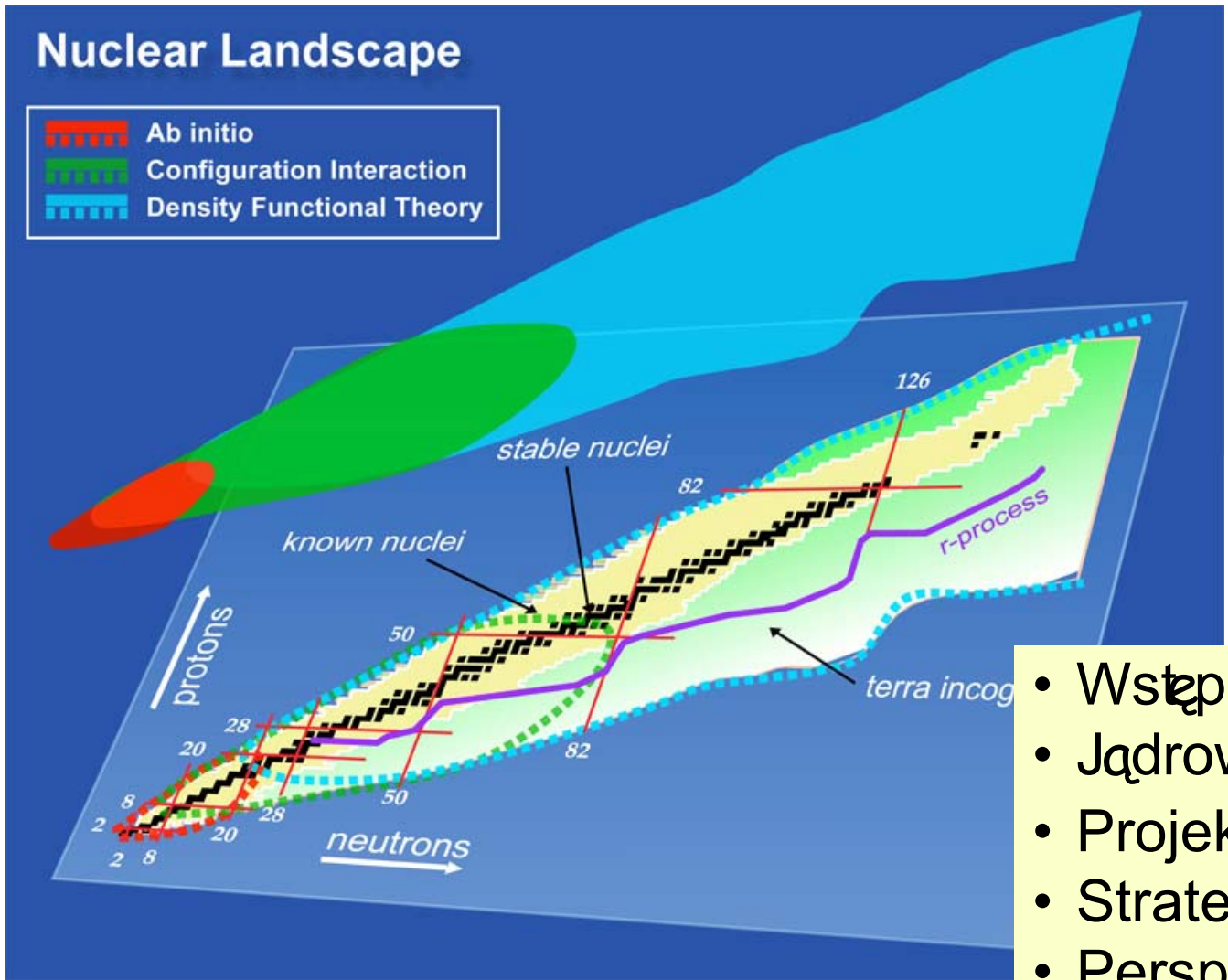
Projekt UNEDF
konstrukcja mikroskopowego jądrowego funkcjonału gęstości

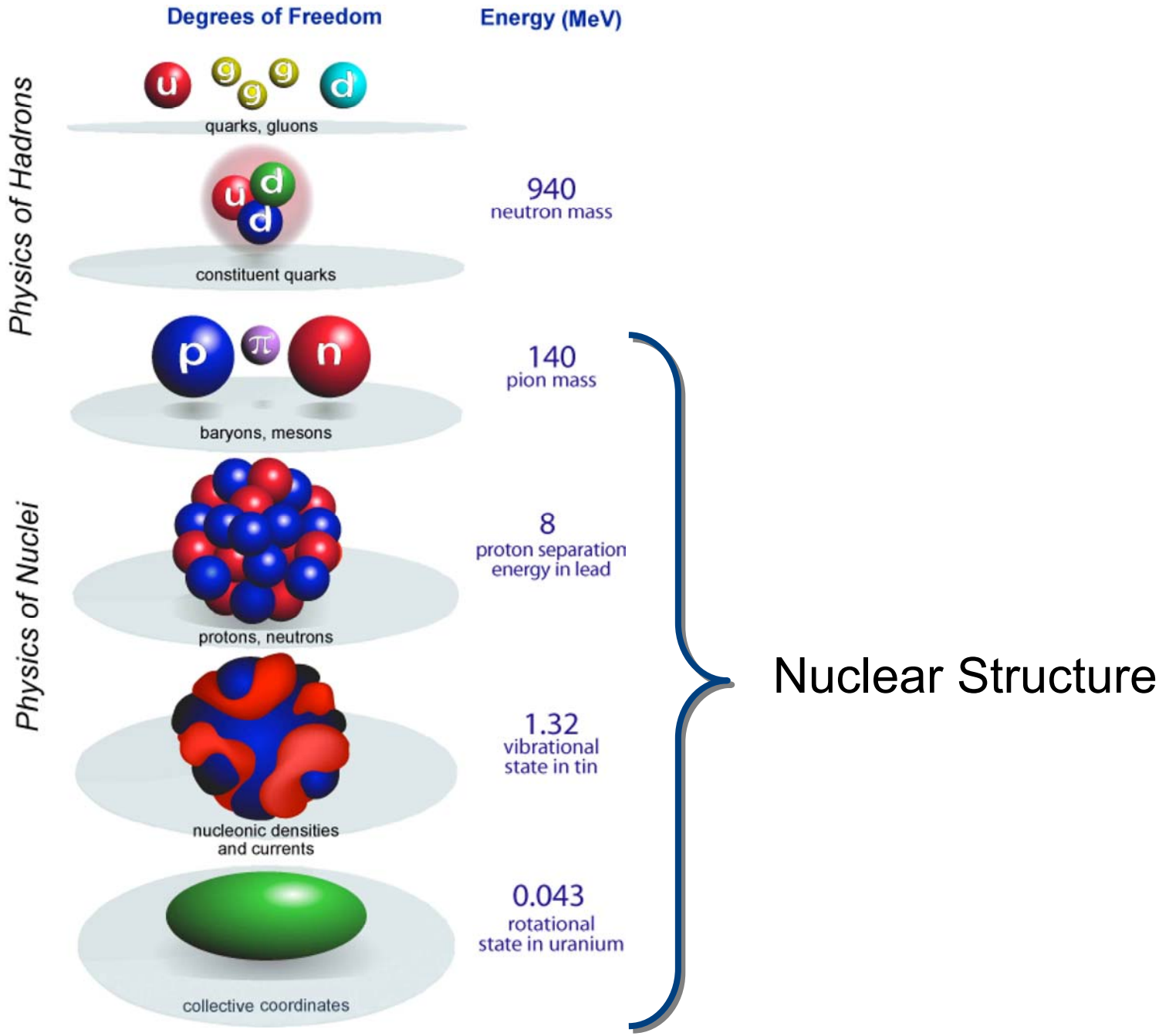
Witold Nazarewicz (Tennessee-Warszawa-Paisley)

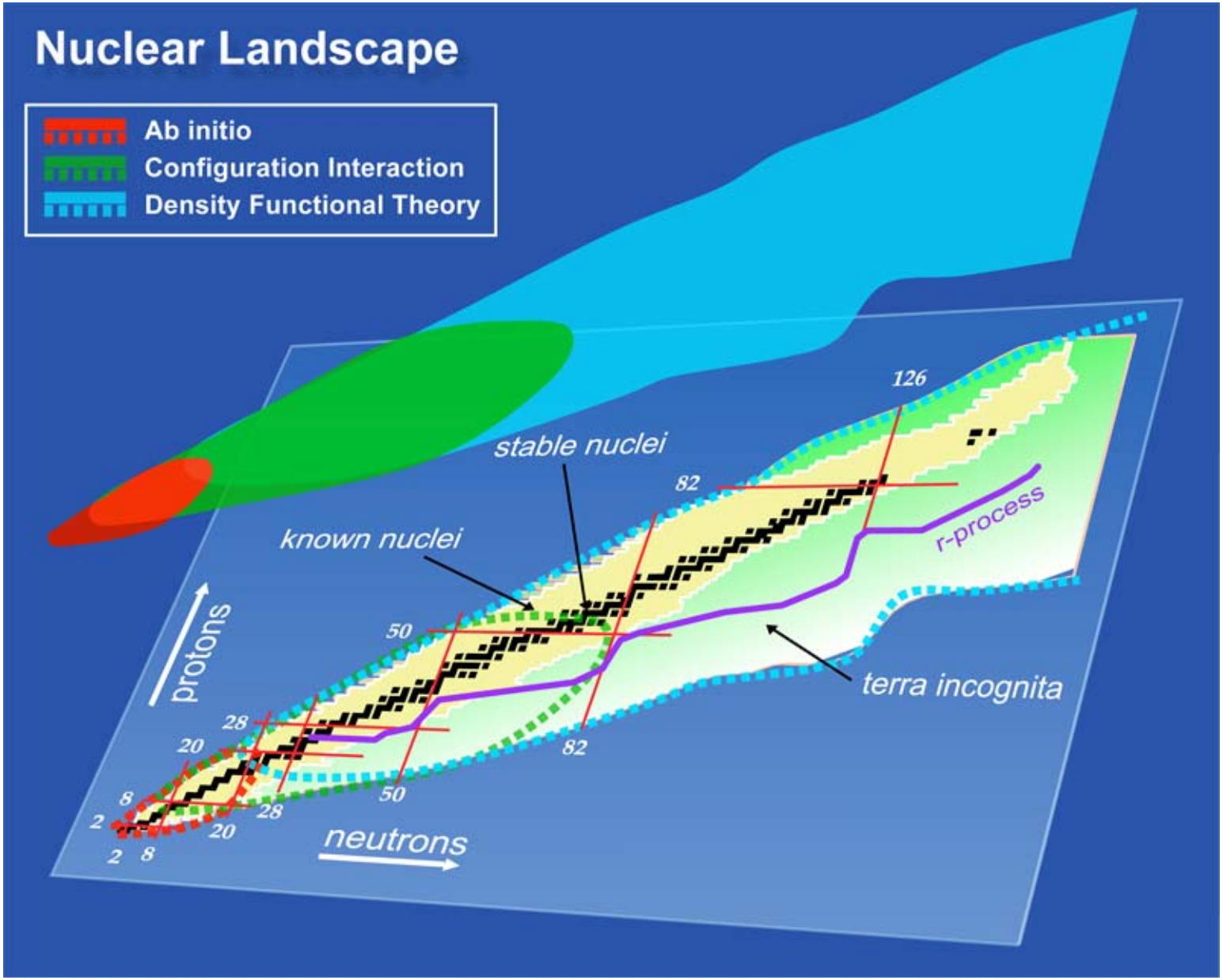
UW, Warszawa, 19 marca 2008



- Wstęp
- Jądrowa teoria DFT
- Projekt UNEDF
- Strategia obliczeniowa
- Perspektywy

Introduction

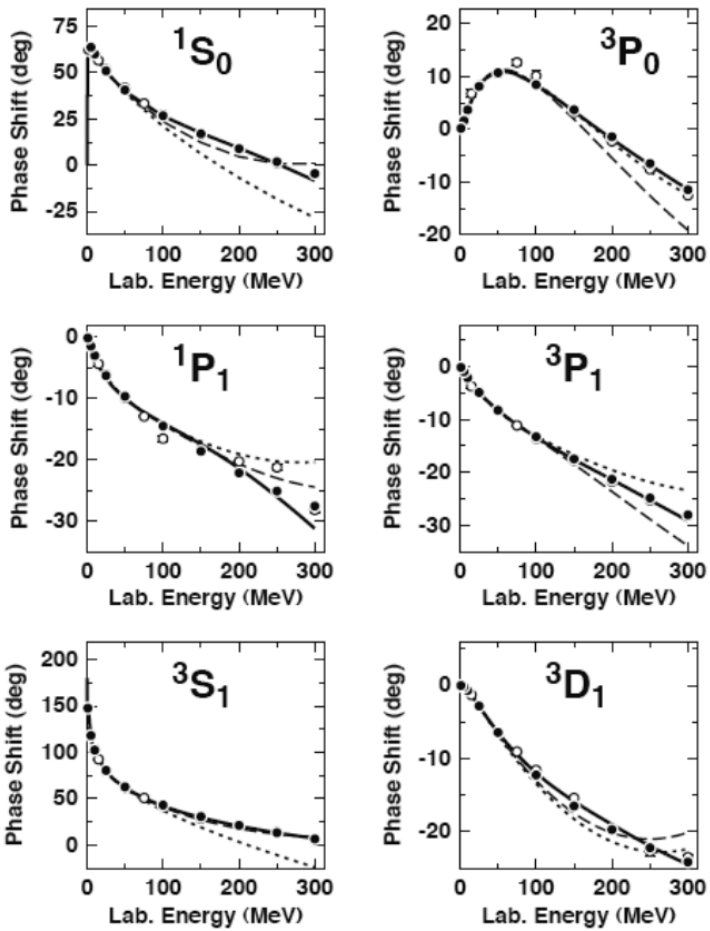

Degrees of Freedom
Energy (MeV)
Physics of Hadrons
Physics of Nuclei
u
g
g
g
d
quarks, gluons
u
d
d
constituent quarks
940
neutron mass
p
π
n
baryons, mesons
140
pion mass
protons, neutrons
8
proton separation energy in lead
nucleonic densities and currents
1.32
vibrational state in tin
collective coordinates
0.043
rotational state in uranium
Nuclear Structure



number of nuclei ~ number of processors!

