Immersion freezing in particle-based cloud μ-physics models

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

1: agh.edu.pl
2: atmos.illinois.edu
3: pnnl.gov
4: giss.nasa.gov
5: stonybrook.edu

funding:

Mini-workshop on particle-based cloud modeling 2025, Kobe, Sep 26th 2025

Immersion freezing: bacteria and the Olympics

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

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RESEARCH ARTICLE
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The unstable ice nucleation properties of Snomax® bacterial particles

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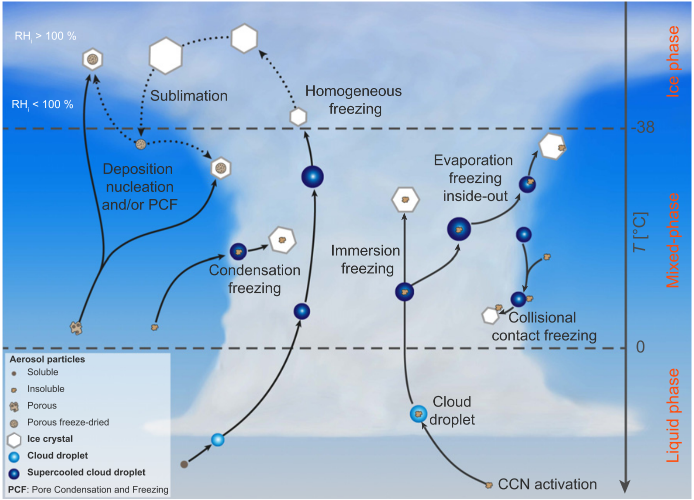
Key Points:
- Very ice active Snomax protein aggregates are fragile and their ice nucleation ability decreases over months of freezer storage
- Partitioning of ice active protein aggregates into the immersion oil reduces the droplet's measured freezing temperature
- Caution is warranted in the use of

Abstract Snomax® is often used as a surrogate for biological ice nucleating particles (INPs) and has recently been proposed as an INP standard for evaluating ice nucleation methods. We have found the immersion freezing properties of Snomax particles to be substantially unstable, observing a loss of ice nucleation ability

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`

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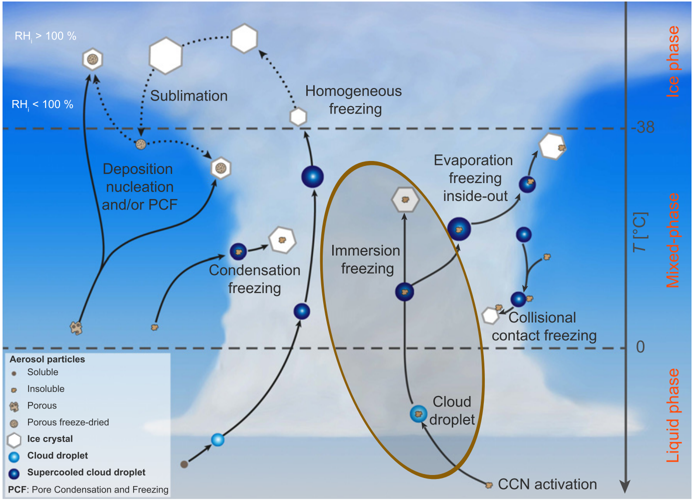

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Marshall et al. 1961, Nubila 4(1)

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.

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

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

Poisson counting process with rate r:

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

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

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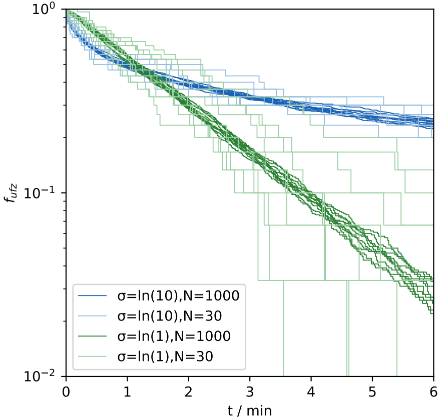
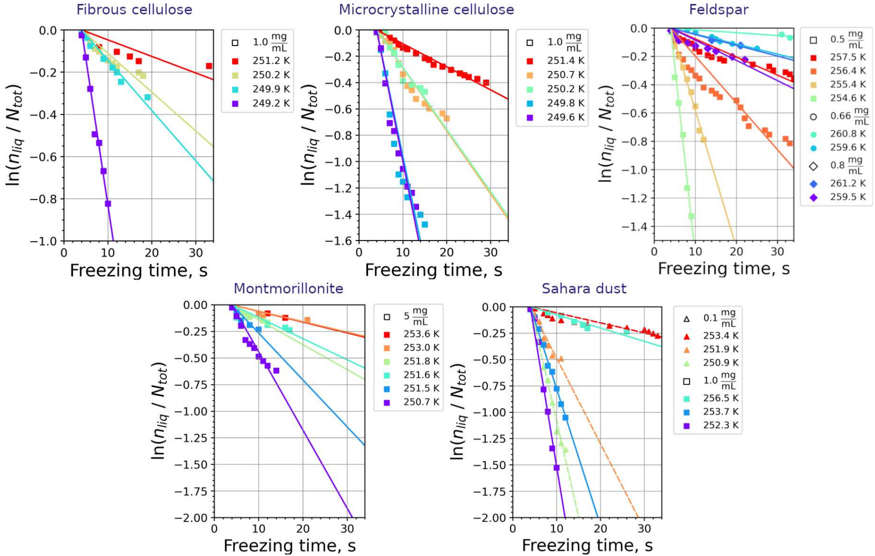
Monte Carlo: const J_{het}, lognormal A



(as in Alpert & Knopf 2016, Fig. 1a)

Szakáll et al. 2021, ACP 21: isothermal experiments (IPA, Mainz)



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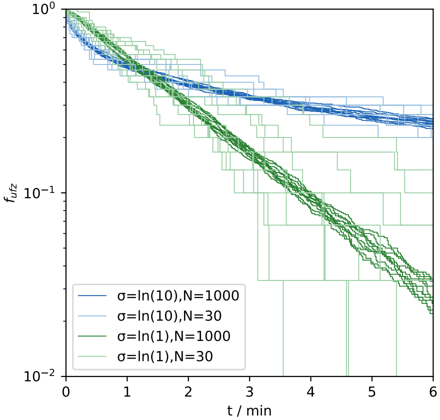

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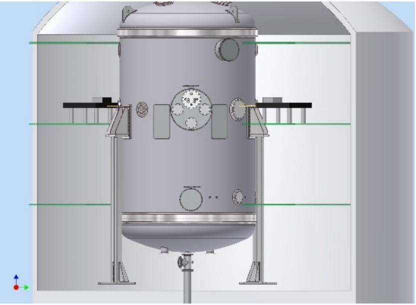
AIDA @ KIT



