Energy Density Functionals for Nuclei

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For references and more details, see:

- unedf.org  UNEDF SciDAC Collaboration
  Universal Nuclear Energy Density Functional
   U.S. DEPARTMENT OF ENERGY
- "Toward ab initio density functional theory for nuclei," arXiv:0906.1463
- J. Phys. G: "Open Problems in Nuclear Structure" (online May, 2010)

Outline

Overview: EDF's and DFT

The UNEDF project

New developments: Constraints, optimization, . . .

Non-empirical EDF's and ab-initio DFT

Summary

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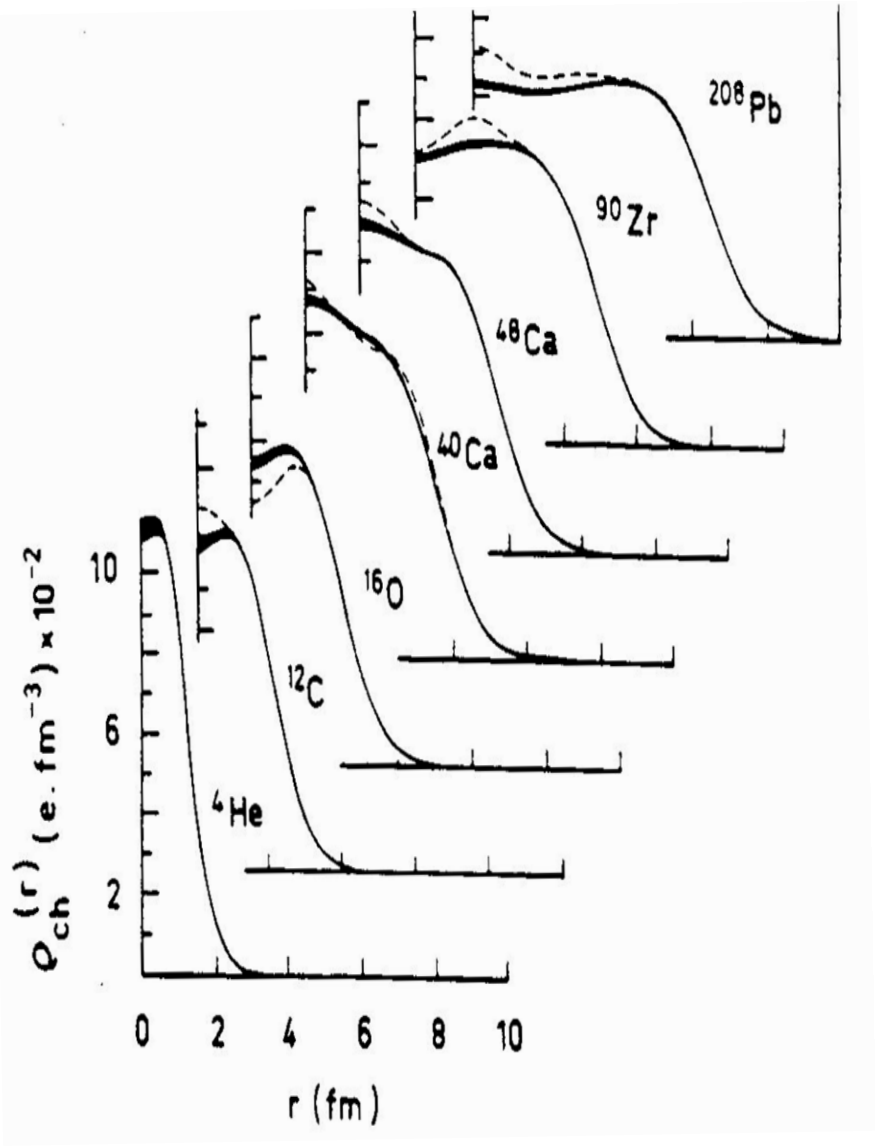
Density functional theory (DFT) as justification for energy density functional (EDF) approach

- Hohenberg-Kohn: There exists an energy functional $E_{v_{\text{ext}}}[\rho]$ of $\rho(\mathbf{x})$ for external potential v_{ext}:

$$E_{v_{\text{ext}}}[\rho] = F_{\text{HK}}[\rho] + \int d\mathbf{x}\, v_{\text{ext}}(\mathbf{x})\rho(\mathbf{x})$$

  Minimize $\Longrightarrow E_{gs}, \rho_{gs}$

- Useful if you can approximate the energy functional; suggests a hunting license for EDF's
- F_{HK} is *universal* (same for any external v_{ext}), so should be able to add any v_{ext} we want!
- Kohn-Sham (KS) DFT: Introduce orbitals for $\rho(\mathbf{x})$



Unraveling the magic of DFT [Kutzelnigg (2008)]

- Wavefunction-based: for anti-symmetric A-body $|\Psi\rangle$, find $E_{gs} = \min_{\Psi} \langle\Psi|\widehat{H}|\Psi\rangle$ (CI, CC use a single-particle basis for $|\Psi\rangle$)
- DFT: fermion densities as basic variables
  - Common but misleading statements:

"All information about a quantum mechanical ground state is contained in its electron density ρ."

"The energy is completely expressible in terms of the density alone."

  - At odds with kinetic and interaction energies needing $(1, 2, \cdots)$–particle density matrices!

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  - At odds with kinetic and interaction energies needing $(1, 2, \cdots)$–particle density matrices!
- Key: WF formulation deals with *single, fixed Hamiltonian*, E stationary to density matrix (or Ψ) variations, not just $\rho(\mathbf{x})$
- DFT: Consider a *family* of Hamiltonians $\widehat{H}[v] \longrightarrow E[v]$, then

$$F_{\rm HK}[\rho] = \min_{v}\{E[v] - \int d\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x})\} \text{ and}$$

$$E[v] = \min_{\rho}\{F[\rho] + \int d\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x})\} \equiv \min_{\rho}\{E_v[\rho]\}$$

$\Longrightarrow$ DFT is based on *Legendre transforms* (see arXiv:0906.1463)

Challenges for nuclear DFT (cf. Coulomb DFT)

- Difficult conventional nuclear Hamiltonians
  - Sources of non-perturbative physics for NN interaction
    1. Strong short-range repulsion ("hard core")
    2. Iterated tensor interactions (e.g., from pion exchange)
    3. Near zero-energy bound states (e.g., deuteron)
  - Non-negligible many-body forces
- Non-trivial implementation issues
  - Essential role of pairing (so like HFB rather than HF)
  - Important long-range correlations
  - Some observables we want are not KS-DFT observables
  - We don't have a v_{ext}!
  - Symmetry breaking in finite, self-bound systems (translation, rotation, number, . . .)
    $\Longrightarrow$ What about symmetry restoration?

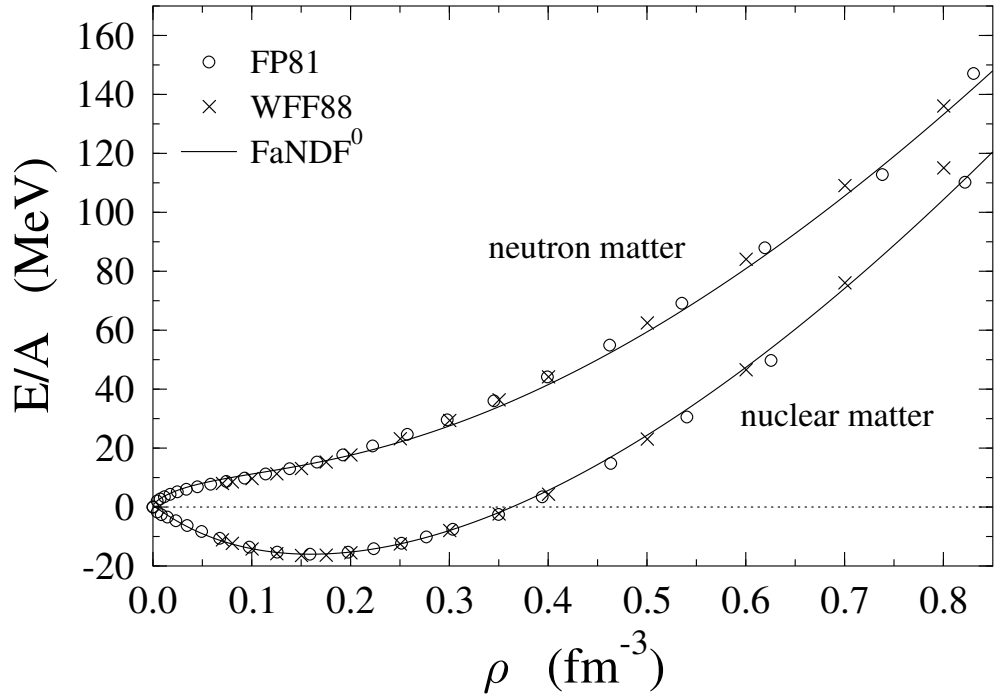
Paths to a nuclear energy functional (EDF)

1. Improve empirical energy functional (Skyrme, Gogny or RMF)
2. Emulate Coulomb DFT: LDA based on precision calculation of uniform system $E[\rho] = \int d\mathbf{r}\, \mathcal{E}(\rho(\mathbf{r}))$ plus constrained gradient corrections ($\nabla\rho$ factors)

   - Fayans and collaborators (e.g., nucl-th/0009034)

     $$\mathcal{E}_v = \tfrac{2}{3}\epsilon_F\rho_0\left[a_+^v\frac{1-h_{1+}^v x_+^{1/3}}{1-h_{2+}^v x_+^{1/3}}x_+^2 + a_-^v\frac{1-h_{1-}^v x_+^{1/3}}{1-h_{2-}^v x_+^{1/3}}x_-^2\right]$$

     where $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$
   - Neutron drops in traps
   - SLDA+ (Bulgac et al.)



3. Construct Kohn-Sham DFT with EFT-based, RG-softened V's

   UNEDF plan: Try them all, mix and match, . . .

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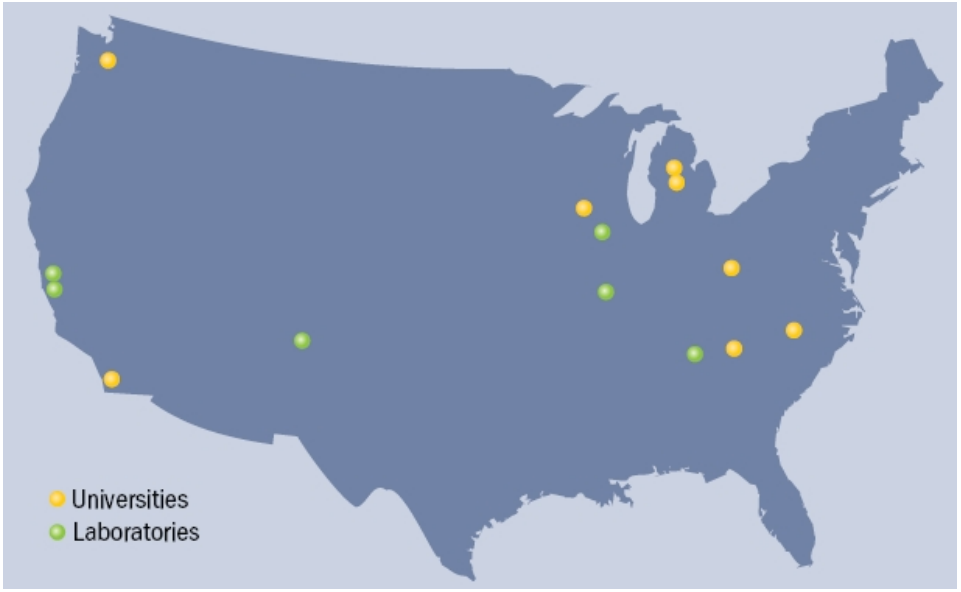
SciDAC 2 Project: *Building a Universal Nuclear Energy Density Functional*



- Collaboration of physicists, applied mathematicians, and computer scientists $\Longrightarrow$ prototype for FRIB theory
- Funding in US but international collaborators also

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

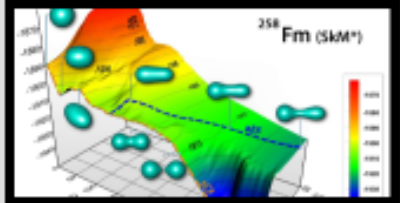
- Understand nuclear properties "for element formation, for properties of stars, and for present and future energy and defense applications"
- Scope is all nuclei with particular interest in reliable calculations of unstable nuclei and in reactions
  $\Longrightarrow$ Density functional theory (DFT) is method of choice
- Order of magnitude improvement over present capabilities
  $\Longrightarrow$ precision calculations of masses, ...
- Maximum predictive power with well-quantified uncertainties
- Connected to the best microscopic physics

[See unedf.org for background, references, and highlights.]

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

MTEX



SRG+MFD

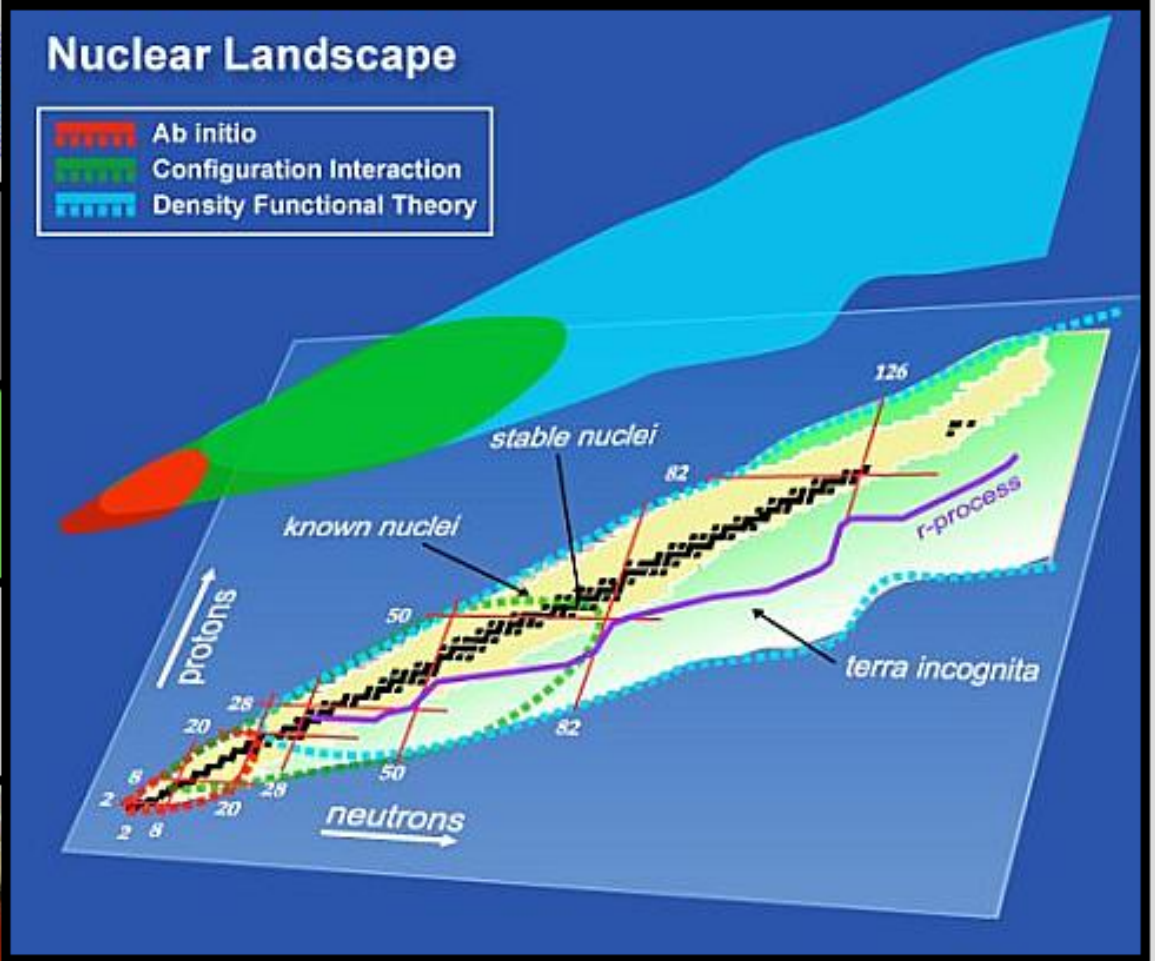
λ =4.0 fm^{-1} λ =2.0 fm^{-1}

^{4}He + n

NCSM/RGM

Jaguar

MADNESS



UNEDF is a collaboration of physicists, computer scientists and applied mathematicians using high-performance computing to explore the nuclear landscape. Point to the buttons at left to highlight computational sub-projects; click for details. Refresh for more.

Good News

UNEDF collaborators Steve Pieper and Bob Wiringa awarded APS Bonner Prize

The Tom W. Bonner Prize is the highest award for research given by the APS Division of Nuclear Physics. Full details on the award to Steve and Bob are available.

DOE awards 40 million processor hours for computational nuclear structure

For the third straight year, the DOE INCITE program awarded a large number of hours for UNEDF computational nuclear physics projects. More details are available.

Announcements (see also Meetings and Job Postings and News Archive)

Leadership Class Configuration Interaction (LCCI) Code Meeting

San Diego State University, San Diego, CA
March 11-13, 2010 (contact James Vary)

Fourth LACM-EFES-JUSTIPEN workshop at Oak Ridge National Laboratory

March 15-17, 2010 (with additional days March 18, 19 for more individual collaborations)

Annual UNEDF Collaboration Meeting, MSU

June 21-25, 2010

Argonne Computational Postdoctoral Fellowships

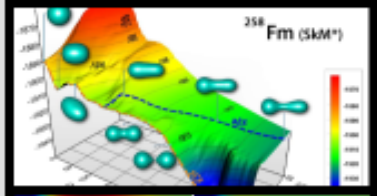
For more information on UNEDF, please contact witek@utk.edu
For a popular description of UNEDF, see the SciDAC Review article

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

Tools:
- SVN Repository
- Public Codes
- Web-based
- DFT Database
- More Databases
  - Mass Tables
  - 2+ States
  - Fission Barriers
  - GDR and E1
- Mass Explorer
- VNC Viewers

MTEX



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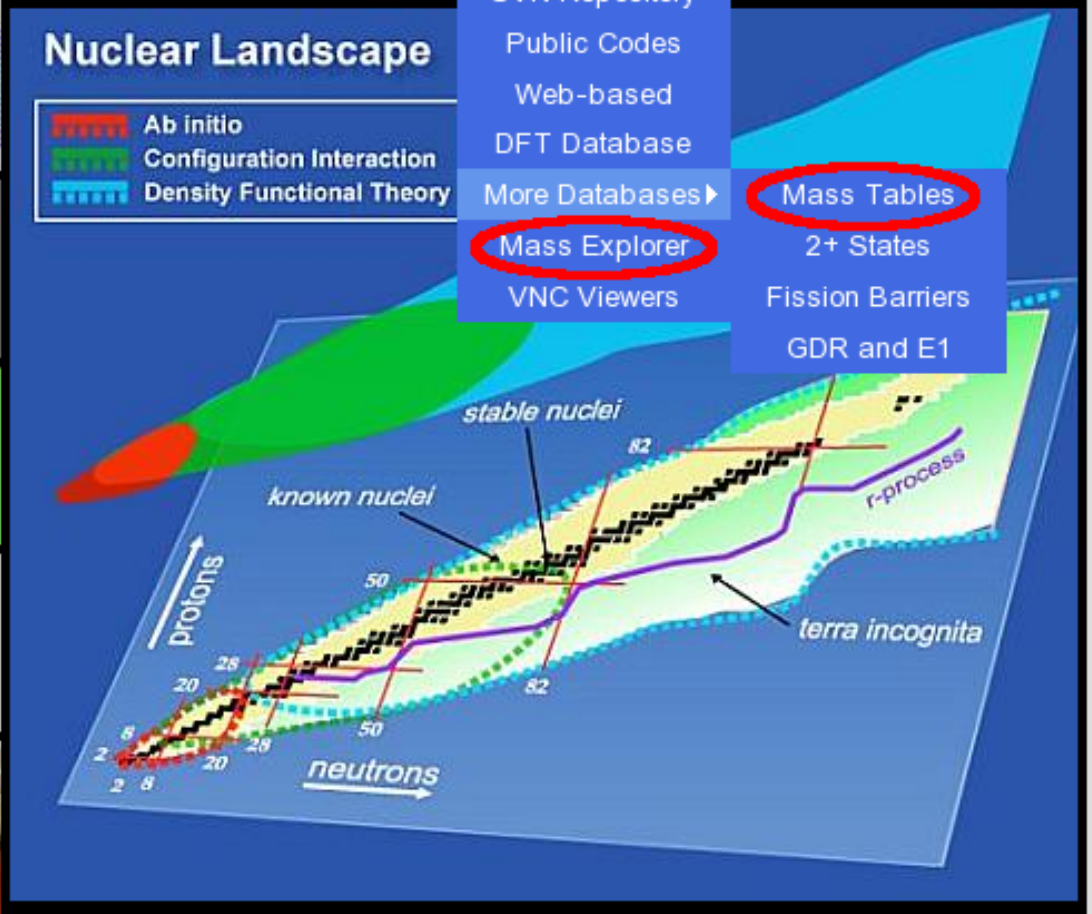

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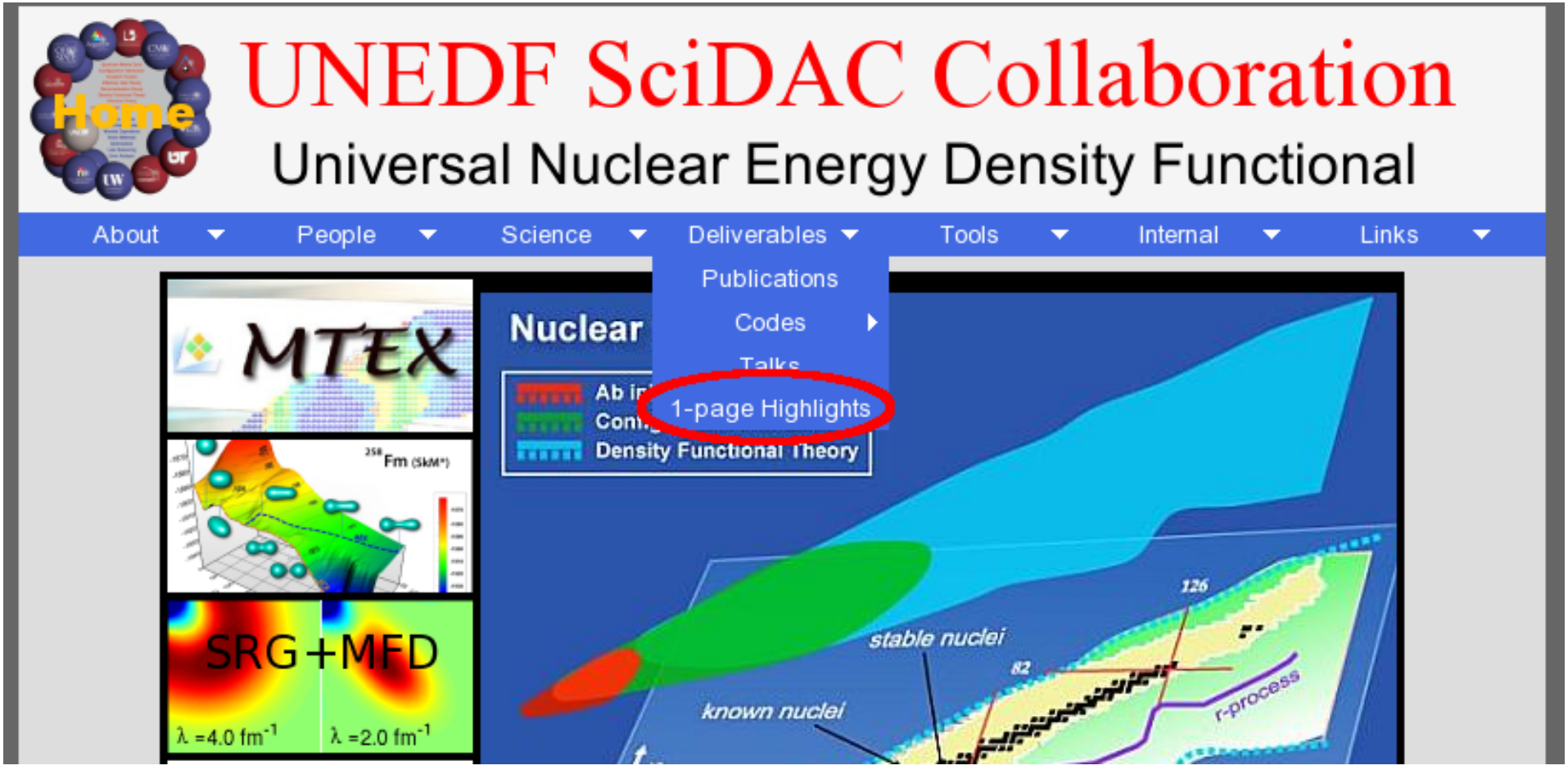
Highlights of research on unedf.org



- One-slide summaries targeted for broad audience
- Notes with details and references

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

UNEDF One-Page Highlights

On this page are links to one-slide summaries of UNEDF-related research accomplishments, plus notes giving contacts and references along with brief explanations of the technical details. All are in pdf format. See also the UNEDF Highlights" page.

