



Engineering Fortran-to-Python Bindings in C++ with nanobind[_json] and cibuildwheel



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Gracjan Adamus @ EuroSciPy 2026



Gracjan Adamus
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Sylwester Arabas

#whoami

- Third-year Applied Computer Science student @ AGH



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- President of KNI Kernel



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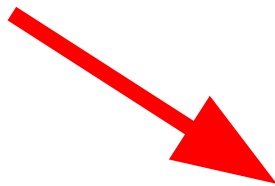
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- Griger5 @ Github



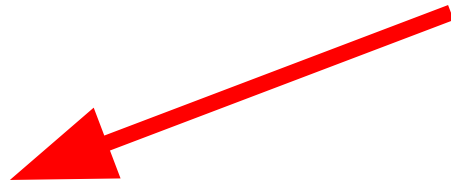
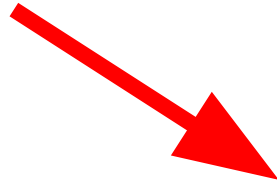
Background



Background



Background



Background



I contribute here!



PartMC



PartMC



- Particle-resolved Monte Carlo code for atmospheric aerosol simulation

PartMC



- Particle-resolved Monte Carlo code for atmospheric aerosol simulation
- Developed at University of Illinois Urbana-Champaign



PartMC



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- Developed for more than 20 years!



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- Developed for more than 20 years!
- More than 4000 citations in research papers



UNIVERSITY OF
ILLINOIS
URBANA - CHAMPAIGN

PartMC



- Particle-resolved Monte Carlo code for atmospheric aerosol simulation
- Developed at University of Illinois Urbana-Champaign
- Developed for more than 20 years!
- More than 4000 citations in research papers
- Written in the object-oriented paradigm, in Fortran 90



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PyPartMC: A maintainable Python interface

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- Usable as a single Python script or a notebook
- **pip** installable



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- We wanted a uniform interface across languages
- Using unmodified PartMC code and no shell
- No need for auxiliary files
- Usable as a single Python script or a notebook
- **pip** installable
- Available on Linux, macOS, Windows, Linux-ARM



```

import numpy as np

import PyPartMC as ppmc
from PyPartMC import si

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

```



```
import numpy as np
```

```
import PyPartMC as ppmc  
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```

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

```
aero_dist = ppmc.AeroDist(  
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            "diam_type": "geometric",  
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            "diam_type": "geometric",  
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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")
```



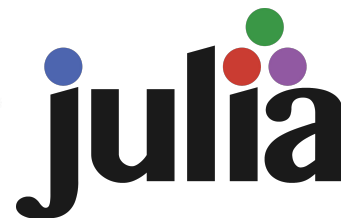
```
using Pkg  
Pkg.add("PyCall")
```

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

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



```
import numpy as np
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```
import PyPartMC as ppmc  
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aero_data = ppmc.AeroData(  
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)
```

```
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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")
```

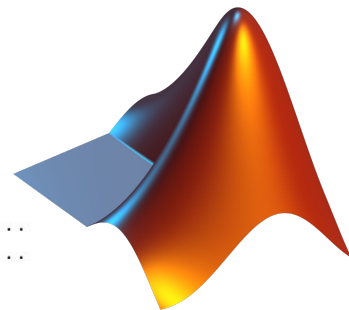


```
ppmc = py.importlib.import_module('PyPartMC');  
si = py.importlib.import_module('PyPartMC').si;
```

```
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,  
    py.dict(pyargs("BC", py.tuple({1800 * si.kg/si.m^3, 0, 1e-3 * si.kg/si.mol,  
})));
```

```
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 ...  
        )), ...  
        "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{:}])))
```



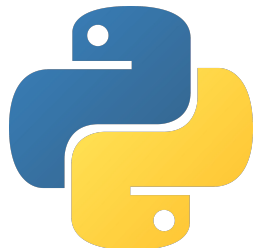
```
import numpy as np
```

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

```
aero_dist = ppmc.AeroDist(  
    aero_data,  
    [{  
        "cooking": {  
            "mass_frac": [{ "OC": [1]}],  
            "diam_type": "geometric",  
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            "geom_mean_diam": 8.64 * si.nm,  
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        },  
        "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")
```



```
auto aero_data = std::make_shared<AeroData>(nlohmann::json({  
    { {"OC", {1000.0 * si::kg / (si::m * si::m * si::m), 0.0, 1e-3 * si::kg /  
    { {"BC", {1800.0 * si::kg / (si::m * si::m * si::m), 0.0, 1e-3 * si::kg /  
})));
```

```
auto aero_dist = AeroDist(  
    aero_data,  
    nlohmann::ordered_json::array({  
        nlohmann::ordered_json::object({  
            {"cooking", {  
                {"mass_frac", nlohmann::ordered_json::array({ nlohmann::ordered  
                {"diam_type", "geometric"},  
                {"mode_type", "log_normal"},  
                {"num_conc", 3200.0 / (si::cm * si::cm * si::cm)},  
                {"geom_mean_diam", 8.64 * si::nm},  
                {"log10_geom_std_dev", 0.28}  
            }},  
            {"diesel", {  
                {"mass_frac", nlohmann::ordered_json::array({ nlohmann::ordered  
                {"diam_type", "geometric"},  
                {"mode_type", "log_normal"},  
                {"num_conc", 2900.0 / (si::cm * si::cm * si::cm)},  
                {"geom_mean_diam", 50.0 * si::nm},  
                {"log10_geom_std_dev", 0.24}  
            }},  
        })  
    })  
);
```

```
int n_part = 100;  
auto aero_state = AeroState(aero_data, n_part, "nummass_source");  
AeroState::dist_sample(aero_state, aero_dist, 1.0, 0.0, true, true);  
  
auto masses = AeroState::masses(aero_state, {}, {});  
auto num_concs = AeroState::num_concs(aero_state);  
double total_mass = std::inner_product(std::begin(num_concs), std::end(num_concs),  
  
std::cout << std::scientific << total_mass << " # kg/m3\n";
```



```
import numpy as np
```

```
import PyPartMC as ppmc  
from PyPartMC import si
```

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

```
aero_dist = ppmc.AeroDist(  
aero_data,  
[  
    "cooking": {  
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        "diam_type": "geometric",  
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    }  
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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")
```



