



# PyPartMC

aerosol dynamics package:

Sylwester Arabas<sup>1</sup>, Zach D'Aquino<sup>2</sup>, Jeff Curtis<sup>2</sup>, Nicole Riemer<sup>2</sup>, Matt West<sup>3</sup>  
& [Py]PartMC contributors

Jan 26<sup>th</sup> 2024  
Columbia University, New York

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<sup>3</sup>Mechanical Science & Engineering, University of Illinois at Urbana-Champaign ([mechse.illinois.edu](http://mechse.illinois.edu))

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- ▶ maintainer & developer:
  - ▶ [github.com/numba-mpi](https://github.com/numba-mpi)
  - ▶ [github.com/open-atmos/{PySDM,PyMPDATA,PyPartMC}](https://github.com/open-atmos/{PySDM,PyMPDATA,PyPartMC})





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aerosol dynamics package:  
engineering Python-to-Fortran bindings  
in C++, for use in Julia and Matlab

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# plan of the talk

PyPartMC: context / statement of need

PyPartMC: goals and status

PyPartMC: design & implementation outline

PyPartMC: demo

PyPartMC: summary



<https://lagrange.mechse.illinois.edu/partmc/>



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- ▶ Monte-Carlo aerosol dynamics simulation package



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- ▶ Monte-Carlo aerosol dynamics simulation package
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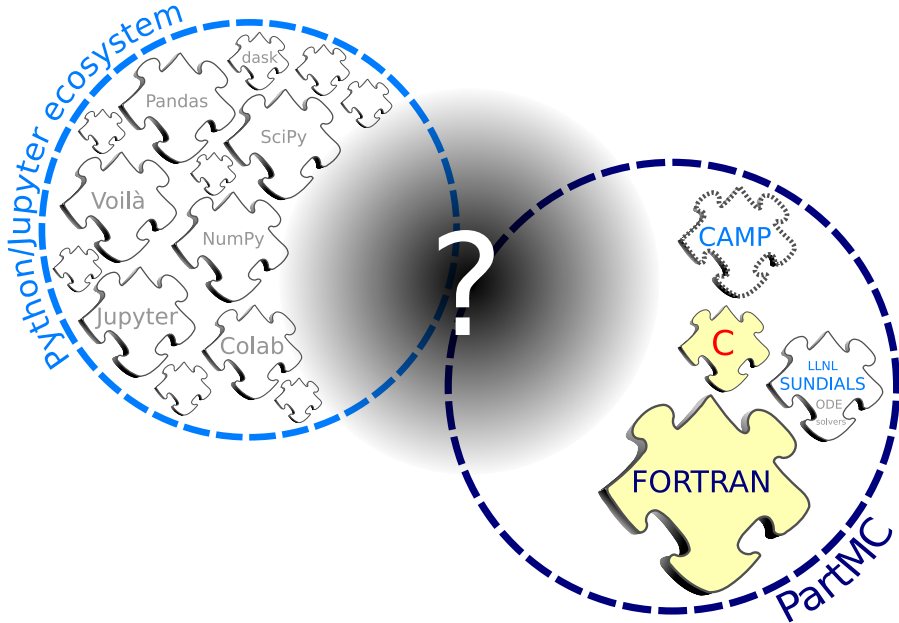
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- ▶ object-oriented architecture, F90, extensive automated test suite



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## project goals

- ▶ **lower the entry threshold for installing and setting up of PartMC**  
down to `pip install PyPartMC`, i.e., no manual dependency installation,  
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## project goals

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- ▶ ensure the same experience on Linux, macOS & Windows
- ▶ **lower the entry threshold for usage with Jupyter-based example notebooks**
- ▶ streamline the dissemination of paper-result reproducers (peer review)

status of the project: v1.0 in Dec 2023 (started 2021)

# SoftwareX



ORIGINAL SOFTWARE PUBLICATION

## PyPartMC: A Pythonic interface to a particle-resolved, Monte Carlo aerosol simulation framework

Zachary D'Aquino • Sylwester Arabas • Jeffrey H. Curtis • Akshunna Vaishnav • Nicole Riemer   • Matthew West

Open Access • Published: December 23, 2023 • DOI: <https://doi.org/10.1016/j.softx.2023.101613>



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## PyPartMC 1.0.1



```
pip install PyPartMC
```



Released: Dec 16, 2023

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pybind11 — Seamless operability between C++11 and Python

docs passing docs stable chat on glitter Discussions Ask CI passing build passing

latest packaged version 2.11.1 pypi v2.11.1 conda-forge v2.11.0 python 3.6 | 3.7 | 3.8 | 3.9 | 3.10 | 3.11 | 3.12

[Setuptools example](#) • [Scikit-build example](#) • [CMake example](#)

**pybind11** is a lightweight header-only library that exposes C++ types in Python and vice versa, mainly to create Python bindings of existing C++ code. Its goals and syntax are similar to the excellent [Boost.Python](#) library by David Abrahams: to minimize boilerplate code in traditional extension modules by inferring type information using compile-time introspection.

