Supercooling super-droplets:
on particle-based modelling of immersion freezing

S. Arabas[1,2], J.H. Curtis[1], I. Silber[3], A. Fridlind[4], D.A Knopf[5], M. West[1] & N. Riemer[1]

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funding:
ASR Atmospheric System Research

Environmental Science and Engineering Seminar

Caltech, Feb 9 2022

aerosol-cloud interactions: a conceptual picture

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background image: `vitsly.ru` / Hokusai

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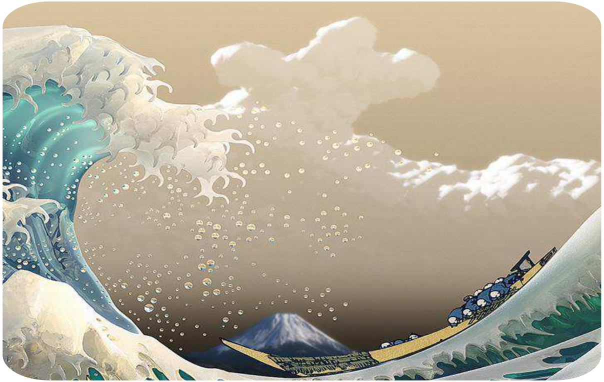

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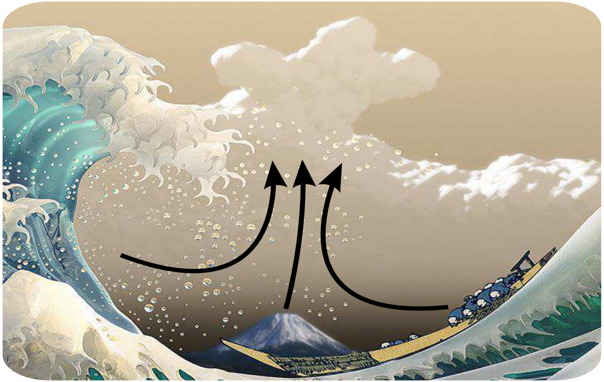
- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei



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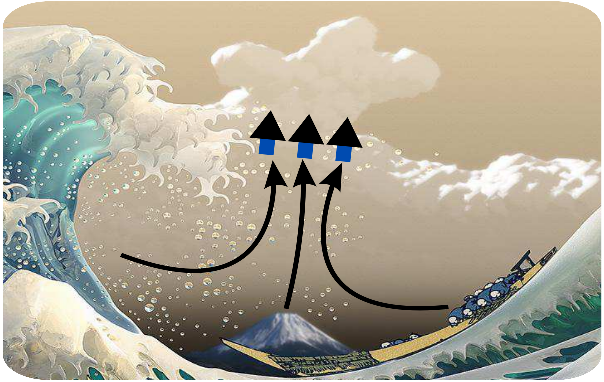

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two-way interactions:
- aerosol characteristics influence cloud microstructure
- cloud processes influence aerosol size and composition

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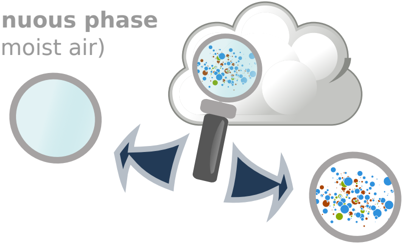
modelling cloud μ-physics: Eulerian vs. Lagrangian approaches

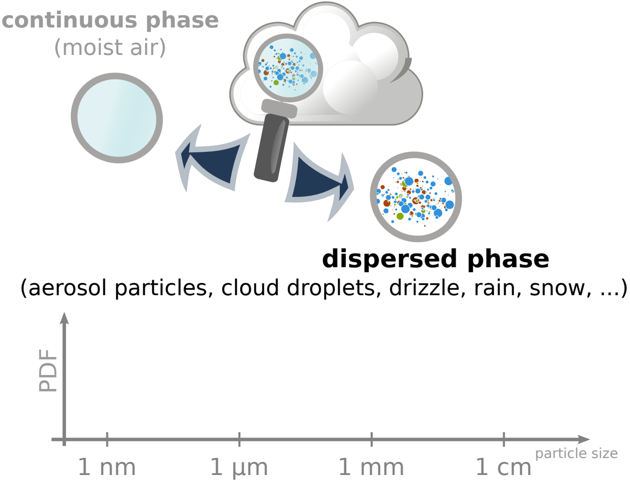
modelling cloud μ-physics: Eulerian vs. Lagrangian approaches

continuous phase
(moist air)



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

modelling cloud μ-physics: Eulerian vs. Lagrangian approaches



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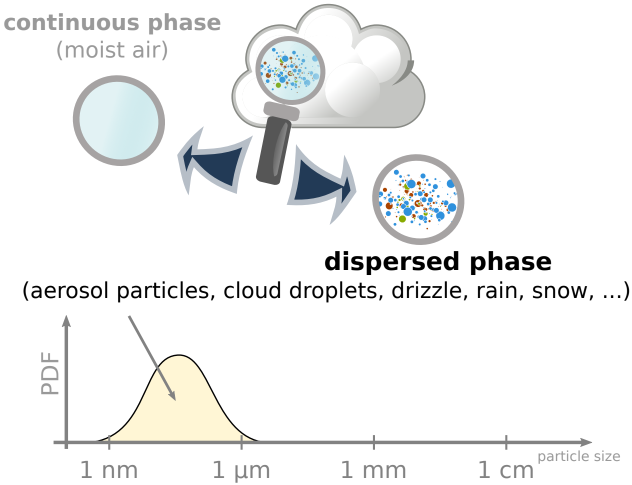

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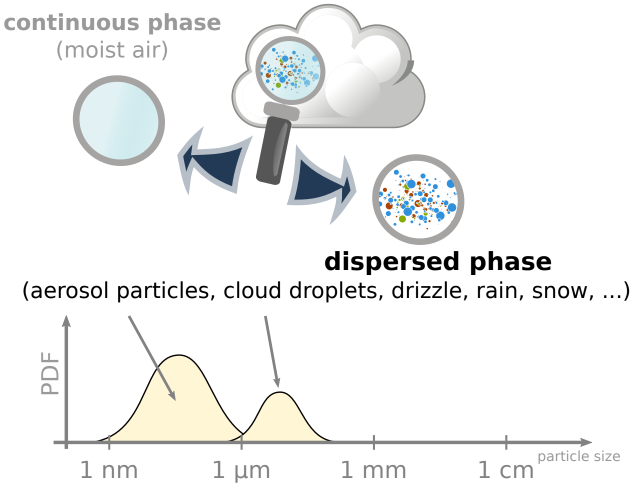

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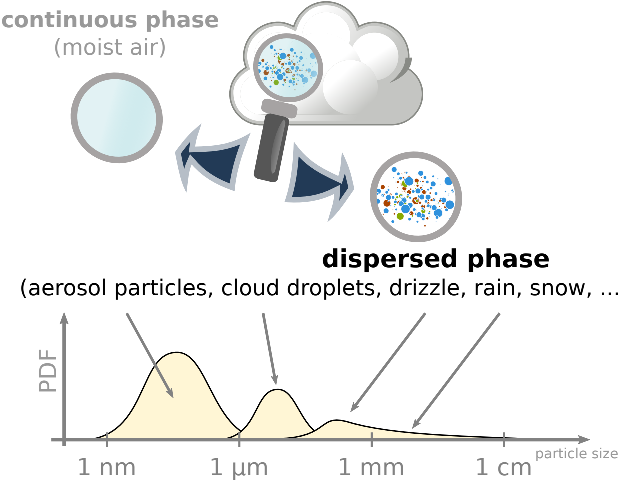

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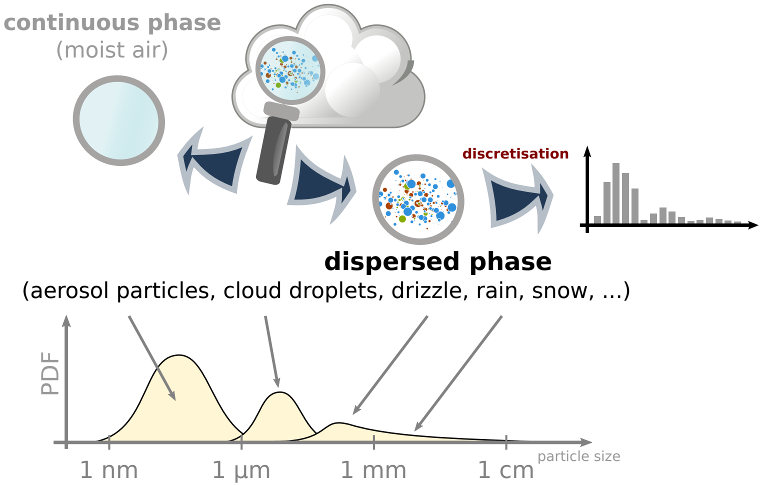

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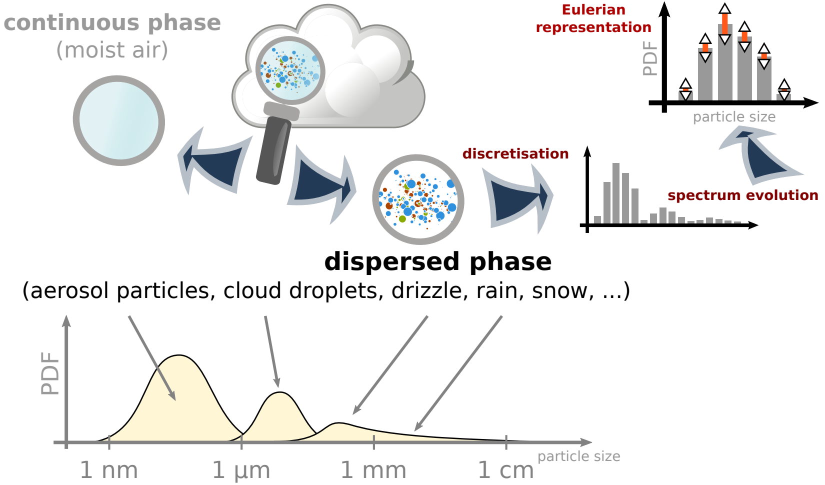

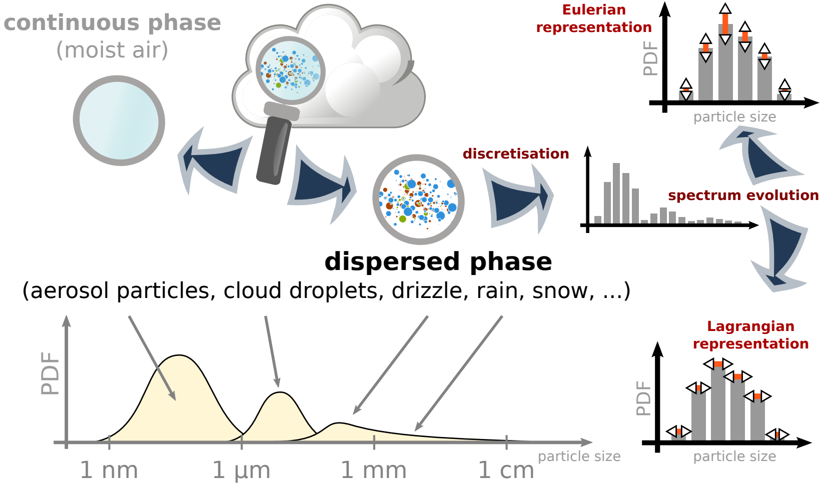
continuous phase
(moist air)
Eulerian
representation
PDF
particle size
discretisation
spectrum evolution
dispersed phase
(aerosol particles, cloud droplets, drizzle, rain, snow, ...)
PDF
1 nm
1 μm
1 mm
1 cm
particle size
Lagrangian
representation
PDF
particle size

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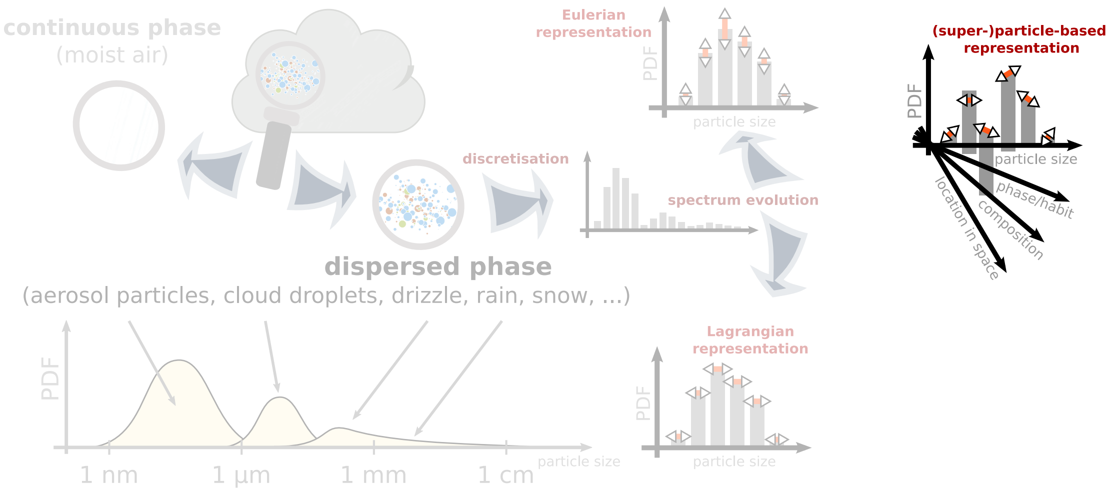

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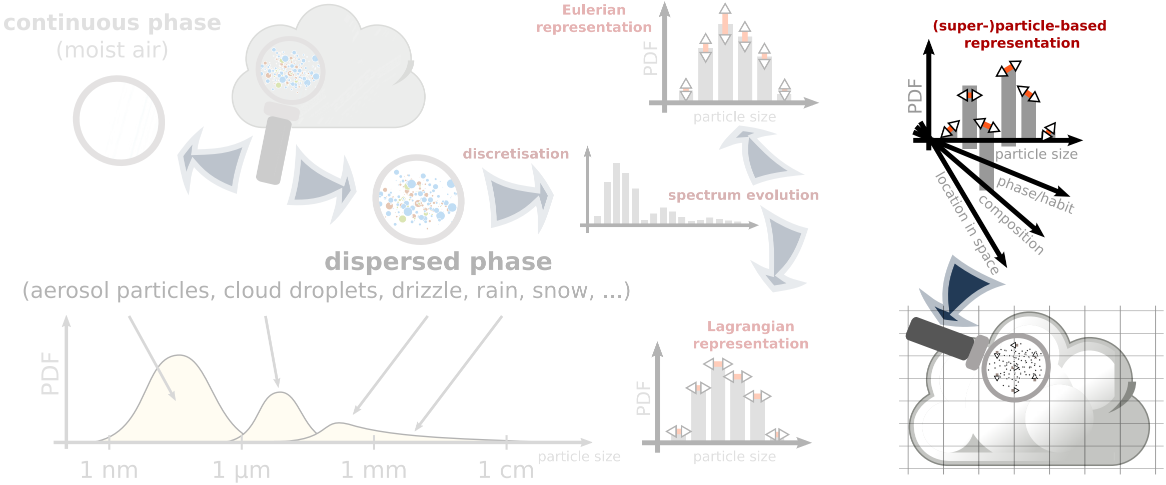

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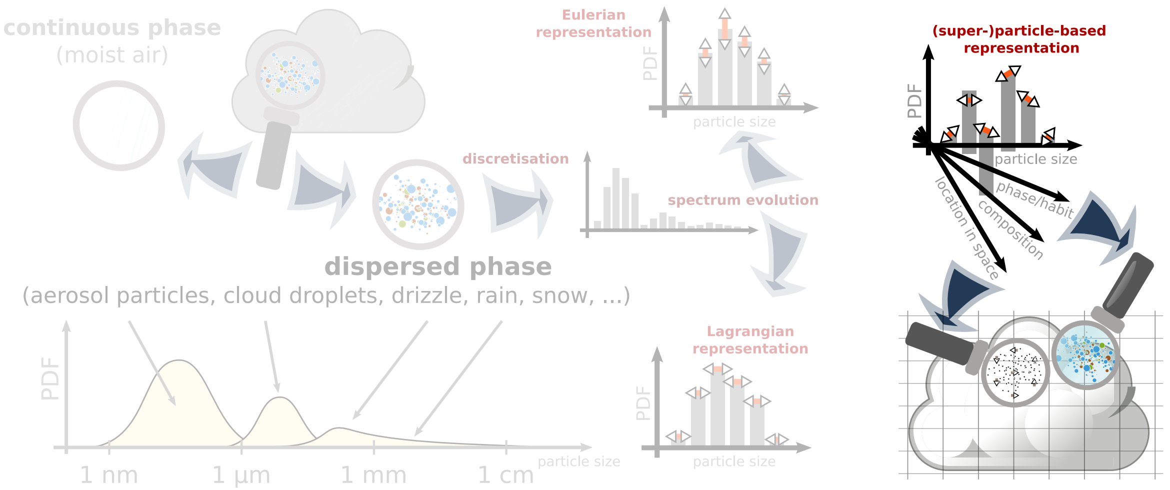