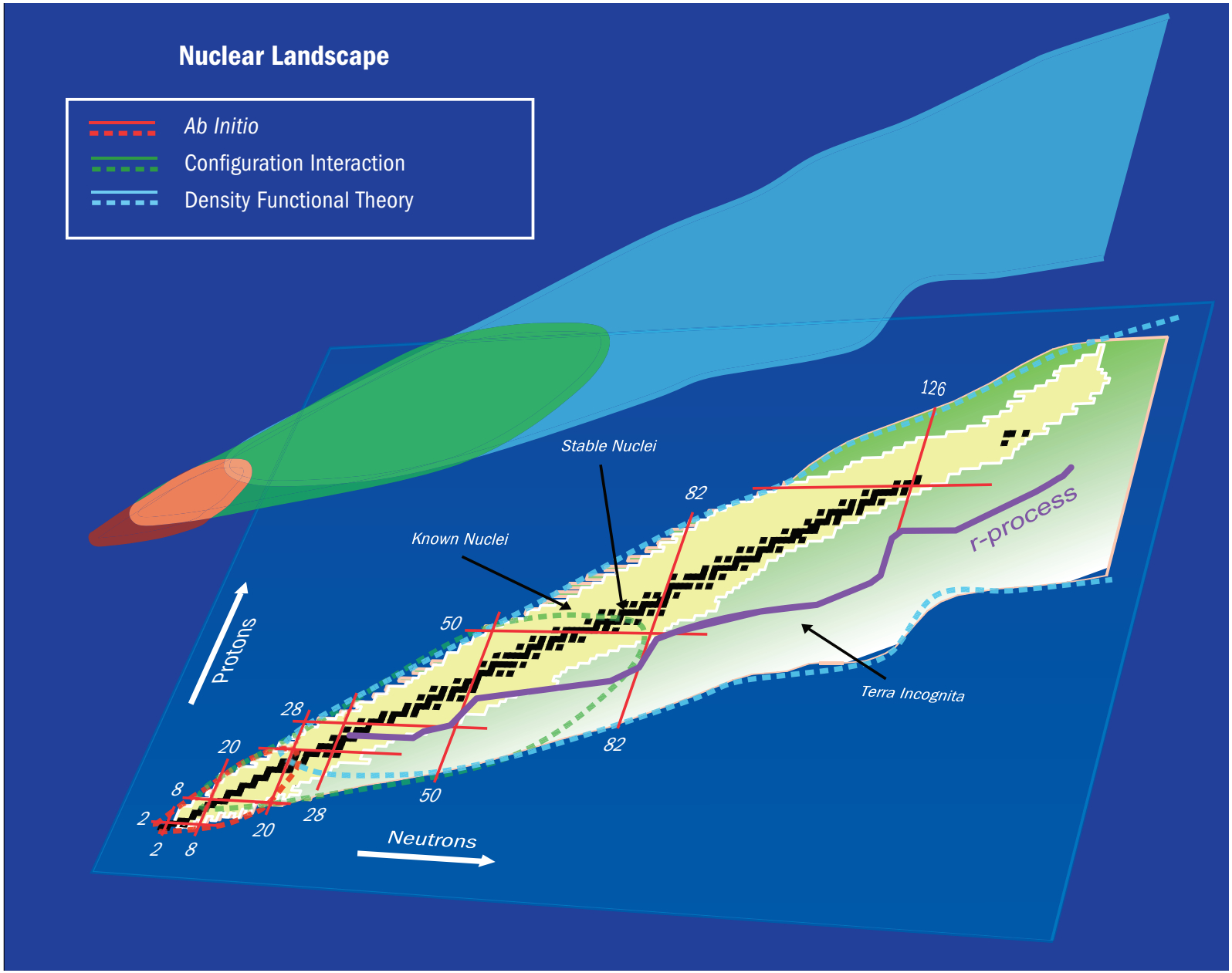
- UNEDF-TOPS eigensolver collaboration: Breakthrough nuclear science [notes]
- Microscopic description of nuclear fission [notes]
- Building medium-mass atomic nuclei from scratch: coupled cluster [notes]
- Computing masses of atomic nuclei [notes]
- Discovering the secrets buried in theories [notes]
- The uNclear Nuclear Pairing [notes]
- For atomic nuclei, three's a crowd: Enabling microscopic calculations of nuclei [notes]
- Building the UNEDF from the ground up [notes]
- Towards improved cross sections on medium and heavy unstable nuclides [notes]
- High-performance code for nuclear level density [notes]
- Predictions for Proton-Dripping Fluorine-14 [notes]
- Ab initio no-core shell model (NCSM) and resonating-group method (RGM)

For more information on UNEDF, please contact witek@utk.edu
For a popular description of UNEDF, see the SciDAC Review article

Major UNEDF research areas

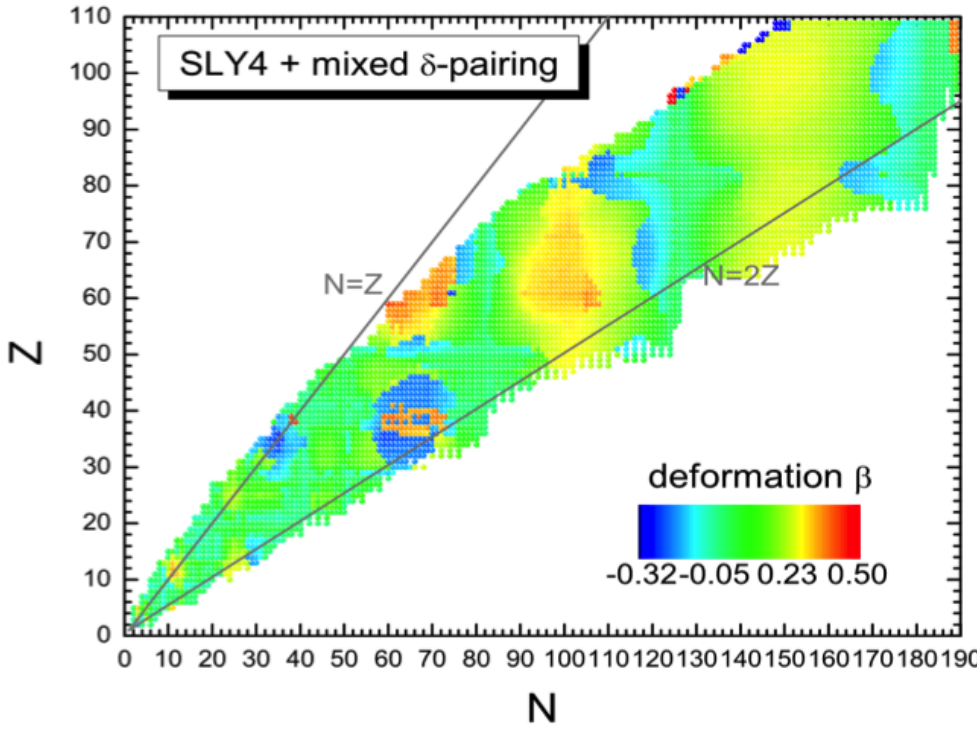
1. Ab initio structure — Nuclear wf's from microscopic NN$\cdots$N
   - Methods: GFMC/AFMC, CI (NCSM/NCFC), CC
   - Interactions: AV18/ILx, chiral EFT $\longrightarrow$ $V_{\mathrm{low}\,k}$, V_{SRG}
2. Ab initio energy functionals — DFT from microscopic NN$\cdots$N
   - Cold atoms — superfluid LDA+ $\Longrightarrow$ nuclear DFT
   - χEFT $\longrightarrow$ $V_{\mathrm{low}\,k}$ $\longrightarrow$ MBPT $\longrightarrow$ DME functional
3. DFT applications — Technology to calculate observables
   - Skyrme HFB+ for all nuclei (solvers)
   - Fitting functionals to data (e.g., correlation analysis)
4. DFT extensions — Long-range correlations, excited states, ...
   - Alphabet soup: LACM, GCM, TDDFT, QRPA, CI, ...
5. Reactions – coupled channels, optical potentials ...
   - Ab initio reactions: NCSM+RGM

Universal Nuclear Energy Density Functional



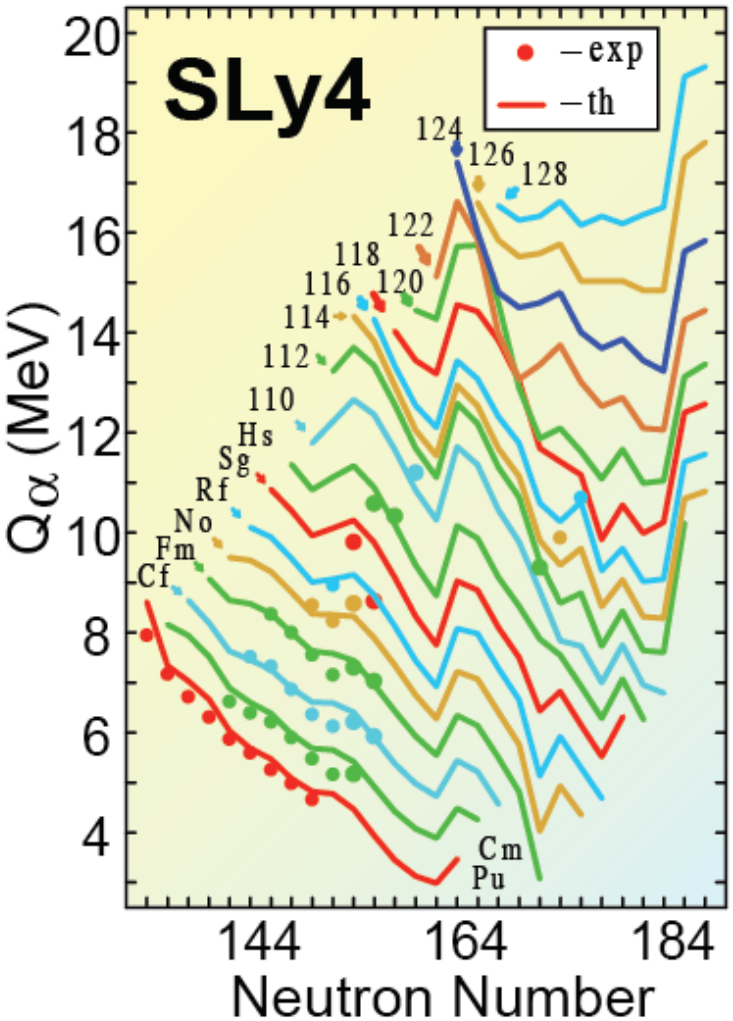
Large-scale mass table calculations [M. Stoitsov et al.]

- One Skyrme functional (∼10–20 parameters) describes all nuclei from few-body to superheavies
- 9,210 nuclei in less than one day on ORNL Jaguar (Cray XT4)
- Under development: optimization and correlation analysis tools
- Extending optimization dataset to symmetry-unresticted nuclei to constrain time-odd terms

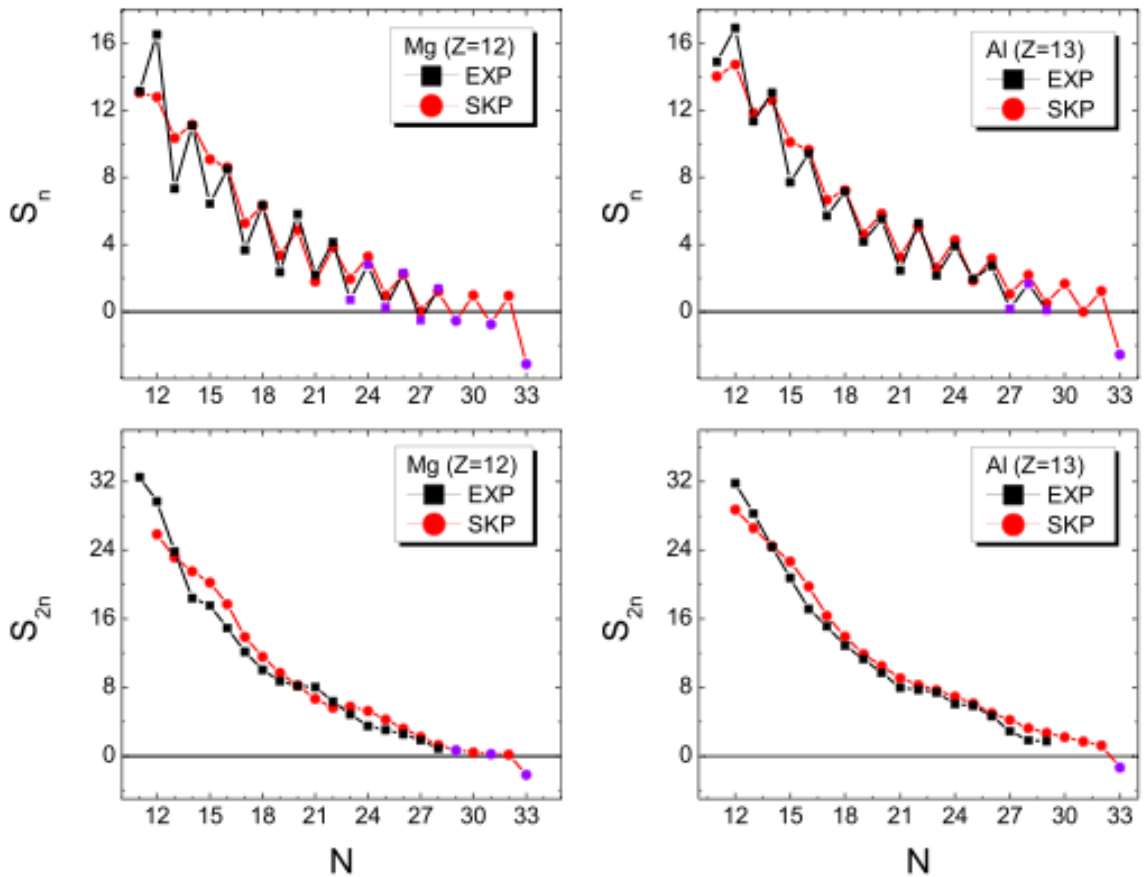


Nuclear DFT: works well for BE differences

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



Stoitsov et al., 2008



- Global DFT mass calculations: HFB mass formula: $\Delta m \sim 700$keV

Issues with empirical EDF's

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No (fully) systematic organization of terms in the EDF
- Difficult to estimate theoretical uncertainties (extrapolation)
- Where are the pions?
- What's the connection to many-body forces?
- Pairing part of the EDF not treated on same footing
- and so on ...

$\Longrightarrow$ Extend conventional EDF form and analysis

$\Longrightarrow$ Turn to microscopic many-body theory for guidance

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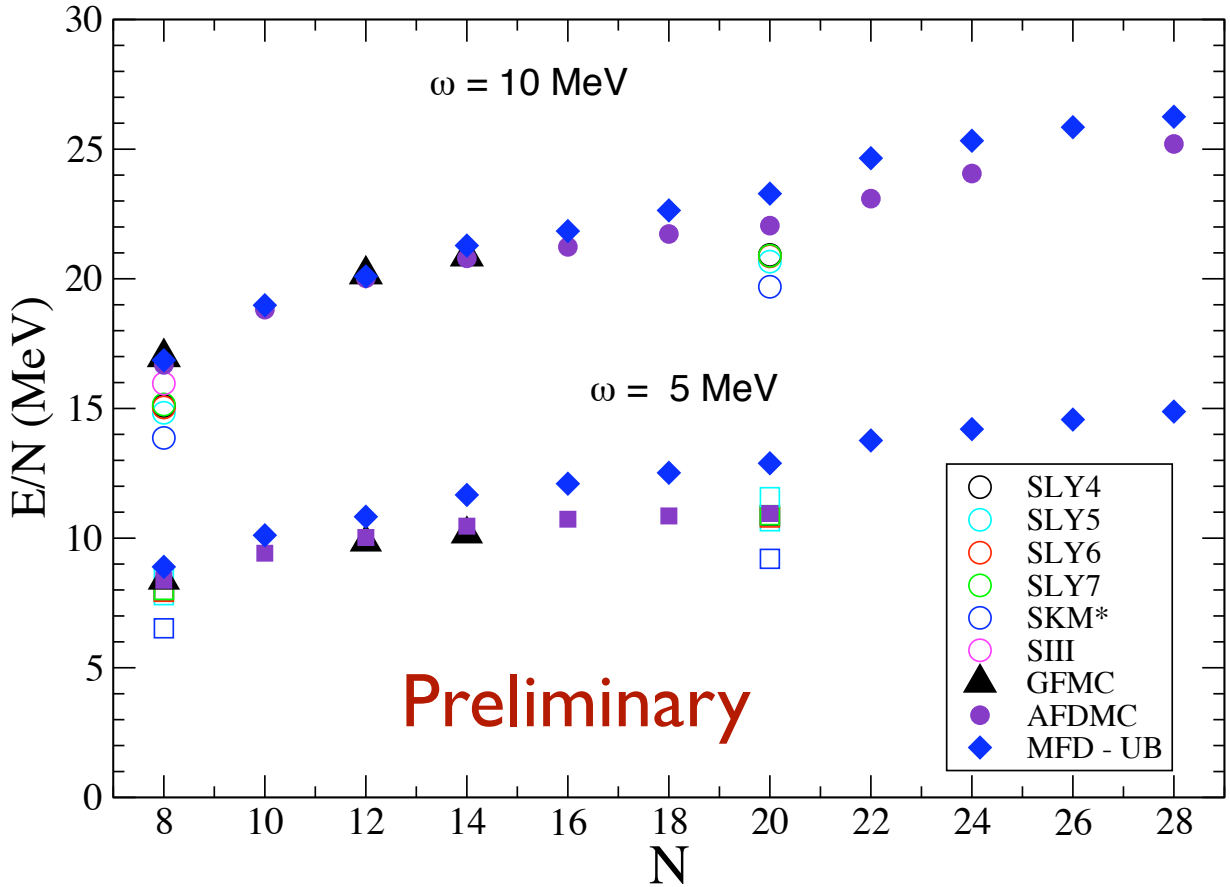
Constraints from external potentials (preliminary)

- Ab initio: neutrons in external potentials ("neutron drops")
  - Here: GFMC, AFDMC (Carlson et al.); NCFC/MFDn (Maris et al.)



