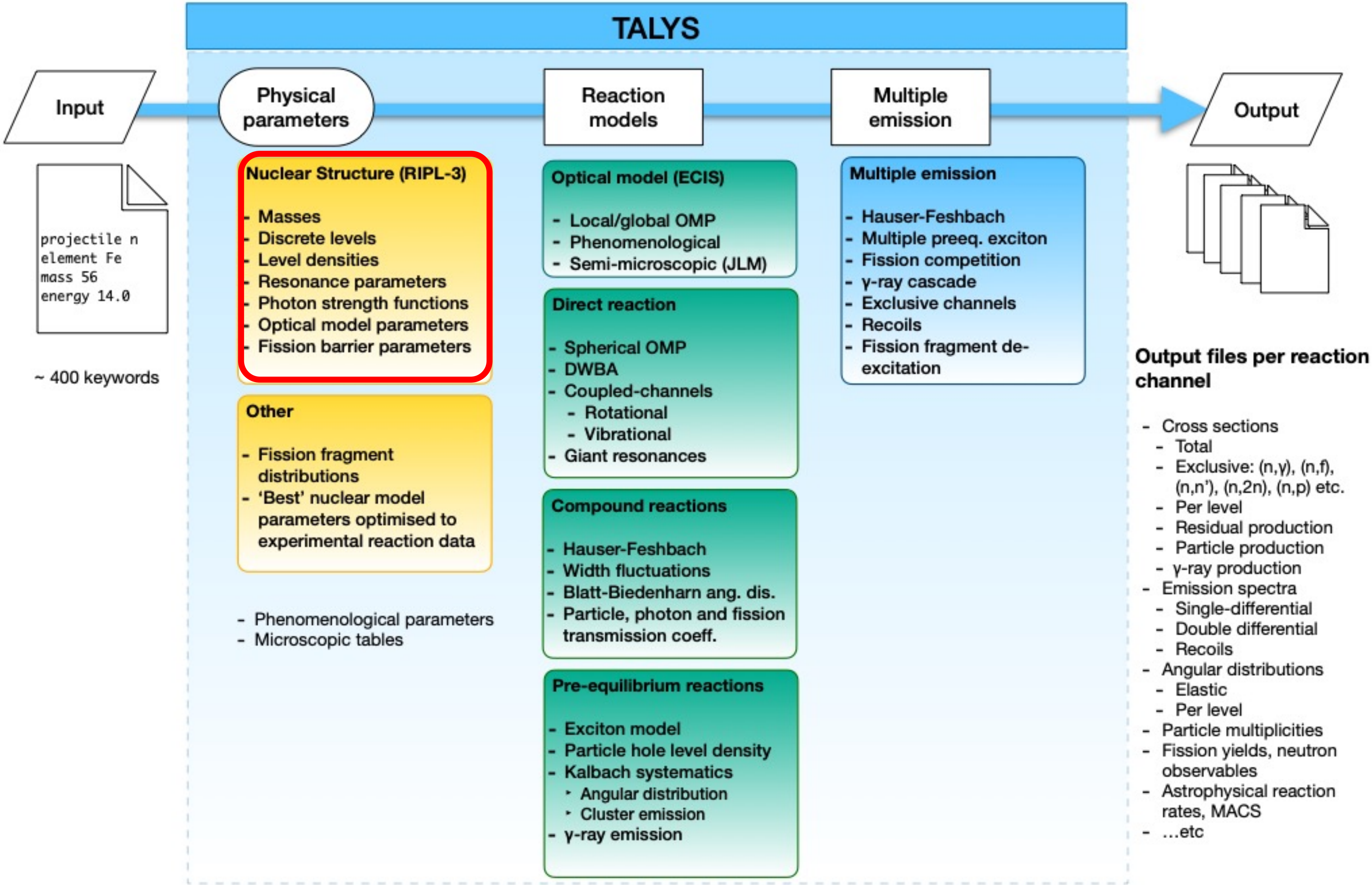
Nuclear Structure Ingredients for reaction models

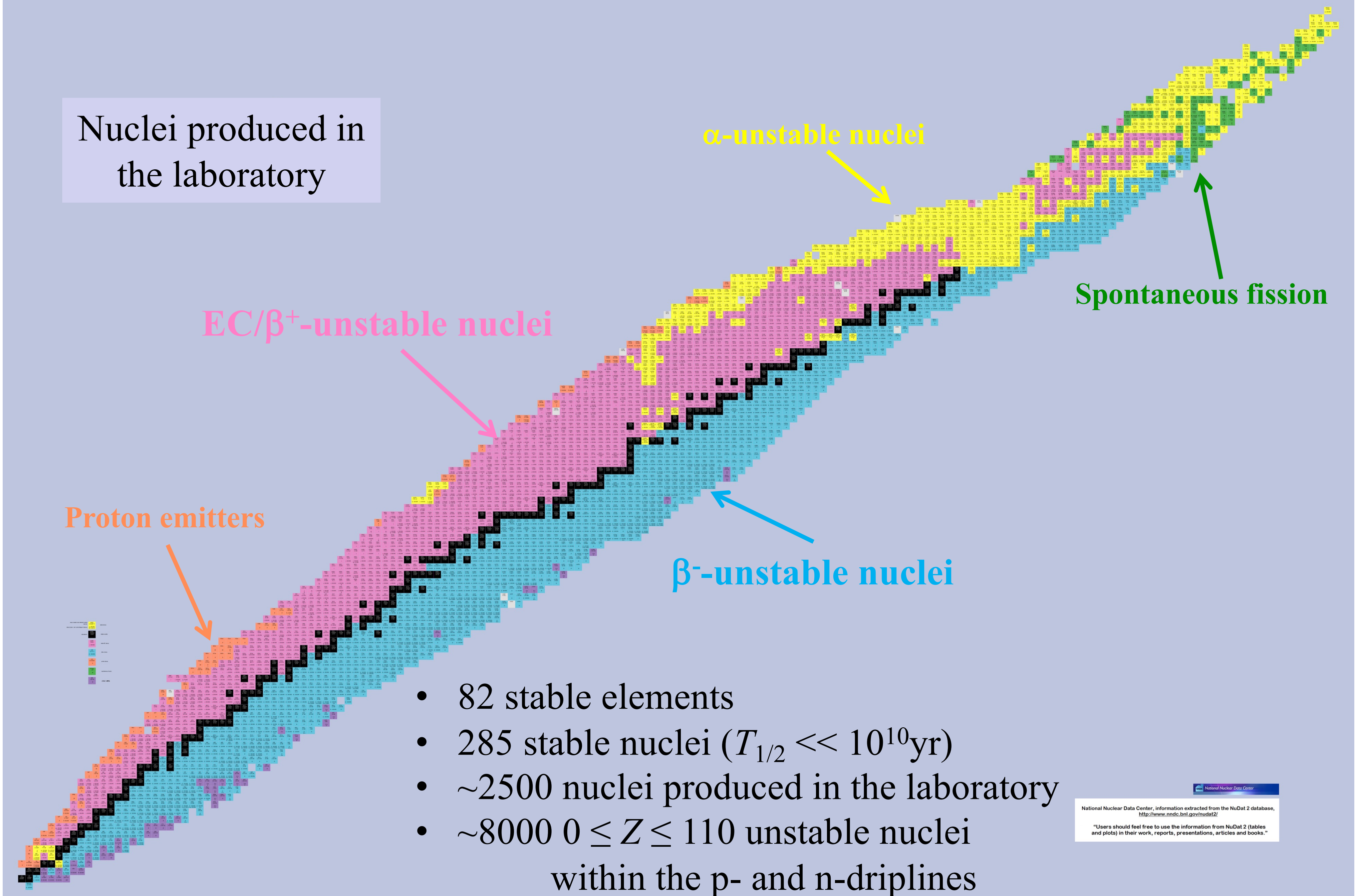
Lecture 1

- Nuclear ingredients for reaction models
    - Models available
    - Masses and their importance
- Masses of nuclei
    - Experimental masses
    - Mass models
        - Liquid-drop models
        - Mean-field models

TALYS code scheme

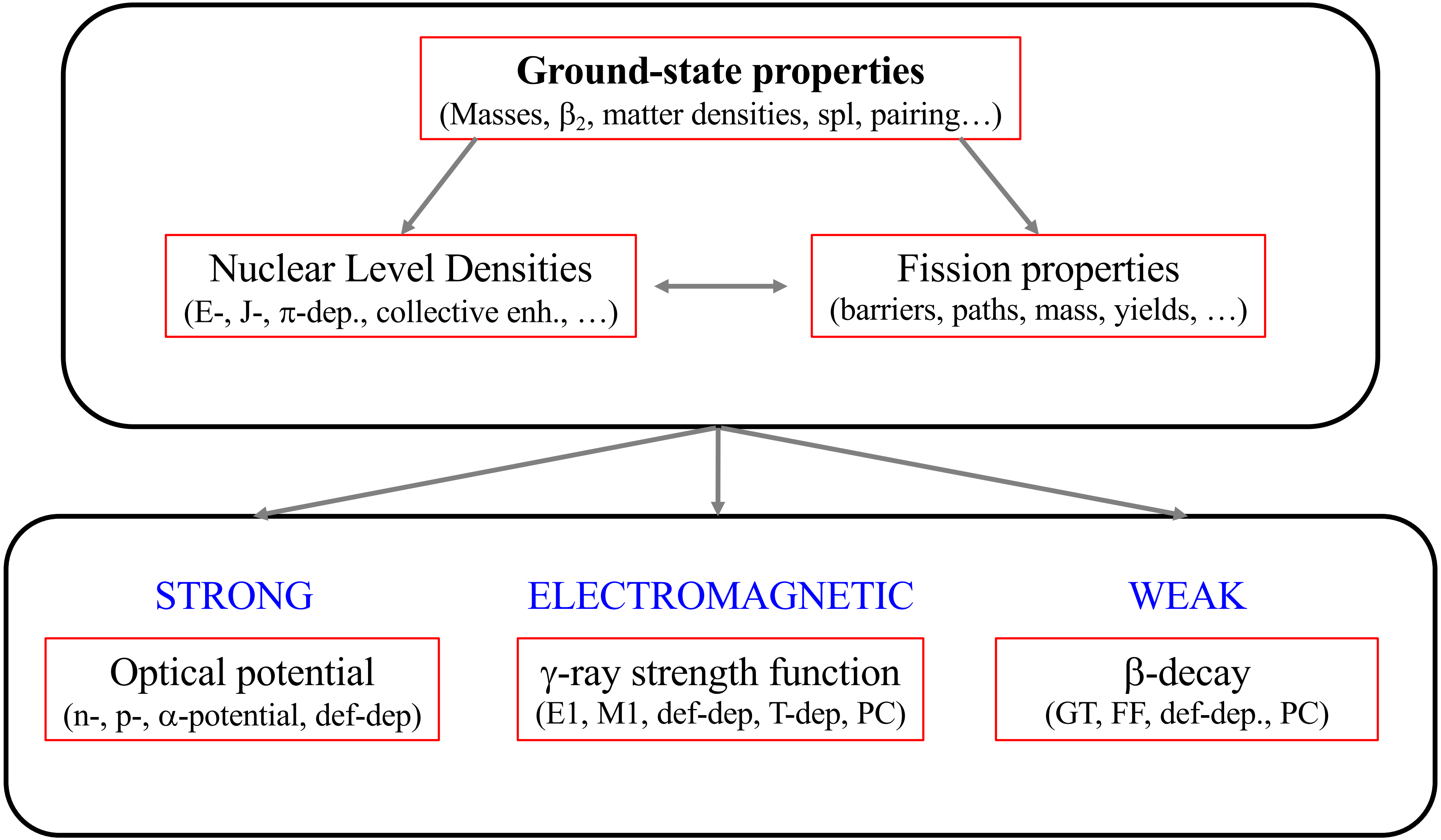


Nuclei produced in the laboratory



- 82 stable elements
- 285 stable nuclei ($T_{1/2} << 10^{10}$yr)
- ~2500 nuclei produced in the laboratory
- ~8000 $0 \leq Z \leq 110$ unstable nuclei within the p- and n-driplines

Nuclear inputs to nuclear reaction codes (e.g TALYS)



Experimental data or Constraints from measurements

Ground-state properties
(Masses, β_2, matter densities, spl, pairing…)

Masses, radii, Q_2, J^π, ...

Nuclear Level Densities
(E-, J-, π-dep., collective enh., …)

n-spacings (D_0,D_1), level scheme

Fission properties
(barriers, paths, mass, yields, …)

Barriers, width, σ_f, T_{sf}…

STRONG

Optical potential
(n-, p-, α-potential, def-dep)

S_0 n-strength
Reaction/Differential xs

ELECTROMAGNETIC

γ-ray strength function
(E1, M1, def-dep, T-dep, PC)

(γ,abs), (γ,n), …
(γ,γ'), Oslo, $<\Gamma_\gamma>$, …

WEAK

β-decay
(GT, FF, def-dep., PC)

β^-, β^+ half-lives,
GT, $P_{\beta dn}$,$P_{\beta df}$

→ cf Lecture of Stephan Pomp

RIPL-2

RIPL-2
Reference Input Parameter Library

Related links: NDS-home CD-ROMs RIPL-1 ENSDF NuDat EMPIRE-II

Coordinated by the IAEA Nuclear Data Section

CONTENTS

Release Date: April 20, 2003

RIPL-2 library contains input parameters for theoretical calculations of nuclear reactions involving light particles such as n, p, d, t, 3-He, 4-He, and gammas at incident energies up to about 100 MeV. The library contains **nuclear masses, deformations, matter densities, discrete levels and decay schemes, spacings of neutron resonances, optical model potentials, level density parameters, Giant Resonance parameters, gamma-ray strength-functions, and fission barriers**. It also includes extensive database of level densities, gamma-ray strength-functions and fission barriers calculated with microscopic approaches. Several computer codes are provided in order to facilitate use of the library.

RIPL-2 has been developed under an international project coordinated by the IAEA Nuclear Data Section as a continuation of the RIPL-1 project concluded in1997. The original scope of RIPL-2 was to test and validate RIPL-1 database. In the course of work most of the recommended files were extended and many new were added. On the other hand, a number of so called 'other' files from RIPL-1 are not included in RIPL-2. Testing of these files was not at the level typical for the RIPL-2 files but they may still be a valuable source of additional information. Therefore, RIPL-1 remains available although use of the RIPL-2 data is generally recommended.

RIPL-2 data are organized into segments, which can be accessed through the **Contents of RIPL-2** or through the navigation bar on the left. The **(ftp)** links next to segment names provide direct (ftp-like) access to the RIPL-2 directories. Entire segments (tarred and gzipped) can be downloaded by clicking on a file with a proper segment name and .tgz extension (e.g., masses.tgz). These files are placed in their respective RIPL-2 directories.

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Etc ….

RIPL-3

International Atomic Energy Agency
Nuclear Data Services
Section Données Nucléaires, AIEA

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Archive
- RIPL-1
- RIPL-2
- CRP (RIPL-3)

Related Links
- Nuclear Data Services
- Nuclear Data on CD's
- ENSDF
- NuDat
- EMPIRE-II
- Nuclear Data Sheets

Reference Input Parameter Library (RIPL-3)

R. Capote, M. Herman, P. Oblozinsky, P.G. Young, S. Goriely, T. Belgya, A.V. Ignatyuk, A.J. Koning, S. Hilaire, V.A. Plujko, M. Avrigeanu, O. Bersillon, M.B. Chadwick, T. Fukahori, Zhigang Ge, Yinlu Han, S. Kailas, J. Kopecky, V.M. Maslov, G. Reffo, M. Sin, E.Sh. Soukhovitskii and P. Talou

Nuclear Data Sheets - Volume 110, Issue 12, December 2009, Pages 3107-3214

RIPL discrete levels database updated in August 2015 - it contains the correction for +X,.. levels

Documents
- RIPL-2 Handbook
- Ducuments listing (ftp)

Segments (ftp)
- MASSES (ftp)
- LEVELS (ftp)
- RESONANCES (ftp)
- OPTICAL (ftp)
- DENSITIES (ftp)
- GAMMA (ftp)
- FISSION (ftp)
- CODES (ftp)

Introduction | MASSES | LEVELS | RESONANCES | OPTICAL | DENSITIES | GAMMA | FISSION | CODES | Contacts

Introduction

We describe the physics and data included in the Reference Input Parameter Library, which is devoted to input parameters needed in calculations of nuclear reactions and nuclear data evaluations. Advanced modelling codes require substantial numerical input, therefore the International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of validated nuclear-model input parameters, referred to as the Reference Input Parameter Library (RIPL). A final RIPL coordinated research project (RIPL-3) was brought to a successful conclusion in December 2008, after 15 years of challenging work carried out through three consecutive IAEA projects. The RIPL-3 library was released in January 2009, and is available on the Web through *http://www-nds.iaea.org/RIPL-3/*. This work and the resulting database are extremely important to theoreticians involved in the development and use of nuclear reaction modelling (ALICE, EMPIRE, GNASH, UNF, TALYS) both for theoretical research and nuclear data evaluations.

The numerical data and computer codes included in RIPL-3 are arranged in seven segments: **MASSES** contains ground-state properties of nuclei for about 9000 nuclei, including three theoretical predictions of masses and the evaluated experimental masses of Audi *et al.* (2003). **DISCRETE LEVELS** contains 118 datasets (Z from 0 to 117) with all known level schemes, electromagnetic and γ-ray decay probabilities available from ENSDF in April 2014. **NEUTRON RESONANCES** contains average resonance parameters prepared on the basis of the evaluations performed by Ignatyuk and Mughabghab. **OPTICAL MODEL** contains 495 sets of phenomenological optical model parameters defined in a wide energy range. When there are insufficient experimental data, the evaluator has to resort to either global parameterizations or microscopic approaches. Radial density distributions to be used as input for microscopic calculations are stored in the MASSES segment. **LEVEL DENSITIES** contains phenomenological parameterizations based on the modified Fermi gas and superfluid models and microscopic calculations which are based on a realistic microscopic single-particle level scheme. Partial level densities formulae are also recommended. All tabulated total level densities are consistent with both the recommended average neutron resonance parameters and discrete levels. **GAMMA** contains parameters that quantify giant resonances, experimental gamma-ray strength functions and methods for calculating gamma emission in statistical model codes. The experimental GDR parameters are represented by Lorentzian fits to the photo-absorption cross sections for 102 nuclides ranging from ^{51}V to ^{239}Pu. **FISSION** includes global prescriptions for fission barriers and nuclear level densities at fission saddle points based on microscopic HFB calculations constrained by experimental fission cross sections.

RIPL-2/3

MASSES – (ftp)
– Mass Excess
– GS Deformations
– Nucl. Matter Densities

LEVELS – (ftp)
– Level Schemes
– Level Parameters

RESONANCES – (ftp)

OPTICAL – (ftp)
– OM Parameters
– Deform. Parameters
– Codes

DENSITIES – (ftp)
– Total Level Densities
– Single–Particle Levels
– Partial Level Densities

GAMMA – (ftp)
– GDR Parameters
– Exp. Strength–Fun.
– Micro. Strength–Fun.
– Codes
– Plot of GDR Shape

FISSION – (ftp)
– Barriers
– Level Densities

Ground-state properties
- Audi-Wapstra atomic mass evaluation
- Mass formulas including deformation and matter densities

Discrete Level Scheme including J, π, γ-transition and branching
- 2546 nuclear decay schemes
- 115346 levels
- 12956 spins assigned
- 159323 γ-transitions

ENSDF-II

Average Neutron Resonance Parameters
- average spacing of resonances ---> level density at $U=S_n$
- neutron strength function ---> optical model at low energy
- average radiative width ---> γ-ray strength function

Optical Model Potentials from neutron to ^{4}He
- Standard OMP parameters
- Deformation parameters
- E- and A-dependent global models (formulas and codes)

Nuclear Level Densities (formulas, tables and codes)
- Spin- and parity-dependent level density fitted to D_0
- Single-particle level schemes for NLD calculations
- Partial p-h level density

γ-strength function (E1, M1)
- GDR parameters and low-energy E1 & M1 strength
- E1 & M1 strength function (formulas, tables and codes)

Fission parameters
- Fitted fission barriers and corresponding NLD
- Fission barriers (tables and codes)
- NLD at fission saddle points (tables)

Nuclear Applications

Different possible approaches depending on the nuclear applications

PHENOMENOLOGICAL DESCRIPTIONS

ACCURACY
(reproduce exp.data)

Concern of applied physics

New concern of some applications

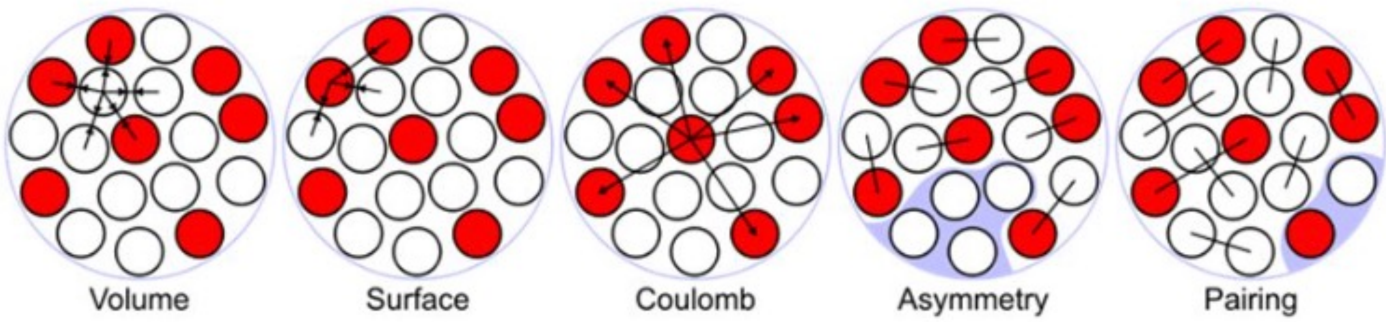
Phenomenological models
(Parametrized formulas, Empirical Fits)
Classical models
(e.g Liquid drop, Droplet)
Semi-classical models
(e.g Thomas - Fermi)
mic-mac models
(e.g Classical with micro corrections)
semi-microscopic
(e.g microscopic models with phenomenological corrections)
fully microscopic
(e.g mean field, shell model, QRPA)

RELIABILITY
(Sound physics)

Concern of fundamental physics

GLOBAL MICROSCOPIC DESCRIPTIONS

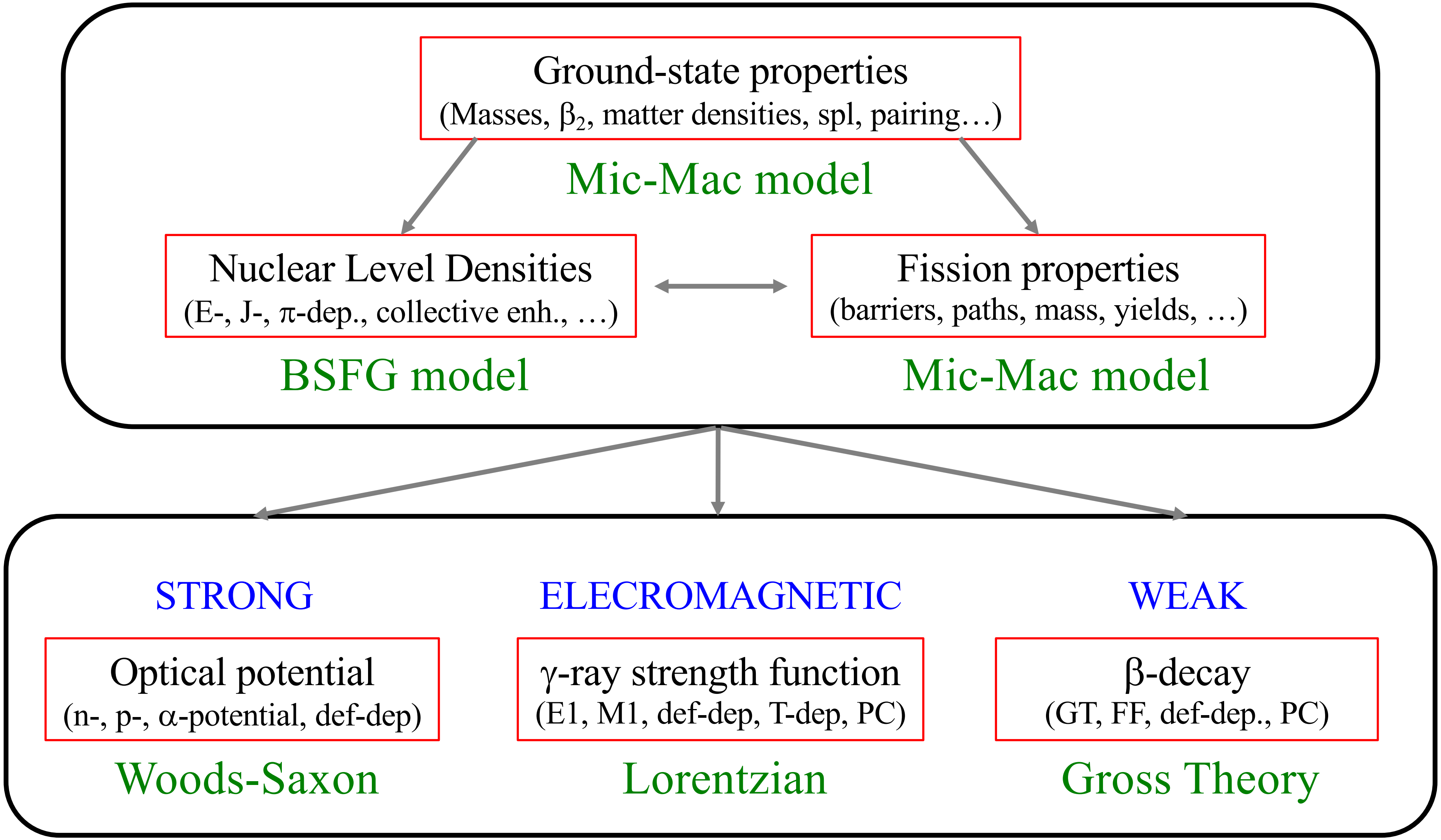
The macroscopic liquid-drop description of the nucleus



$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

Phenomenological description at the level of integrated properties (Volume, Surface, …) with quantum "microscopic" corrections added in a way or another (shell effects, pairing, etc...)