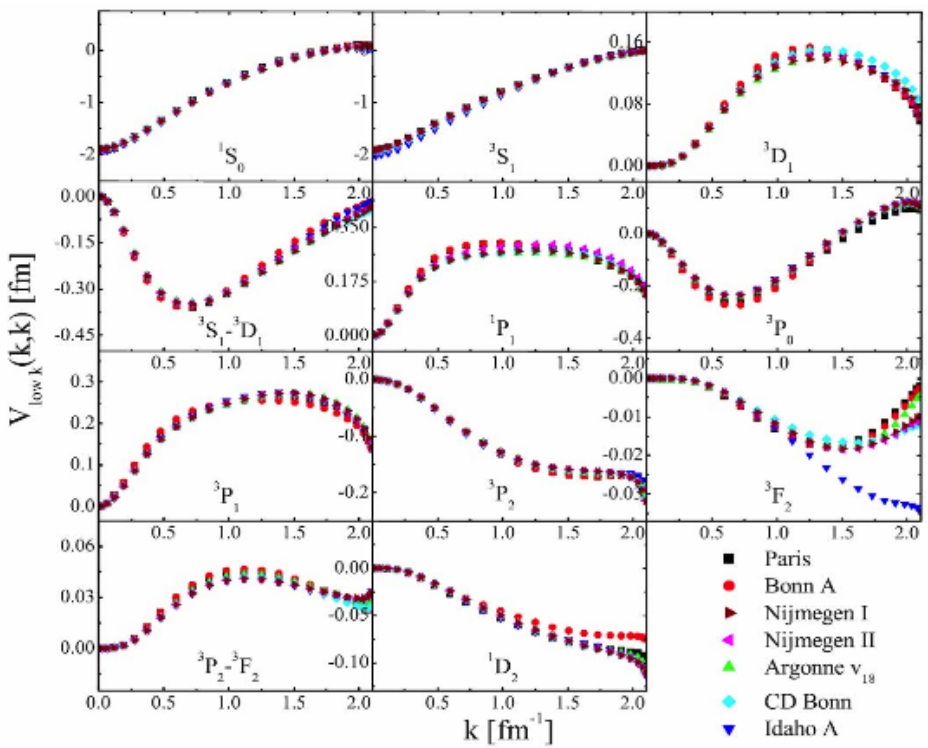
Nuclear Structure: the interaction

Effective-field theory (χPT) potentials



N^{3}LO: Entem et al., PRC68, 041001 (2003)
Epelbaum, Meissner, et al.

$V_{low\text{-}k}$: can it describe low-energy observables?



Bogner, Kuo, Schwenk, Phys. Rep. 386, 1 (2003)

- **Quality two- and three-nucleon interactions exist**
  - **Not uniquely defined (local, nonlocal)**
  - **Soft and hard-core**

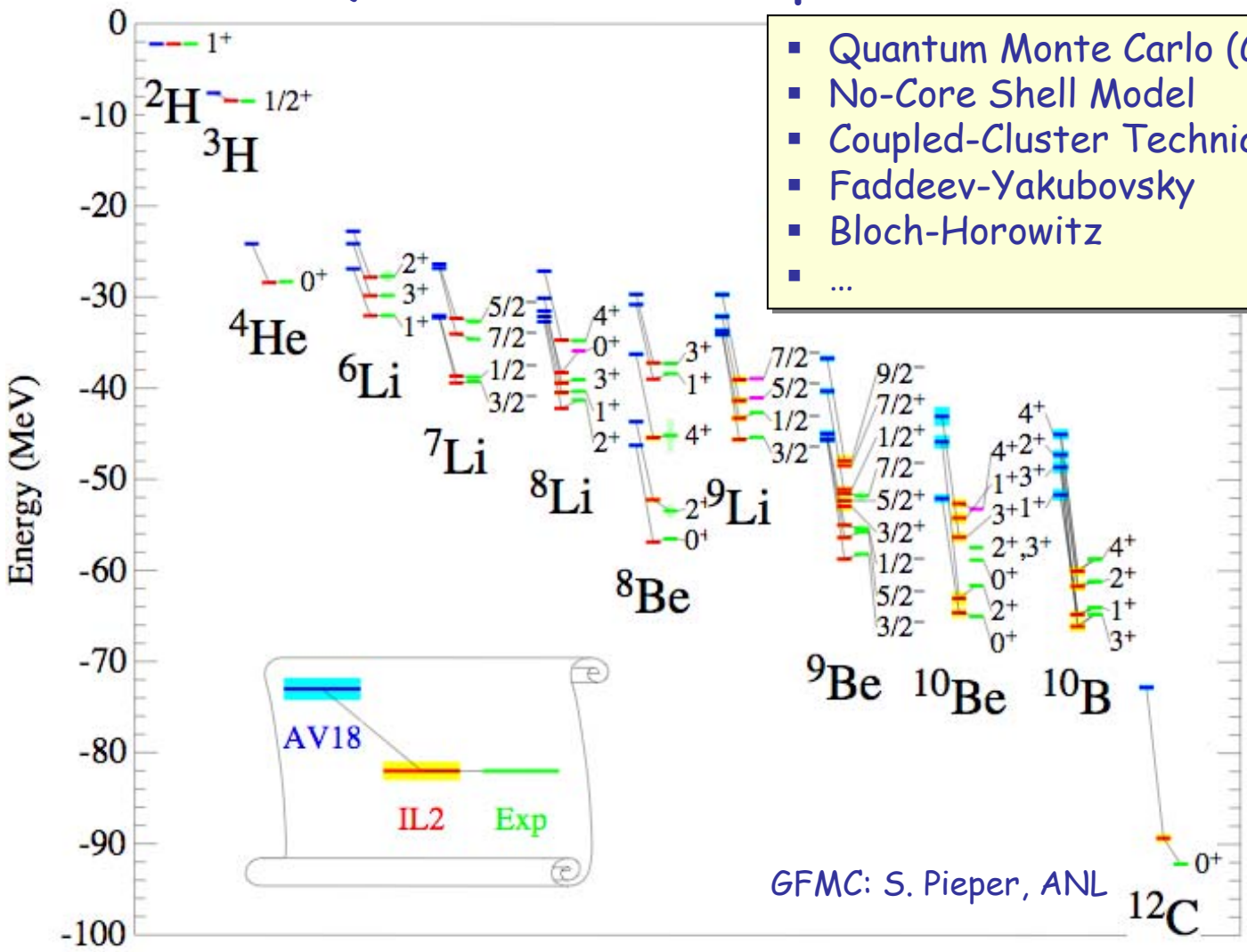
(Nuclear) Many-Body Physics: "Old" vs. "New"

One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof's and Hamiltonians
Find the "best" potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid (hide) divergences	Exploit divergences (cutoff dependence as tool)
Choose diagrams by "art"	Power counting determines diagrams and truncation error

Ab initio: GFMC, NCSM, CCM

(nuclei, neutron droplets, nuclear matter)

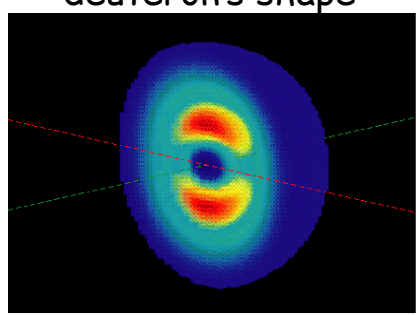
- Quantum Monte Carlo (GFMC) ^{12}C
- No-Core Shell Model ^{13}C
- Coupled-Cluster Techniques ^{16}O
- Faddeev-Yakubovsky
- Bloch-Horowitz
- …



Input:

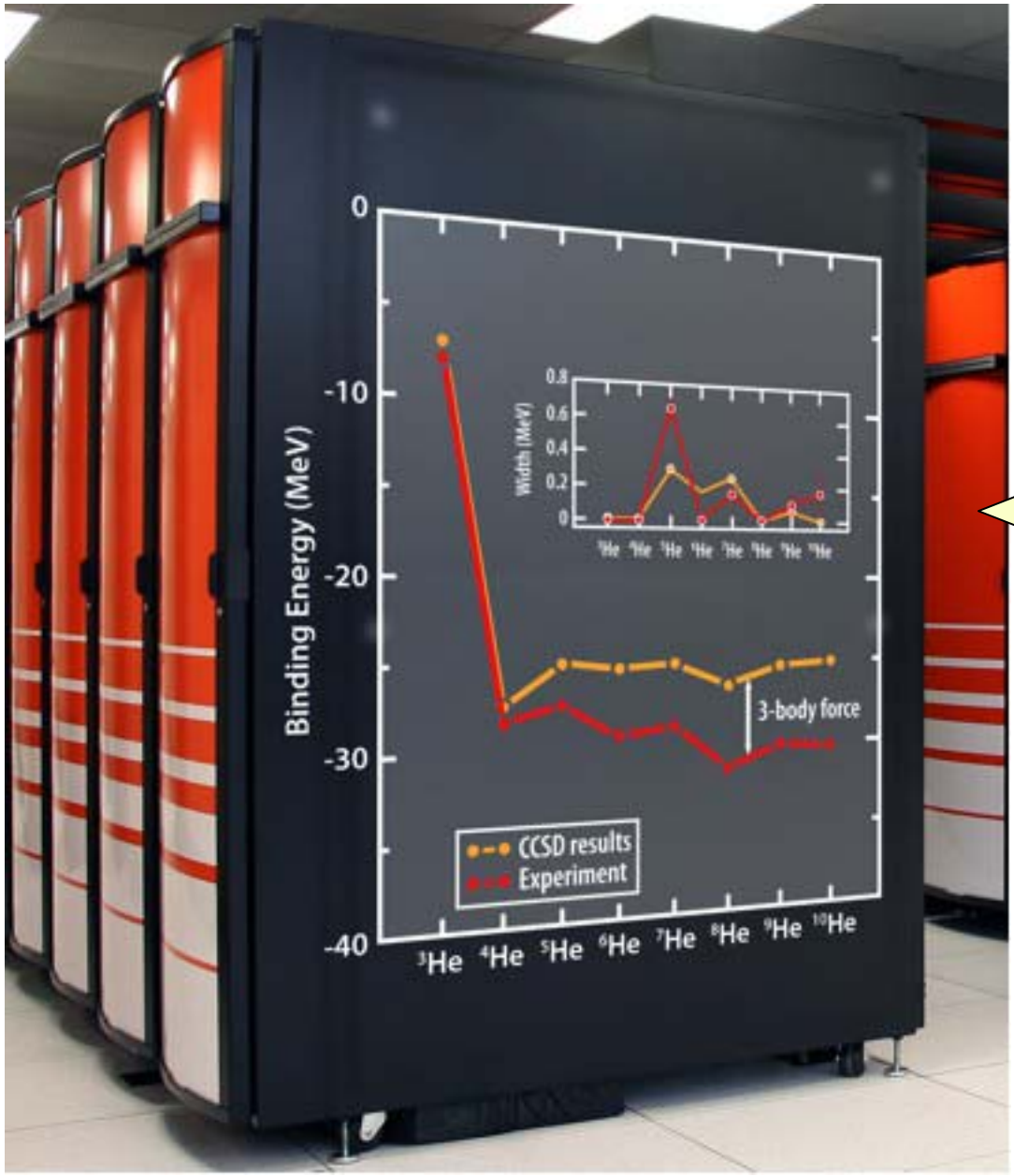
- Excellent forces based on the phase shift analysis
- EFT based nonlocal chiral NN and NNN potentials

deuteron's shape



The nucleon-based description works to <0.5 fm

1-2% calculations of A = 6 – 12 nuclear energies are possible excited states with the same quantum numbers computed



