Data to Constrain EDF

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UNEDF Annual Meeting, Pack Forest, WA, June2008

Technology to calculate observables

- Global properties
- Spectroscopy

DFT Solvers

Functional form

→ Functional optimization

→ Estimation of theoretical errors

...with Nicolas Schunck

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

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

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

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
12. P.-H. Heenen
13. T. Kawano
14. A. Kerman
15. P. Kluepfel
16. N. Itagaki
17. M. Ito
18. T. Lesinski
19. M. Matsuo
20. K. Matsuyanagi
21. P. Möller
22. J. Moré
23. N. Michel
24. N. Nikolov
25. T. Nakatsukasa
26. H. A. Nam
27. W. Nazarewicz
28. T. Otsuka
29. J. Pei
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")	×						
1		×					
Binding energies of ^{16}O and ^{208}Pb			×				
Binding energies of $^{120-132}Sn$				×			
Average pairing gap					×		

Fitting strategies

bulk observables of finite nuclei

E_b binding energies r, R radii σ surface

free χ^2-fit

⇓

infinite matter

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

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 Vpn)
- 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 throughtout and each variable is properly declared. The Fortran 90 code is also explicitly modular for better insertion into other codes.

Spherical

- lZsph
- Bsph
- R0sp
- SIGs
- RMS

Deformed

- lZdef
- Bdef
- dBde
- b2de

Super-def

- lZsup
- Bsup
- ESD

```
           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
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
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)