- Compare vs. Skyrme EDF for two different oscillator ω's
  - For larger ω, Skyrme energies too low and radius too small
    $\Longrightarrow$ more repulsive isovector gradient terms needed?
  - Much more to come! (including CC, ab initio DFT)

Skyrme generalizations based on EFT principles

- Ability to use local densities based on short range of nuclear interactions compared to variations in local and non-local density matrix $\Longrightarrow$ use separation of scales

- Density functional

$$E = \int d^3\mathbf{r} \left[\frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_{\rm Skyrme}(\rho_0,\rho_1,\tau_0,\tau_1,\mathbf{s}_0,\mathbf{s}_1,\ldots) + \mathcal{H}_{\rm Coul.}(\rho_{\rm p}) \right]$$

- Densities

$$\rho = \sum\nolimits_i \varphi_i^\dagger \varphi_i, \qquad \tau = \sum\nolimits_{i,\mu} (\nabla_\mu \varphi_i^\dagger)(\nabla_\mu \varphi_i), \qquad \mathbf{j},\ \mathbf{J}: \text{currents}$$
$$\mathbf{s}_\nu = \sum\nolimits_i \varphi_i^\dagger \sigma_\nu \varphi_i, \qquad \mathbf{T}_\nu = \sum\nolimits_{i,\mu} (\nabla_\mu \varphi_i^\dagger)\sigma_\nu(\nabla_\mu \varphi_i), \qquad \rho_0 = \rho_{\rm n} + \rho_{\rm p}, \quad \rho_1 = \rho_{\rm n} - \rho_{\rm p}, \ \ldots$$

- Strong interaction energy density $\mathcal{H}_{\rm Skyrme}$

$$\begin{aligned}
\mathcal{H}_0^{\rm even} &= C_0^\rho(\rho_0)\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^\tau\rho_0\tau_0 + C_0^J\mathbf{J}_0^2 + C_0^{\nabla J}\rho_0\boldsymbol{\nabla}\cdot\mathbf{J}_0,\\
\mathcal{H}_1^{\rm even} &= C_1^\rho(\rho_0)\rho_1^2 + C_1^{\Delta\rho}\rho_1\Delta\rho_1 + C_1^\tau\rho_1\tau_1 + C_1^J\mathbf{J}_1^2 + C_1^{\nabla J}\rho_1\boldsymbol{\nabla}\cdot\mathbf{J}_1,\\
\mathcal{H}_0^{\rm odd} &= C_0^s(\rho_0)\mathbf{s}_0^2 + C_0^{\Delta s}\mathbf{s}_0\cdot\Delta\mathbf{s}_0 + C_0^{sT}\mathbf{s}_0\cdot\mathbf{T}_0 + C_0^j\mathbf{j}_0^2 + C_0^{\nabla j}\mathbf{s}_0\cdot(\boldsymbol{\nabla}\times\mathbf{j}_0),\\
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\end{aligned}$$

- Expand in densities and gradients
- Includes time-odd fields $\Longrightarrow$ new domain to explore
- Gogny EDF can be accurately cast in same form [arXiv:1002.3646]

Energy density functional for spherical nuclei (II)

We can write the N^{3}LO spherical energy density as a sum of contributions from zero, second, fourth, and sixth orders:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{H}_6,$$

where

$$\mathcal{H}_0 = C_{00}^0 R_0 R_0,$$

$$\begin{aligned}\mathcal{H}_2 &= C_{20}^0 R_0 \Delta R_0 + C_{02}^0 R_0 R_2 \\ [0.5ex] &+ C_{11}^0 R_0 \vec{\nabla}\cdot\vec{J}_1, + C_{01}^1 \vec{J}_1^2,\end{aligned}$$

Energy densities $\mathcal{H}_0$ and $\mathcal{H}_2$ correspond, of course, to the standard Skyrme functional with $C_{00}^0 = C^\rho$, $C_{20}^0 = C^{\Delta\rho}$, $C_{02}^0 = C^\tau$, $C_{11}^0 = C^{\nabla J}$, and $C_{01}^1 = C^{J1}$. At fourth order, the energy density reads

$$\begin{aligned}\mathcal{H}_4 &= C_{40}^0 R_0 \Delta^2 R_0 + C_{22}^0 R_0 \Delta R_2 \\ &+ C_{04}^0 R_0 R_4 + C_{02}^2 R_2 R_2 \\ &+ D_{22}^0 R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D_{02}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{2ab} \\ &+ C_{21}^1 \vec{J}_1 \cdot \Delta \vec{J}_1 + C_{03}^1 \vec{J}_1 \cdot \vec{J}_3 \\ &+ D_{21}^1 \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C_{31}^0 R_0 \Delta\left(\vec{\nabla}\cdot\vec{J}_1\right) + C_{13}^0 R_0 \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C_{11}^2 R_2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + D_{11}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{1b},\end{aligned}$$

At sixth order, the energy density reads

$$\begin{aligned}\mathcal{H}_6 &= C_{60}^0 R_0 \Delta^3 R_0 + C_{42}^0 R_0 \Delta^2 R_2 \\ &+ C_{24}^0 R_0 \Delta R_4 + C_{06}^0 R_0 R_6 \\ &+ C_{22}^2 R_2 \Delta R_2 + C_{04}^2 R_2 R_4 \\ &+ D_{42}^0 R_0 \Delta \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D_{24}^0 R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{4ab} \\ &+ D_{22}^2 R_2 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + E_{22}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \overleftrightarrow{R}_{2ab} \\ &+ F_{22}^2 \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_c \overleftrightarrow{R}_{2cb} + E_{04}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{4ab} \\ &+ C_{41}^1 \vec{J}_1 \cdot \Delta^2 \vec{J}_1 + C_{23}^1 \vec{J}_1 \cdot \Delta \vec{J}_3 \\ &+ C_{05}^1 \vec{J}_1 \cdot \vec{J}_5 + C_{03}^3 \vec{J}_3 \cdot \vec{J}_3 \\ &+ D_{41}^1 \vec{J}_1 \cdot \Delta \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) + D_{23}^1 \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ E_{23}^1 \sum_{abc} \vec{J}_{1a} \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D_{03}^3 \sum_{abc} \overleftrightarrow{J}_{3abc} \overleftrightarrow{J}_{3abc} \\ &+ C_{51}^0 R_0 \Delta^2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + C_{33}^0 R_0 \Delta \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C_{15}^0 R_0 \left(\vec{\nabla}\cdot\vec{J}_5\right) + C_{31}^2 R_2 \Delta \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C_{13}^2 R_2 \left(\vec{\nabla}\cdot\vec{J}_3\right) + C_{11}^4 R_4 \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ D_{33}^0 R_0 \sum_{abc} \vec{\nabla}_a \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D_{13}^2 \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_c \overleftrightarrow{J}_{3abc} \\ &+ D_{31}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \vec{\nabla}_a \vec{J}_{1b} + E_{13}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{3b} \\ &+ D_{11}^4 \sum_{ab} \overleftrightarrow{R}_{4ab} \vec{\nabla}_a \vec{J}_{1b} \\ &+ E_{31}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_b \left(\vec{\nabla}\cdot\vec{J}_1\right).\end{aligned}$$

The energy densities above are given in terms of 50 coupling constants $C_{mn}^{n'}$, $D_{mn}^{n'}$, $E_{mn}^{n'}$, and $F_{mn}^{n'}$.

B.G. Carlsson *et al.*, C 78, 044326 (2008)

Power Counting in Skyrme and RMF Functionals

Can we control the explosion of terms in generalized functionals?

- Old chiral NDA analysis:
  [Friar et al., rjf et al.]

$$c\left[\frac{\psi^\dagger\psi}{f_\pi^2\Lambda}\right]^l\left[\frac{\nabla}{\Lambda}\right]^n f_\pi^2\Lambda^2$$

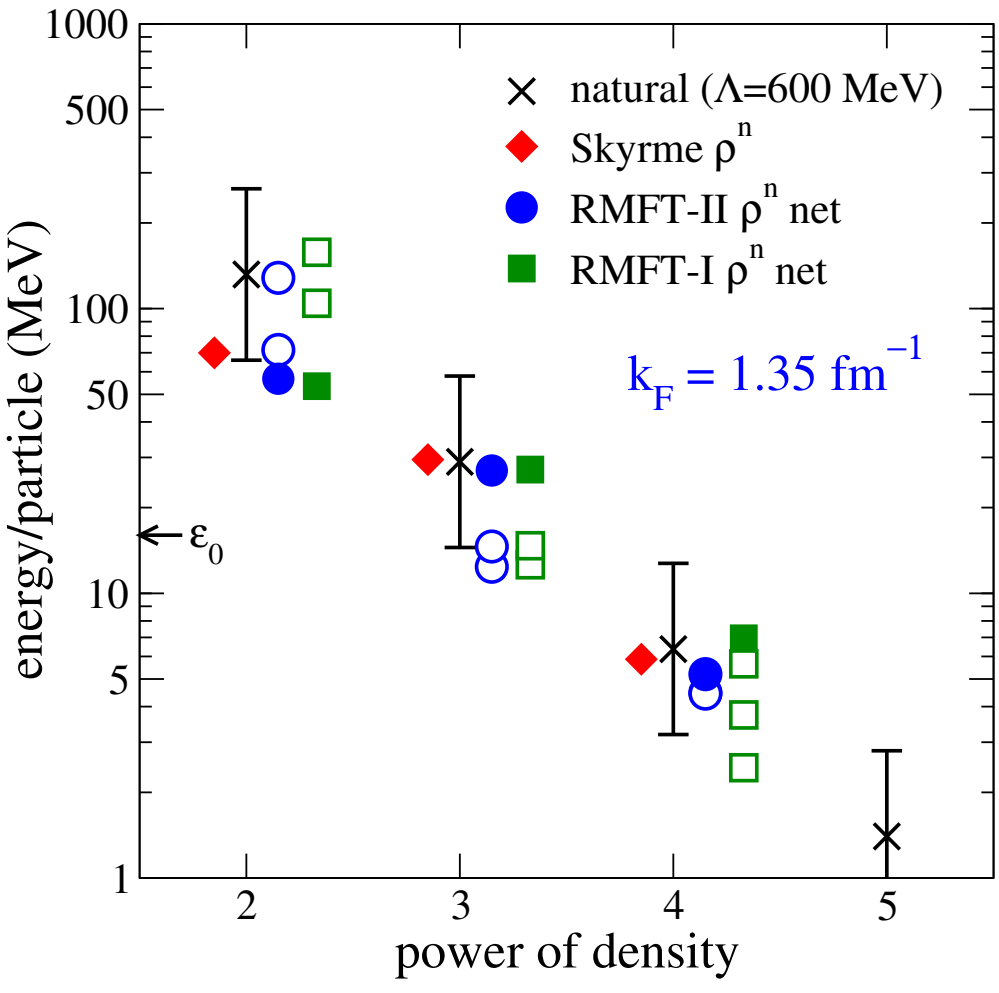
$$\begin{aligned}\rho &\longleftrightarrow \psi^\dagger\psi\\ \Longrightarrow\quad \tau &\longleftrightarrow \nabla\psi^\dagger\cdot\nabla\psi\\ \mathbf{J} &\longleftrightarrow \psi^\dagger\nabla\psi\end{aligned}$$

- Density expansion?

$$\frac{1}{7}\leq\frac{\rho_0}{f_\pi^2\Lambda}\leq\frac{1}{4}$$

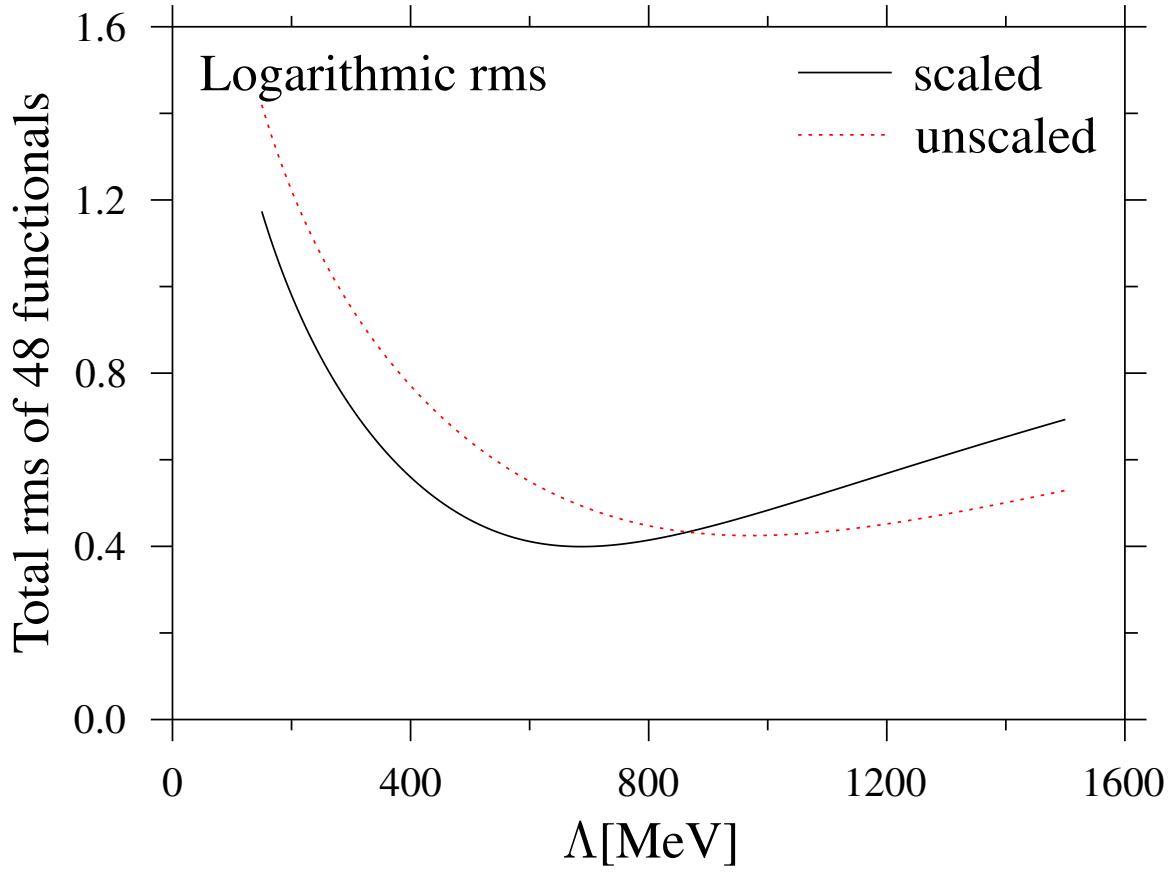
for $1000\geq\Lambda\geq 500$

- Also gradient expansion



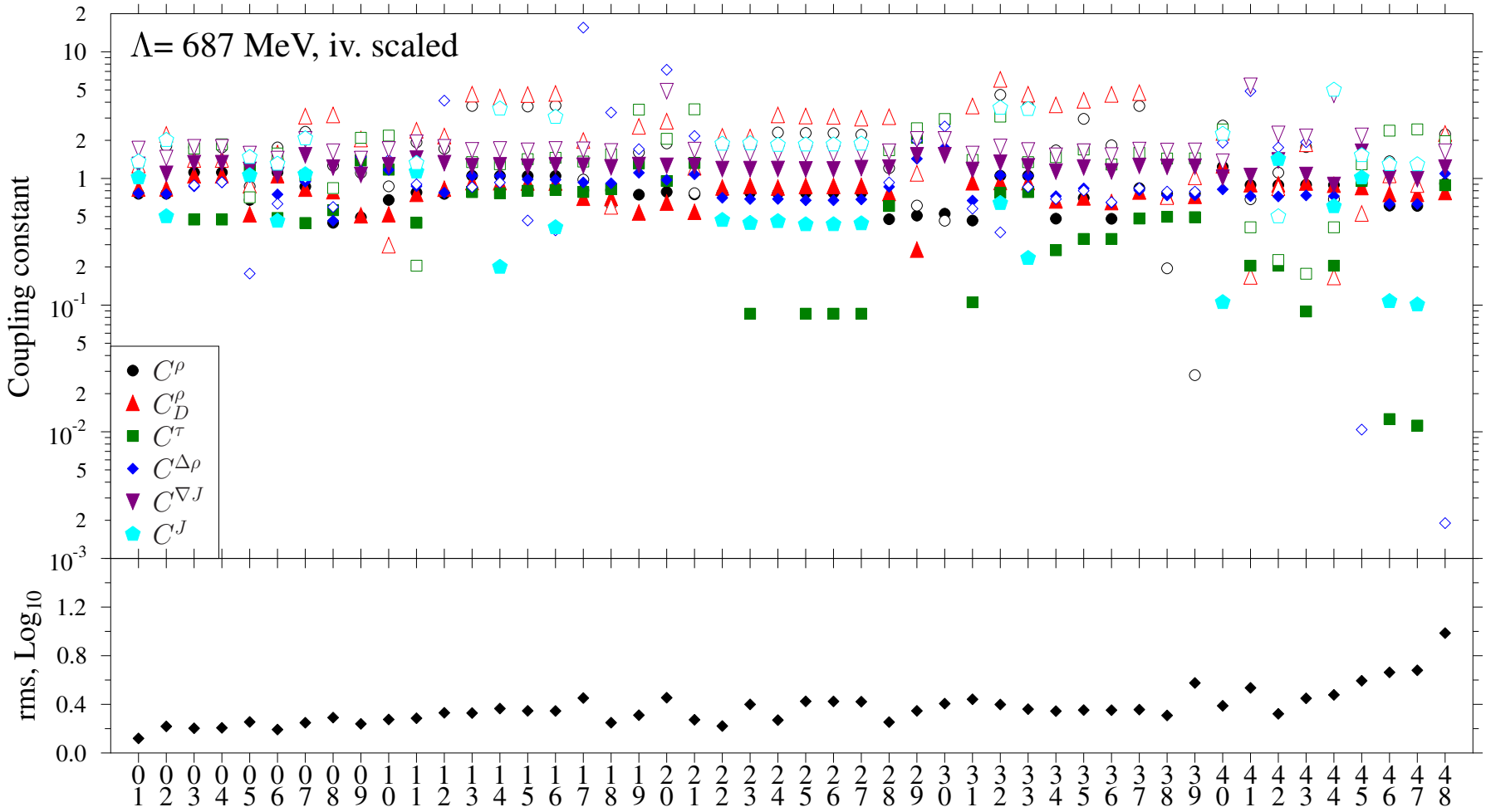
Naturalness revisited (M. Kortelainen et al.)

- Apply natural units scaling to 48 Skyrme functionals
- Look for optimal Λ by deviations from unity:



- $\Lambda \approx 600$ MeV consistent with previous analysis
- What can we use this for?

Signatures of incomplete optimization (massexplorer.org)



- Unnaturally small $C_1^{\Delta\rho}$ in RATP, SkMP; C_0^{τ} in SkX
- Unnaturally large $C_1^{\Delta\rho}$ in SKI1; C_0^{τ} in SkX
- Guide for future fitting attempts with generalized EDF's

Quantified constraints from new observables

(P.G. Reinhard, W. Nazarewicz, arXiv:1002.4140)

- Do new observables bring new information to an EDF?
- Example: What is the information content of the neutron skin?
- Pearson product-moment correlation coefficient

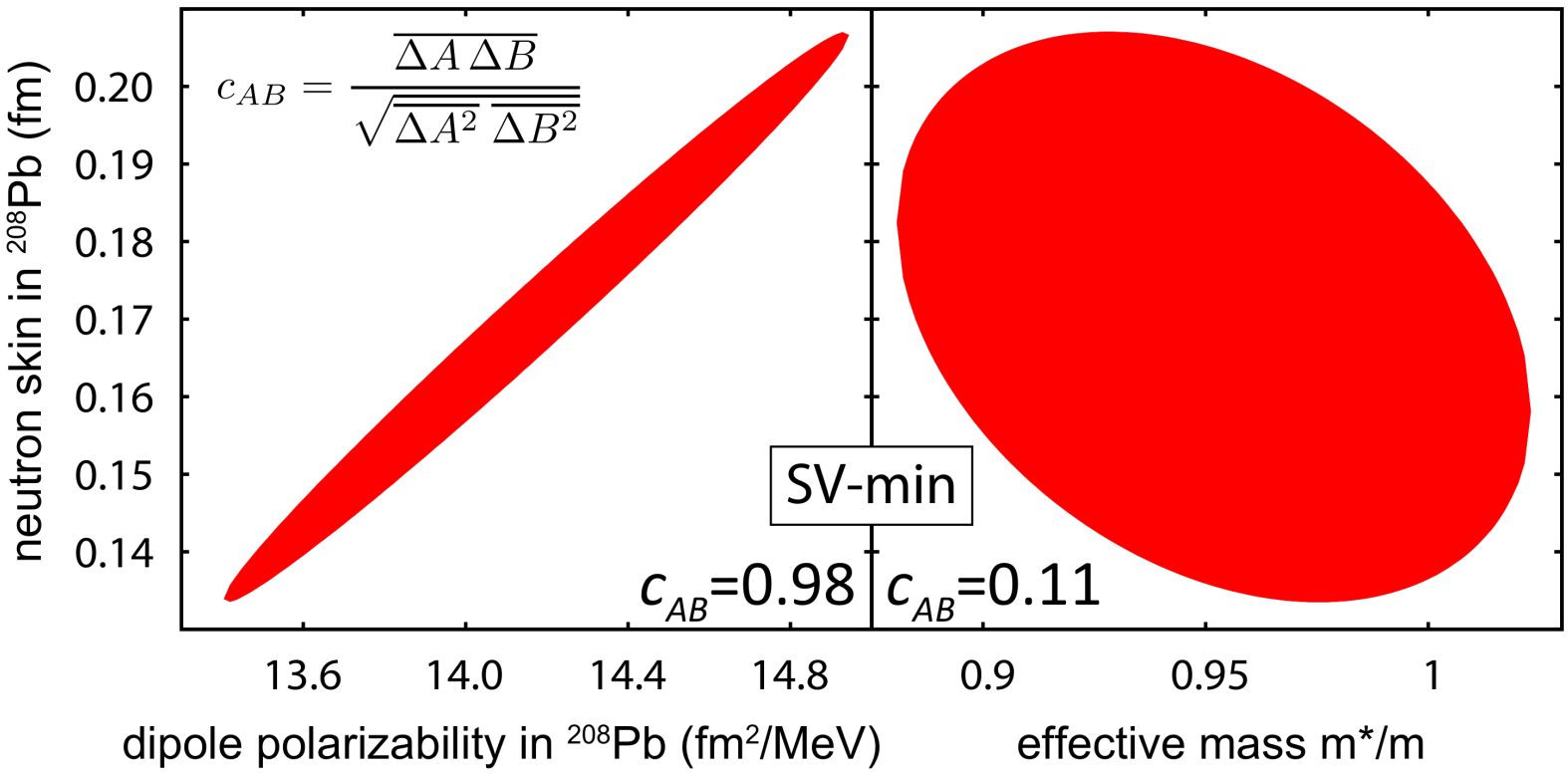
$$c_{AB} = \frac{\overline{\Delta A\, \Delta B}}{\sqrt{\overline{\Delta A^2}\;\overline{\Delta B^2}}} = \begin{cases} 1 & \text{full alignment/correlation} \\ 0 & \text{not aligned/statistically independent} \end{cases}$$

  where A and B are two observables.