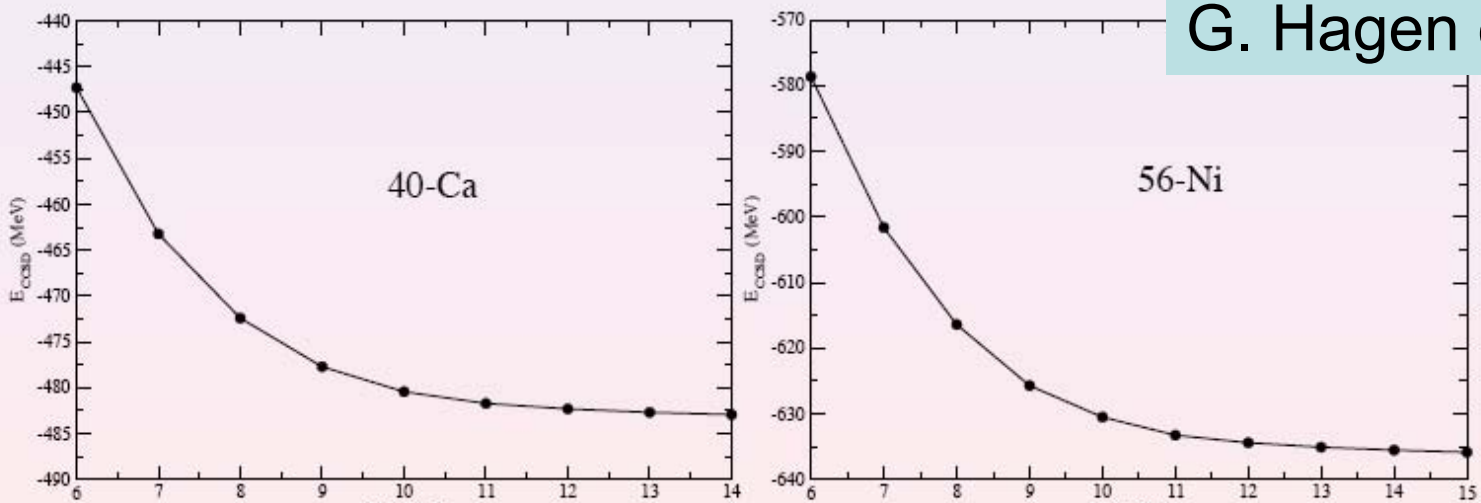
Coupled Cluster Theory

David J. Dean, "Beyond the nuclear shell model", Physics Today **60**, 48 (2007).

http://www.phy.ornl.gov/theory/papenbro/workshop_Jan2008/hagen.pdf

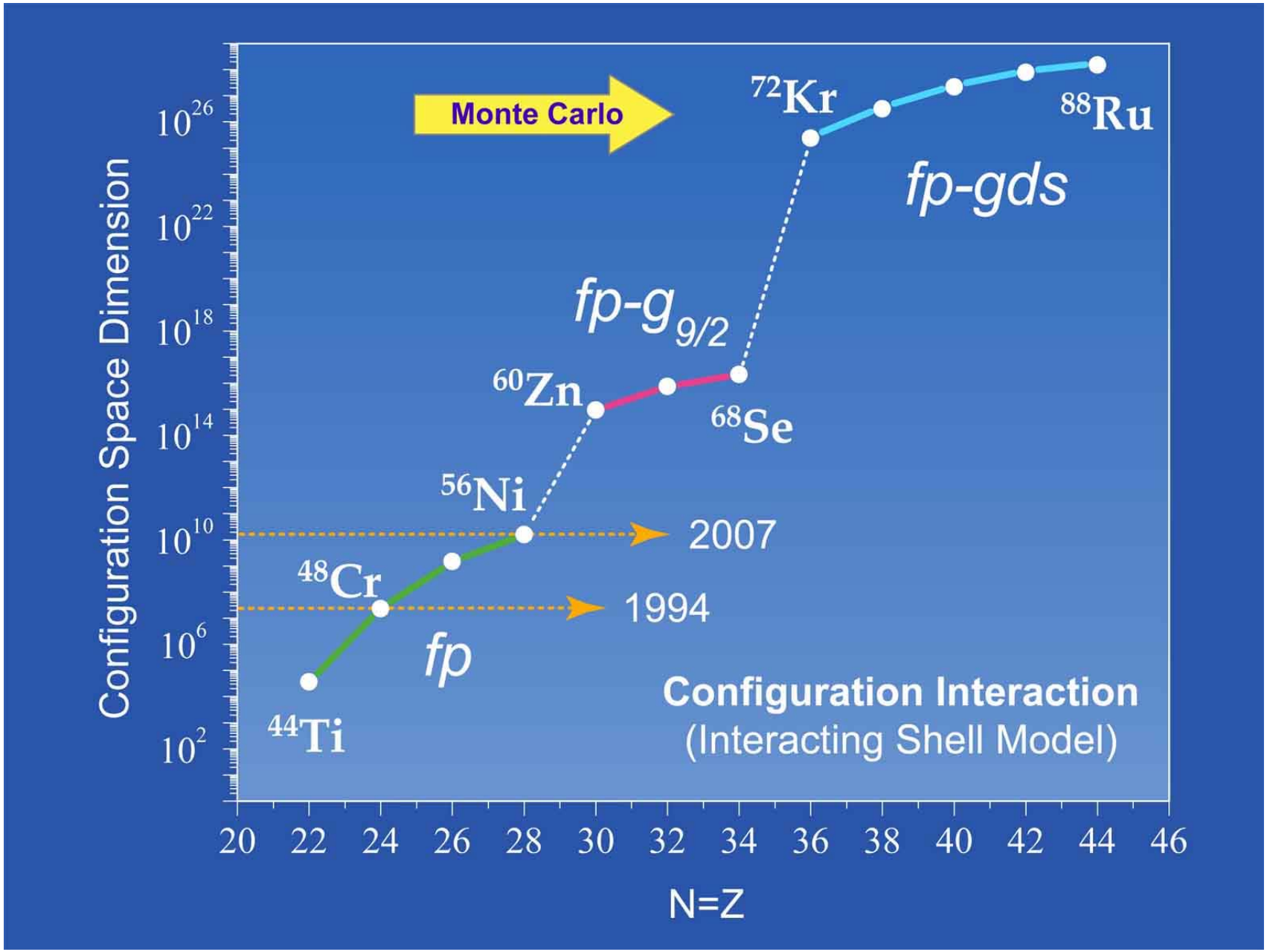
Converged results for ^{40}Ca and ^{56}Ni, using N^{3}LO evolved down to $\lambda = 2.5\mathrm{fm}^{-1}$ from similarity renormalization group theory.

G. Hagen et al.



CCSD results using N^{3}LO at 500 MeV cutoff.

N	^{16}O	^{12}C	^{14}C	^{28}S	^{40}Ca	^{48}Ca	^{56}Ni
10	-99.73	-48.44	-71.97	-142.50	-275.09	-292.05	-246.73
11	-100.67	-49.19	-72.78	-145.24	-281.48	-305.46	-269.63
12	-100.82	-49.29	-72.90	-147.62	-286.54	-310.86	-276.33
13	-101.08	-49.56	-73.15	-148.06	-287.77	-314.65	-283.81
14	-101.12	-	-	-	-289.72	-316.42	-285.82


Monte Carlo
^{72}Kr
^{88}Ru
fp-gds
fp-g$_{9/2}$
^{60}Zn
^{68}Se
^{56}Ni
2007
^{48}Cr
1994
fp
^{44}Ti
Configuration Interaction
(Interacting Shell Model)
Configuration Space Dimension
10^{26}
10^{22}
10^{18}
10^{14}
10^{10}
10^{6}
10^{2}
20 22 24 26 28 30 32 34 36 38 40 42 44 46
N=Z

Nuclear DFT

Density Functional Theory

(introduced for many-electron systems)

The Hohenberg-Kohn theorem states that the ground state electron density minimizes the energy functional:

$$E\left[\rho(\vec{r})\right] = F\left[\rho(\vec{r})\right] + \int \rho(\vec{r}) V_{ion}(\vec{r}) d^3 r$$

an universal functional

P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas", Phys. Rev. **136**, B864 (1964)
M. Levy, Proc. Natl. Acad. Sci (USA) **76**, 6062 (1979)

The original HK proof applies to systems with nondegenerate ground states. It proceeds by *reductio ad absurdum,* using the variational principle. A more general proof was given by Levy.

- The minimum value of *E* is the ground state electronic energy
- Since *F* is a unique functional of the charge density, the energy is uniquely defined by ρ
- Electron density is the fundamental variable
- proof of the Hohenberg-Kohn theorem is not constructive, hence the form of the universal functional *F* is not known

Since the density can unambiguously specify the potential, then contained within the charge density is the total information about the ground state of the system. Thus what was a **4N(3N)-variable problem** (where N is the number of electrons, each one having three Cartesian variables and electron spin) is reduced to the **four (three) variables** needed to define the charge density at a point.

Density Functional Theory

Kohn-Sham equations

W. Kohn and L.J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," Phys. Rev. **140**, A1133 (1965)

$$\rho(\vec{r}) \equiv \sum_i n_i \left|\phi(\vec{r})\right|^2$$

$$T\left[\rho(\vec{r})\right] = \frac{\hbar^2}{2m} \sum_i n_i \int \left|\vec{\nabla}\phi_i(\vec{r})\right|^2 d^3r$$

- Takes into account shell effects
- The link between *T* and ρ is indirect, via the orbitals ϕ
- The occupations n determine the electronic configuration

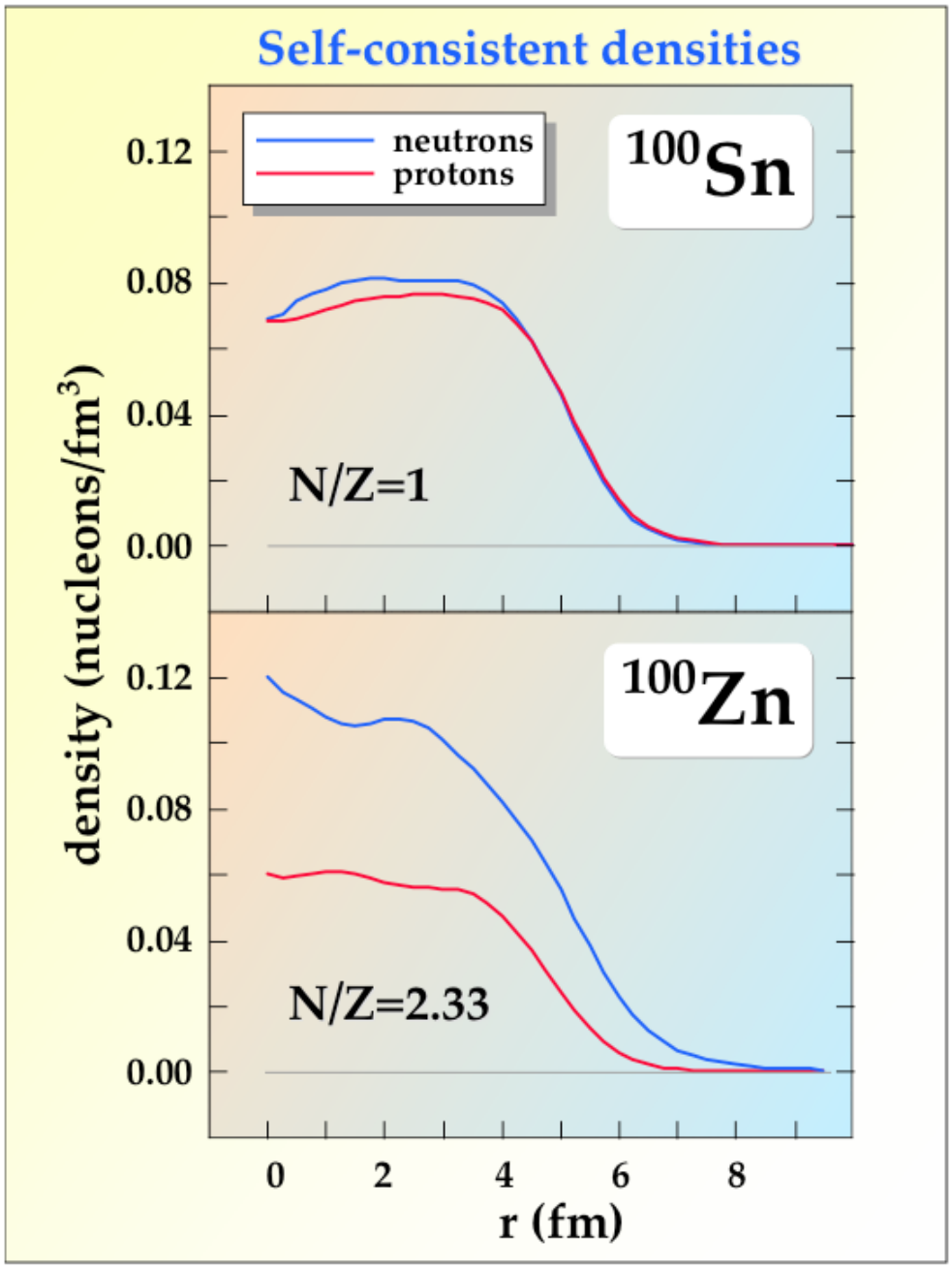
Orbitals ϕ form a complete set. The occupations *n* are given by the Pauli principle (e.g., *n*=2 or 0). The variation of the functional can be done through variations of individual s.p. trial functions with a constraint on their norms. It *looks* like HF, but $\langle\Psi|\hat{H}|\Psi\rangle$ is replaced by *E[ρ]*.

