

Methods & Tools for Modelling of Atmospheric Cloud μ -Physics

habilitation in “Earth and related environmental sciences” discipline submitted to Jagiellonian Univ.

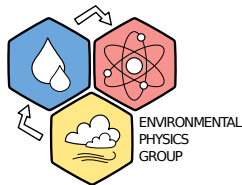
Sylwester Arabas

21 November 2025

AGH Faculty of Physics and Appl. CS Seminar



AGH



Sylwester Arabas: μ -CV

(PhD in Physics, University of Warsaw, 2013)



Institute of Geophysics, Faculty of Physics,
University of Warsaw
(“adiunkt” 2014–2015)

(2015–2018: three-year non-academic employment period)



Institute of Computer Science and Computational Mathematics,
Faculty of Mathematics and Computer Science, Jagiellonian University
(“adiunkt” 2018–2021 & 2022–2023)



Department of Atmospheric Sciences,
University of Illinois Urbana-Champaign, USA
(“postdoc” 2021–2022)



Environmental Physics Group, Faculty of Physics and Applied Computer Science,
AGH University of Krakow
(„adiunkt” since 2023)

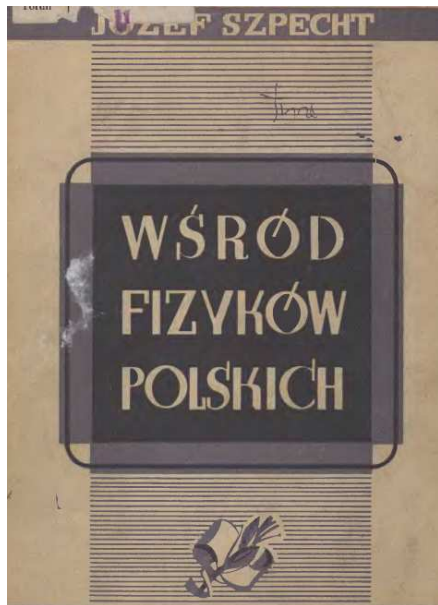
atmospheric cloud μ -physics models

cloud := colloid of water droplets/crystals in air; colloidal instability $\rightsquigarrow$ precipitation

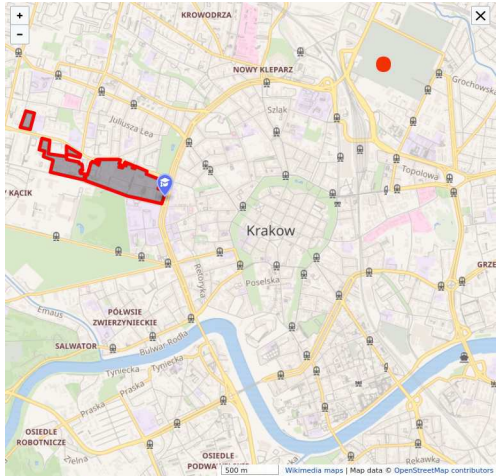


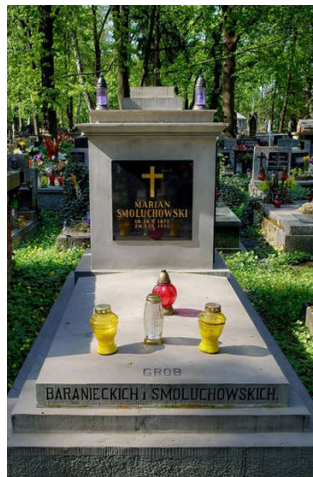
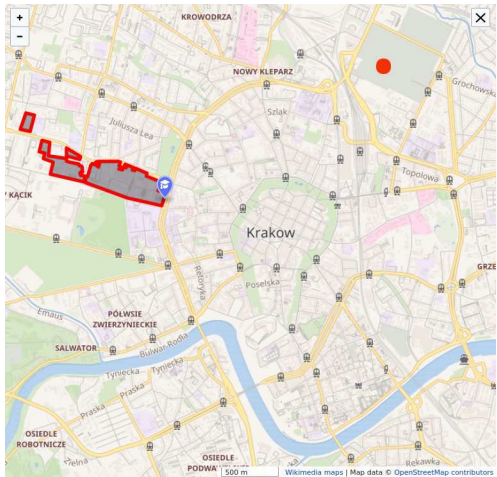
“Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain”

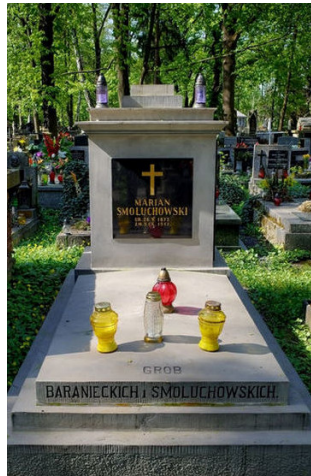
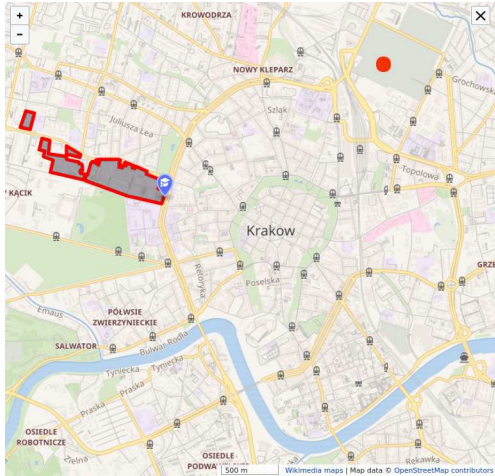
(photo: Yevgen Timashov / National Geographic)



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Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen.

Von

M. v. Smoluchowski.

(Mit 3 Figuren im Text.)

(Eingegangen am 8. 9. 16.)

I. Einleitung.

So sehr auch bis heute die Literatur über Koagulation kolloider Lösungen angewachsen ist, sind doch unsere Kenntnisse betreffs des quantitativen Verlaufs, sowie betreffs des Mechanismus des Koagulationsprozesses äusserst mangelhaft. Die meisten Forscher begnügen sich mit qualitativen Beobachtungen oder stellen ihre Messungsreihen in Tabellen oder Kurvenform¹⁾ dar, da die mathematische Wiedergabe derselben auf aussergewöhnliche Schwierigkeiten stösst.

In den interessanten Arbeiten²⁾ von S. Miyazawa, N. Ishizaka, H. Freundlich, J. A. Gann wird allerdings eine formelmässige Zusammenfassung des empirischen Versuchsmaterials, sowie eine Aufklärung desselben nach Analogie mit den Gesetzen der chemischen Kinetik angestrebt. Aber klare Gesetzmässigkeiten haben sich bisher auf diese Weise nicht ergeben, und wurden sogar gewisse, anfangs aufgestellte Gesetzformeln (Paine, Freundlich und Ishizaka) bei exakterer Prüfung (Freundlich und Gann) als unhaltbar zurückgenommen³⁾.

Die Erfolglosigkeit der bisherigen Versuche, auf dem empirisch-induktiven Wege zu einem Verständnis der hier geltenden Gesetze zu gelangen, kann man nun als einen Grund auffassen, einmal den um-

¹⁾ Vgl. z. B.: A. Galecki, Zeitschr. f. anorg. Chemie 74, 174 (1912); Kolloid-Zeitschr. 10, 169 (1912); A. Lottermoser, Kolloid-Zeitschr. 15, 145 (1914); H. H. Paine, Kolloidchem. Beihfte 4, 24 (1912); Kolloid-Zeitschr. 11, 115 (1912).

²⁾ S. Miyazawa, Journ. Chem. Soc. Tokio 33, 1179, 1210 (1912); N. Ishizaka, Zeitschr. f. physik. Chemie 83, 97 (1915); H. Freundlich u. N. Ishizaka, ebendort 85, 393 (1915); Kolloid-Zeitschr. 12, 230 (1915); J. Gann, Kolloidchem. Beihfte 8, 64 (1916).

³⁾ Siehe Abschnitt VI.

Zeitschrift f. physik. Chemie. XCII.

1911. 2782.

PHYSIK DER ERDE

VON DR. M. P. RUDZKI
O. PROFESSOR AN DER UNIVERSITÄT KRAKAU

MIT SECHZIG ABBILDUNGEN
IM TEXT UND FÜNF TAFELN



LEIPZIG 1911 · CHR. HERM. TAUCHNITZ

Maurycy Pius Rudzki

From Wikipedia, the free encyclopedia

Maurycy Pius Rudzki (b. 1862, d. 1916) was the first person to call himself a professor of geophysics. He held the Chair of Geophysics at the Jagiellonian University in Kraków, and established the Institute of Geophysics there in 1895. His research specialty was elastic anisotropy, as applied to wave propagation in the earth, and he established many of the fundamental results in that arena. ^[1]

Maurycy Pius Rudzki

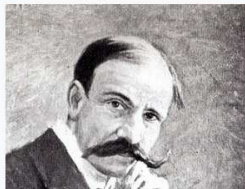


Maurycy Pius Rudzki

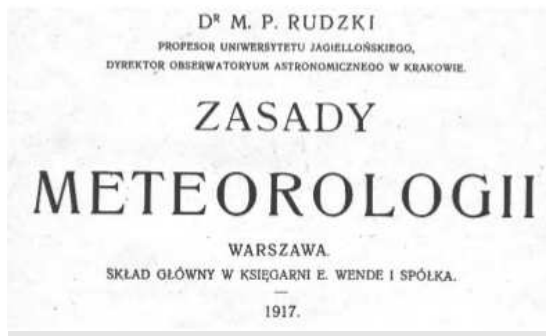
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Maurycy Pius Rudzki



“Principles of Meteorology” book (1917)



Rudzki 1917: Principles of Meteorology



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Revue internationale de physique théorique - Revue internationale de physique expérimentale

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<http://pbc.gda.pl/dlibra/docmetadata?id=18434> (translated)

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modelling coagulation: SCE & SDM

Smoluchowski's coagulation equation (SCE)

droplet concentration (continuous): $c(x, t) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$

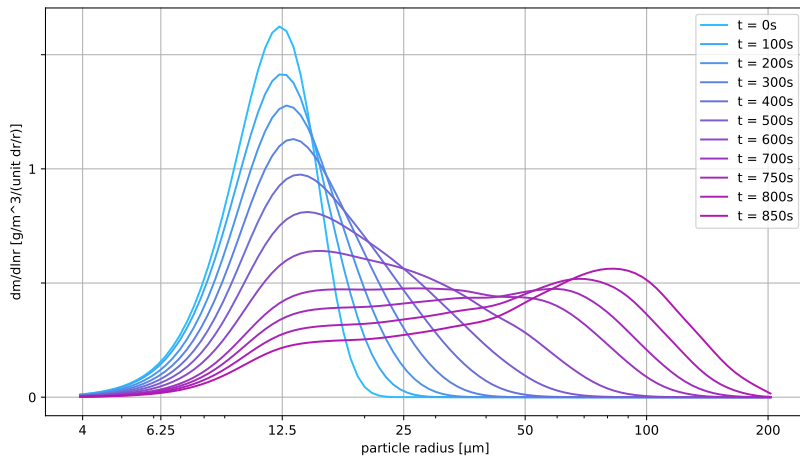
collision kernel: $a(x_1, x_2) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$

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

droplet concentration (discrete): $c_i = c(x_i)$

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

cloud droplet collisional growth





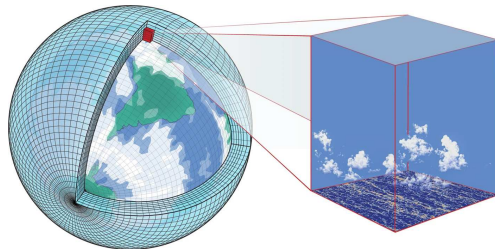
“Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain”

(photo: Yevgen Timashov / National Geographic)



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

(photo: Yevgen Timashov / National Geographic)



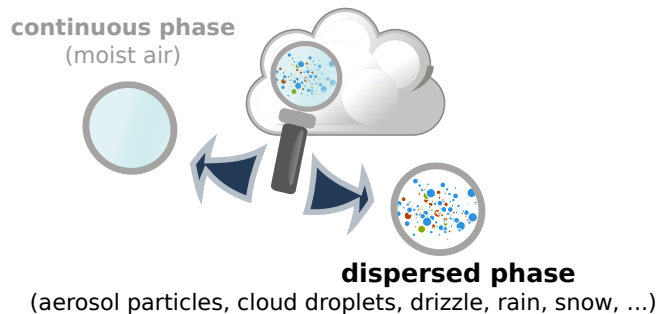
“Grid cells in a global climate model and a large-eddy simulation of shallow cumulus clouds at 5 m resolution”

(fig. from Schneider et al. 2017)

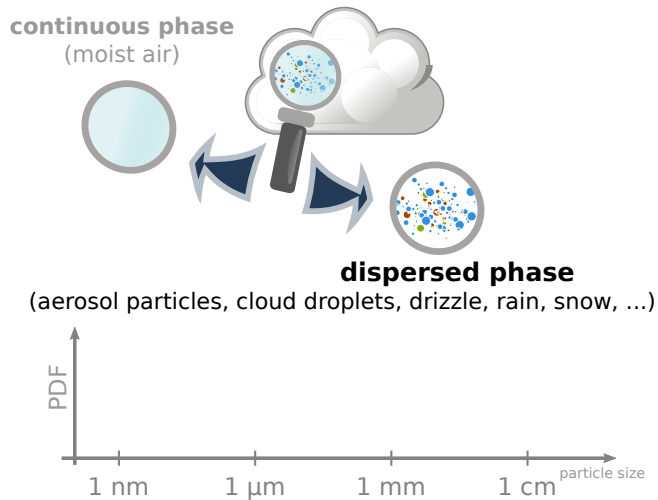
Eulerian vs. Lagrangian microphysics



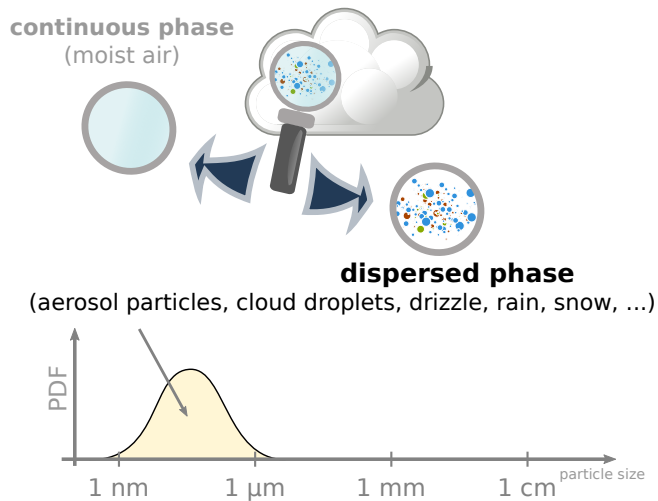
Eulerian vs. Lagrangian microphysics



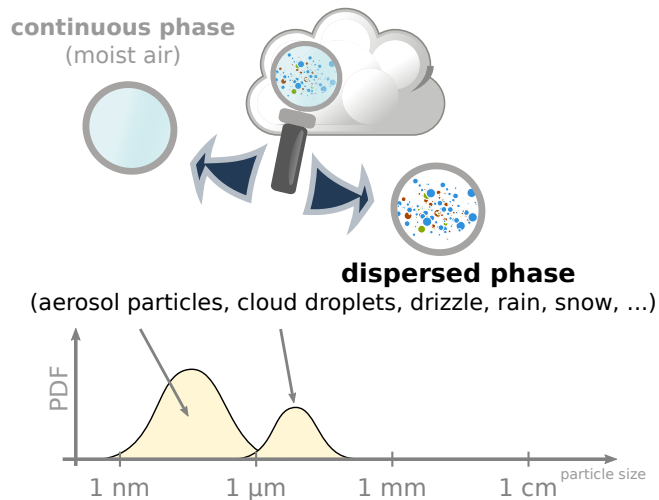
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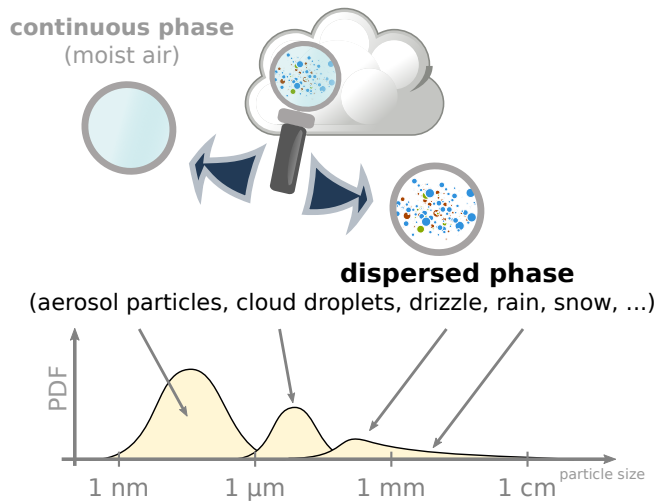
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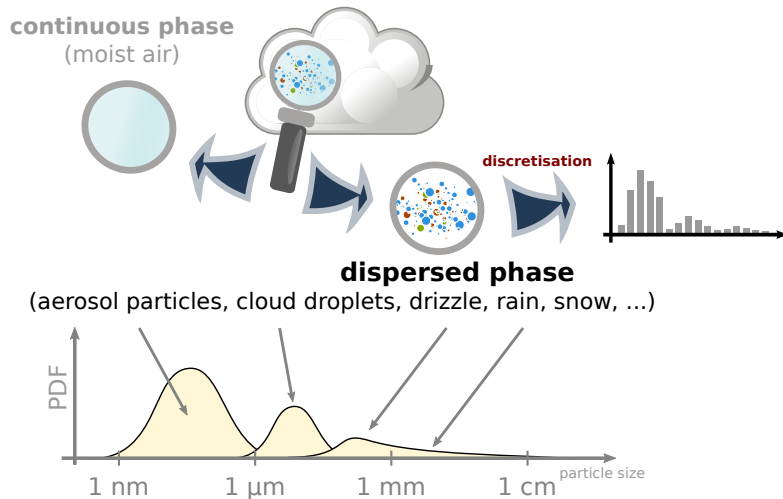
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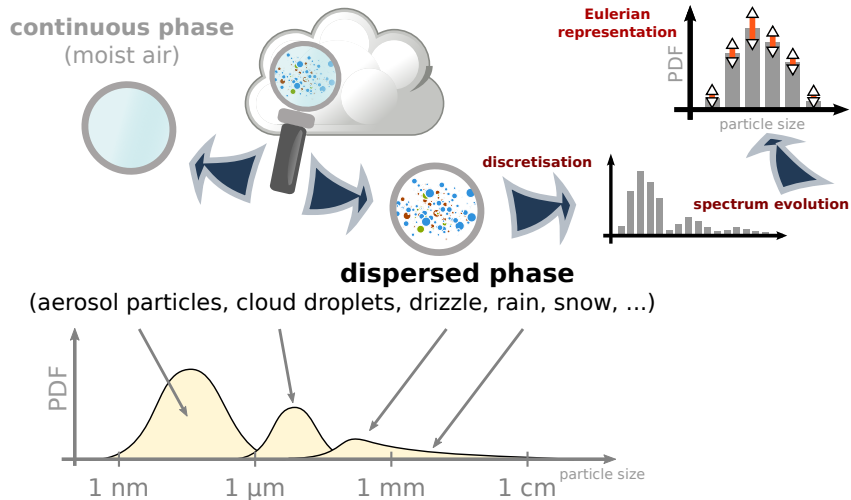
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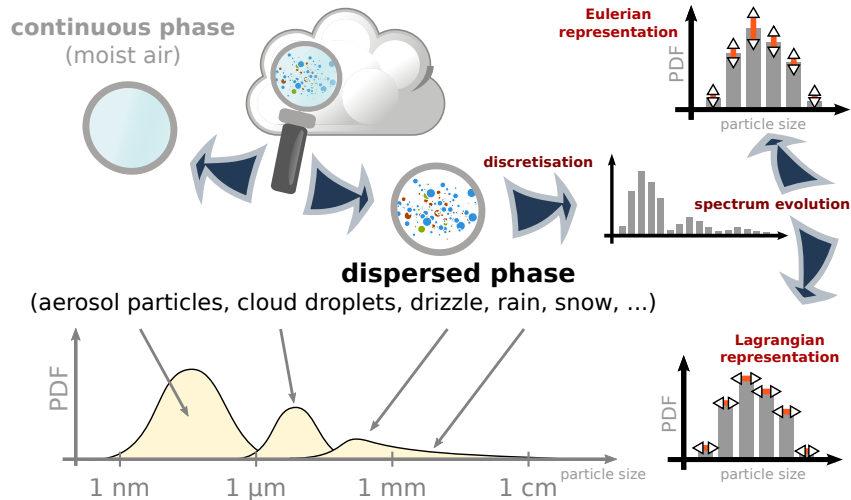
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Eulerian vs. Lagrangian microphysics



