

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

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**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

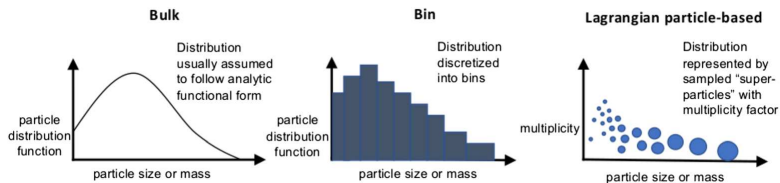
Hugh Morrison ✉, Marcus van Lier-Walqui, Ann M. Fridlind, Wojciech W. Grabowski, Jerry Y. Harrington, Corinna Hoose, Alexei Korolev, Matthew R. Kumjian, Jason A. Milbrandt, Hanna Pawlowska, Derek J. Posselt, Olivier P. Prat, Karly J. Reimel, Shin-Ichiro Shima, Bastiaan van Dierenhoven, Lulin Xue

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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

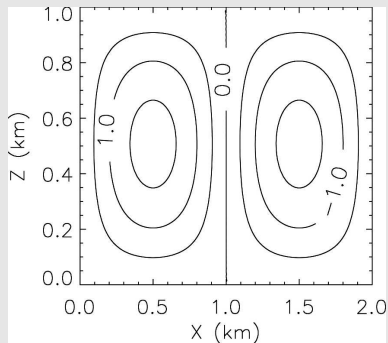
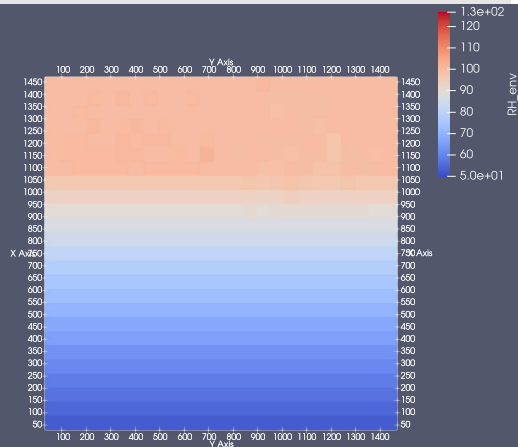
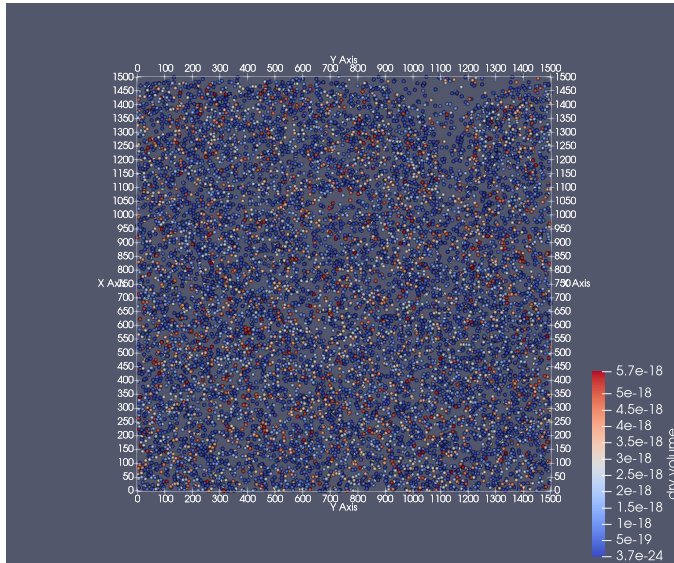


FIG. 1. Time-invariant vertical velocity for the stratocumulus case (contour interval is 0.5 m s<sup>-1</sup>).

