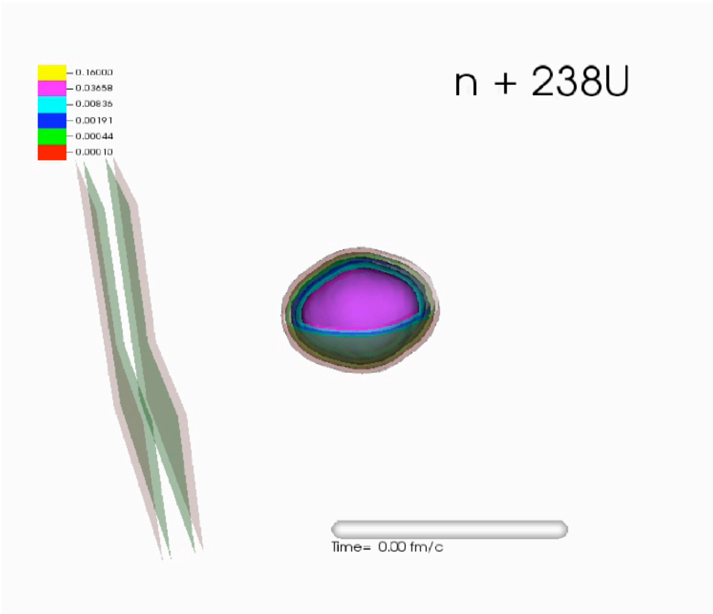
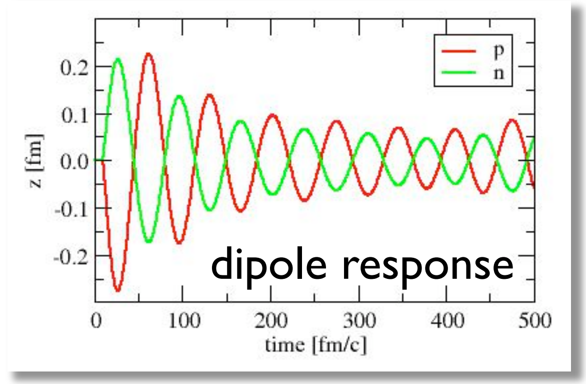




TIME-DEPENDENT APPROACH TO NUCLEAR SYSTEMS

IONEL STETCU
DEPARTMENT OF PHYSICS
UNIVERSITY OF WASHINGTON

Collaborators: A. Bulgac, M.M. Forbes, P. Magierski, Y.-L. (Alan) Luo, K.J. Roche
C. Bertulani and K. Nakatsukasa

UNEDF meeting, Lansing, June 2011

Funding

◆ DOE Grants DE-FG02-07ER41457 (SciDAC-UNEDF) and DE-FG02-97ER41014 (UW NT group)

◆ 40 million CPU hrs. FY 2010 DOE/ASCR Joule Metric on Computational Effectiveness (used ~70 million CPU hrs on jaguarpf.ccs.ornl.gov)

◆ NSF: hyak.washington.edu

◆ DOE: franklin.nersc.gov, hopper.nersc.gov (+5 million CPU hrs)

TD formalism applications

- Nuclear physics:
  - induced fission
  - heavy-ion collisions
  - neutron scattering/capture
  - pairing vibrations
  - electromagnetic response
- Neutron star crust: dynamics of vortices, vortex pinning mechanism
- Cold atoms physics, optical lattices

Limitations:

- only one-body observables can be described accurately
- the results depend on how good the functional is
- large computational resources necessary

RPA and linear response

RPA: small correlations on top of mean-field + excited states 1p-1h

$$|\psi_0\rangle = |HF\rangle + |2p-2h\rangle$$

$$|\nu\rangle \approx |1p-1h\rangle$$

$$\langle\nu|F|\psi_0\rangle = \sum_{ph}(F_{hp}X^{\nu}_{ph} + F_{ph}X^{\nu}_{ph})$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = E_\nu \begin{pmatrix} X_\nu \\ -Y_\nu \end{pmatrix}$$

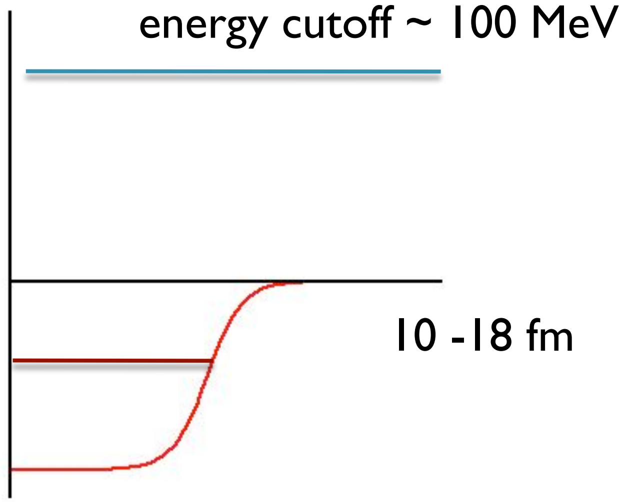
- violates the Pauli principle mainly for non-collective states
- separates the spurious states associated w/ broken symmetry in mean field

Linear response from TD-DFT: e... ly a mod... xcited states

$$i\hbar\dot{\rho} = [h[\rho] + f(t), \rho] \longrightarrow \left\{ \left(\cdots A^* \right) \cdots \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} \delta\rho^{ph} \\ \delta\rho^{hp} \end{pmatrix} = -\begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

- Pauli principle preserved
- separates the spurious states associated w/ broken symmetries in mean field
- description of s.p. excitations

Challenges for QRPA



HF: #s.p. states = # particles

HFB: #q.p. >> # particles
~ 2,500

QRPA: dimension ~ (# q.p.)^2 ~ 10^7

very difficult for today's computers:
- non-Hermitian matrix
- middle of the spectrum