"Macroscopic" Nuclear Inputs

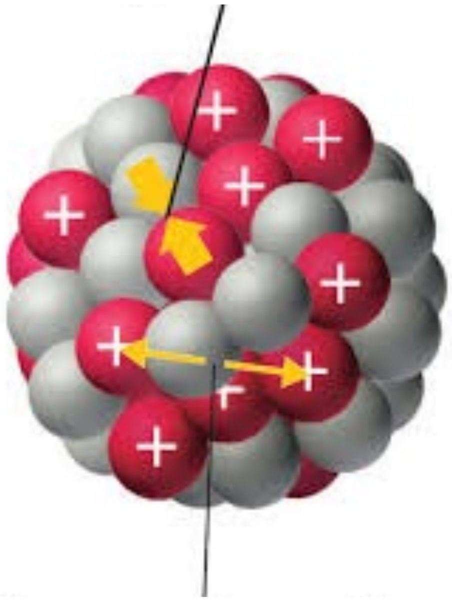


A more « microscopic » description of the nucleus

e.g. Mean-Field

$$E_{MF} = \int \mathcal{E}_{nuc}(\mathbf{r}) d^3\mathbf{r} + \int \mathcal{E}_{coul}(\mathbf{r}) d^3\mathbf{r}$$

Strong nuclear force



Electrostatic repulsion

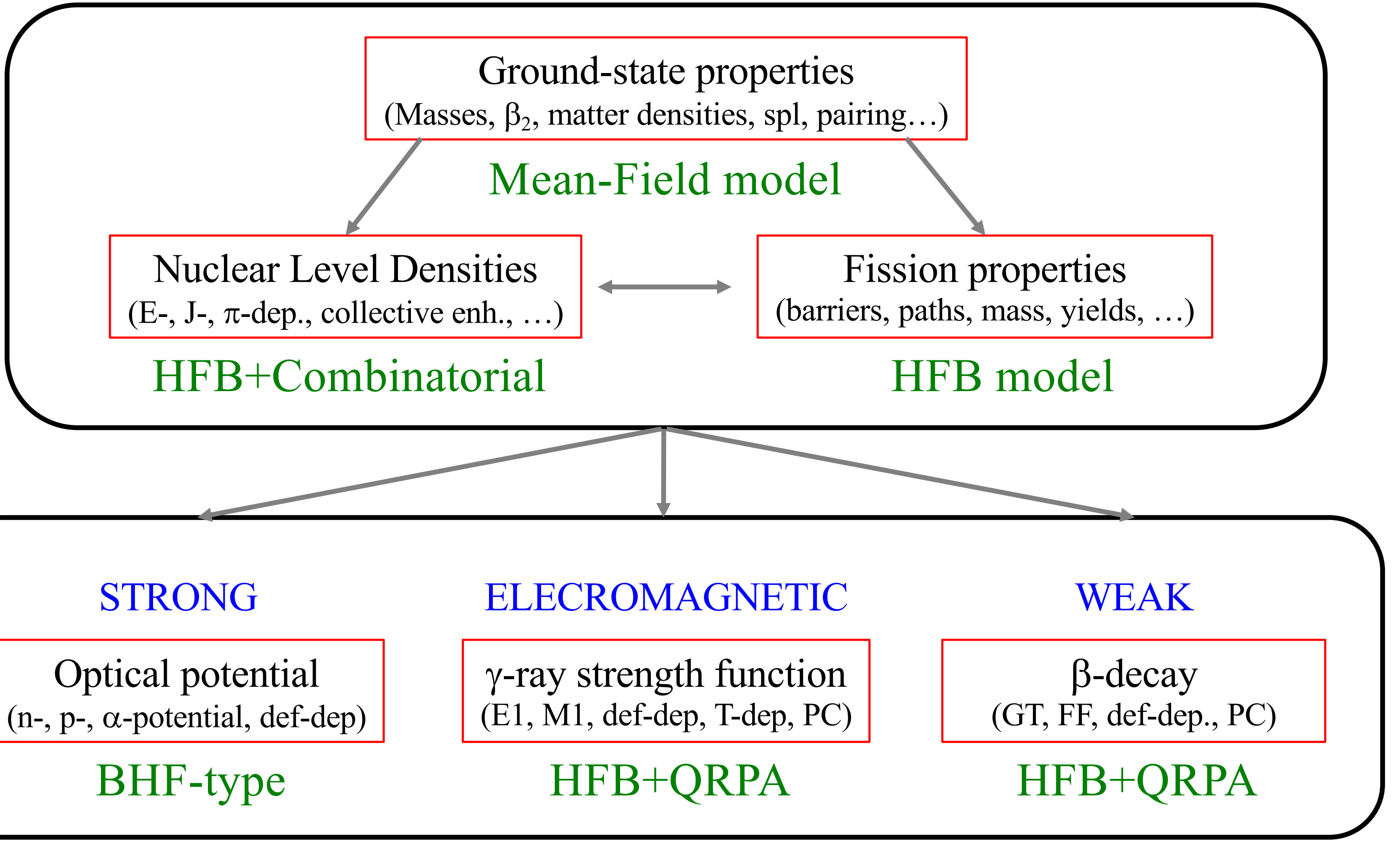
obtained on the basis of an Energy Density Functional generated by an effective n-n interaction !

$$\begin{aligned}
\mathcal{E}_{\rm Sky} = & \sum_{q=n,p} \frac{\hbar^2}{2M_q}\tau_q + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_{q=n,p}\rho_q^2\right] + \frac{1}{4}t_1\left\{\left(1+\frac{1}{2}x_1\right)\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right]\right. \\
& \left. -\left(\frac{1}{2}+x_1\right)\sum_{q=n,p}\left[\rho_q\tau_q + \frac{3}{4}(\nabla\rho_q)^2\right]\right\} + \frac{1}{4}t_2\left\{\left(1+\frac{1}{2}x_2\right)\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right] + \left(\frac{1}{2}+x_2\right)\right. \\
& \left. \times \sum_{q=n,p}\left[\rho_q\tau_q - \frac{1}{4}(\nabla\rho_q)^2\right]\right\} + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{1}{2}x_3\right)\rho^2 - \left(\frac{1}{2}+x_3\right)\sum_{q=n,p}\rho_q^2\right] \\
& + \frac{1}{4}t_4\left\{\left(1+\frac{1}{2}x_4\right)\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right] - \left(\frac{1}{2}+x_4\right)\sum_{q=n,p}\left[\rho_q\tau_q + \frac{3}{4}(\nabla\rho_q)^2\right]\right\}\rho^\beta \\
& + \frac{\beta}{8}t_4\left[\left(1+\frac{1}{2}x_4\right)\rho(\boldsymbol{\nabla}\rho)^2 - \left(\frac{1}{2}+x_4\right)\boldsymbol{\nabla}\rho\cdot\sum_{q=n,p}\rho_q\boldsymbol{\nabla}\rho_q\right]\rho^{\beta-1} + \frac{1}{4}t_5\left\{\left(1+\frac{1}{2}x_5\right)\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right]\right. \\
& \left. + \left(\frac{1}{2}+x_5\right)\sum_{q=n,p}\left[\rho_q\tau_q - \frac{1}{4}(\nabla\rho_q)^2\right]\right\}\rho^\gamma - \frac{1}{16}(t_1x_1+t_2x_2)\,J^2 + \frac{1}{16}(t_1-t_2)\sum_{q=n,p}J_q^2 \\
& - \frac{1}{16}(t_4x_4\rho^\beta + t_5x_5\rho^\gamma)J^2 + \frac{1}{16}(t_4\rho^\beta - t_5\rho^\gamma)\sum_{q=n,p}J_q^2 + \frac{1}{2}W_0\left(\boldsymbol{J}\cdot\boldsymbol{\nabla}\rho + \sum_{q=n,p}\boldsymbol{J}_q\cdot\boldsymbol{\nabla}\rho_q\right).
\end{aligned}$$

Still *phenomenological*, but at the level of the effective n-n interaction

Obviously more complex, but models have now reached stability and **accuracy** !

“Microscopic” Nuclear Inputs



MASSES
&
Nuclear structure properties

Masses of cold nuclei

Nuclear masses, or equivalently binding energies, enter all chapters of applied nuclear physics. Their knowledge is indispensable in order to evaluate the rate and the energetics of any nuclear transformation.

The *nuclear mass* of a nucleus ($Z, A=Z+N$) is defined as

$$M_{\mathrm{nuc}}c^2 = N\,M_n c^2 + Z\,M_p c^2 - B$$

M_p= 938.272 MeV/c^2
M_n= 939.565 MeV/c^2

where M_n is the neutron mass, M_p the proton mass and B the nuclear binding energy (B>0)

The *atomic mass* includes in addition the mass and binding of the Z electrons

$$M_{\mathrm{at}}c^2 = M_{\mathrm{nuc}}c^2 + Z\,M_e c^2 - B_e$$

where M_e is the electron mass, and B_e the atomic binding energy of all the electrons

The number of nucleons ($A=Z+N$) is also conserved by a nuclear reaction. For this reason, the atomic mass M_{at} is usually replaced by the ***mass excess Δm*** defined by

$$\Delta m_{ZA} = \left(M_{\mathrm{at}} - A m_u\right)c^2 = \left[M_{\mathrm{at}}(\mathrm{amu}) - A\right]m_u c^2$$

where m_u is *the atomic mass unit* (amu) defined as 1/12 of the atomic mass of the neutral ^{12}C atom

$$m_u = 1.66\ 10^{27}\ \mathrm{kg} = 931.494\ \mathrm{MeV/c^2}$$

The mass excess is generally expressed in MeV through

$$\Delta m_{ZA} = 931.494\left[M_{\mathrm{at}}(\mathrm{amu}) - A\right]\ \mathrm{MeV}$$

To determine the atomic mass, the nuclear binding energy must be estimated from the nuclear force.

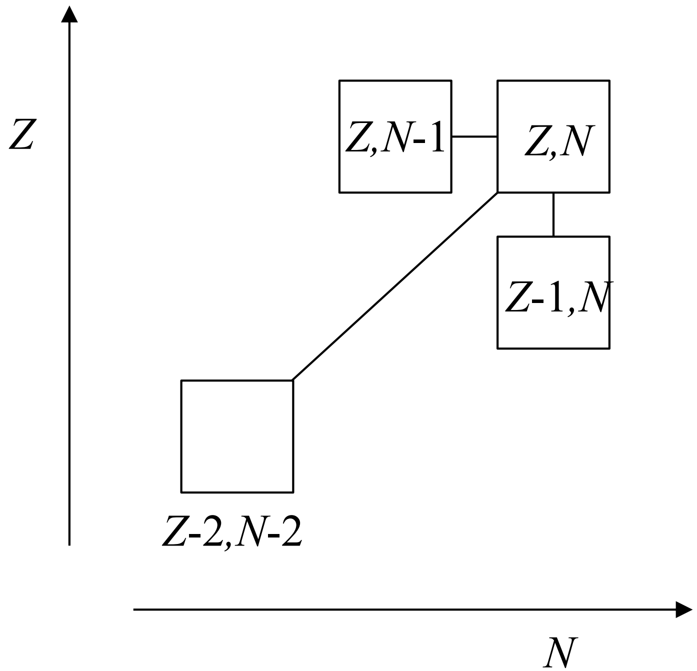
Importance of nuclear masses in the determination of the nuclear stability

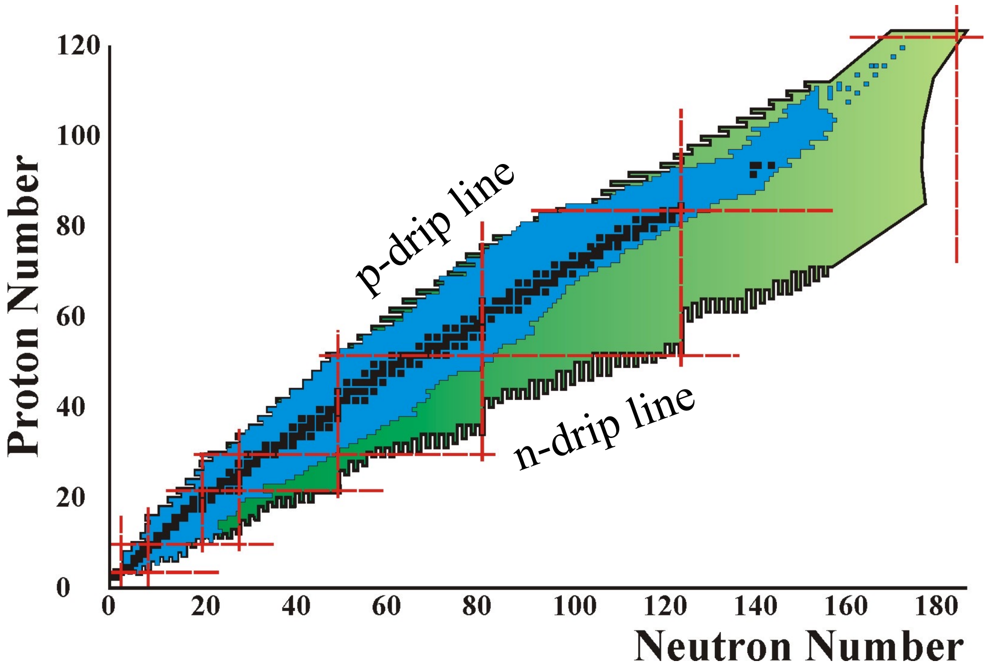
M(Z,N)

$S_n = M(Z,N-1) + M_n - M(Z,N) < 0$ → n-drip line

$S_p = M(Z-1,N) + M_p - M(Z,N) < 0$ → p-drip line

$Q_\alpha = M(Z-2,N-2) + M_\alpha - M(Z,N) < 0$ → α-unstable





β-unstable nuclei

β decay: $p \leftrightarrow n$ conversion within a nucleus via the weak interaction

Modes (for a proton/neutron in a nucleus):

- β^+ decay $\quad p \longrightarrow n + e^+ + \nu_e$
- electron capture $\quad e^- + p \longrightarrow n + \nu_e$

} Favourable for n-deficient nuclei

- β^- decay $\quad n \longrightarrow p + e^- + \bar{\nu}_e$ — Favourable for n-rich nuclei

On earth, only these 3 modes can occur. In particular, electron capture (EC) involves orbital electrons.

Q-values for decay of nucleus *(Z,N)*:

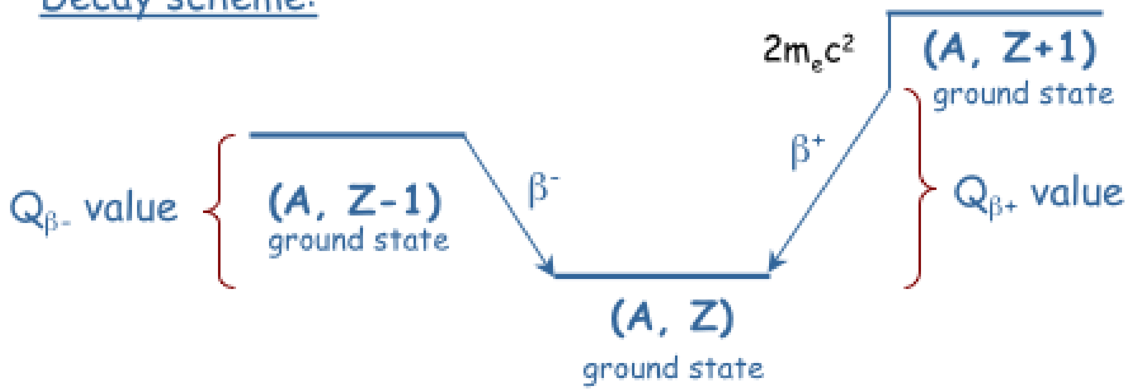
$$Q_{\beta+}/c^2 = M_{nuc}(Z,N) - M_{nuc}(Z\text{-}1,N\text{+}1) - M_e = M_{at}(Z,N) - M_{at}(Z\text{-}1,N\text{+}1) - 2M_e$$

$$Q_{EC}/c^2 = M_{nuc}(Z,N) - M_{nuc}(Z\text{-}1,N\text{+}1) + M_e = M_{at}(Z,N) - M_{at}(Z\text{-}1,N\text{+}1)$$

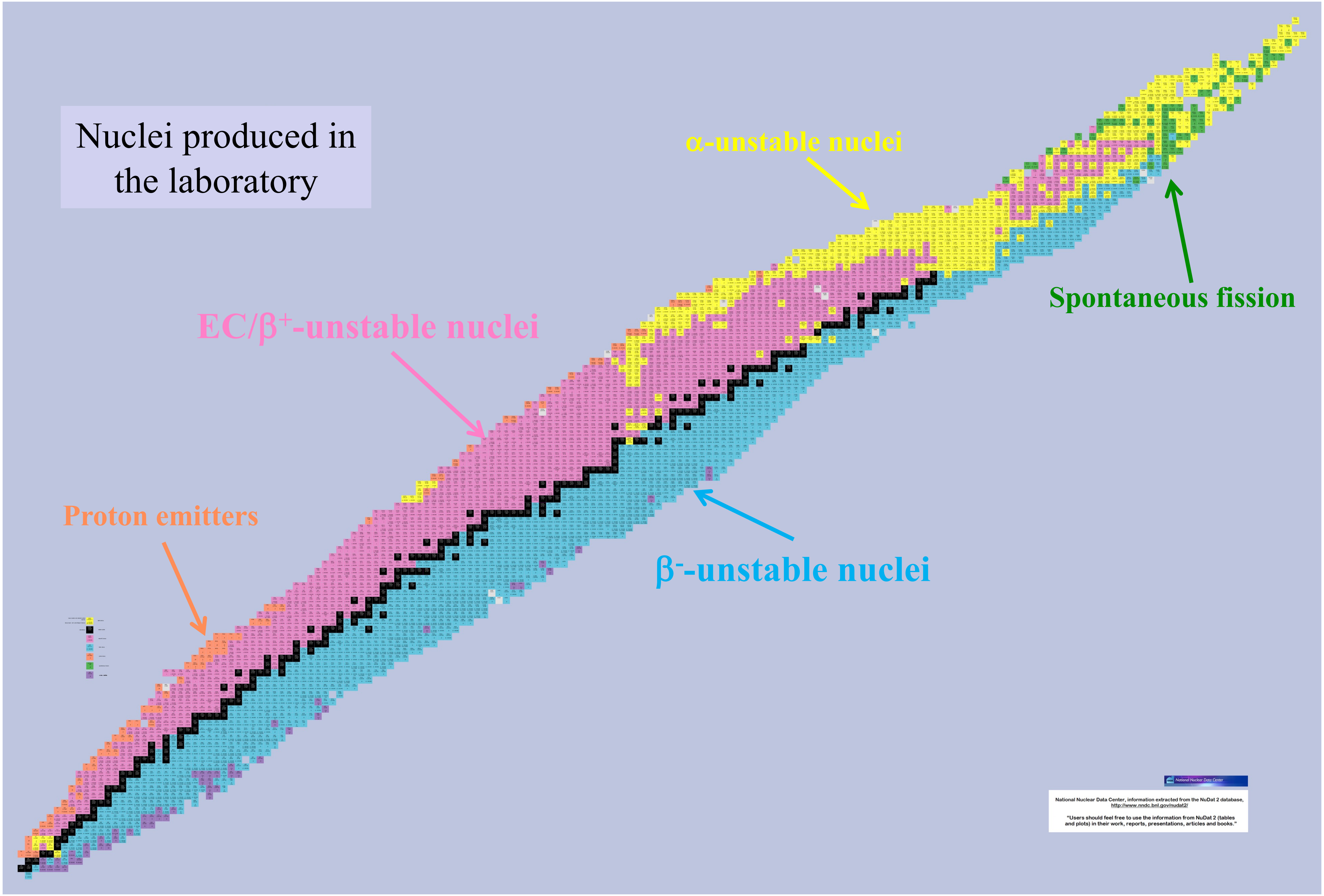
$$Q_{\beta-}/c^2 = M_{nuc}(Z,N) - M_{nuc}(Z\text{+}1,N\text{-}1) - M_e = M_{at}(Z,N) - M_{at}(Z\text{+}1,N\text{-}1)$$

Note: $Q_{EC} = Q_{\beta+} + 2M_ec^2$
$= Q_{\beta+} + 1.022$ MeV

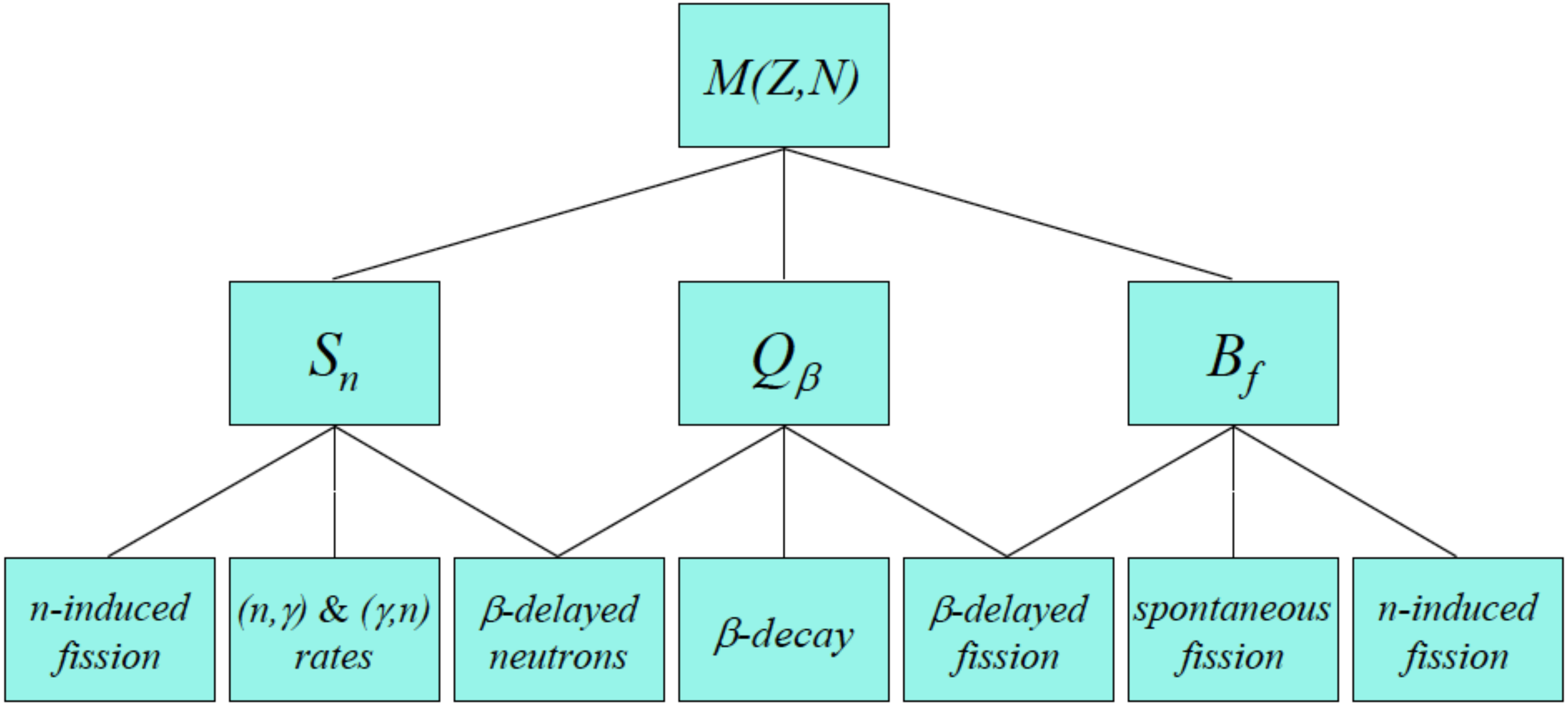
Decay scheme:



