# PyPartMC

## engineering Python-to-Fortran bindings in C++, for use in Julia and Matlab

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

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agh.edu.pl

FOSDEM '24, ULB, Brussels

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PartMC

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

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- Monte-Carlo aerosol dynamics simulation package

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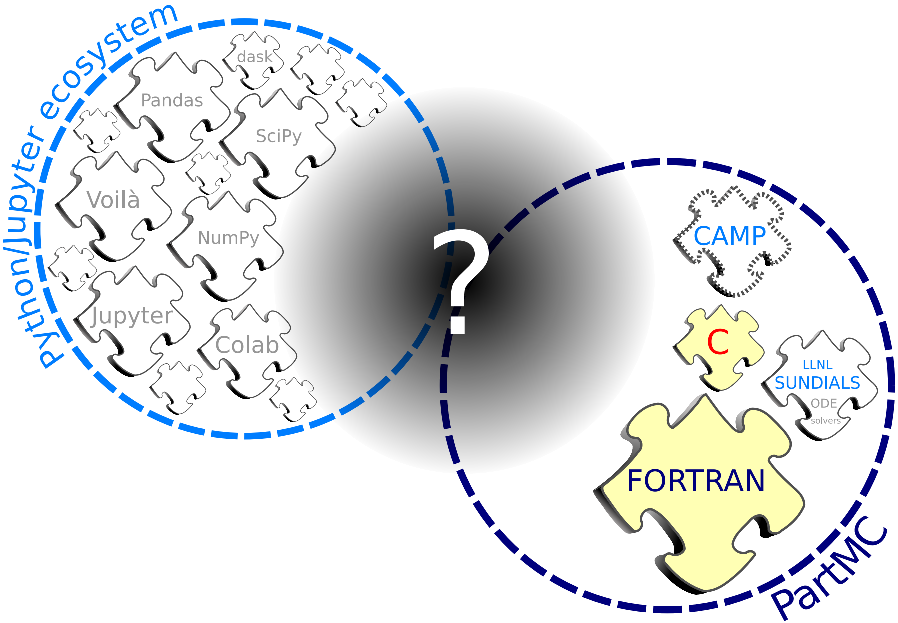
- object-oriented architecture, F90, extensive automated test suite
- usage poses challenges, e.g., to students intending to use it from Jupyter notebooks (dependencies, compilation, updates, automation usually through shell, multi-text-file i/o, output analysis requiring bringing in Fortran, ...)


Python/Jupyter ecosystem
dask
Pandas
SciPy
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Jupyter
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?
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C
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SUNDIALS
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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, no compilation, user doesn't even need to know FORTRAN is involved

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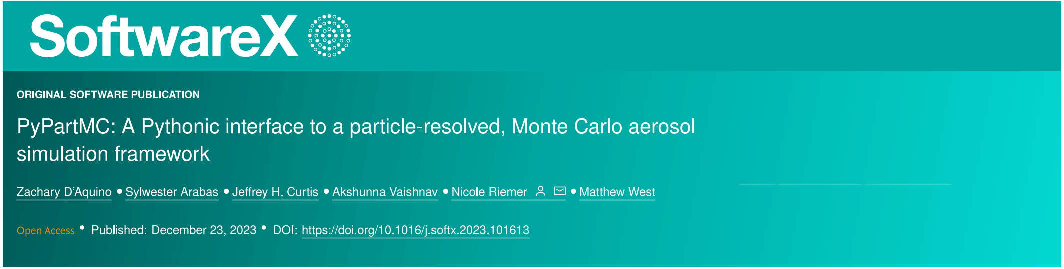
- **lower the entry threshold for usage with Jupyter-based example notebooks**
- streamline the dissemination of paper-result reproducers (peer review)

