

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

S. Arabas¹, J.H. Curtis², I. Silber³, A. Fridlind⁴, D.A Knopf⁵, M. West² & N. Riemer²

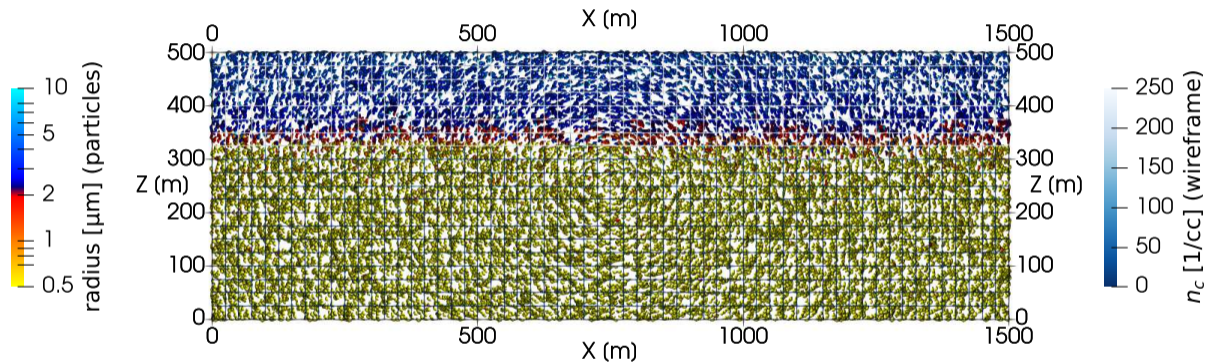


2023 ARM/ASR Joint User Facility/PI Meeting, Rockville, MD

Breakout session: Primary and secondary ice production and impacts on mixed-phase and ice clouds

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 30 s (spin-up till 600.0 s)



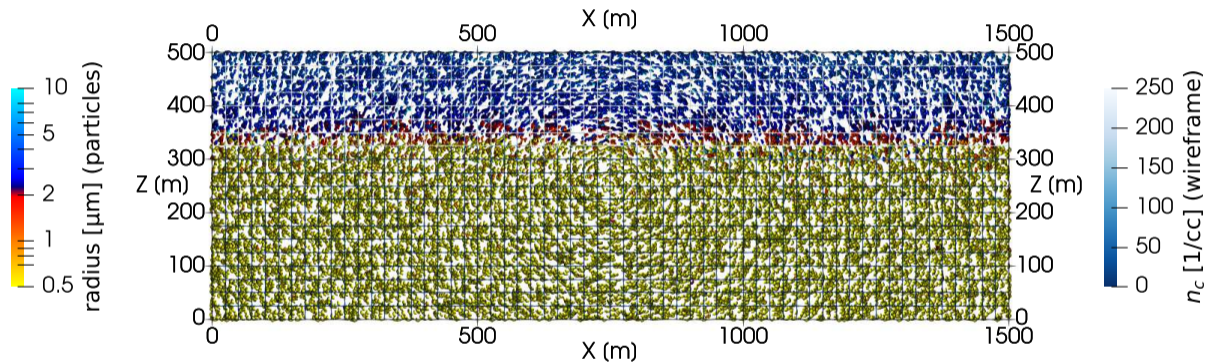
16+16 super-particles/cell for INP-rich + INP-free particles

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

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 60 s (spin-up till 600.0 s)



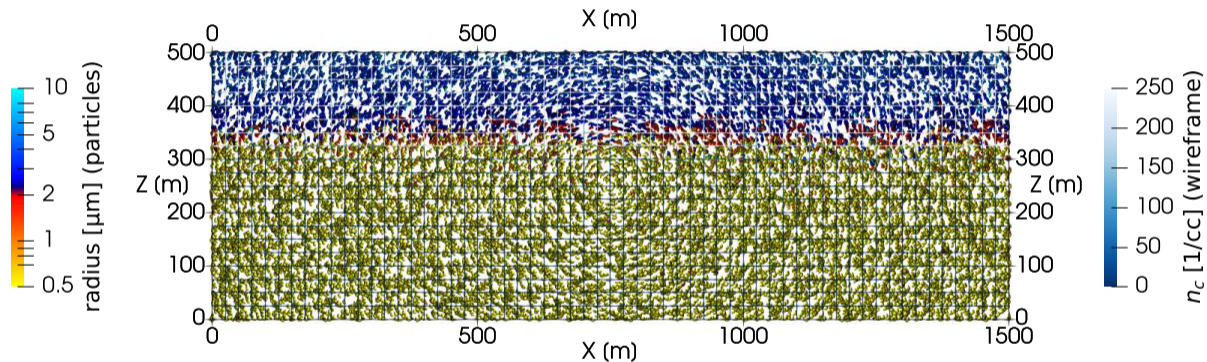
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 90 s (spin-up till 600.0 s)



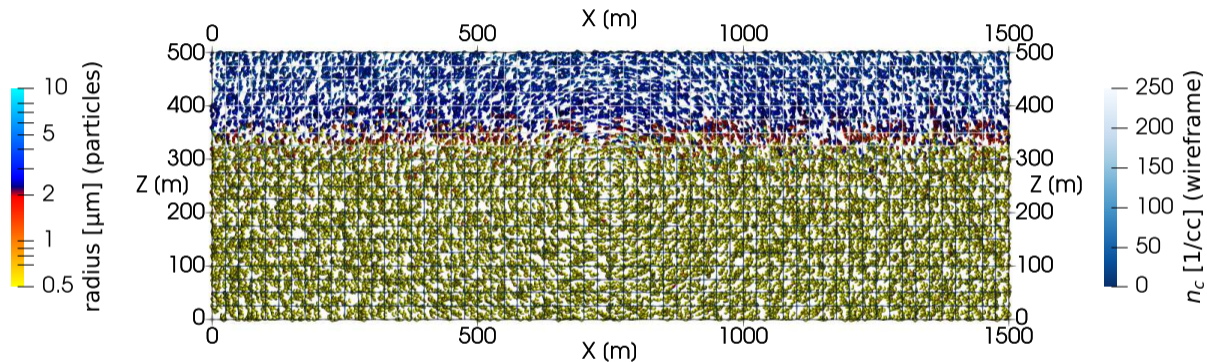
16+16 super-particles/cell for INP-rich + INP-free particles

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 120 s (spin-up till 600.0 s)



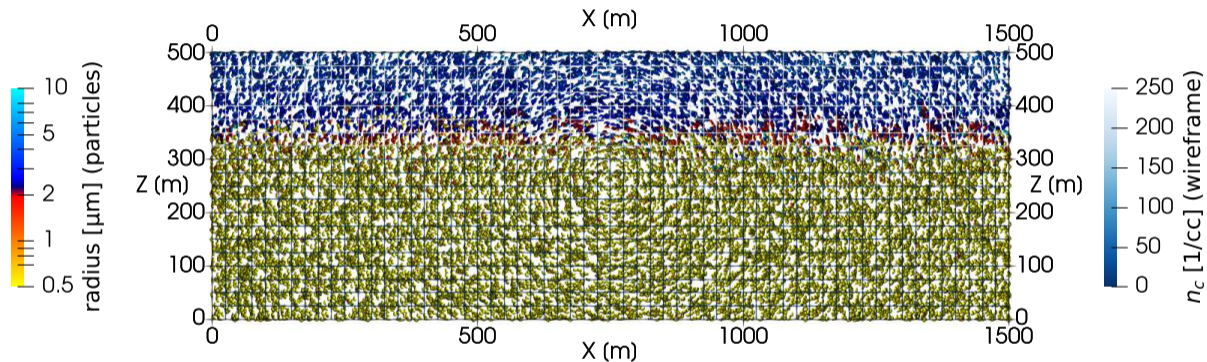
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 150 s (spin-up till 600.0 s)



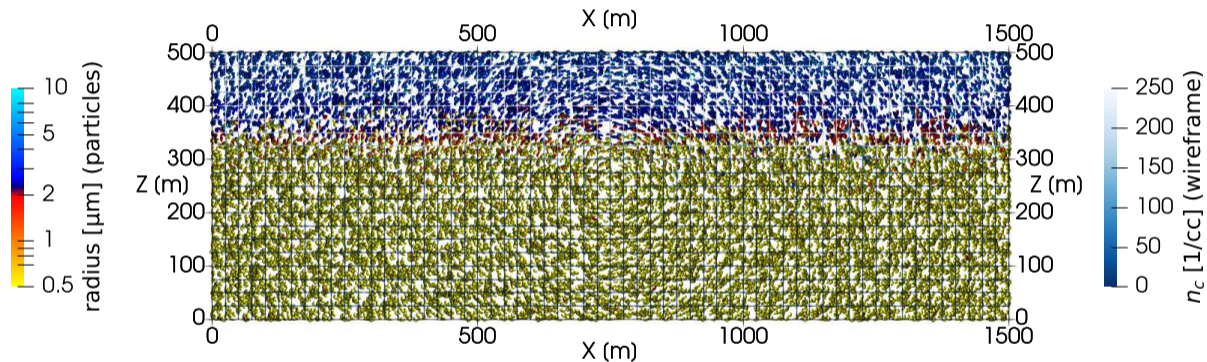
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 180 s (spin-up till 600.0 s)



