Building a Universal Nuclear Energy Density Functional

nn , nnn interactions:
AV-18, Vlow-k , EFT

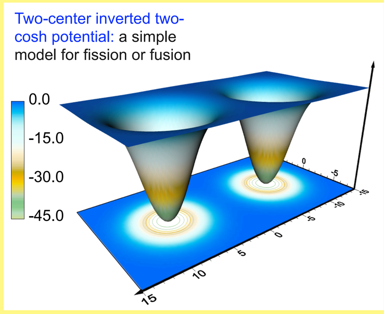
ab initio theory of light nuclei(A<=16)
coupled cluster, no core shell model, Green's function Monte Carlo

density functional theory (A>16)
global properties

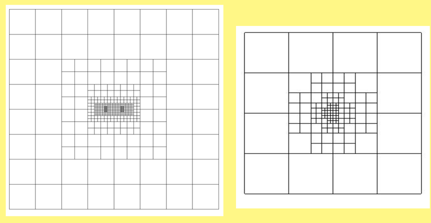
dynamic extensions of density functional theory
LACM, QRPA, TDDFT
level densities

low energy reaction theory
Hauser - Feshbach, Feshbach-Kerman-Koonin
fusion / fission processes
masses , energy distributions

Viewing The Nucleus -Like A Jpeg Picture !



The jpeg picture format is based on the use of wavelet-based techniques to optimize compression. Adaptive 3D multiresolution methods based on wavelet expansions have been applied to describe the structure of atoms and molecules within the MADNESS framework.

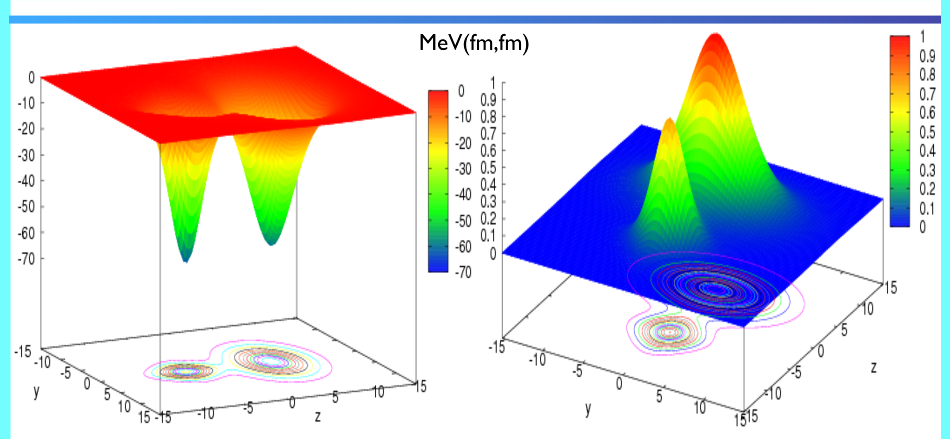


Adaptive support of basis functions. A 2-D slice of the 3-D multiresolution approximation of the inverted two-cosh potential with spin-orbit term (left) and the adaptive support of one of the 3-D wave functions (right).

