Super-droplet μ-physics: a probabilistic look at modelling clouds and the immersion freezing process

Sylwester Arabas
AGH University of Krakow, Poland

July 3 2025 (Institute for Physics of the Atmosphere @uni-mainz.de)

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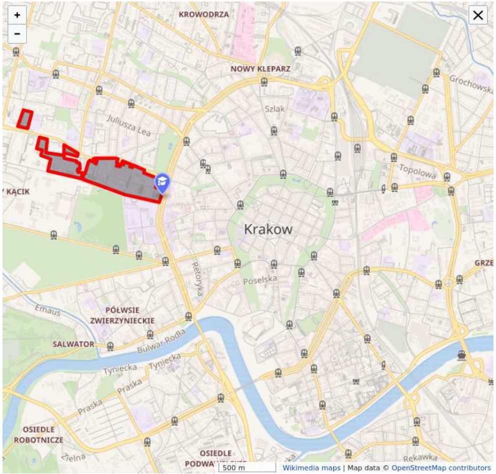
ENVIRONMENTAL PHYSICS GROUP

zfs.agh.edu.pl

AGH campus in Kraków and the ”neighbourhood”..



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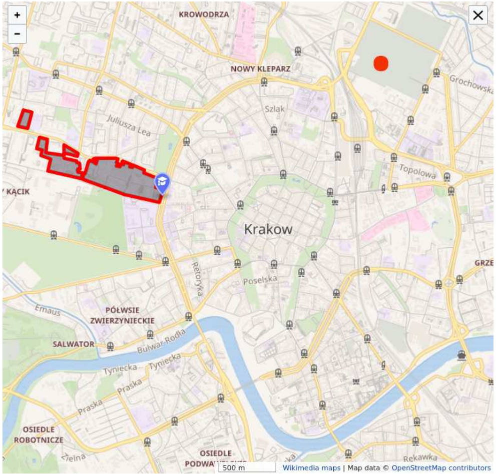

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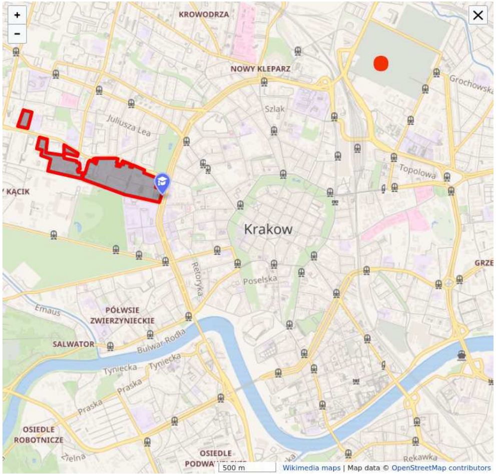

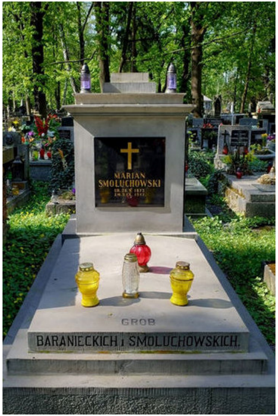

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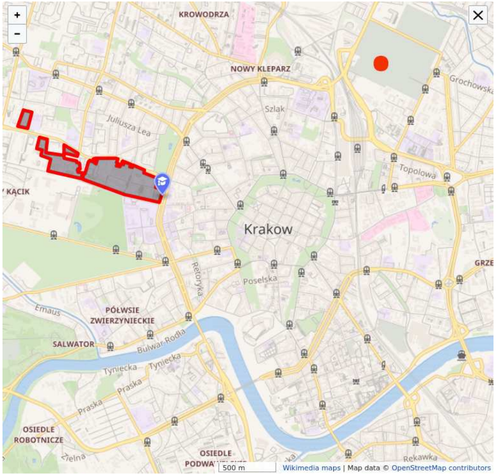
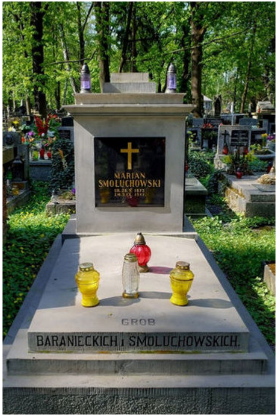
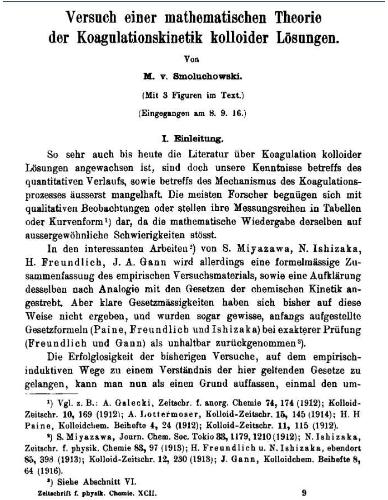




cloud μ-physics models in 1910s?

Smoluchowski & Rudzki



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 Kurvenform[1]) dar, da die mathematische Wiedergabe derselben auf aussergewöhnliche Schwierigkeiten stösst.

In den interessanten Arbeiten[2]) 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 zurückgenommen[3]).

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-

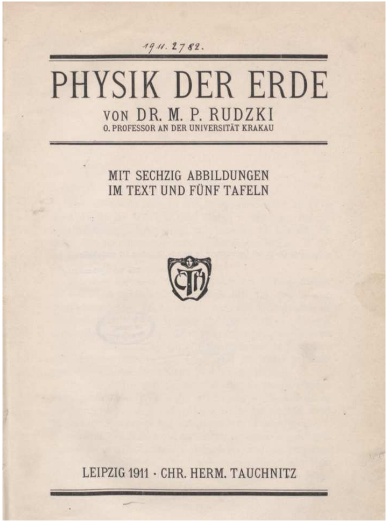
[1]) Vgl. z. B.: A. Galecki, Zeitschr. f. anorg. Chemie **74**, 174 (1912); Kolloid-Zeitschr. **10**, 169 (1912); A. Lottermoser, Kolloid-Zeitschr. **15**, 145 (1914); H. H Paine, Kolloidchem. Beihefte **4**, 24 (1912); Kolloid-Zeitschr. **11**, 115 (1912).

[2]) S. Miyazawa, Journ. Chem. Soc. Tokio **33**, 1179, 1210 (1912); N. Ishizaka, Zeitschr. f. physik. Chemie **83**, 97 (1913); H. Freundlich u. N. Ishizaka, ebendort **85**, 398 (1913); Kolloid-Zeitschr. **12**, 230 (1913); J. Gann, Kolloidchem. Beihefte **8**, 64 (1916).

[3]) Siehe Abschnitt VI.

(Smoluchowski 1918,

DOI:10.1515/zpch-1918-9209)



(available at U. Mainz Zentralbibliothek)

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]

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Maurycy Pius Rudzki

"Principles of Meteorology" book (1917)

Dr M. P. RUDZKI

PROFESOR UNIWERSYTETU JAGIELLOŃSKIEGO,

DYREKTOR OBSERWATORYUM ASTRONOMICZNEGO W KRAKOWIE.

ZASADY

METEOROLOGII

WARSZAWA.

SKŁAD GŁÓWNY W KSIĘGARNI E. WENDE I SPÓŁKA.

—

1917.

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modelling coagulation: SCE & SDM

Smoluchowski's coagulation equation (SCE)

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

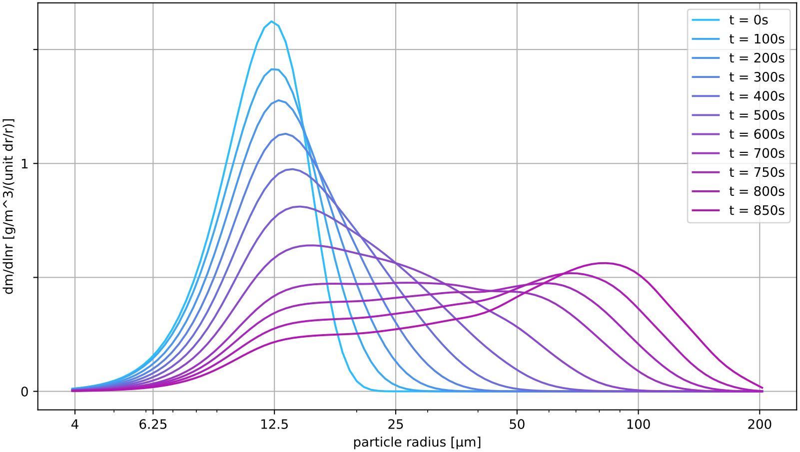
collision kernel: $a(x_1, x_2) : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$

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

droplet concentration: $c_i = c(x_i)$

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

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”

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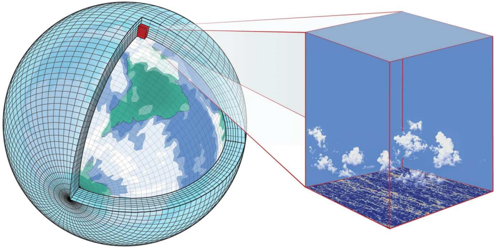


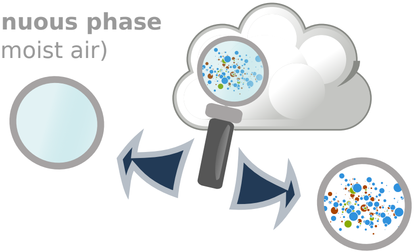
“Grid cells in a global climate model and a large-eddy simulation of shallow cumulus clouds at 5 m resolution”

(fig. from Schneider et al. 2017)

Eulerian vs. Lagrangian microphysics

Eulerian vs. Lagrangian microphysics

continuous phase
(moist air)



dispersed phase
(aerosol particles, cloud droplets, drizzle, rain, snow, ...)

Eulerian vs. Lagrangian microphysics

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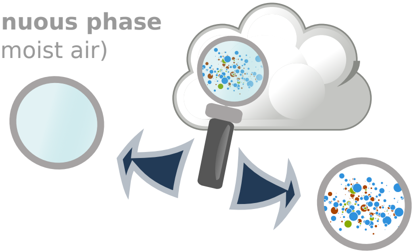

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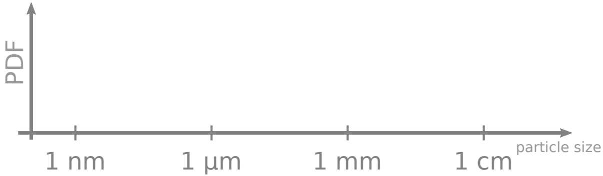

Eulerian vs. Lagrangian microphysics

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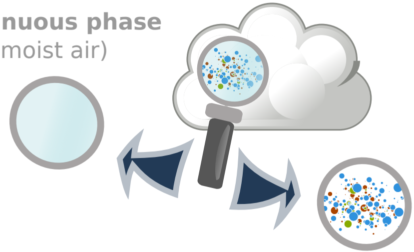

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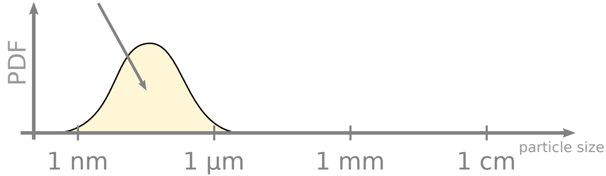

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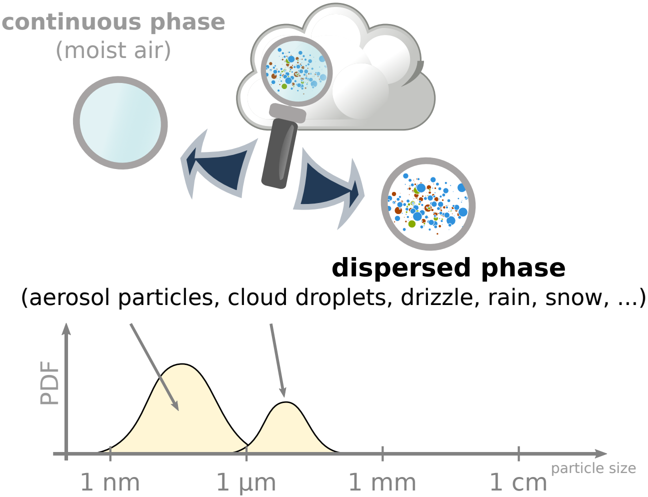

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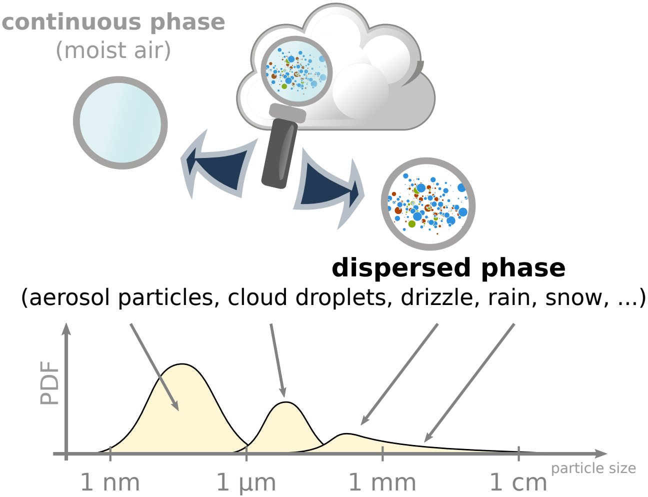

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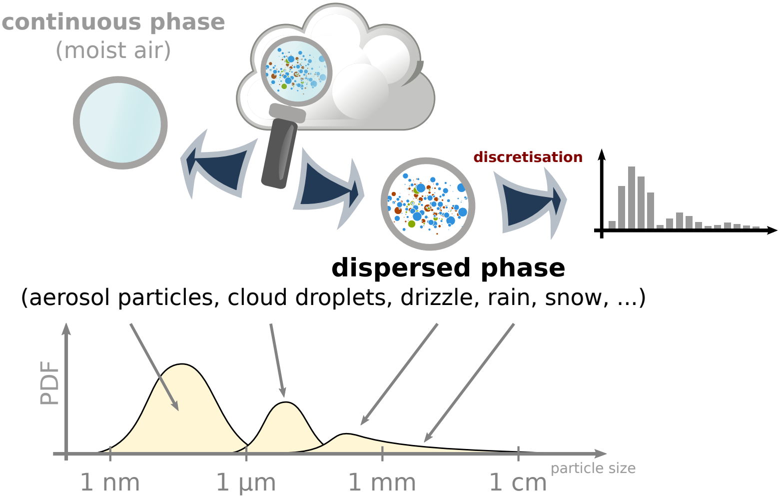

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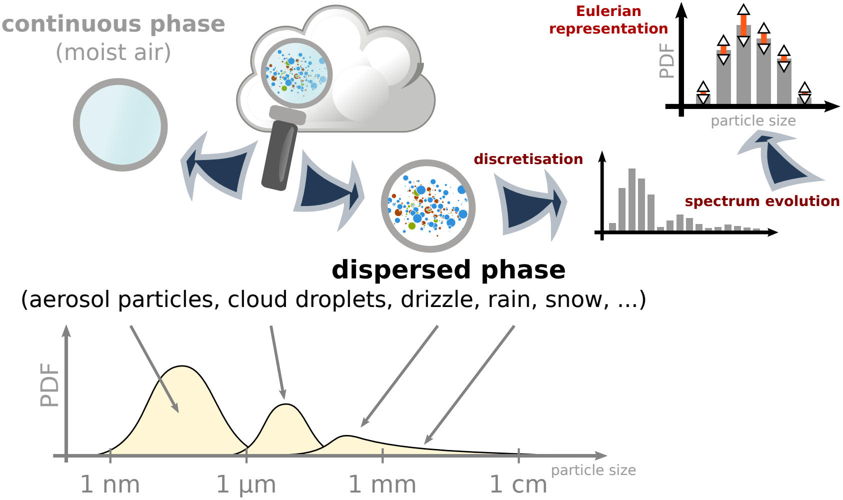

