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

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# Schedule

- Day 1 (08 Apr):
  - Octopus basics tutorial series
- Day 2 (09 Apr):
  - Optical absorption tutorial series
- Day 3 (10 Apr):
  - Solids tutorial series
- Day 4 (11 Apr):
  - Maxwell tutorials
- Day 5 (13 Apr):
  - BerkeleyGW tutorials

# The Octopus code

**Purpose**: simulate the dynamics of electrons and nuclei under the influence of external time-dependent fields in the framework of Time-Dependent Density Functional Theory (TDDFT)

- DFT with many functionals (from `Libxc`), Hartree-Fock, Hartree, RDMFT
- Fortran 2008, C, C++, OpenCL/CUDA and some Python and Perl.
- extensive use of mathematical libraries: `BLAS/LAPACK`, `FFTW`, `GSL`, etc.
- Interfaces to external libraries: `libxc`, `libvdwxc`, `wannier90`, `berkeleygw`, etc.
- Free open-source software (GNU Public License).
- Current version is 16.0.
- Framework to implement and test new ideas

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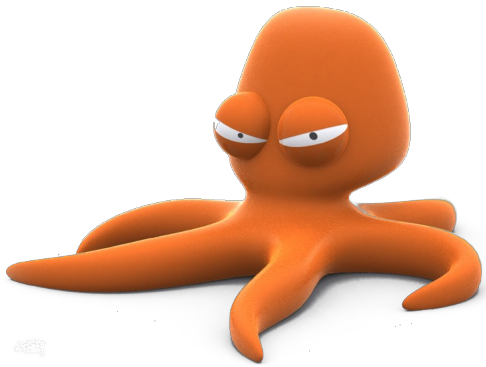

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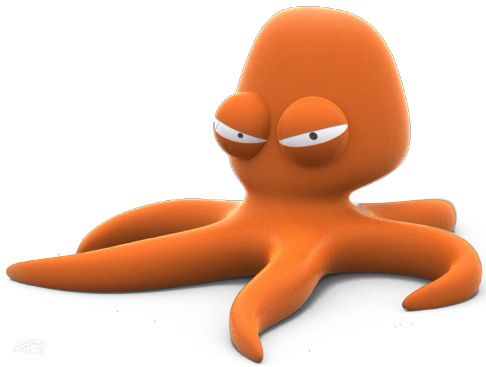

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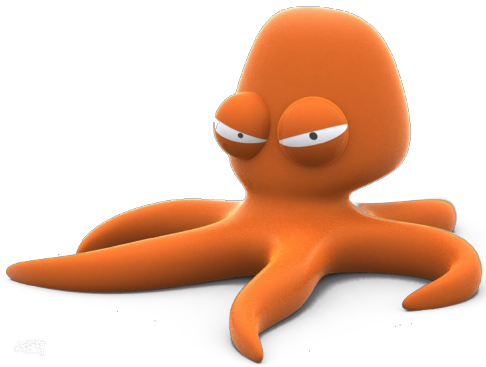

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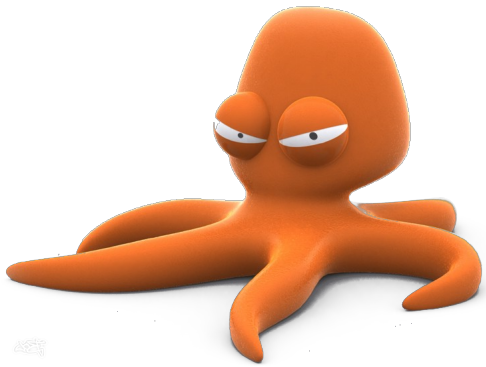

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  - van der Waals interactions

