Brief introduction to ASE

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Overview of ASE

ASE is a free (LGPLv2.1+) toolkit to set up and control atomistic calculations in a fully scripted environment using Python.

Main features

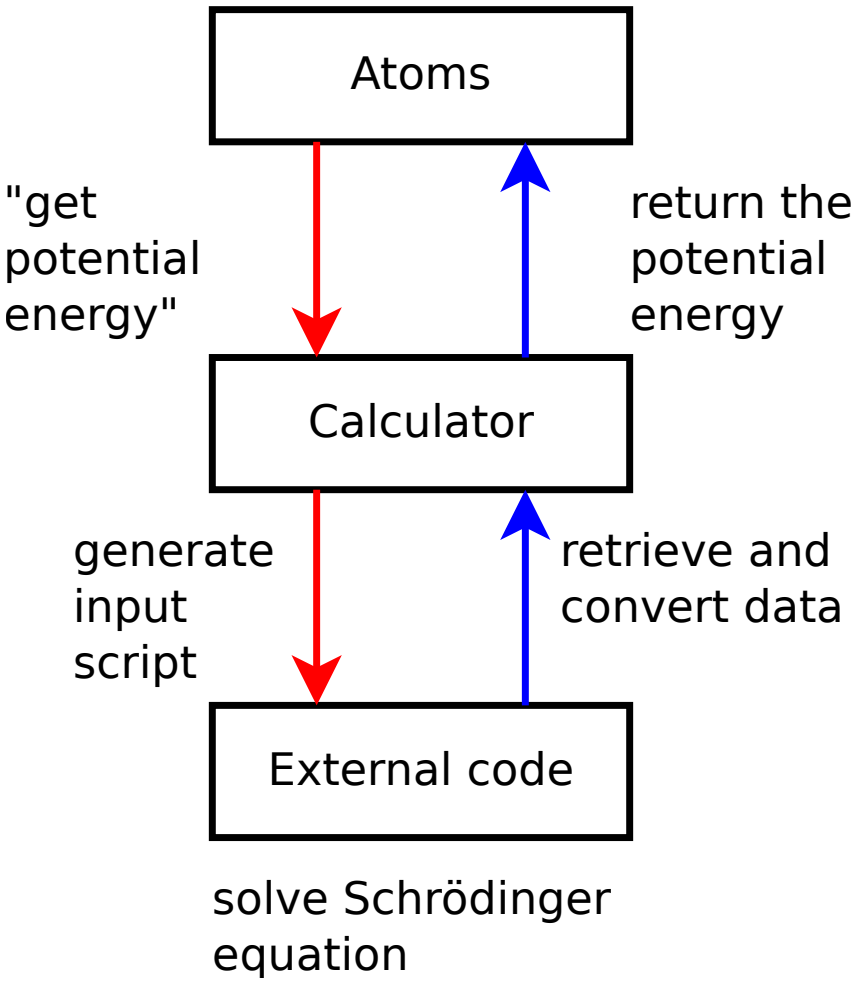
- The `Atoms` object: A collection of atoms
- Calculators: Capable of calculating energies and forces of atoms, often using an external code as backend
- Algorithms working with atoms/calculators: Structure optimization, molecular dynamics, basin hopping, minima hopping, nudged elastic band, ...
- Many utilities: Build crystals, surfaces, ...
- Read/write structures in many formats
- Also: GUI, command-line utilities

Example: Structure optimization

```
from ase import Atoms
from ase.optimize import BFGS
from gpaw import GPAW

system = Atoms('H2O', positions=[[-1, 0, 0],
                                 [1, 0, 0],
                                 [0, 0, 1]])
system.center(vacuum=3.0)
system.calc = GPAW(mode='lcao', basis='dzp')

opt = BFGS(system,
           trajectory='opt.traj',
           logfile='opt.log')
opt.run(fmax=0.05)
```

