Python bindings for libcloudph++

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Abstract

This technical note introduces the Python bindings for libcloudph++. The libcloudph++ is a C++ library of algorithms for representing atmospheric cloud microphysics in numerical models. The bindings expose the complete functionality of the library to the Python users. The bindings are implemented using the Boost.Python C++ library and use NumPy arrays. This note includes listings with Python scripts exemplifying the use of selected library components. An example solution for using the Python bindings to access libcloudph++ from Fortran is presented.

1 Introduction

This paper describes how to use the libcloudph++ from the Python¹ programming language. The libcloudph++² is a free and open-source C++ library of algorithms for representing cloud microphysics in atmospheric numerical models. A detailed description of the library and its C++ interface has been described in [4]. In short, the library covers three numerical schemes describing processes occurring in warm clouds (i.e. in the absence of ice). The represented processes cover cloud-droplet condensational growth and formation of rain drops through collisions and coalescence. The first implemented scheme is a simplistic, so-called single-moment bulk scheme that allows predicting the total mass of cloud water and of rain water in a volume of air. The second scheme is a double-moment bulk scheme that adds prediction of the number concentration of cloud droplets and rain drops. The third scheme is based on the concept of particle tracking. The particle-based scheme implemented in libcloudph++ represents collisional growth of particles using a probabilistic Monte-Carlo type model. Furthermore, it is implemented for use on both multiple CPU threads as well as on a GPU.

Access to libcloudph++ from Python is provided through so-called bindings. The bindings to libcloudph++ allow using the library from Python, without requiring the user to interact with the native C++ interface. The Python bindings significantly facilitate the use of the library and add relatively little runtime overhead (particularly in the case of the resource-intensive particle-based scheme). Python has simpler syntax than C++, its philosophy emphasises succinct code (see [3] for a geoscience-relevant case study comparing Python, C++ and Fortran). Moreover, Python is widespread across the atmospheric science community [7]. The vast availability of software packages for interfacing Python codes from other languages [6] makes the Python bindings a good starting point for using libcloudph++ from other languages, for instance from Fortran. Arguably, the embraced approach makes the best out of salient features of two languages by using:

C++ for implementing numerically-intensive concurrency-enabled algorithms for both CPU and GPU, and encapsulating them in a library;

Python for equipping the library with rapid-development features and for interfacing with other languages.

This note is intended as a companion to the documentation of the library presented in [4] and is structured as follows. Section 2 presents the programming interface of the Python bindings. It includes examples of Python code with calls to two out of four components of the library, namely the commons (section 2.1) and the single-moment bulk scheme (section 2.2). Section 3 exemplifies how to use the Python bindings to call the libcloudph++ from Fortran. Appendix A describes how to obtain and install libcloudph++ and the Python bindings.

2 Summary of the Python interface

All elements of the Python bindings for libcloudph++ are contained in the libcloudphxx Python package. Naming of the package components closely follows the native C++ interface. The Python package contents are summarised in Table 1 and described through examples in the following subsections.

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Table 1: Contents of the libcloudphxx Python package. The a,b,c,d notation indicates that b,c,d are all attributes of a. The blk2m and lgrngn modules listed at the bottom of the table are part of the bindings but are not described in this note.

| item                                    | type     | summary                                      | example      |
|-----------------------------------------|----------|----------------------------------------------|--------------|
| git_revision                            | string   | version number                               | Lst. 1       |
| common                                  | module   |                                              |              |
| common.<R_v, R_d, eps, c_pd, c_pv, g, p_1000, rho_v> | floats   | physical constants                           | Lst. 2       |
| common.th_std2dry(th, rv)               | function | converts \( \theta \) to \( \theta_d \)      | Lst. 3       |
| common.th_dry2std(th, rv)               | function | converts \( \theta_d \) to \( \theta \)       | Lst. 3       |
| common.T(th_d, rh_d)                    | function | implements Eq. A14 in [4]                    | Lst. 3       |
| common.p(th, rv, T)                     | function | implements Eq. A15 in [4]                    | Lst. 3       |
| common.p_vs(T)                          | function | implements Eq. 15 in [2]                     | Lst. 4       |
| common.rw3_cr(rd3, kappa, T)            | function | critical radius cubed [8]                    | Lst. 6,10,11 |
| common.S_cr(rd3, kappa, T)              | function | critical saturation [8]                      | Lst. 6,10,11 |
| blk2m                                  | module   |                                              |              |
| blk2m.opts_t                           | class    | scheme options                               | Lst. 8       |
| blk2m.opts_t.<cond,cevp,revp,conv,accr,sedi> | bools   | process toggling flags                      | Lst. 8       |
| blk2m.opts_t.r_c0                      | float    | autoconversion threshold                     | Lst. 8       |
| blk2m.opts_t.r_eps                     | float    | saturation adjustment tolerance              | Lst. 8       |
| blk2m.adj_cellwise(opts, \( \rho_d \), \( \theta_d \), \( r_v \), \( r_c \), \( r_f \), \( \Delta f \)) | function | condensation                                 | Lst. 9       |
| blk2m.rha_cellwise(opts, \( r_c \), \( r_f \), \( r_v \)) | function | coalescence                                  |              |
| blk2m.rha_columnwise(opts, \( r_f \), \( \rho_d \), \( r_v \), \( \Delta z \)) | function | sedimentation                                |              |
| lgrngn                                  | module   |                                              |              |