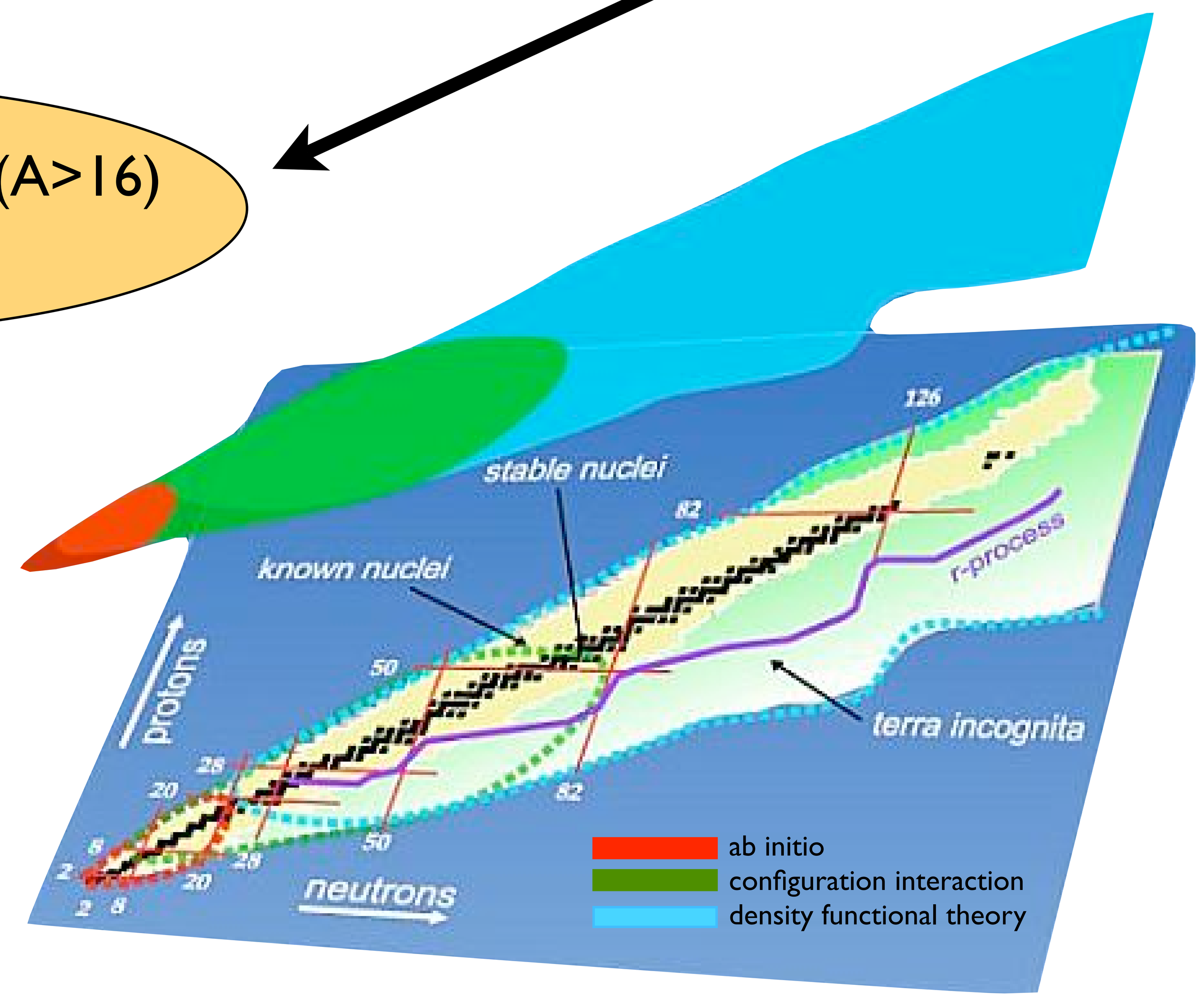
Nuclear physicists, applied mathematicians and computer scientists have applied the MADNESS framework to solve a number of problems within the nuclear energy density functional theory.

MADNESS makes it possible to treat, in a unique formalism and with a user-defined accuracy, a plethora of nuclear phenomena as diverse as fission and fusion, involving extremely elongated shapes and evolving topologies, as well as spatially extended halo systems, and superfluidity.