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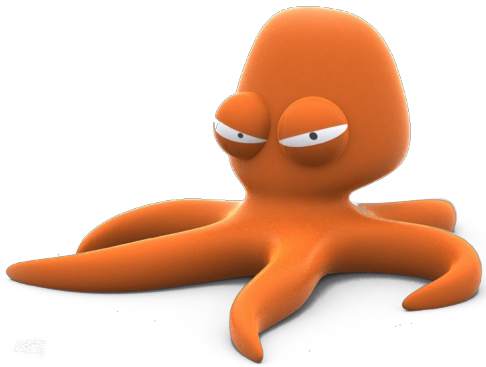
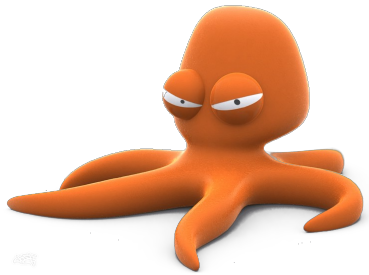
- Move to object oriented design



# The Octopus code

- `https://octopus-code.org`
- `https://gitlab.com/octopus-code`

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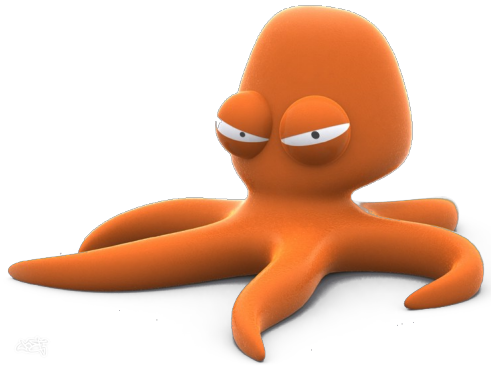

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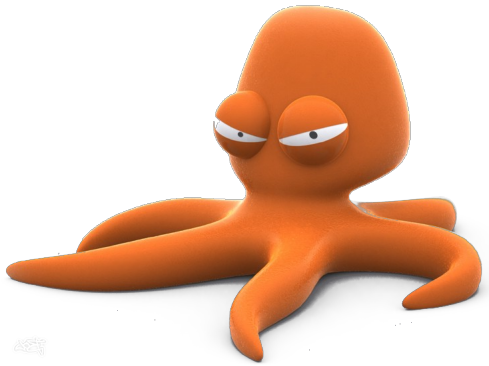

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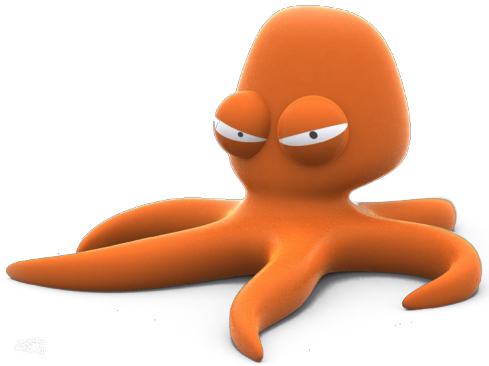

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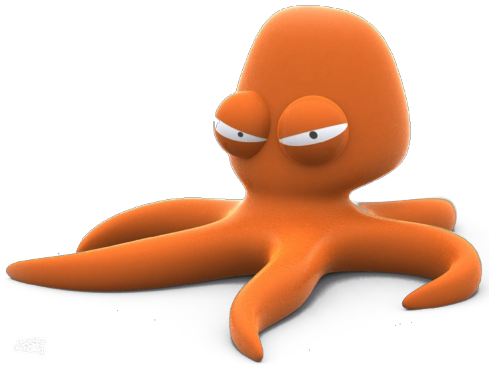

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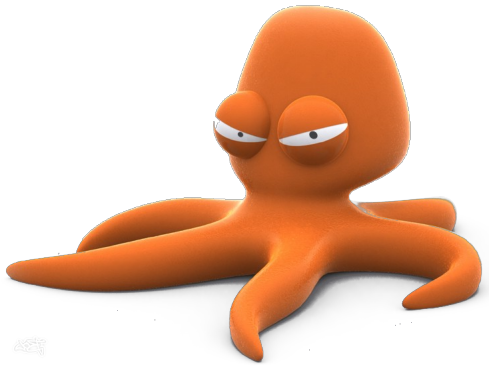