```
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, .false., aero_dist)  
call spec_file_close(f_aero_dist)
```

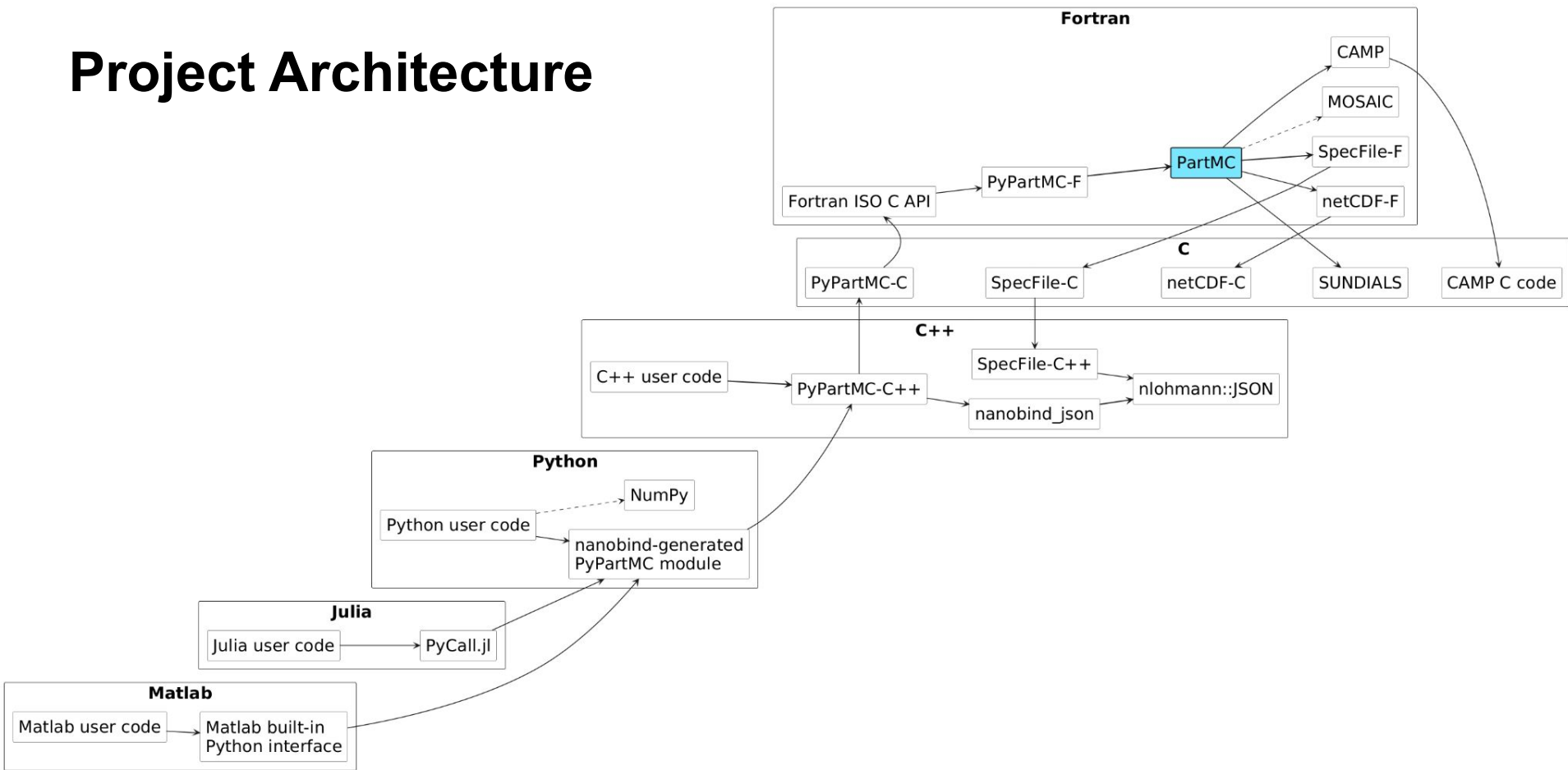
```
call aero_state_zero(aero_state)  
call fractal_set_spherical(aero_data%fractal)  
call aero_state_set_weight(aero_state, aero_data, &  
AERO_STATE_WEIGHT_NUMMASS_SOURCE)  
call aero_state_set_n_part_ideal(aero_state, dble(n_part))  
call aero_state_add_aero_dist_sample(aero_state, aero_data, & 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



Project Architecture







More than 36000 lines of code!



More than 12000 lines of code!



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Over a 200 files



More than 12000 lines of code!

Over 120 files



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Reported code coverage: 77%



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Reported code coverage: 77%

Languages



Fortran 48.9%	Python 44.2%
Gnuplot 2.7%	Shell 2.1%
HTML 0.8%	CMake 0.6%
Other 0.7%	



More than 12000 lines of code!

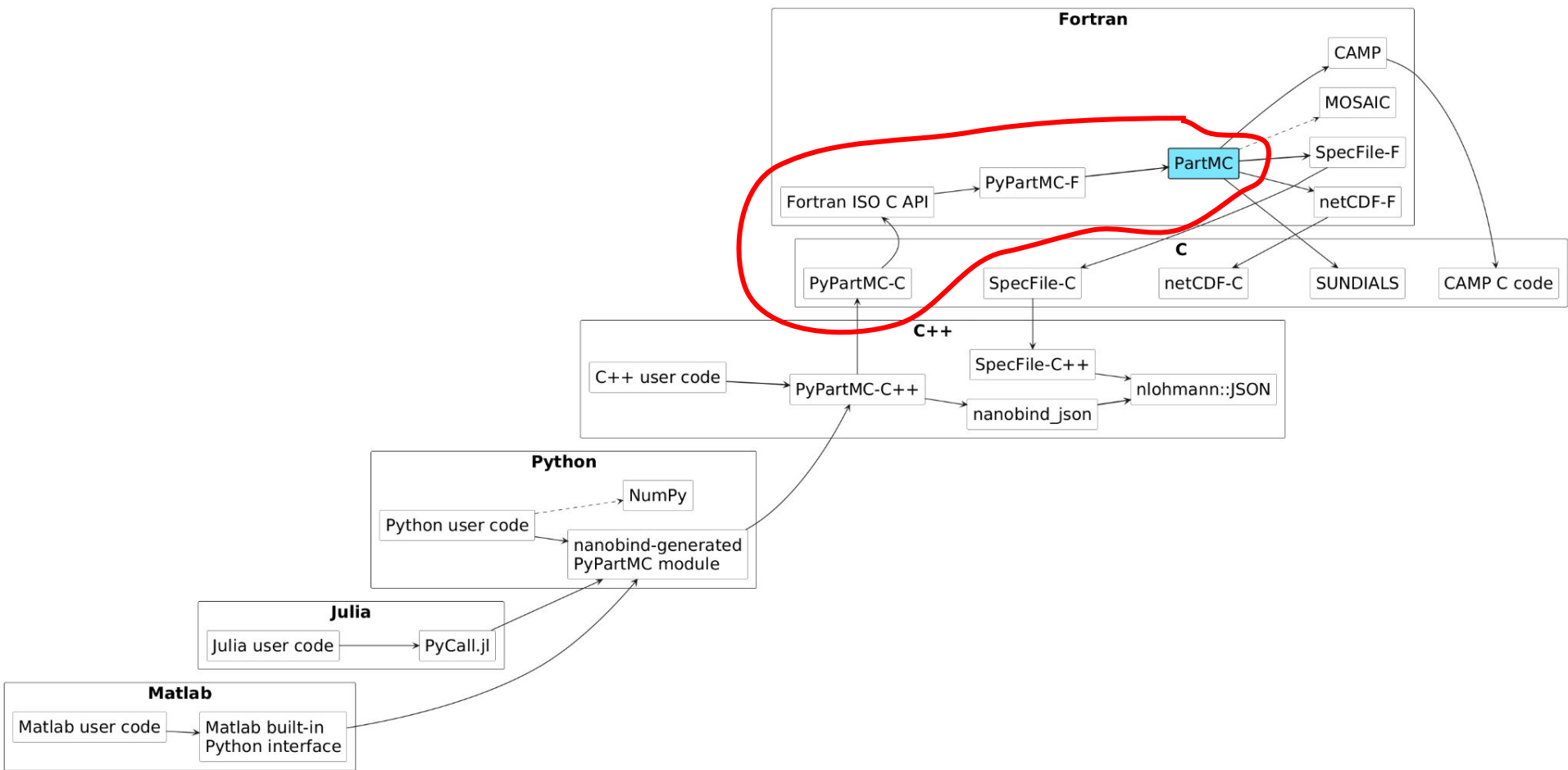
Over 120 files

Reported code coverage: 92%

Languages



C++ 34.2%	Python 31.2%
Fortran 28.9%	CMake 5.7%



Fortran ISO C bindings

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Unified compiler-agnostic interface

