open-source Python projects for particle-based aerosol/cloud microphysics modelling

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Feb 28 2023

DACoPT meeting @ INRIA Sofia Antipolis

Smoluchowski's coagulation equation (SCE)

concentration of particles of size x at time t: $c(x,t)$: $\mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$

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$$\dot{c}(x) = \frac{1}{2} \int_0^x a(y, x-y) c(y) c(x-y) dy - \int_0^\infty a(y,x) c(y) c(x) dy + \dots \tag{1}$$

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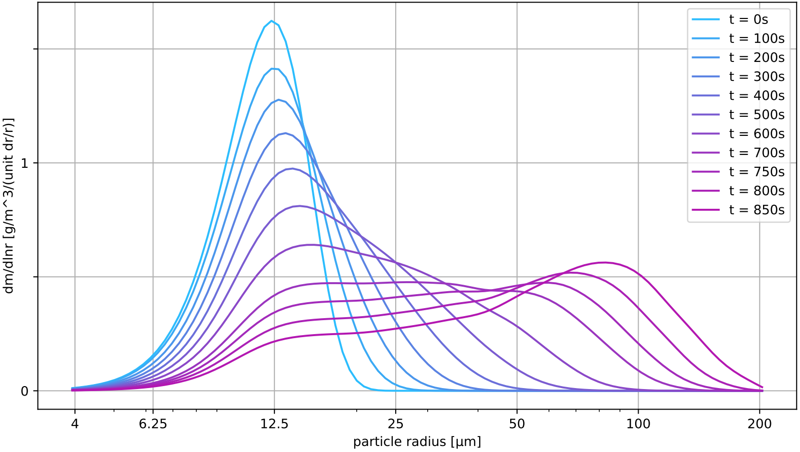
discretised particle concentration: $c_i = c(x_i)$ where $x_i = i \cdot x_0$

$$\dot{c}_i = \frac{1}{2}\sum_{k=1}^{i-1} a(x_k, x_{i-k})c_k c_{i-k} - \sum_{k=1}^{\infty} a(x_k, x_i)c_k c_i + \dots \tag{2}$$

cloud droplet collisional growth



Bartman et al. 2021, LNCS (doi:10.1007/978-3-030-77964-1_2)

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

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

(photo: Yevgen Timashov / National Geographic)

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Shima et al. 2020 (doi:10.5194/gmd-13-4107-2020): mixed-phase

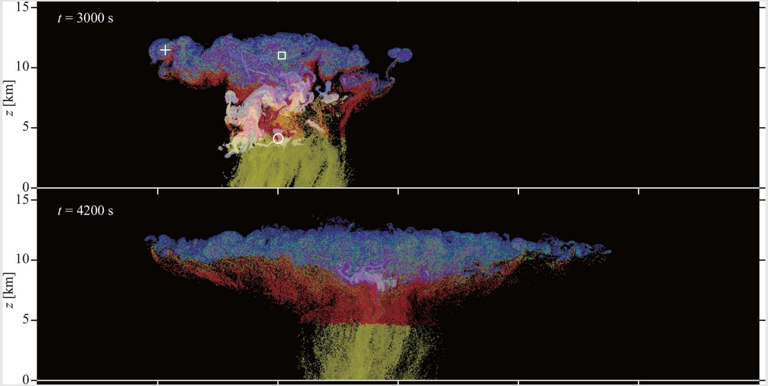

Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic predicted ice particles (Sects. 7.3 and 9.1). See also Movie 1 in the video supplement.

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interpretation	
concentration "c_i" in size bin "i"	besides c_i, each "particle" i carries other physicochemical attributes, e.g. position (x_i, y_i, z_i)

super-particles as an alternative to bulk or bin μ-phyics

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

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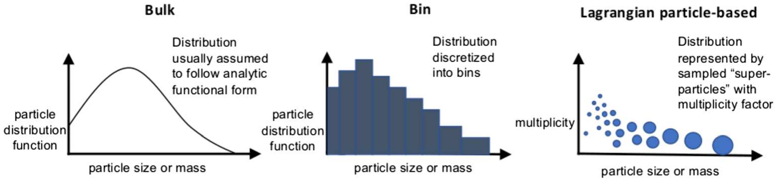

Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

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- **curation**: open licensing (GPL), public versioned development (Github)
  KPI: instant and anonymous execution on commodity environment

PySDM: 2D kinematic Sc test (Morrison & Grabowski '07)

2D flow field

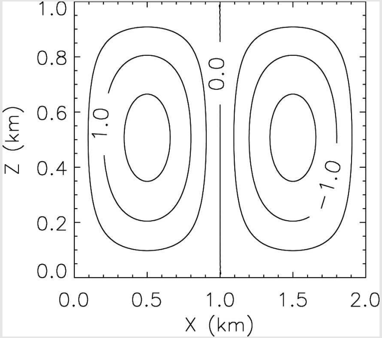
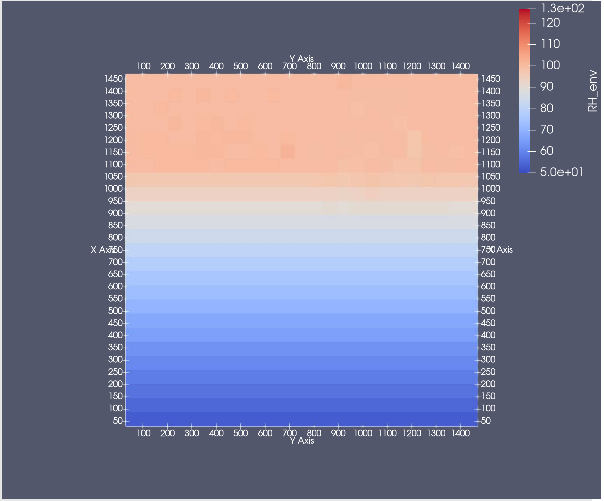
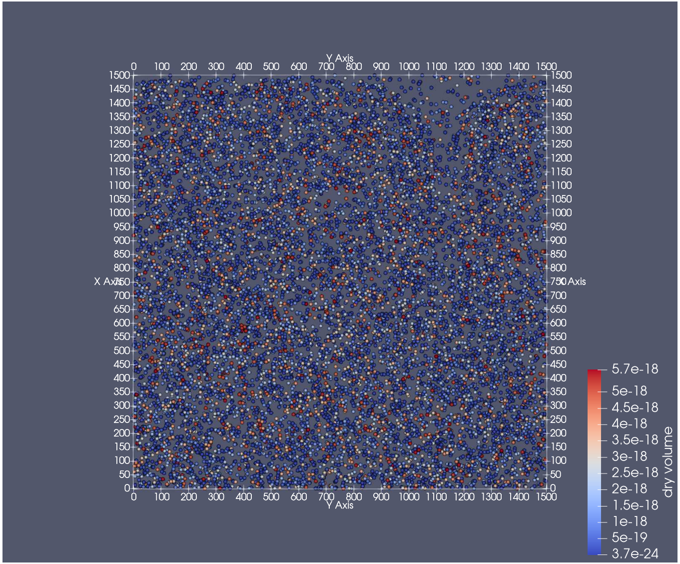


FIG. 1. Time-invariant vertical velocity for the stratocumulus case (contour interval is 0.5 m s^{-1}).

RH profile at t=0



particle attribute initialisation: dry/wet volume



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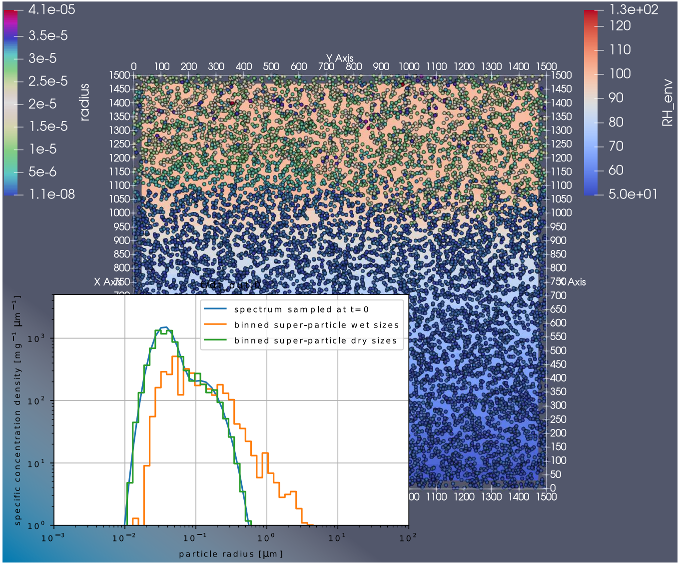
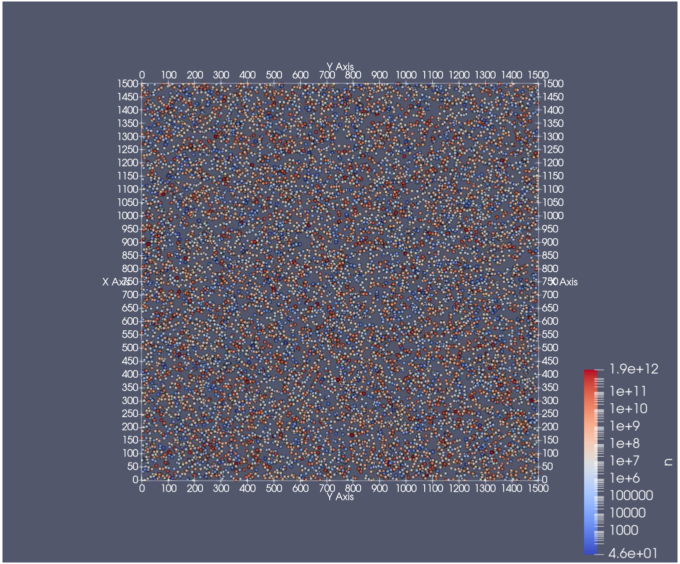
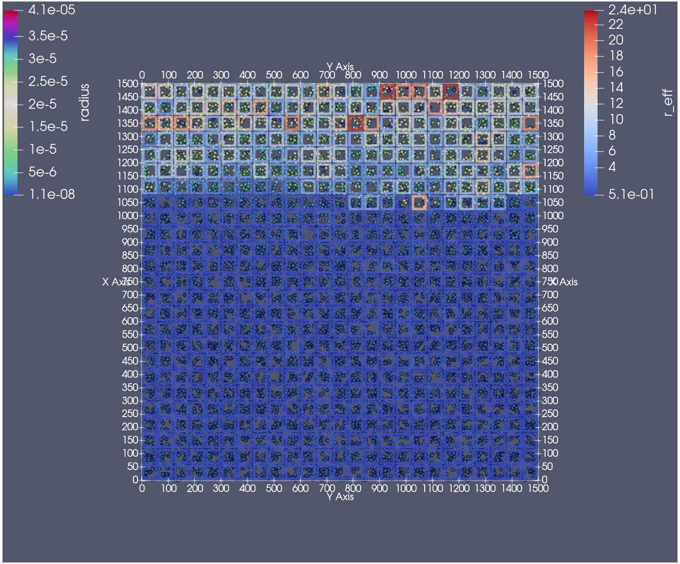


particle attribute initialisation: multiplicity



particle attribute evolution: droplet radius



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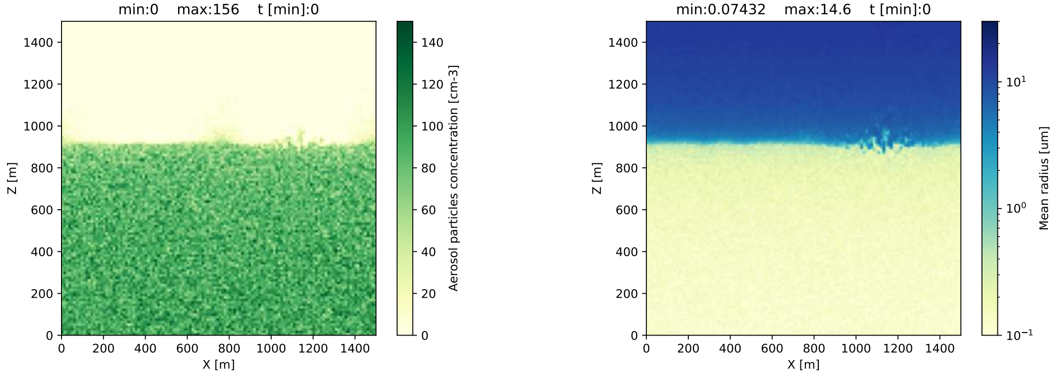

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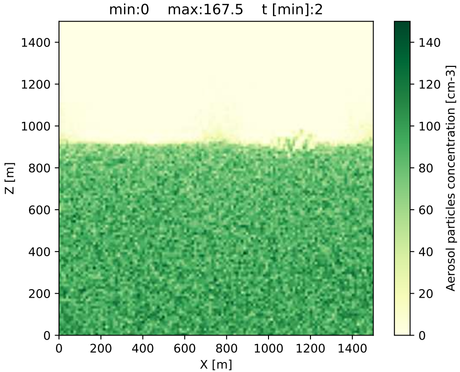

