Large scale static and time-dependent Hartree-Fock calculations with twist-averaged boundary conditions

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NUCLEI
Nuclear Computational Low-Energy Initiative

Nuclear Pasta Matter

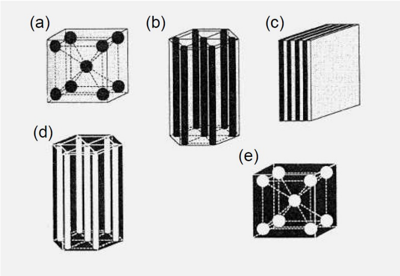


Figure: several pasta shapes (Oyamatsu et. al.)

- nuclear pasta appears at approx. $\rho = 1/8\,\rho_0\,, \quad \rho_0 \approx 0.16\mathrm{fm}^{-3}$
- several shapes appear like "spaghetti" (rod-like) shapes (b) or "lasagna" (slab-like) shapes (c)
- at higher densities inverted pasta appears (holes have rod-like or sphere-like structure) (d and e)

Sites for Nuclear Pasta

Neutron star

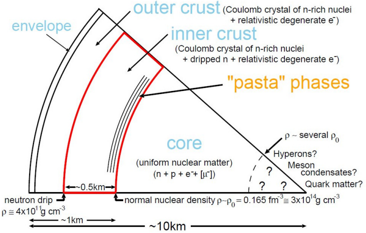


Figure: schematic picture of a neutron star (G. Watanabe et. al.)

- in inner crust of neutron stars
- proton fraction of $X_p \lesssim 0.1$
- thickness of the layer is about 100m

Core Collapse Supernovae

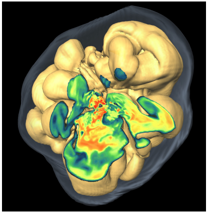


Figure: Supernova calculation (Janka et al.)

- after 100 msec central density reaches ρ_0
- core reaches temperatures of several MeV
- total amount ~20% of total mass

→ periodic boundary conditions

Twist-Averaged Boundary Conditions

strictly periodic boundary conditions introduce finite volume-effects!!!

- Floquet-Bloch theorem

$$\psi_{\alpha\boldsymbol{q}}(\boldsymbol{r},t) = \underbrace{u_{\alpha\boldsymbol{q}}(\boldsymbol{r},t)}_{\text{periodic}}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{r}}$$

- resulting boundary conditions

$$\psi_{\alpha\boldsymbol{\theta}}(\boldsymbol{r}+\boldsymbol{T}_i,t) = e^{\mathrm{i}\theta_i}\psi_{\alpha\boldsymbol{\theta}}(\boldsymbol{r},t)$$

- periodic BC is just one solution ($\theta_i = 0$)
- averaging of observables

$$\langle\hat{O}(t)\rangle = \frac{1}{8\pi^3}\iiint_0^{2\pi} d^3\boldsymbol{\theta}\,\langle\Psi_{\boldsymbol{\theta}}(t)|\hat{O}|\Psi_{\boldsymbol{\theta}}(t)\rangle$$

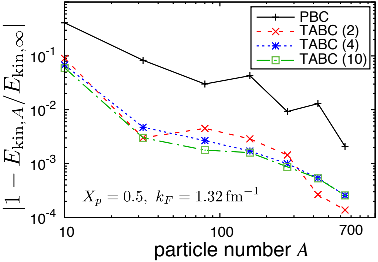


Figure: kinetic energy for periodic and twist-averaged boundary conditions.
BS, W. Nazarewicz PRC 92, 045806 (2015)

The Hartree-Fock Code Sky3D

- equidistant lattice with about 1fm lattice spacing
- full 3d, no symmetry assumptions
- using FFT for derivatives
- state of the art Skyrme forces
- exact treatment of Coulomb force (non-periodic Coulomb possible)

Static Iterations

Solving the Schrödinger equations for a single Slater determinant in the mean-field approximation

$$\hat{h}_{(\boldsymbol{\theta})}\psi_{\alpha\boldsymbol{\theta}}(\boldsymbol{r}) = \epsilon_{\alpha\boldsymbol{\theta}}\psi_{\alpha\boldsymbol{\theta}}(\boldsymbol{r})$$