- Fit EDF couplings $\mathbf{p} = \{p_1, \ldots, p_F\}$ with a $\chi^2(\mathbf{p})$ function
- Find uncertainties and correlation from curvature about minimum, $\mathcal{M}_{ij} = \partial_{p_i}\partial_{p_j}\chi^2|_{\mathbf{p}_0}$ with $\chi^2(\mathbf{p}_0) = \chi^2_{\min}$:

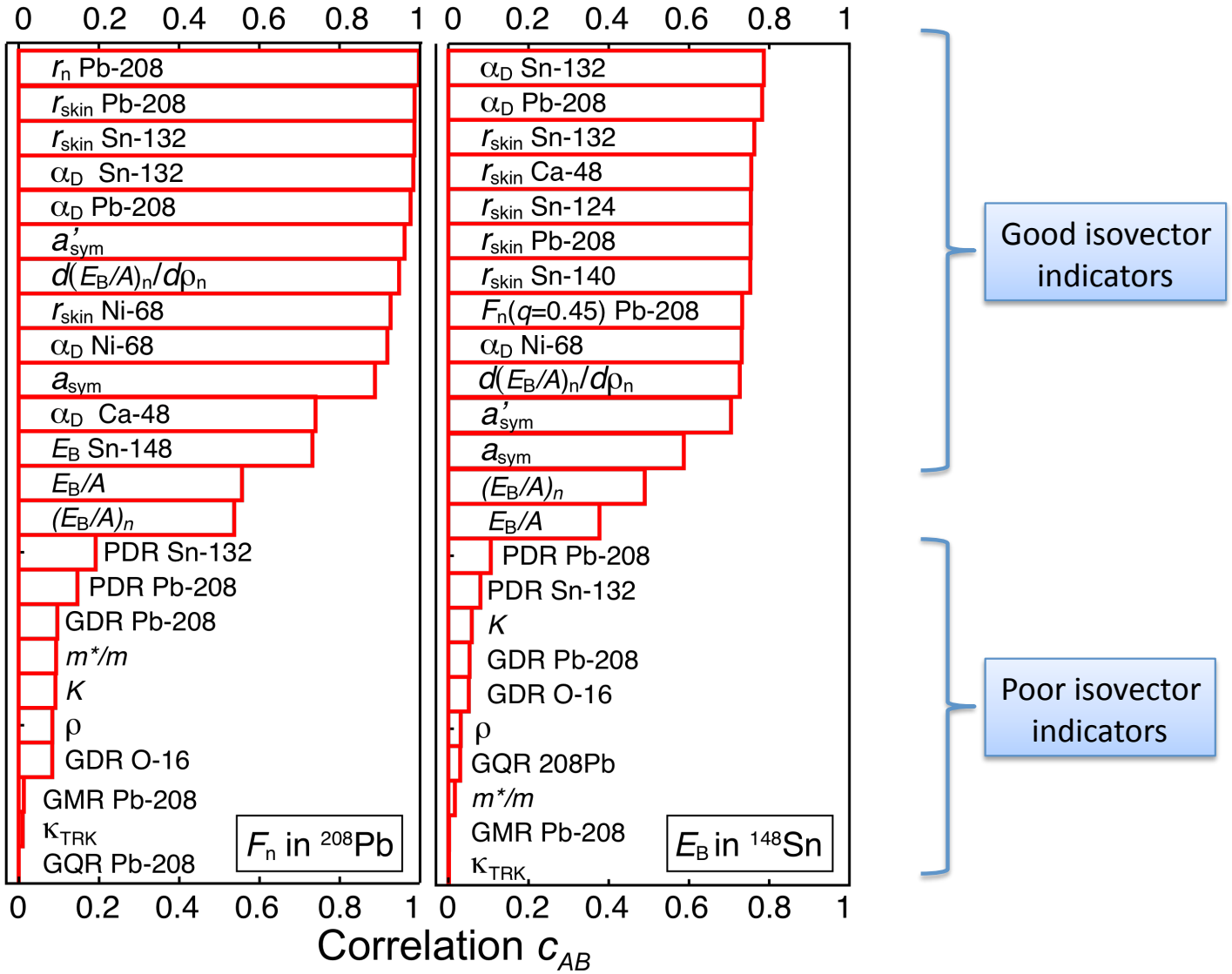
$$\overline{\Delta A^2} = \sum_{ij} \partial_{p_i} A (\widehat{\mathcal{M}}^{-1})_{ij} \partial_{p_j} A|_{\mathbf{p}_0} \quad \text{and} \quad \overline{\Delta A\, \Delta B} = \sum_{ij} \partial_{p_i} A (\widehat{\mathcal{M}}^{-1})_{ij} \partial_{p_j} B|_{\mathbf{p}_0}$$

Correlation example



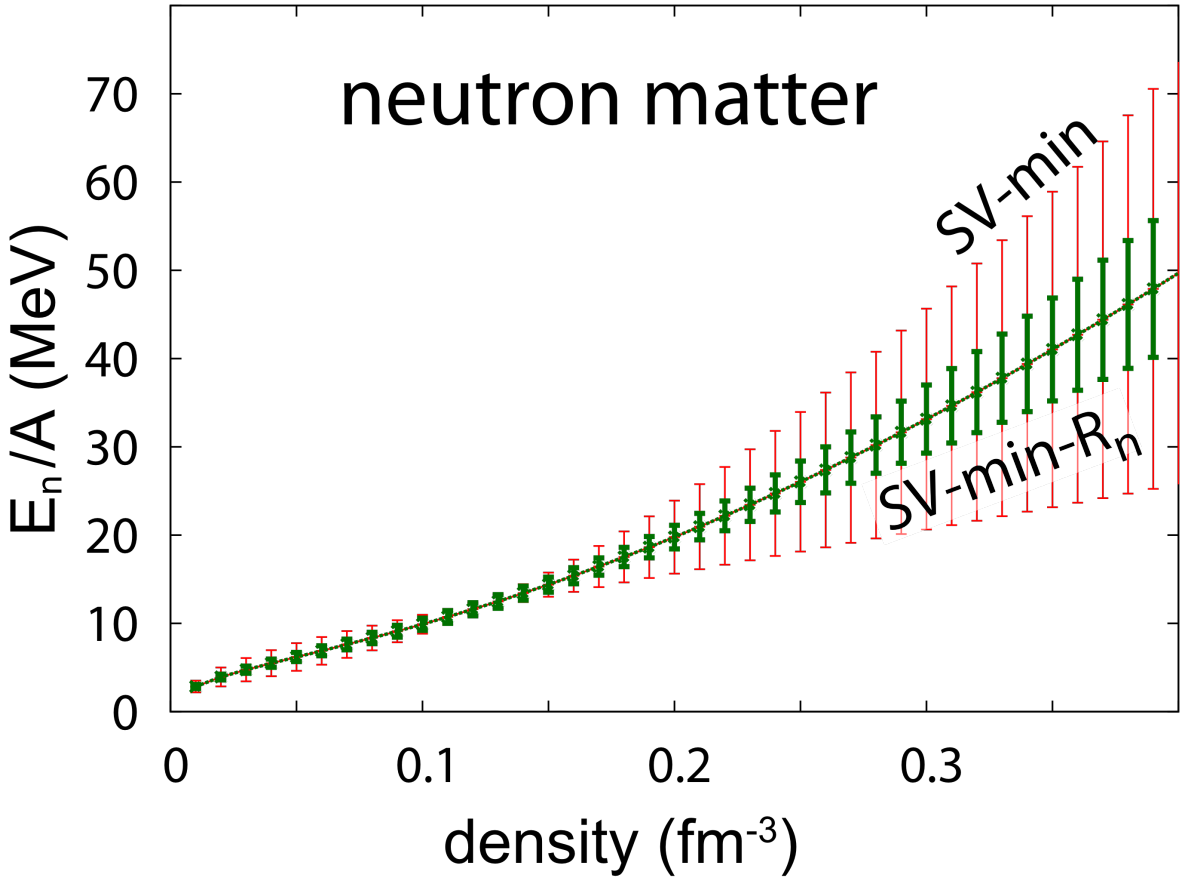
- Filled areas are regions of parameter reasonable domain **p** (where $\chi^2 = \chi^2_{\min} + 1$)
- left: dipole polarizability and neutron skin in ^{208}Pb
- right: m^*/m in nuclear matter and neutron skin in ^{208}Pb

Correlation with observables



- left: neutron form factor $F_n(q = 0.45\,\mathrm{fm}^{-1})$ in ^{208}Pb
- right: binding energy of heavy neutron-rich nucleus ^{148}Sn

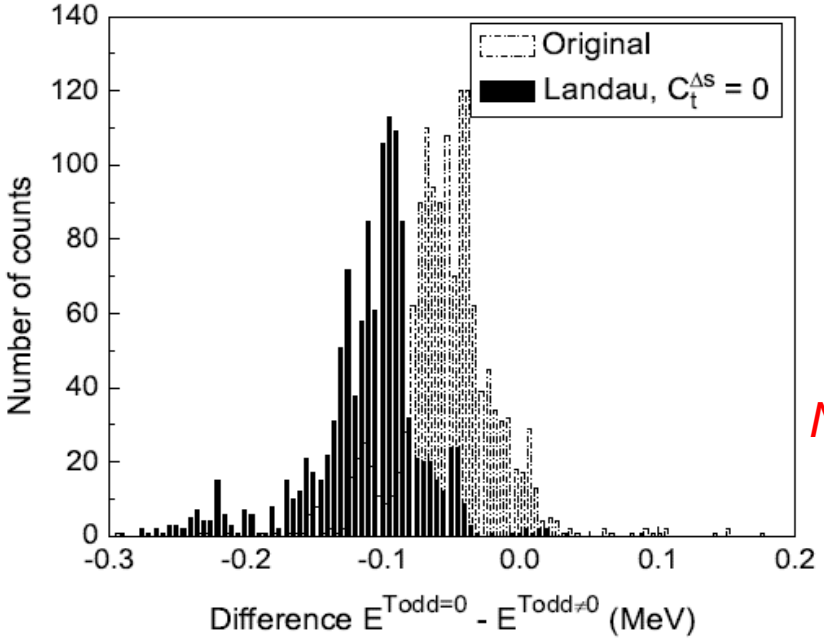
Impact of precise measurement of neutron skin



EOS extrapolation errors

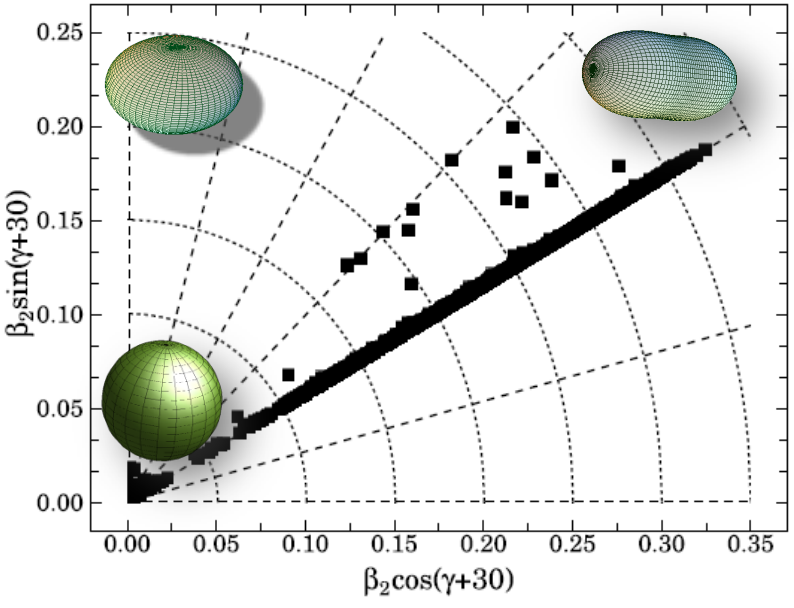
- Original EDF is SV-min from P. Klüpfel et al.
- New EDF SV-min-R_n by adding neutron radius in ^{208}Pb with adopted error 0.02 fm to fit observables
- Uncertainties for isovector indicators shrink by factor of 2

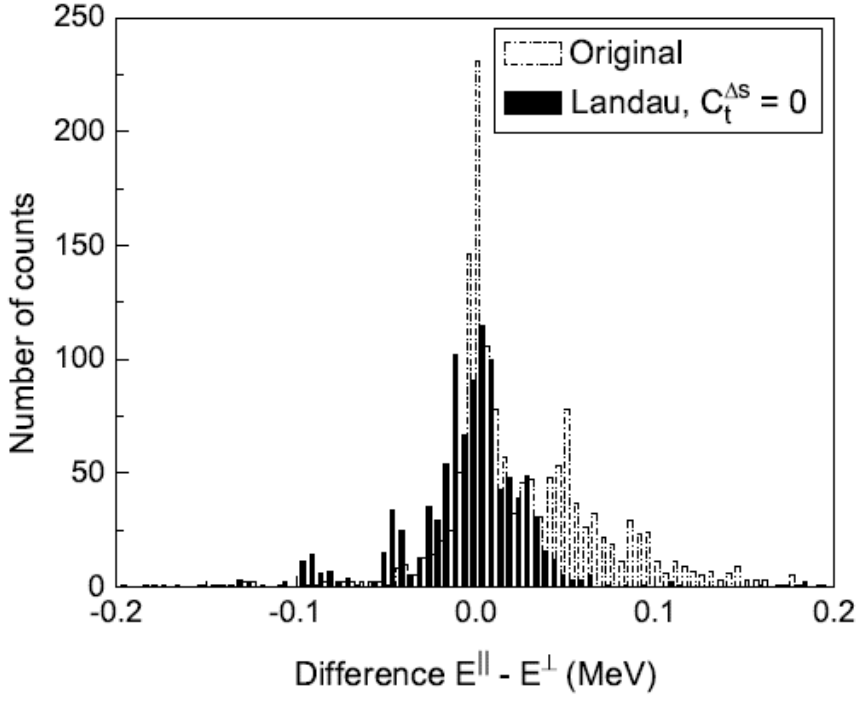
Effects of Time-odd Fields of EDF



- N = 14 full spherical shells (Ns = 680 states)
- Full HFB calculations, including all time-odd terms, in 24 different configurations for 91 nuclei of the rare earth
- 3 different Skyrme interactions, SkP, SIII, SLy4

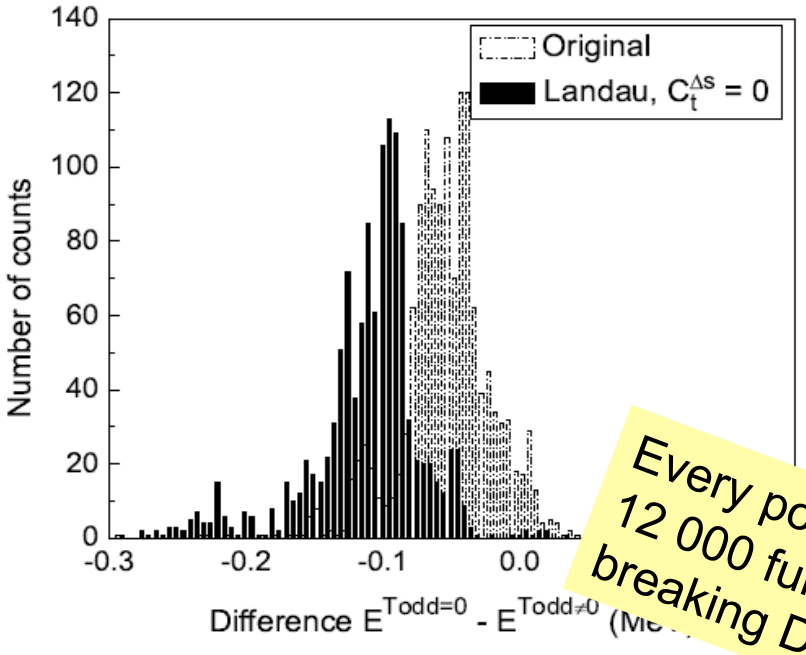
*N. Schunck et al., Phys. Rev. C **81**, 024316 (2010)*





Effect of orientation on time-odd terms

Effects of Time-odd Fields of EDF



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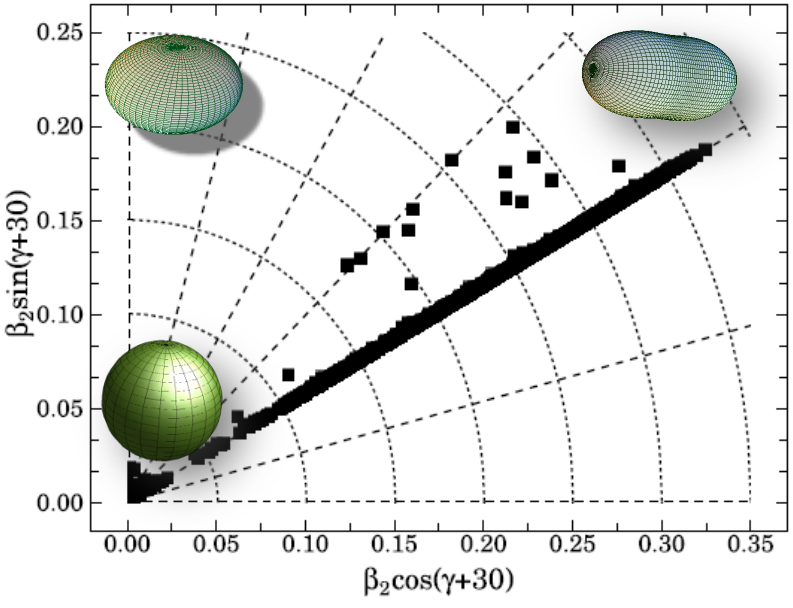
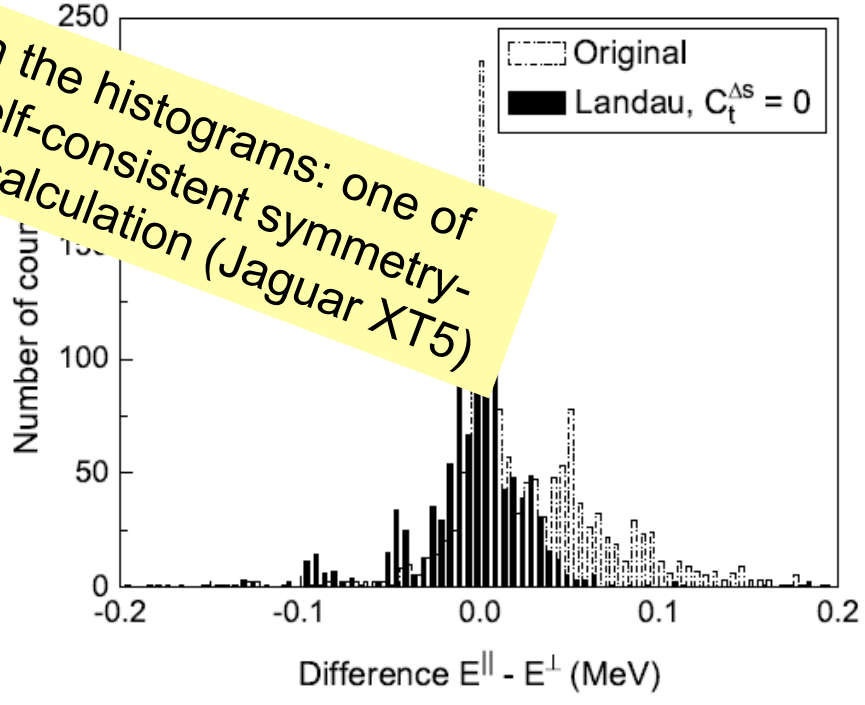
*N. Schunck et al., Phys. Rev. C **81**, 024316 (2010)*

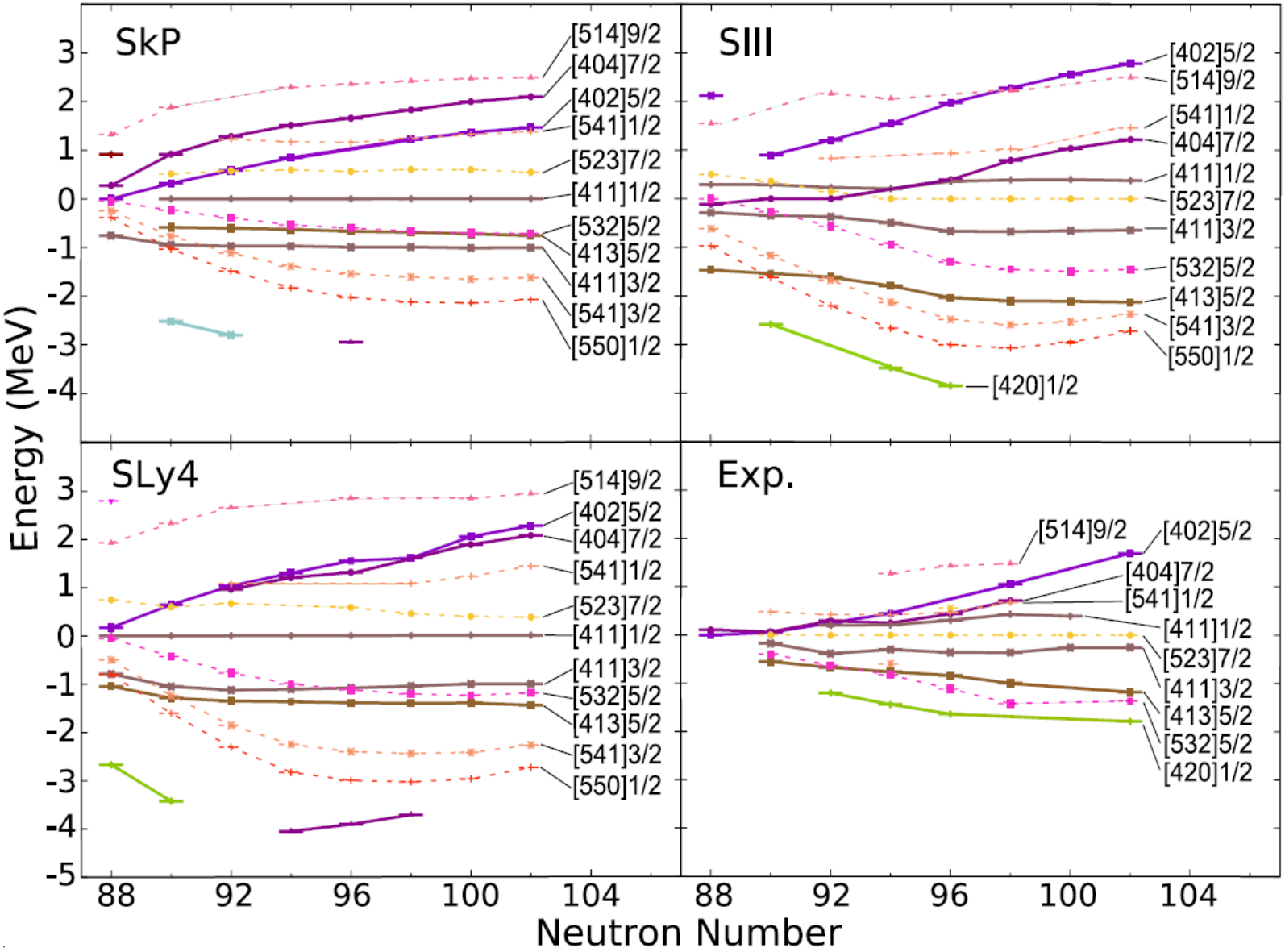
Every point in the histograms: one of 12 000 fully self-consistent symmetry-breaking DFT calculation (Jaguar XT5)





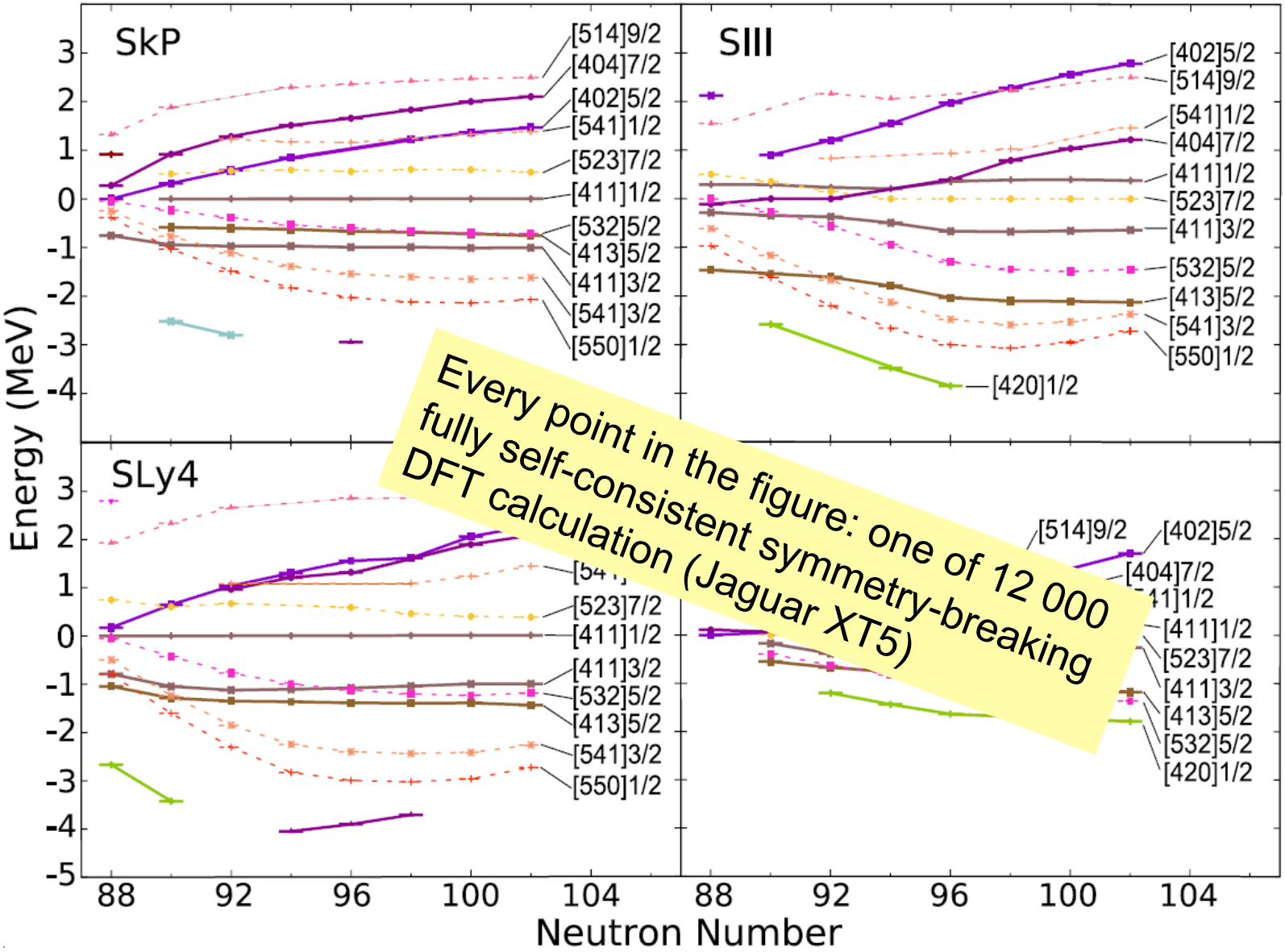
Effect of orientation on time-odd terms

Odd-proton States in Mass A~150



One quasi-particle states in Ho isotopes with 3 different Skyrme interactions.
All time-odd fields included as originally prescribed by each interaction