Eulerian vs. Lagrangian microphysics



PDEs

ODEs

Lagrangian microphysics: early works (0D)

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THE GROWTH OF CLOUD DROPS IN UNIFORMLY COOLED AIR

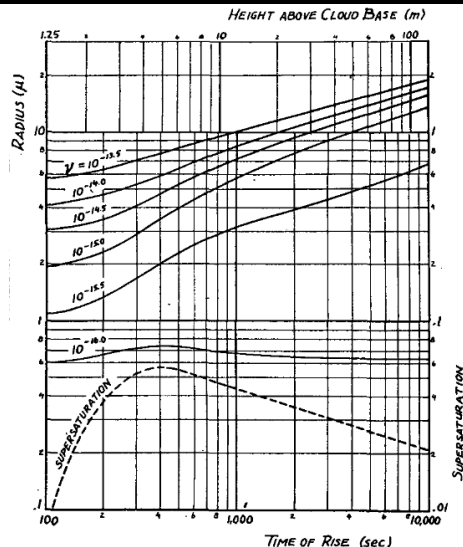
By Wallace E. Howell¹

Blue Hill Meteorological Observatory, Harvard University²

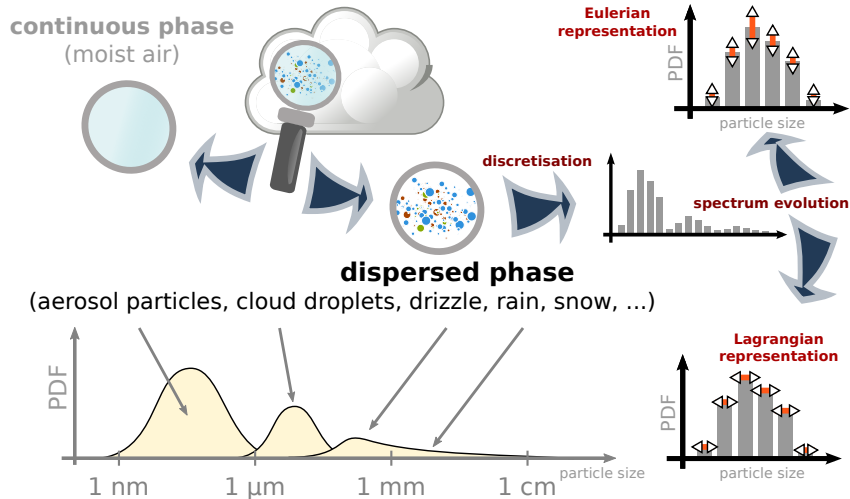
(Manuscript received 10 June 1948)

ABSTRACT

Recent studies of precipitation, aircraft icing, and visibility through fog have focussed attention on the physical constitution of clouds, a subject to which knowledge of the drop-size spectrum and its origin would be an important contribution. The drop-size spectrum resulting when air containing condensation nuclei is uniformly cooled may be computed, leading to a differential equation for the growth of a cloud drop which cannot be integrated analytically. A numerical method of integration is therefore employed.



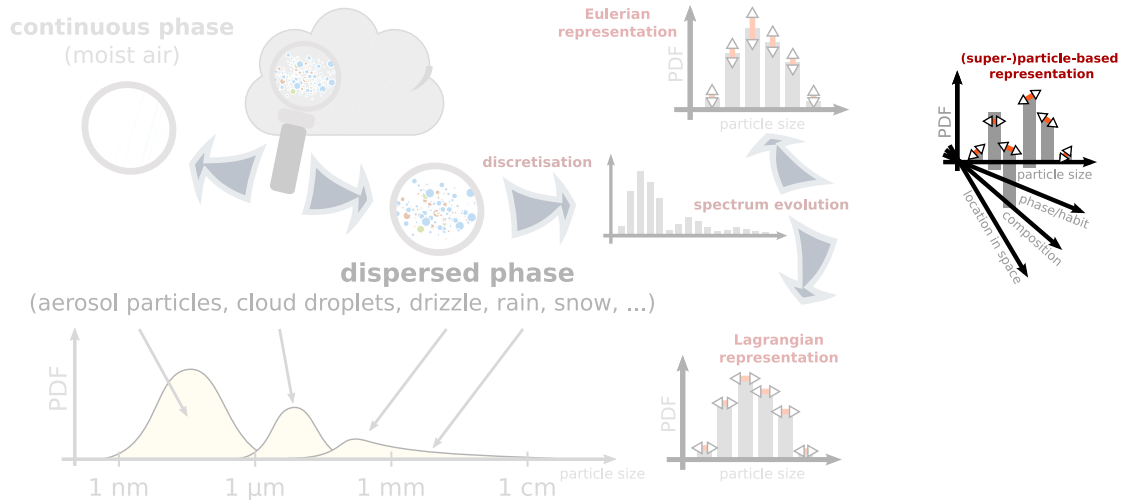
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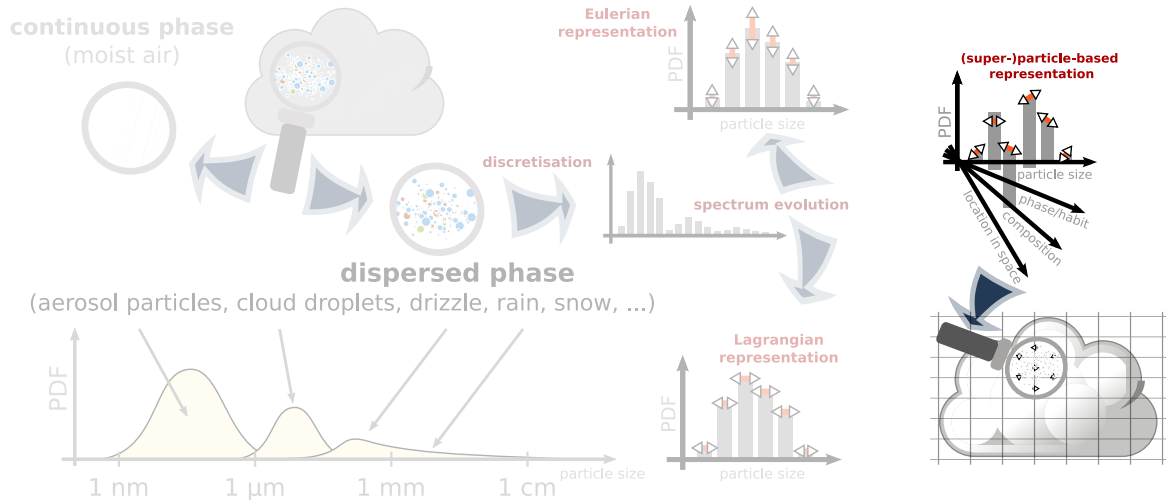
PDEs

ODEs

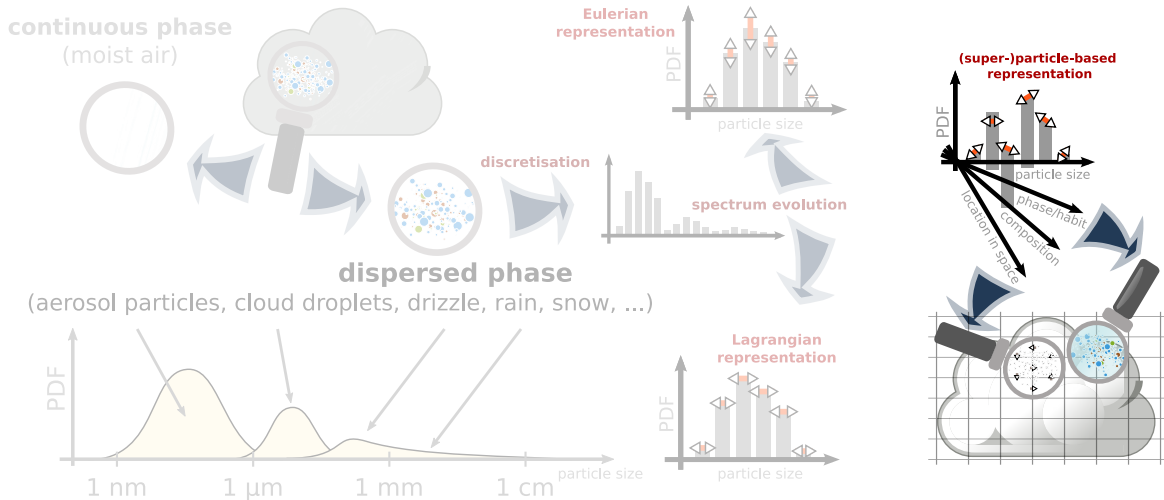
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Eulerian vs. Lagrangian microphysics



JOURNAL OF THE ATMOSPHERIC SCIENCES

A Numerical Experiment on Stochastic Condensation Theory

TERRY L. CLARK AND W. D. HALL

National Center for Atmospheric Research,¹ Boulder, CO 80307

(Manuscript received 30 August 1978, in final form 20 November 1978)

ABSTRACT

A three-dimensional numerical model is used to study the effect of small-scale supersaturation fluctuations on the evolving droplet distribution in the first 150 m above cloud base. The primary purpose of this research is to determine whether the irreversible coupling between the thermodynamics and dynamics due to finite phase relaxation time scales τ_s is sufficient to produce significant small-scale horizontal variations in supersaturation. Thus, the paper is concerned only with this internal source for thermodynamic variability. All other source terms, such as the downgradient flux of the variance of thermodynamic fields, have purposely been neglected.

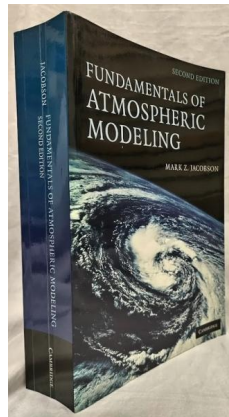
Lagrangian particle experiments were run in parallel with the basic Eulerian model. The purpose of these experiments is to relax some of the microphysical parameterization assumptions with respect to assumed distribution shape and as a result add credibility to the results of distribution broadening.

Eulerian vs. Lagrangian microphysics: a (probabilistic) breakthrough

pre-2009:

„advantage of the full-moving size structure is that core particle material is preserved during growth ... second advantage ... it eliminates numerical diffusion ... [but] nucleation, coagulation ... cause problems ... the full-moving structure is not used in three-dimensional models”^a

„the use of a fixed grid allows for an easy implementation of collision processes, which is not possible for a moving grid (Lagrangian) approach”^b



^a Jacobson 2005: Fundamentals of Atmospheric Modeling

^b Simmel & Wurzler 2006: Condensation and activation in sectional cloud microphysical models

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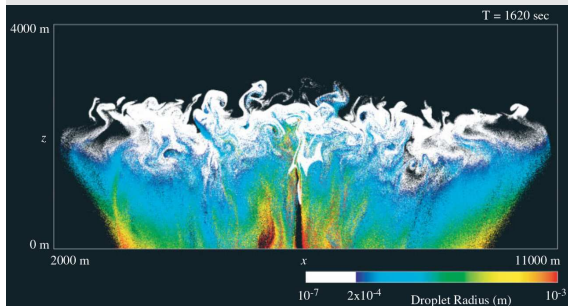
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Super-droplet simulation of a shallow convective cloud
(figure: Shima et al. 2009, QJRMS)

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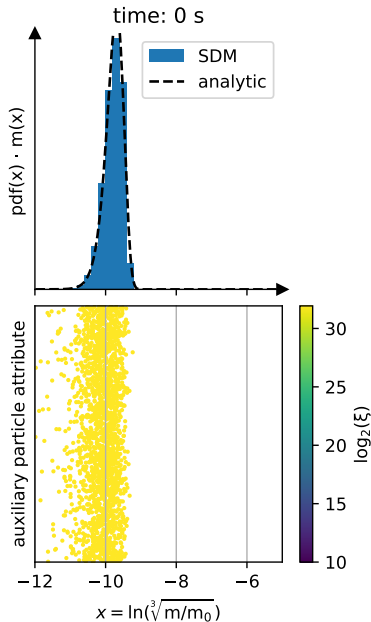
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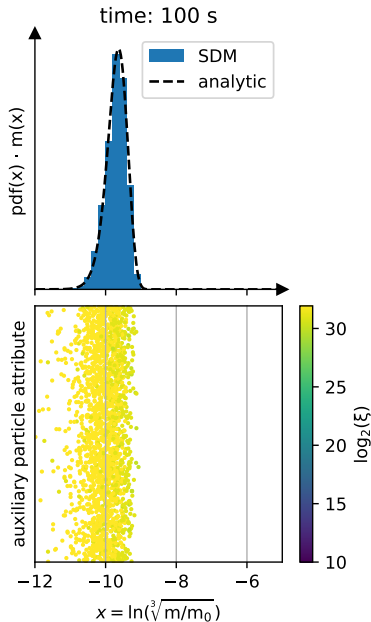
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interpretation	
concentration " c_i " in size bin " i "	besides c_i , each "particle" i carries other physicochemical attributes, e.g. position (x_i, y_i, z_i)