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



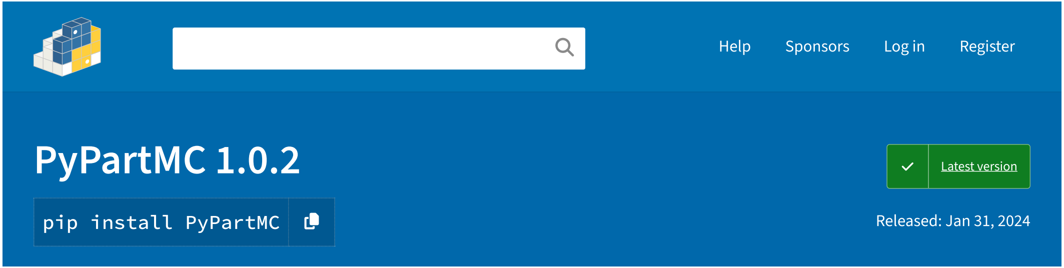
SoftwareX

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



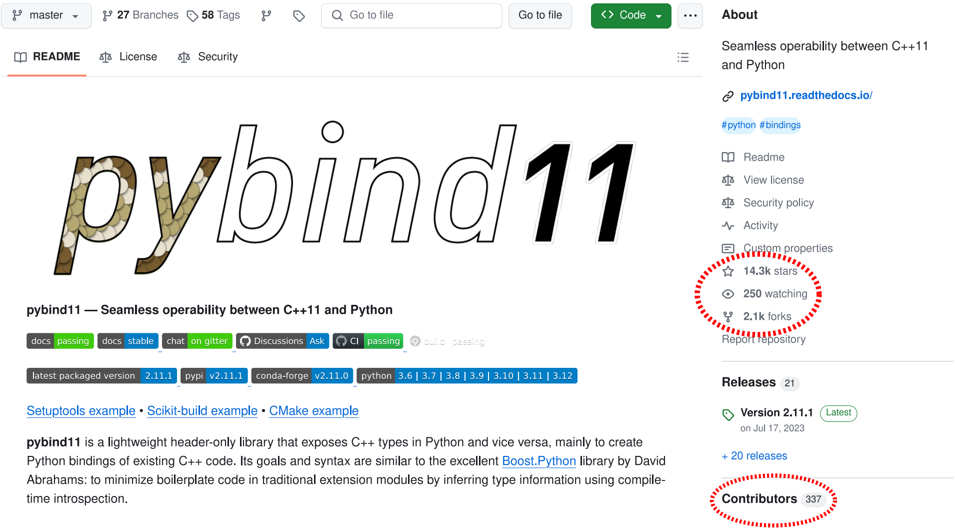
PyPartMC 1.0.2

```
pip install PyPartMC
```

✓ Latest version

Released: Jan 31, 2024

# pybind11



master | 27 Branches | 58 Tags | Go to file | Go to file | Code

README | License | Security

pybind11 — Seamless operability between C++11 and Python

docs passing | docs stable | chat on gitter | 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/

#python #bindings

- Readme
- View license
- Security policy
- Activity
- Custom properties
- **14.3k** stars
- **250** watching
- **2.1k** forks