(https://www.imk-aaf.kit.edu/, photo: KIT/Ottmar Möhler)

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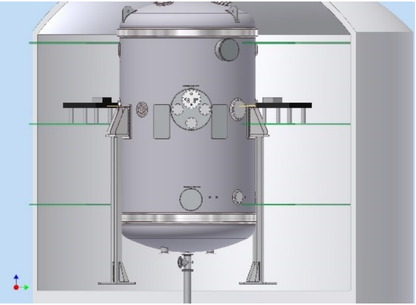

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AIDA cooling rate: ca. $0.5\,{}^{K}/_{min}$

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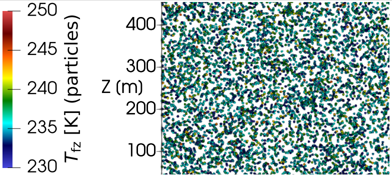

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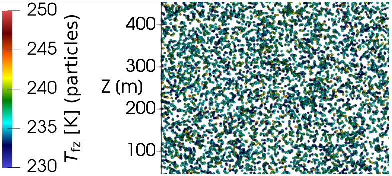

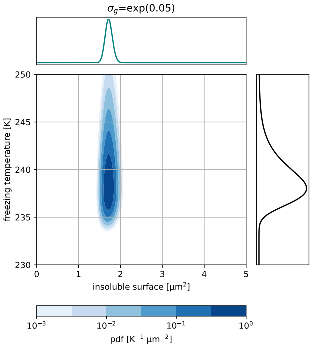

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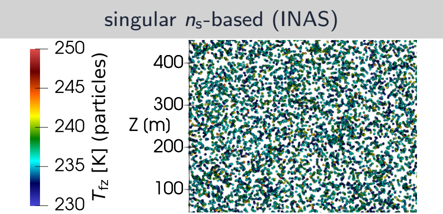

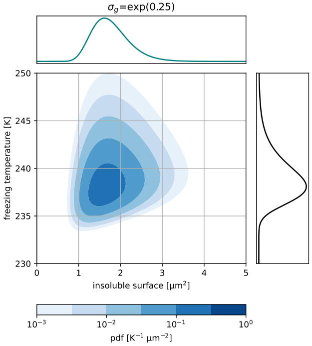

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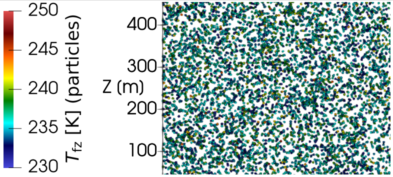

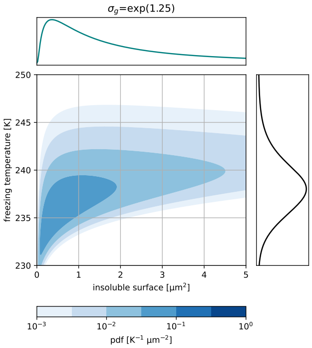

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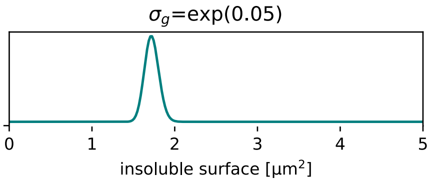
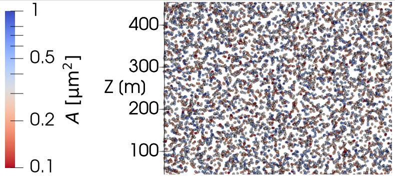


time-dependent J_{het}-based (ABIFM)



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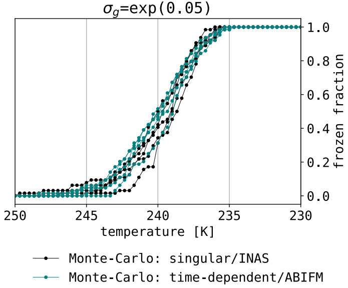
AIDA cooling rate: $0.5\ {}^{K}/_{min}$



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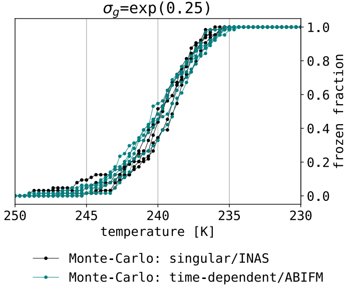

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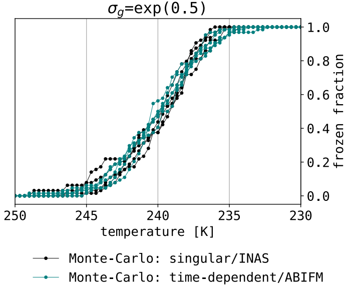

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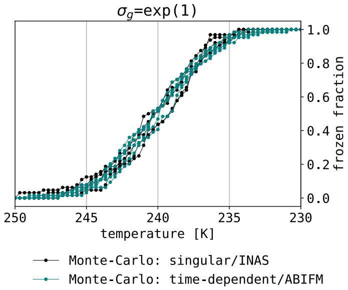

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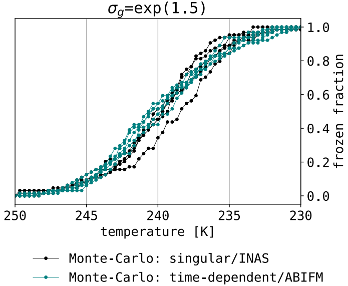

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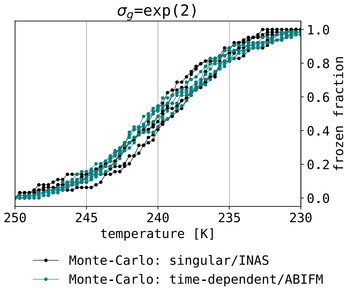

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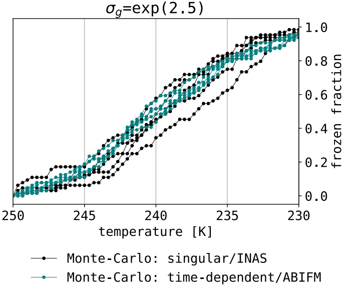

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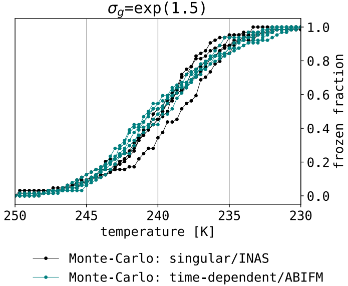