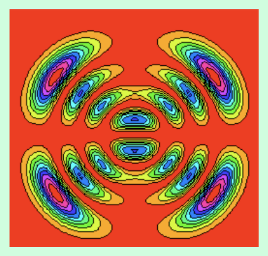
Lattice (sinc) Density Functional Theory Solver $



particle-hole (p-h) potential pairing (p-p) potential



Frontier Nuclear Science Enabled by SciDAC *

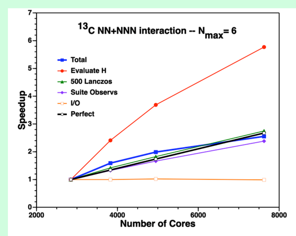


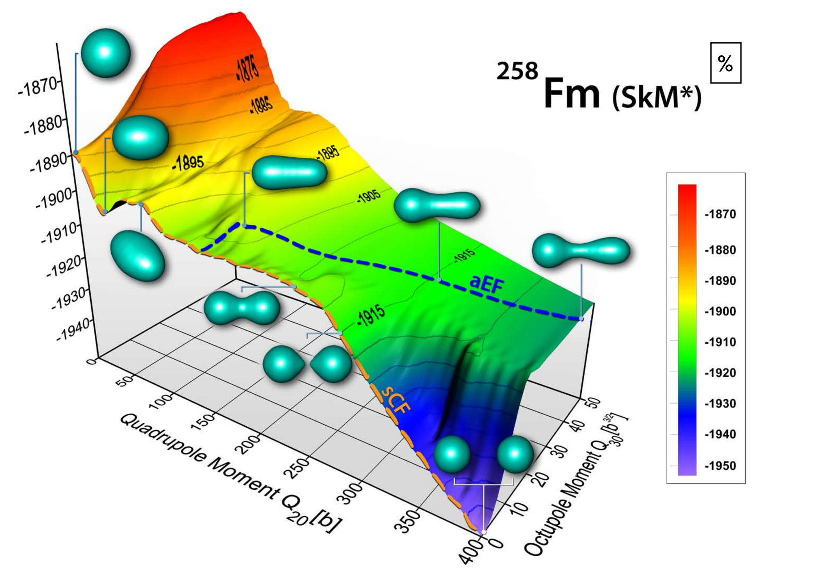
Exotic nuclei with atomic number 14, not previously discovered but important for stellar processes, are predicted to exist for short life-times through advanced simulations using MFDn, a parallel code for configuration interaction modeling in a harmonic oscillator basis (see fig. on left).

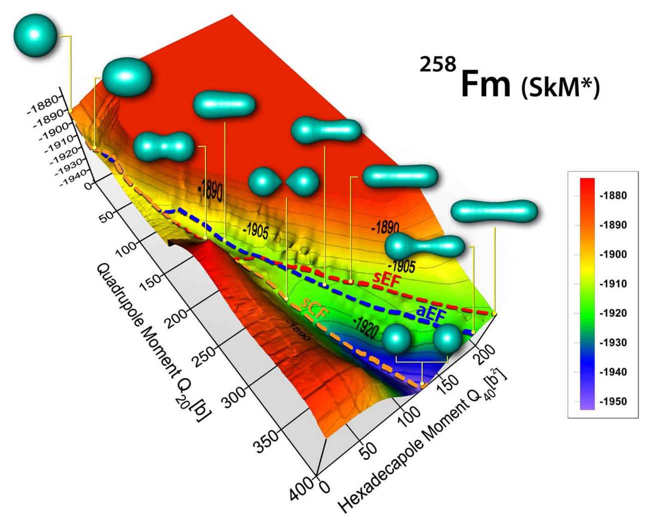
Collaboration among Physics, Applied Mathematics, and Computer Science enabled the simulations through critical improvements in MFDn by a factor of 4-6 on the Cray XT4, equivalent of 3-5 years of progress in computing hardware.

Improvements in MFDn include new data structures, new parallel blocking and combinatorial algorithms, and enhanced inner loop and I/O performance.

