

PySDM v1: particle-based cloud modelling package for warm-rain microphysics and aqueous chemistry

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


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Introduction

PySDM is an open-source Python package for simulating the dynamics of particles undergoing condensational and collisional growth, interacting with a fluid flow and subject to chemical composition changes. It is intended to serve as a building block for process-level as well as computational-fluid dynamics simulation systems involving representation of a continuous phase (air) and a dispersed phase (aerosol), with PySDM being responsible for representation of the dispersed phase. For major version 1 (v1), the development has been focused on atmospheric cloud physics applications, in particular on modelling the dynamics of particles immersed in moist air using the particle-based approach to represent the evolution of the size spectrum of aerosol/cloud/rain particles. The particle-based approach contrasts the more commonly used bulk and bin methods in which atmospheric particles are segregated into multiple categories (aerosol, cloud and rain) and their evolution is governed by deterministic dynamics solved on the same Eulerian grid as the dynamics of the continuous phase. Particle-based methods employ discrete computational (super) particles for modelling the dispersed phase. Each super particle is associated with a set of continuously-valued attributes evolving in Lagrangian manner. Such approach is particularly well suited for using probabilistic representation of particle collisional growth (coagulation) and for representing processes dependent on numerous particle attributes which helps to overcome the limitations of bulk and bin methods ([Morrison et al., 2020](#)).

The PySDM package core is a Pythonic high-performance implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth ([Shima et al., 2009](#)), hence the name. The SDM is a probabilistic alternative to the mean-field approach embodied by the Smoluchowski equation, for a comparative outline of both approaches see Bartman & Arabas (2021). In atmospheric aerosol-cloud interactions, particle collisional growth is responsible for the formation of rain drops through collisions of smaller cloud droplets (warm-rain process) as well as for aerosol washout.

Besides collisional growth, PySDM includes representation of condensation/evaporation of water vapour to/from the particles. Furthermore, representation of dissolution and, if applicable, dissociation of trace gases (sulfur dioxide, ozone, hydrogen peroxide, carbon dioxide, nitric acid, and ammonia) is included to model the subsequent aqueous-phase oxidation of the dissolved sulfur dioxide. Representation of the chemical processes follows the particle-based formulation of Jaruga & Pawlowska (2018).

The usage examples are built on top of four different environment classes included in PySDM v1 which implement common simple atmospheric cloud modelling frameworks: box, adiabatic

44 parcel, single-column, and 2D prescribed flow kinematic models.

45 In addition, the package ships with tutorial code depicting how PySDM can be used from Julia
 46 and Matlab using the PyCall.jl and the Matlab-bundled Python interface, respectively. Two
 47 exporter classes are available as of time of writing enabling storage of particle attributes and
 48 gridded products in the VTK format and storage of gridded products in netCDF format.

49 Dependencies and supported platforms

50 PySDM essential dependencies are: NumPy, SciPy, Numba, Pint, and ChemPy which are all free
 51 and open-source software available via the PyPI platform. PySDM releases are published at
 52 the PyPI Python package index allowing installation using the pip package manager (i.e.,
 53 `pip install PySDM`).

54 PySDM has two alternative parallel number-crunching backends available: multi-threaded CPU
 55 backend based on Numba (Lam et al., 2015) and GPU-resident backend built on top of
 56 ThrustRTC (Yang, 2020). The optional GPU backend relies on proprietary vendor-specific
 57 CUDA technology, the accompanying non-free software and drivers; ThrustRTC and CURandRTC
 58 packages are released under the Anti-996 license.

59 The usage examples for Python were developed embracing the Jupyter interactive platform
 60 allowing control of the simulations via web browser. All Python examples are ready for use
 61 with the mybinder.org and the Google Colab platforms.

62 Continuous integration infrastructure used in the development of PySDM assures the targeted
 63 full usability on Linux, macOS, and Windows environments. Compatibility with Python versions
 64 3.7 through 3.9 is maintained as of the time of writing. Test coverage for PySDM is reported
 65 using the codecov.io platform. Coverage analysis of the backend code requires execution
 66 with JIT-compilation disabled for the CPU backend (e.g., using the `NUMBA_DISABLE_JIT=1`
 67 environment variable setting). For the GPU backend, a purpose-built FakeThrust class is
 68 shipped with PySDM which implements a subset of the ThrustRTC API and translates C++
 69 kernels into equivalent Numba parallel Python code for debugging and coverage analysis.