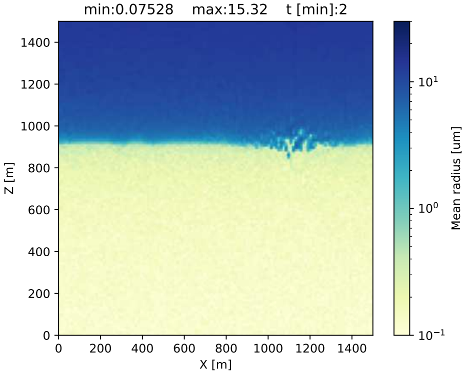

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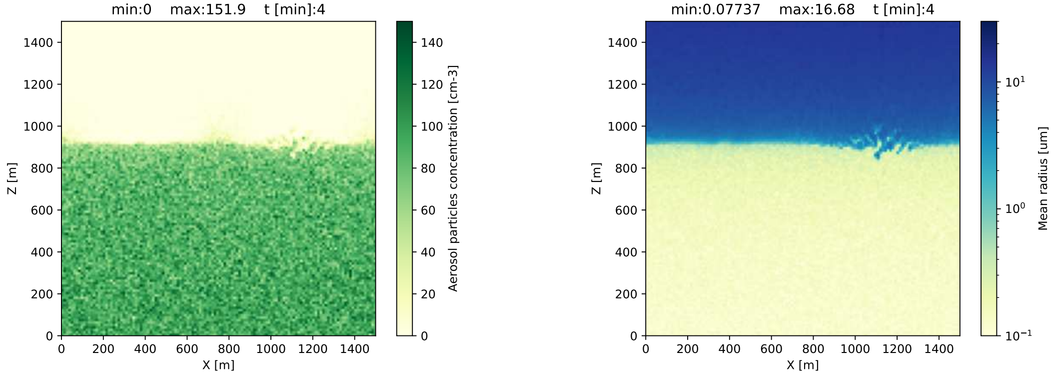

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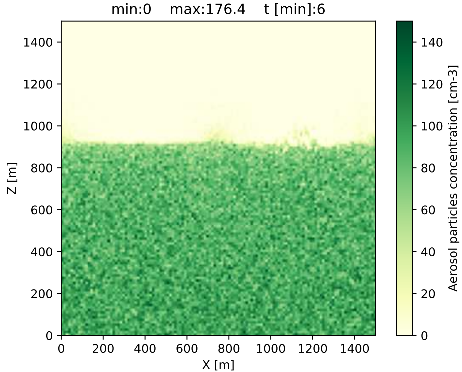

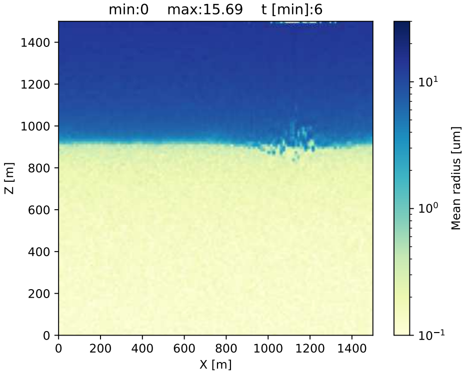

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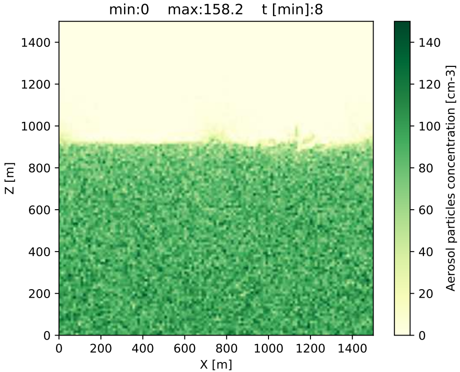

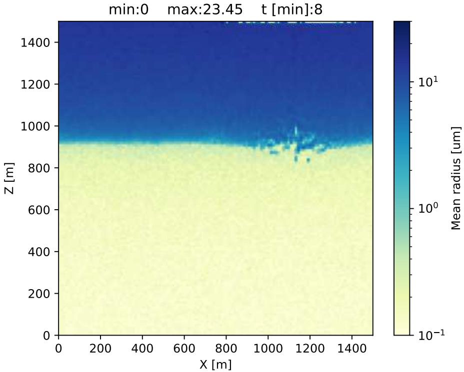

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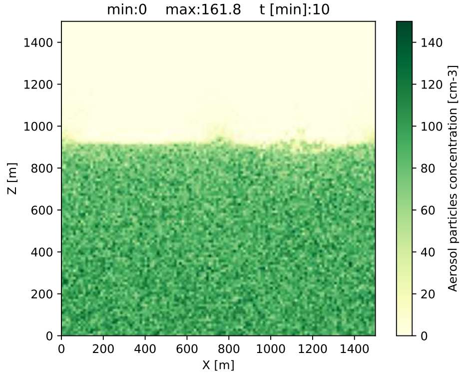

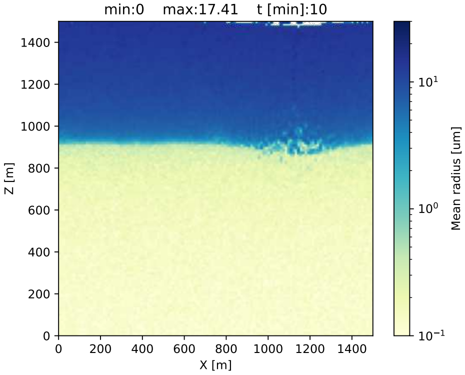

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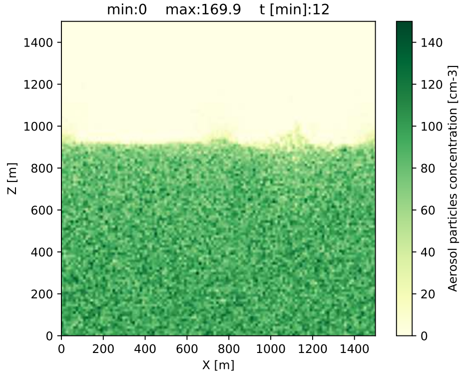

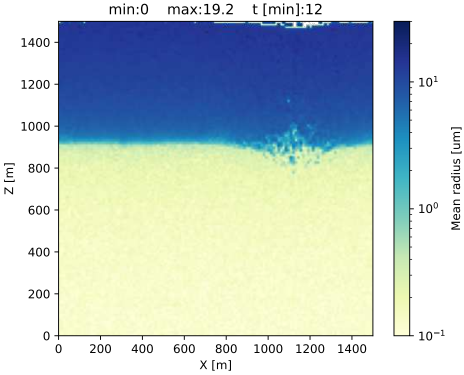

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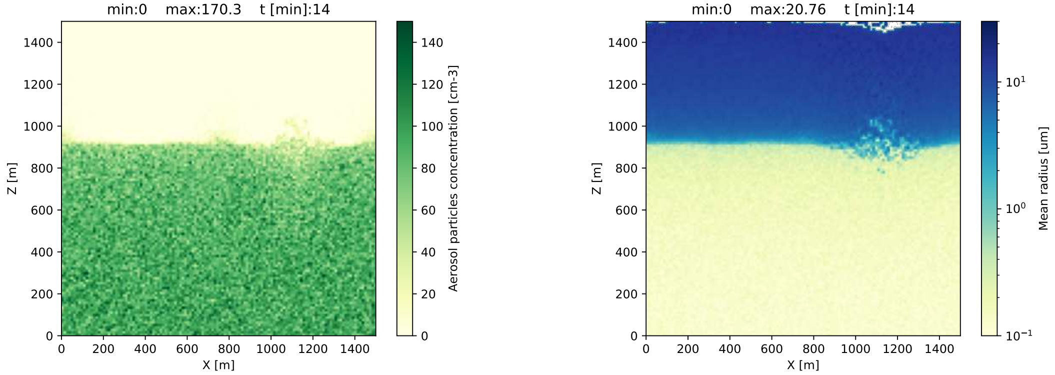

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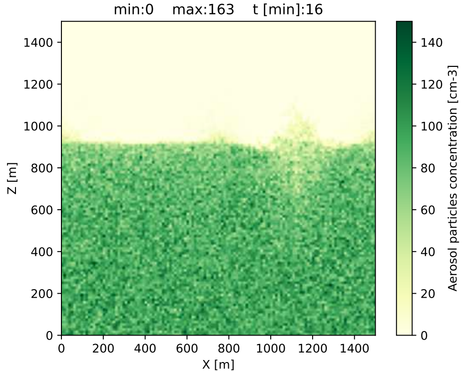

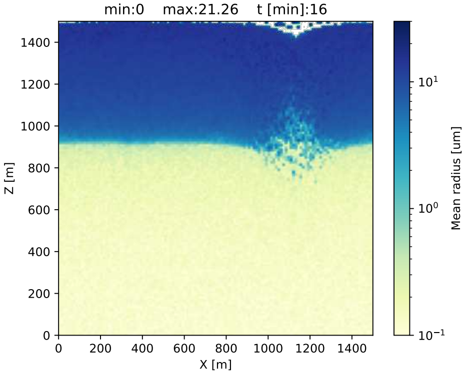

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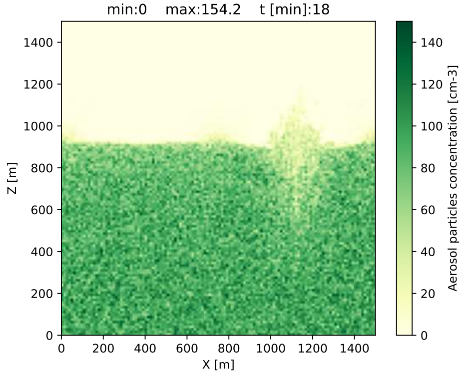

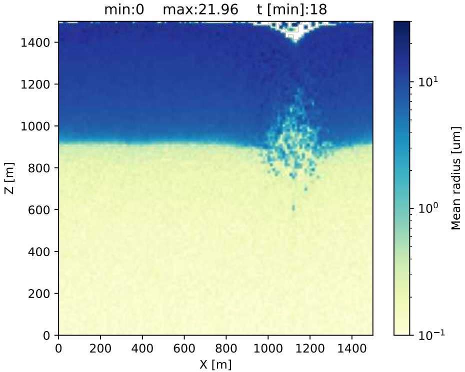

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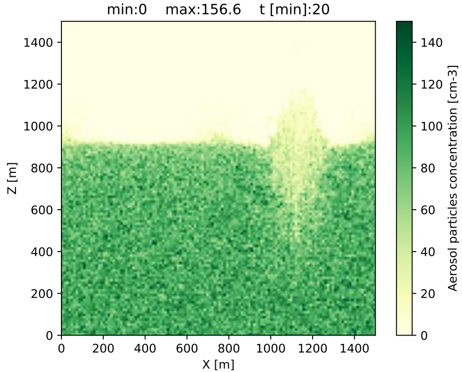

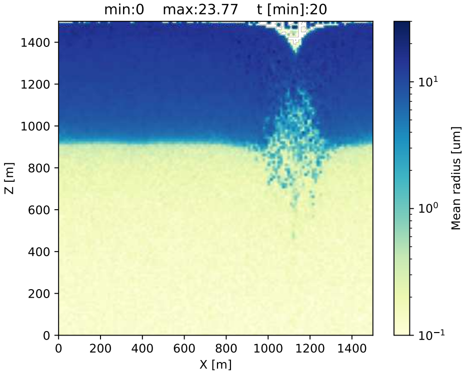

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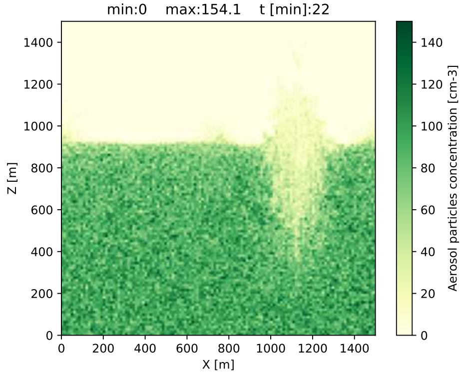

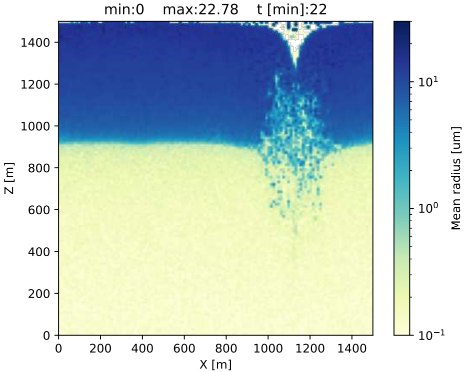

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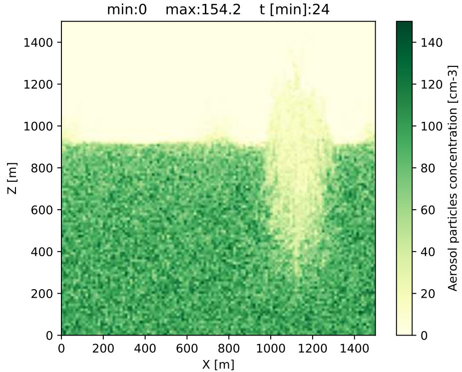