Nuclei produced in the laboratory



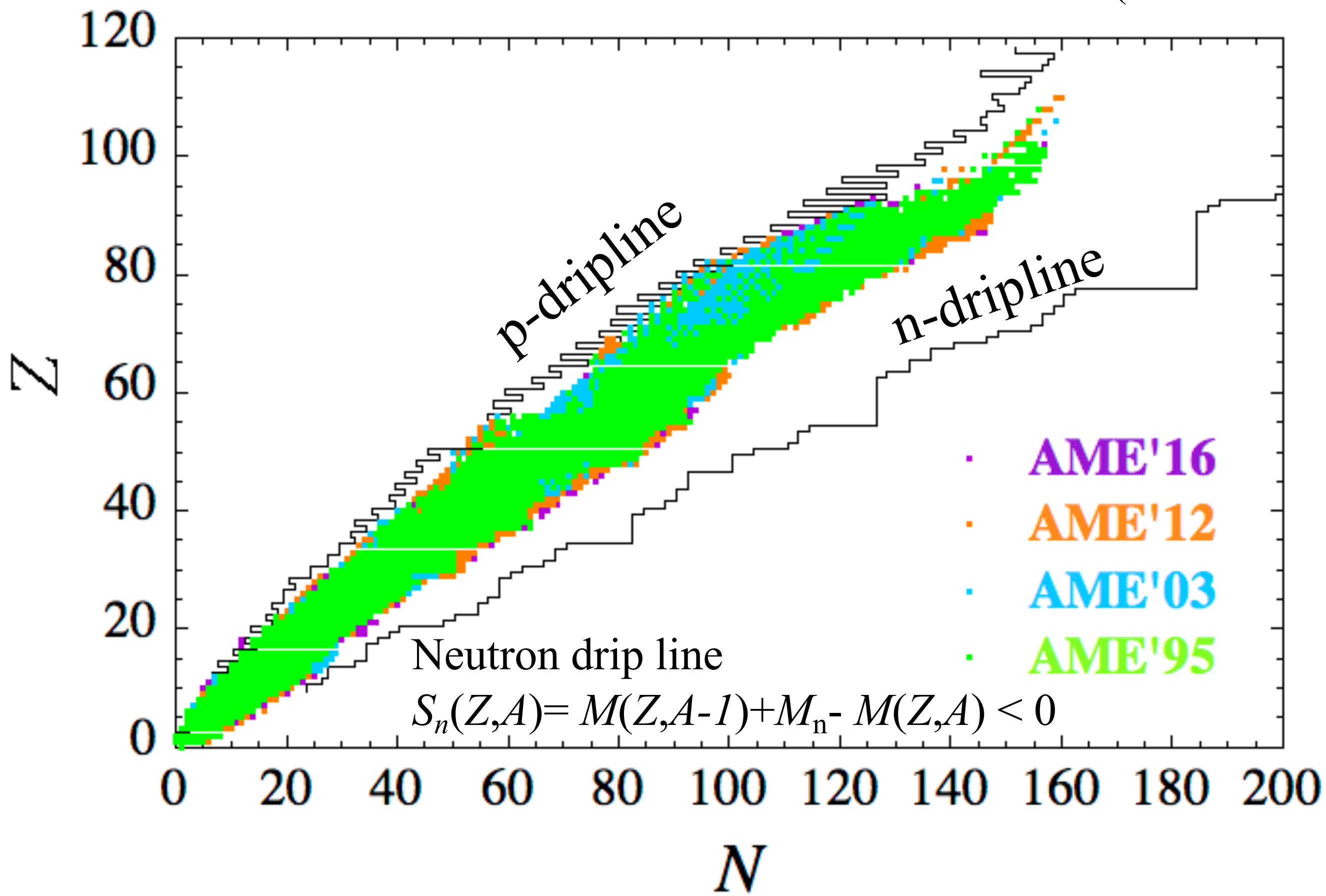
Importance of nuclear masses in the determination of the reaction & decay processes (Q-values)



Experimental masses

About 2550 nuclear masses available *experimentally* (AME2020).
Nuclear (astrophysics) applications require ~ 8000 $0 \le Z \le 110$ masses

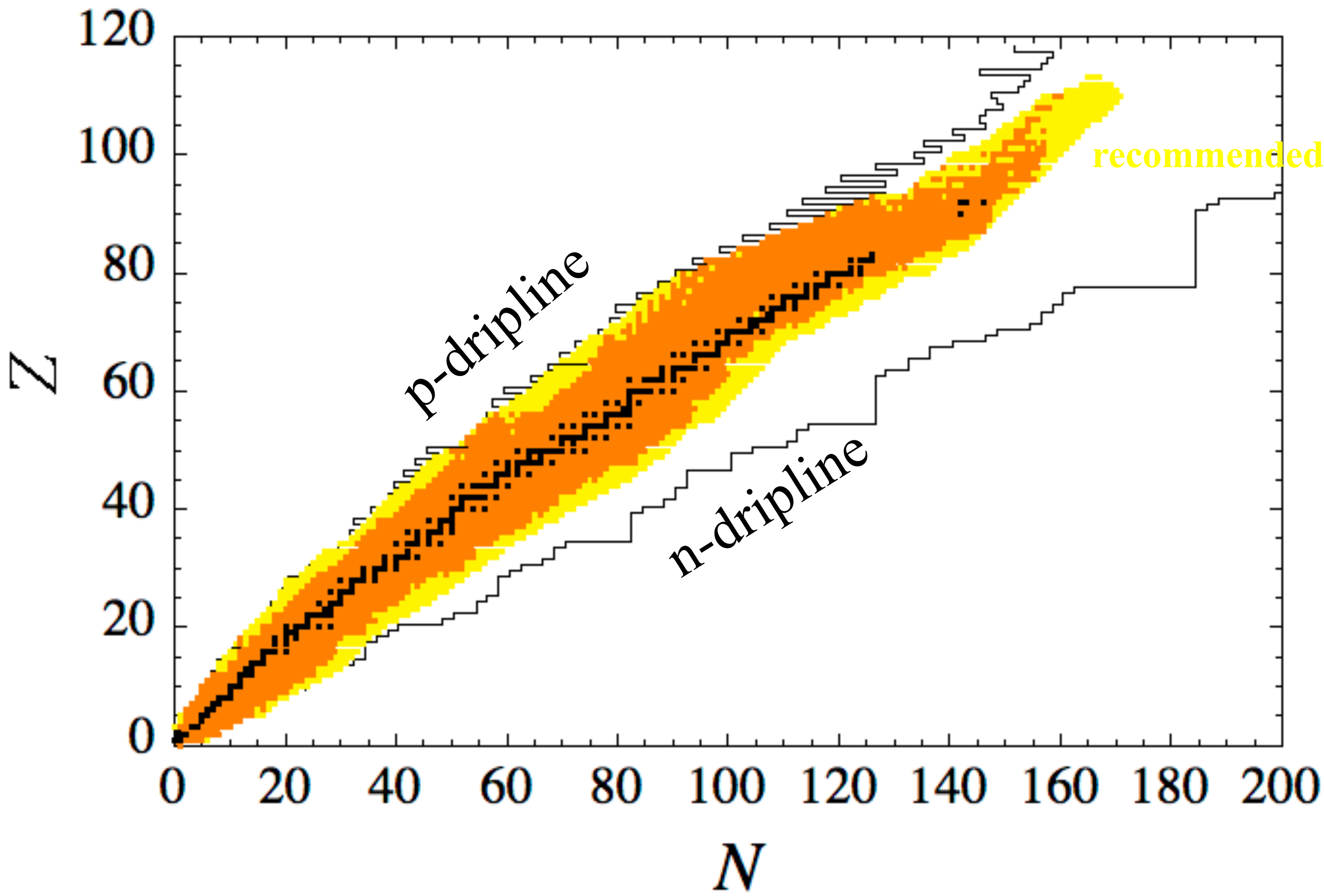
(AME: Atomic Mass Evaluation)



In AME 2003 (wrt 1995): 289 new masses with 242 new p-rich and 47 new n-rich
In AME 2012 (wrt 2003): 225 new masses with 96 new p-rich and 129 new n-rich
In AME 2016 (wrt 2012): 60 new masses with 25 new p-rich and 35 new n-rich
In AME 2020 (wrt 2016): 52 new masses with 34 new p-rich and 40 new n-rich (22 rejected)

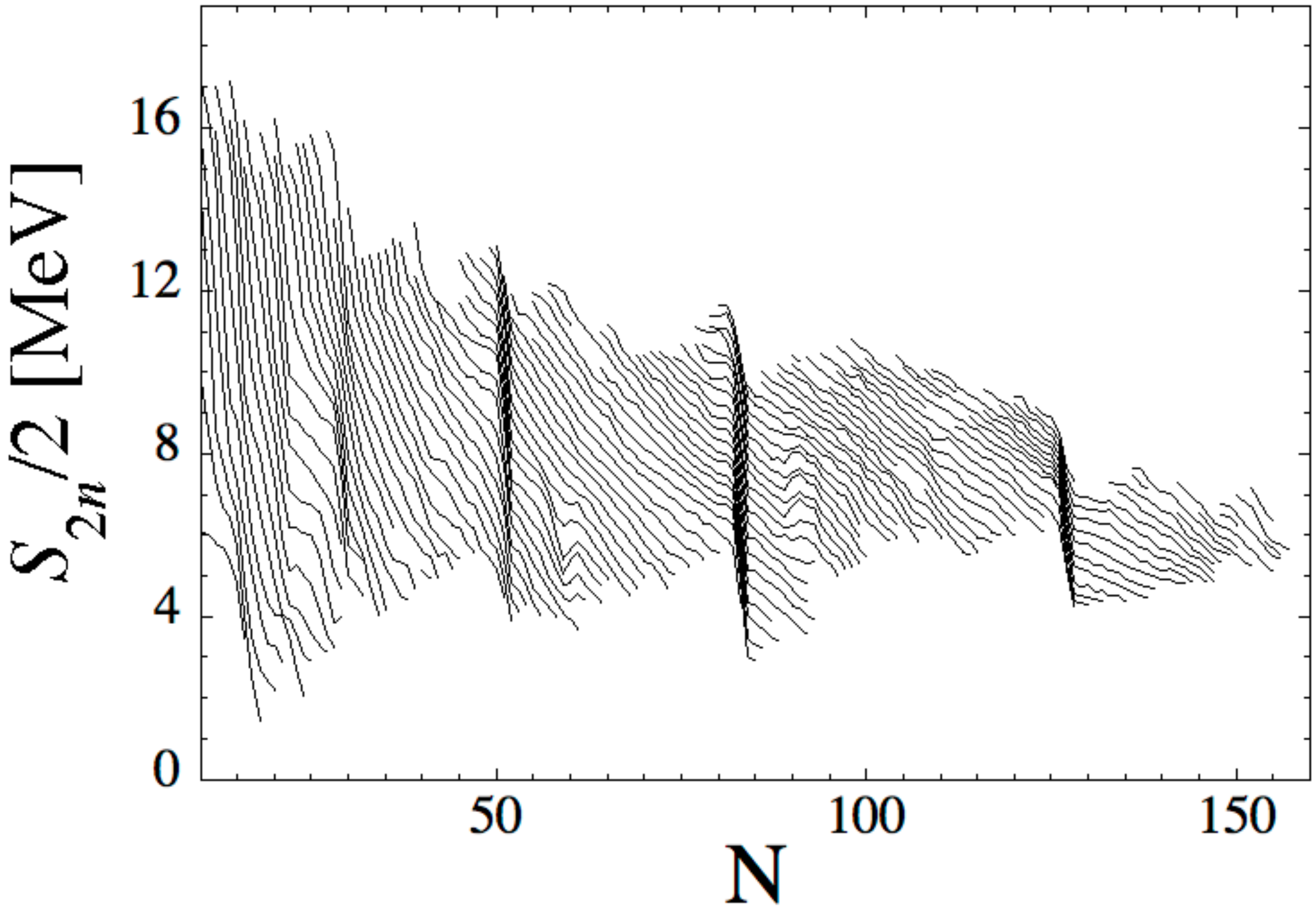
In the Atomic Mass Evaluation (2020)

- 2550 experimentally known masses
- 3558 « recommended » masses = 2550 known + 1008 *extrapolated* masses assuming a smooth mass surface in the vicinity of known masses



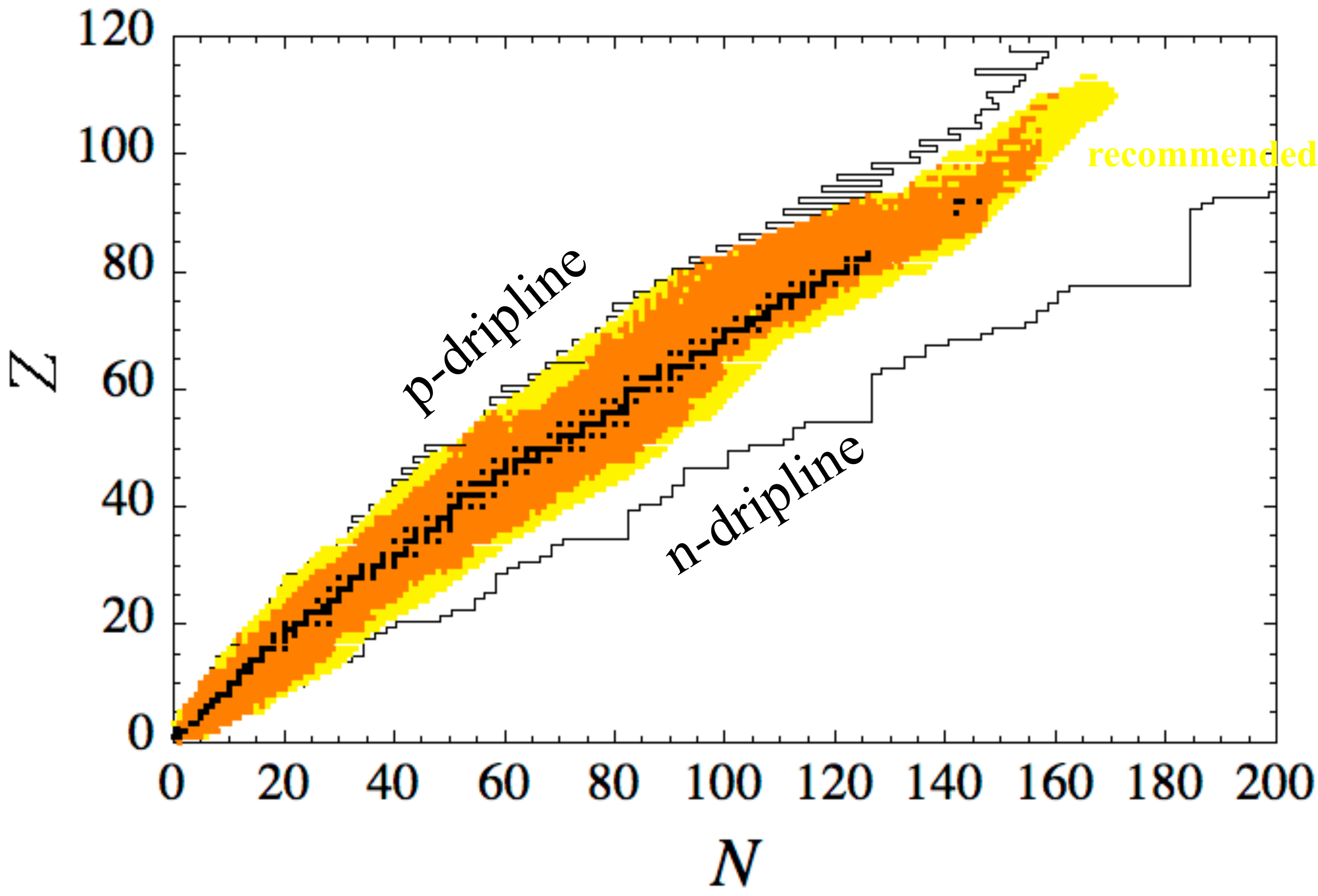
Smooth trend in experimental nuclear masses away from shell closures, shape transitions and Wigner cusps along the N=Z line; in particular in the systematics of S_{2n}, S_{2p}, Q_α

$$S_{2n}(Z,N) = M(Z,N\text{-}2) + 2M_n - M(Z,N)$$



By Default TALYS includes the “recommended” AME (3558) masses !

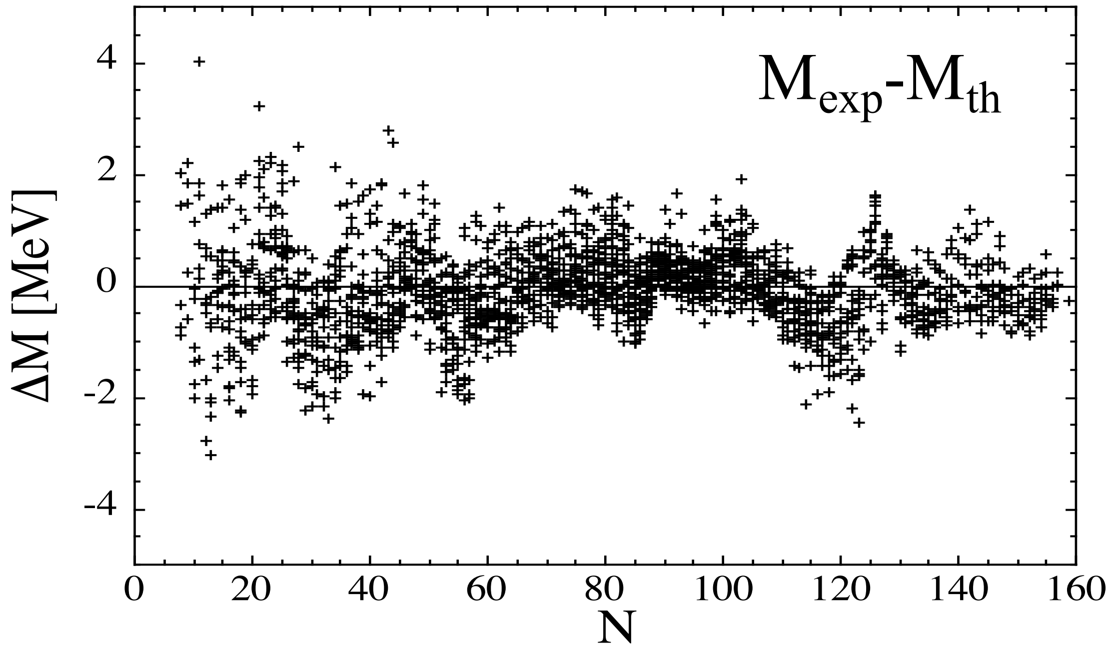
What about the mass of the ~6000 nuclei experimentally unknown ?



Nuclear mass model

1. Fit the parameters of the mass model to all 2457 ($Z,N \geq 8$) experimental masses from AME'20

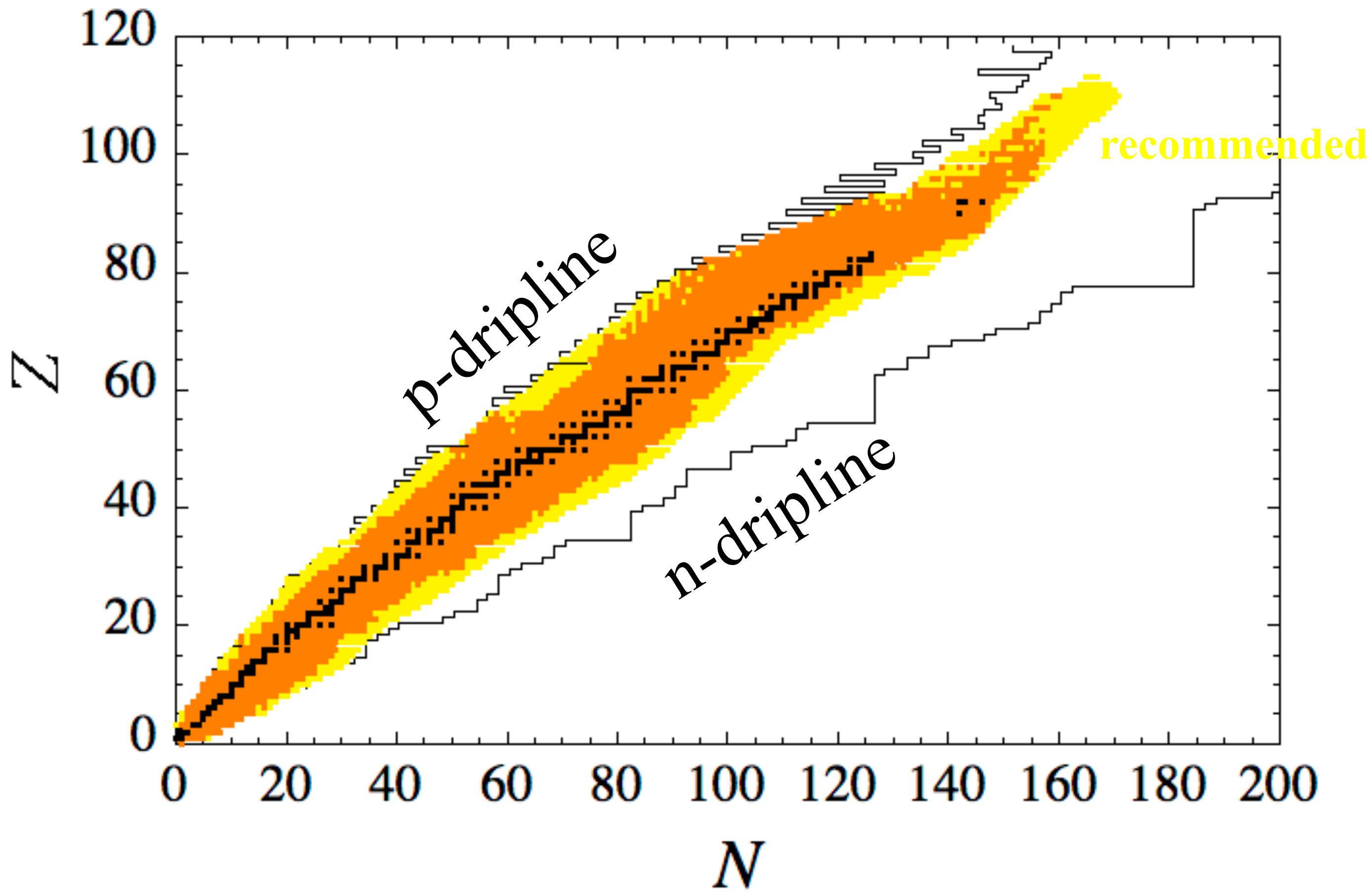
rms deviation of the order of 0.5 - 0.8 MeV on the 2457 *experimental* **masses** (Note B ~ 100-1000 MeV)



2. Extrapolation to the remaining ~6000 nuclei

On major question always remains: How can we trust the extrapolation, what is the accuracy far away from stability ??

What about the mass of the ~6000 nuclei experimentally unknown ?



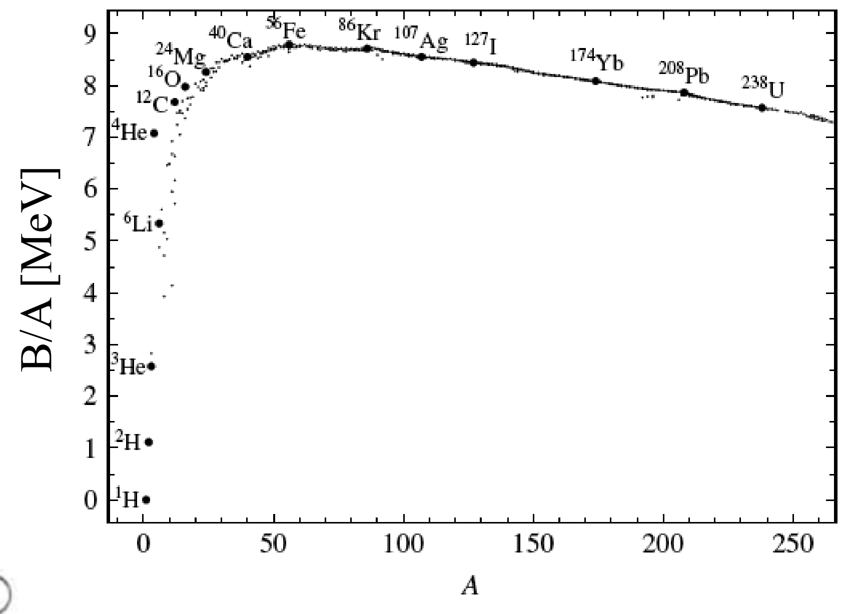
The nuclear mass is given by

$$M_{\text{nuc}}c^2 = N\,M_n c^2 + Z\,M_p c^2 - B$$

The nuclear binding energy must be estimated from the nuclear force binding nucleons inside the nucleus.