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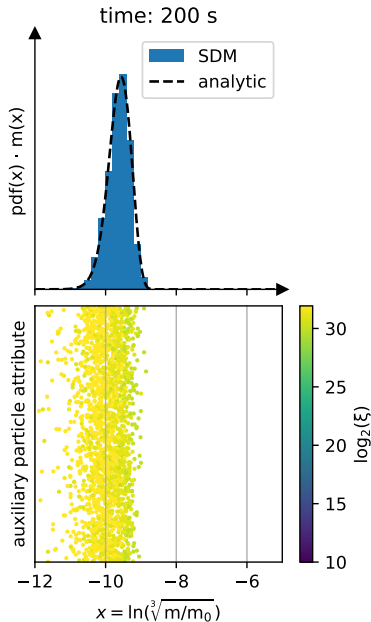
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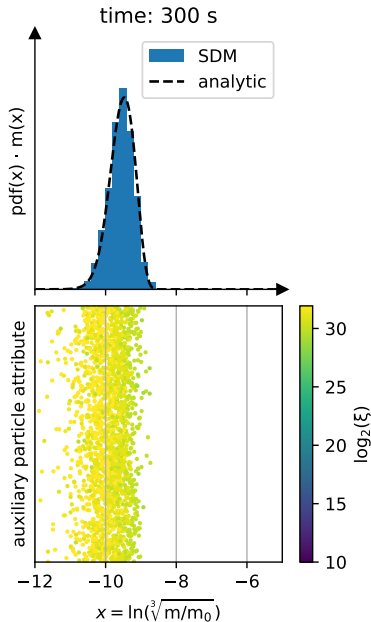
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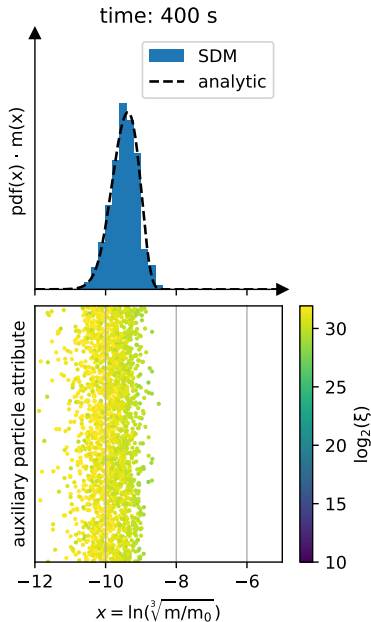
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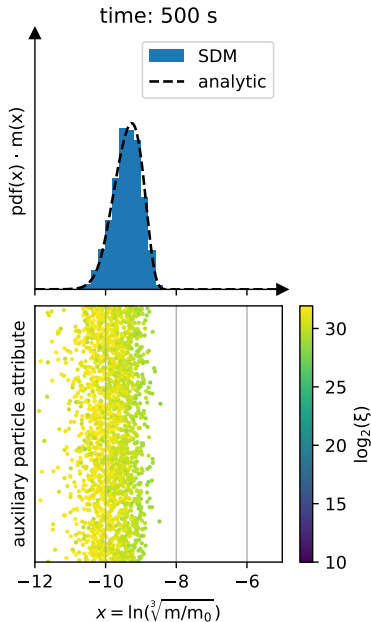
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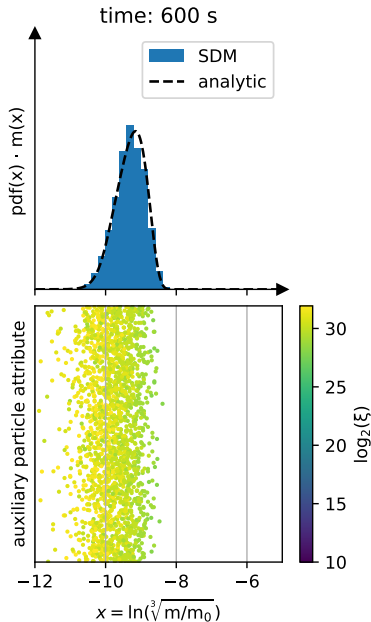
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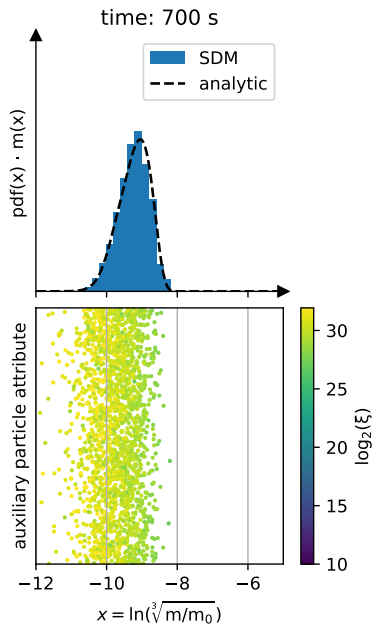
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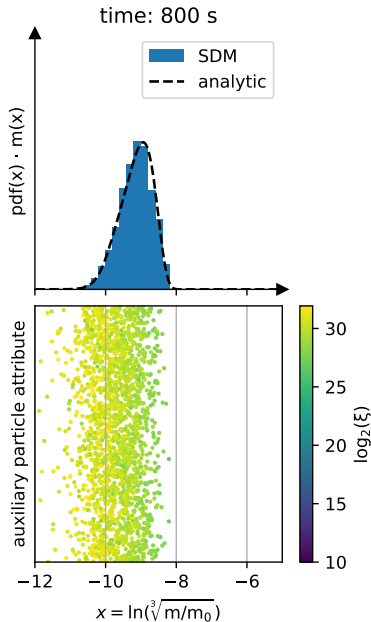
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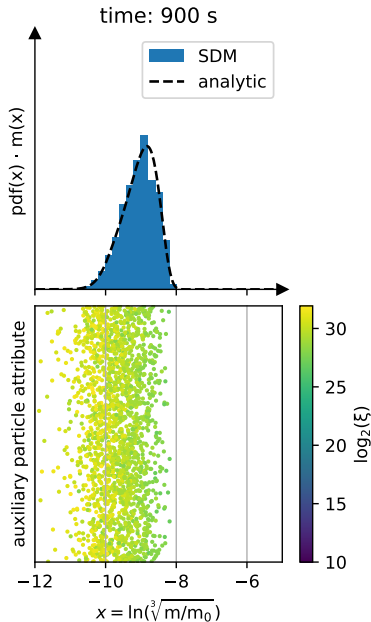
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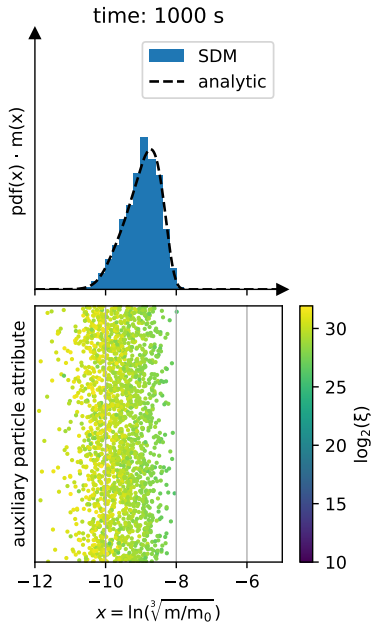
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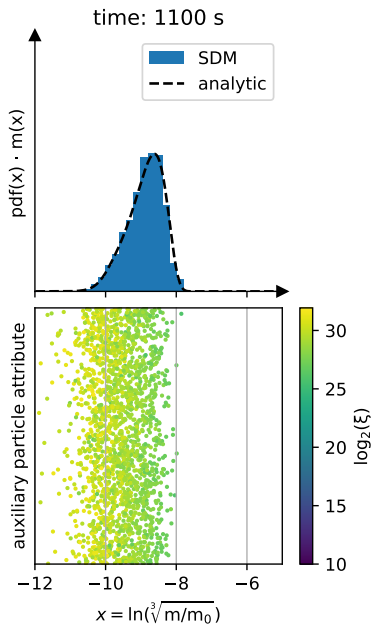
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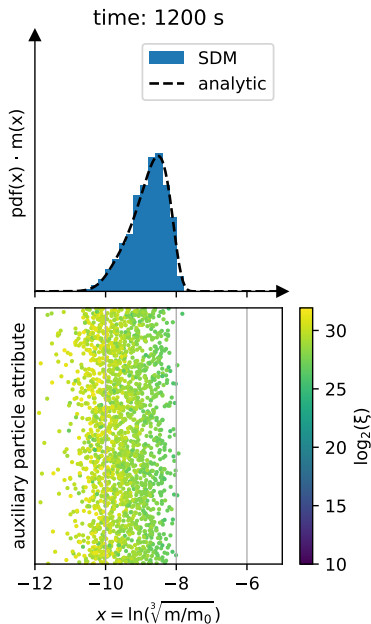
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12    pairs = rng.permutation(n_s)[: 2 * n_pair]
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14    p_ratio = n_s * (n_s - 1) / 2 / n_pair
15    for α, (j, k) in enumerate(pairs.reshape(-1, 2)):
16        p_jk = kern(m[j], m[k]) * Δt / Δv
17        if ξ[j] < ξ[k]:
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20        γ = p_α // 1 + (p_α - p_α // 1) > φ[α]
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27                ξ[j] = ξ[k] // 2
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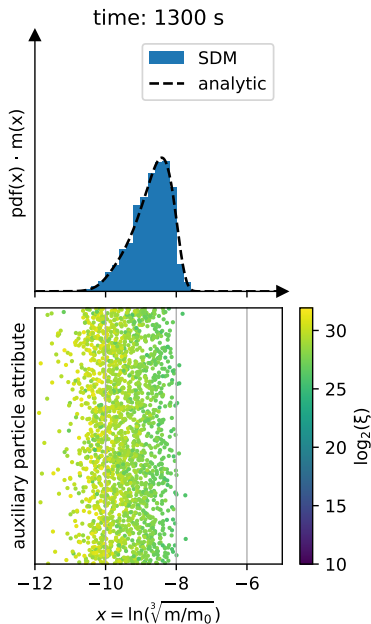
```

```

1 def sdm(*,
2     rng: np.random.Generator,
3     ξ: abc.MutableSequence[int],
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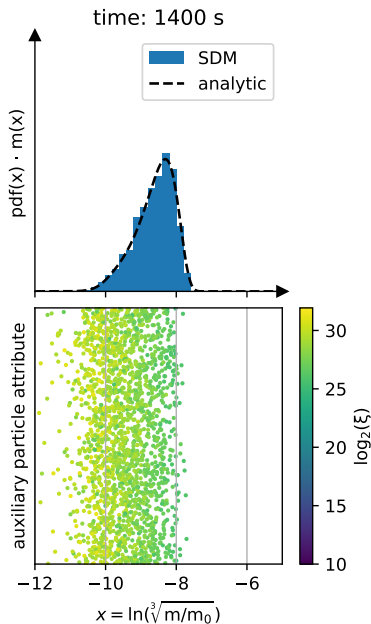
```



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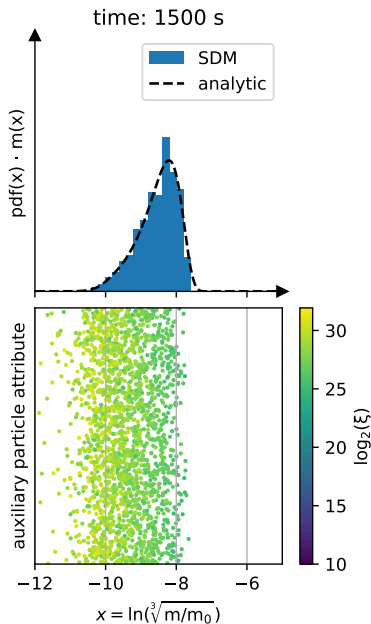
```



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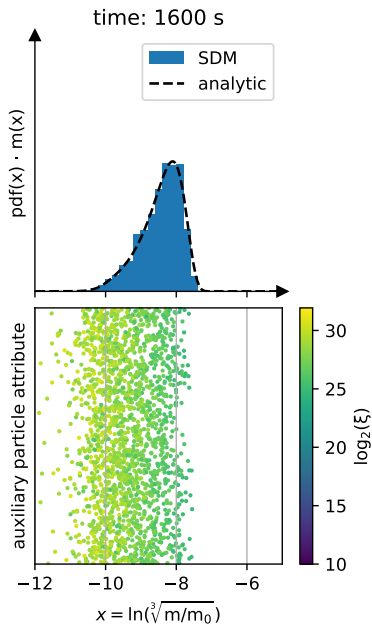
```



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30                m[j] = m[k]

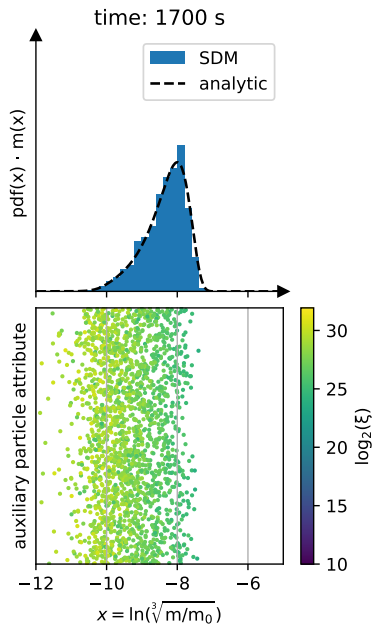
```



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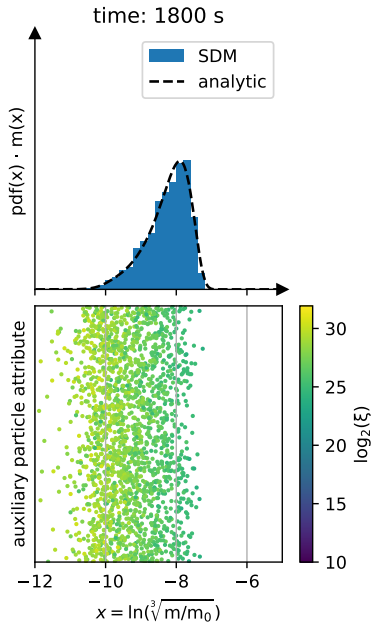
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```

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2     rng: np.random.Generator,
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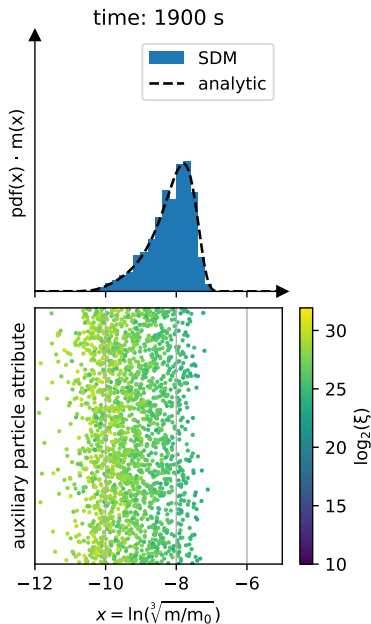
```



```

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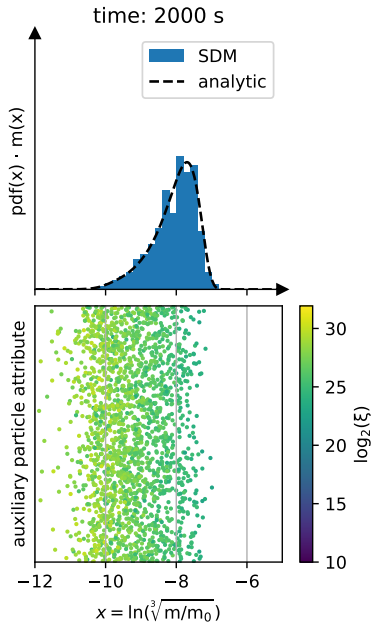
```



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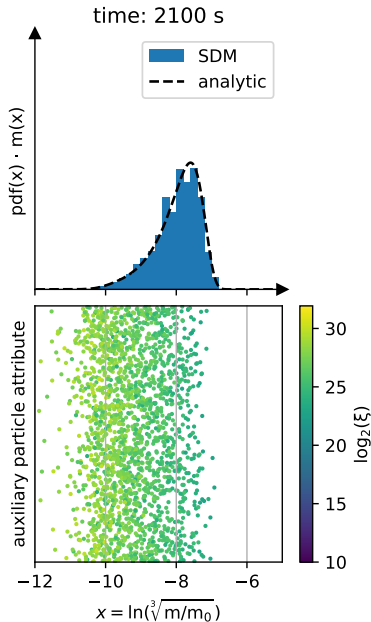
```

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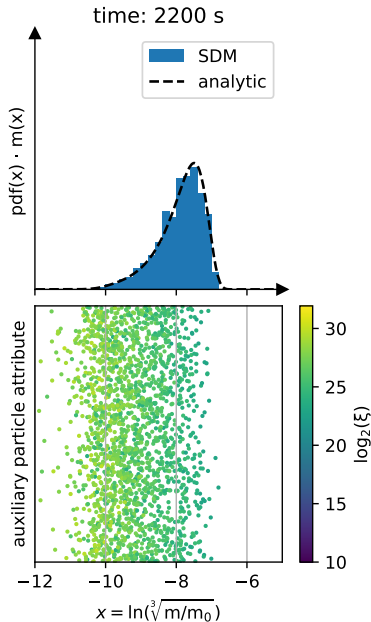
```



```

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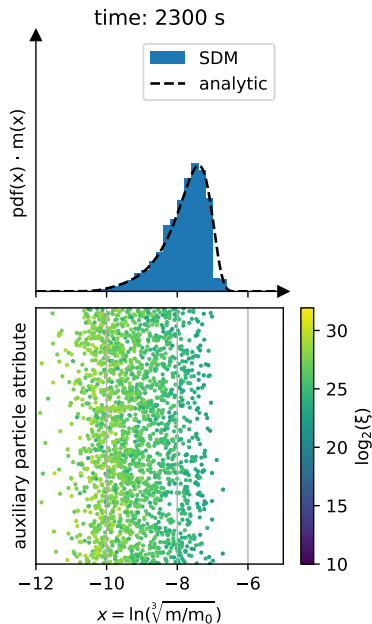
```



```

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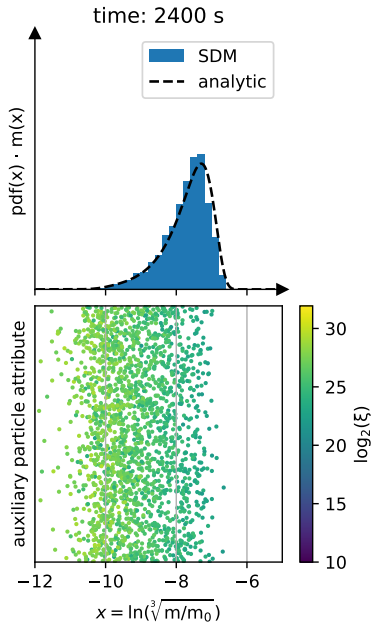
```



```

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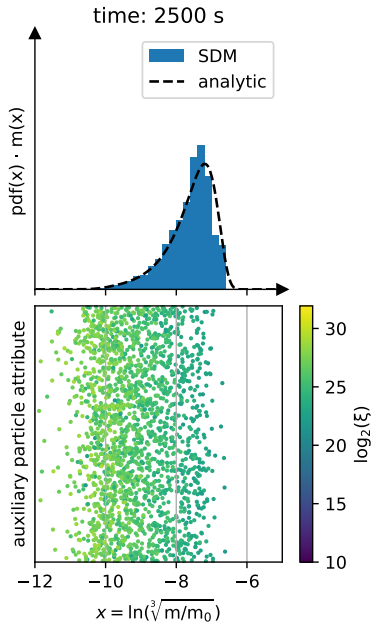
```



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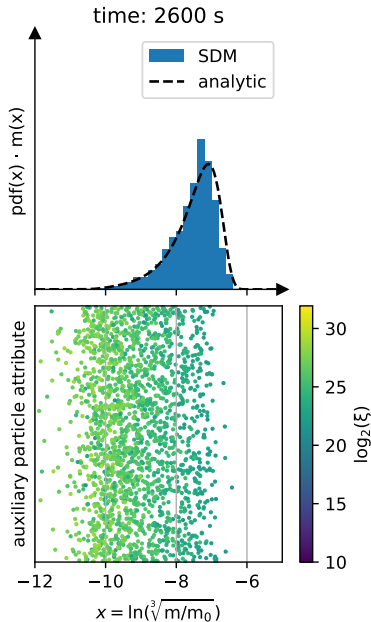
```



