

PySDM: current/future features and how to get involved as a contributor!

Sylwester Arabas

AGH University of Krakow, Poland

PySDM contributors:

S. Azimi, **P. Bartman**, B. Bhalla, S. Bhiogade, **O. Bulenok**, K. Derlatka, I. Dula,
A. Jaruga, **E. de Jong**, B. Mackay, A. Makulska, M. Mints, **C. Singer**, R.X. Ward, ...

Jan 26 2024

Columbia University, New York

context: aerosol-cloud-precipitation interactions (scales!)



“Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain”

(photo: Yevgen Timashov / National Geographic)

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

Hugh Morrison ✉, Marcus van Lier-Walqui, Ann M. Fridlind, Wojciech W. Grabowski, Jerry Y. Harrington, Corinna Hoose, Alexei Korolev, Matthew R. Kumjian, Jason A. Milbrandt, Hanna Pawlowska, Derek J. Posselt, Olivier P. Prat, Karly J. Reimel, Shin-Ichiro Shima, Bastiaan van Diedenhoven, Lulin Xue

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Journal of Advances in Modeling Earth Systems 10.1029/2019MS001689

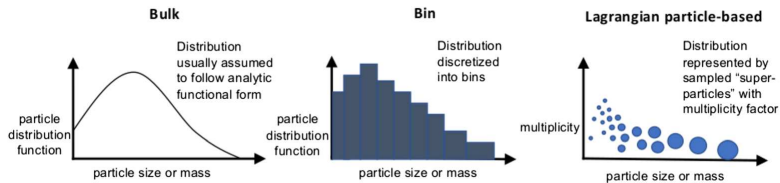


Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

super-particles: example 2D kinematic Sc test (Morrison & Grabowski '07)

2D flow field

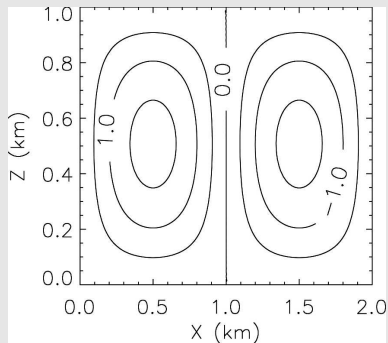
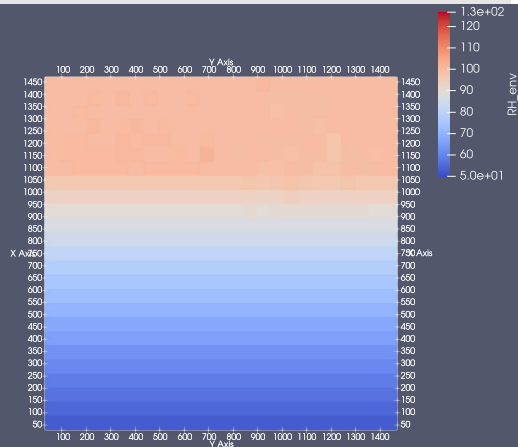
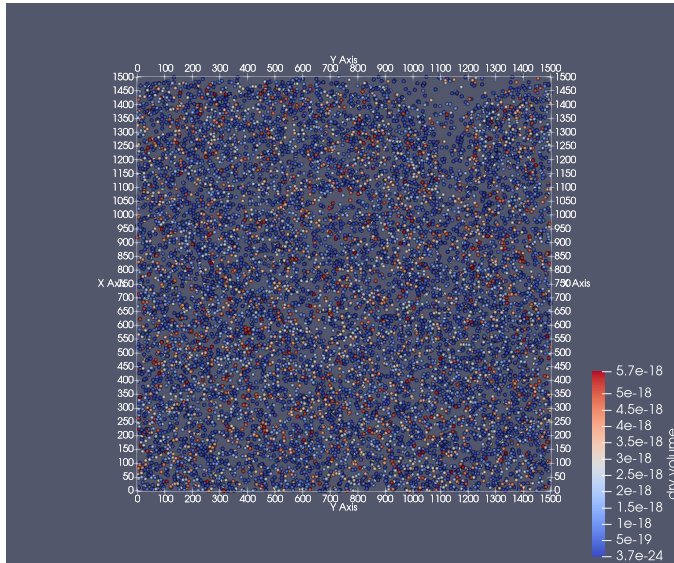


FIG. 1. Time-invariant vertical velocity for the stratocumulus case (contour interval is 0.5 m s⁻¹).