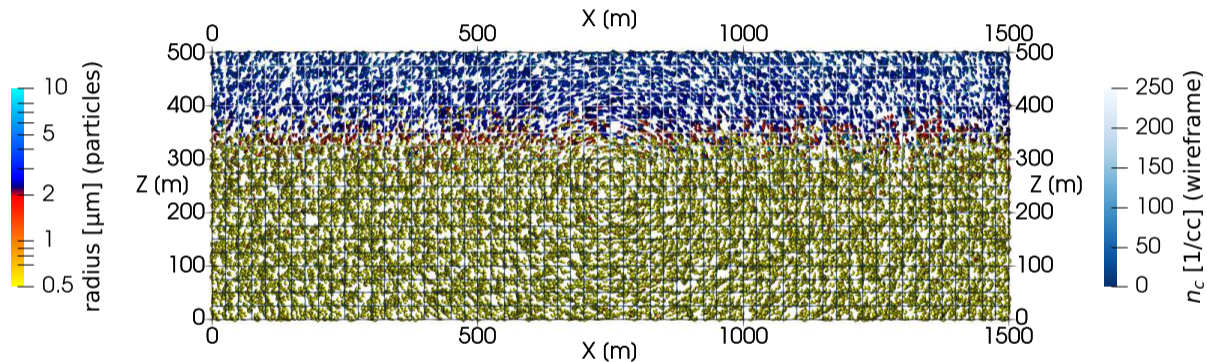
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 210 s (spin-up till 600.0 s)



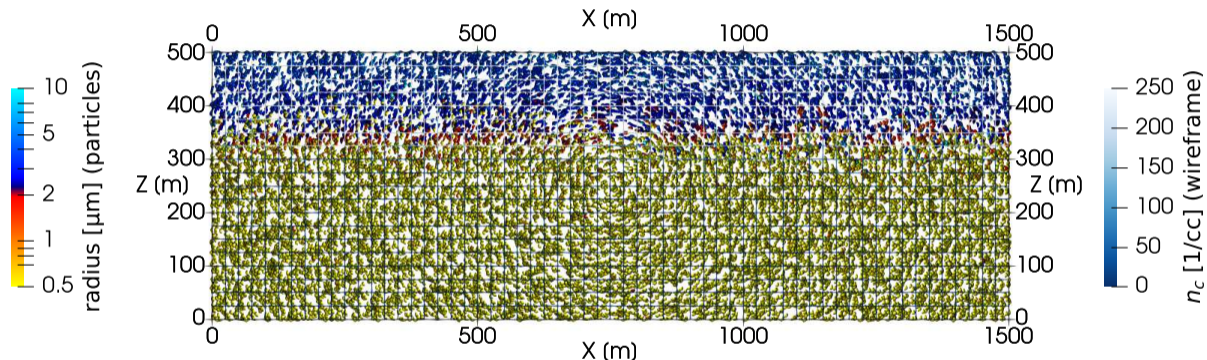
16+16 super-particles/cell for INP-rich + INP-free particles

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 240 s (spin-up till 600.0 s)



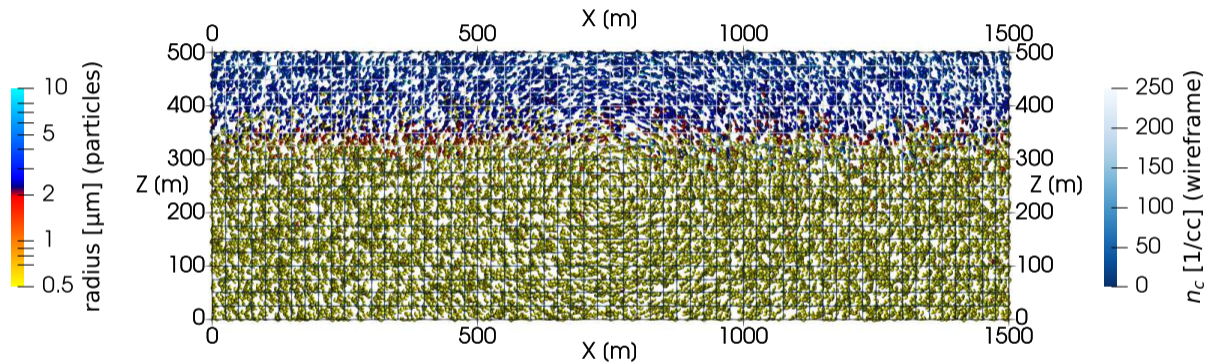
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 270 s (spin-up till 600.0 s)



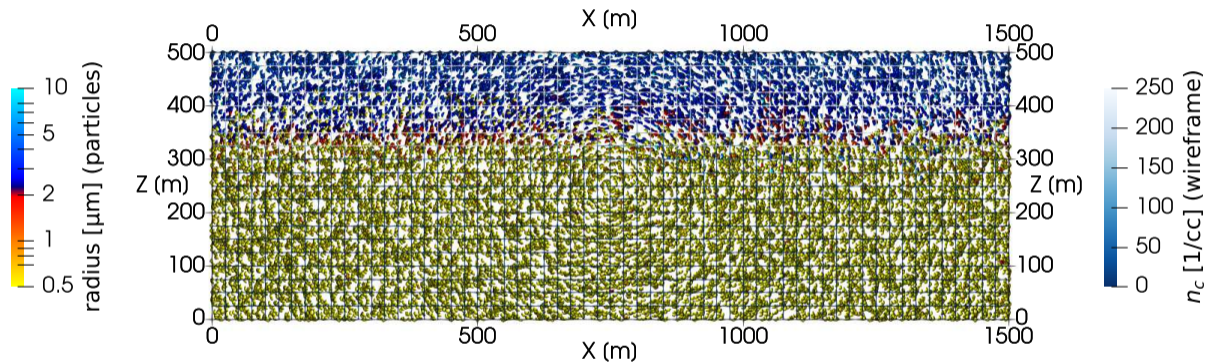
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 300 s (spin-up till 600.0 s)



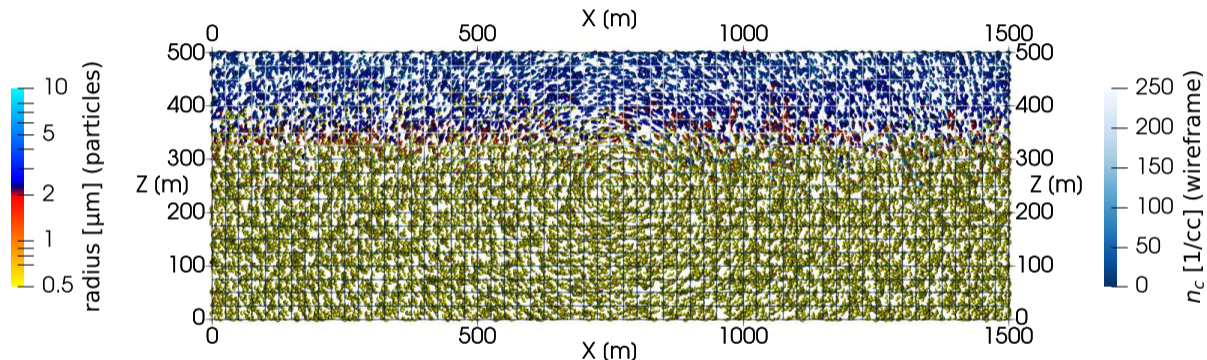
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 330 s (spin-up till 600.0 s)



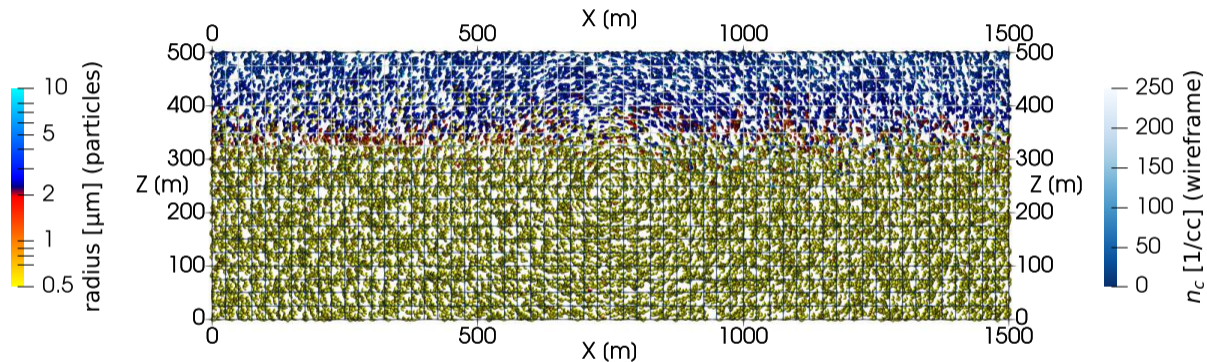
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 360 s (spin-up till 600.0 s)



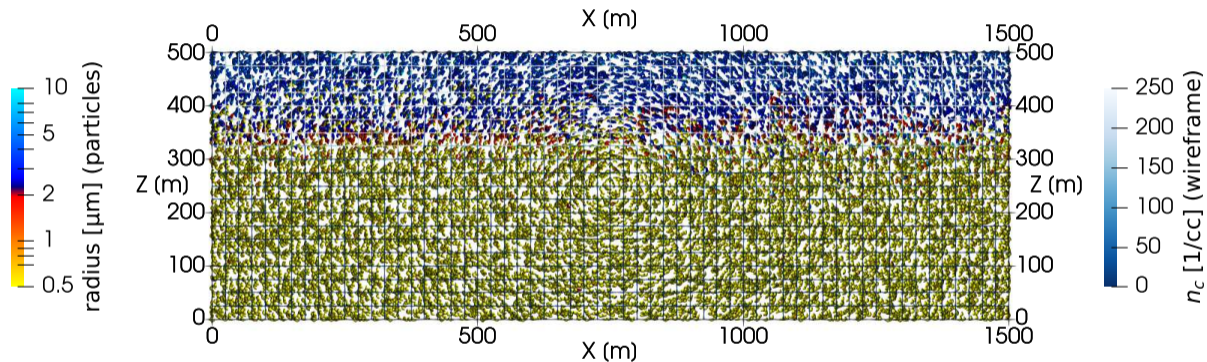
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 390 s (spin-up till 600.0 s)