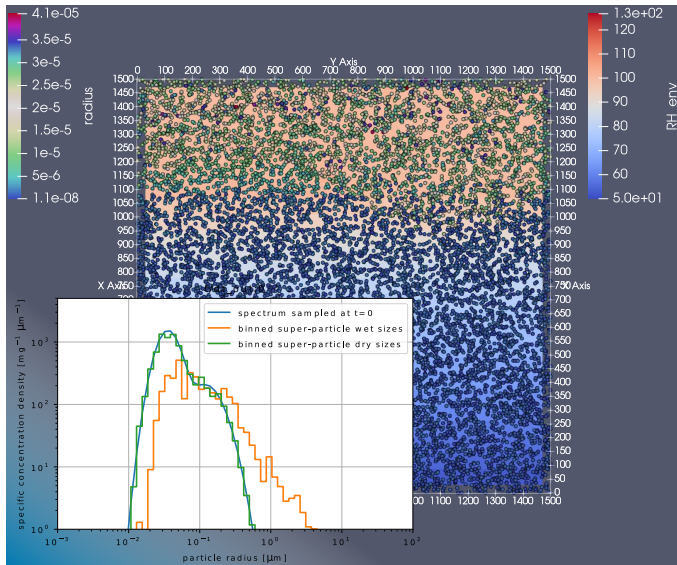
## RH profile at t=0



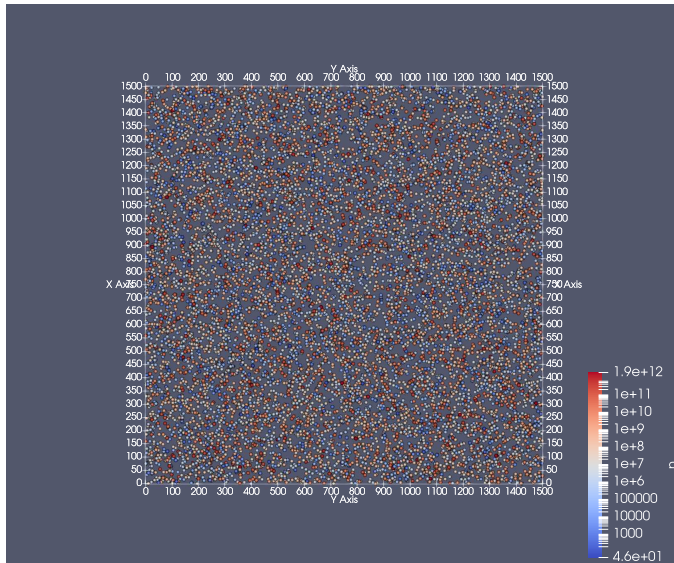
## super-particle attribute initialisation: dry/wet volume



# super-particle attribute initialisation: dry/wet volume

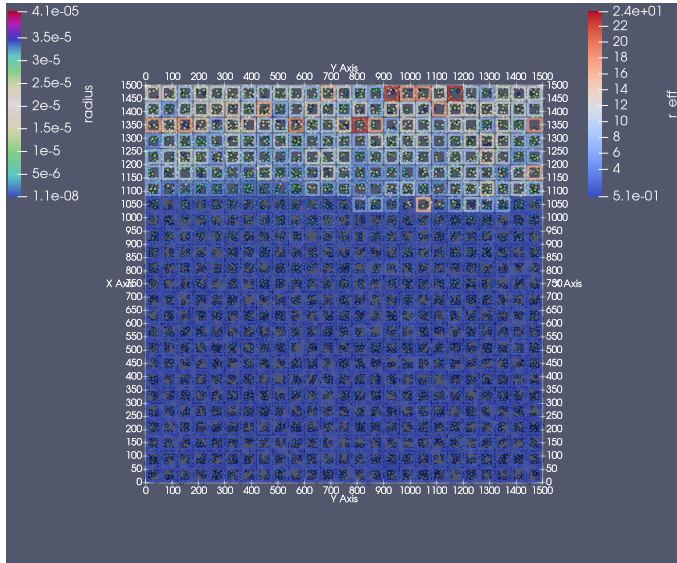


# super-particle attribute initialisation: multiplicity





# 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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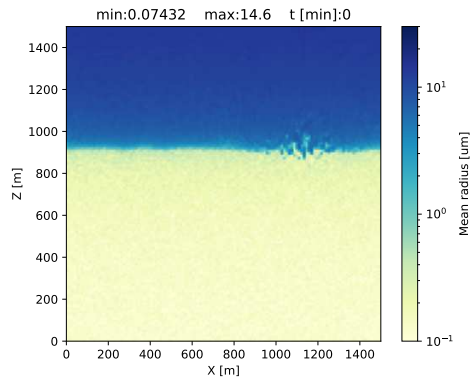
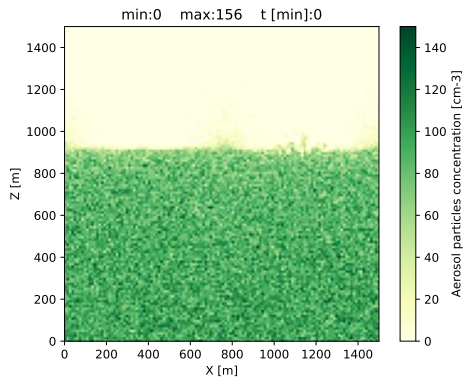
- applicable in research on aerosol-cloud-interactions (and beyond)  
KPI: reproduction of results from classic and recent literature
- **easy to reuse:** code (Python), examples (Jupyter), extensibility (modular, high test coverage)  
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KPI: user feedback & contributions
- **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