Time evolution

Evolving the initial state (Slater determinant) in time with the time evolution operator:

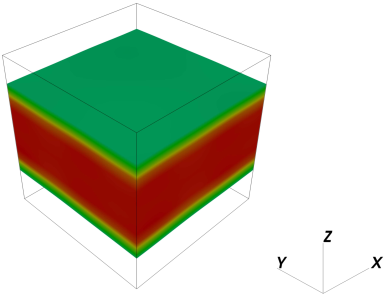
$$\psi_{\alpha\boldsymbol{q}}(\boldsymbol{r},t) = e^{-\mathrm{i}\hat{H}t/\hbar}\psi_{\alpha\boldsymbol{q}}(\boldsymbol{r},t=0)$$

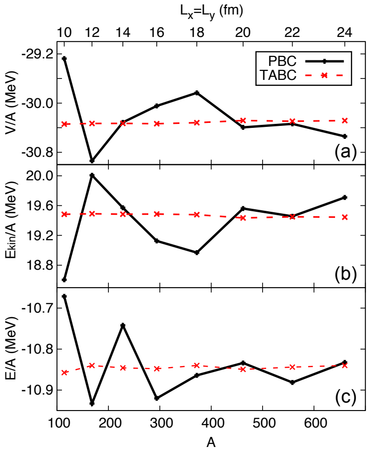
Setup

Initialization of the static calculations with

- lowest plane wave states (spin saturated)
- $X_P = 1/3$
- additional potential for the first 200 iterations which forces the matter to form a specific shape

Slab varying $L_x = L_y$

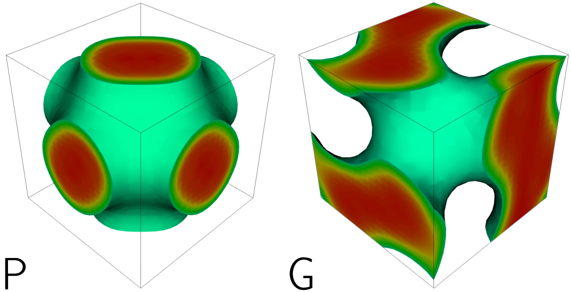




- $\phi_{\rm slab}(x, y, z) = \phi_0 \cos(2\pi x/L)$
- Vary box length in translational invariant directions
- $\rho = 0.07\mathrm{fm}^{-3}$

BS, W. Nazarewicz PRC 92, 045806 (2015)

Minimal surfaces



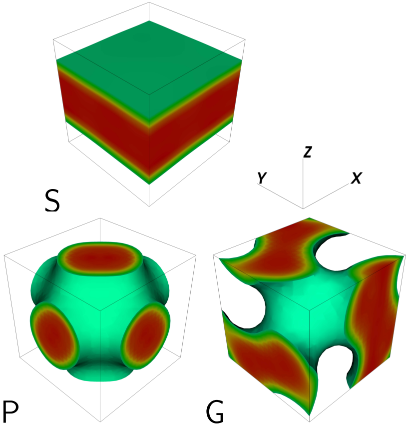
- local minimal surface for given boundary conditions
- divides space into two equal subspaces

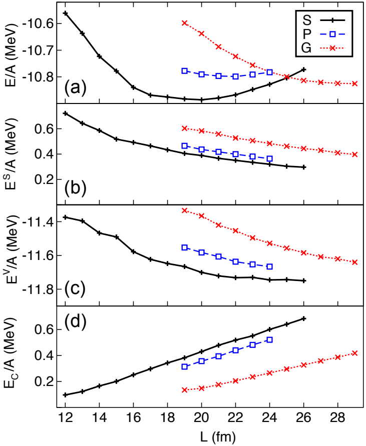
First order nodal approximation potentials:

P: $\phi_{\mathrm{P}}(x, y, z) = \phi_0(\cos x + \cos y + \cos z)$

G: $\phi_{\mathrm{G}}(x, y, z) = \phi_0(\cos x \sin y + \cos y \sin z + \cos z \sin x)$

Which is the ground state shape?