After successful installation (see appendix A), the program given in Listing 1 will print the version number of the library expressed as a git revision id.

```
import libcloudphxx
print libcloudphxx.git_revision
```

2.1 Commons

The libcloudphxx.common module contains a collection of physical constants and formulæ. The constants exposed through the Python bindings can be printed with the instructions in Listing 2.

```
from libcloudphxx import common
print "R_d", common.R_d # gas constant for dry air
print "R_v", common.R_v # gas constant for water vapour
print "eps", common.eps # ratio of the above
print "c_pd", common.c_pd # specific heat of dry air
print "c_pv", common.c_pv # specific heat of water vapour
print "g", common.g # acceleration due to gravity
print "p_1000", common.p_1000 # reference pressure of 1000 hPa
print "rho_w", common.rho_w # density of water
```

As of the current release, there are seven formulæ available in the common module of the Python bindings, see Table 1. The first four functions convert the thermodynamic variables used in libcloudph++ (dry-air potential temperature \( \theta_d \), dry-air density \( \rho_d \), water vapour mixing ration \( r_v \)) to other commonly used variables (for details, see appendix A in [4]). Listing 3 presents example use of two functions for converting between the \( \theta_d \) and the standard potential temperature. It also depicts how to use the functions for diagnosing the temperature \( T \) as a function of \( \theta_d \) and \( \rho_d \), and for diagnosing the pressure \( p \) as a function of \( \rho_d \), \( r_v \) and \( T \) (eqs. A14 and A15 in [4]).

```
from libcloudphxx import common

tht = 300 # K
r_v = .01 # kg/kg

tht_d = common.th_std2dry(tht, r_v)
assert(tht == common.th_dry2std(tht_d, r_v))

rho_d = 1 # kg / m3
T = common.T(tht_d, rho_d)
p = common.p(rho_d, r_v, T)
```

The \( p_{vs}(T) \) function calculates the saturated vapour pressure as a function of temperature using an analytic solution to the Clausius-Clapeyron equation used in the library. Listing 4 depicts example use of this function to calculate the boiling temperature of water for atmospheric pressure of 500 hPa. Output of the program is given in Listing 5.

Note that the formulæ implemented in the common module accept and return only double-precision scalars, hence the need to use NumPy arrays even for single-equation problems).

The last two functions available in the common module compute the critical radius and the critical saturation (see chapter 5 in [5]) using the kappa-Kühler parameterisation of hygroscopicity of water-solution droplets [8]. Listing 6 shows an example Python
script generating a table of values of critical radius and supersaturation for five different nucleus radii (compare Table 5.1 in [5]). Output of the script is given in Listing 7.

2.2 Single-moment bulk scheme

Access to the single-moment bulk scheme implemented in libcloudph++ is provided through the libcloudphxx.blk1m module. The single-moment scheme extends the set of model state variables by adding two mass mixing ratios, namely the cloud water mixing ratio $r_c$ and the rain water mixing ratio $r_r$.

Options of the scheme that can be altered at runtime are grouped as attributes of the blk1m.opts_t class. The default values of all options are set upon creating an instance of opts_t, see Listing 8.