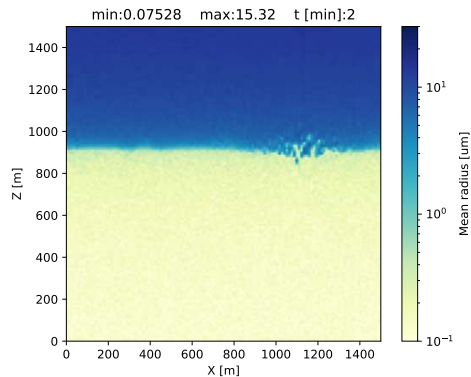
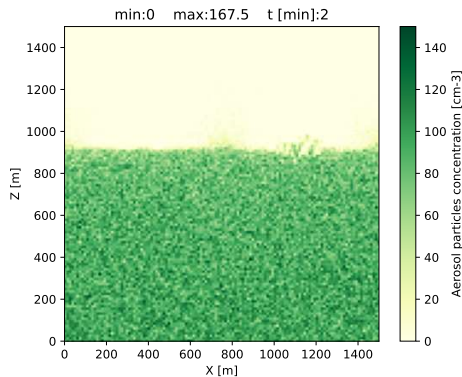
Computational particles:  $2^{21}$



# sample aerosol-cloud-precipitation interactions simulation

Computational grid: 128x128

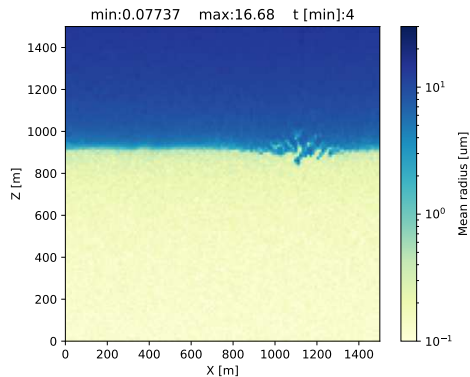
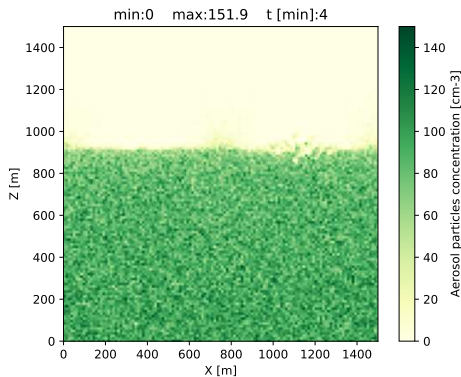
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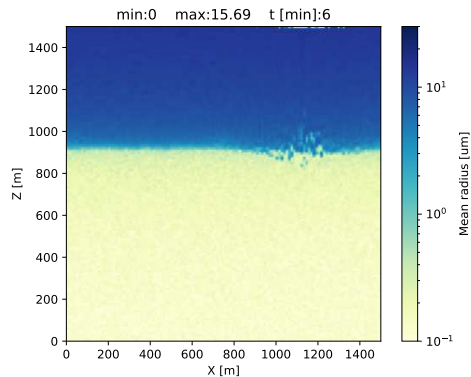
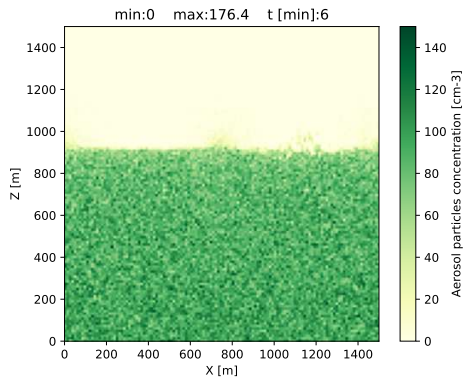
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# sample aerosol-cloud-precipitation interactions simulation