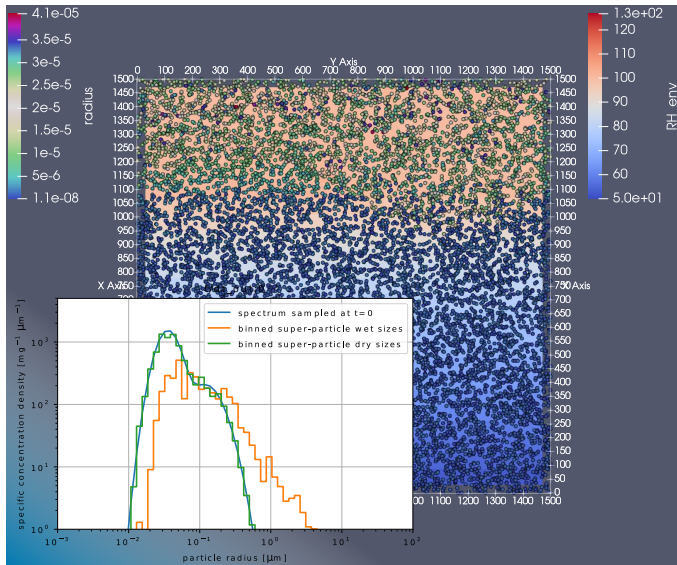
RH profile at t=0



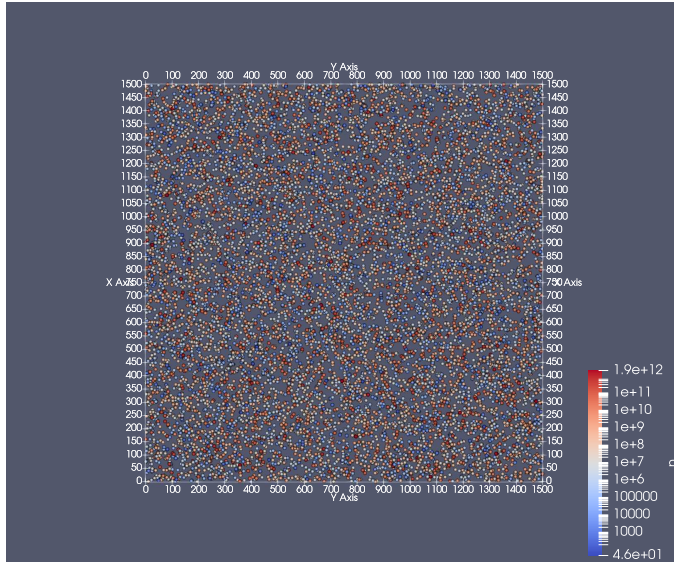
super-particle attribute initialisation: dry/wet volume



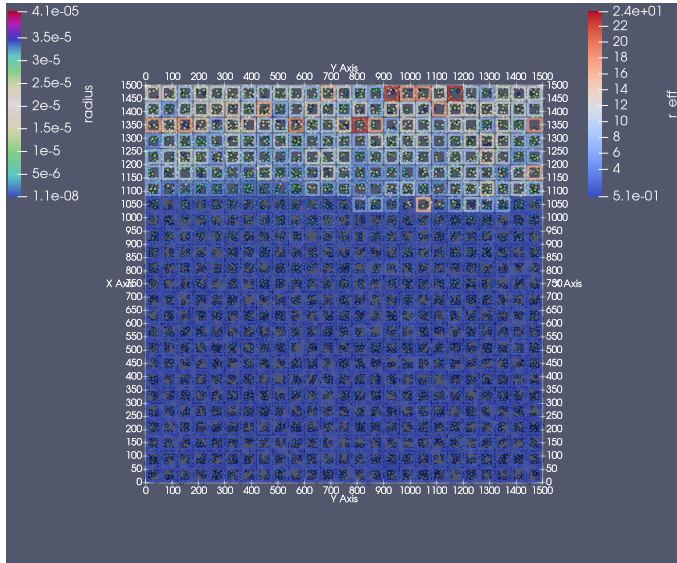
super-particle attribute initialisation: dry/wet volume



super-particle attribute initialisation: multiplicity



super-particle attribute evolution (droplet radius) and "products"



SDM

PySDM

PySDM goals:

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- applicable in research on aerosol-cloud-interactions (and beyond)
KPI: reproduction of results from classic and recent literature

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- **easy to reuse:** code (Python), examples (Jupyter), extensibility (modular, high test coverage)
interoperability (other languages, i/o), leveraging modern hardware (GPUs, multi-core CPUs)
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- **accessibility:** seamless Linux/macOS/Windows installation (pip)
KPI: continuous integration on all targeted platforms

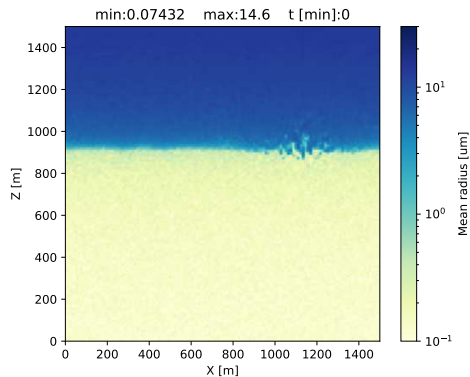
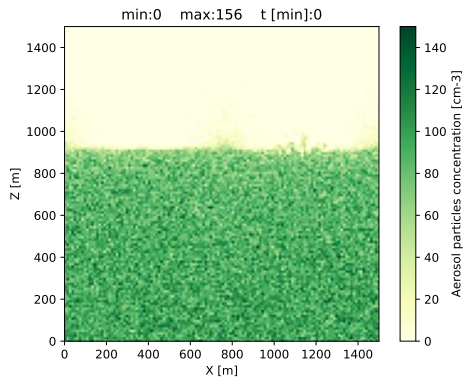
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- **accessibility:** seamless Linux/macOS/Windows installation (pip)
KPI: continuous integration on all targeted platforms
- **curation:** open licensing (GPL), public versioned development (Github)
KPI: instant and anonymous execution on commodity environment

sample aerosol-cloud-precipitation interactions simulation

Computational grid: 128x128

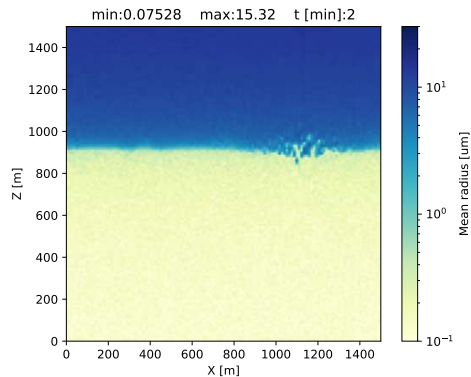
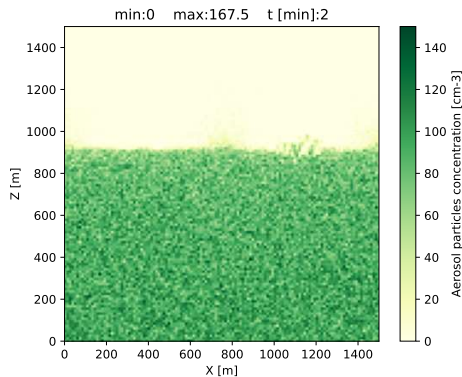
Computational particles: 2^{21}