70 The Pint dimensional analysis package is used for unit testing. It allows asserting on the
 71 dimensionality of arithmetic expressions representing physical formulae. In order to enable JIT
 72 compilation of the formulae for simulation runs, a purpose-built FakeUnitRegistry class that
 73 mocks the Pint API reducing its functionality to SI prefix handling is used by default outside
 74 of tests.

75 API in brief

76 In order to depict PySDM API with a practical example, the following listings provide sample
 77 code roughly reproducing the Figure 2 from the Shima et al. (2009) paper in which the SDM
 78 algorithm was introduced.

79 It is a coalescence-only set-up in which the initial particle size spectrum is exponential and is
 80 deterministically sampled to match the condition of each super particle having equal initial
 81 multiplicity, with the multiplicity denoting the number of real particles represented by a single
 82 computational particle:

```
from PySDM.physics import si
from PySDM.initialisation.sampling import spectral_sampling
from PySDM.initialisation.spectra import Exponential

N_SD = 2 ** 17
initial_spectrum = Exponential(
    norm_factor=8.39e12, scale=1.19e5 * si.um ** 3)
```

```
attributes = {}
sampling = spectral_sampling.ConstantMultiplicity(initial_spectrum)
attributes['volume'], attributes['n'] = sampling.sample(N_SD)
```

83 In the above snippet, the `si` is an instance of the `FakeUnitRegistry` class. The exponential
 84 distribution of particle volumes is sampled at 2^{17} points in order to initialise two key attributes
 85 of the super-droplets, namely their volume and multiplicity. Subsequently, a `Builder` object
 86 is created to orchestrate dependency injection while instantiating the `Particulator` class of
 87 `PySDM`:

```
import numpy as np
from PySDM.builder import Builder
from PySDM.environments import Box
from PySDM.dynamics import Coalescence
from PySDM.dynamics.collisions.collision_kernels import Golovin
from PySDM.backends import CPU
from PySDM.products import ParticleVolumeVersusRadiusLogarithmSpectrum
```

```
builder = Builder(n_sd=N_SD, backend=CPU())
builder.set_environment(Box(dt=1 * si.s, dv=1e6 * si.m ** 3))
builder.add_dynamic(Coalescence(collision_kernel=Golovin(b=1.5e3 / si.s)))
```

```
radius_bins_edges = np.logspace(
    start=np.log10(10 * si.um),
    stop=np.log10(5e3 * si.um),
    num=32
)
products = (ParticleVolumeVersusRadiusLogarithmSpectrum(
    radius_bins_edges=radius_bins_edges,
    name='dv/dlnr'
),)
particulator = builder.build(attributes, products)
```

88 The backend argument may be set to an instance of either CPU or GPU what translates to
 89 choosing the multi-threaded Numba-based backend or the ThrustRTC-based GPU-resident
 90 computation mode, respectively. The employed `Box` environment corresponds to a zero-
 91 dimensional framework (particle positions are neglected). The `SDM` Monte-Carlo coalescence
 92 algorithm is added as the only dynamic in the system (other dynamics available as of time of
 93 writing represent condensational growth, particle displacement, aqueous chemistry, ambient
 94 thermodynamics, and Eulerian advection). Finally, the `build()` method is used to obtain
 95 an instance of the `Particulator` class which can then be used to control time-stepping and
 96 access simulation state through the products registered with the builder. A minimal simulation
 97 example is depicted below with a code snippet and a resultant plot (Figure 1):

```
from PySDM.physics.constants_defaults import rho_w
from matplotlib import pyplot

for step in [0, 1200, 2400, 3600]:
    particulator.run(step - particulator.n_steps)
    pyplot.step(
        x=radius_bins_edges[:-1] / si.um,
        y=particulator.products['dv/dlnr'].get().squeeze() * rho_w/si.g,
        where='post', label=f"$t = \{step\}s$")

pyplot.xscale('log')
pyplot.xlabel(r'particle radius [$\mu$ m]')
pyplot.ylabel("$dm/dlnr$ [g/m$^3$/(unit dr/r)]")
```

```
pyplot.legend()
pyplot.show()
```

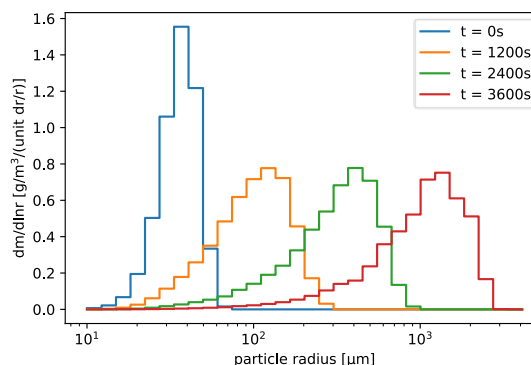


Figure 1: Sample plot generated with the code snippets included in the paper.

