UT-BATTELLE

Odd-mass Calculations: Status, Problems and Perspectives

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1 International Conferences

- *Nuclear DFT: Questions And Challenges*, W. Nazarewicz, First FIDIPRO-JSPS Workshop On Energy Density Functionals In Nuclei, Keurusselka, Finland, October 25-27, 2007
- *Nuclear Structure '07: Exciting, Broad, Relevant*, W. Nazarewicz, Fourth International Conference on Fission and Properties of Neutron-Rich Nuclei, Sanibel Island, Florida, Nov 11-17, 2007
- *Spectroscopy Of Odd-Mass Nuclei In Energy Density Functional Theory,* N. Schunck, 2nd LACM-EFES-JUSTIPEN Workshop, ORNL, Oak Ridge, Jan. 23-25, 2008
- *Computing Atomic Nuclei*, W. Nazarewicz, IOP Annual Nuclear Physics Group Conference, Liverpool, UK, April 1, 2008.
- *Science Of Rare Isotopes: Connecting Nuclei With The Universe*, W. Nazarewicz, plenary talk, 2008 APS April Meeting St. Louis, Missouri, April 12, 2008.
- *Odd-Even Mass Nuclei In Energy Density Functional Theory,* N. Schunck, APS April Meeting, St Louis, Apr. 10-15, 2008
- *Towards The Spectroscopy Of Odd-Mass Nuclei In Density Functional Theory,* N. Schunck, Carnegie 2008 Conference: Nuclear Structure at the Extremes, University of West Scotland, Paisley, May. 7-10, 2008
- *Large-scale mass table calculations with the UNEDF project*, M. Stoitsov, Mass Olympics, ECT* Workshop, May 26-30, 2008
- *Spectroscopy Of Odd-Mass Nuclei In Energy Density Functional Theory,* N. Schunck, Nuclear Structure 2008, MSU, Jun. 12-16, 2008

2

Publications And Meetings

Organization of the Workshop on the *Determination of the Nuclear Energy Functional: Optimization Strategy, Essential Experimental Data and Chi-Square Metric*, Oak Ridge, Jan. 22, 2008.

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

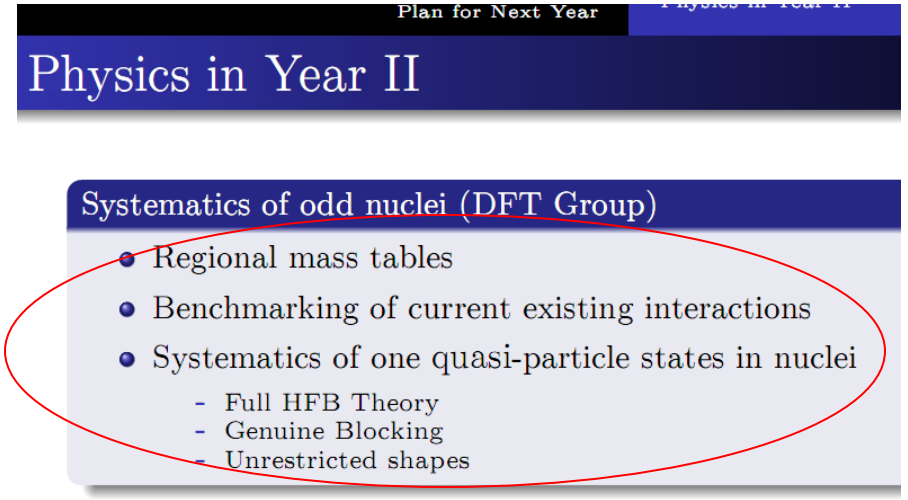
Name	Title of Contribution	File
K. Bennaceur	Stability Criteria for Skyrme Energy Functionals	Bennaceur.pdf
J. Moré (1)	Validation of Models	More_1.pdf
J. Moré (2)	Parameter Estimation in Nuclear Fission	More_2.pdf
T. Lesinski	Minimization Algorithms for Local and Global Minima Search	Lesinski.pdf

