1. What is Density Functional Theory?
2. Motivation
3. Deliverables for Nuclear Physics
4. Scientific Organizational Structure
5. Challenges
6. Near-term goals
7. Milestones

Density Functional Theory--What is it?

Conceptual   --Ask me later

Practical --Kohn&Sham, 1965

Define a set of N orbitals $\phi_i(r); \ i = 1, .., N$

Minimize with respect to the orbital functions

$$\int \left(\sum_i \frac{|\nabla \phi_i|^2}{2m} + V(\{\phi\}) \right) d^3r \qquad \qquad n(r) = \sum_i^N |\phi_i(r)|^2$$
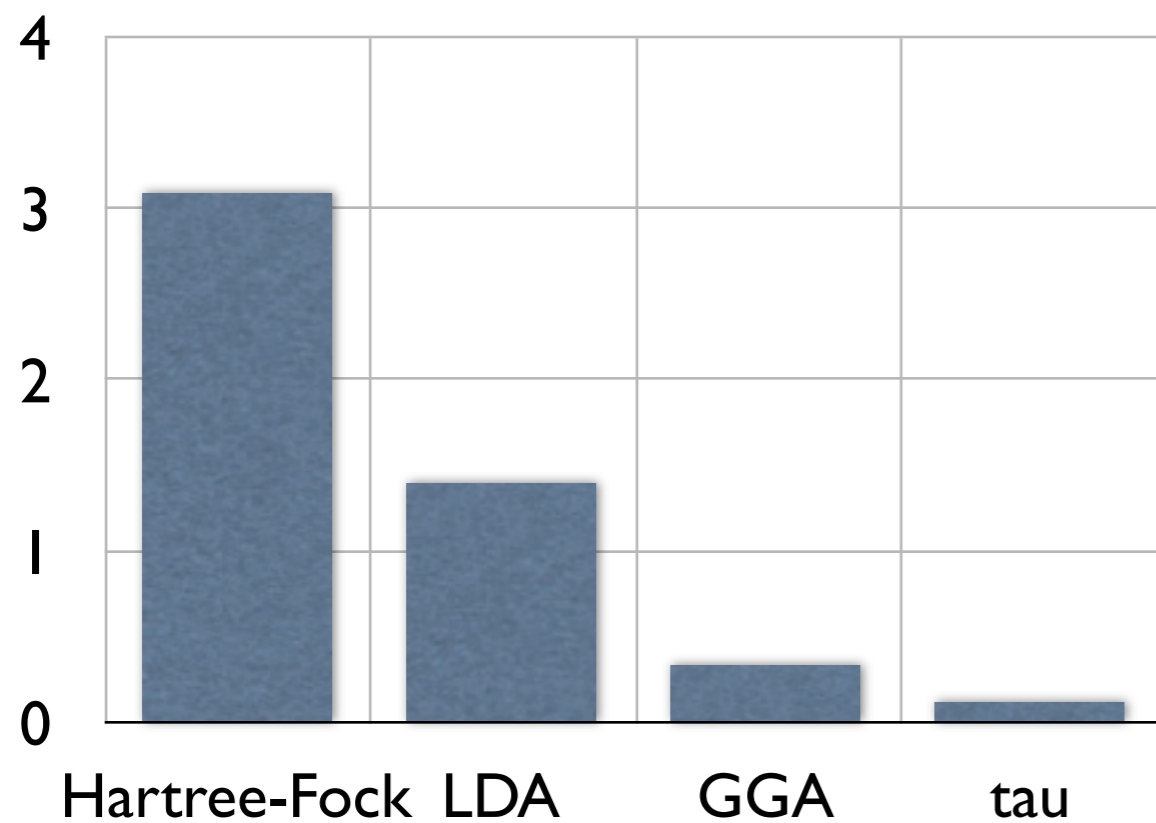
Kohn-Sham equations

$$-\frac{\hbar^2 \nabla^2}{2m} \phi_i + \frac{\delta V}{\delta n} \phi_i = \epsilon_i \phi_i$$

$$V = V_{ext}(r)n(r) + \frac{e^2}{2} \int d^3r' \frac{n(r)n(r')}{|r - r'|} + \mathcal{E}_{xc}[n]$$