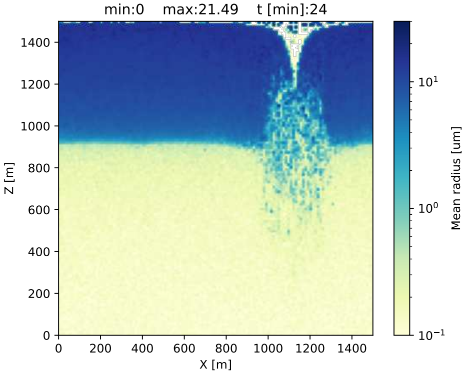

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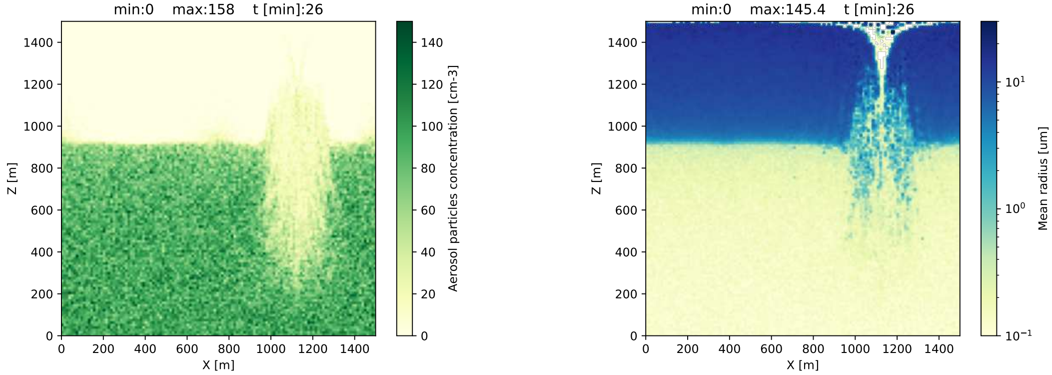

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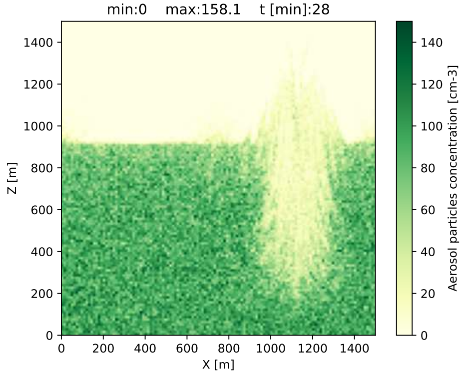

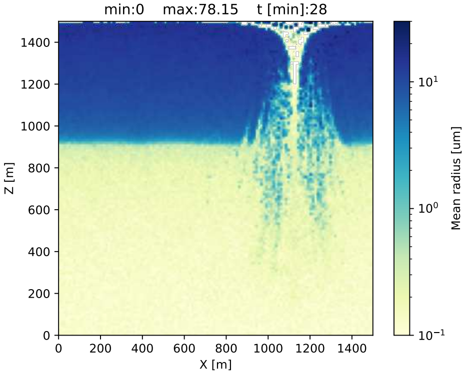

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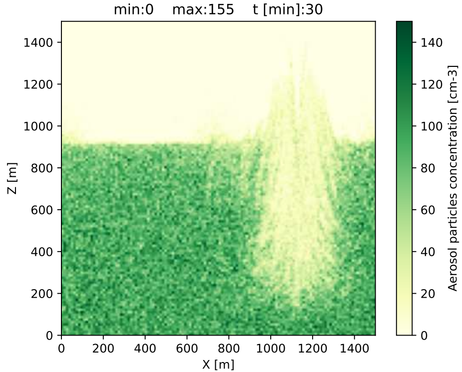

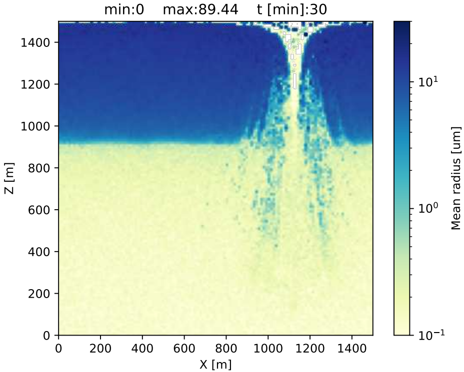

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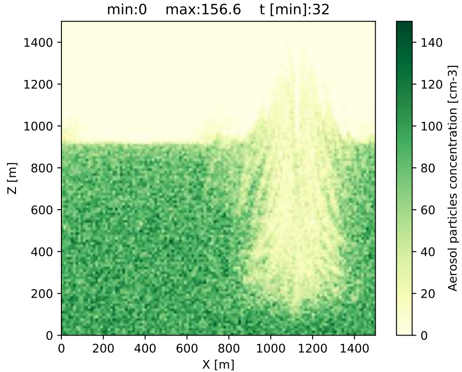

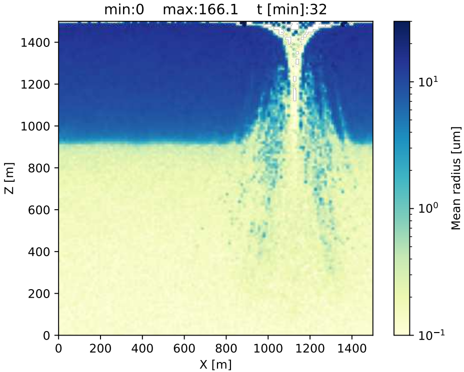

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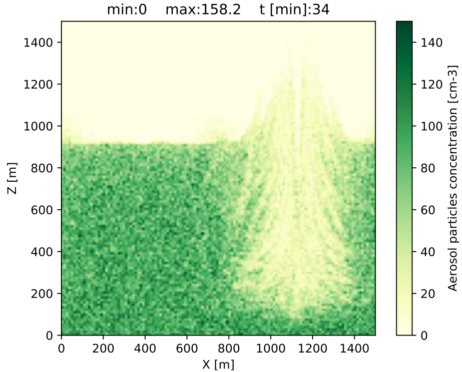

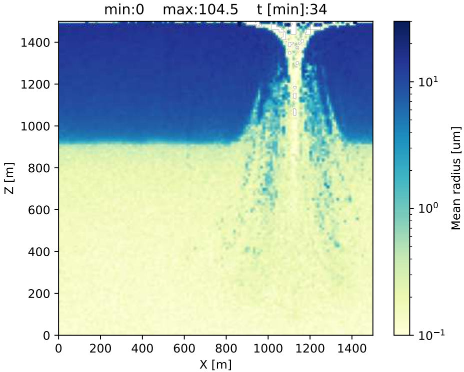

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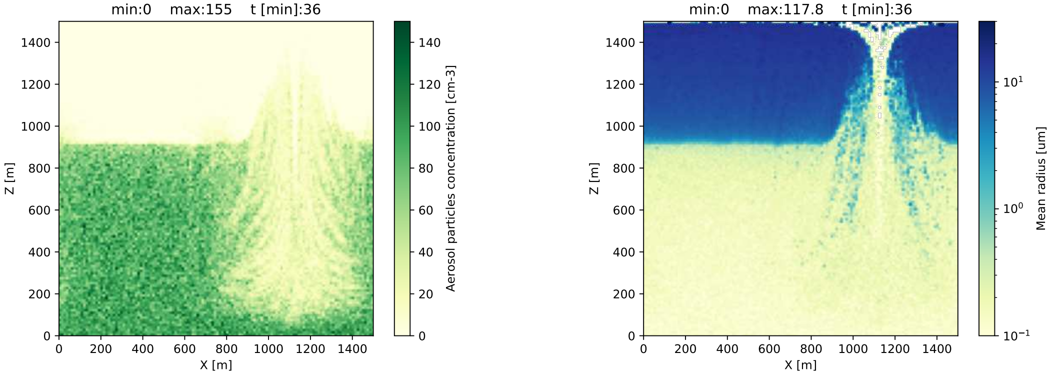

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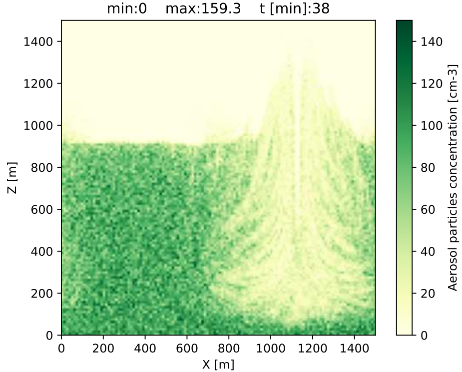
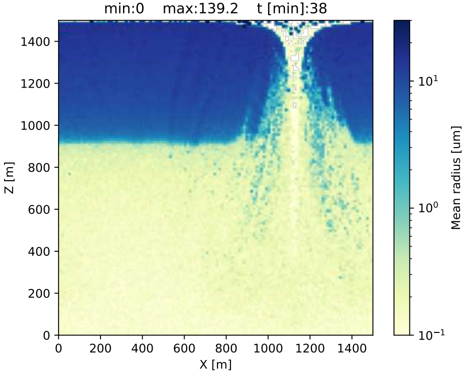


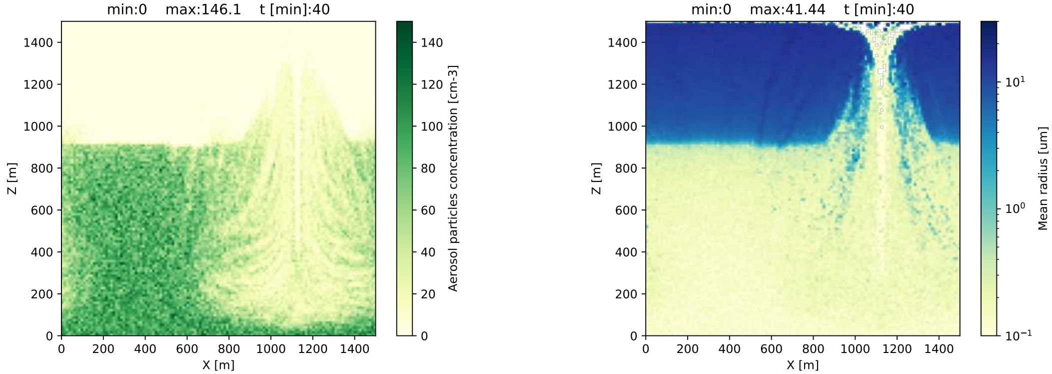


Simulation & visualisation: Piotr Bartman (MSc thesis @ WMiI UJ)

sample aerosol-cloud-precipitation interactions simulation

Computational grid: 128x128

Computational particles: 2^{21}



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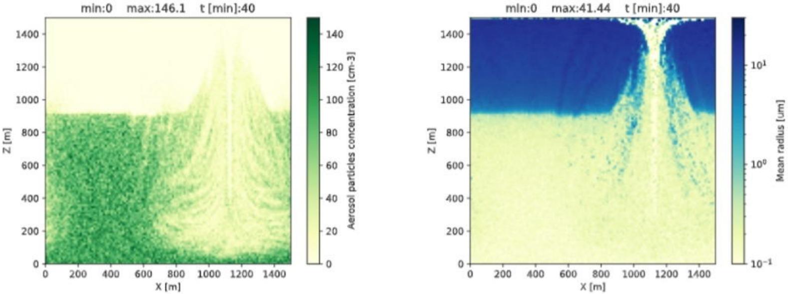
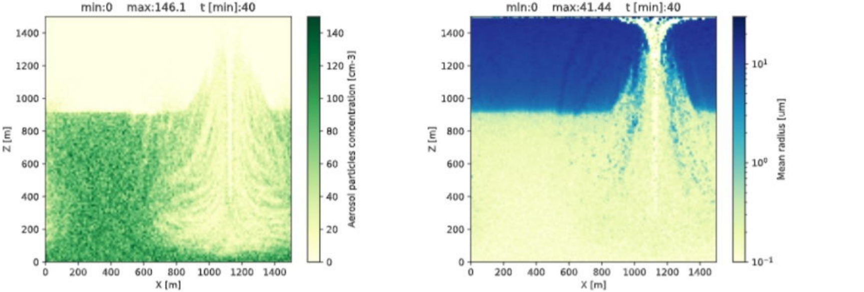
PySDM:



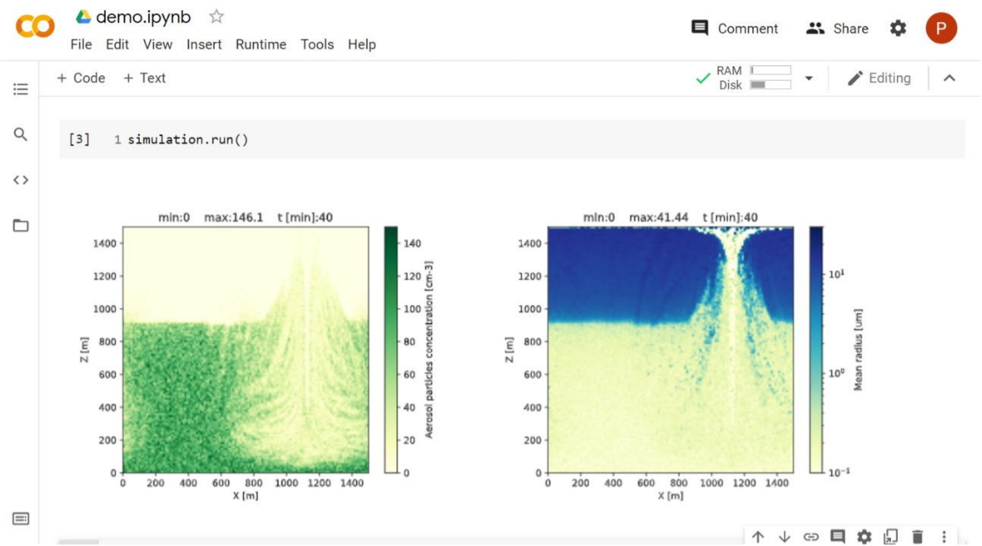
min:0 max:146.1 t [min]:40
Z [m]
X [m]
Aerosol particles concentration [cm-3]
min:0 max:41.44 t [min]:40
Z [m]
X [m]
Mean radius [um]