sample aerosol-cloud-precipitation interactions simulation

Computational grid: 128x128

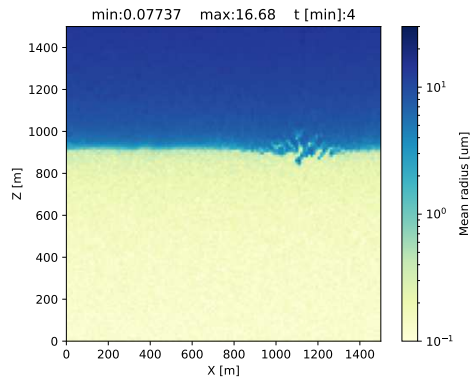
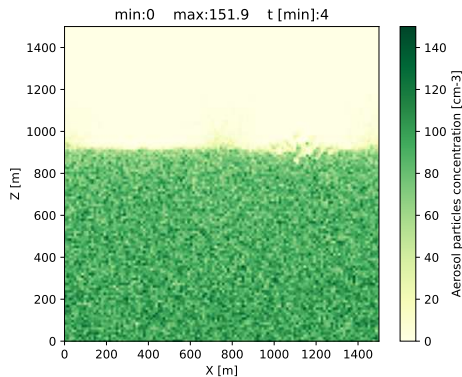
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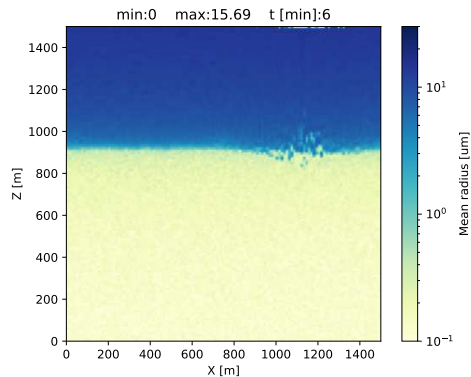
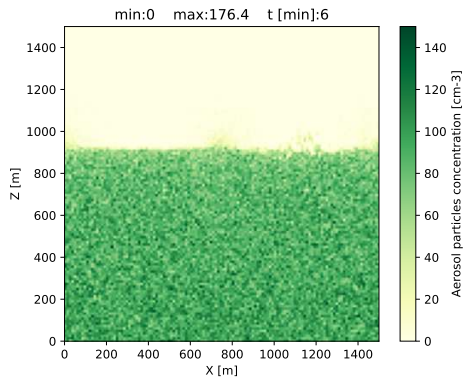
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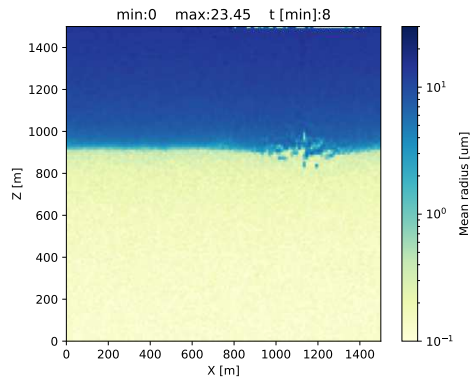
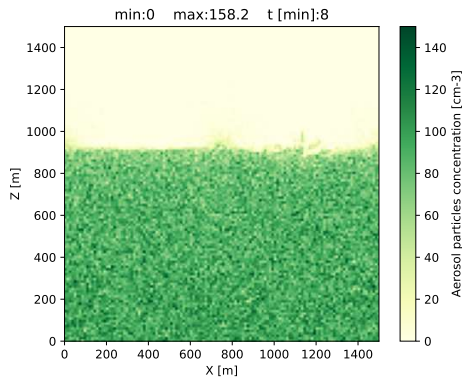
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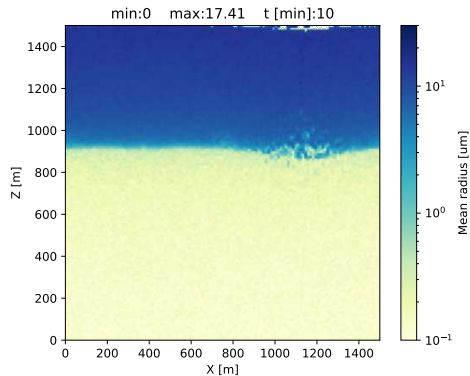
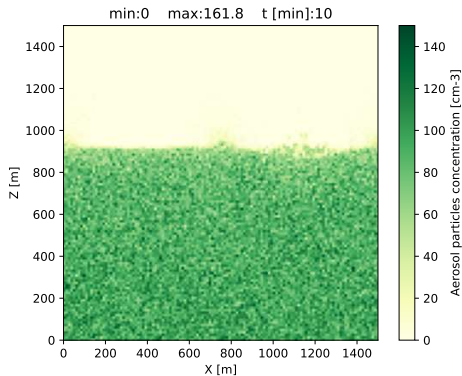
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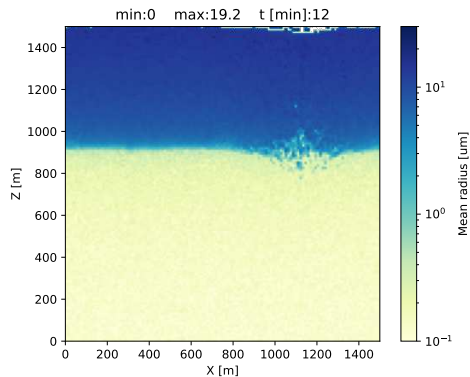