Usage examples

The PySDM examples are shipped in a separate package that can also be installed with pip (pip install PySDM-examples) or conveniently experimented with using Colab or mybinder.org platforms (single-click launching badges included in the PySDM README file). The examples are based on setups from literature, and the package is structured using bibliographic labels (e.g., PySDM_examples.Shima_et_al_2009).

All examples feature a settings.py file with simulation parameters, a simulation.py file including logic analogous to the one presented in the code snippets above for handling composition of PySDM components using the Builder class, and a Jupyter notebook file with simulation launching code and basic result visualisation.

Box environment examples

The Box environment is the simplest one available in PySDM, and the PySDM-examples package ships with two examples based on it. The first is an extension of the code presented in the snippets in the preceding section and reproduces Fig. 2 from the seminal paper of Shima et al. (2009). Coalescence is the only process considered, and the probabilities of collisions of particles are evaluated using the Golovin additive kernel, which allows to compare the results with analytical solution of the Smoluchowski equation (included in the resultant plots).

The second example based on the Box environment, also featuring collision-only setup, reproduces several figures from the work of Berry (1966) involving more sophisticated collision kernels representing such phenomena as the geometric sweep-out and the influence of electric field on the probability of collisions.

Adiabatic parcel examples

The Parcel environment shares the zero-dimensionality of Box (i.e., no particle physical coordinates considered), yet provides a thermodynamic evolution of the ambient air mimicking adiabatic displacement of an air parcel in hydrostatically stratified atmosphere. Adiabatic cooling during the ascent results in supersaturation which triggers activation of aerosol particles (condensation nuclei) into cloud droplets through condensation. All examples based on the Parcel environment utilise the Condensation and AmbientThermodynamics dynamics.

The simplest example uses a monodisperse particle spectrum represented with a single super-droplet and reproduces simulations described in Arabas & Shima (2017) where an ascent-descent scenario is employed to depict hysteresis behaviour of the activation/deactivation phenomena.

A polydisperse lognormal spectrum represented with multiple super-droplets is used in the example based on the work of Yang et al. (2018). Simulations presented involve repeated ascent-descent cycles and depict the evolution of partitioning between activated and unactivated particles. Similarly, polydisperse lognormal spectra are used in the example based on Lowe et al. (2019), where additionally each lognormal mode has a different hygroscopicity. The Lowe et al. (2019) example features representation of droplet surface tension reduction by organics.

Finally, there are two examples featuring adiabatic parcel simulations involving representation of the dynamics of chemical composition of both ambient air and the droplet-dissolved substances, in particular focusing on the oxidation of aqueous-phase sulfur. The examples reproduce the simulations discussed in Kreidenweis et al. (2003) and in Jaruga & Pawlowska (2018).

Kinematic (prescribed-flow) examples

Coupling of PySDM with fluid-flow simulation is depicted with both 1D and 2D prescribed-flow simulations, both dependent on the PyMPDATA package (Bartman et al., 2021) implementing the MPDATA advection algorithm. For a review on MPDATA, see e.g., Smolarkiewicz (2006).

Usage of the kinematic_1d environment is depicted in an example based on the work of Shipway & Hill (2012). The kinematic_2d environment is showcased with an interactive user interface which allows study of aerosol-cloud interactions in a drizzling stratocumulus setup based on the works of Morrison & Grabowski (2007) and Arabas et al. (2015).

