PyPartMC

A Pythonic interface to a particle-resolved Monte Carlo aerosol simulation framework

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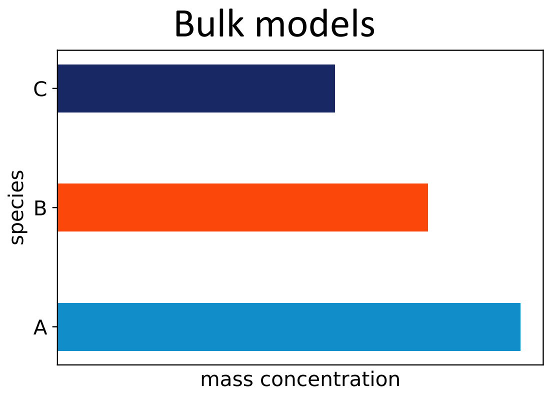
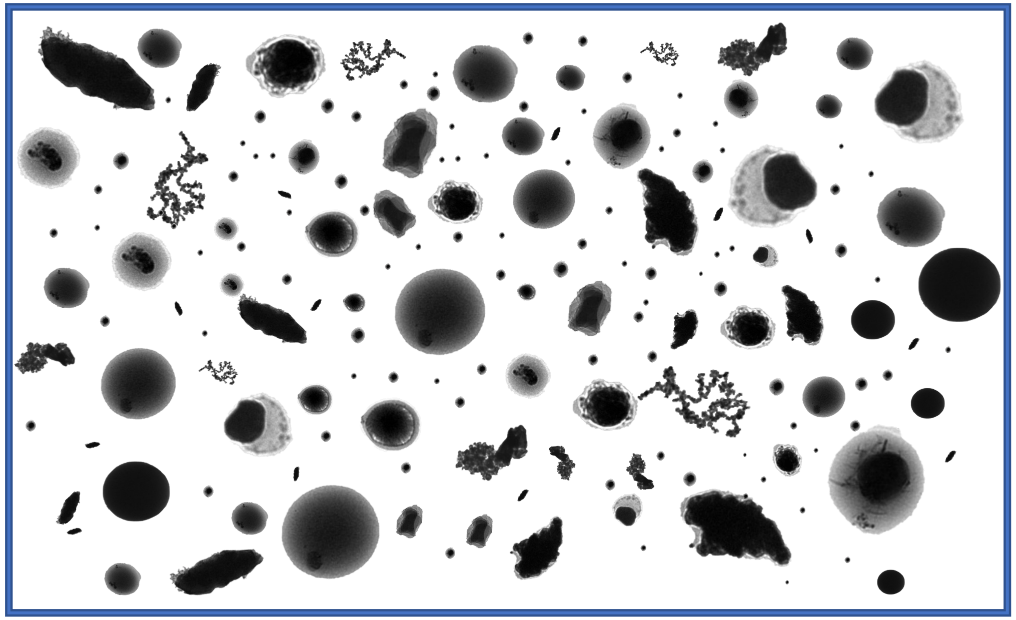
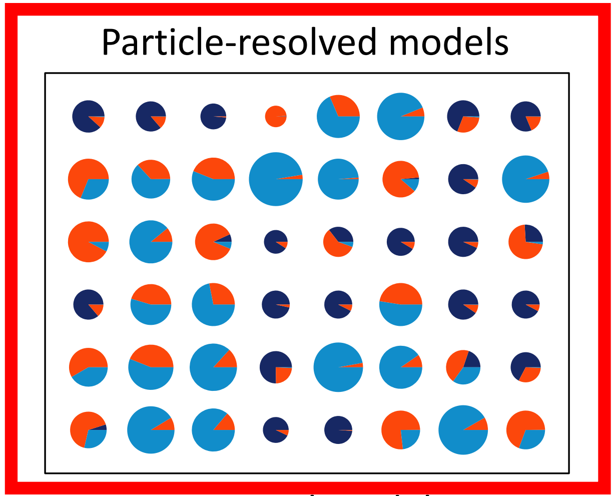
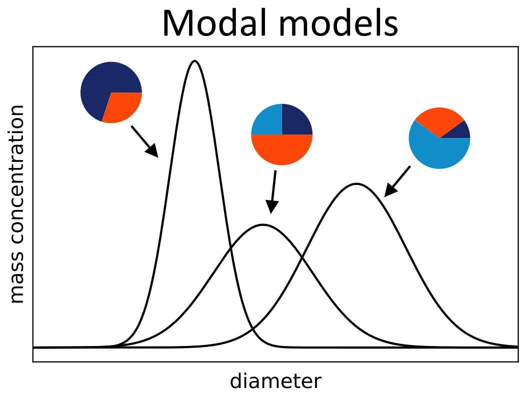
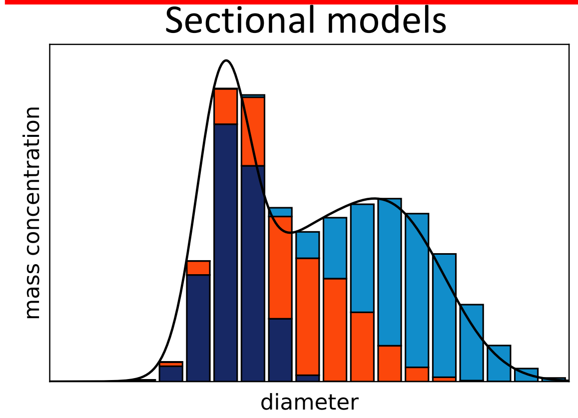
Particle-resolved modeling