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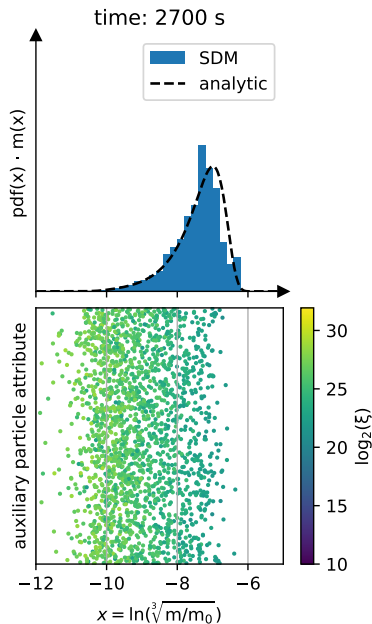
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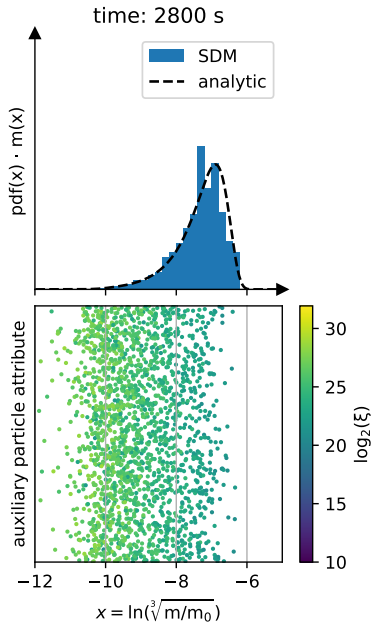
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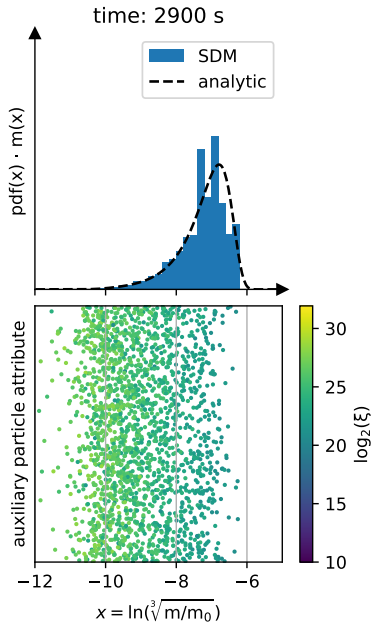
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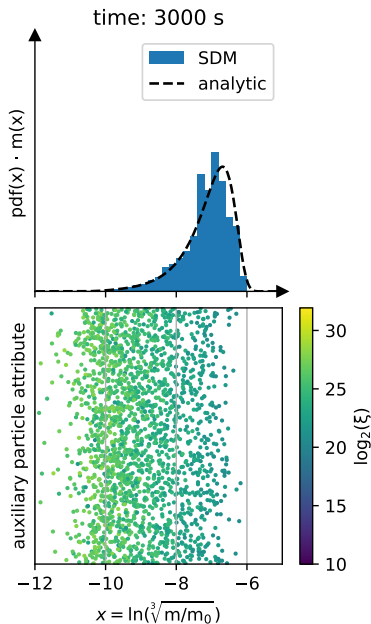
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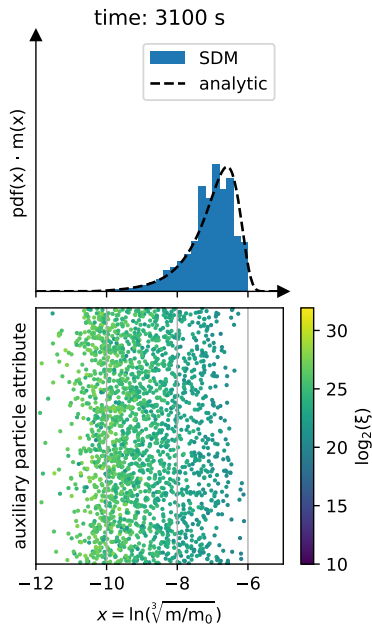
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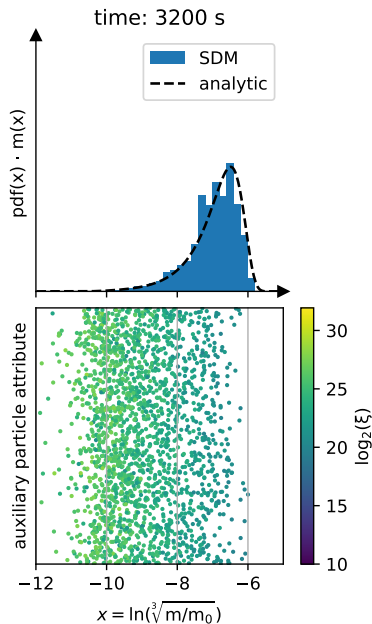
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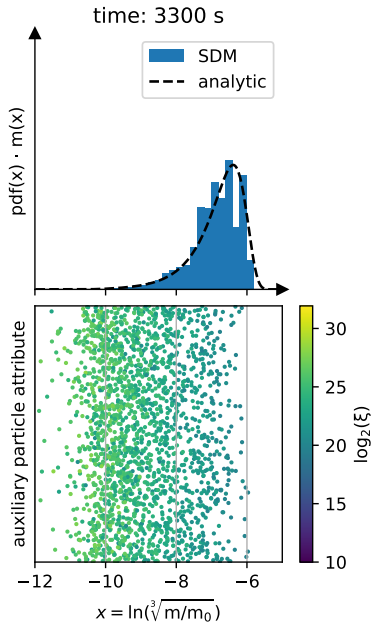
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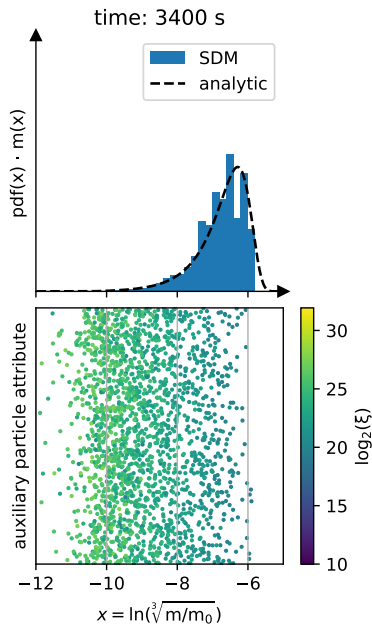
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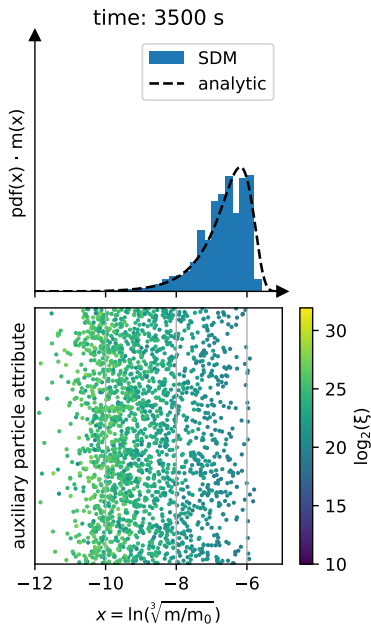
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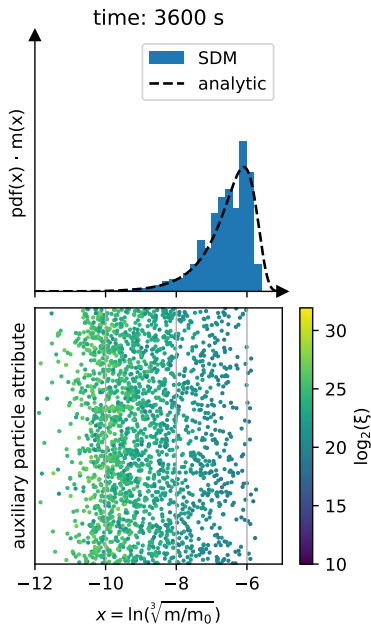
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Shin-ichiro Shima

The super-droplet method for the numerical simulation of clouds and precipitation: a particle-based and probabilistic microphysics model coupled with a non-hydrostatic model

[PDF] from arxiv.org
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Authors S Shima, Kanya Kusano, Akio Kawano, Tooru Sugiyama, Shintaro Kawahara

Publication date 2009/7/1

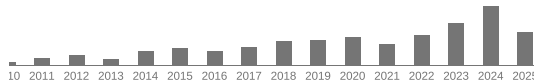
Journal Quarterly Journal of the Royal Meteorological Society

Volume 135

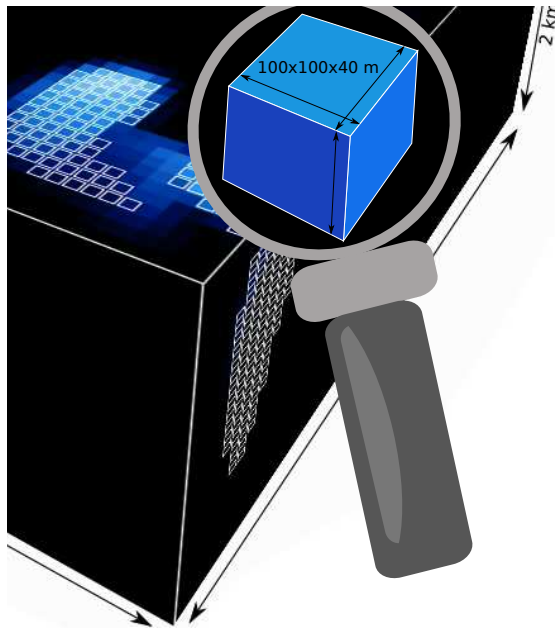
Issue 642

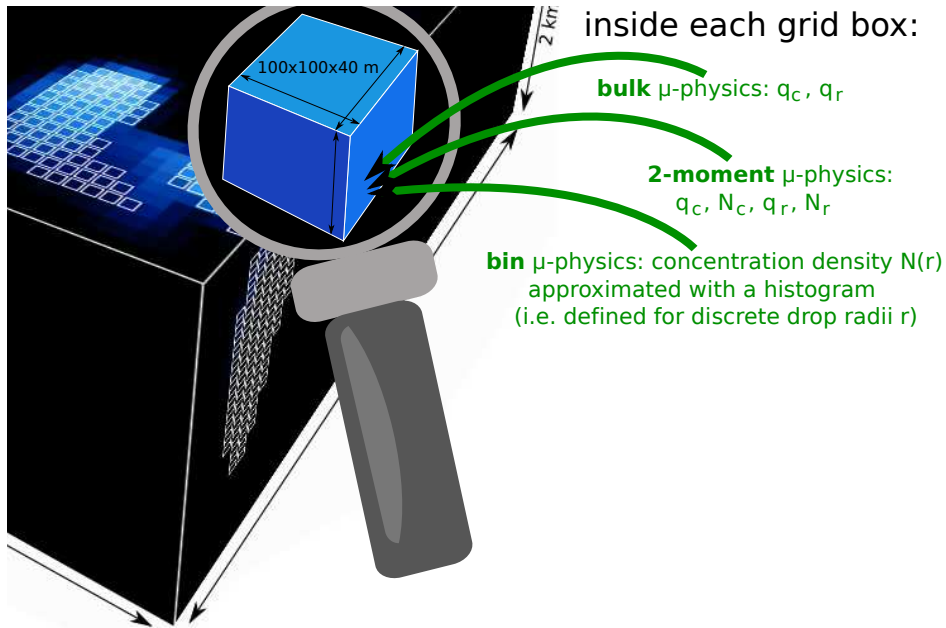
Pages 1307-1320

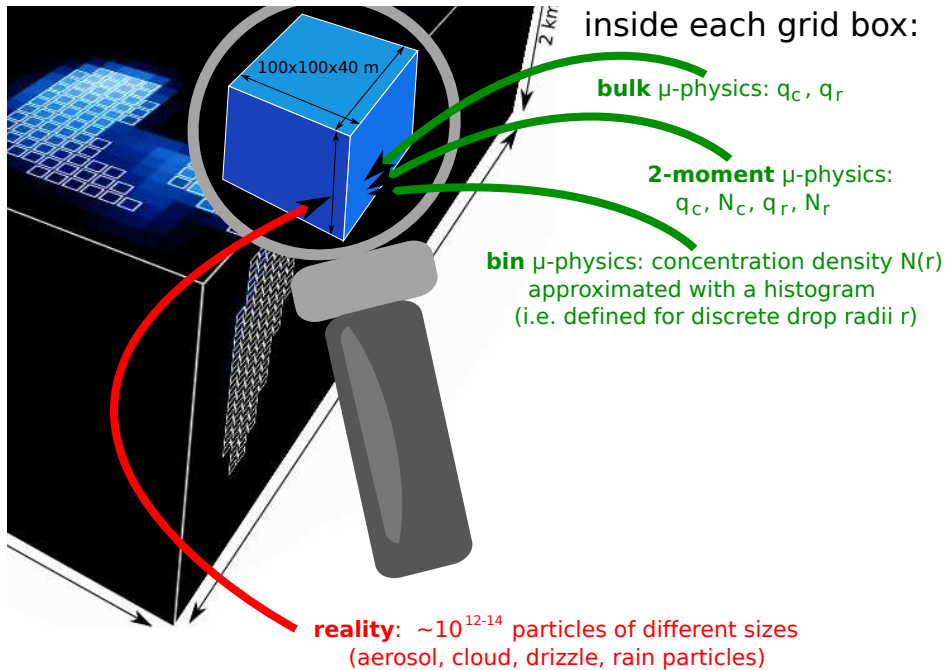
Total citations Cited by 309

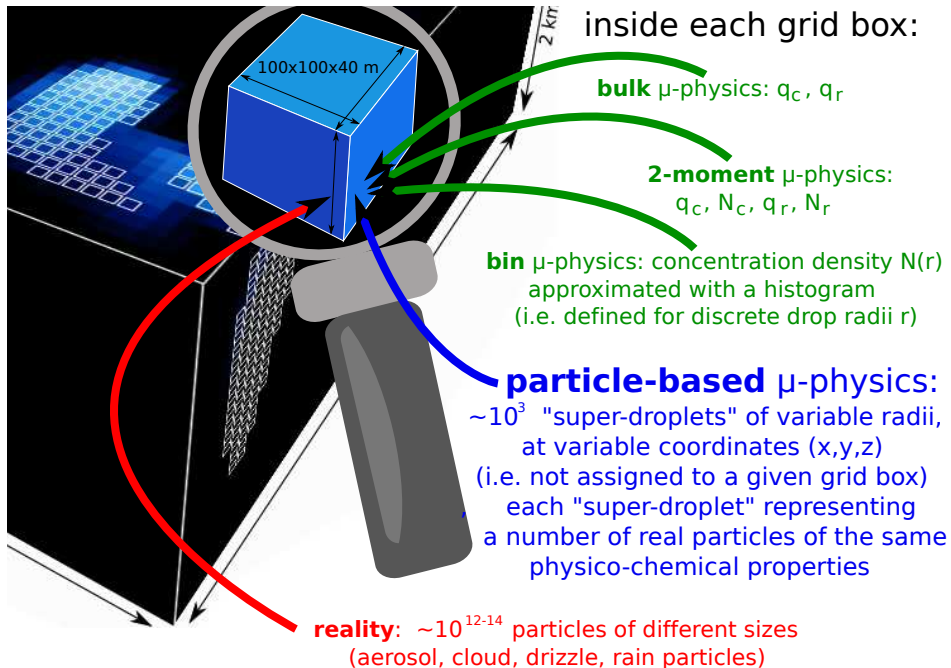


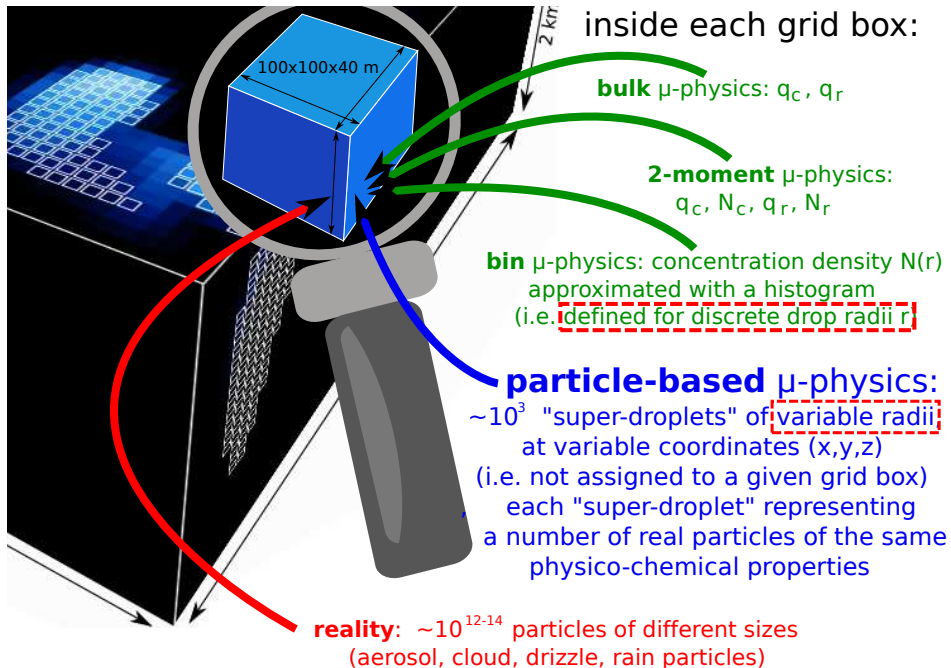
Arabas & Shima 2013: SDM in LES











model validation: Fast-FSSP (Forward Scattering Spectrometer Probe)

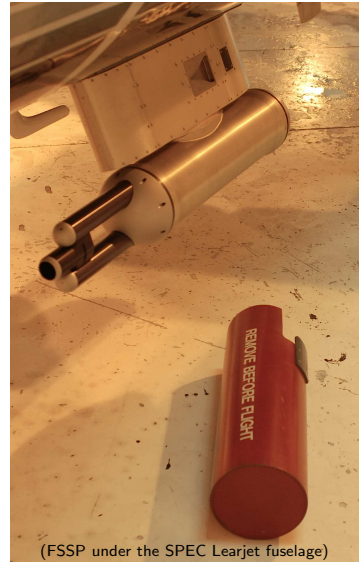
- measures laser light scattered by cloud droplets



(FSSP under the SPEC Learjet fuselage)

model validation: Fast-FSSP (Forward Scattering Spectrometer Probe)

- measures laser light scattered by cloud droplets
- single-particle counter



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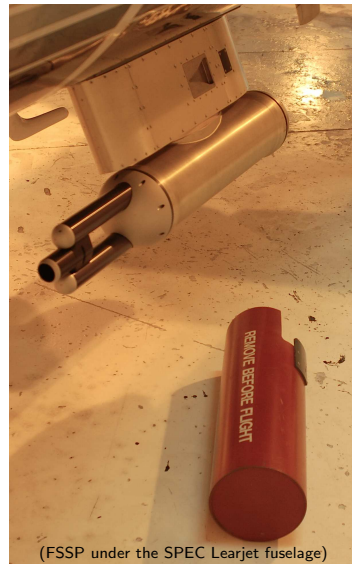
- measures laser light scattered by cloud droplets
- single-particle counter
- range: 2 – 50 μm in diameter



(FSSP under the SPEC Learjet fuselage)

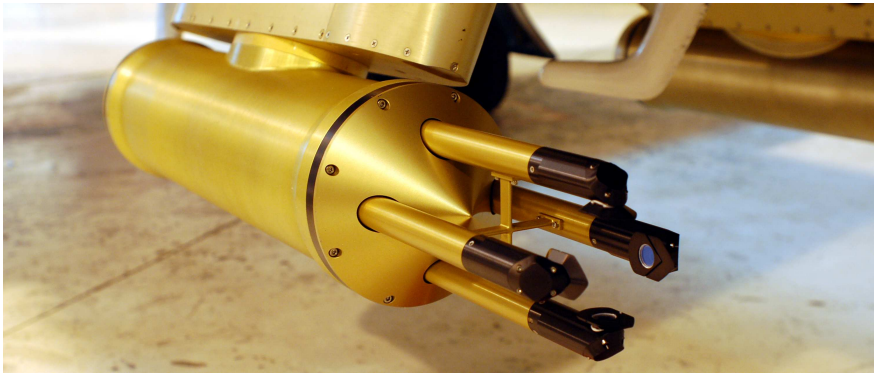
model validation: Fast-FSSP (Forward Scattering Spectrometer Probe)

- measures laser light scattered by cloud droplets
- single-particle counter
- range: $2 - 50\ \mu m$ in diameter
- developed by Météo-France



(FSSP under the SPEC Learjet fuselage)

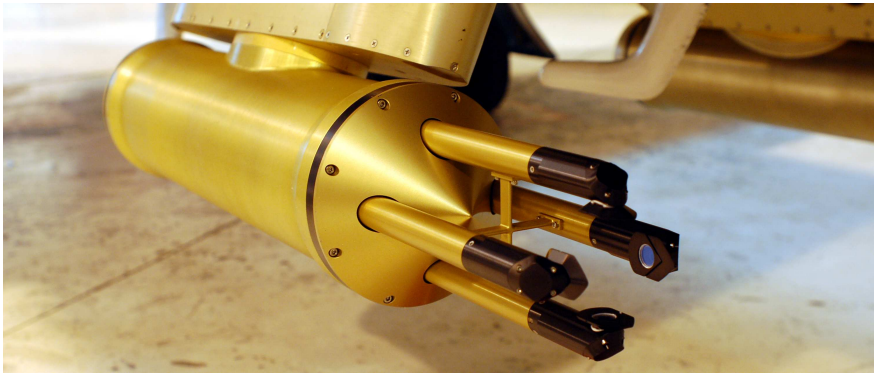
model validation: OAP-2DS (2-dimensional "stereo" optical array probe)