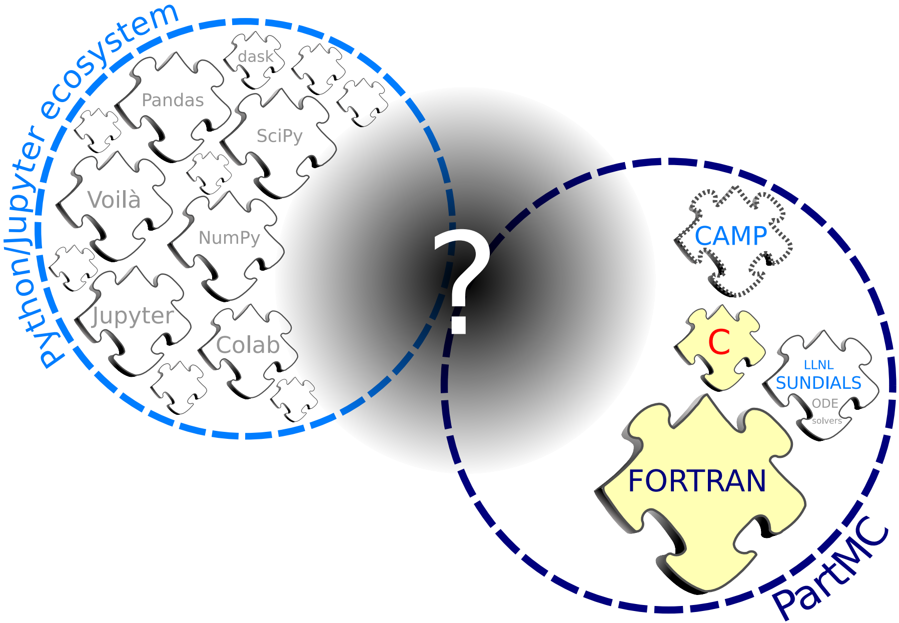
Report repository

**Releases** 21

**Version 2.11.1** Latest
on Jul 17, 2023

+ 20 releases

**Contributors** 337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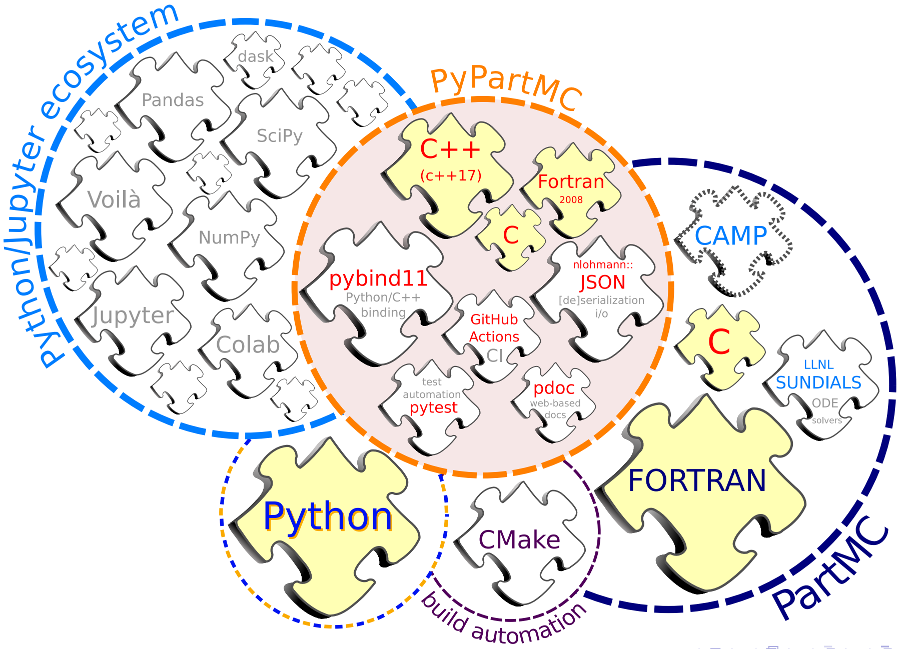

Python/Jupyter ecosystem

dask

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Jupyter

Colab

PyPartMC

C++
(c++17)

Fortran
2008

C

pybind11
Python/C++
binding

nlohmann::
JSON
[de]serialization
i/o

GitHub
Actions
CI

test
automation
pytest

pdoc
web-based
docs

PartMC

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solvers

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Python

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build automation

# developer perspective

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

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  ⇝ minimising effort to accommodate future additions to PartMC

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- freeing of Python-allocated PartMC FORTRAN types through Python Garbage Collector
- 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

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

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  & backports of C++20 features to C++17 (multilinux!): span, string_view, optional

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

# user perspective: Fortran (PartMC)

### c: Fortran code

```fortran
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)

```python
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": {
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            "geom_mean_diam": 8.64 * si.nm,
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        }
    },
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            "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")
```

### b: Julia code (with embedded data)

```julia
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,
      "geom_mean_diam" => 50 * si.nm,
      "log10_geom_std_dev" => .24,
    )
  )
))

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)

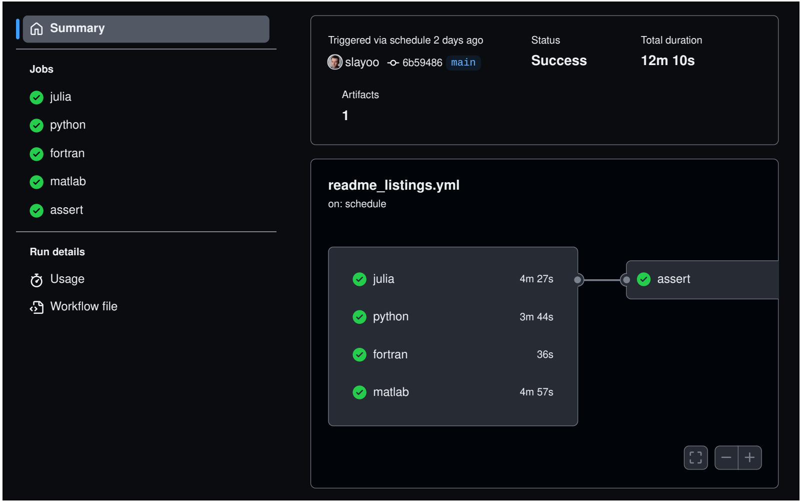
```
ppmc = py.importlib.import_module('PyPartMC');
si = py.importlib.import_module('PyPartMC').si;

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}))), ...
      }), ...
      "diam_type", "geometric", ...
      "mode_type", "log_normal", ...
      "num_conc", 2900 / si.cm^3, ...
      "geom_mean_diam", 50 * si.nm, ...
      "log10_geom_std_dev", .24 ...
    )) ...
  )) ...
}));

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{:}]))
```