Broyden's Method in Nuclear Structure Calculations, A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck, and M. V. Stoitsov, *Submitted to Phys. Rev. C*

3 Physics and CS Involved

Goal: Benchmark existing Skyrme functionals on odd-mass nuclei to assess their performance and probe (poorly known) time-odd terms

Theoretical framework: symmetry-unrestricted "Skyrme-like" HFB theory

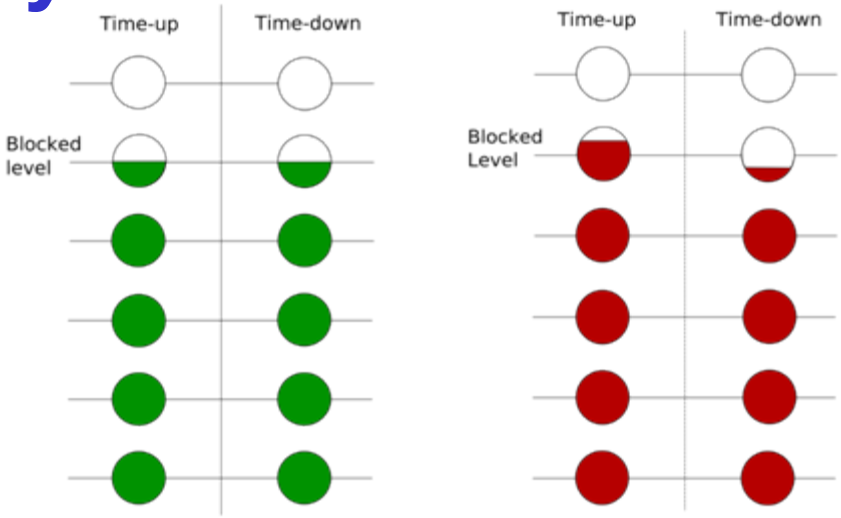


- The Physics:
  - Rare-earth region: Probing single-particle spectrum in a deformed mean-field traces back to spherical j-shells
  - Choice and fit of the pairing interaction and handling of pairing collapse in HFB theory via the Lipkin-Nogami prescription (see George's talk)
  - Probing time-odd terms
- Computing issues:
  - Choice of optimal even-even core
  - Stability of even-even and odd-even calculations
  - Automatic handling of blocked states
  - Data post-processing software

⇐ Exact blocking prescription

4 Odd Nuclei in "Skyrme-like" HFB

- Exact blocking prescription requires broken time-reversal symmetry
- Time-odd part of the functional becomes active



$$\mathcal{H}_t^{even}(\vec{r}) = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\overleftrightarrow{J}^2 + C_t^{\nabla J}\rho_t\vec{\nabla}\cdot\vec{J}$$

$$\mathcal{H}_t^{odd}(\vec{r}) = C_t^{s}\vec{s}_t^2 + C_t^{\Delta s}\vec{s}_t\cdot\Delta\vec{s}_t + C_t^{T}\vec{s}_t\cdot\vec{T}_t + C_t^{j}\vec{j}^2 + C_t^{\nabla j}\vec{s}_t\cdot\left(\vec{\nabla}\wedge\vec{j}_t\right)$$