Terasaki and Engel, PRC **82** (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
dimension ~ 160,000 (j-dependent)

in TDHFB: $$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} \approx \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \exp(-iEt) + \begin{pmatrix} \delta u(t) \\ \delta v(t) \end{pmatrix}$$

# of evolved wfs. = # of q.p.
numerical advantage: can be easily parallelized

need latest generation computers to run

QRPA and TD

	QRPA	TD-SLDA
Dimensions	# qp. squared	# qp
Truncation	identification of spurious states difficult	N/A
Galilean invariance	(usually) not implemented	trivial (in functional)

Terasaki and Engel, PRC **82** (2010) 034326
QRPA w/ axial symmetry for ^{172}Yb
Energies of spurious states: 0.3 – 1.5 MeV

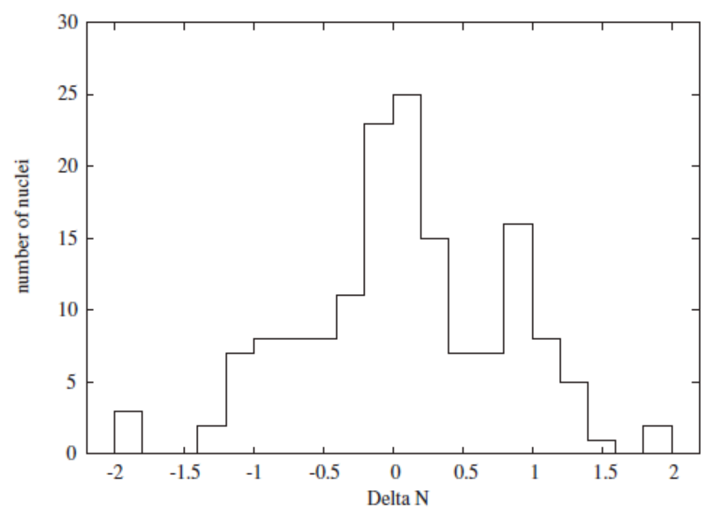


FIG. 1. Particle-hole character of the lowest 2^+ solutions. The histogram displays the quantity ΔN defined in Eq. (1) for 155 nuclei in the SLy4 data set (one of which we drop—see text). The values $-2, 0, +2$ correspond to excitations of hole-hole, particle-hole, and particle-particle character, respectively.

Terasaki, Engel, Bertsch, PRC **78** (2008) 044311

Induced fission

PHYSICAL REVIEW C VOLUME 17, NUMBER 3 MARCH 1978

Dynamics of induced fission*

J. W. Negele†
Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

S. E. Koonin†
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125

P. Möller‡ and J. R. Nix
Theoretical Division, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87545

A. J. Sierk†
W. K. Kellogg Radiation Laborat
and Theoretical Division, Los Alamos Scier

Induced fission of ^{236}U is calculated
reflection symmetry and omitting the
the appropriate initial condition an
calculations. Although dynamic mea
predicted observables are consistent v
with macroscopic models indicate th
observables similar to those of the me
fundamentally different.

VI. SUMMARY AND CONCLUSIONS

Subject to the limitations of axial symmetry and the omission of the spin-orbit interaction, the time-dependent mean-field approximation has been successfully applied to the fission of ^{236}U. The resulting fission dynamics has all the expected qualitative features and, given the uncertainty in

Nuclear energy functionals

- Ab initio: DME (Negele, Vautherin, Furnstahl, Bogner, ...)
- Phenomenological functionals:

$$\mathcal{E}(\vec{r}) = \frac{1}{2M_n}\tau_n(\vec{r}) + \frac{1}{2M_p}\tau_p(\vec{r}) - \Delta(\vec{r})\nu_c(\vec{r})$$
$$+ \sum_{T=0,1} \Big(C_T^{\rho}\rho_T^2 + C_T^{\Delta}\rho_T\nabla^2\rho_T + C_\gamma\rho_0^\gamma\rho_T^2$$
$$+C_T^{\tau}(\rho_T\tau_T - \vec{j}_T^2) + C_T^{\nabla J}(\rho_T\vec{\nabla}\cdot\vec{J} + \vec{s}_T\times\vec{j}_T)\Big)$$

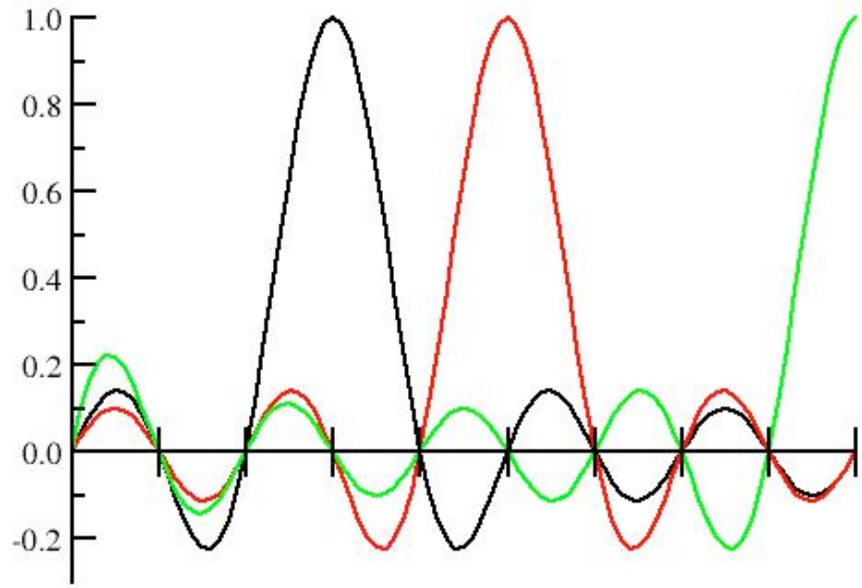
Galilean invariance

$$h(\vec{r}) = -\nabla\frac{\hbar^2}{2m(\vec{r})}\nabla + U(\vec{r}) + i\vec{\sigma}\cdot\vec{V}(\vec{r}) + i\vec{V}_1(\vec{r})\cdot\nabla + i\vec{W}(\vec{r})\cdot(\vec{\sigma}\times\nabla)$$