Odd-proton States in Mass A~150



One quasi-particle states in Ho isotopes with 3 different Skyrme interactions.
All time-odd fields included as originally prescribed by each interaction

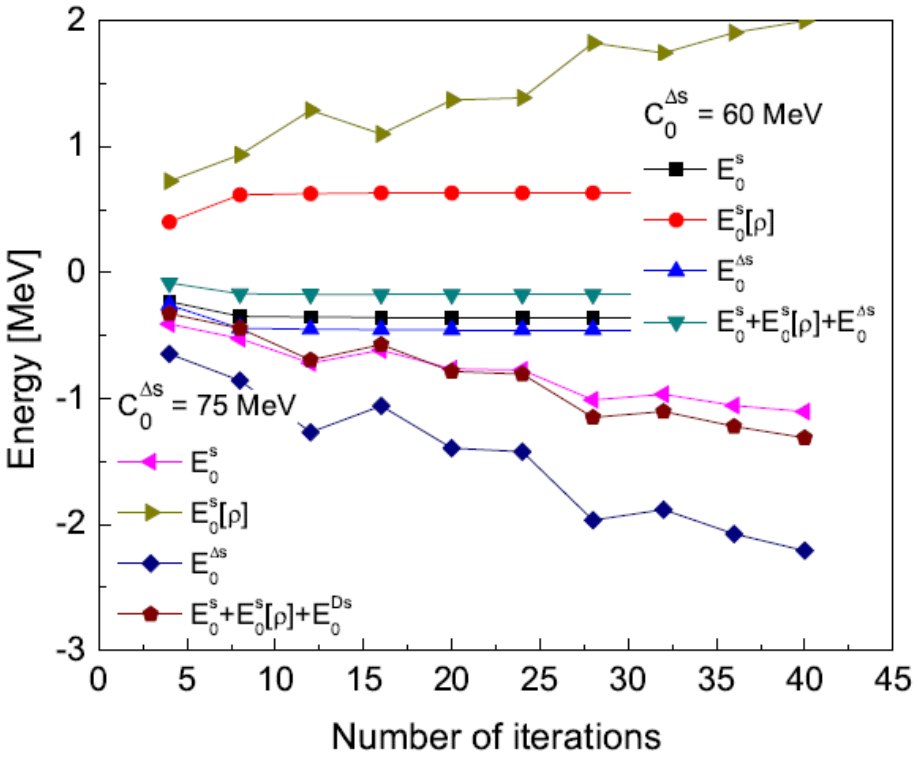
Finite-size spin instabilities

T. Lesinski, N. Schunck, M. Kortelainen, T. Duguet

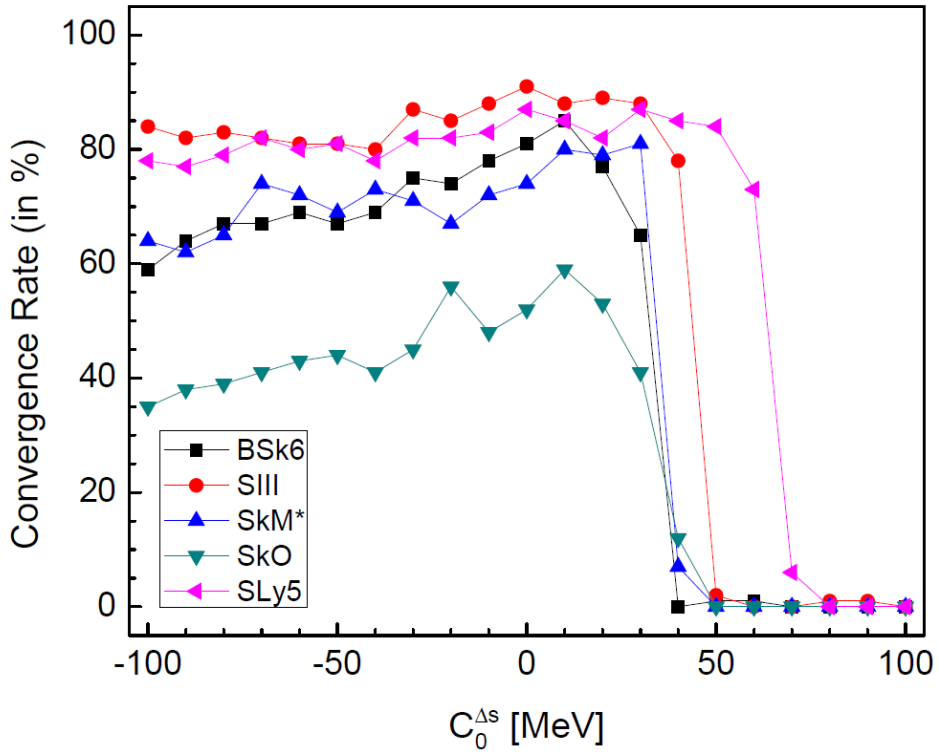
- Response of the nucleus to a perturbation with finite momentum q studied in the RPA theory

$$Q^{(\alpha)} = e^{-i\omega t} \sum_a e^{i\mathbf{q}.\mathbf{r}_a} \Theta_a^{(\alpha)}$$

- Channels: scalar-isoscalar, scalar-isovector, vector-isoscalar, vector-isovector, etc.



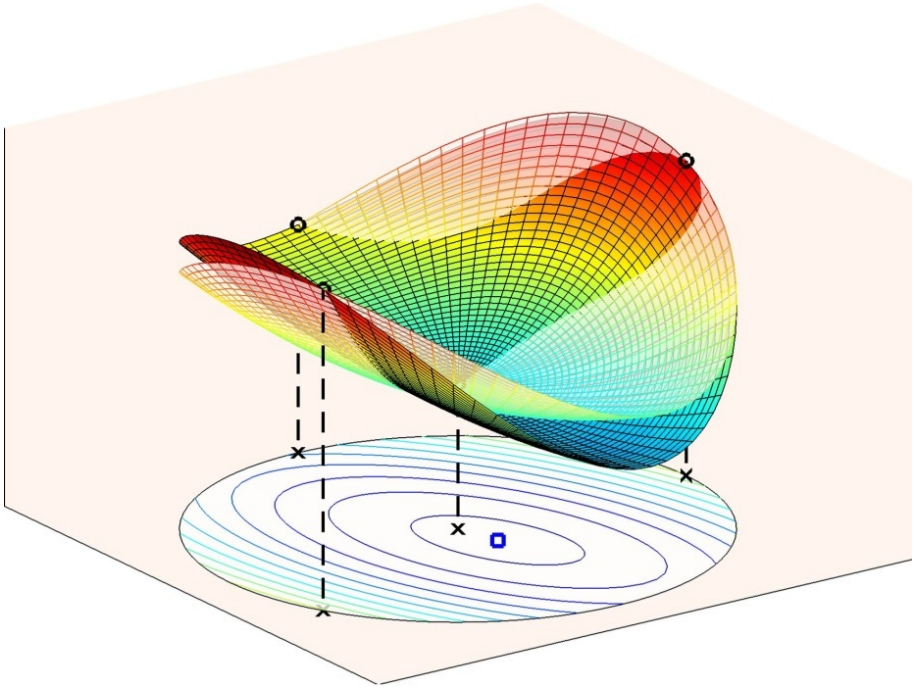
Every point: Convergence rate of the HFB calculation over 100 blocked states in $^{157\text{-}165}$Ba, 10 500 points total (NERSC Franklin XT4)

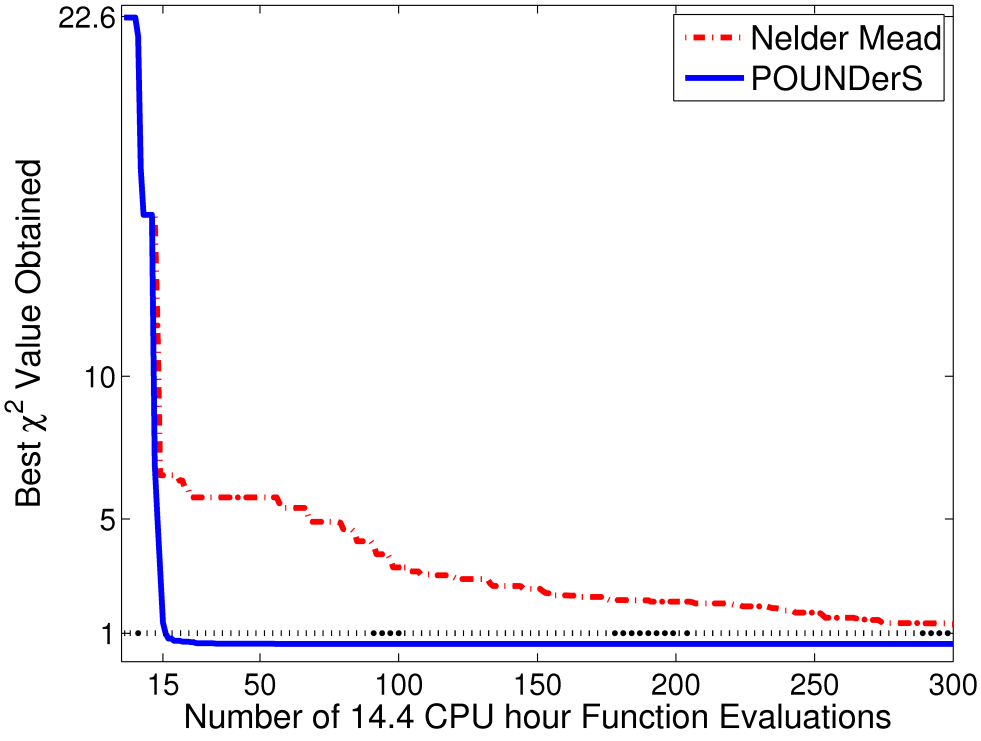


Contributions of different channels of the Skyrme functional to the total energy as function of iterations for the [521]3/2 blocked state in ^{157}Ba with the SLy5 force.

Novel optimization algorithms (ANL + ORNL)

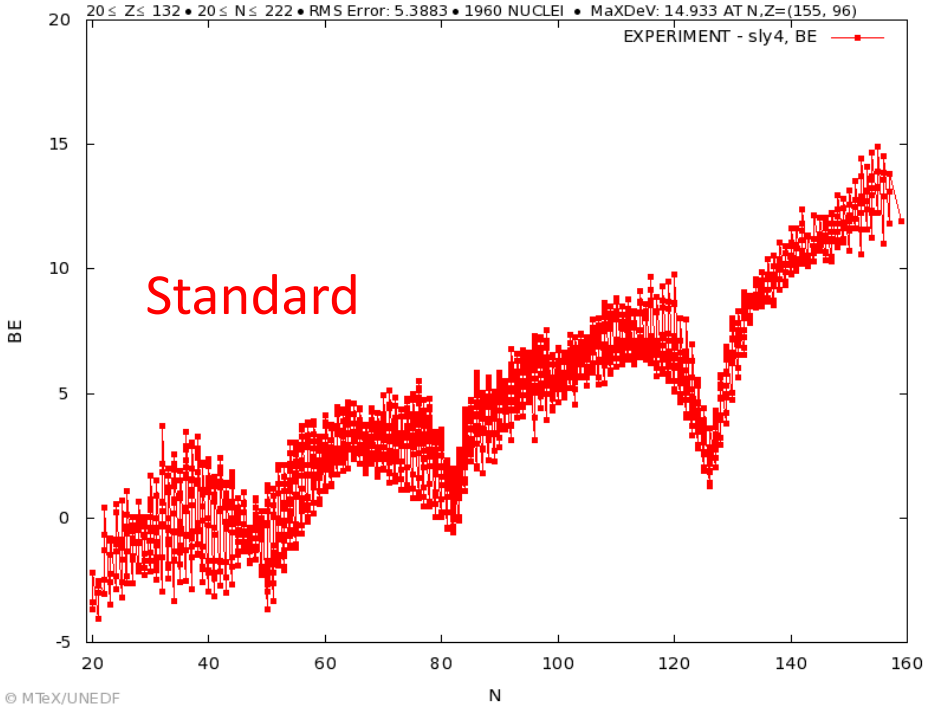
- Computational cost of optimization is high because some nuclei can take hours to compute (so restrict to spherical)
- New model-based optimization: minimize local approximation to exact function

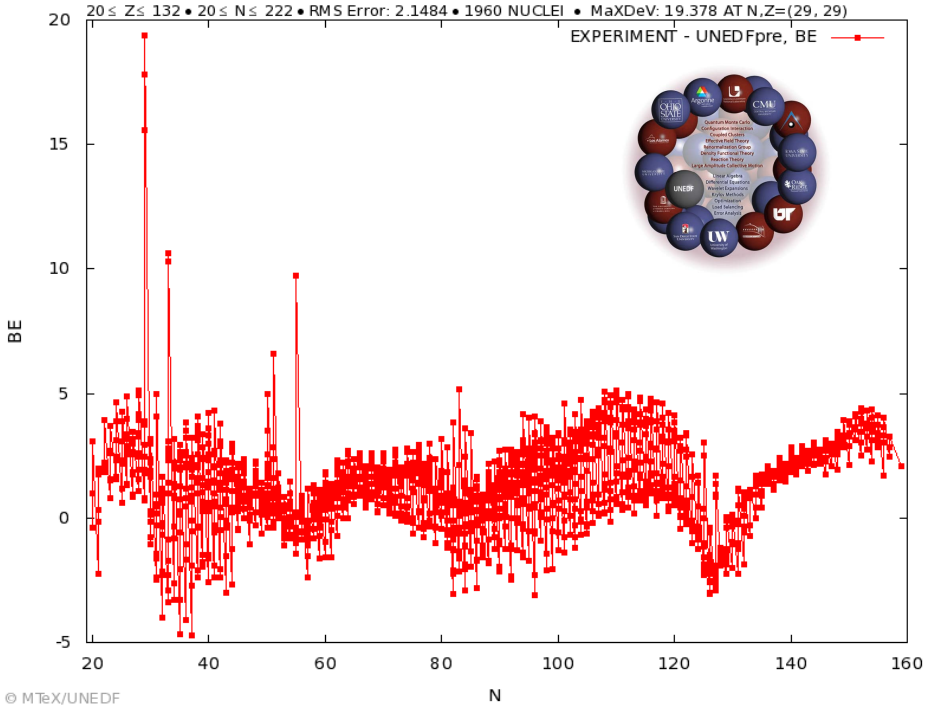




- POUNDerS algorithm greatly outperforms conventional method
- Opens the door to EDF optimization with non-spherical nuclei

Novel optimization algorithms: Test case

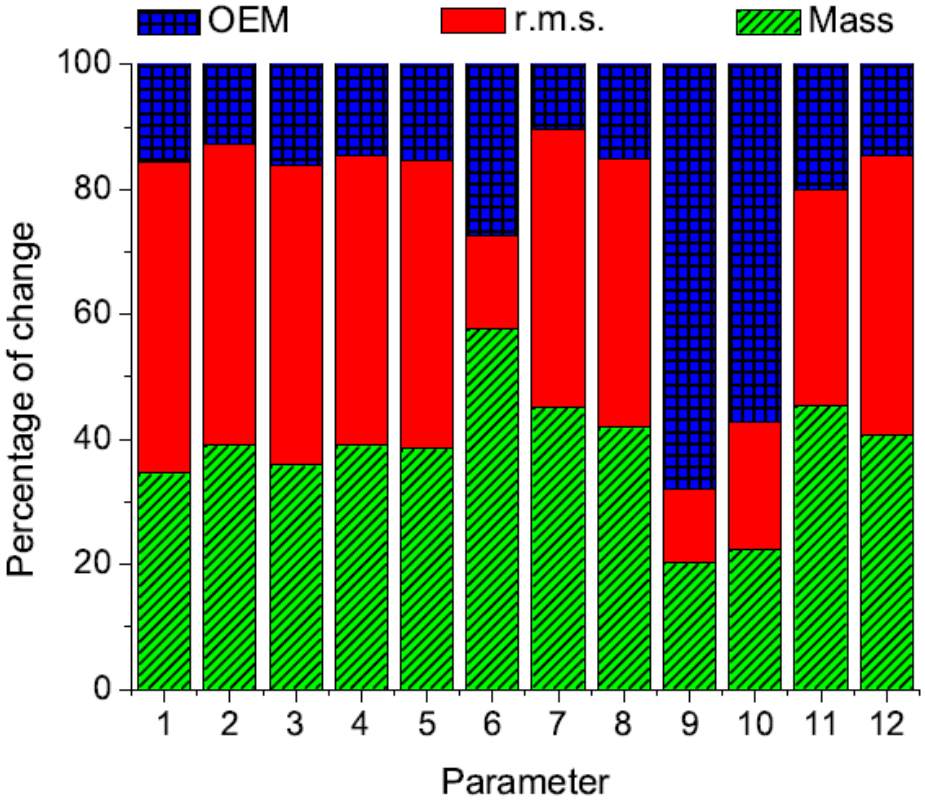


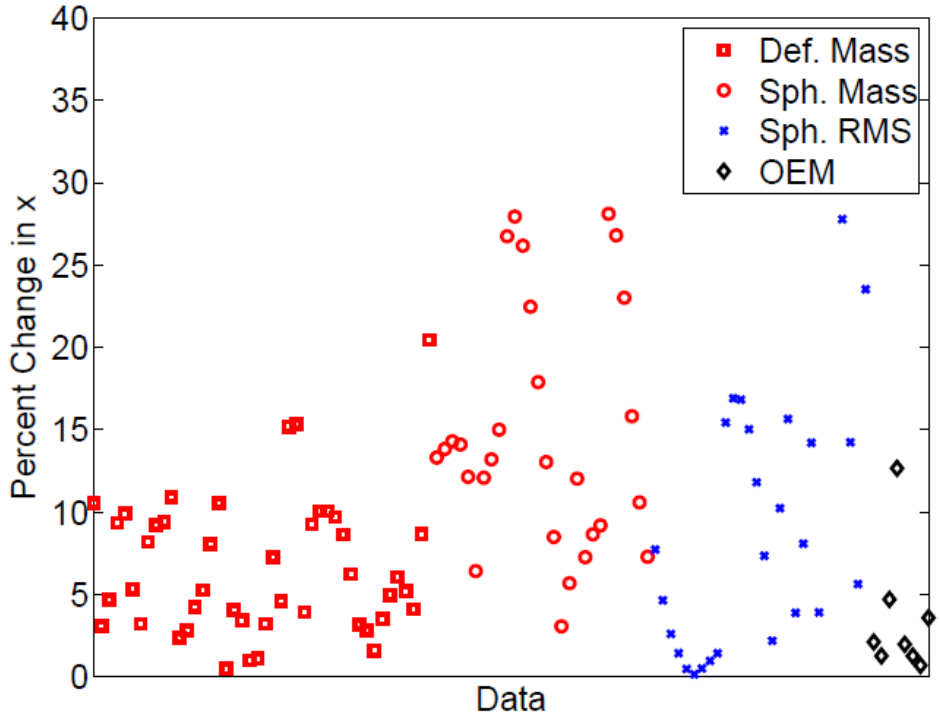


- left: Deviation between theoretical and experimental nuclear masses for the SLy4 Skyrme EDF using HFBTHO solver
- right: Same for UNEDFpre EDF parametrization
- Close to conventional Skyrme accuracy limit

Theoretical error bars from statistical analysis

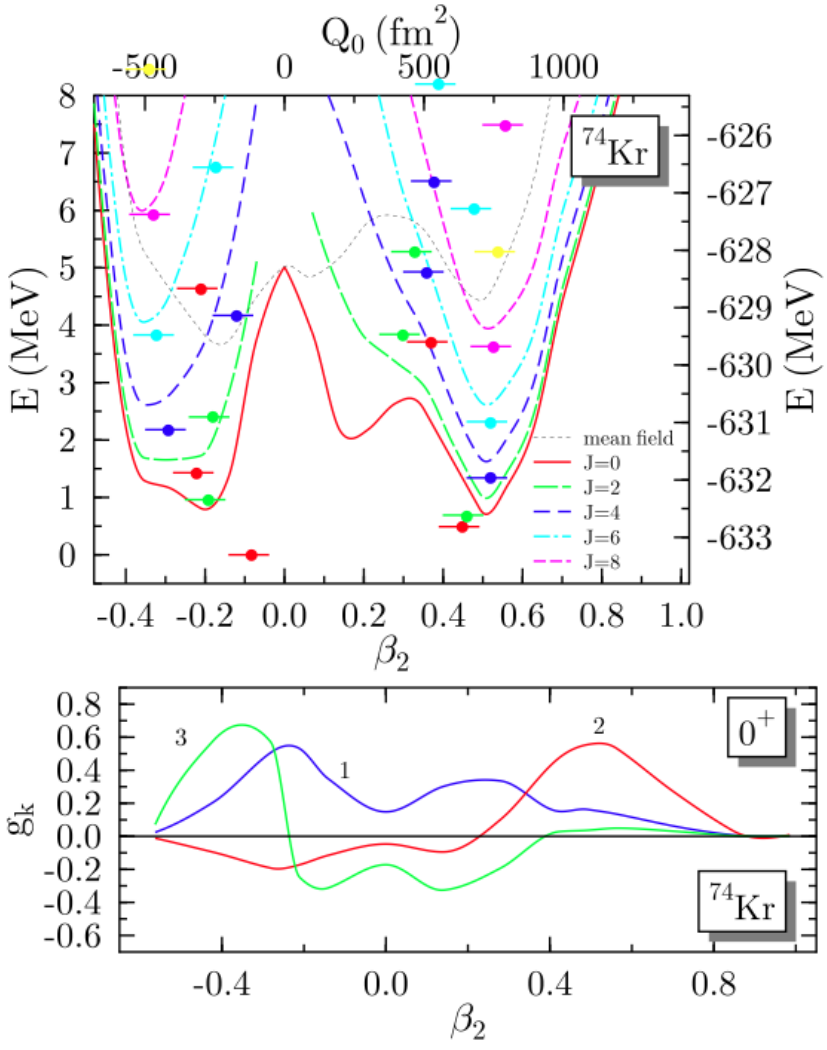
- EDF analyzed using surrogate (model-based) approach
- Method is highly scalable (e.g., $>$ 5000 cores on Franklin)