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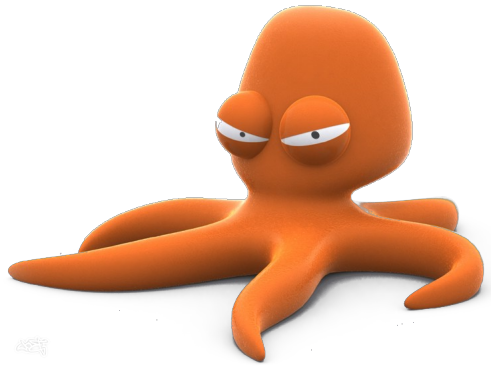

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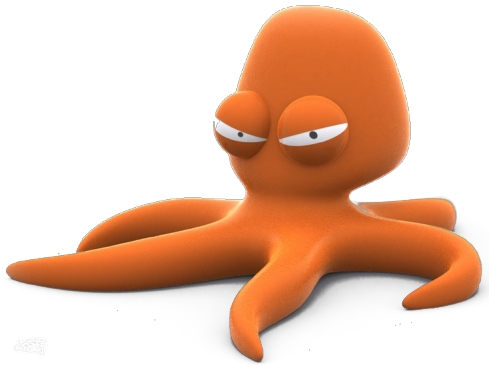

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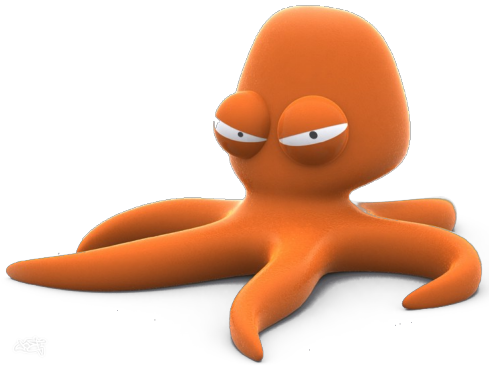

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- Many other features

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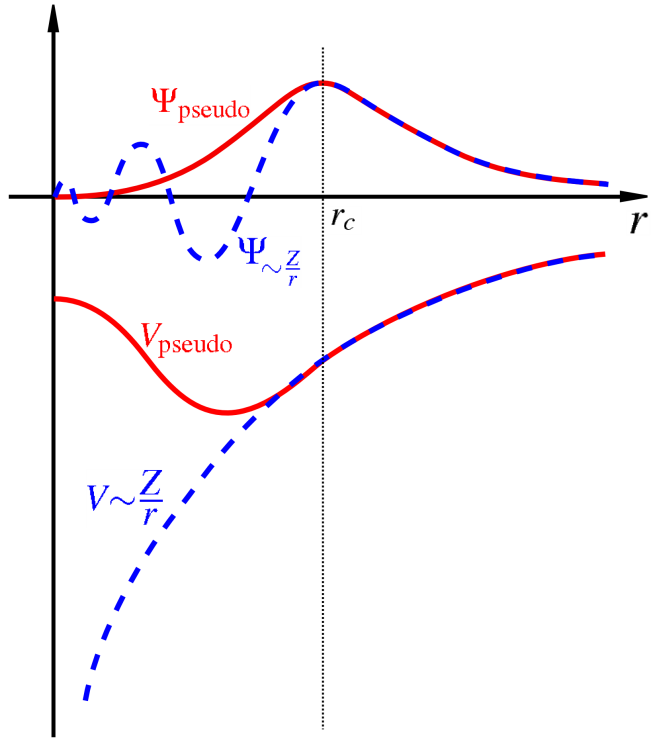