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Unified compiler-agnostic interface

```
use iso_c_binding
```

Fortran ISO C bindings

Unified compiler-agnostic interface

```
use iso_c_binding
```

```
subroutine f_aero_data_len(ptr_c, len) bind(C)
  type(aero_data_t), pointer :: ptr_f => null()
  type(c_ptr), intent(in) :: ptr_c
  integer(c_int), intent(out) :: len

  call c_f_pointer(ptr_c, ptr_f)
  len = aero_data_n_spec(ptr_f)
end subroutine
```

Fortran ISO C bindings

Unified compiler-agnostic interface

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use iso_c_binding
```

```
subroutine f_aero_data_len(ptr_c, len) bind(C)
  type(aero_data_t), pointer :: ptr_f => null()
  type(c_ptr), intent(in) :: ptr_c
  integer(c_int), intent(out) :: len

  call c_f_pointer(ptr_c, ptr_f)
  len = aero_data_n_spec(ptr_f)
end subroutine
```

PartMC
function



Fortran ISO C bindings

Unified compiler-agnostic interface

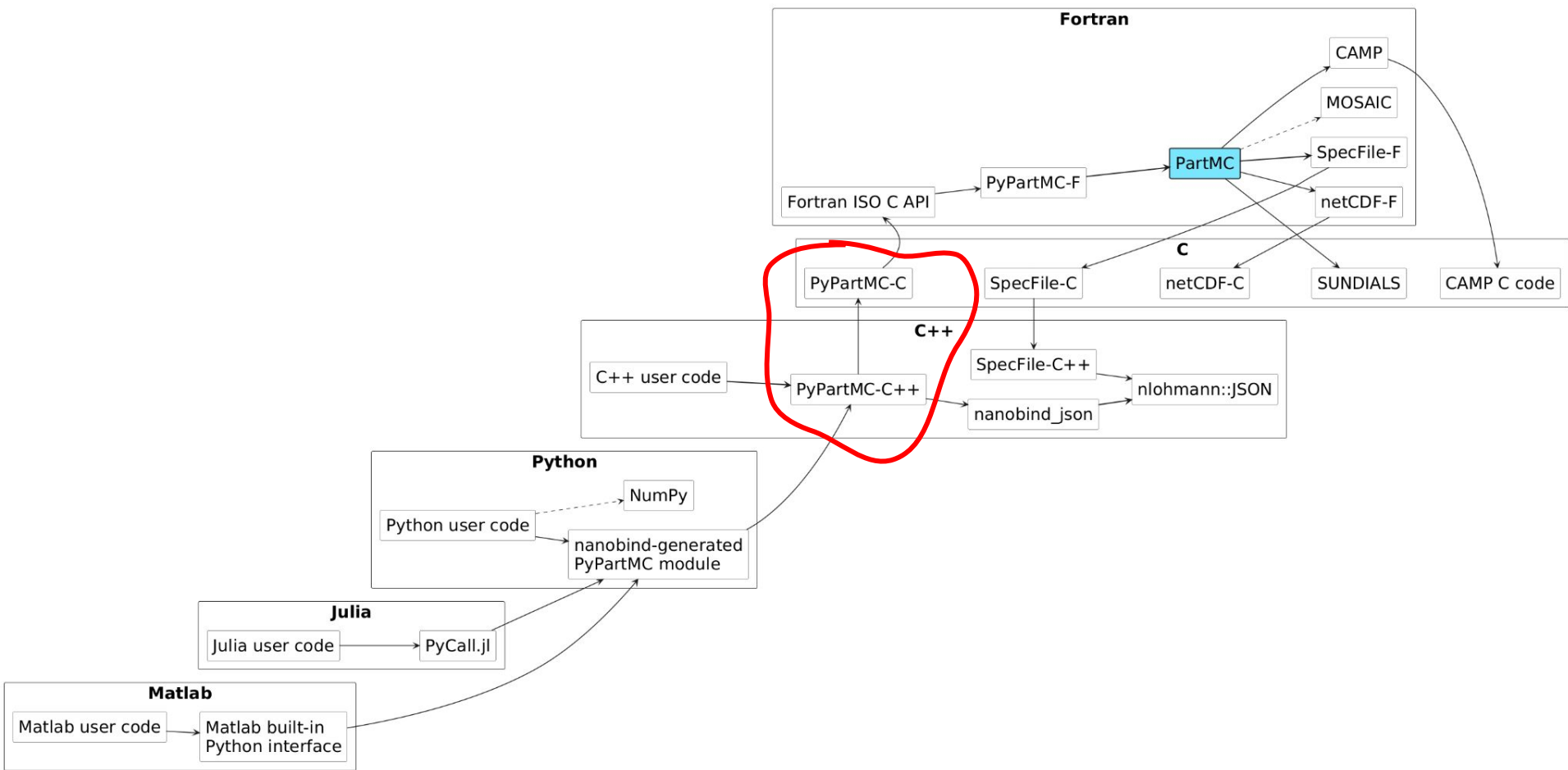
```
use iso_c_binding
```

```
subroutine f_aero_data_len(ptr_c, len) bind(C)
  type(aero_data_t), pointer :: ptr_f => null()
  type(c_ptr), intent(in) :: ptr_c
  integer(c_int), intent(out) :: len

