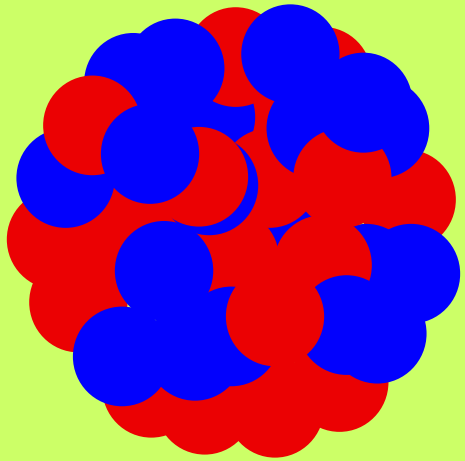
UNEDF Project: Towards a Universal Nuclear Energy Density Functional

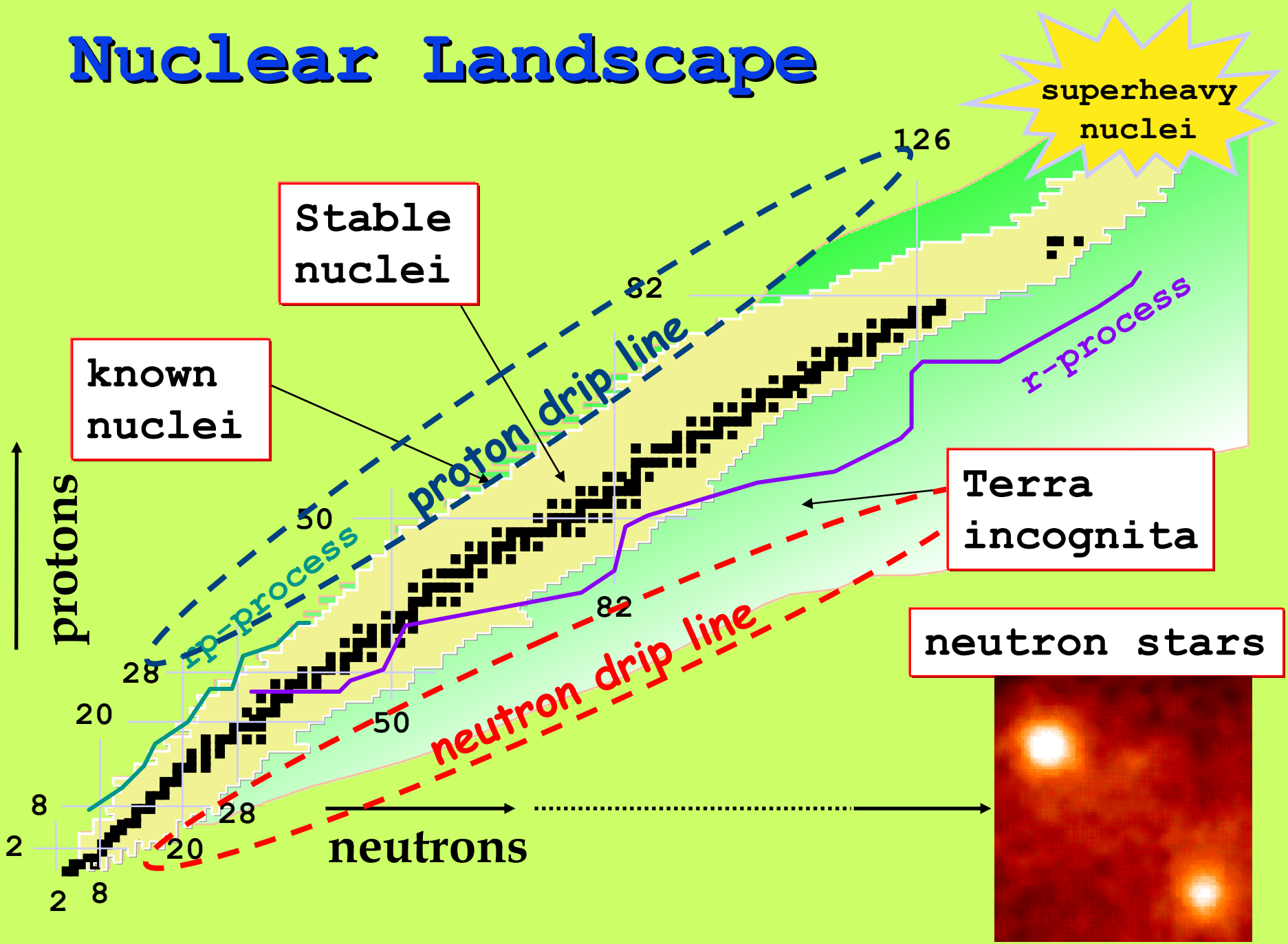
Atomic nucleus



Piotr Magierski

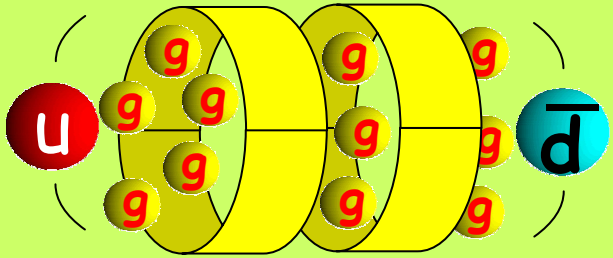
Warsaw University of Technology/University of Washington

Nuclear Landscape

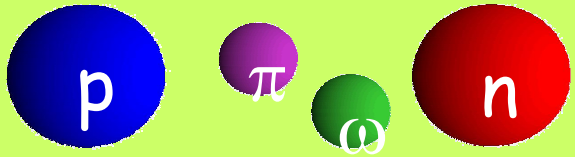


What are the basic degrees of freedom of a nuclear system?

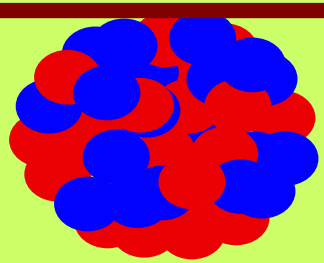
It depends on the energy scale we are interested?



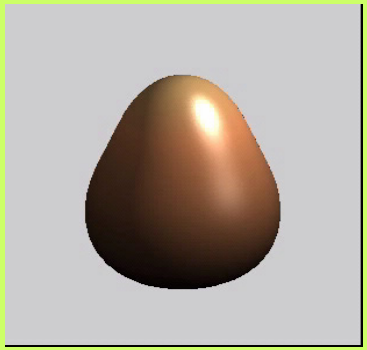
Quarks and gluons
QCD energy scale: 1000MeV