The DFT Success Story

Average error for simple molecules

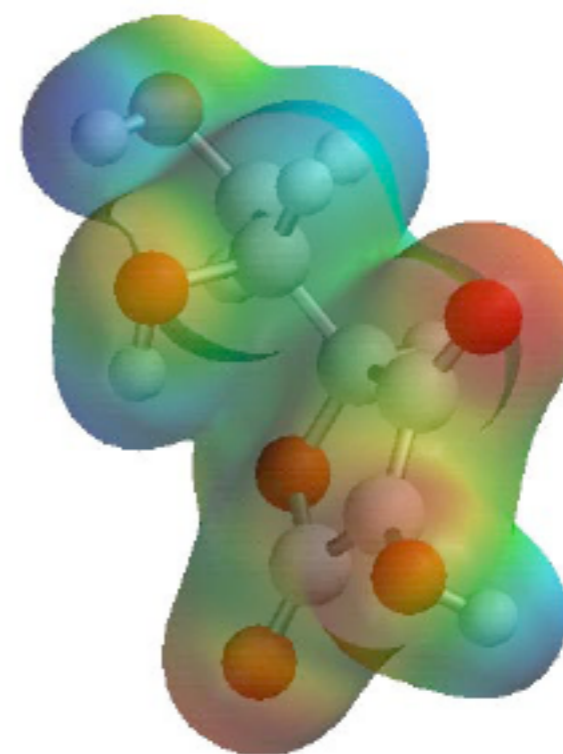|	
Hartree-Fock	1929
LDA	1965
GGA	1989
tau	1999

Image of vitamin C from Nobel Foundation website

What do we want to know?

Binding Energies

Nucleosynthesis

Interactions with neutrons

Inelastic cross sections: For some intermediate mass nuclei (e.g., ^{23}Na or ^{56}Fe) inelastic scattering cross-section accuracies of the order of 10% are needed. Moreover, there exists a general need to improve the knowledge of inelastic scattering for actinides. Relevant experiments have proven particularly difficult. It would be worthwhile for the basic science community to investigate whether current challenges could be met with new and innovative measurement techniques.
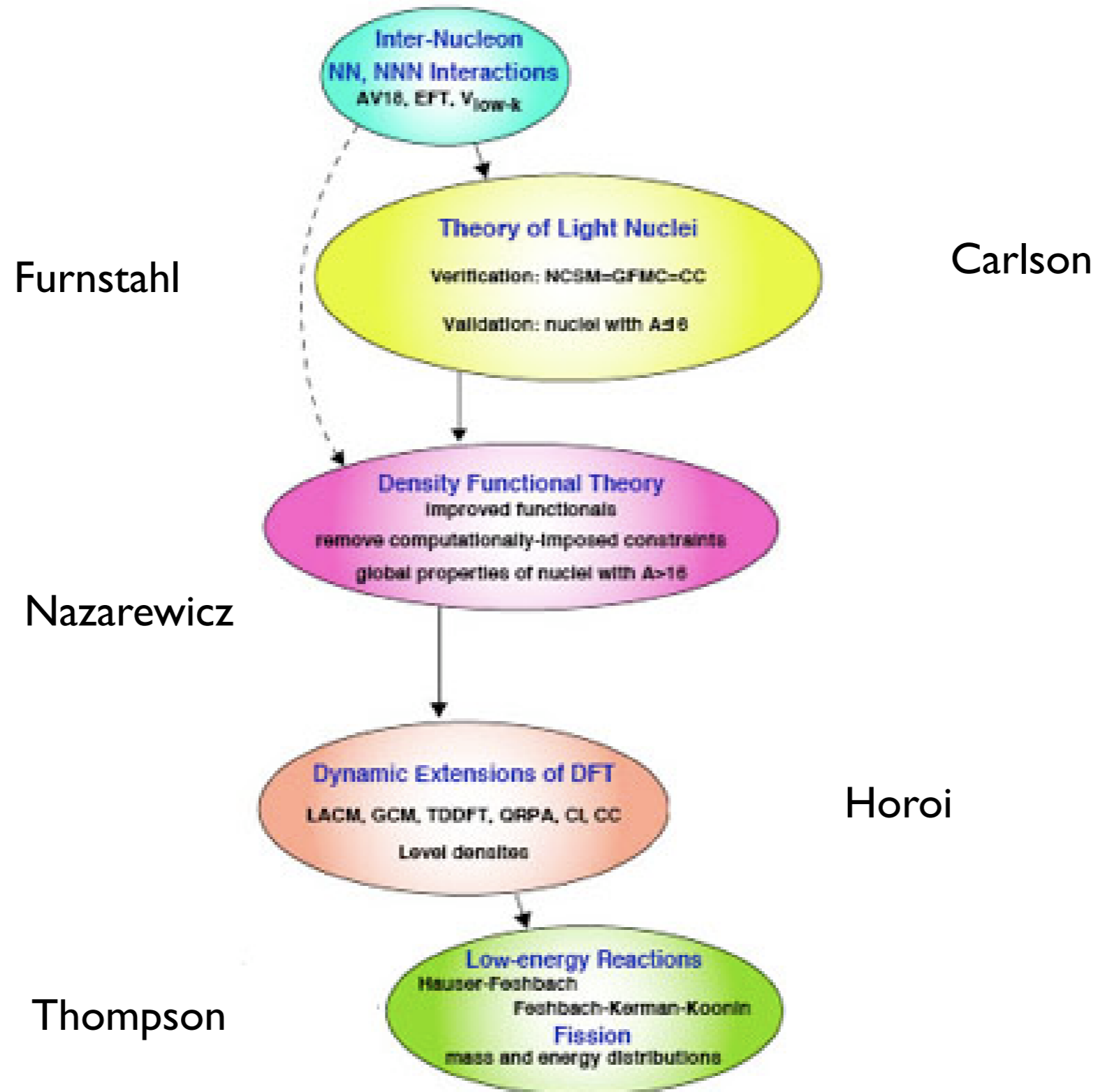
From the report "Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles", 2006