PySDM: Pythonic

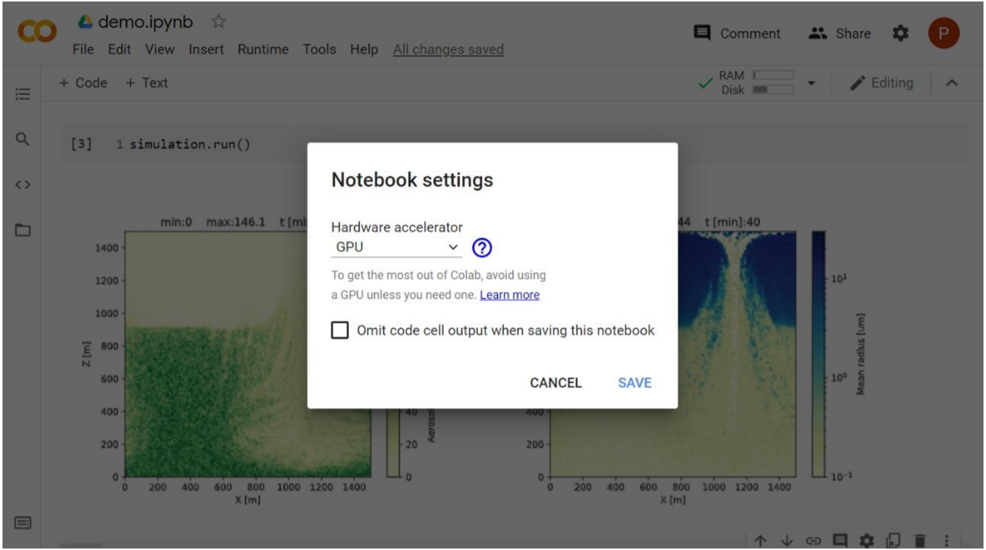
```
[3]  1 simulation.run()
```



PySDM: Pythonic, Jupyter-friendly



PySDM: Pythonic, Jupyter-friendly, GPU-enabled



PySDM: packages

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PySDM 2.15

`pip install PySDM`

Latest version

Released: Dec 30, 2022

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 | OpenHub | JOSS 10.21105/joss.03219 | DOI 10.5281/zenodo.7640495

EU Funding by FNP | PL Funding by NCN | US DOE Funding by ASR

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PySDM: users

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

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M Bieli, ORA Dunbar, EK De Jong… - Journal of Advances …, 2022 - Wiley Online Library

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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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first 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

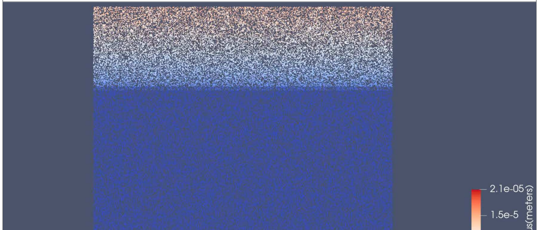
This PR includes a coupling logic for ClimateMachine.jl and PySDM.

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-caltech
- tapios

Assignees

trontrytel

Labels

Microphysics

Projects

None yet

Milestone

No milestone

Development

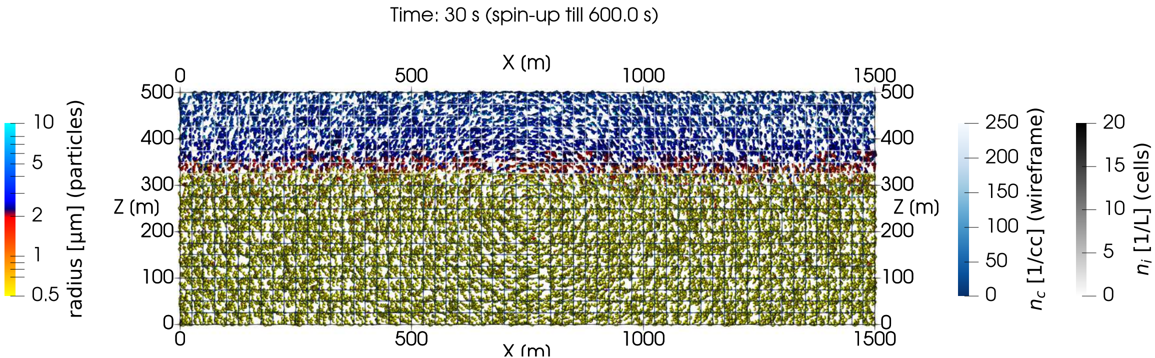
Successfully merging this pull request may close these issues.

None yet

teaser: Monte-Carlo immersion freezing in PySDM (singular or time-dependent)

https://www.reuters.com/markets/commodities/making-snow-stick-wind-challenges-winter-games-slope-makers-2021-11-29/

PySDM: particle-based μ-physics + prescribed-flow test (PyMPDATA)



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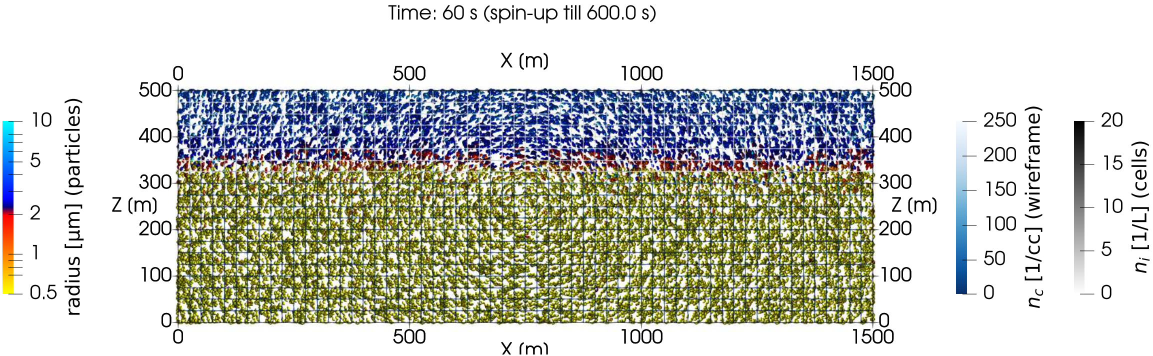

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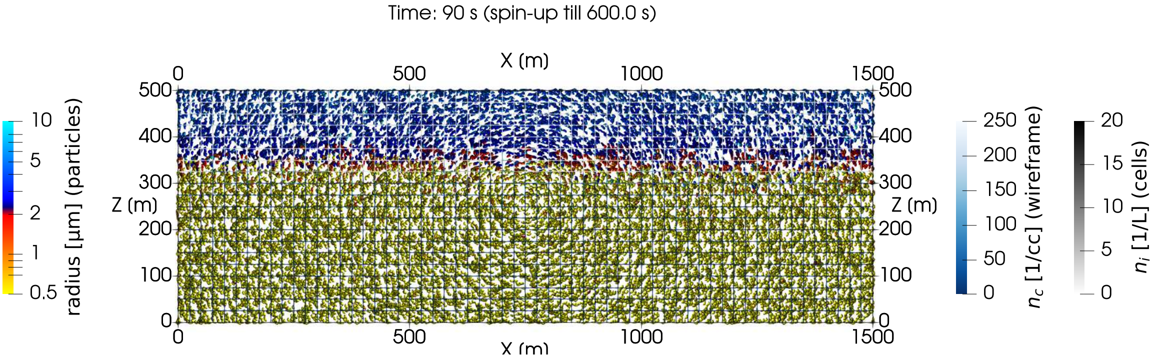

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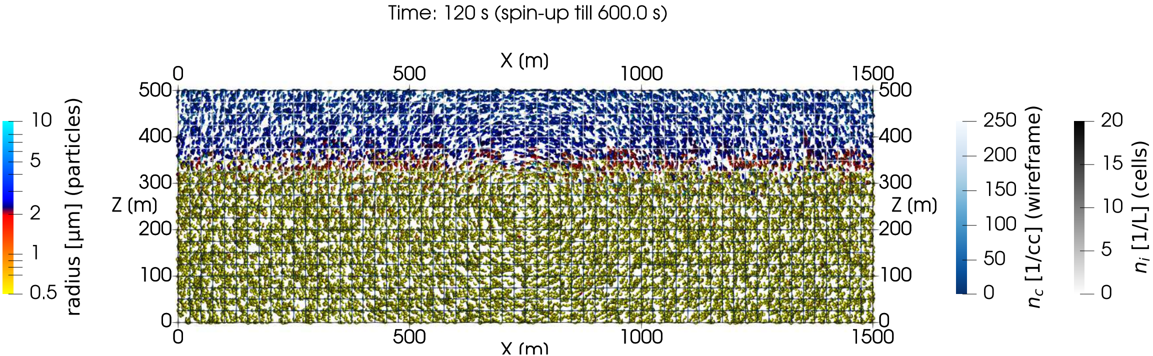

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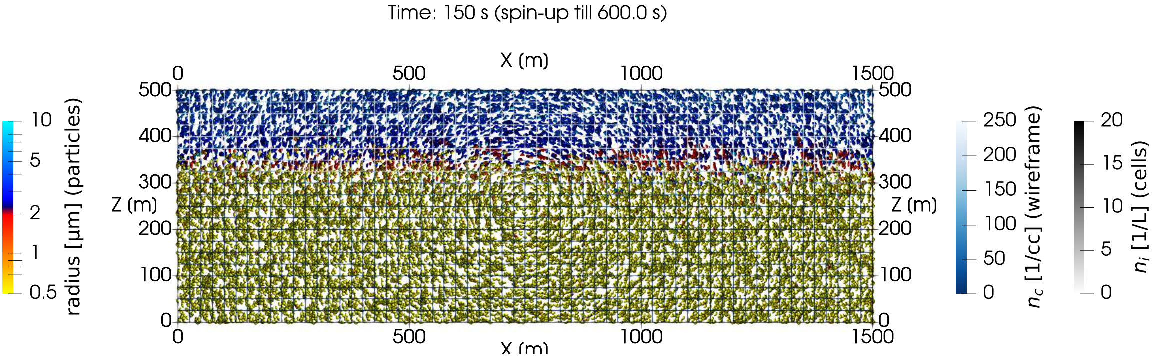

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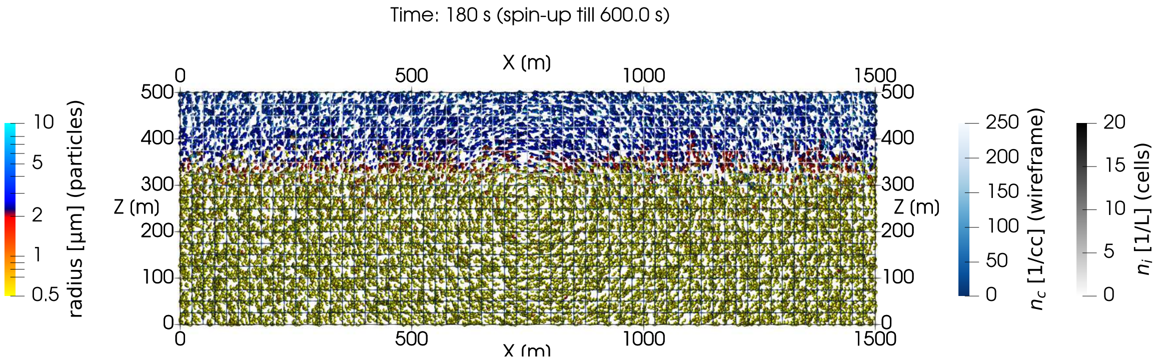

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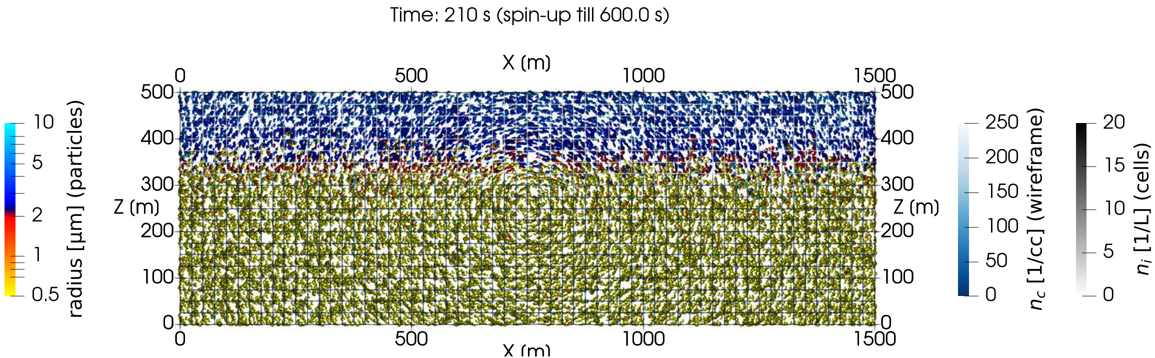

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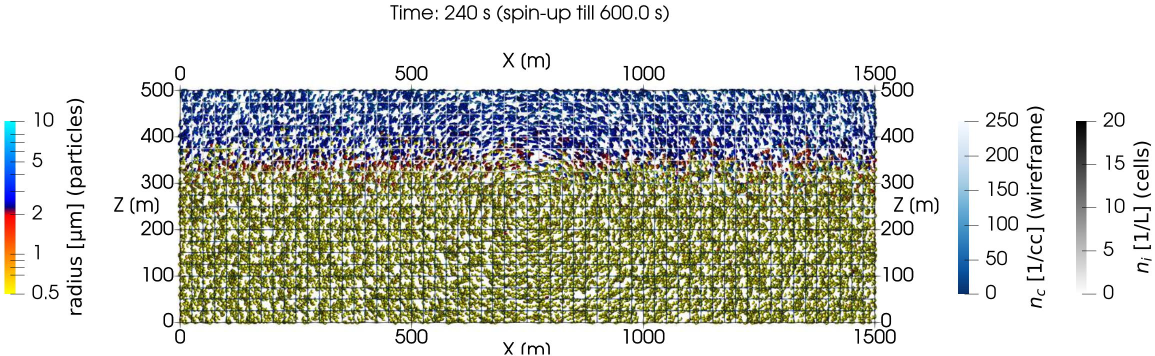