$$\left\{\hat{T} + V_{KS}(\vec{r})\right\}\phi_i(\vec{r}) = E_i\phi_i(\vec{r})$$ **Kohn-Sham equation**

$$V_{KS}(\vec{r}) = V_H\left[\rho(\vec{r})\right] + V_{xc}\left[\rho(\vec{r})\right]$$ **Kohn-Sham potential (local!)**

$$V_{xc}\left[\rho(\vec{r})\right] = \frac{\delta}{\delta\rho(\vec{r})} E_{xc}(\rho)$$ ← has to be evaluated approximately

Mean-Field Theory ⇒ Density Functional Theory



Nuclear DFT

- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.

Nuclear Local s.p. Densities and Currents

$$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\,\sigma\tau;\vec{r}\,\sigma\tau)$$ 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 $(\rho_1 = \rho_n - \rho_p)$

$$\vec{s}_0(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\,\sigma\tau;\vec{r}\,\sigma'\tau)\sigma_{\sigma'\sigma}$$ 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

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

+ analogous p-p densities and currents

Construction of the functional

Perlinska et al., Phys. Rev. C 69, 014316 (2004)

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

p-h density p-p density

Most general second order expansion in densities and their derivatives

$$\begin{aligned}
\chi_0(r) &= C_0^{\rho}\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^{\tau}\rho_0\tau_0 + C_0^{J0}J_0^2 + C_0^{J1}J_0^2 + C_0^{J2}\underline{J}_0^2 + C_0^{\nabla J}\rho_0\nabla\cdot J_0 \\
&+ C_0^{s}s_0^2 + C_0^{\Delta s}s_0\cdot\Delta s_0 + C_0^{T}s_0\cdot T_0 + C_0^{j}j_0^2 + C_0^{\nabla j}s_0\cdot(\nabla\times j_0) + C_0^{\nabla s}(\nabla\cdot s_0)^2 + C_0^{F}s_0\cdot F_0, \\
\chi_1(r) &= C_1^{\rho}\vec{\rho}^2 + C_1^{\Delta\rho}\vec{\rho}\circ\Delta\vec{\rho} + C_1^{\tau}\vec{\rho}\circ\vec{\tau} + C_1^{J0}\vec{J}^2 + C_1^{J1}\vec{J}^2 + C_1^{J2}\underline{\vec{J}}^2 + C_1^{\nabla J}\vec{\rho}\circ\nabla\cdot\vec{J} \\
&+ C_1^{s}\vec{s}^2 + C_1^{\Delta s}\vec{s}\cdot\circ\Delta\vec{s} + C_1^{T}\vec{s}\cdot\circ\vec{T} + C_1^{j}\vec{j}^2 + C_1^{\nabla j}\vec{s}\cdot\circ(\nabla\times\vec{j}) + C_1^{\nabla s}(\nabla\cdot\vec{s})^2 + C_1^{F}\vec{s}\cdot\circ\vec{F},
\end{aligned}$$

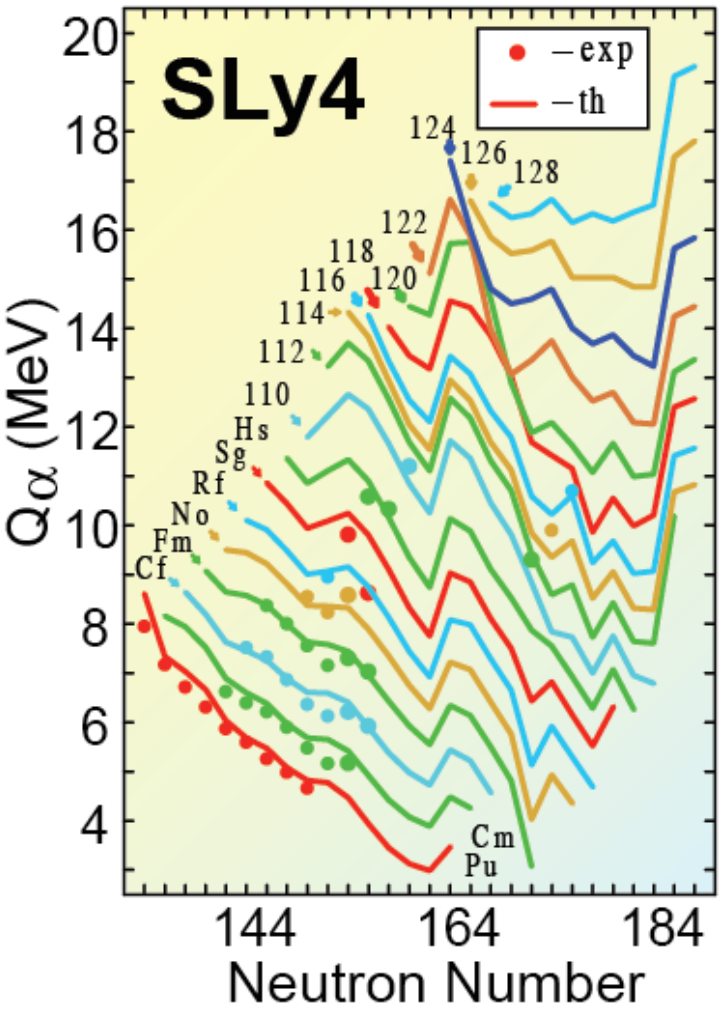
$$\begin{aligned}
\breve{\chi}_0(r) &= \breve{C}_0^{s}|\breve{s}_0|^2 + \breve{C}_0^{\Delta s}\Re(\breve{s}_0^{*}\cdot\Delta\breve{s}_0) + \breve{C}_0^{T}\Re(\breve{s}_0^{*}\cdot\breve{T}_0) \\
&+ \breve{C}_0^{j}|\breve{j}_0|^2 + \breve{C}_0^{\nabla j}\Re(\breve{s}_0^{*}\cdot(\nabla\times\breve{j}_0)) + \breve{C}_0^{\nabla s}|\nabla\cdot\breve{s}_0|^2 + \breve{C}_0^{F}\Re(\breve{s}_0^{*}\cdot\breve{F}_0), \\
\breve{\chi}_1(r) &= \breve{C}_1^{\rho}|\breve{\vec{\rho}}|^2 + \breve{C}_1^{\Delta\rho}\Re(\breve{\vec{\rho}}^{*}\circ\Delta\breve{\vec{\rho}}) + \breve{C}_1^{\tau}\Re(\breve{\vec{\rho}}^{*}\circ\breve{\vec{\tau}}) \\
&+ \breve{C}_1^{J0}|\breve{\vec{J}}|^2 + \breve{C}_1^{J1}|\breve{\vec{J}}|^2 + \breve{C}_1^{J2}|\underline{\breve{\vec{J}}}|^2 + \breve{C}_1^{\nabla J}\Re(\breve{\vec{\rho}}^{*}\circ\nabla\cdot\breve{\vec{J}}).
\end{aligned}$$

pairing functional

Not all terms are equally important. Some probe specific observables

Nuclear DFT: works well for differences

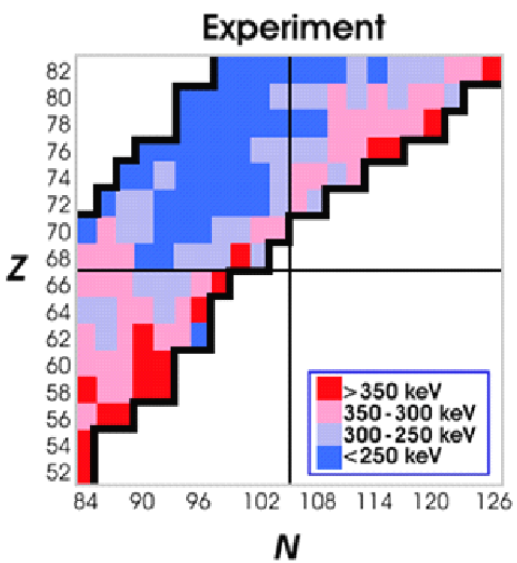
S. Cwiok, P.H. Heenen, W. Nazarewicz
Nature, 433, 705 (2005)

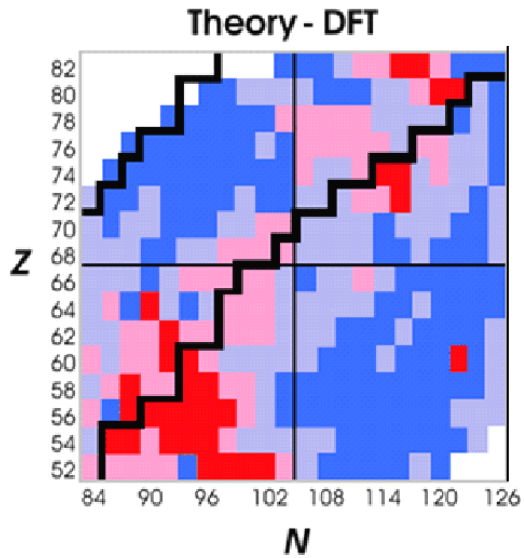


Stoitsov et al., PRL 98, 132502 (2007)