Radioactive decay properties

Fission properties

Scientific Organization of UNEDF

Inter-Nucleon
NN, NNN Interactions
AV18, EFT, V_{low-k}

Theory of Light Nuclei
Verification: NCSM=GFMC=CC
Validation: nuclei with A≤16

Furnstahl

Carlson

Density Functional Theory
improved functionals
remove computationally-imposed constraints
global properties of nuclei with A>16

Nazarewicz

Dynamic Extensions of DFT
LACM, GCM, TDDFT, QRPA, CI, CC
Level densities

Horoi

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

Thompson

Challenges we face

The functional itself

The DFT solver

Extensions for dynamics

Reactions with DFT input

Utilizing leadership class machines

Building blocks: Nuclear Local 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 $\quad \left(\rho_0 = \rho_n + \rho_p \right)$

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

isovector (T=1) density $\quad \left(\rho_1 = \rho_n - \rho_p \right)$

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

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

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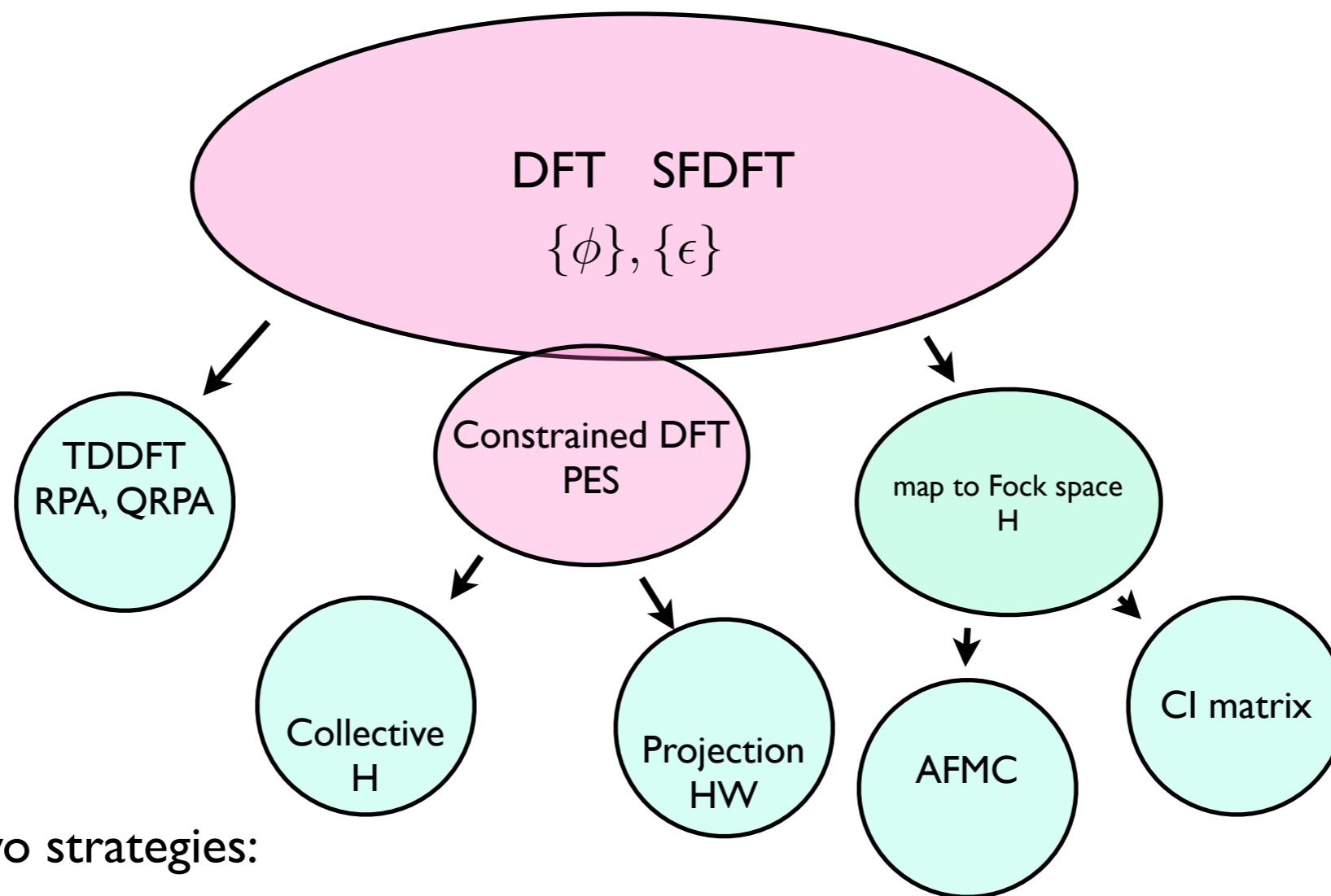
current density

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

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

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

kinetic spin density

+ analogous p-p densities and currents

Need to go beyond DFT for dynamics, excited states

DFT   SFDFT
$\{\phi\}, \{\epsilon\}$

TDDFT
RPA, QRPA

Constrained DFT