Baryons and mesons
Energy scale: 100MeV



Nucleons
Energy scale: 10MeV

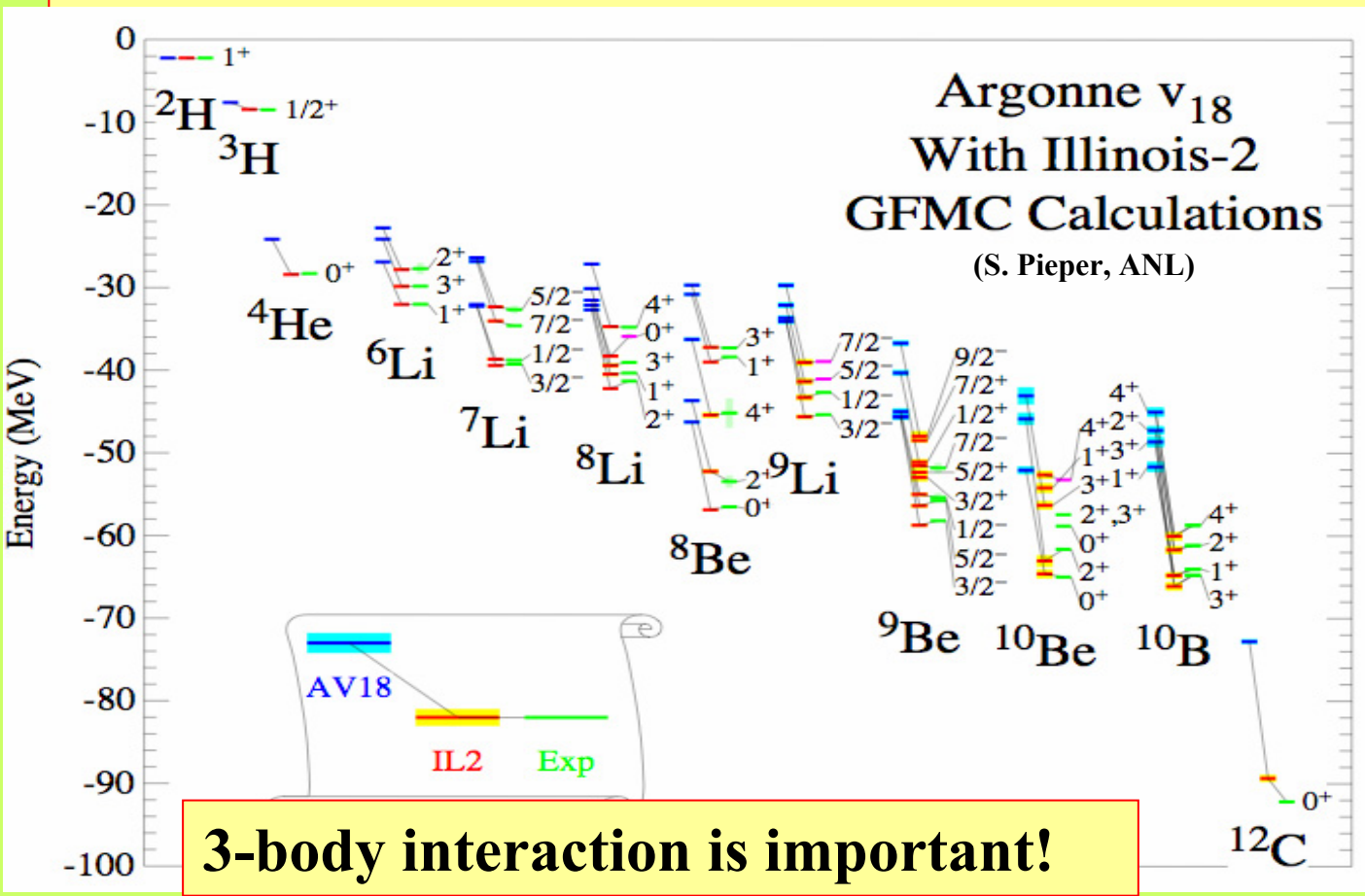


Collective degrees of freedom: 0.1-1MeV

Nucleon-nucleon (N-N) interaction is an effective interaction

$$V = V_{central} + V_{spin} + V_{tensor} + V_{spin-orbit} + V_{3-body}$$

N-N force can be determined (except for the three-body term) from the proton-proton and proton-neutron scattering experiments with some guidance coming from QCD (symmetries).



3-body interaction is important!

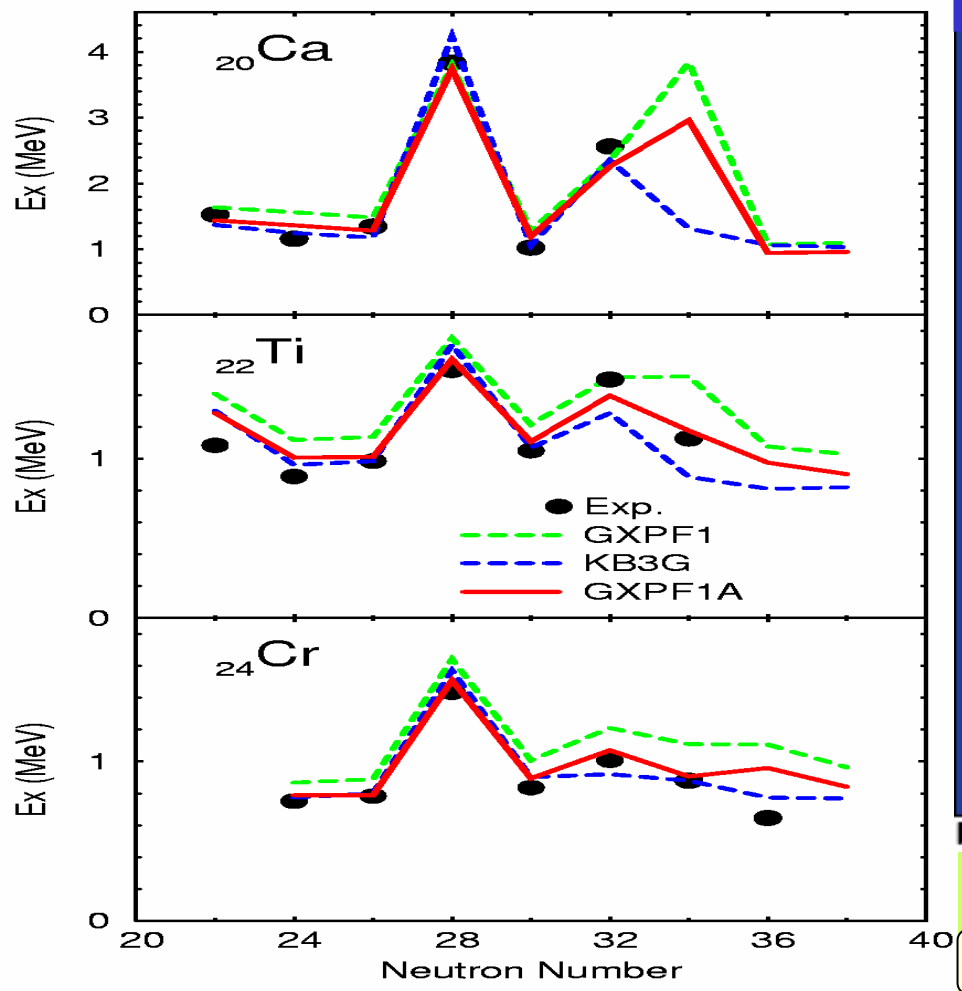
Results of solving Schroedinger eq. with N-N potential.

Blue – only two-body terms included.
Red – two-body and three-body terms.
Green – experiment.

Configuration Interaction (CI)

For heavier nuclei one may solve (stationary) Schroedinger equation in a limited many-body basis (configuration space).

Excitation energies of the lowest 2^+ states. Size of the basis:~10^9



Size of the basis grows rapidly with the number of protons and neutrons.

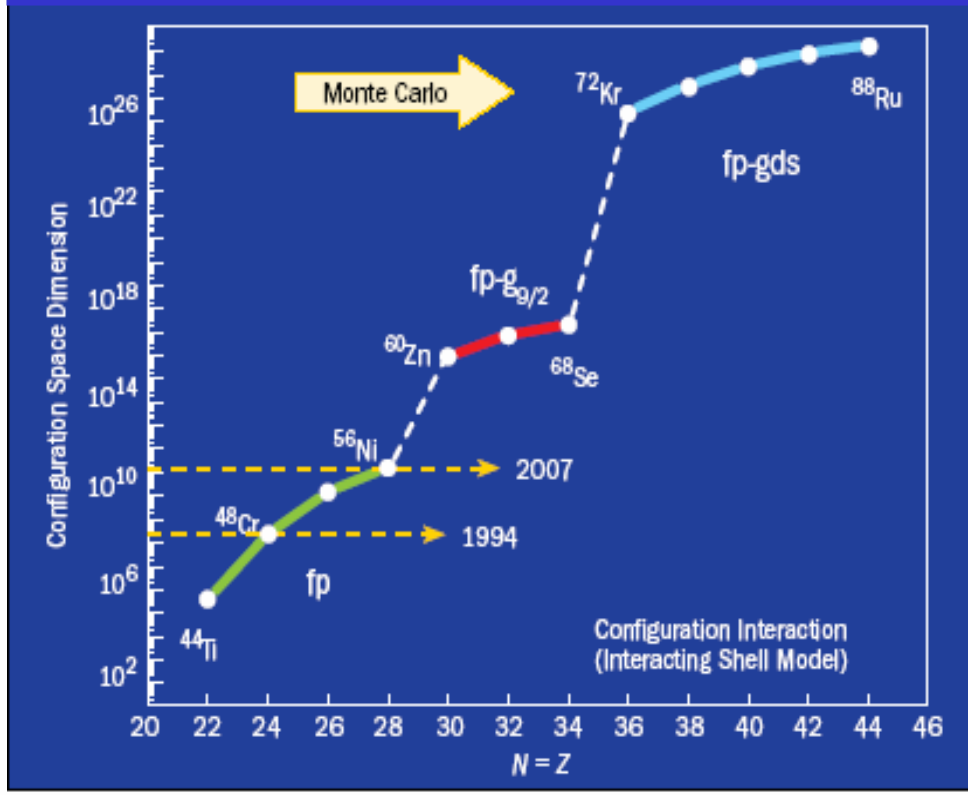


Figure 6. *Configuration space dimension of the interacting shell model for fp-shell nuclei.*

Honma, Otsuka et al., PRC69, 034335 (2004)

Can we calculate the wave function for medium and heavy nuclei?

The radius of a nucleus of mass number A (number of nucleons) is of the order of $R = r_0 A^{1/3}, \; r_0 \approx 1.2\, fm$

In order to make a reliable calculation of the wave function we have to consider a volume at least of the order of

$$V \geq (2R)^3 = 8 r_0^{\,3} A$$

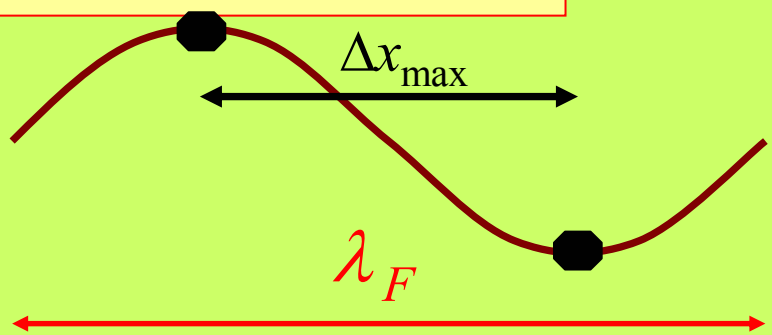
How many points inside the volume V do we need?