- Vary 'physical' direction
- $\rho = 0.07125 \mathrm{fm}^{-3}$

BS, W. Nazarewicz PRC 92, 045806 (2015)

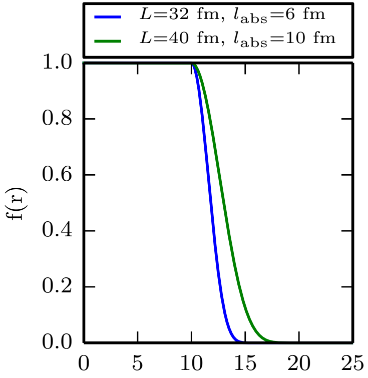
Problems for 3d TD-DFT for vibrating finite nuclei

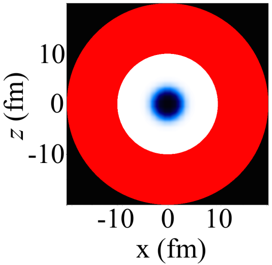
- spurious finite-volume effects due to limited box sizes
- usually periodic or reflecting boundary conditions
  1. evaporated matter is reflected at boundaries or enters box from opposite side
  2. k-space is quantized according to box length
- problem can be solved in 1d with very large boxes
- or in 3d with absorbing boundary conditions

Absorbing boundary conditions (ABC)

masking function: $\psi_\alpha \to \psi_\alpha f(r)$ with (equivalent to imaginary potential)

$$f(r) = \begin{cases} 1 & \text{if } r < L/2 - l_{\mathrm{abs}} \\ \cos\left(\frac{\pi}{2}\frac{r - L/2 + l_{\mathrm{abs}}}{l_{\mathrm{abs}}}\right)^p & \text{if } L/2 - l_{\mathrm{abs}} < r \le L/2 \\ 0 & \text{if } x \ge L/2 \end{cases}$$





Low energy excitations in ^{16}O

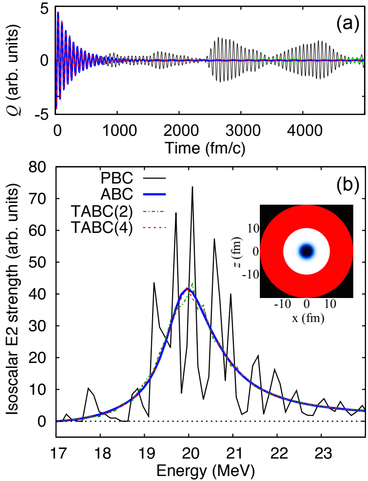


Figure: ^{16}O isoscalar quadrupole excitation with $E^* = 3$ MeV

BS, W. Nazarewicz, P.-G. Reinhard PRC 93, 054304 (2016)