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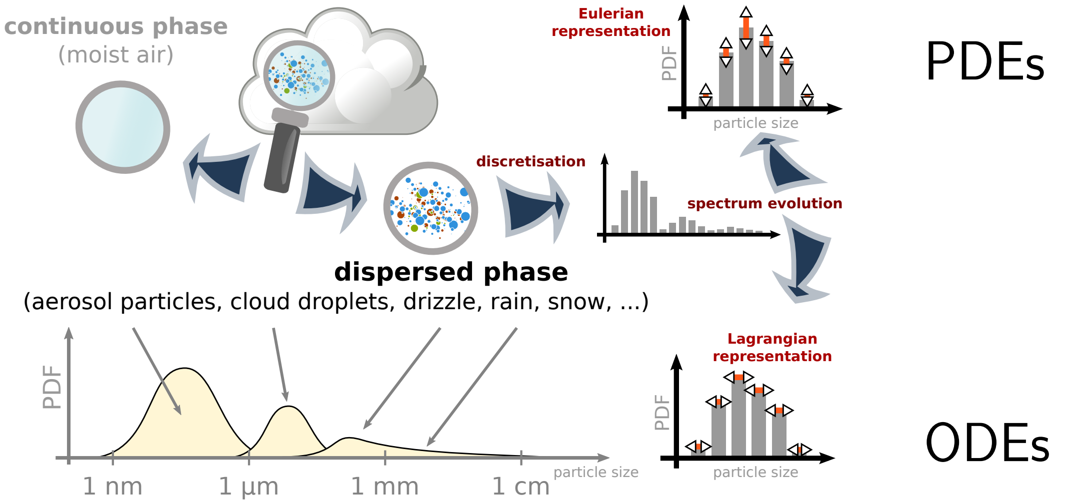


Lagrangian microphysics: early works (0D)

JOURNAL OF METEOROLOGY

THE GROWTH OF CLOUD DROPS IN UNIFORMLY COOLED AIR

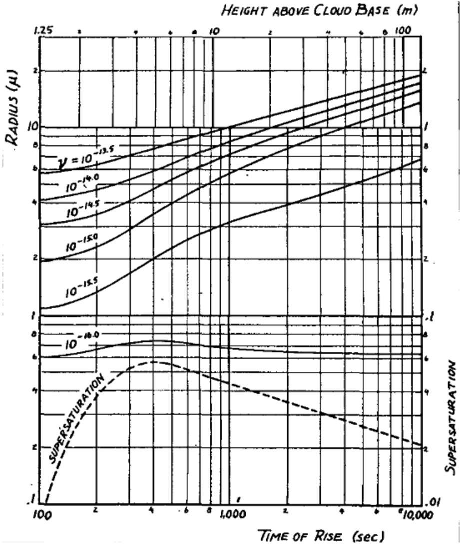
By *Wallace E. Howell*[1]

Blue Hill Meteorological Observatory, Harvard University[2]

(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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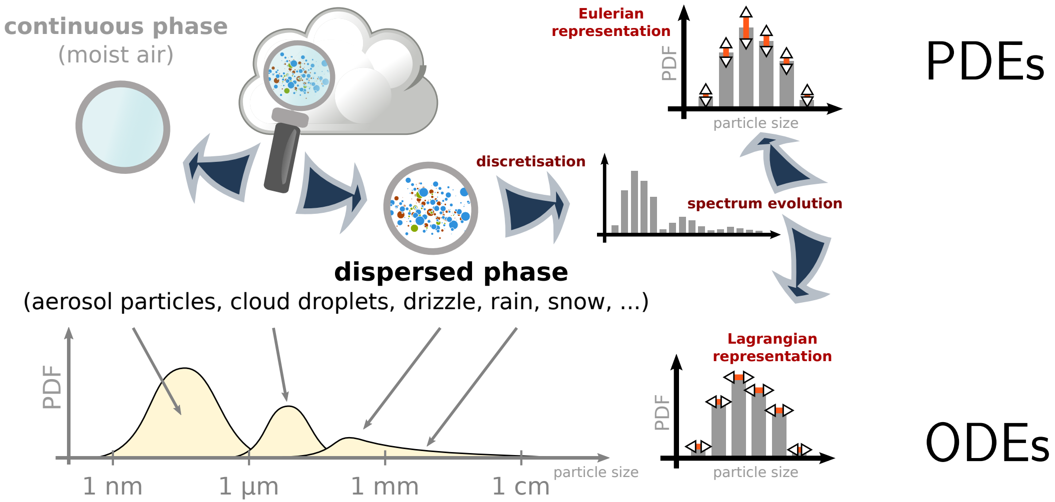
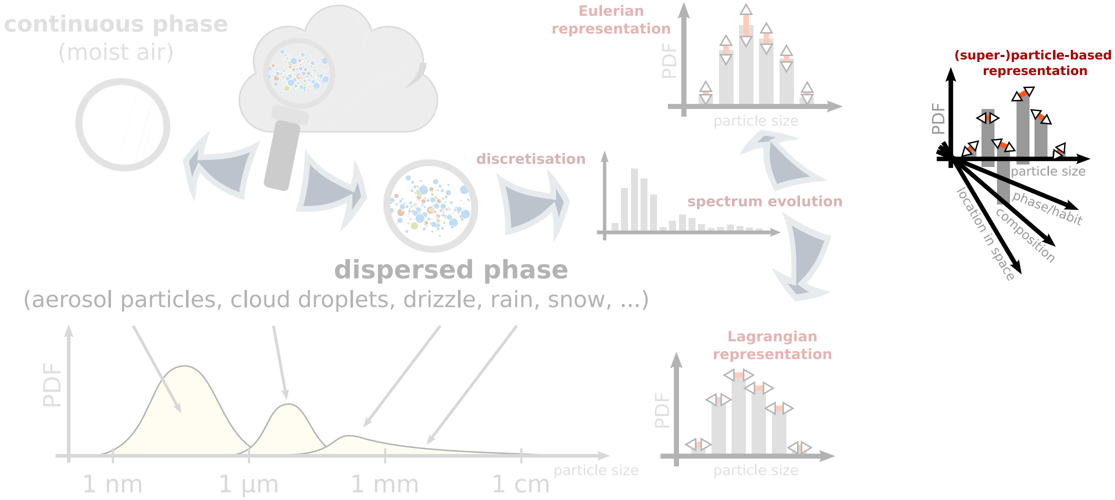
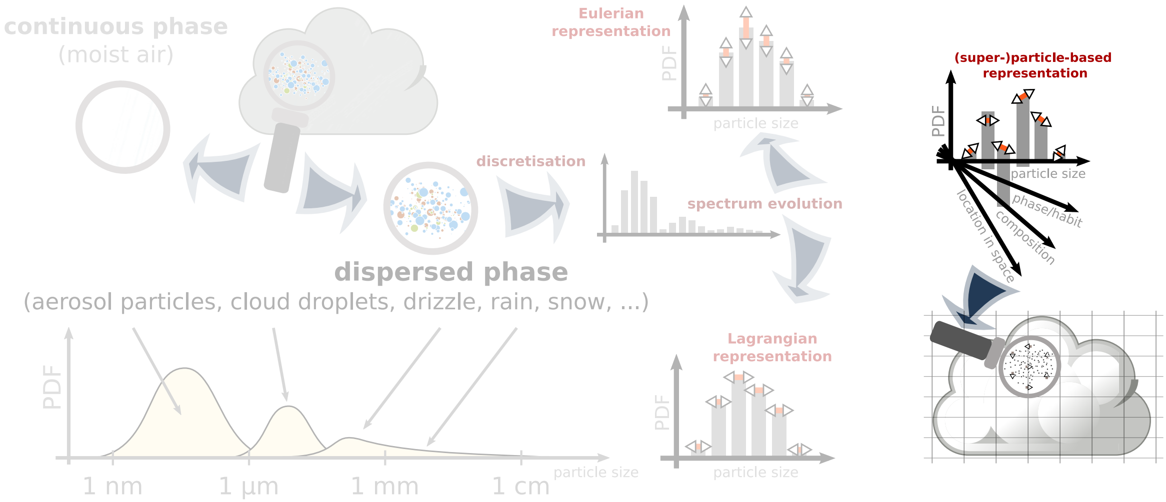



continuous phase
(moist air)
dispersed phase
(aerosol particles, cloud droplets, drizzle, rain, snow, ...)
PDF
1 nm
1 µm
1 mm
1 cm
particle size
discretisation
Eulerian
representation
PDF
particle size
spectrum evolution
Lagrangian
representation
PDF
particle size
(super-)particle-based
representation
PDF
particle size
phase/habit
composition
location in space

Eulerian vs. Lagrangian microphysics



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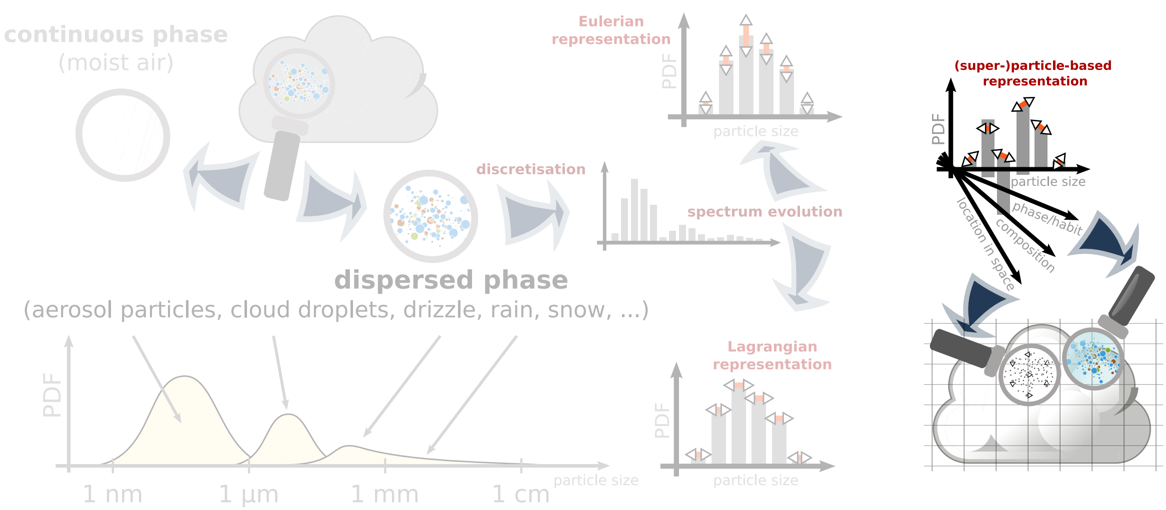

Lagrangian microphysics: early works (3D)

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

Eulerian vs. Lagrangian microphysics: a (probabilistic) breakthrough

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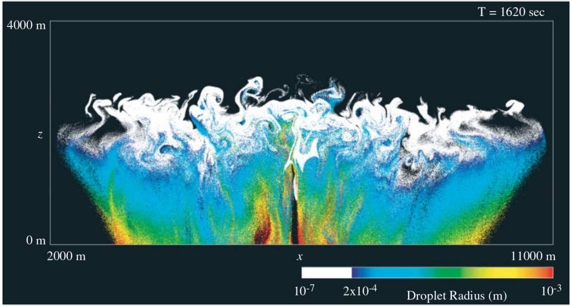
Shima 2009: Monte-Carlo particle-based collision algorithm for cloud simulations



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

[a] Jacobson 2005: Fundamentals of Atmospheric Modeling

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

SCE (naïve impl)	SDM
method type	
mean-field, deterministic	Monte-Carlo, stochastic

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

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

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

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

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AGU ADVANCING EARTH AND SPACE SCIENCE
Journal of Advances in Modeling Earth Systems 10.1029/2019MS001689

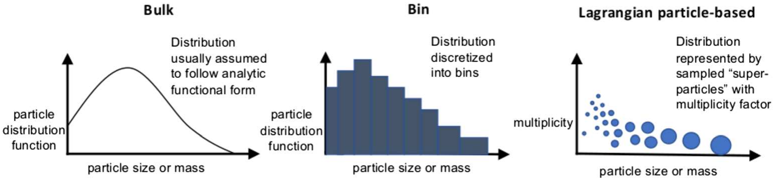

Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

PySDM: SDM implementation for reproducible research & active learning

PySDM

PySDM goals:

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

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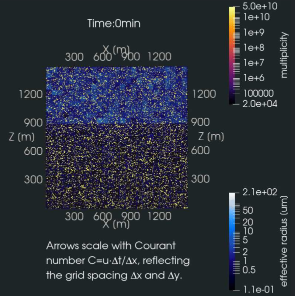
  KPI: continuous integration on all targeted platforms
- **curation**: open licensing (GPL), public versioned development (Github), archival (Zenodo)
  KPI: instant and anonymous execution of arbitrary version in commodity environments

PySDM

Documentation

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

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Monte-Carlo collisional breakup (constant super-droplet number formulation)

Geosci. Model Dev., 16, 4193–4211, 2023
https://doi.org/10.5194/gmd-16-4193-2023

Geoscientific Model Development
Open Access
Development and technical paper

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

Emily de Jong[1], John Ben Mackay[2,a], Oleksii Bulenok[3], Anna Jaruga[4], and Sylwester Arabas[5,b,c]

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[b]formerly at: Department of Atmospheric Sciences, University of Illinois Urbana-Champaign, Urbana, IL, USA
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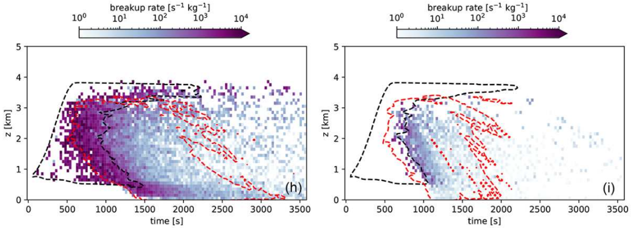

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Sajjad Azimi & Anna Jaruga @caltech.edu calibration of bulk model using PySDM, ...

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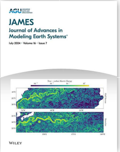
Training Warm-Rain Bulk Microphysics Schemes Using Super-Droplet Simulations

Sajjad Azimi, Anna Jaruga, Emily de Jong, Sylwester Arabas, Tapio Schneider

First published: 26 July 2024 | https://doi.org/10.1029/2023MS004028



Volume 16, Issue 7
July 2024
e2023MS004028
This article also appears in:
The CliMA Earth System Model

Abstract

Cloud microphysics is a critical aspect of the Earth's climate system, which involves processes at the nano- and micrometer scales of droplets and ice particles. In climate modeling, cloud microphysics is commonly represented by bulk models, which contain simplified process rates that require calibration. This study presents a framework for calibrating warm-rain bulk schemes using high-fidelity super-droplet simulations that provide a more accurate and physically based representation of cloud and precipitation processes. The calibration framework employs ensemble Kalman methods including Ensemble Kalman Inversion and Unscented Kalman Inversion to calibrate bulk microphysics schemes with probabilistic super-droplet simulations. We demonstrate the framework's effectiveness by calibrating a single-moment bulk scheme, resulting in a reduction of data-model mismatch by more than 75% compared to the model with initial parameters. Thus, this study demonstrates a powerful tool for enhancing the accuracy of bulk microphysics schemes in atmospheric models and improving climate modeling.

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SA @illinois.edu (now @agh.edu.pl) immersion freezing, . . .

particle-based modelling of immersion freezing

Monte-Carlo SCE alternatives: e.g., SDM by Shima et al.