## About

Seamless operability between C++11 and Python

[pybind11.readthedocs.io/](https://pybind11.readthedocs.io/)

[#python](#) [#bindings](#)

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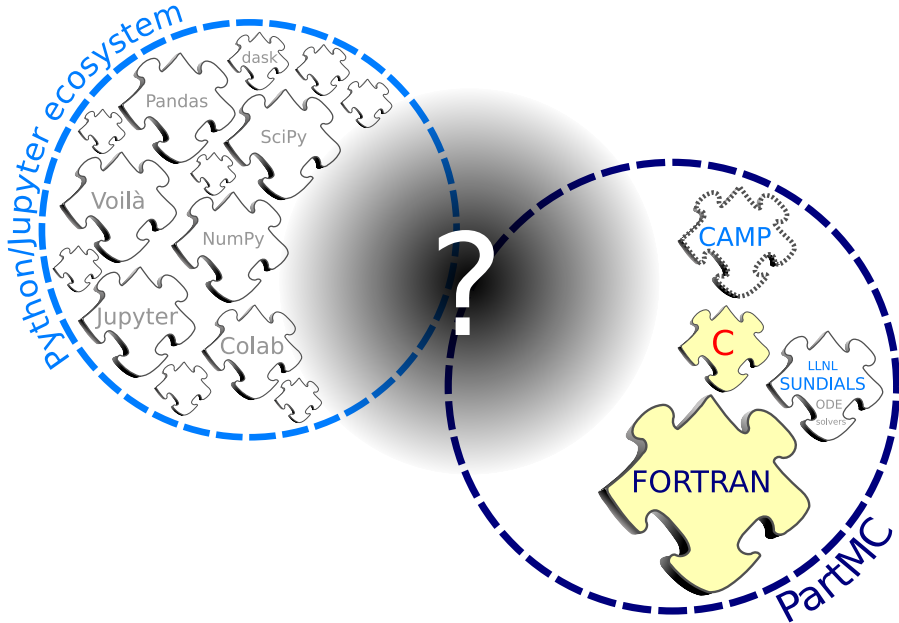
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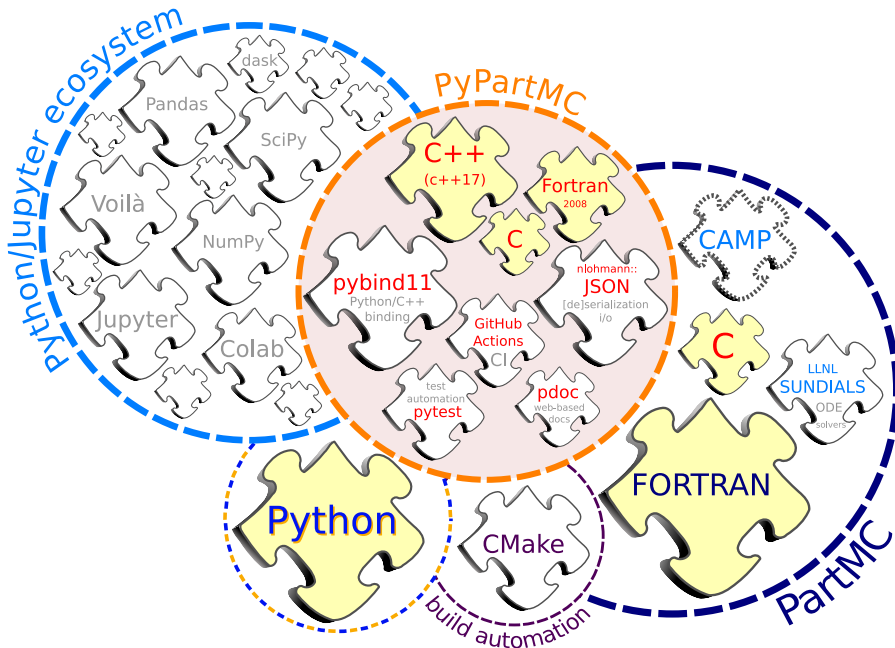
## Releases 21