(OAP-2DS under the SPEC Learjet fuselage)

- registers shadows of particles on two photodiode arrays

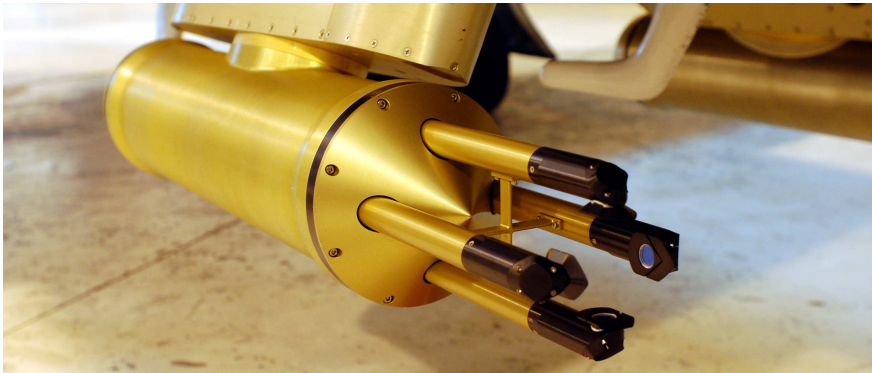
model validation: OAP-2DS (2-dimensional "stereo" optical array probe)



(OAP-2DS under the SPEC Learjet fuselage)

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- multiple droplets at a time, particle spectra via image analysis

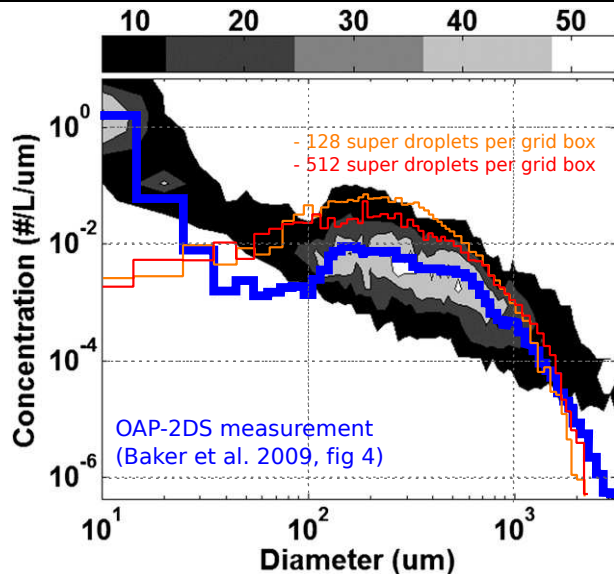
model validation: OAP-2DS (2-dimensional "stereo" optical array probe)



(OAP-2DS under the SPEC Learjet fuselage)

- registers shadows of particles on two photodiode arrays
- multiple droplets at a time, particle spectra via image analysis
- sizes cloud, drizzle and rain particles (5–3000 μm diam.)

model validation: OAP-2DS spectra vs. RICO SDM simulations



data in the plot based on:

- measurements (Baker et al.)
→ ca. 10h of research flight
- simulation (Arabas & Shima)
→ ca. 10h on ES2 (~100 TFLOPS)

PySDM: JIT-compiled SDM

(open-source Python package)

100%  python™ open-source code:



PySDM goals:

- implementation of SDM + particle-based/Monte-Carlo models of other cloud processes

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KPI: reproduction of results from classic literature, use in new research

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- **accessibility**: seamless Linux/macOS/Windows Intel/ARM installation (pip)
KPI: continuous integration on all targeted platforms

PySDM goals:

- implementation of SDM + particle-based/Monte-Carlo models of other cloud processes
- applicable in research on aerosol-cloud-interactions (and beyond)
KPI: reproduction of results from classic literature, use in new research
- **easy to reuse**: code (100% Python), documentation, examples/tutorials (Jupyter), extensibility (modular, high test coverage), interoperability (other languages, i/o), leveraging modern hardware (GPUs, multi-core CPUs)
KPI: user feedback & multi-institutional contributions
- **accessibility**: seamless Linux/macOS/Windows Intel/ARM installation (pip)
KPI: continuous integration on all targeted platforms
- **curation**: open licensing (GPL), public versioned development (Github), archival (Zenodo)
KPI: instant and anonymous execution of arbitrary version in commodity environments

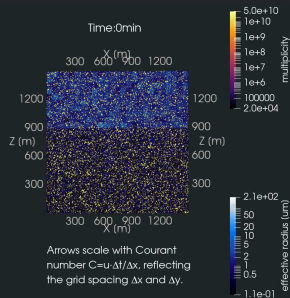


Documentation

PySDM

What is PySDM?

PySDM is a package for simulating the dynamics of population of particles undergoing diffusional and collisional growth (and breakage). The package features a Pythonic high-performance (multi-threaded CPU & CUDA GPU) implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth (Shima et al. 2009), hence the name. 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 (a.k.a. super-droplet) approach to represent aerosol/cloud/rain microphysics. The key goal of PySDM is to enable rapid development and independent reproducibility of simulations in cloud microphysics while being free from the two-language barrier commonly separating prototype and high-performance research code. PySDM ships with a set of examples reproducing results from literature and serving as tutorials. The animation shown here depicts a flow-coupled simulation in which the flow is resolved using PySDM's sibling project: PyMPDATA. The examples include also single-column setups (with PyMPDATA used for advection) as well as adiabatic cloud parcel model setups (with PySDM alone sufficient to constitute a microphysics-resolving cloud parcel model in Python).



Jupyter notebook setting up and running the above PySDM simulation and generating the visualisation using Paraview

**collisional breakup for (Py)SDM:
de Jong et al. 2023**

Geosci. Model Dev., 16, 4193–4211, 2023
<https://doi.org/10.5194/gmd-16-4193-2023>
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Geoscientific
Model Development
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EGU

Development and technical paper

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

Emily de Jong¹, John Ben Mackay^{2,a}, Oleksii Bulenok³, Anna Jaruga⁴, and Sylwester Arabas^{5,b,c}

¹Department of Mechanical and Civil Engineering, California Institute of Technology, Pasadena, CA, USA

²Scripps Institution of Oceanography, San Diego, CA, USA

³Faculty of Mathematics and Computer Science, Jagiellonian University, Kraków, Poland

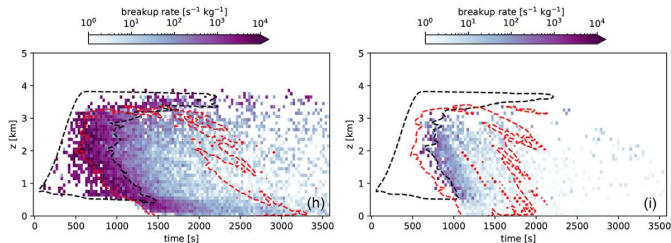
⁴Department of Environmental Science and Engineering, California Institute of Technology, Pasadena, CA, USA

⁵Faculty of Physics and Applied Computer Science, AGH University of Krakow, Kraków, Poland

^aformerly at: Department of Environmental Science and Engineering, California Institute of Technology, Pasadena, CA, USA

^bformerly at: Department of Atmospheric Sciences, University of Illinois Urbana-Champaign, Urbana, IL, USA

^cformerly at: Faculty of Mathematics and Computer Science, Jagiellonian University, Kraków, Poland



[Home](#) / [News](#) / Emily de Jong Receives the 2025 Centennial Prize for Best Thesis in MCE

Emily de Jong Receives the 2025 Centennial Prize for Best Thesis in MCE

June 11, 2025

Emily de Jong, a PhD Candidate in Mechanical Engineering, receives the award for her thesis, "Cloudy with a Chance of Microphysics: Modeling Droplet Collisions for the Climate Scale." She is advised by [Tapio Schneider](#), Theodore Y. Wu Professor of Environmental Science and Engineering.



Centennial Prize for the Best Thesis in Mechanical and Civil Engineering

Awarded each year to a candidate for the degree of Doctor of Philosophy in applied mechanics, civil engineering or mechanical engineering whose doctoral thesis is judged to be the most original and significant by a faculty committee appointed annually by the Executive Officer for Mechanical and Civil Engineering.

Congratulations Emily de Jong!

California Institute of Technology

1200 East California Boulevard
Pasadena, California 91125

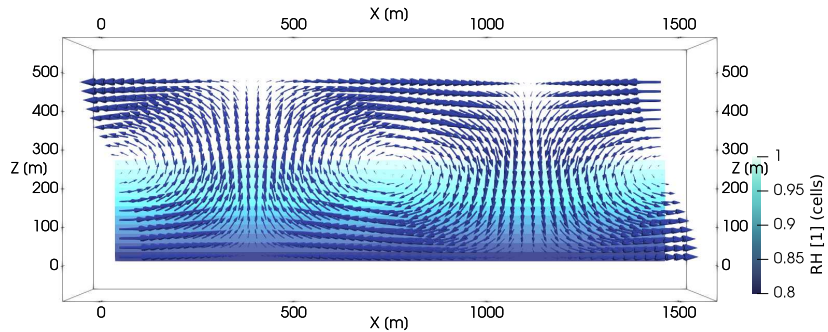
Monte-Carlo immersion freezing in (Py)SDM

immersion freezing: bacteria and the Olympics



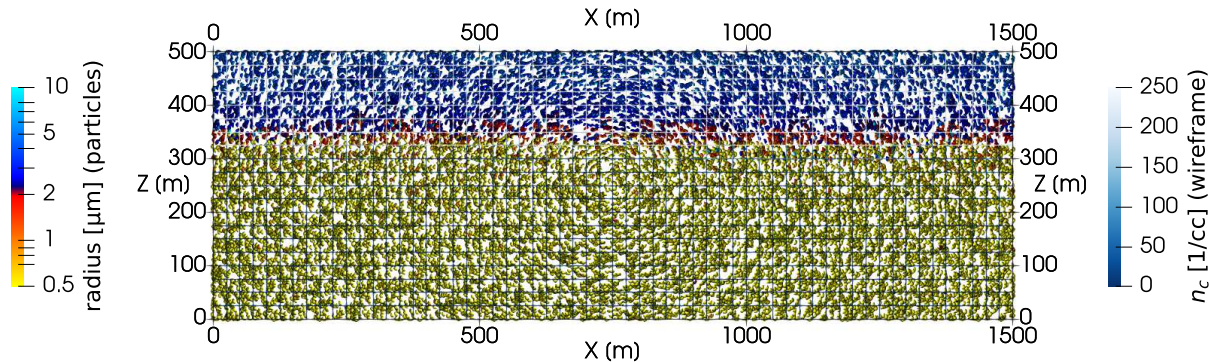
[https://www.reuters.com/markets/commodities/
making-snow-stick-wind-challenges-winter-games-slope-makers-2021-11-29/](https://www.reuters.com/markets/commodities/making-snow-stick-wind-challenges-winter-games-slope-makers-2021-11-29/)

immersion freezing: singular vs. time-dependent in flow-coupled simulation



immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

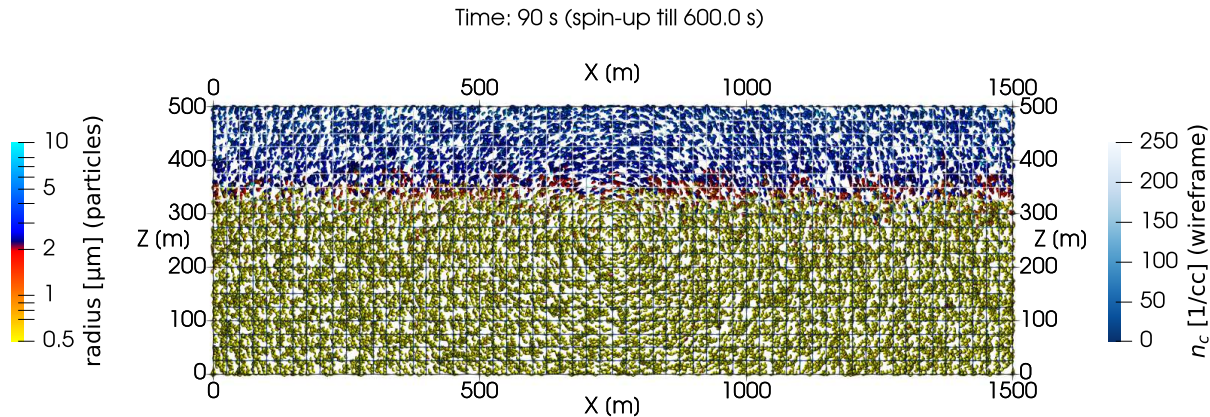


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

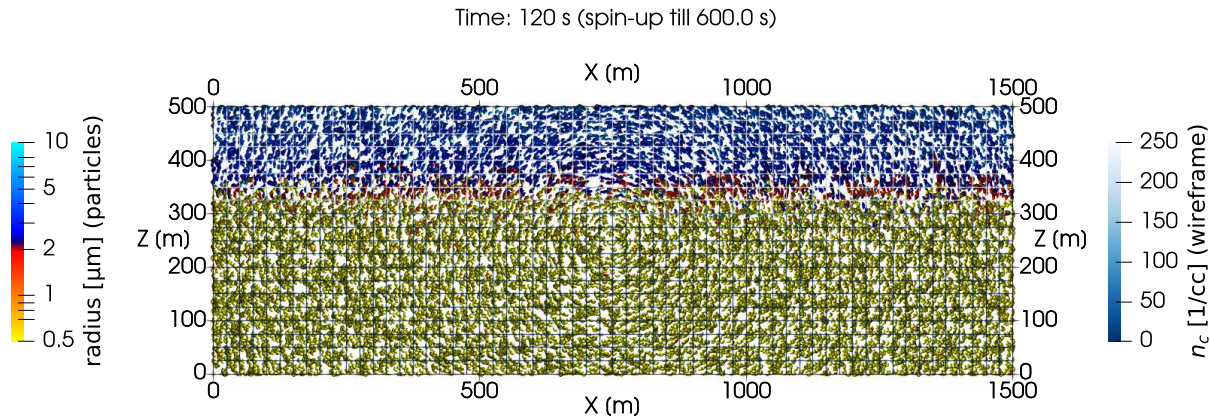


16+16 super-particles/cell for INP-rich + INP-free particles

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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



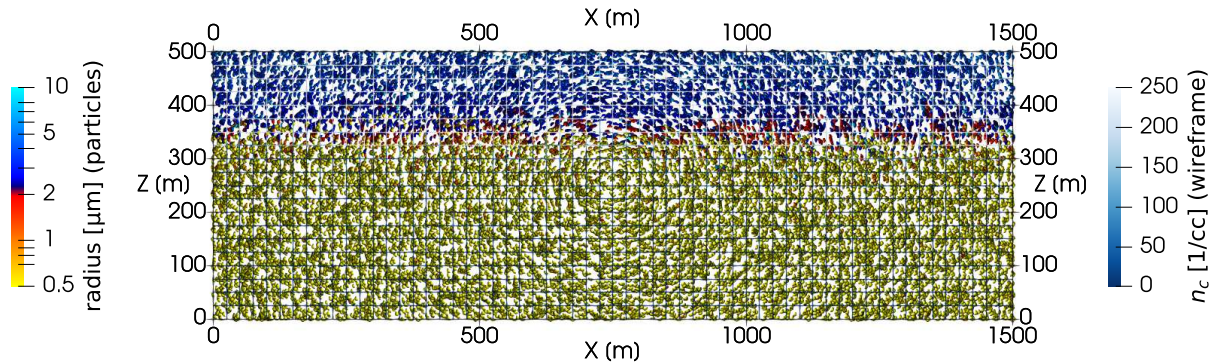
16+16 super-particles/cell for INP-rich + INP-free particles

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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

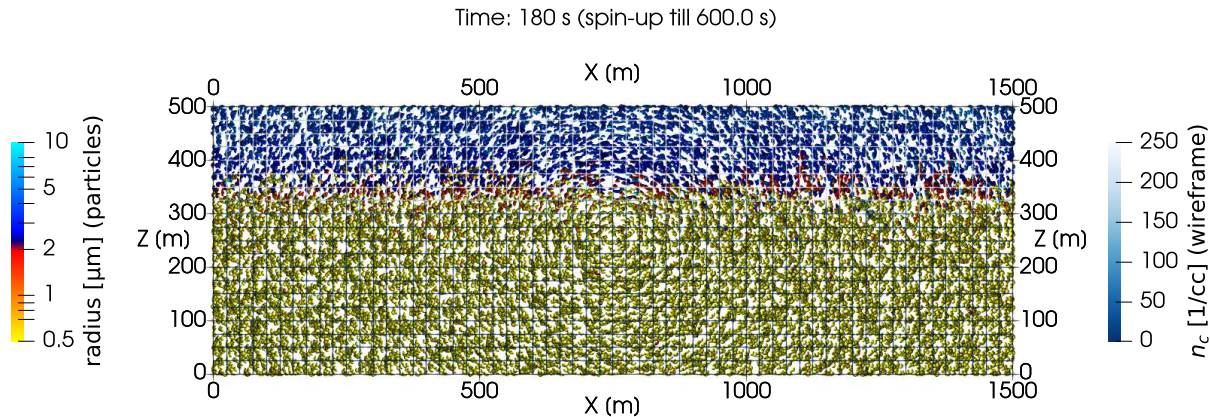


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



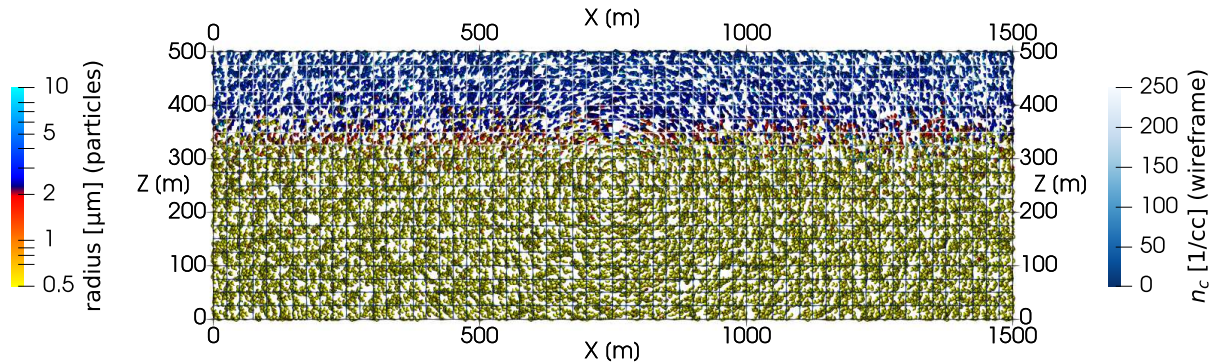
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