  call c_f_pointer(ptr_c, ptr_f)
  len = aero_data_n_spec(ptr_f)
end subroutine
```

PartMC
function

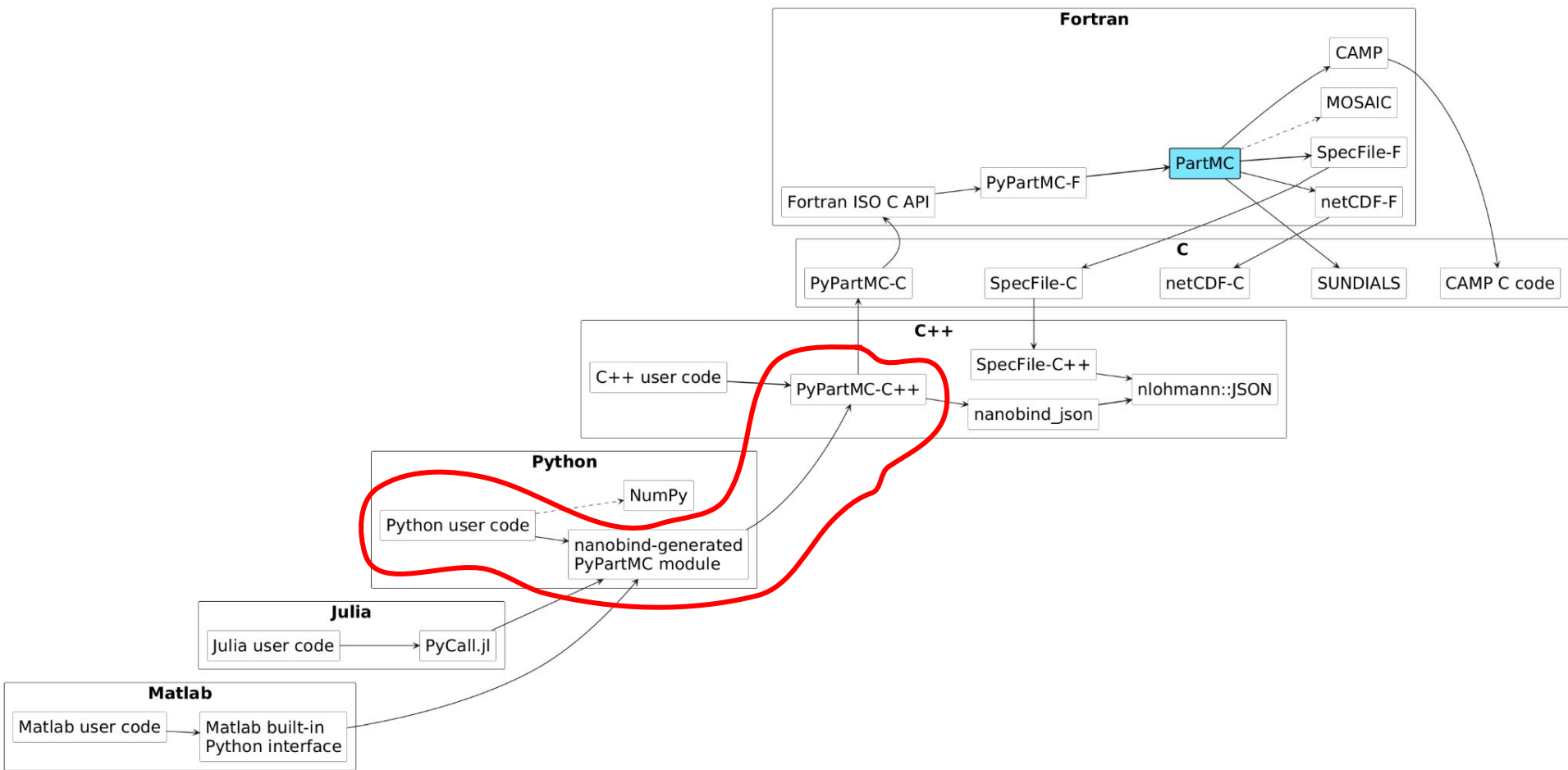
```
void f_aero_data_len(const void *ptr, int *len) noexcept;
```



Calling C from C++

Calling C from C++

```
extern "C"  
void f_aero_data_len(  
    const void *ptr,  
    int *len) noexcept;
```



nanobind



nanobind

- Created by Wenzel Jakob, associate professor at EPFL



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- Successor to his previous project - **pybind11**



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- Exposes C++ to Python and vice versa



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- A convenient wrapper over Python's C API (**Python.h**)



nanobind

- Created by Wenzel Jakob, associate professor at EPFL
- Successor to his previous project - **pybind11**
- Exposes C++ to Python and vice versa
- A convenient wrapper over Python's C API (**Python.h**)
- Minimal boilerplate



nanobind

```
NB_MODULE(_PyPartMC, m) {  
    m.doc() = R"pbdoc(  
        PyPartMC is a Python interface to PartMC.  
    )pbdoc";  
  
    m.def("run_part", &run_part, "Do a particle-resolved Monte Carlo simulation.");  
    m.def("run_part_timestep", &run_part_timestep, "Do a single time step.");  
  
    nb::class_<AeroDist>(m, "AeroDist")  
        .def(nb::init<std::shared_ptr<AeroData>, const nlohmann::ordered_json&>())  
        .def_prop_ro("n_mode", &AeroDist::get_n_mode,  
            "Number of aerosol modes in the distribution.")  
        .def_prop_ro("num_conc", &AeroDist::get_total_num_conc,  
            "Total number concentration of a distribution (#/m^3).")  
        .def("mode", AeroDist::get_mode,  
            "Return the mode of a given index.")  
    ;  
}
```

```

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

```

nanobind: Custom Type Casters

nanobind: Custom Type Casters

```
template <typename Type>  
struct type_caster<tl::optional<Type>> :  
optional_caster<tl::optional<Type>> {};
```

```

template <typename Type> struct type_caster<std::valarray<Type>> {
    NB_TYPE_CASTER(std::valarray<Type>, const_name("[") + const_name("std::valarray") + const_name("]"))

    using Caster = make_caster<Type>;

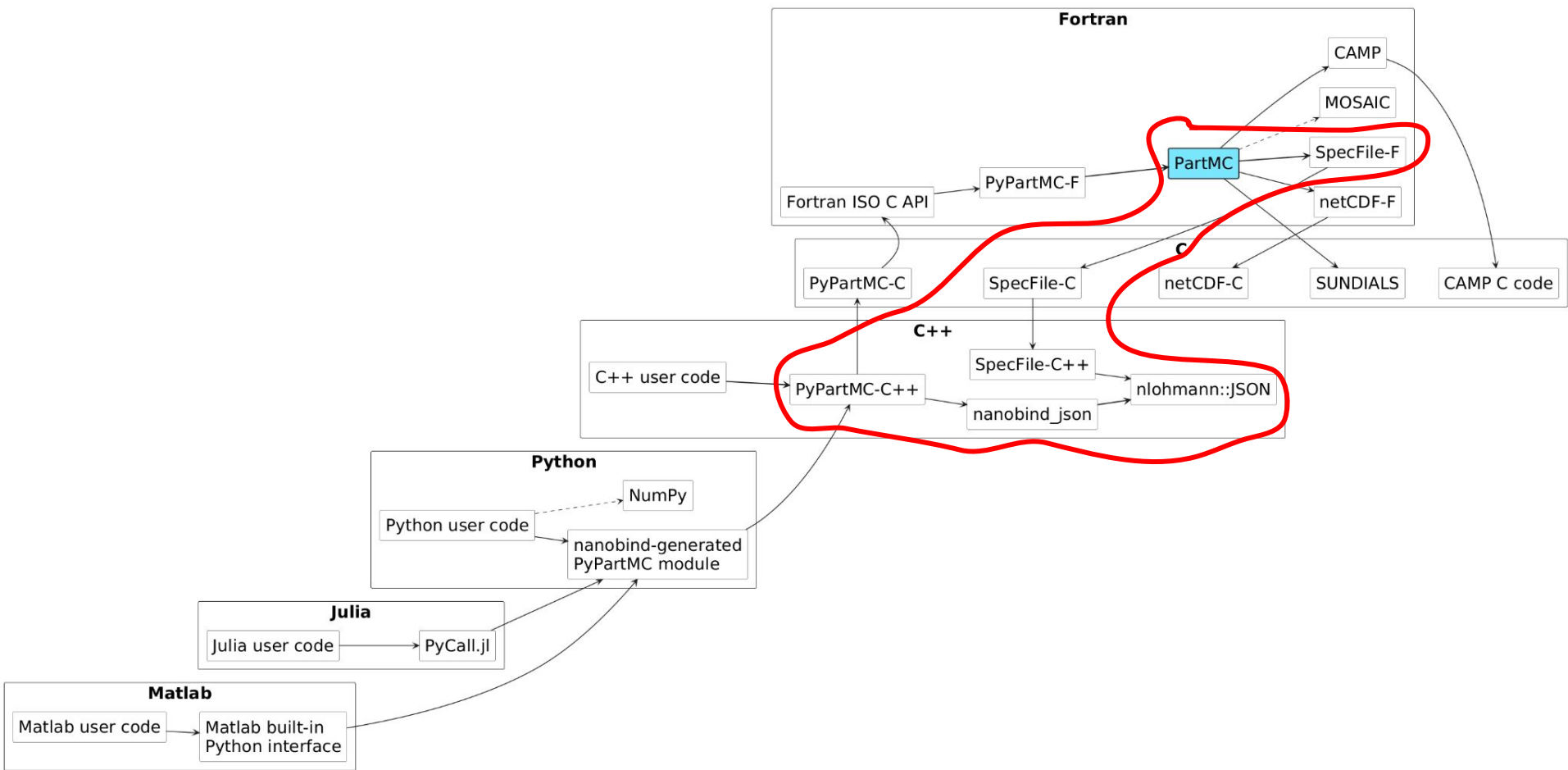
    bool from_python(handle src, uint8_t flags, cleanup_list *cleanup) noexcept {
        if (nb::isinstance<nb::list>(src)) {
            try {
                auto py_array = nb::cast<nb::list>(src);
                size_t size = py_array.size();