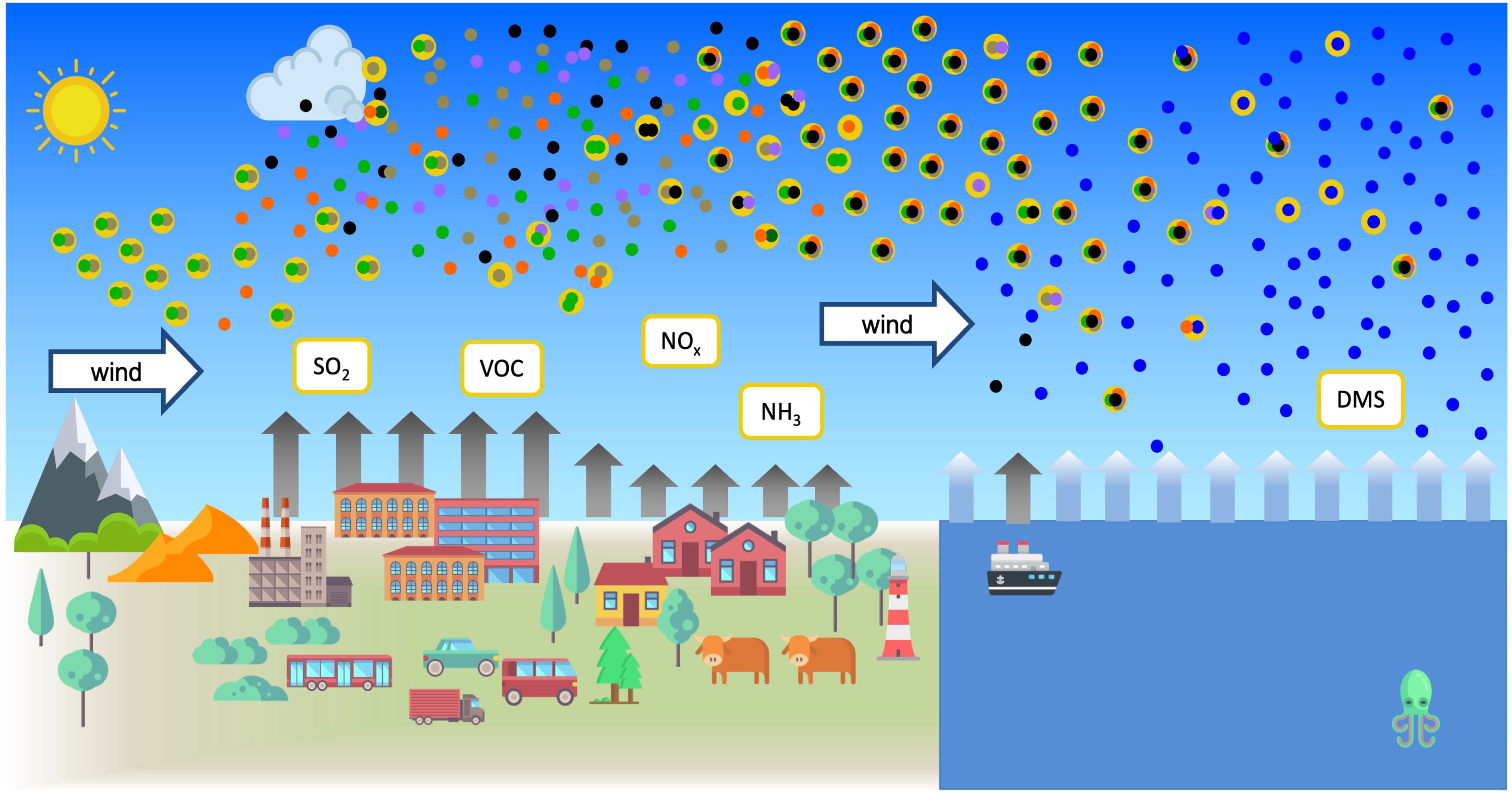








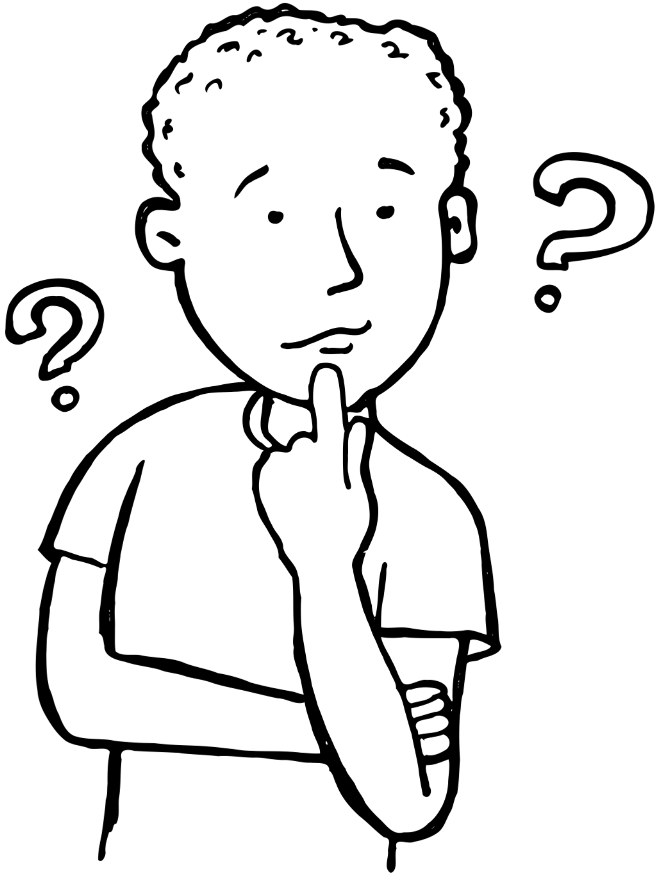
PartMC

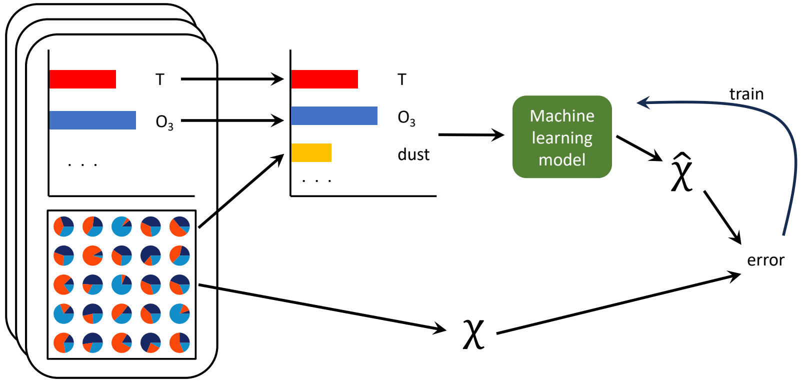


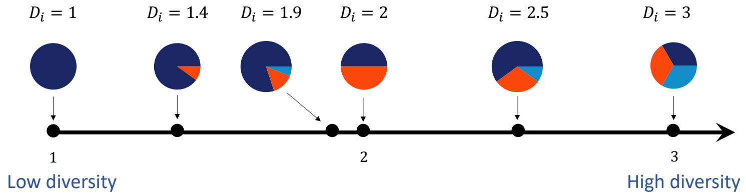
- Emission from primary sources
- Brownian coagulation
- Nucleation scavenging
- Dry deposition

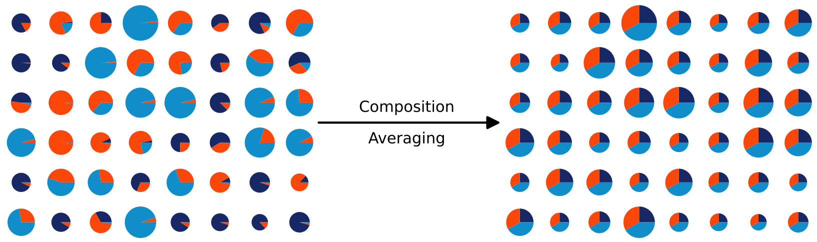
Riemer, Ault, West, Craig, Curtis, *Rev. Geophys.*, 2019

Why do we need PyPartMC?