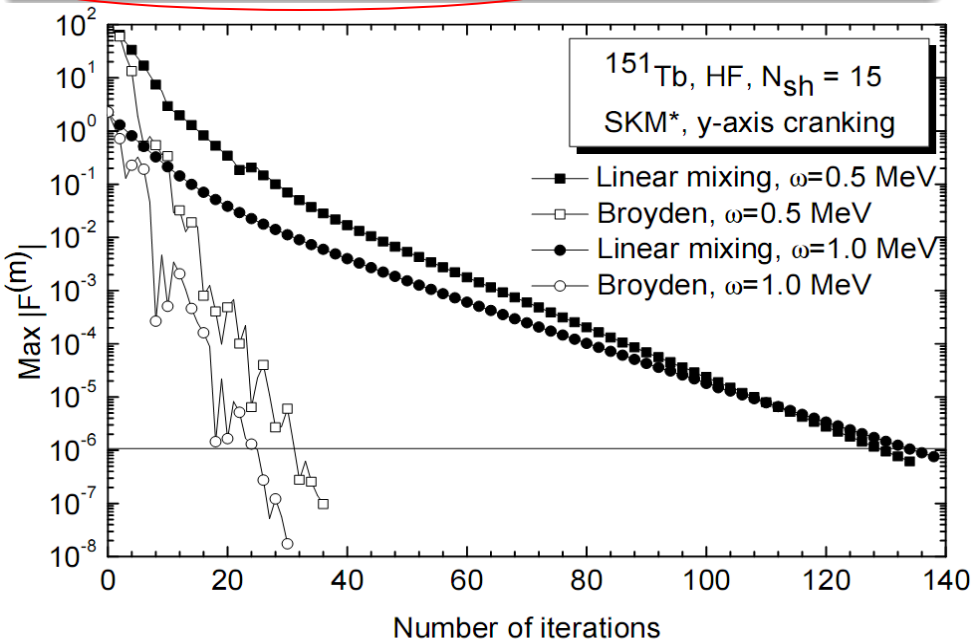
- Standard fits of functionals based on nuclear/neutron matter + doubly-magic closed shells nuclei ⇒ Can not constrain time-odd terms (among others)
- Local gauge invariance of HFB wave-function fixes C^T $(=-C^J)$, C^j $(=-C^\tau)$ and $C^{\nabla j}$ $(=+C^{\nabla J})$ - Also implies Galilean invariance of Skyrme interaction
- Genuine Skyrme functionals imply all C^s, $C^{\Delta s}$, C^T, C^j and $C^{\nabla j}$ are uniquely determined from the parameters of the interaction
- Varying C^s and $C^{\Delta s}$ implies Skyrme-like, gauge-invariant energy functionals

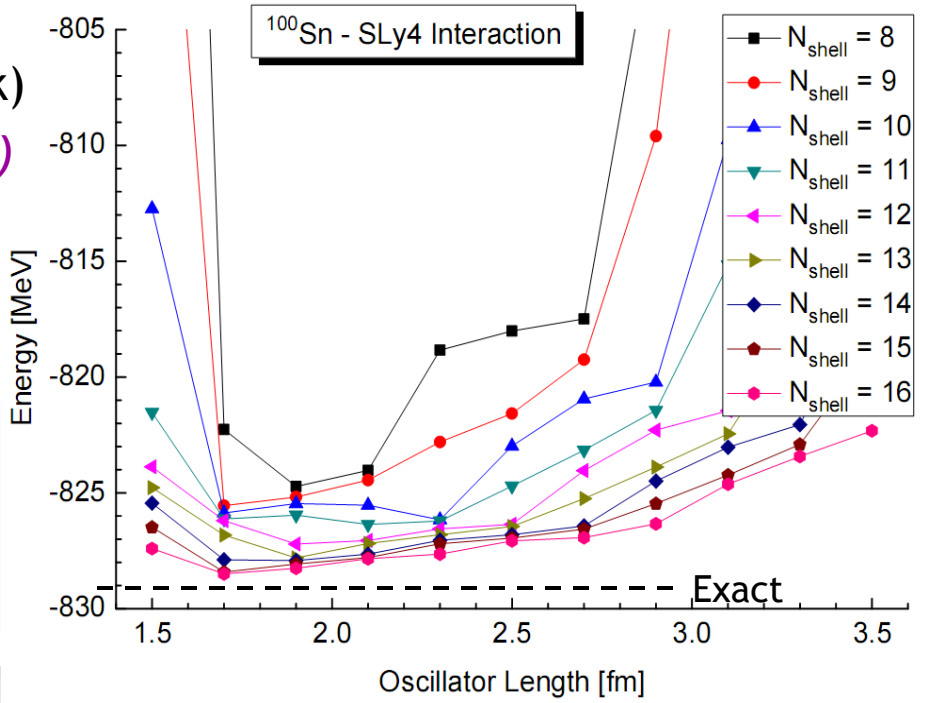
DFT Solver: HFODD

- Modified Broyden Method (see Mario's talk)
- *Optimization of Broyden (see Jorge's talk)*
- New features:
  - Isospin projection (W. Satuła)
  - Exact Coulomb exchange (J. Dobaczewski)