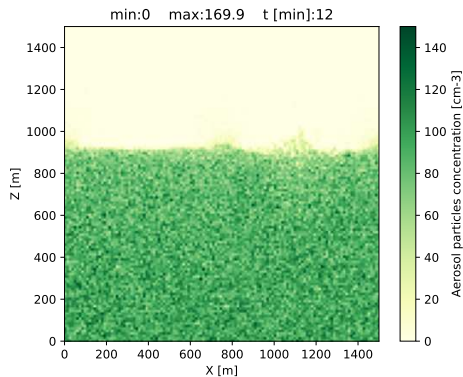
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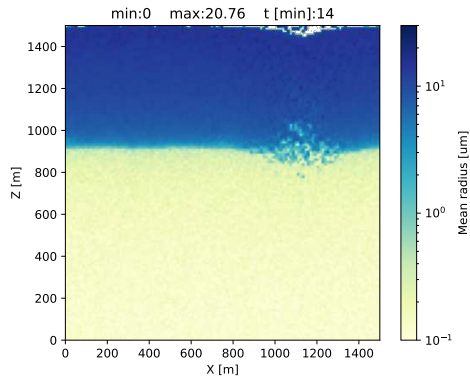
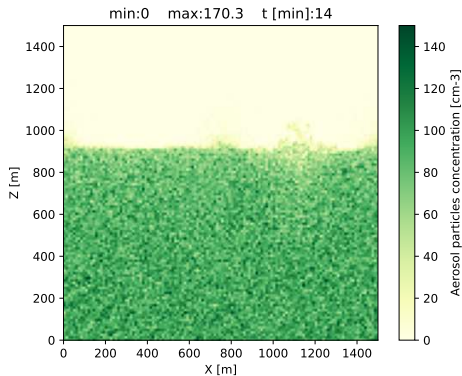
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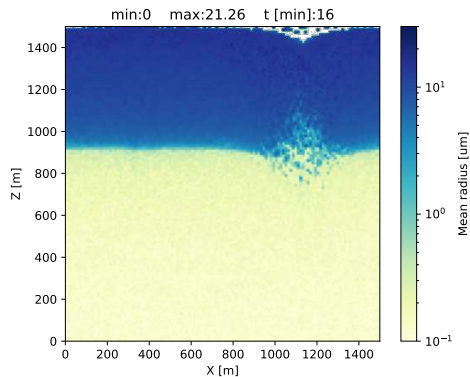
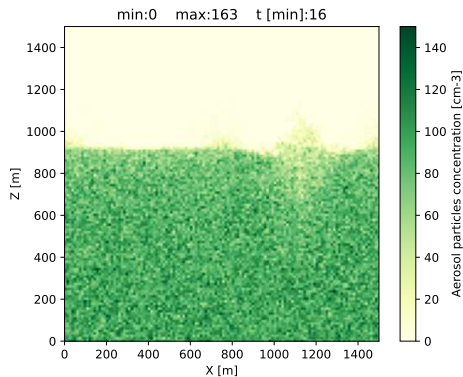
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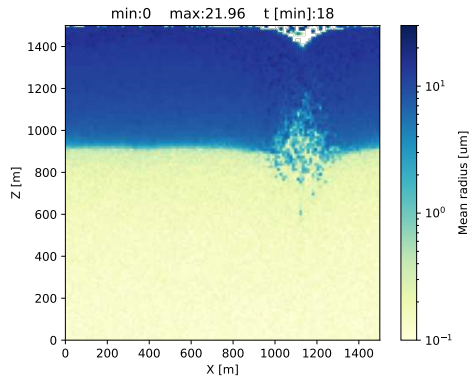
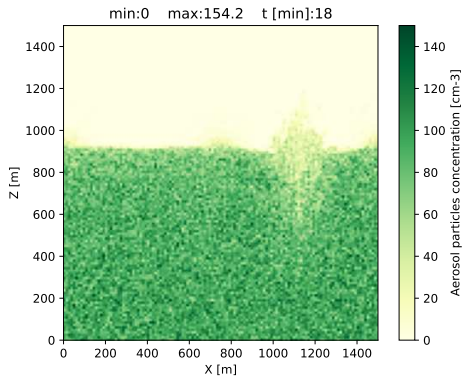
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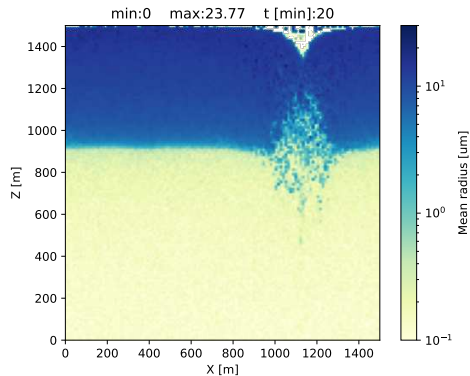
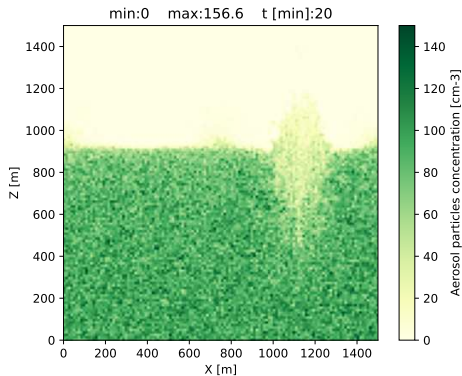
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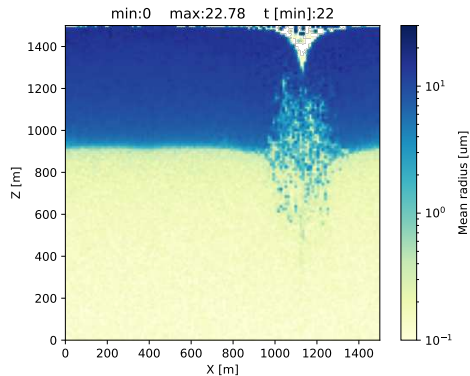
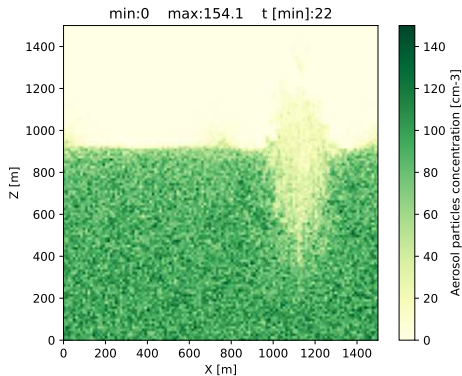