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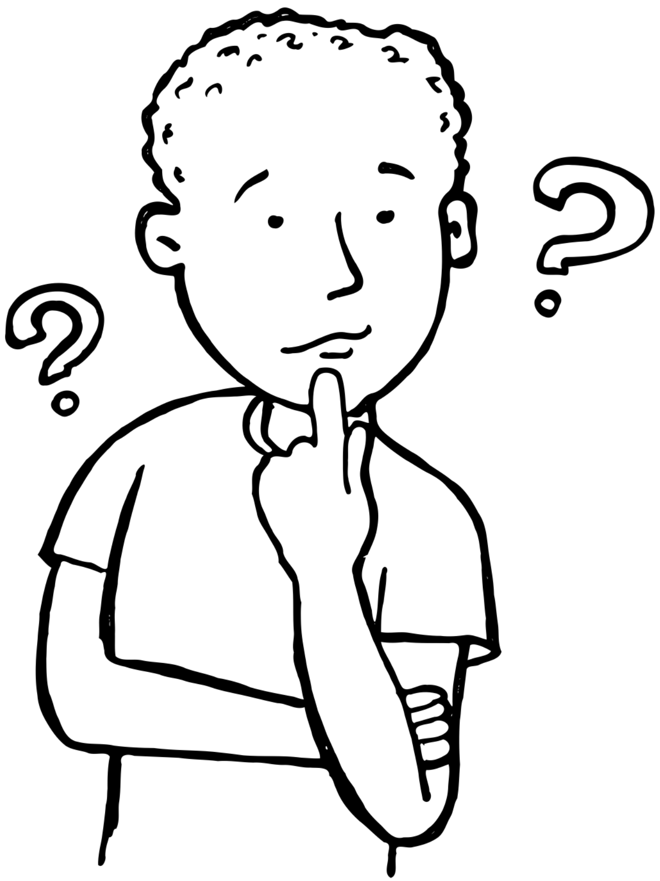
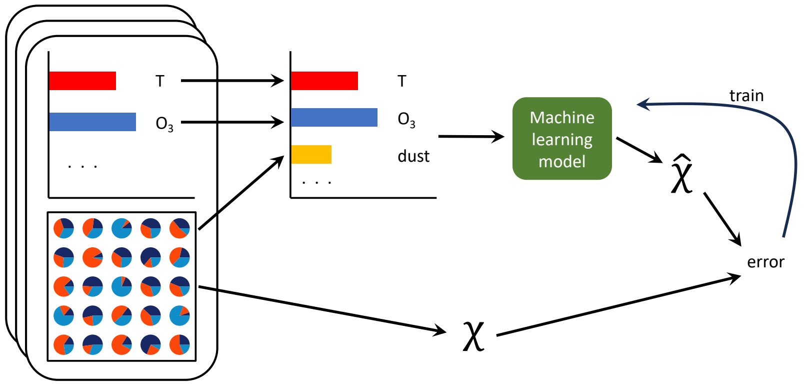
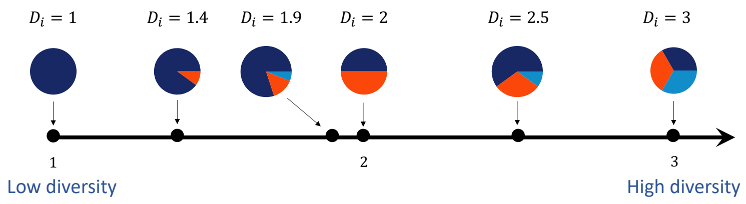
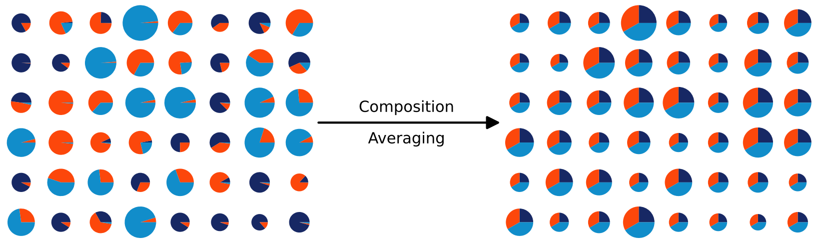
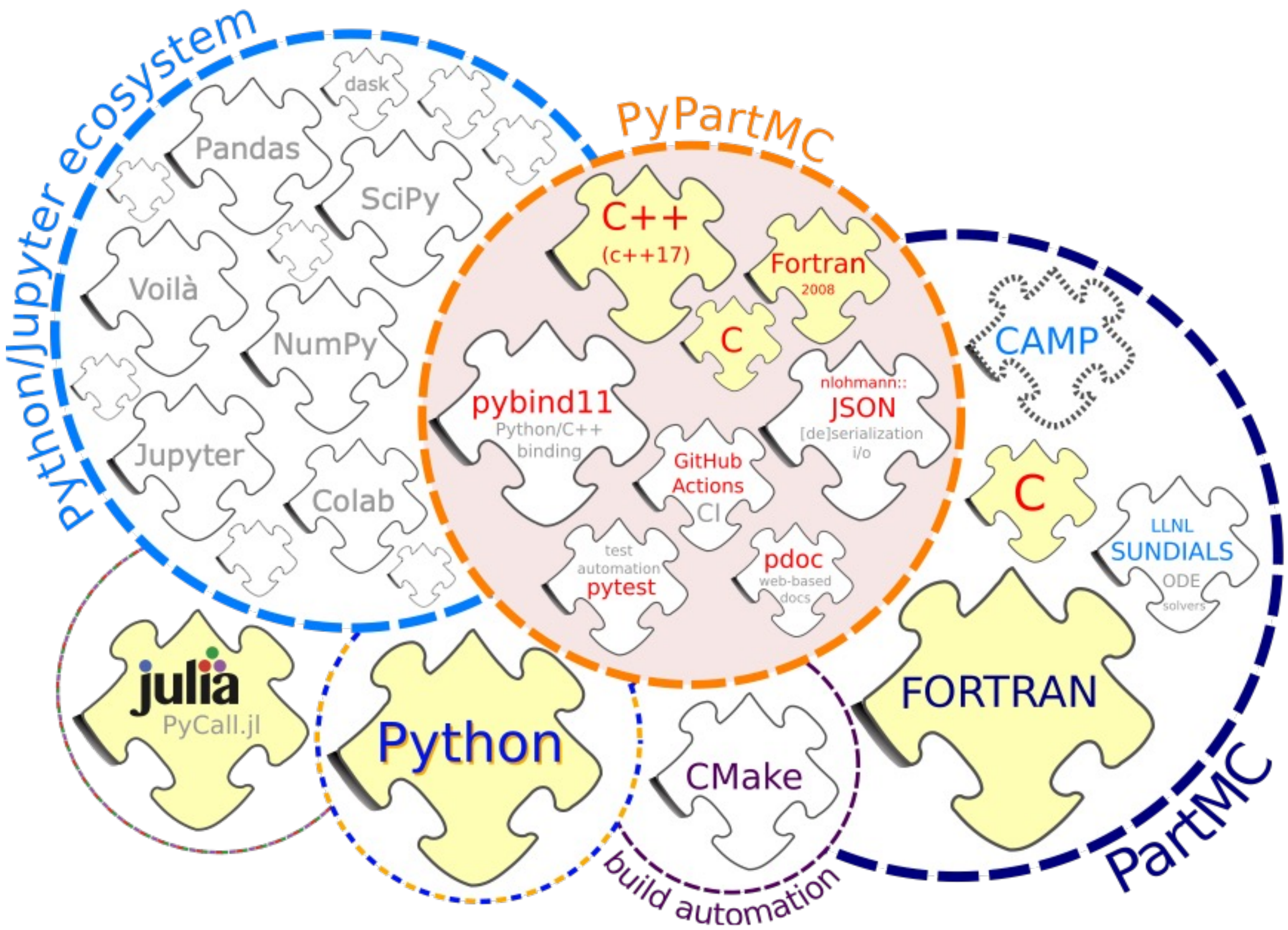