Shima et al. 2009 (doi:10.1002/qj.441): warm-rain

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

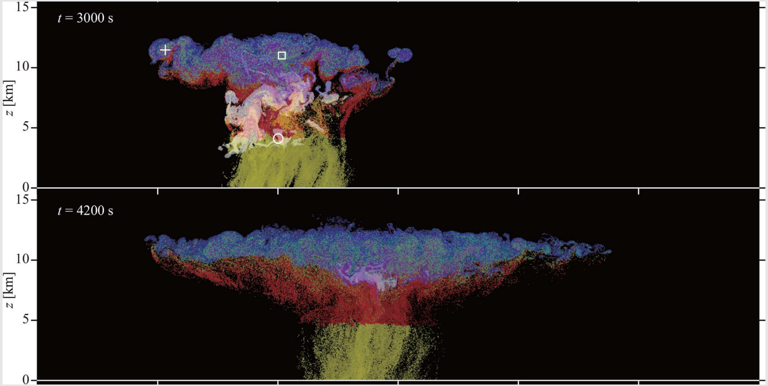
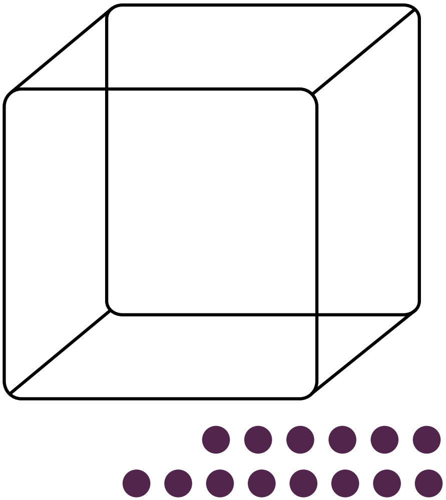
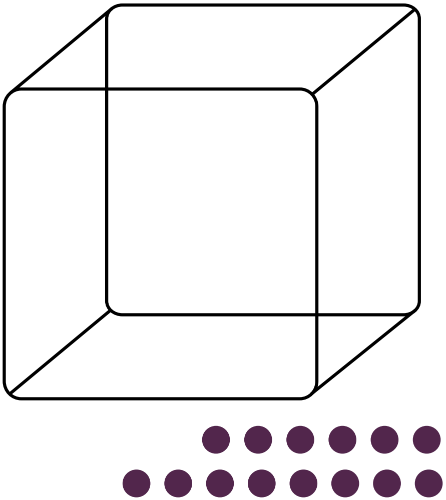


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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



Domain randomly populated with "μ-physics information carriers"

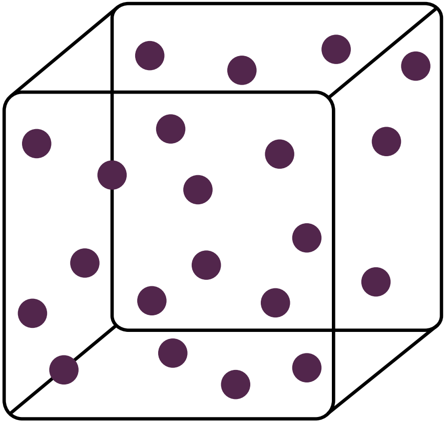
(super particles / super droplets)



Domain randomly populated with "μ-physics information carriers"

(super particles / super droplets)

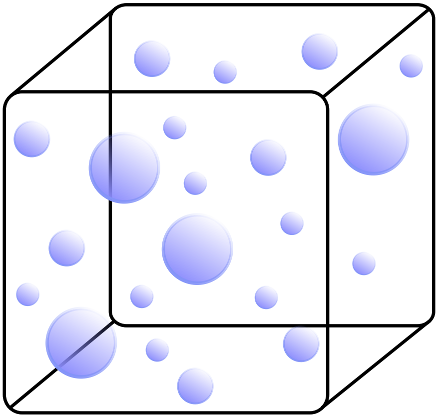
carrier attributes:



Domain randomly populated with "μ-physics information carriers"
(super particles / super droplets)

carrier attributes:

- location

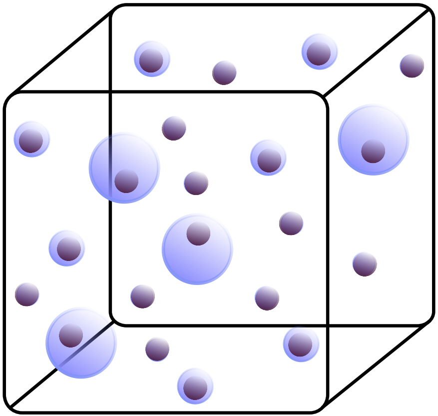


Domain randomly populated with "μ-physics information carriers"

(super particles / super droplets)

carrier attributes:

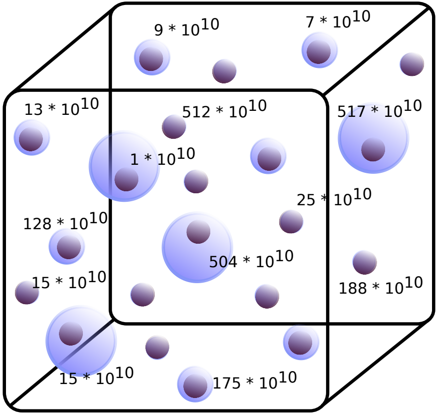
- location
- wet radius



Domain randomly populated with "μ-physics information carriers"
(super particles / super droplets)

carrier attributes:

- location
- wet radius
- CCN/INP size



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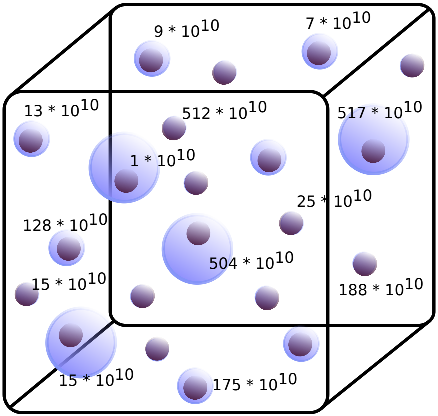
carrier attributes:

- location
- wet radius
- CCN/INP size
- multiplicity



Domain randomly populated with "μ-physics information carriers"

(super particles / super droplets)

carrier attributes:

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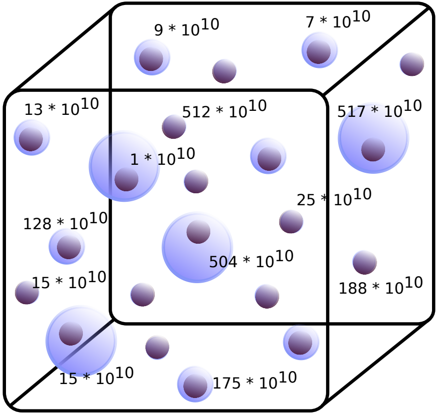

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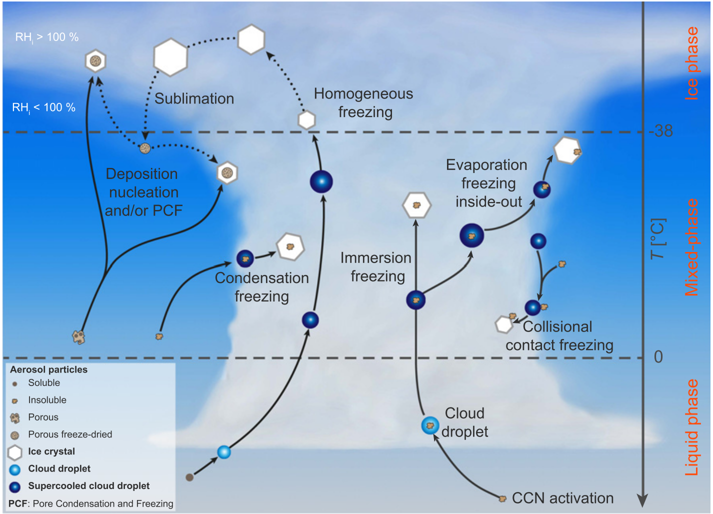
- ...
- freezing temperature?
- freezing rate (temperature)?



Kanji et al. 2017, graphics F. Mahrt, https://doi.org/10.1175/AMSMONOGRAPHS-D-16-0006.1

Journal of Geophysical Research: Atmospheres

RESEARCH ARTICLE
10.1002/2016JD025251

Key Points:
- Very ice active Snomax protein aggregates are fragile and their ice nucleation ability decreases over months of freezer storage
- Partitioning of ice active protein aggregates into the immersion oil reduces the droplet's measured freezing temperature
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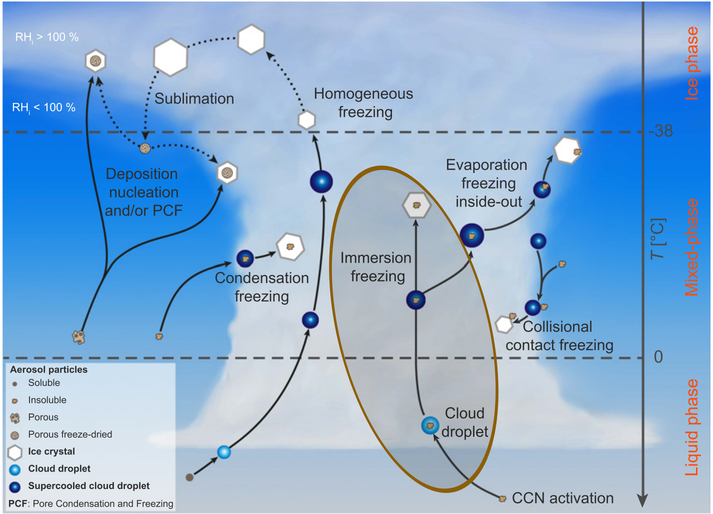

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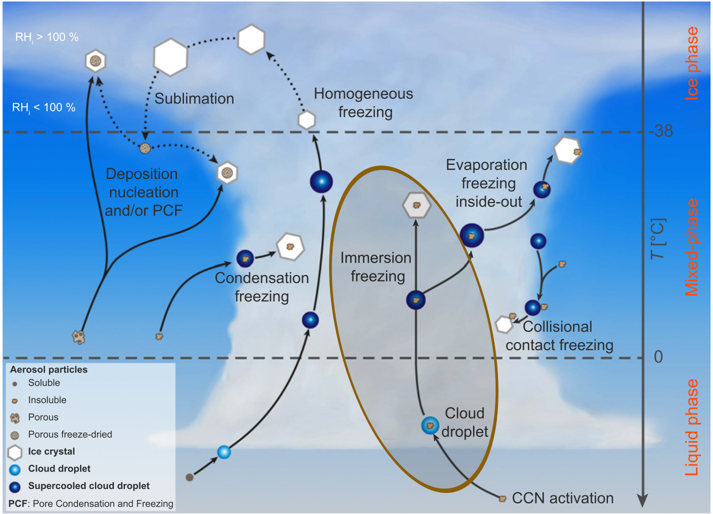

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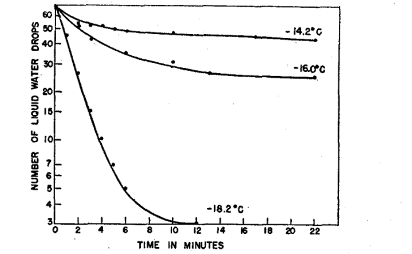
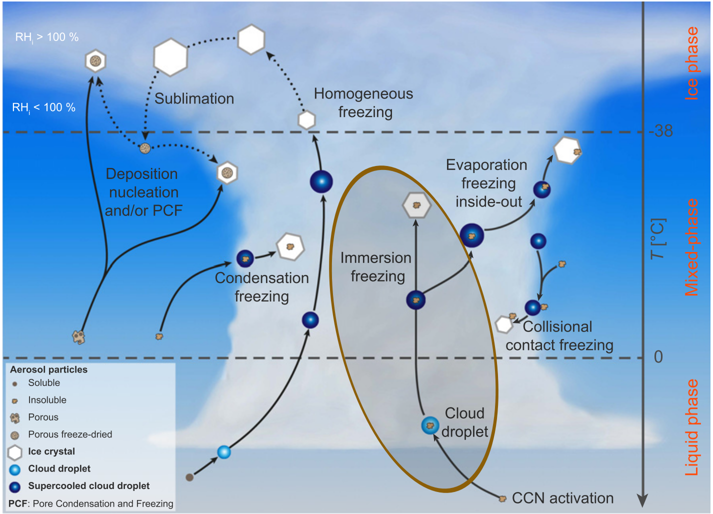


Fraction of water drops remaining unfrozen as a function of time.



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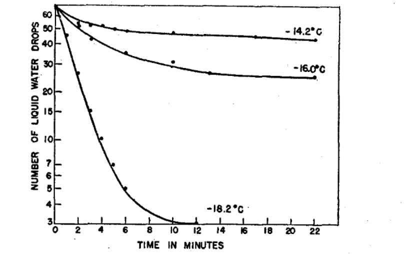

Fraction of water drops remaining unfrozen as a function of time.

Vali 2014 (ACP)

"Interpretations of the experimental results face considerable difficulties ... two separate ways of interpreting the same observations; one assigned primacy to time the other emphasized the temperature-dependent impacts of the impurities ... dichotomy – the stochastic and singular models"

Marshall et al. 1961 (Nubila 4:1)

Heterogeneous Nucleations is a Stochastic Process

by

J. S. MARSHALL

McGill University, Montreal, Canad.

Presented at the International Congress on the Physics of Clouds (Hailstorms) at Verona 9-13 August 1960.

http://cma.entecra.it/Astro2_sito/doc/Nubila_1_1961.pdf

theory (in modern notation)

(Bigg '53, Langham & Mason '58, Carte '59, Marshall '61)

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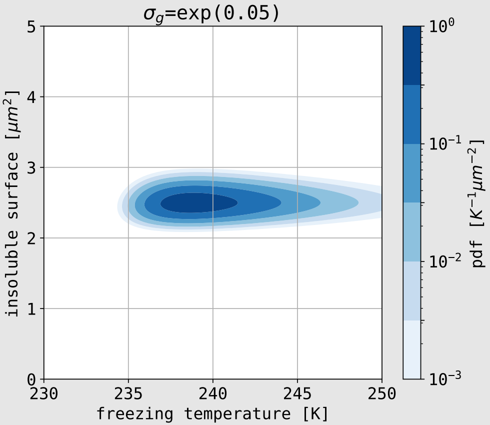

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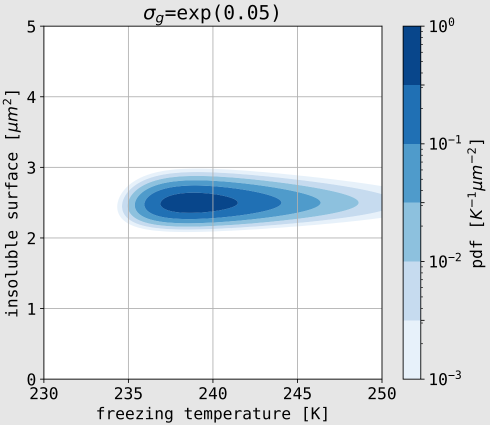

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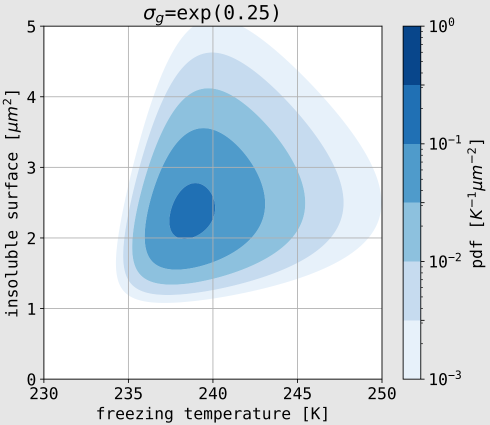

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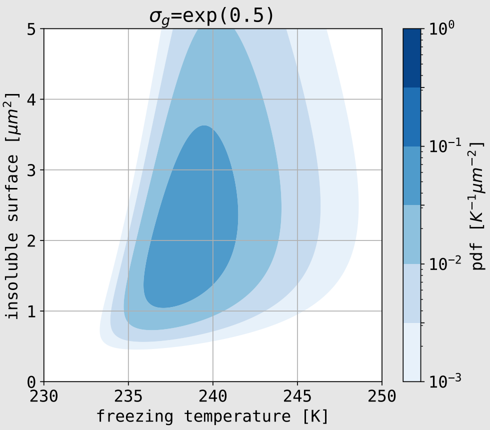

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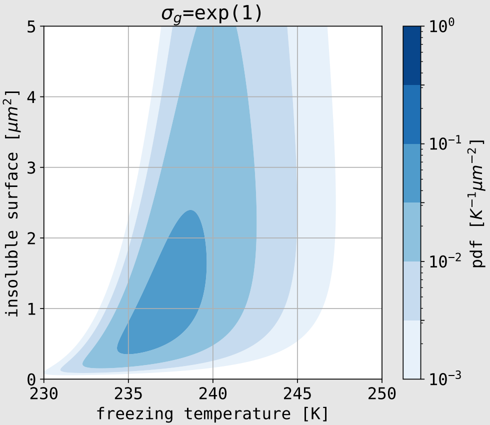