Figure 2 presents a snapshot from the 2D simulation performed with a setup described in detail in Arabas et al. (2015). Each plot depicts a 1.5 km by 1.5 km vertical slab of an idealised atmosphere in which a prescribed single-eddy non-divergent flow is forced (updraft in the left-hand part of the domain, downdraft in the right-hand part). The left-hand plot shows the distribution of aerosol particles in the air. The upper part of the domain is covered with a stratocumulus-like cloud formed on aerosol particles above the flat cloud base at the level where relative humidity goes above 100%. Within the cloud, the aerosol concentration is thus reduced. The middle plot depicts the wet radius of particles. Particles larger than 1 micrometre in diameter are considered as cloud droplets, particles larger than 50 micrometres in diameter are considered as drizzle (unlike in bin or bulk models, such categorisation is employed for analysis only and not within the particle-based model formulation). Concentration of drizzle particles forming through collisions is depicted in the right-hand panel. A rain shaft forms in the right part of the domain where the downward flow direction amplifies particle sedimentation. Precipitating drizzle drops collide with aerosol particles washing out the sub-cloud aerosol. Most of the drizzle drops evaporate before reaching the bottom of the domain depicting the virga phenomenon and the resultant aerosol resuspension.

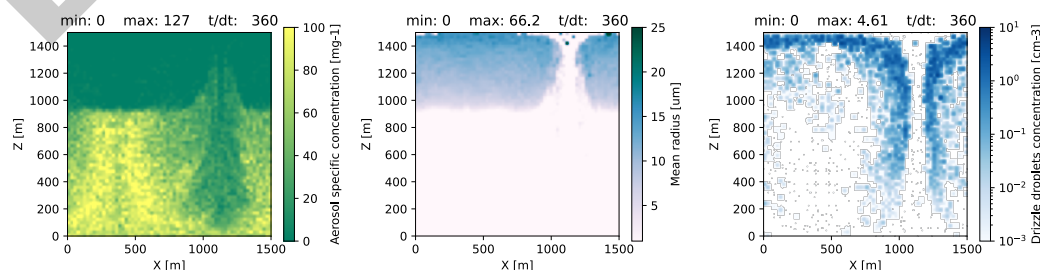


Figure 2: Results from a 2D prescribed-flow simulation using the Arabas et al. (2015) example.

Selected relevant recent open-source developments

The SDM algorithm implementations are part of the following open-source packages (of otherwise largely differing functionality):

- libcloudph++ in C++ (Arabas et al., 2015; Jaruga & Pawlowska, 2018) with Python bindings (Jarecka et al., 2015);
- SCALE-SDM in Fortran, (Sato et al., 2018);
- PALM LES in Fortran, (Maronga et al., 2020);
- LCM1D in Python/C, (Unterstrasser et al., 2020);
- Pencil Code in Fortran, (Brandenburg et al., 2021);
- NTLF in Fortran, (Richter et al., 2021).
- superdroplet in Python (Cython and Numba), C++, Fortran and Julia (<https://github.com/darochen/superdroplet>);

A list of links directing to SDM-related files within the above projects' repositories is included in the PySDM README file.

Python packages for solving the dynamics of aerosol particles with discrete-particle (moving-sectional) representation of the size spectrum include (both depend on the Assimulo package for solving ODEs):

- pyrcel, (Rothenberg & Wang, 2017);
- PyBox, (Topping et al., 2018).

Summary

The key goal of the reported endeavour was to equip the cloud modelling community with a solution enabling rapid development and independent reproducibility of simulations while being free from the two-language barrier commonly separating prototype and high-performance research code. The key advantages of PySDM stem from the characteristics of the employed Python language which enables high performance computational modelling without trading off such features as:

succinct syntax – the snippets presented in the paper are arguably close to pseudo-code;

portability depicted in PySDM with continuous integration Linux, macOS and Windows;

interoperability depicted in PySDM with Matlab and Julia usage examples requiring minimal amount of biding-specific code;

multifaceted ecosystem depicted in PySDM with one-click execution of Jupyter notebooks on mybinder.org and colab.research.google.com platforms;

availability of tools for modern hardware depicted in PySDM with the GPU backend.

PySDM together with a set of developed usage examples constitutes a tool for research on cloud microphysical processes, and for testing and development of novel modelling methods. PySDM is released under the GNU GPL v3 license.

Author contributions

PB had been the architect and lead developer of PySDM v1 with SA taking the role of main developer and maintainer over the time. PySDM 1.0 release accompanied PB's MSc thesis prepared under the mentorship of SA. MO contributed to the development of the condensation solver and led the development of relevant examples. GŁ contributed the initial draft of the aqueous-chemistry extension which was refactored and incorporated into PySDM under guidance from AJ. KG and BP contributed to the GPU backend. CS and AT contributed to

the examples. OB contributed the VTK exporter. The paper was composed by SA and PB and is partially based on the content of the PySDM README file and PB's MSc thesis.

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