Lagrangian approaches: moving-sectional, particle-based, probabilistic

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super-particles as a probabilistic alternative to bulk or bin μ-physics

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COMMISSIONED MANUSCRIPT
10.1029/2019MS001689

Key Points:
- Microphysics is an important component of weather and climate models, but its representation in current models is highly uncertain

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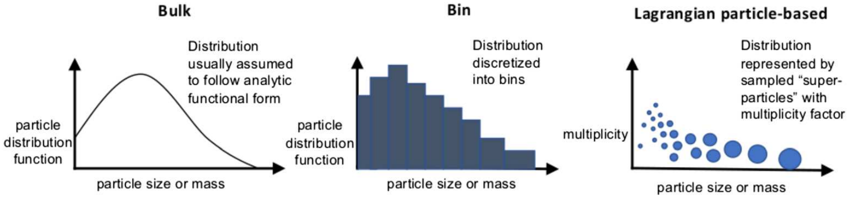

Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

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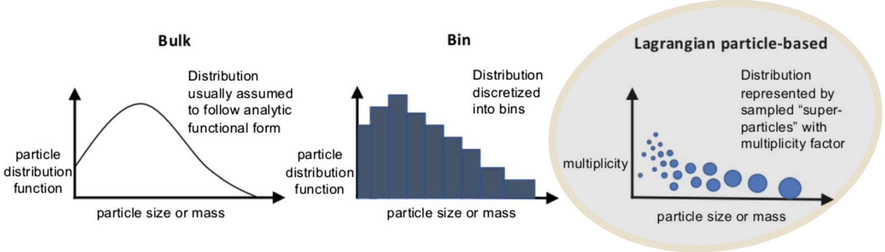

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plan of the talk

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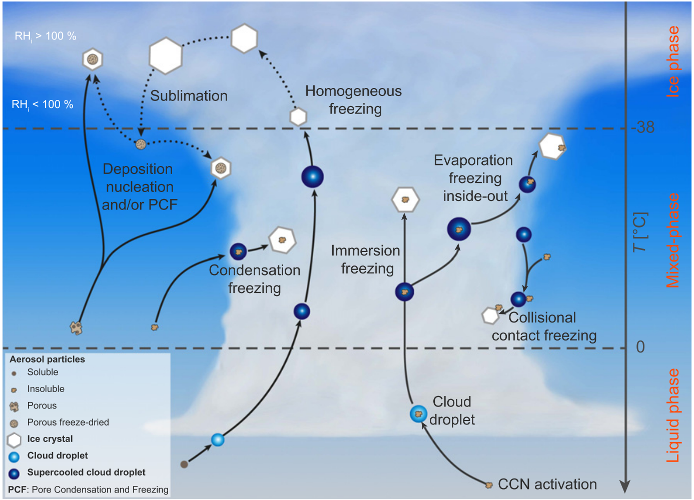
cloud μ-microphysics: Eulerian vs. Lagrangian

immersion freezing: singular vs. stochastic

implications, summary & outlook

plan of the talk

immersion freezing and other ice crystal formation pathways in clouds



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

Shima, Sato, Hashimoto & Misumi 2020 (GMD):
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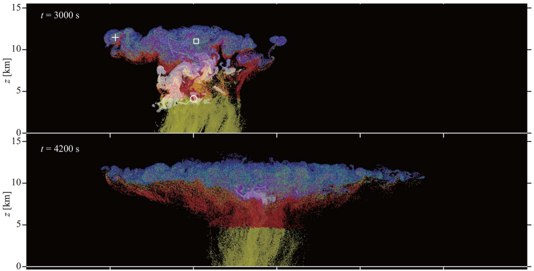

Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

Shima et al. '20 particle-based mixed-phase μ-physics

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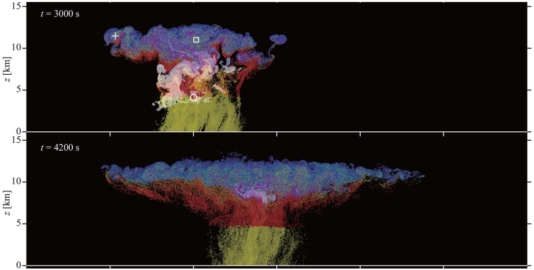

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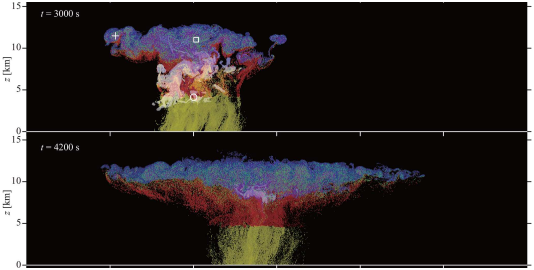

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- Eulerian component: momentum, heat, moisture budget
- Lagrangian component: super particles representing aerosol, water droplets, ice particles (porous spheroids)

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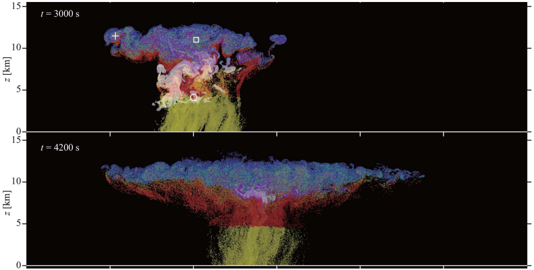

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Shima et al. '20 particle-based mixed-phase μ-physics

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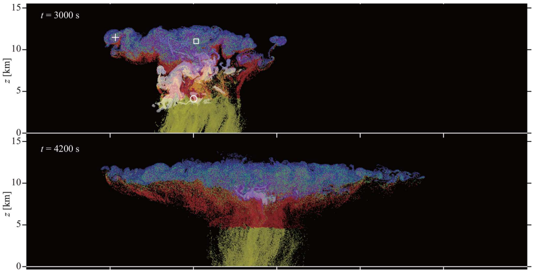

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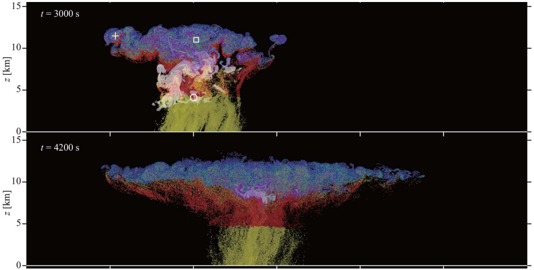

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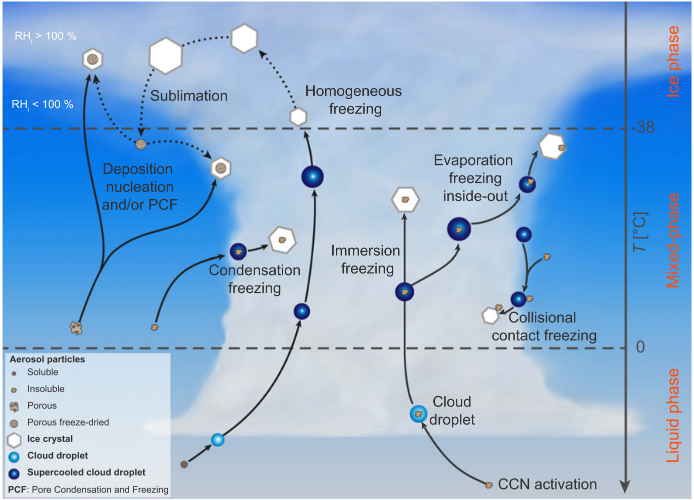
immersion freezing and other ice crystal formation pathways in clouds



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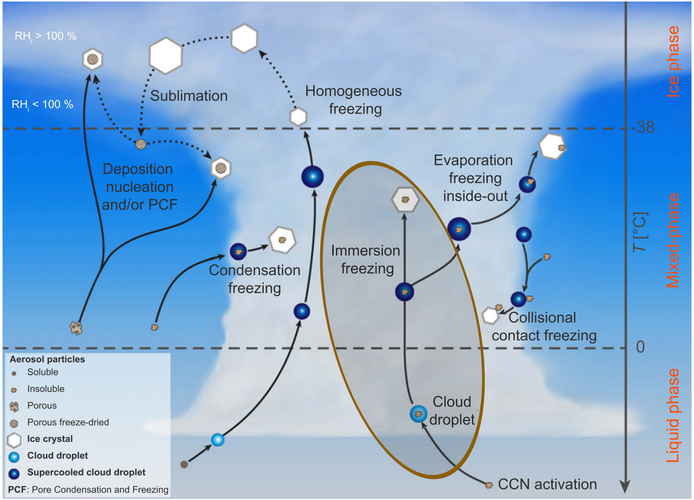

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RESEARCH ARTICLE

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Key Points:

- Very ice active Snomax protein aggregates are fragile and their ice nucleation ability decreases over months of freezer storage
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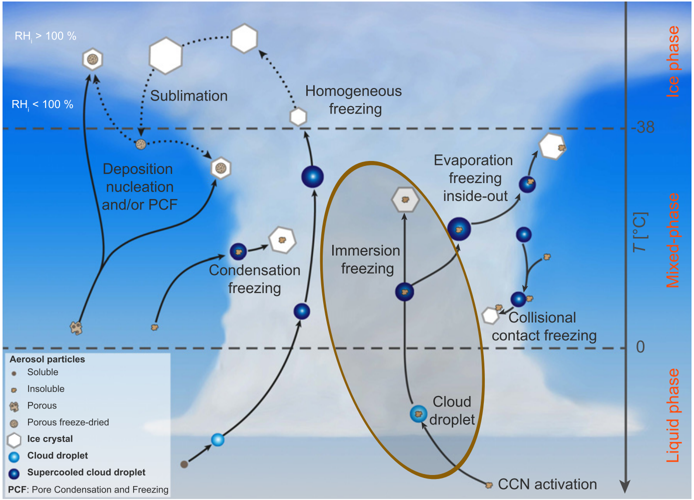

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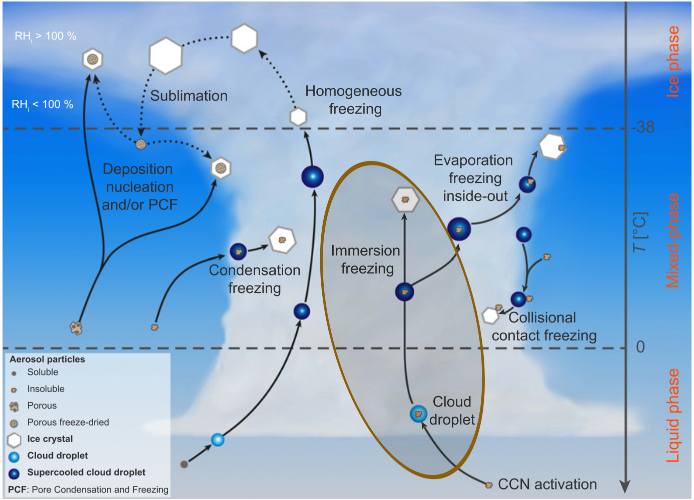

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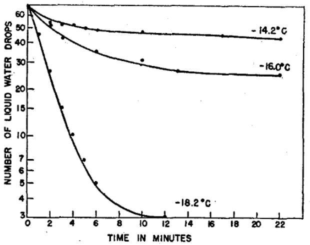

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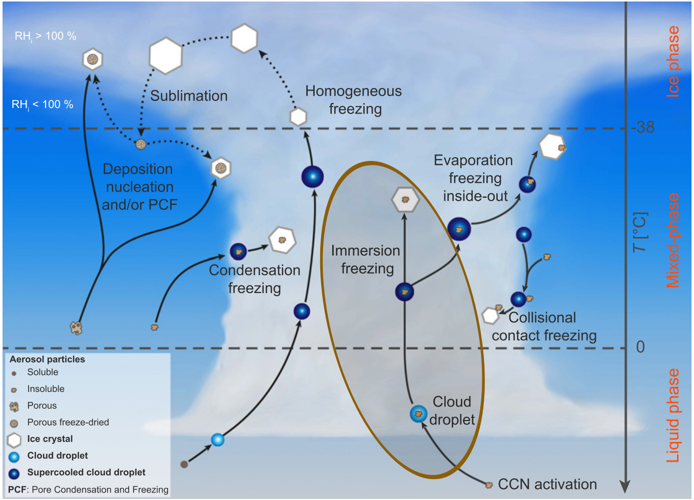

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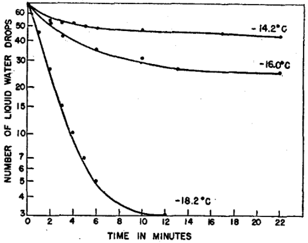

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Vali 2014 (ACP)

"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"

Poissonian model of freezing & Ice Nucleation Active Sites (INAS)

theory (in modern notation)
(Bigg '53, Langham & Mason '58, Carte '59, Marshall '61)

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Poisson counting process with rate r:

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

freezing temperature T_{fz} as a super-particle attribute

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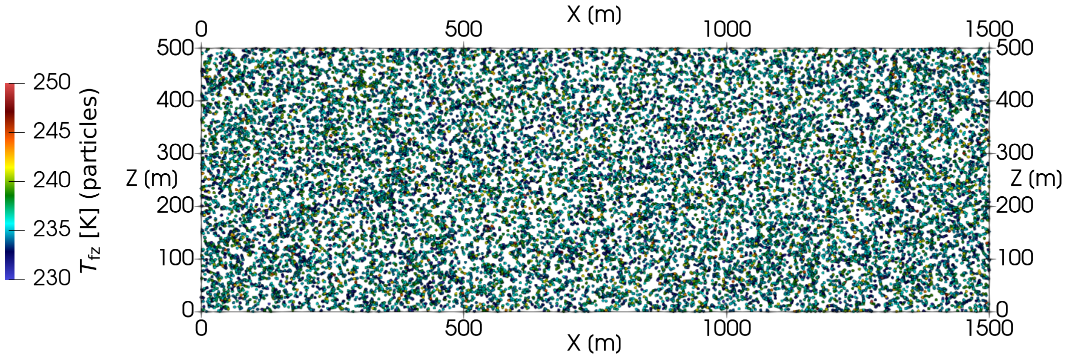

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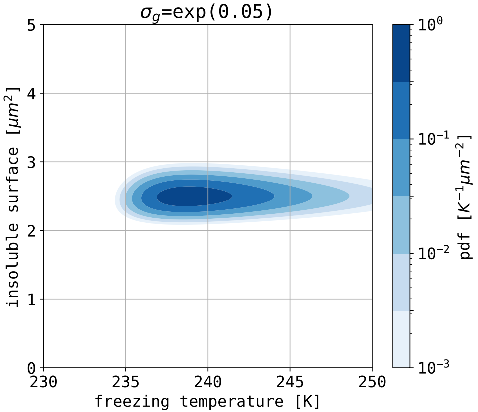

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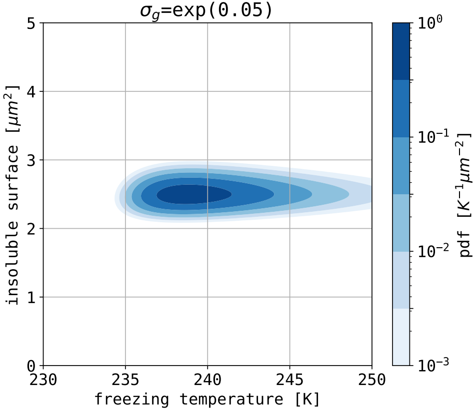