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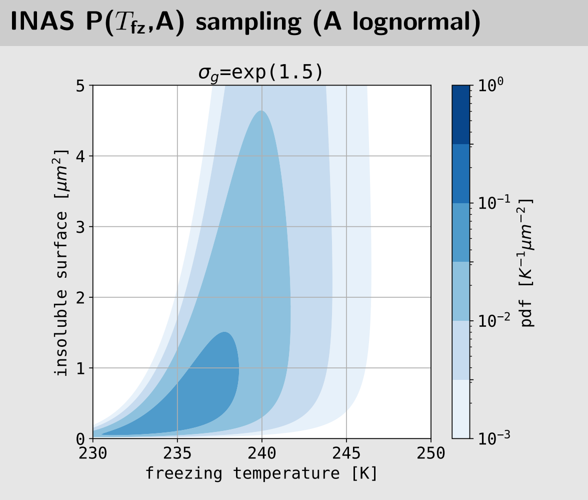

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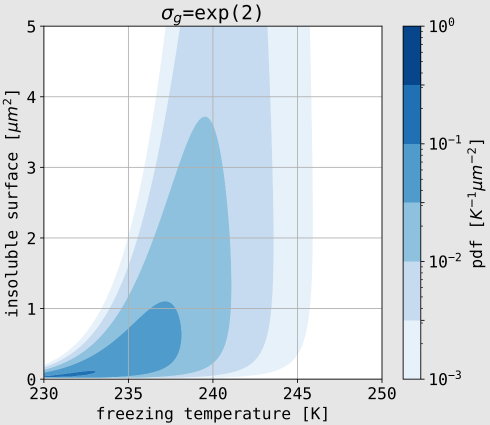

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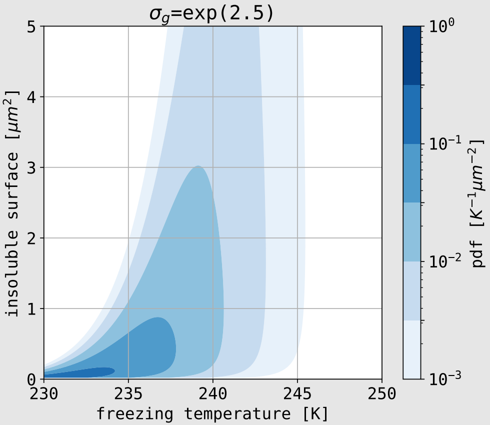

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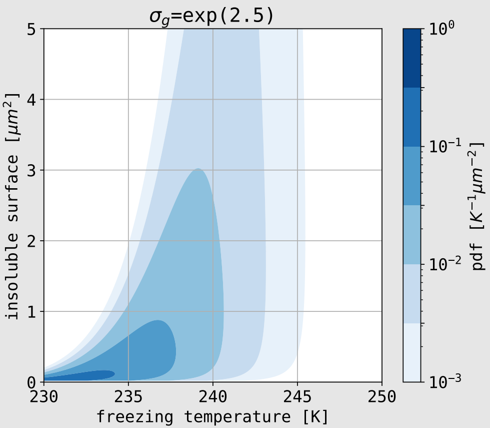

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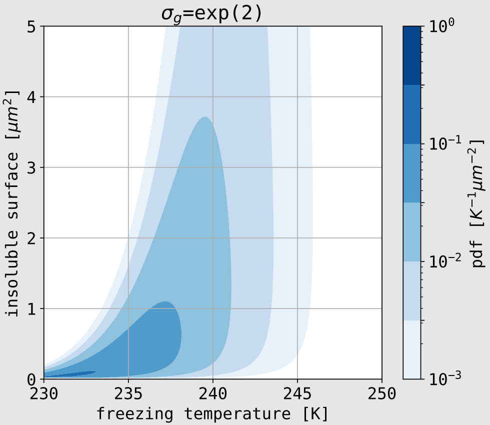

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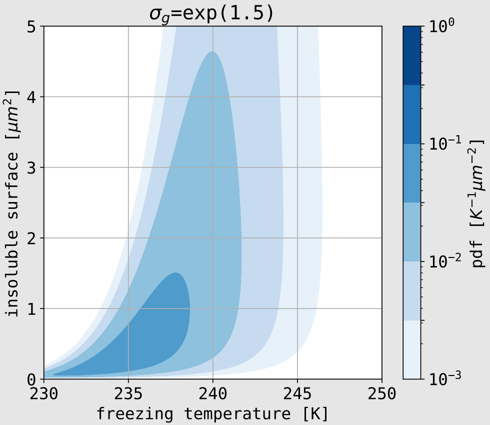

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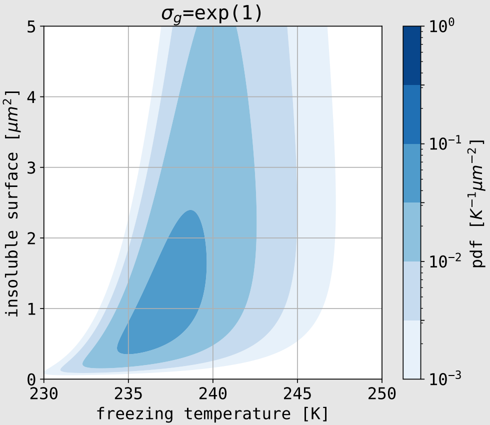

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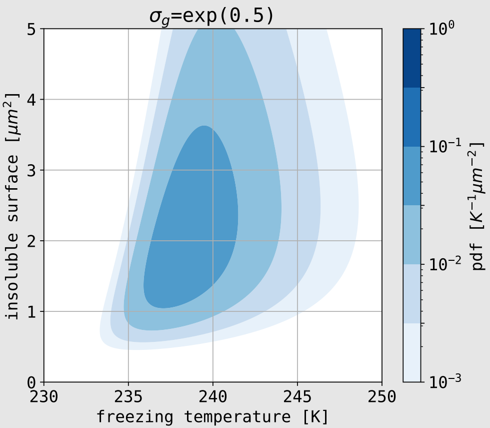

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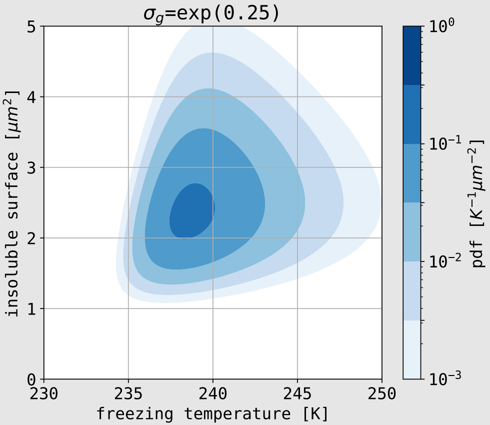

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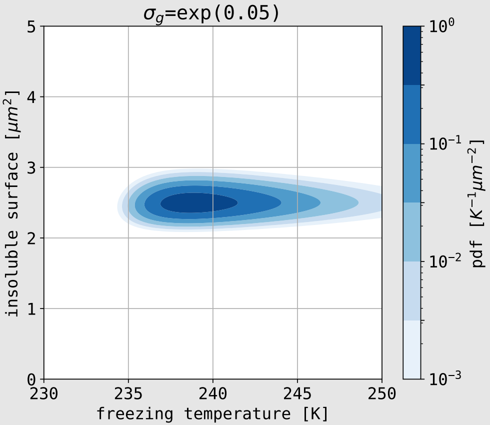

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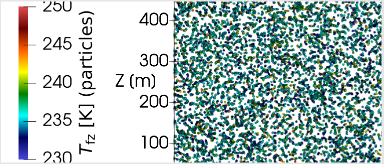
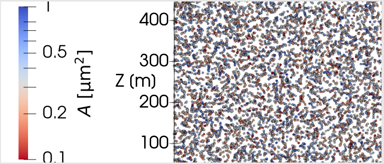


time-dependent (ABIFM)



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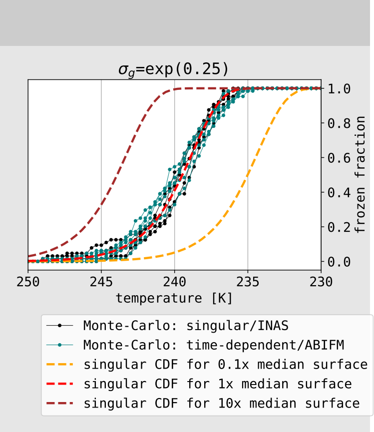

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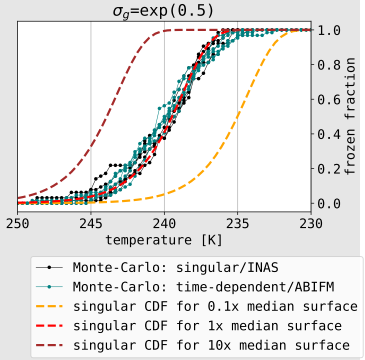

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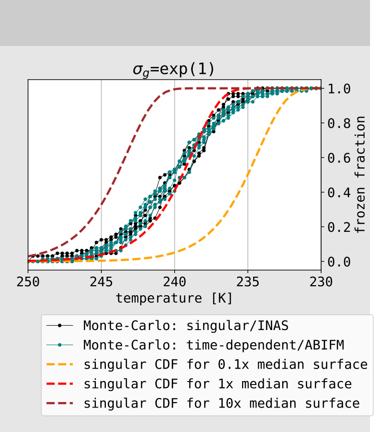

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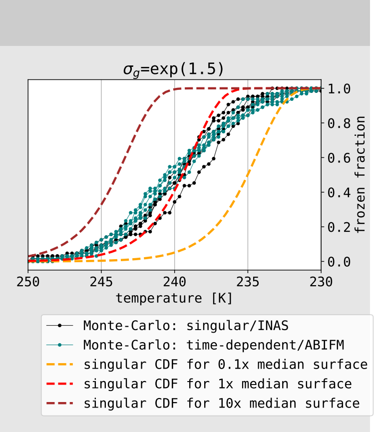

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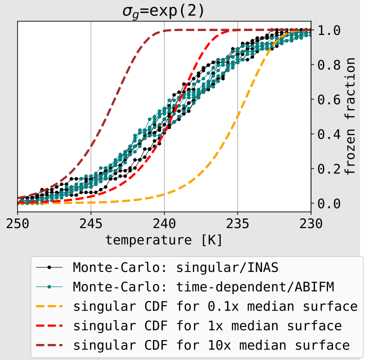

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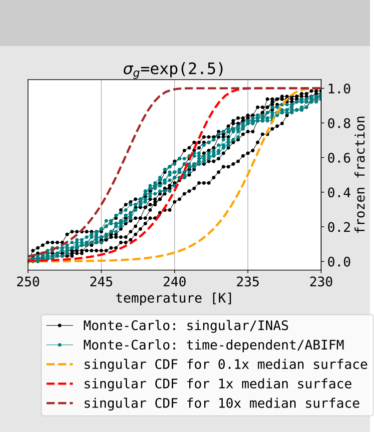

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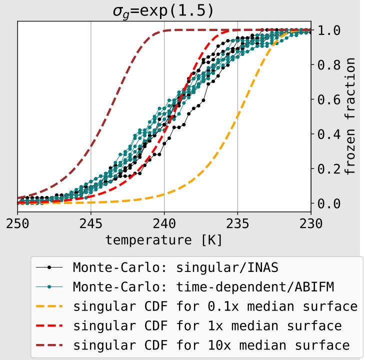

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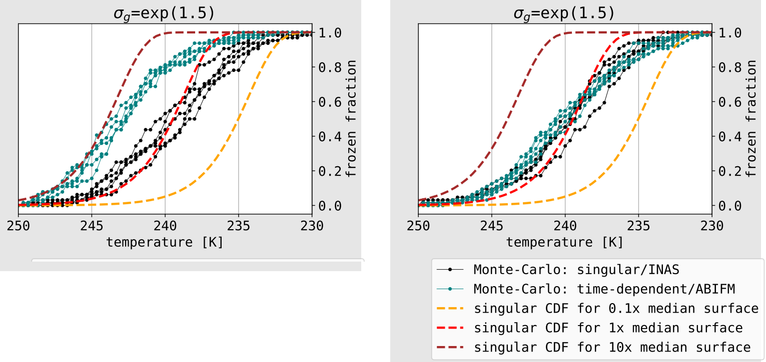

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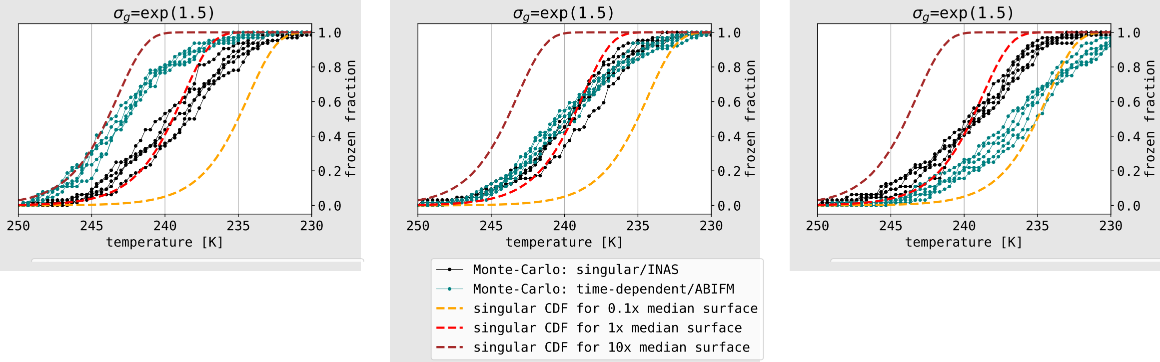

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INAS: $$I(T) = n_s(T) = \exp(a \cdot (T - T_{0°C}) + b)$$

experimental $n_s(T)$ fits: e.g., Niemand et al. 2012

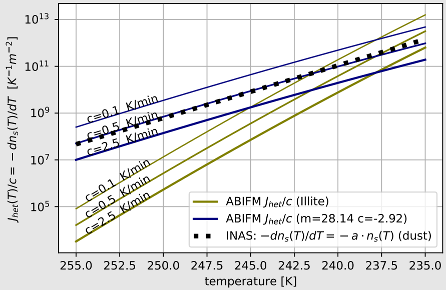
for a constant cooling rate $c = dT/dt$:

$$\ln(1 - P(A,t)) = -\frac{A}{c}\int_{T_0}^{T_0+ct} J_{\text{het}}(T')dT' = -A \cdot I(T)$$

$$\frac{dn_s(T)}{dT} = a \cdot n_s(T) = -\frac{1}{c} J_{\text{het}}(T)$$

experimental fits: INAS n_s (Niemand et al. '12)

ABIFM J_{het} (Knopf & Alpert '13)



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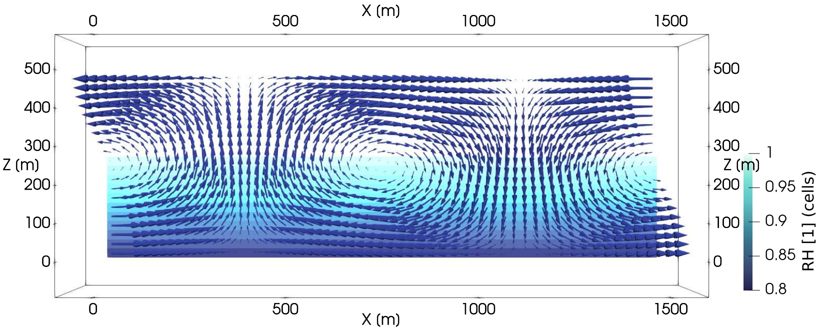