The nuclear force is not known from first principles, but deduced from

- nucleon-nucleon interaction
- deuterium properties
- curve of the binding energy per nucleon



The binding energy per nucleon is a smooth curve, almost A-independent for $A>12$: $B/A \sim 8 - 8.5$ MeV/nucleon

This implies that the interaction between nucleons is

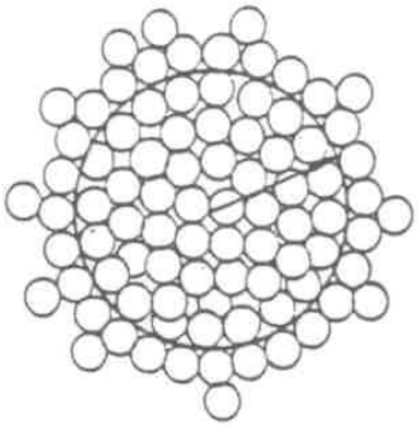
- charge independent
- saturated in nuclei

(one nucleon in the nucleus interacts with only a limited number of nucleons)

Volume term: $B/A \sim$ cst

→ roughly constant density of nucleons inside the nucleus with a relatively sharp surface

→ radius of the nucleus $R \sim A^{1/3}$



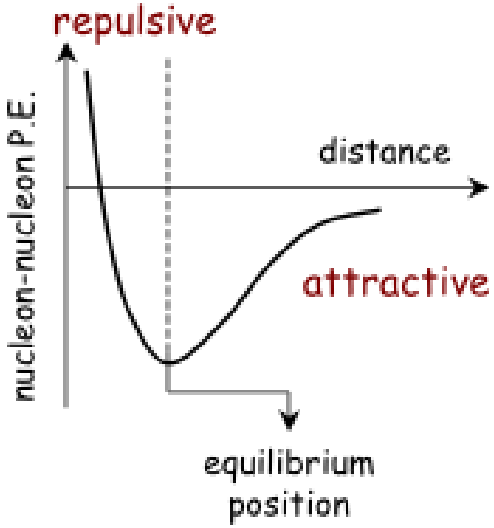
Characteristic of the nuclear force

Short range: strongly attractive component on a short range

Repulsive core: repulsive component at very short distances (<0.5 fm)

⟶ average separation between nucleons leading to a saturation of the nuclear force

Charge symmetric: the nuclear force is isospin independent



Global mass models

	Reliability	Accuracy
• Macroscopic-Microscopic Approaches		
Liquid drop model (Myers & Swiateki 1966)	– –	+ +
Droplet model (Hilf et al. 1976)	– –	+ +
FRDM model (Moller et al. 1995, 2012)	+ –	+ +
KUTY model (Koura et al. 2000)	+ –	+ +
Weizsäcker-Skyrme model (Wang et al. 2011)	+ –	+++
Approximation to Microscopic models		
Shell model (Duflo & Zuker 1995)	+	+++
ETFSI model (Aboussir et al. 1995)	+	+ +
• Mean Field Model		
Hartree-Fock-BCS model (2000)	+ +	+ +
Hartree-Fock-Bogolyubov model (2010)	+ + +	+ +
Relativistic Hartree-Bogolyubov	+ + +	– +

Nuclear mass models

Nuclear mass models provide all basic nuclear ingredients:

Mass excess (Q-values), deformation, GS spin and parity

but also

single-particle levels, pairing strength, density distributions, … in the GS
as well as non-equilibrium (e.g fission path, isomeric) configuration

Building blocks for the prediction of ingredients of relevance in the determination of nuclear reaction cross sections, β-decay rates, … such as

- nuclear level densities
- γ-ray strengths
- optical potentials
- fission probabilities & yields
- etc …

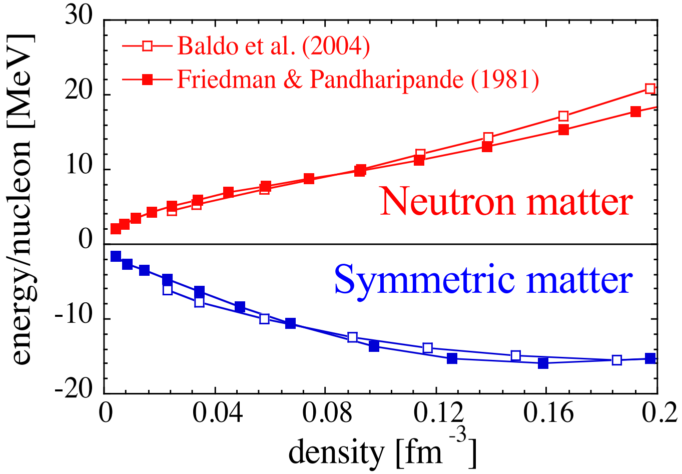
***as well as for the nuclear/neutron matter Equation of State* (NEUTRON STARS)**

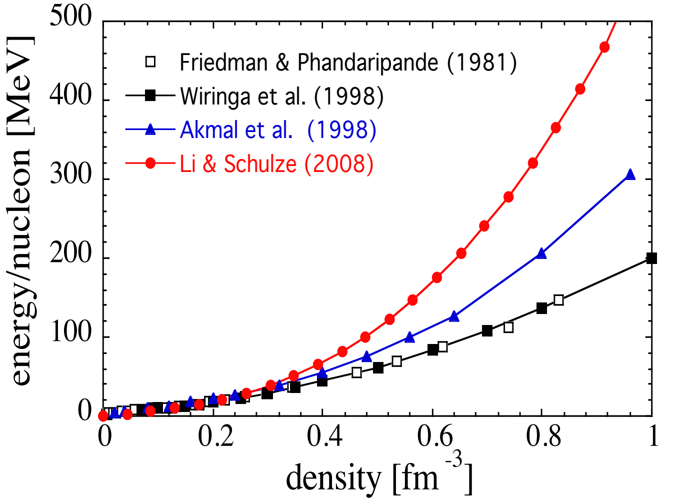
The criteria to qualify a mass model should NOT be restricted to the rms deviation wrt to exp. masses, but also include
- the quality of the underlying physics (sound, coherent, "microscopic", …)
- all the observables of relevance in the specific applications of interest

Challenge for modern mass models: to reproduce as many observables as possible

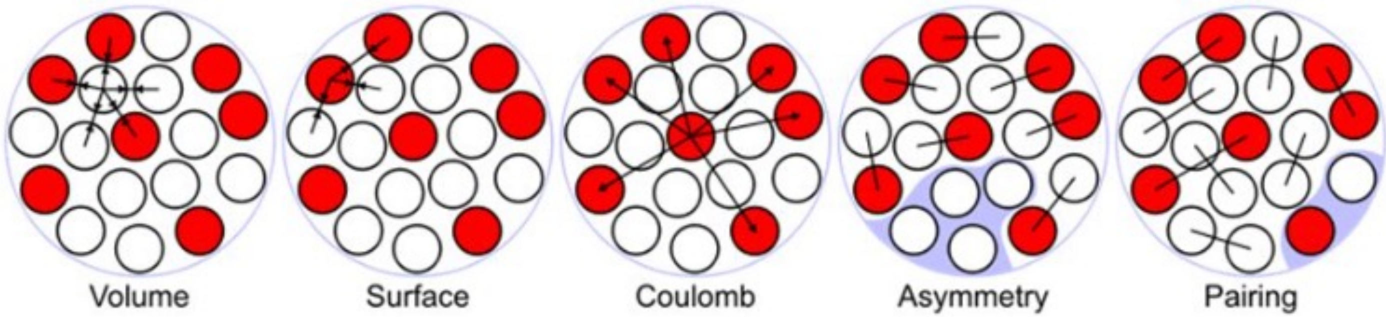
- **2457 experimental masses** from AME'2020 → rms ~ 500-800keV
- 782 exp. charge radii (rms ~ 0.03fm), charge distributions, as well as ~26 n-skins
- Isomers & Fission barriers (scan large deformations)
- Symmetric infinite nuclear matter properties
  - $m^* \sim 0.6 - 0.8$ (BHF, GQR) & $m^*_n(\beta) > m^*_p(\beta)$
  - $K \sim 230 - 250$ MeV (breathing mode)
  - E_{pot} from BHF calc. & in 4 (S,T) channels
  - Landau parameters $F_l(S,T)$
    - stability condition: $F_l^{ST} > -(2l+1)$
    - empirical $g_0 \sim 0$; $g_0' \sim 0.9\text{-}1.2$
    - sum rules $S_1 \sim 0$; $S_2 \sim 0$
  - Pairing gap (with/out medium effects)
  - Pressure around $2\text{-}3\rho_0$ from heavy-ion collisions
- Infinite neutron matter properties
  - $J \sim 29 - 32$MeV
  - E_n/A from realistic BHF-like calculations
  - Pairing gap
  - Stability of neutron matter at all polarizations
- Giant resonances
  - ISGMR, IVGDR, ISGQR
- Additional model-dependent properties
  - Nuclear Level Density (pairing-sensitive)
  - Properties of the lowest 2^+ levels (519 e-e nuclei)
  - Moment of inertia in superfluid nuclei (back-bending)

~ model-dependent





The macroscopic liquid-drop description of the nucleus



$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

Phenomenological description at the level of integrated properties (Volume, Surface, …) with quantum "microscopic" corrections added in a way or another (shell effects, pairing, etc...)

The semi-empirical liquid drop mass model: (Bethe-Weizsäcker Formula, 1935): The nucleus is described as a collection of neutrons and protons forming a liquid drop of an incompressible fluid

$$B(Z,A) = a_V A$$

Volume Term: each nucleon gets bound by about the same energy

$$-a_s A^{2/3}$$

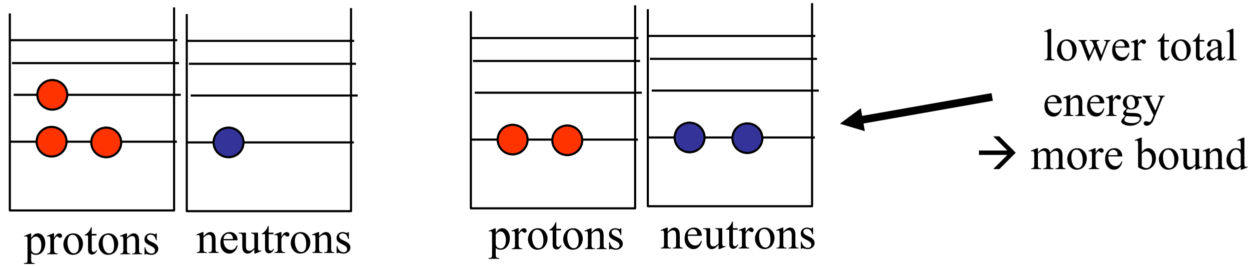
Surface Term: ~ surface area (surface nucleons are less bound)

$$-a_{coul} \frac{Z^2}{A^{1/3}}$$

Coulomb term: Coulomb repulsion leads to a reduction of the binding: uniformly charged sphere has $E=3/5\ Q^2/R$

$$-a_{sym} \frac{(N-Z)^2}{A}$$

Asymmetry term: Pauli principle applied to nucleons: symmetric filling of p,n potential levels has the lowest energy (omitting Coulomb)



$$+\delta \begin{cases} +\Delta & \text{ee} \\ 0 & \text{oe/eo} \\ -\Delta & \text{oo} \end{cases}$$

Pairing correlation effect due to the attractive character of the nucleon force: each orbit can be occupied by 2 nucleons

Pairing term: $\Delta \sim 12/A^{1/2}$[MeV]

even number of like-nucleons are favoured

(e=even, o=odd referring to Z, N respectively)

In summary, the binding energy can be written as

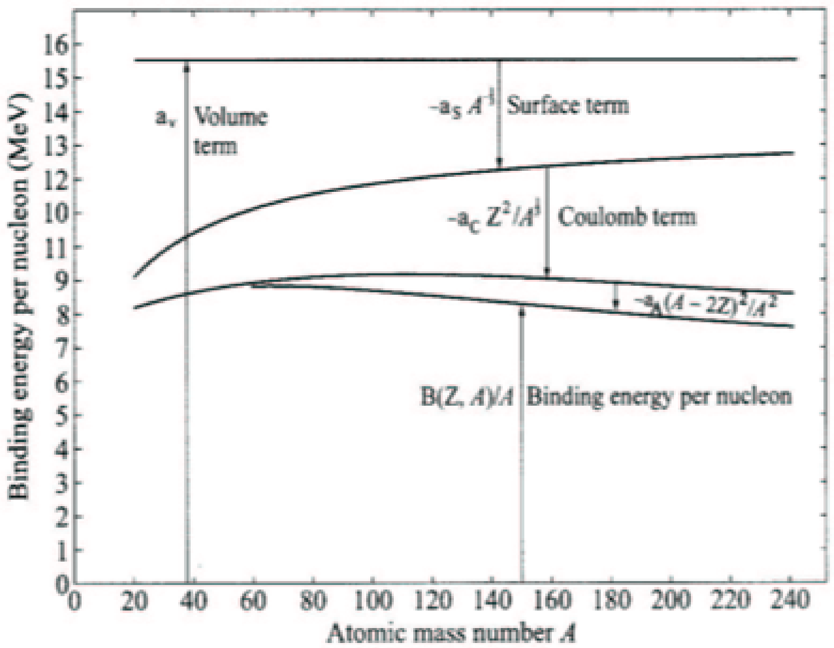
$$B(Z,A) = a_V A - a_S A^{2/3} - a_{coul} Z^2 A^{-1/3} - a_{sym} \left(\frac{N-Z}{A} \right)^2 A + \delta$$

Or equivalently, the internal energy per nucleon $e = -B/A$

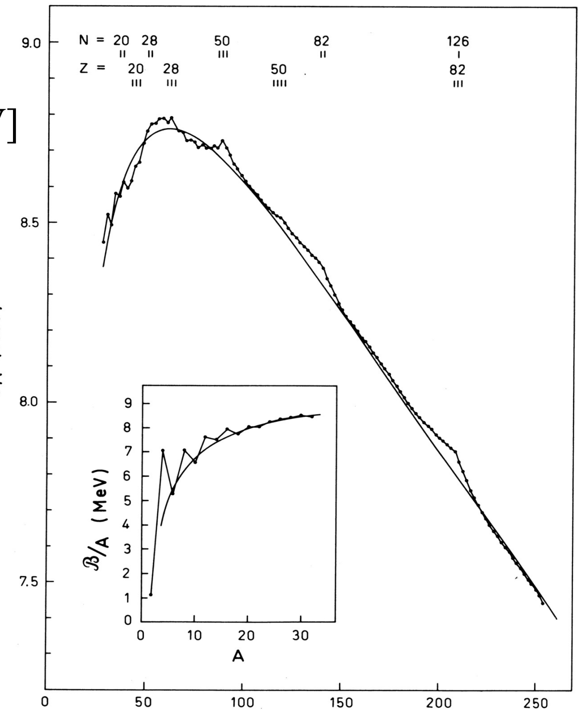
$$e(Z,A) = -a_V + a_S A^{-1/3} + a_{coul} Z^2 A^{-4/3} + a_{sym} \left(\frac{N-Z}{A} \right)^2 - \delta / A$$

$$\Rightarrow e = e_0 + f\left(Z - Z_0\right)^2$$ mass parabola

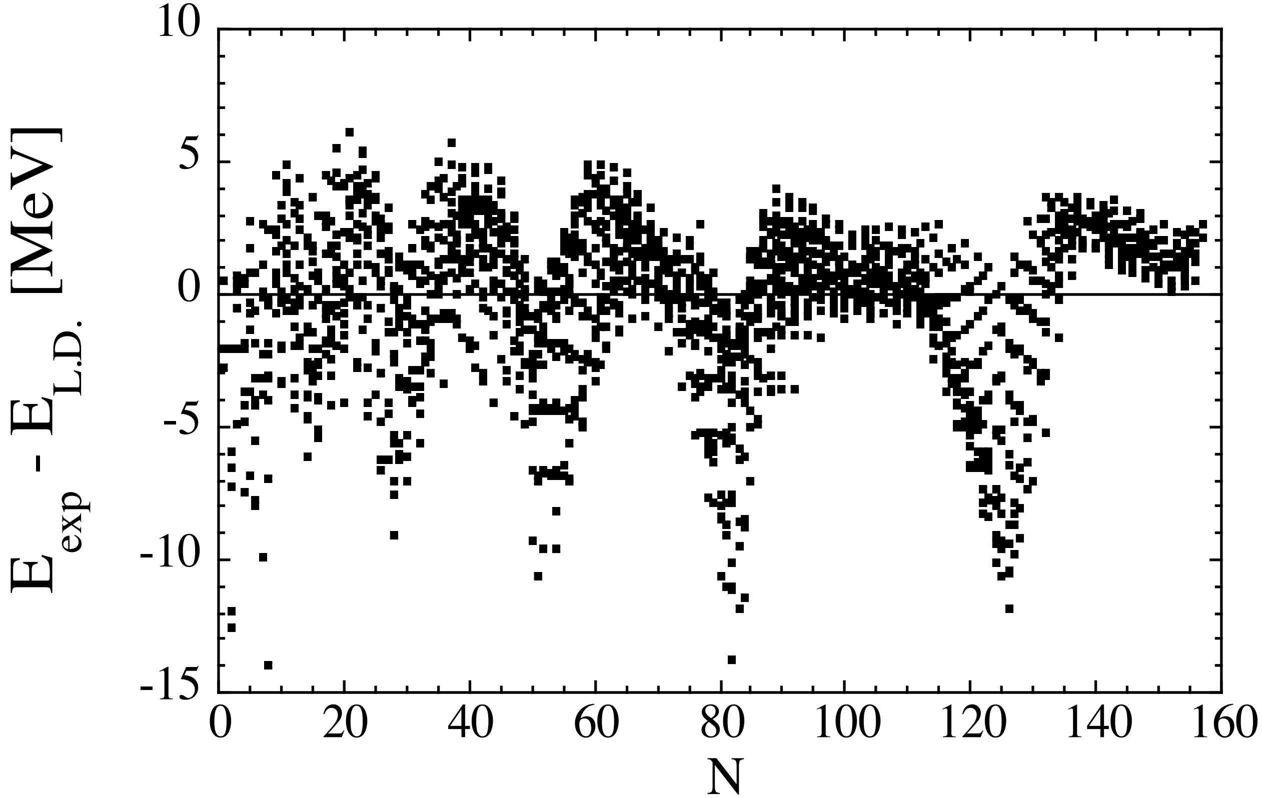
A fit to experimental masses lead to
a_V~ 15.85MeV; a_S~ 18.34 MeV; a_{coul}~ 0.71 MeV; a_{sym}~ 92.86 MeV
or
a_V~ 15.7MeV; a_S~ 17.2 MeV; a_{coul}~ 0.70 MeV; a_{sym}~ 23.3 MeV



Binding energy per nucleon
Experimental data versus liquid drop



Some missing energy : $\delta W = E_{\text{exp}} - E_{\text{LD}}$ → Shell correction energy



For nuclei with exp. masses only

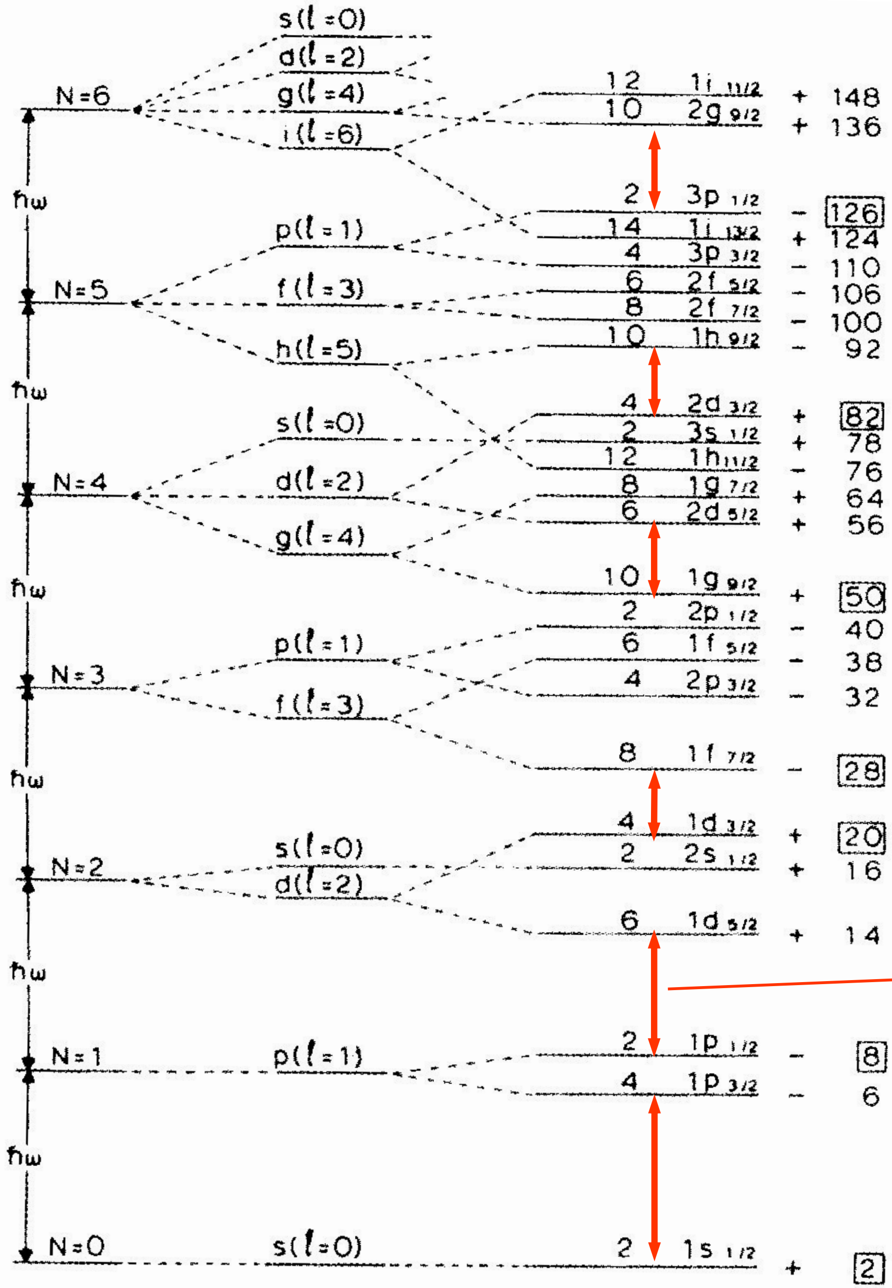
$$B(Z,A) = a_V A - a_S A^{2/3} - a_{coul} Z^2 A^{-1/3} - a_{sym}\left(\frac{N-Z}{A}\right)^2 A + \delta - \delta W$$

The shell effect

Shell model: single-particle energy levels are not equally spaced

→

need to add shell correction term $\delta W(Z,N)$



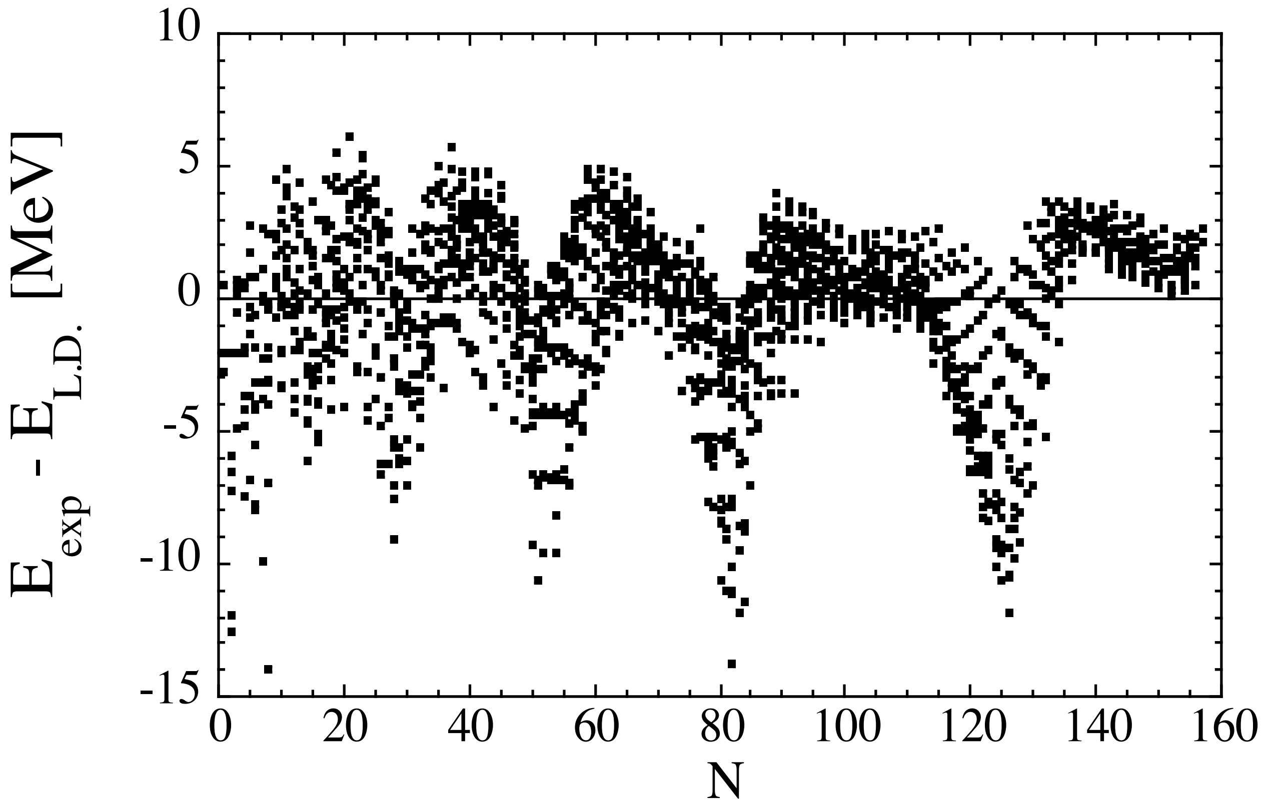
less bound than average

more bound than average.

shell gaps

Magic numbers

Shell correction energy: $\delta W = E_{exp} - E_{LD}$



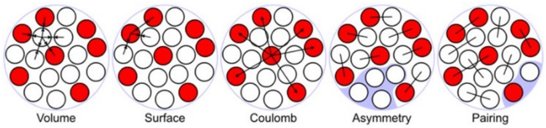
For nuclei with exp. masses only

$$B(Z,A) = a_V A - a_S A^{2/3} - a_{coul} Z^2 A^{-1/3} - a_{sym}\left(\frac{N-Z}{A}\right)^2 A + \delta - \delta W$$

But it remains difficult to predict reliably and accurately shell correction energies on the basis of simple analytical formula (e.g Myers & Swiatecki 1966) for experimentally unknown nuclei. Need more microscopic approaches like mean field theories, shell model, … to put the extrapolation on a safe footing. In particular, it is not clear if the *N*=28, 50, 82, 126 magic numbers remain in the neutron-rich region !