                value.resize(size);

                for (size_t i = 0; i < size; i++) {
                    value[i] = nb::cast<Type>(py_array[i]);
                }

                return true;
            }
            catch (...) {
                PyErr_Clear();
                return false;
            }
        }
        else if (nb::isinstance<nb::ndarray<Type, nb::ndim<1>>>(src)) {

```



Spec files

≡ aero_emit_dist.dat ×

scenarios > 1_urban_plume > ≡ aero_emit_dist.dat

```
1 mode_name paved_road
2 mass_frac aero_emit_comp_pavedrd.dat # composition proportions of species
3 diam_type geometric # type of diameter specified
4 mode_type log_normal # type of distribution
5 num_conc 5.03E+03 # particle number concentration (#/m^2)
6 geom_mean_diam 1.42e-6 # geometric mean diameter (m)
7 log10_geom_std_dev 0.11 # log_10 of geometric std dev of diameter
8
9 mode_name cooking
10 mass_frac aero_emit_comp_cooking.dat # composition proportions of species
11 diam_type geometric # type of diameter specified
12 mode_type log_normal # type of distribution
13 num_conc 9.0E+06 # particle number concentration (#/m^2)
14 geom_mean_diam 8.64e-8 # geometric mean diameter (m)
15 log10_geom_std_dev 0.28 # log_10 of geometric std dev of diameter
16
17 mode_name diesel
18 mass_frac aero_emit_comp_diesel.dat # composition proportions of species
19 diam_type geometric # type of diameter specified
20 mode_type log_normal # type of distribution
21 num_conc 1.6E+08 # particle number concentration (#/m^2)
22 geom_mean_diam 5e-8 # geometric mean diameter (m)
23 log10_geom_std_dev 0.24 # log_10 of geometric std dev of diameter
24
25 mode_name gasoline
26 mass_frac aero_emit_comp_gasol.dat # composition proportions of species
27 diam_type geometric # type of diameter specified
28 mode_type log_normal # type of distribution
29 num_conc 5.00E+07 # particle number concentration (#/m^2)
30 geom_mean_diam 5e-8 # geometric mean diameter (m)
31 log10_geom_std_dev 0.24 # log_10 of geometric std dev of diameter
```

Why JSONs?

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```
AERO_MODE_CTOR_LOG_NORMAL_FULL = {  
    "test_mode": {  
        "mass_frac": [{"SO4": [1]}],  
        "diam_type": "geometric",  
        "mode_type": "log_normal",  
        "num_conc": 100 / si.m**3,  
        "geom_mean_diam": 2 * si.um,  
        "log10_geom_std_dev": np.log10(1.6),  
    }  
}  
  
AERO_MODE_CTOR_EXP = {  
    "test_mode": {  
        "mass_frac": [{"H2O": [1]}],  
        "diam_type": "geometric",  
        "mode_type": "exp",  
        "num_conc": 1e9 / si.m**3,  
        "diam_at_mean_vol": 20 * si.um,  
    }  
}  
  
AERO_MODE_CTOR_SAMPLED = {  
    "test_mode": {  
        "mass_frac": [{"H2O": [1]}],  
        "diam_type": "geometric",  
        "mode_type": "sampled",  
        "size_dist": [  
            {"diam": [1, 2, 3, 4]},  
            {"num_conc": [100, 200, 300]},  
        ],  
    }  
}
```

nanobind_json

nanobind_json

- We needed JSON operability for nanobind

nanobind_json

- We needed JSON operability for nanobind
- We found an unmaintained and broken nanobind_json package

nanobind_json

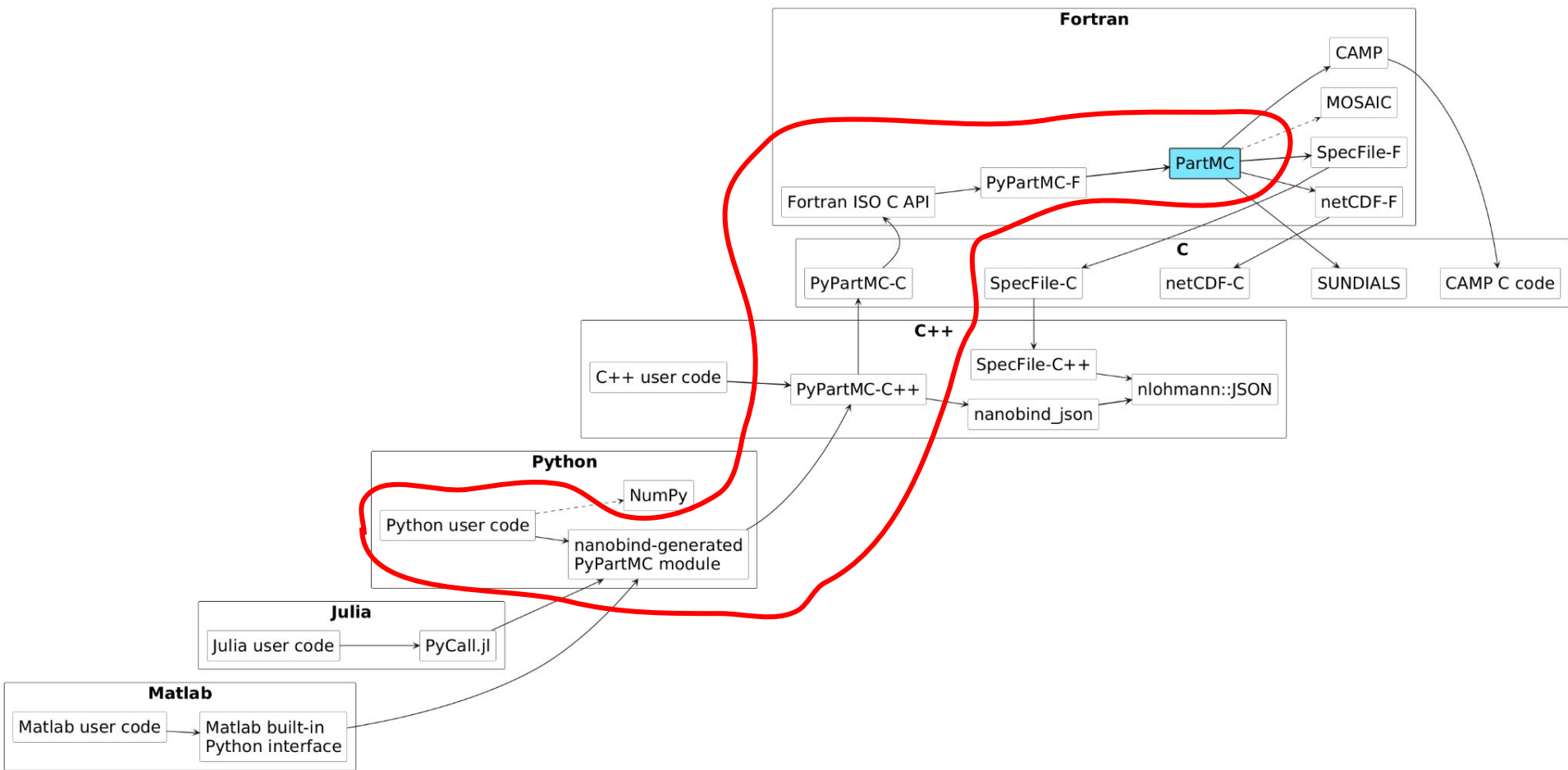
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- So we adopted it, and I became its maintainer!