# github.com/open-atmos/PyPartMC/actions/



Summary

**Jobs**

- ✓ julia
- ✓ python
- ✓ fortran
- ✓ matlab
- ✓ assert

**Run details**

- Usage
- Workflow file

Triggered via schedule 2 days ago

slayoo 6b59486 `main`

Status

**Success**

Total duration

**12m 10s**

Artifacts

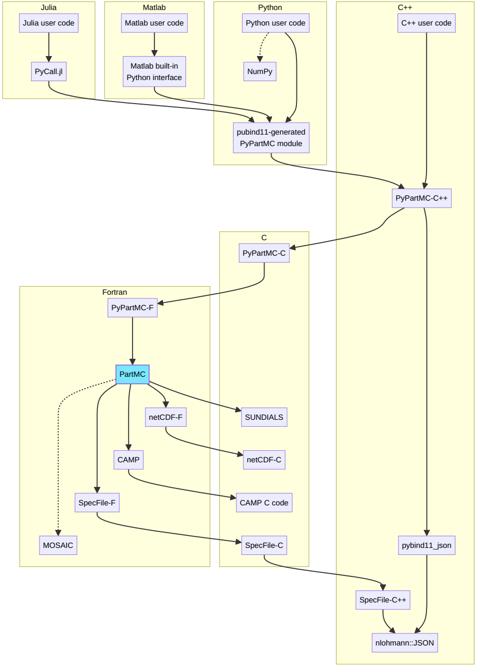
**1**

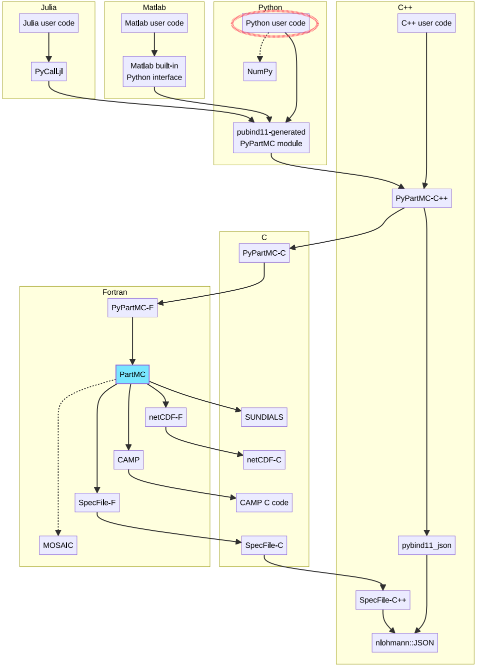
**readme_listings.yml**

on: schedule

| | |
|---|---|
| ✓ julia | 4m 27s |
| ✓ python | 3m 44s |
| ✓ fortran | 36s |
| ✓ matlab | 4m 57s |

✓ assert


Julia
Julia user code
PyCall.jl
Matlab
Matlab user code
Matlab built-in Python interface
Python
Python user code
NumPy
pubind11-generated PyPartMC module
C++
C++ user code
PyPartMC-C++
C
PyPartMC-C
Fortran
PyPartMC-F
PartMC
netCDF-F
SUNDIALS
netCDF-C
CAMP
CAMP C code
SpecFile-F
SpecFile-C
MOSAIC
pybind11_json
SpecFile-C++
nlohmann::JSON



```
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]},
))
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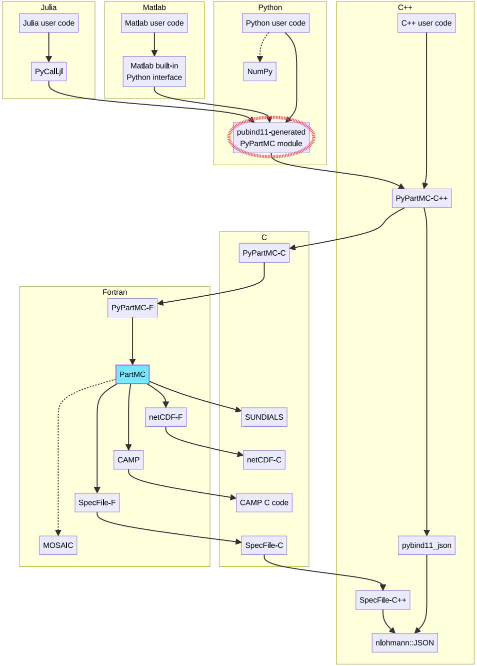
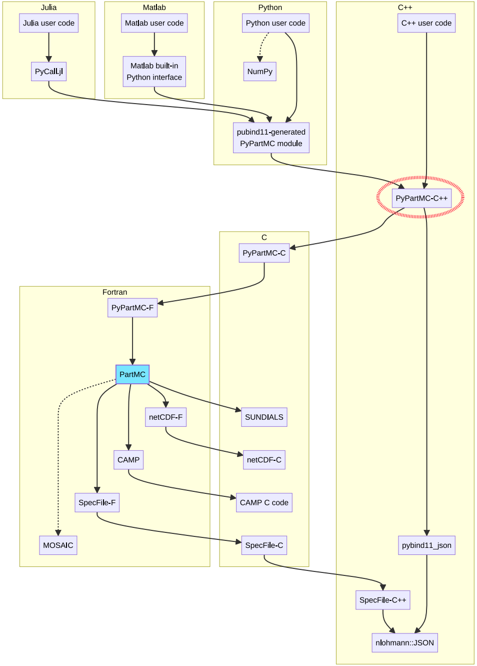