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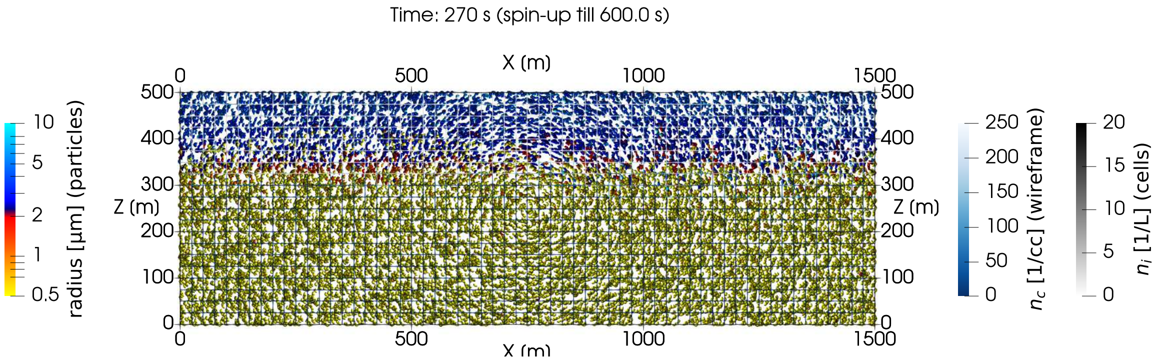

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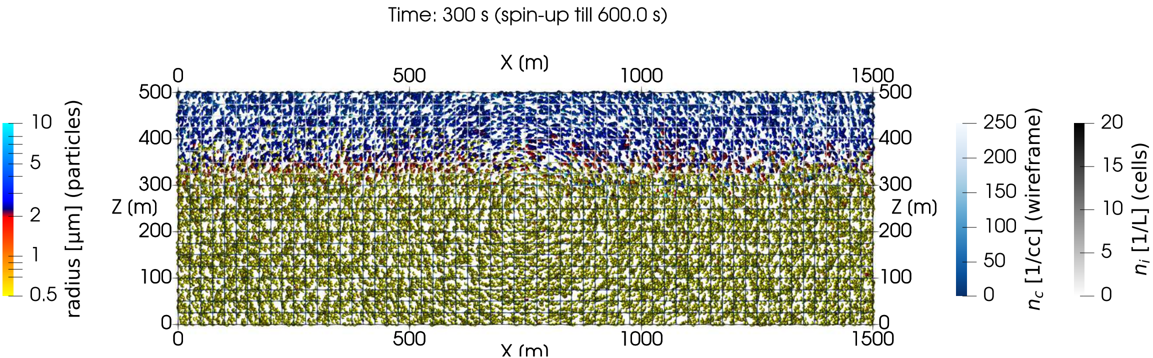

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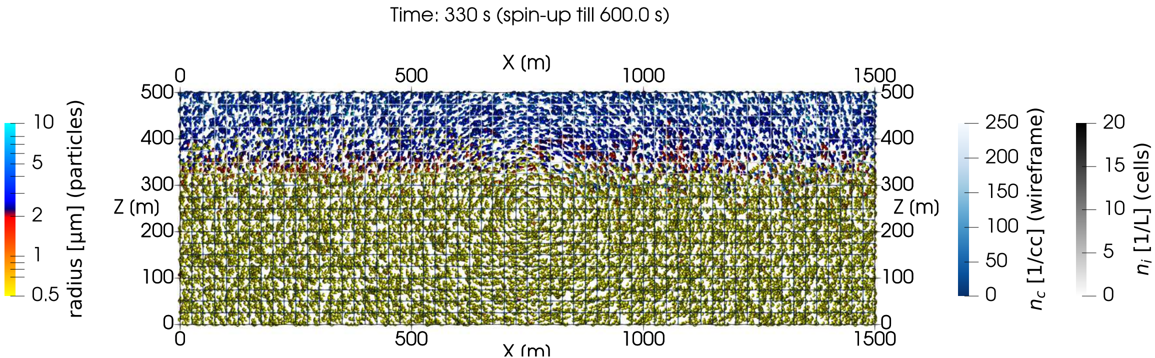

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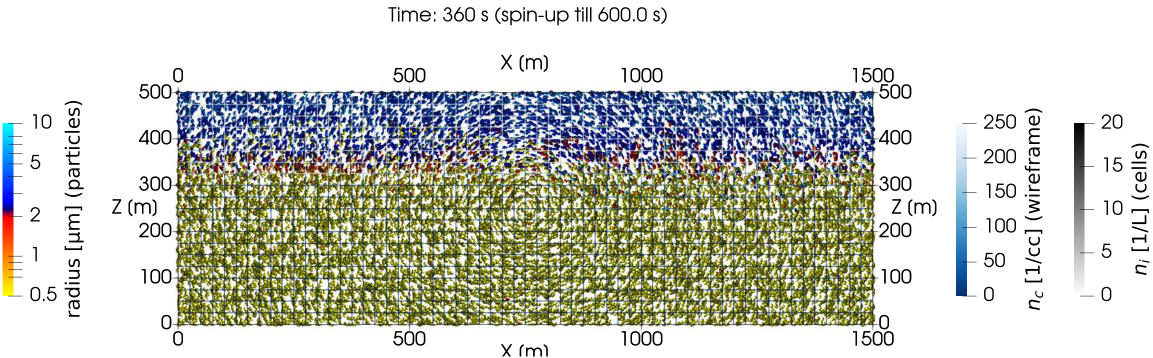

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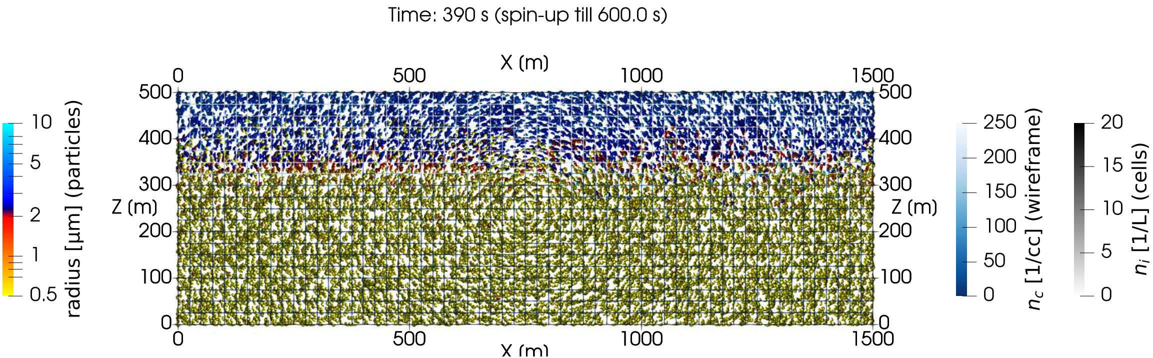

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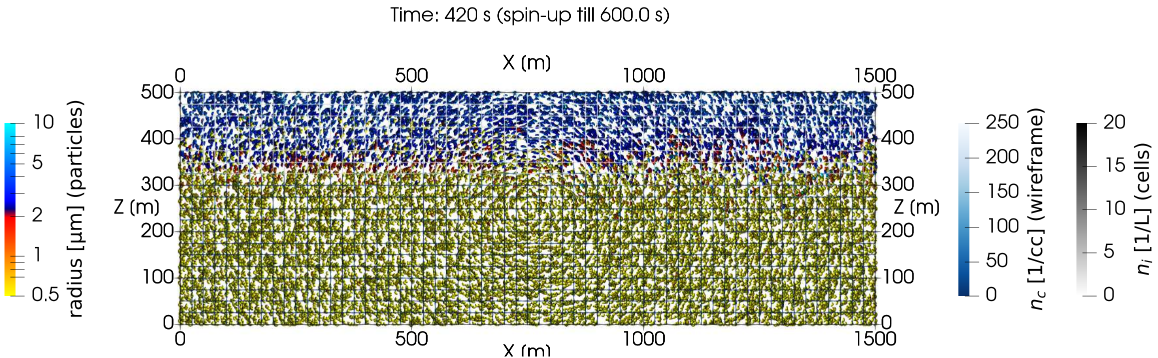

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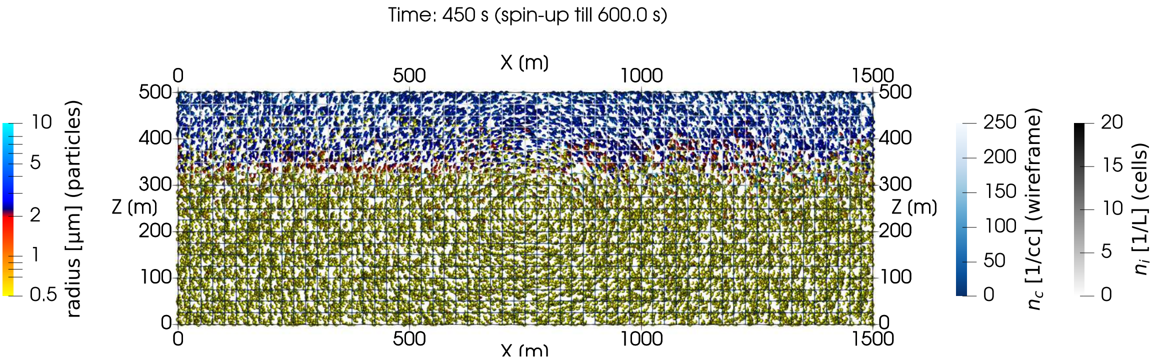

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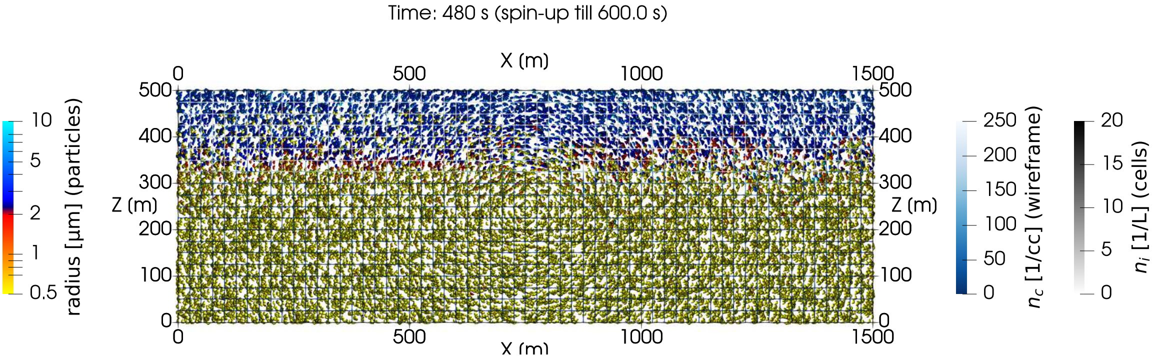

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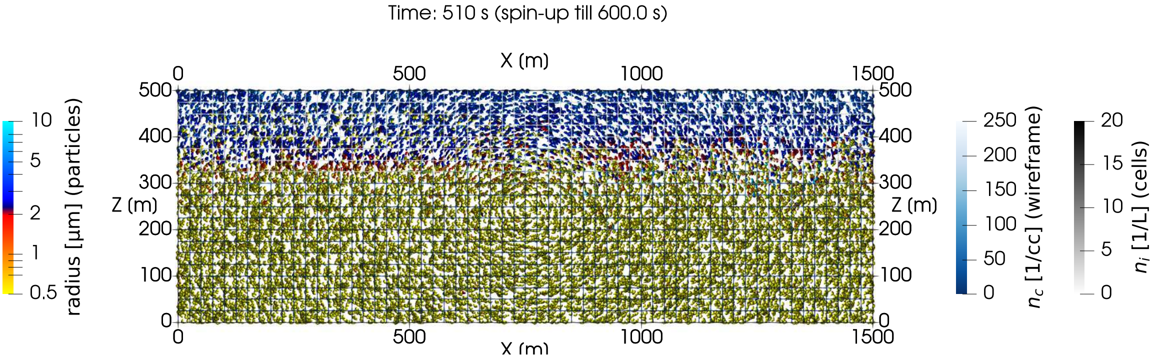

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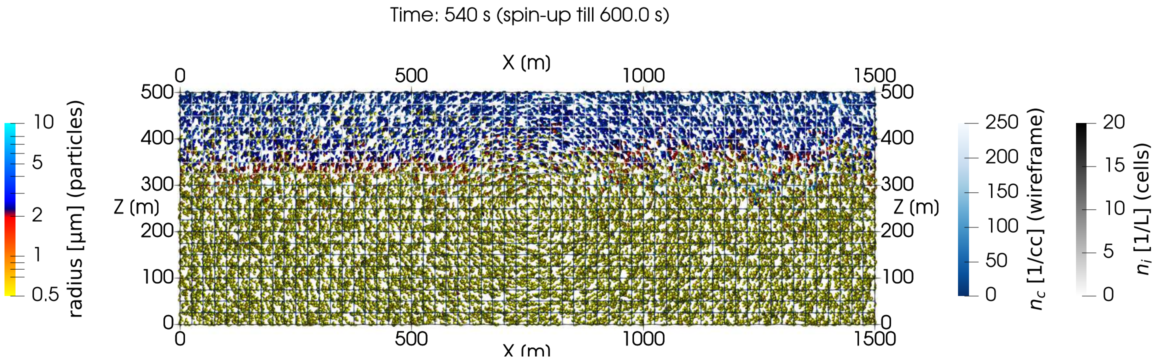