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Is there a way to pass JSON objects between Python and C++?

Yes, an unofficial, currently maintained, package supporting that can be found [here](#). It is based on a similar package for `pybind11` called `pybind11_json`.



Code coverage for a multi-language codebase

Code coverage for a multi-language codebase

```
- run: |  
  set -xe  
  CMAKE_ARGS="-DCMAKE_CXX_FLAGS=--coverage \  
  |         -DCMAKE_C_FLAGS=--coverage \  
  |         -DCMAKE_Fortran_FLAGS=--coverage" \  
  pip install --config-settings=build-dir=build -e .[tests]  
  pytest -We tests  
  lcov --capture --directory ./build/CMakeFiles/_PyPartMC.dir/ \  
  |     --output-file coverage.info --no-external
```

Garbage Collection of Fortran Objects

Garbage Collection of Fortran Objects

```
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
```

Garbage Collection of Fortran Objects

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

Garbage Collection of Fortran Objects

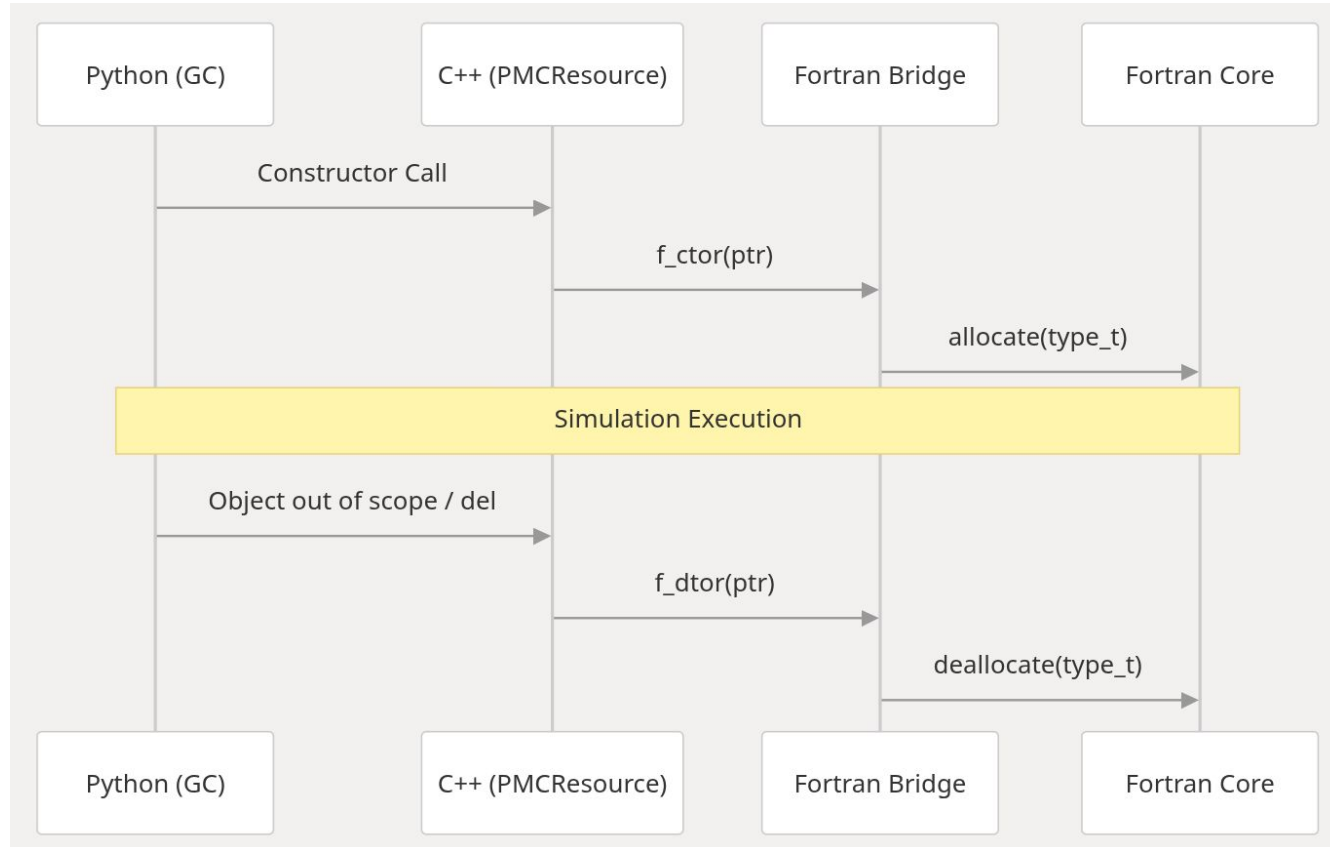
```
class PMCTest {  
    void *ptr;  
    void (*f_ctor)(void*);  
    void (*f_dtor)(void*);  
  
    PMCTest(const PMCTest&) = delete;  
    PMCTest& operator= (const PMCTest&) = delete;  
  
public:  
    PMCTest(  
        decltype(f_ctor) f_ctor,  
        decltype(f_dtor) f_dtor  
    ) :  
        f_ctor(f_ctor),  
        f_dtor(f_dtor)  
    {  
        this->f_ctor(&this->ptr);  
    }  
};
```