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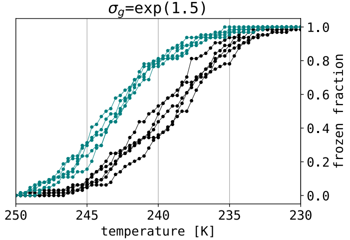

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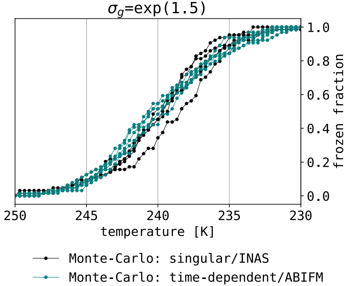

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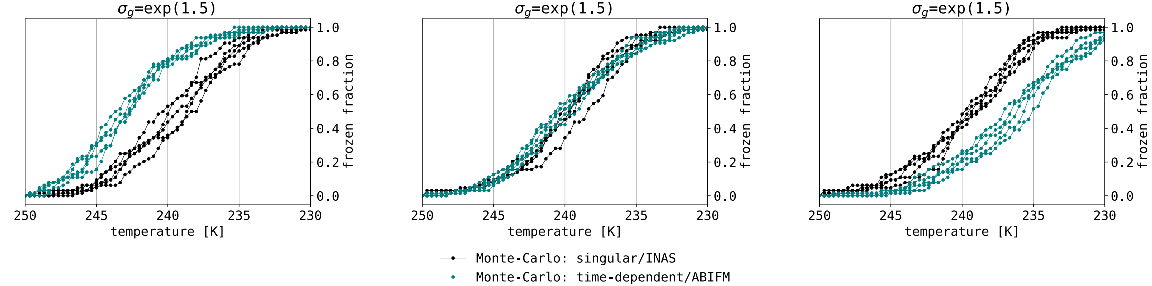

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$$\ln(1-P) = -rt$$

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

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

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

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

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

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

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Knopf & Alpert '13

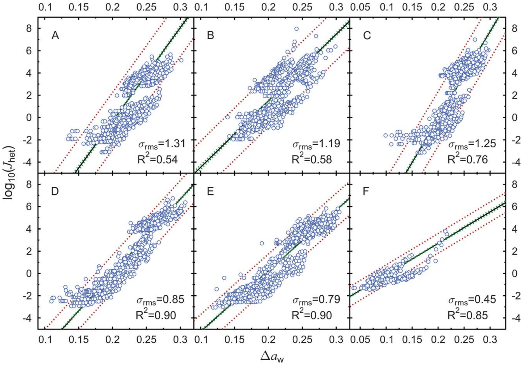

Fig. 3 The decadal log of the heterogeneous ice nucleation rate coefficients, $\log_{10}(J_{het})$, are shown as a function of Δa_w for individually analysed freezing events, initiated by the different IN types investigated in this study and previous work.[41,43,57,66,73,75,78,95] $\text{Log}_{10}(J_{het})$ are shown for (A) *Nannochloris atomus*, (B) *Thalassiosira pseudonana*, (C) Pahokee Peat, (D) Leonardite, (E) Illite, and (F) 1-nonadecanol. The solid black line is a linear fit where dashed green and red lines represent confidence intervals and prediction bands at 95% level. The root mean square error, σ_{rms}, and the adjusted coefficient of determination, R^2, are given in each panel.

Kanji et al. '17

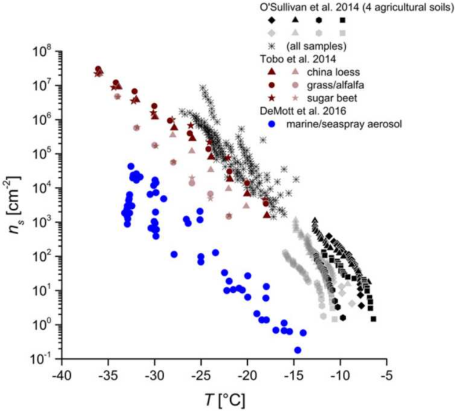

FIG. 1-6. Ice nucleation active site densities n_s as a function of temperature for H_2O_2 (hydrogen peroxide) treated (lighter-shaded symbols) and untreated (dark symbols) agricultural soil dusts in comparison to the n_s of marine aerosol. Differences between various black symbols are for organic content (OC). High OC (12.7 wt%)

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

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

Poisson counting process with rate r:

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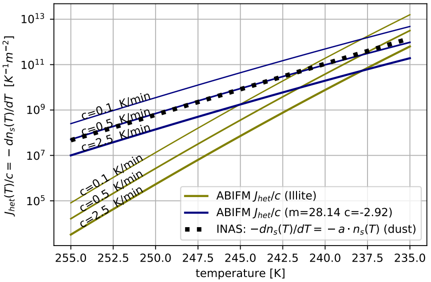
ABIFM J_{het} (Knopf & Alpert '13)



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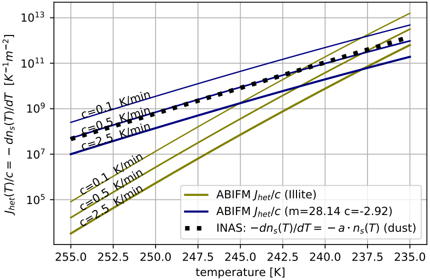

Poissonian model of freezing & Ice Nucleation Active Sites (INAS)

Is it a problem?

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

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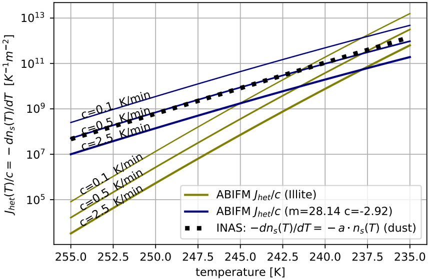

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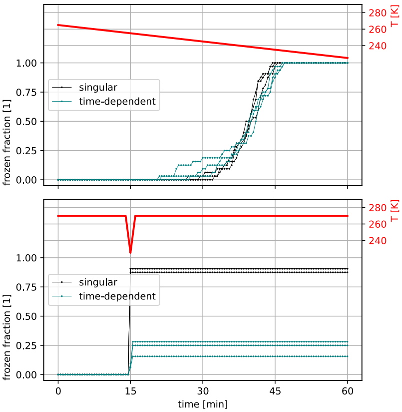
Immersion Freezing in Particle-Based Aerosol-Cloud Microphysics: A Probabilistic Perspective on Singular and Time-Dependent Models

Sylwester Arabas[1], Jeffrey H. Curtis[2], Israel Silber[3,4], Ann M. Fridlind[5], Daniel A. Knopf[6], Matthew West[7], and Nicole Riemer[2]