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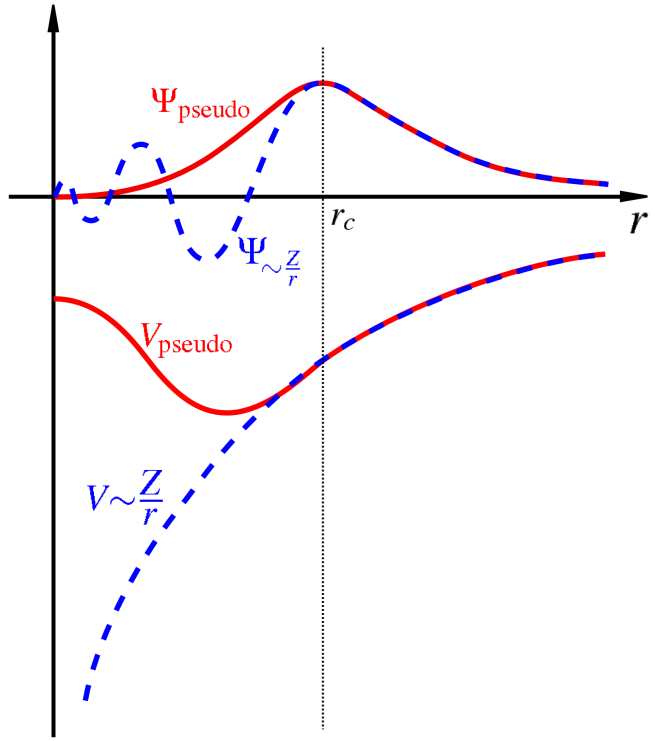

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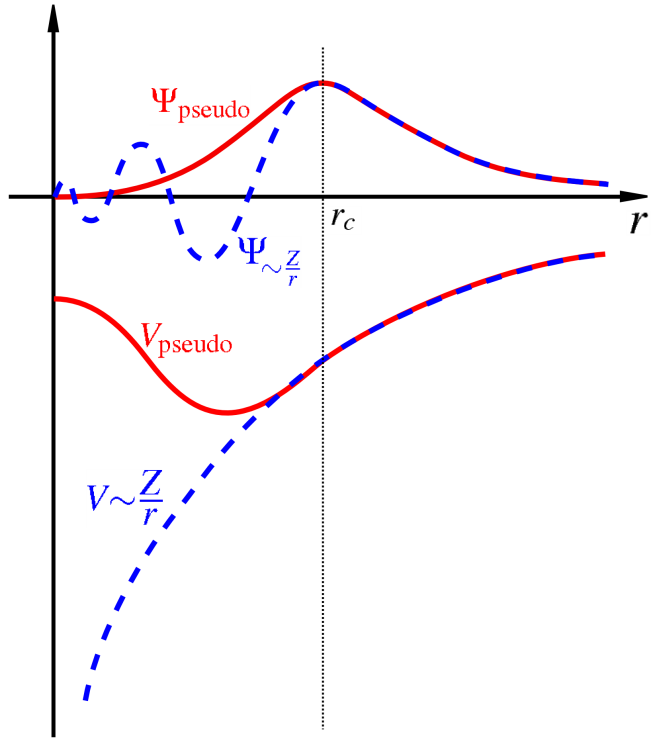

