

Data to Constrain EDF

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Technology to calculate observables

- Global properties
- Spectroscopy

DFT Solvers

Functional form

Functional optimization

Estimation of theoretical errors



...with Nicolas Schunck

**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

Skx
SkP

| 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

SkI...
SGII

| 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 |

Participants

1. A. Afanasjev
2. K. Bennaceur
3. C. Bertulani
4. A. Brown
5. G. Colo
6. D. Dean
7. J. Dobaczewski
8. Y. Enyo
9. P. Fallon
10. R. Furnstahl
11. B. Gebremariam
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14. A. Kerman
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16. N. Itagaki
17. M. Ito
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21. P. Möller
22. J. Moré
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25. T. Nakatsukasa
26. H. A. Nam
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30. M. Ploszajczak
31. H. Sagawa
32. J. Sarich
33. N. Schunck
34. S. Shlomo
35. M. Stoitsov
36. J. Terasaki
37. I. Thompson
38. T. Uesaka
39. U. Utsuno
40. J. Vary
41. E. Vigezzi

The aim of the January meeting at ORNL was to prepare the development of the next generation of functionals by discussing various aspects pertaining to the optimization of the EDF. In particular, we addressed the questions:

- What essential experimental data should be taken into account for the EDF optimization ?
- What optimization techniques should be used ?
 - Importance of pseudo data (e.g., INM properties)
 - Stability conditions
 - Static and dynamic properties
 - Choice of weights in χ^2
 - Minimization algorithms
 - Optimization validation
 - Error estimation and error propagation

Example: The Matrix – SkP case

| | Skyrme binding energy, saturation density incompressibility, enhancement factor, isospin symmetry energy at ρ_0 and $\rho_0/2$; (6 parameters) | Effective Mass | Skyrme surface energy | Spin-orbit strength W_0 | Average pairing matrix element |
|---|--|----------------|-----------------------|---------------------------|--------------------------------|
| NM binding energy saturation density incompressibility, enhancement factor, isospin symmetry energy at ρ_0 and $\rho_0/2$; (6 “observables”) | X | | | | |
| 1 | | X | | | |
| Binding energies of ^{16}O and ^{208}Pb | | | X | | |
| Binding energies of $^{120-132}\text{Sn}$ | | | | X | |
| Average pairing gap | | | | | X |

Fitting strategies

bulk observables of finite nuclei

E_b binding energies r, R radii σ surface

free χ^2 -fit



infinite matter

$a_{\text{sym}}, K_{\infty}, m^*/m, \kappa$

nuclear matter properties (NMP)



**big extrapolation
errors for NMP**

(correlations between NMP)

χ^2 -fit with **constrained NMP**



additional observables

a posteriori computation of

level splittings, giant resonances,
SHE, ...



**optimal choice of
NMP**

Outcome

DFT-UNEDF Working Group

**Determination of the Nuclear Energy functional:
Database of Experimental Data and Related Software**

[Introduction](#)

[Experimental Data Table](#)

[Software](#)

[Credits and
Documentation](#)

<http://orph02.phy.ornl.gov/workshops/lacm08/UNEDF/database.html>

A website containing the tabulated experimental data that could be used to fit the nuclear EDF and to compare various EDF parametrizations

- Peter Kluepfel (masses and radii of spherical nuclei)
- Gianluca Colo (giant monopole and dipole resonance)
- Jun Terasaki (2+ states and B(E2) values)
- Mario Stoitsov (axially-deformed nuclei deformations and V_{pn})
- Ludovic Bonneau (odd-mass spins and parity)
- Wojtek Satula (terminating states)

Last Modification: June, 18, 2008

This page is maintained by N. Schunck, in collaboration with J. Dobaczewski and W. Nazarewicz

Experimental Data Table

Spherical Nuclei

- Masses, r.m.s. radii, diffraction radii and surface thickness
- Giant monopole and dipole resonance in ^{90}Zr , ^{116}Sn and ^{208}Pb
- Experimental energy of the first 2+ state and B(E2) value in Ca, Ni, Sn and Pb isotopes

Axially-deformed Nuclei

- Binding energy of well-deformed even-even nuclei. Candidates were selected from a HFB mass-table calculation by M. Stoitsov with the SLy4 interaction according to 2 criteria
 1. The ground-state equilibrium deformation is greater than 0.25
 2. The experimental mass of the nucleus is known
- Super-deformed bandheads and fission isomers
- $V_{pn}(Z,N) = 0.5 * [B(Z,N) - B(Z,N-2) - B(Z-2,N) + B(Z-2,N-2)]$, see M. Stoitsov, R. B. Cakirli, R. F. Casten, W. Nazarewicz and W. Satula, Phys. Rev. Lett. **98**, 132502 (2007)