Recent Mic-Mac mass models

$$E = E_{LD} + E_{micro}$$



$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

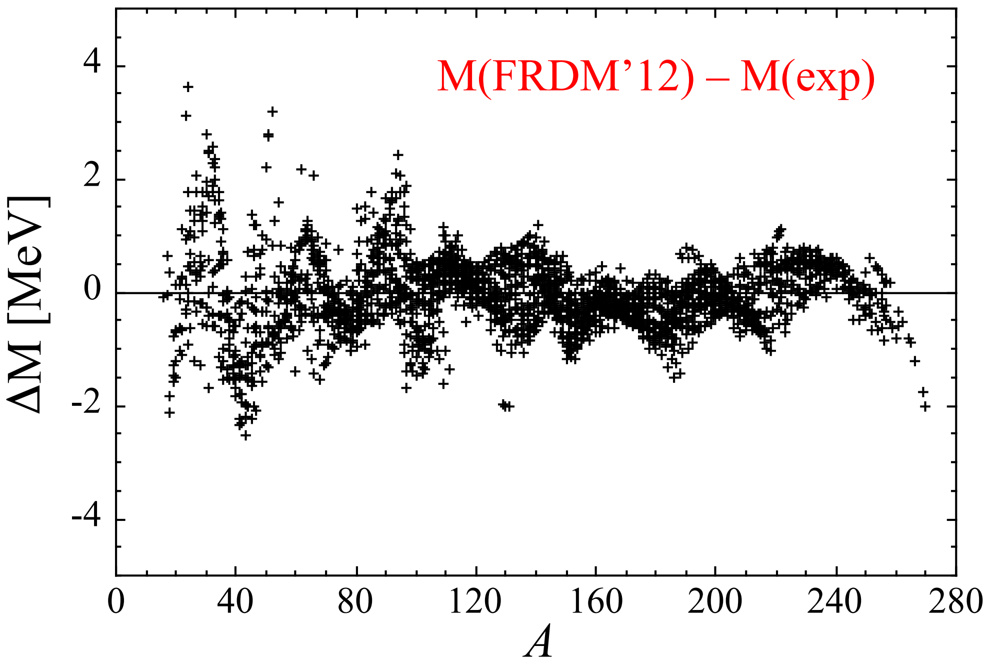
Mic-Mac models : ~ 30 parameters fitted to atomic masses

INCLUDED IN TALYS

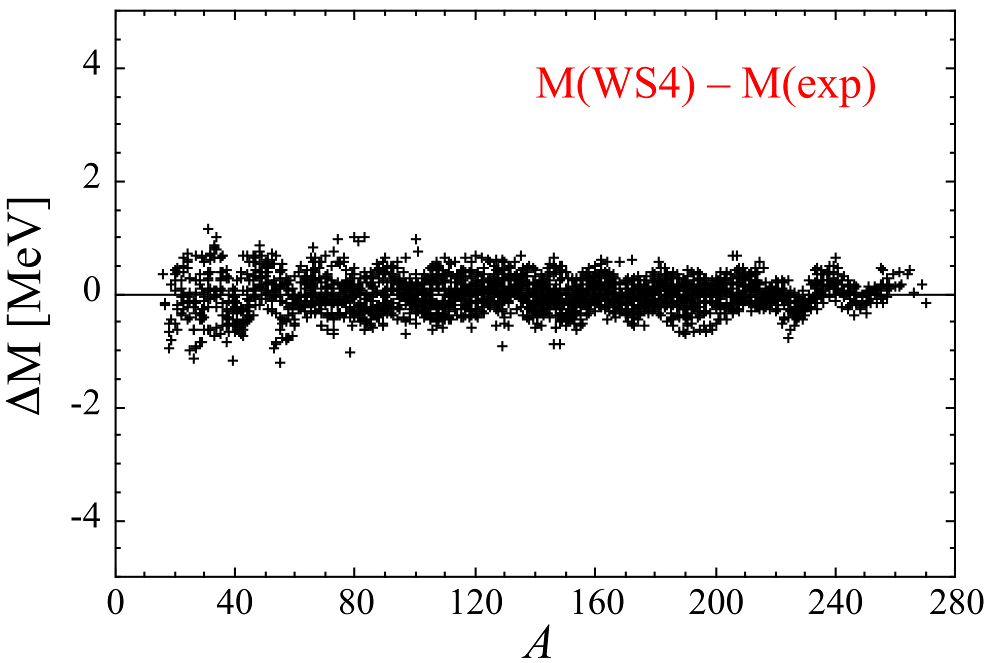
- FRDM'12 : update from FRDM'95 (Möller 2012)
  - σ_{rms} = 0.61 MeV (2457 nuclei in AME'20)

- WS mass formula (Ning Wang et al. 2011 including RBF corr.)
  - WS3: σ_{rms} = 0.34 MeV (2457 nuclei in AME'20)
  - WS4: σ_{rms} = 0.30 MeV (2457 nuclei in AME'20)

RBF: additional ~ 500 parameters to reduce deviations !

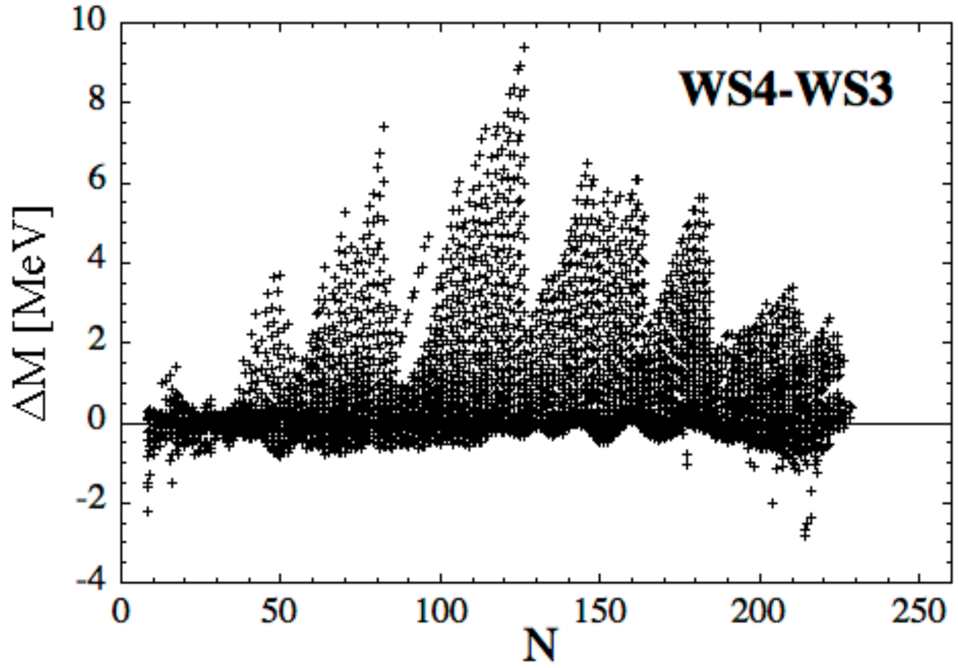


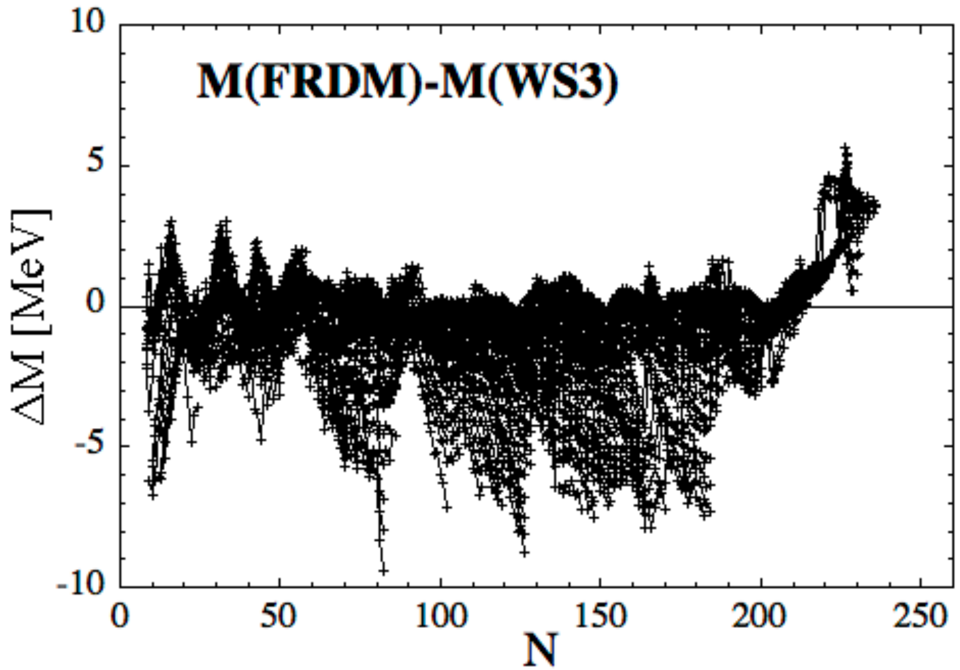
AME'20:
2547 nuclei
with $Z \geq 8$



$M_{RBF}=M_{WS4}+\text{Correction}$

EXTRAPOLATIONS



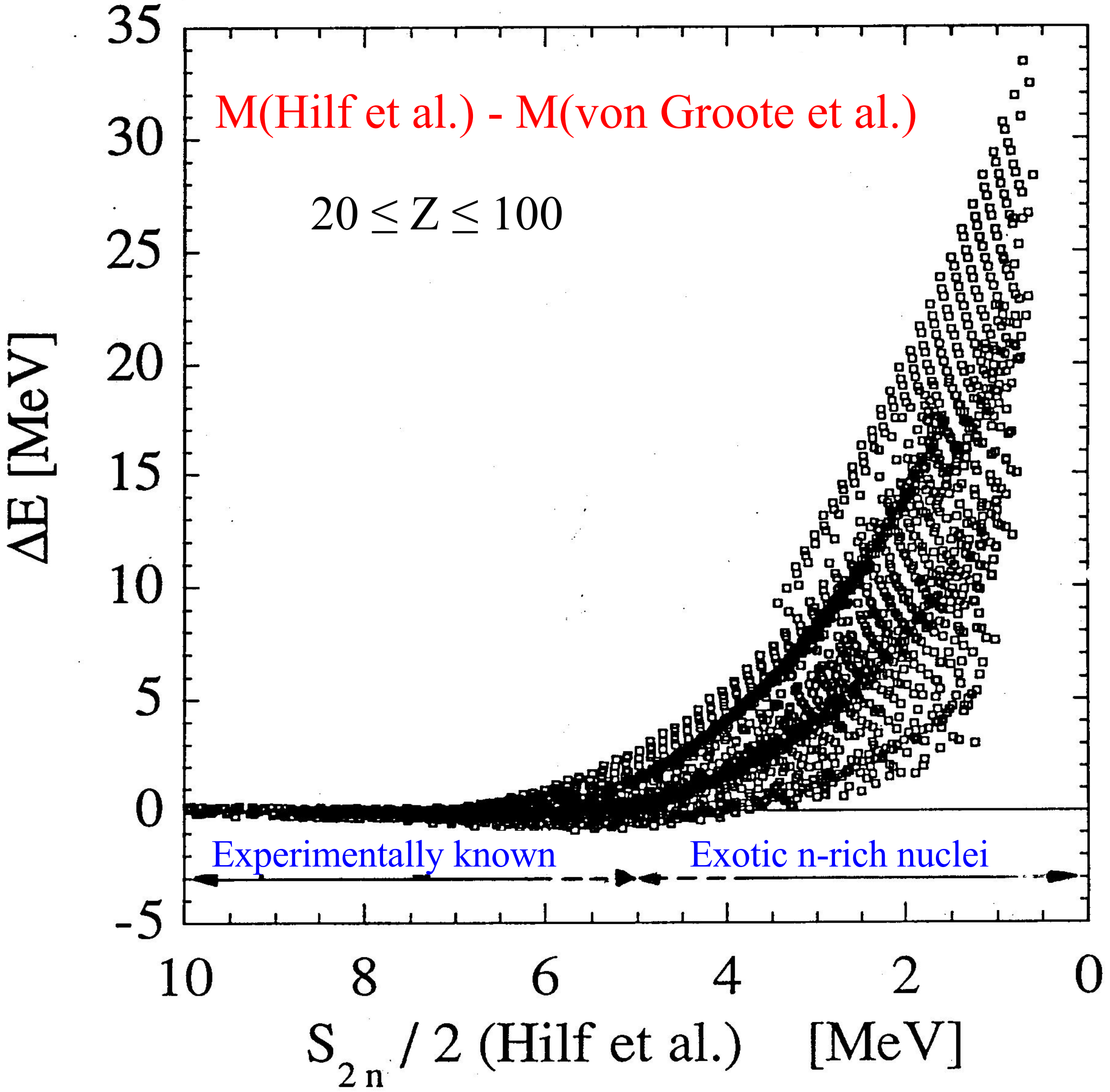


~ 7500 nuclei with $8 \leq Z \leq 124$

Uncertainties in the prediction of masses far away from the experimentally known region

Two identical “droplet models” but with two different parametrizations
Hilf et al. (1976) versus von Groote et al. (1976)

rms deviation on exp masses ~ 670 keV (1976) – 950 keV (2003) – 1020 keV (2012) – 1060 keV (2016)

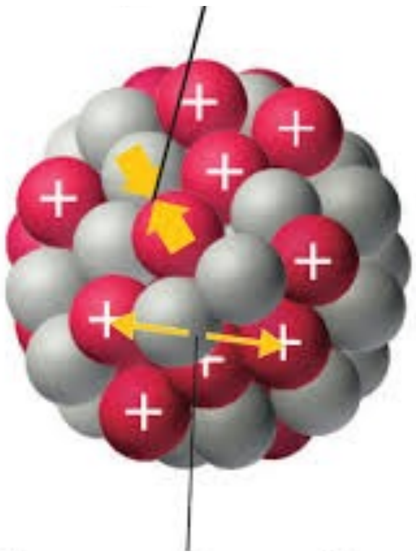


A more « microscopic » description of the nucleus

e.g. Mean-Field

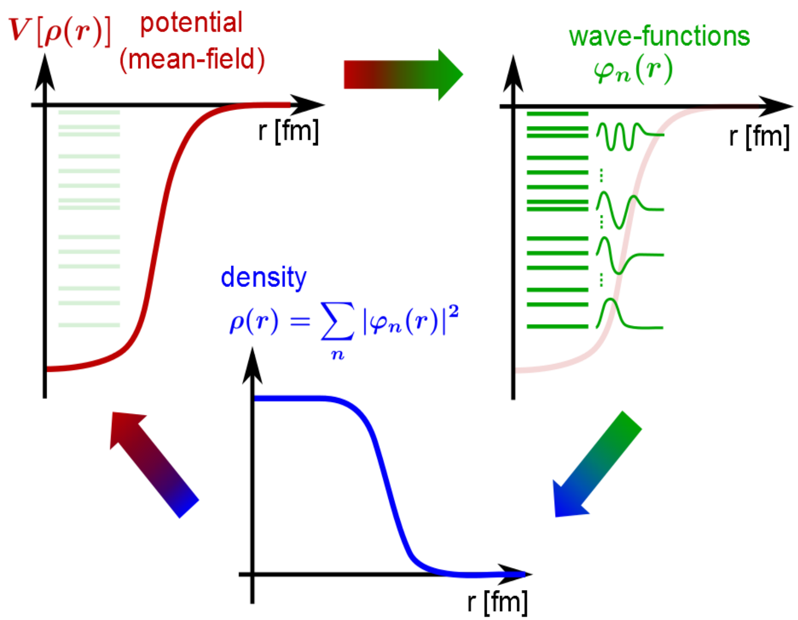
$$E_{MF} = \int \mathcal{E}_{nuc}(\mathbf{r}) d^3\mathbf{r} + \int \mathcal{E}_{coul}(\mathbf{r}) d^3\mathbf{r}$$

Strong nuclear force



Electrostatic repulsion

obtained on the basis of an Energy Density Functional generated by an effective n-n interaction !



Self-consistent mean-field theory

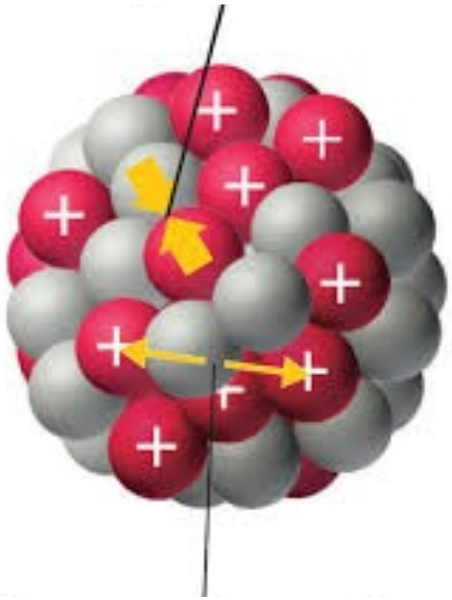
Mean-field: each nucleon moves independently of other nucleons in a central potential *V* representing the interaction of a nucleon with all the other nucleons

A more « microscopic » description of the nucleus

e.g. Mean-Field

$$E_{MF} = \int \mathcal{E}_{nuc}(\mathbf{r})d^3\mathbf{r} + \int \mathcal{E}_{coul}(\mathbf{r})d^3\mathbf{r}$$

Strong nuclear force



Electrostatic repulsion

obtained on the basis of an Energy Density Functional generated by an effective n-n interaction !

$$\begin{aligned}
\mathcal{E}_{\text{Sky}} = & \sum_{q=n,p} \frac{\hbar^2}{2M_q}\tau_q + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_{q=n,p}\rho_q^2\right] + \frac{1}{4}t_1\left\{\left(1+\frac{1}{2}x_1\right)\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right]\right. \\
& \left. -\left(\frac{1}{2}+x_1\right)\sum_{q=n,p}\left[\rho_q\tau_q + \frac{3}{4}(\nabla\rho_q)^2\right]\right\} + \frac{1}{4}t_2\left\{\left(1+\frac{1}{2}x_2\right)\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right] + \left(\frac{1}{2}+x_2\right)\right. \\
& \left. \times \sum_{q=n,p}\left[\rho_q\tau_q - \frac{1}{4}(\nabla\rho_q)^2\right]\right\} + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{1}{2}x_3\right)\rho^2 - \left(\frac{1}{2}+x_3\right)\sum_{q=n,p}\rho_q^2\right] \\
& + \frac{1}{4}t_4\left\{\left(1+\frac{1}{2}x_4\right)\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right] - \left(\frac{1}{2}+x_4\right)\sum_{q=n,p}\left[\rho_q\tau_q + \frac{3}{4}(\nabla\rho_q)^2\right]\right\}\rho^\beta \\
& + \frac{\beta}{8}t_4\left[\left(1+\frac{1}{2}x_4\right)\rho(\nabla\rho)^2 - \left(\frac{1}{2}+x_4\right)\nabla\rho\cdot\sum_{q=n,p}\rho_q\nabla\rho_q\right]\rho^{\beta-1} + \frac{1}{4}t_5\left\{\left(1+\frac{1}{2}x_5\right)\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right]\right. \\
& \left. + \left(\frac{1}{2}+x_5\right)\sum_{q=n,p}\left[\rho_q\tau_q - \frac{1}{4}(\nabla\rho_q)^2\right]\right\}\rho^\gamma - \frac{1}{16}(t_1x_1+t_2x_2)J^2 + \frac{1}{16}(t_1-t_2)\sum_{q=n,p}J_q^2 \\
& - \frac{1}{16}(t_4x_4\rho^\beta + t_5x_5\rho^\gamma)J^2 + \frac{1}{16}(t_4\rho^\beta - t_5\rho^\gamma)\sum_{q=n,p}J_q^2 + \frac{1}{2}W_0\left(J\cdot\nabla\rho + \sum_{q=n,p}J_q\cdot\nabla\rho_q\right).
\end{aligned}$$

Still *phenomenological*, but at the level of the effective n-n interaction
Obviously more complex, but models have now reached stability and **accuracy** !