Computing the 10 lowest eigenstates using the improved MFDn for ^{14}F requires 3 hours on 30,628 Cray XT-4 nodes at ORNL. This would have taken at least 18 hours using previous versions of MFDn.







$$\hat{H}\Psi(\vec{x}) = E\Psi(\vec{x}) \qquad \Psi(\vec{x}) = \{\psi_n(\vec{x})\}\forall n$$

$$\hat{H} = \begin{pmatrix} \hat{h}(\vec{x}) & \hat{\Delta}(\vec{x}) \\ -\hat{\Delta}^\dagger(\vec{x}) & -\hat{h}^*(\vec{x}) \end{pmatrix} \qquad \hat{\Delta}(\vec{x}) = \begin{pmatrix} 0 & \Delta(\vec{x}) \\ -\Delta(\vec{x}) & 0 \end{pmatrix}$$

$$\psi_n(\vec{x}) = \begin{pmatrix} u_n(\vec{x}) \\ v_n(\vec{x}) \end{pmatrix} \quad u_n(\vec{x}) = \begin{pmatrix} u_{n,\uparrow}(\vec{x}) \\ u_{n,\downarrow}(\vec{x}) \end{pmatrix} \quad v_n(\vec{x}) = \begin{pmatrix} v_{n,\uparrow}(\vec{x}) \\ v_{n,\downarrow}(\vec{x}) \end{pmatrix}$$

$$\hat{h}(\vec{x}) = \begin{pmatrix} -\vec{\nabla}\cdot(\frac{\hbar^2}{2m_\uparrow(\vec{x})}\vec{\nabla}) + U_\uparrow(\vec{x}) - \mu_\uparrow & 0 \\ 0 & -\vec{\nabla}\cdot(\frac{\hbar^2}{2m_\downarrow(\vec{x})}\vec{\nabla}) + U_\downarrow(\vec{x}) - \mu_\downarrow \end{pmatrix} - i\hbar(\vec{\sigma}\times\vec{W}(\vec{x}))\cdot\vec{\nabla}$$

$$E_{gs} = \int\{\epsilon_{normal}[\rho_n(\vec{x}),\rho_p(\vec{x})] + \epsilon_{superfluid}[\rho_n(\vec{x}),\rho_p(\vec{x}),\nu_n(\vec{x}),\nu_p(\vec{x})]\}d^3x$$

$$\epsilon_{superfluid}[\rho_n,\rho_p,\nu_n,\nu_p] = g(\rho_p,\rho_n)[|\nu_p|^2+|\nu_n|^2] + f(\rho_p,\rho_n)[|\nu_p|^2-|\nu_n|^2]\frac{\rho_p-\rho_n}{\rho_p+\rho_n}$$

$$\epsilon_{normal}[\rho_n(\vec{x}),\rho_p(\vec{x})] = \epsilon_{normal}[\rho_p(\vec{x}),\rho_n(\vec{x})] \quad g(\rho_p,\rho_n) = g(\rho_n,\rho_p), f(\rho_p,\rho_n) = f(\rho_n,\rho_p)$$

Superfluid Local Density Approximation Applied to Nuclei : a time dependent extension of density functional theory

(Invited Session: A. Bulgac , K. Roche) [special thanks to Y.Yu]

$$i\hbar\partial_t\begin{pmatrix} u_n(\vec{x},t) \\ v_n(\vec{x},t) \end{pmatrix} = \begin{pmatrix} \hat{h}(\vec{x},t) + \hat{V}_{ext}(\vec{x},t) & \hat{\Delta}(\vec{x},t) + \hat{\Delta}_{ext}(\vec{x},t) \\ \hat{\Delta}^\dagger(\vec{x},t) + \hat{\Delta}^\dagger_{ext}(\vec{x},t) & -\hat{h}(\vec{x},t) - \hat{V}_{ext}(\vec{x},t) \end{pmatrix}\begin{pmatrix} u_n(\vec{x},t) \\ v_n(\vec{x},t) \end{pmatrix}$$