Improving the calculations (DFT Group + J. More, J. Sarich)

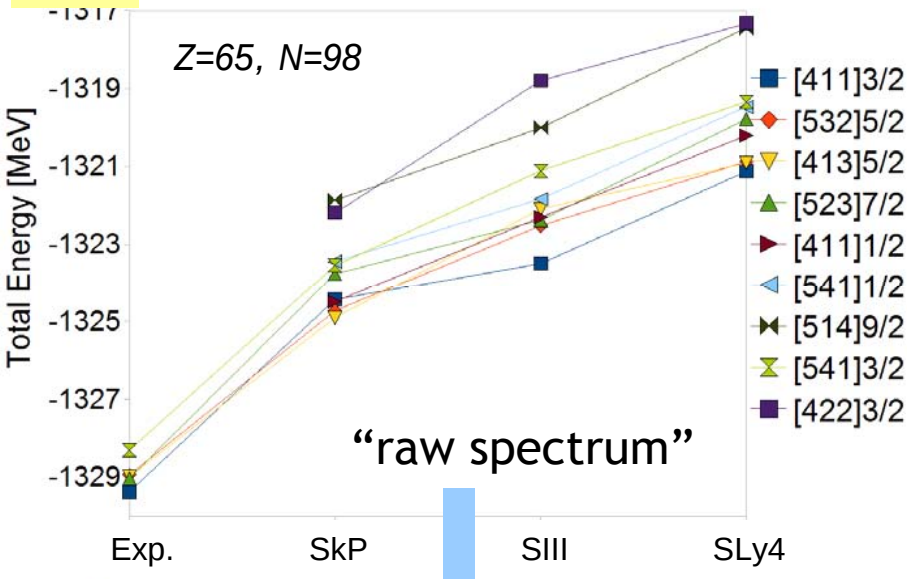
- Optimization of single-processor mode to decrease the time of calculation and cope with Jaguar policies
- Better MPI architecture with "on-the-fly" monitoring to avoid dead-times and idle processors
- Interfacing HFODD with (published) axial code HFB-THO for warm-starting
- Optimization of constrained calculations