Mean Field mass models

$$E = E_{MF} - E_{coll} - E_W$$

$\boldsymbol{E_{MF}}$ **:** HFB or HF-BCS (or HB) main Mean-Field contribution

$\boldsymbol{E_{coll}}$**:** Quadrupole Correlation corrections to restore broken symmetries and include configuration mixing

$\boldsymbol{E_W}$ **:** *Wigner* correction contributes only for nuclei along the $Z \sim N$ line (and in some cases for light nuclei)

Skyrme-HFB	Gogny-HFB	Relativistic MF
rms ~ 0.5-0.8MeV	rms ~ 0.8MeV	rms > 1.1MeV

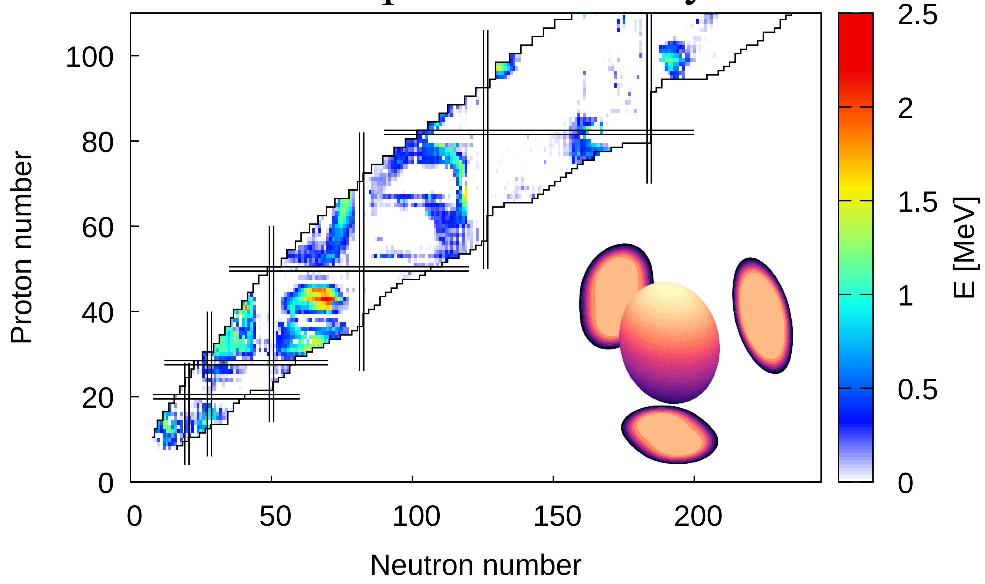
INCLUDED IN TALYS

Progress in mean field (HFB) mass models for astrophysical applications

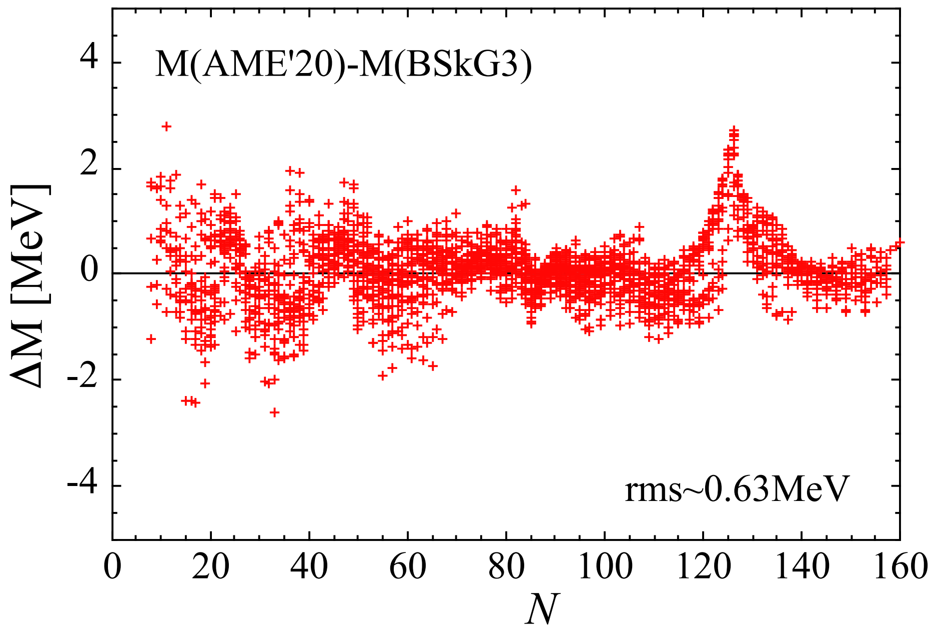
BSkG3: Ryssens et al. (2022)

- Time-reversal breaking
- Triaxial & Octupole deformations
- Fit to Masses, Radii, Fission barriers, INM, ...

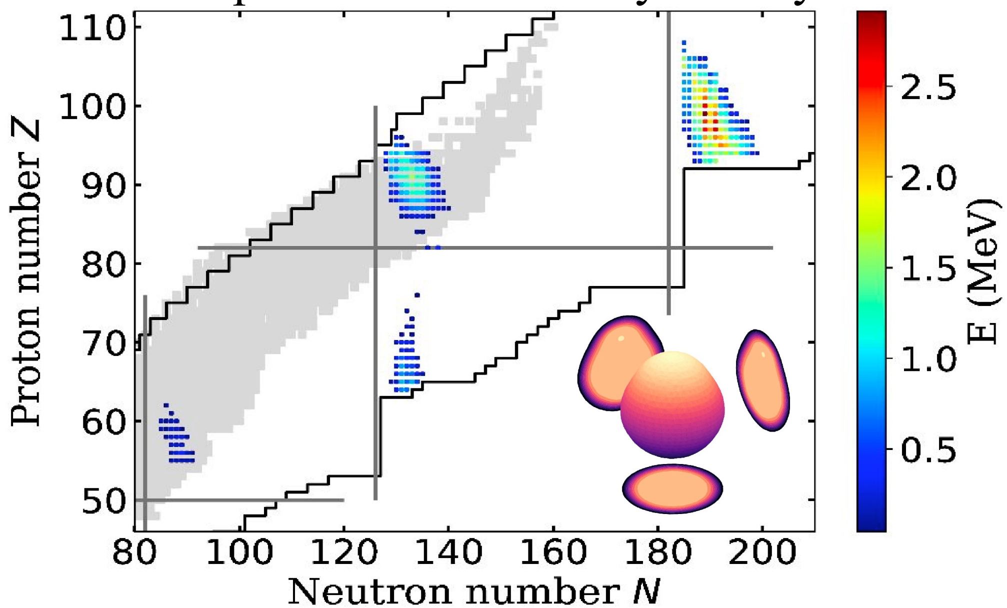
Impact of triaxility



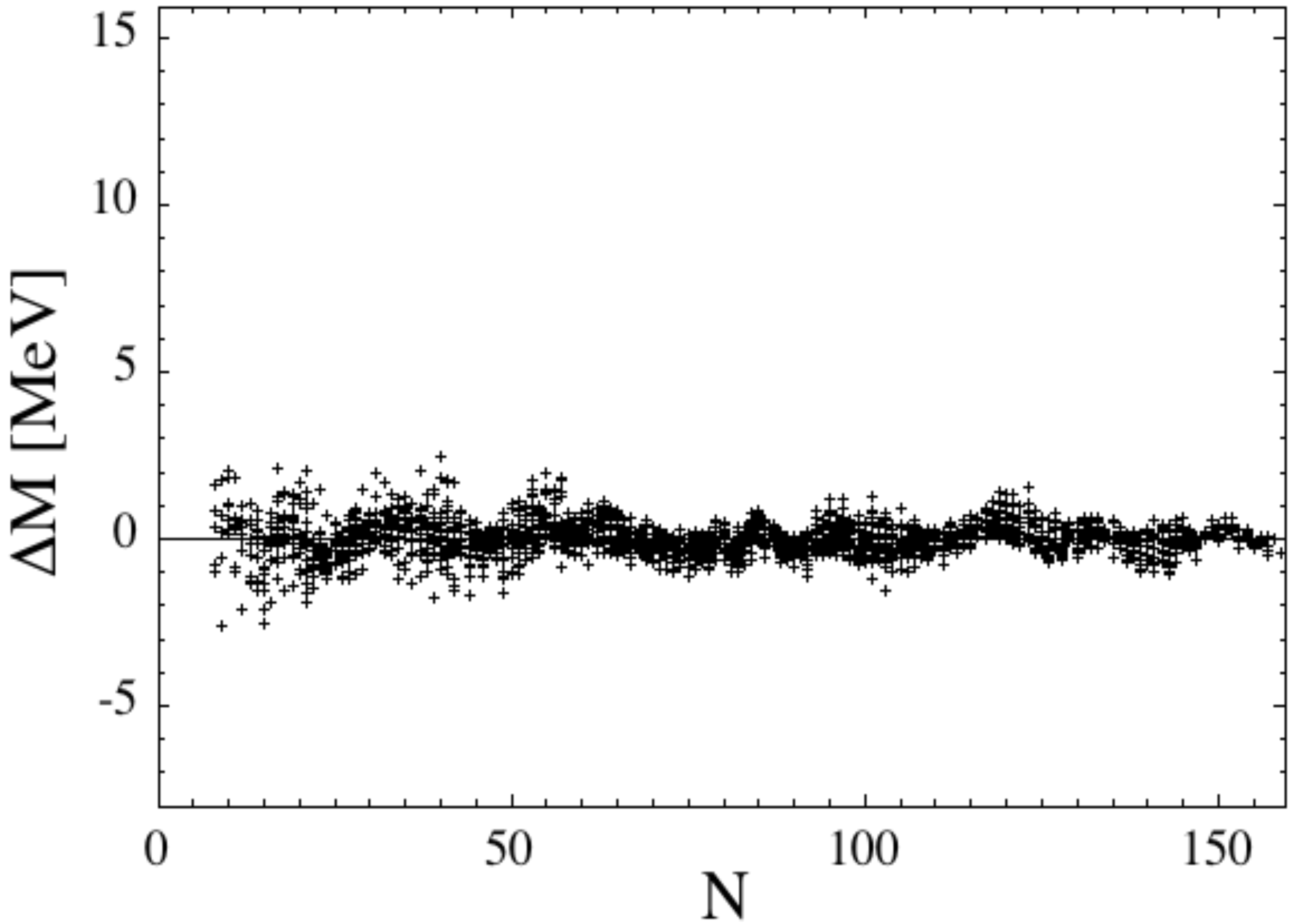
BSkG3: σ(2457nuc)=0.63 MeV



Impact of reflection asymmetry



M(BSk27) – M(exp)

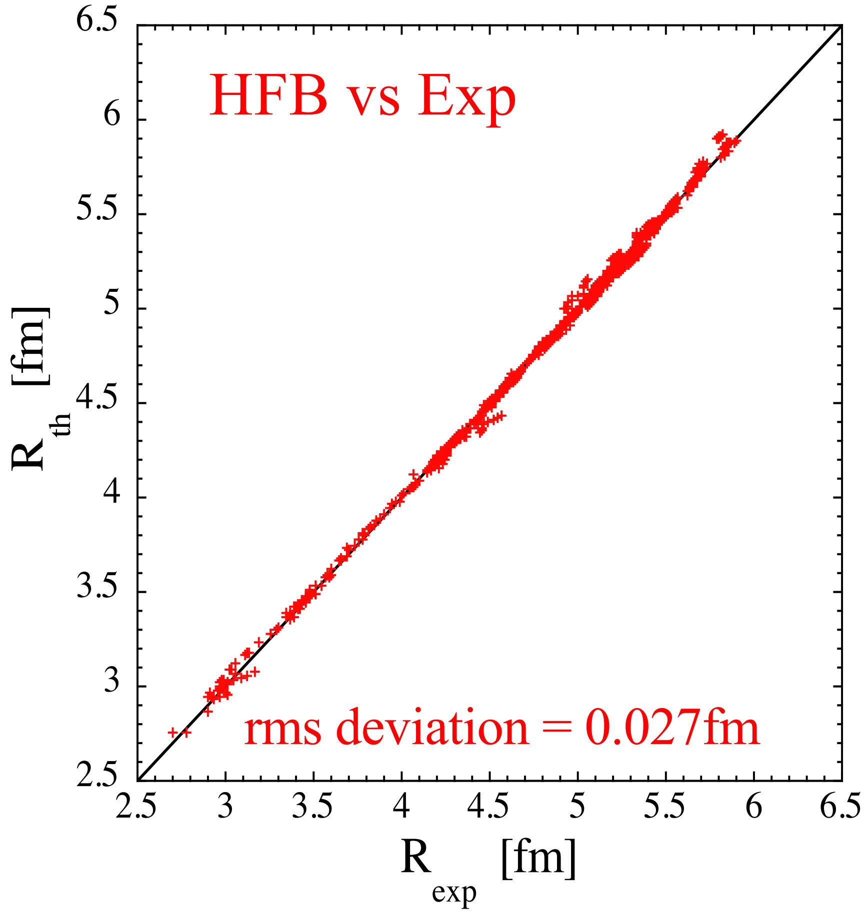


Skyrme and pairing interactions adjusted on all available masses → rms ~ 0.5-0.7 MeV

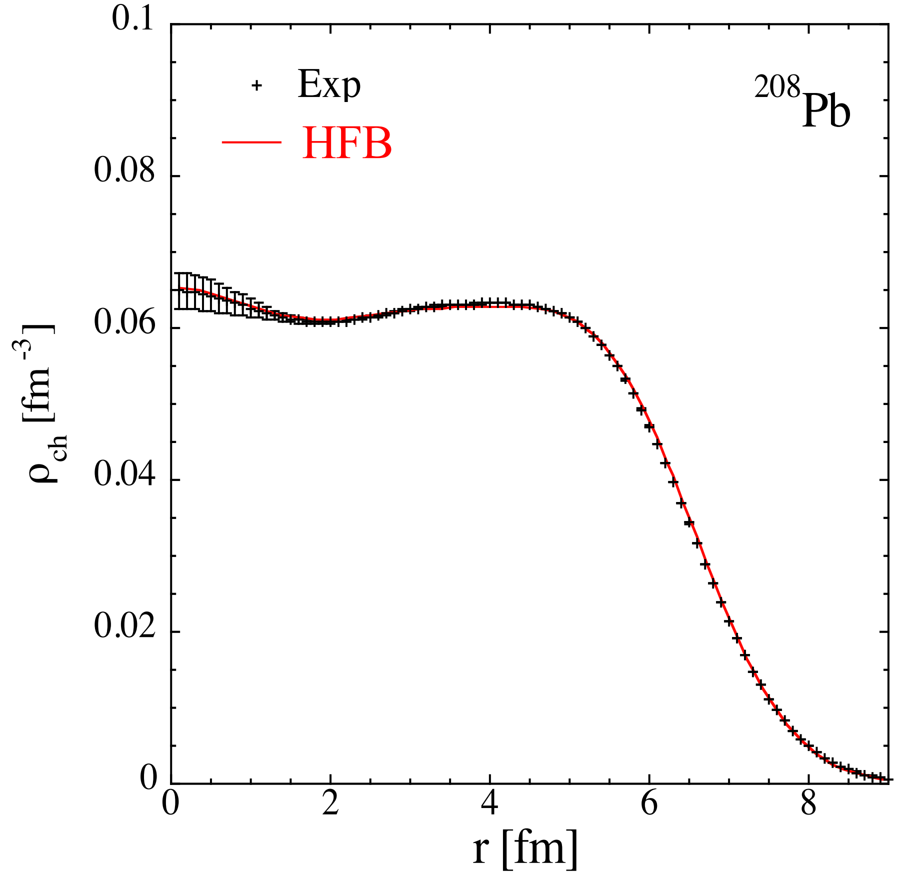
(Only a few Skyrme interactions leading to a competitive mass prection)

Some examples for nuclear structure properties of interest for applications

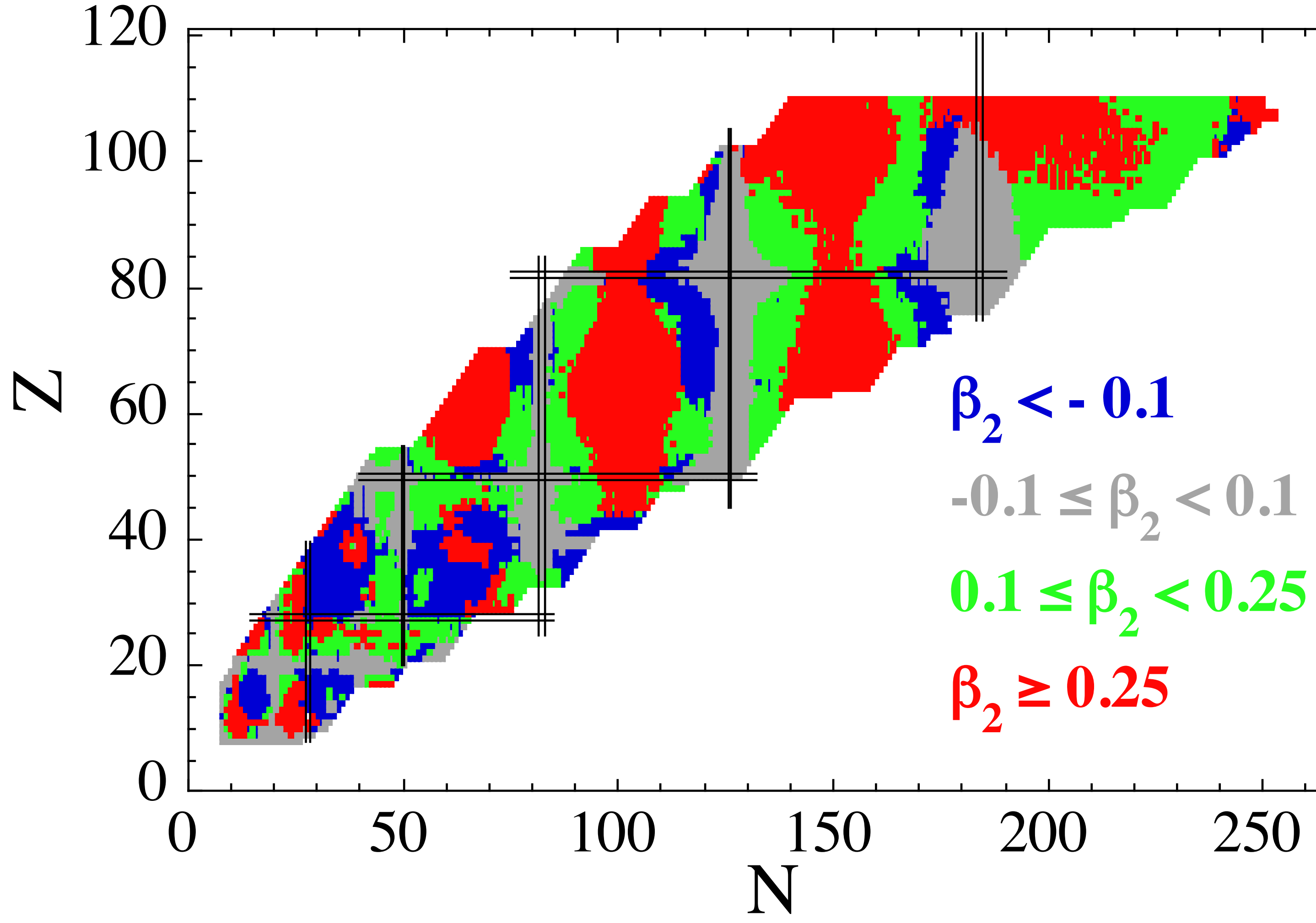
Charge radii for 782 nuclei



Charge distribution of ^{208}Pb



HFB predictions of nuclear deformations



Prediction of GS spins and parities from the single-particle level scheme in the simple "last-filled orbit" approximation

For odd-A nuclei

Spherical nuclei ($\beta_2 \leq 0.05$): ~ 95% spins correctly predicted

Deformed nuclei ($\beta_2 > 0.25$): ~50% spins correctly predicted

For all odd-A and odd-odd nuclei (using Nordheim's rule**)**

Total of **1588** nuclei (experimental J^π from RIPL-3 database)

Spherical spl scheme for $\beta_2 \leq 0.16$

Deformed spl scheme for $\beta_2 > 0.16$

~50% spins correctly predicted

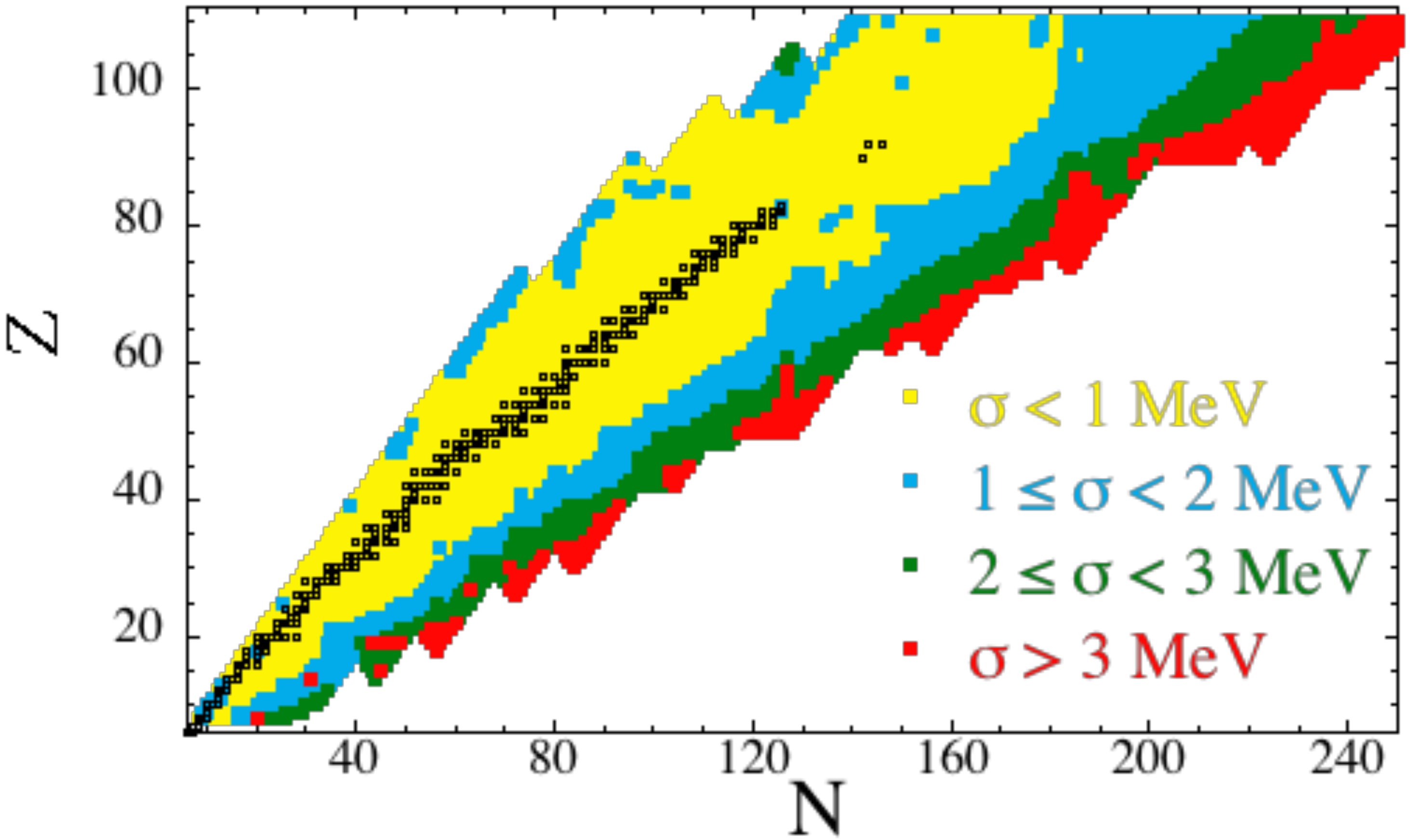
~75% parities correctly predicted

TALYS: Full HFB mass table including predicted GS J^π and deformation (β_2, β_4) for 8508 nuclei with $8 \leq Z \leq 110$

Uncertainties of mass extrapolation in HFB mass models

1σ uncertainties between the 29 HFB mass models

(0.51 < σ_{exp} <0.79 MeV)

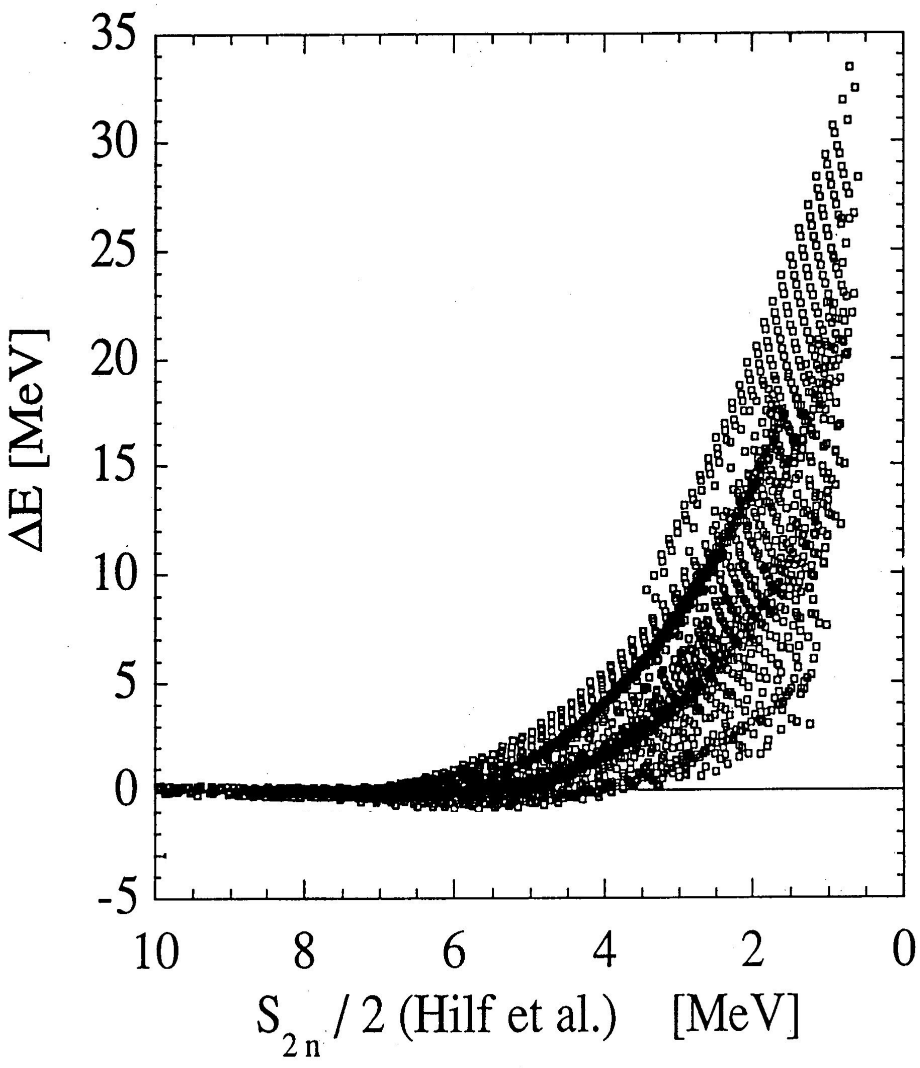


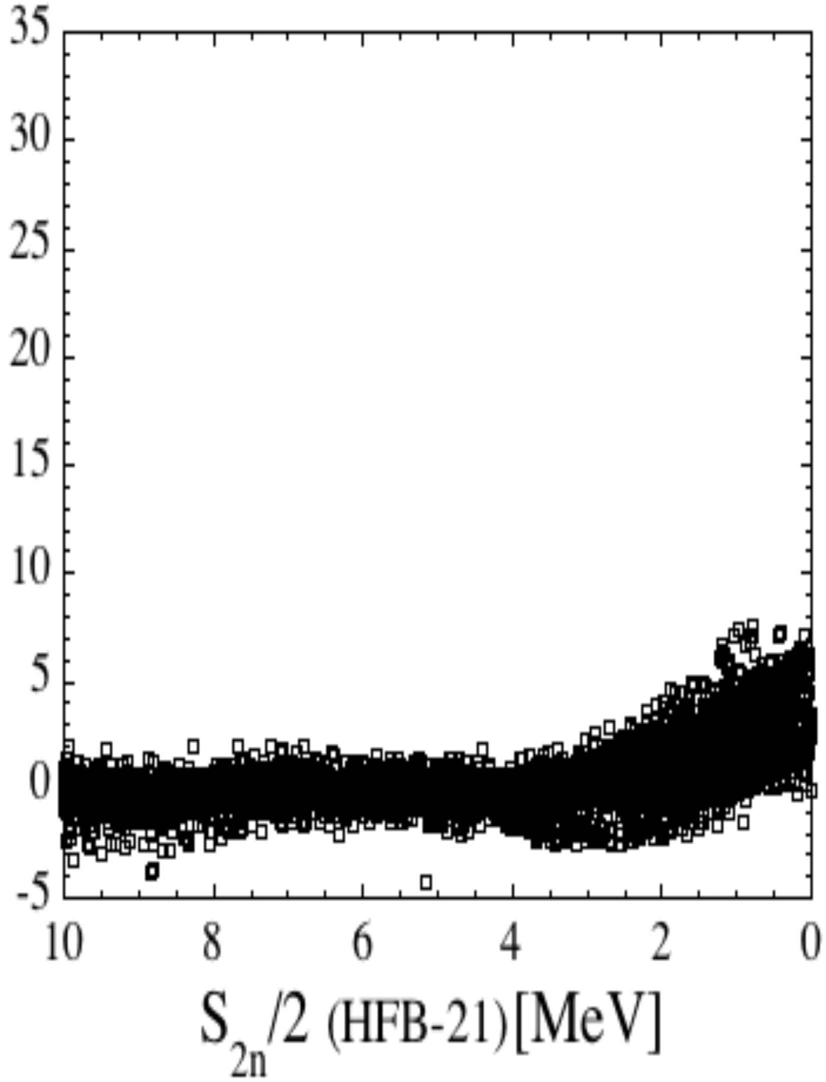
Parameter uncertainties in the droplet vs HFB models

$20 \leq Z \leq 100$

M(Hilf et al.) – M(von Groote et al.)