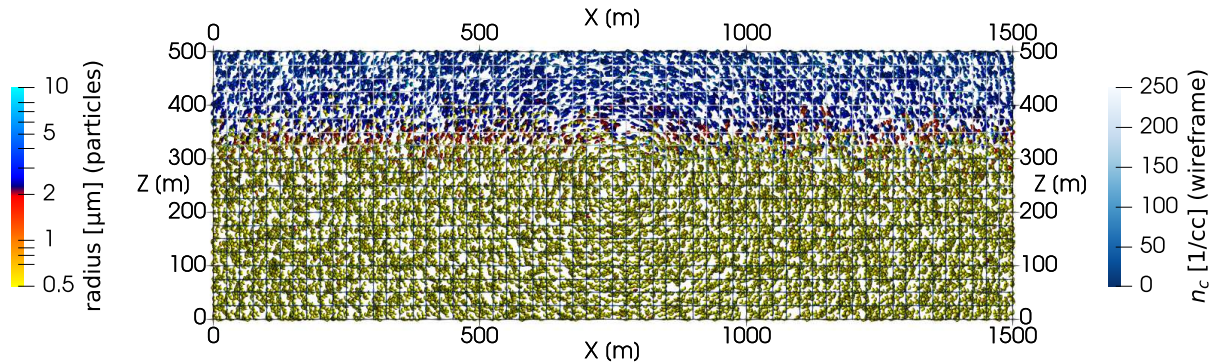
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



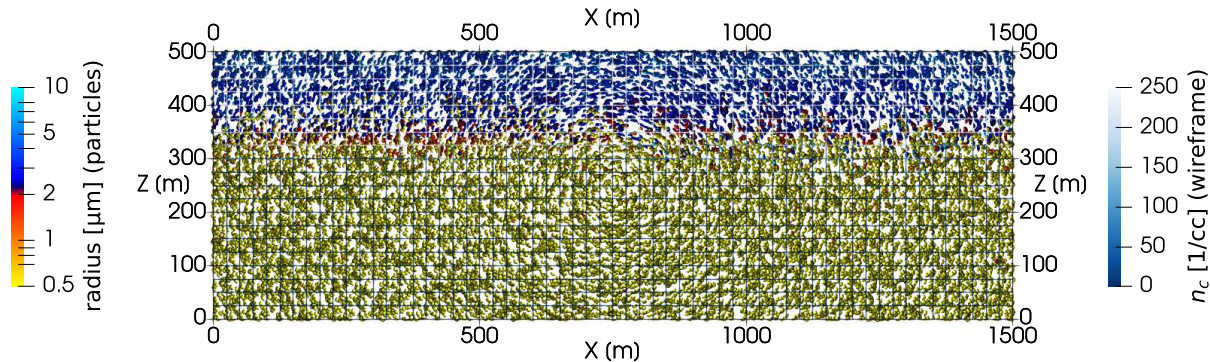
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



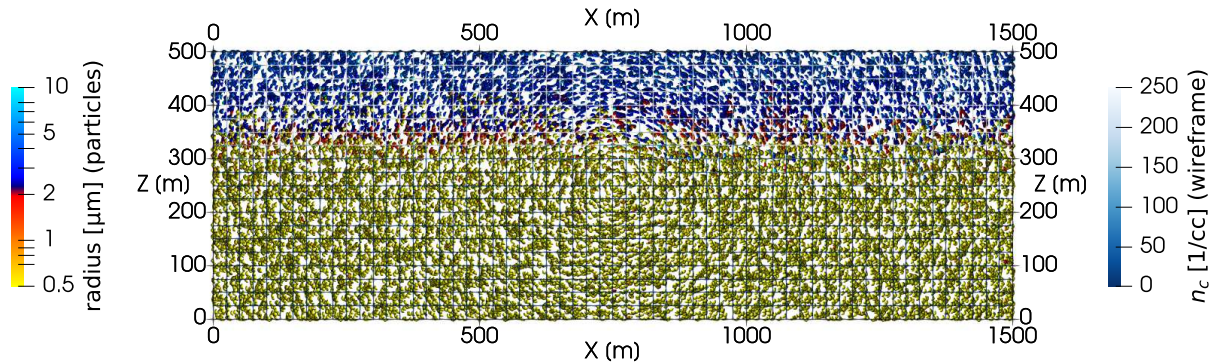
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

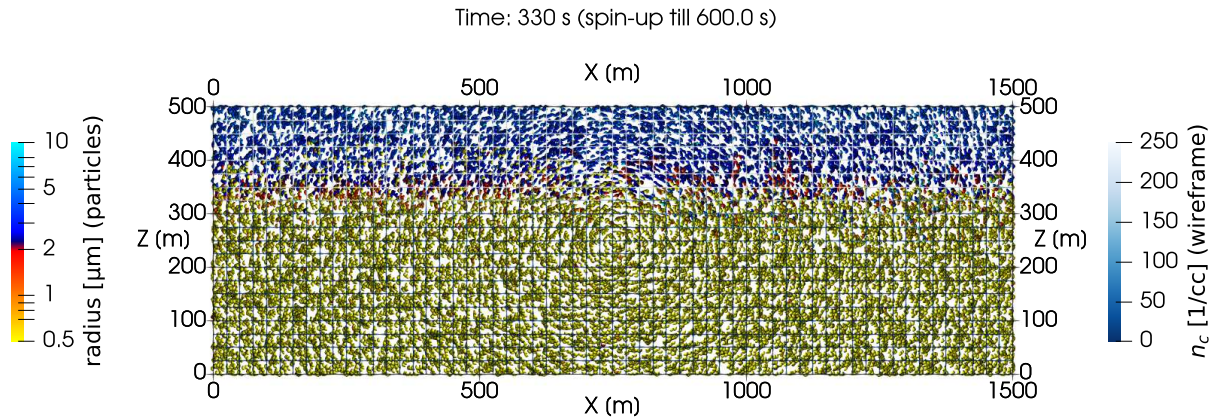


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

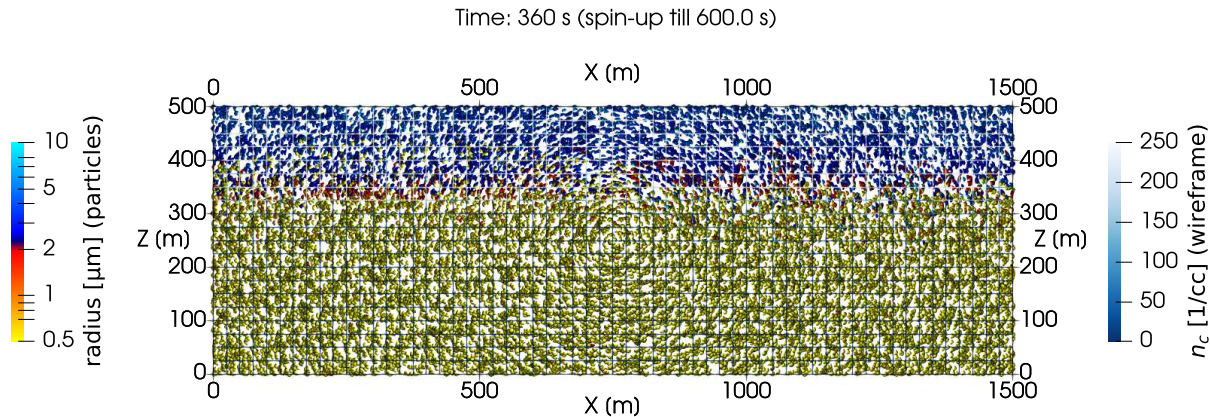


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

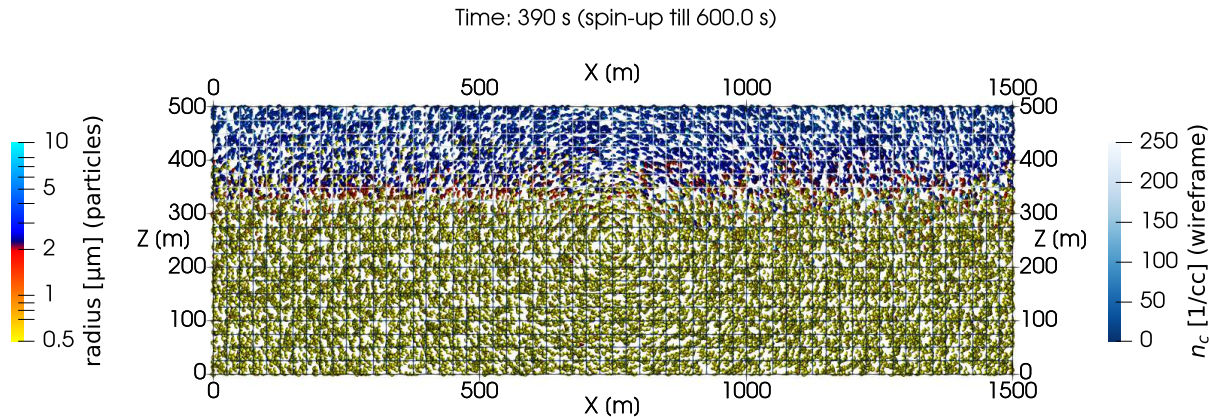


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



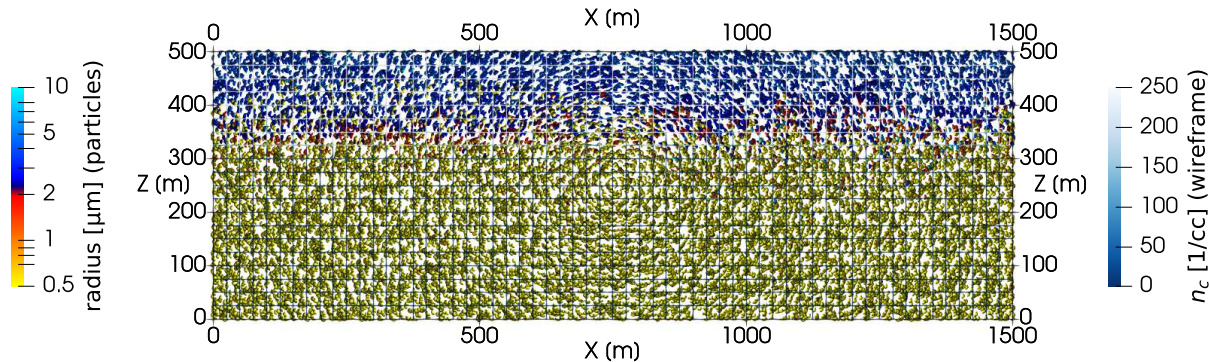
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



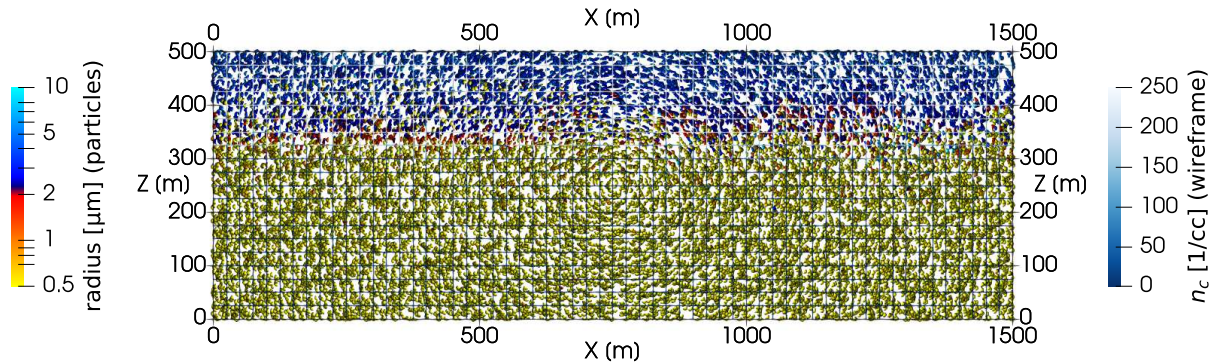
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



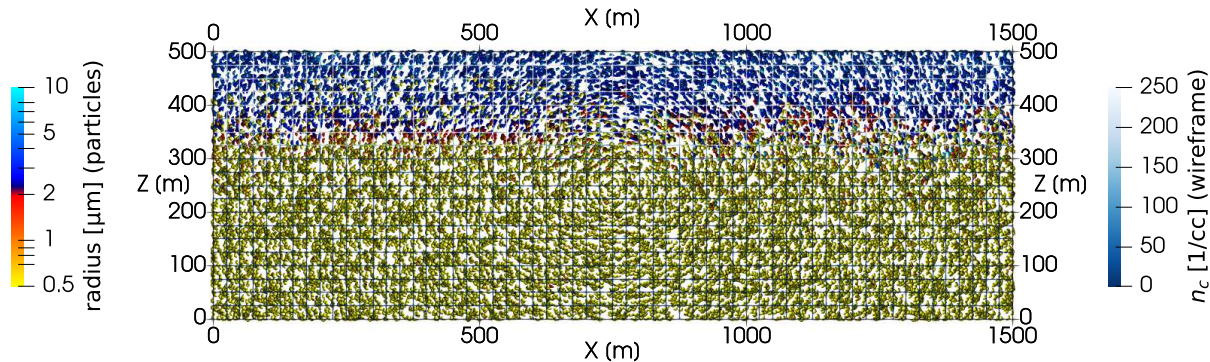
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



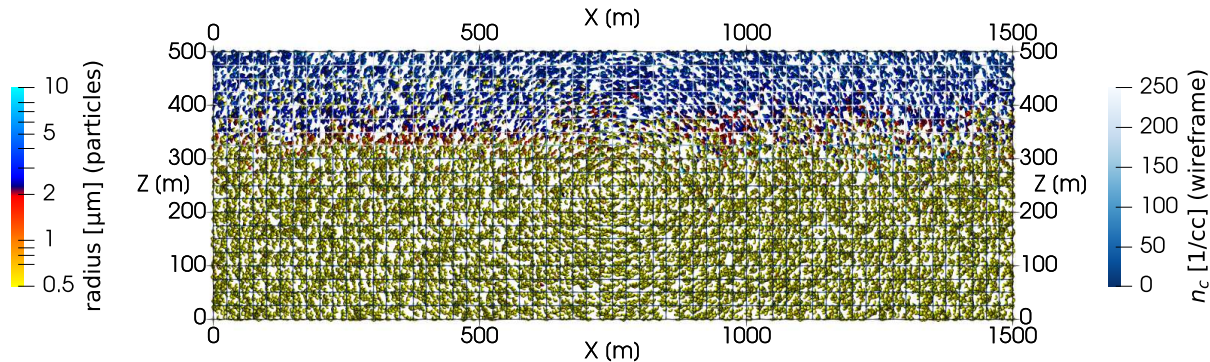
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



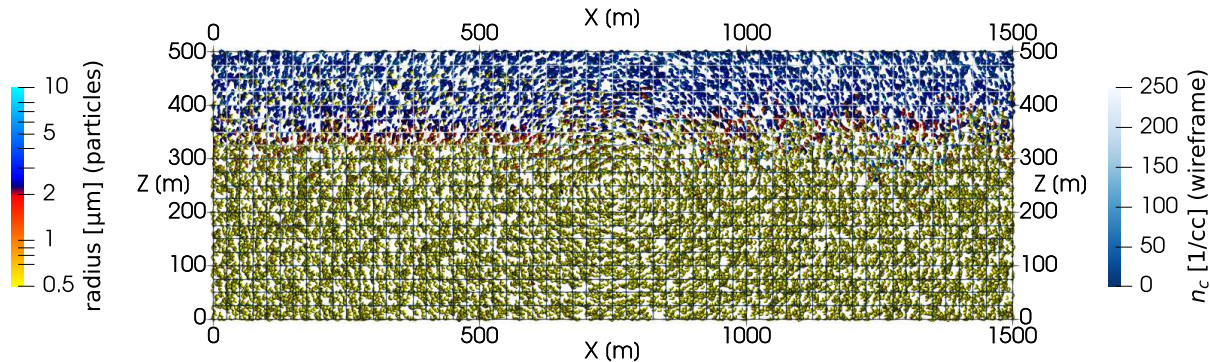
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



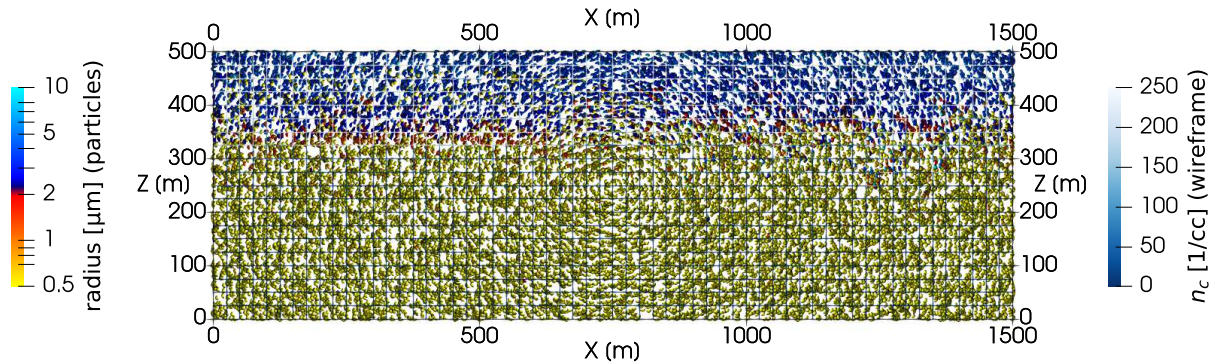
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



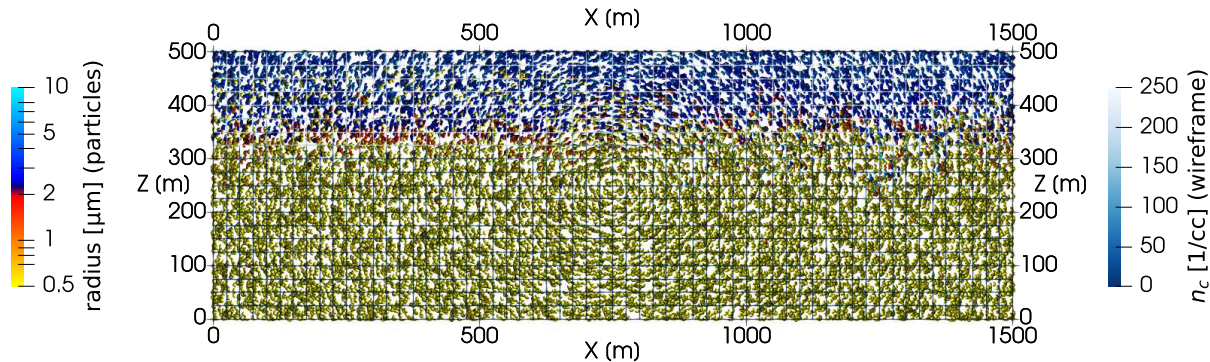
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