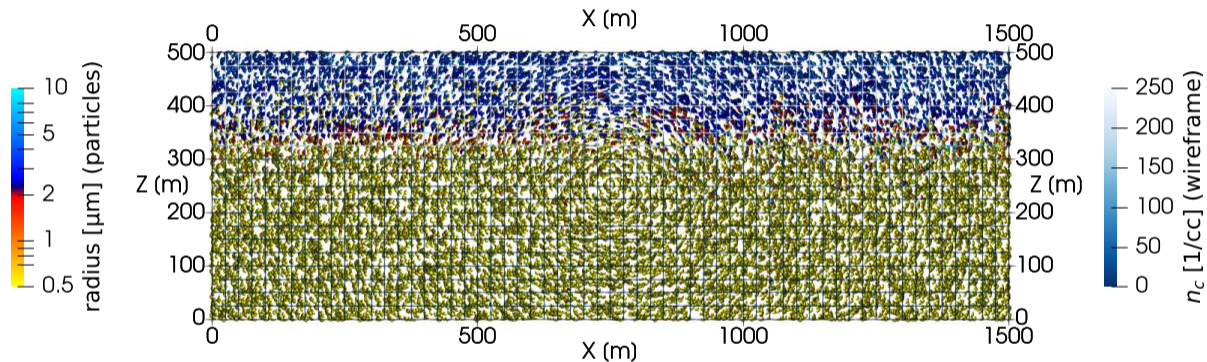
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 420 s (spin-up till 600.0 s)



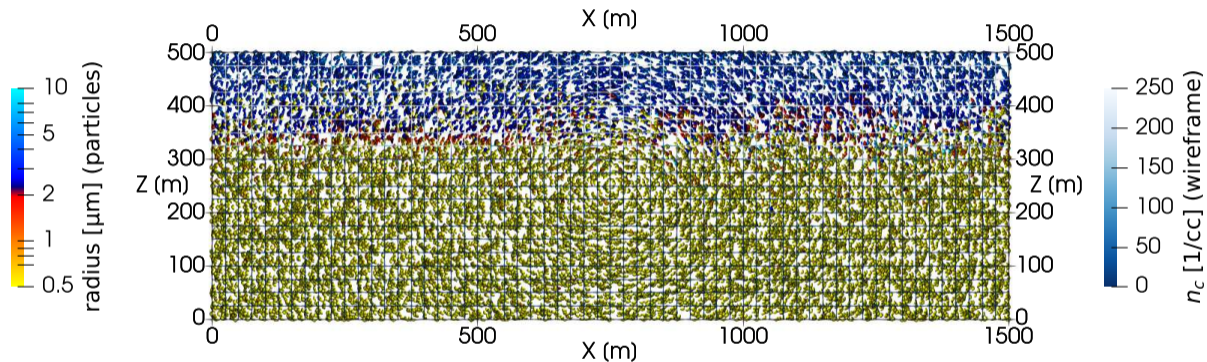
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 450 s (spin-up till 600.0 s)



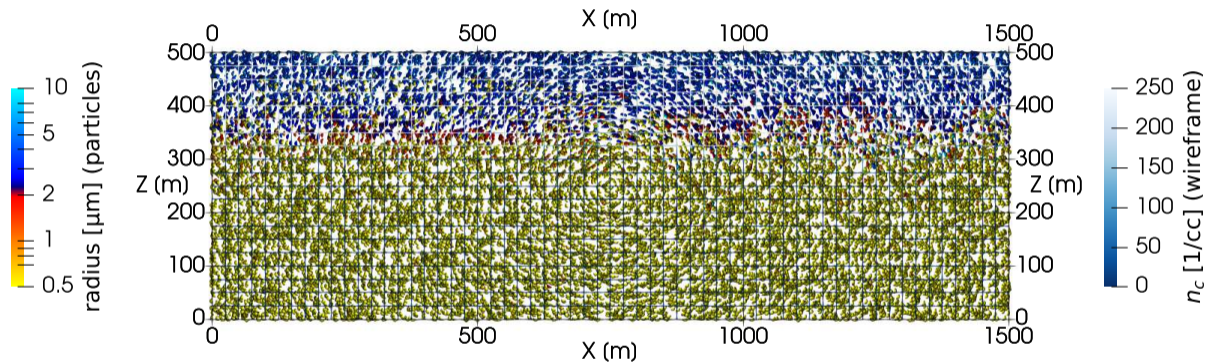
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 480 s (spin-up till 600.0 s)



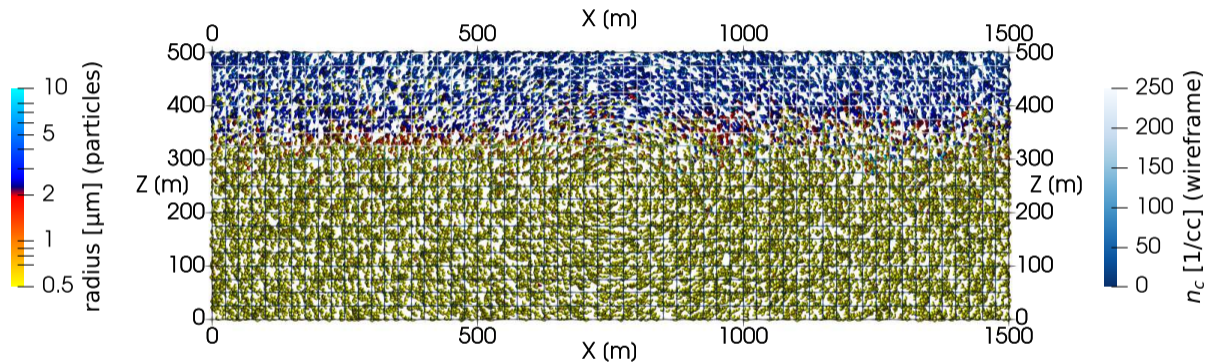
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 510 s (spin-up till 600.0 s)



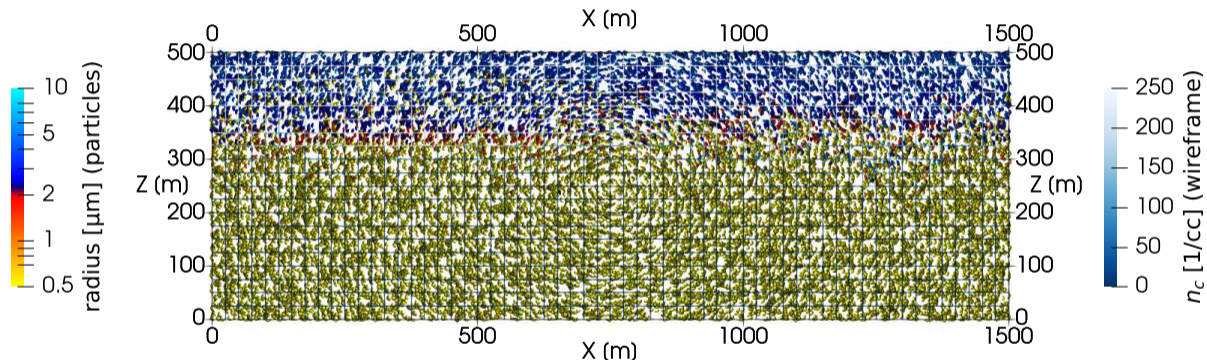
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 540 s (spin-up till 600.0 s)



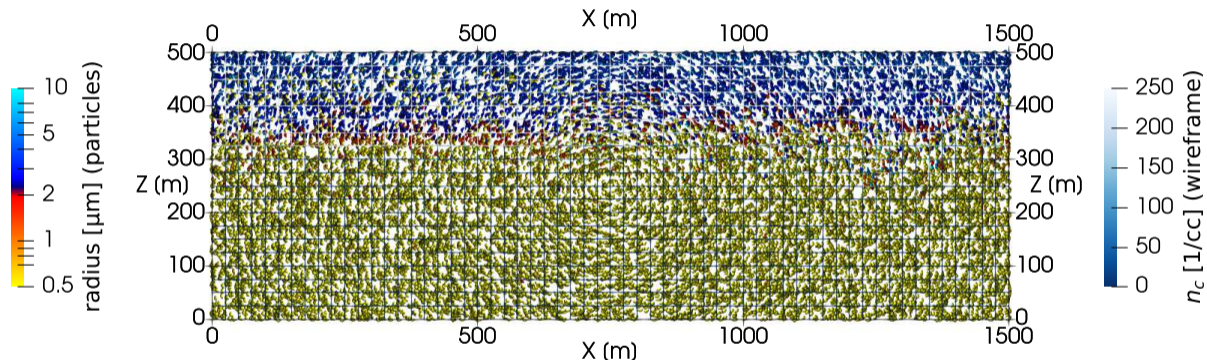
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 570 s (spin-up till 600.0 s)