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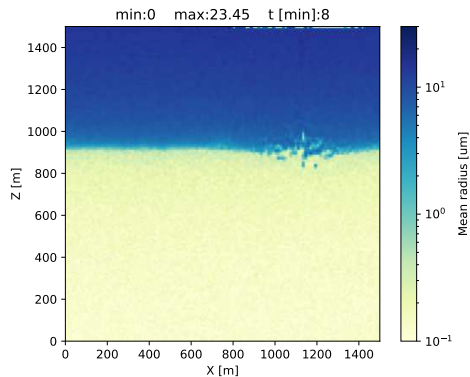
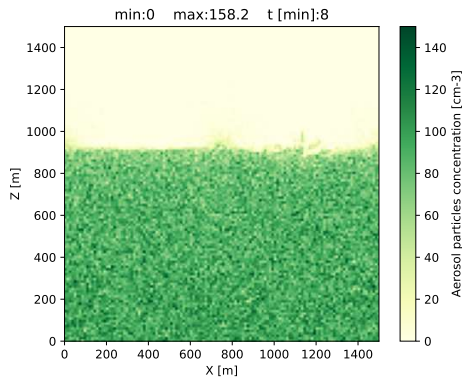
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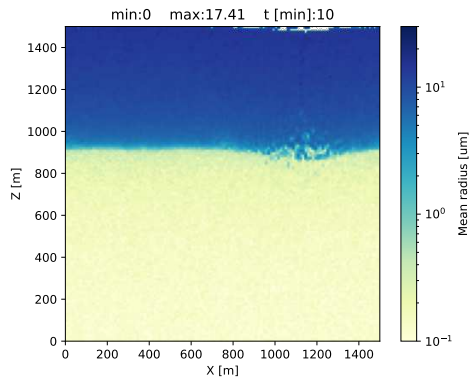
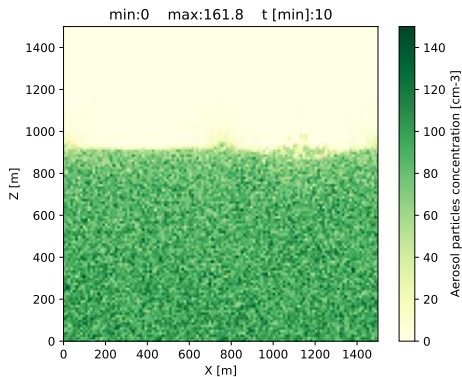
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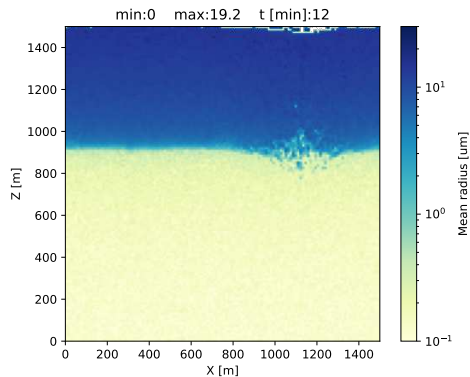
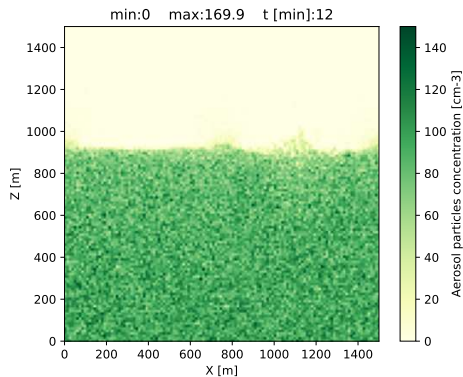
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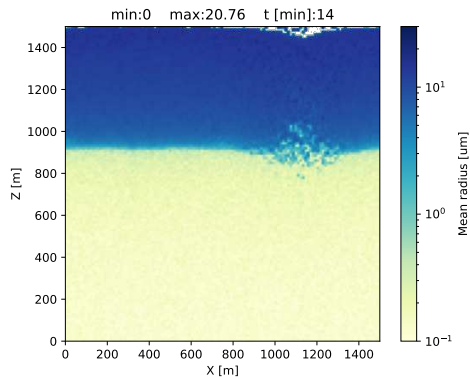
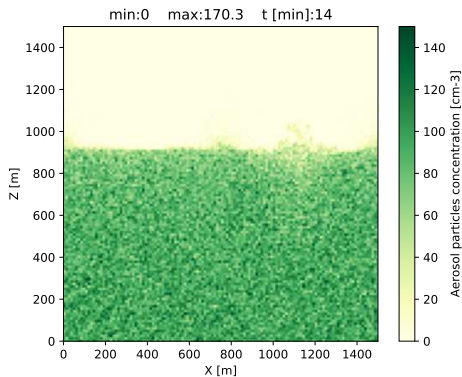
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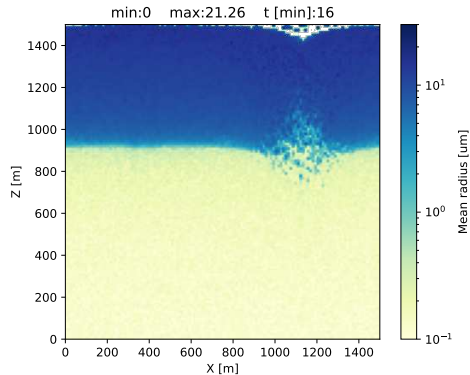
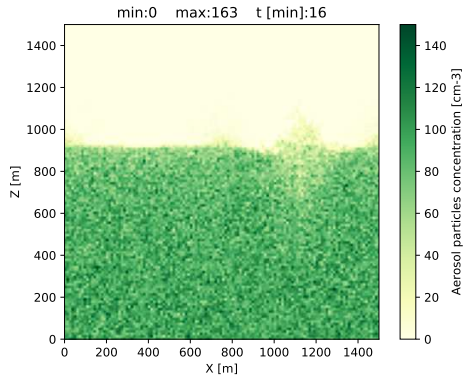