From the Fermi gas model:

$$p_F / \hbar = k_F = \left(\frac{3}{2} \pi^2 \rho \right)^{1/3}, \rho \approx 0.16\, fm^{-3} \text{-nuclear saturation density}$$

$\lambda_F = 2\pi / k_F$ – *Fermi wavelength*

$\Delta x_{\max} = \frac{\lambda_F}{2}$ **Maximum distance between points**



Therefore values of the wave function have to be known at least in

$$\frac{V}{(\Delta x_{\max})^3} = \frac{8(k_F r_0)^3}{\pi^3} A \approx A$$

points

But the wave function depends on A variables (disregarding spin):

$$\Psi\left(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A\right)$$

To store the wave function we need to store A^A complex numbers.

For A=100 it means 10^{200} complex numbers

Not possible now and never will be!!!

Nuclear wave function contains too much information

Instead of wave function one may use a density distribution:

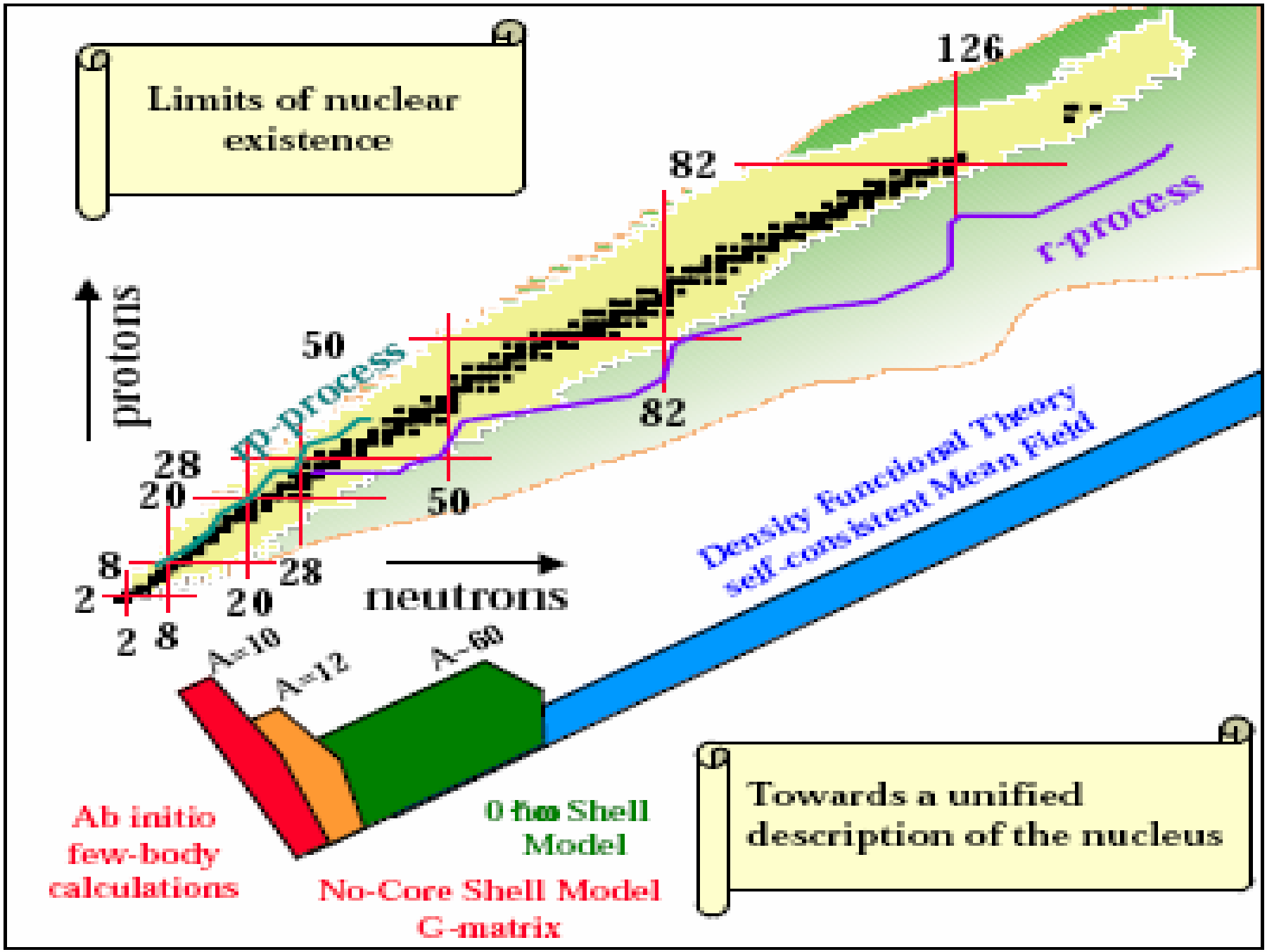
$$\rho(\vec{r},\vec{r}) = \rho(\vec{r}) = \int d^3 r_2 \ldots d^3 r_A \, |\Psi(\vec{r},\vec{r}_2,\ldots,\vec{r}_A)|^2$$

Theorem (Hohenberg & Kohn):

The energy of the nondegenerate ground state of the Fermi system is uniquely determined by its density distribution.

It is sufficient to search for the density functional: $E[\rho(\vec{r})]$

The ground state energy is obtained through the requirement that the functional reaches the minimum value for the ground state density distribution.



From W. Nazarewicz talk

Building blocks of Nuclear Energy Density Functional

In nuclear systems we have to generalize the density functional taking into account also spin and isospin.

$$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)$$ **isoscalar (T=0) density** $(\rho_0 = \rho_n + \rho_p)$

$$\rho_1(\vec{r}) = \rho_1(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)\tau$$ **isovector (T=1) density** $(\rho_1 = \rho_n - \rho_p)$

$$\vec{s}_0(\vec{r}) = \sum \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\sigma_{\sigma'\sigma}$$ **isoscalar spin density**

$$\vec{s}_1(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\sigma_{\sigma'\sigma}\tau$$ **isovector spin density**

$$\vec{j}_T(\vec{r}) = \frac{i}{2}\left(\vec{\nabla}' - \vec{\nabla}\right)\rho_T(\vec{r},\vec{r}')\Big|_{\vec{r}'=\vec{r}}$$ **current density**

$$\vec{\vec{J}}_T(\vec{r}) = \frac{i}{2}\left(\vec{\nabla}' - \vec{\nabla}\right)\otimes \vec{s}_T(\vec{r},\vec{r}')\Big|_{\vec{r}'=\vec{r}}$$ **spin-current tensor density**

$$\tau_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\,\rho_T(\vec{r},\vec{r}')\Big|_{\vec{r}'=\vec{r}}$$ **kinetic density**

$$\vec{\mathbf{T}}_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\;\vec{s}_T(\vec{r},\vec{r}')\Big|_{\vec{r}'=\vec{r}}$$ **kinetic spin density**

Local densities and current

$$\mathcal{H}_T(\vec{r}) = C_T^{\rho}\rho_T^2 + C_T^{s}s_T^2 + C_T^{\Delta\rho}\rho_T\Delta\rho_T + C_T^{\Delta s}\vec{s}_T\Delta\vec{s}_T$$
$$+ C_T^{\tau}\left(\rho_T\tau_T - j_T^2\right) + C_T^{T}\left(\vec{s}_T\cdot\vec{T}_T - \vec{\vec{J}}_T^2\right) + C_T^{\nabla J}\left[\rho_T\vec{\nabla}\cdot\vec{J}_T + \vec{s}_T\cdot\left(\vec{\nabla}\times\vec{j}_T\right)\right]$$

Example: Skyrme Functional

$$E_{tot} = \int\left[\frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\vec{r}) + \mathcal{H}_1(\vec{r})\right]d^3r$$

Total ground-state energy

Pairing field has still to be added...

Construction of the functional

E. Perlinska, S.G. Rohozinski, J. Dobaczewski, and W. Nazarewicz
Phys. Rev. C 69, 014316 (2004)

Density distributions of matter, spin, and current cand be used as fields defining new degrees of freedom that describe the nucleus a a composite particle.