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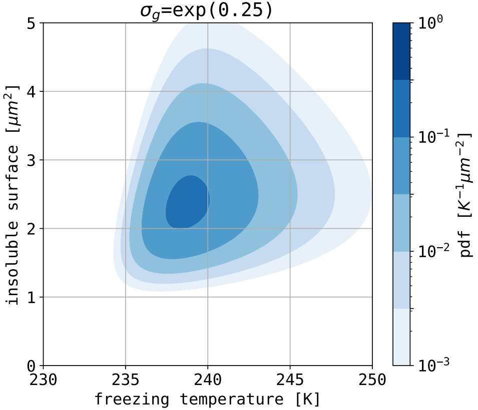

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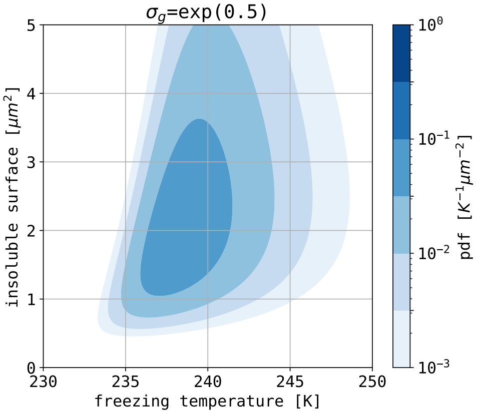

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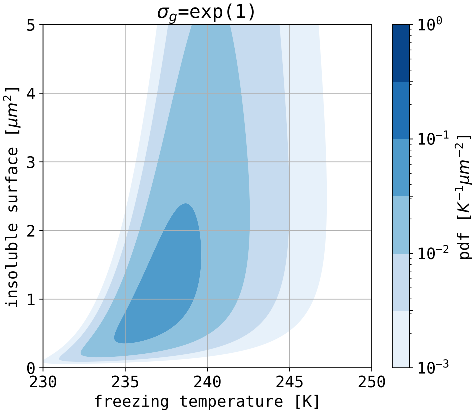

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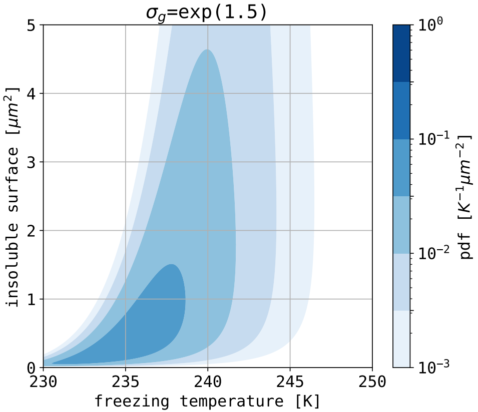

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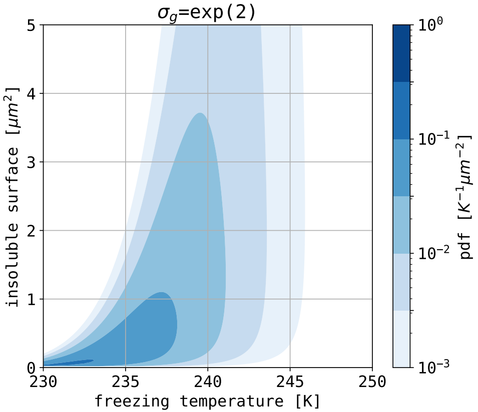

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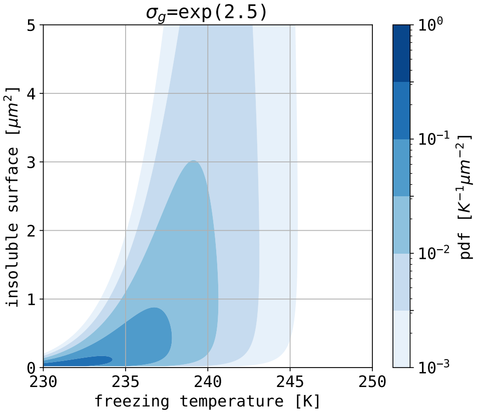

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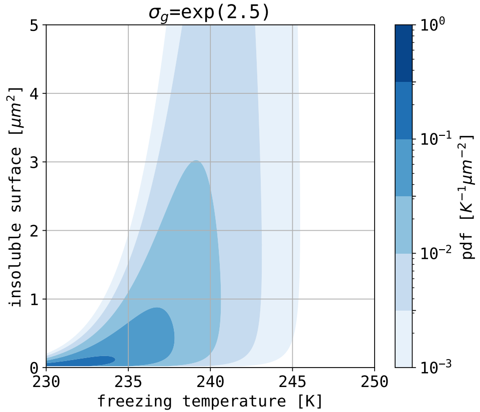
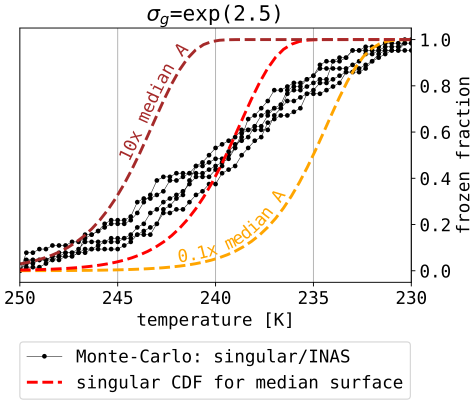


box model (or single grid cell)



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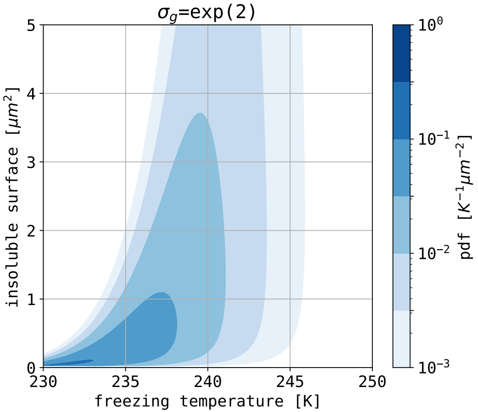

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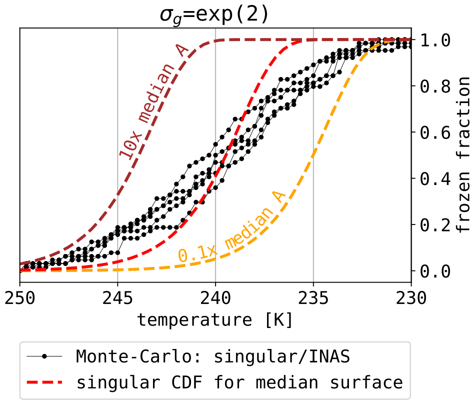

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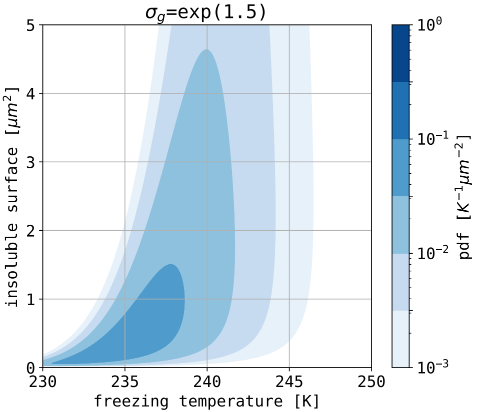

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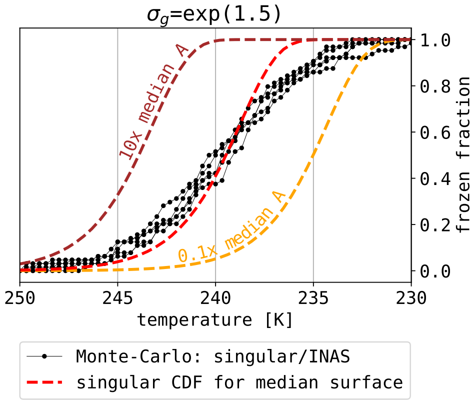

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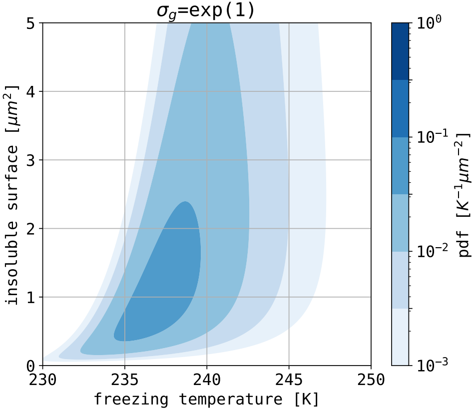

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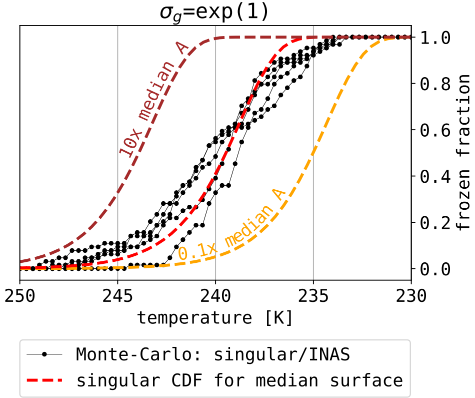

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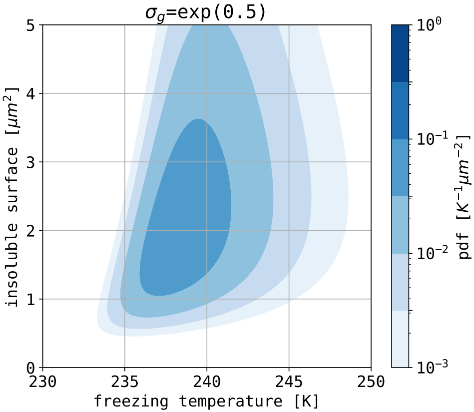

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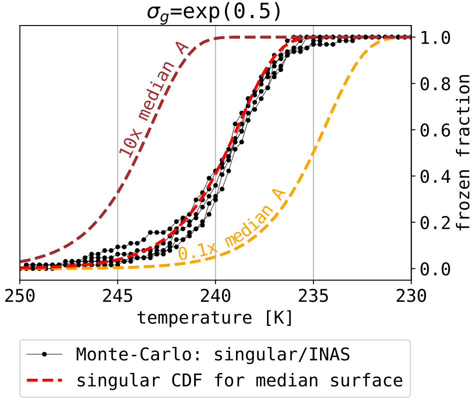

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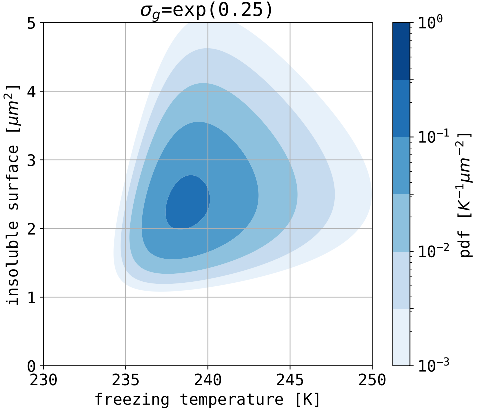

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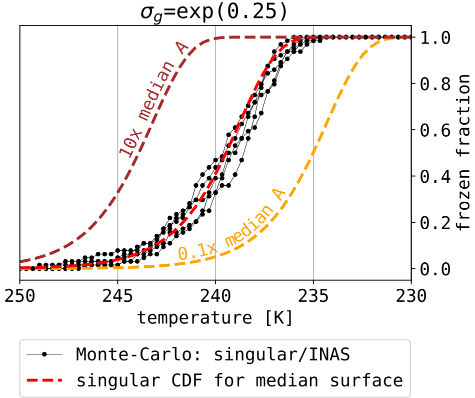

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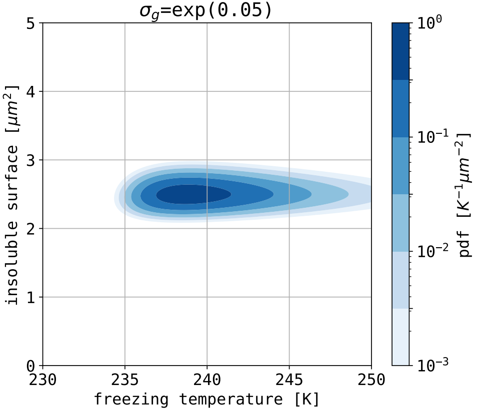

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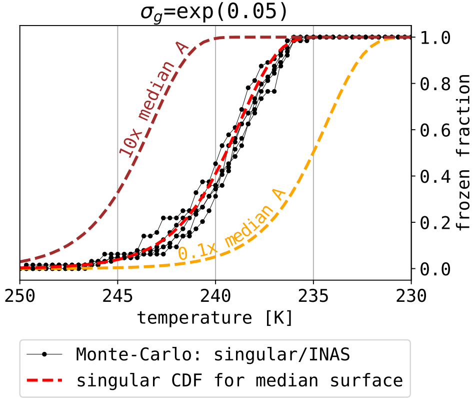

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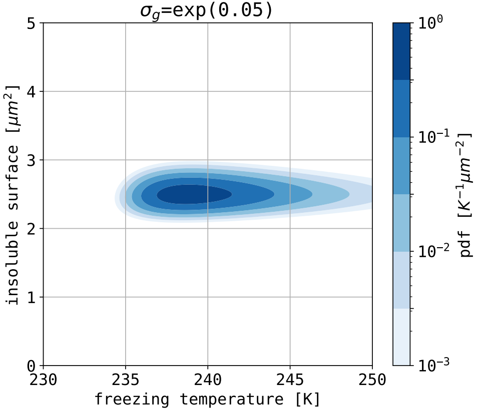

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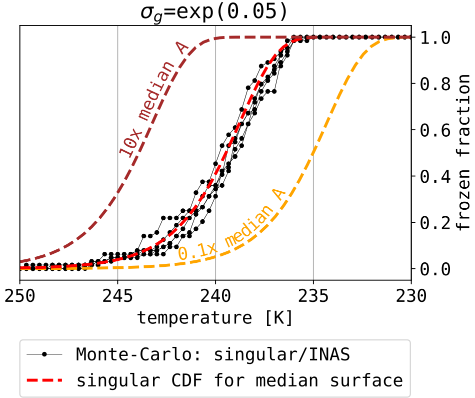

- limitations stemming from monodisperse INP assumption (see also Alpert & Knopf '16)
- singular particle-based model is capable of representing polydisperse INP

particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular:	INAS T_{fz} **as attribute**; initialisation by random sampling from $P(T_{fz}, A)$ with lognormal A (A is not an attribute, initialisation only); freezing if $T(t) < T_{fz}(t = 0)$
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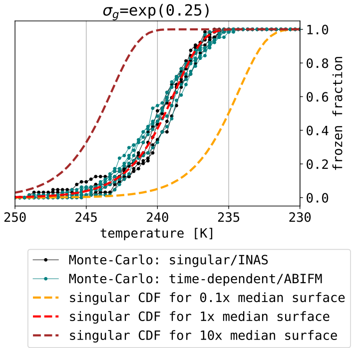

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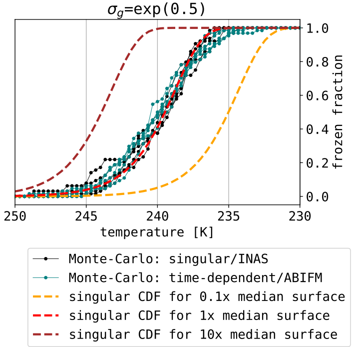

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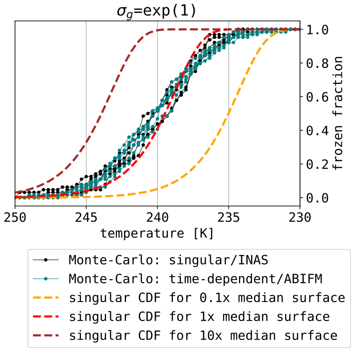

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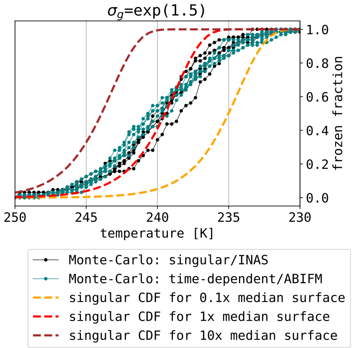