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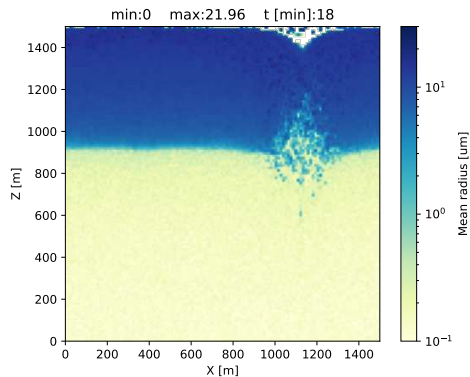
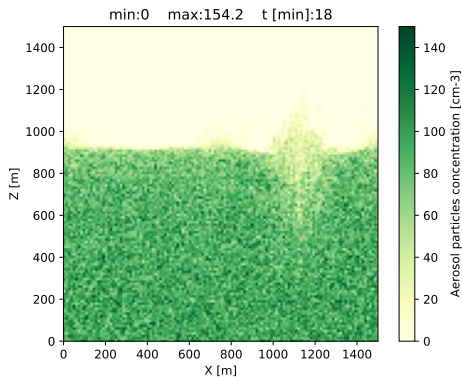
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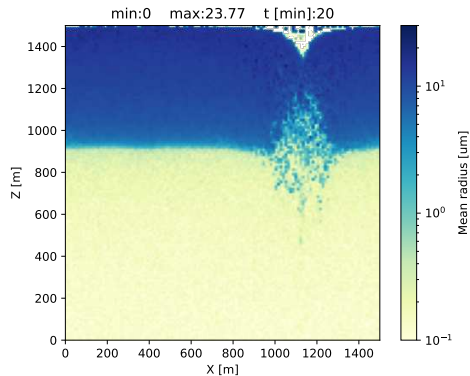
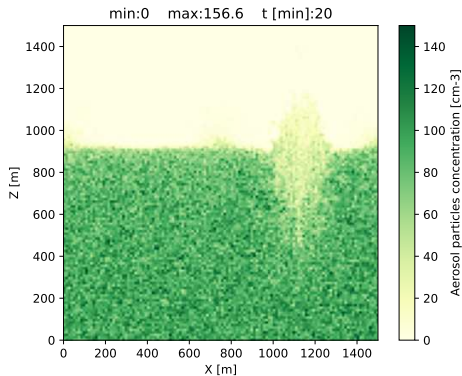
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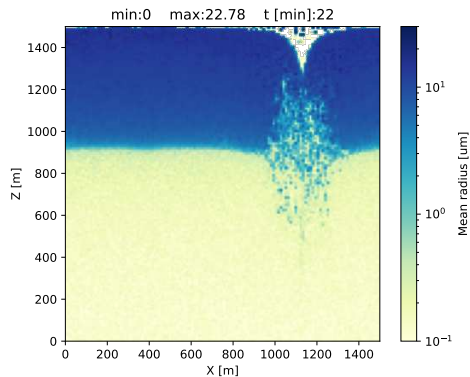
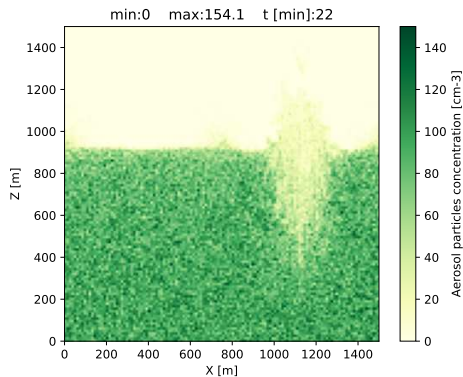
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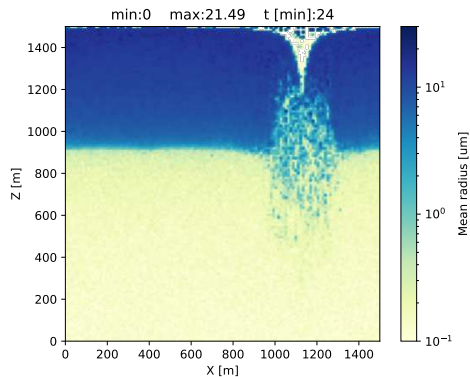
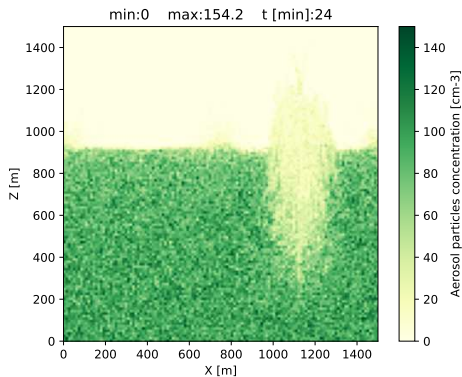