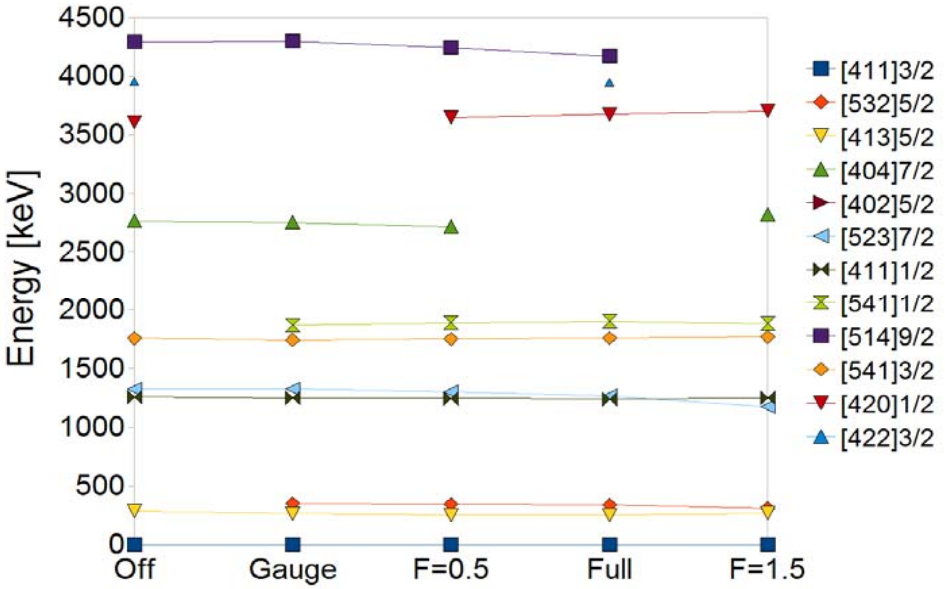




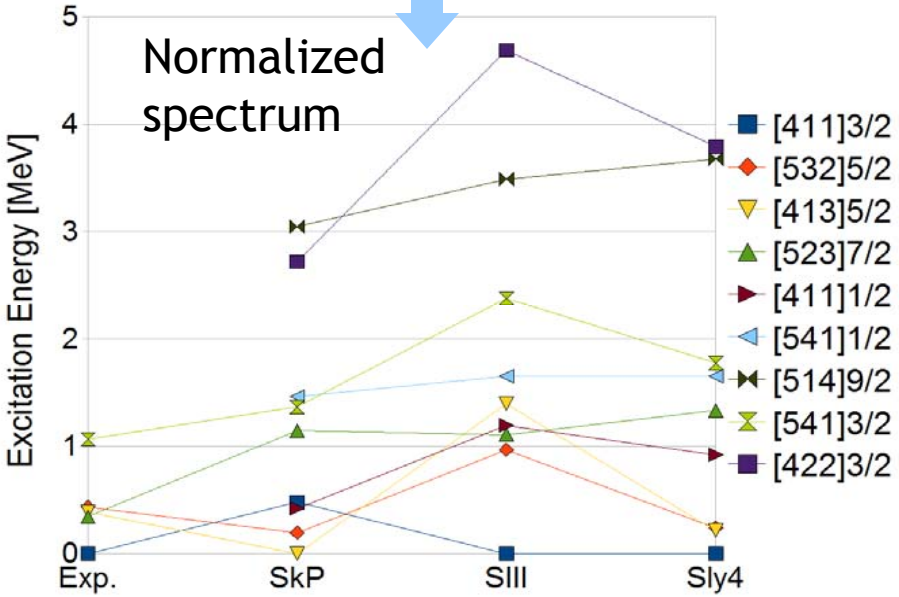
- Truncation scheme: dependence of results on N_{shell}, $\hbar\omega$, deformation of the basis (see NCSM, CC, SM, etc.)
- Reference provided by HFB-AX (Pei, see Mario's talk)
- Error estimate for given model space ⇒ give theoretical error bars