PES

map to Fock space
H

Collective
H

Projection
HW

AFMC

CI matrix

Two strategies:

$$\phi_i \rightarrow \phi_i(t), \phi_i(q), \ldots$$

$$\phi_i \rightarrow a_i^\dagger$$

Near-term goals

Verification

> Methodologies for ab initio wave functions

Global Benchmarking

> 2+ Excited states

> Odd-A mass table

> Pairing energies

Physics Milestones

2.2. Computational

  a) Schroedinger solver with fission-quality accuracy.   (June 2008)
     Note: the outcome of the comparison here may affect the
     choice of algorithms for the final DFT solver.
  b) Medium-mass coupled-cluster calculations within a new
        spherical coding scheme   (Dec. 2008)
  c) DFT solver with fission-quality accuracy   (June 2009)
  d) NCSM solver and analyser program suite   (June 2009)
  e) Parallelized coupled-channel code including 2p2h excitations   (Mar. 2009)
  f) Partially fitted, energy density functional
     with documented global performance   (Dec. 2010)

2.3. DFT

 a) First comparisons of ab initio coupled-cluster and large-configuration
    calculations with the density matrix expansion using the same
    low-momentum NN + fit NNN Hamiltonian   (June 2008)
 b) Delivery of a complete DFT based on above Hamiltonian compatible
    with Skyrme DFT solvers.   (Dec. 2008)
 c) Completed evaluation of adequacy of the density matrix
    expansion (DME) for ab initio functionals.   (June 2009)
 d) Delivery of an energy density functional using a fine-tuned Hamiltonian   (Dec. 2009)