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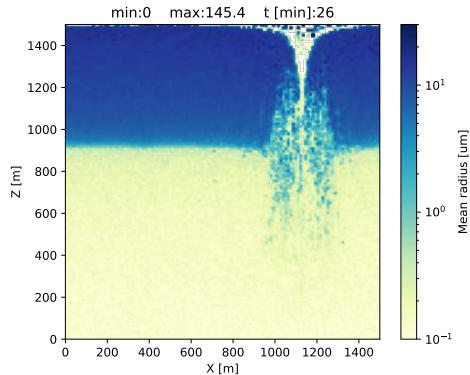
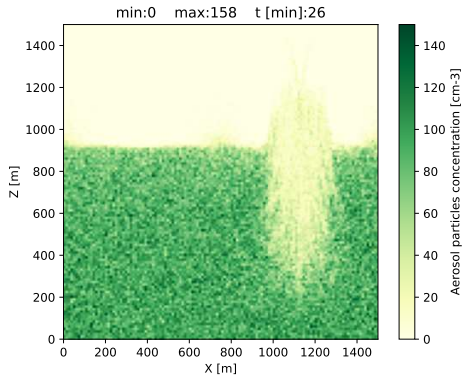
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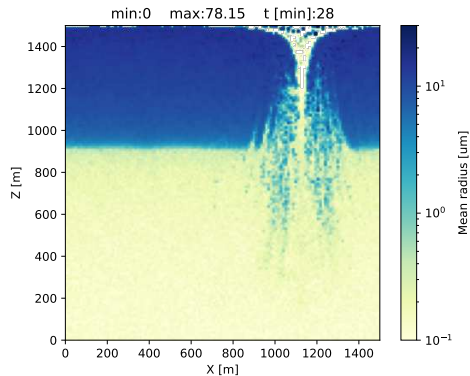
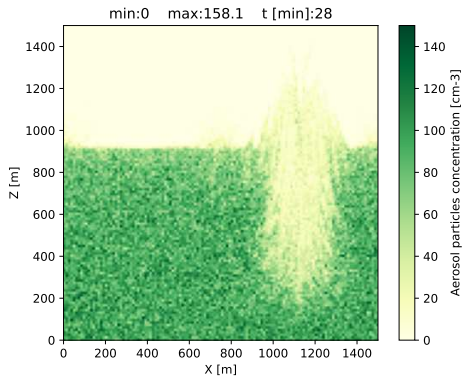
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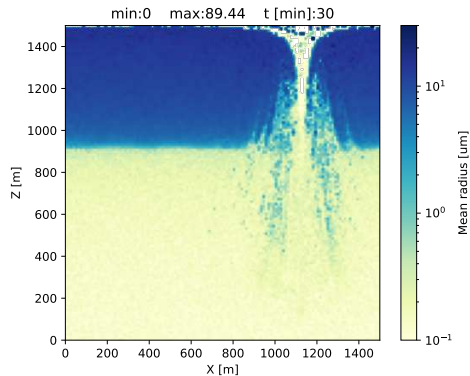
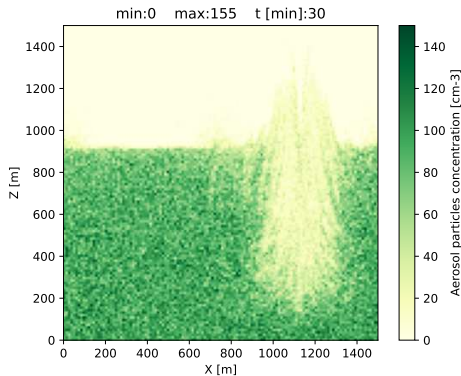
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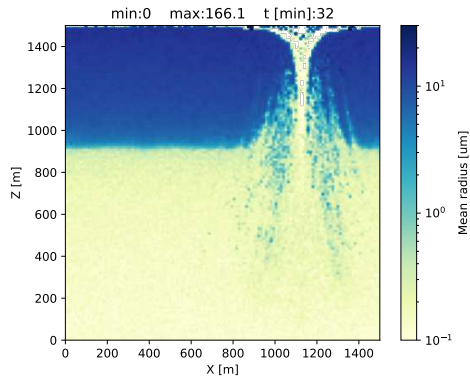
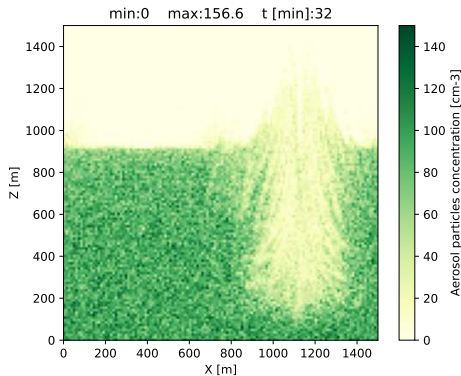