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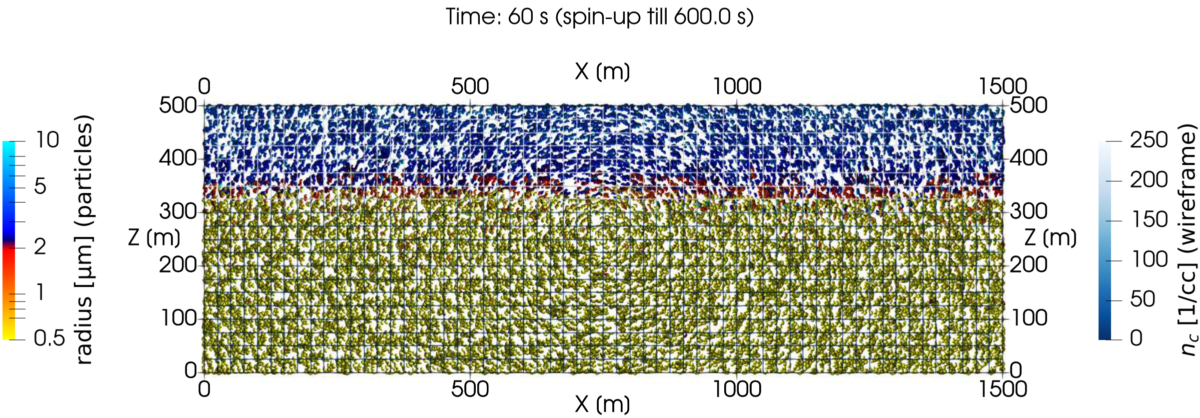

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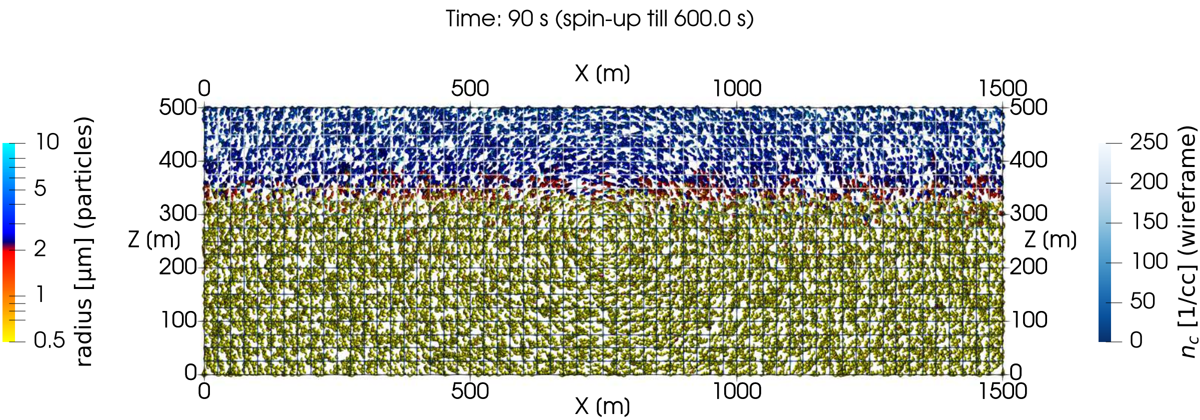

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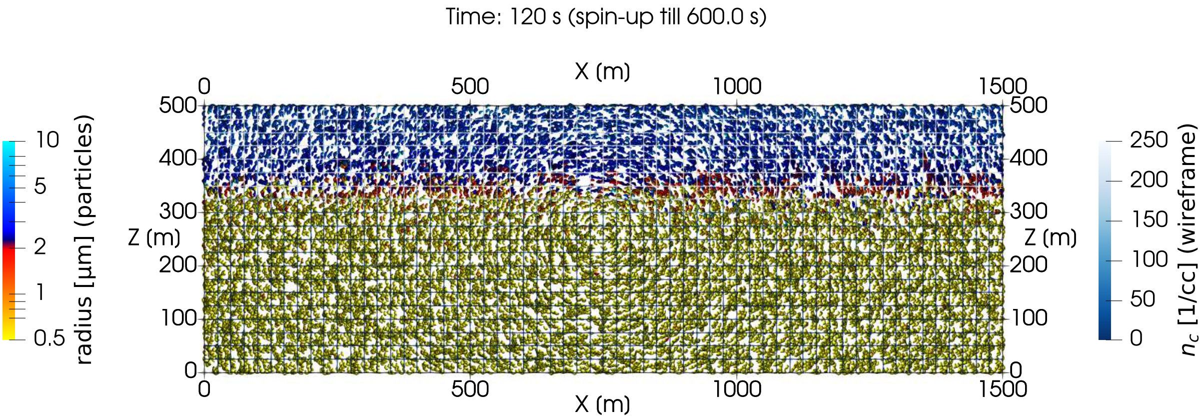

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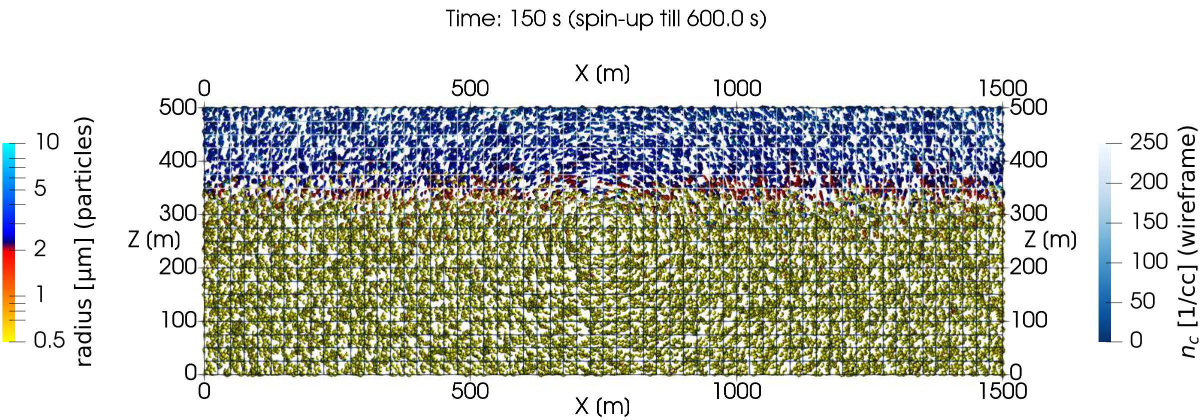

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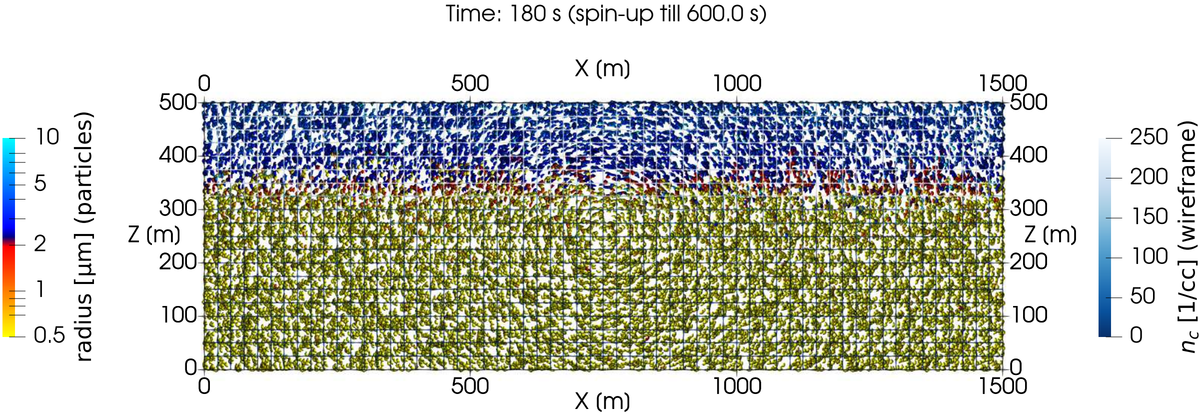

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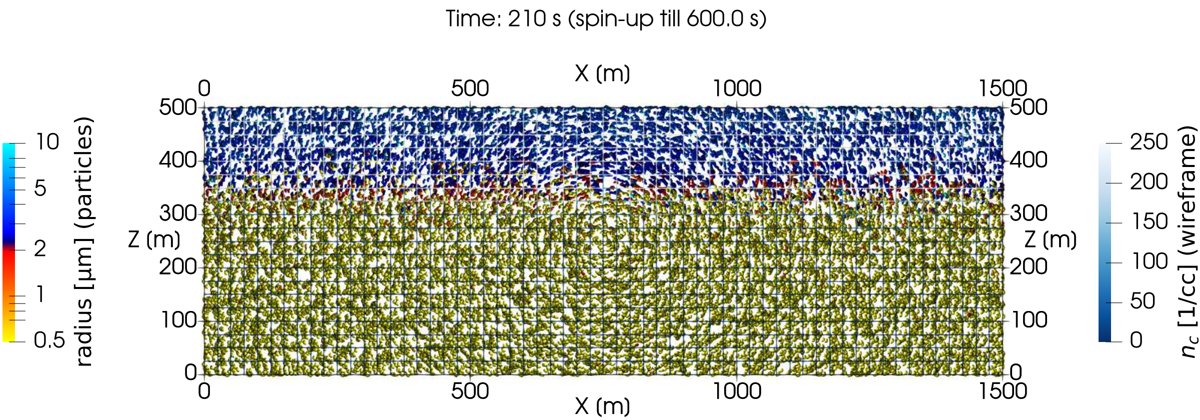

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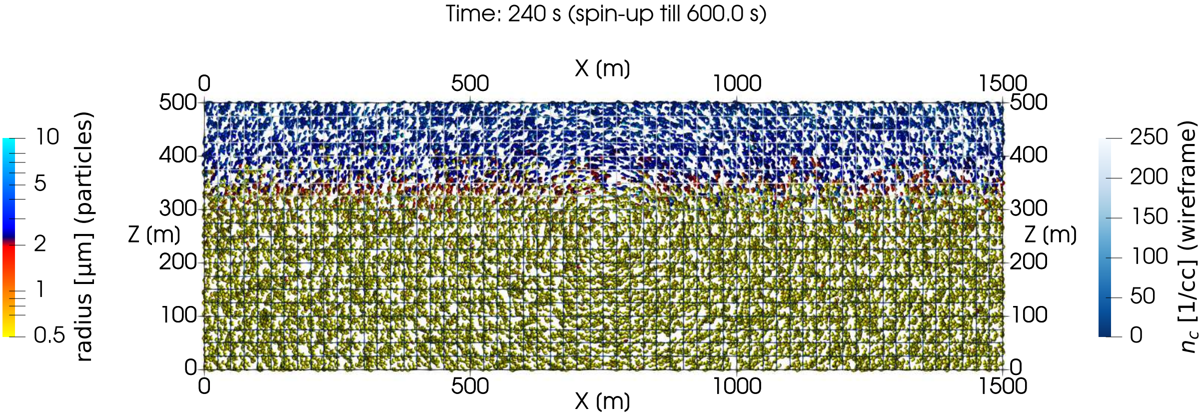

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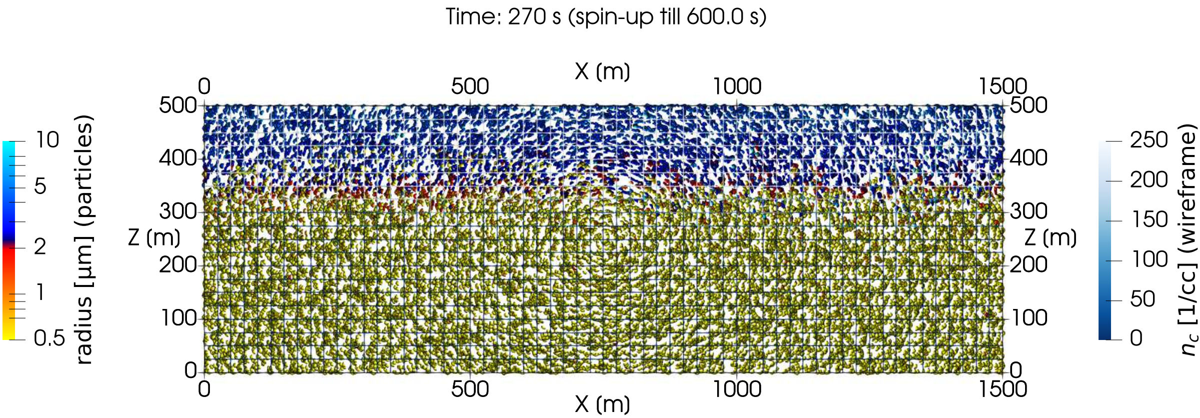

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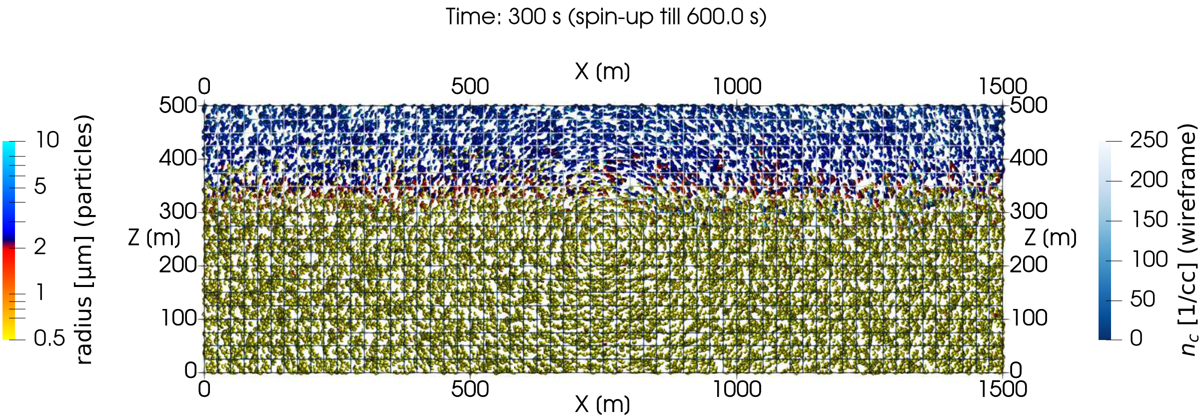

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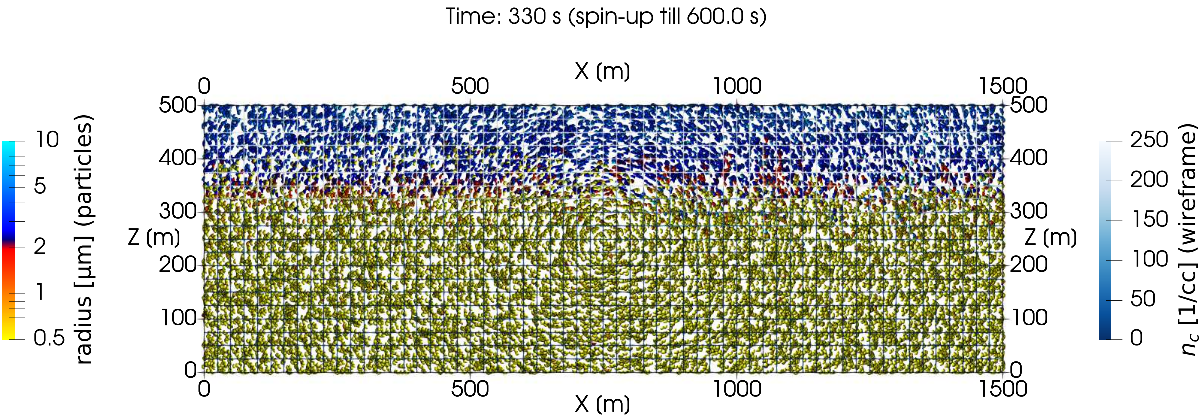