Discrete variable representation

1D basis states
on the lattice

$$\varphi_i(x) = \frac{1}{N} e^{-\frac{i\pi(x-x_i)}{Na}} \frac{\sin\frac{\pi(x-x_i)}{a}}{\sin\frac{\pi(x-x_i)}{Na}}$$



$$\begin{pmatrix} h_{++}-\mu & h_{+-} & 0 & \Delta \\ h_{-+} & h_{--}-\mu & -\Delta & 0 \\ 0 & -\Delta^* & \mu-h^*_{++} & -h^*_{+-} \\ \Delta^* & 0 & -h^*_{-+} & \mu-h^*_{--} \end{pmatrix} \begin{pmatrix} u_+ \\ u_- \\ v_+ \\ v_- \end{pmatrix} = E \begin{pmatrix} u_+ \\ u_- \\ v_+ \\ v_- \end{pmatrix}$$

dimension: 4 $N_x N_y N_z$

Largest calculation: 4x40x40x64=409,600 (~5 hrs on 217,800 cores on jaguarpf)

Lattice representation

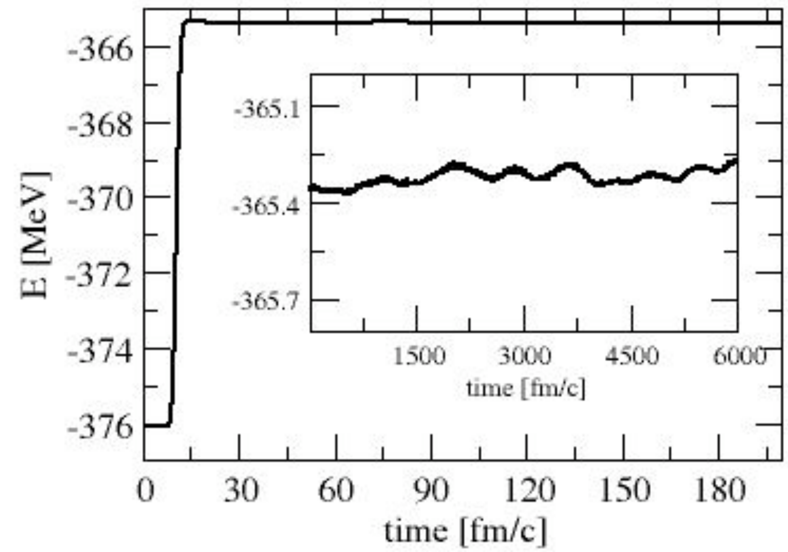
- quasiparticle wavefunctions represented on a lattice
- periodic boundary conditions
- N_x, N_y, N_z spatial points
- unrestricted deformation
- derivatives computed with FFT
- good description of the relevant DOF for E>0
- <u>(almost) unique ability to describe correctly all components of the quasiparticle wavefunctions</u>

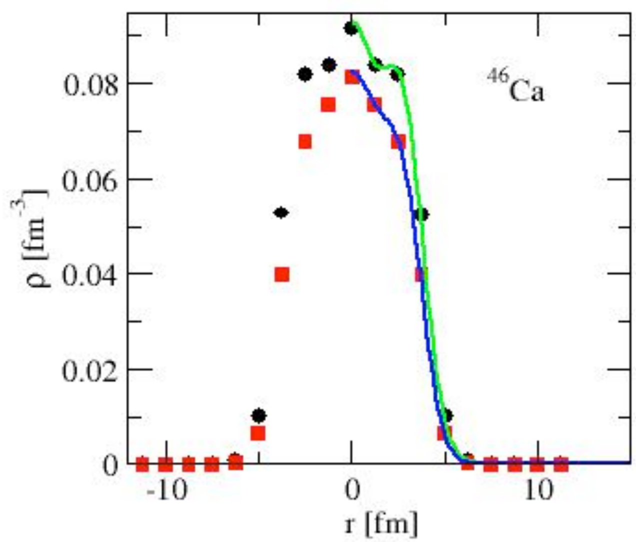
Codes: timeline and status

- 2006: TD code for unitary gas (Bulgac, Yu)
- 2007: TD for unitary gas, parallel version (Roche, Bulgac)
- 2009:
  - static solver (initial conditions) for unitary gas (Magierski, Luo, Roche and Bulgac)
  - production stage for unitary gas
  - nuclear TD code initial implementation, HFBRAD used for initial conditions (Stetcu, Roche, Bulgac)
  - static solver for trapped neutrons (Magierski)
  - static (semi-parallel) solver for protons and neutrons (Stetcu, Magierski)
- 2010:
  - static solver (f90) and interface with the TD code (Stetcu, Roche, Bulgac)
- 2011:
  - static solver C version (Stetcu)
  - production stage for even-even nuclei
  - dynamic solver C version (Stetcu): testing phase

Benchmarks

- tested simple solutions: KE only, KE+constant pairing, SO, etc.
- tested the solutions in the TD code: energy and number of particle conservation within expected numerical precision
- good agreement with HFBRAD for spherical systems





	μ_p (MeV)	μ_n (MeV)	E_{gs} (MeV)
^{30}Mg (SKP)			
HFBRAD:	-5.16	-14.51	-222.75
LATTICE:	-5.24	-14.35	-223.50
^{136}Xe (SLy4)			
HFBRAD:	-5.56	-8.02	-1101.70
LATTICE:	-5.91	-7.99	-1101.49