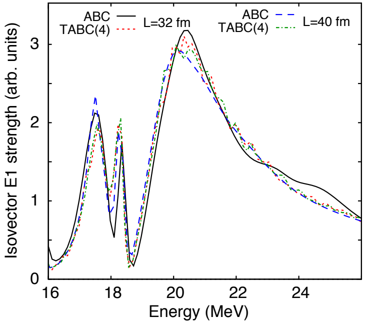


Figure: ^{16}O isovector dipole excitation with $E^* = 1$ MeV

High energy excitations in ^{16}O

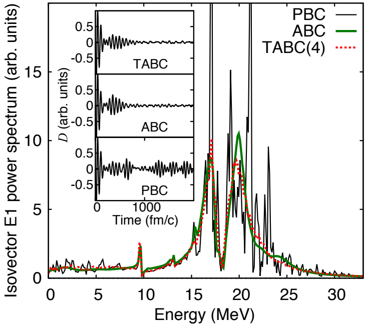


Figure: ^{16}O isovector dipole excitation with $E^* = 20$ MeV

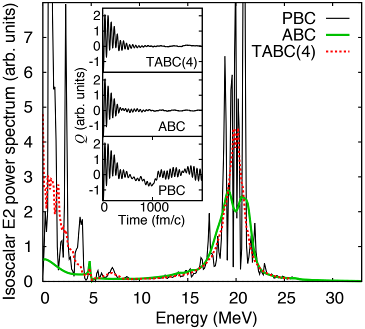


Figure: ^{16}O isoscalar quadrupole excitation with $E^* = 20$ MeV

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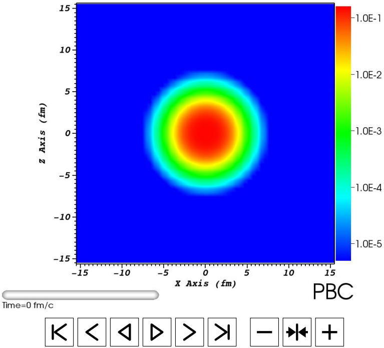
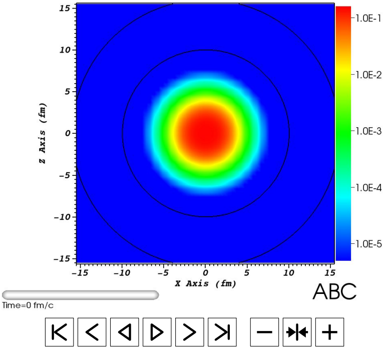
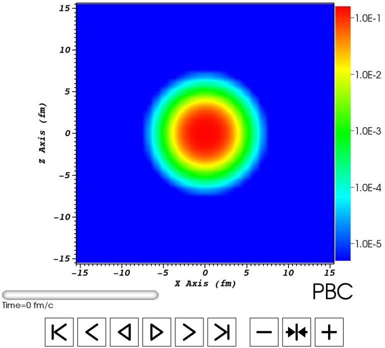
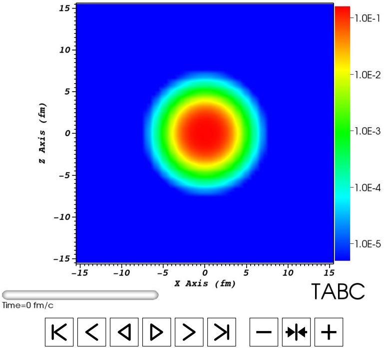
Periodic vs. absorbing boundary conditions





Periodic vs. twist-averaged boundary conditions





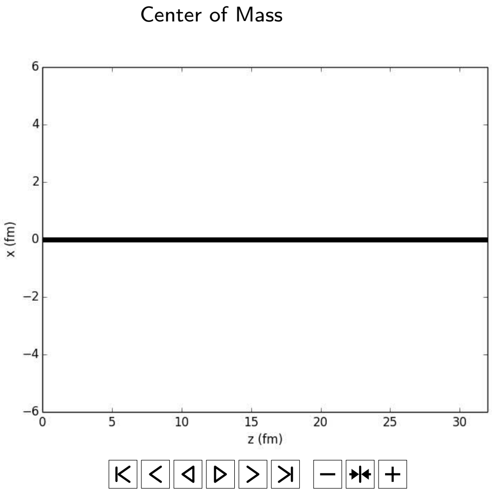
Twist-averaged boundary conditions for excited rod

- rod configuration along z axis
- excitation with

$$\psi \rightarrow \psi \exp(-iS(\boldsymbol{r}))$$

$$S(\boldsymbol{r}) \sim x \sin(2\pi z/l_z)$$

$$v_x \sim \frac{\partial S}{\partial x} \sim \sin(2\pi z/l_z)$$



Conclusion & Outlook

Conclusion:

- TABC is a good method to get answers for strictly periodic systems with small boxes and a small number of particles in static as well as in time-dependent calculations
- for defects of structures which are not strictly periodic we have to go to bigger boxes anyway
- TABC can also be used for finite nuclei if not too many particles are evaporated

Outlook:

- can be used in many other applications for periodic systems e.g. oscillating slabs

Collaborators:
Witek Nazarewicz and Paul-Gerhard Reinhard

Thank you for your attention