Example 2: Structure optimization

```
from ase import Atoms
from ase.optimize import BFGS
from ase.calculators.espresso import Espresso

system = Atoms('H2O', positions=[[-1, 0, 0],
                                 [1, 0, 0],
                                 [0, 0, 1]])
system.center(vacuum=3.0)
system.calc = Espresso(
    ecutwfc=40., pseudo_dir='.', tprnfor=True,
    pseudopotentials={'H': 'H_ONCV_PBE-1.0.upf',
                      'O': 'O_ONCV_PBE-1.0.upf'})
opt = BFGS(system, trajectory='opt.traj',
           logfile='opt.log')
opt.run(fmax=0.05)
```



Interface through file I/O

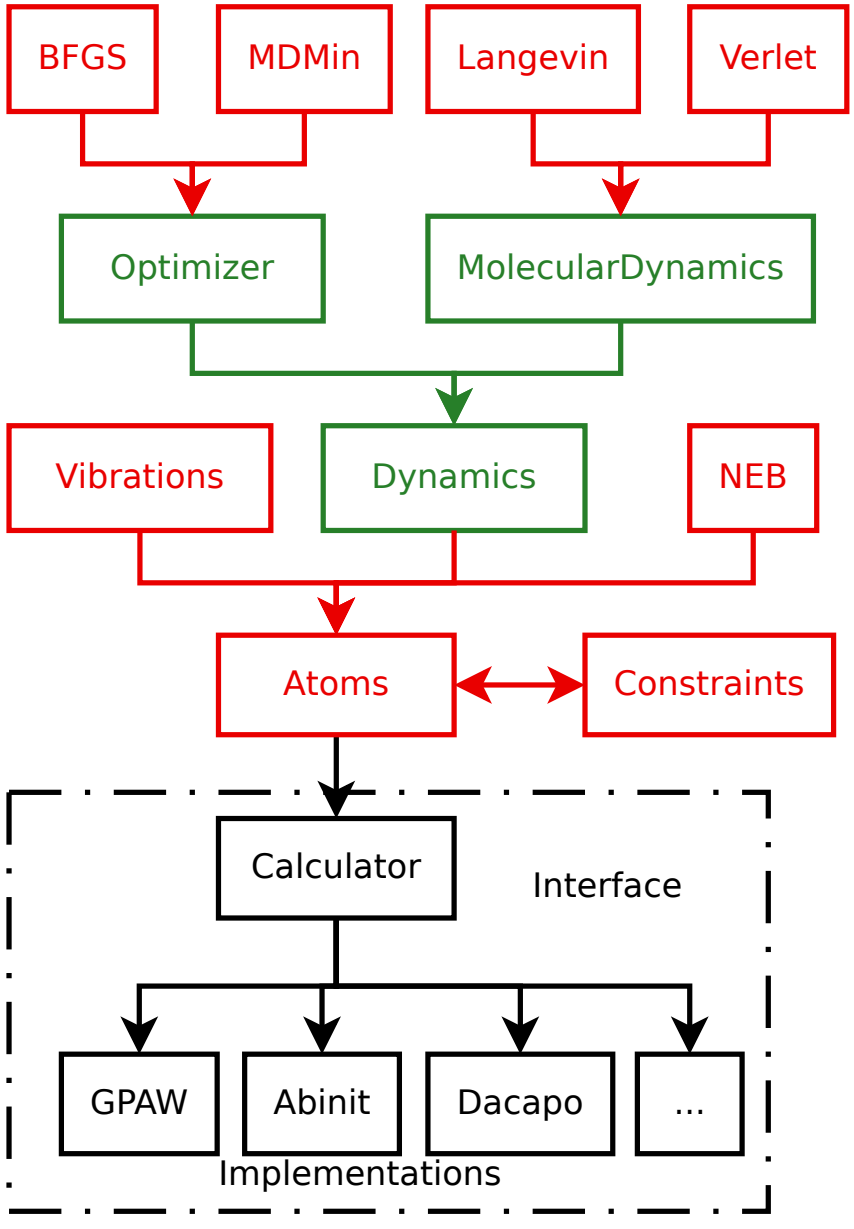
- ASE creates inputfile, runs programme (see figure)