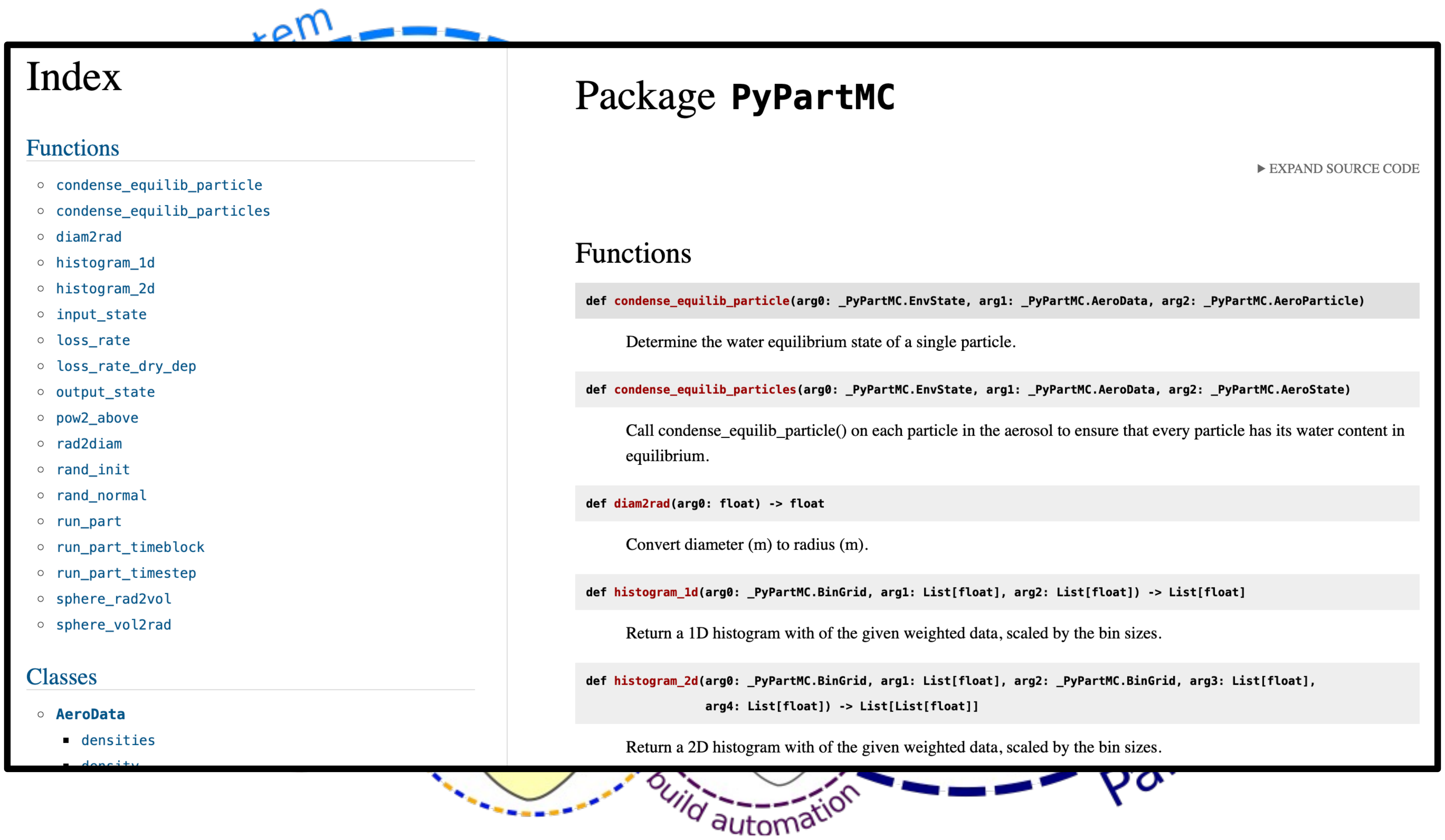




Key technologies



Key technologies



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Classes

- **AeroData**
  - densities

Package **PyPartMC**

▶ EXPAND SOURCE CODE

Functions

```
def condense_equilib_particle(arg0: _PyPartMC.EnvState, arg1: _PyPartMC.AeroData, arg2: _PyPartMC.AeroParticle)
```

Determine the water equilibrium state of a single particle.

```