10.1029/2024MS004770

Testing different cooling-rate profiles in a box model



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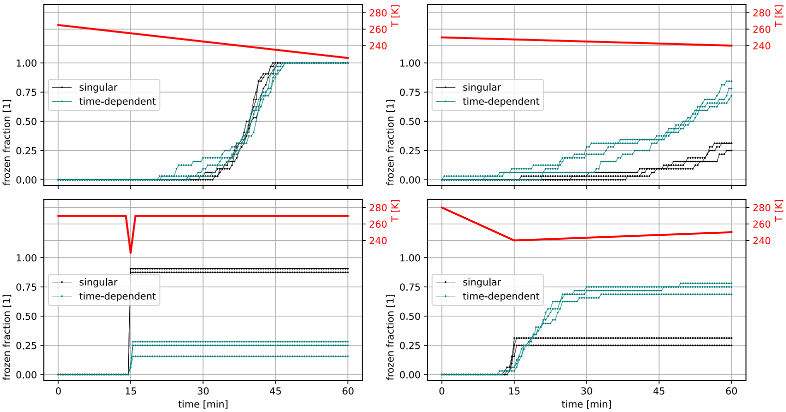

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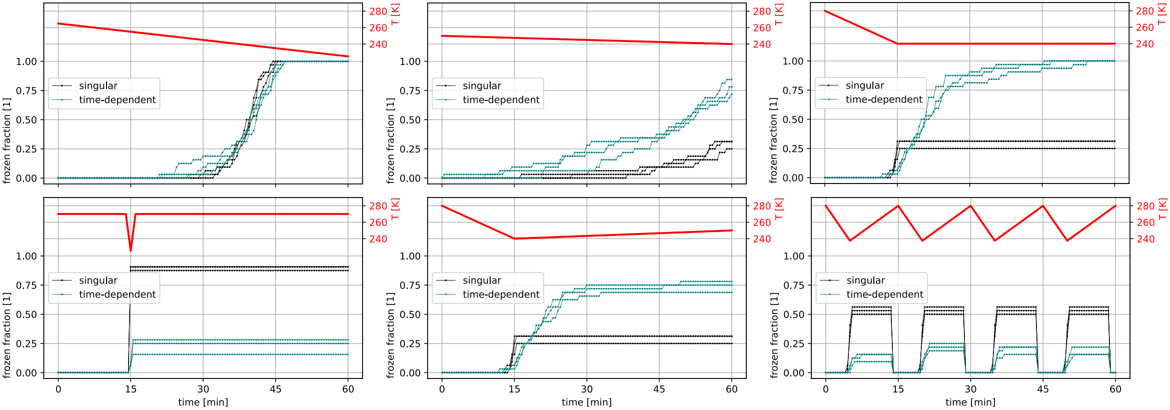
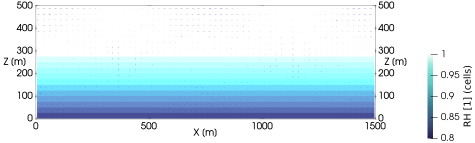


100% python™ open-source code:

GitHub / OPENATMOS / PySDM

Testing three flow regimes and two immersion freezing representations

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



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

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

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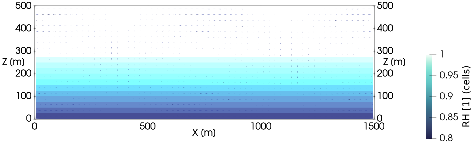

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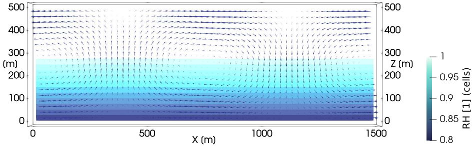

$w_{max} \approx 3$ m/s

Testing three flow regimes and two immersion freezing representations

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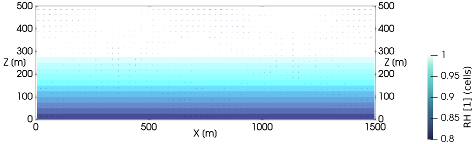

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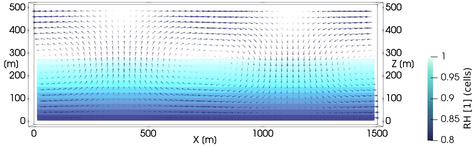

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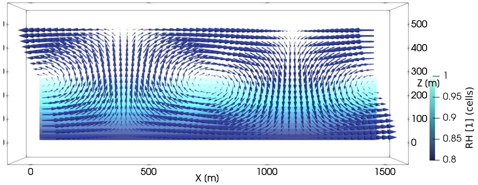

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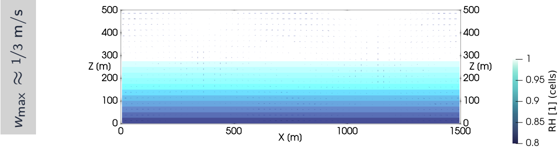
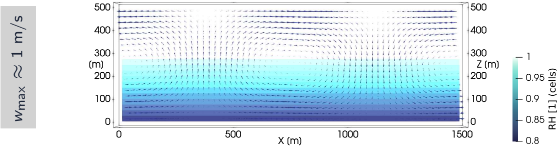
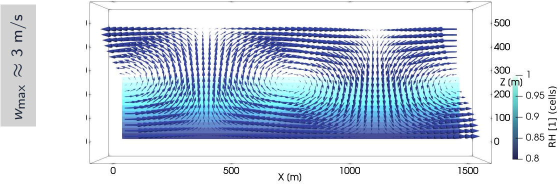
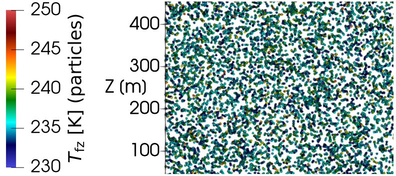