Current lattice implementation (TD)

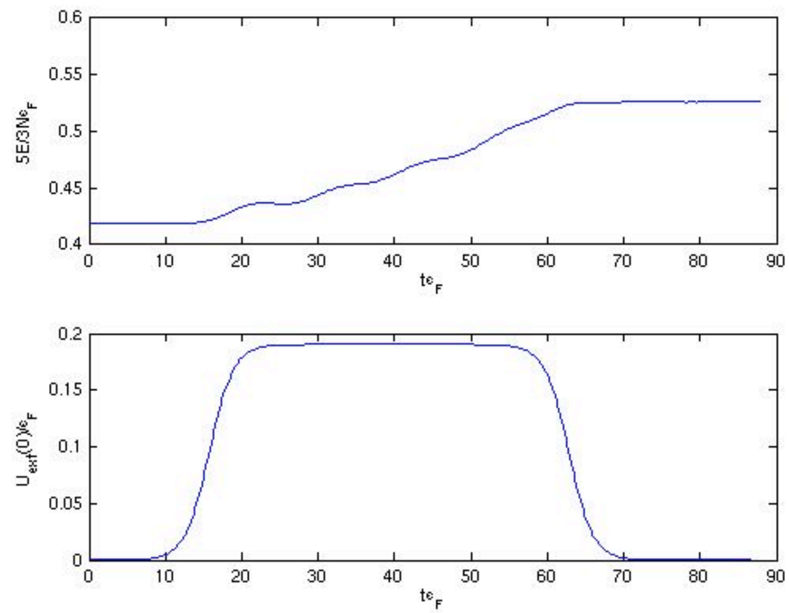
Unitary gas: A. Bulgac and K. Roche, J. Phys. Conf. Series **125** (2008) 012064

Time evolution realized with the multistep predictor-modifier-corrector Adams-Bashford-Milne (ABM) method:

✓ two applications of h per time step (few operations, does not involve matrix multiplication)

✓ fifth order method (very accurate)

✓ very stable numerically for long time intervals



Derivatives are calculated using FFTW

MPI implementation

Very efficient i/o for Check-Point Restart

Small-amplitude dynamics

Formalism

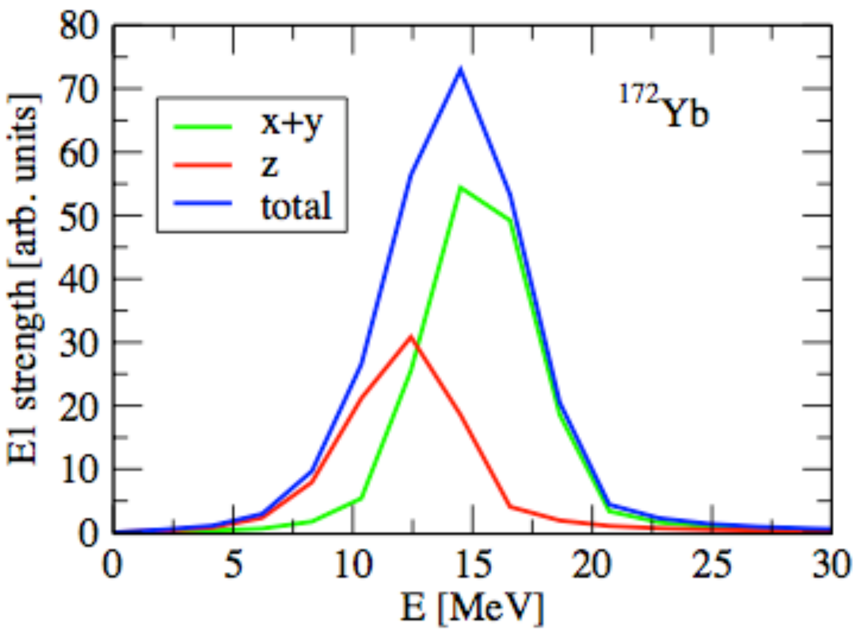
$$H_0\Psi(\vec{r}_1,\cdots,\vec{r}_A) = E_0\Psi(\vec{r}_1,\cdots,\vec{r}_A)$$

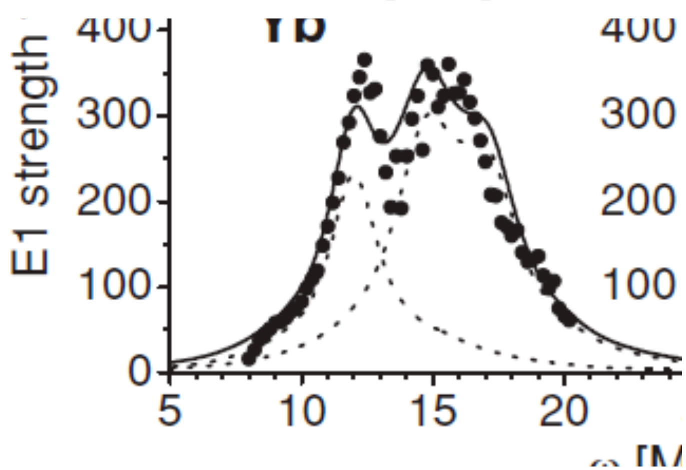
$$V_{ext}(\vec{r},t) = O(\vec{r})f(t)$$

$$\tilde{O}(\omega) = \int d^3r\, O^*(\vec{r})\,\delta\rho(\vec{r},\omega)$$

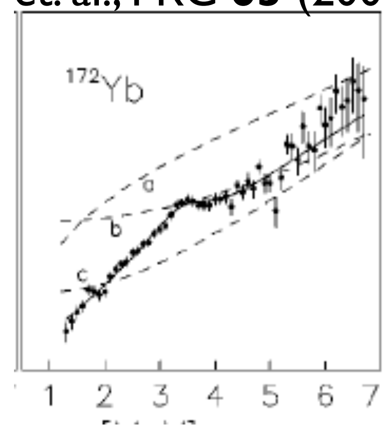
$$\boxed{S(\omega) = \sum_n |\langle\Psi_0|O|\Psi_n\rangle|^2\delta(\omega-\omega_n) = -\frac{1}{\pi}\Im\left(\frac{\tilde{O}(\omega)}{\tilde{f}(\omega)}\right)}$$