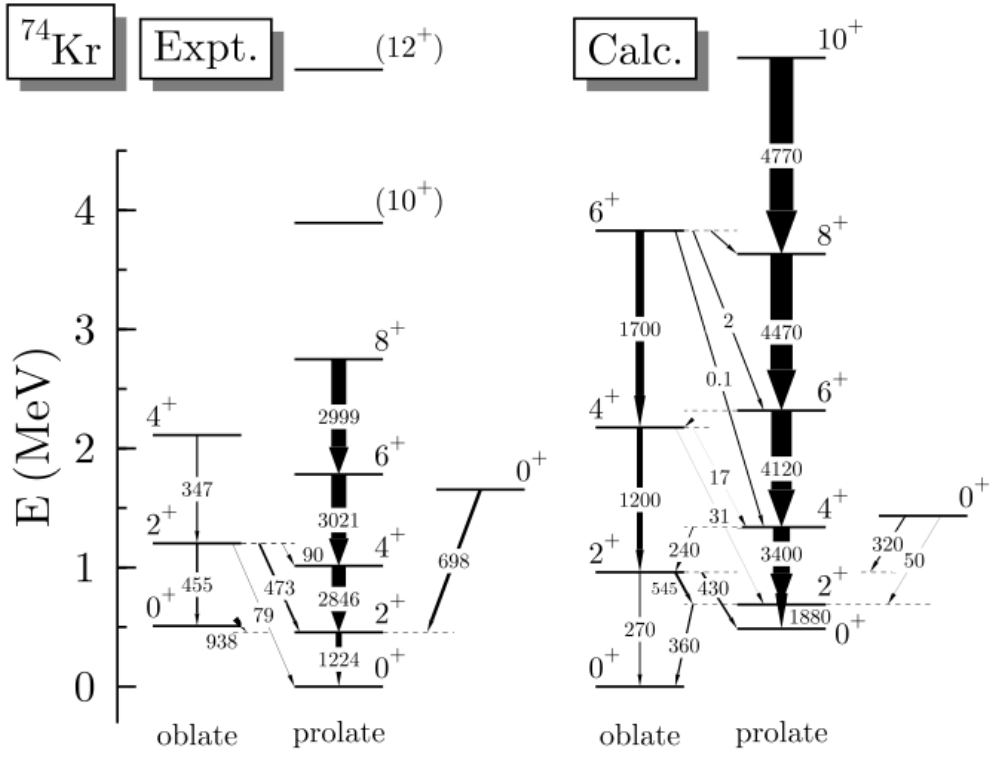




- left: Sensitivity of each parameter to global changes in data
- right: Global sensitivity to specific data changes by 0.1σ
- Standard parametrization is highly correlated $\Longrightarrow$ ideal is N independent parameters unambiguously constrained by data

Nuclear constrained calculations: GCM



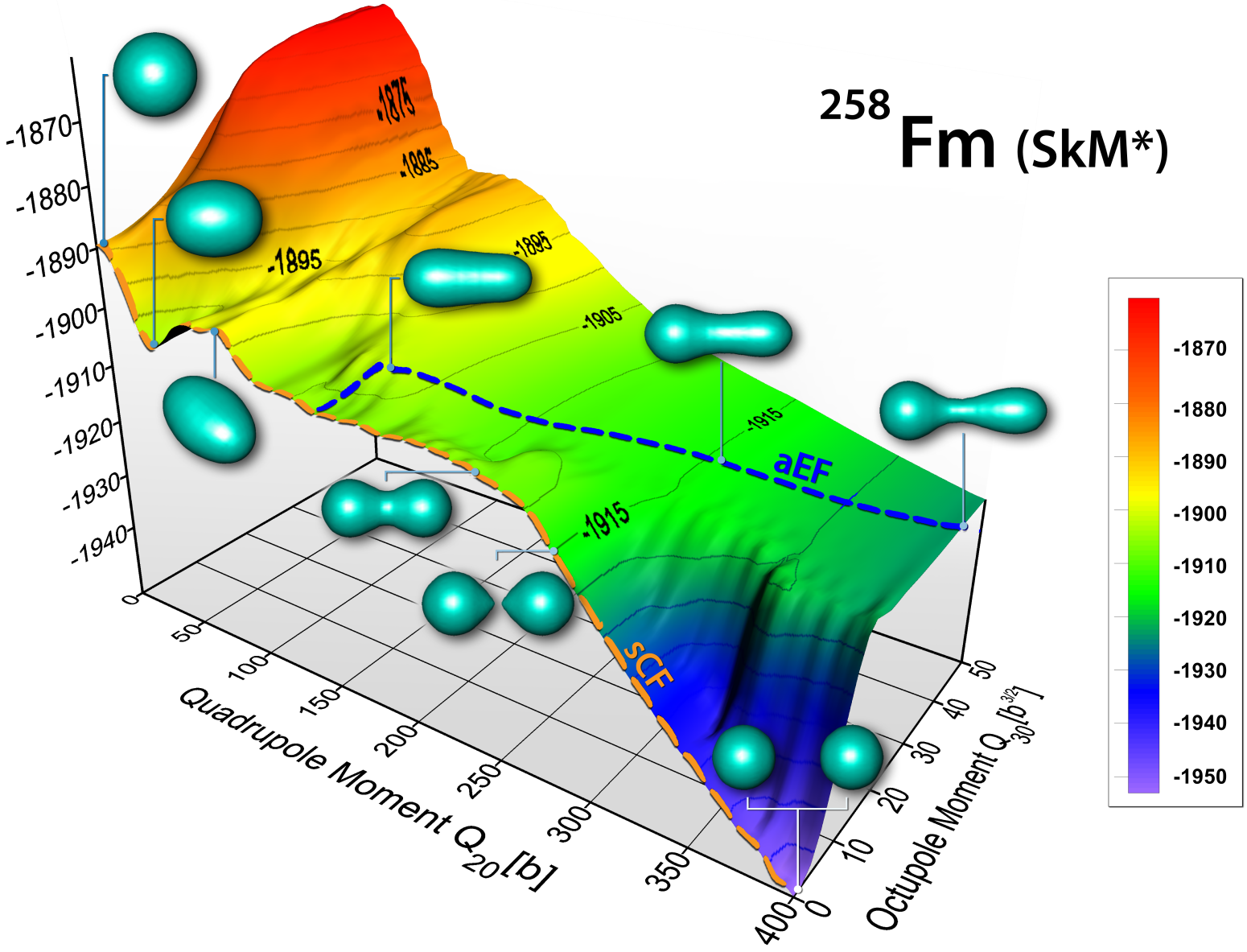


- SLy6+density-dependent pairing
- There are no adjustable parameters. . .

Experiment: E. Clément *et al.* Phys. Rev. C75 (2007) 054313, A. Görgen *et al.* Eur. Phys. J. A26 (2005) 153

M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312.

Nuclear constrained calculations: Deformation energy surface



Augmented Lagrangian Method M.V. Stoitsov et al.

Quadratic Constraint

Nuclear Energy From DFT

$$E(q)$$

Nuclear Quadruple Moment

$$q =< \hat{Q} >$$

Quadratic Lagrangian Function

$$E^{'}(q) = E(q) + \ c\ (q - q_0)^2$$

Nuclear Potential in the Solver

$$U' = U - 2\ c\ (q - q_0)\hat{Q}$$

HFODD, HFBTHO

THE ONLY CHANGE IN THE SOLVER

$$\bar{q}_0(\lambda^k) = q_0 - \frac{\lambda^k}{2c}$$

Augmented Lagrangian Method

Nuclear Energy From DFT

$$E(q)$$

Nuclear Quadruple Moment

$$q =< \hat{Q} >$$

Augmented Lagrangian Function

$$E^{'}(q) = E(q) + \ \lambda\ (q - q_0) + \ c\ (q - q_0)^2$$

Nuclear Potential in the Solver

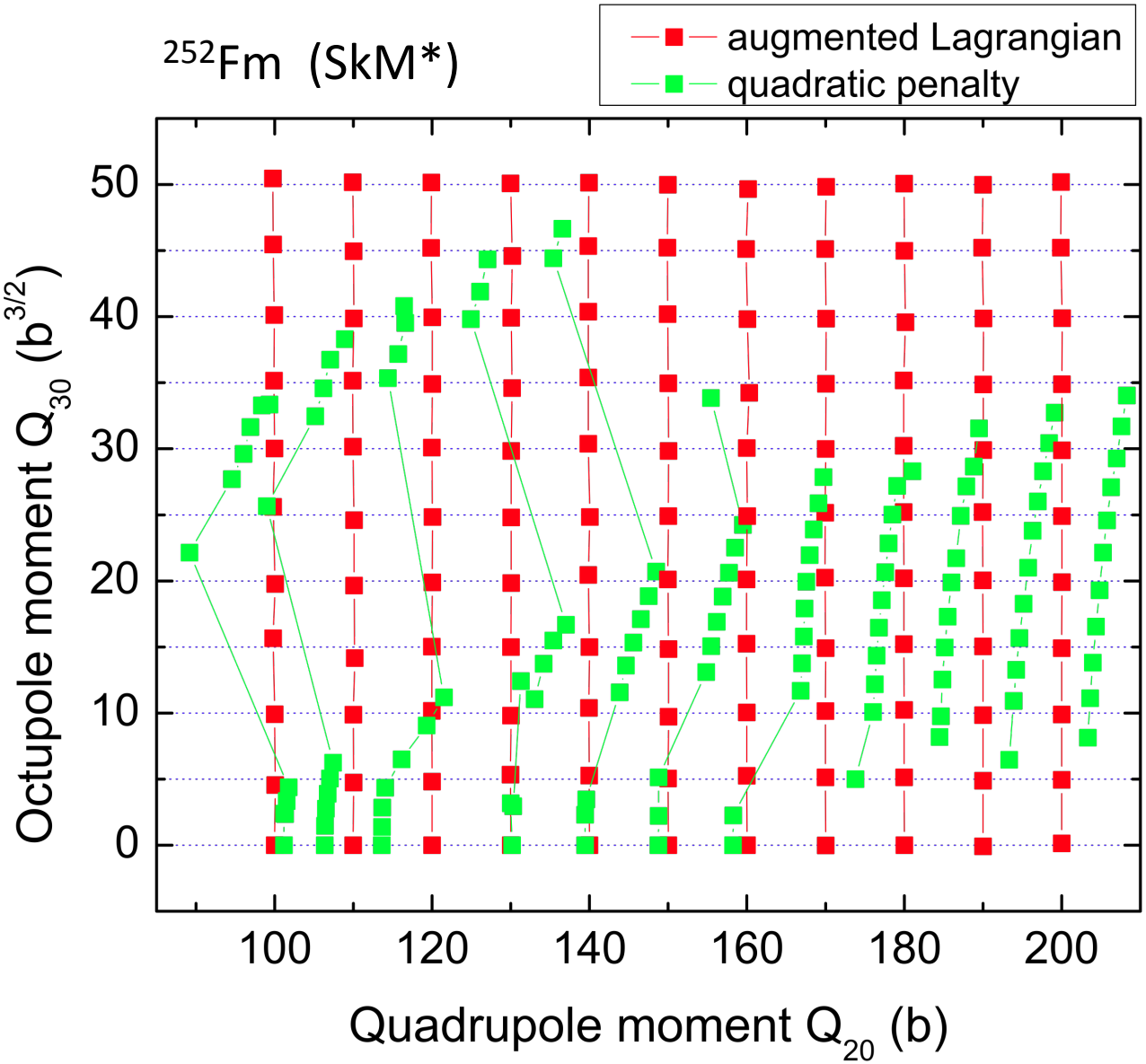
$$U' = U - 2\ c\ \ (q - \bar{q}_0(\lambda))\,\hat{Q}$$

Lagrange Multiplier Iterations

$$\lambda^{k+1} = \lambda^k + 2\ c\ (q - \bar{q}_0(\lambda^k))$$

- Quadratic constraint procedure often fails to deliver requested average value of constrained operator with acceptable accuracy.
- Augmented Lagrangian Method (ALM) has a linear constraint and a quadratic penalty function $\Longrightarrow$ proper convergence

Augmented Lagrangian Method M.V. Stoitsov et al.



- Request solutions at grid points of deformation lattice
- Standard quadratic constraint method fails; ALM succeeds!

Outline

Overview: EDF's and DFT

The UNEDF project

New developments: Constraints, optimization, ...

Non-empirical EDF's and ab-initio DFT

Summary

Historically: Microscopic EDF from G-Matrix

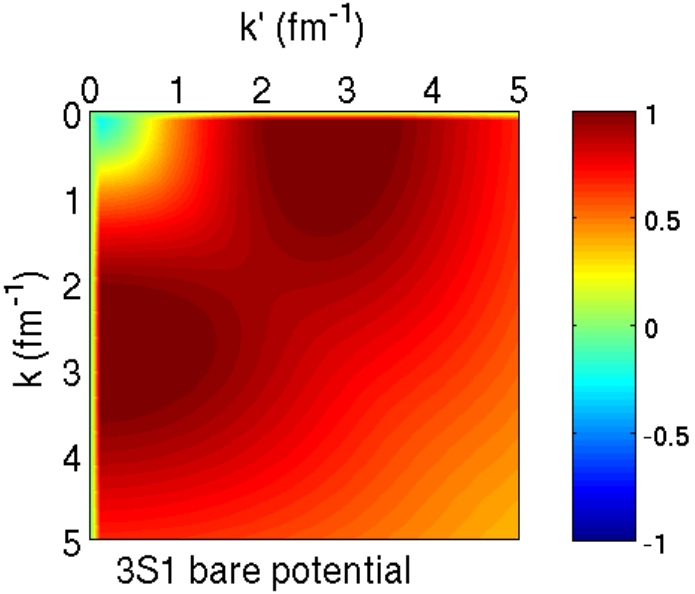
- G-matrix softens highly non-perturbative NN potentials
- Negele/Vautherin density matrix expansion (DME)
  $\Longrightarrow$ Skyrme-like EDF from G-matrix for Hartree-Fock
  - Semi-quantitatively successful
  - Empirical fits far superior $\Longrightarrow$ little further development
- Ab-initio DFT is possible from many-body perturbation theory (MBPT) if convergent and can tune single-particle potential U

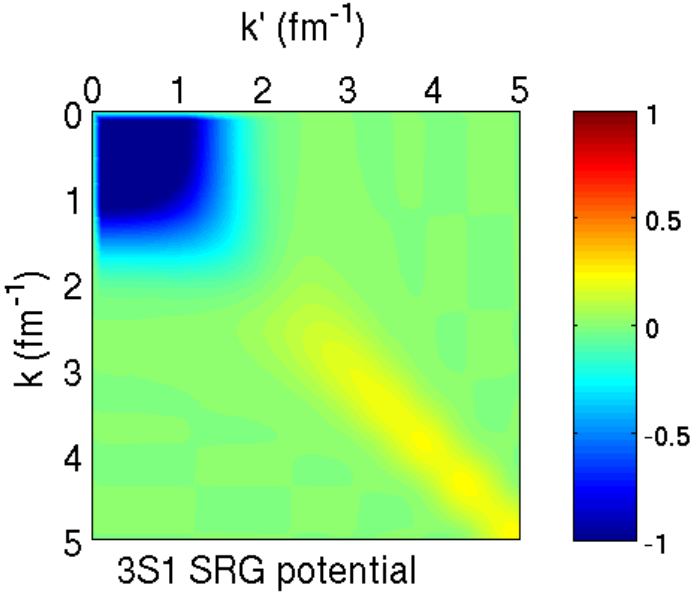
$$H = \underbrace{(T+U)}_{\mathrm{Kohn-Sham}} + (V-U)$$

  - Need to be able to adjust U so density unchanged
  - Recent successes for Coulomb DFT
- But MBPT with G-matrix doesn't work (hole-line expansion)
- New development: low-momentum potentials ($V_{\mathrm{low}\,k}$, V_{SRG})
  - revisit hole-line expansion

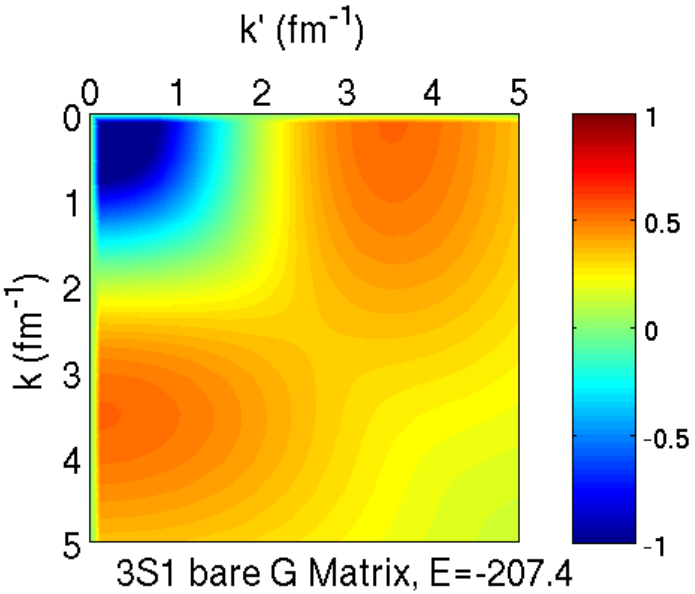
Compare Potential and G Matrix: AV18 vs. V_{SRG}

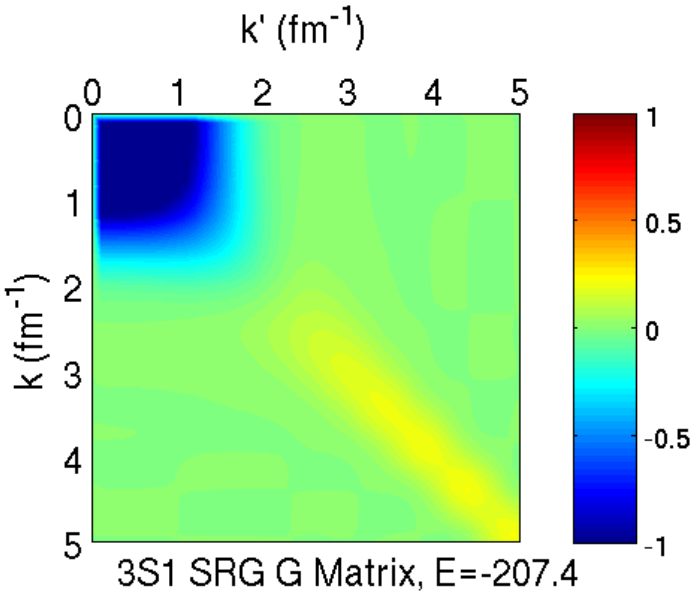
AV18





V_{SRG}

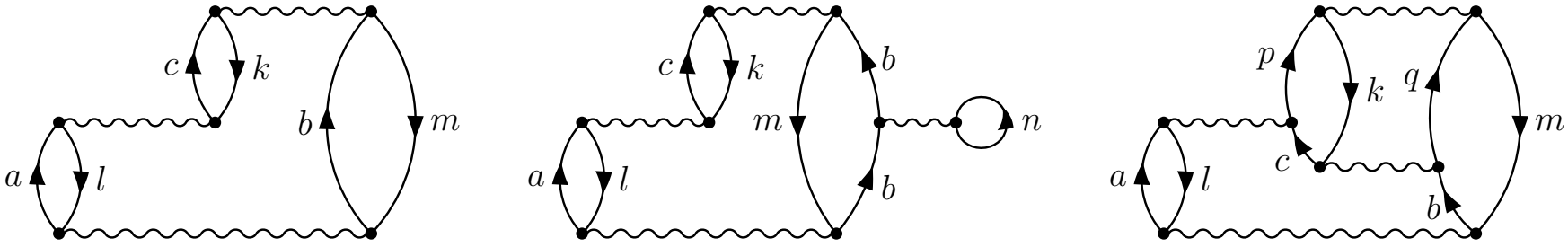




G Matrices

Hole-Line Expansion Revisited (Bethe, Day, ...)

- Consider ratio of fourth-order diagrams to third-order:

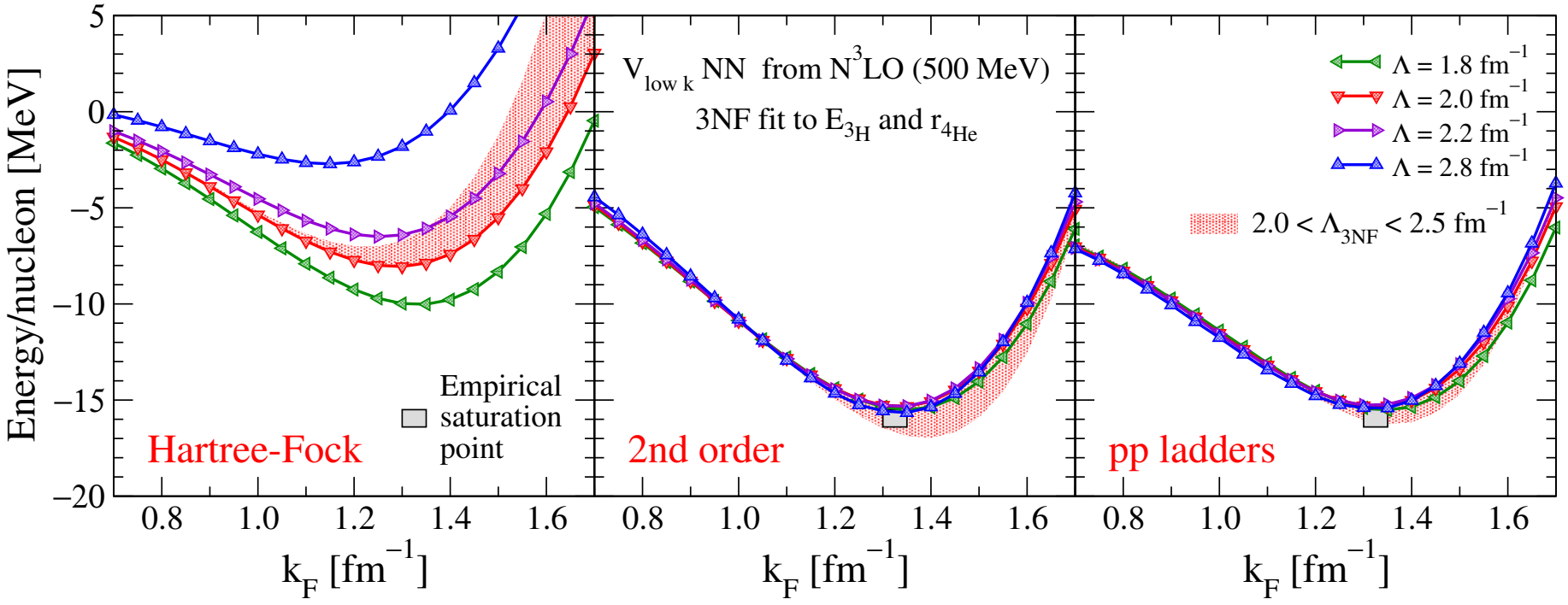


- "Conventional" G matrix still couples low-k and high-k
  - no new hole line $\Longrightarrow$ ratio $\approx -\chi(\mathbf{r}=0) \approx -1 \Longrightarrow$ sum all orders
  - add a hole line $\Longrightarrow$ ratio $\approx \sum_{n\le k_\mathrm{F}} \langle bn|(1/e)G|bn\rangle \approx \kappa \approx 0.15$
- Low-momentum potentials decouple low-k and high-k
  - add a hole line $\Longrightarrow$ still suppressed
  - no new hole line $\Longrightarrow$ also suppressed (limited phase space)
  - freedom to choose single-particle $U \Longrightarrow$ use for Kohn-Sham

  $\Longrightarrow$ Ab initio MBPT and DFT can work!
- (How do we get a Kohn-Sham $V_\mathrm{KS}(\mathbf{x})$ from even HF diagrams?)