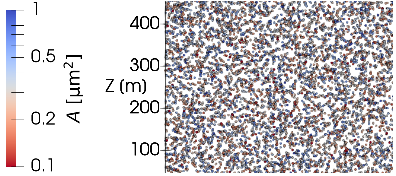




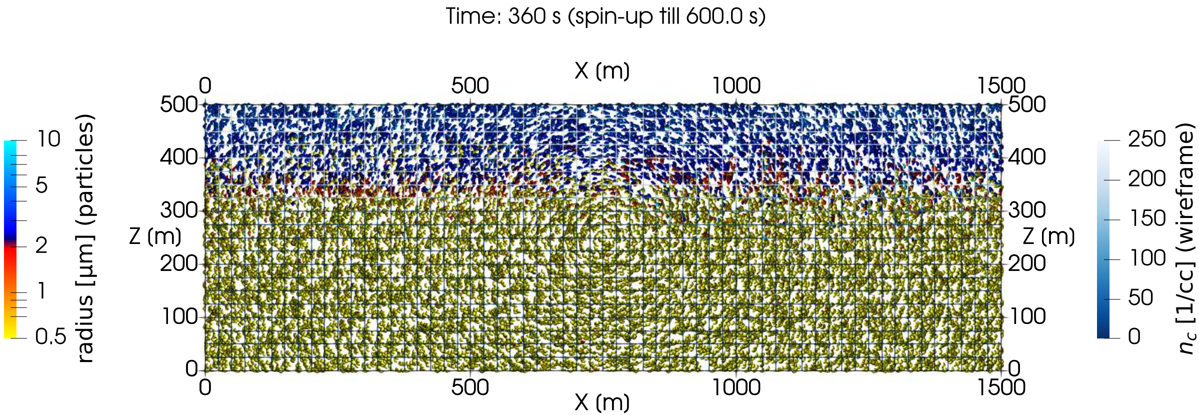
singular (INAS)



time-dependent (J_{het})

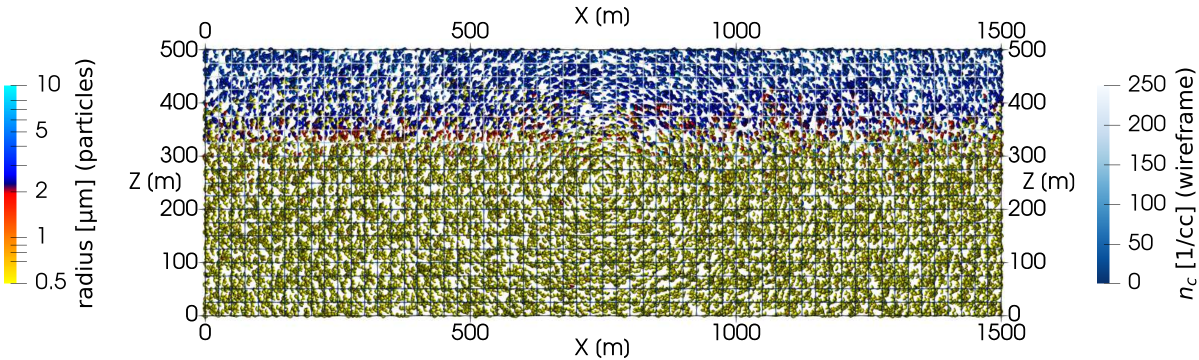


Particle-based μ-physics + prescribed-flow: spin-up



Particle-based μ-physics + prescribed-flow: spin-up

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



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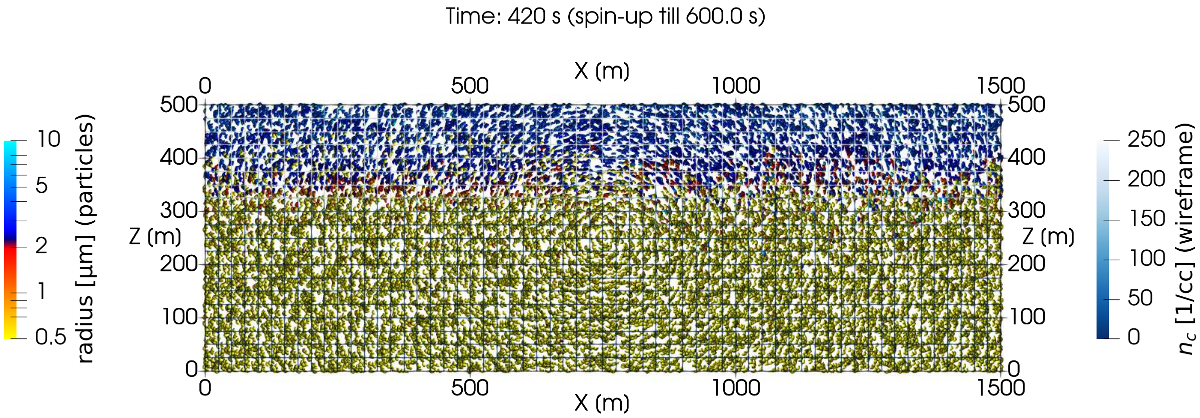

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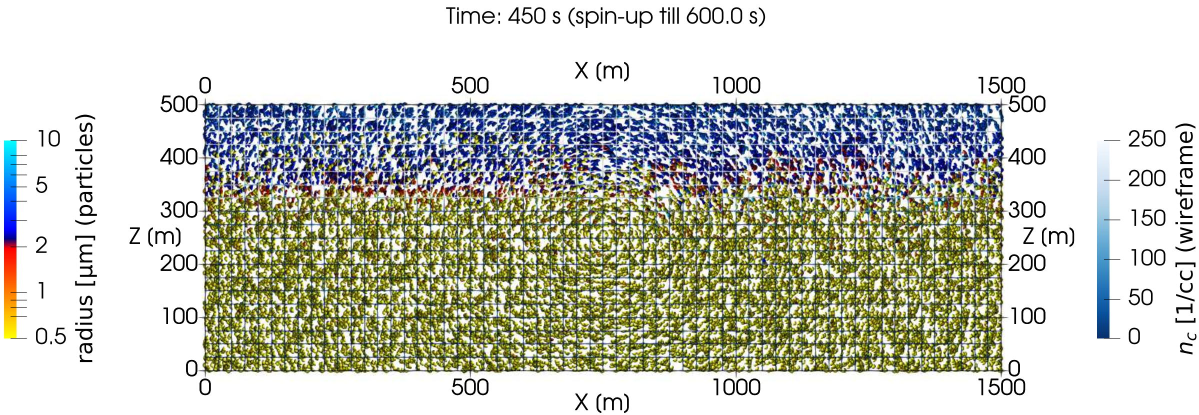

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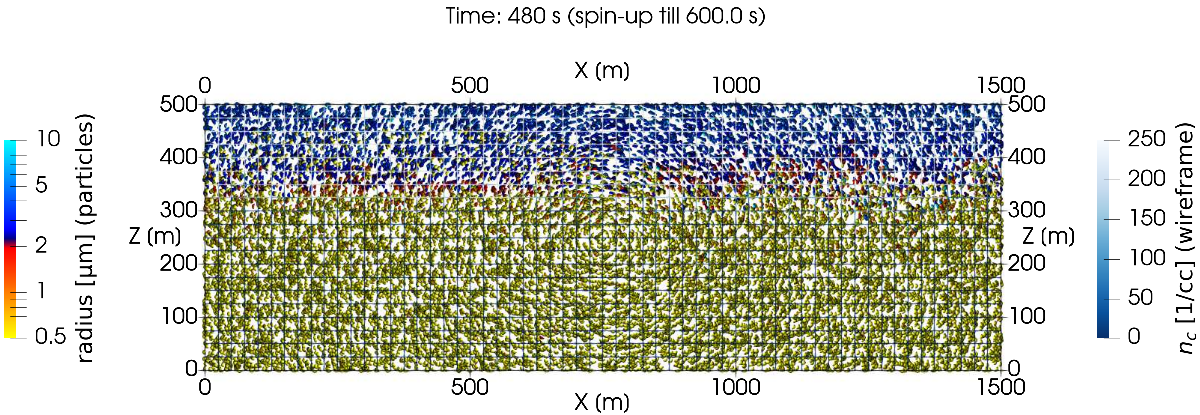

