aerosol dynamics package:

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

Jan 26th 2024
Columbia University, New York

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[2]Atmospheric Sciences, University of Illinois at Urbana-Champaign (atmos.illinois.edu)
[3]Mechanical Science & Engineering, University of Illinois at Urbana-Champaign (mechse.illinois.edu)

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- maintainer & developer:
  - github.com/numba-mpi
  - 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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- highlight: aerosol mixing state evolution

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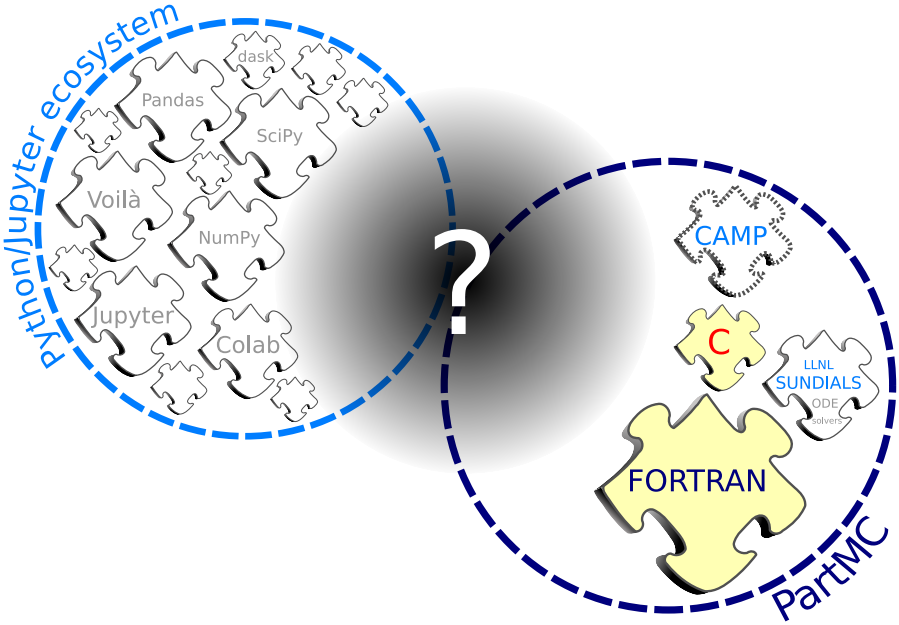
- highlight: aerosol mixing state evolution
- object-oriented architecture, F90, extensive automated test suite


Python/Jupyter ecosystem
dask
Pandas
SciPy
Voilà
NumPy
Jupyter
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?
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- **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**

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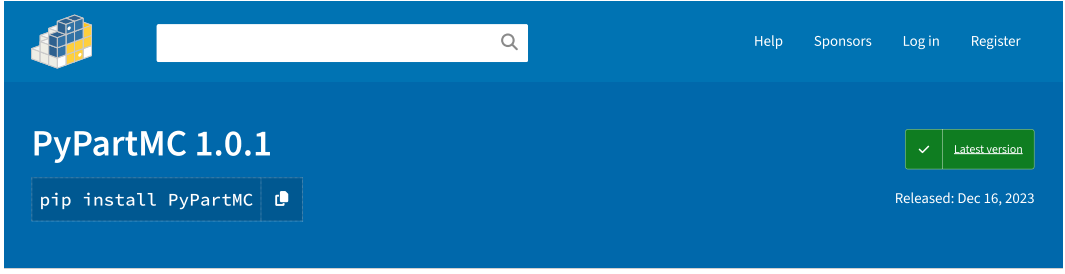
- ensure the same experience on Linux, macOS & Windows
- **lower the entry threshold for usage with Jupyter-based example notebooks**
- streamline the dissemination of paper-result reproducers (peer review)