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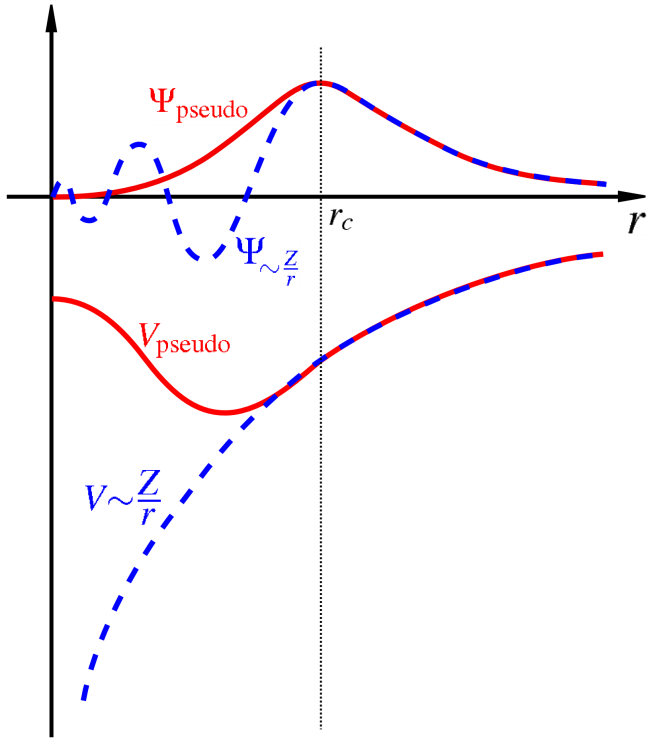

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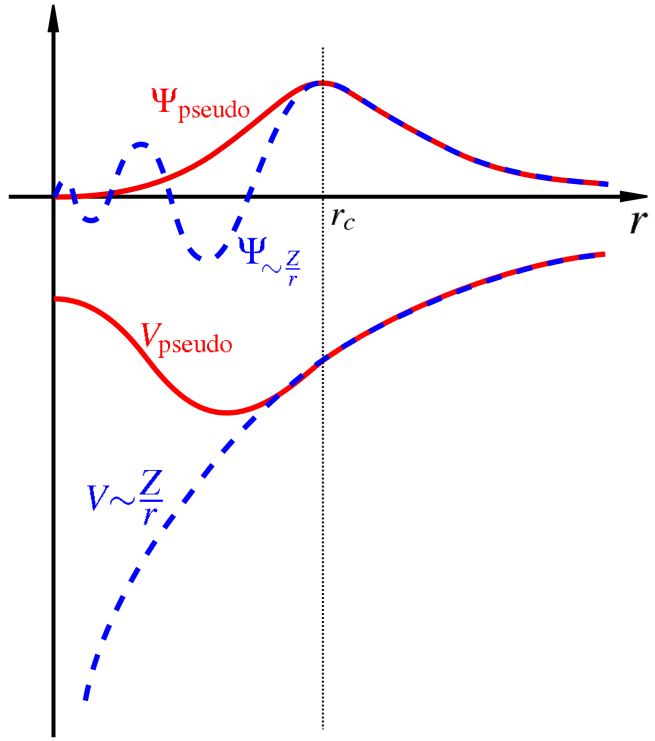


## Norm-conserving pseudo-potentials in Kleinman-Bylander form

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

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# Discretization of the Hamiltonian

We use finite differences to evaluate the Laplacian (kinetic energy):

- Derivative at a point: weighted sum over neighboring points
- General form for the Laplacian:

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

- The coefficients $c_{ij}$ depend on the mesh and number of points used: *the stencil*
- More points $\rightarrow$ more precision

The Hamiltonian becomes a finite-size matrix

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- Very large matrix with lots of zero components (*Sparse*)
- Use iterative solvers where only the application of the matrix is required (various options available in the code)

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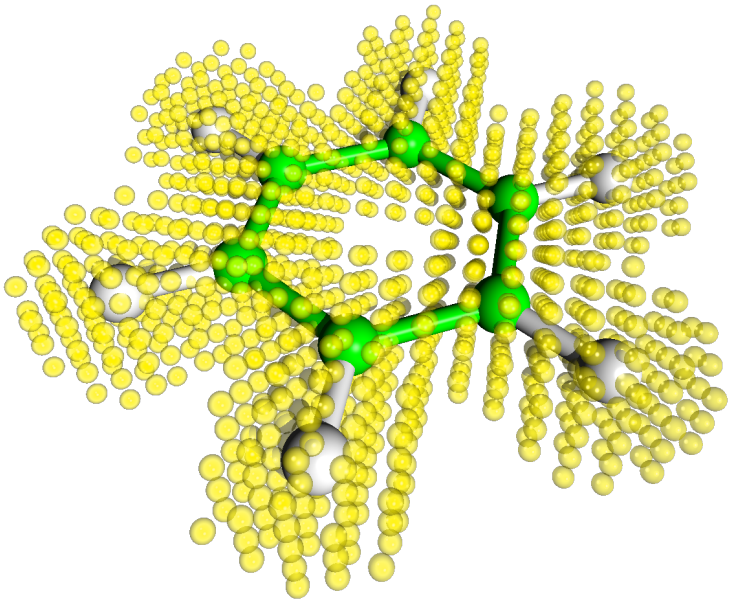
  - etc