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0(\boldsymbol{r}) + \sum_{t=0,1} \left(\chi_t(\boldsymbol{r}) + \breve{\chi}_t(\boldsymbol{r})\right),$$

p-h density p-p density

Most general, second order expansion in densities and their derivatives

The coupling terms depend on density (=higher-order contact terms which represent high-energy phenomena that are not explicitely important in the nuclear scale)

$$\begin{aligned}
\chi_0(\boldsymbol{r}) &= C_0^{\rho}\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^{\tau}\rho_0\tau_0 + C_0^{J0}J_0^2 + C_0^{J1}\boldsymbol{J}_0^2 + C_0^{J2}\underline{J}_0^2 + C_0^{\nabla J}\rho_0\boldsymbol{\nabla}\cdot\boldsymbol{J}_0 \\
&+ C_0^{s}\boldsymbol{s}_0^2 + C_0^{\Delta s}\boldsymbol{s}_0\cdot\Delta\boldsymbol{s}_0 + C_0^{T}\boldsymbol{s}_0\cdot\boldsymbol{T}_0 + C_0^{j}\boldsymbol{j}_0^2 + C_0^{\nabla j}\boldsymbol{s}_0\cdot(\boldsymbol{\nabla}\times\boldsymbol{j}_0) + C_0^{\nabla s}(\boldsymbol{\nabla}\cdot\boldsymbol{s}_0)^2 + C_0^{F}\boldsymbol{s}_0\cdot\boldsymbol{F}_0, \\
\chi_1(\boldsymbol{r}) &= C_1^{\rho}\vec{\rho}^{\,2} + C_1^{\Delta\rho}\vec{\rho}\circ\Delta\vec{\rho} + C_1^{\tau}\vec{\rho}\circ\vec{\tau} + C_1^{J0}\vec{J}^2 + C_1^{J1}\vec{\boldsymbol{J}}^2 + C_1^{J2}\vec{\underline{J}}^{\,2} + C_1^{\nabla J}\vec{\rho}\circ\boldsymbol{\nabla}\cdot\vec{\boldsymbol{J}} \\
&+ C_1^{s}\vec{\boldsymbol{s}}^2 + C_1^{\Delta s}\vec{\boldsymbol{s}}\cdot\circ\Delta\vec{\boldsymbol{s}} + C_1^{T}\vec{\boldsymbol{s}}\cdot\circ\vec{\boldsymbol{T}} + C_1^{j}\vec{\boldsymbol{\jmath}}^2 + C_1^{\nabla j}\vec{\boldsymbol{s}}\cdot\circ(\boldsymbol{\nabla}\times\vec{\boldsymbol{\jmath}}) + C_1^{\nabla s}(\boldsymbol{\nabla}\cdot\vec{\boldsymbol{s}})^2 + C_1^{F}\vec{\boldsymbol{s}}\cdot\circ\vec{\boldsymbol{F}}, \\
\breve{\chi}_0(\boldsymbol{r}) &= \breve{C}_0^{s}|\breve{\boldsymbol{s}}_0|^2 + \breve{C}_0^{\Delta s}\Re\left(\breve{\boldsymbol{s}}_0^{*}\cdot\Delta\breve{\boldsymbol{s}}_0\right) + \breve{C}_0^{T}\Re\left(\breve{\boldsymbol{s}}_0^{*}\cdot\breve{\boldsymbol{T}}_0\right) \\
&+ \breve{C}_0^{j}|\breve{\boldsymbol{\jmath}}_0|^2 + \breve{C}_0^{\nabla j}\Re\left(\breve{\boldsymbol{s}}_0^{*}\cdot(\boldsymbol{\nabla}\times\breve{\boldsymbol{\jmath}}_0)\right) + \breve{C}_0^{\nabla s}|\boldsymbol{\nabla}\cdot\breve{\boldsymbol{s}}_0|^2 + \breve{C}_0^{F}\Re\left(\breve{\boldsymbol{s}}_0^{*}\cdot\breve{\boldsymbol{F}}_0\right), \\
\breve{\chi}_1(\boldsymbol{r}) &= \breve{C}_1^{\rho}|\vec{\breve{\rho}}|^2 + \breve{C}_1^{\Delta\rho}\Re\left(\vec{\breve{\rho}}^{\,*}\circ\Delta\vec{\breve{\rho}}\right) + \breve{C}_1^{\tau}\Re\left(\vec{\breve{\rho}}^{\,*}\circ\vec{\breve{\tau}}\right) \\
&+ \breve{C}_1^{J0}|\vec{\breve{J}}|^2 + \breve{C}_1^{J1}|\vec{\breve{\boldsymbol{J}}}|^2 + \breve{C}_1^{J2}|\vec{\underline{\breve{J}}}|^2 + \breve{C}_1^{\nabla J}\Re\left(\vec{\breve{\rho}}^{\,*}\circ\boldsymbol{\nabla}\cdot\vec{\breve{\boldsymbol{J}}}\right).
\end{aligned}$$

Not all terms are equally important! Some probe specific observables!

Example: pairing mean field

$$\begin{aligned}
\breve{h}_0(\boldsymbol{r};s',s) &= \breve{\boldsymbol{\Sigma}}_0\cdot\hat{\boldsymbol{\sigma}}_{s's} + \tfrac{1}{2i}\left\{\boldsymbol{\nabla}\cdot\breve{\boldsymbol{I}}_0\delta_{s's} + \breve{\boldsymbol{I}}_0\delta_{s's}\cdot\boldsymbol{\nabla}\right\} - \boldsymbol{\nabla}\cdot\left[\breve{C}_0\cdot\hat{\boldsymbol{\sigma}}_{s's}\right]\boldsymbol{\nabla} - \boldsymbol{\nabla}\cdot\breve{\boldsymbol{D}}_0\,\hat{\boldsymbol{\sigma}}_{s's}\cdot\boldsymbol{\nabla}, \\
\vec{\breve{h}}(\boldsymbol{r};s',s) &= \vec{\breve{U}}(\boldsymbol{r})\delta_{s's} + \tfrac{1}{2i}\left\{\boldsymbol{\nabla}\cdot\left[\vec{\mathsf{B}}(\boldsymbol{r})\cdot\hat{\boldsymbol{\sigma}}_{s's}\right] + \left[\vec{\mathsf{B}}(\boldsymbol{r})\cdot\hat{\boldsymbol{\sigma}}_{s's}\right]\cdot\boldsymbol{\nabla}\right\} - \boldsymbol{\nabla}\cdot\vec{\breve{M}}\delta_{s's}\boldsymbol{\nabla}.
\end{aligned}$$

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

5-year project
(Second year just passed)

Director: George Bertsch, University of Washington

Ames National Laboratory - M. Sosonkina
Argonne National Laboratory - M. Pervin, S. Pieper, R. Wiringa, E. (Rusty) Lusk, J. Moré, B. Norris
Lawrence Berkeley National Laboratory - E. Ng, P. Sternberg, C. Yang
Lawrence Livermore National Laboratory - J. Escher, P. Navratil, E. Ormand, S. Quaglioni, G. Stoitcheva, I. Thompson
Los Alamos National Laboratory - J. Carlson, M. Dupuis, T. Kawano, P. Möller
Oak Ridge National Laboratory - G. Arbanas, D. Dean, G. Fann, G. Hagen, K. Roche, W. Shelton
Central Michigan University - Z. Gao, M. Horoi
Iowa State University - P. Maris, J. Vary
Michigan State University - S. Bogner, B. Alex Brown, R. Sen'kov
University of North Carolina at Chapel Hill - J. Engel, J. Terasaki
Ohio State University - R. Furnstahl, L. Platter
San Diego State University - C. Johnson
Texas A&M Commerce - C. Bertulani
University of Tennessee - W. Nazarewicz, T. Papenbrock, N. Schunck, M. Stoitsov
University of Washington - G. Bertsch, A. Bulgac, S.-Y. Chang

M. Bender (Bordeaux, France)
J. Dobaczewski (Warsaw, Poland; Jvyäskylä, Finland)
T. Duguet (Saclay, France),
H. Goutte (Bruyères-le Châtel, France)
P.-H. Heenen (Brussels, Belgium)
P. Magierski (Warsaw, Poland)
T. Nakatsukasa (RIKEN, Japan)
A. Schwenk (TRIUMF, Canada)
A. Shirokov (Moscow State University and Iowa State University)

Color denotes:

- Physics
- Computer Science & Applied Mathematics
- Foreign Collaborators

Sponsoring Agencies

- Scientific Discovery through Advanced Computing (SciDAC)
- Office of Science, the U.S. Department of Energy (DOE)
- National Nuclear Security Administration (NNSA)
- The Office of Advanced Scientific Computing Research (ASCR)