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



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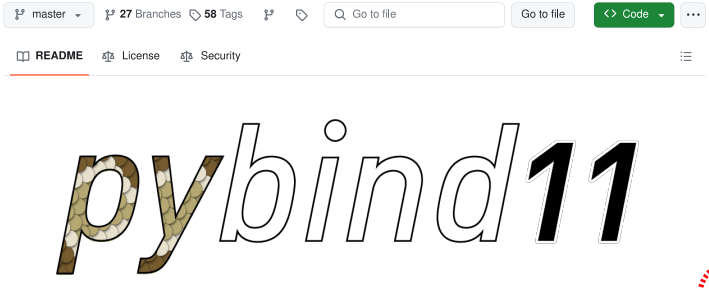
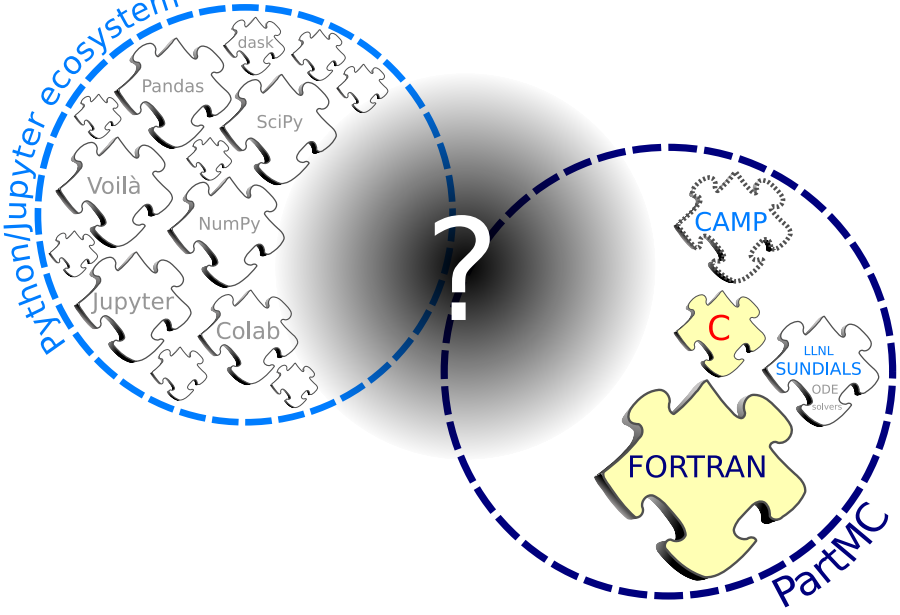
pybind11


master
27 Branches
58 Tags
Go to file
Go to file
Code
README
License
Security
pybind11
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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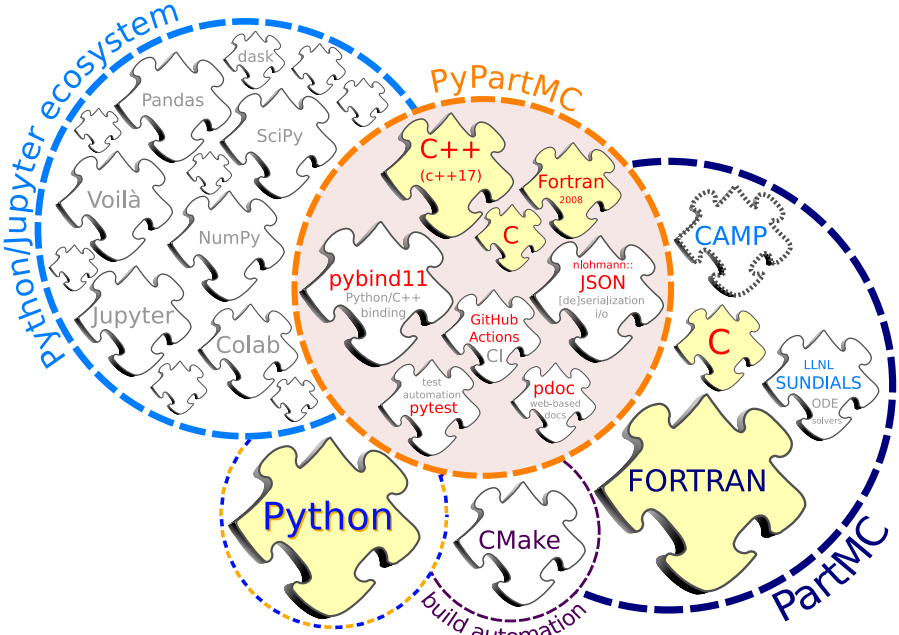
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(c++17)
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- dependency version pinning with git submodules: PartMC (F), CAMP (C/F), json (C++), pybind11 (C++), json-fortran (F), netCDF (C/F), SUNDIALS (F/C), SuiteSparse (C), ...
  & backports of C++20 features to C++17 (multilinux!): span, string_view, optional

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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

```
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)

```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": {
            "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)

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import PyPartMC as ppmc
from PyPartMC import si