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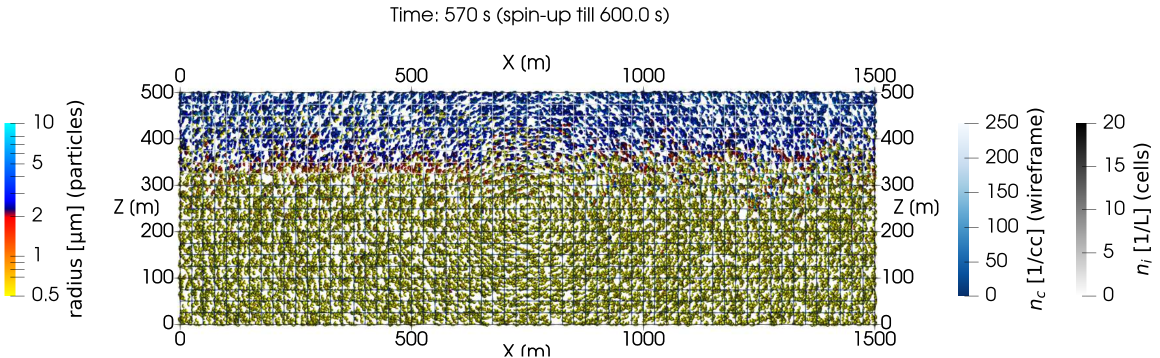

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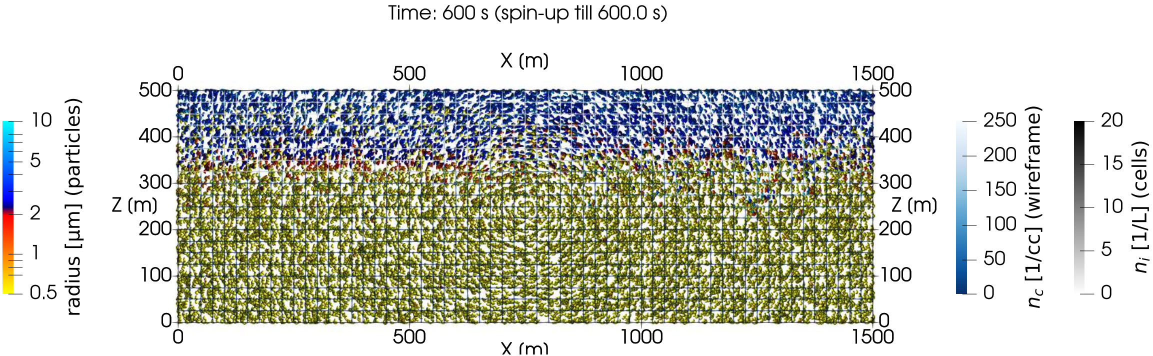

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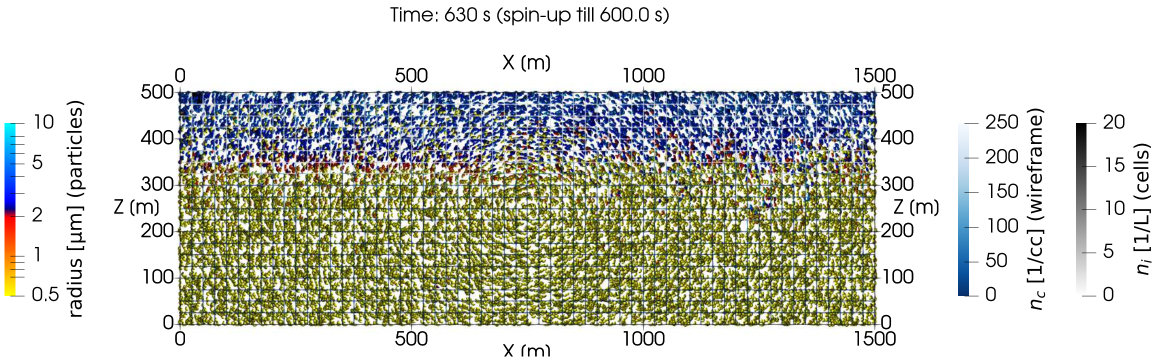

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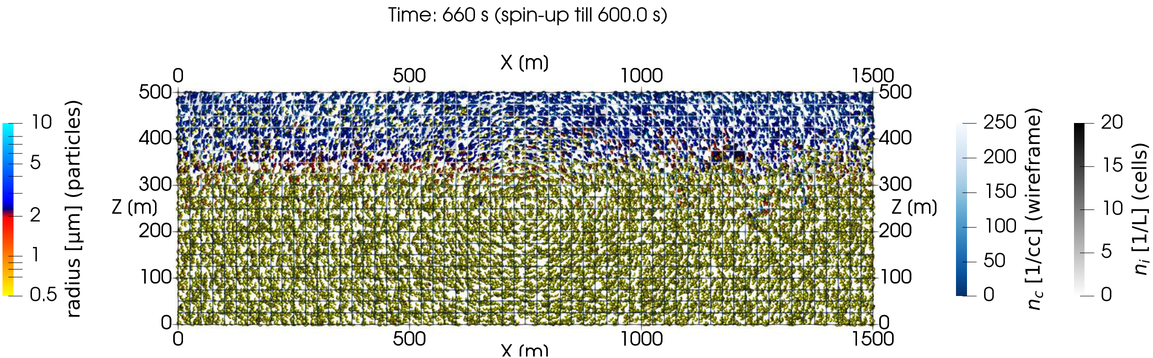

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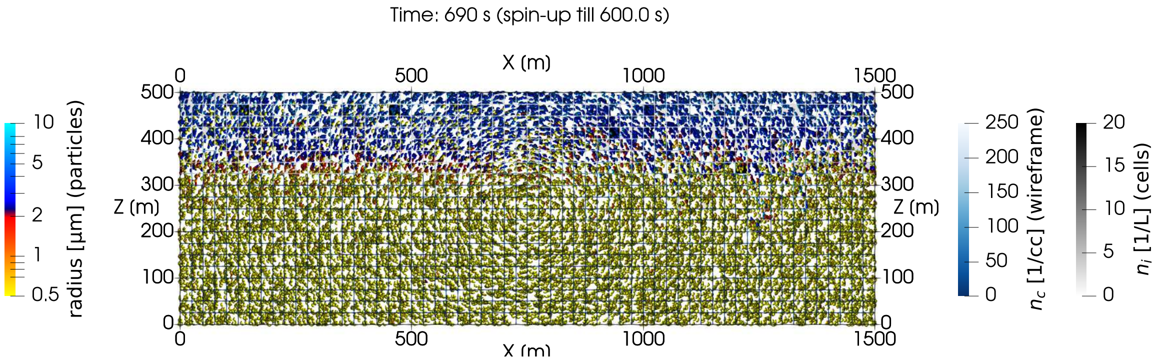

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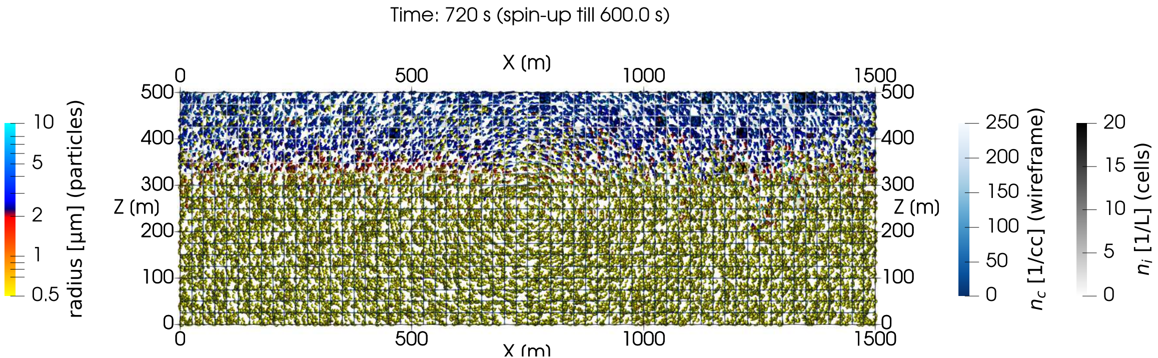

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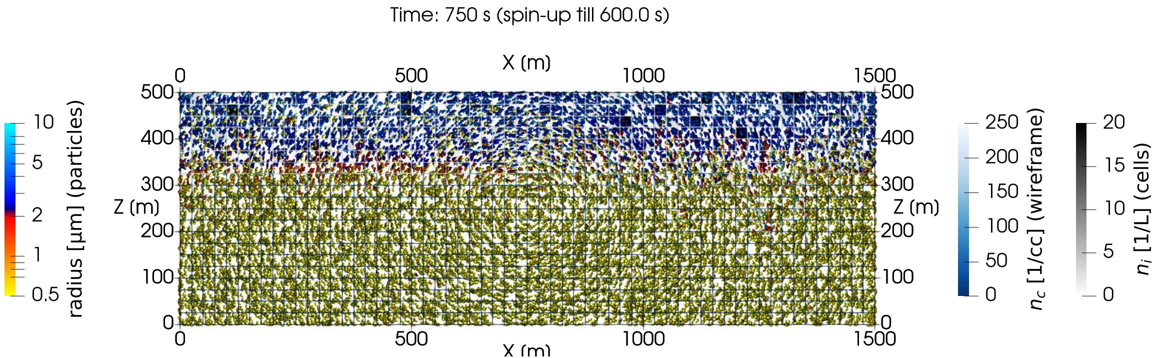

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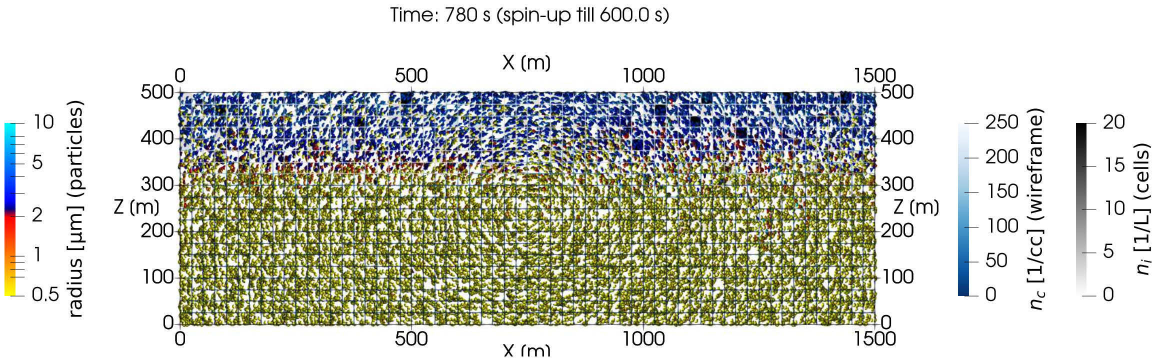

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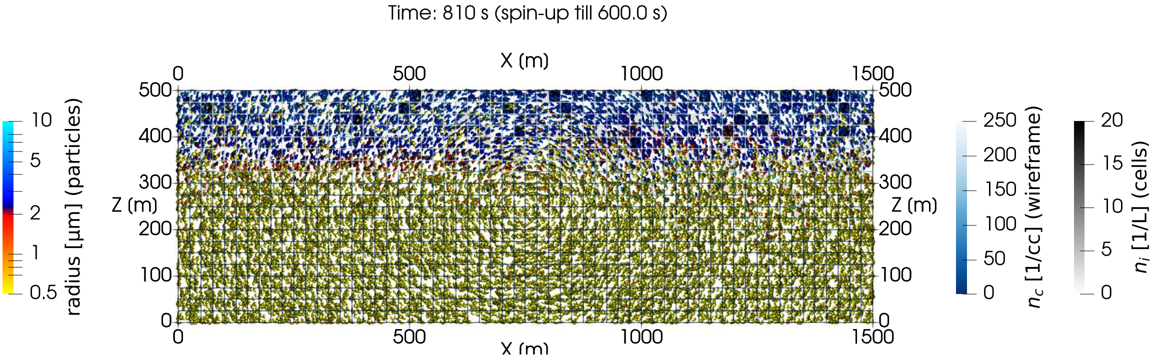

16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (lognormal, $D_g = 0.74$ μm, $\sigma_{\text{g}} = 2.55$)

spin-up = freezing off; subsequently frozen particles act as tracers

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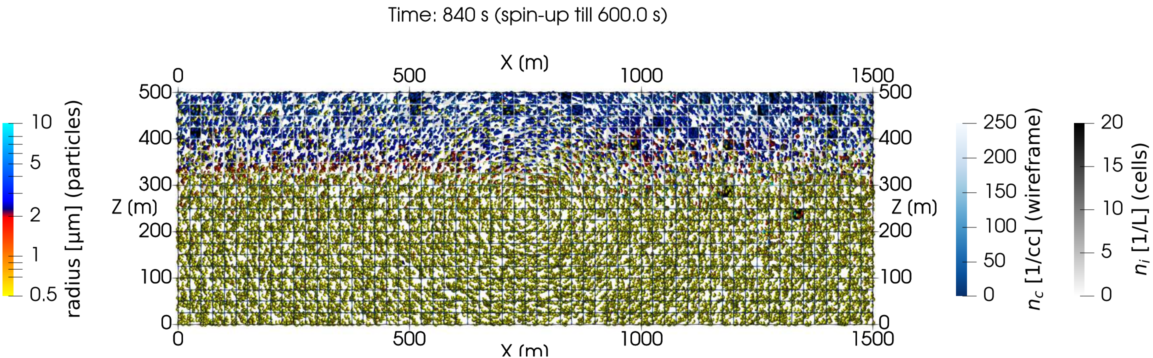