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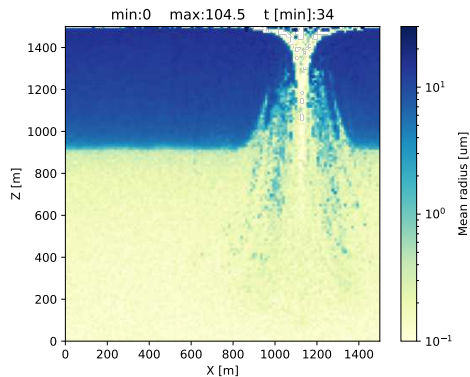
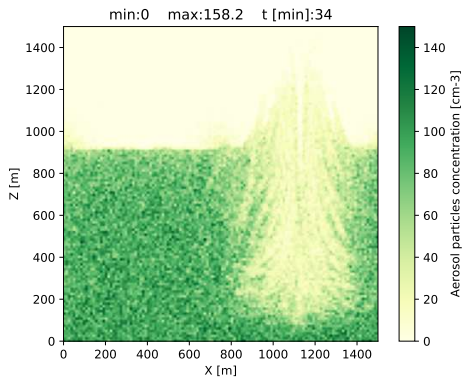
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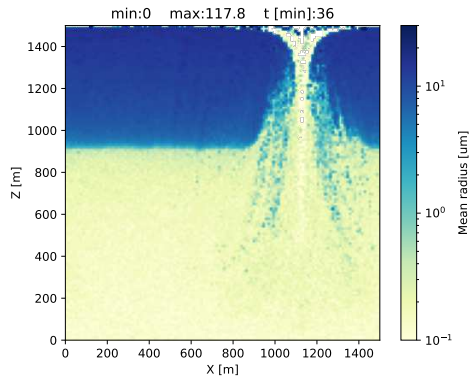
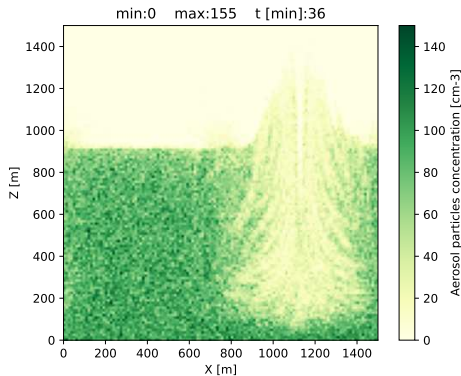
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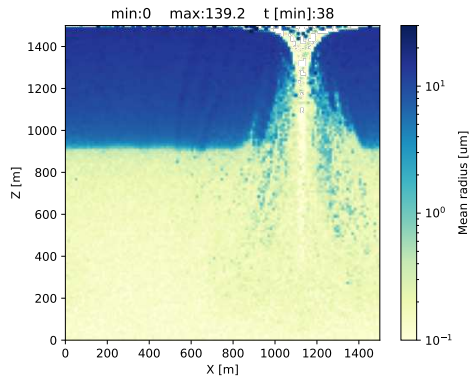
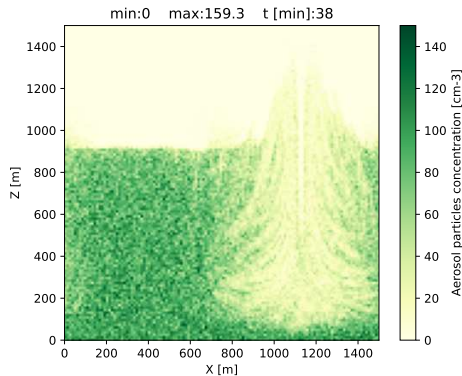
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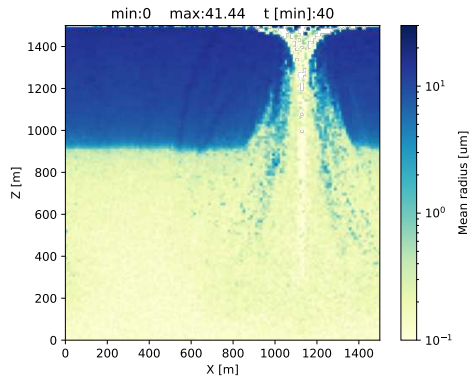
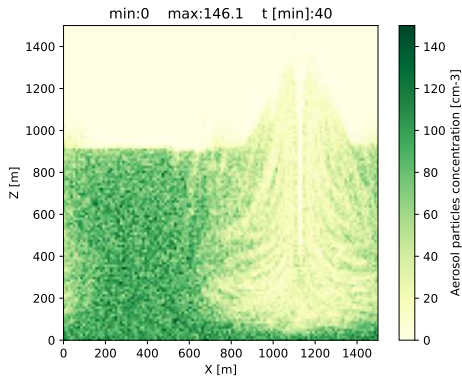
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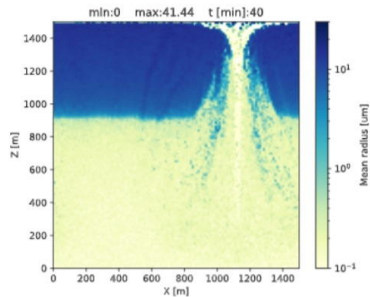
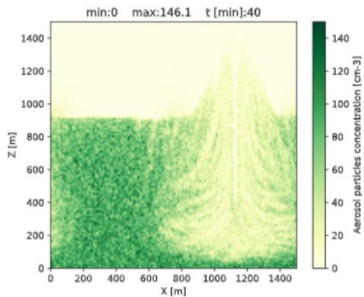


