WOUTER RYSSENS

# 3D Coordinate space simulations with nuclear EDFs

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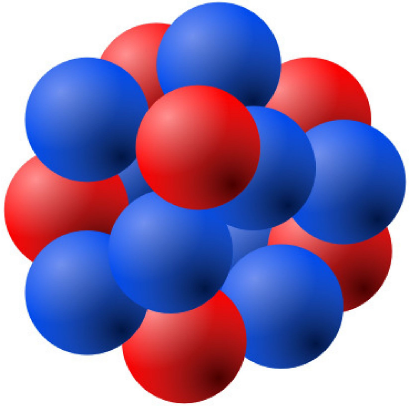
# The structure of this talk

1. Intro: the dense matter many-body problem & EDFs
2. Meshes: what and why?
3. Static calculations in 3D
4. Dynamic calculations
5. Conclusions and perspectives

# The dense matter many-body problem

$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle$$



**Fundamental problems**

1. Complexity of many-body systems
2. Unknown Hamiltonian

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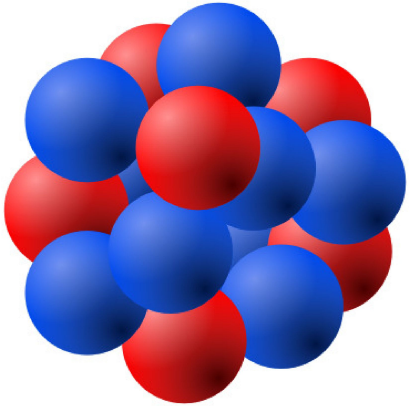

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   -> wavefunction ansätze
2. Unknown Hamiltonian
   -> effective interactions

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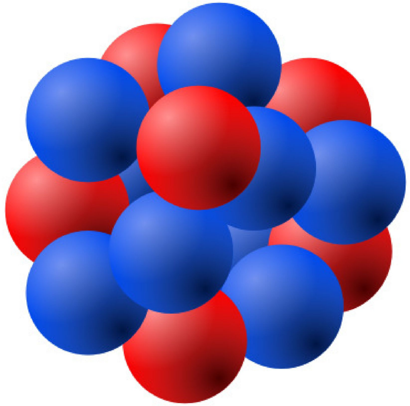

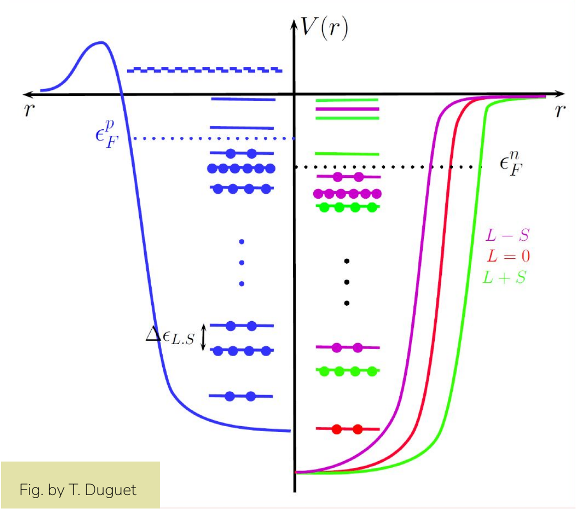


## Fundamental problems

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   -> wavefunction ansätze
2. Unknown Hamiltonian
   -> effective interactions

## Single-particle wavefunctions

- building blocks of all approaches
- simplest use: mean-field states
- their numerical representation determines **A LOT**

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

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

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Local densities and currents of a mean-field wavefunction

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Coupling constants (**10** ~ **25** parameters) fitted to data

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Local densities and currents of a mean-field wavefunction

## Advantages

- ✅ many-body theory, so wavefunctions
- ✅ all observables accessible in theory
- ✅ doable for large amounts of nucleons

Skyrme
Gogny
Fayans
Relativistic
....

# Energy Density Functionals (EDFs)

Energy

Coupling constants (**10** ~ **25** parameters) fitted to data

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

Local densities and currents of a wavefunction

## Advantages

- ✅ many-body theory, so wavefunctions
- ✅ all observables accessible in theory
- ✅ doable for large amounts of nucleons

## Disadvantages

- ❌ needs a 'guess' of the form of the EDF
- ❌ mean-field wavefunctions are too simple
- ❌ requires fitting to experimental data

# Application 1: structure and fission of finite nuclei

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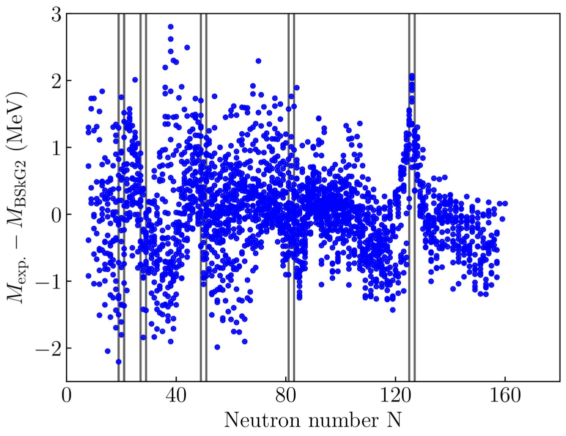
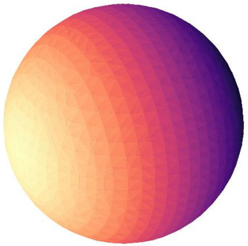



## EDF theory for finite nuclei

- Enormous gaps in our knowledge
  - ~ 2500 masses
  - ~140 spontaneous fission half-lives
  - ~ 800 radii
- only true many-body approach that is applicable at scale



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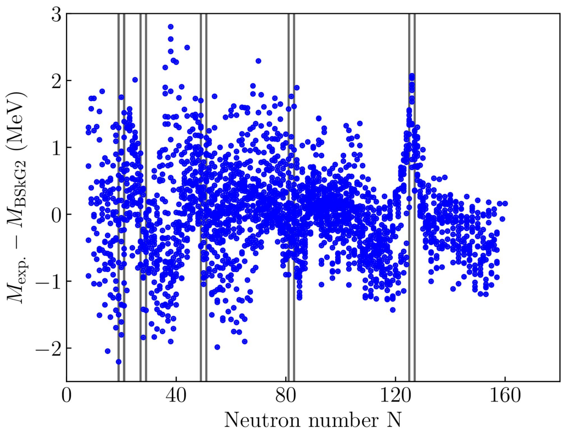