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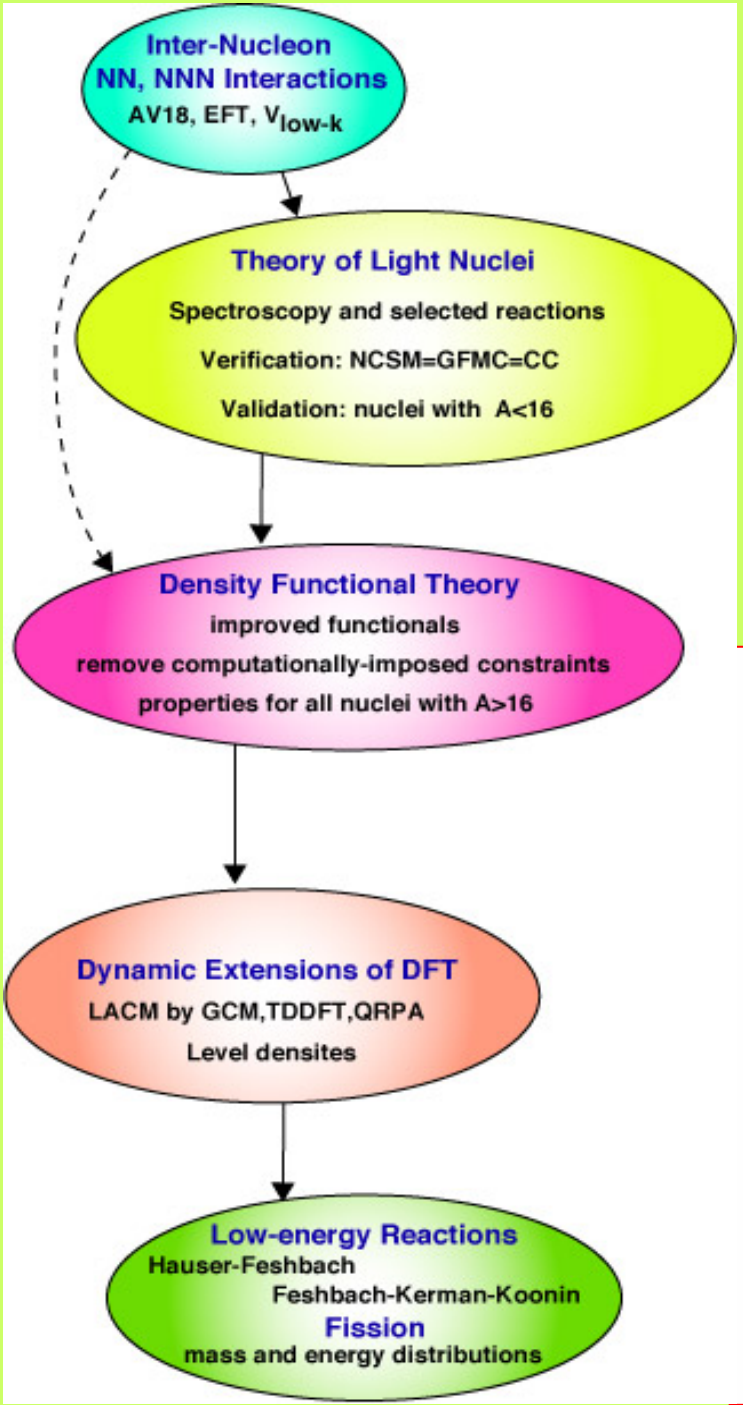
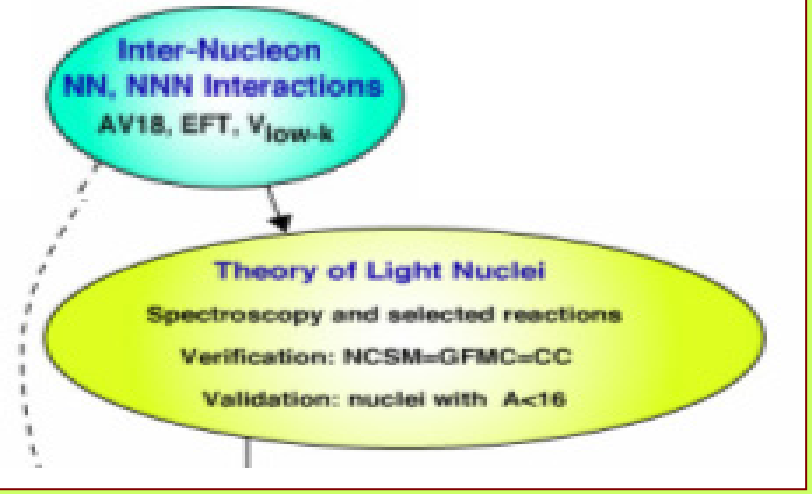


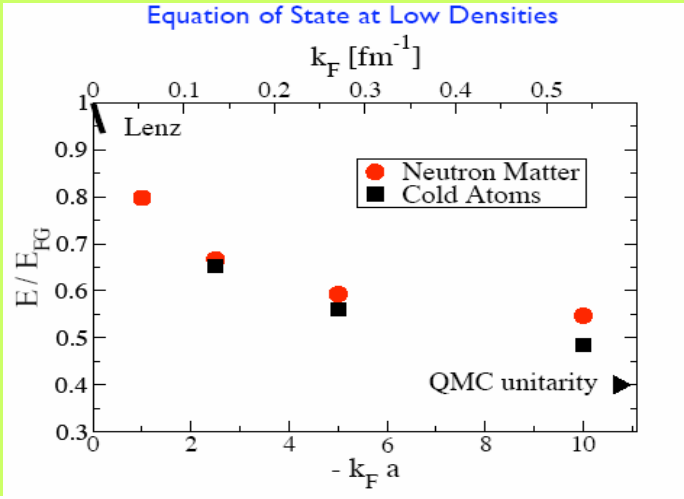
Goals

- First, to find an optimal functional using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- Second, to apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure data.
- Third, to apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.

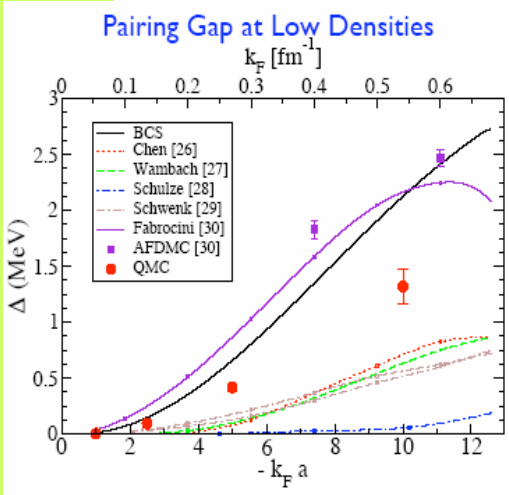


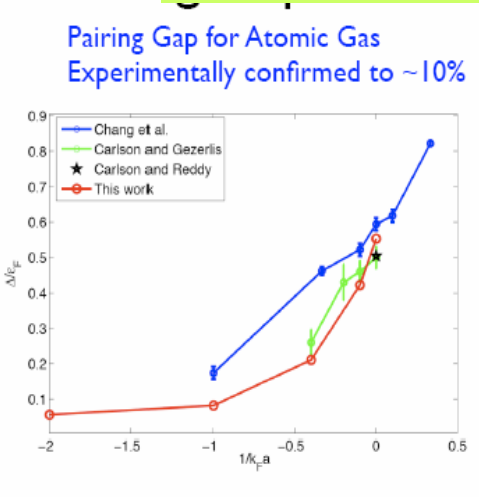
Constraints on the density functional from ab-initio approaches

Equation of state of dilute neutron matter:



Pairing gap in dilute neutron matter:





Ab-initio calculations in medium mass nuclei:

Coupled Cluster (CC) method and Configuration Interaction (CI) method has to agree with each other up to 1% error (in binding energy) for the following nuclei: ^{8}He, ^{16}O, ^{40}Ca.

Ab-inition calculations should agree with Density Functional Theory with respect to:

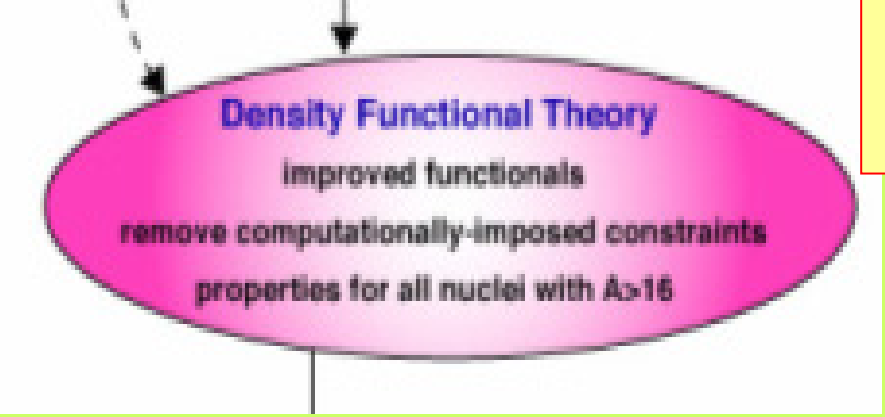
-one body density matrix,

-binding energy,

-energy as a function of various external fields: monopole, quadrupole, etc.

-energy as a function of isospin degree of freedom,

-energy as a function of general density perturbations.