Version 2.11.1 Latest  
on Jul 17, 2023

+ 20 releases

Contributors 337





## solving the challenges

- ▶ written in C/Fortran/C++ as **C++ bindings** to PartMC internals (derived types), Python bindings generated using **pybind11**

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- ▶ JSON-based reimplementation of PartMC "spec-file" i/o module (unmodified code of PartMC uses original API)  
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- ▶ **dependency version pinning with git submodules**: PartMC (F), CAMP (C/F), json (C++), pybind11 (C++), json-fortran (F), netCDF (C/F), SUNDIALS (F/C), SuiteSparse (C), ... & backports of C++20 features to C++17 (multilinux!): span, string\_view, optional

## solving the challenges

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- ▶ all dependencies (incl. Fortran and C++ runtimes) statically linked (single-file install)

# user perspective: Fortran (PartMC)

## c: Fortran code

```
program main
  use pmc_spec_file
  use pmc_aero_data
  use pmc_aero_mode
  use pmc_aero_dist
  use pmc_aero_state

  implicit none

  type(spec_file_t) :: f_aero_data, f_aero_dist
  type(aero_data_t) :: aero_data
  type(aero_dist_t) :: aero_dist
  type(aero_state_t) :: aero_state
  integer, parameter :: n_part = 100
  integer :: n_part_add
  real(kind=dp), dimension(n_part) :: num_concs, masses

  call spec_file_open("aero_data.dat", f_aero_data)
  call spec_file_read_aero_data(f_aero_data, aero_data)
  call spec_file_close(f_aero_data)

  call spec_file_open("aero_dist.dat", f_aero_dist)
  call spec_file_read_aero_dist(f_aero_dist, aero_data, aero_dist)
  call spec_file_close(f_aero_dist)

  call aero_state_zero(aero_state)
  call fractal_set_spherical(aero_data%fractal)
  call aero_state_set_weight(aero_state, aero_data, &
    AERO_STATE_WEIGHT_NUMMASS_SOURCE)
  call aero_state_set_n_part_ideal(aero_state, dble(n_part))
  call aero_state_add_aero_dist_sample(aero_state, aero_data, &
    aero_dist, 1d0, 0d0, .true., .true., n_part_add)

  num_concs = aero_state_num_concs(aero_state, aero_data)
  masses = aero_state_masses(aero_state, aero_data)
  print *, dot_product(num_concs, masses), "# kg/m3"
end
```

## d: aero\_dist.dat file (for Fortran code)

```
mode_name cooking
mass_frac cooking_comp.dat
diam_type geometric
mode_type log_normal
num_conc 3.2e9 # (#/m^3)
geom_mean_diam 8.64e-9 # (m)
log10_geom_std_dev 0.28
```

```
mode_name diesel
mass_frac diesel_comp.dat
diam_type geometric
mode_type log_normal
num_conc 2.9e9 # (#/m^3)
geom_mean_diam 5e-8
log10_geom_std_dev 0.24
```

## e: cooking\_comp.dat file (for Fortran code)

#	proportion
OC	1

## f: diesel\_comp.dat file (for Fortran code)

#	proportion
OC	0.3
BC	0.7

# user perspective: Python (PyPartMC)

## a: Python code (with embedded data)

```
import numpy as np

import PyPartMC as ppmc
from PyPartMC import si

aero_data = ppmc.AeroData((
    # [density, ions in solution, molecular weight, kappa]
    {"OC": [1000 * si.kg/si.m**3, 0, 1e-3 * si.kg/si.mol, 0.001]},
    {"BC": [1800 * si.kg/si.m**3, 0, 1e-3 * si.kg/si.mol, 0]},
))

aero_dist = ppmc.AeroDist(
    aero_data,
    [{
        "cooking": {
            "mass_frac": [{"OC": [1]}],
            "diam_type": "geometric",
            "mode_type": "log_normal",
            "num_conc": 3200 / si.cm**3,
            "geom_mean_diam": 8.64 * si.nm,
            "log10_geom_std_dev": 0.28,
        },
    },
    {
        "diesel": {
            "mass_frac": [{"OC": [0.3]}, {"BC": [0.7]}],
            "diam_type": "geometric",
            "mode_type": "log_normal",
            "num_conc": 2900 / si.cm**3,
            "geom_mean_diam": 50 * si.nm,
            "log10_geom_std_dev": 0.24,
        },
    },
    ],
)

n_part = 100
aero_state = ppmc.AeroState(aero_data, n_part, "nummass_source")
aero_state.dist_sample(aero_dist)
print(np.dot(aero_state.masses, aero_state.num_concs), "# kg/m3")
```