# Boundary conditions

- Optimize the shape of the box to minimize the number of points needed

- Available box shapes:



Benzene molecule in minimal box

# Boundary conditions

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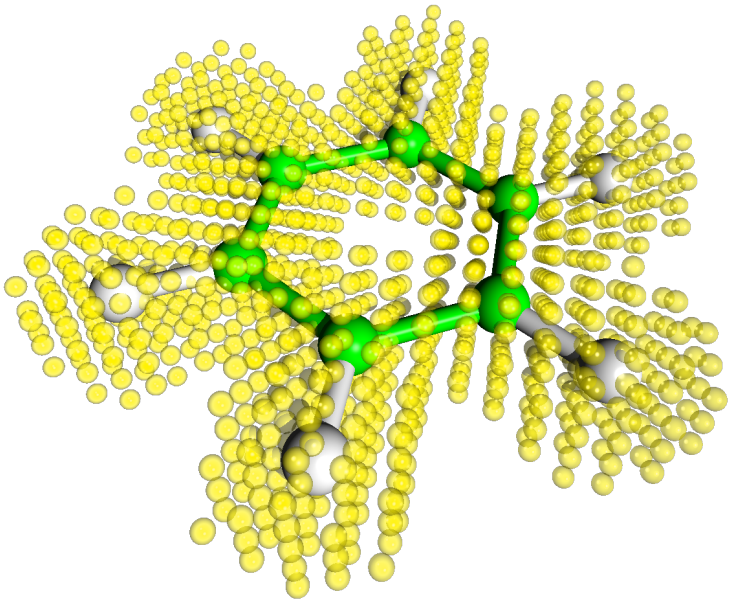
- Available box shapes:
  - Sphere



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# Boundary conditions

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- Available box shapes:
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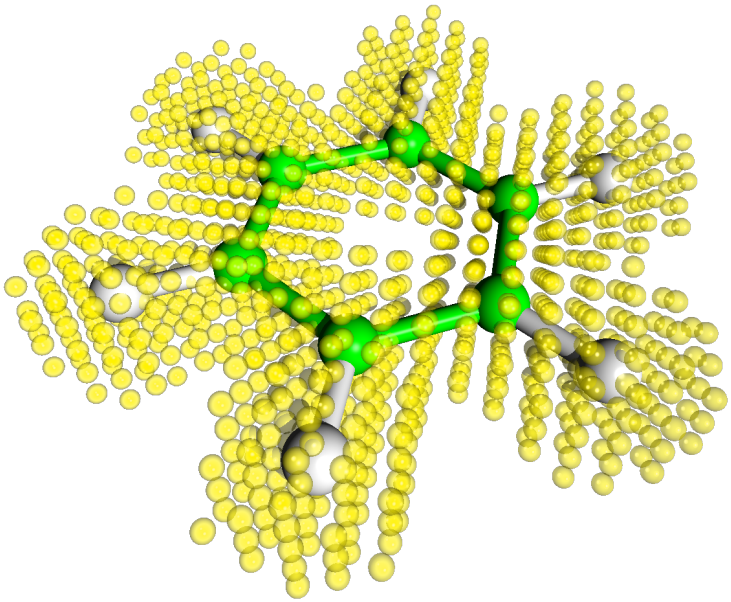
  - Cylinder