```
import os
from contextlib import contextmanager
from pathlib import Path

# https://github.com/diegoferigo/cmake-build-extension/blob/master/src/cmake_build_extension
@contextmanager
def __build_extension_env():
    cookies = []
    # https://docs.python.org/3/whatsnew/3.8.html#bpo-36085-whatsnew
    if hasattr(os, "add_dll_directory"):
        basepath = os.path.dirname(os.path.abspath(__file__))
        dllspath = os.path.join(basepath, "..")
        os.environ["PATH"] = dllspath + os.pathsep + os.environ["PATH"]
        for path in os.environ.get("PATH", "").split(os.pathsep):
            if path and Path(path).is_absolute() and Path(path).is_dir():
                cookies.append(os.add_dll_directory(path))
    try:
        yield
    finally:
        for cookie in cookies:
            cookie.close()

with __build_extension_env():
    import _PyPartMC
    from _PyPartMC import *
    from _PyPartMC import (
        __all__,
        __version__,
        __versions_of_build_time_dependencies__,
    )
```



```
#include "pybind11/pybind11.h"
#include "nlohmann/json.hpp"
#include "pybind11_json/pybind11_json.hpp"

[...]

#include "aero_data.hpp"

[...]

namespace py = pybind11;

[...]

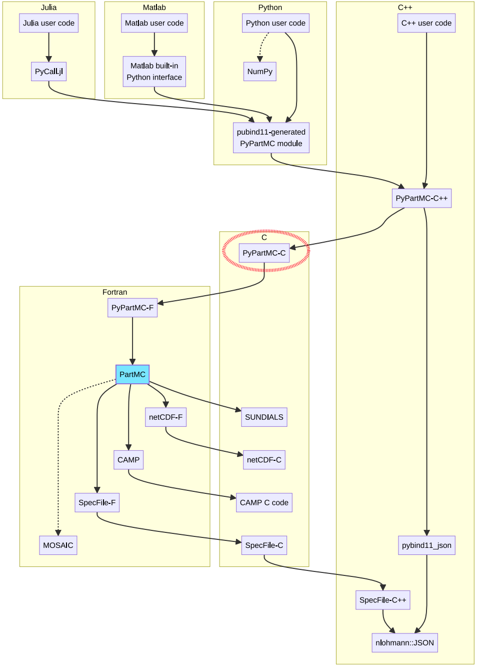
PYBIND11_MODULE(_PyPartMC, m) {

    [...]

    py::class_<
        AeroData,
        std::shared_ptr<AeroData>
    >(m, "AeroData")
        .def(py::init<const nlohmann::json&>())

    [...]

    m.attr("__all__") = py::make_tuple(
        "__version__",
        "AeroData",
        [...]
    );
}
```



```
#pragma once

#include "pmc_resource.hpp"
#include "gimmicks.hpp"

[...]

extern "C" void f_aero_data_ctor(void *ptr) noexcept;
extern "C" void f_aero_data_dtor(void *ptr) noexcept;
extern "C" void f_aero_data_from_json(const void *ptr) noexcept;

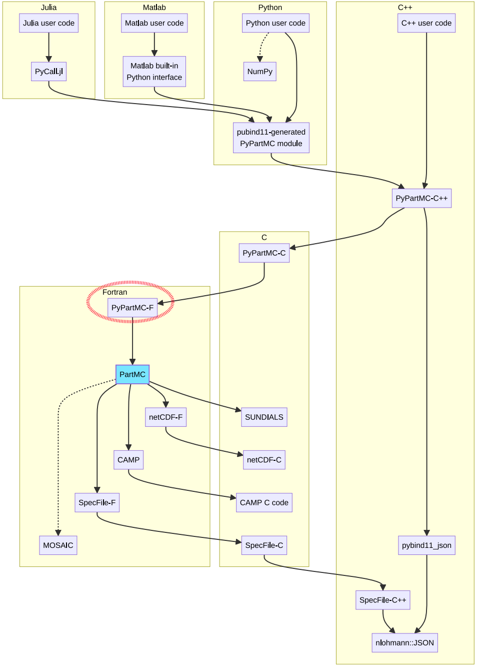
[...]

struct AeroData {
    PMCResource ptr;

    AeroData(const nlohmann::json &json) :
        ptr(f_aero_data_ctor, f_aero_data_dtor)
    {
        if (!InputGimmick::unique_keys(json))
            throw std::runtime_error("Species names must be unique");

        GimmickGuard<InputGimmick> guard(json);
        f_aero_data_from_json(this->ptr.f_arg());
    }