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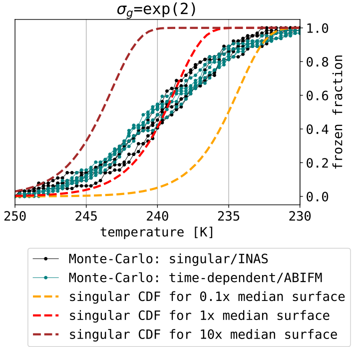

particle-based freezing: singular (Shima et al.) / time-dependent (this work)

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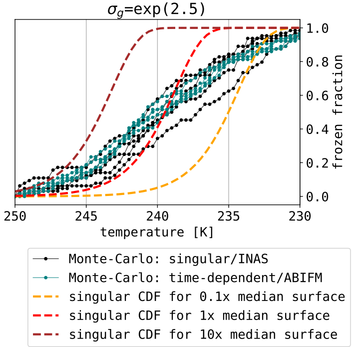

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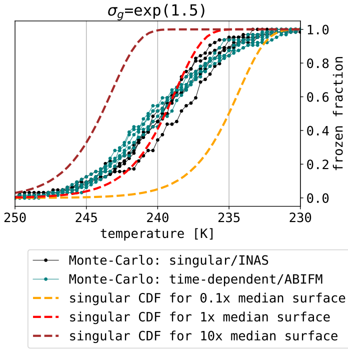
cooling rate: $0.5\ K/min$



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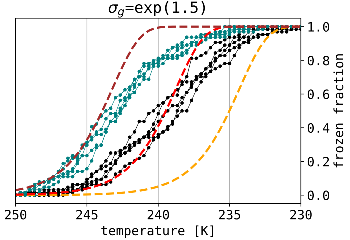

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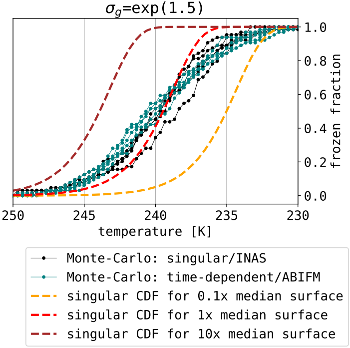

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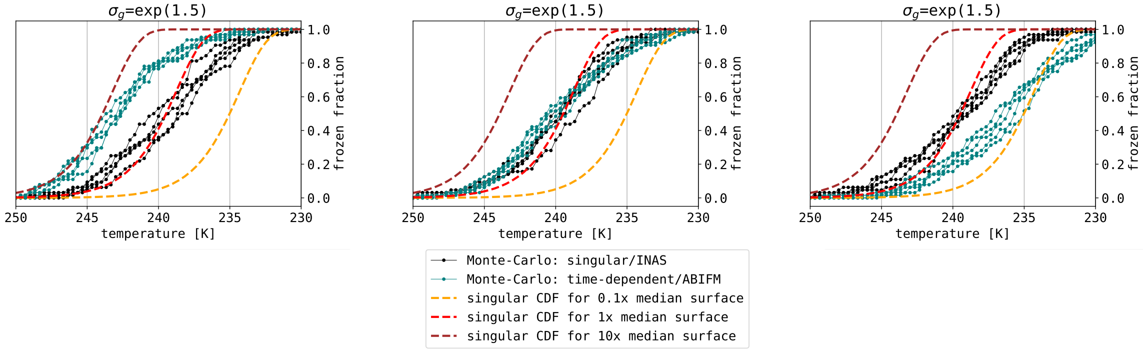
cooling rate: 0.1 $^K/_{min}$ | cooling rate: 0.5 $^K/_{min}$ | cooling rate: 2.5 $^K/_{min}$



theory (in modern notation)
(Bigg '53, Langham & Mason '58, Carte '59, Marshall '61)

Poisson counting process with rate r:

$$P^*(\text{k events in time t}) = \frac{(rt)^k \exp(-rt)}{k!}$$

$$P(\text{one or more events in time t}) = 1 - P^*(k=0,t)$$

$$\ln(1-P) = -rt$$

introducing $J_{\text{het}}(T)$, $T(t)$ and INP surface A:

$$\ln\left(1 - P(A,t)\right) = -A\underbrace{\int_0^t J_{\text{het}}(T(t'))\,dt'}_{I(T)}$$

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

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

Poissonian model of freezing & Ice Nucleation Active Sites (INAS)

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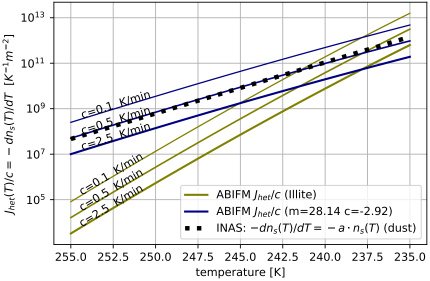
ABIFM J_{het} (Knopf & Alpert '13)



Poissonian model of freezing & Ice Nucleation Active Sites (INAS)

Is it a problem?

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

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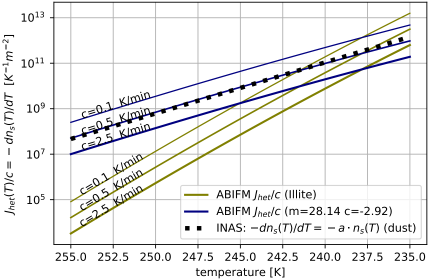
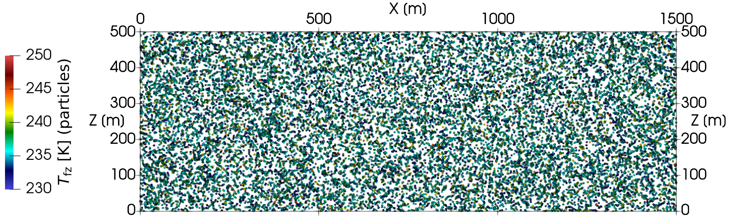


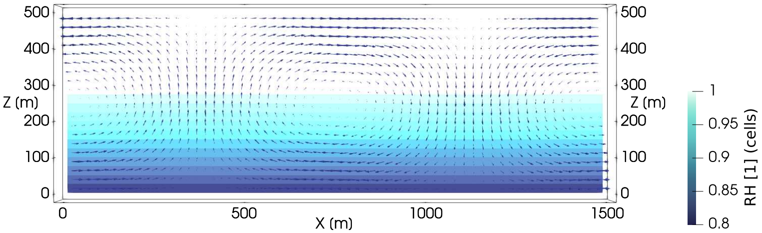
cf. Vali & Stansbury '66; modified singular model (Vali '94, Murray et al. '11)
but the singular ansatz limitation of sampling T_{fz} at t=0 remains

particle-based μ-physics + prescribed-flow test (aka KiD-2D)[a,b,c,d,e]

Lagrangian component (PySDM)



Eulerian component (PyMPDATA)



[a] concept: Gedzelman & Arnold '93
[b] stratiform: Morrison & Grabowski '07
[c] particle-based: Arabas et al. '15
[d] KiD-2D: github.com/BShipway/KiD
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particle-based μ-physics + prescribed-flow test (aka KiD-2D)[a,b,c,d,e]

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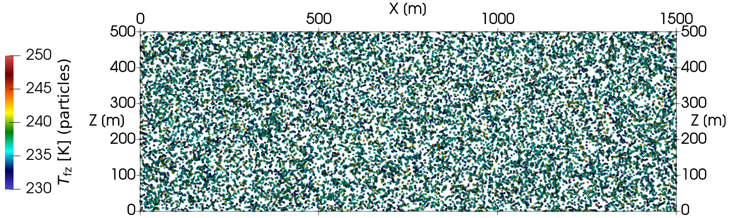

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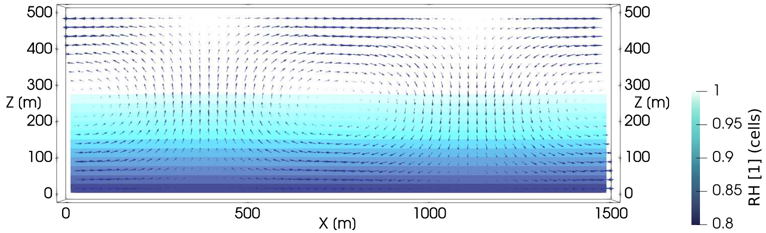

PySDM & PyMPDATA
(Bartman et al. 2022)

- new packages
  (`pip install PySDM PyMPDATA`)
- open-source
  github.com/atmos-cloud-sim-uj
- pure Python, multi-threaded
  (Numba/LLVM JIT)
- Jupyter & Colab friendly
  single-click reproducible in the cloud

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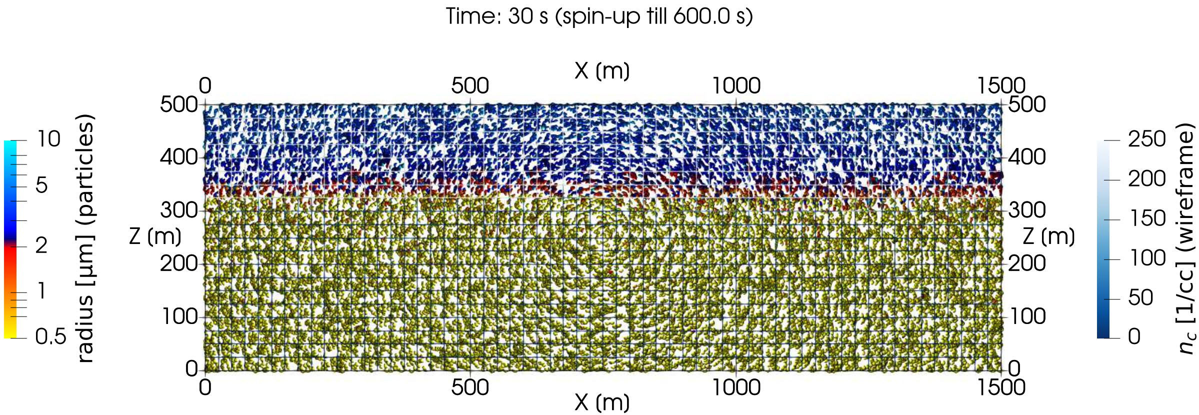
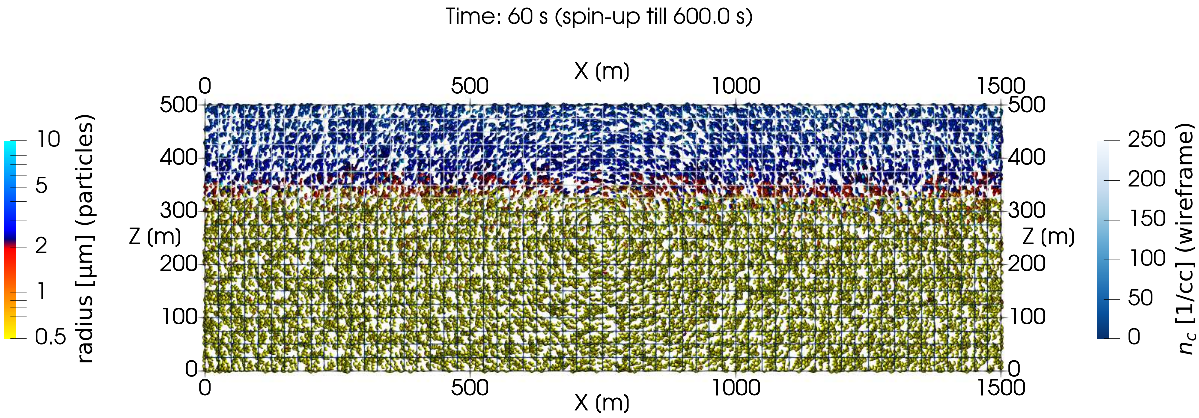


16+16 super-particles/cell for INP-rich + INP-free particles

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

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

particle-based μ-physics + prescribed-flow test



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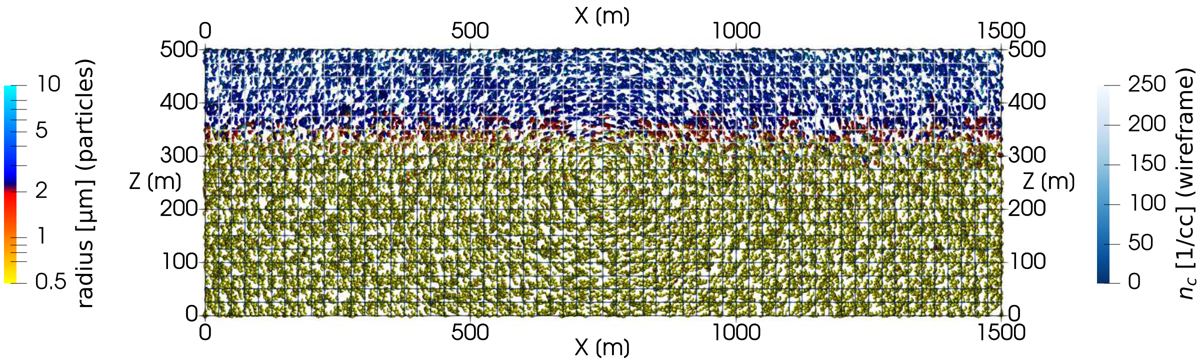
Time: 90 s (spin-up till 600.0 s)



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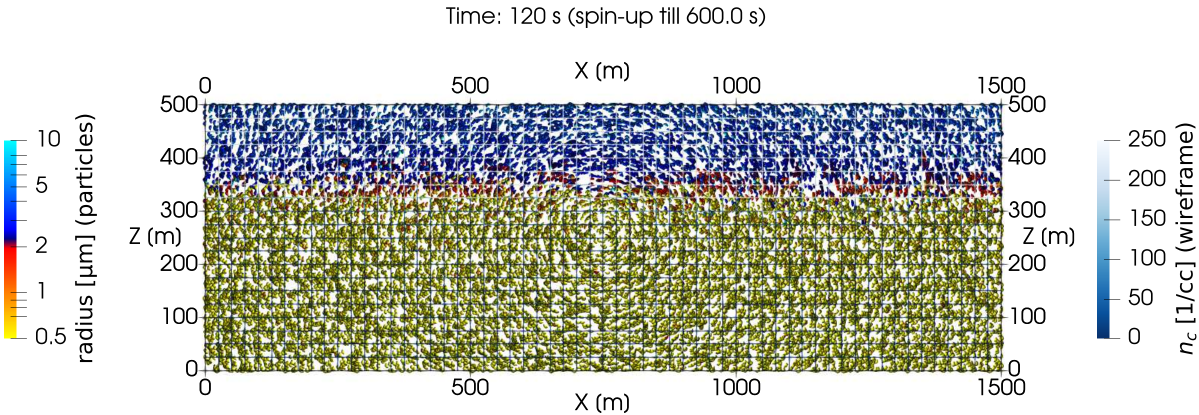

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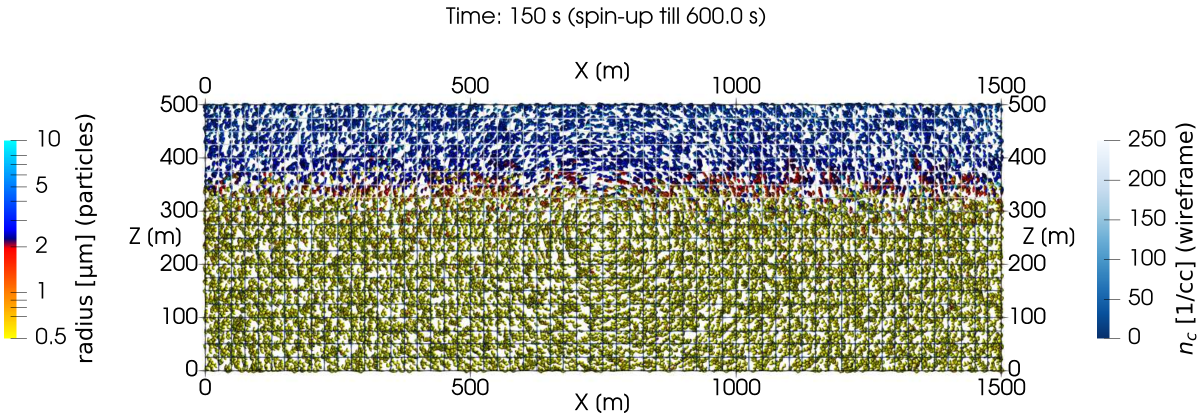