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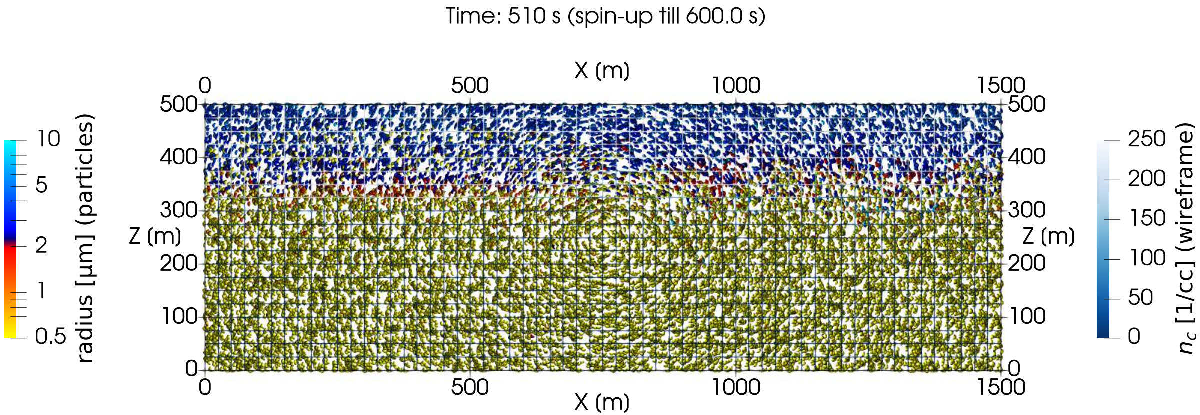

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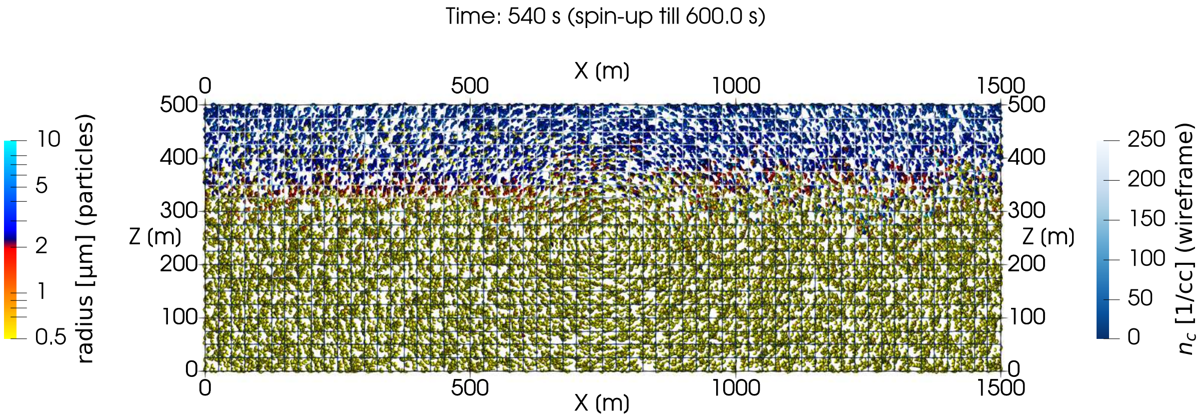

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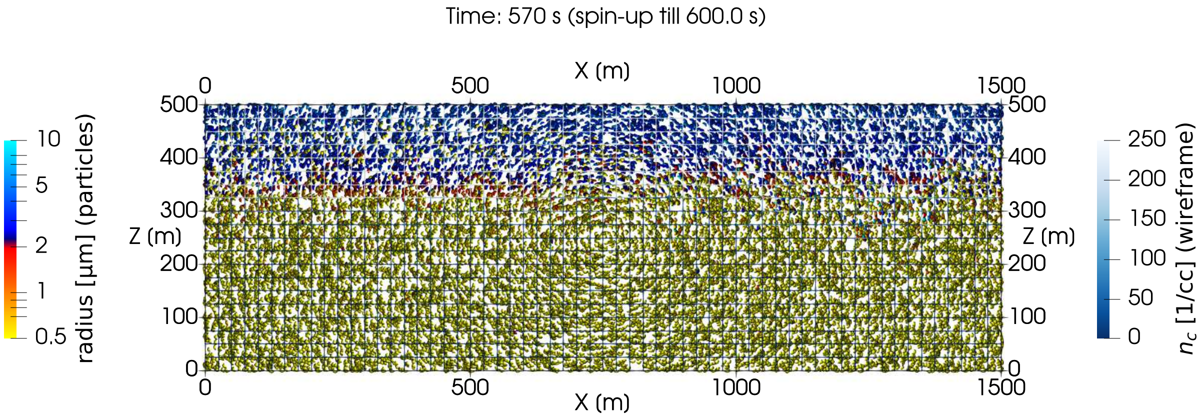