2.4. Reactions

 a) Folding treatment of full target-projectile interaction.   (June 2009)
 b) Dispersive optical potentials for many DFT structure models   (Dec. 2009)
 c) nonlocal exchange and pickup corrections to optical potentials   (June 2010)
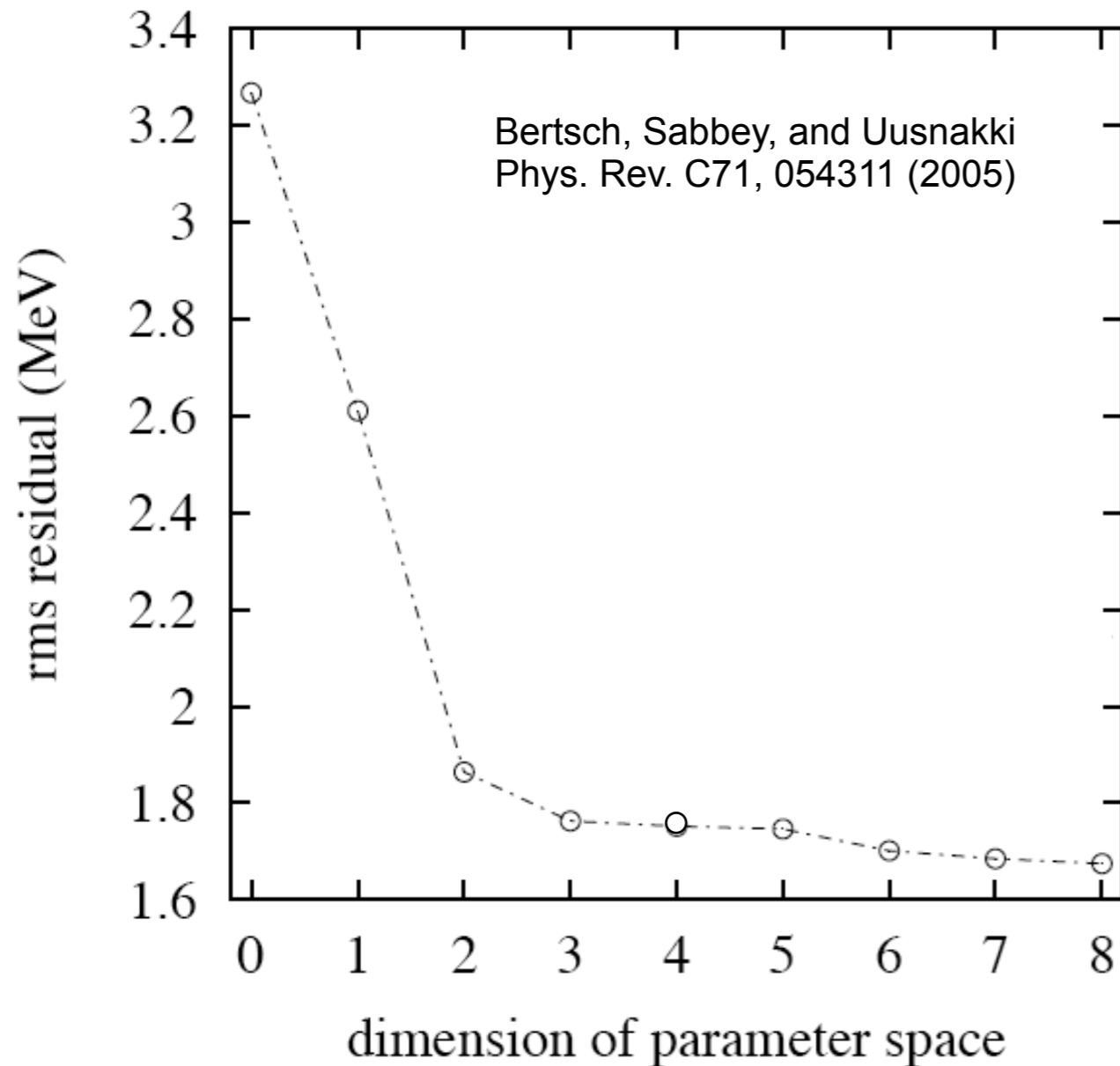
2.5. Final Deliverables (mid 2011)