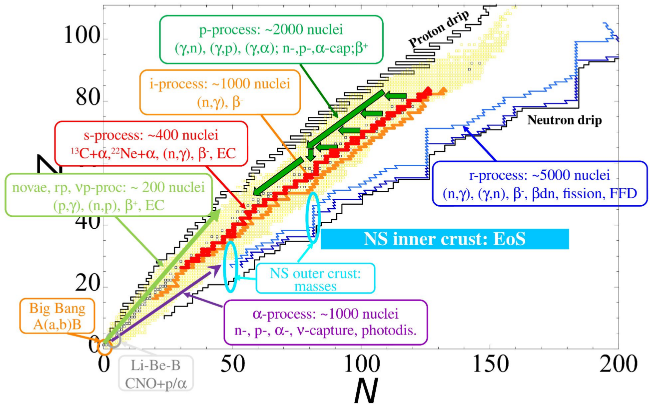


## EDF theory for finite nuclei

- Enormous gaps in our knowledge
  - ~ 2500 masses
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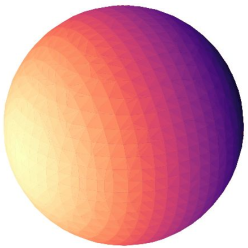
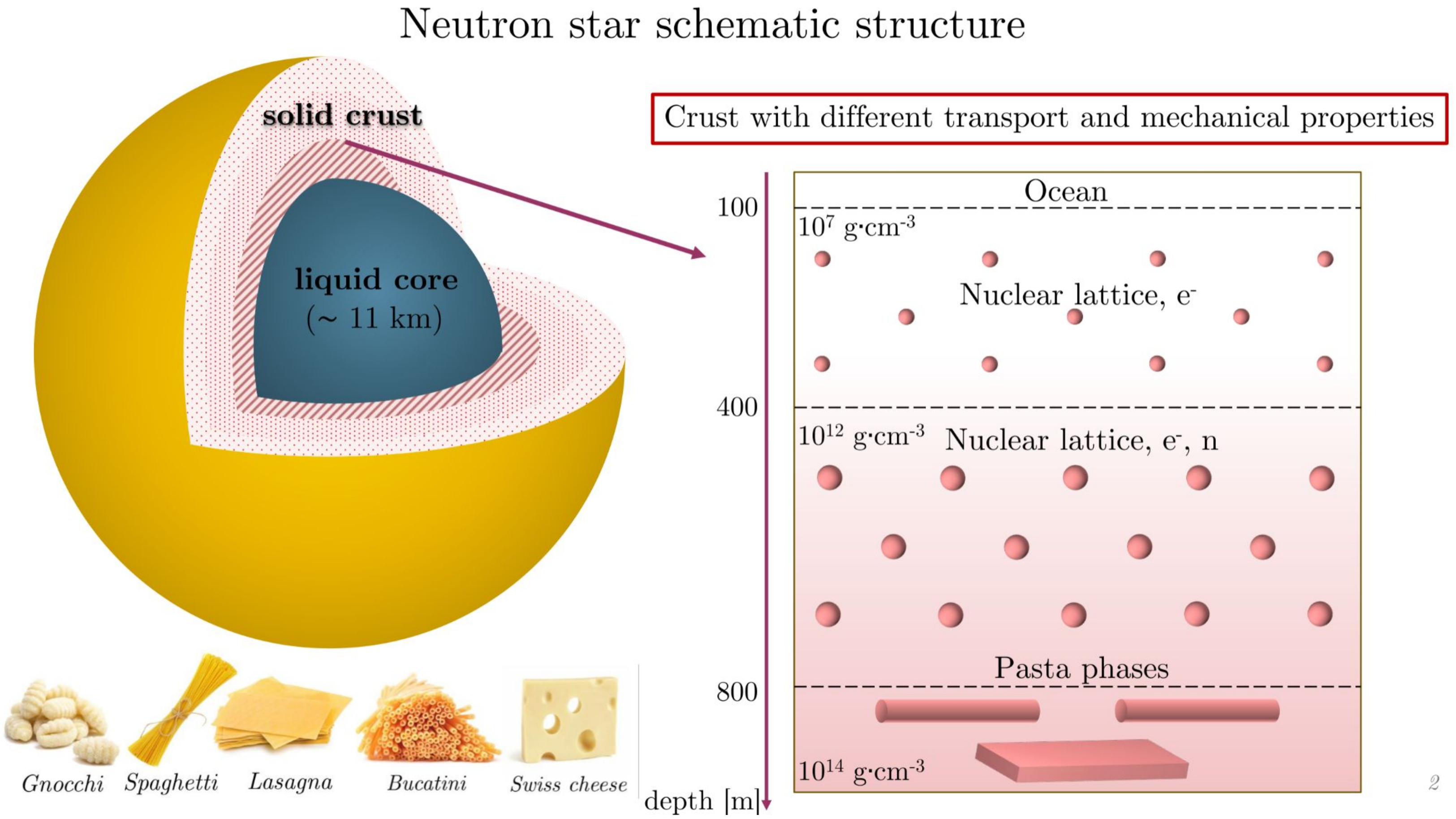
  - ~ 800 radii
- only true many-body approach that is applicable at scale
- necessary for applications!



# Application 2: crusts of neutron stars

Figures courtesy of N. Shchechilin



# Application 2: crusts of neutron stars

Figures courtesy of N. Shchechilin

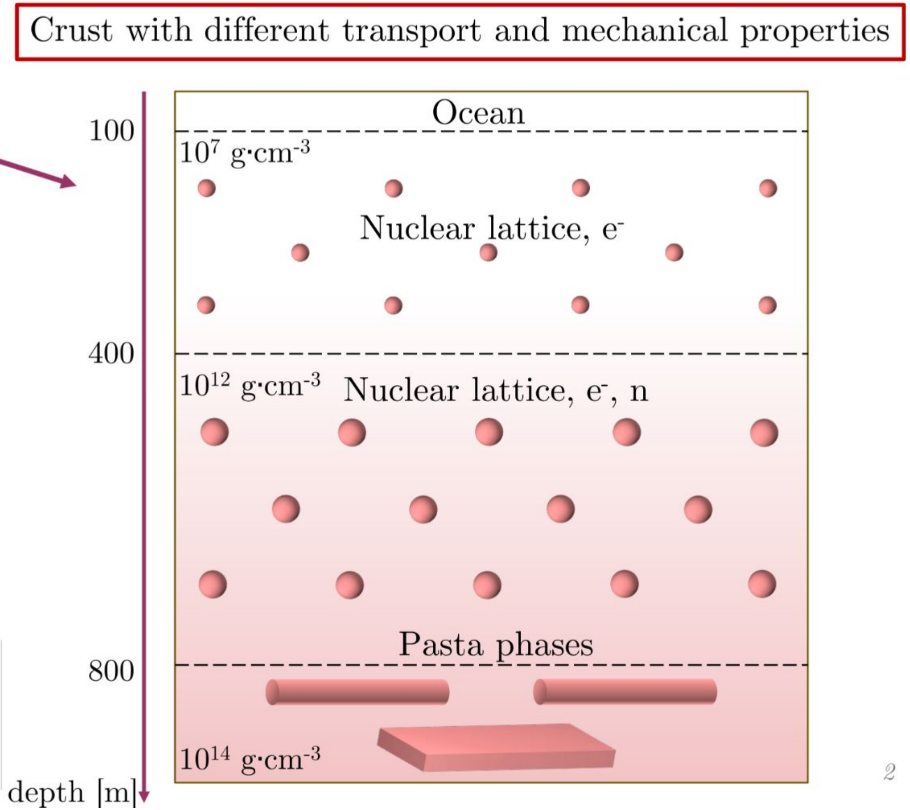
Neutron star schematic structure

The crust represents

- ~10 - 15% of NS radius
- ~ 1% of NS mass

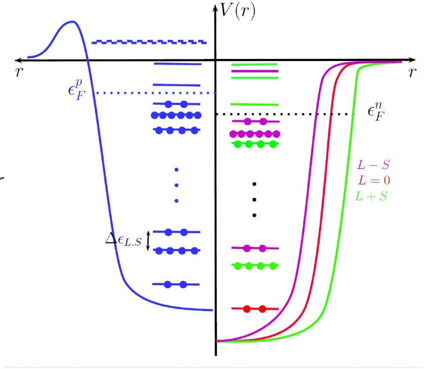
... but impacts:

- neutron star cooling
- magnetic field decay
- gravitational wave emission
- merger ejecta composition
- astroseismology of magnetars



# Meshes; what and why?

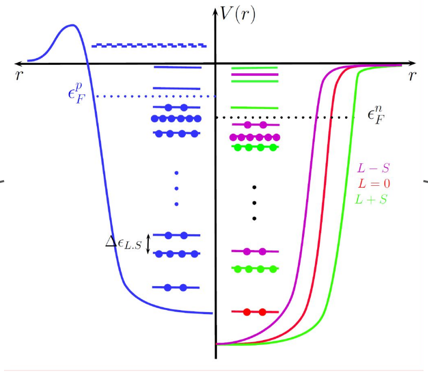
# Representing single-particle wavefunctions




$$\psi_i(\vec{r},\sigma) = \sum_{a=1}^{N} C_{ai}\psi_a(\vec{r},\sigma)$$

$$E(\rho,\tau,\ldots) \rightarrow E(C_{ai})$$

# Representing single-particle wavefunctions

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$$\psi_i(\vec{r}_a,\sigma) \text{ for } a = 1,\ldots,N$$

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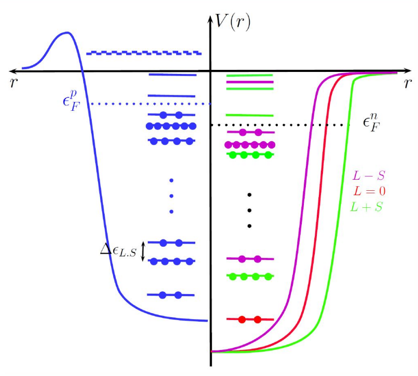


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**Basis expansion**

- suited to specific geometries
- often linked to orthogonal polynomials
- some work can be made analytical
- many flavours of harmonic oscillator

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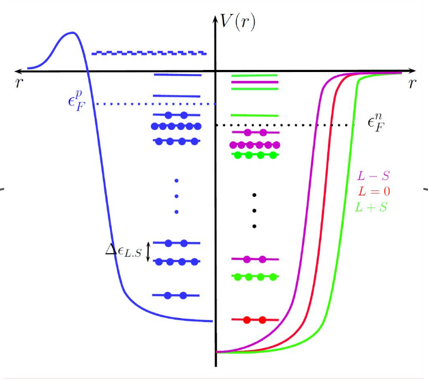


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**Coordinate discretisation**

- potentially **geometry - agnostic**
- sometimes linked to polynomials
- all work is numerical
- Lagrange meshes, Fourier meshes, B-splines, FEM, wavelets, ....

| Derivatives | Collocation of points | Basis = variational? | Boundary conditions | Codes |
|---|---|---|---|---|
| Finite-differences | arbitrary | ❌ | any | EV8 |
| | | | | |
| | | | | |
| | | | | |

## Things to choose

1. mesh points location
2. a way to calculate derivatives
3. a way to calculate integrals


EV8: W. Ryssens et al., CPC **187** (2015).
Sky3D: J.A. Maruhn et. al., CPC **185**, (2014).
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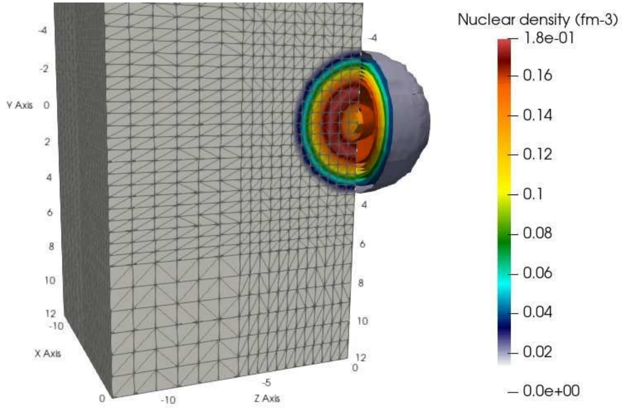

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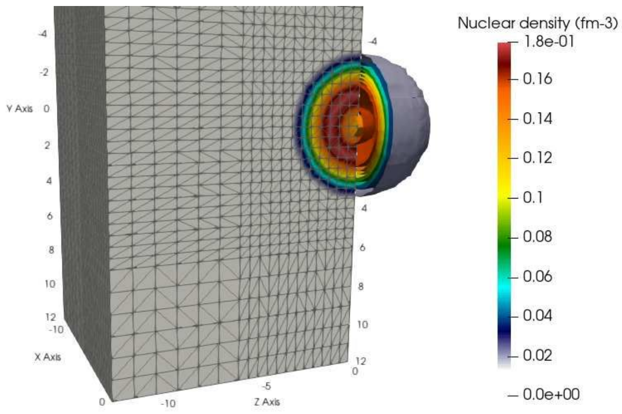

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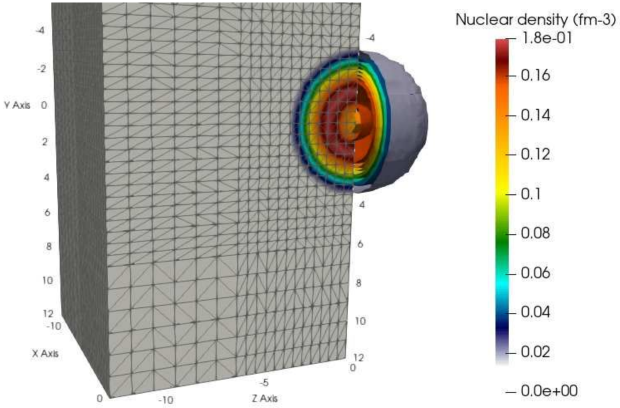

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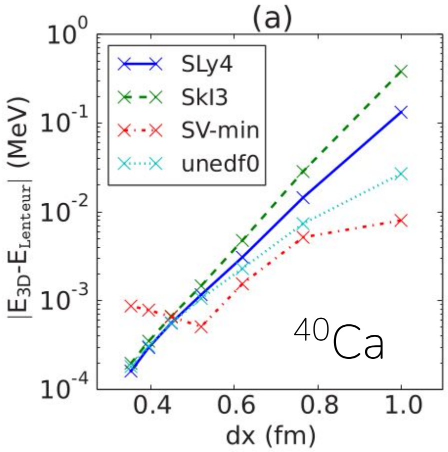


# Mesh (dis)advantages

✅ discretisation error: easily controllable, interpretable

✅

✅

✅

❌

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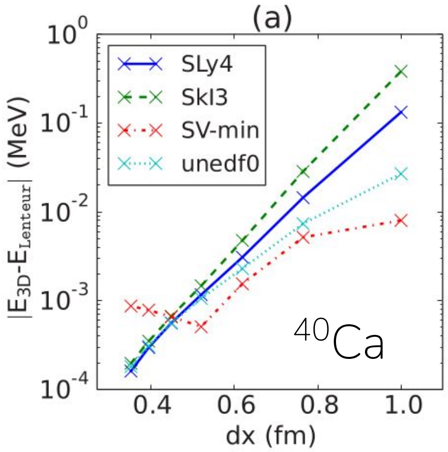