What is needed for ab initio Kohn-Sham DFT?

1. Need MBPT to work with tuned U $[H = (T + U) + (V - U)]$

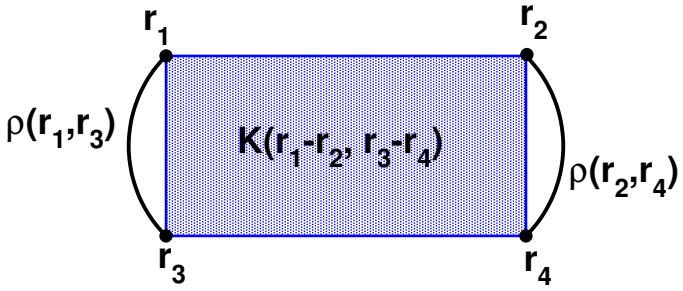


   - (see new results from K. Hebeler et al.)
   - If convergence insensitive to $U \Longrightarrow$ choose so KS density exact
2. Need to calculate $V_{\rm KS}(\mathbf{x})$ from $\delta E[\rho]/\delta\rho(\mathbf{x})$, etc. but diagrams depend non-locally on KS orbitals
   - Density matrix expansion (DME) $\Longrightarrow$ explicit densities
   - Use chain rule $\Longrightarrow$ "optimized effective potential" (OEP)

Density matrix expansion revisited [Negele/Vautherin]

- Dominant MBPT contributions can be put into form

$$\langle V \rangle \sim \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r}_1, \mathbf{r}_3) K(\mathbf{r}_{12}, \mathbf{r}_{34}) \rho(\mathbf{r}_2, \mathbf{r}_4)$$



  - finite range and non-local resummed vertices K (+ NNN)

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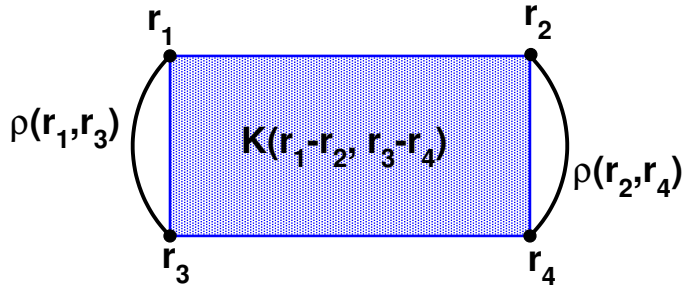
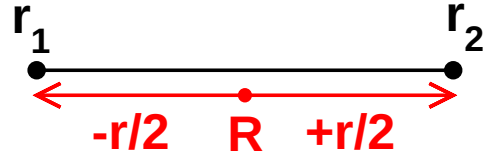


  - finite range and non-local resummed vertices K (+ NNN)
- DME: Expand KS ρ in local operators w/factorized non-locality

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \psi^\dagger_\alpha(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2) = \sum_n \Pi_n(\mathbf{r}) \langle \mathcal{O}_n(\mathbf{R}) \rangle$$



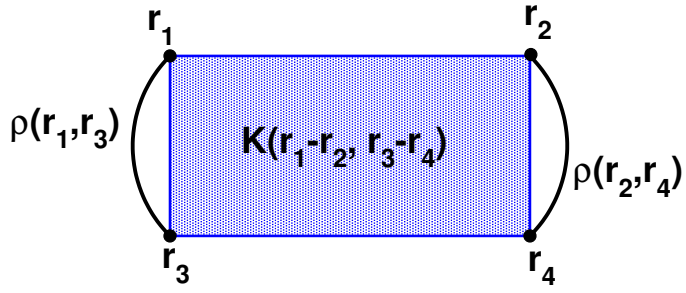
with $\langle \mathcal{O}_n(\mathbf{R}) \rangle = \{\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \cdots\}$ maps $\langle V \rangle$ to Skyrme-like EDF!

- Adds density dependences, isovector, . . . missing in Skyrme

Density matrix expansion revisited [Negele/Vautherin]

- Dominant MBPT contributions can be put into form

$$\langle V \rangle \sim \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r}_1, \mathbf{r}_3) K(\mathbf{r}_{12}, \mathbf{r}_{34}) \rho(\mathbf{r}_2, \mathbf{r}_4)$$



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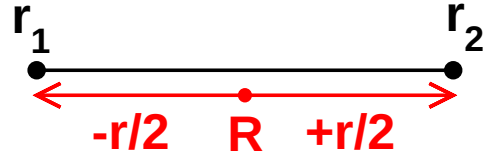
- DME: Expand KS ρ in local operators w/factorized non-locality

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \psi^\dagger_\alpha(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2) = \sum_n \Pi_n(\mathbf{r}) \langle \mathcal{O}_n(\mathbf{R}) \rangle$$



with $\langle \mathcal{O}_n(\mathbf{R}) \rangle = \{\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \cdots\}$ maps $\langle V \rangle$ to Skyrme-like EDF!

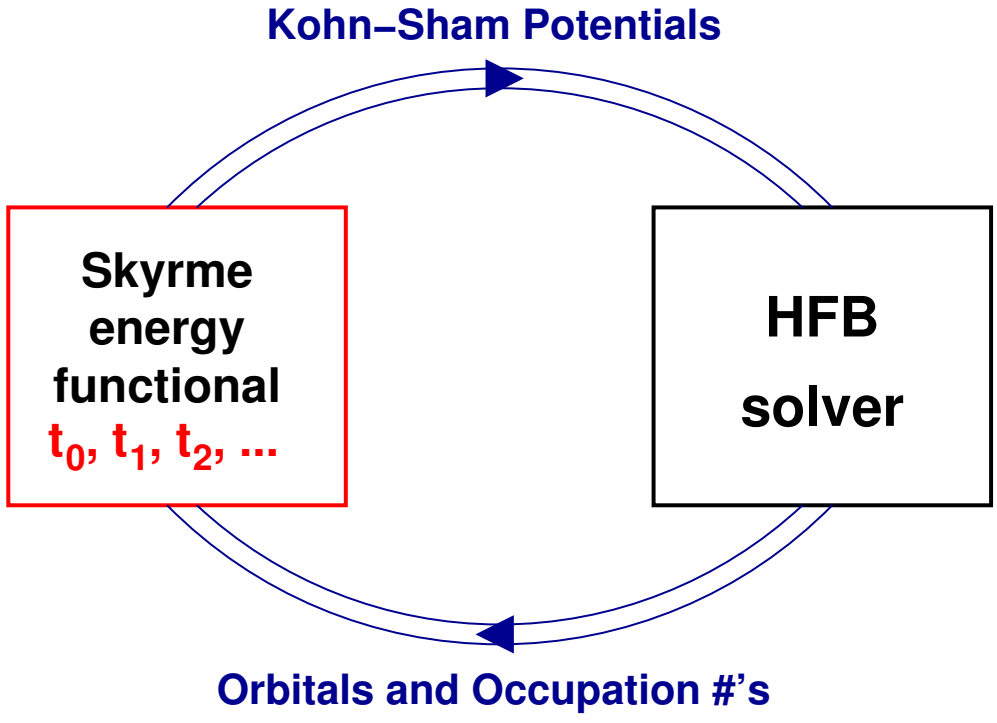
- Adds density dependences, isovector, . . . missing in Skyrme
- Original DME expands about nuclear matter (k-space + NNN)

$$\rho(\mathbf{R}+\mathbf{r}/2, \mathbf{R}-\mathbf{r}/2) \approx \frac{3j_1(sk_F)}{sk_F}\rho(\mathbf{R}) + \frac{35j_3(sk_F)}{2sk_F^3}\left(\frac{1}{4}\nabla^2\rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5}k_F^2\rho(\mathbf{R}) + \cdots\right)$$

Adaptation to Skyrme HFB Implementations

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

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



$$V_{\rm KS}(\mathbf{r}) = \frac{\delta E_{\rm int}[\rho]}{\delta\rho(\mathbf{r})} \iff [-\frac{\nabla^2}{2m} + V_{\rm KS}(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha\psi_\alpha \Longrightarrow \rho(\mathbf{x}) = \sum_\alpha n_\alpha|\psi_\alpha(\mathbf{x})|^2$$

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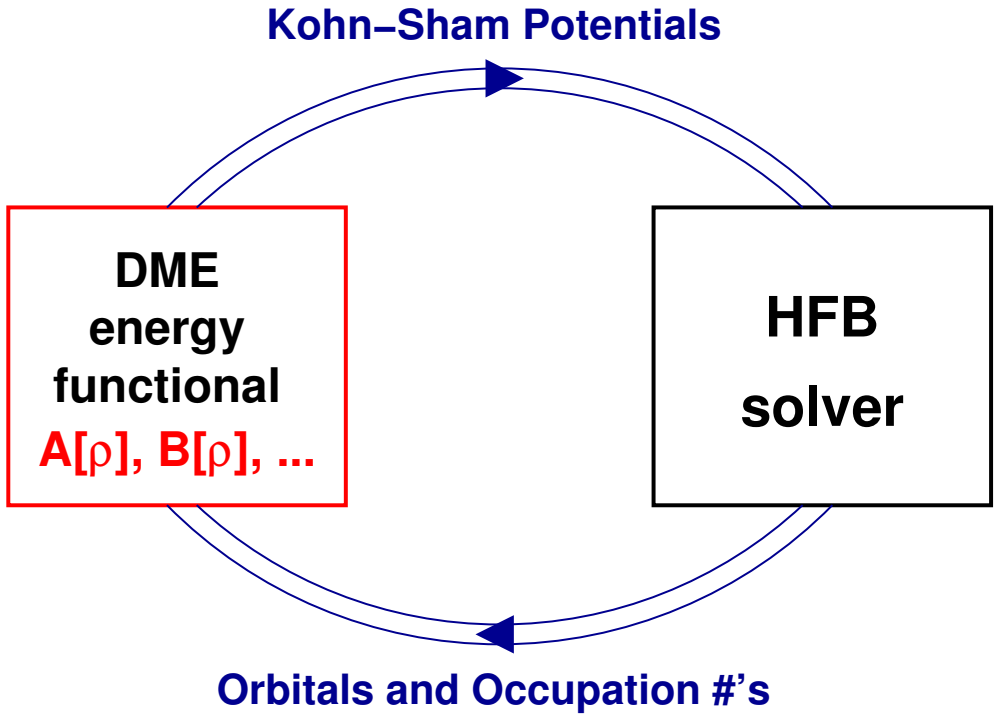

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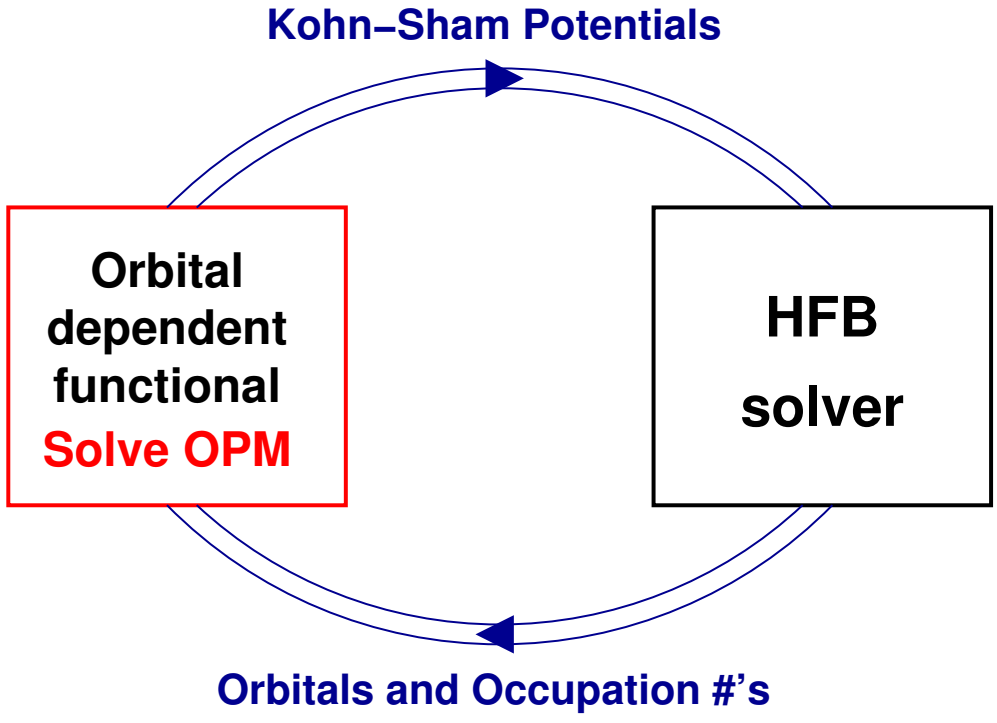

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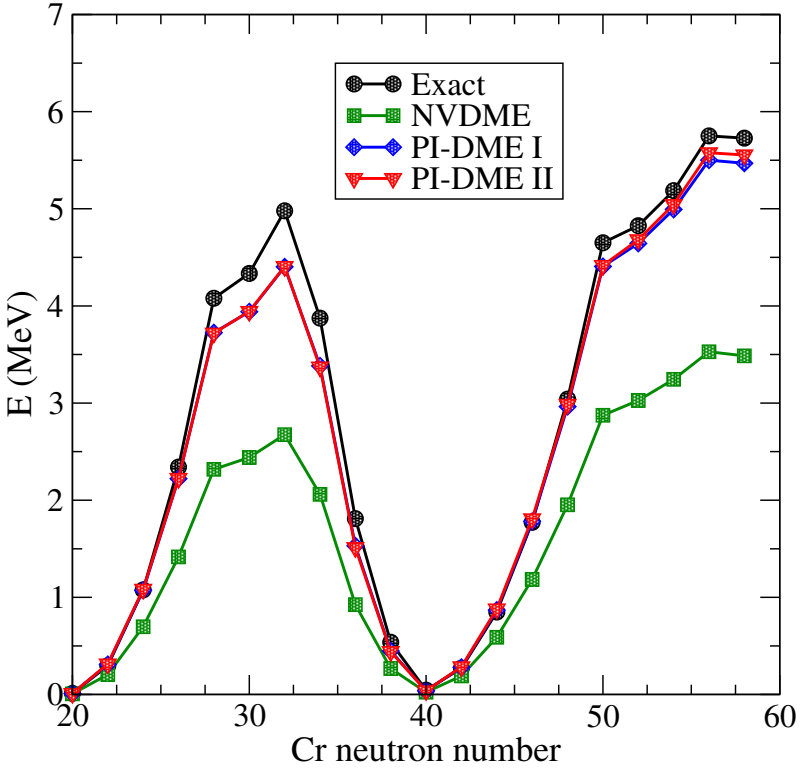
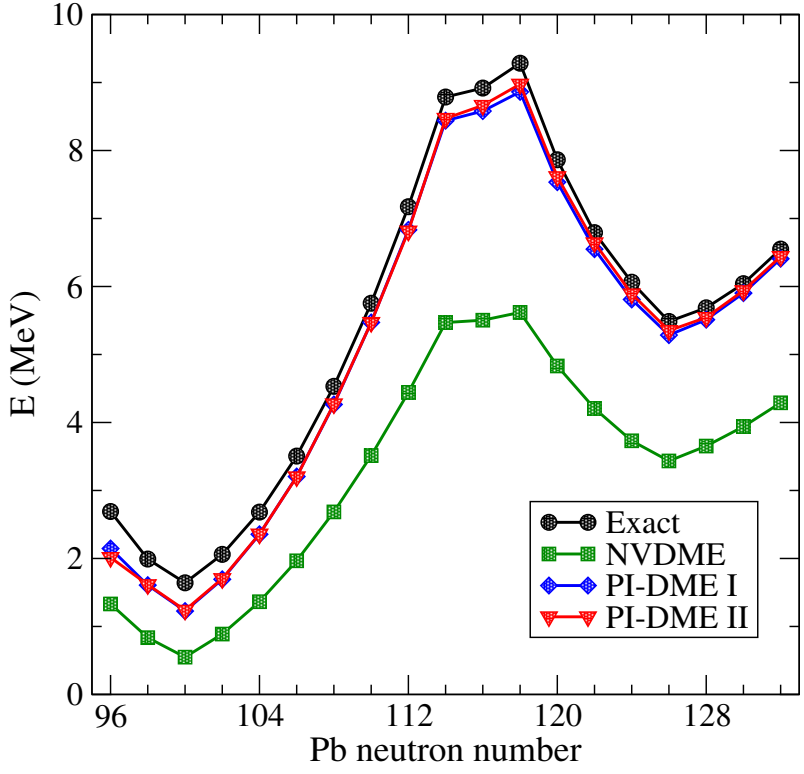
Improved DME for pion exchange [Gebremariam et al.]

- Phase-space averaging for finite nuclei (symmetries, sum rules)
- Focus on long-range interactions $\Longrightarrow$ pion exchange in NN and NNN from chiral effective field theory (χEFT)
- Tests are very promising [arXiv:0910.4979]:

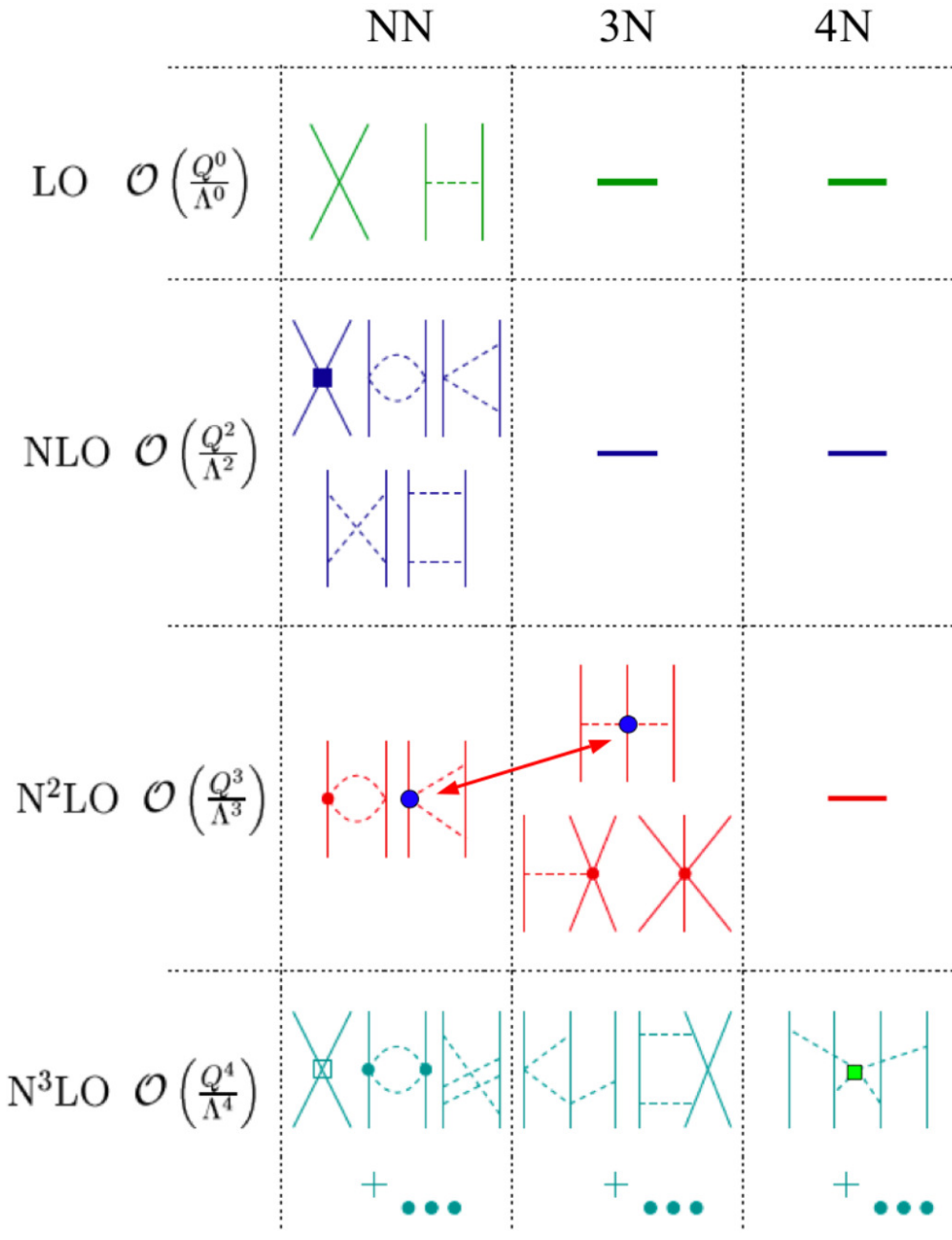




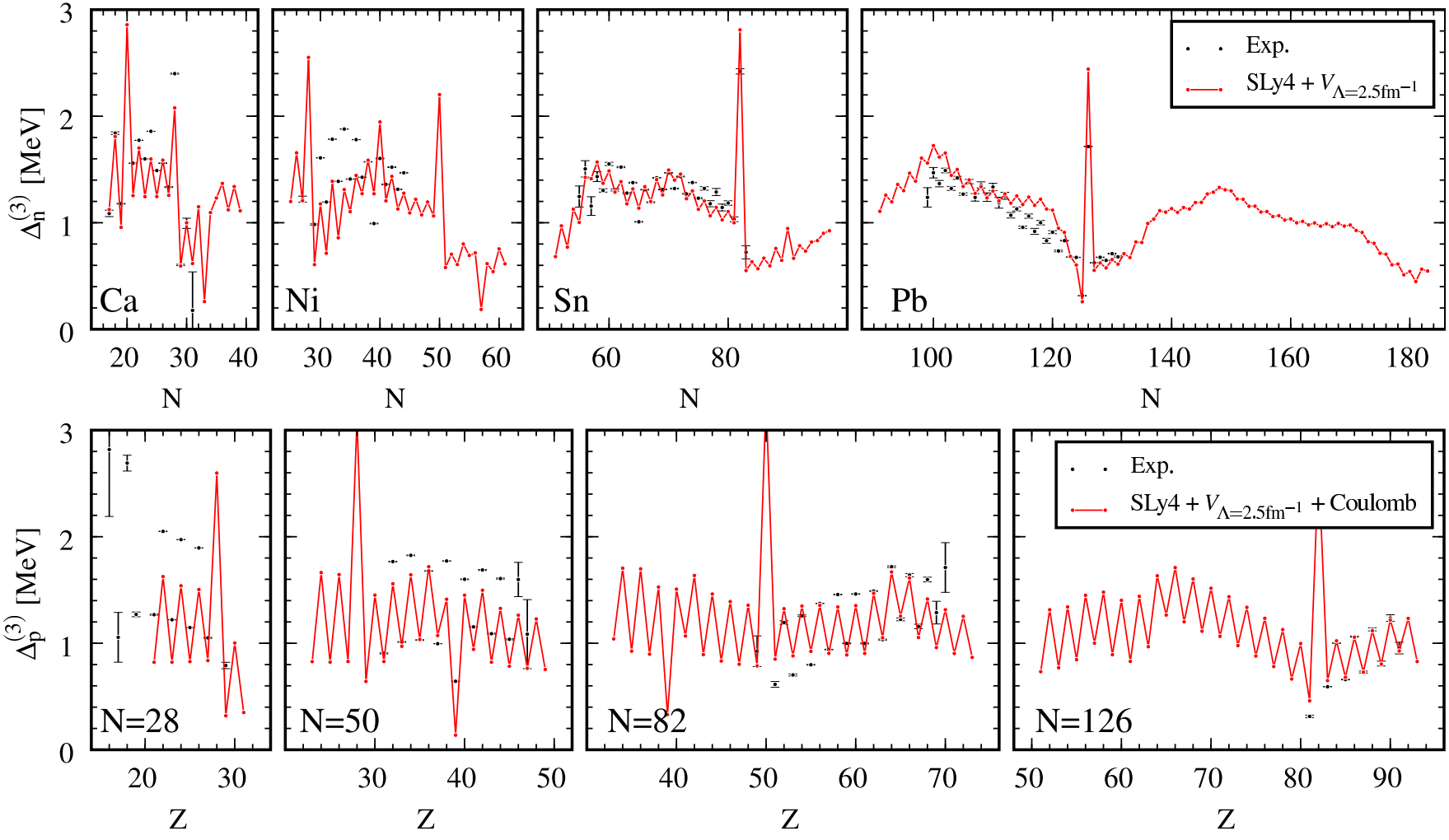
See Scott Bogner's talk!