M(HFB-2) – M(HFB-24)





Another approach to mass models

Gogny-HFB mass table
beyond mean field !

The total binding energy is estimated from

$$E_{tot} = E_{HFB} - E_{Quad}$$

- E_{HFB}: deformed HFB binding energy obtained with a *finite-range* standard Gogny-type force

$$V(1,2)=\sum_{j=1,2} e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_j^2}}(W_j+B_jP_\sigma-H_jP_\tau-M_jP_\sigma P_\tau)$$
$$+t_0\,(1+x_0P_\sigma)\,\delta\,(\vec{r}_1-\vec{r}_2)\left[\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\right]^\alpha$$
$$+i\,W_{LS}\overleftarrow{\nabla}_{12}\,\delta\,(\vec{r}_1-\vec{r}_2)\times\overrightarrow{\nabla}_{12}.\,(\overrightarrow{\sigma}_1+\overrightarrow{\sigma}_2)\,.$$

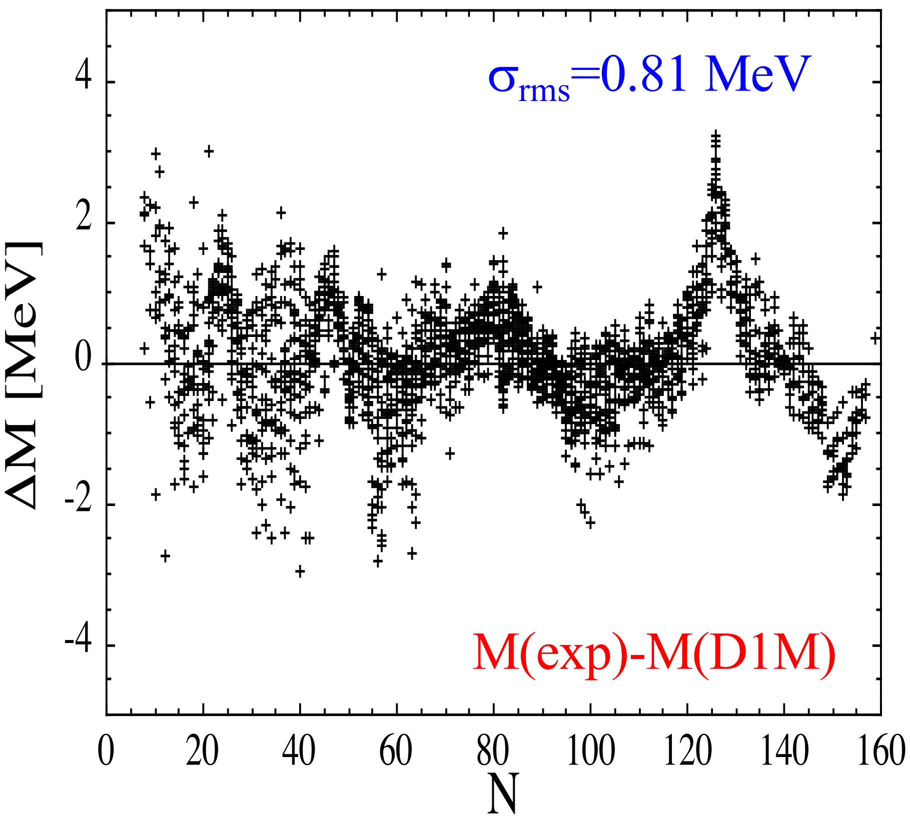
- E_{Quad} : quadrupolar correction energy determined with the *same* Gogny force (no "double counting") in the framework of the GCM+GOA model for the five collective quadrupole coordinates, i.e. rotation, quadrupole vibration and coupling between these collective modes (axial and triaxial quadrupole deformations included)

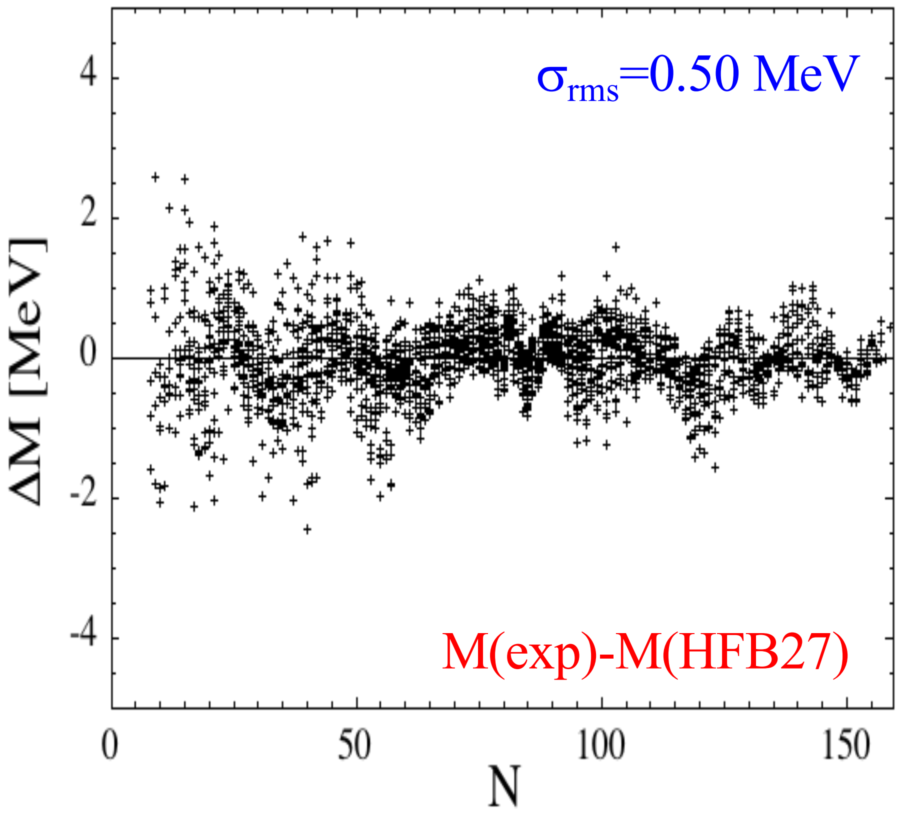
Girod, Berger, Libert, Delaroche

Gogny-HFB mass formula (D1M force)

2457 Masses: σ_{rms}=0.81 MeV (AME'20) with coherent E_{Quad} & E_{HFB} !

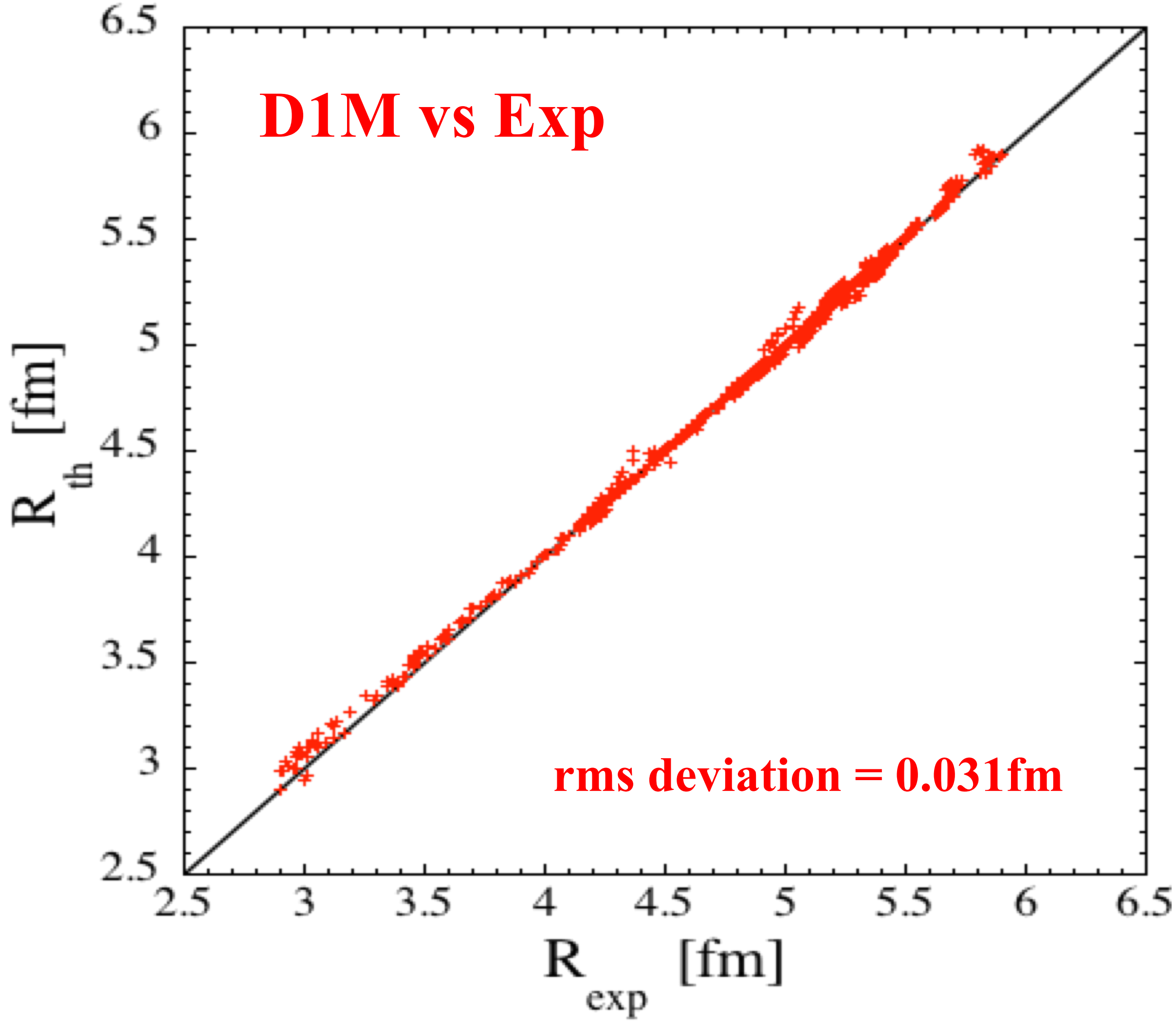
707 Radii: σ_{rms}=0.031 fm (with Quadrupole corrections)





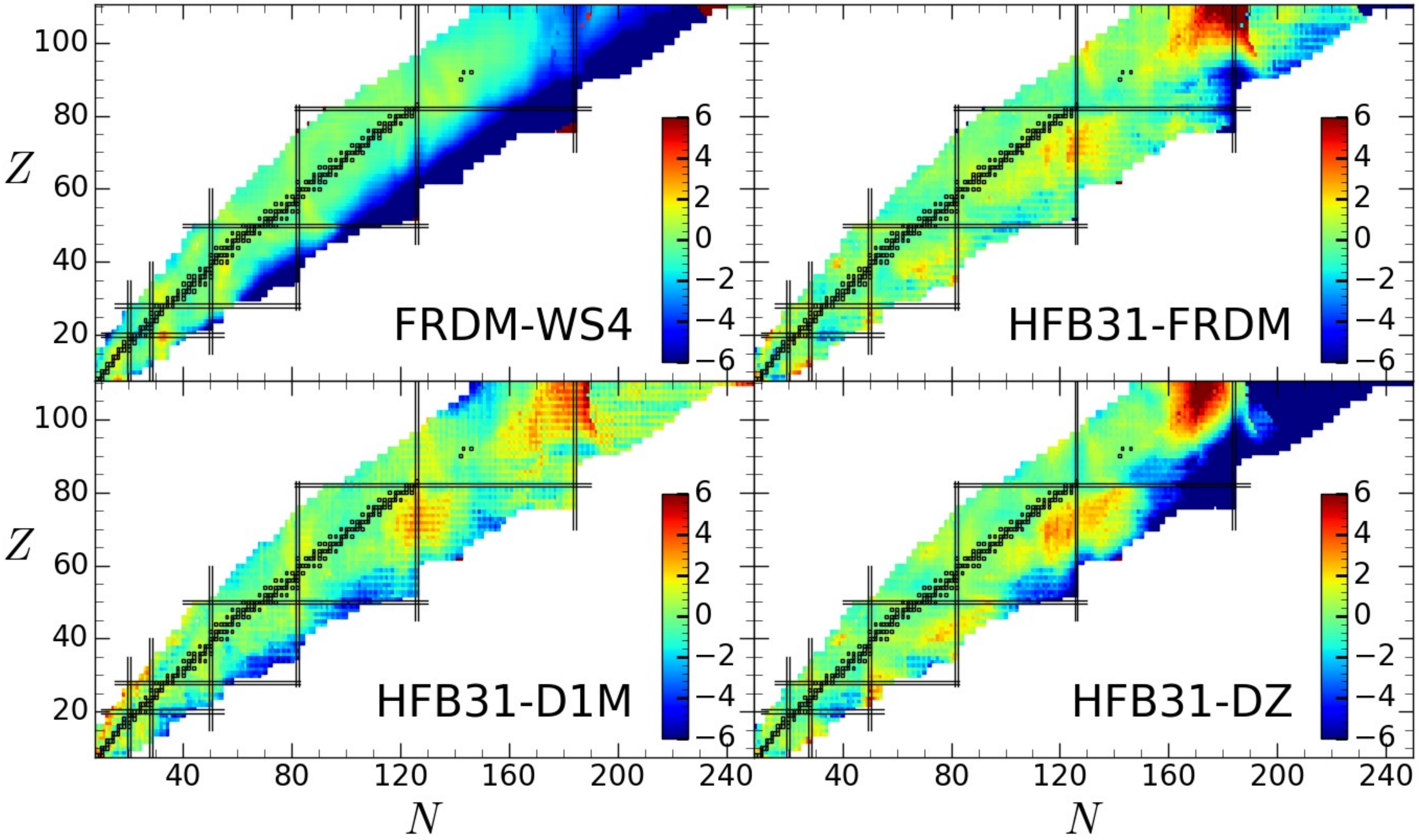
→ It is possible to adjust a Gogny force to reproduce all experimental masses "accurately"

Comparison of charge radii for 707 nuclei



Including the quadrupole correction: $R_{ch} = \sqrt{R_{HFB}^2 + \Delta R_{corr}^2}$

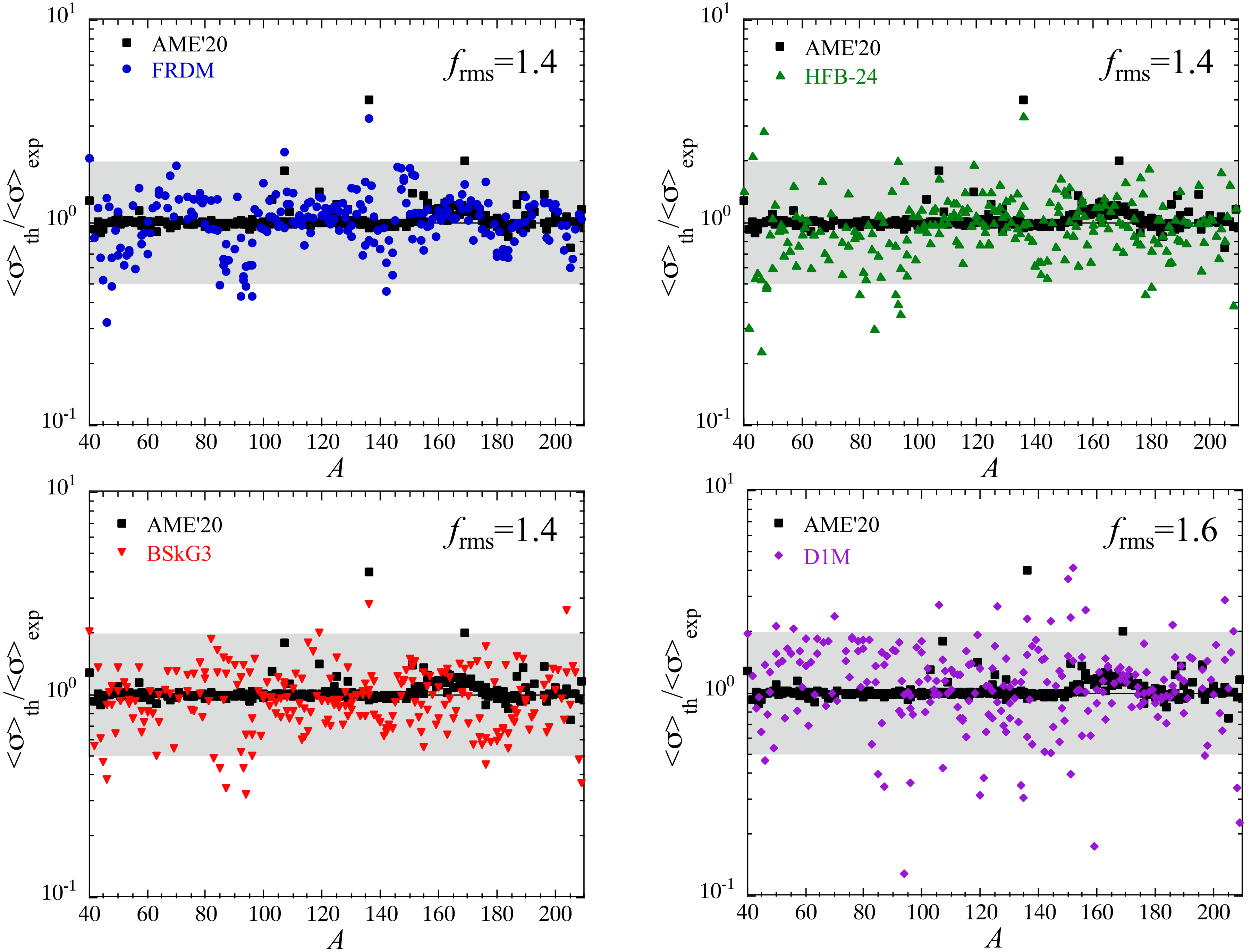
Relative agreement/disagreement between mass models



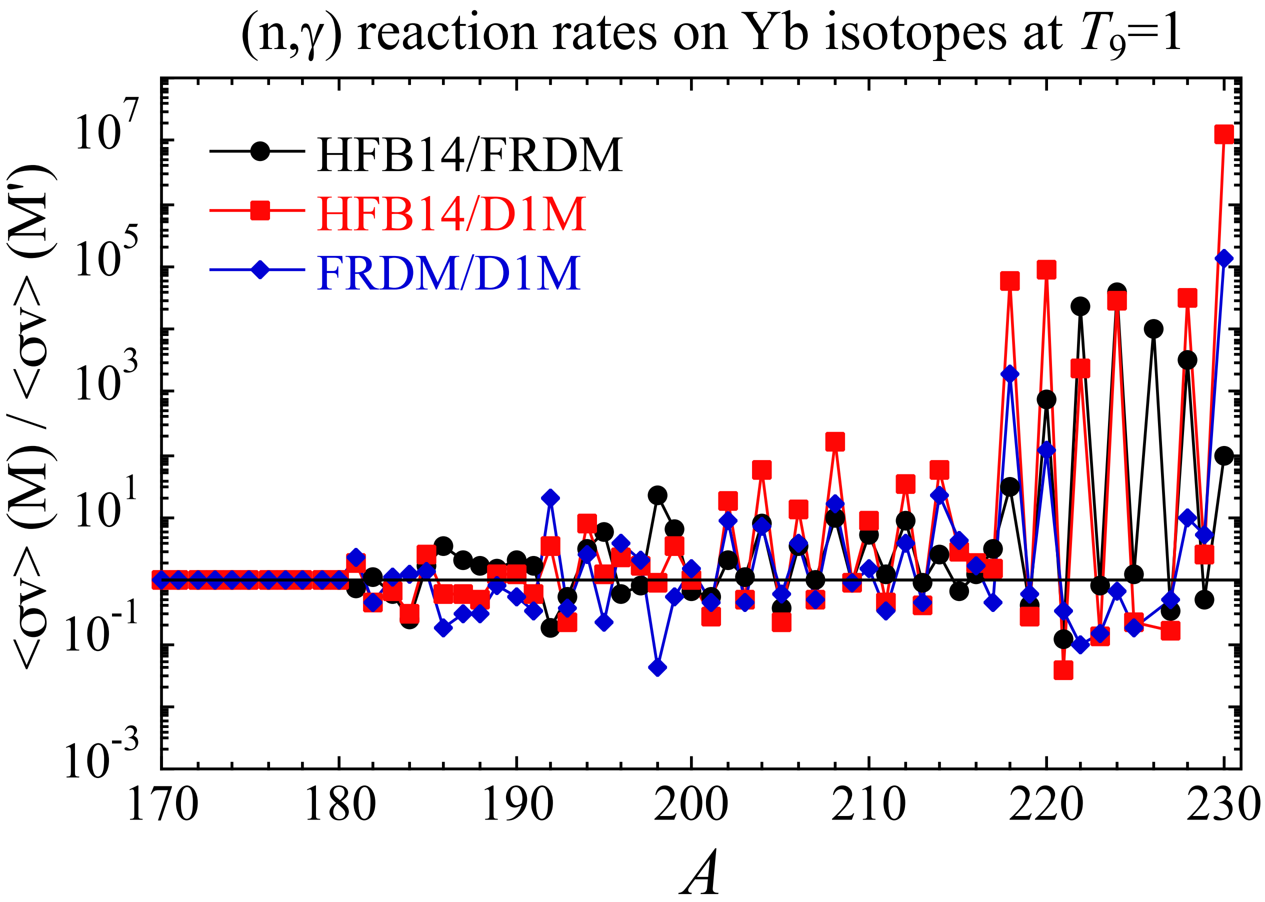
Major differences

- stiffness of the mass parabola
- around magic numbers *N*~126 and *N*~184
- heavy and super-heavy nuclei
- odd-even pairing effects