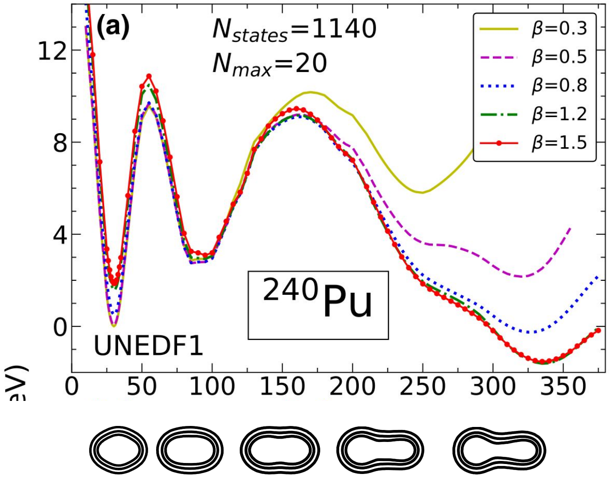


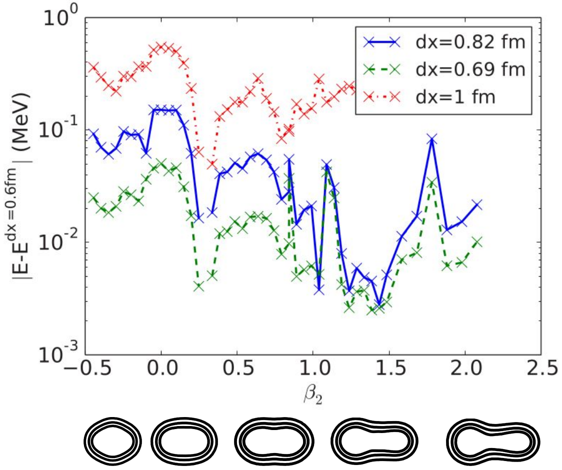


## Mesh (dis)advantages

- ✅ discretisation error: easily controllable, interpretable
- ✅ geometry agnostic: error = shape-independent
- ✅
- ❌

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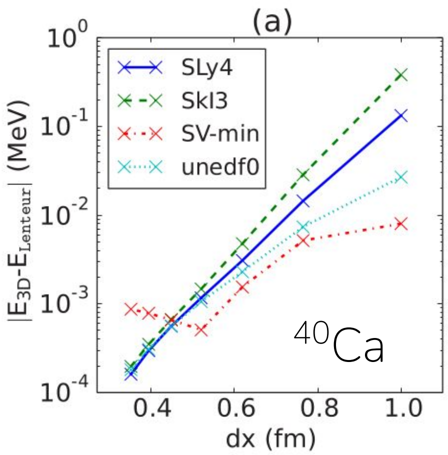


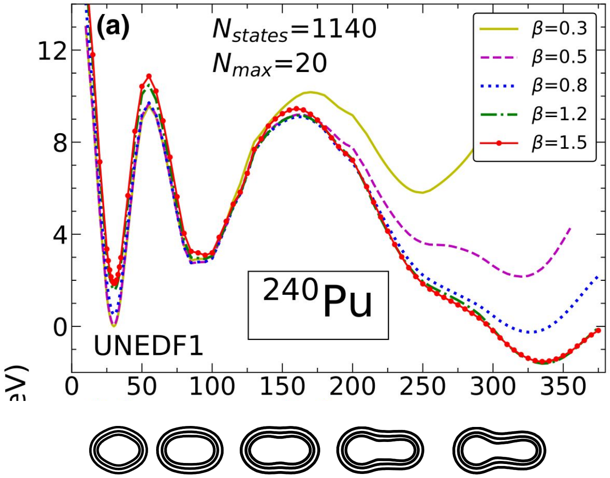


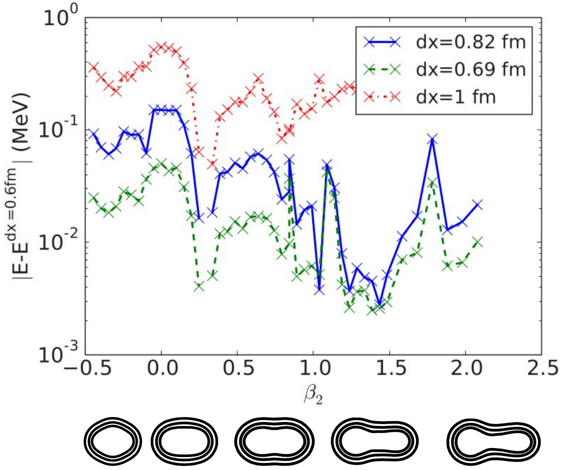


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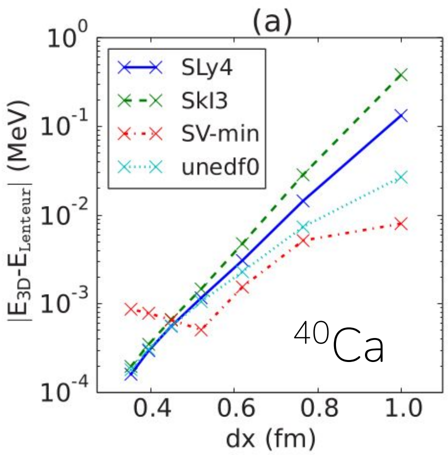


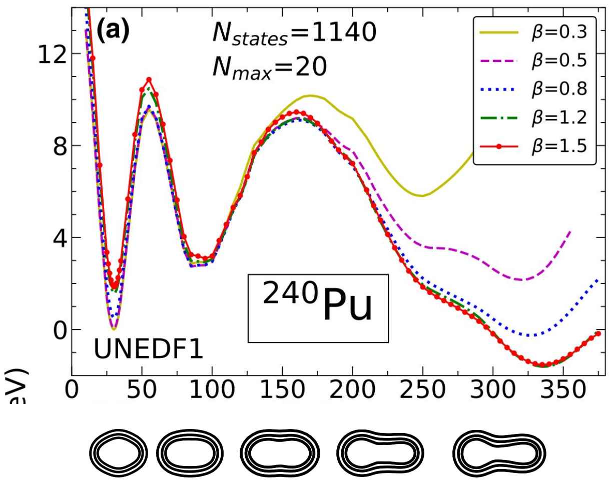


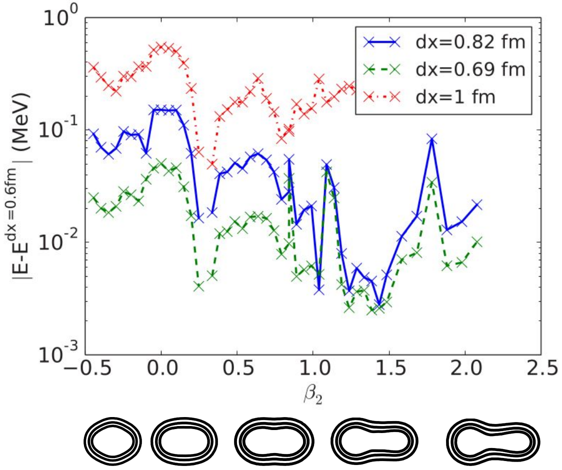


## Mesh (dis)advantages

- ✅ discretisation error: easily controllable, interpretable
- ✅ geometry agnostic: error = shape-independent
- ✅ often easy to code, particularly in 3D
- ❌ computation of exchange terms
  - ➢ “forced” to use zero-range EDFs

$$E_{\mathrm{dir}}=\frac{1}{2}\int\int d^3r d^3r'\,\rho(\mathbf{r},\mathbf{r})v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\mathbf{r}'),$$

$$E_{\mathrm{ex}}=\frac{1}{2}\int\int d^3r d^3r'\,\rho(\mathbf{r},\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\mathbf{r}).$$