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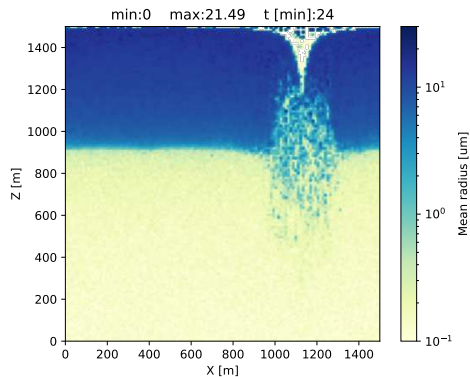
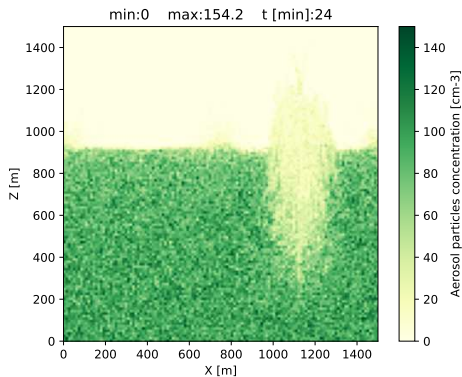
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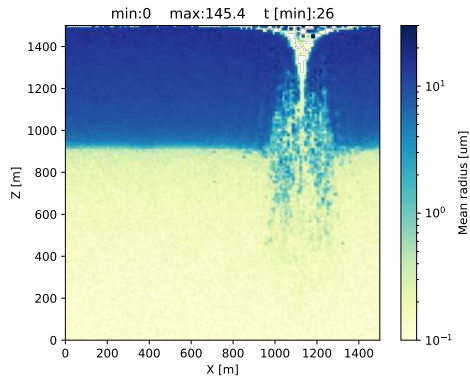
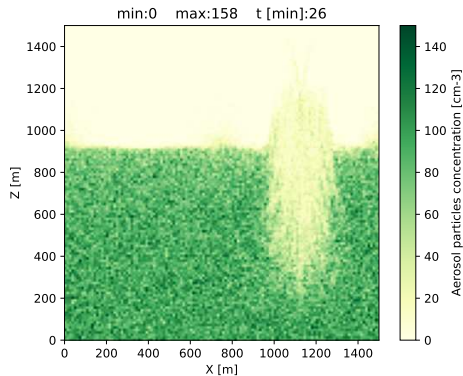
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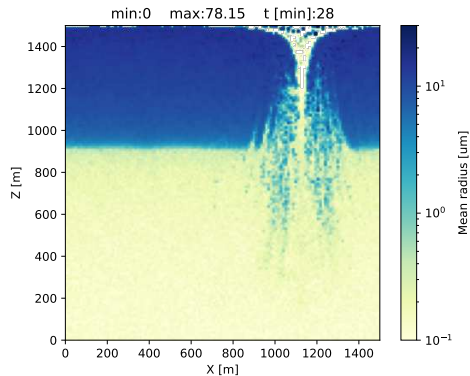
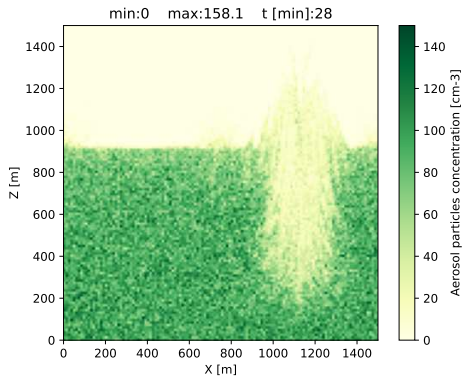
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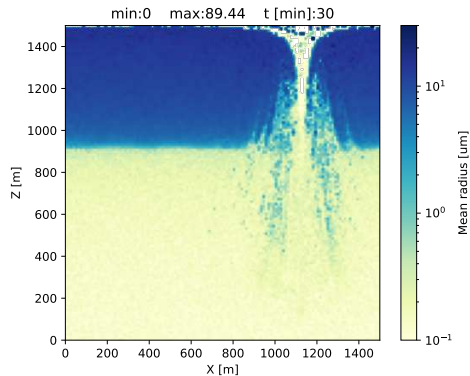
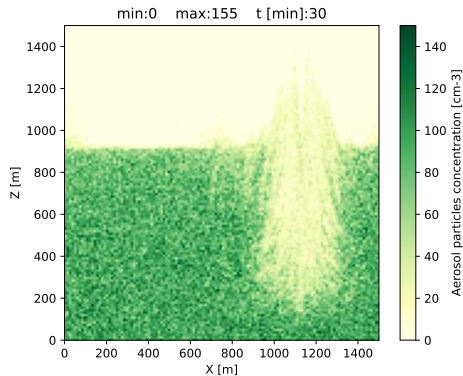
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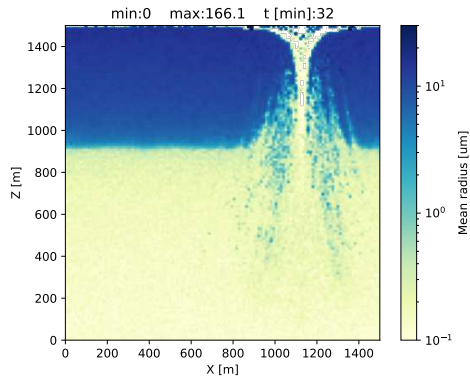
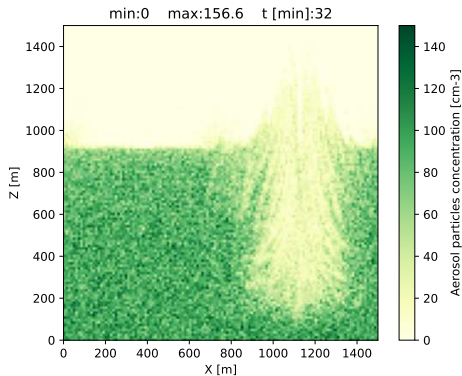