Effects of Time-odd Fields





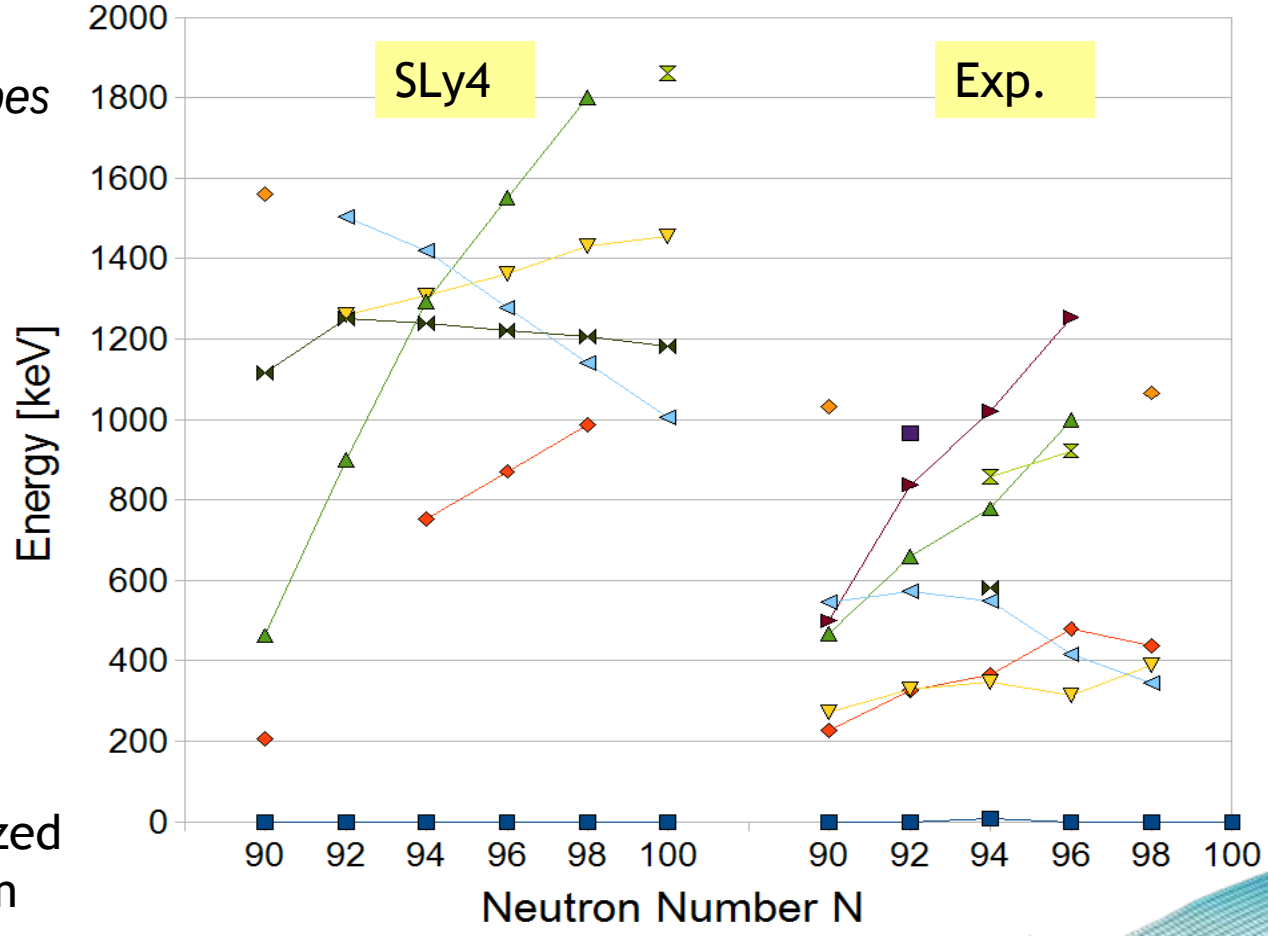
Z=65, N=96 – SLy4 Interaction



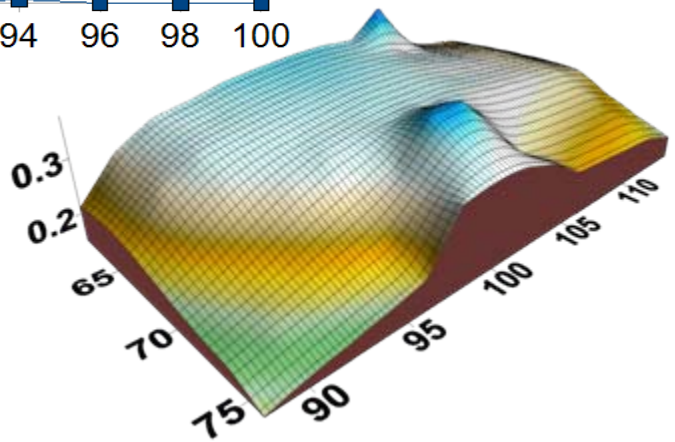
- Effect of time-odd fields of ~ 100 keV (maximum) on q.p. spectra
- Deformation, pairing, interaction far more crucial
- Induced effects (triaxiality) can only be accounted for by symmetry-unrestricted codes

Systematic of Odd-Mass Nuclei

Ho Isotopes (Z=67)