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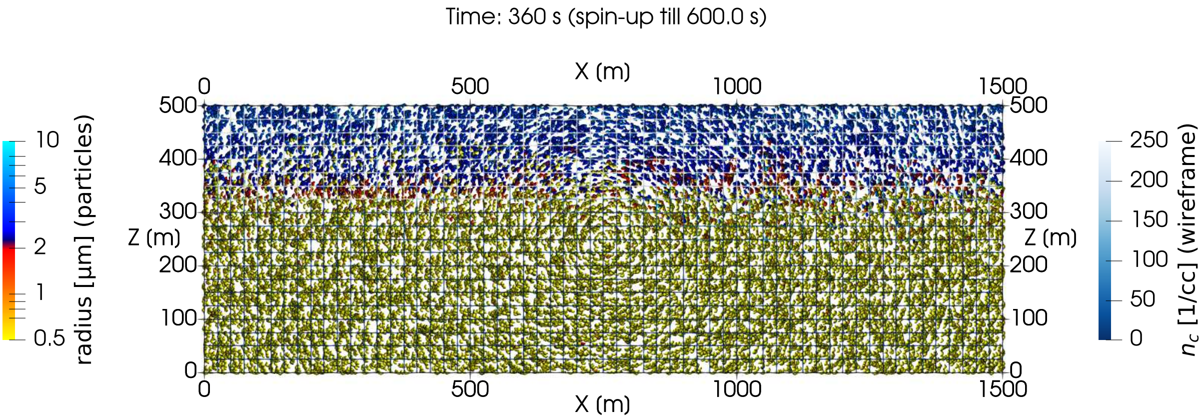

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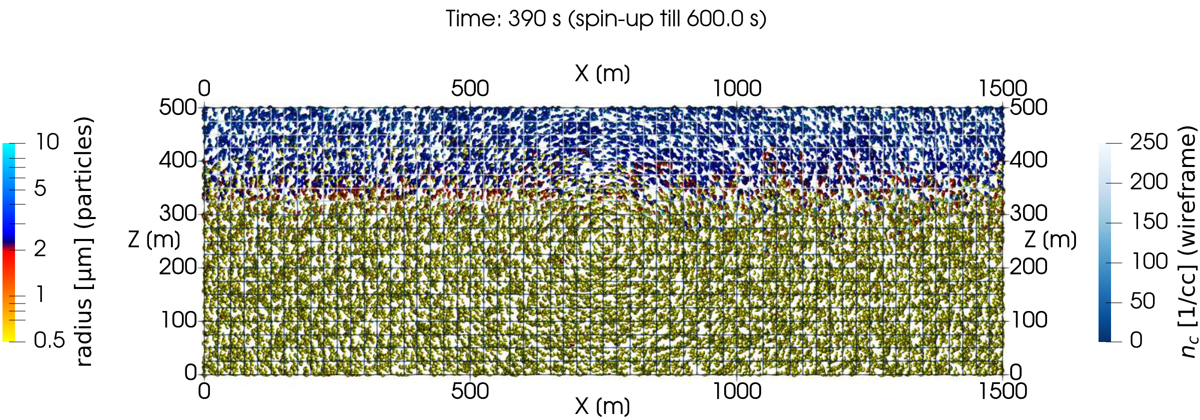

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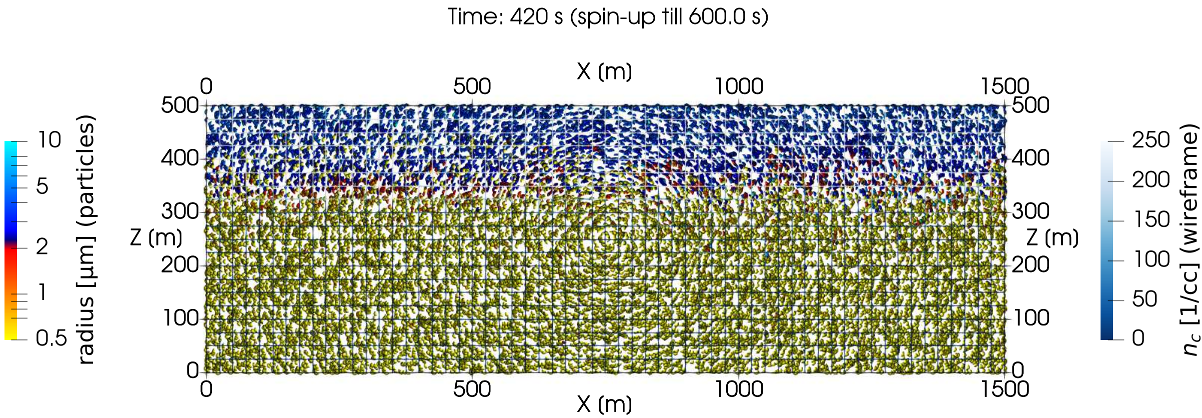

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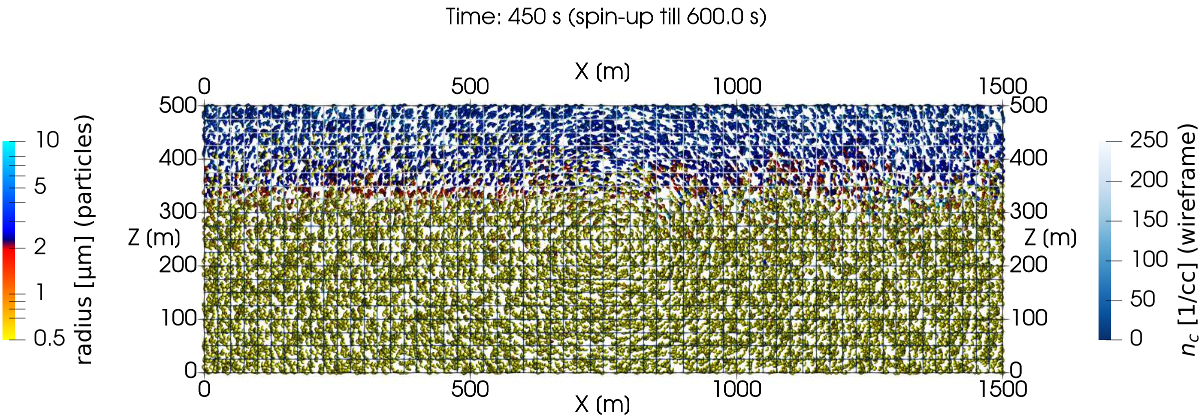

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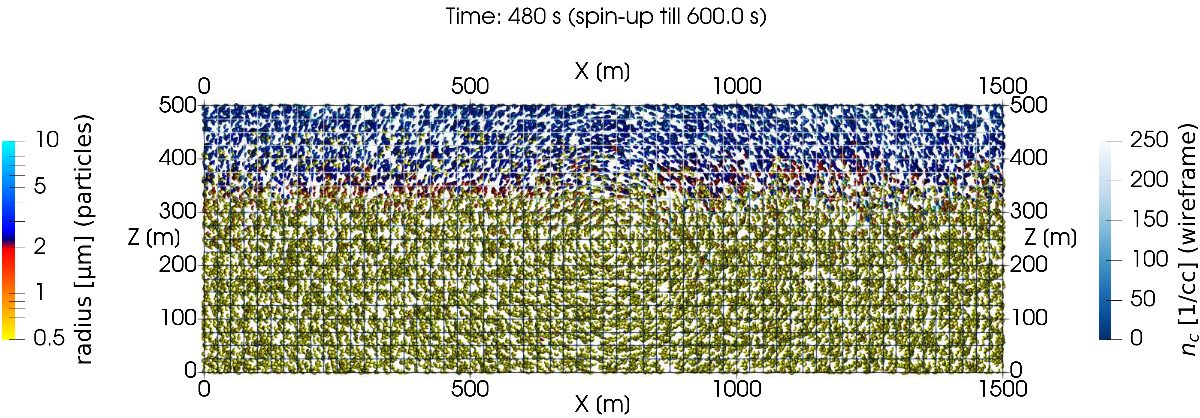

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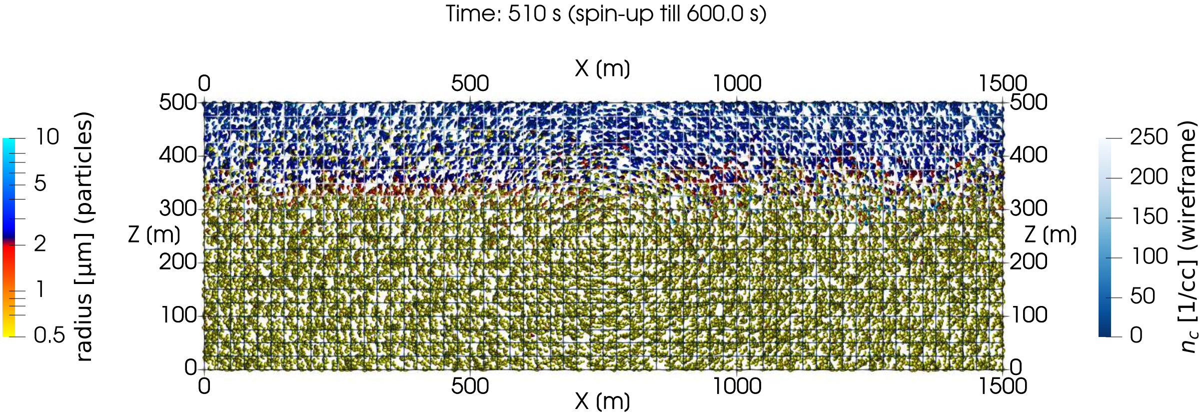

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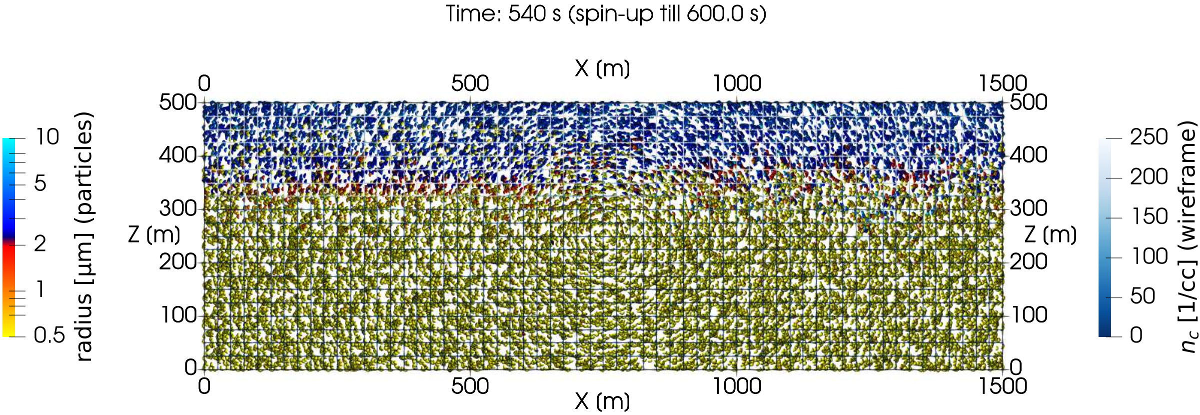

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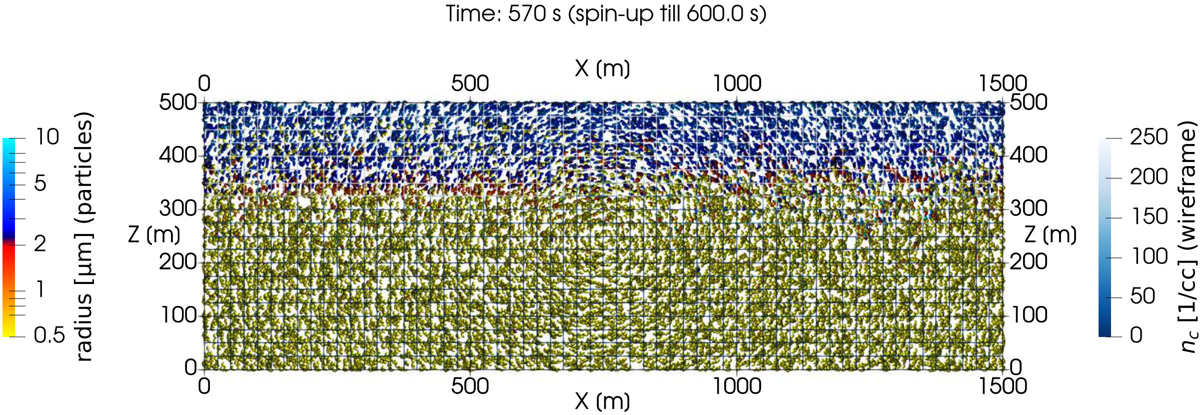

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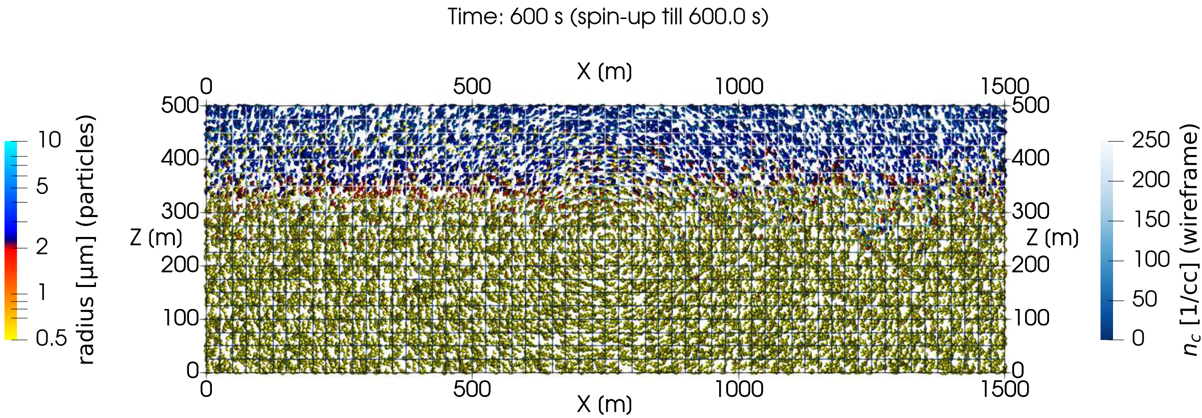

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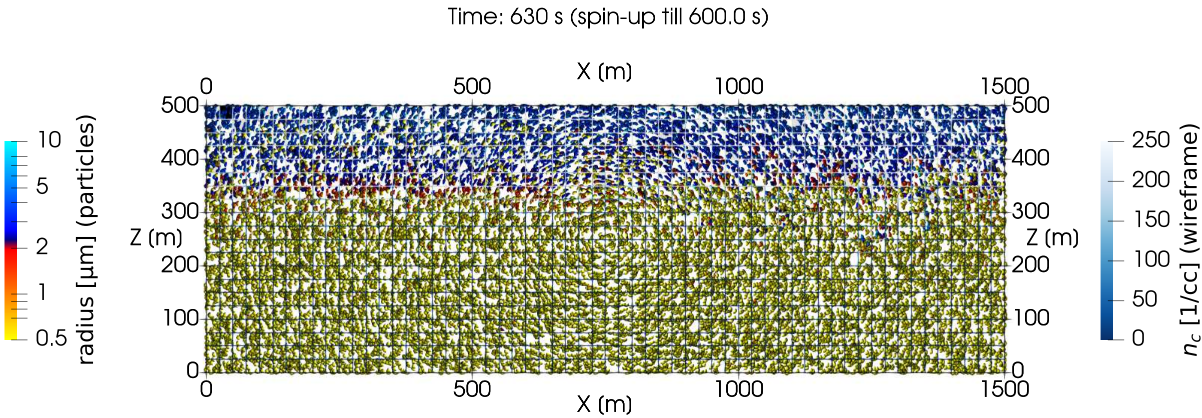

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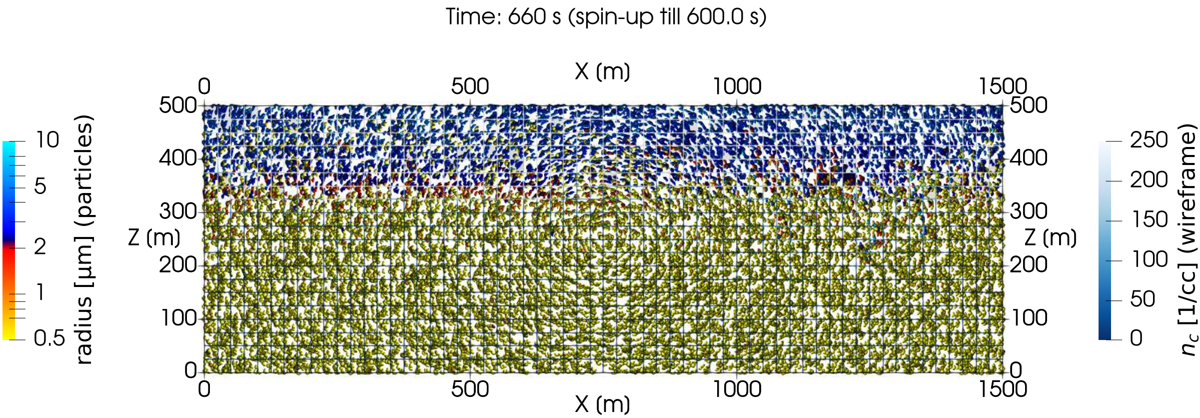