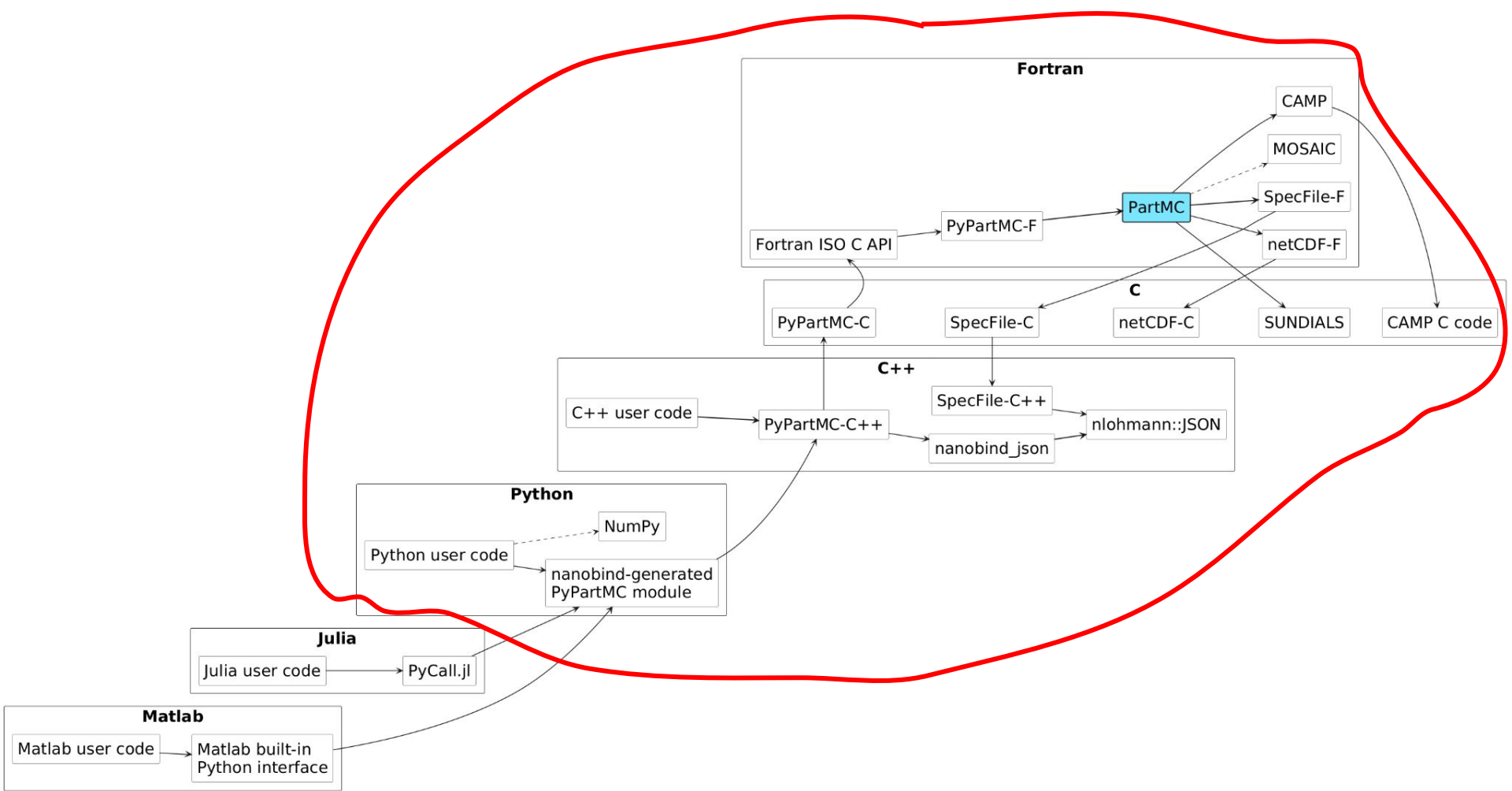
```
~PMCTest() {  
    this->f_dtor(&this->ptr);  
}  
  
const void *f_arg() const {  
    return &this->ptr;  
}  
  
void *f_arg_non_const() {  
    return &this->ptr;  
}  
};
```

Garbage Collection of Fortran Objects

```
struct AeroData {  
    PMCResource ptr;  
  
    AeroData() :  
        ptr(f_aero_data_ctor, f_aero_data_dtor)  
    {}  
}
```

Garbage Collection of Fortran Objects





Quest for a single *pip* install

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To run PartMC, you need to:

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- Install numerous dependencies

✓ gitmodules	
> camp	S
> devops_tests	S
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> json-fortran	S
> nanobind	S
> nanobind_json	S
> netcdf-c	S
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> sundials	S

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Quest for a single *pip* install

To run PartMC, you need to:

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- Perform multi-language compilation
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- **pip install pypartmc**
- Done!
- Or: Single click execution of an example notebook on Google Colab!

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```
function(scoped_sundials_setup_config)
  set(PROJECT_SOURCE_DIR ${SUNDIALS_SOURCE_DIR})
  set(SUNDIALS_PRECISION "double")
  set(SUNDIALS_CINDEX_TYPE "int64_t")

  file(MAKE_DIRECTORY ${CMAKE_BINARY_DIR}/sundials)
  execute_process(
    COMMAND ${Python_EXECUTABLE} "-c" "import sys; print(''.join([line for line in sys.stdin if line.startswith('set(PACKAGE_VERSION_')])))"
    INPUT_FILE ${CMAKE_SOURCE_DIR}/gitmodules/sundials/CMakeLists.txt
    OUTPUT_FILE ${CMAKE_BINARY_DIR}/sundials/CMakeLists.txt
  )
  include(${CMAKE_BINARY_DIR}/sundials/CMakeLists.txt)

  set(PACKAGE_VERSION "${PACKAGE_VERSION_MAJOR}.${PACKAGE_VERSION_MINOR}.${PACKAGE_VERSION_PATCH}")
  include(${SUNDIALS_SOURCE_DIR}/cmake/SundialsSetupConfig.cmake)
endfunction()

scoped_sundials_setup_config()
```

Quest for a single *pip* install

```
if (MINGW)
|   file(WRITE "${CMAKE_BINARY_DIR}/fix_mingw_wstat64.h" "
#pragma once
#include <sys/stat.h>
#ifdef _WIN64
#   undef _wstat64
#   define _wstat64(path, buf) _wstat64((path), (struct _stat64*)(buf))
#endif
")
|   target_compile_options(netcdf_clib PRIVATE
|       -include${CMAKE_BINARY_DIR}/fix_mingw_wstat64.h
|   )
endif()
```

Biggest CMake trickery

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- When migrating from **pybind11** to **nanobind**, our build backend changed too

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- We needed to switch from **setuptools** to **scikit-build-core**
- scikit-build wanted to force installation of all CMake dependencies
- We need the *install()* to work for PyPartMC, but not any other package
- To prevent it, we had to resort to a undocumented CMake feature!

Biggest CMake trickery

 cmake.org/pipermail/cmake/2011-March/043320.html



Mailing List Archives

The archives once hosted here have been removed. They were an important part of our community's history, and we are grateful to everyone who contributed to them over the years.

Biggest CMake trickery

INTERNET ARCHIVE
WayBackMachine

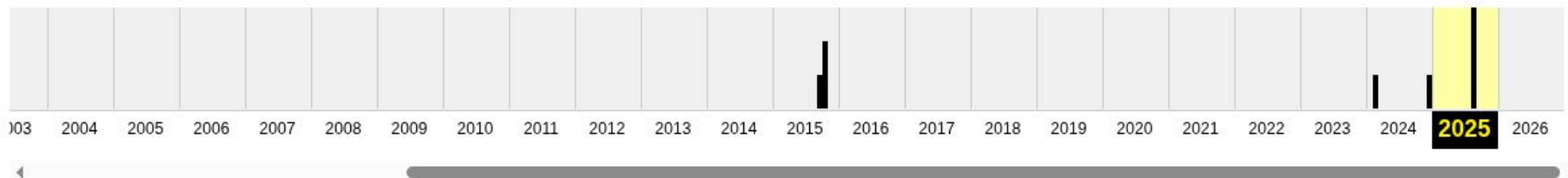
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<https://cmake.org/pipermail/cmake/2011-March/043320.html> ✕

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Biggest CMake trickery

I'm assuming you mean `"_add_library(${name} ${ARGN})"`?

The "override and call original with a leading `_`" is probably not well documented anywhere. While it's useful on occasion, we do not recommend using it if there's an alternate technique that you can use.

When you override a function, there is only one `"_"` original function reference saved in CMake's data structures. So... if you do it more than once, the `_` version now refers to one of the ones you've defined rather than the real "original" one. It's more like the last one.

Biggest CMake trickery