Long-range chiral EFT $\Longrightarrow$ enhanced Skyrme

- Add long-range (π-exchange) contributions in the density matrix expansion (DME)
  - NN/NNN through N^{2}LO [Gebremariam et al.]
- Refit Skyrme parameters for short-range parts
- Test for sensitivities and improved observables (e.g., isotope chains) [ORNL]
- Spin-orbit couplings from 2π 3NF particularly interesting
- Can we "see" the pion in medium to heavy nuclei?



Non-empirical pairing gaps from $V_{\mathrm{low}\,k}$ [Duguet et al.]



- Use Skyrme for particle-hole functional and $V_{\mathrm{low}\,k}$ for pairing
- Leading order and doesn't include NNN, but very promising!

See Scott Bogner's talk!

Orbital Dependent DFT (OEP, OPM, ...) [J. Drut, L. Platter, rjf]

- Construct MBPT for $E_{\rm int}[\rho, \tau, \mathbf{J}, \ldots]$; densities are sums over orbitals solving from Kohn-Sham S-eqn with $V_{\rm KS}(\mathbf{r}), \ldots$
- Self-consistency $\Longrightarrow$ $V_{\rm KS}(\mathbf{r}) = \delta E_{\rm int}[\rho, \ldots]/\delta\rho(\mathbf{r}), \ldots$
  - i.e., Kohn-Sham potential is functional derivative of interacting energy functional (or $E_{\rm xc}$) wrt (all) densities
  - How do we calculate this functional derivative?
- Approximations with explicit $\rho(\mathbf{r})$ dependence: LDA, DME, ...

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- Orbital-dependent DFT $\Longrightarrow$ full derivative via chain rule:

$$V_{\rm KS}(\mathbf{r}) = \frac{\delta E_{\rm int}[\phi_\alpha,\varepsilon_\alpha]}{\delta\rho(\mathbf{r})} = \int d\mathbf{r}'\,\frac{\delta V_{\rm KS}(\mathbf{r}')}{\delta\rho(\mathbf{r})}\sum_\alpha\left\{\int d\mathbf{r}''\left[\frac{\delta\phi^\dagger_\alpha(\mathbf{r}'')}{\delta V_{\rm KS}(\mathbf{r}')}\frac{\delta E_{\rm int}}{\delta\phi^\dagger_\alpha(\mathbf{r}'')} + c.c.\right] + \frac{\delta\varepsilon_\alpha}{\delta V_{\rm KS}(\mathbf{r}')}\frac{\partial E_{\rm int}}{\partial\varepsilon_\alpha}\right\}$$

  - Solve the OPM equation for $V_{\rm KS}$ using $\chi_s(\mathbf{r},\mathbf{r}') = \delta\rho(\mathbf{r})/\delta V_{\rm KS}(\mathbf{r}')$

$$\int d^3r'\,\chi_s(\mathbf{r},\mathbf{r}')\,V_{\rm KS}(\mathbf{r}') = \Lambda_{\rm xc}(\mathbf{r})$$

  - $\Lambda_{\rm xc}(\mathbf{r})$ is functional of the orbitals ϕ_α, eigenvalues ε_α, and $G^0_{\rm KS}$

Outline

Overview: EDF's and DFT

The UNEDF project

New developments: Constraints, optimization, ...

Non-empirical EDF's and ab-initio DFT

Summary

Multi-pronged effort to improve nuclear EDF's

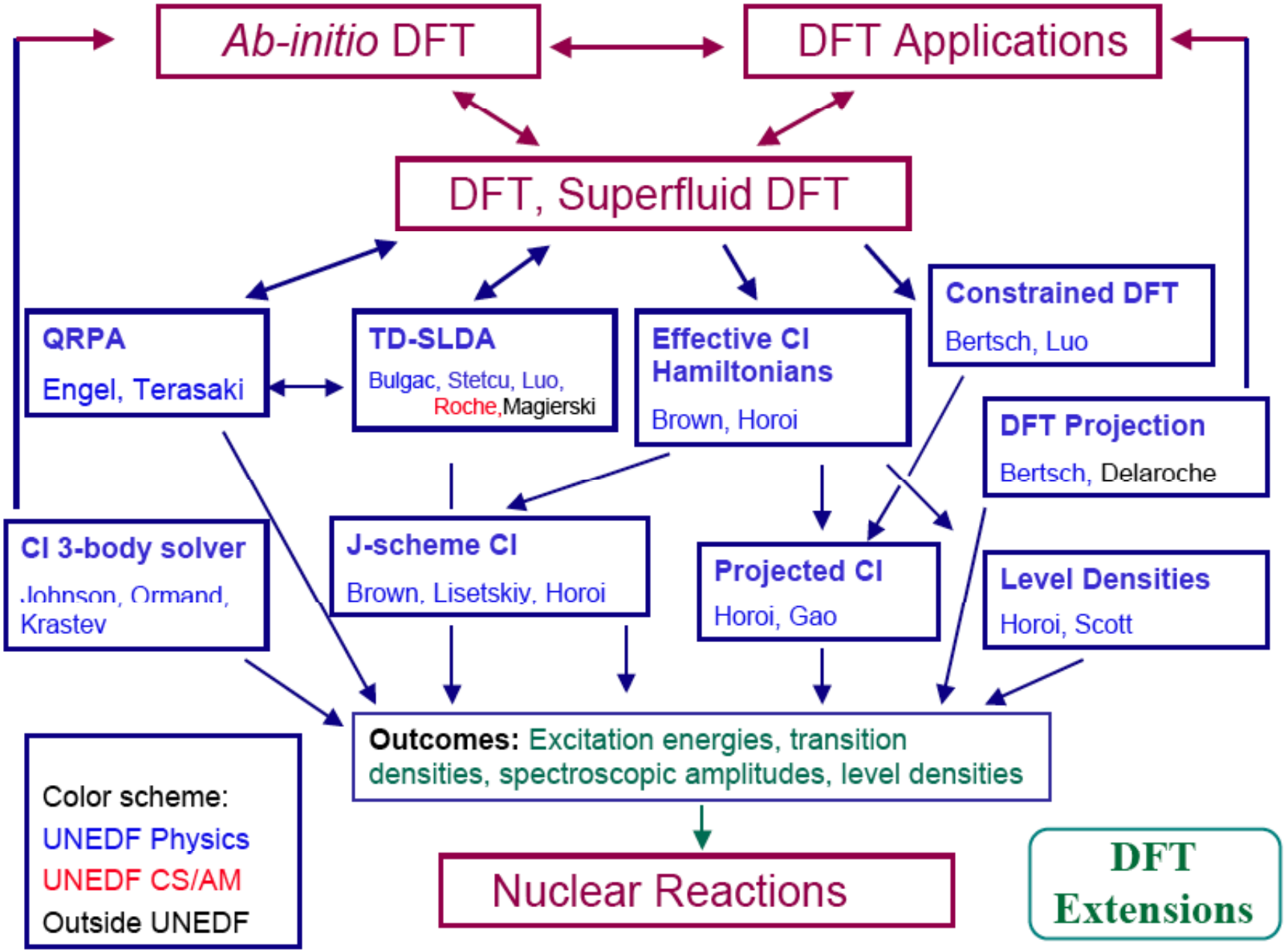
- Worldwide collaborative effort: UNEDF + FIDIPRO + ...
  - SciDAC model is effective
- Strategies
  - Extend existing functionals following EFT principles and using sophisticated correlation analyses
  - Constrain with new data and accurate microscopic calculations (e.g., trapped neutron drops using GFMC/AFMC and NCFC)
  - Develop ab initio functionals using low-momentum interactions
    - Many-body perturbative expansions possible
    - Long-distance chiral physics (EFT expansion)
    - Density matrix expansion (DME) or full orbital-based OEP

Expect many developments in the coming years!

(Some) issues for nuclear DFT to be addressed

- DFT for self-bound systems
  - Does DFT even exist? (HK theorem for intrinsic states?)
  - Effective actions: symmetry breaking and zero modes
  - Game plans proposed:
    - T. Duguet et al.: “multi-reference” projection methods
    - B. Giraud et al.: use harmonic oscillator trap
    - J. Engel, J. Messud et al.: find intrinsic functional
    - J. Braun et al.: deal with zero modes using Fadeev-Popov or BRST methods
- What about single-particle spectra?
  - R. Bartlett: good reproduction for Coulomb systems
  - Connect to Green’s function formulation?
- How to best deal with long-range correlations?
- What about alternative functionals? (e.g., T. Papenbrock)

UNEDF DFT Extensions: Interconnections



Jacob's Ladder: Coulomb DFT [J. Perdew et al.]

"And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . . " [Genesis 28:12]

HEAVEN $\Longrightarrow$ Chemical Accuracy

5. Full orbital-based DFT from MBPT+.
   [E.g., RPA with Kohn-Sham orbitals.]
4. Hyper-GGA includes exact exchange energy density calculated with (occupied) orbitals.
3. Meta-GGA adds (some subset of) $\nabla^2\rho_\uparrow(\mathbf{r})$, $\nabla^2\rho_\downarrow(\mathbf{r})$, $\tau_\uparrow(\mathbf{r})$, and $\tau_\downarrow(\mathbf{r})$.
   [Note: $\tau[\rho]$ is nonlocal; $\tau[\phi_i^{\rm KS}]$ is semi-local.]
2. Generalized gradient approximation (GGA) adds $\nabla\rho_\uparrow(\mathbf{r})$ and $\nabla\rho_\downarrow(\mathbf{r})$.
1. Local spin density approximation (LSDA) with $\rho_\uparrow(\mathbf{r})$ and $\rho_\downarrow(\mathbf{r})$ as ingredients.

Jacob's Ladder: Nuclear DFT [arXiv:0906.1463]

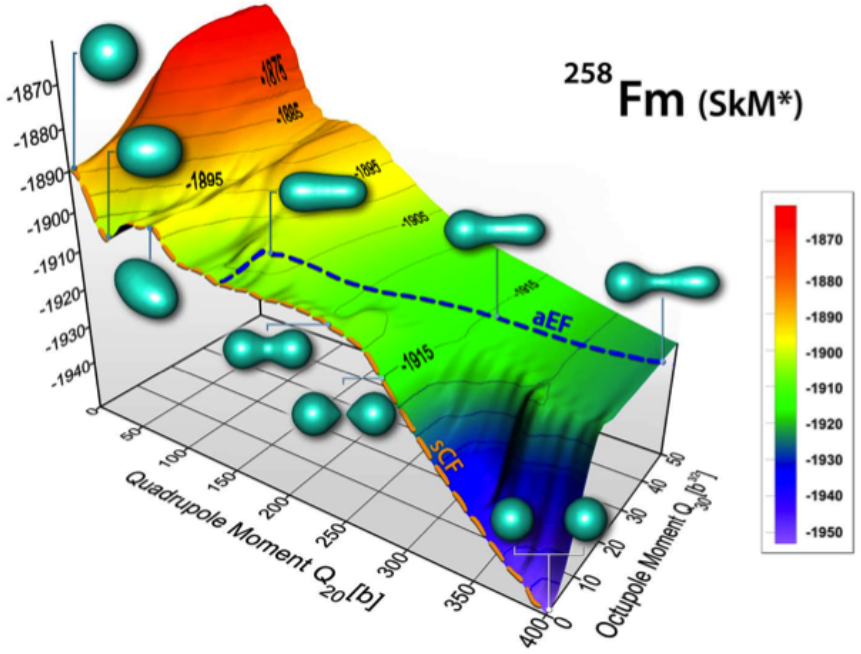
"And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . . " [Genesis 28:12]

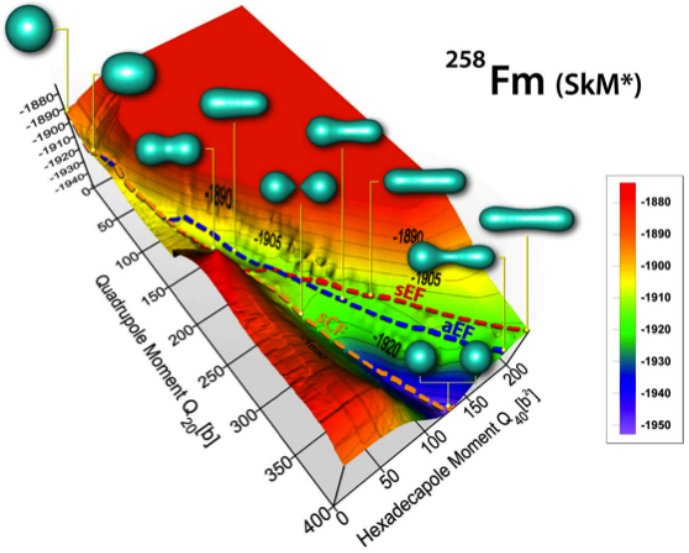
HEAVEN $\Longrightarrow$ UNEDF from NN$\cdots$N (QCD)

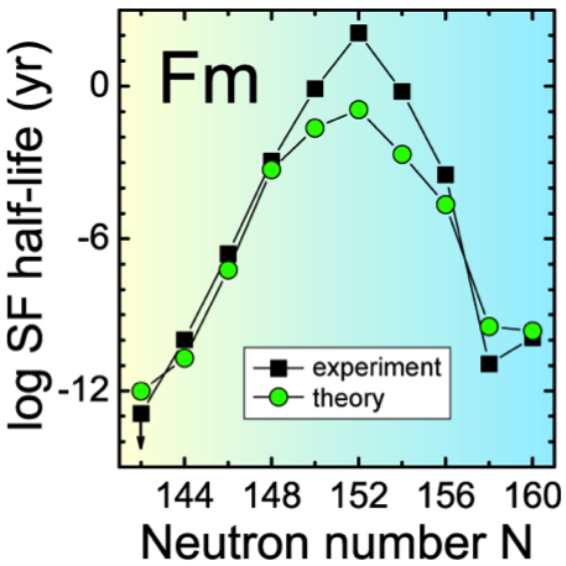
5. Full orbital-based DFT based on [lattice QCD $\Longrightarrow$] chiral EFT $\Longrightarrow$ $V_{\mathrm{low}\,k}$.
4. Complete semi-local functional (e.g., DME) from chiral EFT $\Longrightarrow$ $V_{\mathrm{low}\,k}$.
3. Long-range chiral NN and NNN $\Longrightarrow$ Π–DME $\Longrightarrow$ merged with Skyrme and refit.
2. Generalized Skyrme with $\nabla^n\rho(\mathbf{r})$, $\rho^\alpha(\mathbf{r})$, . . . with constraints (e.g., neutron drops)
1. Conventional Skyrme EDF's [e.g. SLY4].

- Developing 2.–5. in parallel!

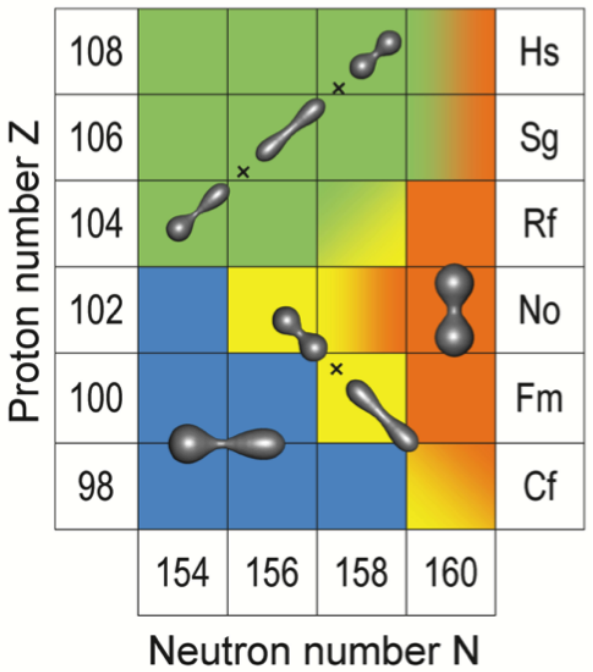
Spontaneous fission: Energy surfaces from DFT







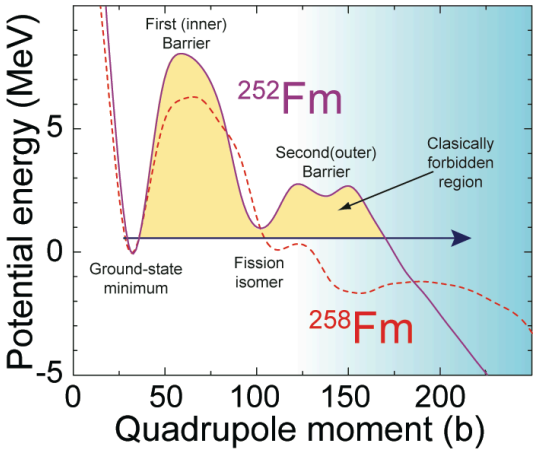
A. Staszczak et al.,
PRC 80, 014309 (2009)



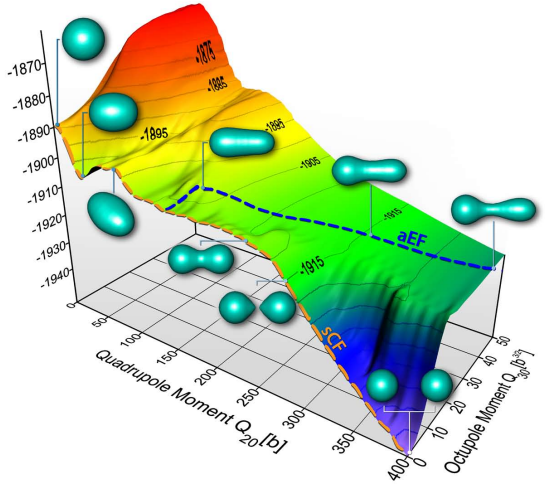
A promising starting point for an extreme scale challenge!

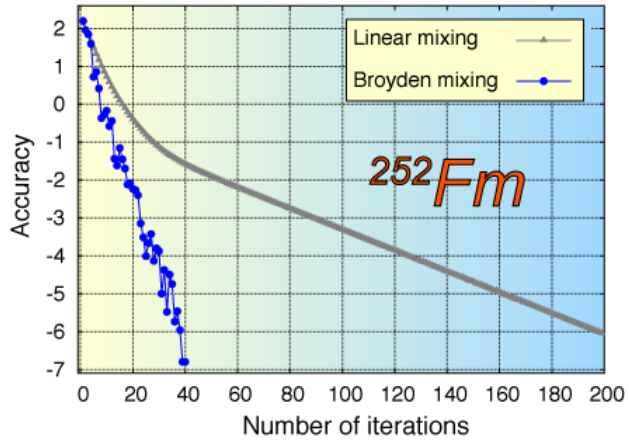
Microscopic description of nuclear fission

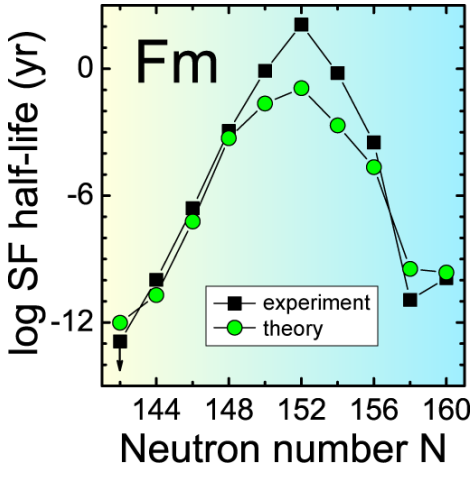
Advanced theoretical methods and high-performance computers may finally unlock the secrets of nuclear fission, a fundamental nuclear decay that is of great relevance to society

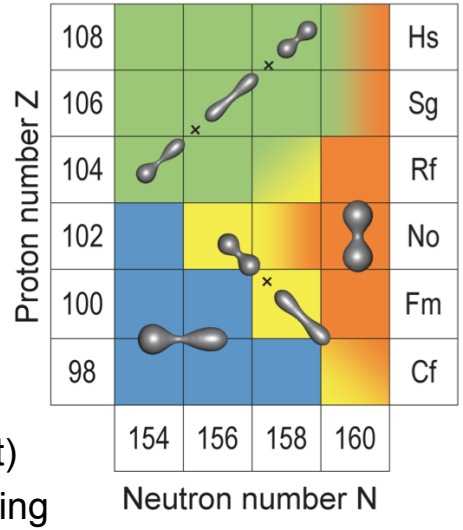


- The nuclear many-body problem is difficult
- Much of the progress in fission theory has been based on phenomenological models
  - This limits our predictive capability
  - … and makes it difficult to estimate the uncertainties









- There are fundamental problems in fission that cry to be solved. Success will impact:
  - Basic science (nuclear structure and astrophysics)
  - Societal applications (energy, defense, environment)
- Fission is a perfect problem for extreme scale computing
- We are developing a *microscopic* model for fission that will be predictive and extendable. The figures show progress:
  - Calculating pathways and half-lives
  - Greatly improving calculation speed