Introduction to Octopus: a real-space (TD)DFT code

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TDDFT 2012, Benasque

[1]Filling in for Xavier Andrade (Harvard).

Introduction

Time-dependent Kohn-Sham equation

$$\begin{aligned} i\frac{\partial}{\partial t}\varphi_n(\boldsymbol{r},t) &= -\nabla^2\varphi_n + V_{\text{eff}}\left[\rho\right](\boldsymbol{r},t)\varphi_n(\boldsymbol{r},t) \\ \rho(\boldsymbol{r},t) &= \sum_n \varphi_n^*(\boldsymbol{r},t)\varphi_n(\boldsymbol{r},t) \end{aligned}$$

- Solve the equations numerically.
- Represent functions and other objects.
- Calculate derivatives and integrals.

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Pseudo-potentials

- The atomic potential is very strong and “hard” (small spacing or high plane-wave cutoff required).
- Core electrons are almost independent of the environment.
- Replace the potential and core electrons by a pseudo-potential.

Norm-conserving pseudo-potentials in Kleinman-Bylander form

$$V = V_{loc} + \sum_{lm} |lm\rangle \left(V_l - V_{loc}\right) \langle lm|$$

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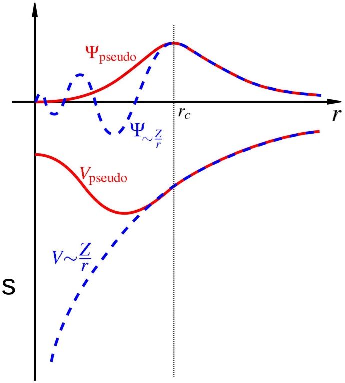

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Real-space grid

- Partial differential equation with infinite degrees of freedom.
- Reduce to a finite number.
- Functions are represented by values on a set of points.
- Point distribution:
- Finite region of the space: *Box*

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Boundary conditions

- For finite systems, functions go to zero.
- Force functions to go to zero on the border of the box.
- The box has to be large enough to contain the functions.
- Other BCs are possible: periodic, zero derivative, open.

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- Optimize the shape of the box to minimize the number of points needed.
- Available box shapes:
  - Minimum box: union of spheres around each atom.
  - Sphere.
  - Cylinder.
  - Parallelepiped.
  - Arbitrary (e.g. 2D image!)

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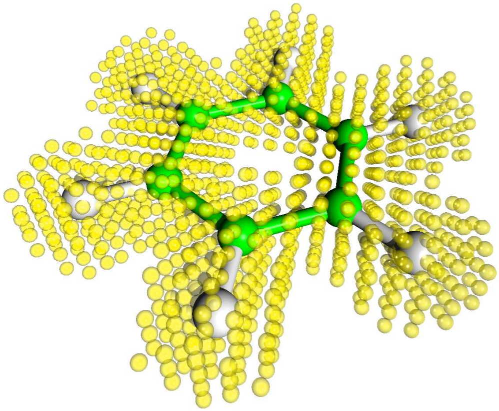
Example: benzene molecule in minimal box



Real-space grid characteristics

- Natural boundary conditions for different problems:
  zero, one, two, or three periodic dimensions for molecules, wires, sheets, and solids.
- Representation used for calculating $V_{\mathrm{xc}}[\rho]$ even with other bases.
- Can systematically improve discretization quality:
  - Decrease the spacing (like increasing plane-wave cutoff)
  - Increase the box size (in finite directions).
- Orthogonal “basis set”.
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Derivatives

- Derivative at a point: sum over neighboring points.
- The coefficients c_{ij} depend on the mesh and number of points used: *the stencil*.
- General form for Laplacian:

$$\nabla^2 f(n_x h, n_y h) = \sum_i^n \sum_j^n \frac{c_{ij}}{h} f(n_x h + ih, n_y h + jh)$$

- Compare definition of derivative:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{\Delta x}$$

- More points $\rightarrow$ more precision.
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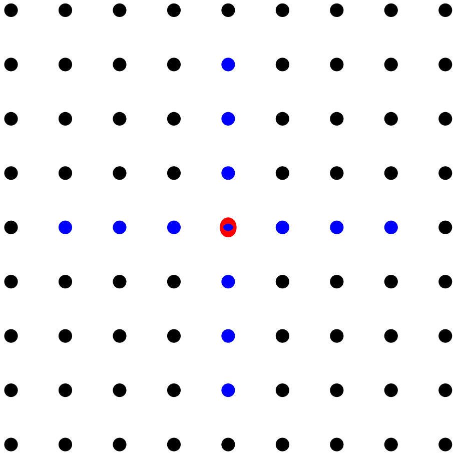
Example of stencil for Laplacian

Symmetric third-order in 2D.