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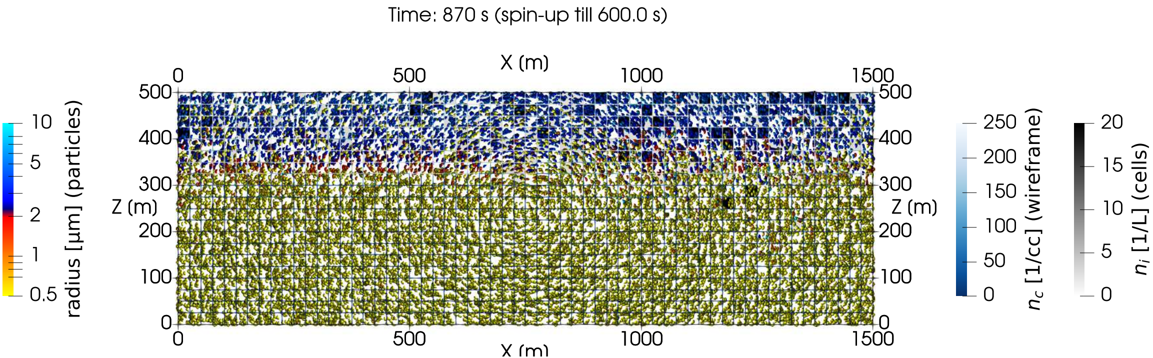

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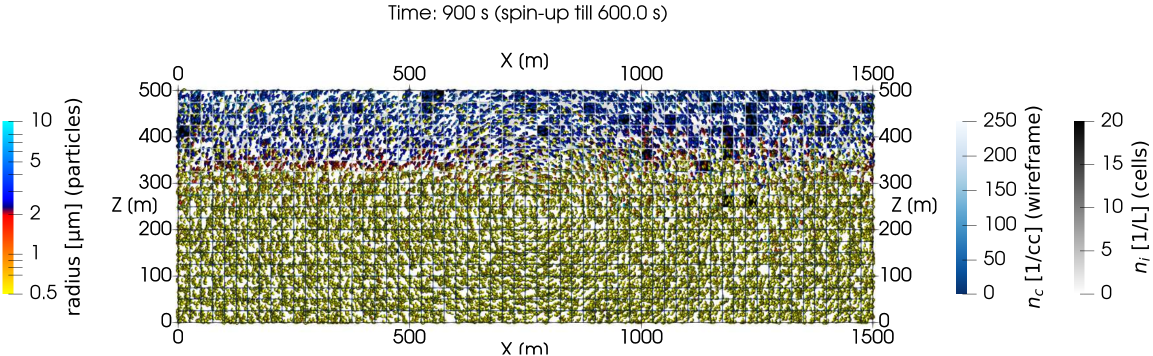

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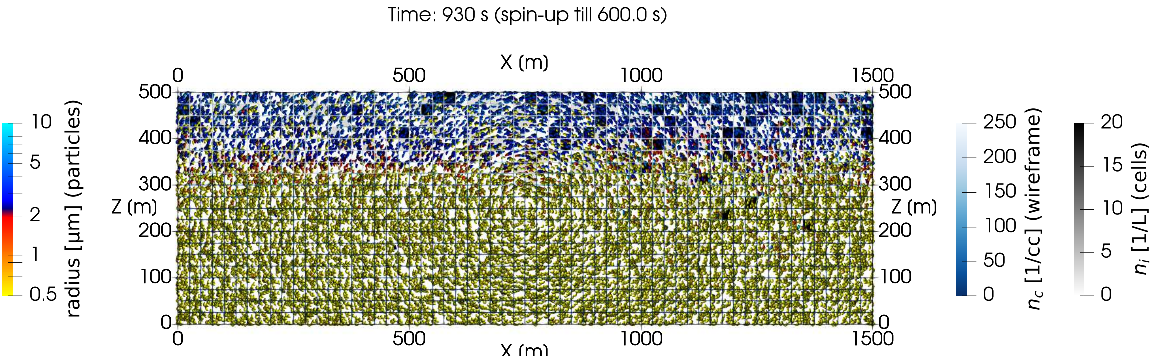

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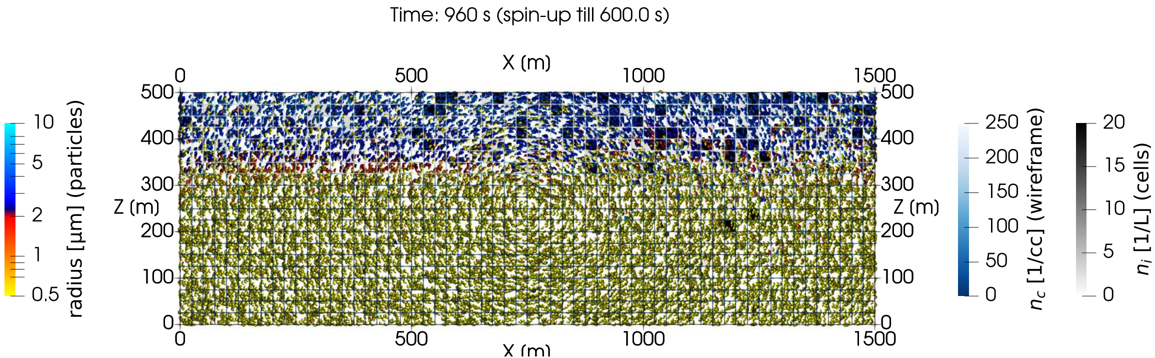

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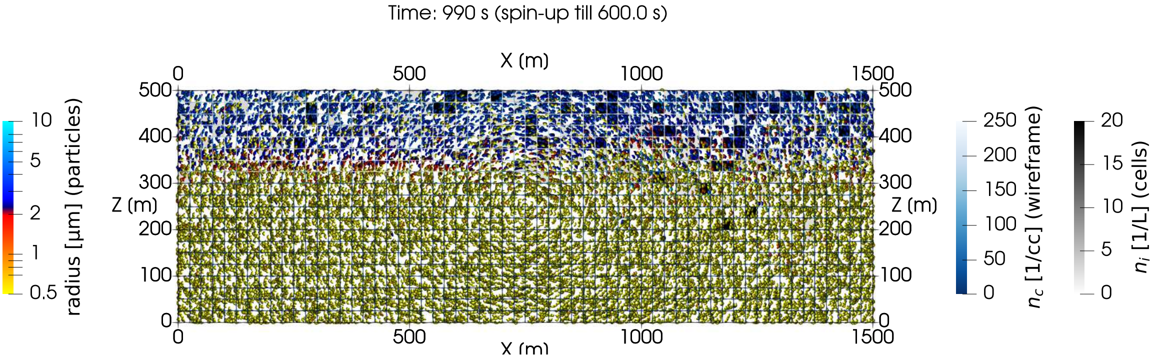

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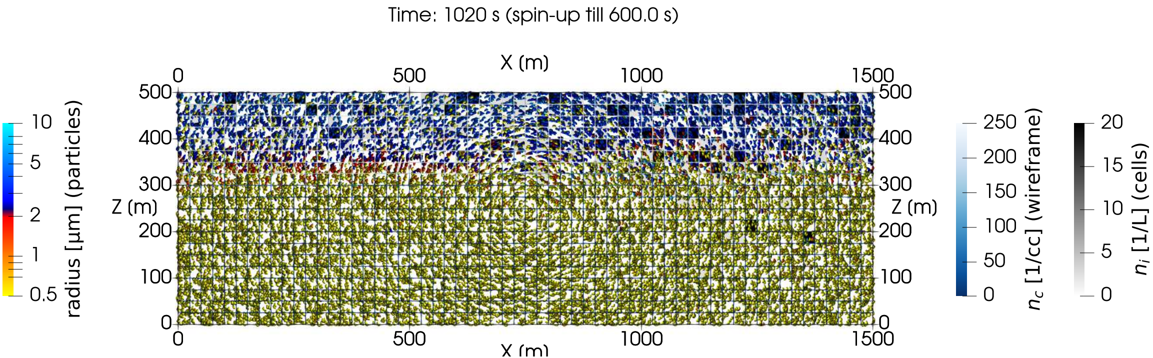

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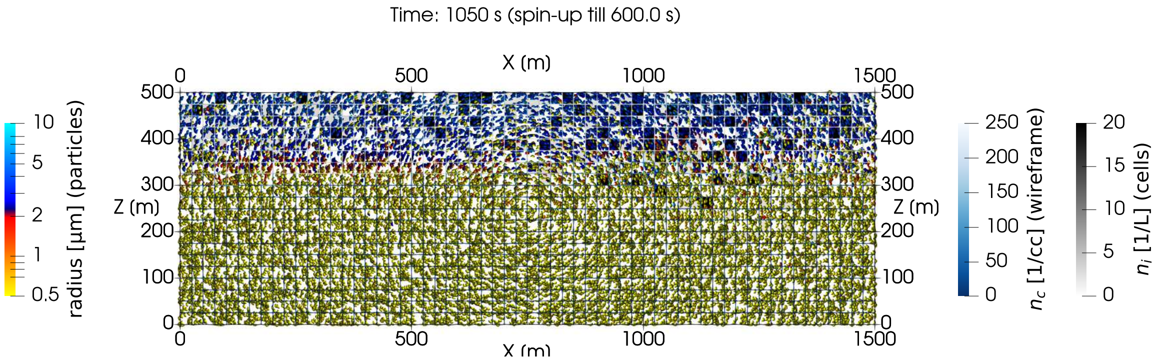

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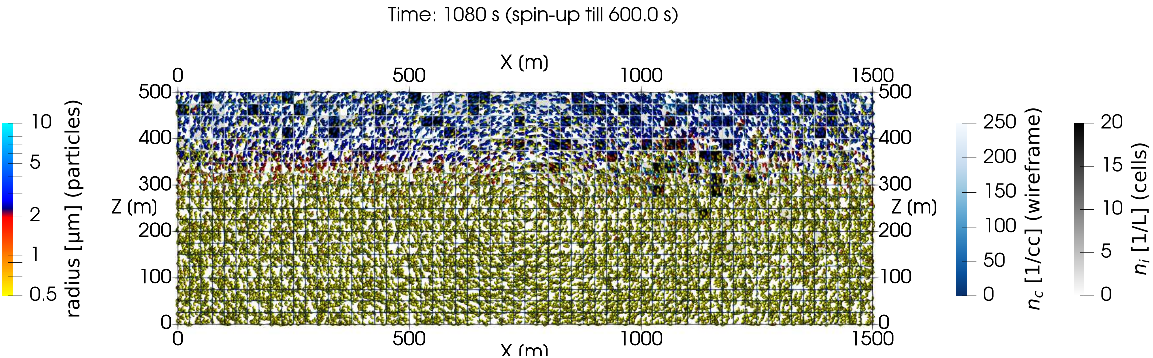

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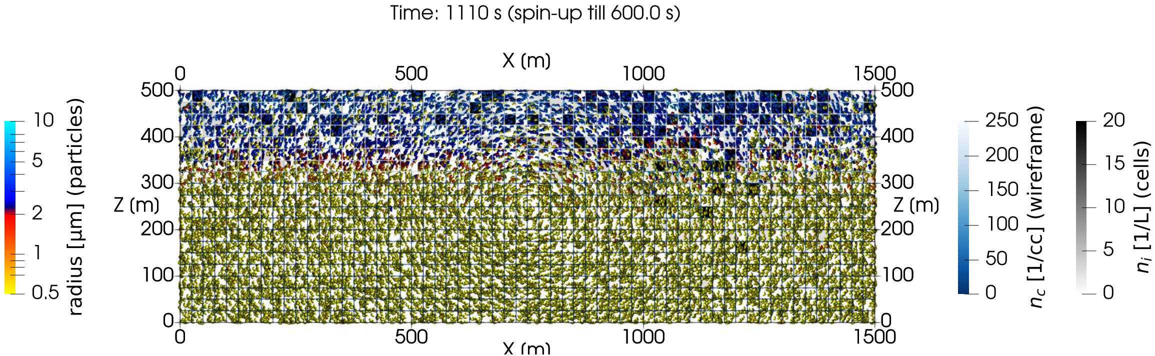

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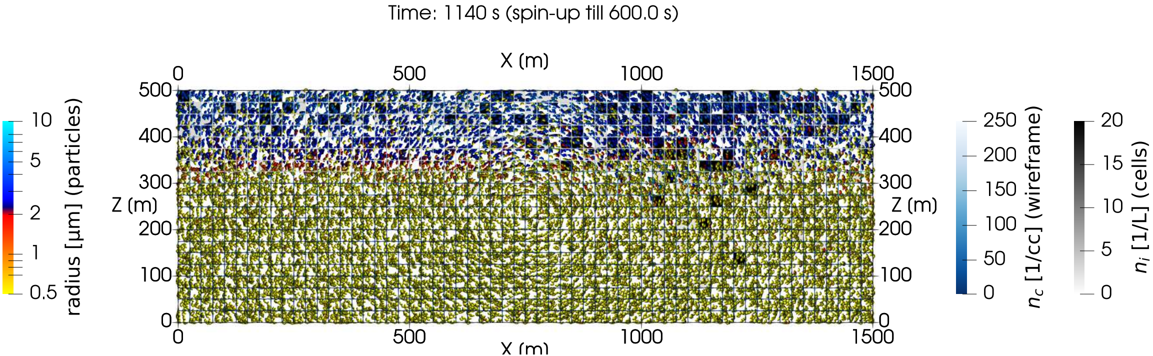