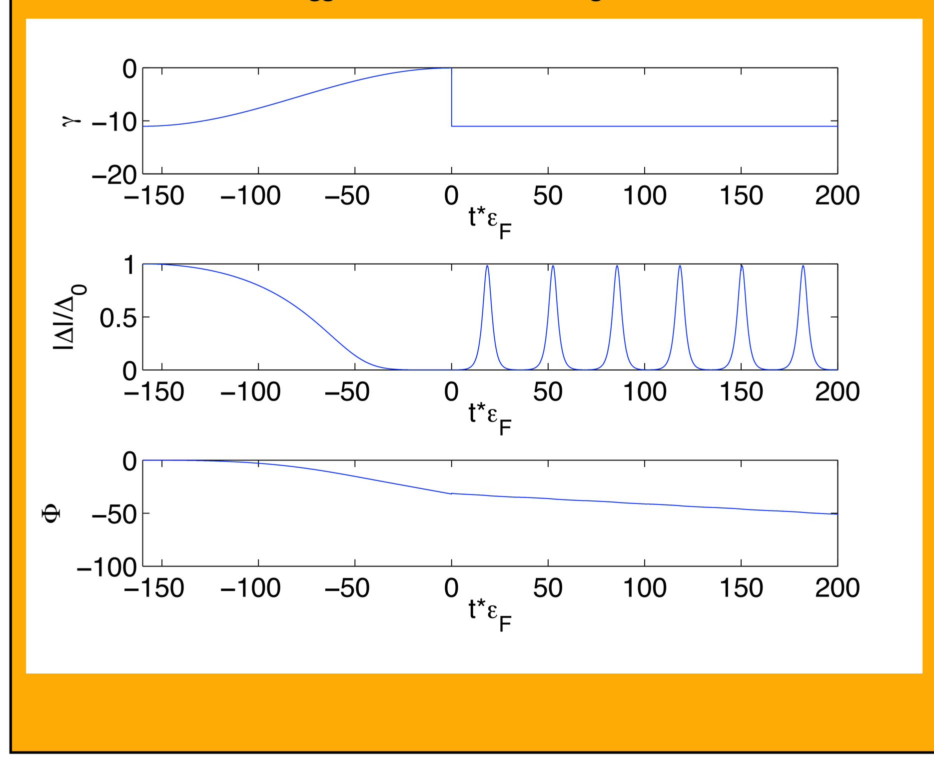
$\psi_n(\vec{x},t) \sim O(4\times N^3)$ $\quad N \in [50,100]$ ~ Number of quasiparticle functions

$[10^3, 10^5]$ ~ Number of time steps per nucleus

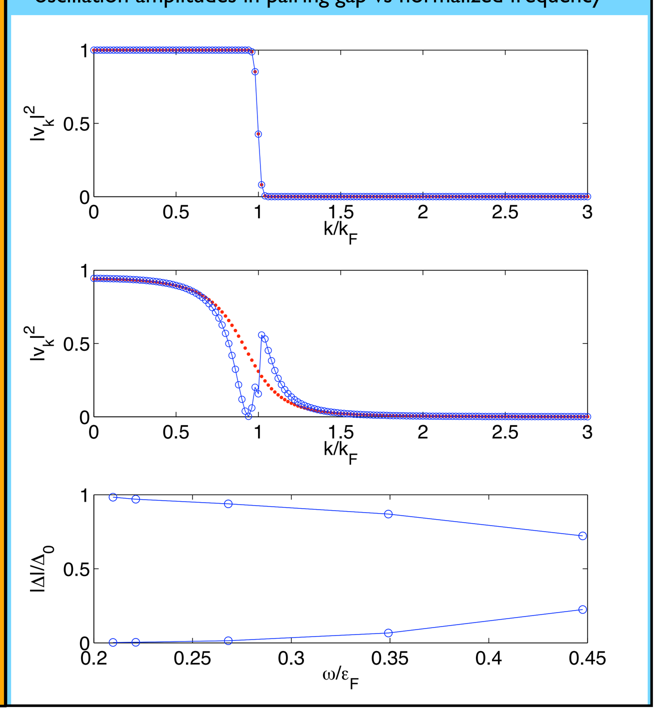
Computation of Observables $\quad Q(\omega) = \sum_\sigma \int Q(\vec{x},\sigma,t)\rho(\vec{x},\sigma,t)e^{i\omega t}d^3x dt$