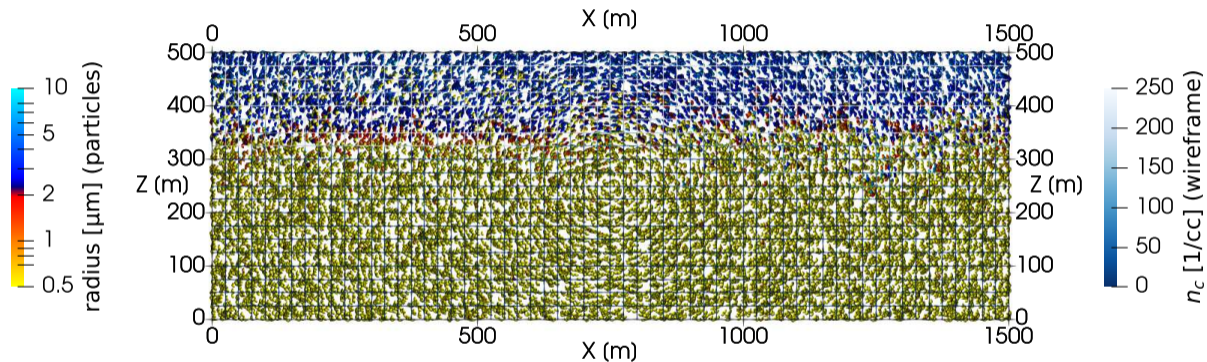
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 600 s (spin-up till 600.0 s)



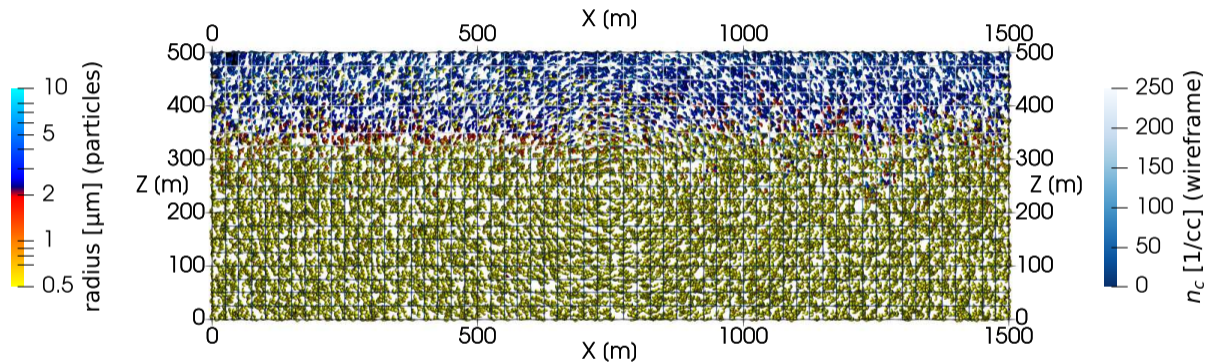
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 630 s (spin-up till 600.0 s)



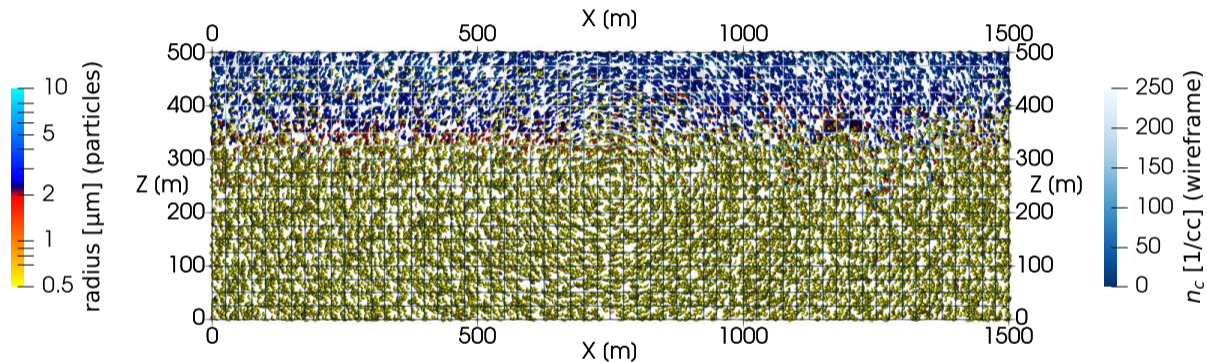
16+16 super-particles/cell for INP-rich + INP-free particles

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 660 s (spin-up till 600.0 s)



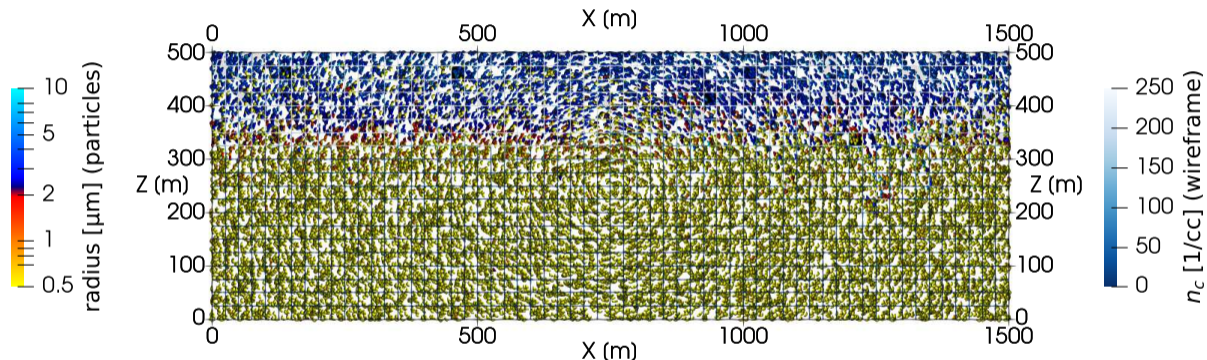
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 690 s (spin-up till 600.0 s)



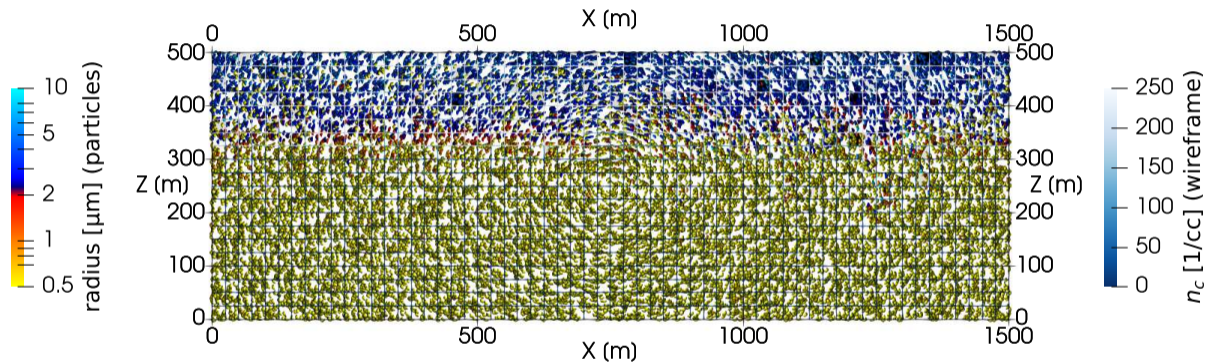
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 720 s (spin-up till 600.0 s)



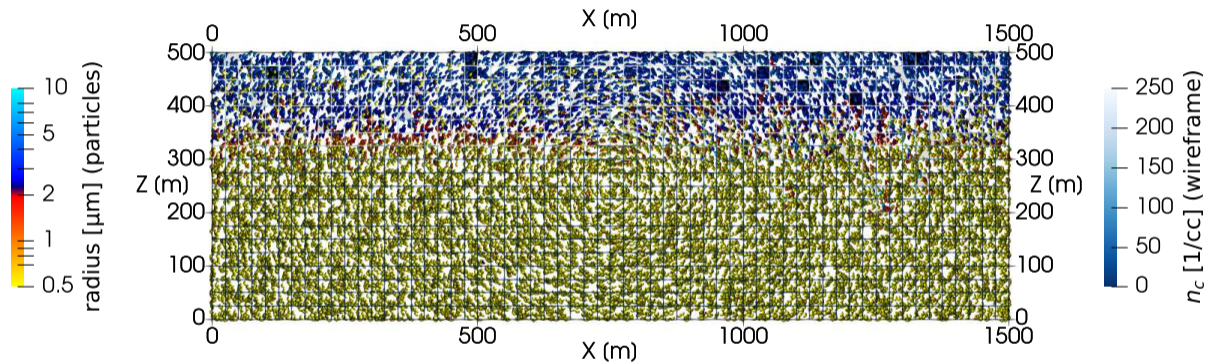
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 750 s (spin-up till 600.0 s)



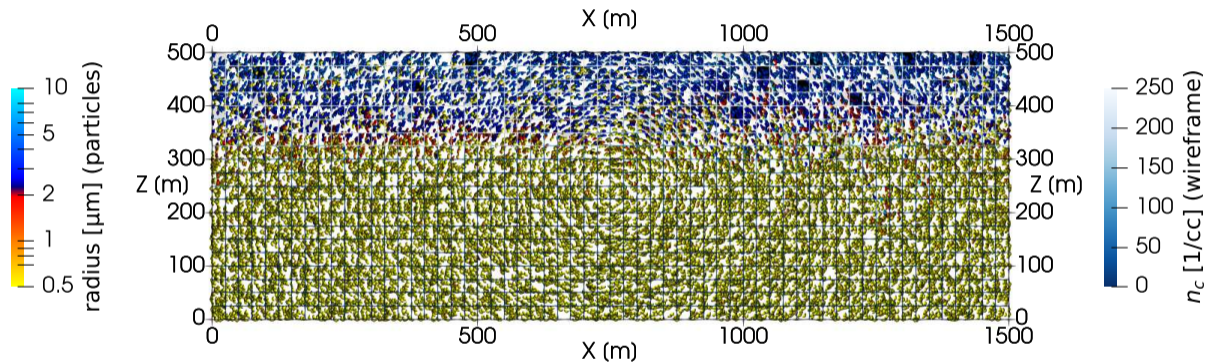
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 780 s (spin-up till 600.0 s)