  a) The performance-documented functional;
  b) The codes to apply the functional to the nuclear energy
       surface including post-fission shapes;
  c) The codes to apply the extension of DFT to nuclear excitations;
  d) Systematic predicted optical potentials including nonlocatities;
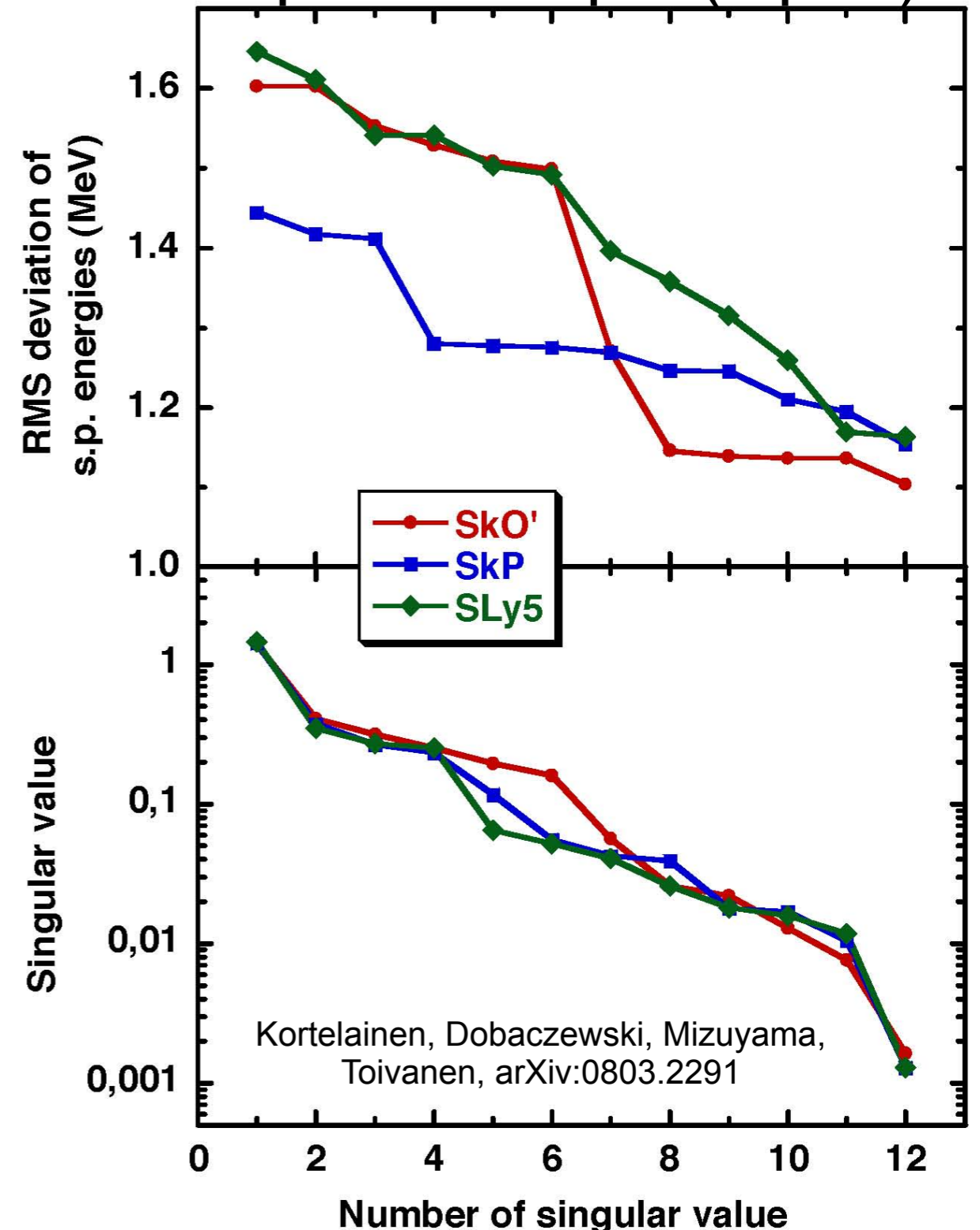 e) DFT-based level densities for neutron reactions.