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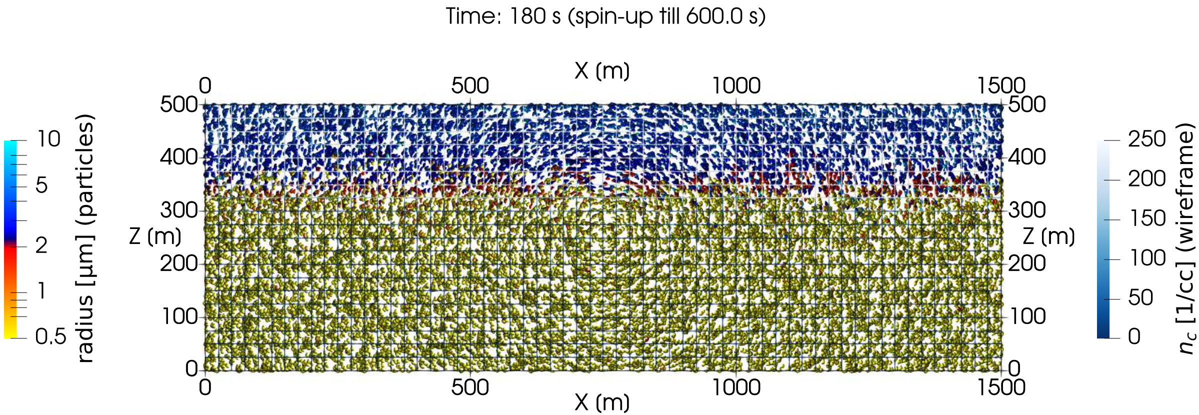

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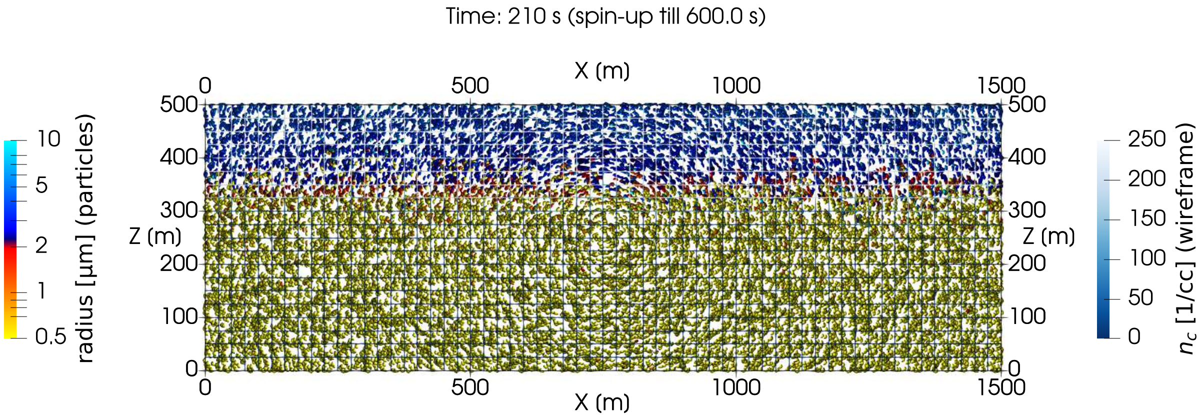

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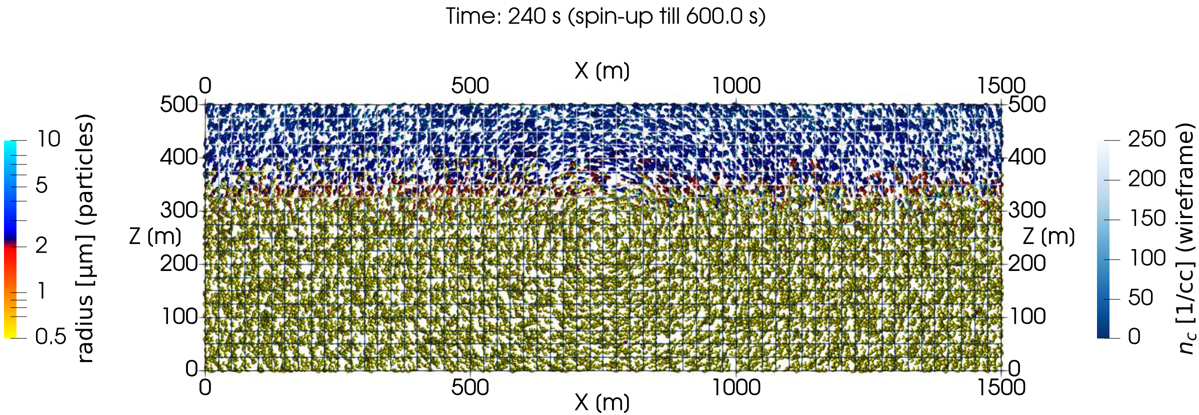

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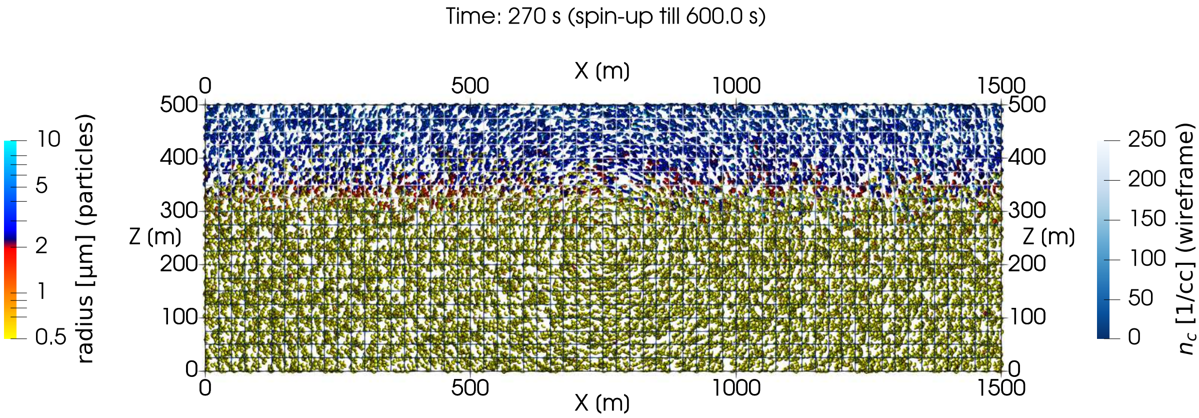

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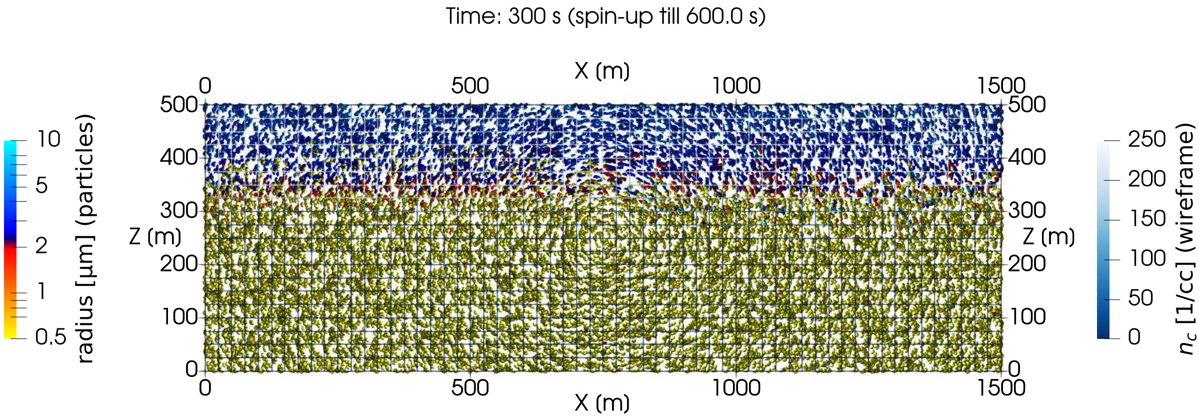

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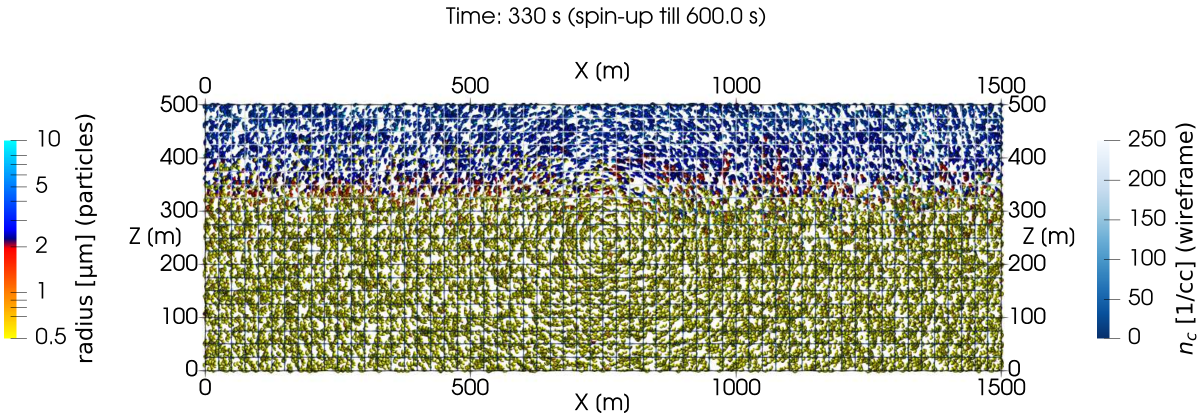

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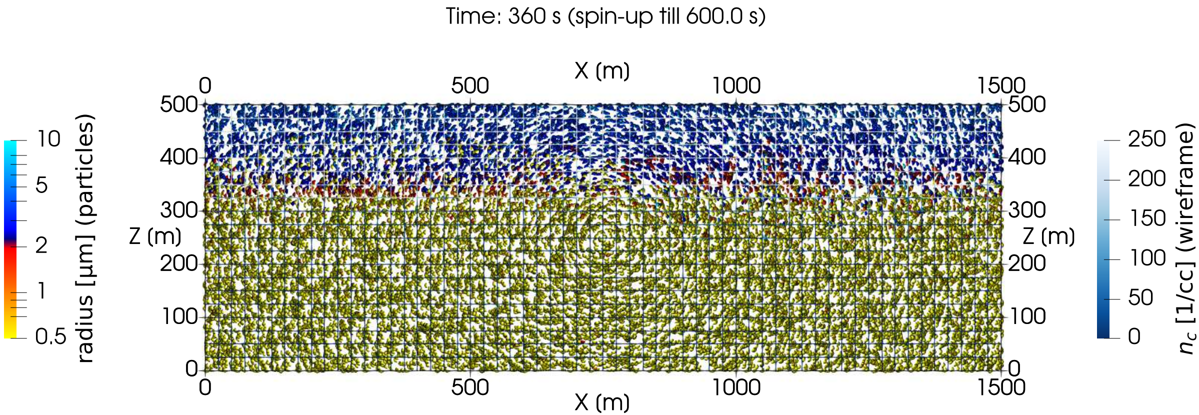

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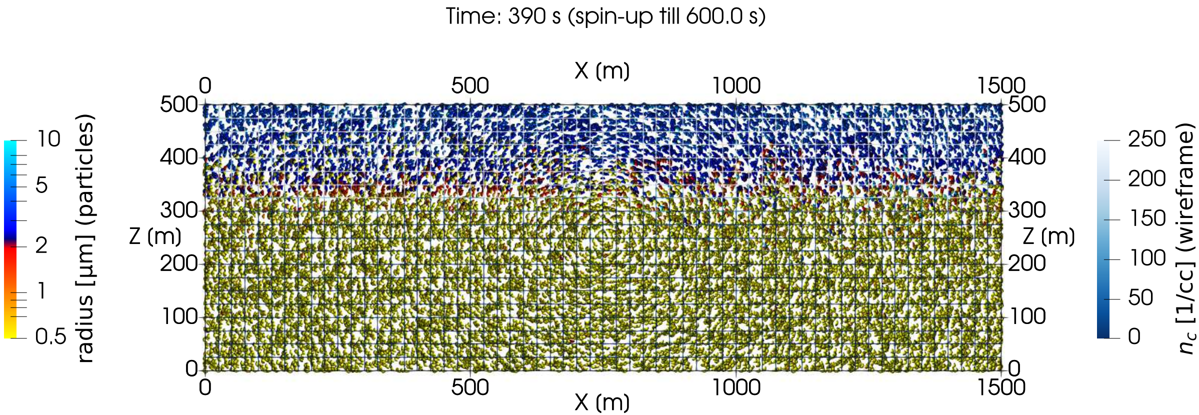

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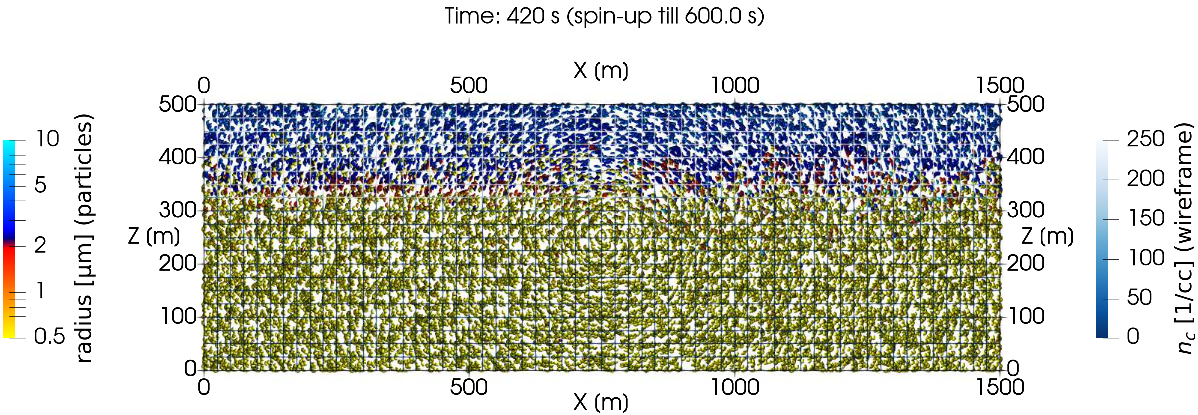

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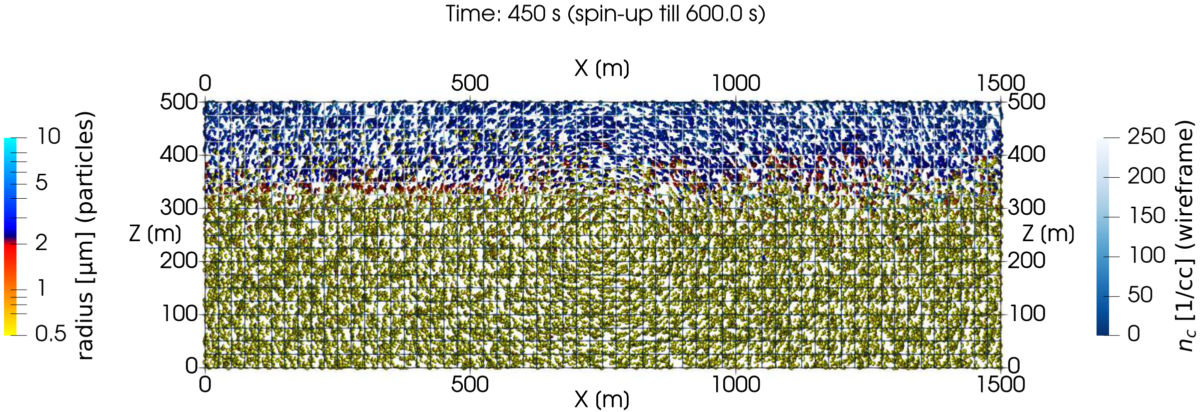