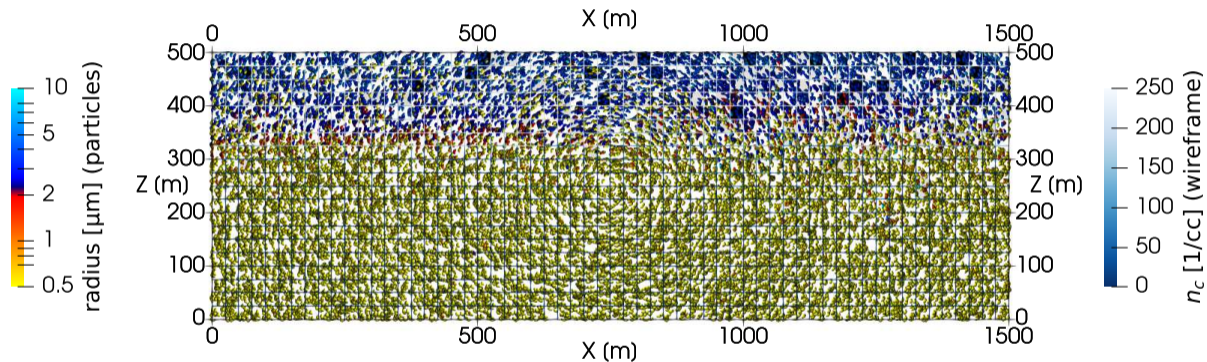
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 810 s (spin-up till 600.0 s)



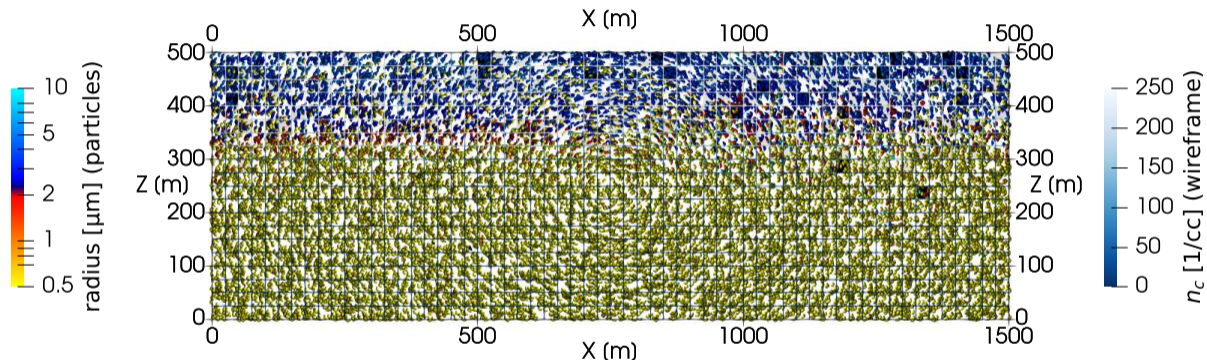
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 840 s (spin-up till 600.0 s)



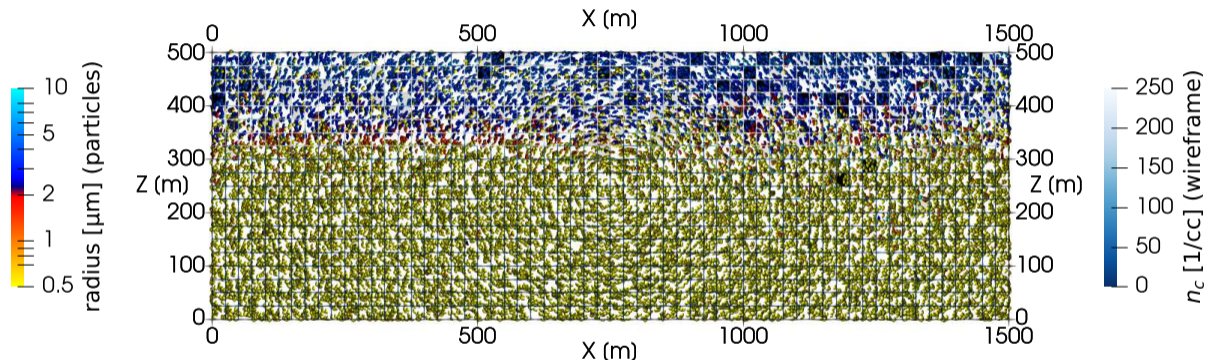
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 870 s (spin-up till 600.0 s)



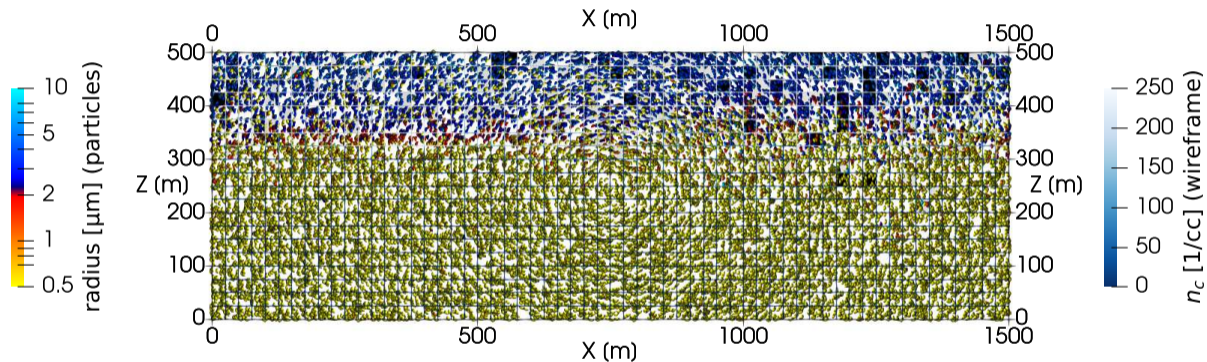
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 900 s (spin-up till 600.0 s)



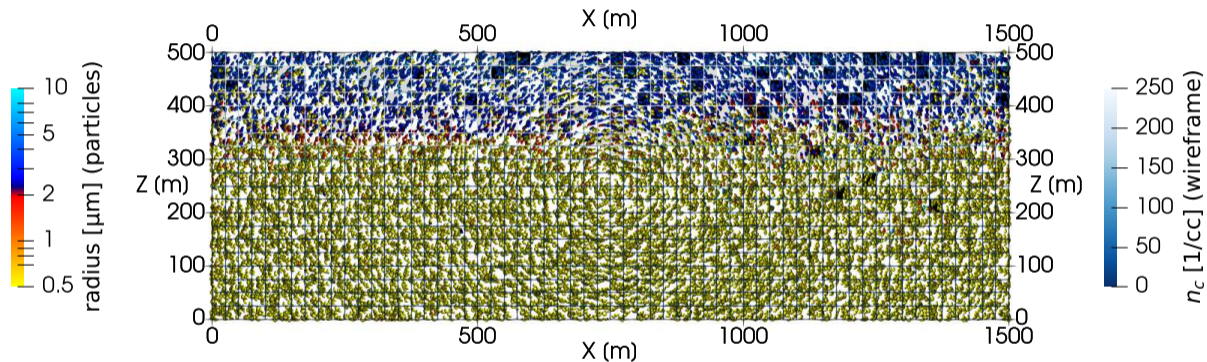
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 930 s (spin-up till 600.0 s)



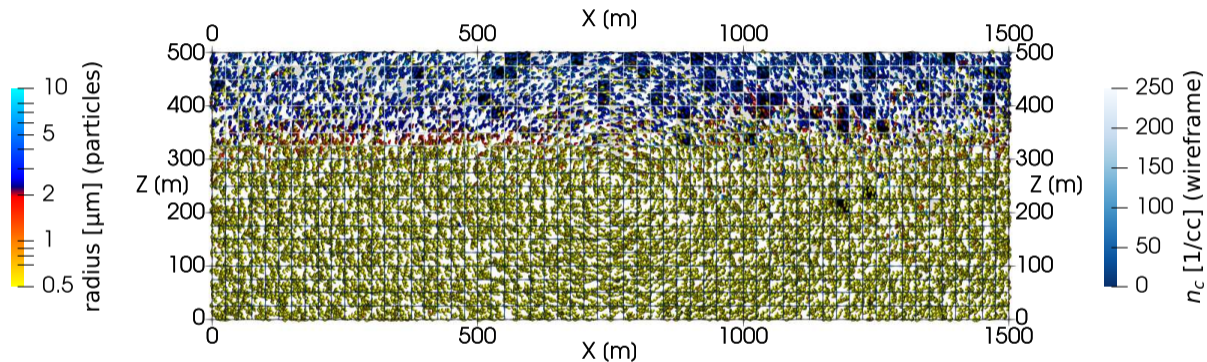
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 960 s (spin-up till 600.0 s)



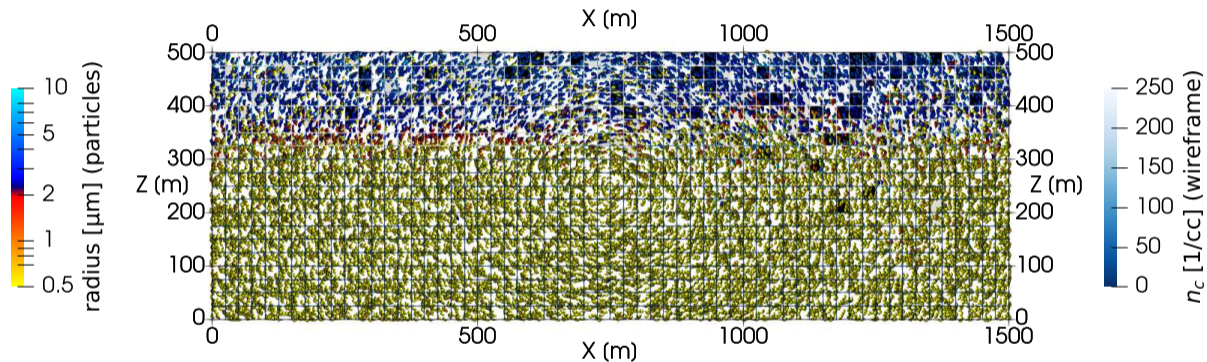
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 990 s (spin-up till 600.0 s)