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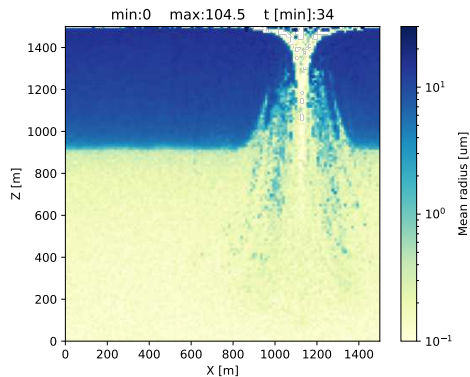
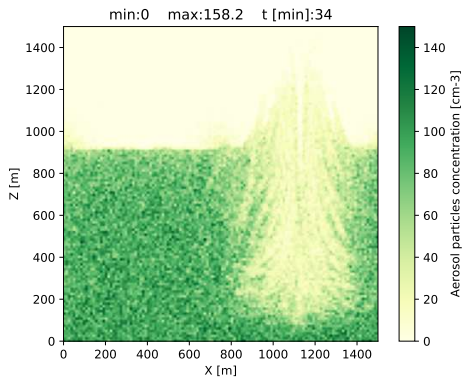
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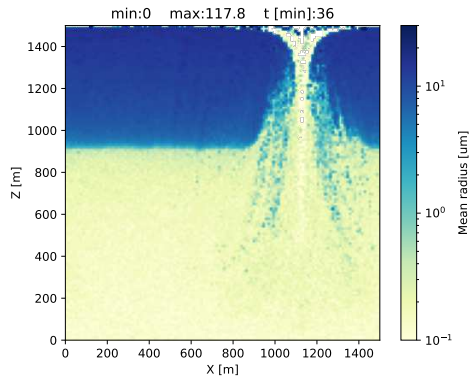
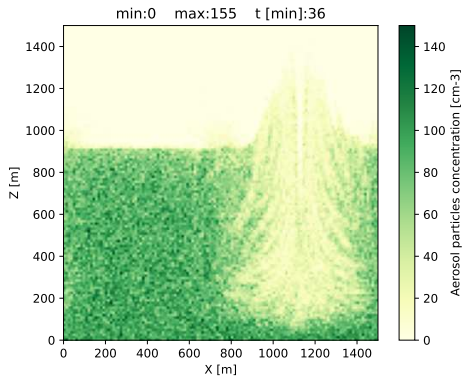
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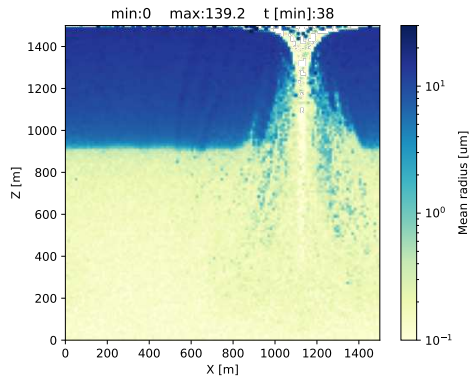
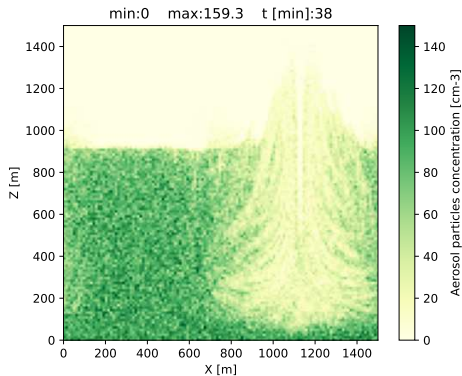
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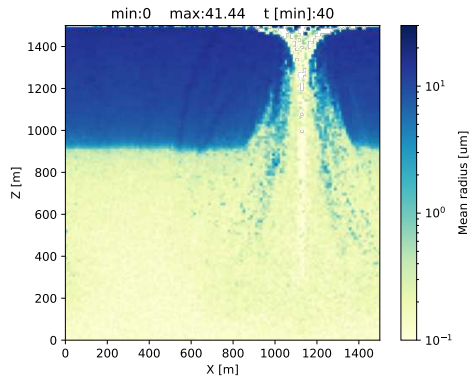
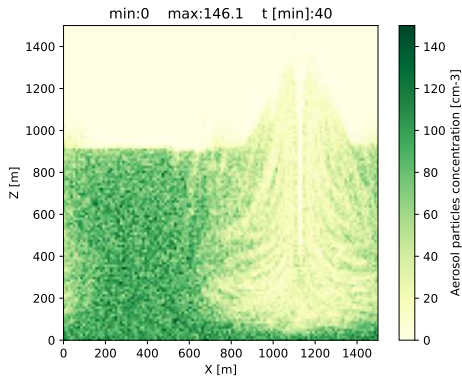
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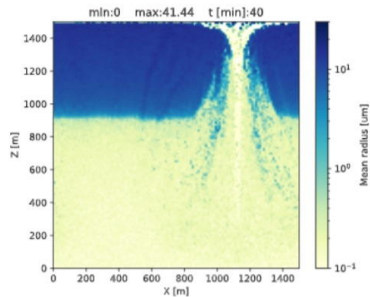
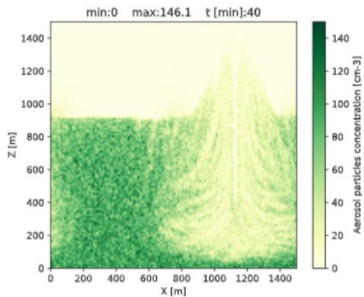