^{172}Yb dipole giant resonance

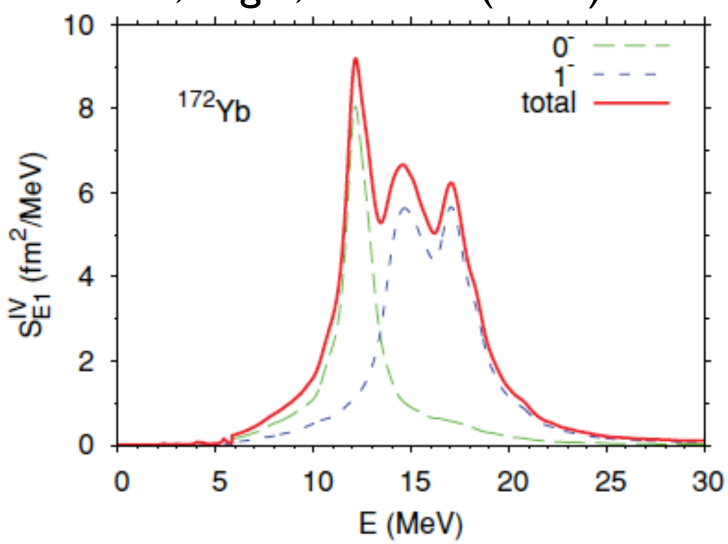




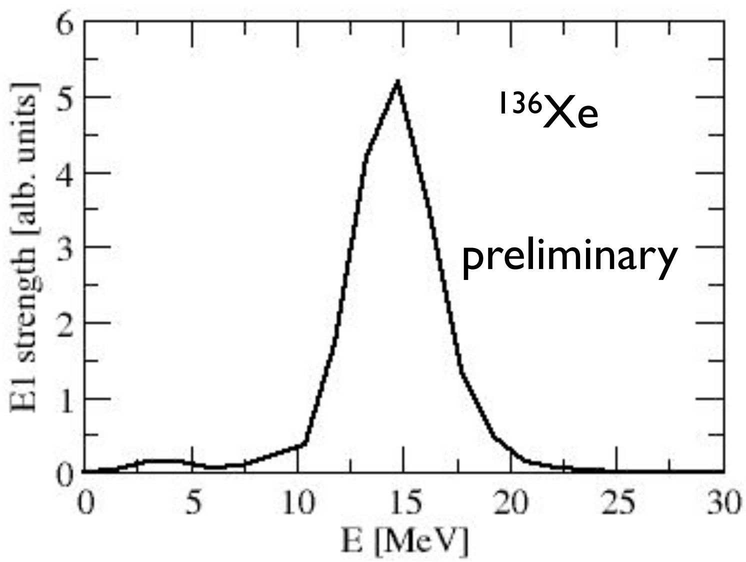
Voinov et. al., PRC **63** (2001) 044313

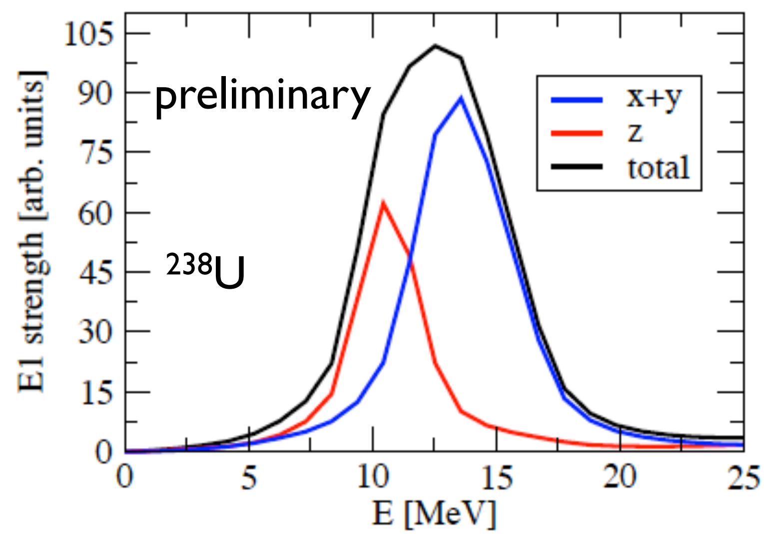


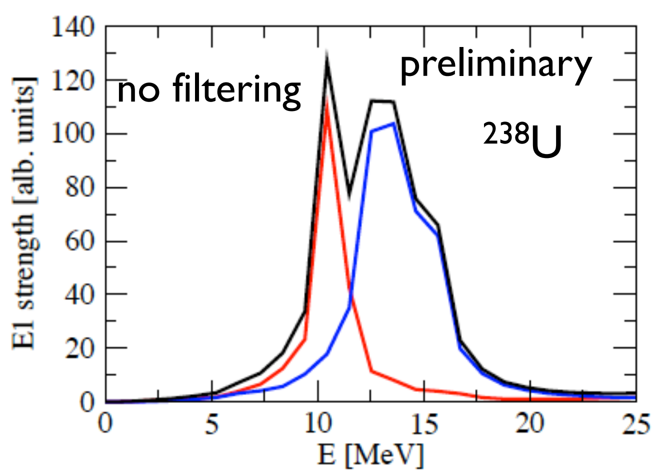
Terasaki, Engel, PRC **82** (2010) 03426