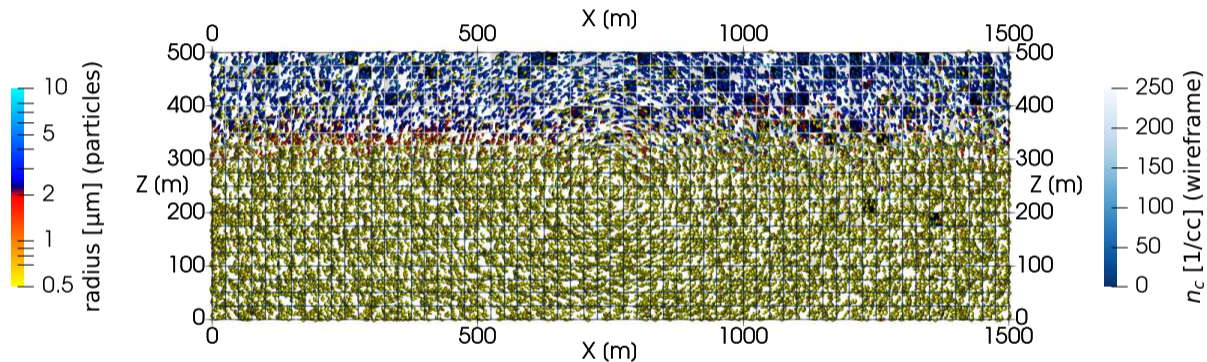
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1020 s (spin-up till 600.0 s)



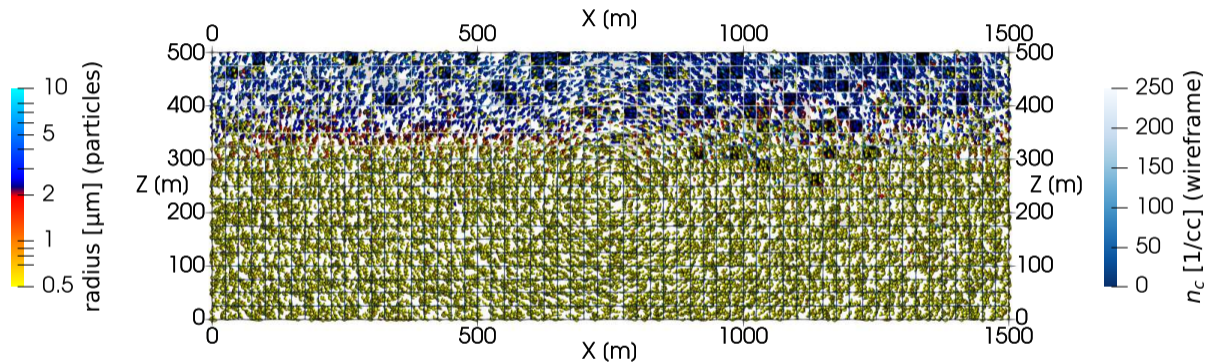
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1050 s (spin-up till 600.0 s)



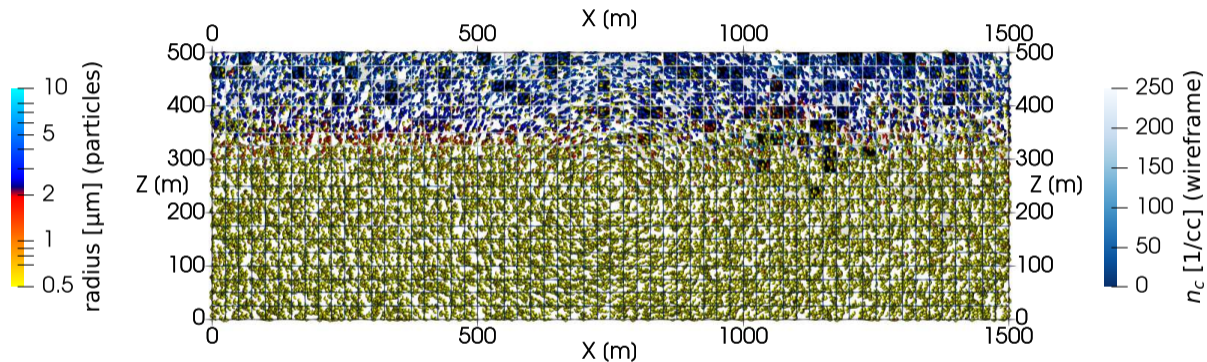
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spin-up = freezing off; subsequently frozen particles act as tracers

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1080 s (spin-up till 600.0 s)



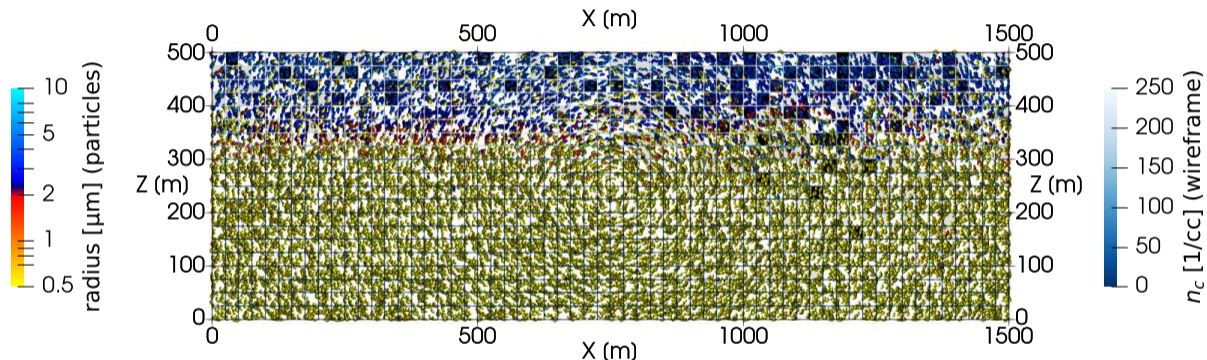
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$N_{\text{aer}} = 300/\text{cc}$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (lognormal, $D_g = 0.74 \mu\text{m}$, $\sigma_g = 2.55$)

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1110 s (spin-up till 600.0 s)



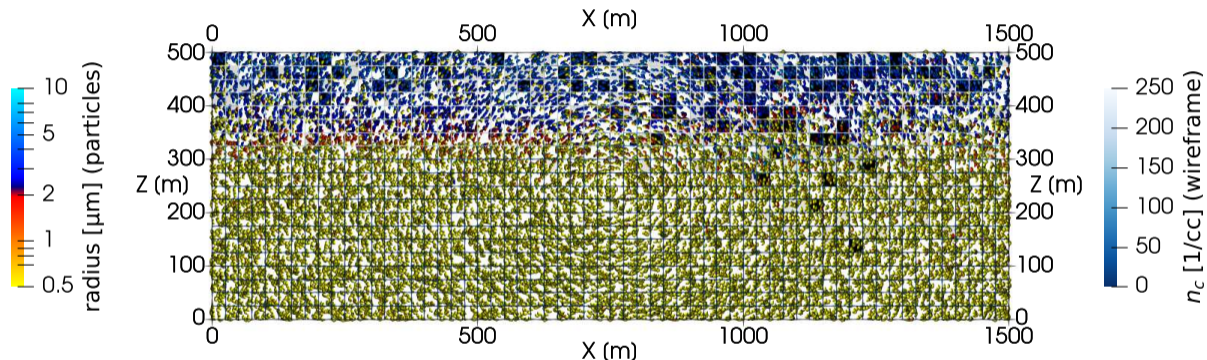
16+16 super-particles/cell for INP-rich + INP-free particles

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

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1140 s (spin-up till 600.0 s)



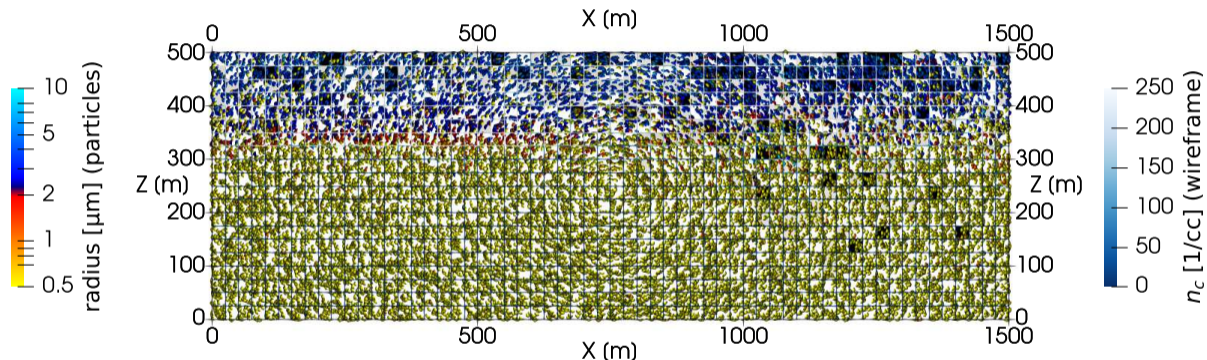
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Time: 1170 s (spin-up till 600.0 s)