Impact of masses on experimental MACS <σ>

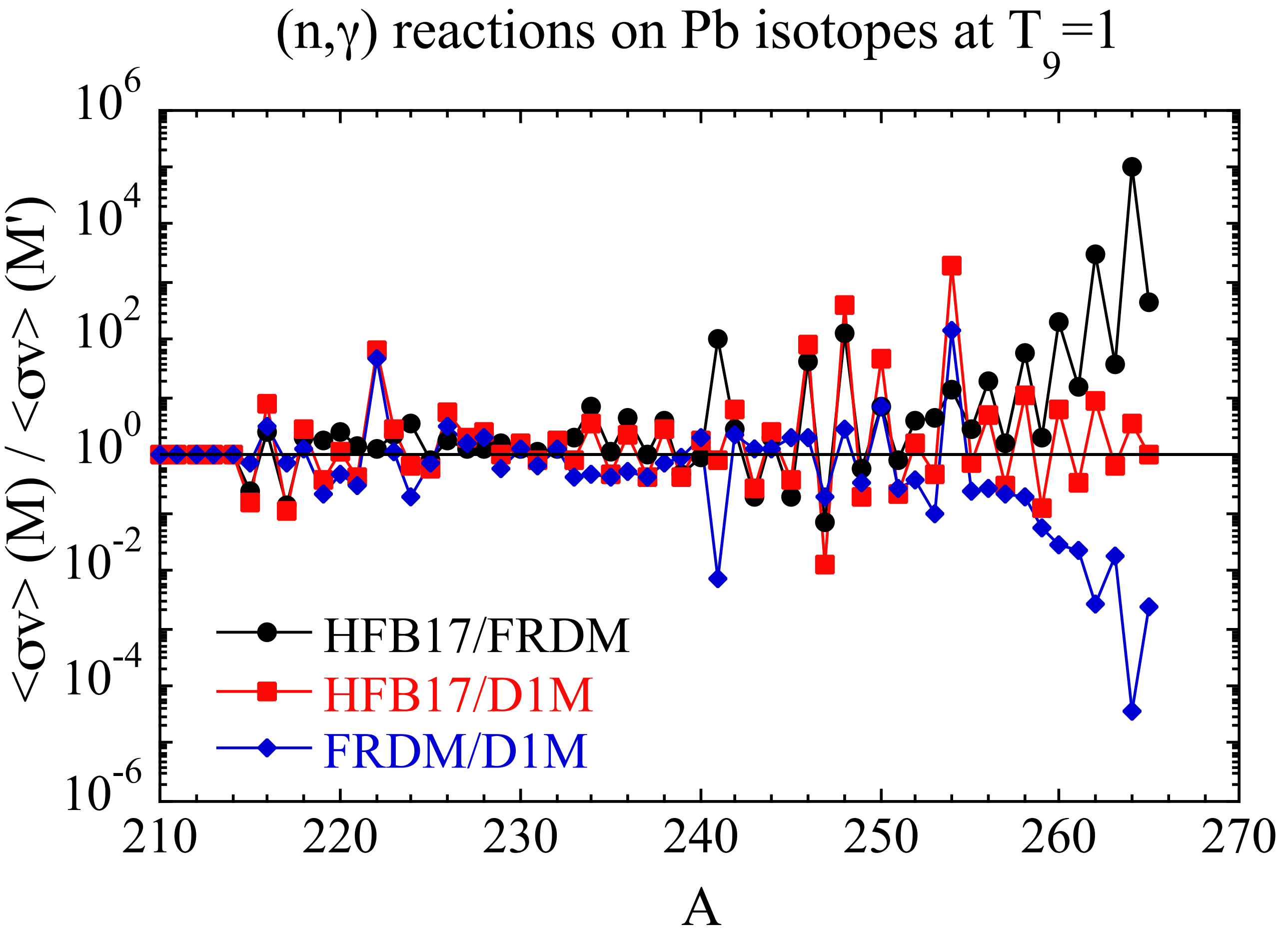


Impact of masses on unknown MACS <σ>



AME'20: masses known till ^{178}Yb

Impact of masses on unknown MACS <σ>



AME'20: masses known till ^{215}Pb

Mass models included in TALYS

- **Default:**
  - Experimental and recommended masses (AME'20)
  - `massmodel=2`: Skyrme-HFB masses, deformations, spins, and parities (HFB-27) → to be replaced by BSkG3 ?

- **Choice:**
  - `massmodel=1`: Finite Range Droplet Model (FRDM) masses and deformations (FRDM'12)
  - `massmodel=3`: Gogny-HFB (D1M) masses, deformation and densities
  - Duflo & Zuker approximation to the Shell Model (for non-tabulated nuclei)

  … or more user-specific choices ...
  e.g. massdir='hfb-32'

⚠ All *Q*-values in reaction codes must be estimated within the same model !

Mass models included in TALYS

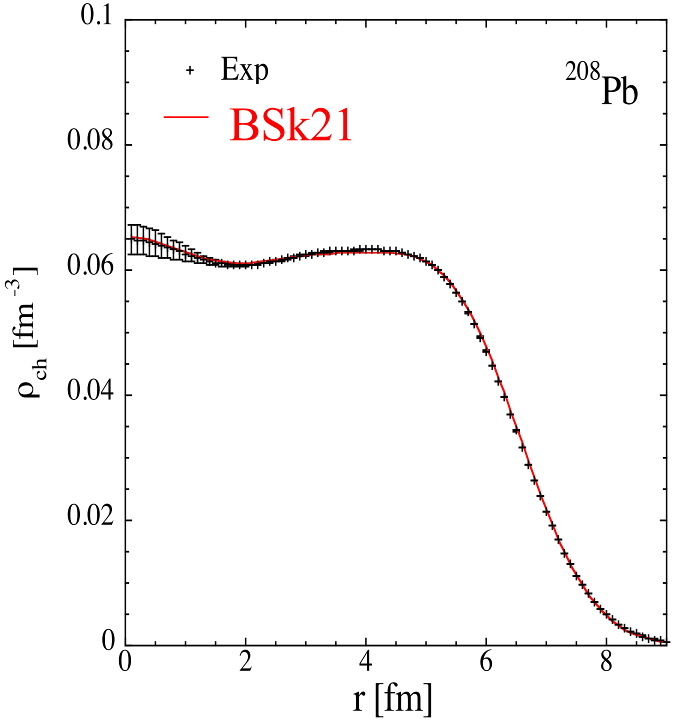
Provides masses but also deformation parameters as well as GS spin and parities

Z	A	M [amu]	M [MeV]	β_2	β_4	J	π	Sym
50	90	90.038334	35.708000	0.0000	0.0000	0.0	1	90Sn
50	91	91.027503	25.619000	-0.0400	0.0100	4.5	1	91Sn
50	92	92.015408	14.352000	0.0000	0.0000	0.0	1	92Sn
50	93	93.005836	5.436000	0.0000	0.0000	4.5	1	93Sn
50	94	93.993988	-5.600000	0.0000	0.0000	0.0	1	94Sn
50	95	94.985581	-13.431000	0.0000	0.0000	4.5	1	95Sn
50	96	95.973592	-24.599000	-0.0400	0.0100	0.0	1	96Sn
50	97	96.965974	-31.695000	0.0000	0.0000	4.5	1	97Sn
50	98	97.955808	-41.165000	0.0000	0.0000	0.0	1	98Sn
50	99	98.946890	-49.472000	0.0500	-0.0100	4.5	1	99Sn
50	100	99.938152	-57.611000	0.0200	0.0000	0.0	1	100Sn
50	101	100.934715	-60.813000	-0.0500	0.0100	2.5	1	101Sn
50	102	101.929810	-65.382000	0.0400	0.0000	0.0	1	102Sn
50	103	102.927732	-67.317000	-0.0900	0.0200	2.5	1	103Sn
50	104	103.922857	-71.858000	0.0600	-0.0100	0.0	1	104Sn
50	105	104.921322	-73.288000	-0.0800	0.0200	2.5	1	105Sn
50	106	105.917163	-77.162000	-0.0900	0.0200	0.0	1	106Sn
50	107	106.915967	-78.276000	-0.0900	0.0100	3.5	1	107Sn
50	108	107.912442	-81.560000	-0.1100	0.0200	0.0	1	108Sn
50	109	108.911800	-82.158000	0.1300	0.0400	3.5	1	109Sn
50	110	109.908689	-85.056000	-0.1200	0.0300	0.0	1	110Sn

Matter densities included in TALYS

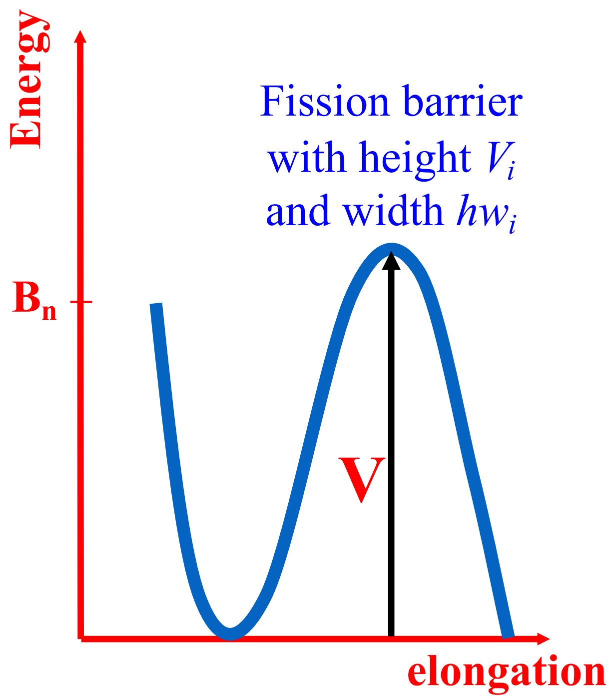
- **Default:**
  - `radialmodel = 2` → Gogny-HFB matter densities (deformed)

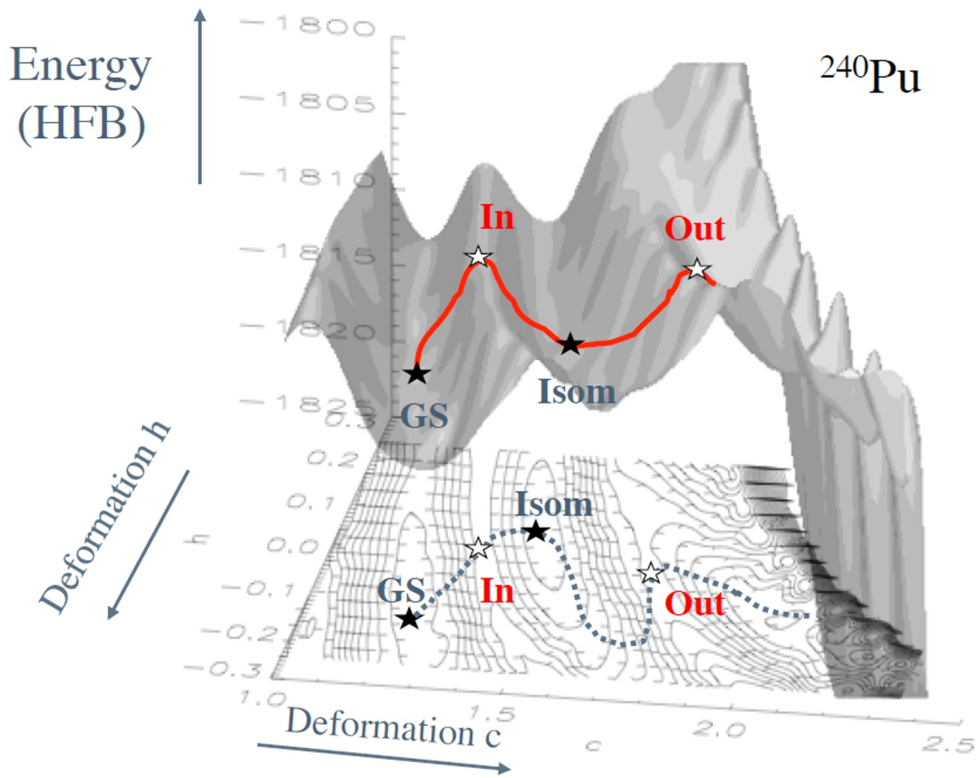
- **Choice:**
  - `radialmodel = 1` → Skyrme-HFB matter densities (spherical)



Nuclear structure in the deformation space

Calculation of the fission path and barriers on the basis of a mass model





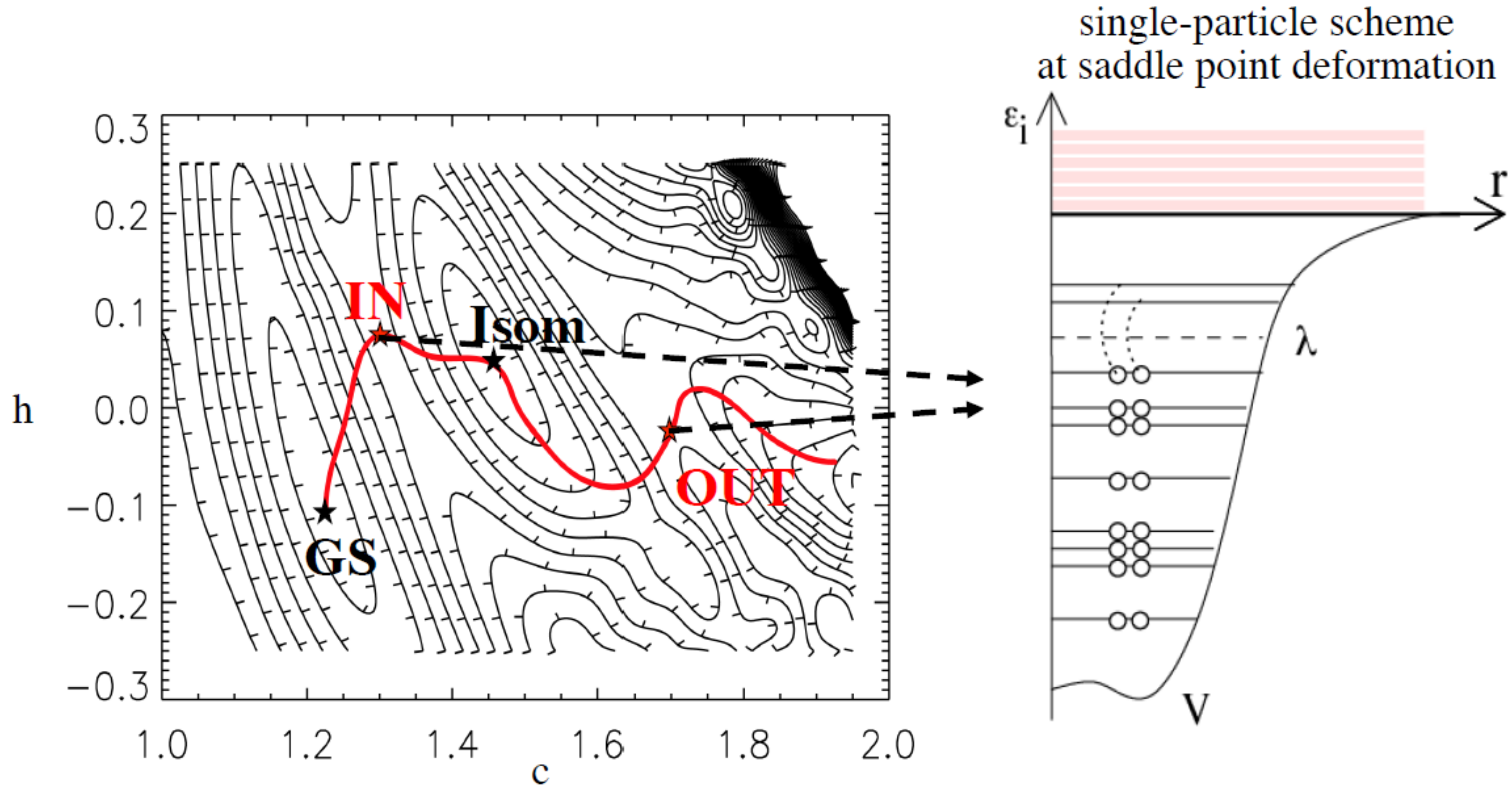
Requires the heights and widths of the fission barriers or more generally the fission path

TALYS can treat triple-hamped fission barriers as well as 1D fission paths

Nuclear structure in the energy space

Nuclear level densities at the saddle points

HFB model provides at each deformation (including saddle points)
all nuclear properties needed to estimate the NLD



But requires a proper description of saddle point properties: SPL, deformation, pairing, MoI, ...

→ cf Lecture of Stephane Hilaire

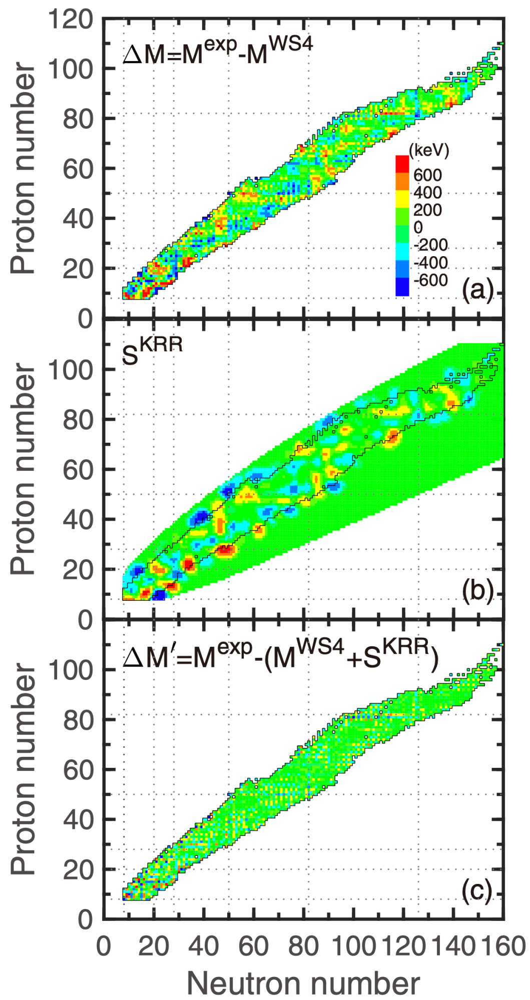
Machine Learning & Nuclear masses

Mass formulas more and more complemented by ML algorithms:
- Baysian Neural Networks
- Kernel Ridge Regression
- Gaussian Processes
- Radial Basis Functions

→ rms to ~ 100-200 keV on all ~2500 known masses

For example

- Wang et al. (2014): WS3/4 with RBF
  → **rms ~ 170 keV**
- Wu et al. (2020, 2021): WS4 with KRR
  → **rms ~ 128 keV**
- Shelley & Pastore (2021) : DZ10 with GP
  → **rms ~ 178 keV**



Wu et al. (2020)

BUT

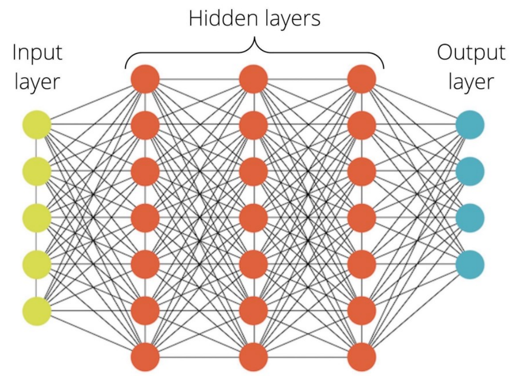
- No mention of number of additional "*hidden*" ML parameters
- Only masses concerned, no other properties (β_2, R, δW, ...)
- Reliability of the extrapolation to unknown masses ?

Test on ML estimate of known masses (no physical model)

(TensorFlow : ~ 5000 "*hidden*" parameters)

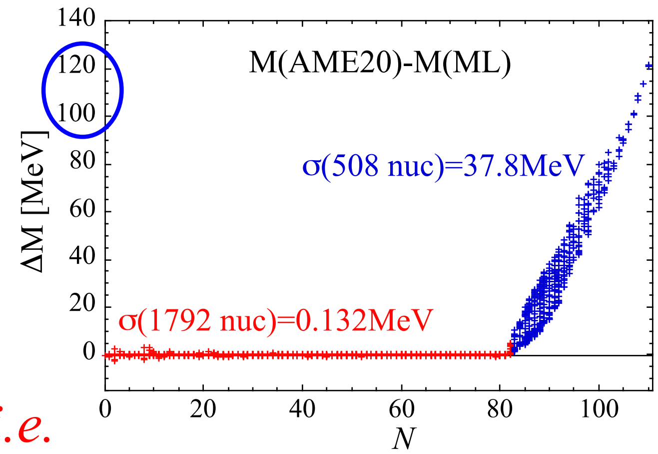
Interpolation test: Random sets of known (AME20) masses

	Nbr	rms[MeV]
TRAIN	2000	0.15
VALIDATION	250	0.59
TEST (not in validation)	250	0.49
ALL	2500	0.28



Extrapolation test: training on $Z < 82$ —> Test on measured $Z \geq 82$

	Nbr	rms[MeV]
TRAIN (*Z*<82)	1792	0.13
VALIDATION (*Z*<82)	250	0.57
TEST (*Z*≥82)	**508**	**37.8**
ALL	2550	16.9



Similar application usually performed wrt "residuals", *i.e.* relative to a given physical model (cf Neufcourt et al. 2018; Niu et al. 2019;Wu et al. 2021)

→ Similar loss of extrapability ? e.g. Capacity to predict new shell effects?

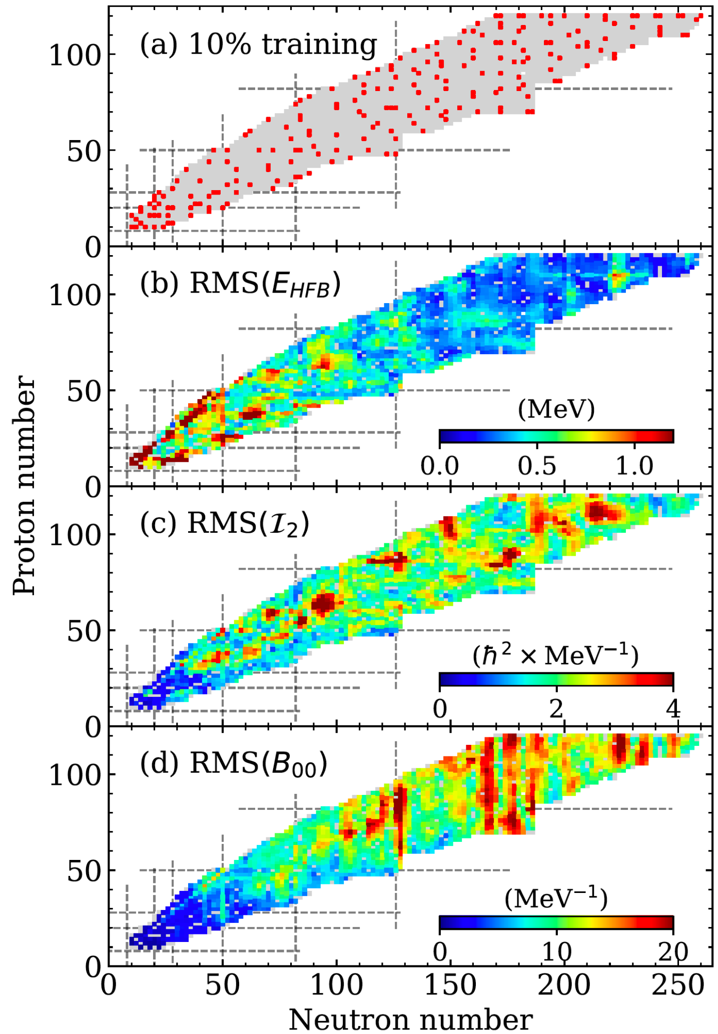
Additionally, successful use of Machine Learning techniques

- **To speed up computer-expensive calculations**
(e.g. HFB +GCM calculations (Lasseri et al. 2020)

↓

High-quality predictions already achieved with only 10% of the total dataset:
rms(E_{HFB}-ML)=0.56MeV on 1890 e-e nuclei

- **To scan the extremely large space of mass model parameters (Scamps et al. 2021)**



CONCLUSION

- Experimental nuclear structure information exist for a limited number of nuclei
- If not experimentally known, be critical about the *accuracy and reliability* of the theoretical model. This is fundamental for nuclear structure properties, i.e. masses, deformation, spin/parities, matter densities, fission properties, ...

These are the building blocks for the prediction of ingredients of relevance in the determination of nuclear reaction cross sections. These include

- nuclear level densities
- γ-ray strengths
- optical potentials
- fission probabilities & yields
- etc …