = rooted in many-body theory

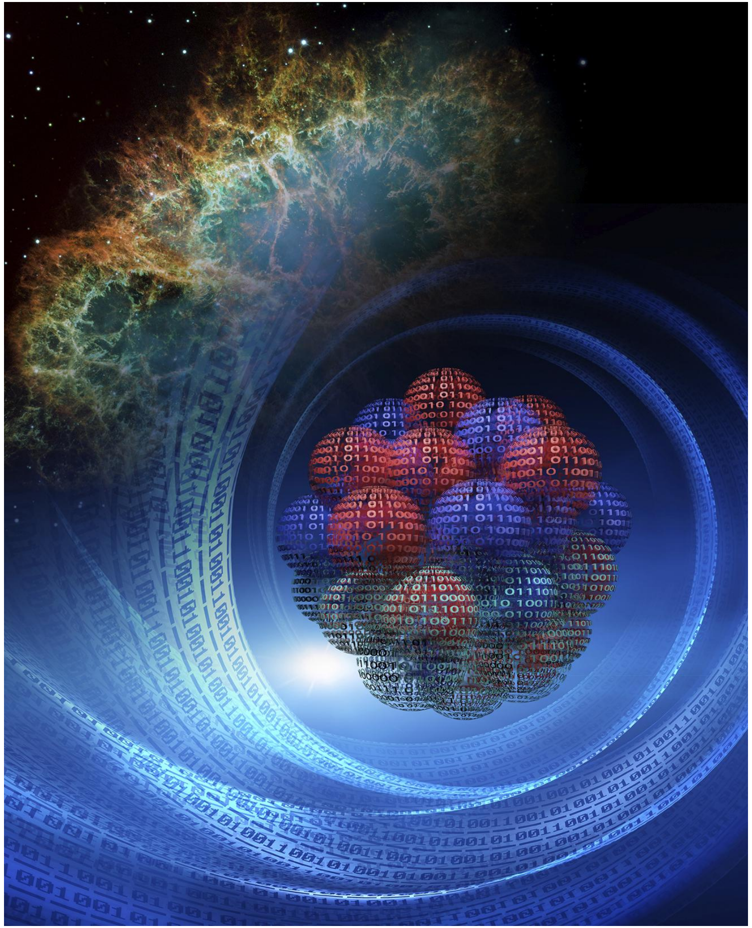
The BSkG models

- excellent description of masses and charge radii
- consistent with NS observations
- unmatched for fission properties
- constant exchange with experiment

The future is promising:

1. fission properties of ~3000 nuclei
2. BSkG5: more with less
3. nuclear pasta with the BSkGs
4. Electromagnetic transitions and β-decay rates

Towards a **consistent** set of microscopic nuclear data!



Thank you for...

...... all the wonderful work!

N. Chamel
S. Goriely
G. Grams
P. Demol
A. Sanchez-Fernandez
N. Shchechilin

S. Hilaire

M. Bender

G. Scamps

S. Bara

+ several experimental teams

Thank you for...

...... all the wonderful work!

ULB

N. Chamel
S. Goriely
G. Grams
P. Demol
A. Sanchez-Fernandez
N. Shchechilin

cea

S. Hilaire

iP2i LES 2 INFINIS LYON

M. Bender

L2IT

G. Scamps

KU LEUVEN

S. Bara

+ several experimental teams

...... the computing time!

CÉCI

EuroHPC Joint Undertaking

Thank you for...

...... all the wonderful work!

N. Chamel
S. Goriely
G. Grams
P. Demol
A. Sanchez-Fernandez
N. Shchechilin

S. Hilaire

M. Bender

G. Scamps

S. Bara

+ several experimental teams

...... the computing time!

...... the funding!

Thank you for...

...... all the wonderful work!

ULB: N. Chamel, S. Goriely, G. Grams, P. Demol, A. Sanchez-Fernandez, N. Shchechilin

cea: S. Hilaire

iP2i: M. Bender

L2IT: G. Scamps

KU LEUVEN: S. Bara

+ several experimental teams

...... the computing time!

CÉCI

EuroHPC Joint Undertaking

...... the funding!

fnrs LA LIBERTÉ DE CHERCHER

EOS THE EXCELLENCE OF SCIENCE

.... your attention!