$$4\delta V_{pn} = +B(Z,N) -B(Z,N-2) -B(Z-2,N) +B(Z-2,N-2)$$

$$\delta V_{pn} \approx \frac{\partial^2 B}{\partial Z \partial N}$$

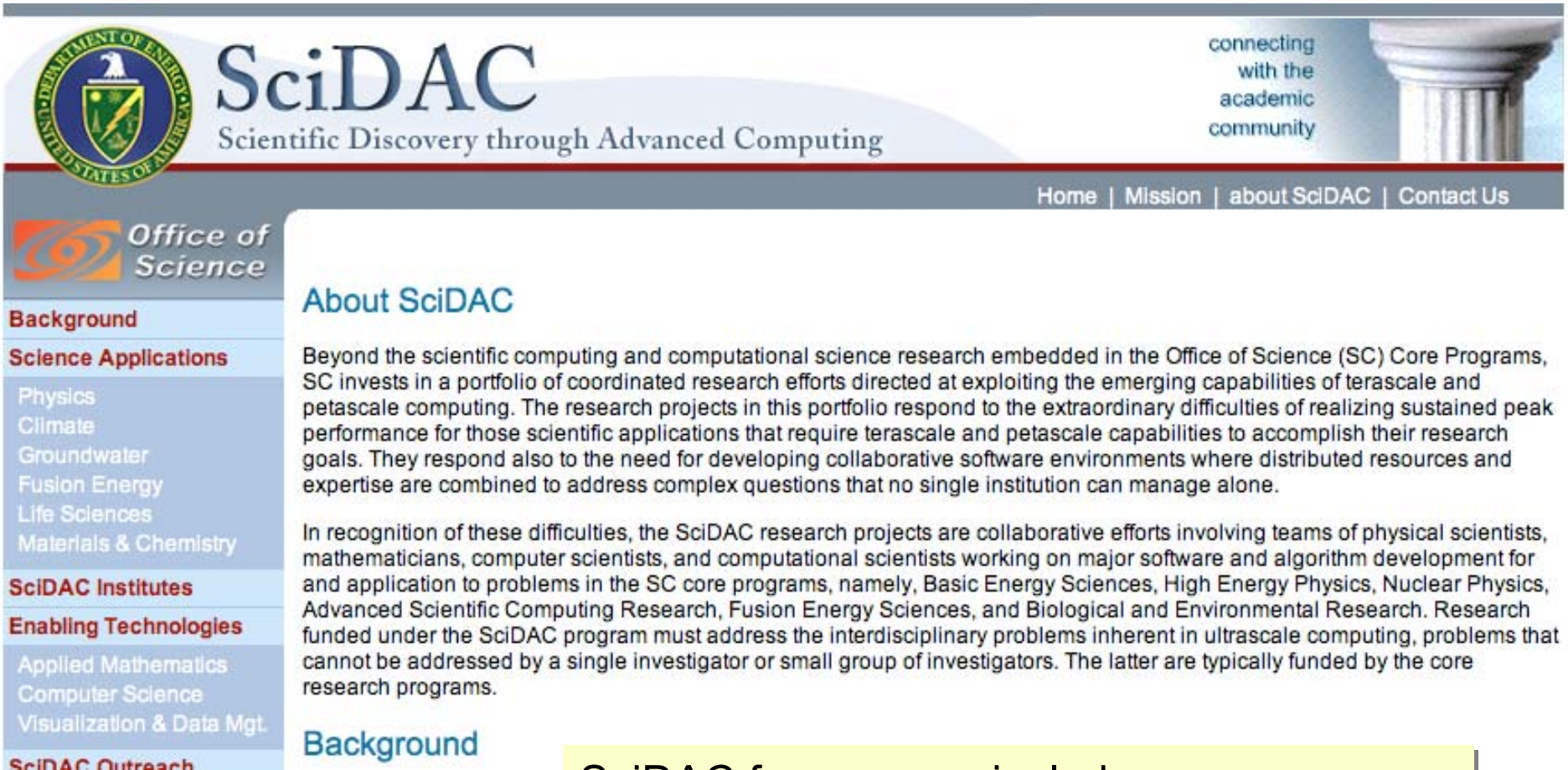




- Global DFT mass calculations: HFB mass formula: Δm~700keV
- Taking advantage of high-performance computers

UNEDF Project

http://www.scidac.gov



1peta=10^{15} flops

SciDAC focus areas include:

- Scientific Challenge Codes
- Computing Systems and Mathematical Software
- Collaboratory Software Infrastructure
- Scientific Computing Hardware Infrastructure
- Scientific Computing Software Infrastructure

SciDAC 2 Project: *Building a Universal Nuclear Energy Density Functional*

- Understand nuclear properties "for element formation, for properties of stars, and for present and future energy and defense applications"
- Scope is all nuclei, with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities
  - ➢ Precision calculations
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

[See http://www.scidacreview.org/0704/html/unedf.html by Bertsch, Dean, and Nazarewicz]

Other SciDAC *Science at the Petascale* Projects

- **Physics (Astro):** Computational Astrophysics Consortium: Supernovae, Gamma Ray Bursts, and Nucleosynthesis, Stan Woosley (UC/Santa Cruz) [$1.9 Million per year for five years]
- **Physics (QCD):** National Computational Infrastructure for Lattice Gauge Theory, Robert Sugar (UC/Santa Barbara) [$2.2 Million per year for five years]
- **Physics (Turbulence):** Simulations of Turbulent Flows with Strong Shocks and Density Variations, Sanjiva Lele (Stanford) [$0.8 million per year for five years]
- **Physics (Petabytes):** Sustaining and Extending the Open Science Grid: Science Innovation on a PetaScale Nationwide Facility, Miron Livny (U. Wisconsin) [$6.1 Million per year for five years]

Universal Nuclear Energy Density Functional

http://unedf.org/

- 15 institutions
- ~50 researchers
  - physics
  - computer science
  - applied mathematics
- foreign collaborators
- annual budget $3M
- 5 years

Major Research Areas

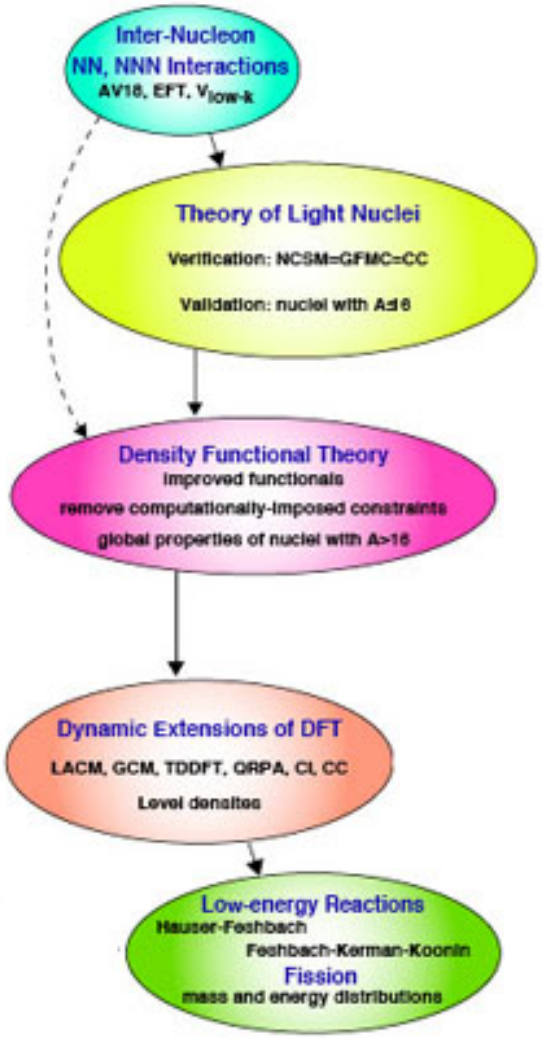
- Ab initio structure — Nuclear wf's from microscopic NN$\cdots$N
  - NCSM/FCI, CC, GFMC/AFMC
  - AV18/ILx, chiral EFT $\longrightarrow$ $V_{\mathrm{low}\,k}$
- Ab initio energy functionals — DFT from microscopic NN$\cdots$N
  - $V_{\mathrm{low}\,k}$ $\longrightarrow$ MBPT $\longrightarrow$ DME
  - Cold atoms — superfluid LDA+ as prototype for nuclear DFT
- DFT applications — Technology to calculate observables
  - Skyrme HFB+ for all nuclei (solvers)
  - Fitting the functional (e.g., correlation analysis)
- DFT extensions — Long-range correlations, excited states
  - LACM, GCM, TDDFT, QRPA, CI
- Reactions – Low-energy reactions, fission, ...

Participating Institutions and Investigators

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)

Universal Nuclear Energy Density Functional



Color denotes:

- Physics
- Computer Science & Applied Mathematics
- Foreign Collaborators

Physics/Computer Science Partnerships

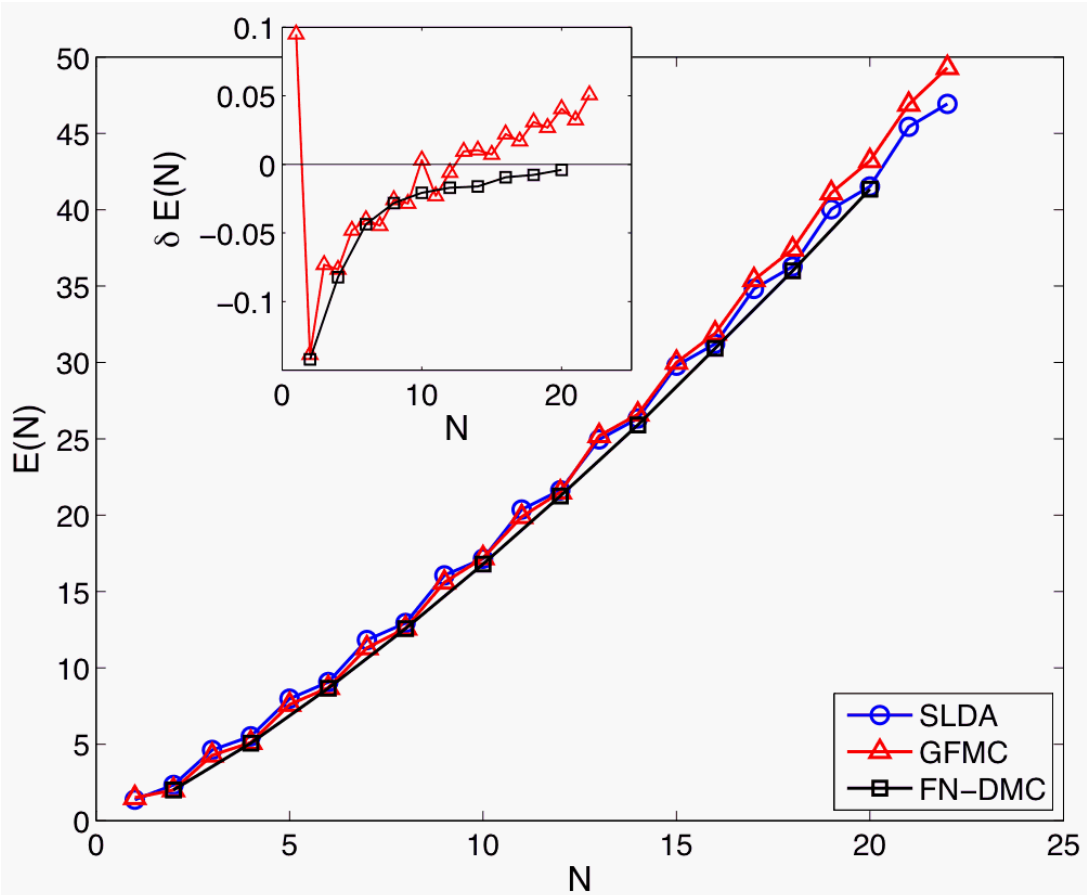
Partnerships have been formed consisting of computer scientists and applied mathematicians linked with specific physicists. In each partnership, the mathematician/computer scientist is addressing a research topic in order to remove a specific barrier to progress on the computational/algorithmic physics side.

- FCI, NCSM — linear algebra
- GFMC — ADLB (load balancing)
- Gridded DFT solver — wavelet basis; sinc basis
- Oscillator DFT solver — efficiency and parallel execution
- Coupled Cluster — NNN interactions
- Coupled Channel — efficiency and parallel execution (proposed)

Can dynamics be incorporated directly into the functional?

Example: **Local Density Functional Theory for Superfluid Fermionic Systems: The Unitary Gas,** *Aurel Bulgac, Phys. Rev. A 76, 040502 (2007)*

$$\mathcal{E}(\mathbf{r}) = \alpha \frac{\tau_c(\mathbf{r})}{2} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\mathbf{r})}{10} + g_{eff}(\mathbf{r})|\nu_c(\mathbf{r})|^2 + V_{ext}(\mathbf{r}) n(\mathbf{r})$$



See also:

Density-functional theory for fermions in the unitary regime
T. Papenbrock
Phys. Rev. A72, 041603 (2005)

Density functional theory for fermions close to the unitary regime
A. Bhattacharyya and T. Papenbrock
Phys. Rev. A 74, 041602(R) (2006)

