# Octopus: Meshes and Grids

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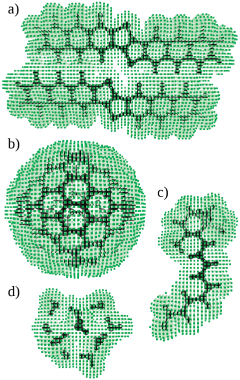
# Real-space methods



# Real-space methods

Finite difference methods:

- Finite simulation volume (simulation box)
- Discretize space within this volume (mesh)
- Represent functions on these mesh points
- Represent derivatives through finite differences
- Boundary conditions

# Simulation box

The simulation box:

- Some finite volume in which we solve the equations
- main function: is a point inside or outside?
- can have different shapes
- can be a combination of boxes (recursively)

# Simulation box

Examples:

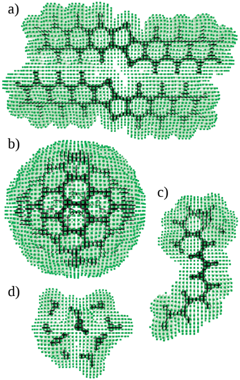
- Parallelepiped
- Sphere
- Cylinder
- Union and Intersection
- Minimum box (union of spheres)

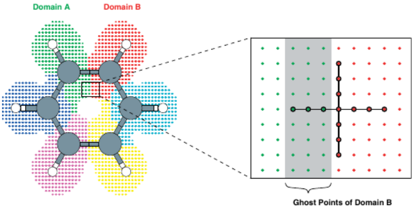
# Simulation box

Implementation:

- In folder `src/boxes/`
- Abstract class `box_t`
- Instance created by factory `box_factory.F90`
- ...

# The mesh



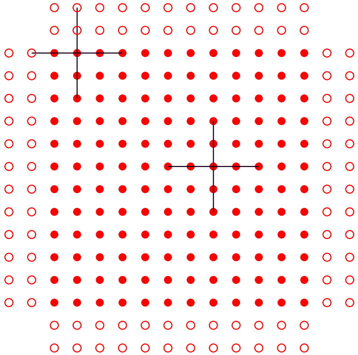



# Real-space mesh

The mesh:

- usually uniform (curvilinear meshes or double grids are possible)
- contained in 'simulation box'
- can be distributed over processes (domain decomposition)
- access via linear indices (local and global index)
- we need some 'extra points':
  - for boundary conditions
  - halo points (ghost points)

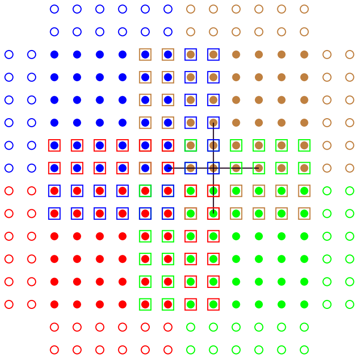
# Boundary points



• inner point
∘ boundary point

- Points in the simulation box
- Stencil for derivatives
- Derivatives close to the boundary: need extra points!
- Boundary points

# Parallel domain decomposition



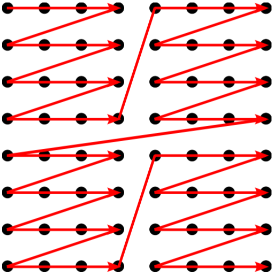
- • local point
- ◦ boundary point
- □ ghost point

- Distribute points over processors
- Derivatives close to the boundary: require communication (slow!!)
- Introduce halo (ghost points) on each processor
- total number of points on a processor: local + boundary + ghost points

- Note: boundary and ghost points are only needed if you need to take a derivative!

# 1D mapping

- Octopus is designed to work in various spatial dimensions.
- memory layout cannot depend on spatial dimensions
- map to 1-dimensional arrays
- cubic mapping or Hilbert curve mapping
- separate inner (local) from boundary (ghost) points
- Usually hidden in low level routines



## Real-space mesh

Memory layout:

- mesh sizes:

| | |
|---|---|
| `np` | number of local 'inner' points |
| `np_part` | number of local 'inner' points + 'ghost' points + boundary points |
| `np_global` | number of global 'inner' points |
| `np_part_global` | number of global 'inner' points + boundary points |

- ordering:
  - inner points first `[1:np]`
  - ghost and boundary points: `[np+1:np_part]`
- mesh points: `mesh%x(1:mesh%np_part, 1:space%dim)`

# Real-space mesh

In the typical case of zero boundary conditions `v(np+1:np_part)` is 0. The two parts are split according to the partitions. The result of this split are local vectors `v_local` on each process which consist of three parts:

- `v_local(1:np_local)` local points.
- `v_local(np_local+1:np_local+np_ghost)` ghost points.
- `v_local(np_local+np_ghost+1:np_local+np_ghost+np_bndry)` boundary points.

# Real-space mesh: in practice

- Low level routines take care of boundary/ghost points.
- Only need to set the values for inner points
- BUT: If you need derivatives of a mesh function,
  it must be allocated as contiguous memory `1:np_part`

# The grid

# Real-space grid

The grid describes a number of things:

- the mesh (the actual points in space)
- the derivatives
- the stencil
- symmetries and the symmetrizer

```
type, extends(mesh_t) :: grid_t
  ! Components are public by default
  type(derivatives_t)     :: der
  type(stencil_t)         :: stencil
  type(symmetries_t)      :: symm
  type(symmetrizer_t)     :: symmetrizer
end type grid_t
```

# Stencils

The stencil describes:

- The points for the derivatives
- Specific stencils: routines to generate coefficients for derivatives

# Derivatives

The derivatives object contains:

- gradient and laplacian operators (`nl_operator_t`)
- boundary conditions

The class provides:

- routines to apply the derivatives to mesh functions and batches
  - apply boundary conditions
  - perform ghost updates