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Kohn-Sham equations

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Discretization of the Hamiltonian

- For the Laplacian (kinetic energy) we use finite differences.
- The local part of the potential can be applied directly.
- The non-local potential is applied in a small spherical grid around the atoms.
- The Hamiltonian becomes a finite-size matrix.

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- We minimize (using conjugate gradient or other method):

Rayleigh-Ritz quotient

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- Response to time-dependent fields: lasers.

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Absorption spectra from time-propagation

- Start from the ground state, with a ‘kick.’

Time-dependent potential

$$V(\boldsymbol{r},t) = \boldsymbol{\kappa}\delta(t) \qquad \Rightarrow \qquad \psi \to \psi e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- Time-propagate and get the dipole $\boldsymbol{d}(t)$ as a function of time.

Polarizability tensor

$$\alpha_{ij}(\omega) = \frac{1}{\kappa_j}\int dt\, e^{i\omega t} d_i(t)$$

Absorption cross section

$$\sigma(\omega) = \frac{4\pi\omega}{c}\Im[\alpha(\omega)]$$

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$$\sigma(\omega) = \frac{4\pi\omega}{c}\Im\left[\alpha(\omega)\right]$$

Absorption spectra from time-propagation

- Start from the ground state, with a 'kick.'

Time-dependent potential

$$V(\boldsymbol{r}, t) = \boldsymbol{\kappa}\delta(t) \qquad \Rightarrow \qquad \psi \to \psi e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- Time-propagate and get the dipole $\boldsymbol{d}(t)$ as a function of time.

Polarizability tensor

$$\alpha_{ij}(\omega) = -\frac{1}{\kappa_i}\int dt\, e^{i\omega t} d_j(t)$$

Absorption cross section

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Octopus[2]

- Fortran 95 and C (+ some Perl utilities).
- Focused on finite systems (periodic systems possible too).
- Norm-conserving pseudopotentials.
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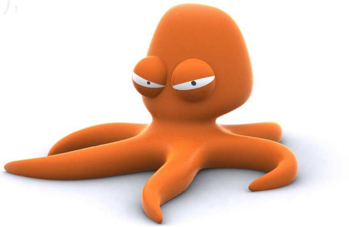

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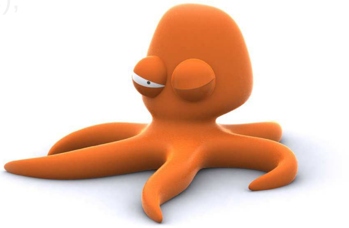

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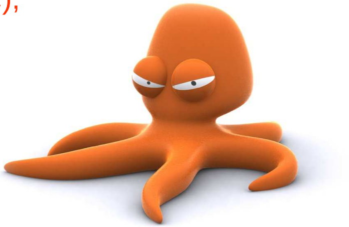

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References

Two papers on the Octopus code:

- A. Castro, H. Appel, Micael Oliveira, C.A. Rozzi, X. Andrade, F. Lorenzen, M.A.L. Marques, E.K.U. Gross, and A. Rubio, “octopus: a tool for the application of time-dependent density functional theory,” *Phys. Stat. Sol. B* **243**, 2465-2488 (2006).
- M.A.L. Marques, Alberto Castro, George F. Bertsch, and Angel Rubio, “octopus: a first-principles tool for excited electron-ion dynamics,” *Comput. Phys. Commun.* **151**, 60-78 (2003).

Pulpo a feira (pulpo a la gallega)

The origin of the name Octopus. (Recipe available in code.)

Octopus[3]

- Ground-state DFT.
- Time-propagation.
- Molecular dynamics (Ehrenfest, Born-Oppenheimer, Car-Parrinello).
- Casida linear response.
- Sternheimer linear response for electromagnetic response, phonons, Van der Waals coefficients.
- Optimal control theory.
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- (Other experimental features.)

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  - Points in the boundaries of each region must be copied to other nodes.
  - Integrals are performed locally and summed over all domains.
  - Efficient and scalable scheme.
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