# Static calculations on 3D meshes

# Dedicated solution techniques

$$[h(\rho), \rho] = i\frac{\partial \rho}{\partial t}$$

**Basis expansion**

**Coordinate space**

# Dedicated solution techniques

$$[h(\rho), \rho] = 0$$

**Basis expansion**

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$$[h(\rho), \rho] = 0$$

= repeated diagonalisation problem of dimension $N_{basis}$

**Basis expansion**

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**Basis expansion**

- exceptional basis selection
  $N_{basis} \approx 20k \sim N^3_{shell}$

**Coordinate space**

- 'smallish' mesh with 32 points in X/Y/Z
  $N_{basis} = 8 * N^3_{mesh} \approx 262k$

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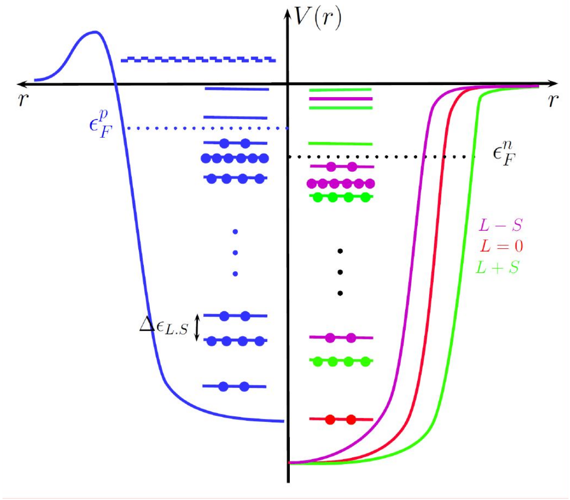


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**Coordinate space**

- ‘smallish’ mesh with 32 points in X/Y/Z
  $N_{basis} = 8 * N^3_{mesh} \approx 262k$
- makes brute force not competitive and memory a concern
- store/solve lowest eigenstates only

# A history of 3D mesh applications

**'76:** Cusson et al.: first static calculations, initialising TD calculations

**'79:** Flocard @ Orsay - Paul Bonche @ CEA

**'80:** Davies: dedicated solution method

**'84:** Heenen & Baye: angular momentum projection

**'85:** Bonche et al. : first use of complete Skyrme interaction

**'94:** Gall et al.: Hartree-Fock-Bogoliubov rendered feasible

**'98:** Matsuse: first use of finite-range Gogny EDF

**'99:** Rutz et al.: first use of relativistic EDFs

**'02:** Magierski & Heenen: first neutron star crust calculations

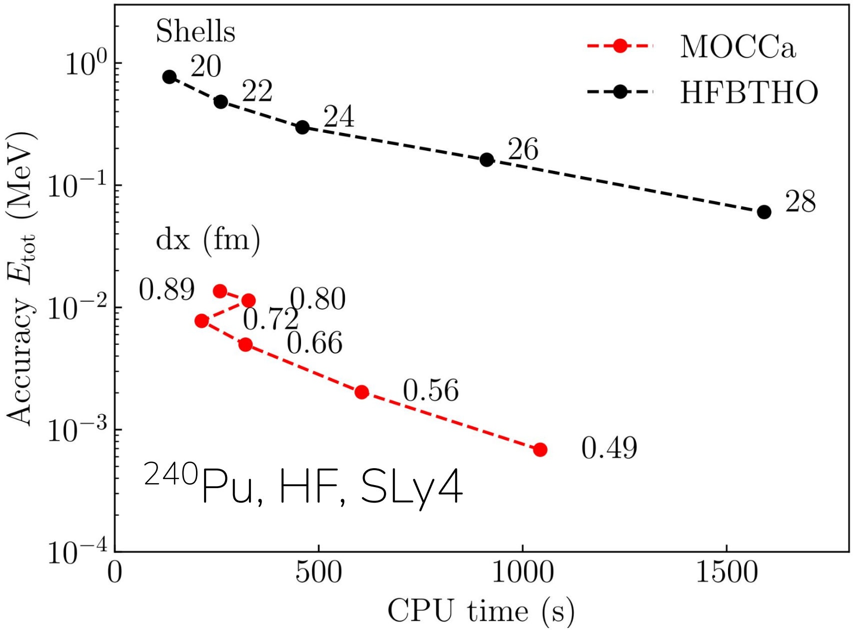
**'03:** Imagawa & Hashimoto: first solution of the linear response equations

**'05:** EV8: first public static code

**'08:** Bulgac & Roche: first full diagonalisation with CPUs

**'16:** S. Yin et al.: leveraging GPU's on large meshes

# CPU & accuracy




## HFBTHO

P. Marevic et al., CPC **267** (2022).

- 2D harmonic oscillator expansion
- default settings
- single CPU
- ULB cluster

## MOCCa

W. Ryssens et al., EPJA **55** (2019).

- 3D Lagrange mesh representation
- default settings
- single CPU
- ULB cluster

# **B**russels-**Sk**yrme-on-a-**G**rid: BSkG

**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).

## BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

| Rms $\sigma$ | BSkG1 | BSkG2 | BSkG3 | BSkG4 |
|---|---|---|---|---|
| Masses [MeV] | 0.741 | | | |
| $S_n$ [MeV] | 0.466 | | | |
| Radii [fm] | 0.024 | | | |
| Prim. barriers [MeV] | | | | |
| Sec. barriers [MeV] | | | | |
| Fission isomers [MeV] | | | | |
| Max. NS mass [$M_\odot$] | | | | |

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|---|---|---|---|---|
| Masses [MeV] | 0.741 | 0.678 | | |
| $S_n$ [MeV] | 0.466 | 0.500 | | |
| Radii [fm] | 0.024 | 0.027 | | |
| Prim. barriers [MeV] | 0.88 | 0.44 | | |
| Sec. barriers [MeV] | 0.87 | 0.47 | | |
| Fission isomers [MeV] | 1.0 | 0.49 | | |
| Max. NS mass [$M_\odot$] | | | | |

## BSkG2

- fit to 45 reference fission barriers
  + 28 fission isomers
- complete time-reversal breaking

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**BSkG1:** G. Scamps et al., EPJA **57**, 333 (2021).
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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).

## BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

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

## BSkG2

- <u>**complete**</u> time-reversal breaking
- fit to 45 reference fission barriers
  + 28 fission isomers

## BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

# **B**russels-**Sk**yrme-on-a-**G**rid: BSkG

**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., EPJA **61,** 35 (2024).

## BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

## BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

| Rms $\sigma$ | 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 |

## BSkG2

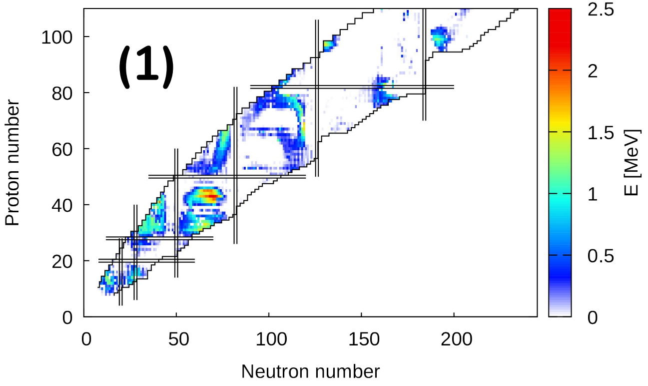
- complete time-reversal breaking
- fit to 45 reference fission barriers + 28 fission isomers

## BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

# Example: static approach to nuclear structure

W. Ryssens et al., PRC 99 (2019).
G. Scamps et al., EPJA **57**, 333 (2021).
W. Ryssens et al., EPJA **58**, 246 (2022).
B. Maass et al. arXiv 2503.07841 (2025).