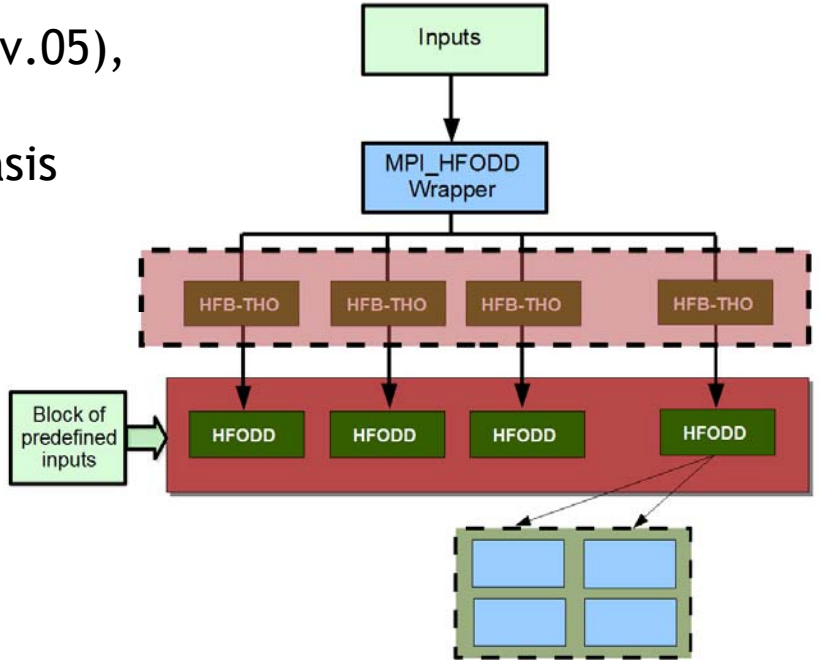
Normalized spectrum



Scale: 10,000+ processors for 5 hours: ~30 blocked configurations, number of interactions $1 \le N \le 24$, ~100 isotopes, optional scaling of time-odd fields

Parallel Wrapper: MPI-HFODD

- HFODD: solves the symmetry-unrestricted HFB problem with Skyrme-like functionals in the deformed, Cartesian, y-simplex conserving, HO basis
- MPI-HFODD version 08:
  - Fully modular Fortran 90 interface
  - HFODD core plus parallel interface with master/slave architecture
  - About 1.2 Gflops/core on Jaguar (before upgrade) and 2 GB memory/core required for standard calculations (~ 1000x1000 matrices)
- Implemented:
  - Various calculation mode: blocking (v.05), pairing fit (v.06), mass table (v.07), fission (v.07), convergence of the basis (v.08)
  - Automatic restart allows re-use of previous set of calculation (v.07)
  - Standard constrained/released HFB introduced (v.07)
  - Full Broyden method (v.08)
  - Automated post-processing scripts



Interface HFB-THO/HFODD

- Restarting HFODD from HFB-THO means:
  - Tremendous gain in time of calculation
  - Accrued numerical stability
  - Taking advantage of existing mass tables
- Procedure:
  - Coordinate + phase transformation (both unitary)
  - Modify HFODD to restart from HFB matrix elements instead of density fields on Gauss-Hermite mesh

Interface in alpha-phase (= it works but can not yet be used for production)

state:	1/2+[4,4,0]		1/2+[4,0,0]		3/2−[5,2,1]	
code:	HFBTHO	HFODD	HFBTHO	HFODD	HFBTHO	HFODD
N_0	14	14	14	14	14	14
$N_{\rm st}$	680	680	680	680	680	680
$b_\perp = b_z$	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697
$E_{\rm qp}$	1.007644	1.008	1.611961	1.612	1.388951	1.387
λ_n	−7.749566	−7.7494	−7.696179	−7.6962	−7.972801	−7.9742
$E_n^{\rm pair}$	−9.294443	−9.2964	−10.397019	−10.3983	−8.703141	−8.7035
Δ_n	1.057516	1.0576	1.120611	1.1207	1.037402	1.0373
r_t	4.689535	4.6895	4.690459	4.6905	4.689510	4.6895
β	−0.025699	−0.0256	0.000000	0.0001	0.015789	0.0147
Q_t	−0.862706	−0.8604	0.000000	0.0036	0.530038	0.4921
$E_n^{\rm kin}$	1360.437867	1360.442751	1362.407077	1362.409601	1358.912567	1358.886614
$E_p^{\rm kin}$	827.317590	827.317961	827.123364	827.123676	827.195176	827.191207
$E_{\rm SO}$	−50.483676	−50.485916	−50.922860	−50.923940	−49.607742	−49.592026
$E_{\rm dir}$	365.743676	365.743774	365.621013	365.621031	365.736277	365.735680
$E_{\rm tot}$	−1024.707275	−1024.707272	−1024.301233	−1024.301252	−1024.415866	−1024.416901