Calculator daemon

- Calculator runs in background
- Read/write using sockets

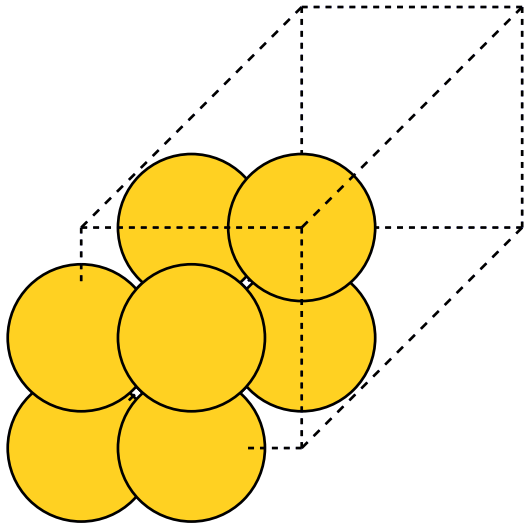
Direct linking

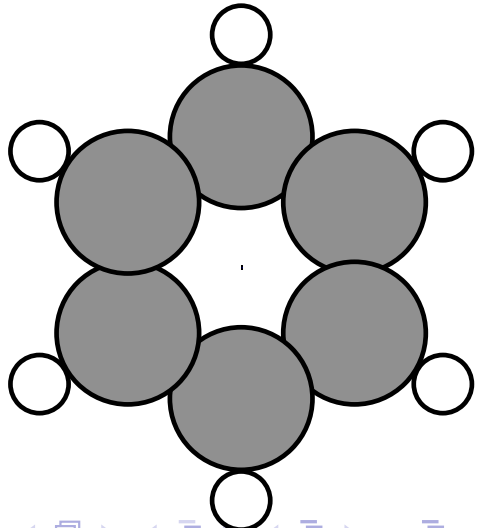
- Everything within one process $\rightarrow$ efficient and flexible
- Also rather complicated


BFGS
MDMin
Langevin
Verlet
Optimizer
MolecularDynamics
Vibrations
Dynamics
NEB
Atoms
Constraints
Calculator
Interface
GPAW
Abinit
Dacapo
...
Implementations