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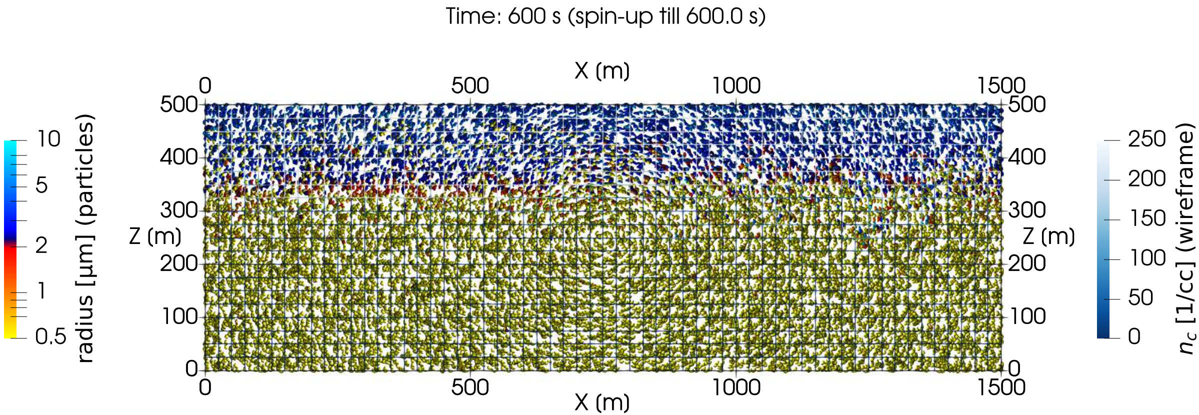
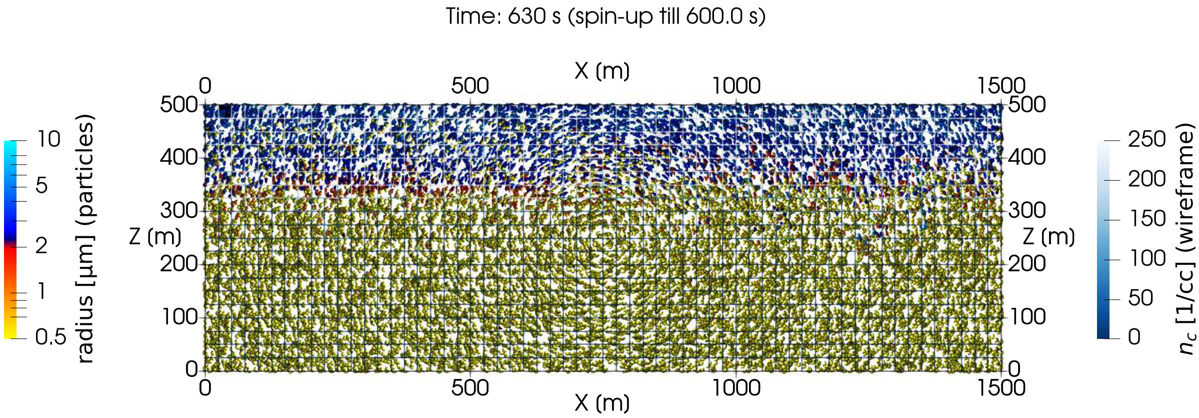


Particle-based μ-physics + prescribed-flow: glaciation



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

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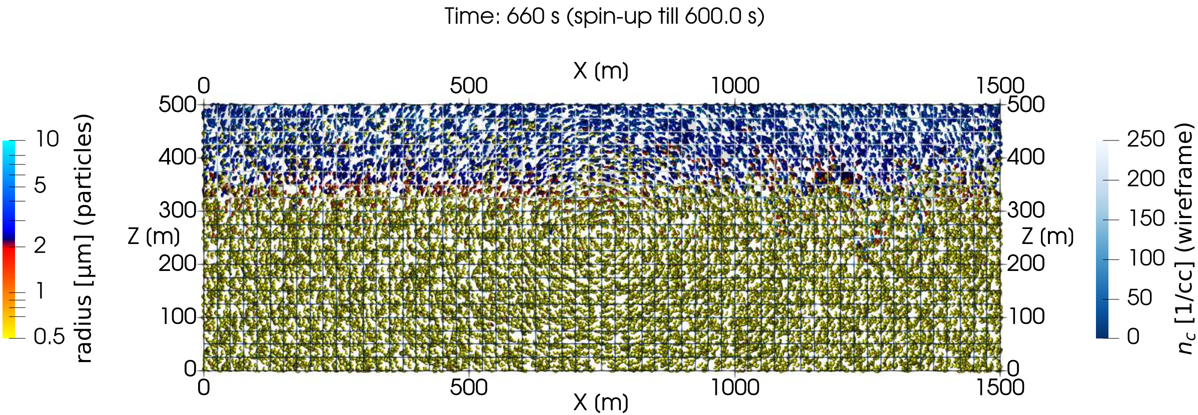

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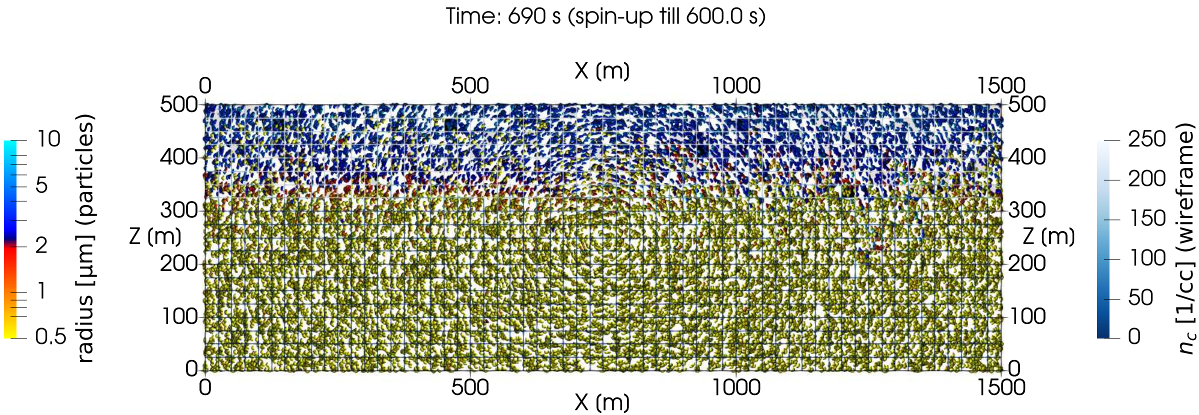

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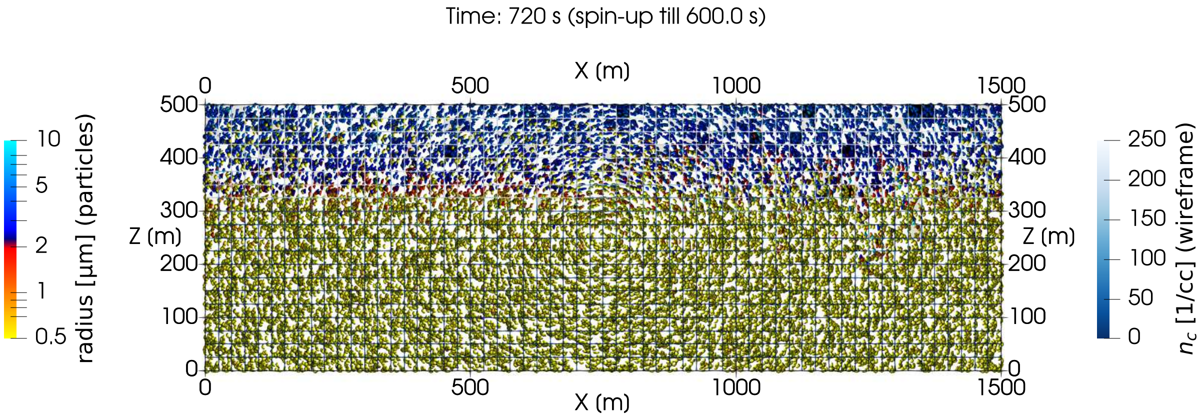