Density Functional Theory (DFT) And Applications

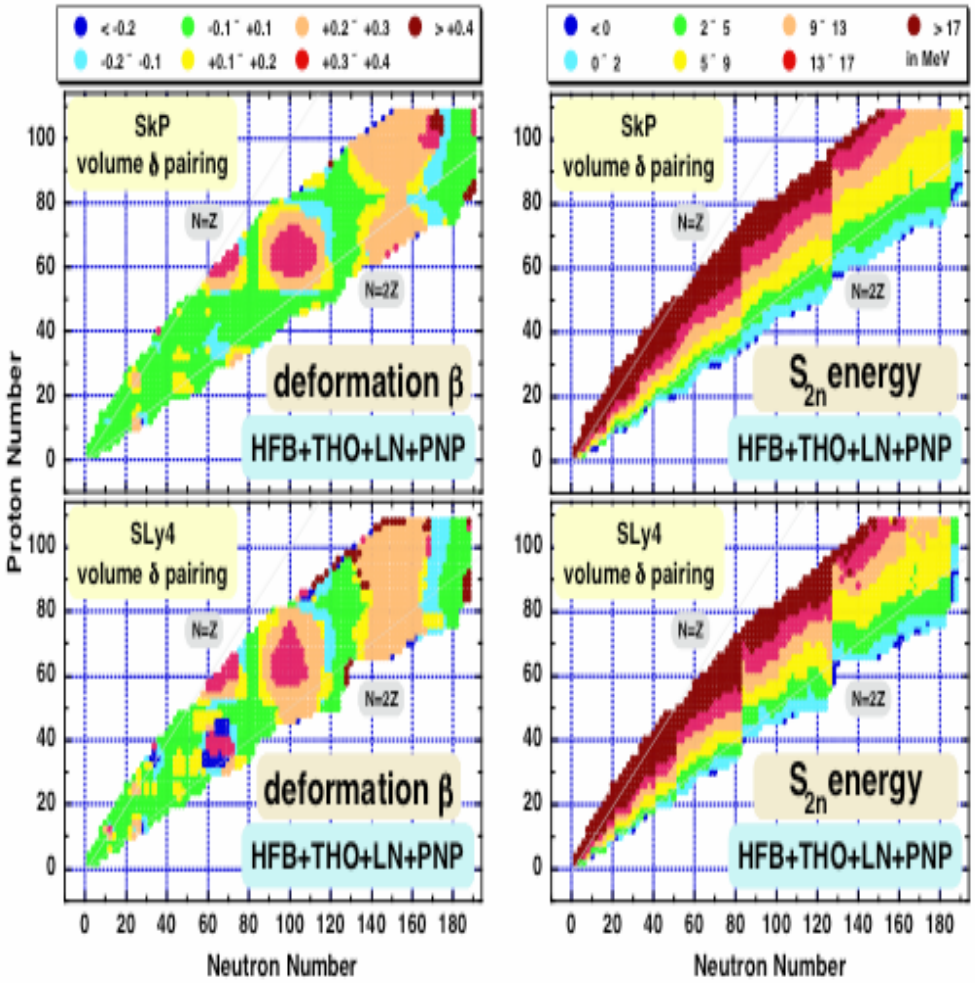
Present status:

- There is entire ZOO of parametrizations of nuclear DFT.
- The role of various terms in DFT is still not well understood.
- DFT works well for differences.
- Dependence of DFT on pairing fields is poorly known.
- Present accuracy of nuclear mass determination is of the order of 700 keV (above 2500 nuclei were calculated).

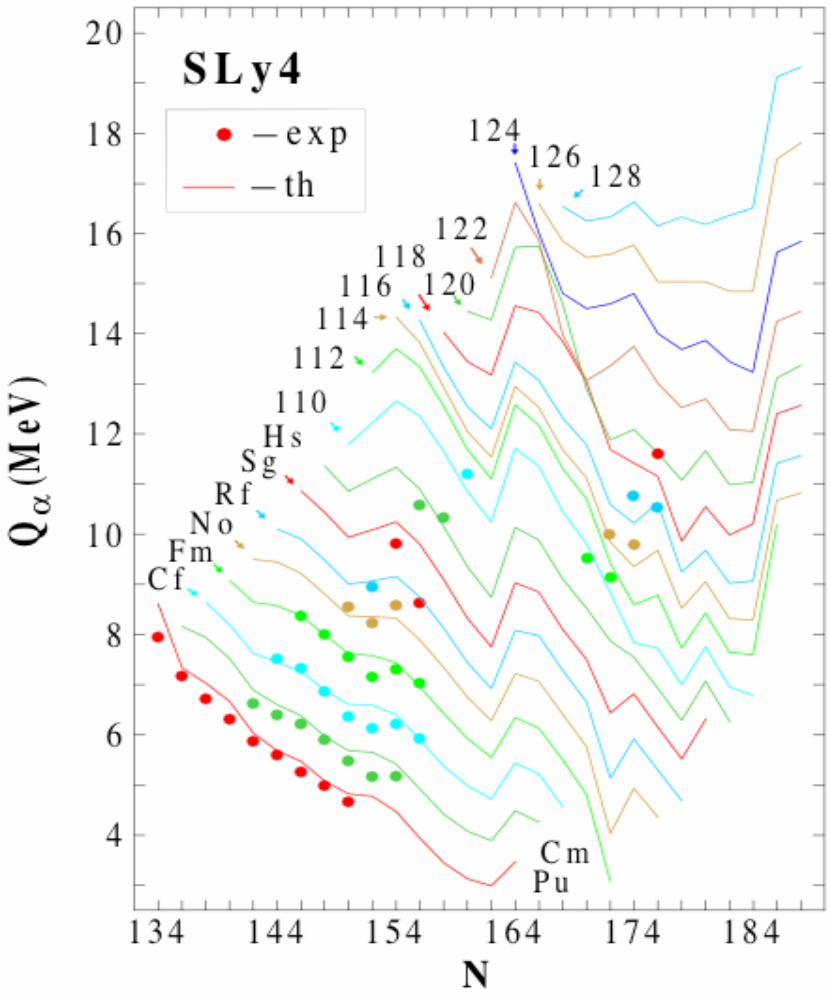
Examples

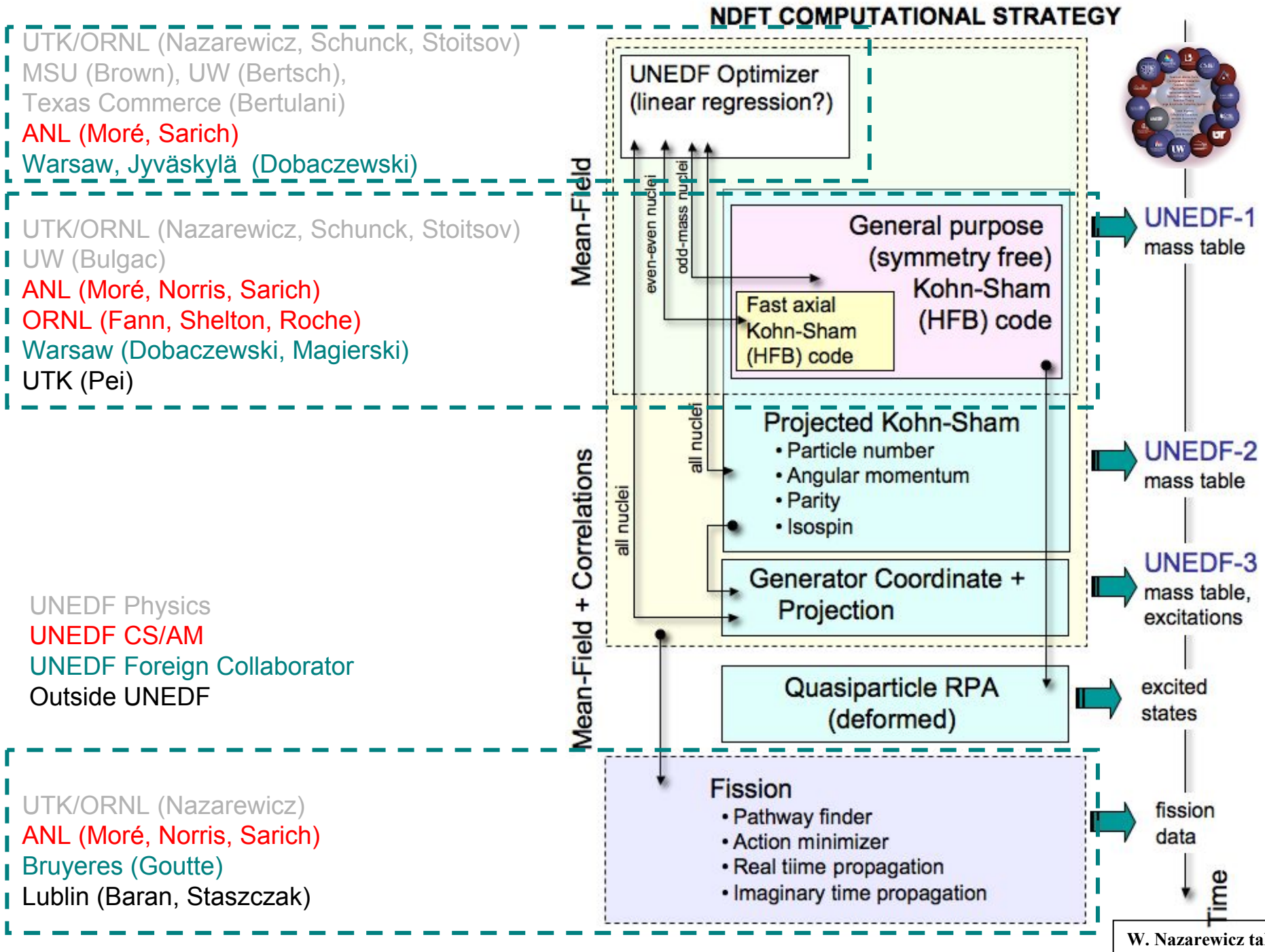
Microscopic Mass Table

Stoitsov et al., PRL 98, 132502 (2007)



S. Cwiok, P.H. Heenen, W. Nazarewicz
Nature, 433, 705 (2005)





W. Nazarewicz talk

Construction of 3-D DFT Solvers

The important part of the project is to develop numerical codes which solve with controllable accuracy the stationary nuclear many-body problem using the energy density functional theory.
The following requirements have to be met:

-No symmetry limitations: any nuclear shape has to be tractable with the same accuracy.