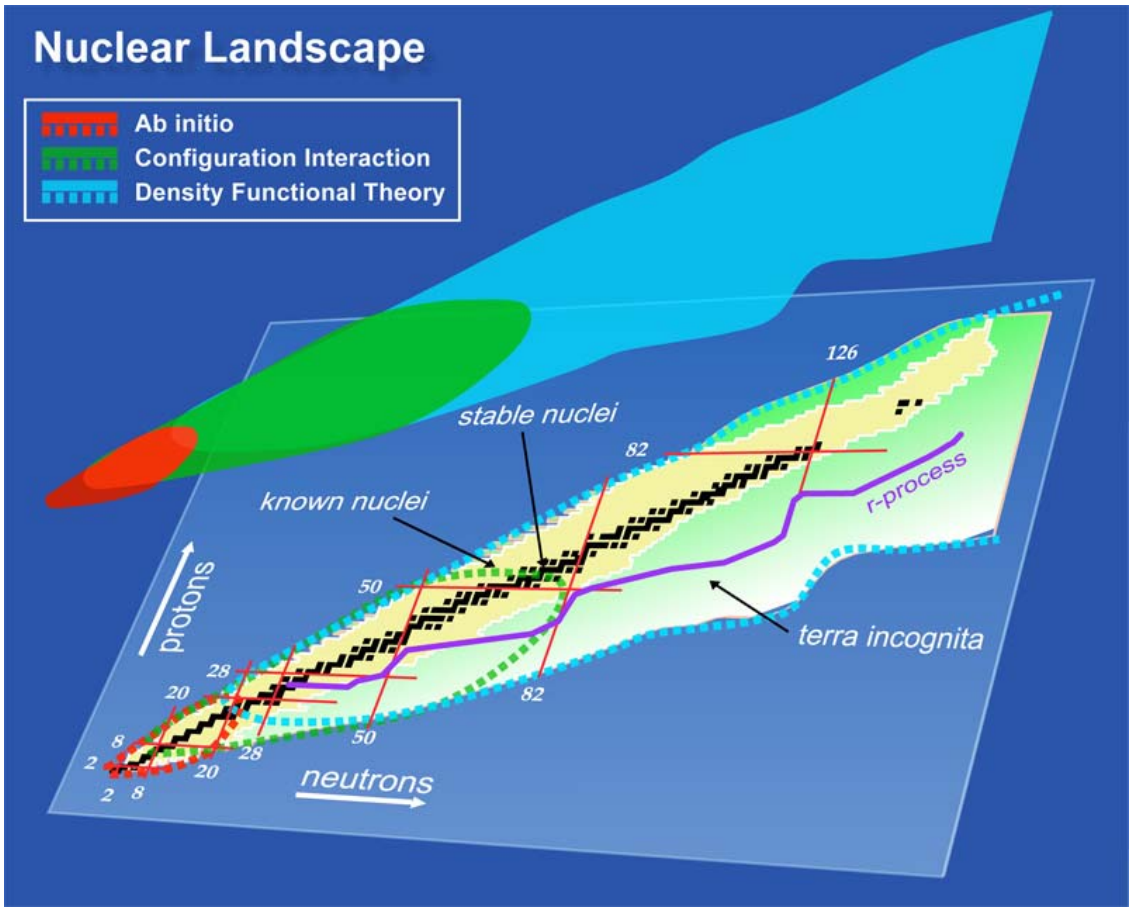
Why us?

There is a zoo of nuclear functionals on the market. What makes us believe we will 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
- Unique experimental data available

Conclusion: we can deliver a well theoretically founded EDF, based on as much as possible ab intio input at this point in time

Building Connections: Bridging Approaches



Ab-initio - Ab-initio

Ab-initio - DFT
- low-density neutron matter
- finite nuclei (DME)

DFT - DFT

Increased coherence

Ab-initio - DFT Connection

UNEDF
Pack Forest meeting

- One-body density matrix is the key quantity to study
- "local DFT densities" can be expressed through ρ(x,x')
- Testing the Density Matrix Expansion and beyond

one-body density matrix:

$$\rho(x,x') = \int \Psi^*(x,x_2,\cdots,x_N)\Psi(x',x_2,\cdots,x_N)dx_2\cdots dx_N$$

$$x = \{\vec{r},s,t\}$$

$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau}\rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)$ 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 $(\rho_1 = \rho_n - \rho_p)$

$\vec{s}_0(\vec{r}) = \sum_{\sigma\sigma'\tau}\rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\sigma_{\sigma'\sigma}$ 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

$\vec{J}_T(\vec{r}) = \frac{i}{2}\left(\vec{\nabla}'-\vec{\nabla}\right)\otimes\vec{s}_T(\vec{r},\vec{r}')\big|_{\vec{r}'=\vec{r}}$ 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

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

UNEDF Homework

- Introduce external potential
  - HO for spherical nuclei (amplitude of zero-point motion=1 fm)
  - 2D HO for deformed nuclei
- Density expressed in COM coordinates
- Calculate ρ(x,x') for ^{12}C, ^{16}O and

^{40,48,60}Ca (CC) ← **isospin**

- Perform Wigner transform to relative and c-o-m coordinates *q* and *s*
- Extract ρ, J, τ
- Analyze data by comparing with results of DFT calculations and low-momentum expansion studies.

- Go beyond I=0 to study remaining densities (for overachievers)

$$\rho(\vec{r},\vec{r}') \approx \rho(\vec{q}) i\vec{s}\cdot\vec{j}(\vec{q}) + \frac{1}{2}s^2\left[\tau(\vec{q}) - \frac{1}{4}\Delta_{\vec{q}}\rho(\vec{q})\right], \quad \vec{q} = \frac{\vec{r}+\vec{r}'}{2}, \ \vec{s} = \vec{r}-\vec{r}'$$

Negele and Vautherin:
PRC 5, 1472 (1972)

Density Matrix Expansion for RG-Evolved Interactions

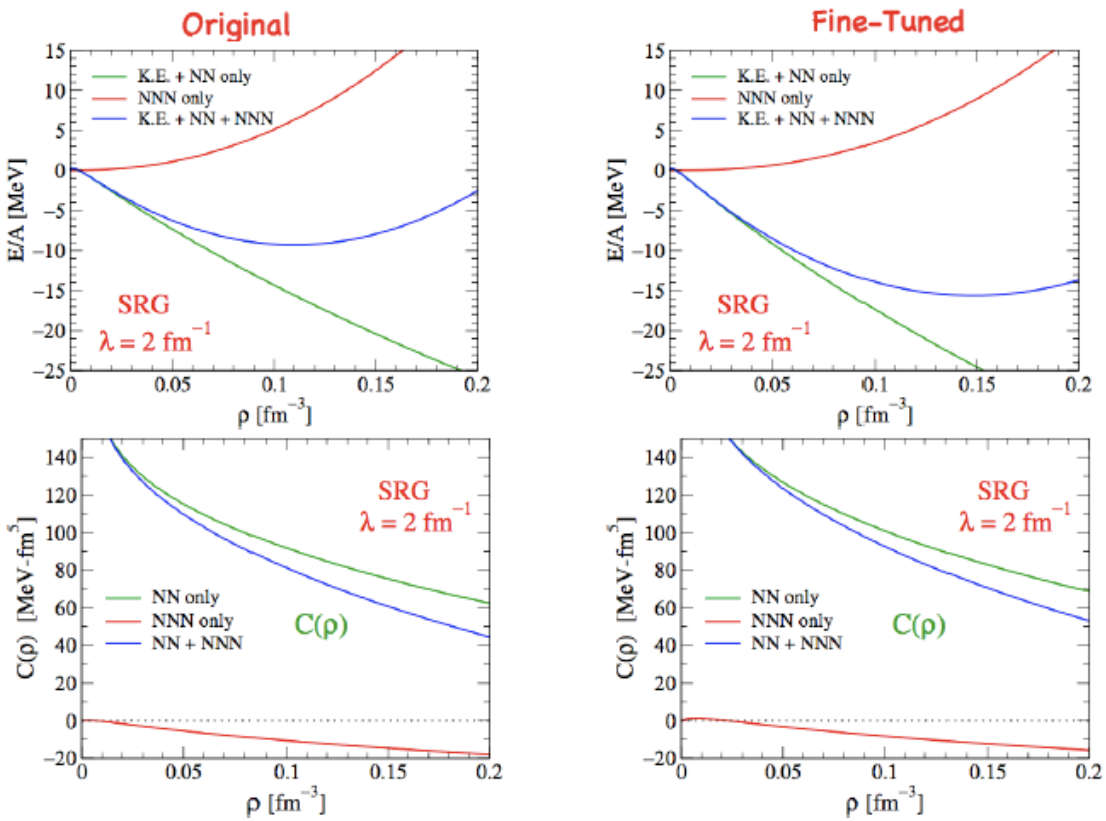
S.K. Bogner, R.J. Furnstahl et al.

Skyrme-like EDF's from the DME

$$\mathcal{E} = \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1+5t_2)\rho\tau + \frac{1}{64}(9t_1-5t_2)|\nabla\rho|^2 + \cdots \quad \text{Skyrme}$$

$$\mathcal{E} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots \quad \text{DME}$$

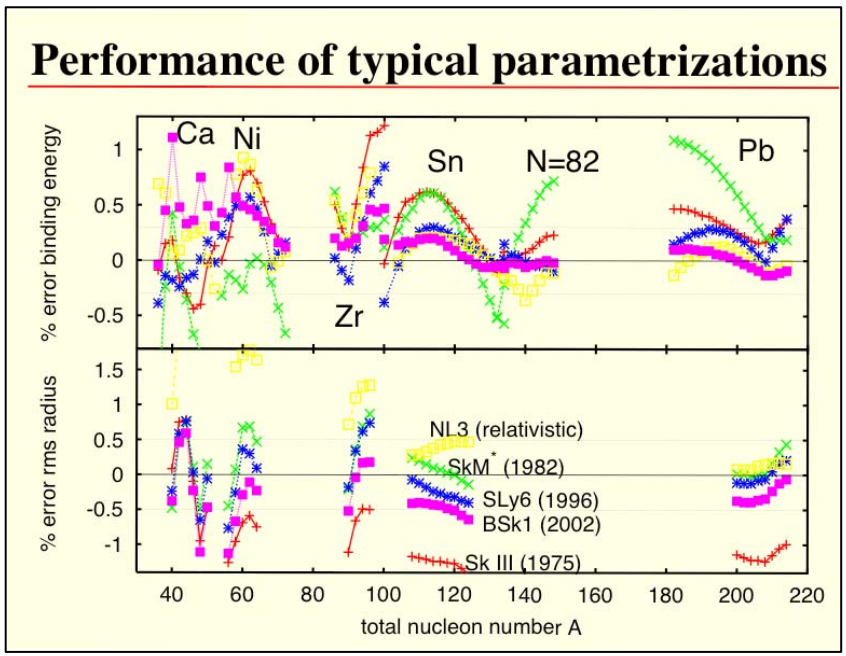
DME ABC Functions



see also:
EFT for DFT
R.J. Furnstahl
nucl-th/070204

DFT Mass Formula
(can we go below 500 keV?)

P.G. Reinhard 2004



- need for error and covariance analysis (theoretical error bars in unknown regions)
- a number of observables need to be considered (masses, radii, collective modes)
- different terms sensitive to particular data
- only data for selected nuclei should be used

How to optimize the search? SVD can help…

Fitting theories of nuclear binding energies
G. F. Bertsch, B. Sabbey and M. Uusnakki,
Phys. Rev. C71, 054311(2005)

Theory	r.m.s residual	$a_v(c)$	$a_s(c)$
SLy4 [8]	1.75	-16.06	32.0
SkP-based [11]	1.75	-16.11	31.1
BSk4-based [12]	1.65	-16.03	29.6
Skxce-based [13]	1.55	-16.10	31.0
LD	3.1	-15.6	23.3