sample aerosol-cloud-precipitation interactions simulation

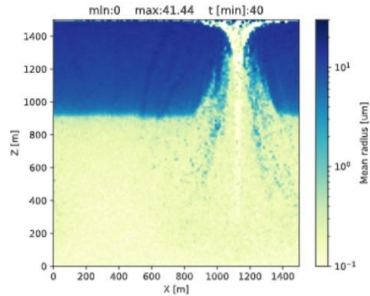
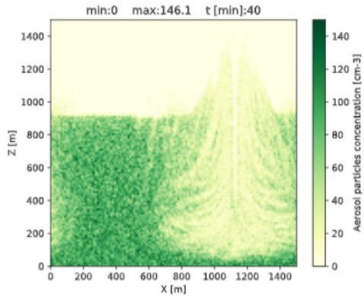
Computational grid: 128x128

Computational particles: 2^{21}





```
[3] 1 simulation.run()
```



PySDM: Pythonic, Jupyter-friendly



demo.ipynb ☆

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RAM

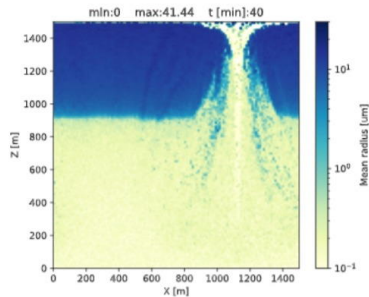
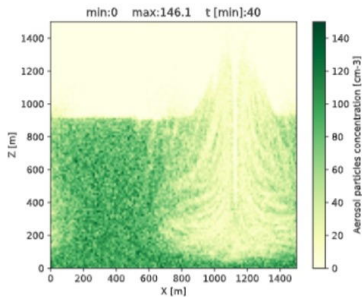
Disk



Editing



```
[3] 1 simulation.run()
```



PySDM: Pythonic, Jupyter-friendly, GPU-enabled

Learn more'. At the bottom of the dialog is a checkbox labeled 'Omit code cell output when saving this notebook'. The background shows a Jupyter Notebook with a code cell containing '[3] 1 simulation.run()' and two 2D plots. The left plot is titled 'min:0 max:146.1 t[mi]' and the right plot is titled '44 t[min]:40'. Both plots show a color map of 'Mean radius [um]' on a logarithmic scale from 10^-1 to 10^1. The x-axis is labeled 'X [m]' and the y-axis is labeled 'Z [m]'."/>

demo.ipynb ☆

File Edit View Insert Runtime Tools Help All changes saved

+ Code + Text

RAM ✓ Disk

Editing

[3] 1 simulation.run()

Notebook settings

Hardware accelerator
GPU ?

To get the most out of Colab, avoid using a GPU unless you need one. [Learn more](#)

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CANCEL SAVE


min:0 max:146.1 t[mi]

44 t[min]:40

Mean radius [um]

X [m]

Z [m]



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PySDM 2.40

`pip install PySDM`

✓ [Latest version](#)

Released: Jan 22, 2024

Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab

Navigation

- Project description**
- [Release history](#)
- [Download files](#)

Project links

- [Homepage](#)

Project description

PySDM

Python 3

LLVM

Numba

CUDA

ThrustRTC

Linux

macOS

Windows

Jupyter

Maintained?

yes

Open Hub

PySDM

JOSS

10.21105/joss.03219

DOI

10.5281/zenodo.10549422

EU Funding by

FNP

PL Funding by

NCN

US DOE Funding by

ASR

License

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tests+artifacts+pypl

passing

build

passing

codecov

82%

pypl package

2.40

API docs

pdoc3

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

☐ [Search within citing articles](#)

An Efficient Bayesian Approach to Learning Droplet Collision Kernels: Proof of Concept Using “Cloudy,” a New n -Moment Bulk Microphysics Scheme

M Bieli, ORA Dunbar, EK De Jong... - [Journal of Advances ...](#), 2022 - [Wiley Online Library](#)

The small-scale microphysical processes governing the formation of precipitation particles cannot be resolved explicitly by cloud resolving and climate models. Instead, they are ...