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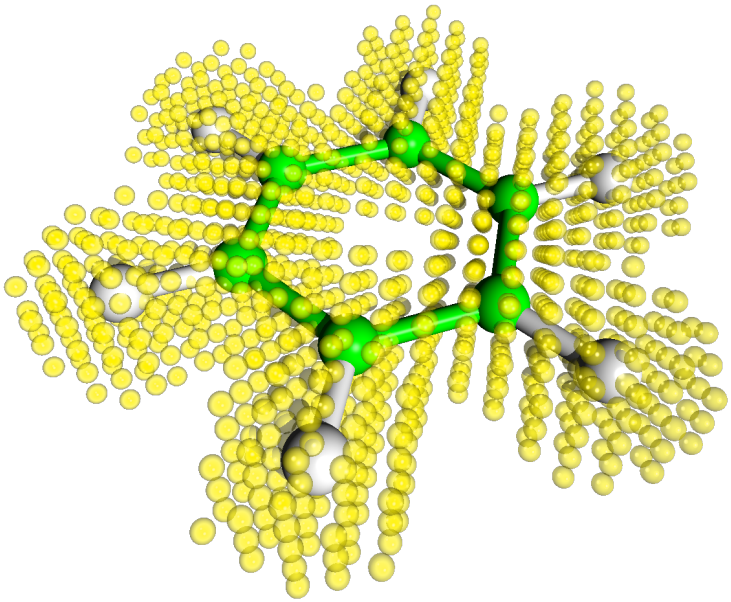

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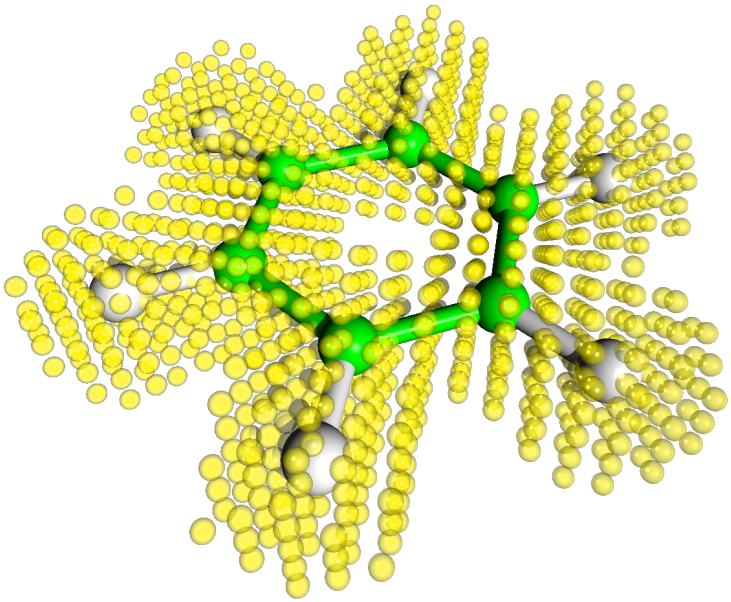

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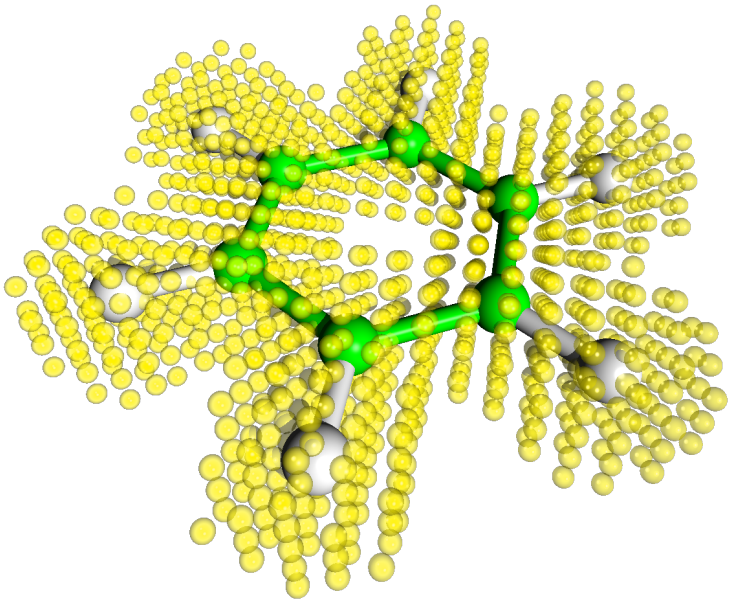
  - Arbitrary (*e.g.* 2D image!)