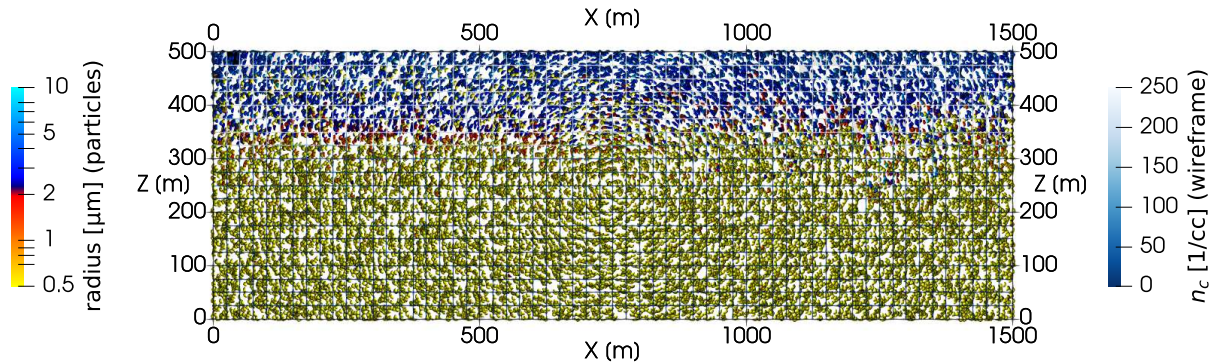
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



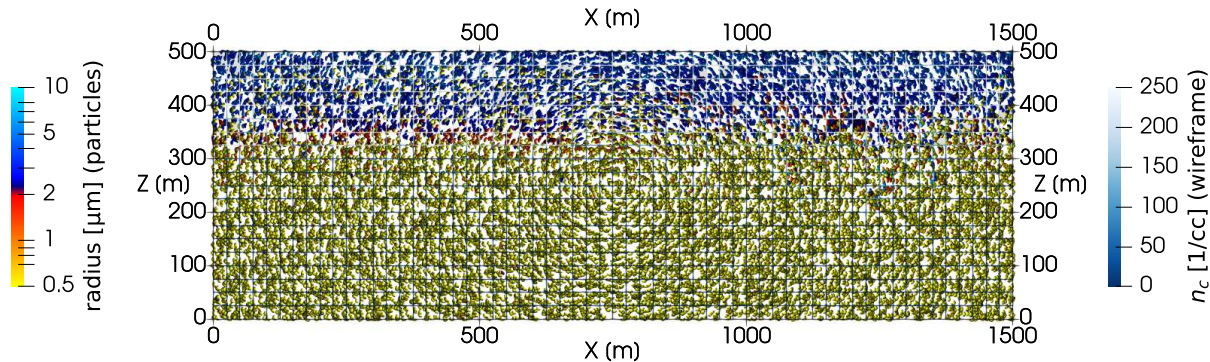
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

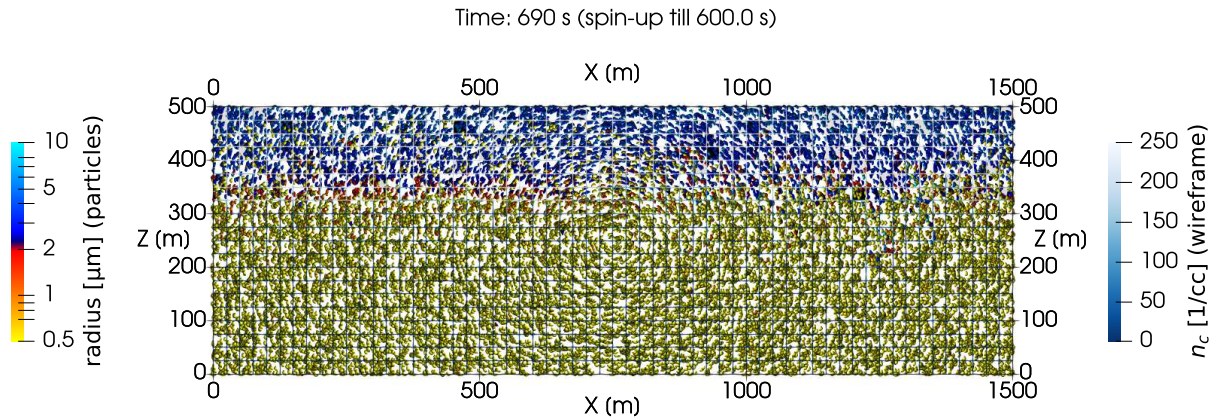


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



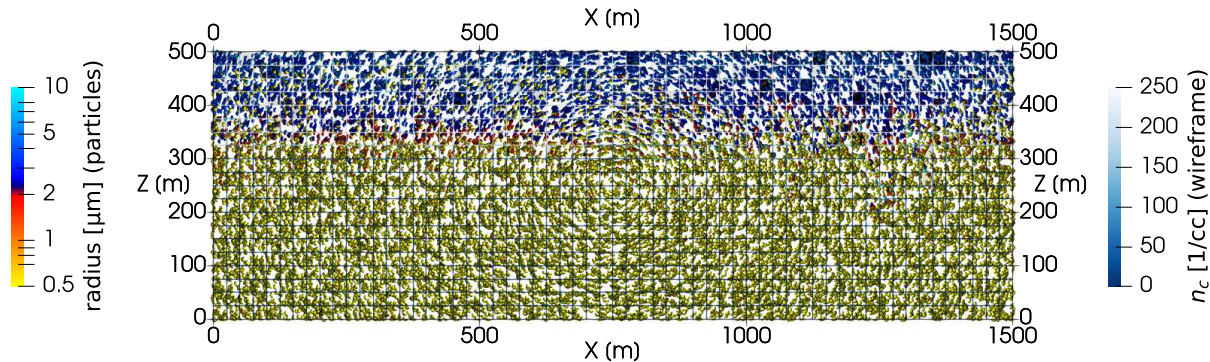
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



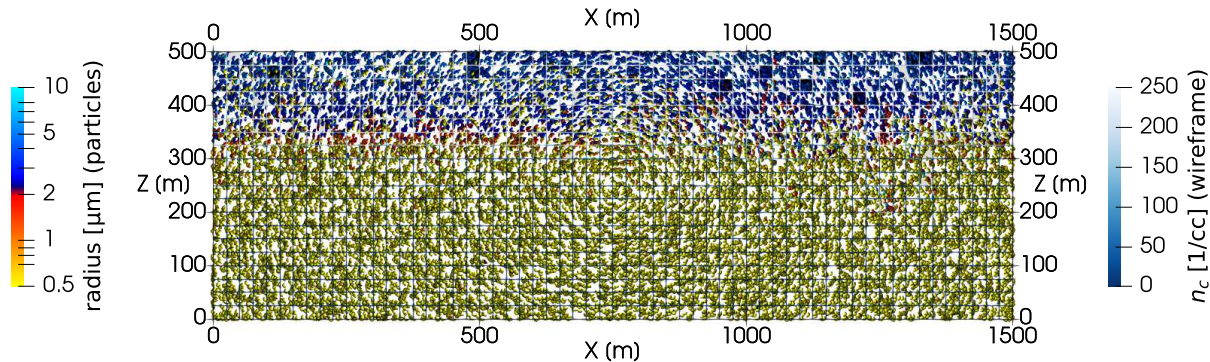
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



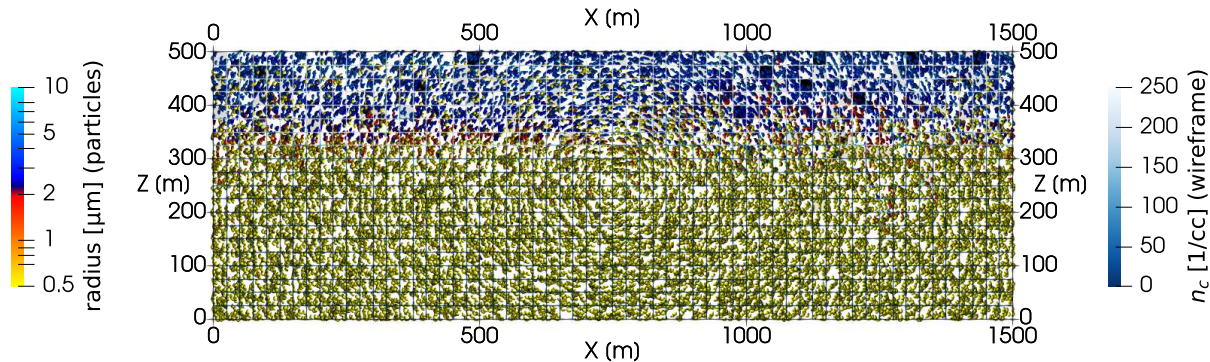
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



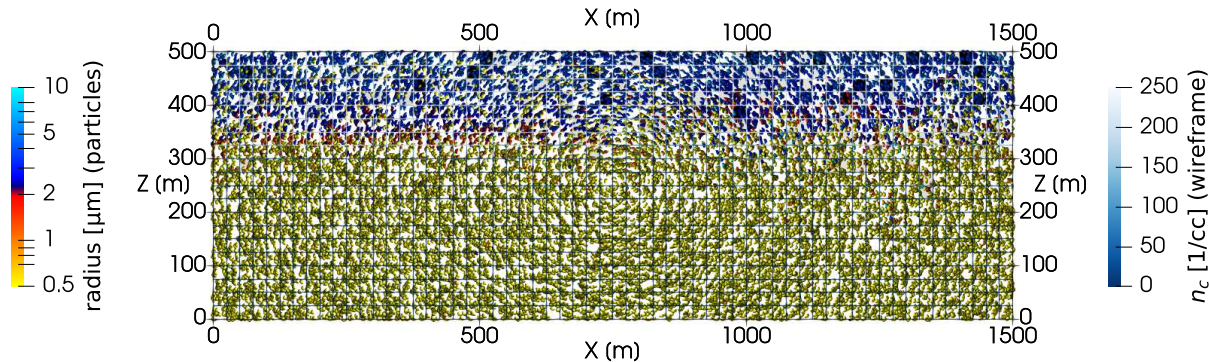
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



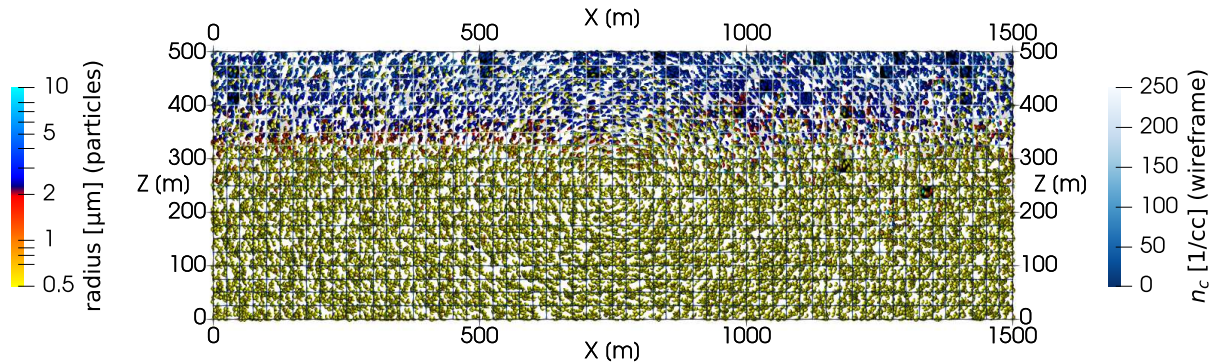
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



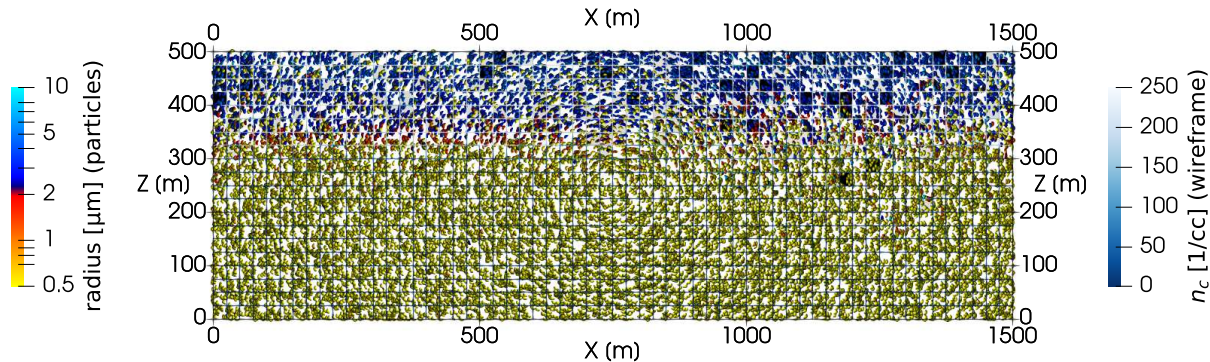
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

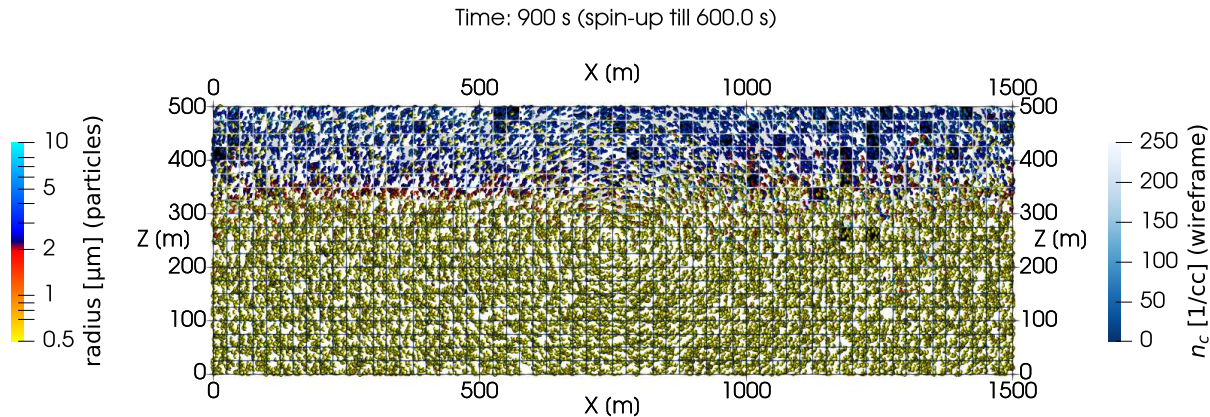


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

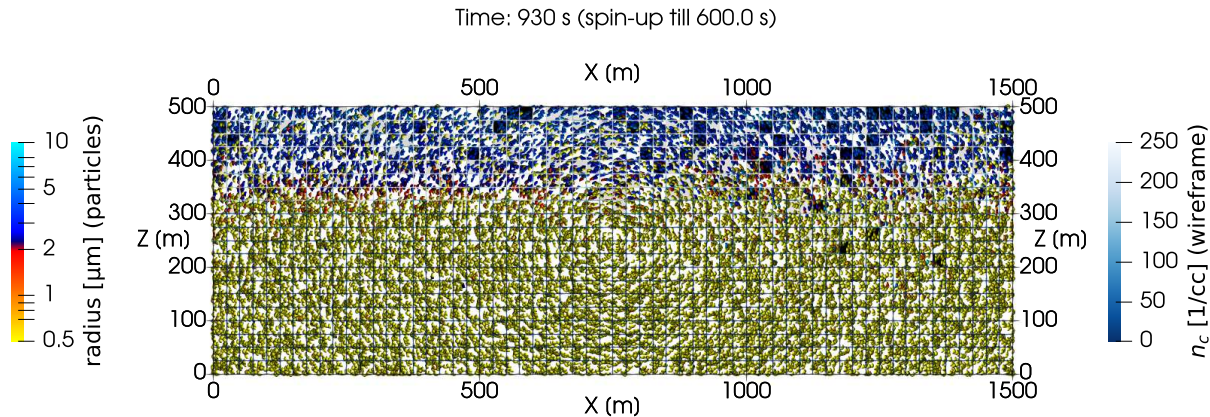


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



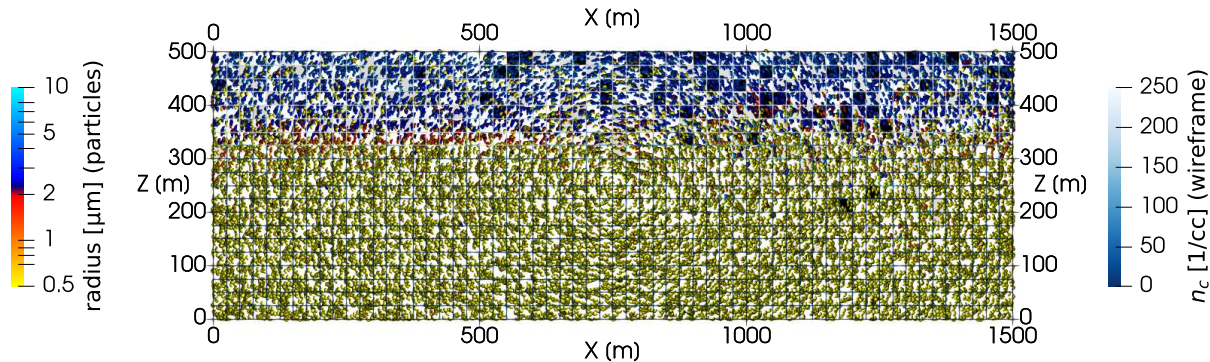
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$N_{\text{aer}} = 300/\text{cc}$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (lognormal, $D_g = 0.74 \mu\text{m}$, $\sigma_g = 2.55$)

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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