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PyPartMC: A Pythonic interface to a particle-resolved, Monte Carlo aerosol simulation framework

Z D'Aquino, S Arabas, JH Curtis, A Vaishnav, N Riemer... - [SoftwareX](#), 2024 - [Elsevier](#)

PyPartMC is a Pythonic interface to PartMC, a stochastic, particle-resolved aerosol model implemented in Fortran. Both PyPartMC and PartMC are free, libre, and open-source ...

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Breakups are complicated: An efficient representation of collisional breakup in the superdroplet method

E de Jong, JB Mackay, A Jaruga, S Arabas - [EGUsphere](#), 2022 - [egusphere.copernicus.org](#)

A key constraint of particle-based methods for modeling cloud microphysics is the conservation of total particle number, which is required for computational tractability. The ...

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Immersion freezing in particle-based aerosol-cloud microphysics: a probabilistic perspective on singular and time-dependent models

S Arabas, JH Curtis, I Silber, A Fridlind... - [arXiv preprint arXiv ...](#), 2023 - [arxiv.org](#)

Cloud droplets containing ice-nucleating particles (INPs) may freeze at temperatures above than the homogeneous freezing threshold. This process, referred to as immersion freezing ...

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Spanning the gap from bulk to bin: A novel spectral microphysics method

EK De Jong, T Bischoff, A Nadim... - [Journal of Advances in ...](#), 2022 - [Wiley Online Library](#)

Microphysics methods for climate models and numerical weather prediction typically track one, two, or three moments of a droplet size distribution for various categories of liquid, ice ...

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coupling with an external CFD code (Oleksii Bulenok)

(<https://github.com/CliMA/ClimateMachine.jl/pull/2244>)

PySDM and ClimateMachine coupling examples in Kinematic setup #2244

<> Code

 **Open** abulenok wants to merge 16 commits into `CliMA:master` from `abulenok:ob-pysdmachine` 

 Conversation 32

 Commits 16

 Checks 10

 Files changed 17

+2,528 -1 



abulenok commented on 27 Oct 2021

Contributor

This PR includes a coupling logic for `ClimateMachine.jl` and `PySDM`.

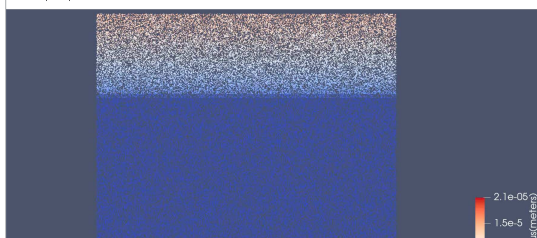
PySDM is a particle-based aerosol/cloud microphysics package written entirely in Python.

This PR depicts how Python modules can be leveraged within `ClimateMachine.jl` including the continuous integration setup.










The initial set of tests included here is based on the kinematic 2D example previously used as a test case in both `PySDM` and `ClimateMachine.jl`. In the tests added in this PR, `ClimateMachine.jl` handles air motion and total water transport, while `PySDM` handles representation of aerosol and liquid water transport as well as phase changes leading to formation of cloud water.

Output from `PySDM` is handled using VTK files. Example animation with an evolution of radius computed from particle properties is shown below:

 output.mp4



Reviewers

-  slayoo 
-  charleskawczynski 
-  claresinger 
-  jakebolewski 
-  edejong-callech 
-  tapios 

Assignees

-  trontrytel

Labels

- Microphysics

Projects

- None yet

Milestone

- No milestone

Development

Successfully merging this pull request may close these issues.

- None yet

Literature Reference	Cond/Evap	Collisions	Isotopes	Breakup	Transport	Chemistry	Freezing	Comments/keywords
no-environment								
Pierchala et al. 2022			x					theoretical curves for a lab experiment
OD box environment								
Shima et al. 2009		x						Golovin kernel example
Berry 1967		x						Several different kernels
Bieli et al. 2022		x		x				
de Jong et al. 2023		x		x				
Alpert & Knopf 2016							x	
OD parcel environment								
Kreidenweis et al. 2003	x					x		"Hoppel" gap
Jaruga & Pawlowska 2018	x					x		"Hoppel" gap
Lowe et al. 2019	x							surfactants
Yang et al. 2018	x							ripening (depending on the definition)
Graf et al. 2019	x		x					
Grabowski and Pawlowska 2023	x							ripening (not named so in the paper)
Arabas and Shima 2017	x							monodisperse, activation/deactivation cycle
Abdul-Razzak & Ghan 2000	x							parcel vs. activation parameterisation
1D single-column kinematic env.								
Shipway & Hill 2012	x	x			x			KiD 1D
deJong et al. 2023 (figures 6-8)	x	x		x	x			
2D prescribed-flow environment								
Arabas et al. 2015	x	x			x			includes GUI
Arabas et al. 2023 (figure 11)	x	x			x		x	Paraview script example

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- could we organise a PySDM hackathon/workshop/school/...?

Thank you!

github.com/open-atmos/PySDM

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- Foundation for Polish Science
- Polish National Science Centre
- DoE ASR
- Eric and Wendy Schmidt & Heising-Simons Foundation
- ...