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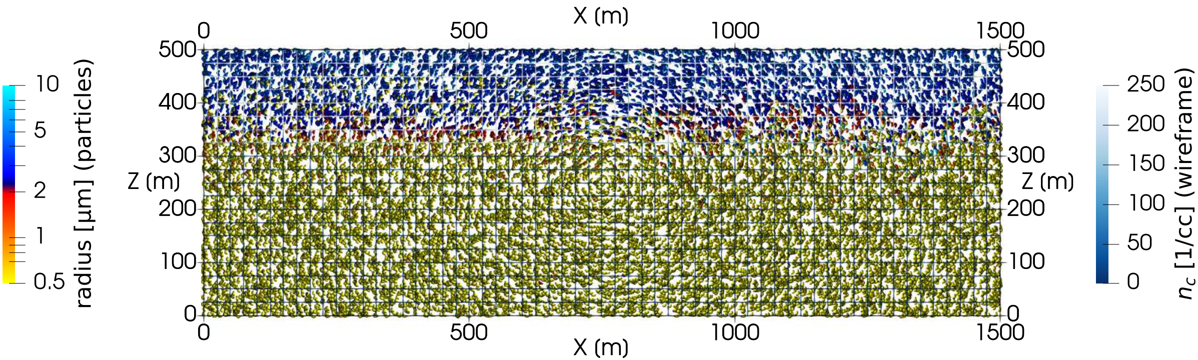
Time: 480 s (spin-up till 600.0 s)



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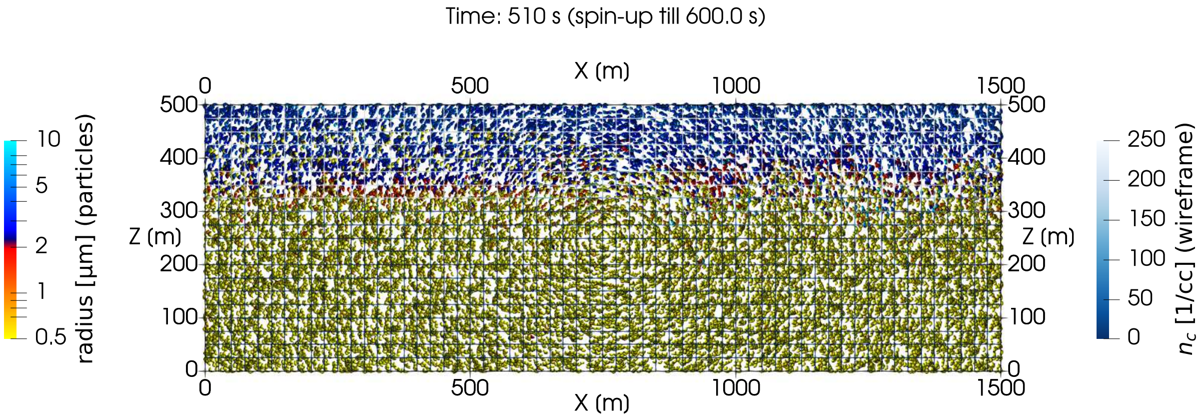

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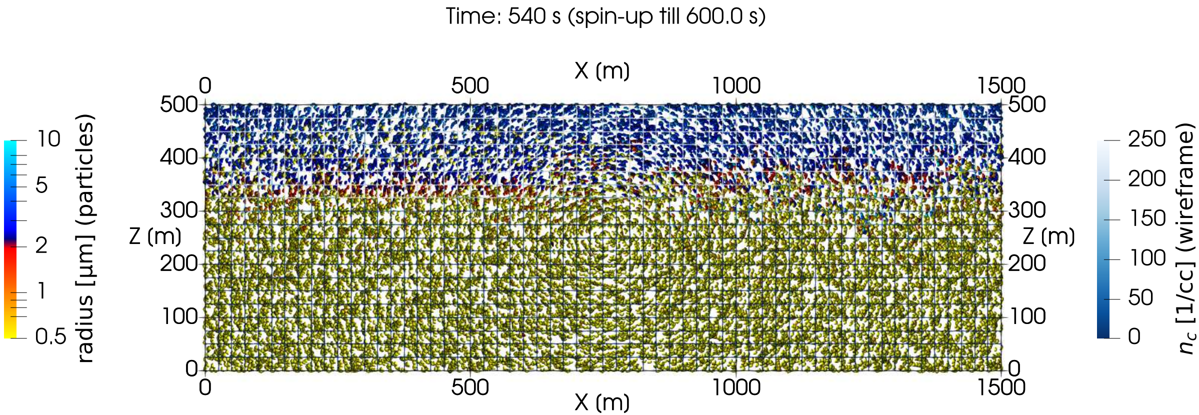

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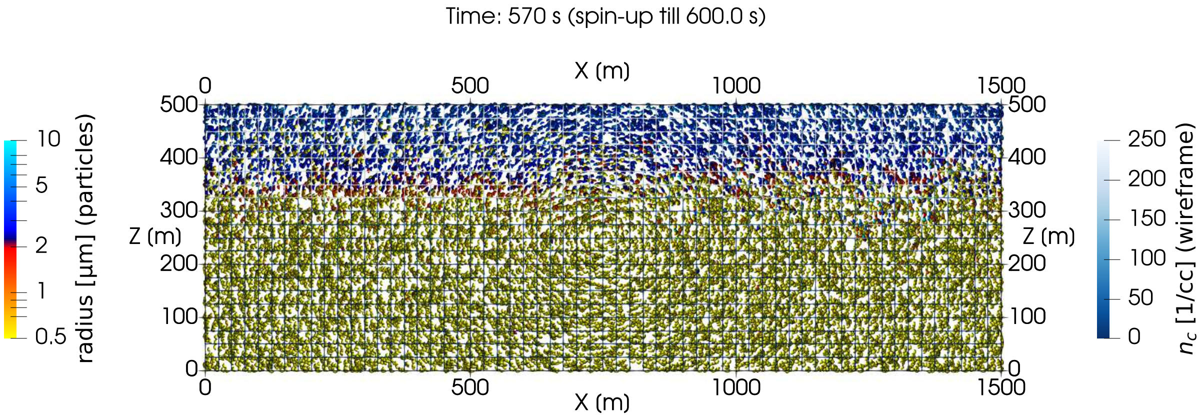

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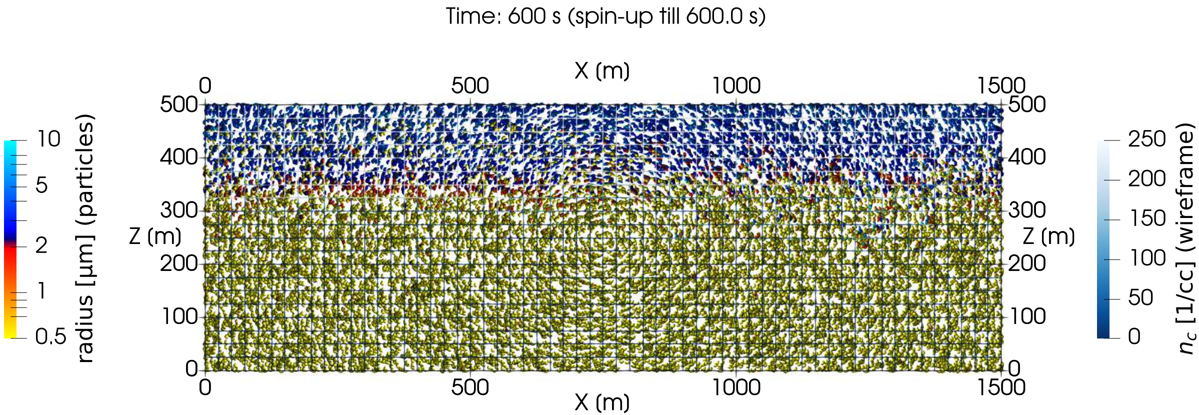

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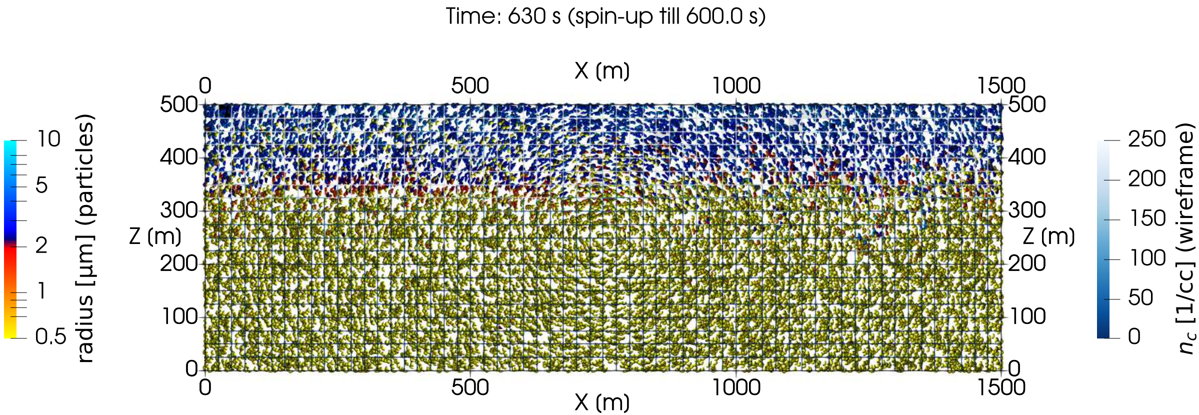
spin-up = freezing off; subsequently frozen particles act as tracers

particle-based μ-physics + prescribed-flow test



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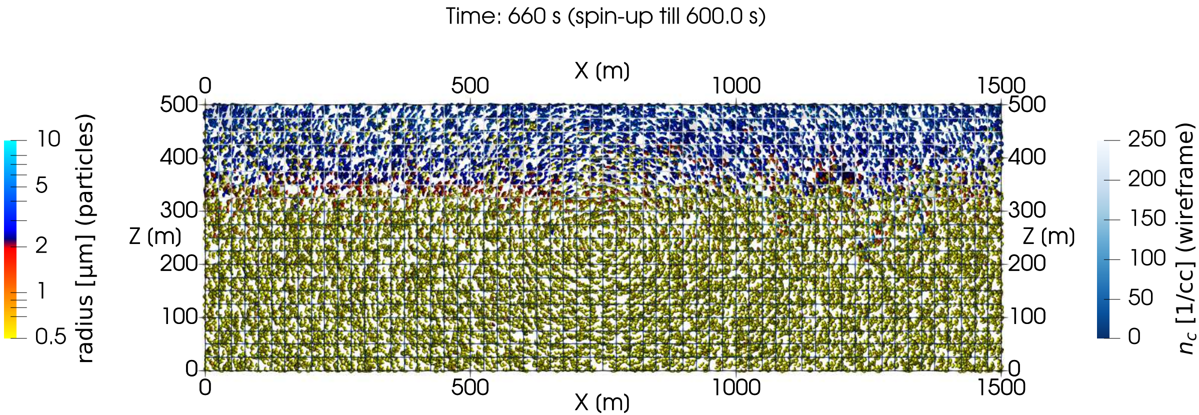

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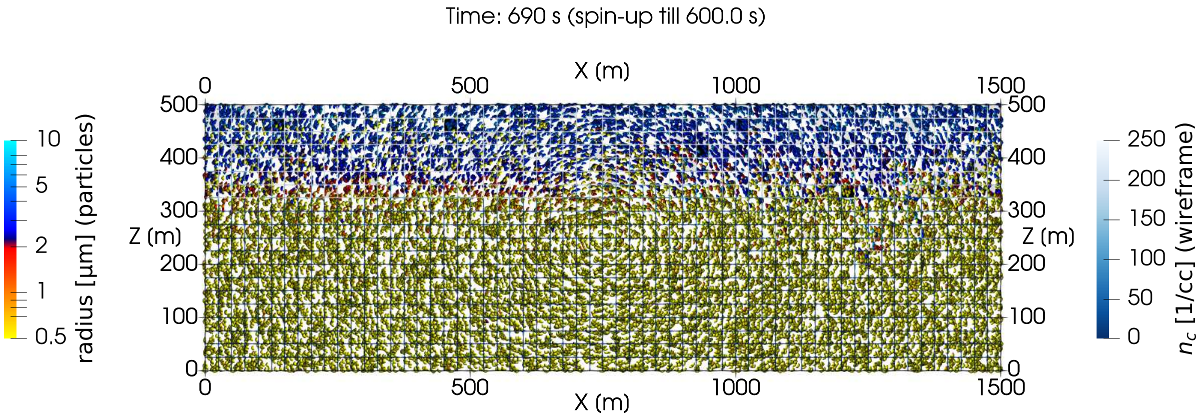

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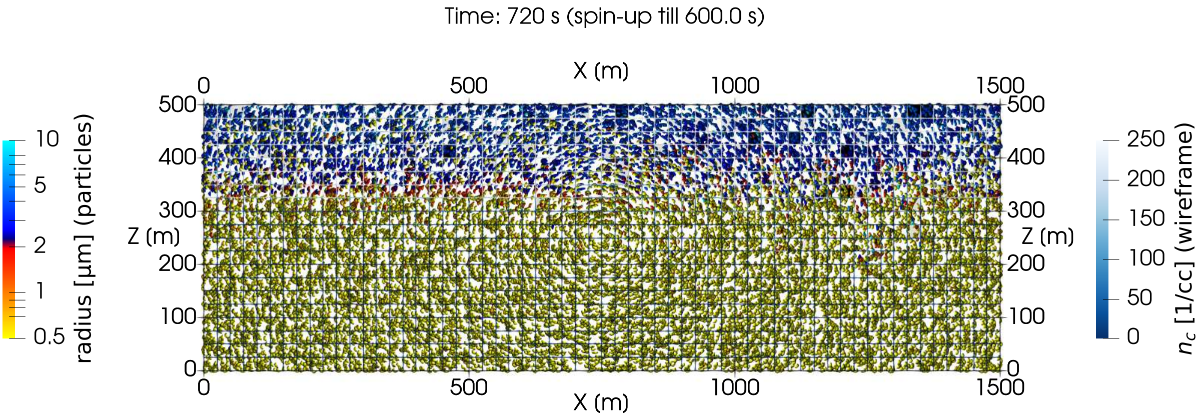

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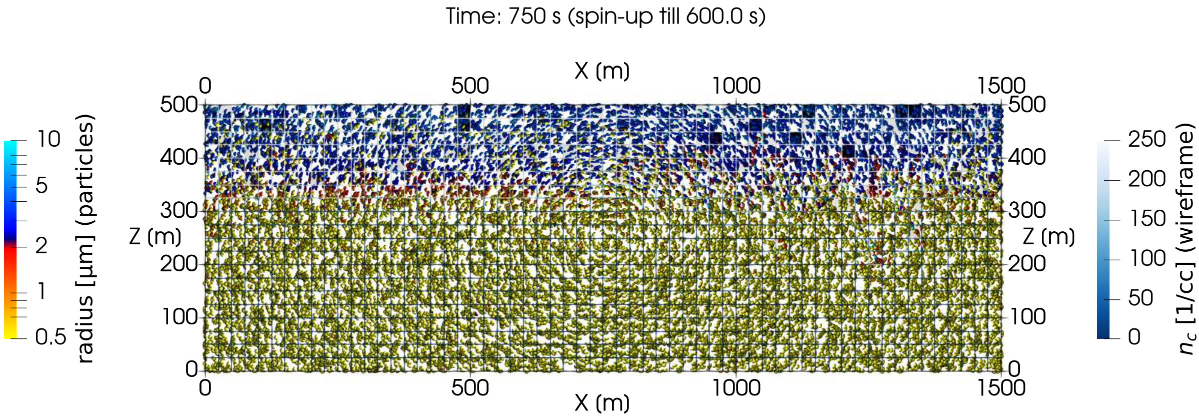

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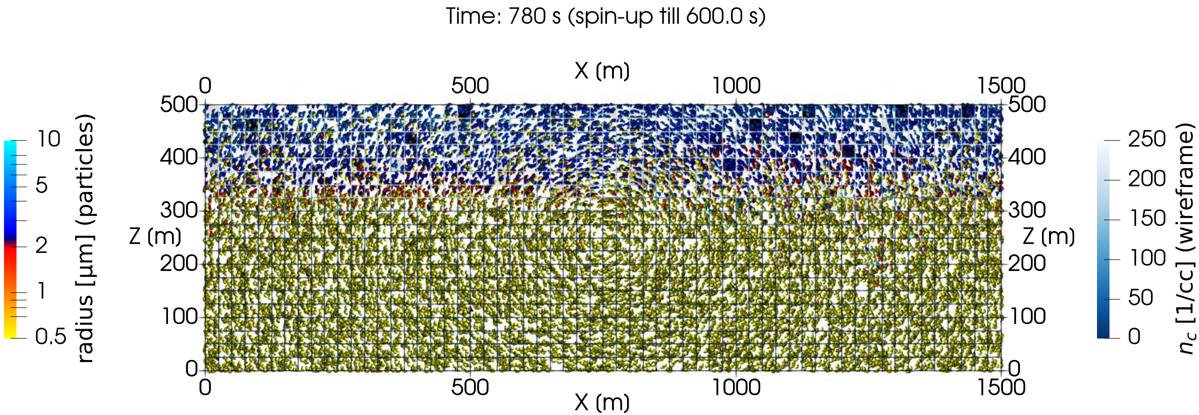