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# Time propagation

Propagation of the wavefunctions in time:

$$\varphi_i(\boldsymbol{r}, t + \Delta t) = \hat{T}\exp\left\{-\mathrm{i}\int_t^{t+\Delta t} \mathrm{d}t\, \hat{H}\varphi_i(\boldsymbol{r}, t)\right\}$$

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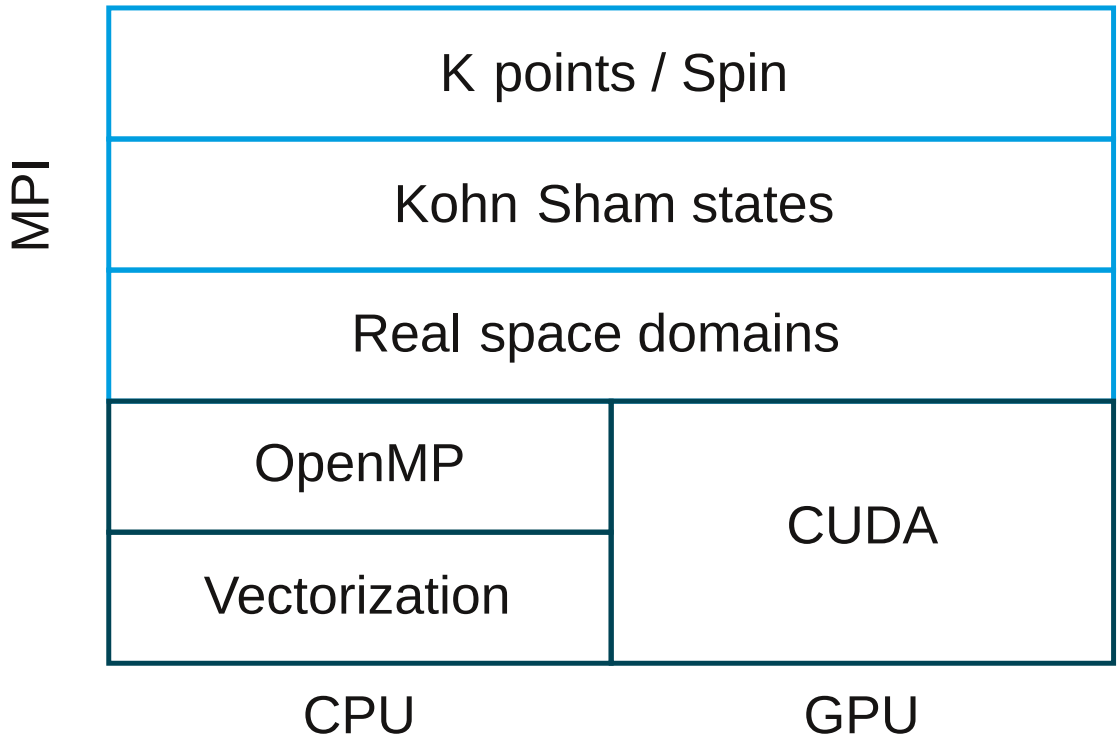
- See e.g. tutorials on optical absorption

# Parallelisation strategy



# The tutorials

You can find the tutorials under this link:
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Have fun!