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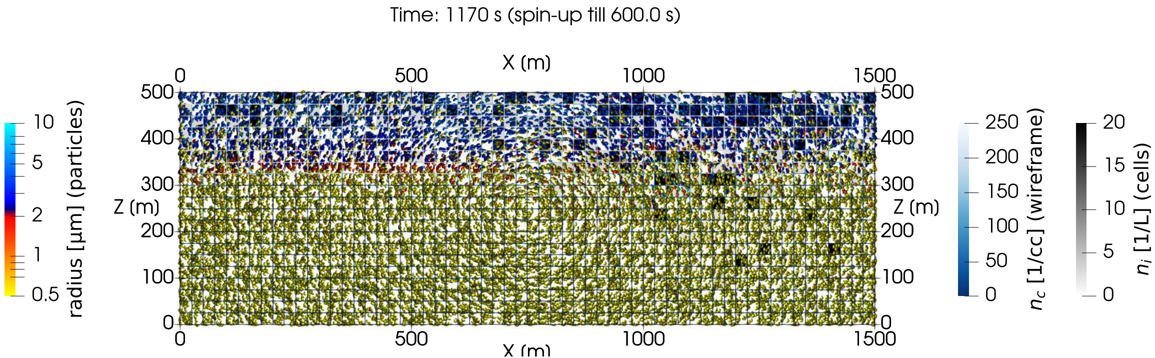

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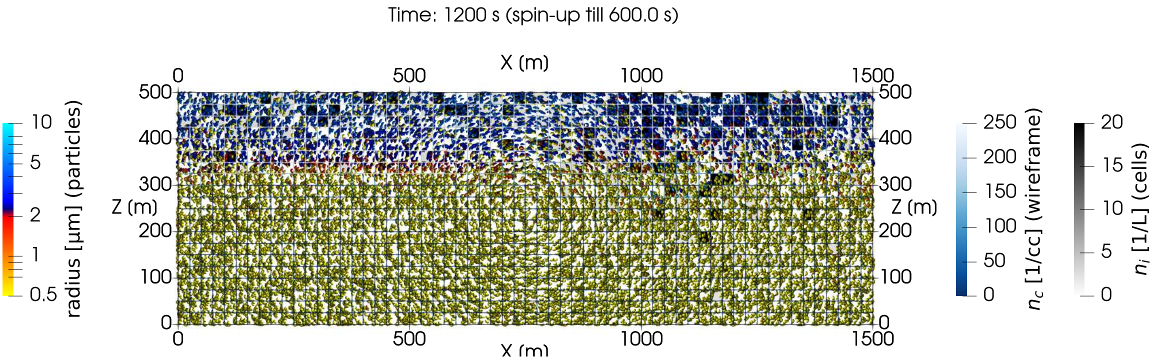

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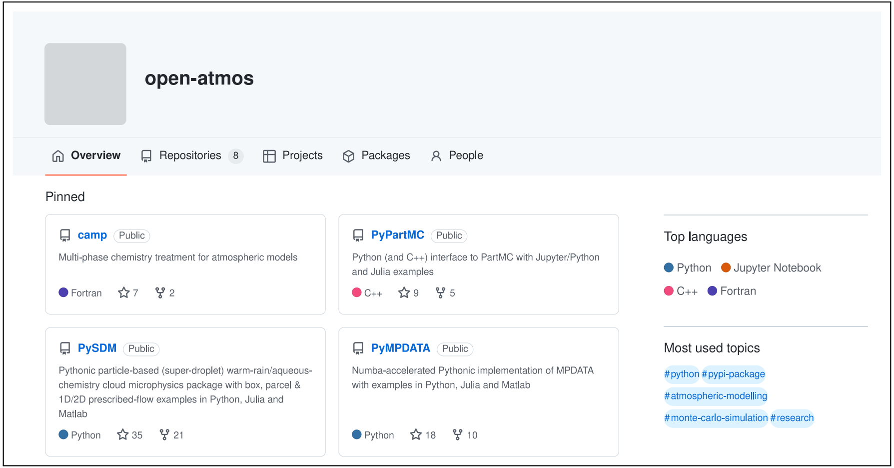
https://github.com/open-atmos



CAMP: BSC, NCAR, UIUC, UCI

PyPartMC: UIUC

PySDM: Jagiellonian, Caltech, UIUC

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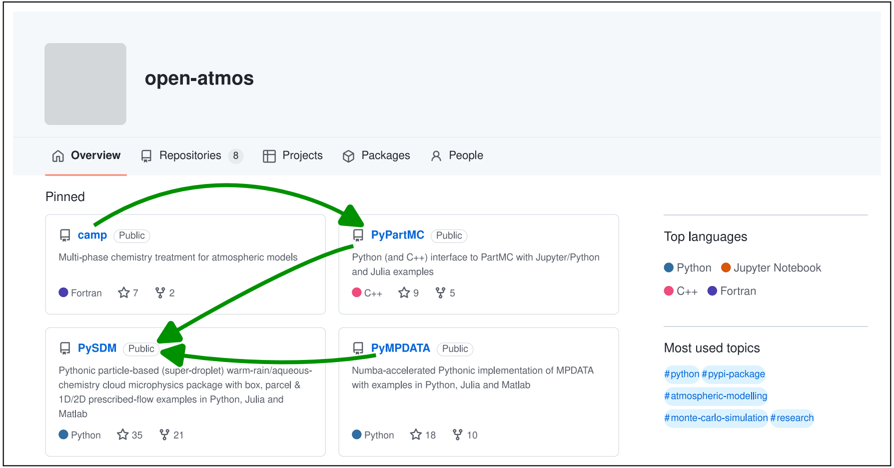

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PySDM: Jagiellonian, Caltech, UIUC

PyMPDATA: Jagiellonian

compdyn/partmc: Particle-resolved stochastic atmospheric aerosol model

PartMC: Particle-resolved Monte Carlo code for atmospheric aerosol simulation

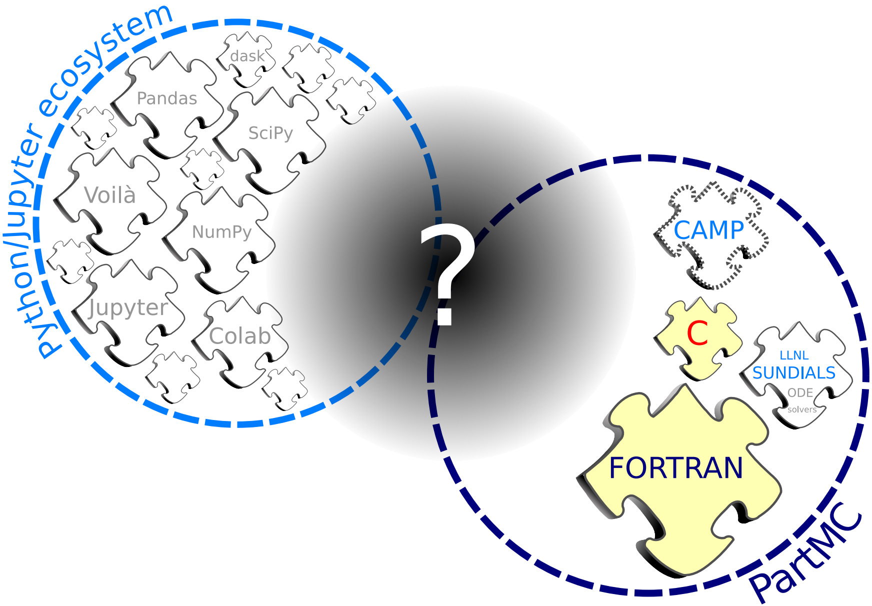
version v2.6.1 docker build automated CI passing license GPL-2.0 DOI 10.5281/zenodo.6144610

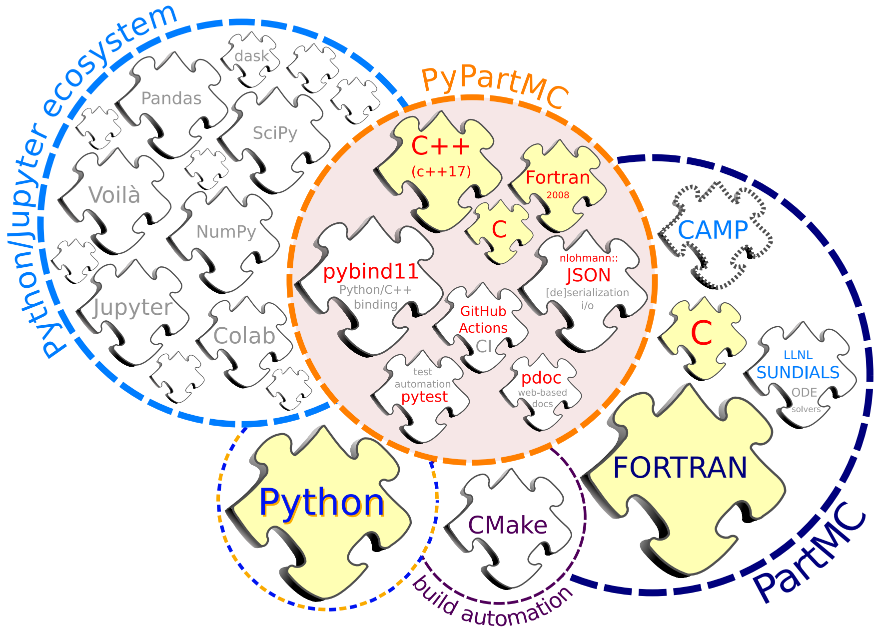
Version 2.6.1
Released 2022-02-18

Source: https://github.com/compdyn/partmc

Homepage: http://lagrange.mechse.illinois.edu/partmc/

Cite as: M. West, N. Riemer, J. Curtis, M. Michelotti, and J. Tian (2022) PartMC, version v2.6.1, DOI 10.5281/zenodo.6144610


Python/Jupyter ecosystem
dask
Pandas
SciPy
Voilà
NumPy
Jupyter
Colab
?
CAMP
C
LLNL
SUNDIALS
ODE
solvers
FORTRAN
PartMC



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(c++17)
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C
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Python/C++
binding
nlohmann::
JSON
[de]serialization
i/o
GitHub
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CI
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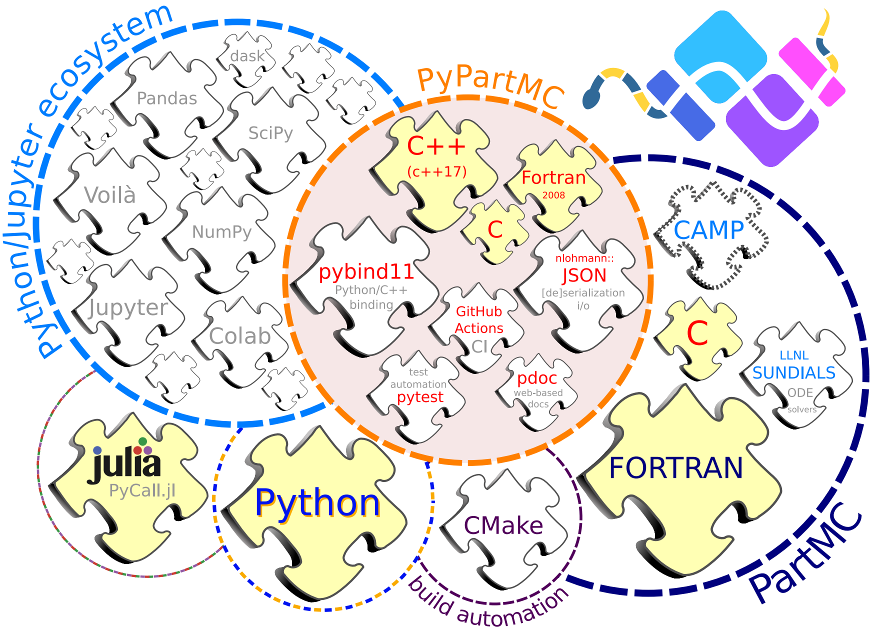
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pytest
pdoc
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PartMC
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PyCall.jl
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CMake
build automation

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PyPartMC 0.0.25

```
pip install PyPartMC
```

Latest version

Released: Feb 21, 2023

Python interface to PartMC

Navigation

- Project description
- Release history
- Download files

Project links

- Documentation
- Source

Project description

PyPartMC (pre-alpha!)

PyPartMC is a Python interface to [PartMC](), a particle-resolved Monte-Carlo code for atmospheric aerosol simulation. Since PyPartMC is implemented in C++, it also constitutes a C++ API to the PartMC Fortran internals; the Python API can be used from other environments - see, e.g., Julia example below.

US DOE Funding by ASR | License GPL v3 | Copyright UIUC | Maintained? yes | tests passing | API docs pdoc3

- super-particle-count conserving probabilistic collisional breakup (Emily de Jong @Caltech)
  - $\rightsquigarrow$ https://doi.org/10.5194/egusphere-2022-1243

doctoral network links/prospects

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  - (super-)particle advection and sedimentation
  - collision kernel (mixed-phase!)

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  - collision kernel (mixed-phase!)

- Python/Jupyter ecosystem in coursework/workshop context – PySDM already used at:
  - "Modelling of Atmospheric Clouds" course at the Jagiellonian Univ.
  - "ESE 134. Cloud and Boundary Layer Dynamics" course at Caltech
  - "High-Performance Computing Summer School" at Univ. Kobe

Merci de votre attention

sylwester.arabas@uj.edu.pl (soon @agh.edu.pl)

collaborators:

N. Riemer, M. West, J. Curtis, Z. D'Aquino, ... (UIUC),

P. Bartman & O. Bulenok, ... (Jagiellonian),

E. de Jong, C. Singer, A. Jaruga, ... (Caltech)

...

funding:

Foundation for Polish Science, Poland's National Science Centre, US DOE (ASR)