## The 3D nature of nuclei

1. impacts masses / binding energies

# Example: static approach to nuclear structure

W. Ryssens et al., PRC 99 (2019).
G. Scamps et al., EPJA **57**, 333 (2021).
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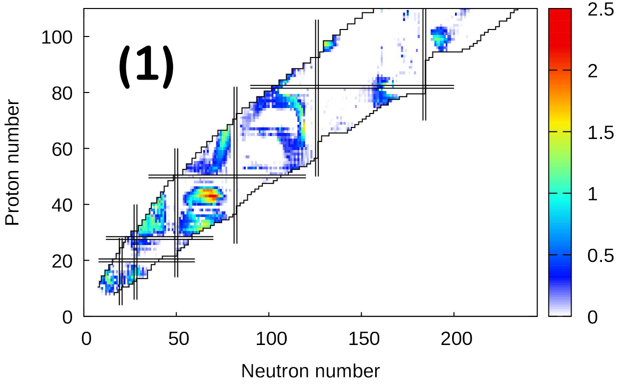


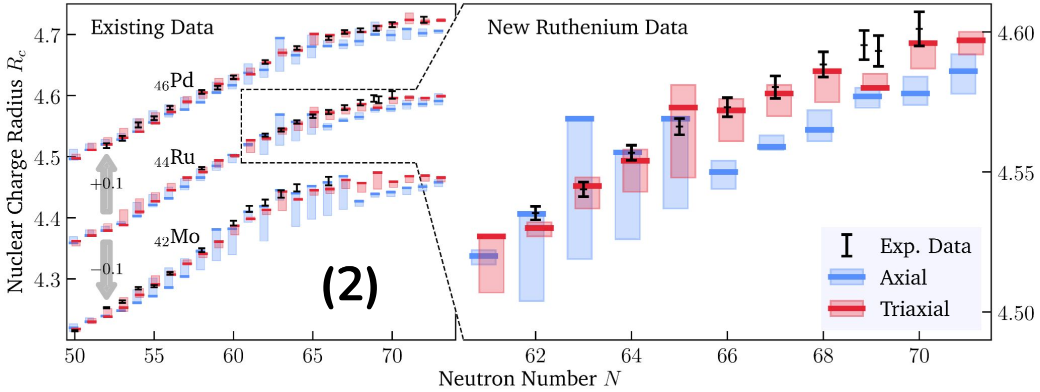


## The 3D nature of nuclei

1. impacts masses / binding energies
2. impacts charge radii

# Example: static approach to nuclear structure

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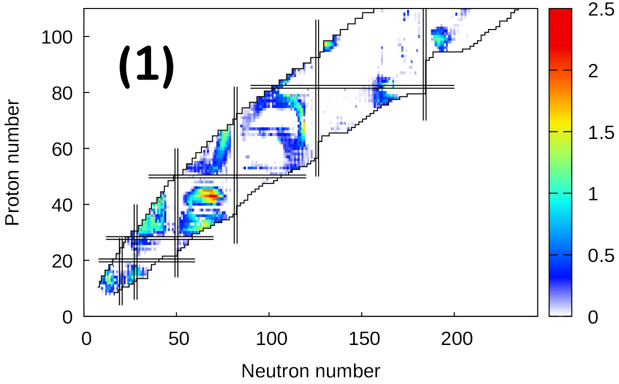
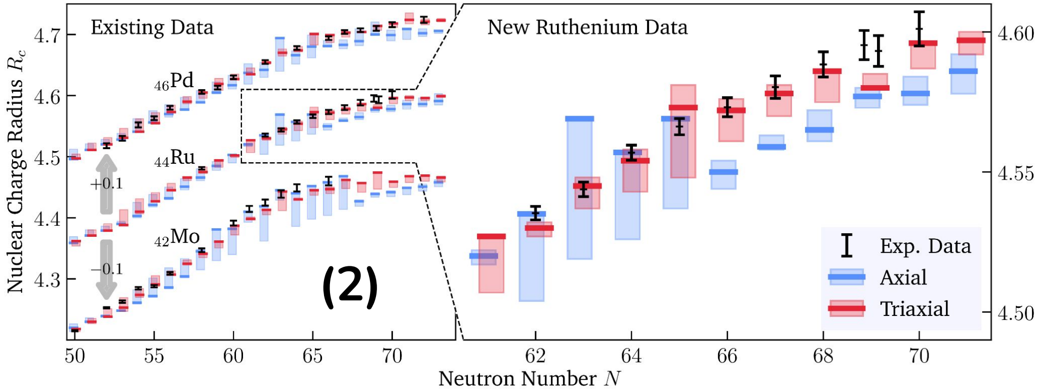
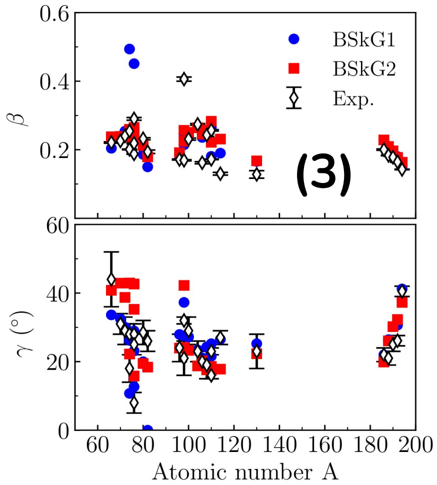



## The 3D nature of nuclei

1. impacts masses / binding energies
2. impacts charge radii
3. is visible in experiment directly