    [...]
};
```



```fortran
module PyPartMC_aero_data
  use iso_c_binding
  use pmc_aero_data
  implicit none

  contains

  subroutine f_aero_data_ctor(ptr_c) bind(C)
    type(aero_data_t), pointer :: ptr_f => null()
    type(c_ptr), intent(out) :: ptr_c

    allocate(ptr_f)
    call fractal_set_spherical(ptr_f%fractal)
    ptr_c = c_loc(ptr_f)
  end subroutine

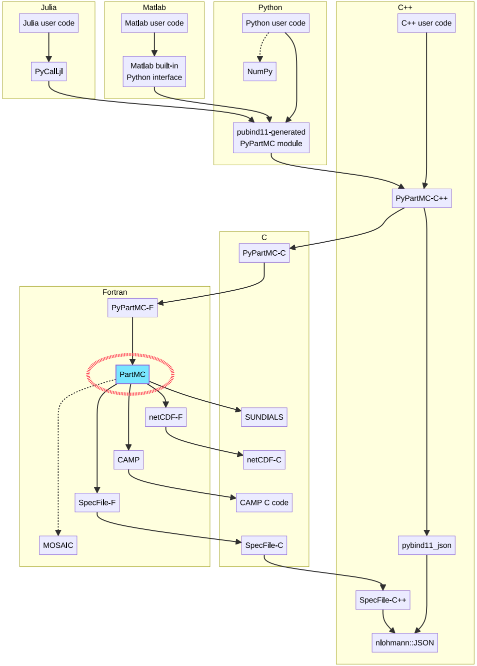
  subroutine f_aero_data_dtor(ptr_c) bind(C)
    type(aero_data_t), pointer :: ptr_f => null()
    type(c_ptr), intent(in) :: ptr_c

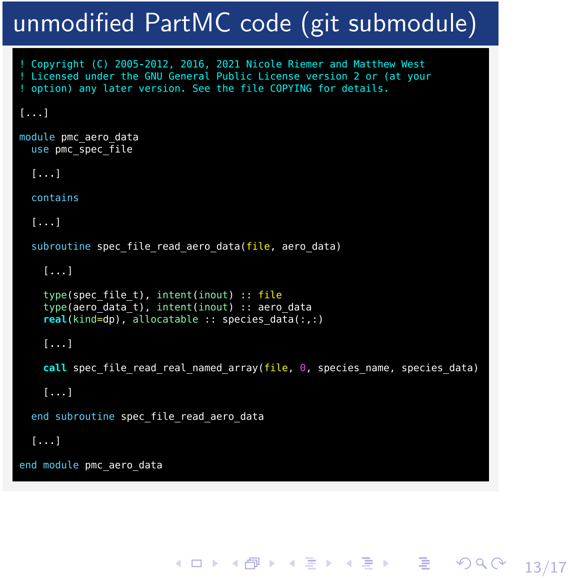
    call c_f_pointer(ptr_c, ptr_f)
    deallocate(ptr_f)
  end subroutine

  subroutine f_aero_data_from_json(ptr_c) bind(C)
    type(aero_data_t), pointer :: ptr_f => null()
    type(c_ptr), intent(in) :: ptr_c
    type(spec_file_t) :: file
    call c_f_pointer(ptr_c, ptr_f)
    call spec_file_read_aero_data(file, ptr_f)
  end subroutine

  [...]

end module
```





## unmodified PartMC code (git submodule)

```
! Copyright (C) 2005-2012, 2016, 2021 Nicole Riemer and Matthew West
! Licensed under the GNU General Public License version 2 or (at your
! option) any later version. See the file COPYING for details.

[...]

module pmc_aero_data
  use pmc_spec_file

  [...]

  contains

  [...]

  subroutine spec_file_read_aero_data(file, aero_data)

    [...]

    type(spec_file_t), intent(inout) :: file
    type(aero_data_t), intent(inout) :: aero_data
    real(kind=dp), allocatable :: species_data(:,:)

    [...]

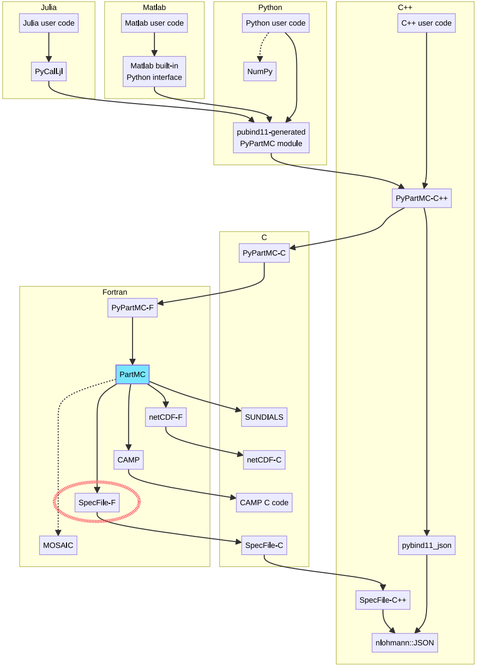
    call spec_file_read_real_named_array(file, 0, species_name, species_data)