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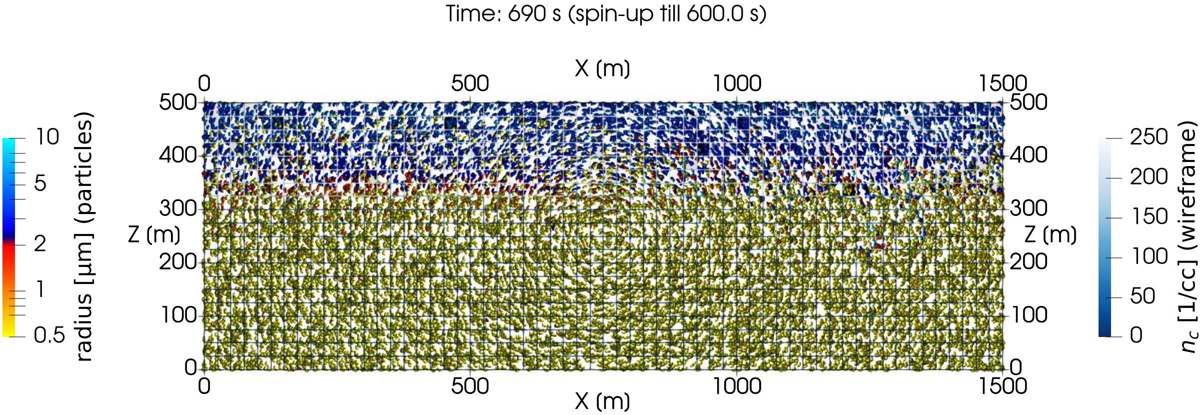

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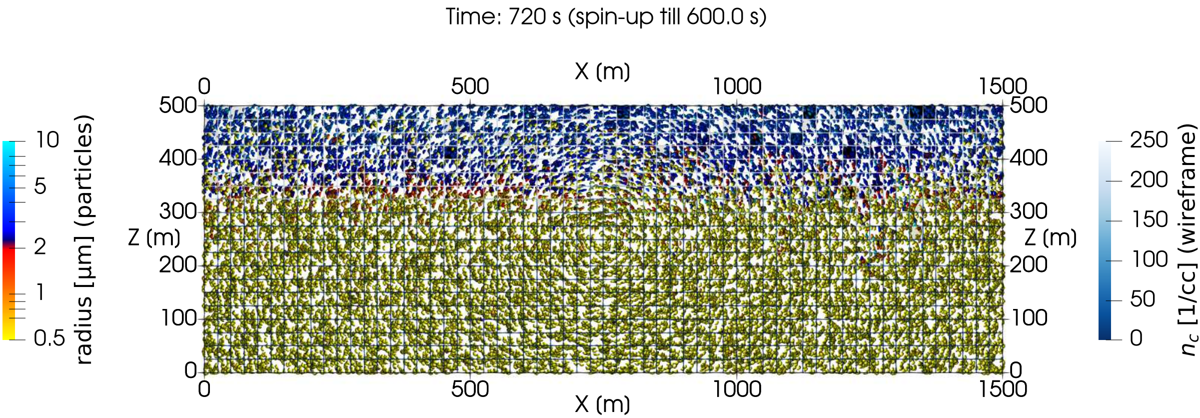

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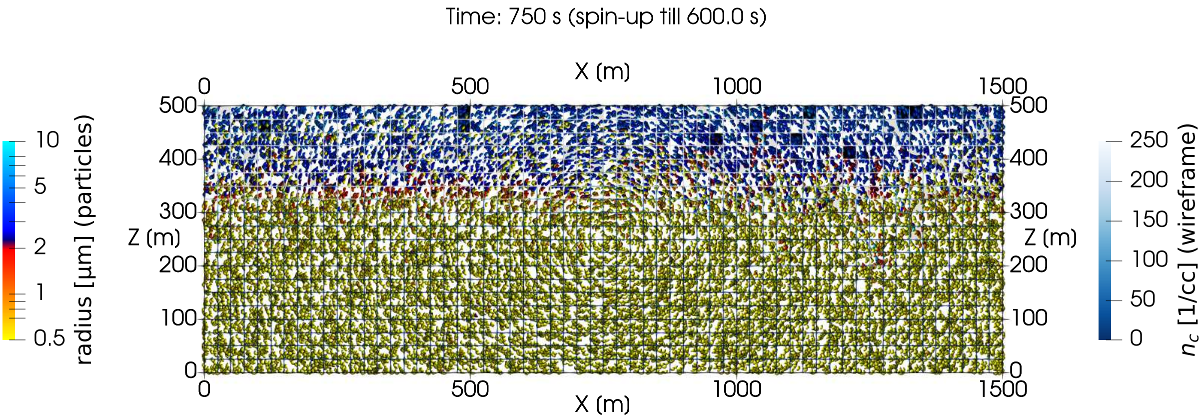

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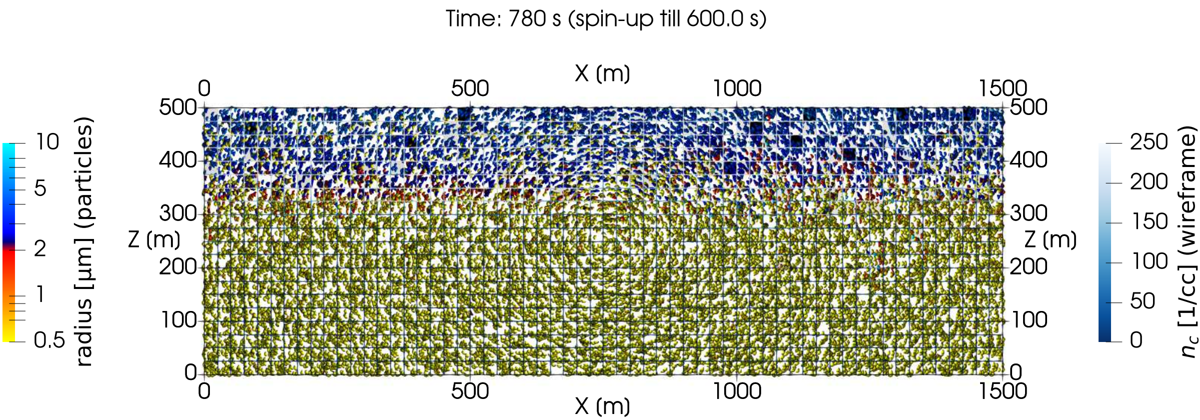

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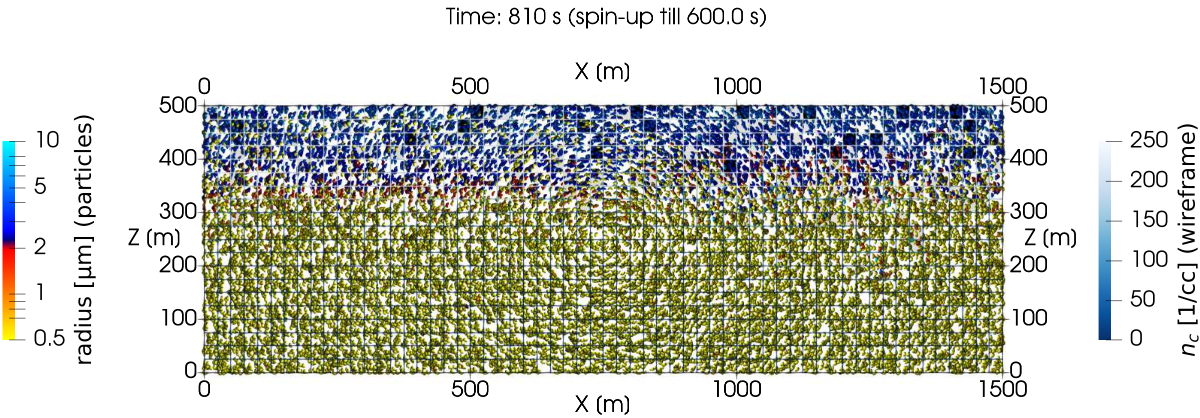

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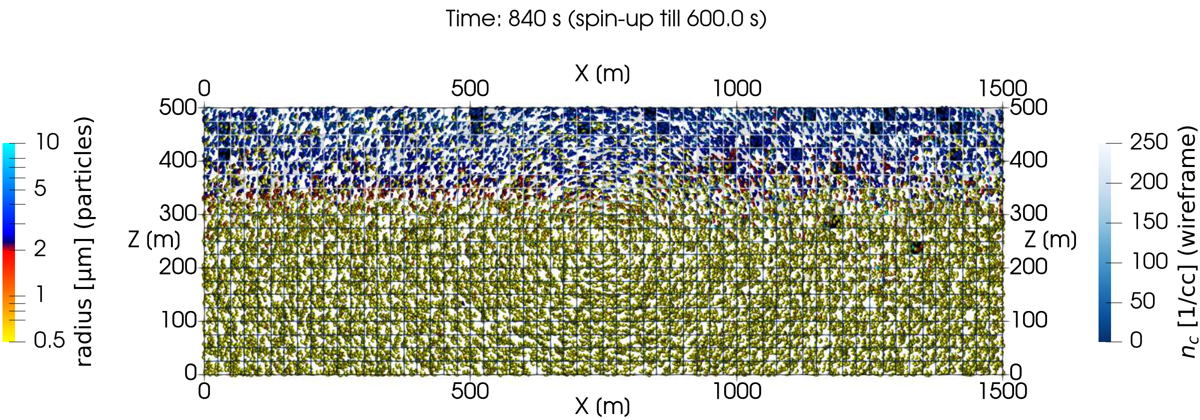

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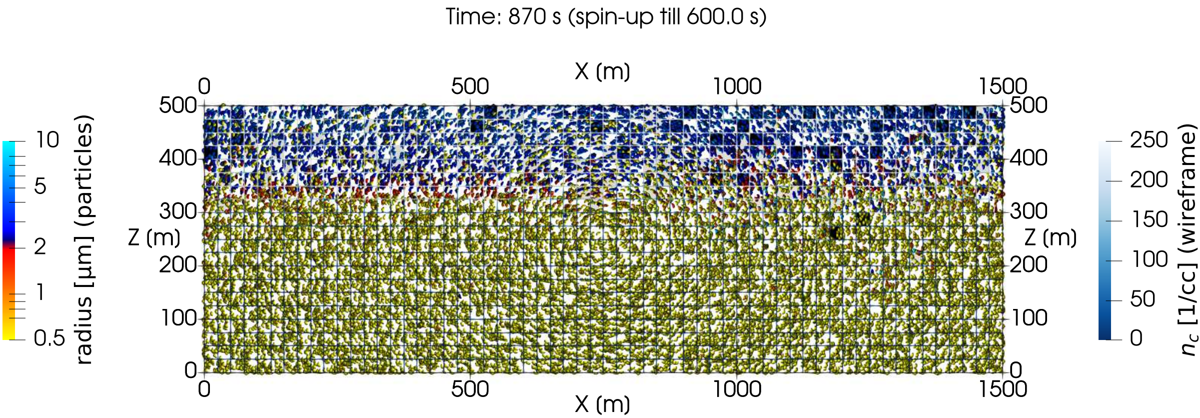

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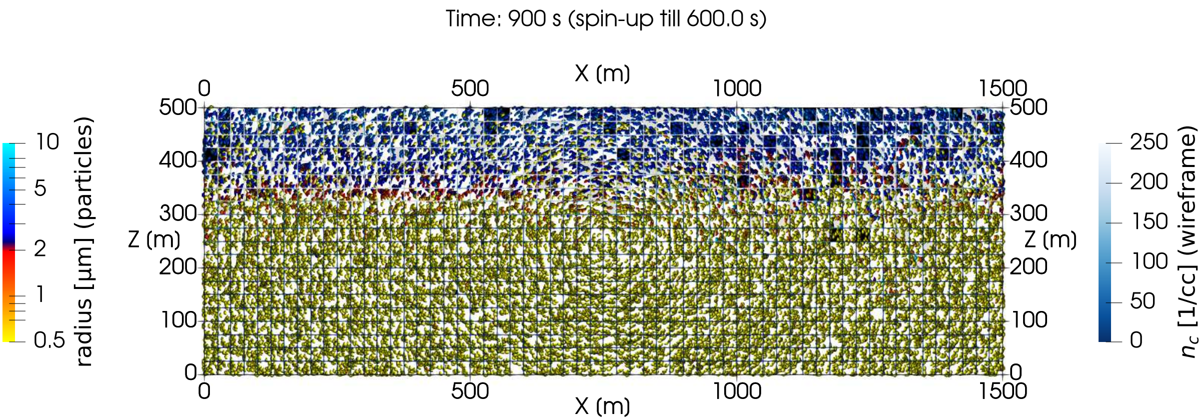

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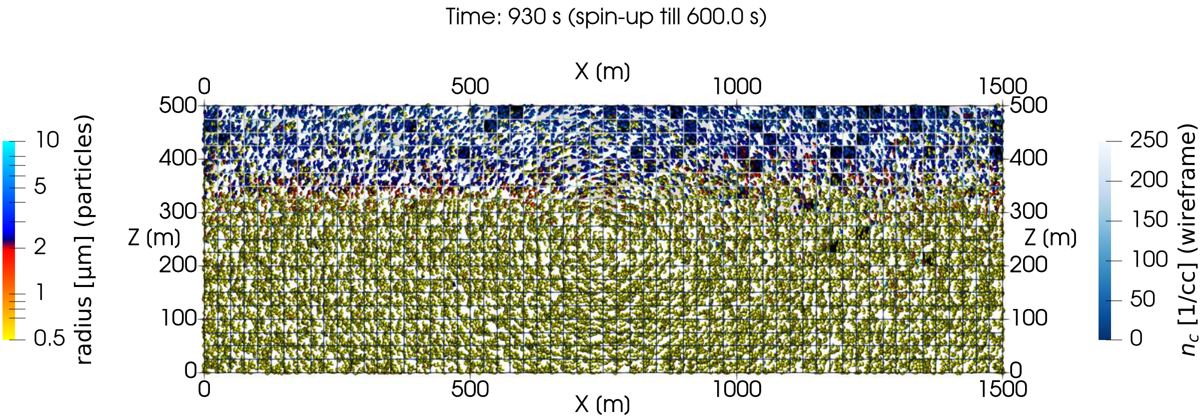

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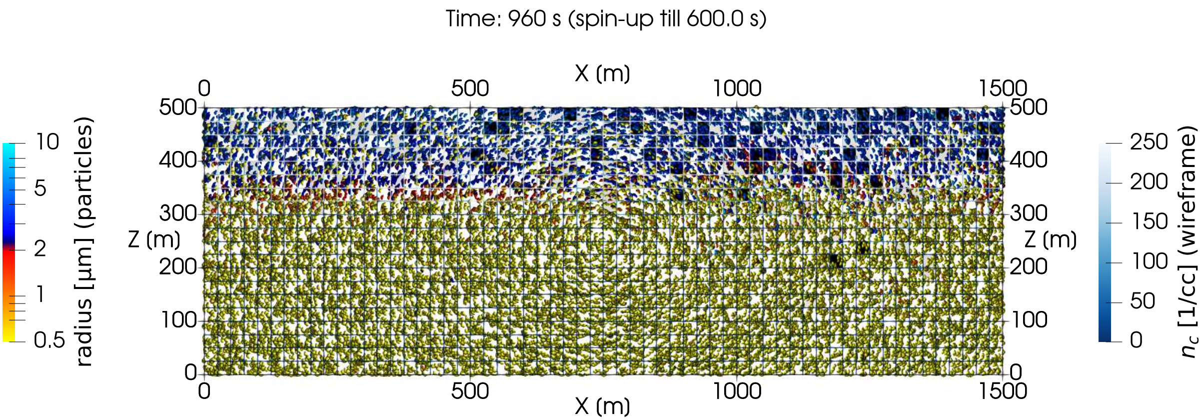