HFB-THO: Axial

Cylindrical coordinates

Time-reversal symmetry

j-block diagonalization

HFODD: symmetry-unrestricted

Cartesian coordinates

Y-simplex eigenbasis

No time-reversal symmetry

Full diagonalization

Are We On Track ?

Improving the calculations (DFT Group + J. More, J. Sarich)

- Optimization of single-processor mode to decrease the time of calculation and cope with Jaguar policies *Done*
- Better MPI architecture with "on-the-fly" monitoring to avoid dead-times and idle processors *Partly Done*
- Interfacing HFODD with (published) axial code HFB-THO for warm-starting *Done*
- Optimization of constrained calculations *Done*

Systematics of odd nuclei (DFT Group)

- Regional mass tables *Done*
- Benchmarking of current existing interactions *Done*
- Systematics of one quasi-particle states in nuclei *Done*
  - Full HFB Theory
  - Genuine Blocking
  - Unrestricted shapes

Construction of a Minimizer (DFT Group)

- Construction of a χ^2 function of the C parameters of the functional

$$\xi^2 = \sum_{\text{nuclei}} \sum_{\text{observables } i} w_i (O_i^{exp} - O_i^{the})^2$$

Partly Done, See Witek's talk

- Determination of the observables O_i and of the weights w_i

Work Plan (Year 2-3)

- Have a DFT package combining HFB-THO and HFODD available for large-scale calculations
- *Optimize full diagonalization of "large" (4,000 × 4,000) matrices in HFODD*
  - *Take advantage of N-core architecture*
  - *Increase speed for large bases (fission, heavy nuclei)*
  - *Overcome current memory limitations*
- *Optimize Broyden method (Cf. Jorge's talk) to improve stability/convergence*
- *ALDB ? (Fission pathways, blocked states vs. experimental q.p. energy, etc.)*

Open Question to CS: (How) Can We Parallelize a Self-Consistent Iterative Process ?

Deliverables for next year (strictly related to studies of odd-mass nuclei)

- Paper 1 on odd nuclei: Methodology and Theoretical Models
  - Demonstrate fine-tuning role of time-odd terms
  - Benchmark equal-filling approximation against exact blocking
- Paper 2 on odd nuclei: Systematic and comparison with experiment
  - Deformed rare-earth
  - Deformed actinides

Work Plan (Year 4-5)

Years 4 and 5 should be devoted to the determination of new functionals

- *Choice, implementation and optimization of parameter estimation techniques*
- *Error estimate and propagation: how reliable is our functional ?*
- Link DFT package (HFB-THO/HFODD) to minimization codes
- The following experimental observables require, to some extent, symmetry-unrestricted codes (see Witek's talk):
  - Fission barriers (triaxiality, parity-breaking)
  - $V_{pn}(Z,N) = 0.5 * [B(Z,N) - B(Z,N-2) - B(Z-2,N) + B(Z-2,N-2)]$,
  - 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 (cranking, time-odd)
  - 1q.p. excited states of odd-mass heaviest elements
- Observation that time-odd terms seem negligible for q.p. spectra imply that fitting strategy may have to be built on two-steps approach
  - First class of χ^2 functions based on (large) subset of experimental data and involving HFBTHO mode
  - Second class for fine-tuning time-odd coupling constants (involving HFODD mode)