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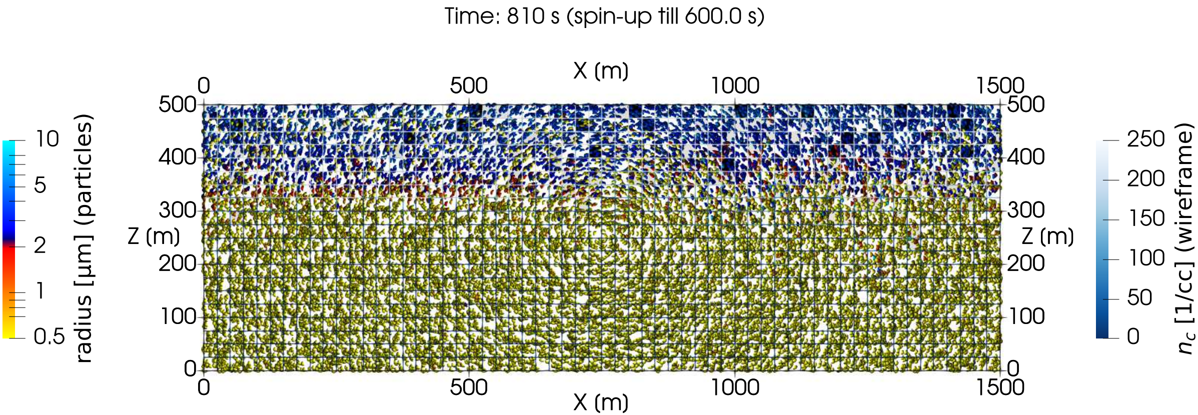

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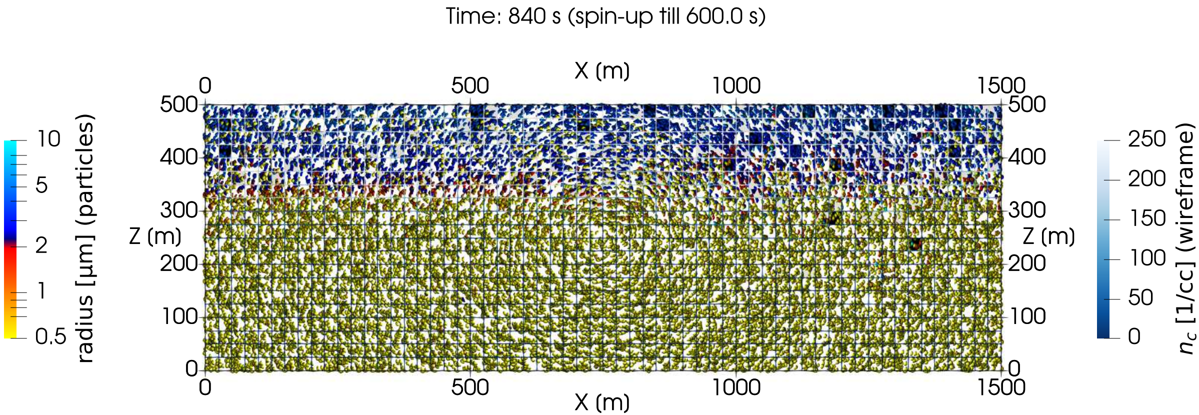

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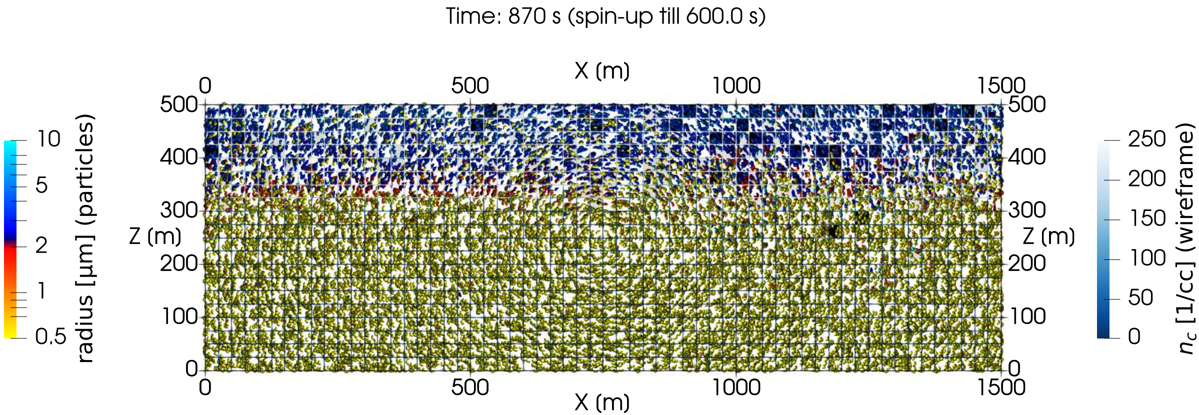

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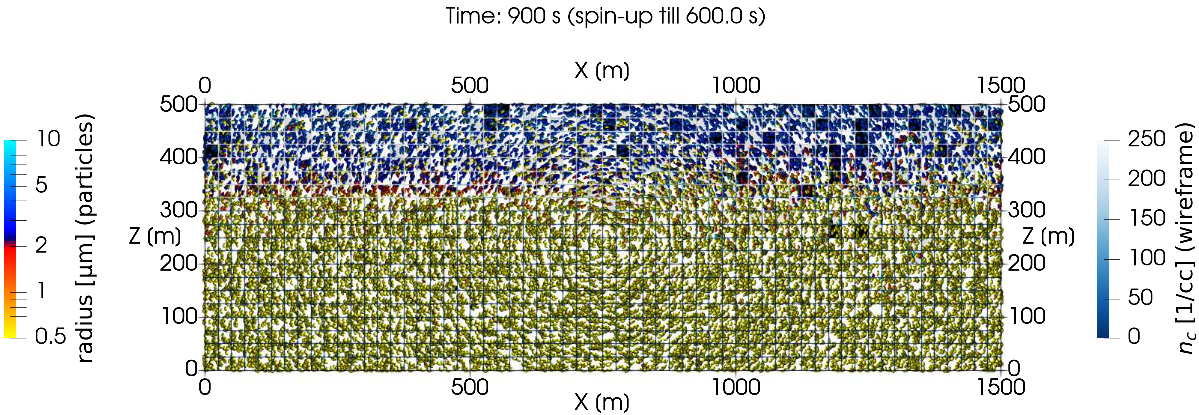

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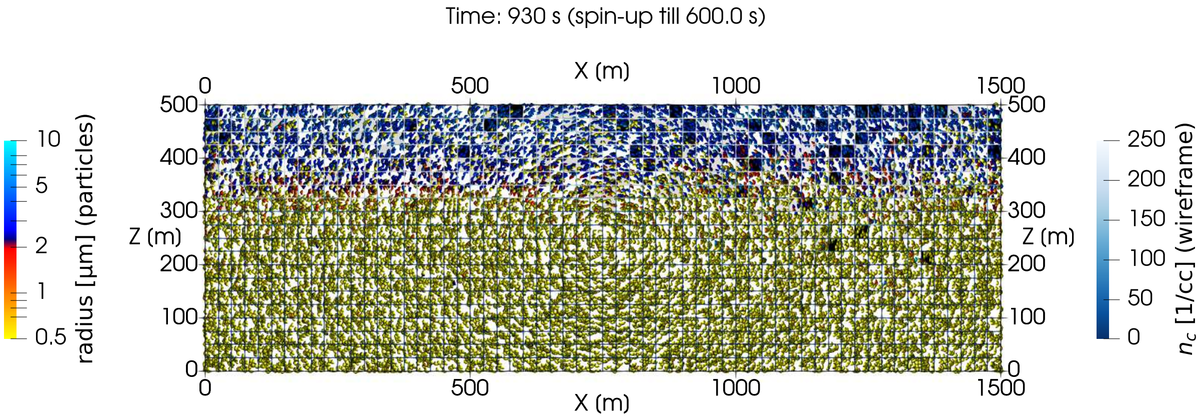

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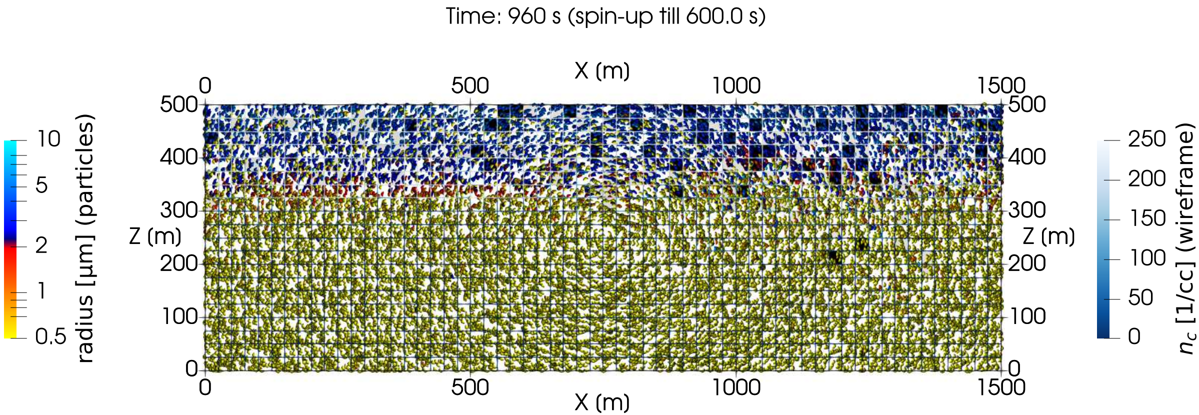

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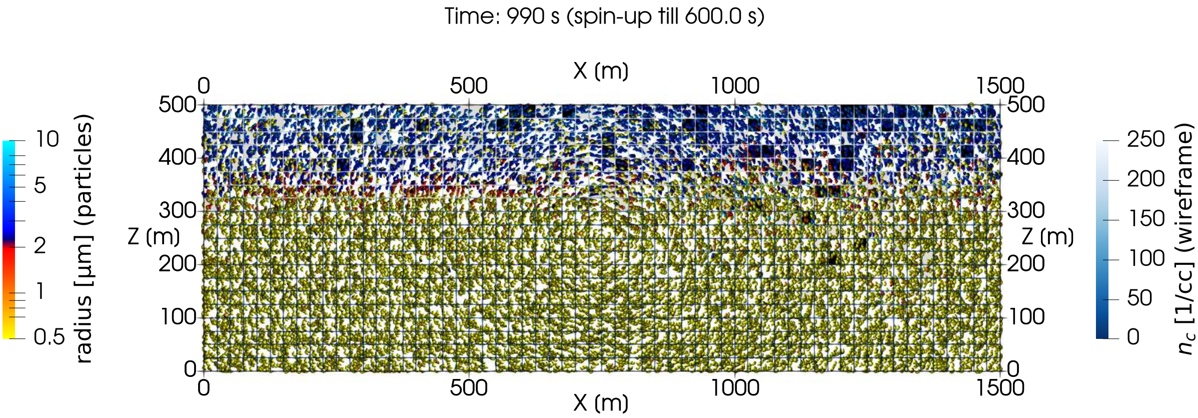

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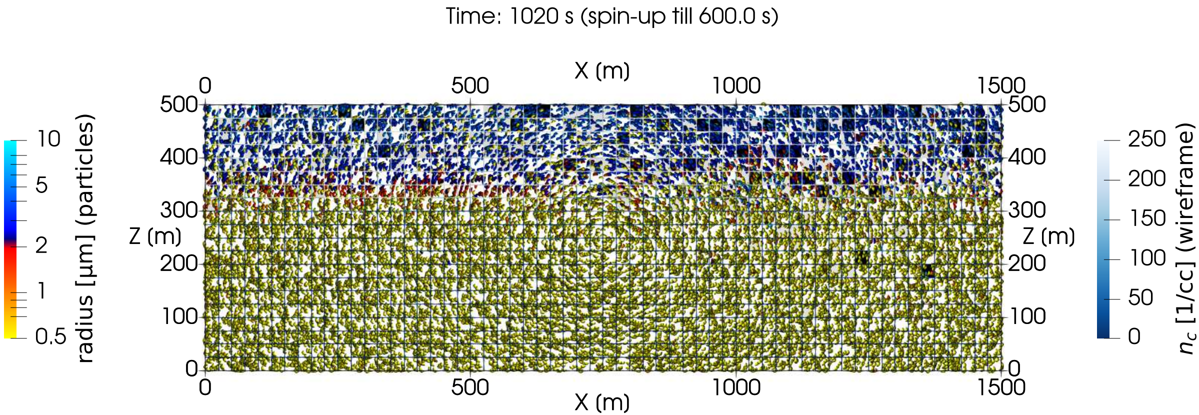

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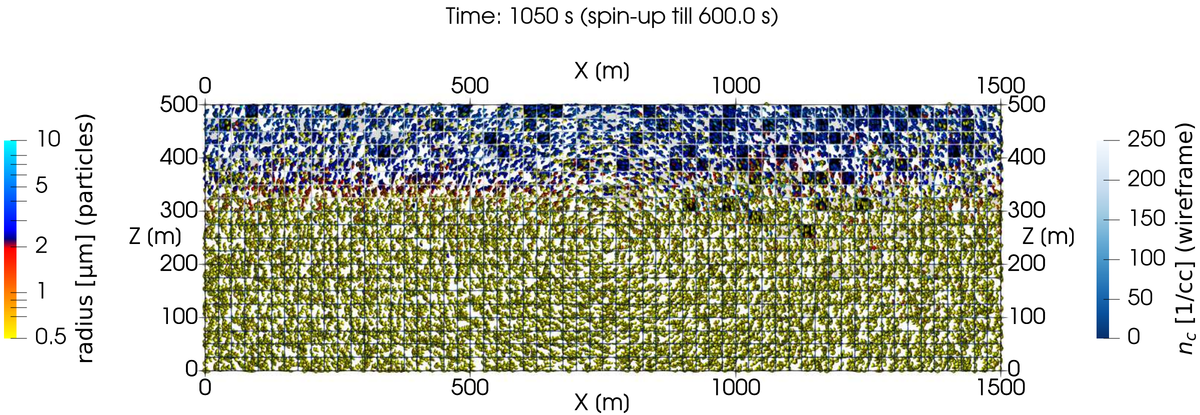

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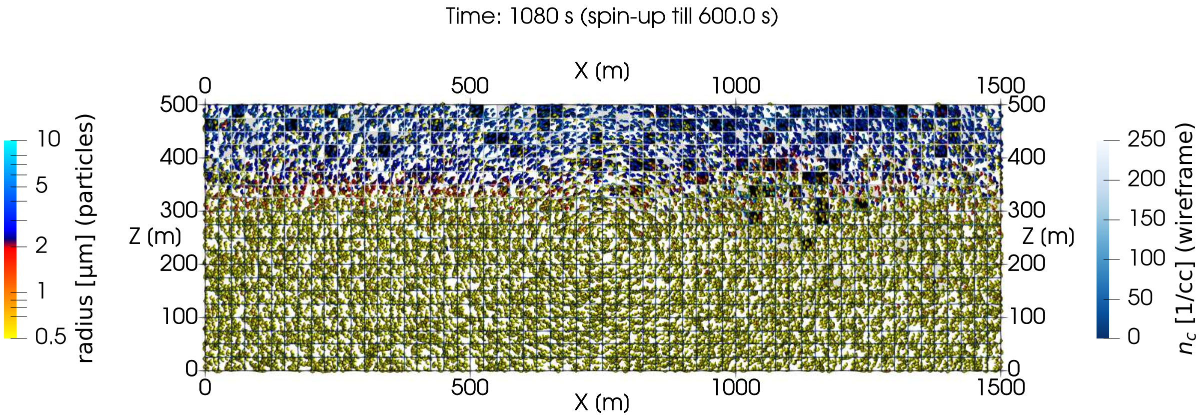