def condense_equilib_particles(arg0: _PyPartMC.EnvState, arg1: _PyPartMC.AeroData, arg2: _PyPartMC.AeroState)
```

Call condense_equilib_particle() on each particle in the aerosol to ensure that every particle has its water content in equilibrium.

```
def diam2rad(arg0: float) -> float
```

Convert diameter (m) to radius (m).

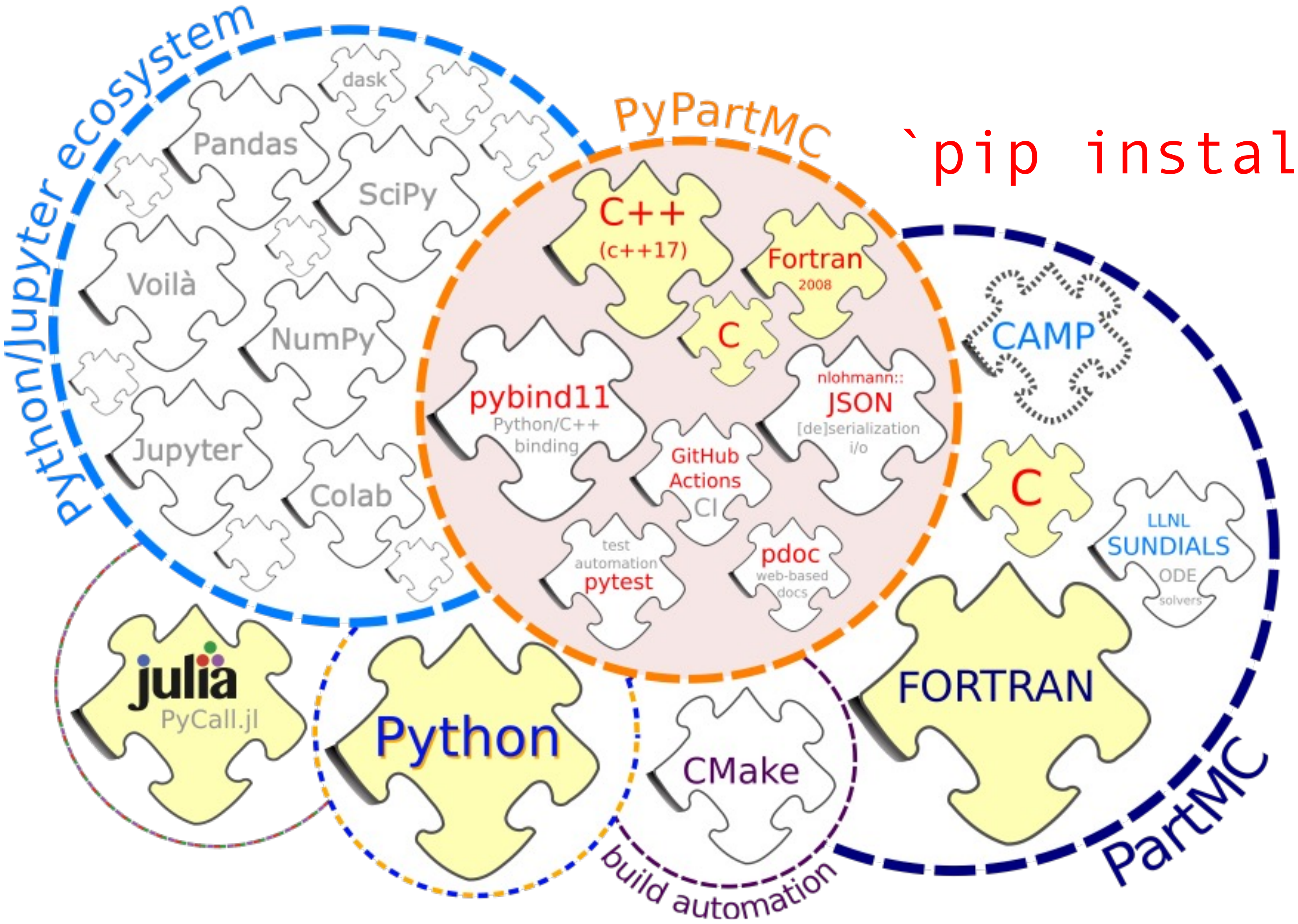
```
def histogram_1d(arg0: _PyPartMC.BinGrid, arg1: List[float], arg2: List[float]) -> List[float]
```