Among the options, there are Boolean flags for toggling condensation (cond), cloud-water evaporation (cevp), rain-water evaporation (revp), autoconversion of cloud water into rain (conv), accretion of cloud water by rain (accr) and sedimentation of rain (sedi). There $r_c0$ controls the threshold on cloud water mixing ratio above which autoconversion begins. The $r_eps$ is the absolute tolerance in terms of mass mixing ratio that controls the number of iterations within the saturation adjustment procedure. For further details, see description of Listing 3.1 in [4]. An instance of opts_t is expected as the first argument of the functions that constitute the interface of the single-moment scheme.

The blk1m.adj_cellwise() function implements the saturation adjustment procedure. It models the condensational growth of cloud droplets as well as the evaporation of water from cloud droplets and rain drops. An example calling sequence is presented in Listing 9 which is assumed to be a continuation of the code in Listing 8. The adj_cellwise() function expects: an instance of opts_t, five NumPy arrays of the model variables and a value of timestep dt. The five arrays are expected to contain values of the dry-air density $\rho_d$, that is not altered in the call, and four model state variables $\theta_d$, $r_v$, $r_c$, $r_r$. A call to adj_cellwise() modifies the state variables. In the presented example, the arrays have only one element what corresponds to a parcel-model set-up. If multi-element arrays are given, the saturation adjustment procedure is applied on each element.

The rhs_cellwise() and rhs_columnwise() functions implement representation of the collision-coalescence and the rain-sedimentation processes, respectively. They both take five arguments, and they both expect the first one to be an instance of opts_t.
For `rhs_cellwise()`, the next two arguments are `NumPy` arrays to which the tendencies of cloud- and rain-water mixing ratio will be added. The last two arguments are `NumPy` arrays storing cloud- and rain-water mixing ratios; these will not be modified.

For `rhs_columnwise()`, the second argument is a `NumPy` array to which the tendency of rain-water mixing ratio will be added. The third argument is expected to be a `NumPy` array with values of dry-air density. The array can have the same shape as other arrays, or can be a single-column array. The fourth argument is expected to be a `NumPy` array of rain-water mixing ratios and will not be modified. The last argument is the vertical grid spacing. The second and the third dimensions are treated as the vertical ones for 2-D and 3-D arrays, respectively. It is assumed that the indices of the array increase with height.

### 3 Accessing `libcloudph++` from Fortran via Python

Python is an efficient “glue” language for coupling codes written in different programming languages. In this section, we present an example solution for accessing `libcloudph++` from Fortran using the Python bindings. It is implemented using the CFFI (C Foreign Function Interface) Python package and the ISO C BINDING module that is part of the Fortran 2003 standard. Despite the fact that both CFFI and ISO C BINDING are intended for interfacing code written in the C language, the presented solution does not require a C compiler.

```python
from cffi import FFI
from libcloudphxx import common

ffi = FFI()
lib = ffi.dlopen("test.so")
ffi.cdef("void main(void*);")

@ffi.callback("double(double,double,double)"
def rw3_cr(rd3, kappa, T):
    return common.rw3_cr(rd3, kappa, T)

@ffi.callback("double(double,double)"
def S_cr(rd3, kappa, T):
    return common.S_cr(rd3, kappa, T)

lib.main(rd3, kappa, T)
```

The code exemplifying the use of `libcloudph++` from Fortran is presented in Listings 10 and 11. The code prints the same table as the one from Listing 6 but doing the calls to `libcloudph++` from Fortran.

The central idea is to provide a common addressing space for Python and Fortran, so that it is possible to refer to the Python code from Fortran and vice versa. To implement such C++/Python/Fortran coupling, the Fortran code is compiled as a shared library to be loaded from Python.

Example commands to compile and execute the codes from Listings 10 and 11 are presented in Listing 12. First, the `gfortran` compiler is instructed to compile `test.f` into a shared library `test.so`. Second, the Python script is run being instructed to include the current directory (“.”) in the shared-library search path. Consequently, even though the goal is to call Python from Fortran, the control flow starts in Python.

In the Python code in Listing 10, the `test.so` library is loaded by using the CFFI’s interface to the `dlopen()` system call. In order to enable accessing the Fortran subroutine `main`, the datatypes of the arguments of `main` are specified using the CFFI’s `cdef` function. The `void*` pointers are interpreted as function pointers within `main`. The CFFI “callback” mechanism is used to create callback objects for which Fortran-compatible function pointers can be obtained. The callback objects are defined as functions with the definition prepended with a `@ffi.callback` decorator. The decorator includes the C signature of the function. The signature specifies the datatypes of the return value and of the arguments. The callback objects defined in this way are then passed as arguments to `main`.