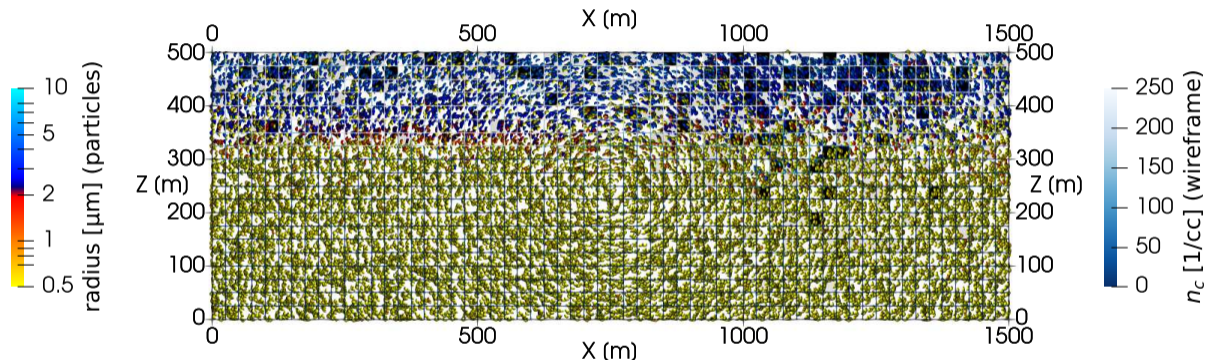
16+16 super-particles/cell for INP-rich + INP-free particles

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

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

particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1200 s (spin-up till 600.0 s)



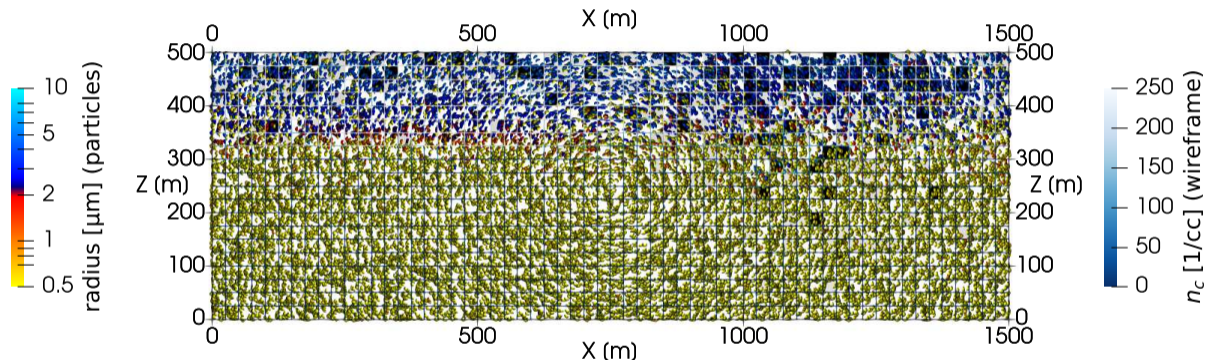
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spin-up = freezing off; subsequently frozen particles act as tracers

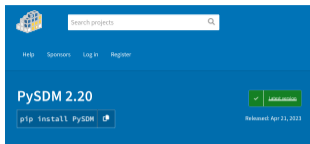
particle-based probabilistic aerosol-cloud μ -physics (super droplets)

Time: 1200 s (spin-up till 600.0 s)



100% Python, 100% open-source, 100% runs "in the cloud" (Google Colab, jupyterhub, ...)

new open-source HPC Python packages



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

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Project description

Release history

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- GitHub statistics:
- Stars: 40
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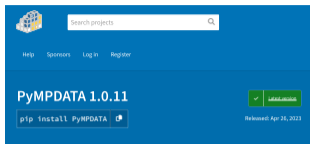
Project description

PySDM



PySDM is a package for simulating the dynamics of population of particles. It is intended to serve as a building block for simulation systems modelling fluid flows involving a dispersed phase, with PySDM being responsible for representation of the dispersed phase. Currently, the development is focused on atmospheric cloud physics applications, in particular on modelling the dynamics of particles immersed in moist air using the particle-based (aka a super-droplet) approach to represent aerosol/cloud/val microphysics. The package features a Pythonic high-performance implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth (Sinha et al. 2009), hence the name.

PySDM has two alternative parallel number-crunching backends available: multi-threaded CPU backend based on [Numba](#) and GPU-resident backend built on top of [Thrust](#). The [Numba](#) backend (aka [SDM](#)) features multi-threaded parallelism for multi-core CPUs, it uses the just-in-time compiler technique based on the LLVM infrastructure. The [Thrust](#) backend (aka [GPU](#)) offers



Numba-accelerated Pythonic implementation of MPDATA with examples in Python, Julia and Matlab

Navigation

Project description

Release history

Download files

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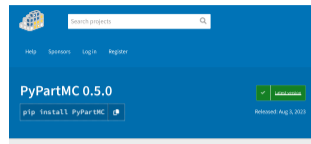
Project description

PyMPDATA



PyMPDATA is a high-performance Numba-accelerated Pythonic implementation of the MPDATA algorithm of Smolarkiewicz et al. used in geophysical fluid dynamics and beyond. MPDATA numerically solves generalised transport equations - partial differential equations used to model conservation/balance laws, scalar transport problems, convection diffusion phenomena. As of the current version, PyMPDATA supports homogeneous transport in 1D, 2D and 3D using structured meshes, optionally generalised by employment of a Jacobian of coordinate transformation. PyMPDATA includes implementation of a set of MPDATA variants including the non-oscillatory option, infinite-gauge, divergence-free, double-pass donor cell (DPDC) and third-order terms options. It also features support for integration of Fickian terms in advection diffusion problems using the pseudo-transport velocity approach. In 2D and 3D simulations, domain-decomposition is used for multi-threaded parallelism.

PyMPDATA is engineered purely in Python targeting both performance and usability, the latter encompassing research users, developers' and maintainers' perspectives. From researcher's perspective, PyMPDATA offers hassle-free



Python interface to PartMC

Navigation

Project description

Release history

Download files

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- Documentation
- Source
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 - Open PRs: 3

View statistics for this project via [Libraries.io](#) or by using [our tool](#).

[Download on PyPI](#)

Project description



PyPartMC

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



TL;DR (try in a Jupyter notebook)



```
! pip install PyPartMC
Support: PyPartMC
```

Jupyter notebooks with examples

- Urban plume scenario demo (as in [DustMC](#)):
[Urban plume](#) [Scenario Demo](#) [Open in Colab](#) [Search results](#)
- Dry-Wet Particle Size Equilibration with PartMC and PySDM:
[Dry-Wet Particle Size Equilibration](#) [Open in Colab](#) [Search results](#) [View on GitHub](#)

new open-source HPC Python packages

PySDM 2.20

pip install PySDM

Released: Apr 21, 2023

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

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Project description

Release history

Download files

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Project description

PySDM



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PyMPDATA 1.0.11

pip install PyMPDATA

Released: Apr 21, 2023

Numba-accelerated Pythonic implementation of MPDATA with examples in Python, Julia and Matlab

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PyMPDATA



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PyPartMC 0.5.0

pip install PyPartMC

Released: Aug 3, 2023

Python interface to PartMC

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[View on SourceForge](#)
[View on Docker](#)
[View on CSD](#)

Project description



PyPartMC

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TL;DR (try in a Jupyter notebook)



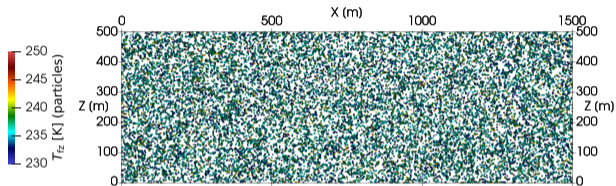
```
! pip install PyPartMC
! pip install PyPartMC
```

Jupyter notebooks with examples

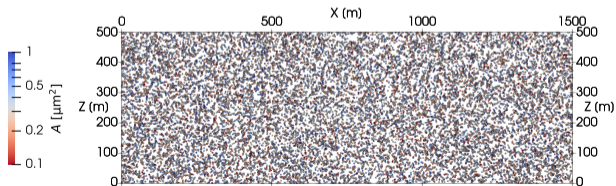
- Urban plume scenario demo (as in [DustMC](#)):
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- Dry-Wet Particle Size Equilibration with PartMC and PySDM:
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Monte-Carlo immersion freezing: singular vs. time-dependent

singular Monte-Carlo (as in Shima et al. '20)



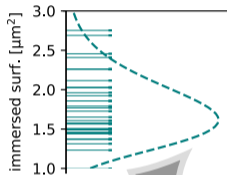
time-dependent Monte-Carlo (as in Alpert & Knopf '16)



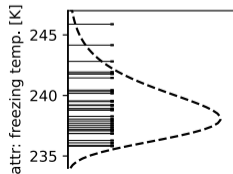
Monte-Carlo immersion freezing: singular vs. time-dependent

particle attribute sampling

random sampling of immersed surface for each particle



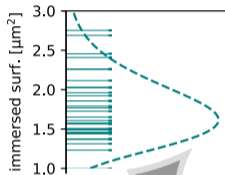
random sampling of freezing temperatures
(conditional distribution for a given surface)



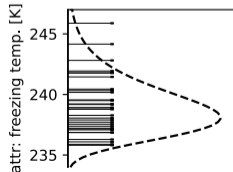
Monte-Carlo immersion freezing: singular vs. time-dependent

particle attribute sampling

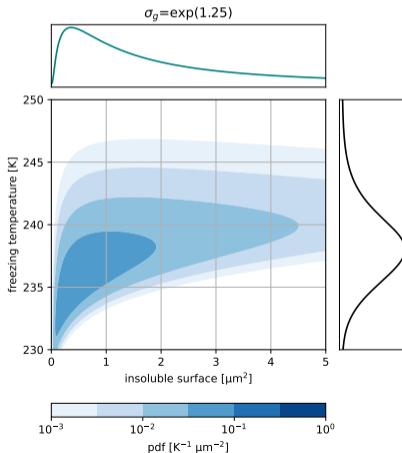
random sampling of immersed surface for each particle