Symmetry-unrestricted

- Ground-state spin and parity for odd-mass nuclei (odd-even, even-odd and odd-odd)
- High-K terminating states in f-p shell nuclei
- 1q.p. excited states of odd-mass heaviest elements

Software (Version 01, June 18, 2008)

We supply the database itself in the form of an Ascii file, as well as the necessary Fortran 77 and Fortran 90 subroutines to read the files. Each of the modules can be used "as is" in existing programs.

| File | Fortran 77 | Fortran 90 |
|--------------------------|-------------------------|---------------------------|
| Test Program | main.f | main.f90 |
| Input/Output Module | input.f | input.f90 |
| Database | | |

The entire package (fortran source and file) is also available below in the form of zip archive (unzip *.zip to decompress):

| Fortran 77 | Fortran 90 |
|---|---|
| ExpDataTablePackage_F77.zip | ExpDataTablePackage_F90.zip |

The programs supplied here open the data file, read all records and fill out a number of arrays with the data that are read. All the relevant arrays are listed below, together with a short description for each of them. This list can also be found in the form of comments in each source file. In Fortran 77, we use implicit declaration of variables (variables whose name starts by I-N are integers by default, others are real by default). In Fortran 90 the *Implicit None* instruction is used throughout and each variable is properly declared. The Fortran 90 code is also explicitly modular for better insertion into other codes.

Spherical

- |Zsph
- Bsph
- R0sph
- SIGs
- RMS

| | | | | | | |
|------------|-----|-----|-------------|---------------|---------|------------------------------------|
| | 108 | 160 | -1955.59595 | 0.53600 | 0.35506 | |
| | 108 | 162 | -1969.38000 | 0.27000 | 0.34422 | |
| | 108 | 164 | -1981.24805 | 0.54400 | 0.33152 | |
| | 108 | 166 | -1993.62402 | 0.54799 | 0.31692 | |
| SDSTATES : | Z | N | B [MeV] | ESD(0+) [MeV] | | Reference |
| | 12 | | | | | |
| | 18 | 18 | -306.71600 | 4.329 | | Nucl. Phys. A682, 1c (2001) |
| | 20 | 20 | -342.05200 | 5.212 | | Phys. Rev. Lett. 87, 222501 (2001) |
| | 30 | 30 | -514.99000 | 7.500 | | Phys. Rev. Lett. 82, 3400 (1999) |
| | 66 | 86 | -1245.33000 | 7.500 | | Phys. Rev. Lett. 88, 042501 (2002) |
| | 80 | 112 | -1519.11700 | 5.300 | | Phys. Rev. Lett. 77, 1707 (1996) |
| | 80 | 114 | -1535.44000 | 6.017 | | Phys. Rev. Lett. 73, 777 (1994) |
| | 82 | 110 | -1508.09700 | 4.011 | | Phys. Rev. C49, 2849 (1994) |
| | 82 | 112 | -1525.89100 | 4.640 | | Phys. Rev. C55, 2819 (1997) |
| | 82 | 114 | -1543.18600 | 5.630 | | ANU-P/1667 (2005) |
| | 92 | 144 | -1790.40900 | 2.750 | | |
| | 92 | 146 | -1801.68900 | 2.557 | | |
| | 96 | 146 | -1823.34800 | 1.900 | | |

Deformed

- |Zdef
- Bdef
- dBdef
- b2def

| | | | | |
|------------|----|-----|---------|--------------|
| MONOPRES : | Z | N | E [MeV] | DeltaE [MeV] |
| | 3 | | | |
| | 40 | 50 | 17.81 | 0.35 |
| | 50 | 66 | 15.83 | 0.06 |
| | 82 | 126 | 14.18 | 0.11 |
| DIPOLRES : | Z | N | E [MeV] | |
| | 3 | | | |
| | 40 | 50 | 16.74 | |
| | 50 | 66 | 15.68 | |
| | 82 | 126 | 13.63 | |

Super-def

- |Zsup
- Bsup
- ESD

| | | | | |
|------------|-----|---|------|--------|
| ODDNUCLE : | Z | N | Spin | Parity |
| | 630 | | | |
| | 6 | 5 | 1.5 | -1 |
| | 6 | 7 | 0.5 | -1 |
| | 6 | 9 | 0.5 | 1 |
| | 7 | 4 | 0.5 | 1 |
| | 7 | 6 | 0.5 | -1 |
| | 7 | 8 | 0.5 | -1 |

Recent Work

Variations on a theme by Skyrme

P. Klüpfel, P. -G. Reinhard, T.J. Bürvenich and J. A. Maruhn
arXiv:0804.3385 (April 2008)

Error analysis of nuclear mass fits

J. Toivanen, J. Dobaczewski, M. Kortelainen and K. Mizuyama
arXiv:0806.1914 (June 2008)