# Example: static approach to nuclear structure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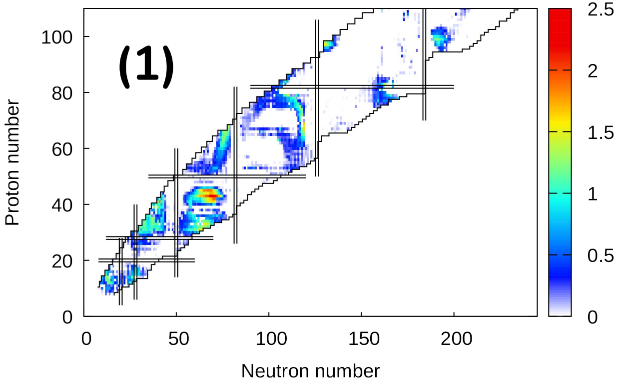
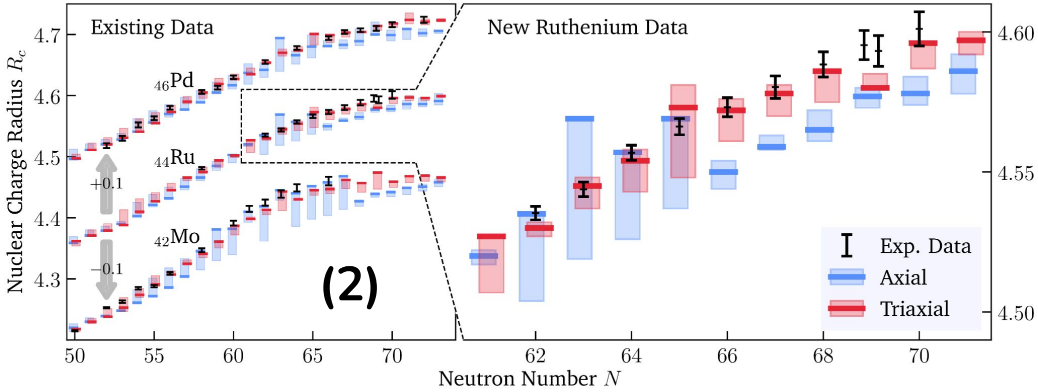
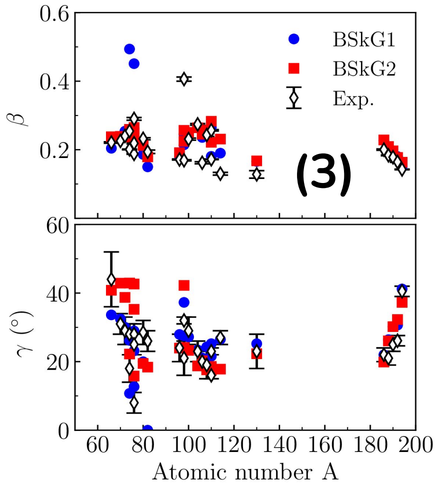
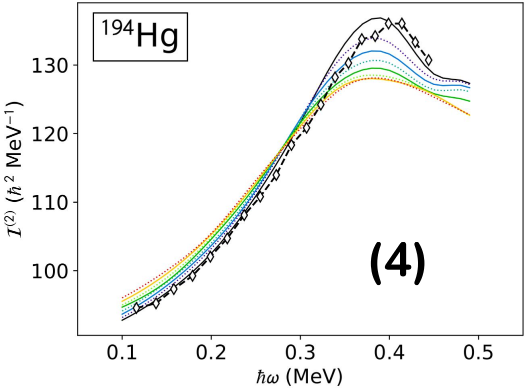


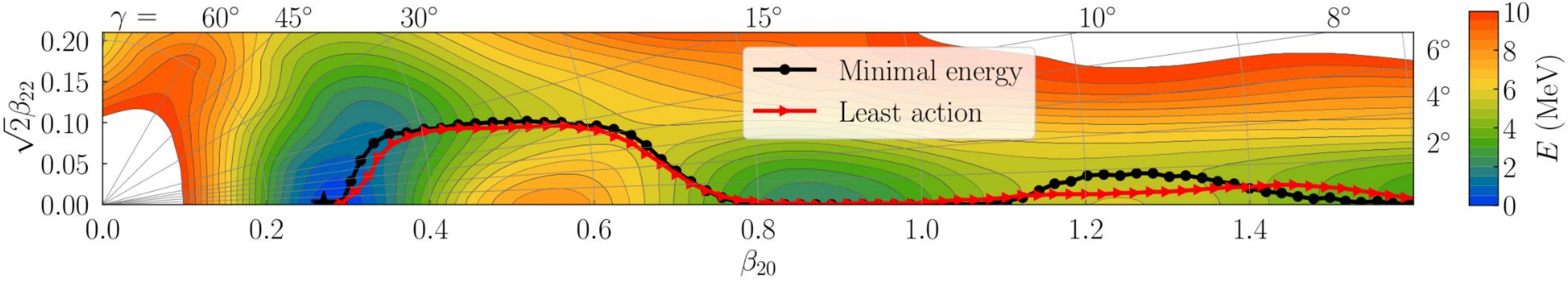

## The 3D nature of nuclei

1. impacts masses / binding energies
2. impacts charge radii
3. is visible in experiment directly
4. is required to study e.g. rotational bands