Build and view structures

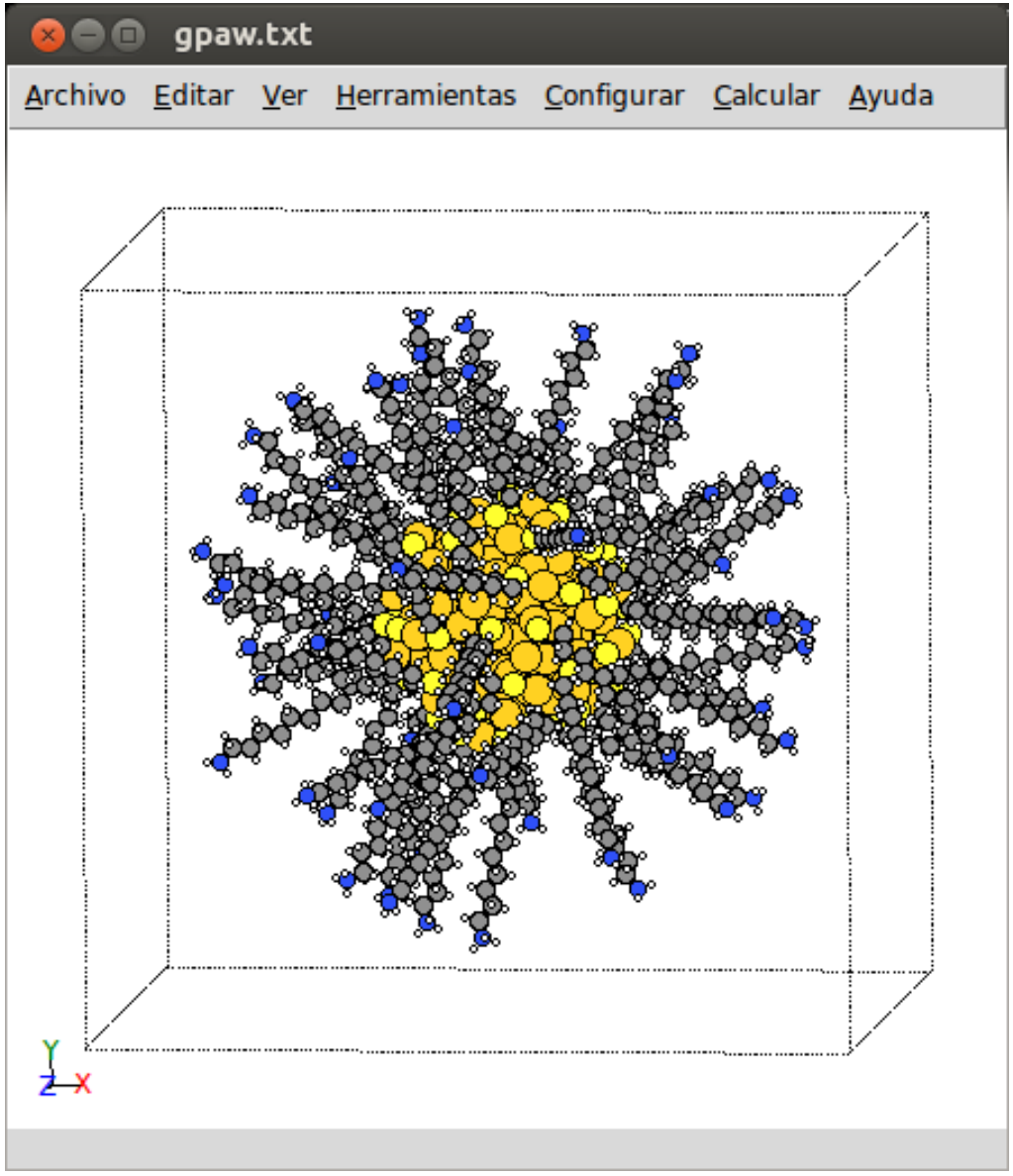
```
from ase import Atoms
from ase.visualize import view

a = 2.04
gold = Atoms('Au', pbc=True,
             cell=[[0, a, a],
                   [a, 0, a],
                   [a, a, 0]])
print(gold)
view(gold.repeat((2, 2, 2)))

from ase.build import molecule
view(molecule('C6H6'))
```





Try the ASE GUI

- Run `ase gui` (previously: `ase-gui`)
- Build nanoparticle or something else
- Select, move atoms (Ctrl+M)
- Save to your favourite format



More on ASE

- Started as an object-oriented Python interface to the old ultrasoft pseudopotential planewave code Dacapo
- S.R. Bahn, K.W. Jacobsen, "An object-oriented scripting interface to a legacy electronic structure code". Computing in Science & Engineering, 4(3):56–66, 2002.
- BDFL: Jens Jørgen Mortensen, DTU Physics
- Very large number of contributors
- New reference paper: A.H. Larsen, J.J. Mortensen *et al.*, 2017 *J. Phys. Condens. Matter* **29** 273002, 2017. "The Atomic Simulation Environment – A Python library for working with atoms". (Also available as Psi-k Highlight of the Month, January 2017)

Concluding remarks

- Web page: `https://wiki.fysik.dtu.dk/ase/`
- Gitlab: `https://gitlab.com/ase/ase`
- Mailing lists, IRC:
  `https://wiki.fysik.dtu.dk/ase/contact.html`