    [...]

  end subroutine spec_file_read_aero_data

  [...]

end module pmc_aero_data
```



```
module pmc_spec_file
    [...]

    interface
        [...]

        subroutine c_spec_file_read_real_named_array_data( &
            row, &
            names_data, names_size, &
            vals_data, vals_size &
        ) bind(C)
            import c_double
            character, intent(in) :: names_data
            real(c_double), intent(out) :: vals_data
            integer, intent(in) :: row, vals_size, names_size
        end subroutine

        [...]
    end interface

    [...]

    subroutine spec_file_read_real_named_array(file, max_lines, names, vals)
        [...]

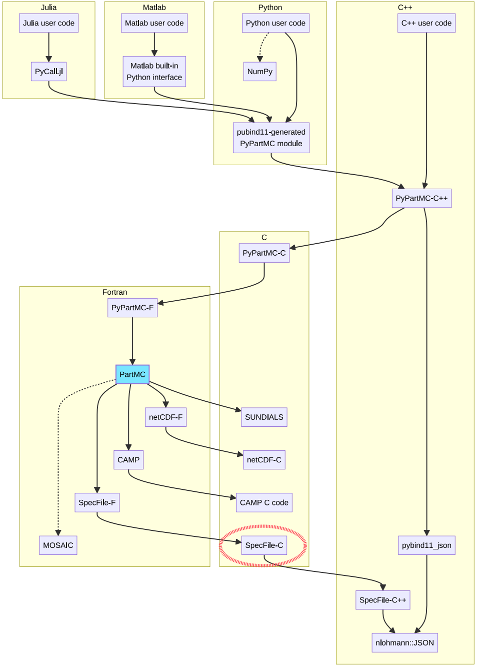
        do row = 1, n_rows
            [...]

            call c_spec_file_read_real_named_array_data( &
                row, &
                names(row), name_size, &
                vals_row(1), size(vals, 2) &
            )
            [...]

        end do
        [...]

    end subroutine
    [...]

end module
```



Julia

Julia user code

PyCall.jl

Matlab

Matlab user code

Matlab built-in Python interface

Python

Python user code

NumPy

pubind11-generated PyPartMC module

C++

C++ user code

PyPartMC-C++

C

PyPartMC-C

Fortran

PyPartMC-F

PartMC

netCDF-F

SUNDIALS

netCDF-C

CAMP

CAMP C code

SpecFile-F

MOSAIC

SpecFile-C

pybind11_json

SpecFile-C++

nlohmann::JSON

```
#include "gimmicks.hpp"

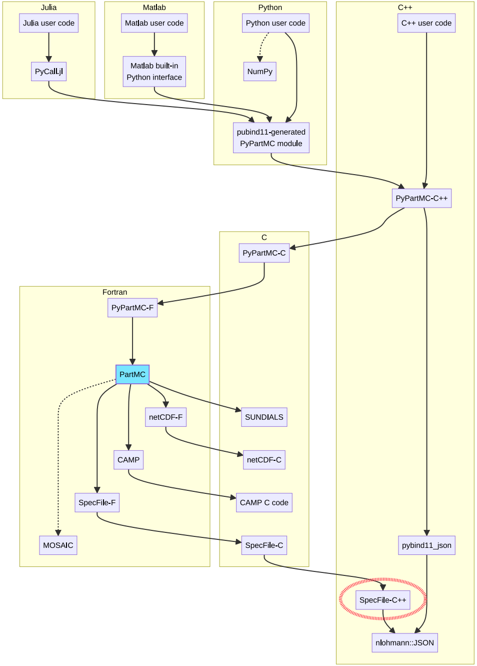
[...]