-No assumed time-reversal invariance: odd and even nuclear systems are treated on the same footing.

-Coordinate representation (DVR basis or adaptive basis): The wave function and nuclear densities are represented on the spatial lattice.

-Parallelization: The code is supposed to run on the largest contemporary computer clusters and therefore the computational task has to be efficiently split into many processors.

Computational issues (solved thanks to Physics-Computer Science partnership).

- Optimization techniques for nuclear structure DFT codes
- Solving large-scale systems of nonlinear equations
- Evaluation of performance and scalability in DFT calculations
- Evaluation of derivative-free methods for noisy, nonlinear problems
- 3-D adaptive multi-resolution method for atomic nuclei (Madness)

Example: Computational Complexity of Large Scale Mass Table Calculations

M. Stoitsov; HFB+LN mass table, HFBTHO

Even-Even Nuclei

- The SkM* mass table contains 2525 even-even nuclei
- A single processor calculates each nucleus 3 times (prolate, oblate, spherical) and records all nuclear characteristics and candidates for blocked calculations in the neighbors
- Using 2,525 processors - about 4 CPU hours (1 CPU hour/configuration)

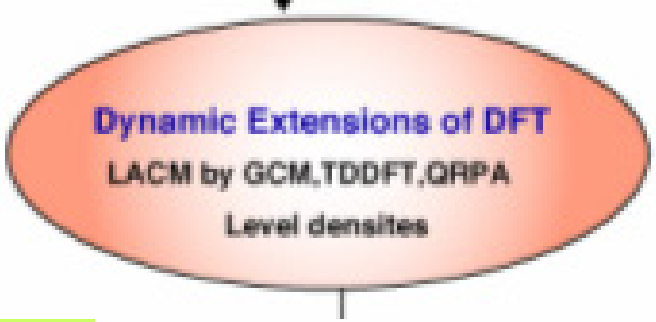
Jaguar Cray XT4 at ORNL

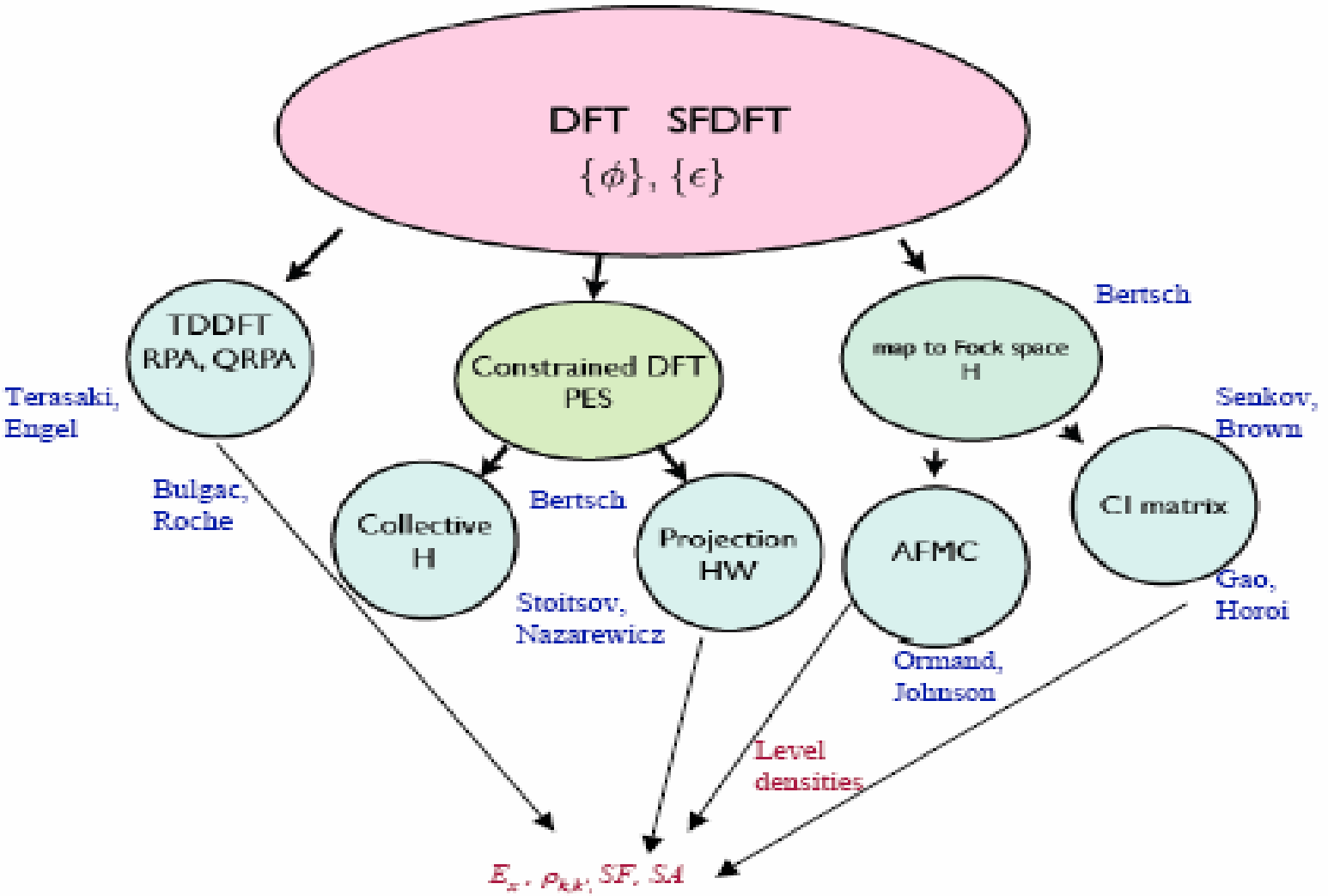
All Nuclei

- 9,210 nuclei
- 599,265 configurations
- Using 3,000 processors - about 25 CPU hours