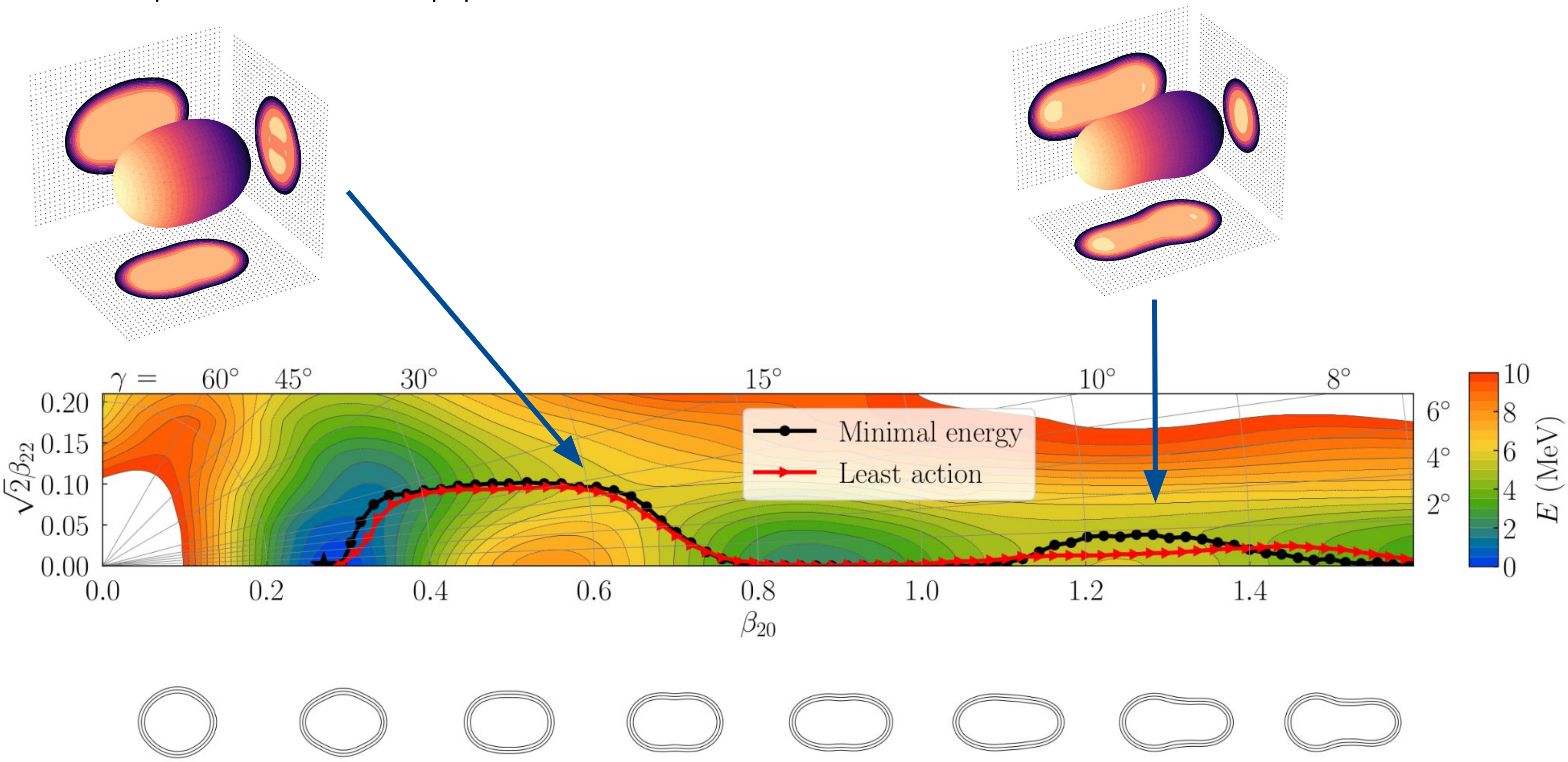


# Example: static approach to fission




# Example: static approach to fission



# Example: static approach to nuclear pasta

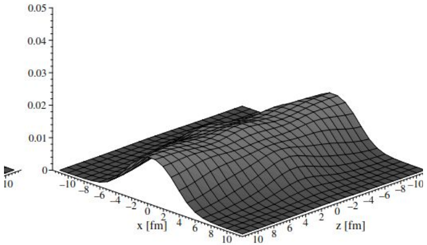
**2002**
~600 nucleons
~(20 fm)$^3$

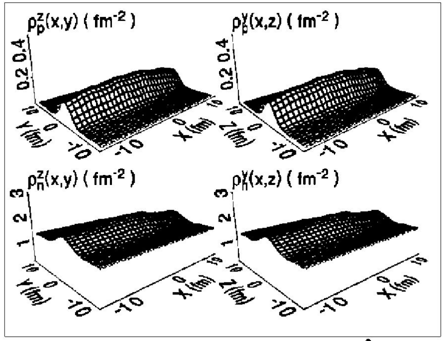
**2007**
~600 nucleons
~(20 fm)$^3$

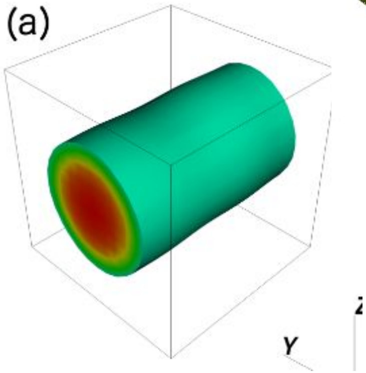
**2015**
~1500 nucleons
~(26 fm)$^3$

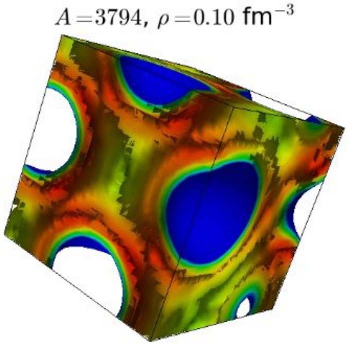
**2017**
~4000 nucleons
~(33 fm)$^3$

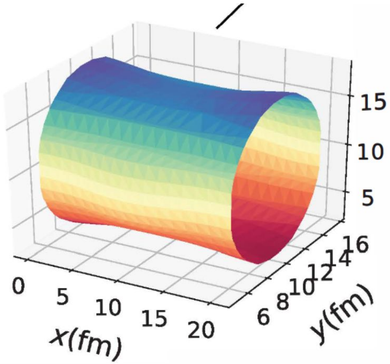
**2021**
~1200 nucleons
~20 fm$^3$



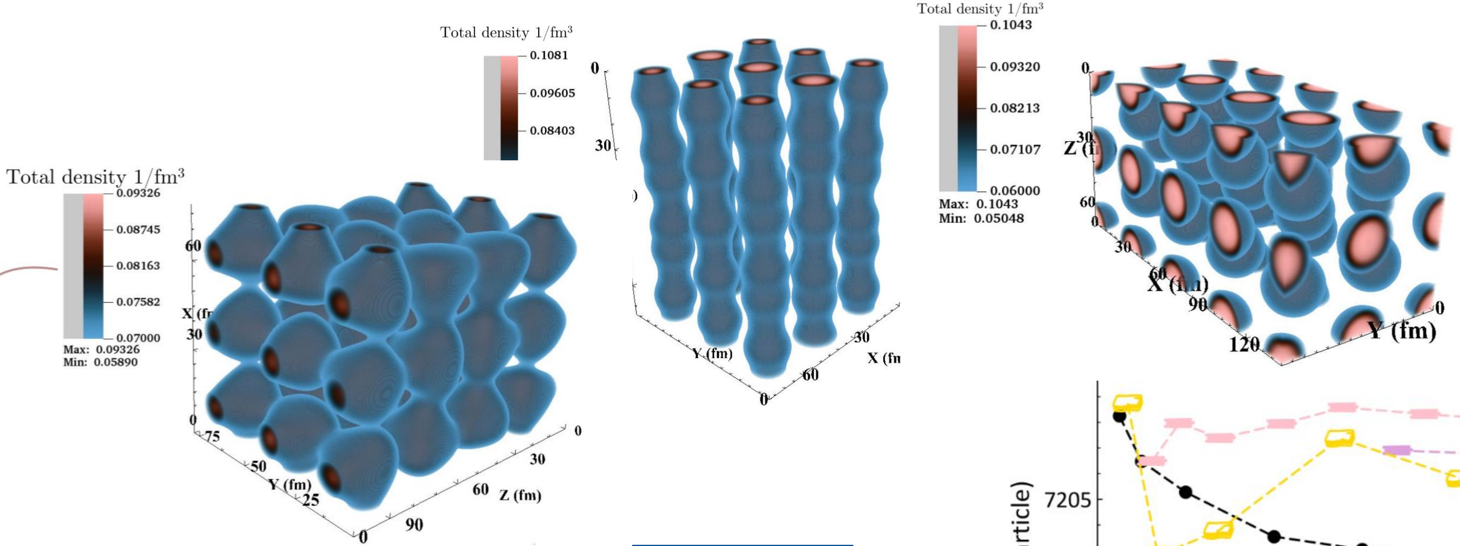



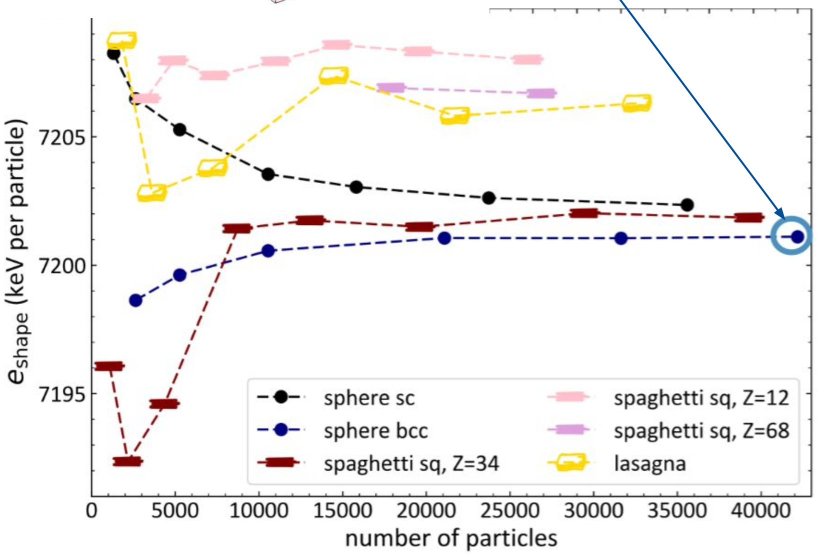


P. Magierski & P.-H. Heenen, PRC **65** (2002).
P. Gögelein & H. Müther, PRC **76** (2007).
B. Schuetrumpf & W. Nazarewicz, PRC **92** (2015).
Fattoyev et al., PRC **95** (2017).
W. Newton et al., PRC **105**(2021).

# Example: static approach to nuclear pasta

Figures courtesy of N. Shchechilin






- $10^6$ $fm^3$ volume, up to 50000 particles
- hundreds of thousands of CPU hours
- necessary to beat finite box-size effects
- manageable because of EU HPCs!