Global calculations of ground-state spins and parities for odd-mass nuclei

L. Bonneau, P. Quentin, and P. Möller, Phys. Rev. C 76, 024320 (2007)

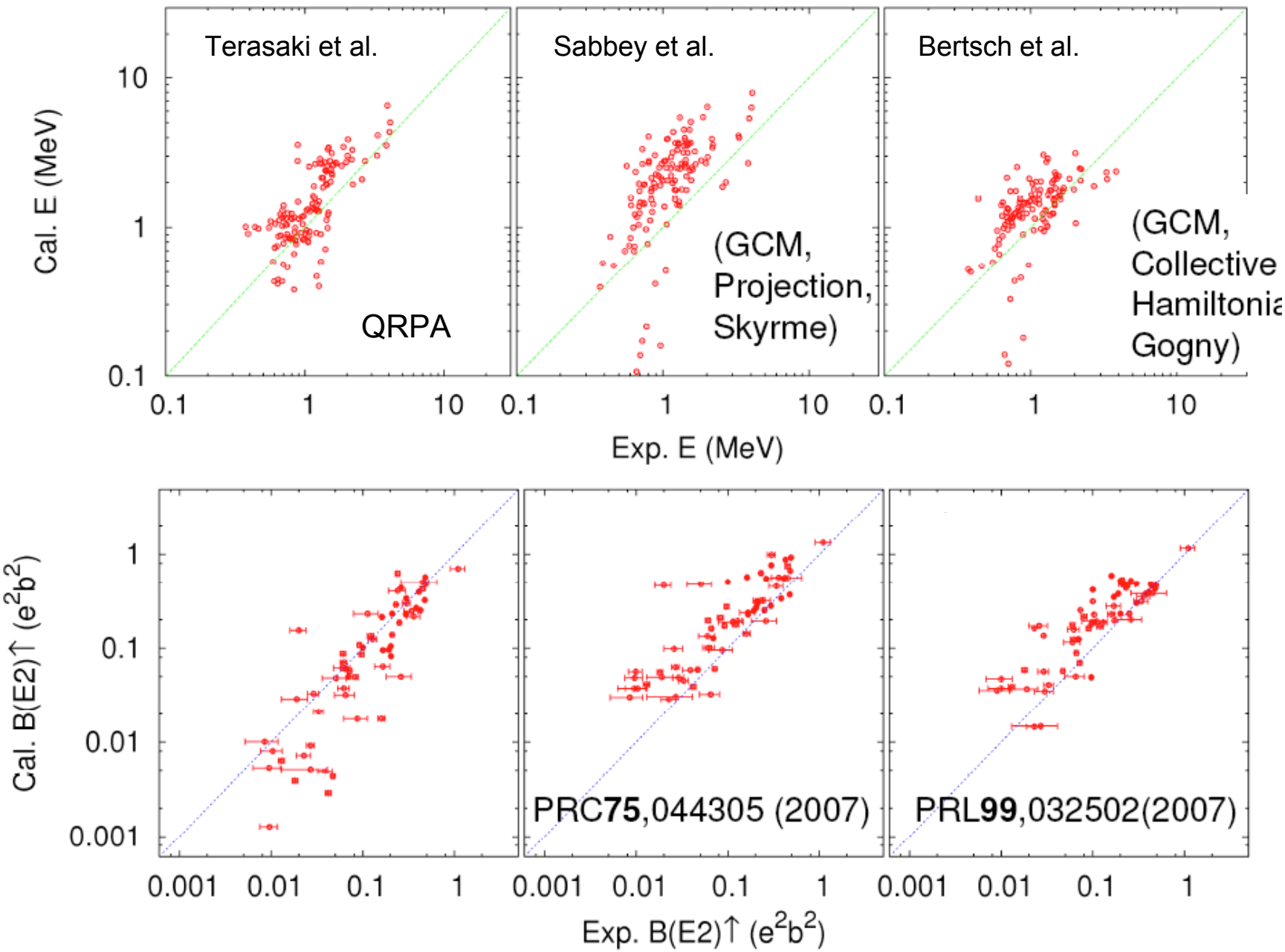
GS SPINS AND PARITIES

RESULTS

Comparison including all nuclei such that $V_{PO} \geqslant 2$ MeV and $|\beta_2| \notin [0.01; 0.1]$

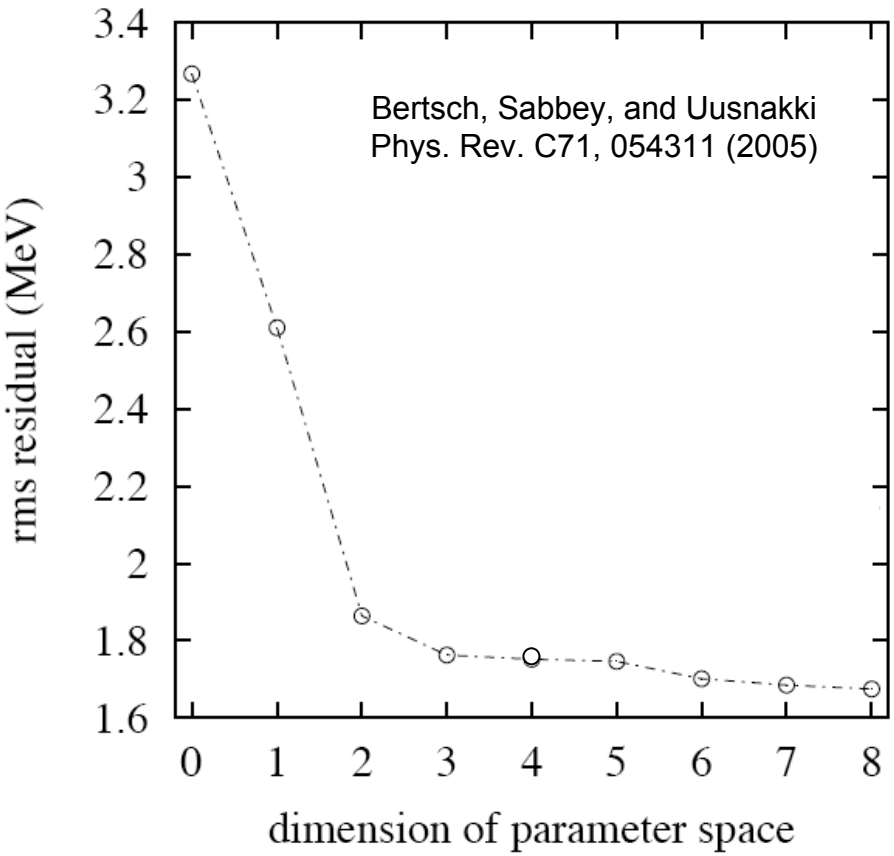
Model	Sph.	Def.	Total
SIII	83.9%*(90.8%)*	40.5% *(61.5%)*	66.4% *(79.0%)*
	183*(+15)*/218	60*(+31)*/148	242*(+46)*/365
SkM*	76.2%*(89.2%)*	37.5% *(61.8%)*	63.3% *(80.0%)*
	218*(+37)*/286	54*(+35)*/144	272*(+72)*/430
SLy4	77.8%*(85.8%)*	39.3% *(60.7%)*	64.1% (77.6%)
	186*(+19)*/239	57*(+32)*/140	243*(+51)*/379
FRDM	90.9%	41.5%	51.5%
	90/99	137/318	227/417

Global calculations of the lowest 2^+ states

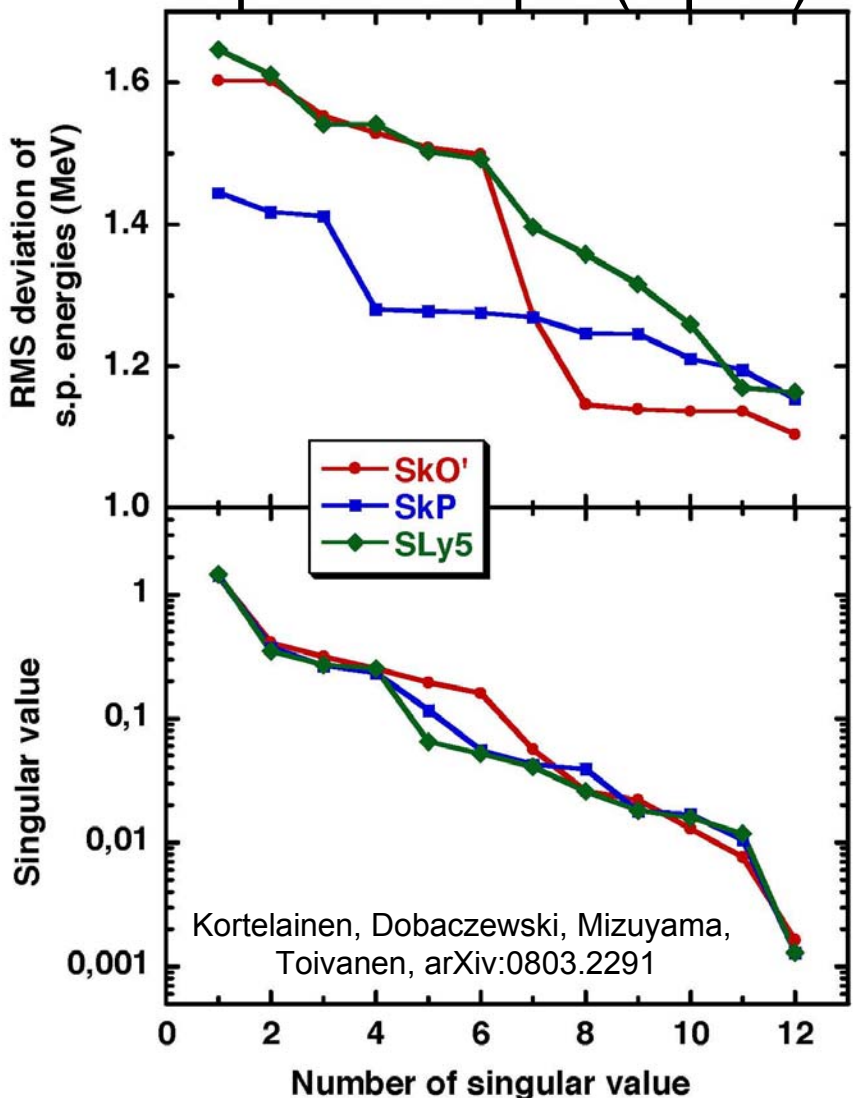


How many parameters are really needed?

Global (masses)



Spectroscopic (s.p.e.)



New optimization strategy and protocol needed

DFT-UNEDF Workshop

Determination of the Nuclear Energy functional: Optimization Strategy, Essential Experimental Data and Chi-Squared Metrics

Joint Institute for Heavy Ion Research, ORNL,
Oak Ridge, TN-37831, USA
January 22, 2008

41 participants

Talks

Name	Title of Contribution	File
A. Brown	Strategies for Extracting Optimal Effective Hamiltonians for CI and Skyrme EDF Applications	Brown.ppt
J. Dobaczewski	Spectroscopic-Quality Energy Density Functional and How to Get There	Dobaczewski.ppt

Choice of Experimental Observables

Name	Title of Contribution	File
A. Afanasjevs	Terminating States: Can They Be Used to Constrain DFT ?	Afanasjevs.pdf
G. Colo	Constraints from Collective States	Colo.ppt
P. Kluepfel	Best Mean-Field Nuclei for Fits	Kluepfel_1.pdf
P. Kluepfel	Fitting Strategies	Kluepfel_2.pdf
H. Sagawa	Constraints to Universal Energy Density Functionals by Giant Resonances	Sagawa.ppt
N. Schunck	Large Deformations in DFT Fits	Schunck_1.ppt
N. Schunck	Quasi-particle Spectra in DFT Fits	Schunck_2.ppt
J. Terasaki	QRPA Calculation in Fitting Process of Functional	Terasaki.ppt
J. Vary	Ab-initio calculations with an external field - initial results	Vary.ppt

Minimization and Algorithms

Name	Title of Contribution	File
K. Bennaceur	Stability Criteria for Skyrme Energy Functionals	Bennaceur.pdf
J. Moré (1)	Validation of Models	More_1.pdf
J. Moré (2)	Parameter Estimation in Nuclear Fission	More_2.pdf
T. Lesinski	Minimization Algorithms for Local and Global Minima Search	Lesinski.pdf