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

aero_dist = ppmc.AeroDist(
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        }
    },
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    }],
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```

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,
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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( ...
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      "mass_frac", py.tuple({py.dict(pyargs("OC", py.tuple({1})))}), ...
      "diam_type", "geometric", ...
      "mode_type", "log_normal", ...
      "num_conc", 3200 / si.cm^3, ...
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    )) ...
  )), ...
  py.dict(pyargs( ...
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      "mass_frac", py.tuple({ ...
        py.dict(pyargs("OC", py.tuple({.3}))), ...
        py.dict(pyargs("BC", py.tuple({.7}))), ...
      }), ...
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      "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{:}]))
```
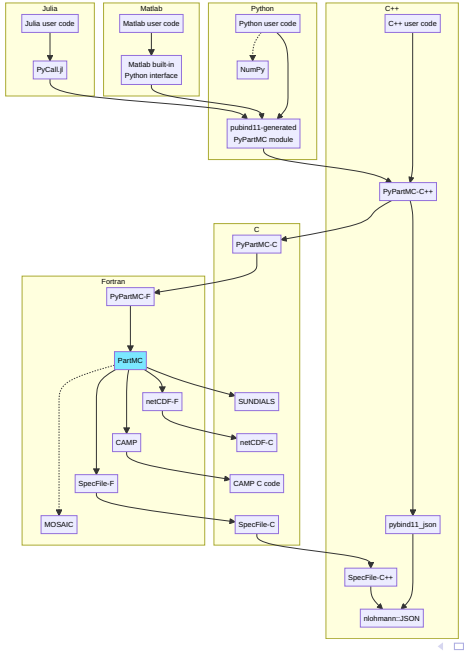
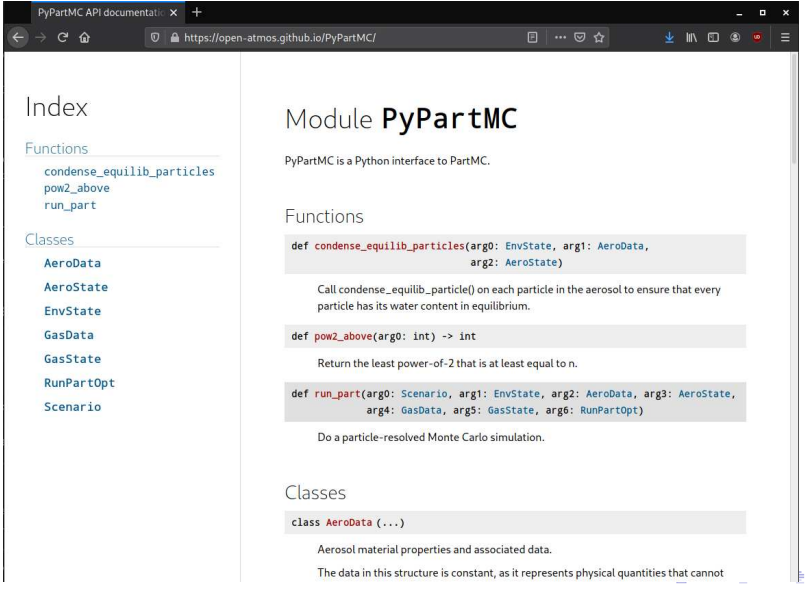


Julia
Julia user code
PyCall.jl
Matlab
Matlab user code
Matlab built-in Python interface
Python
Python user code
NumPy
pubind11-generated PyPartMC module
C++
C++ user code
PyPartMC-C++
C
PyPartMC-C
Fortran
PyPartMC-F
PartMC
netCDF-F
SUNDIALS
CAMP
netCDF-C
SpecFile-F
CAMP C code
MOSAIC
SpecFile-C
pybind11_json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

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



plan of the talk

PyPartMC: context / statement of need

PyPartMC: goals and status

PyPartMC: design & implementation outline

PyPartMC: demo

PyPartMC: summary

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- exception propagation from C++ through Fortran to C++ compiler dependent

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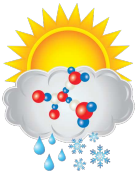
- offering users (students) a single-language familiar quick-start environment

acknowledgements

funding:



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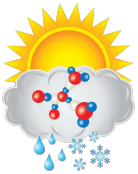

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Thank you for your attention!

pypi.org/p/PyPartMC
github.com/open-atmos/PyPartMC
doi:10.1016/j.softx.2023.101613