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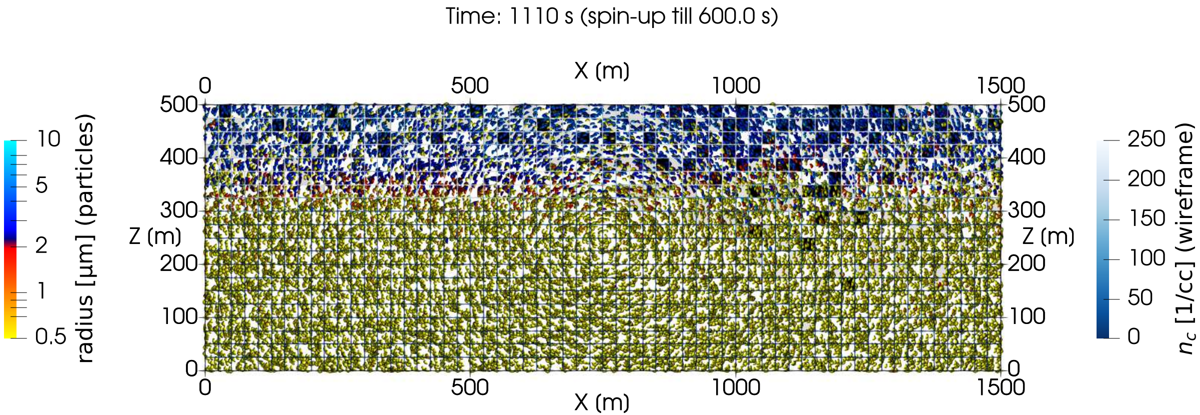

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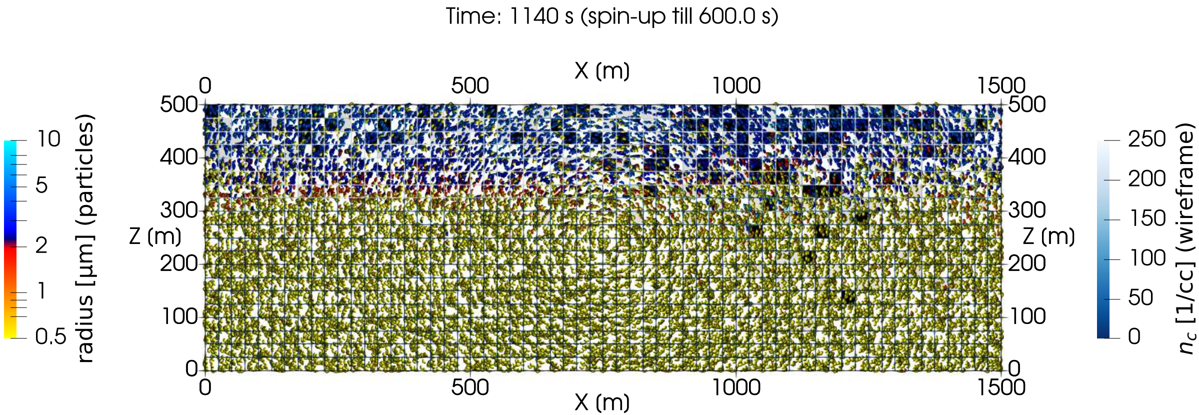

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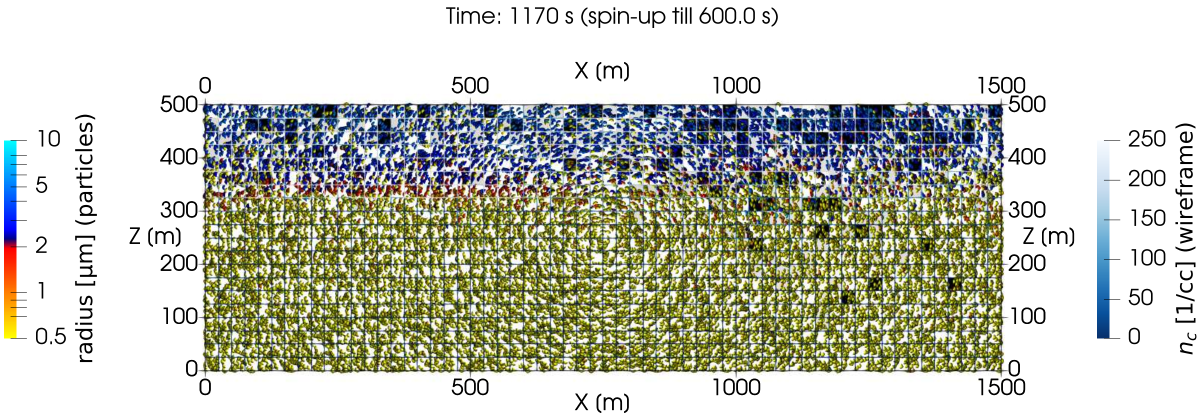

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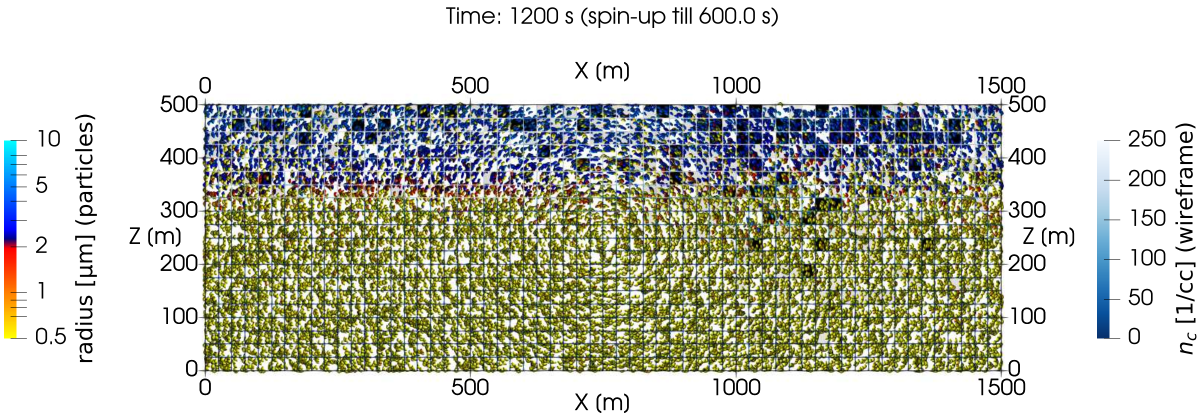

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testing three flow regimes and two immersion freezing representations

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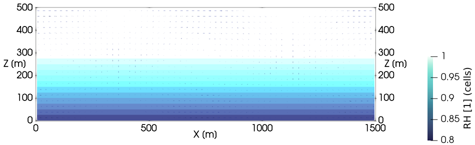

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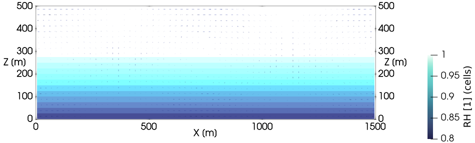

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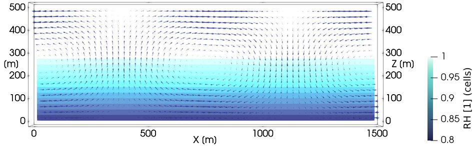

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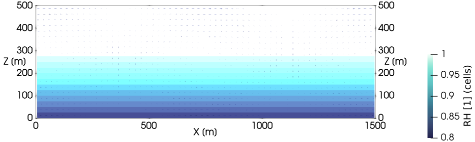

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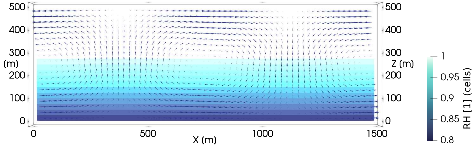

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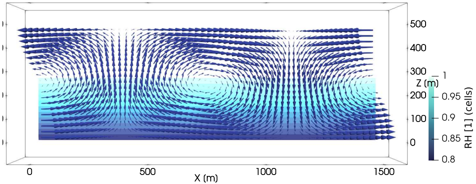

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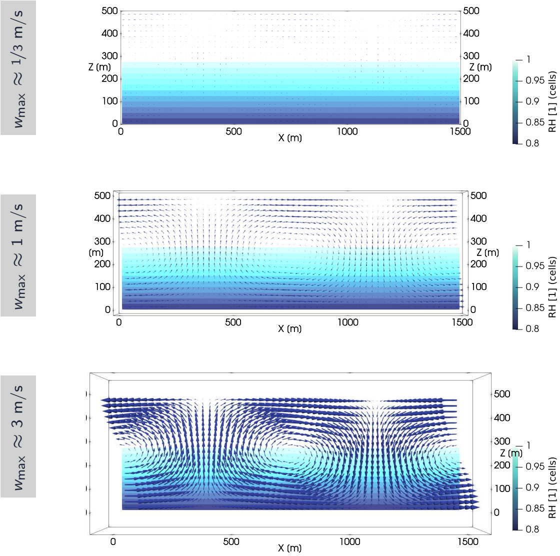

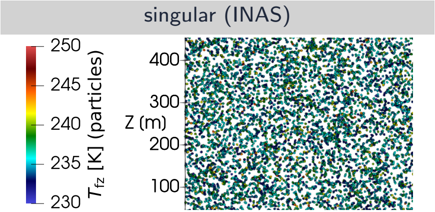

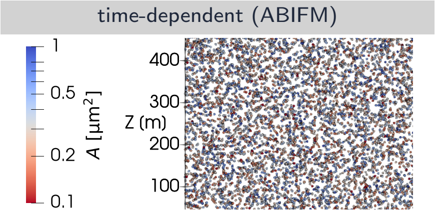

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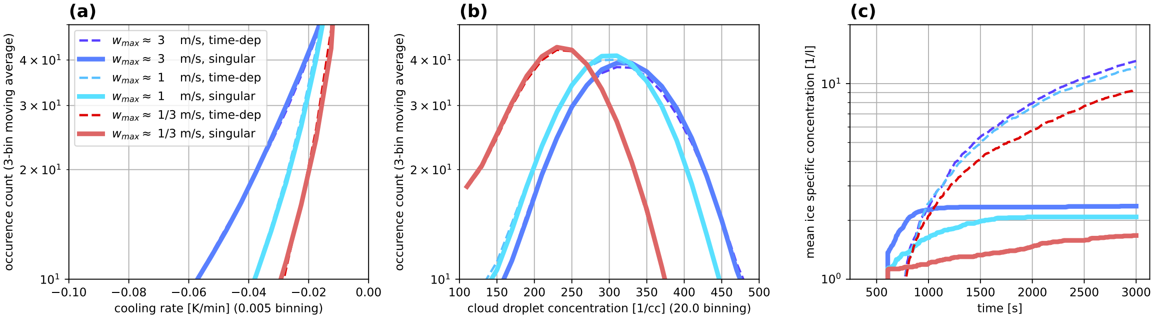

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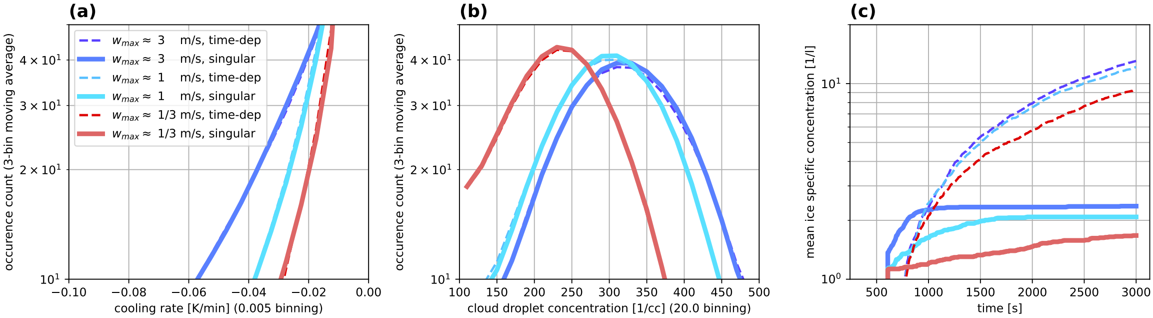

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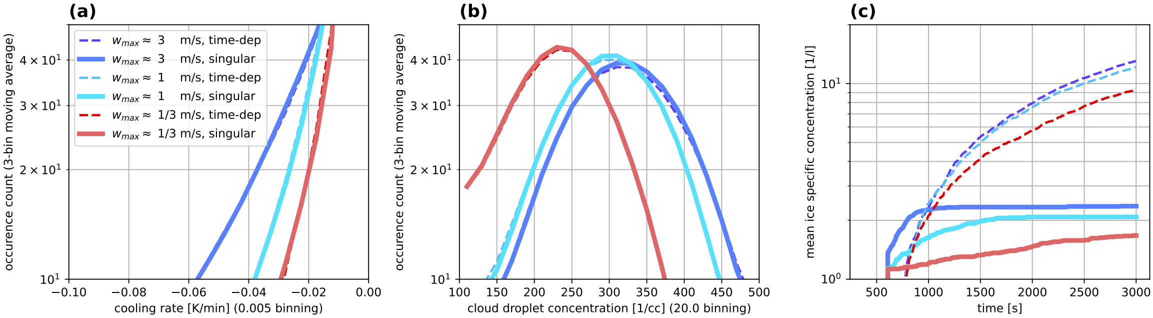

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plan of the talk

aerosol-cloud interactions: a conceptual picture

cloud μ-microphysics: Eulerian vs. Lagrangian

immersion freezing: singular vs. stochastic

implications, summary & outlook

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Opinion: Cloud-phase climate feedback and the importance of ice-nucleating particles

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Atmospheric Chemistry and Physics
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EGU
Atmos. Chem. Phys., 21, 665–679, 2021
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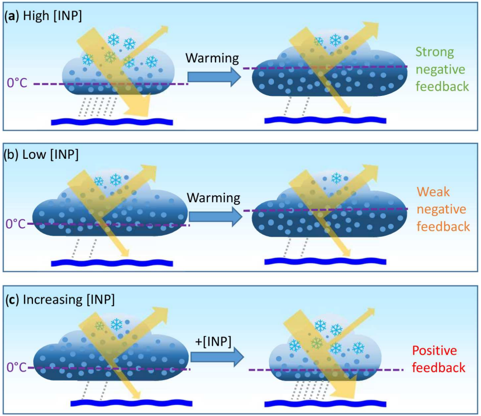

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INPs, cloud-phase feedback, modelling challenges

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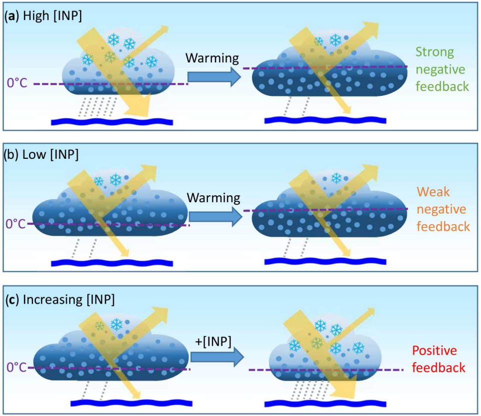

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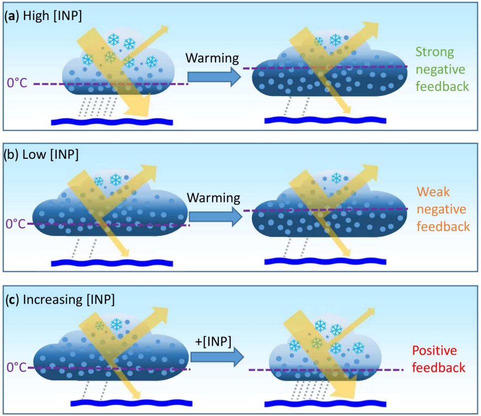

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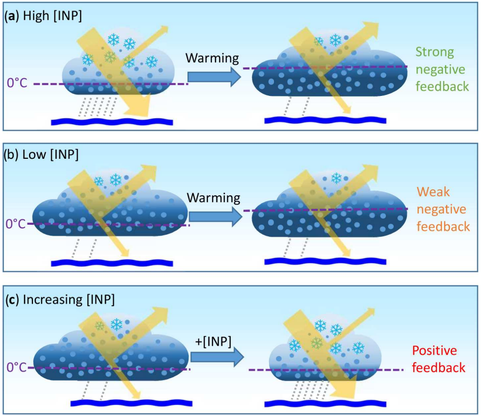

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- *"must also represent the INP removal processes, which in turn depend on a correct representation of the microphysics"*

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ASR Atmospheric System Research
DOE ASR grant no. DE-SC0021034

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Thank you for the invitation!