http://orph02.phy.ornl.gov/workshops/lacm08/unedf.html

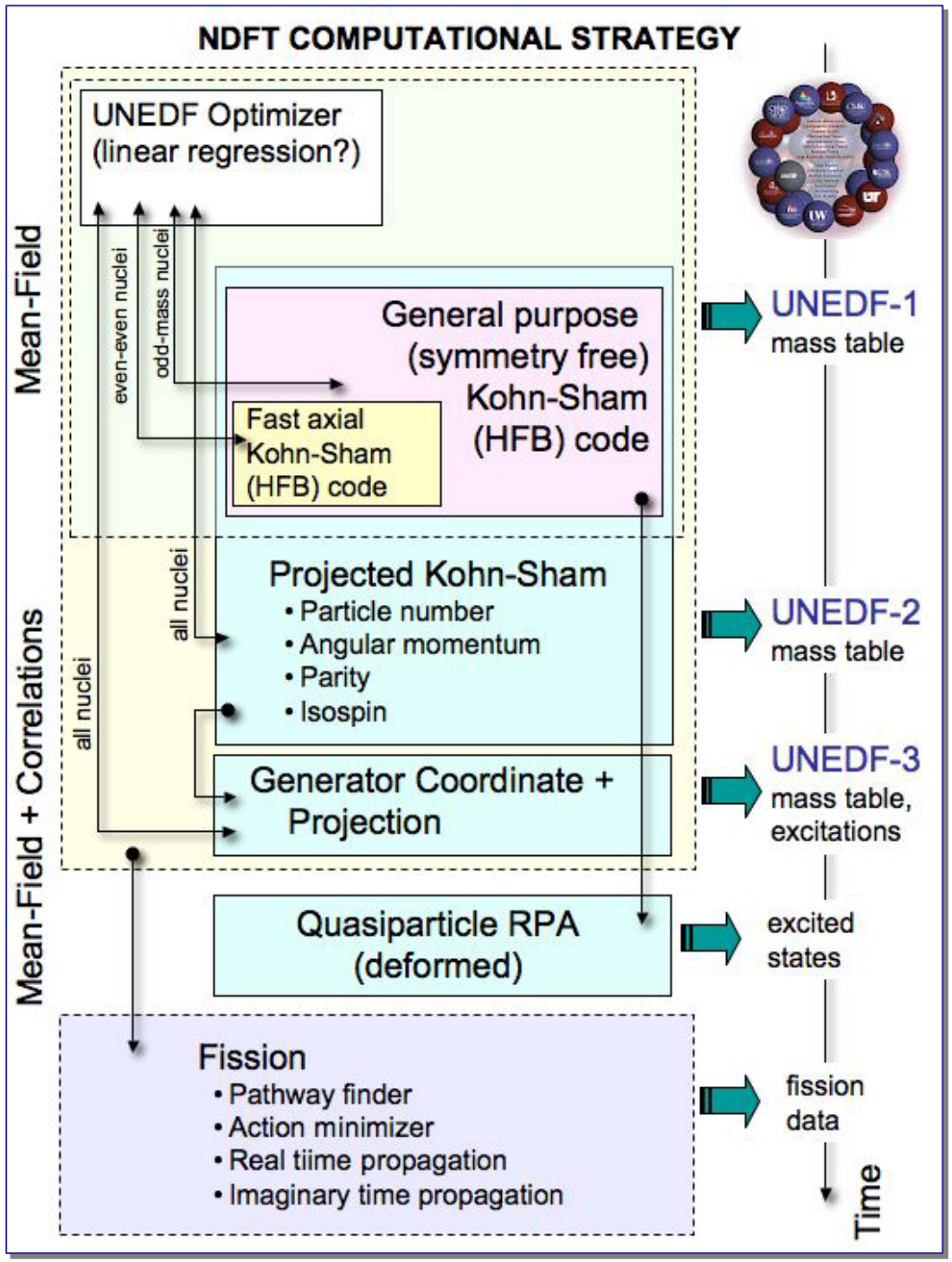
Computational Strategy

Ab Initio DFT: Parallel Development

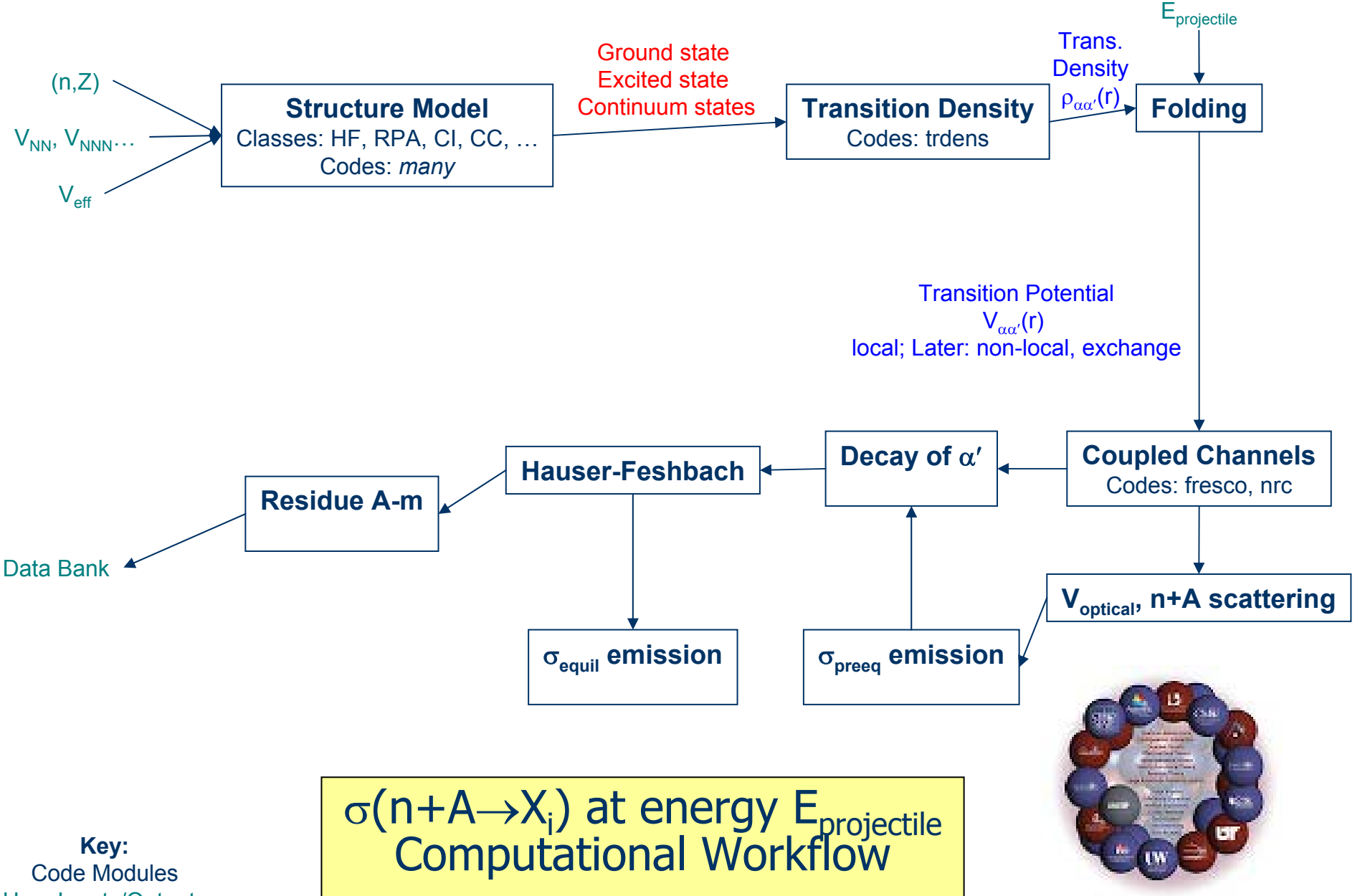
1. Momentum-space Renormalization Group (RG) methods to evolve chiral NN and NNN potentials to more perturbative forms as inputs to nuclear matter and ab initio methods (coupled cluster, NCSM).
2. Controlled nuclear matter calculations based on the RG-improved interactions, as ab initio input to Skyrme EDF benchmarking and microscopic functional.
3. Approximate DFT functional, initially by adapting density matrix expansion (DME) to RG-improved interactions.
4. Adaptation to Skyrme codes and allowance for fine tuning.

Points of emphasis:

- Systematic upgrade path with existing and developing technology
- Theoretical error bars on interaction (vary EFT Λ and order of calculation) and on implementation (vary SRG λ or $V_{\mathrm{low}\,k}$ Λ)


NDFT COMPUTATIONAL STRATEGY
Mean-Field
Mean-Field + Correlations
UNEDF Optimizer
(linear regression?)
even-even nuclei
odd-mass nuclei
General purpose
(symmetry free)
Kohn-Sham
(HFB) code
Fast axial
Kohn-Sham
(HFB) code
UNEDF-1
mass table
all nuclei
all nuclei
Projected Kohn-Sham
• Particle number
• Angular momentum
• Parity
• Isospin
UNEDF-2
mass table
Generator Coordinate +
Projection
UNEDF-3
mass table,
excitations
Quasiparticle RPA
(deformed)
excited
states
Fission
• Pathway finder
• Action minimizer
• Real tiime propagation
• Imaginary time propagation
fission
data
Time

From Ian Thompson



$\sigma(n+A \rightarrow X_i)$ at energy $E_{projectile}$ Computational Workflow

Key:
Code Modules
User Inputs/Outputs
Exchanged Data
Need Clarification

From Ian Thompson

Connections to computational science

Jaguar Cray XT4 at ORNL
No. 2 on Top500

- 11,706 processor nodes
- Each compute/service node contains 2.6 GHz dual-core AMD Opteron processor and 4 GB/8 GB of memory
- Peak performance of over 119 Teraflops
- 250 Teraflops after Dec.'07 upgrade
- 600 TB of scratch disk space

1Teraflop=10^{12} flops
1peta=10^{15} flops (next 2-3 years)
1exa=10^{18} flops (next 10 years)

Example: Large Scale Mass Table Calculations

Science scales with processors

M. Stoitsov

Jaguar@ OAK RIDGE National Laboratory

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)

All Nuclei

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

Perspectives

What is needed/essential?

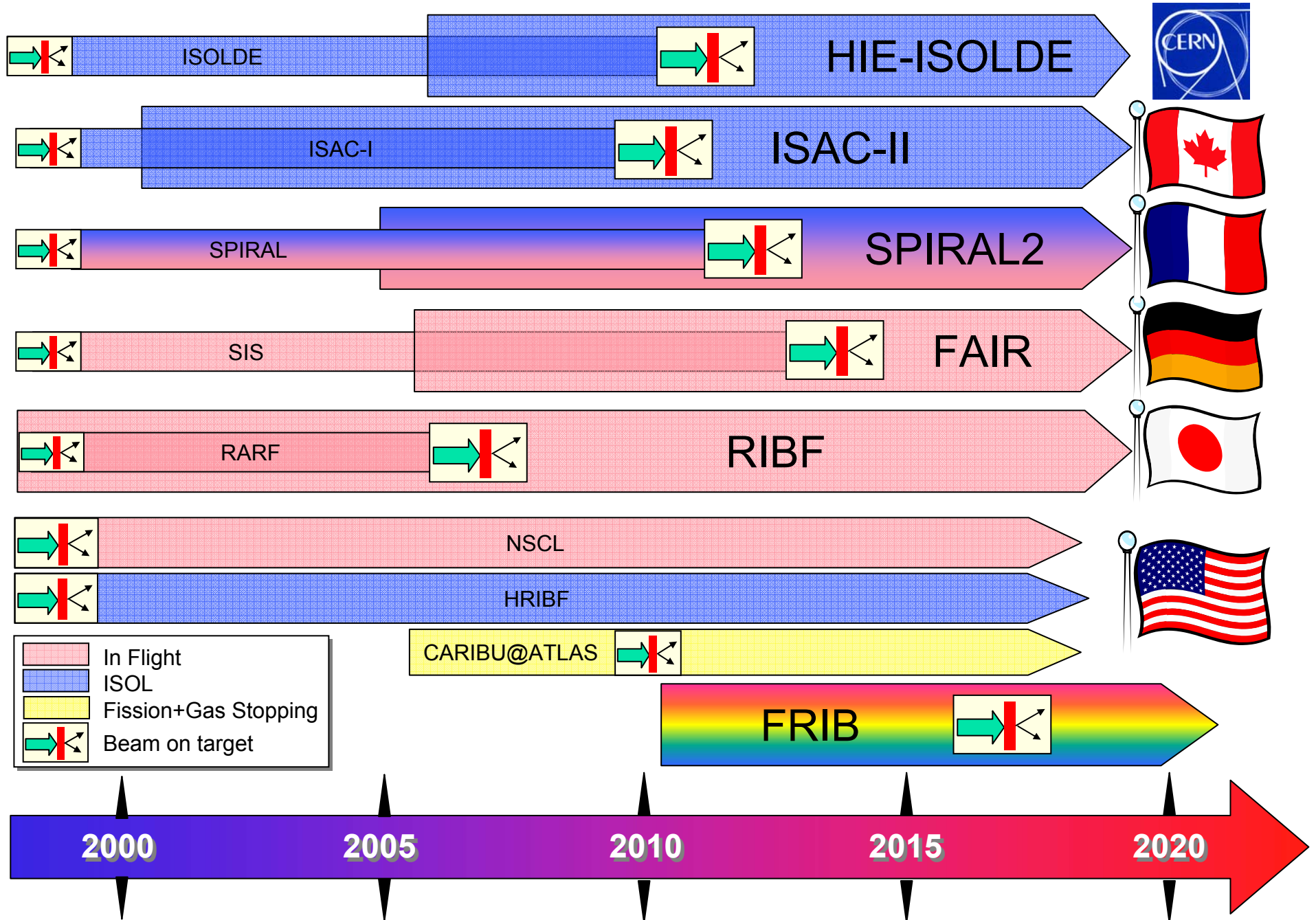
- Young talent
- Focused effort
- Large collaborations

UNEDF

- Data from *terra incognita*
  RNB facilities provide strong motivation!

- High-performance computing

Radioactive Ion Beam Facilities Timeline



Conclusions

- **Exciting** science; old paradigms revisited
- **Interdisciplinary** (quantum many-body problem, cosmos,…)
- **Relevant** to society (energy, medicine, national security, …)

- Theory gives the mathematical formulation of our understanding and predictive ability
- New-generation computers provide unprecedented opportunities
- Large coherent international theory effort is needed to make a progress

Guided by data on short-lived nuclei, we are embarking on a comprehensive study of all nuclei based on the most accurate knowledge of the strong inter-nucleon interaction, the most reliable theoretical approaches, and the massive use of the computer power available at this moment in time. **The prospects look good.**

Thank You