Return a 1D histogram with of the given weighted data, scaled by the bin sizes.

```
def histogram_2d(arg0: _PyPartMC.BinGrid, arg1: List[float], arg2: _PyPartMC.BinGrid, arg3: List[float],
            arg4: List[float]) -> List[List[float]]
```

Return a 2D histogram with of the given weighted data, scaled by the bin sizes.

Key technologies



`pip install PyPartMC`

PartMC

```fortran
module pmc_aero_particle

  type aero_particle_t
     !> Constituent species volumes [length # of species] (m^3).
     real(kind=dp), allocatable :: vol(:)
  end type aero_particle_t

contains

  !> Total volume of the particle (m^3).
  elemental real(kind=dp) function aero_particle_volume(aero_particle)

     !> Particle.
     type(aero_particle_t), intent(in) :: aero_particle

     aero_particle_volume = sum(aero_particle%vol)

  end function aero_particle_volume

end module
```

PyPartMC

```fortran
module PyPartMC_aero_particle
  use iso_c_binding
  use pmc_aero_particle
  implicit none

  contains

  subroutine f_aero_particle_volume(ptr_c, vol) bind(C)
    type(aero_particle_t), pointer :: ptr_f => null()
    type(c_ptr), intent(in) :: ptr_c
    real(c_double), intent(out) :: vol

    call c_f_pointer(ptr_c, ptr_f)

    vol = aero_particle_volume(ptr_f)
  end subroutine

end module
```

```cpp
extern "C" void f_aero_particle_volume(const void *ptr, double *vol) noexcept;

namespace py = pybind11;
struct AeroParticle {
    static auto volume(const AeroParticle &self) {
        double vol;
        f_aero_particle_volume(
            self.ptr.f_arg(),
            &vol
        );
        return vol;
    }
}
```

```cpp
PYBIND11_MODULE(_PyPartMC, m) {
    pybind11::class_<AeroParticle>(m, "AeroParticle",
        R"pbdoc(
             Single aerosol particle data structure.

             The \c vol array stores the total volumes of the different
             species that make up the particle.
        )pbdoc"
    )
        .def_property_readonly("volume", AeroParticle::volume,
            "Total volume of the particle (m^3).")
}
```

```python
import PyPartMC as ppmc
from PyPartMC import si
import gc

class TestAeroParticle:

    @staticmethod
    def test_volume():
        aero_data_arg = (
            {"H2O": [1000 * si.kg / si.m**3,
             1, 18e-3 * si.kg / si.mol, 0]}
        )
        aero_data = ppmc.AeroData(aero_data_arg)
        volumes = [1e-6]
        sut = ppmc.AeroParticle(aero_data, volumes)
        aero_data = None
        gc.collect()

        vol = sut.volume

        assert vol == sum(volumes)
```

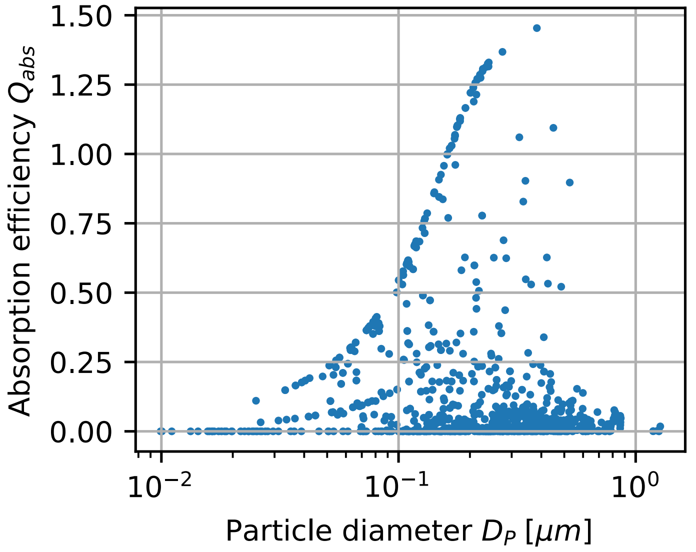
- PyPartMC operates with unmodified PartMC
- Data remains in underlying PartMC Fortran types
- Modularity of PartMC allows wrapping structure to work
- C++ wrappers allow pybind11 to automate API generation