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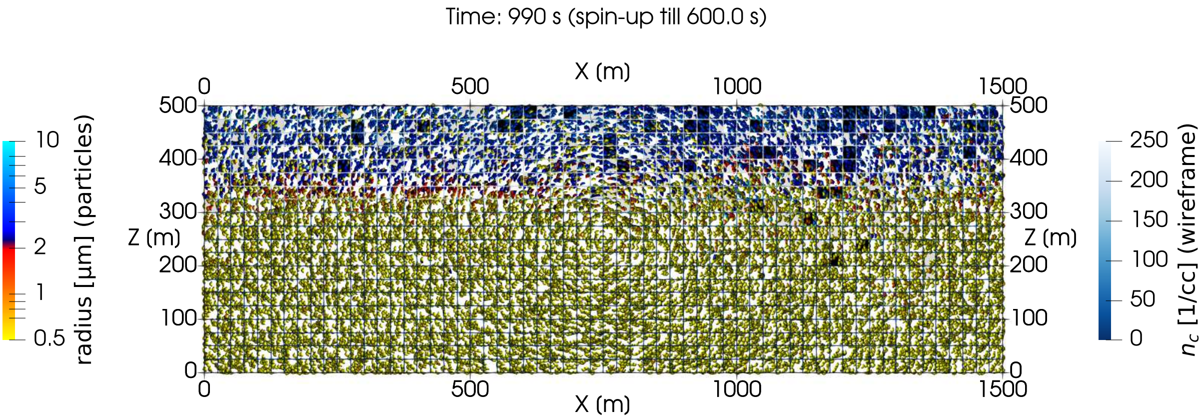

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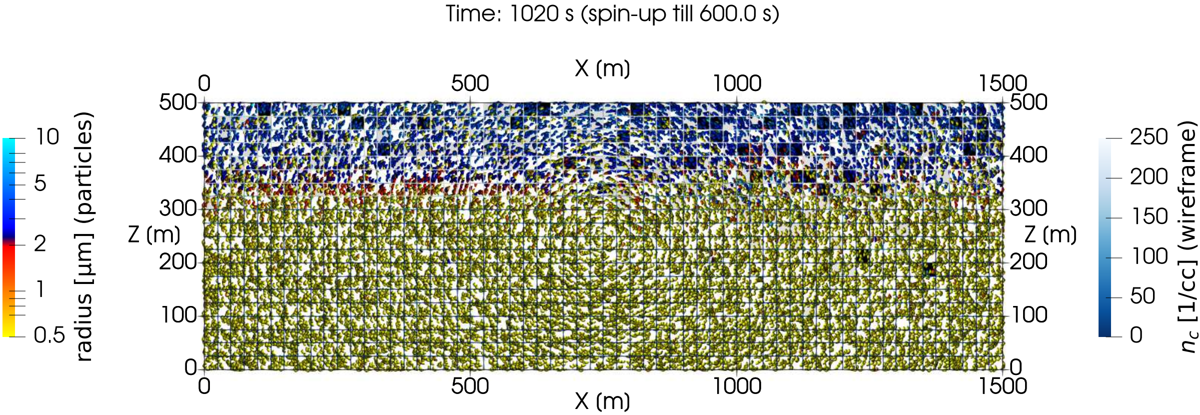

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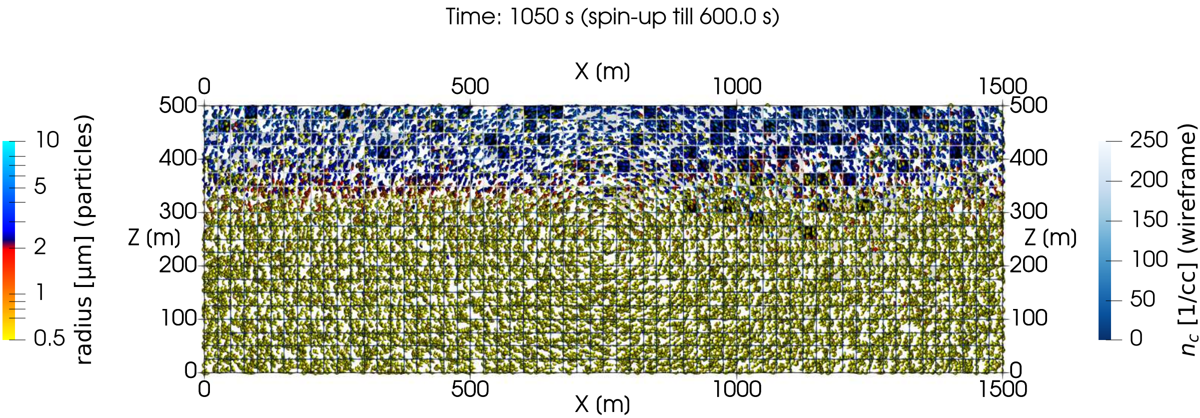

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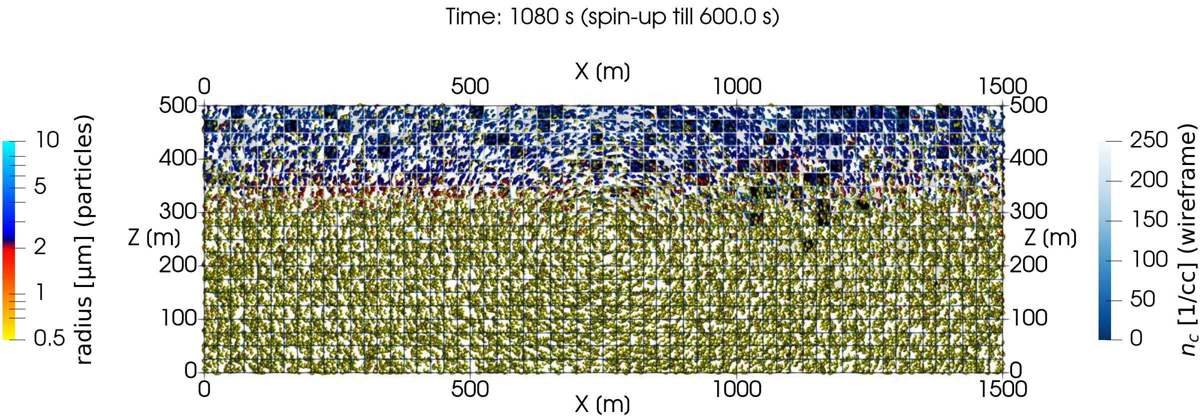

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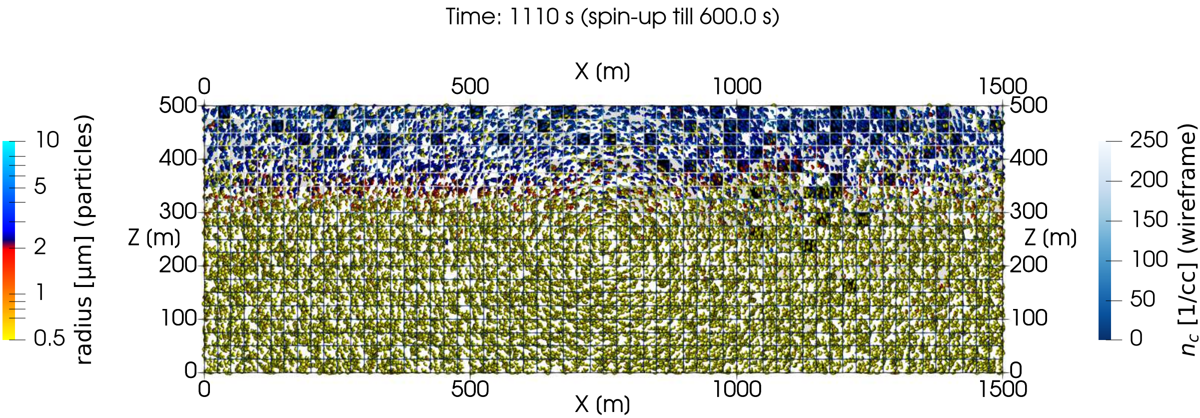
spin-up = freezing off; subsequently frozen particles act as tracers

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



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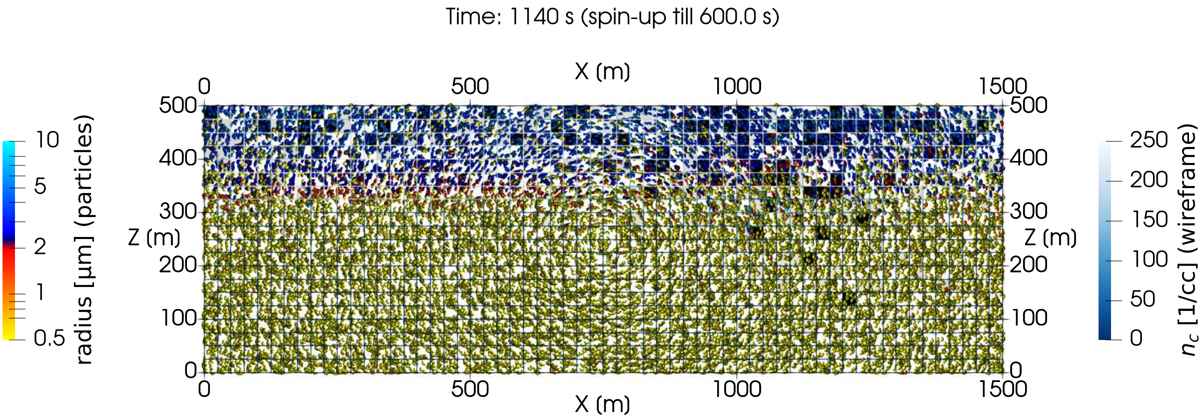

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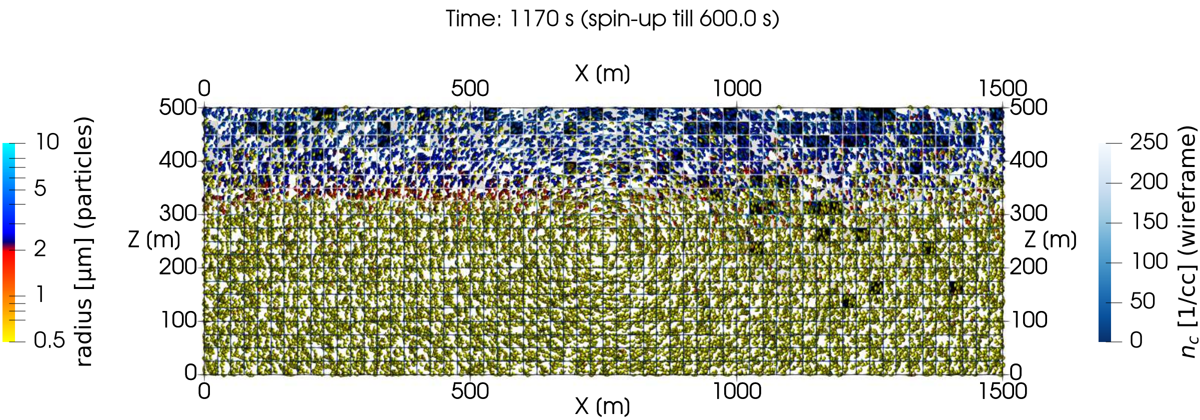

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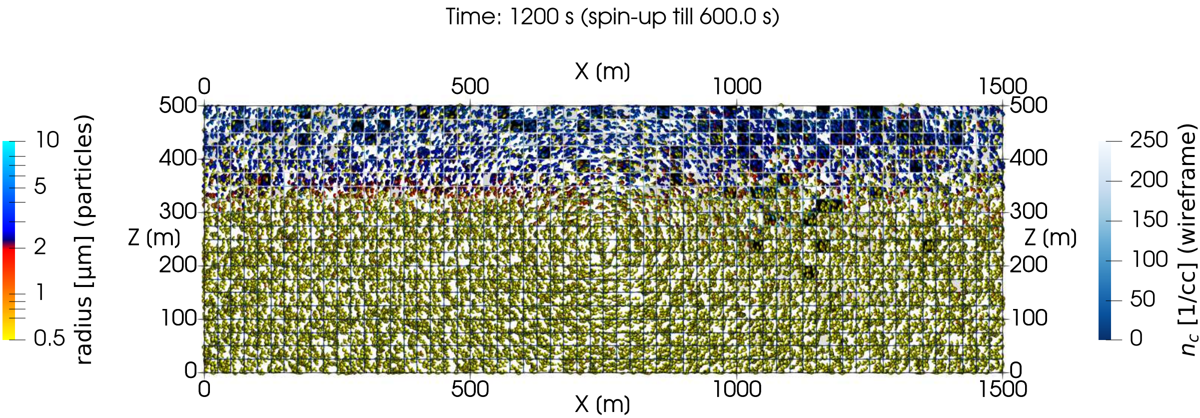

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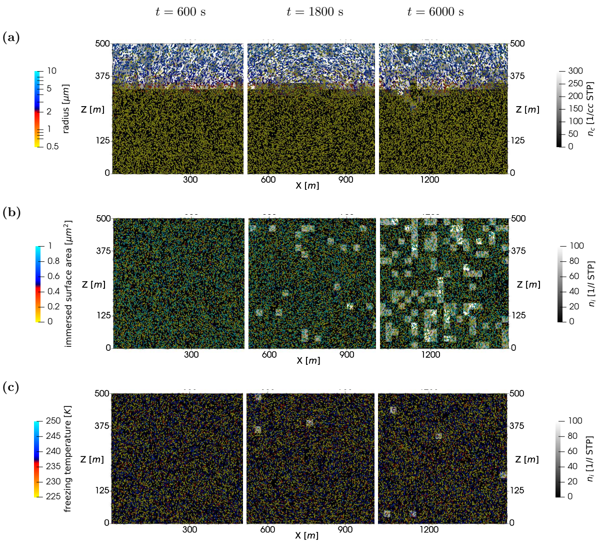

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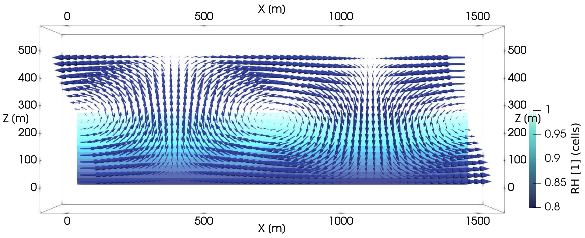
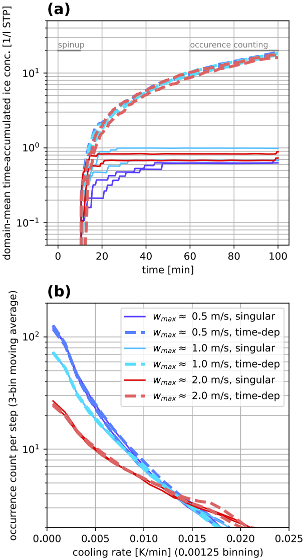


⇝ singular model not robust to flow regimes

⇝ working with Tim on extending to ice growth



PySDM@Kraków funding:

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NATIONAL SCIENCE CENTRE POLAND

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AMS Annual Meeting @Houston (25-29 Jan 2026) session

AMS 2026

106TH ANNUAL MEETING

AMERICAN METEOROLOGICAL SOCIETY

25-29 JANUARY 2026 | HOUSTON, TX & ONLINE

18th Symposium on Aerosol–Cloud– Climate Interactions

Third Symposium on Cloud Physics

Abstracts are due by **14 August 2025 at 5:00 PM ET**

SUBMIT ABSTRACT

Joint Sessions

- Advances in numerical modeling of aerosol-cloud interactions: moment-, bin- and particle-resolved methods and beyond

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Thank you for your attention!

sylwester.arabas@agh.edu.pl