Remarkable example of LACM using the time dependent lattice technique: homogeneous unitary Fermi gas [special thanks to S.Yoon]

Higgs Mode of the Pairing Field



(top two)oscillation between almost normal state and superfluid state and corresponding quasiparticle distribution, red is equilibrium state; (bottom)maximum and minimum oscillation amplitudes in pairing gap vs normalized frequency



- •all nuclei (even, odd, spherical,deformed)
- •any quantum numbers of (Q)RPA modes
- •fully self-consistent and no imposed symmetries
- •probe excited state properties of nuclei
- •new space-time lattice code, designed with lattice dft solver$ connection
- •plave wave basis, discrete Fourier transforms (FFTW) for gradients, derivatives
- •multi-step (predictor-modifier-corrector) time algorithm , O(h^5)
- •numerically conserved constants of the motion
- •Fortran and C versions fully consistent
- •same codes run on laptop (no MPI) or parallel (w/MPI) computers
- •out-of-core version exists in C language

Outstanding Computational Scaling Properties : Cray XT4 National Center for Computational Sciences - ORNL

STRONG SCALING EXAMPLE

N^3 = 30^3

PEs (jaguarcnl)	576	1152	1728	2304
<NWF / PE>	48	24	16	12
[s]/ts	56.2	28.8	19.3	14.92 (14.05)

N^3 = 40^3

PEs (jaguar)	942 (x4)	1884(x4)	2826(x4)	3768(x4)
<NWF/PE>	70	36	24	17
[s] / 10 time steps	296.15	153.31	103.17	77.02 (74.03)
Total INS	7.87635E+14	8.15353E+14	8.15732E+14	8.10577E+14
max(INS(PE))	8.38278E+11	4.25906E+11	2.83689E+11	2.13813E+11
Total FLOP	1.84227E+14	1.84997E+14	1.85766E+14	1.86536E+14
max(INS(FLOP))	1.9578E+11	99655061696	66696994580	50218692684

WEAK SCALING EXAMPLE

N^3	30^3	40^3	50^3
quasiparticles	28288	66796	130528
PEs	168(x4)	942(x4)	3626(x4)
[s] / 10 time steps	297.31	296.15	319.03
Total INS	1.41538E+14	7.87635E+14	3.13385E+15
Total FLOP	3.3787E+13	1.84227E+14	8.22772E+14
Total BYTES	5.37701E+11	3.00957E+12	1.14865E+13
t(50^3)/t(40^3) = 1.077	PE/PE=3.849	INS/INS=3.97	FLOP/FLOP=4.46
t(50^3)/t(30^3) = 1.073	PE/PE=21.583	INS/INS=22.14	FLOP/FLOP=24.35
t(40^3)/t(30^3) = .996	PE/PE=5.607	INS/INS=5.564	FLOP/FLOP=5.45

Out-of-Core (OOC) Variant to Manage Memory Demand

N^3	Quasiparticles	BYTEs	BYTEs (OOC)
30^3	28288	5.37701E+11	44280000
40^3	66796	3.00957E+12	104960000
50^3	130528	1.14865E+13	205000000
60^3	226156	3.43902E+13	354240000
70^3	359056	8.6702E+13	562520000
80^3	535516	1.93026E+14	839680000
90^3	763824	3.92007E+14	1195560000
100^3	1046604	7.36809E+14	1640000000
110^3	1393008	1.30528E+15	2182840000
120^3	1808172	2.19966E+15	2833920000
130^3	2299056	3.55592E+15	3603080000

60x60x60 ~ current in-core problem size limit on Cray XT4 at ORNL

! , G. Fann et al
$, P. Magierski et al
%, W. Nazarewicz et al
*, J. Vary, E. Ng et al

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