Ultimate goal:

Order-of-magnitude improvement of global systematics with respect to near-term benchmarks.
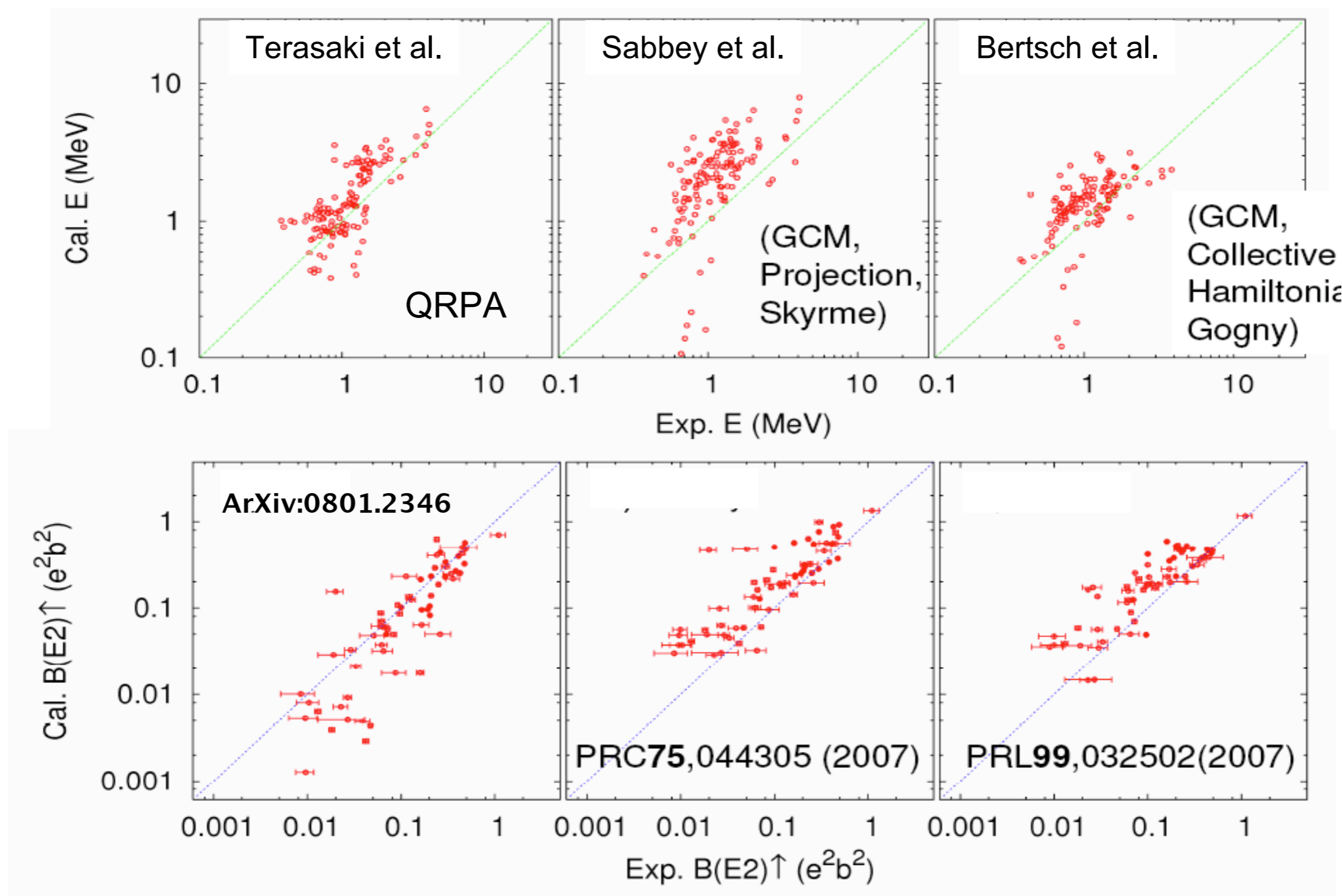
How many parameters are really needed?

Spectroscopic (s.p.e.)

Global (masses)

Bertsch, Sabbey, and Uusnakki
Phys. Rev. C71, 054311 (2005)

Kortelainen, Dobaczewski, Mizuyama,
Toivanen, arXiv:0803.2291

New optimization strategy and protocol needed

Global calculations of the lowest 2$^+$ states

Terasaki et al.

Sabbey et al.

Bertsch et al.

QRPA

(GCM, Projection, Skyrme)

(GCM, Collective Hamiltonian Gogny)

ArXiv:0801.2346

PRC**75**,044305 (2007)

PRL**99**,032502(2007)

Deformed QRPA code including general Skyrme functional in progress (Terasaki, Engel)