Example using external package

User-defined function employs the PyMieScatt package to compute optical properties at each timestep

```
def aero_state_compute_optical(aero_state_optical):
    wl = 550.0 # unit: nm
    refr_shell = 1.52+0*1j
    refr_core = 1.82+0.74*1j
    diams_core = np.array(aero_state_optical.diameters(include=["BC"])) * 1e9 # unit: nm
    diams_total = np.array(aero_state_optical.diameters()) * 1e9 # unit: nm

    qsca_part = np.zeros(len(aero_state_optical))
    qabs_part = np.zeros(len(aero_state_optical))
    for i_part in range(len(aero_state_optical)):
        val = PyMieScatt.MieQCoreShell(refr_core,
                                        refr_shell,
                                        wl,
                                        diams_core[i_part],
                                        diams_total[i_part],
                                        asDict=True
                                        )
        qsca_part[i_part] = val['Qsca']
        qabs_part[i_part] = val['Qabs']

    cross_section = np.pi * (diams_total / 2 / 1e9)**2

    num_concs = aero_state_optical.num_concs
    B_abs = np.sum(qabs_part * cross_section * num_concs)
    B_sca = np.sum(qsca_part * cross_section * num_concs)

    return (diams_total, qsca_part, qabs_part, B_sca, B_abs)
```

```
for i_block in range(1,N_BLOCKS+1):
    i_next = int(N_STEPS_PER_BLOCK * i_block)
    ppmc.run_part_timeblock(
        scenario,
        env_state,
        aero_data,
        aero_state,
        gas_data,
        gas_state,
        run_part_opt,
        camp_core,
        photolysis,
        i_time,
        i_next,
        0,
    )
    time[i_block] = env_state.elapsed_time
    diameters, qsca, qabs, Bsca[i_block], Babs[i_block] = aero_state_compute_optical(aero_state)
    i_time = i_next + 1
```



Time stepping in Fortran

process_simulation_output.ipynb

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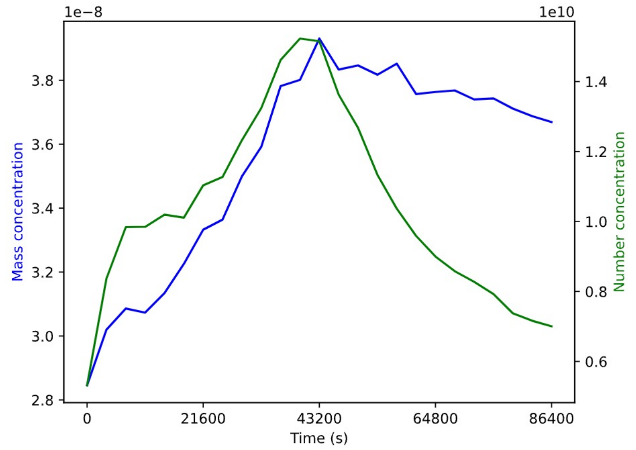
[44]
```
ppmc.run_part(scenario, env_state, aero_data,
         aero_state, gas_data, gas_state,
         run_part_opt, camp_core,photolysis,
)
```

Time stepping in Fortran

```
N_TIMES = 25
num_conc = np.zeros(N_TIMES)
mass_conc = np.zeros(N_TIMES)
time = np.zeros(N_TIMES)
for i_time in range(N_TIMES):
    filename = ppmc.input_state(f"urban_plume_0001_{i_time+1:08}.nc",
                                aero_data, aero_state, gas_data, gas_state,
                                env_state)
    num_conc[i_time] = aero_state.total_num_conc
    mass_conc[i_time] = aero_state.total_mass_conc

plt.plot(time, mass_conc, "b", label="mass conc")
plt.ylabel("Mass concentration", color='b')
plt.xlabel("Time (s)")
plt.twinx()
plt.plot(time, num_conc, "g", label="num conc")
plt.xticks(np.linspace(0, time[-1], 5))
plt.ylabel("Number concentration", color='g')
show_plot()
```

Processes data from outputted netCDF files and use matplotlib to visualize



- Entire simulation runs in Google Colab
- Choice in time stepping control
- Data generation and processing in a single notebook

More than just a wrapper!

GitHub

Documentation

Atmospheric
System Research