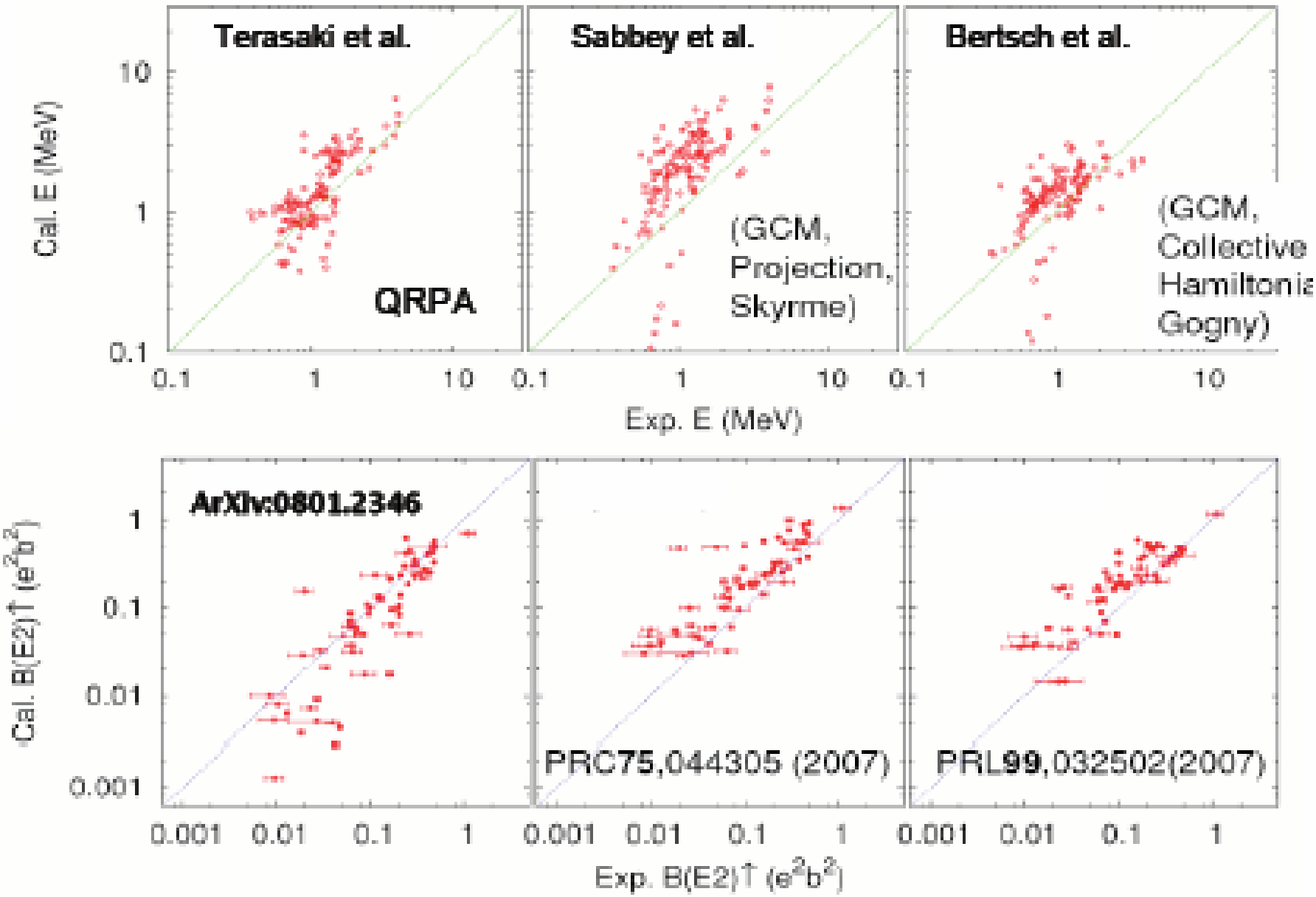
Number of processors > number of nuclei!

Dynamic extension of Density Functional Theory





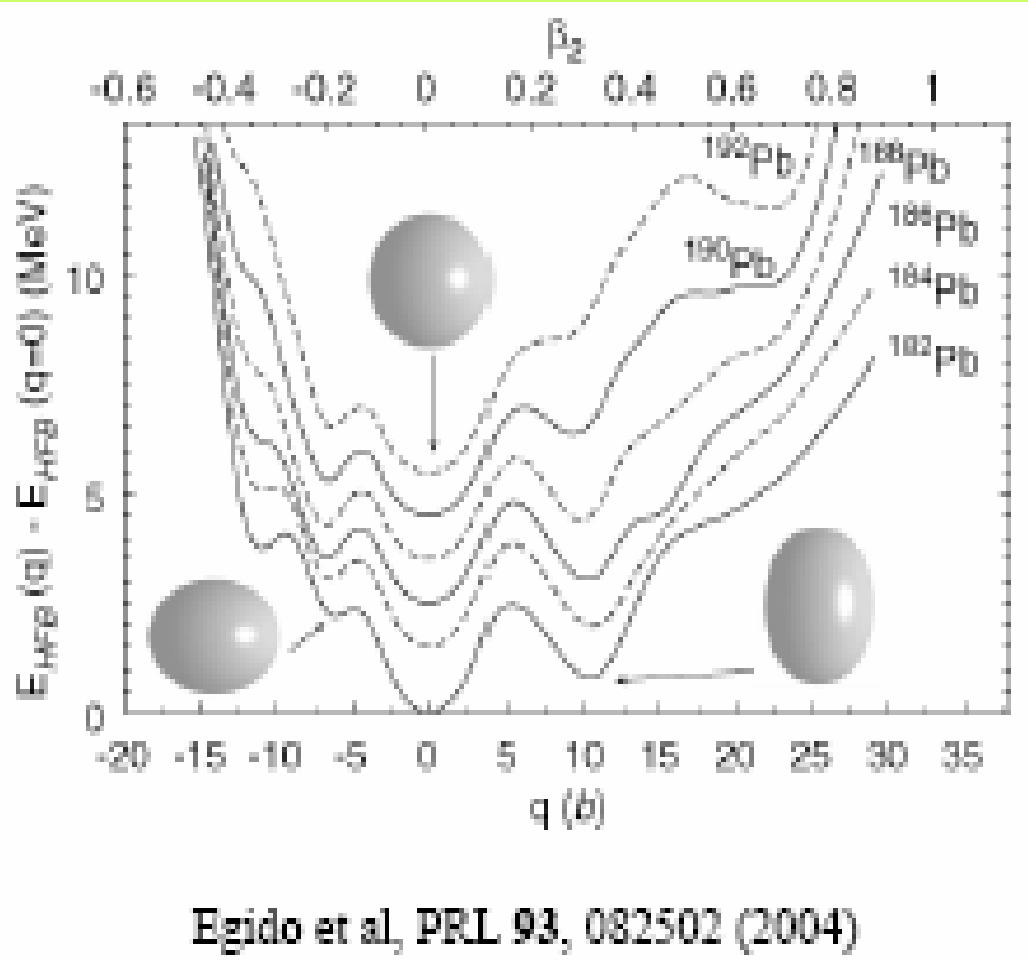
Global calculations of the lowest 2^+ states (present status)



See also Ela Ganioğlu's talk later today

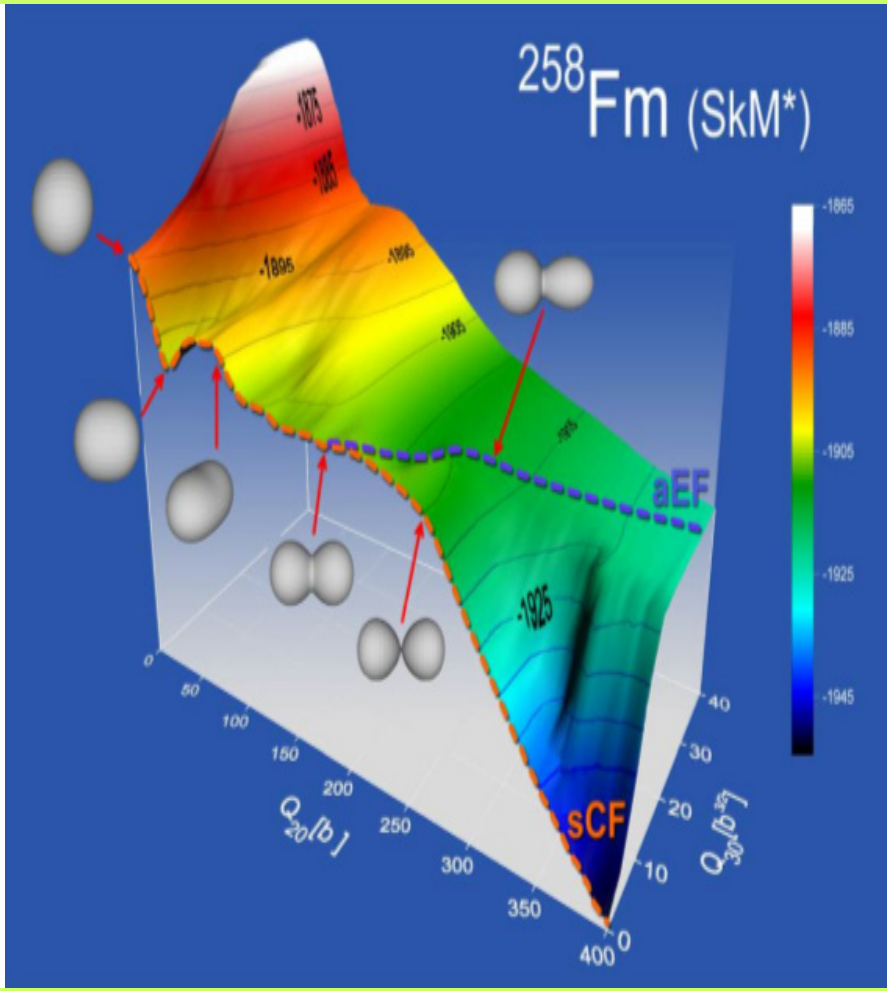
Main challenges

Description of shape coexistence:



Egido et al, PRL 93, 082502 (2004)

Descipription of spontaneous fission process:



What makes us believe we can make a breakthrough?

- Solid microscopic foundation
  - ❖ link to ab-initio approaches
  - ❖ limits obeyed (e.g., unitary regime)
- Unique opportunities provided by coupling to CS/AM
- Comprehensive phenomenology probing crucial parts of the functional
  - ❖ different observables probing different physics
- Stringent optimization protocol providing not only the coupling constants but also their uncertainties (theoretical errors)
- Unprecedented international effort

Conclusion:
we can deliver a well theoretically founded Energy Density Functional, of spectroscopic quality, for structure and reactions, based on as much as possible ab initio input at this point in time.