# user perspective: Python (PyPartMC) & Julia (via PyCall.jl)

## a: Python code (with embedded data)

```
import numpy as np

import PyPartMC as ppmc
from PyPartMC import si

aero_data = ppmc.AeroData((
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    {"OC": [1000 * si.kg/si.m**3, 0, 1e-3 * si.kg/si.mol, 0.001]},
    {"BC": [1800 * si.kg/si.m**3, 0, 1e-3 * si.kg/si.mol, 0]},
))

aero_dist = ppmc.AeroDist(
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        "cooking": {
            "mass_frac": [{"OC": [1]}],
            "diam_type": "geometric",
            "mode_type": "log_normal",
            "num_conc": 3200 / si.cm**3,
            "geom_mean_diam": 8.64 * si.nm,
            "log10_geom_std_dev": 0.28,
        },
    },
    {
        "diesel": {
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            "diam_type": "geometric",
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            "num_conc": 2900 / si.cm**3,
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        },
    },
])

n_part = 100
aero_state = ppmc.AeroState(aero_data, n_part, "nummass_source")
aero_state.dist_sample(aero_dist)
print(np.dot(aero_state.masses, aero_state.num_concs), "# kg/m3")
```

## b: Julia code (with embedded data)

```
using Pkg
Pkg.add("PyCall")

using PyCall
ppmc = pyimport("PyPartMC")
si = ppmc["si"]

aero_data = ppmc.AeroData((
    # (density, ions in solution, molecular weight, kappa)
    Dict{"OC"=>(1000 * si.kg/si.m^3, 0, 1e-3 * si.kg/si.mol, 0.001)},
    Dict{"BC"=>(1800 * si.kg/si.m^3, 0, 1e-3 * si.kg/si.mol, 0)})
))

aero_dist = ppmc.AeroDist(aero_data, (
    Dict(
        "cooking" => Dict(
            "mass_frac" => (Dict{"OC" => (1,)},),
            "diam_type" => "geometric",
            "mode_type" => "log_normal",
            "num_conc" => 3200 / si.cm^3,
            "geom_mean_diam" => 8.64 * si.nm,
            "log10_geom_std_dev" => .28,
        ),
    ),
    Dict(
        "diesel" => Dict(
            "mass_frac" => (Dict{"OC" => (.3,)}, Dict{"BC" => (.7,)}),
            "diam_type" => "geometric",
            "mode_type" => "log_normal",
            "num_conc" => 2900 / si.cm^3,
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        ),
    ),
))

n_part = 100
aero_state = ppmc.AeroState(aero_data, n_part, "nummass_source")
aero_state.dist_sample(aero_dist)
print(aero_state.masses' aero_state.num_concs, "# kg/m3")
```