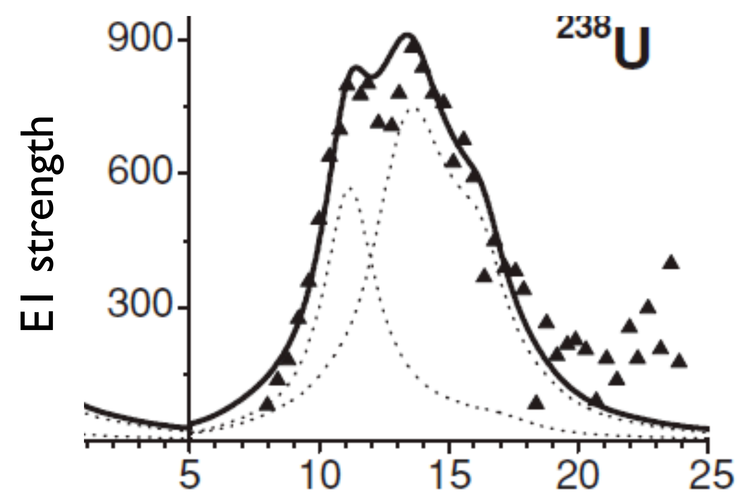


Dipole response ^{136}Xe and ^{238}U

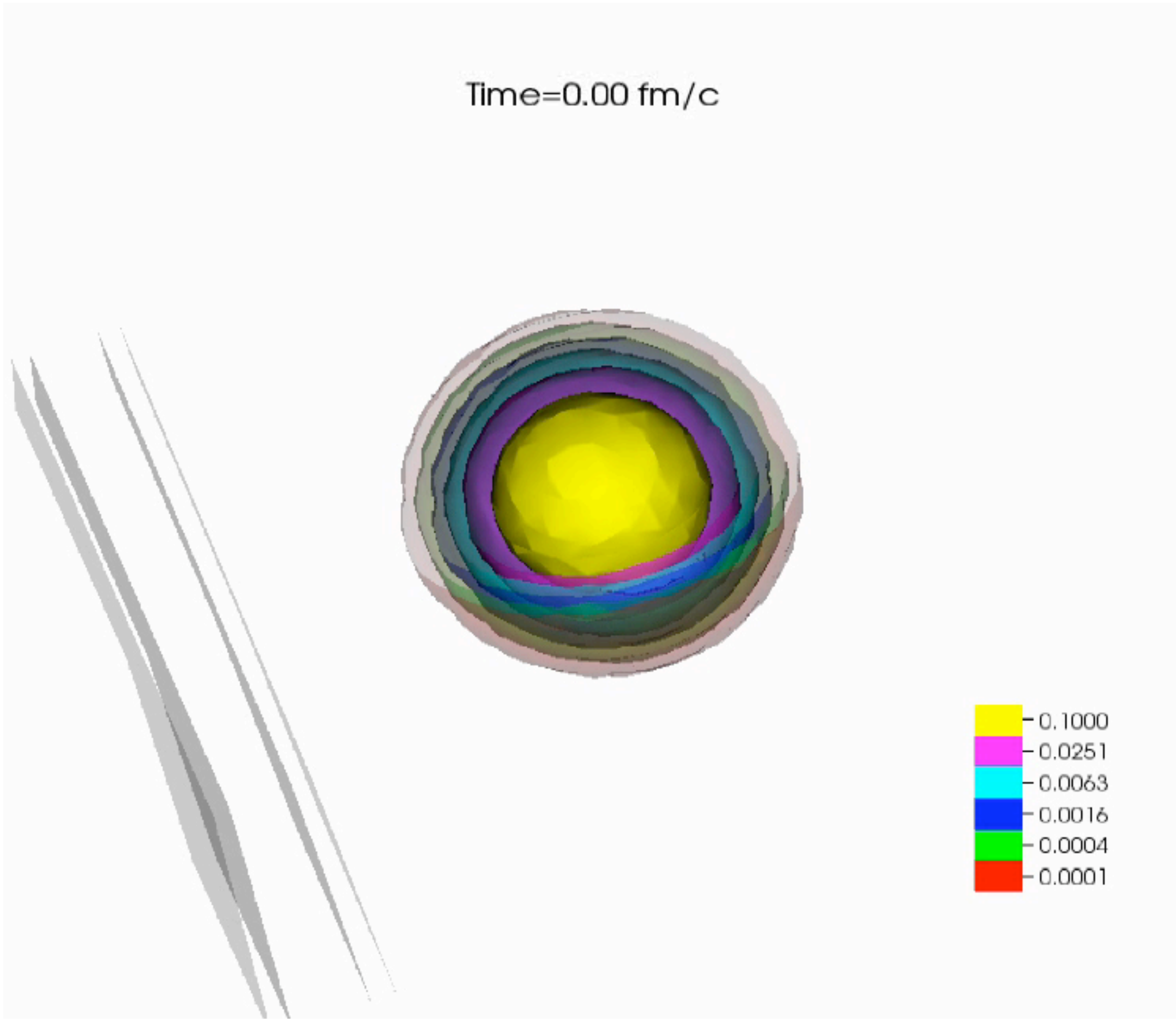








n (flux)-^{126}Sn process

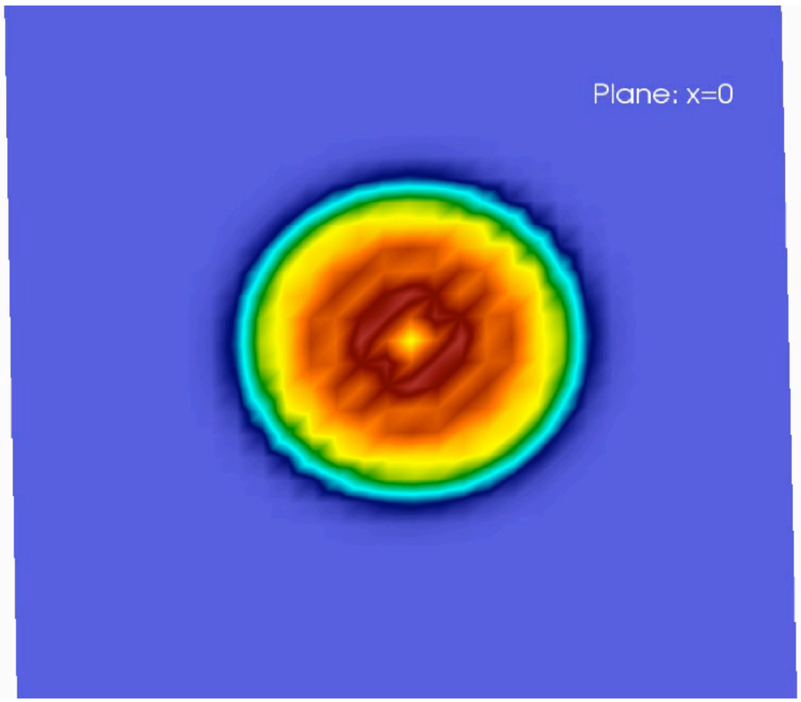


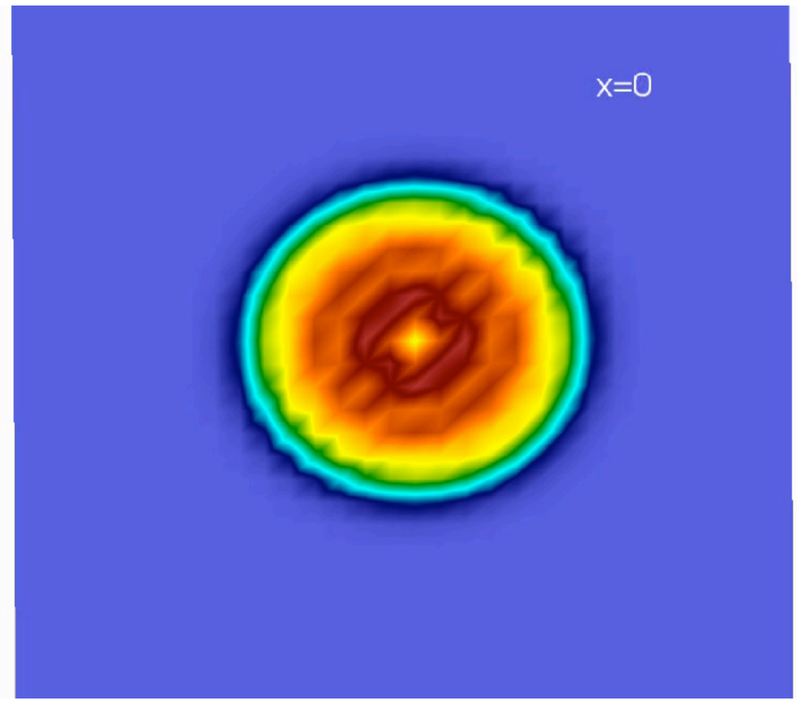
Large amplitude collective motion

Several simulations at:
http://www.phys.washington.edu/groups/qmbnt/index.html

Coulomb excitation: ^{280}Cf

isovector density 32^3

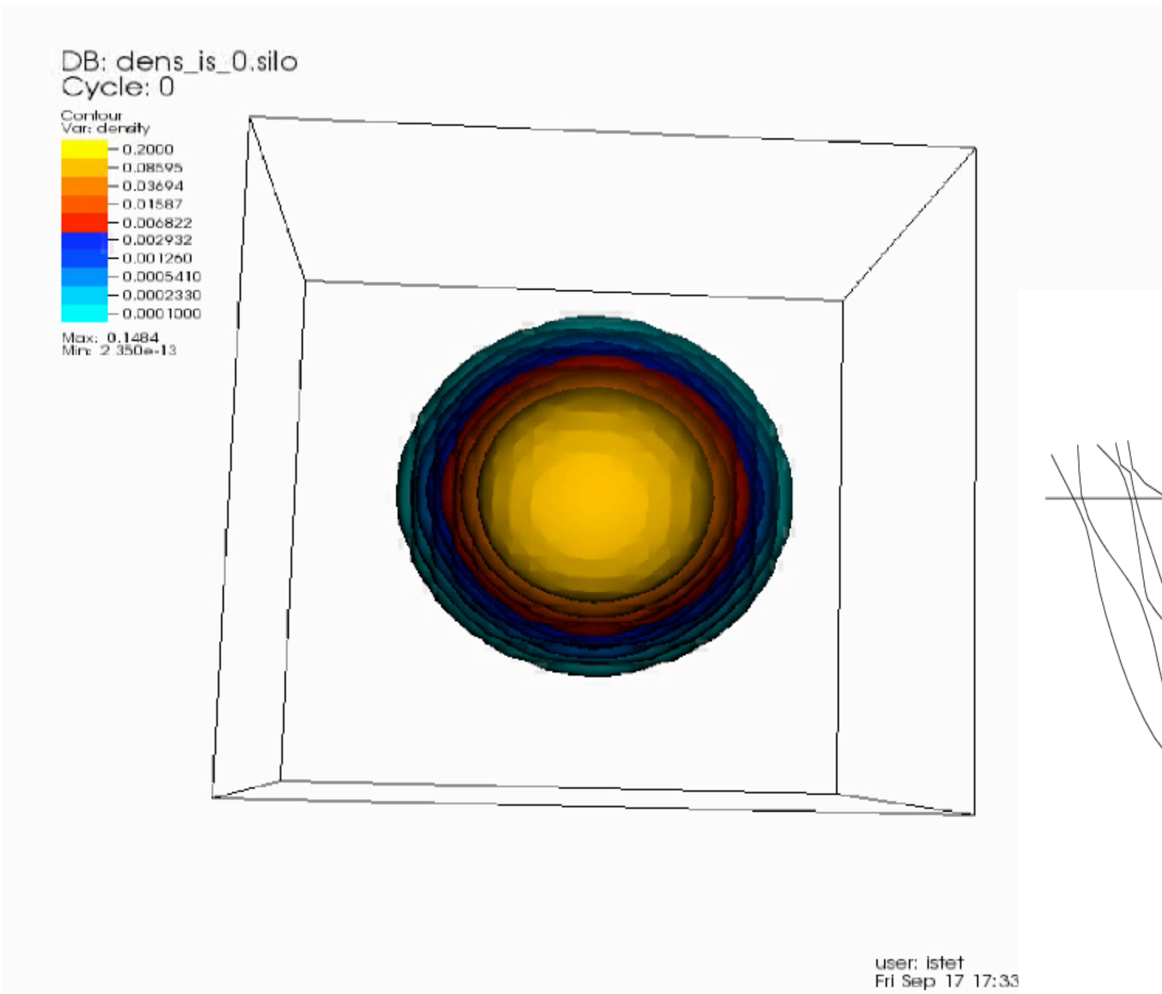


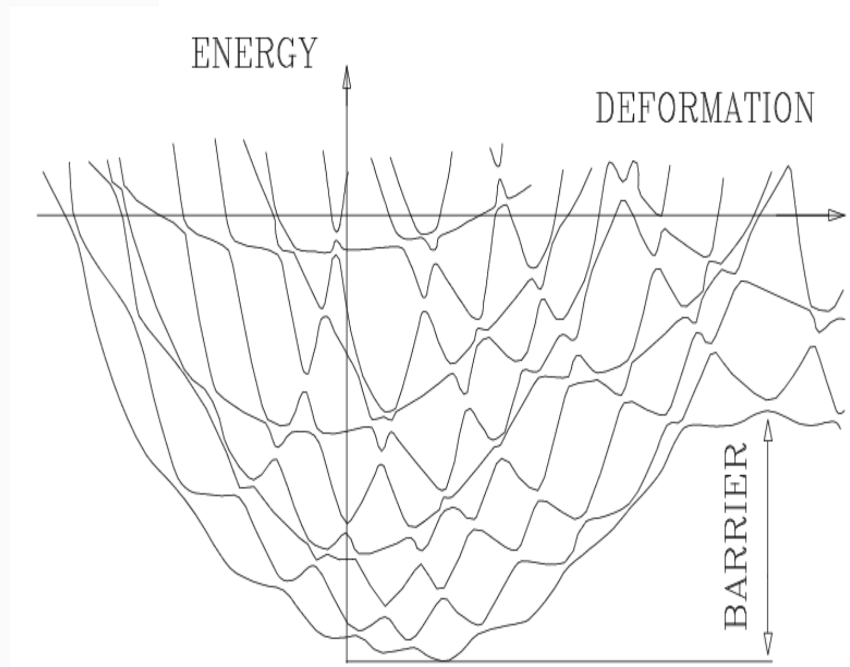


1 projectile

2 projectiles

First induced fission simulation





Summary and outlook

- Static and dynamic SLDA software developed (nuclear physics and Fermi gases)
  - efficient utilization of the largest computers (jaguarpf and hopper)
  - fortran 90 and C versions