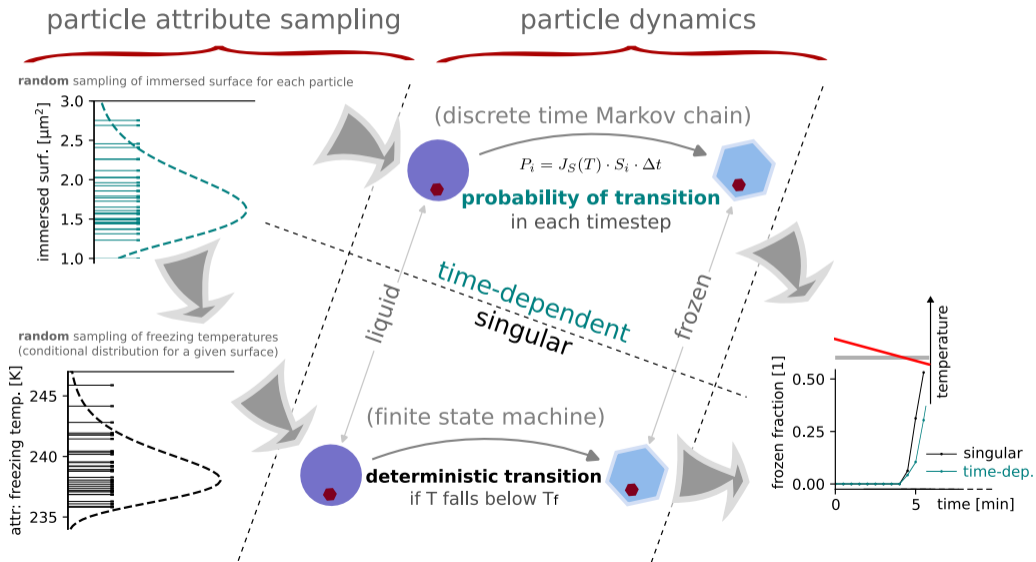
random sampling of freezing temperatures
(conditional distribution for a given surface)



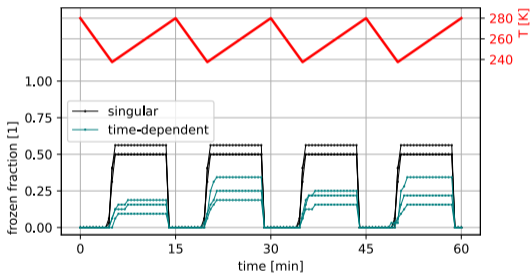
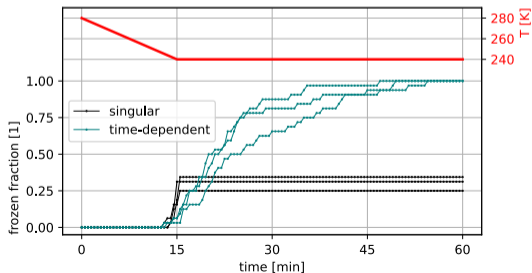
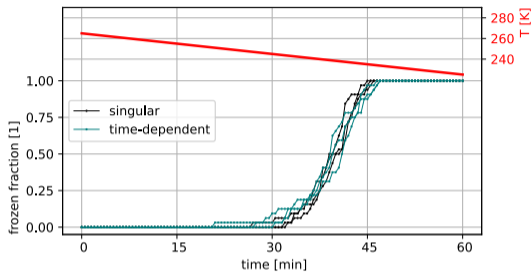
for singular: sampling from
INAS-derived pdf



Monte-Carlo immersion freezing: singular vs. time-dependent

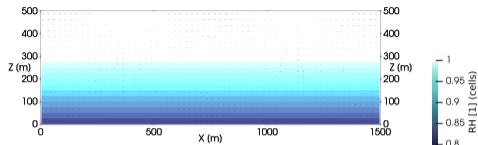


cooling-rate response (box model): singular vs. time-dependent



cooling-rate response (2D flow): singular vs. time-dependent

$w_{\max} \approx 1/3 \text{ m/s}$

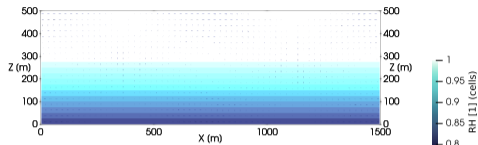


$w_{\max} \approx 1 \text{ m/s}$

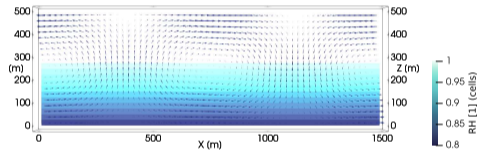
$w_{\max} \approx 3 \text{ m/s}$

cooling-rate response (2D flow): singular vs. time-dependent

$w_{\max} \approx 1/3 \text{ m/s}$



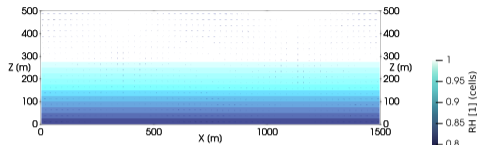
$w_{\max} \approx 1 \text{ m/s}$



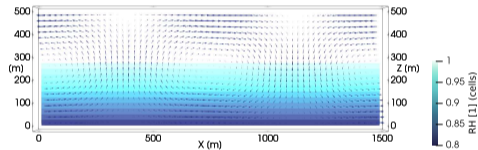
$w_{\max} \approx 3 \text{ m/s}$

cooling-rate response (2D flow): singular vs. time-dependent

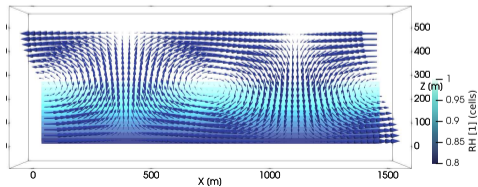
$w_{\max} \approx 1/3 \text{ m/s}$



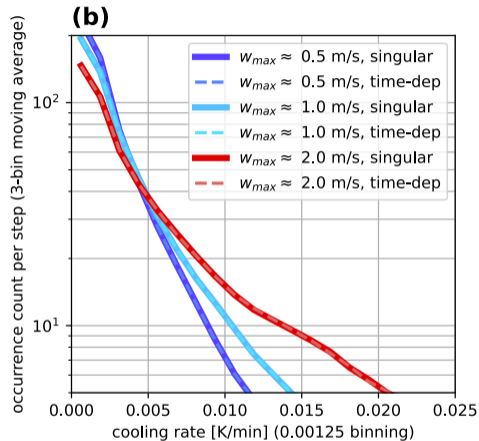
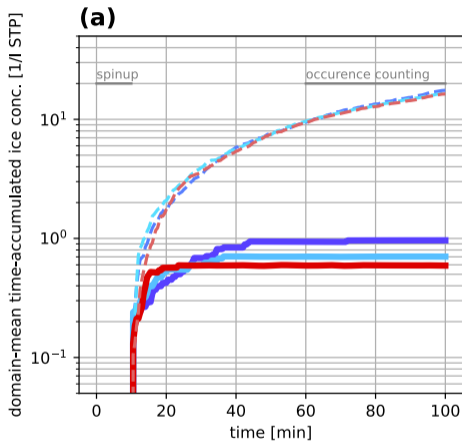
$w_{\max} \approx 1 \text{ m/s}$



$w_{\max} \approx 3 \text{ m/s}$

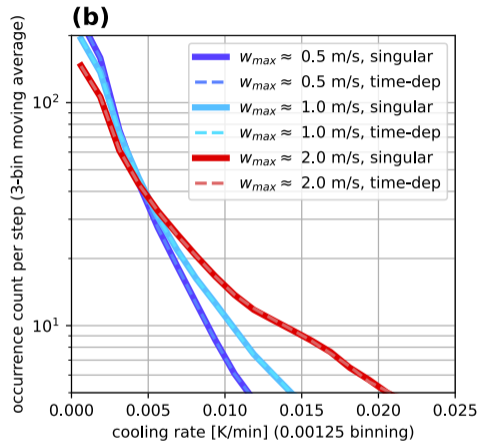
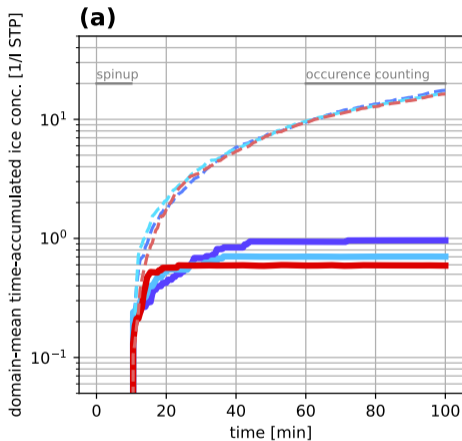


cooling-rate response (2D flow): singular vs. time-dependent



► singular vs. time-dependent markedly different (as in box model for $c \ll 1K/min$)

cooling-rate response (2D flow): singular vs. time-dependent



- ▶ singular vs. time-dependent markedly different (as in box model for $c \ll 1K/min$)
- ▶ diverse cooling rates even in a simple flow (far from $c \sim 1 K/min$ for AIDA)

stay tuned: Arabas et al. 2023
(in prep.; e-print uploaded to arXiv)

100% Python & open-source: github.com/open-atmos

contact:

sylwester.arabas@agh.edu.pl