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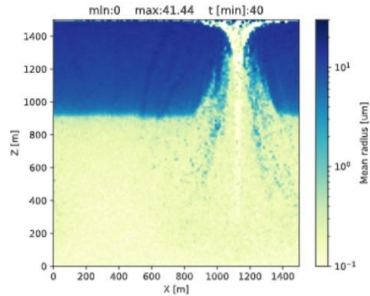
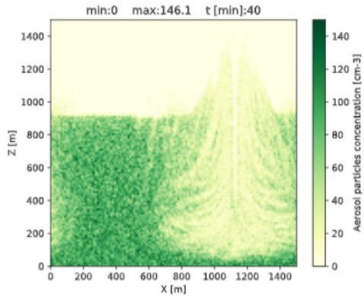
Computational grid: 128x128

Computational particles:  $2^{21}$





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



# PySDM: Pythonic, Jupyter-friendly



demo.ipynb ☆

File Edit View Insert Runtime Tools Help



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RAM

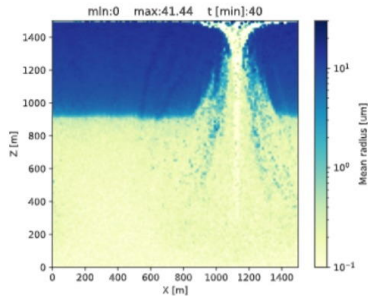
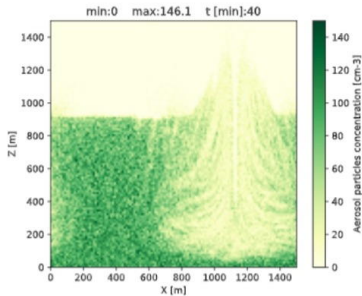
Disk



Editing



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





# PySDM: Pythonic, Jupyter-friendly, GPU-enabled

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](#)

☐ Omit code cell output when saving this notebook

CANCEL SAVE

min:0 max:146.1 t[mi]

1400  
1200  
1000  
800  
600  
400  
200  
0

Z [m]

0 200 400 600 800 1000 1200 1400

X [m]

Aerosol

40  
20  
0


44 t[min]:40

10<sup>1</sup>  
10<sup>0</sup>  
10<sup>-1</sup>

Mean radius [um]


0 200 400 600 800 1000 1200 1400

X [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 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 GPL v3

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 ...

☆ [Save](#) [Cite](#) [Cited by 7](#) [Related articles](#) [All 13 versions](#)

### 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 ...

☆ [Save](#) [Cite](#) [Cited by 1](#) [Related articles](#)

### 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`.

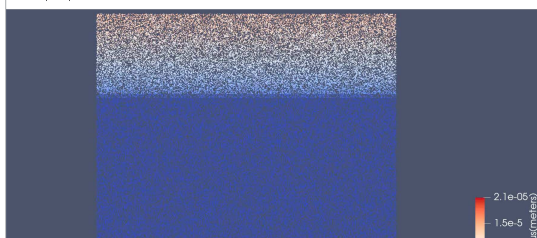
PySDM is a particle-based aerosol/cloud microphysics package written entirely in Python.

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
<b>no-environment</b>								
Pierchala et al. 2022			x					theoretical curves for a lab experiment
<b>OD box environment</b>								
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	
<b>OD parcel environment</b>								
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
<b>1D single-column kinematic env.</b>								
Shipway & Hill 2012	x	x			x			KiD 1D
deJong et al. 2023 (figures 6-8)	x	x		x	x			
<b>2D prescribed-flow environment</b>								
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](https://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
- ...