- First linear response calculations in heavy nuclei, with the pairing included properly
- Future applications:
  - dipole response of ^{172}Yb: survey of functionals (pygmy resonance?)
  - relativistic Coulomb excitation of ^{136}Xe
  - electromagnetic response of heavy nuclei (spherical, axially symmetric, triaxial)
  - low-energy nuclear reactions
  - (induced) fission
  - stochastic TD-SLDA: mass and energy distributions of emerging fission fragments (exascale computing needed)

Additional slides

Pairing Renormalization

$$\nu(\vec{r}) = \sum_k u(\vec{r}) v_k^*(\vec{r}) \qquad \tau(\vec{r}) = \sum_k |\vec{\nabla} v_k(\vec{r})|^2$$

$$\mathcal{E}_S \stackrel{def}{=} -\Delta(\vec{r})\nu_c(\vec{r}) = g_{eff}(\vec{r})|\nu_c(\vec{r})|^2$$

A. Bulgac and Y. Yu, Phys. Rev. Lett. **88** (2002) 042504
Regularization: using Thomas Fermi approximated free-wave Green's function to subtract out the divergent term.

$$\frac{1}{g_{eff}(\vec{r})} = \frac{1}{g[\rho(\vec{r})]} - \frac{m(\vec{r})k_c(\vec{r})}{2\pi^2\hbar^2}\left\{1 - \frac{k_F(\vec{r})}{2k_c(\vec{r})}\ln\frac{k_c(\vec{r}) + k_F(\vec{r})}{k_c(\vec{r}) - k_F(\vec{r})} + \frac{k_1^2(\vec{r})}{24k_c^2(\vec{r})}\left(1 - \frac{k_c(\vec{r})}{k_F(\vec{r})}\ln\frac{k_F(\vec{r}) + k_c(\vec{r})}{\kappa(\vec{r})}\right)\right\}$$

$$|\vec{V}(\vec{r})|^2 = \frac{\hbar^2 k_1^2(\vec{r})}{2m(\vec{r})} \qquad E_c + \mu = \frac{\hbar^2 k_c^2(\vec{r})}{2m(\vec{r})} + U(\vec{r}) \qquad \mu = \frac{\hbar^2 k_F^2(\vec{r})}{2m(\vec{r})} + U(\vec{r})$$