## user perspective: Matlab (built-in Python bridge)

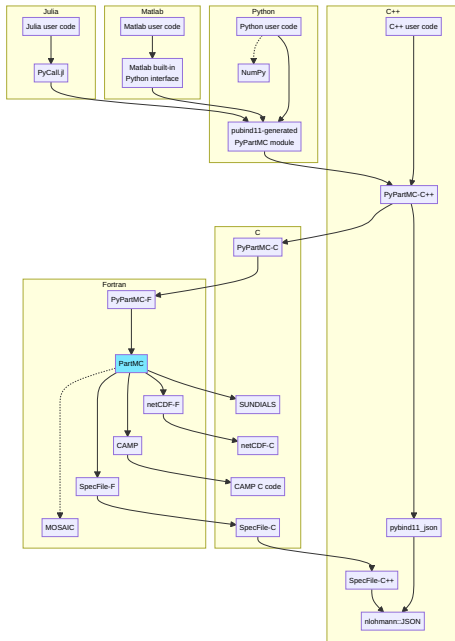
```
ppmc = py.importlib.import_module('PyPartMC');
si = py.importlib.import_module('PyPartMC').si;

aero_data = ppmc.AeroData(py.tuple({ ...
    py.dict(pyargs("OC", py.tuple({1000 * si.kg/si.m^3, 0, 1e-3 * si.kg/si.mol, 0.001}))), ...
    py.dict(pyargs("BC", py.tuple({1800 * si.kg/si.m^3, 0, 1e-3 * si.kg/si.mol, 0}))) ...
}));

aero_dist = ppmc.AeroDist(aero_data, py.tuple({ ...
    py.dict(pyargs( ...
        "cooking", py.dict(pyargs( ...
            "mass_frac", py.tuple({py.dict(pyargs("OC", py.tuple({1})))), ...
            "diam_type", "geometric", ...
            "mode_type", "log_normal", ...
            "num_conc", 3200 / si.cm^3, ...
            "geom_mean_diam", 8.64 * si.nm, ...
            "log10_geom_std_dev", .28 ...
        )) ...
    )), ...
    py.dict(pyargs( ...
        "diesel", py.dict(pyargs( ...
            "mass_frac", py.tuple({ ...
                py.dict(pyargs("OC", py.tuple({.3}))), ...
                py.dict(pyargs("BC", py.tuple({.7}))), ...
            )), ...
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            "num_conc", 2900 / si.cm^3, ...
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        )) ...
    )) ...
}));

n_part = 100;
aero_state = ppmc.AeroState(aero_data, n_part, "nummass_source");
aero_state.dist_sample(aero_dist);
masses = cell(aero_state.masses());
num_concs = cell(aero_state.num_concs());
fprintf('%g # kg/m3\n', dot([masses{:}], [num_concs{:}])))
```





PyPartMC API documentation

+

← → ↺ 🏠

🔒 https://open-atmos.github.io/PyPartMC/

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📄 📁 📄 📄 📄

Index

Functions

condense\_equilib\_particles  
pow2\_above  
run\_part

Classes

AeroData  
AeroState  
EnvState  
GasData  
GasState  
RunPartOpt  
Scenario

Module **PyPartMC**

PyPartMC is a Python interface to PartMC.

Functions

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

Call condense\_equilib\_particle() on each particle in the aerosol to ensure that every particle has its water content in equilibrium.

```
def pow2_above(arg0: int) -> int
```

Return the least power-of-2 that is at least equal to n.

```
def run_part(arg0: Scenario, arg1: EnvState, arg2: AeroData, arg3: AeroState,  
            arg4: GasData, arg5: GasState, arg6: RunPartOpt)
```

Do a particle-resolved Monte Carlo simulation.

Classes

```
class AeroData (...)
```

Aerosol material properties and associated data.

The data in this structure is constant, as it represents physical quantities that cannot

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PyPartMC: design & implementation outline

**PyPartMC: demo**

PyPartMC: summary

<https://github.com/open-atmos/PyPartMC>

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- ▶ offering users (students) a single-language familiar environment (Colab, ARM JupyterHub)

## PyPartMC: Removing barriers in aerosol modeling

### Submitter

Riemer, Nicole — University of Illinois Urbana-Champaign

West, Matthew — University of Illinois at Urbana-Champaign

### Area of research

Aerosol Processes

### Journal Reference

D'Aquino Z, S Arabas, J Curtis, A Vaishnav, N Riemer, and M West. 2024. "[PyPartMC: A Pythonic interface to a particle-resolved, Monte Carlo aerosol simulation framework](#)." *SoftwareX*, 25, 101613, 10.1016/j.softx.2023.101613.

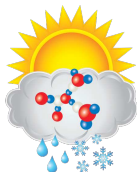
## Science

PartMC is a powerful open-source tool for aerosol simulations. However, it requires knowledge of shell and CMake, C and Fortran compilers, and installation and configuration of several C and Fortran dependencies. This is a significant hurdle for those with little experience in computation. PyPartMC offers a single-step installation process of PartMC and all dependencies through the pip Python package manager on Linux, macOS, and Windows. It provides streamlined access to the unmodified and versioned Fortran internals of the PartMC codebase from both Python and other interoperable environments (e.g., Julia through PyCall).

## Impact

- Ability to run PartMC simulations in the cloud, including using the ARM Jupyter Hub.

funding:



**ASR**  
Atmospheric  
System Research



NATIONAL SCIENCE CENTRE  
POLAND

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## Thank you for your attention!

[pypi.org/p/PyPartMC](https://pypi.org/p/PyPartMC)

[github.com/open-atmos/PyPartMC](https://github.com/open-atmos/PyPartMC)

[doi:10.1016/j.softx.2023.101613](https://doi.org/10.1016/j.softx.2023.101613)