```
macro(install)  
endmacro(install)
```

Biggest CMake trickery

```
macro(install)  
endmacro(install)
```

```
_install(TARGETS _PyPartMC LIBRARY DESTINATION PyPartMC)
```

Are git submodules maintainable?

Are git submodules maintainable?

Yes!

Are git submodules maintainable?

Yes!

```
version: 2
updates:
  - package-ecosystem: "github-actions"
    directory: "/"
    schedule:
      interval: "weekly"
  - package-ecosystem: "pre-commit"
    directory: "/"
    schedule:
      interval: "weekly"
  - package-ecosystem: "git submodule"
    directory: "/"
    schedule:
      interval: "weekly"
```

Are git submodules maintainable?

Yes!

```
version: 2
updates:
  - package-ecosystem: "github-actions"
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    directory: "/"
    schedule:
      interval: "weekly"
  - package-ecosystem: "git submodule"
    directory: "/"
    schedule:
      interval: "weekly"
```

Dependabot

Dependabot creates pull requests to keep your dependencies secure and up-to-date.

You can opt out at any time by removing the `.github/dependabot.yml` config file.

[View update status](#)[Dismiss](#)

Packaging: cibuildwheel

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- Created and maintained by **Python Packaging Authority**



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- Easily create Python wheels for different operating systems and architectures!



Packaging: cibuildwheel

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- Easily create Python wheels for different operating systems and architectures!
- Wheels available for all modern Python versions in CPython (3.9-3.14) and PyPy (3.9-3.11)



Packaging: cibuildwheel

- Created and maintained by **Python Packaging Authority**
- Easily create Python wheels for different operating systems and architectures!
- Wheels available for all modern Python versions in CPython (3.9-3.14) and PyPy (3.9-3.11)
- Build wheels, test your code, and upload it to PyPI all in your **CI workflow!**



Packaging: cibuildwheel

- ✓ Build wheels on ubuntu-latest
- ✓ Build wheels on ubuntu-24.04-arm
- ✓ Build wheels on macos-14
- ✓ Build wheels on macos-15
- ✓ Build wheels on macos-15-intel
- ✓ Build wheels on windows-latest

Packaging: cibuildwheel

- ✓ Build wheels on ubuntu-latest
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- ✓ Build wheels on macos-15-intel
- ✓ Build wheels on windows-latest

Building cp313-manylinux_x86_64 wheel

CPython 3.13 manylinux x86_64

▶ Setting up build environment...

✓ 0.09s

▶ Building wheel...

✓ 179.37s

▶ Repairing wheel...

✓ 2.45s

No audit required for this wheel, as it is not abi3

▶ Testing wheel...

✓ 13.50s

✓ cp313-manylinux_x86_64 finished in 3 minutes

Building cp314-manylinux_x86_64 wheel

CPython 3.14 manylinux x86_64

▶ Setting up build environment...

✓ 0.09s

▶ Building wheel...

✓ 178.12s

▶ Repairing wheel...

✓ 2.44s

No audit required for this wheel, as it is not abi3

▶ Testing wheel...

✓ 14.39s

✓ cp314-manylinux_x86_64 finished in 3 minutes

CI example

```
- name: Install cibuildwheel
  run: python -m pip install cibuildwheel

- name: Build and test wheels
  env:
    # skip 32-bit, musllinux, and free-threaded builds
    CIBW_SKIP: "*-win32 *-manylinux_i686 *musllinux* cp3??t-*"
    CIBW_BEFORE_BUILD_WINDOWS: pip install delvewheel
    CIBW_ENVIRONMENT_WINDOWS: >-
      CMAKE_ARGS="-DCMAKE_MAKE_PROGRAM=D:/a/_temp/msys64/mingw64/bin/ninja.exe"
      CMAKE_PROGRAM_PATH="D:/a/_temp/msys64/usr/bin"
      CMAKE_GENERATOR="Ninja"
      TEMP="D:/a/_temp/"
    CIBW_REPAIR_WHEEL_COMMAND_WINDOWS: delvewheel repair -w {dest_dir} {wheel}
    CIBW_BEFORE_BUILD_MACOS: brew reinstall gcc; pip install --only-binary=llvmlite llvmlite
    CIBW_ENVIRONMENT_MACOS: MACOSX_DEPLOYMENT_TARGET=`sw_vers -productVersion` SYSTEM_VERSION_COMPAT=0
    CIBW_TEST_REQUIRES: pytest pytest-order
    CIBW_TEST_COMMAND: pytest -v -s -We -p no:unraisableexception {package}/tests
  run: python -m cibuildwheel --output-dir dist
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CI example

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- name: Install cibuildwheel
  run: python -m pip install cibuildwheel

- name: Build and test wheels
  env:
    # skip 32-bit, musllinux, and free-threaded builds
    CIBW_SKIP: "*-win32 *-manylinux_i686 *musllinux* cp3??t-*"
    CIBW_BEFORE_BUILD_WINDOWS: pip install delvewheel
    CIBW_ENVIRONMENT_WINDOWS: >-
      CMAKE_ARGS="-DCMAKE_MAKE_PROGRAM=D:/a/_temp/msys64/mingw64/bin/ninja.exe"
      CMAKE_PROGRAM_PATH="D:/a/_temp/msys64/usr/bin"
      CMAKE_GENERATOR="Ninja"
      TEMP="D:/a/_temp/"
    CIBW_REPAIR_WHEEL_COMMAND_WINDOWS: delvewheel repair -w {dest_dir} {wheel}
    CIBW_BEFORE_BUILD_MACOS: brew reinstall gcc; pip install --only-binary=llvmlite llvmlite
    CIBW_ENVIRONMENT_MACOS: MACOSX_DEPLOYMENT_TARGET=`sw_vers -productVersion` SYSTEM_VERSION_COMPAT=0
    CIBW_TEST_REQUIRES: pytest pytest-order
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    CIBW_ENVIRONMENT_MACOS: MACOSX_DEPLOYMENT_TARGET=${CIBW_PLATFORM} SYSTEM_VERSION_COMPAT=0
    CIBW_TEST_REQUIRES: pytest pytest-order
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- Enjoy!

Useful links

- PyPartMC Github: <https://github.com/open-atmos/PyPartMC>
- PyPartMC SoftwareX article: <https://doi.org/10.1016/j.softx.2023.101613>
- nanobind_json Github: https://github.com/Griger5/nanobind_json

Thank you!