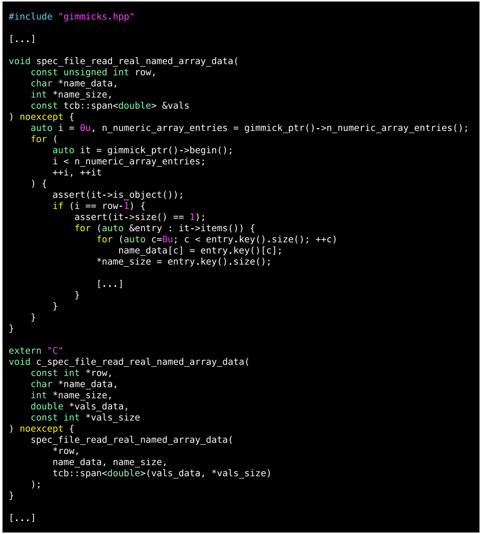
void spec_file_read_real_named_array_data(
    const unsigned int row,
    char *name_data,
    int *name_size,
    const tcb::span<double> &vals
) noexcept {
    auto i = 0u, n_numeric_array_entries = gimmick_ptr()->n_numeric_array_entries();
    for (
        auto it = gimmick_ptr()->begin();
        i < n_numeric_array_entries;
        ++i, ++it
    ) {
        assert(it->is_object());
        if (i == row-1) {
            assert(it->size() == 1);
            for (auto &entry : it->items()) {
                for (auto c=0u; c < entry.key().size(); ++c)
                    name_data[c] = entry.key()[c];
                *name_size = entry.key().size();

                [...]
            }
        }
    }
}

extern "C"
void c_spec_file_read_real_named_array_data(
    const int *row,
    char *name_data,
    int *name_size,
    double *vals_data,
    const int *vals_size
) noexcept {
    spec_file_read_real_named_array_data(
        *row,
        name_data, name_size,
        tcb::span<double>(vals_data, *vals_size)
    );
}

[...]
```





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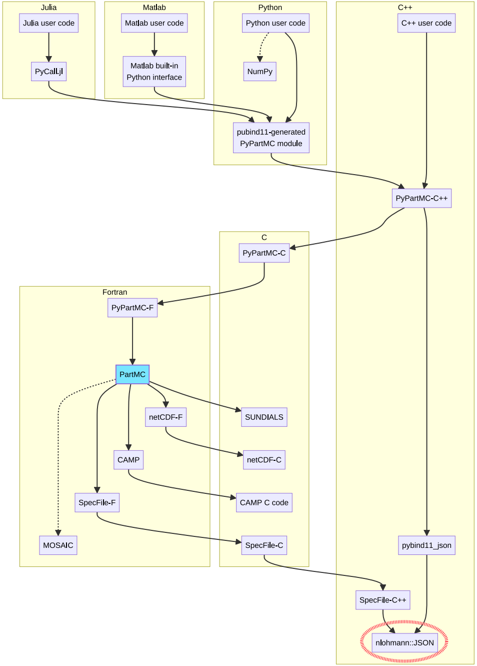
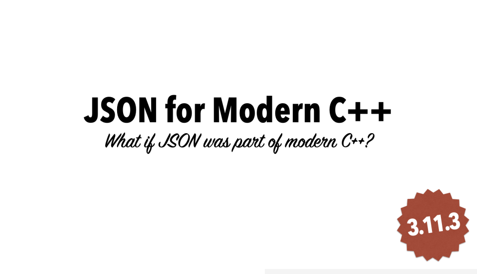
    const int *vals_size
) noexcept {
    spec_file_read_real_named_array_data(
        *row,
        name_data, name_size,
        tcb::span<double>(vals_data, *vals_size)
    );
}

[...]
```

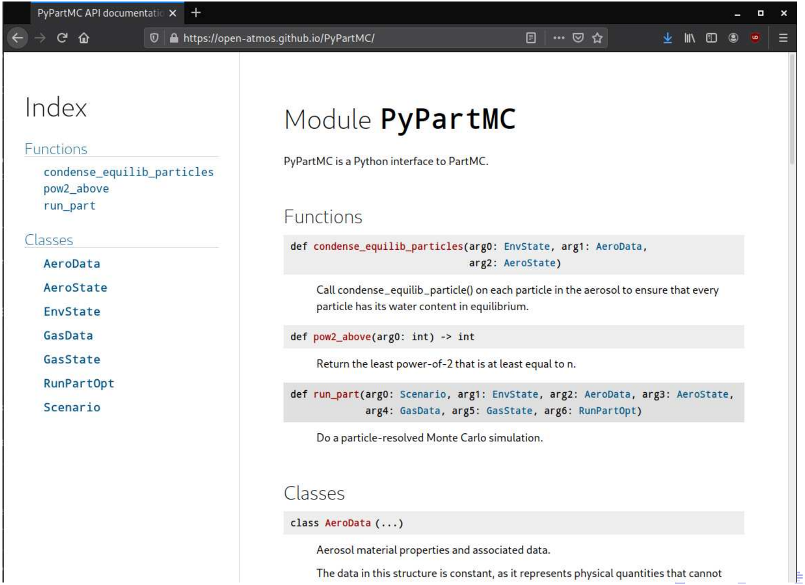


## json.nlohmann.me

JSON for Modern C++



# PyPartMC API docs: `https://open-atmos.github.io/PyPartMC/`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## Index

### Functions

### Classes

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

PyPartMC

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# acknowledgements

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Thank you for your attention!

pypi.org/p/PyPartMC
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