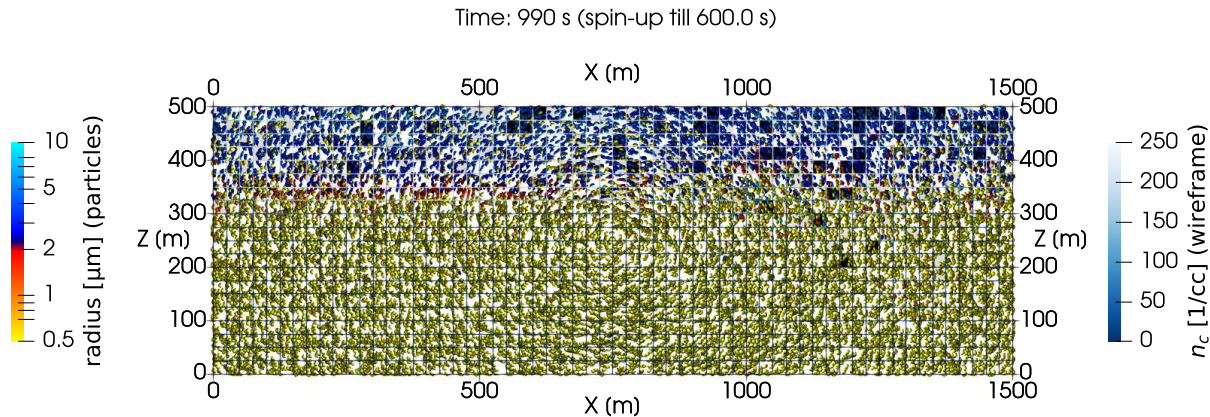


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



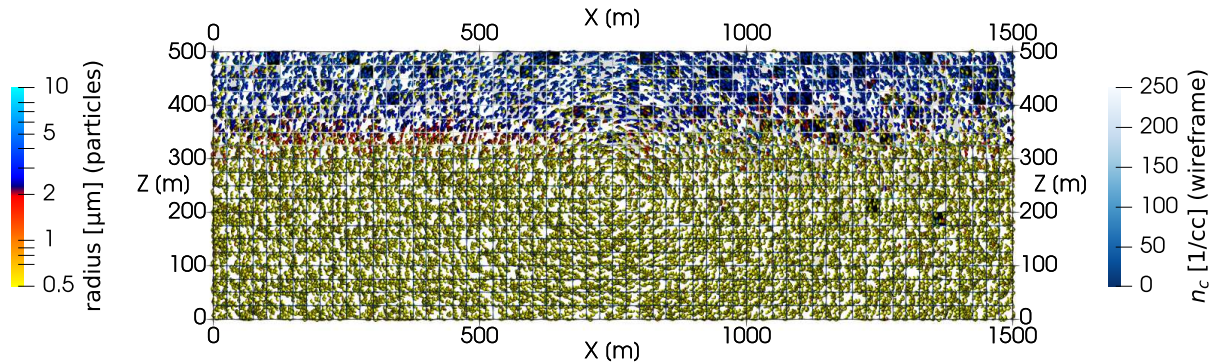
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spin-up = freezing off; subsequently frozen particles act as tracers

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



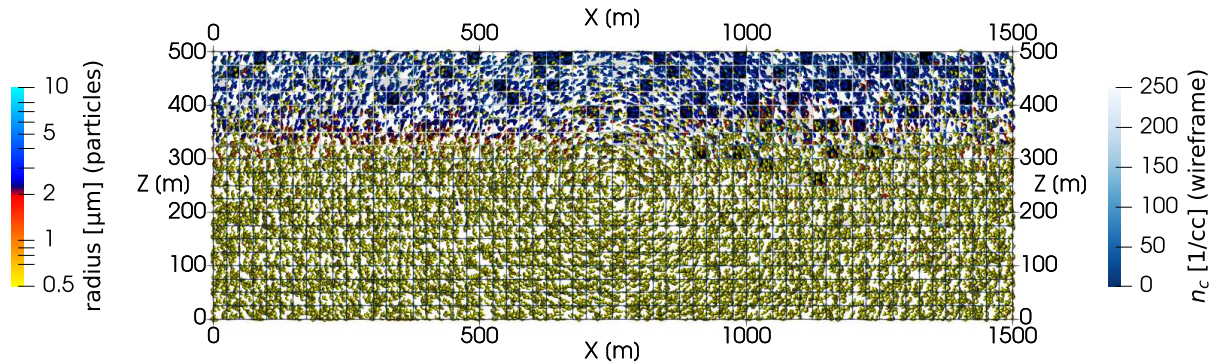
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

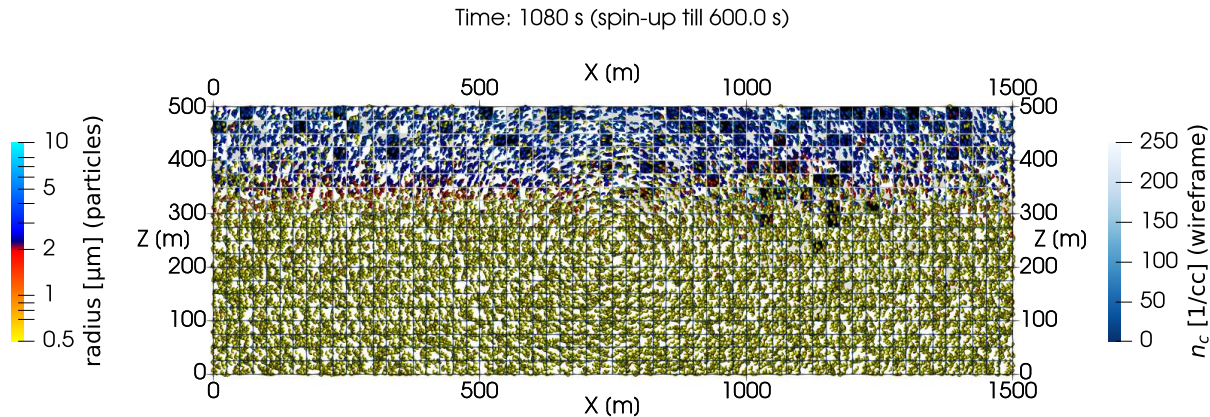


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



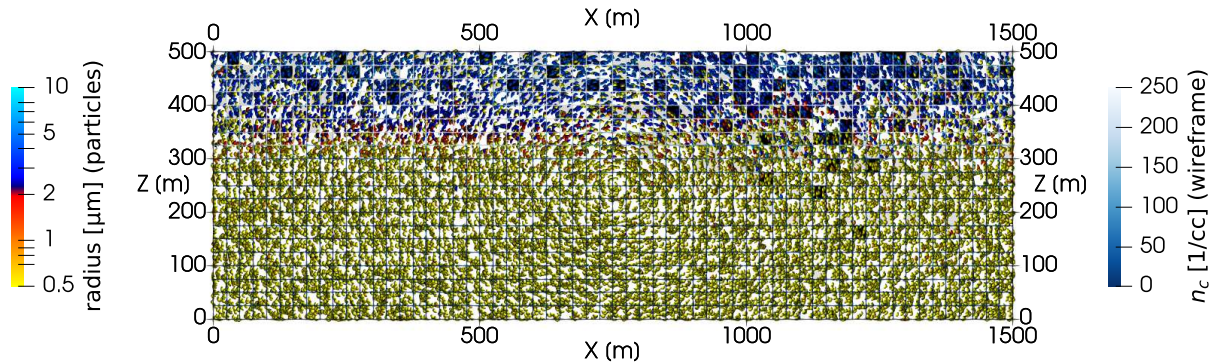
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spin-up = freezing off; subsequently frozen particles act as tracers

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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

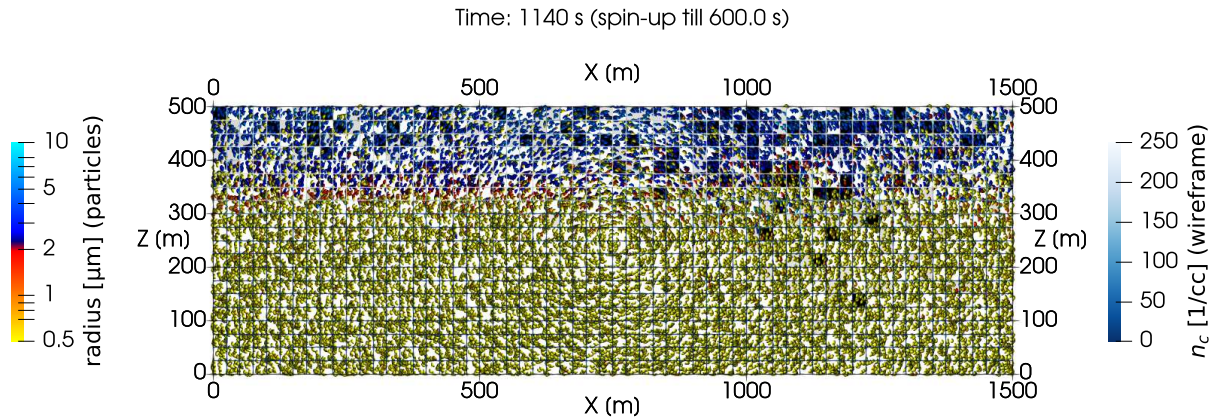


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation



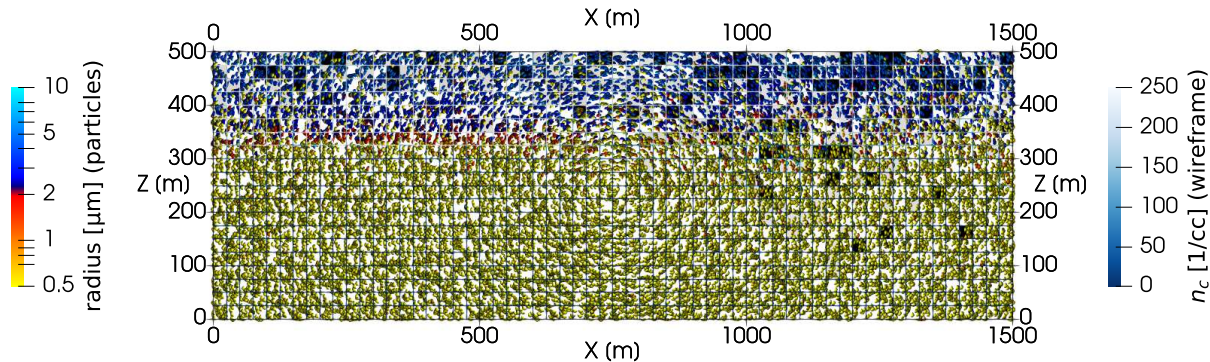
16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/\text{cc}$ (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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

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



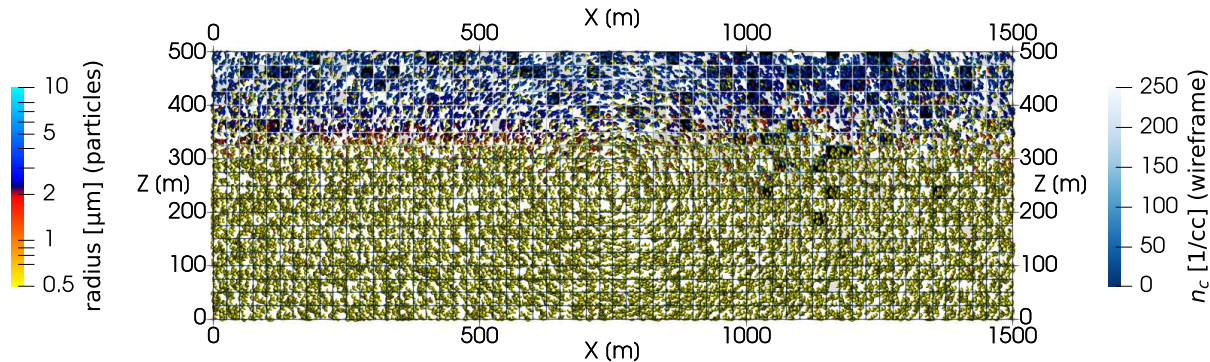
16+16 super-particles/cell for INP-rich + INP-free particles

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

immersion freezing: singular vs. time-dependent in flow-coupled simulation

Time: 1200 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

**PySDM companion packages:
PyMPDATA & Numba-MPI**



[Help](#) [Docs](#) [Sponsors](#) [Log in](#) [Register](#)

pympdata-mpi 0.1.1

`pip install pympdata-mpi`

 [Latest version](#)

Released: Apr 4, 2025

PyMPDATA + numba-mpi coupler sandbox

Navigation

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

Project description

PyMPDATA-MPI

Python 3 LLVM Numba Linux macOS Maintained? yes

PL Funding by [NCN](#) License [GPL v3](#) Copyright [Jagiellonian University](#) DOI [10.5281/zenodo.10866521](#)

 pull requests 7 open

 pull requests 131 closed

 issues 14 open

 issues 36 closed

 tests+pyPI no status

pyPI package 0.1.1

docs [gdoc.dler](#)

 codecov 72%

PyMPDATA-MPI constitutes a [PyMPDATA](#) + [numba-mpi](#) coupler enabling numerical solutions of transport equations with the MPDATA numerical scheme in a hybrid parallelisation model with both multi-threading and MPI distributed memory communication. PyMPDATA-MPI adapts to API of PyMPDATA offering domain decomposition logic.

Verified details

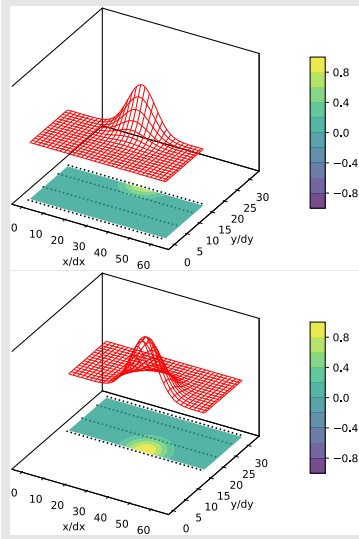
These details have been [verified by PyPI](#)

Maintainers

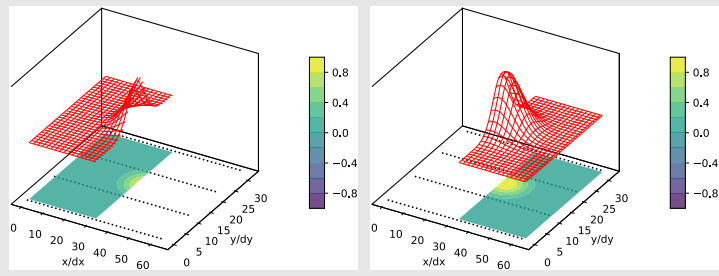
 [Sfonxu](#)

PyMPDATA-MPI: customisable hybrid threading + MPI parallelisation

threading dim = MPI dim



threading dimension $\neq$ MPI dimension



Derlatka et al. 2024 (SoftwareX, doi:10.1016/j.softx.2024.101897)



Original software publication

Numba-MPI v1.0: Enabling MPI communication within Numba/LLVM JIT-compiled Python code

Kacper Derlatka ^{a 1}, Maciej Manna ^{a 2}, Oleksii Bulenok ^{a 3}, David Zwicker ^b, Sylwester Arabas ^c  

^a Faculty of Mathematics and Computer Science, Jagiellonian University in Kraków, Poland

^b Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

^c Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland

<https://doi.org/10.1016/j.softx.2024.101897> 

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Abstract

The numba-mpi package offers access to the Message Passing Interface (MPI) routines from Python code that uses the Numba just-in-time (JIT) compiler. As a result, high-performance and multi-threaded Python code may utilize MPI communication facilities without leaving the JIT-compiled code blocks, which is not possible with the mpi4py package, a higher-level Python interface to MPI. For debugging or code-coverage analysis purposes, numba-mpi retains full functionality of the code even if the JIT compilation is disabled.

habilitation application

A: Methods and Tools for Modelling of Atmospheric Cloud Microphysics:

- A1:** Arabas, Pawlowska 2011
"Adaptive method of lines for multi-component aerosol condensational growth and CCN activation"
Geosci. Model Dev. (EGU)
- A2:** Arabas, Shima 2013
"Large-Eddy Simulations of Trade Wind Cumuli Using Particle-Based Microphysics with Monte Carlo Coalescence"
J. Atmos. Sci. (AMS)
- A3:** Arabas, Jaruga, Pawlowska, Grabowski 2015
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students in Kraków:

kudos team & contributors!

Graduate Students (@agh.edu.pl)



[Agnieszka Zaba](#)

Ongoing PhD project co-advised with [Miroslaw Zimnoch](#) (prior: MSc in Mathematics, AGH, 2023, BEng in Applied Mathematics, Wrocław University of Science and Technology, 2018)



[Konrad Bożioch](#)

Ongoing MSc project (major: Computer Science & Intelligent Systems; prior: BEng in Computer Science & Intelligent Systems, AGH, 2024)

Undergraduate Students (@fis.agh.edu.pl)



[Gracjan Adamus](#)

Ongoing internship (major: Applied Computer Science, AGH)



[Daria Klimaszczyńska](#)

Ongoing BEng project (major: Technical Physics, AGH; prior: BEng in Nanomaterials Engineering, AGH)



[Aleksandra Strzabala](#)

Ongoing BEng project (major: Micro- and Nanotechnologies in Biophysics, AGH)



[Michał Wroński](#)

Ongoing BEng project (major: Micro- and Nanotechnologies in Biophysics, AGH)

Alumni (@agh.edu.pl & @uj.edu.pl)



[Emma Ware](#)

Completed Erasmus+ traineeship in 2024/25 at AGH (from U. California Davis)



[Paweł Magnuszewski](#)

Completed MSc project in 2025 (major: Computer Science & Intelligent Systems, AGH)



[Michał Kowalczyk](#)

Completed BEng project in 2025 (major: Technical Physics, AGH)



[Weronika Romaniec](#)

Completed a (visual identity design) summer internship at AGH in 2024 (from Social Informatics, AGH)



[Sanket Bhogade](#)

PhD student at AGH (2023-2024)



[Agnieszka Makulska](#)

Completed a summer internship at AGH in 2023 (from Physics, Univ. Warsaw)



[Kacper Derlaśka](#)

Completed MSc project in 2023 (major: Computer Science, Jagiellonian Univ.)



[Oleksii Bulenok](#)

Completed MSc project in 2023 (major: Computer Science, Jagiellonian Univ.)



[Piotr Bartman-Szwarc](#)

Completed MSc project in 2020 (major: Computer Science, Jagiellonian Univ.)



[Michael Oleś](#)

Completed MSc project in 2020 (major: Physics, Jagiellonian Univ.)

PySDM, PyMPDATA and Numba-MPI contributors:

- [caltech.edu](#): Sajjad Azimi, Ben Mackay & Anna Jaruga
- [colorado.edu](#): Clare Singer
- [columbia.edu](#): Jatan Buch
- [ds.mpg.de](#): David Zwicker
- [exeter.ac.uk](#): Daniel Partridge
- [imgw.pl](#): Maciej Manna

- [lnl.gov](#): Emily de Jong
- [mpimet.mpg.de](#): Clara Bayley
- [okayama-u.ac.jp](#): Grzegorz Łazarski
- [uni-mainz.de](#): Tim Lüttmer
- [uw.edu.pl](#): Agnieszka Makulska
- [washington.edu](#): Jason Barr

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We are a team of students, researchers and developers at the [AGH University of Krakow](#) 🇵🇱 in Poland 🇵🇱. Our activities concern free/libre and open-source software for [atmospheric sciences](#) 🌍, and [cloud physics](#) ☁️ in particular. We develop example-rich tools to support reproducible [computational science](#), while promoting best practices in [research software engineering](#). Our team contributes to the open-source ecosystem we rely on. We explore modern, transferable technologies that are useful both within and beyond academia. Most of the projects we develop, maintain, and contribute to are hosted at github.com/open-atmos (while the [Kraków](#) airport IATA ✈️ code is KRK, hence **open-atmos-krk** 😊). Before moving to the [AGH Environmental Physics Group](#) in 2023, we had been based at the [Institute of Computer Science and Computational Mathematics, Jagiellonian University in Kraków](#).



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Thank you for your attention!

sylwester.arabas@agh.edu.pl