In the Fortran code in Listing 11, the definition of subroutine `main` is preceded by a definition of an interface to a three-argument function. Both the interface and the `main` subroutine are assigned with the `bind(c)` attribute which ensures CFFI-compatible naming of functions in the shared library.

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<http://cffi.readthedocs.org/>
The arguments to main are defined as C function pointers. Within main, the three-argument function interface is used to define two Fortran function pointers rw3_cr and S_cr. The Fortran function pointers are associated with the C ones by calling the c_f_procpointer subroutine (defined in the standard ISO_C_BINDING module). Afterwards, the rw3_cr and S_cr can be used as any other function in Fortran.

Output from execution of the two commands from Listing 12 is presented in Listing 13. It matches the result obtained with Python code from listing 6 presented in Listing 7.

### Listing 13

|     |     |     |     |
|-----|-----|-----|-----|
| rd  | um  | r*  | S−1 |
| 0.22E−01 | 0.19 | 0.39 |
| 0.48E−01 | 0.61 | 0.13 |
| 0.10 | 1.9 | 0.40E−01 |
| 0.22 | 6.1 | 0.12E−01 |
| 0.48 | 19. | 0.40E−02 |

### 4 Remarks

The presented bindings to libcloudph++ provide access to the library from Python, a de-facto standard interpreted language in science. Availability of the bindings enlarges the potential user base of libcloudph++. It also enlarges the range of the library applications by offering the possibility to couple libcloudph++ with numerous existing Python packages, e.g. with SciPy or CFFI as exemplified in this paper.

The presented C++/Python/Fortran coupling method is, to the authors’ knowledge, a novel approach. While not being straightforward, it has the advantage of offering productivity-oriented features of an interpreted language, even though the addressed problem concerns coupling of two compiled languages.

### A Obtaining and installing the bindings

The Python bindings for libcloudph++ are shipped with the library. The library uses CMake for build and test automation. Besides CMake, the library code depends on several components of the Boost C++ library collection and on the Thrust C++ library. If available, the library will be compiled with support for parallelisation of the particle-based algorithm using OpenMP and CUDA.

Listing 14 gives a set of commands that result in downloading the current development version of the library, compilation, execution of test programs, and installation of the library and Python bindings on the system. For reference on how to use non-default compiler or how to use non-default paths, see documentation of CMake and the README file shipped with libcloudph++.

### Listing 14

```bash
git clone http://github.com/igfuw/libcloudphxx
cd libcloudphxx
mkdir build; cd build
make ...
make all test
sudo make install
```

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### References

[1] D. Abrahams and R. Grosse-Kunstleve. “Building Hybrid Systems With Boost Python”. C/C++ Users Journal 21 (7 2003).

[2] S. Arabas and H. Pawlowska. “Adaptive method of lines for multi-component aerosol condensational growth and CCN activation”. Geosci. Model. Dev. 4 (2011), pp. 15–31. doi: 10.5194/gmd-4-15-2011.

[3] S. Arabas, D. Jarecka, A. Jaruga, and M. Fijalkowski. “Formula translation in Blitz++, NumPy and modern Fortran: A case study of the language choice tradeoffs”. Sci. Prog. 22 (2014), pp. 201–222. doi: 10.3233/SPR-140379.

[4] S. Arabas, A. Jaruga, H. Pawlowska, and W. Grabowski. “libcloudph++ 1.0: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++”. Geosci. Model. Dev. (2015). submitted, arXiv:1310.1905.

[5] J. Curry and P. Webster. Thermodynamics of Atmospheres and Oceans. Academic Press, 1999.

[6] H. Langtangen. “Combining Python with Fortran, C, and C++”. In: Python Scripting for Computational Science. Springer, 2008, pp. 189–226. isbn: 978-3-540-73915-9.

[7] J. W.-B. Lin. “Why Python Is the Next Wave in Earth Sciences Computing”. Bull. Amer. Meteor. Soc. 93 (2012), pp. 1823–1824. doi: 10.1175/BAMS-D-12-00148.1.

[8] M. Petters and S. Kreidenweis. “A single parameter representation of hygroscopic growth and cloud condensation nucleus activity”. Atmos. Chem. Phys. 7 (2007), pp. 1961–1971. doi: 10.5194/acp-7-6273-2008.