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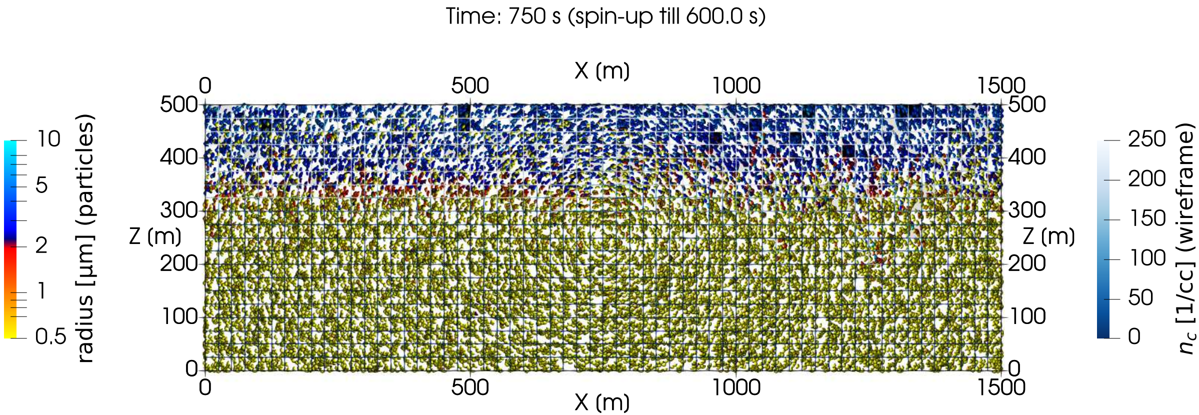

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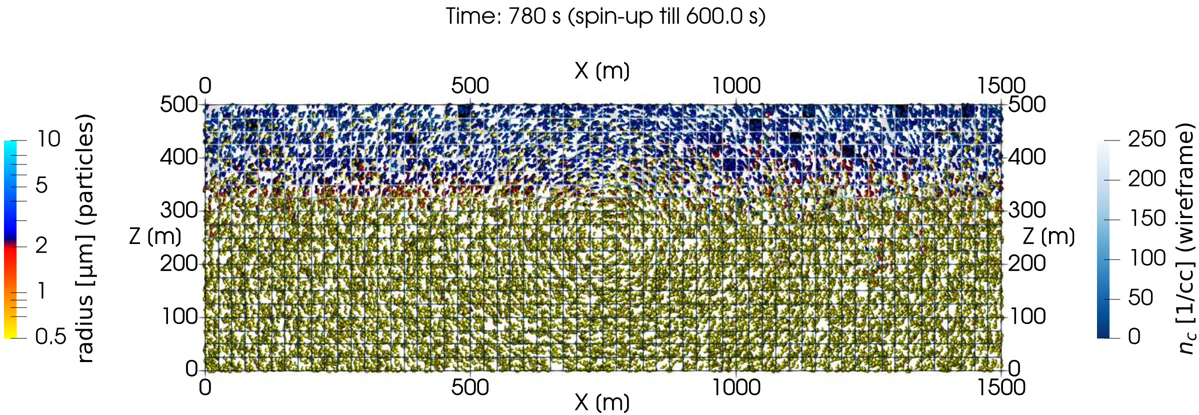

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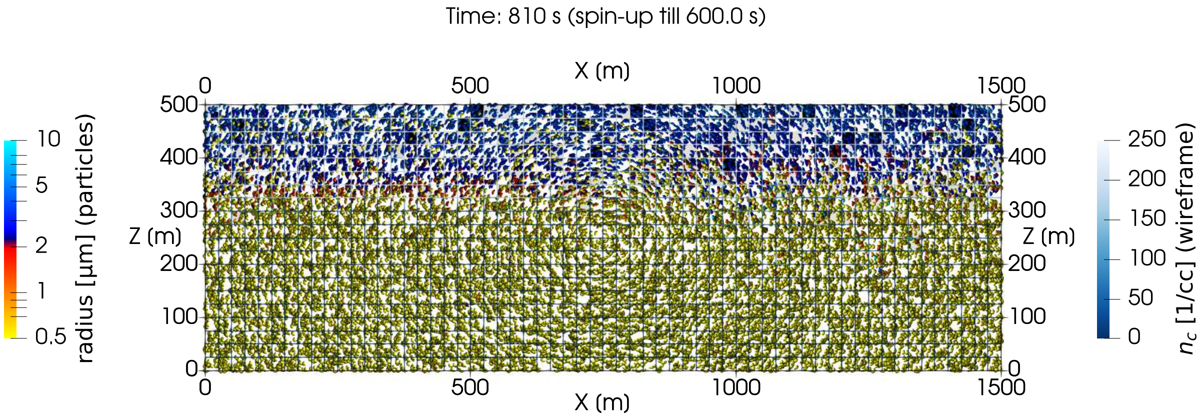

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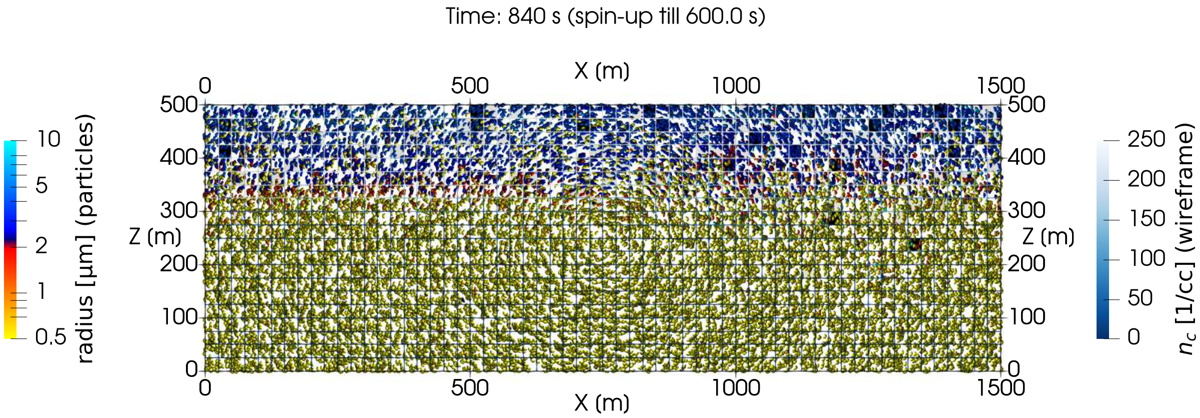

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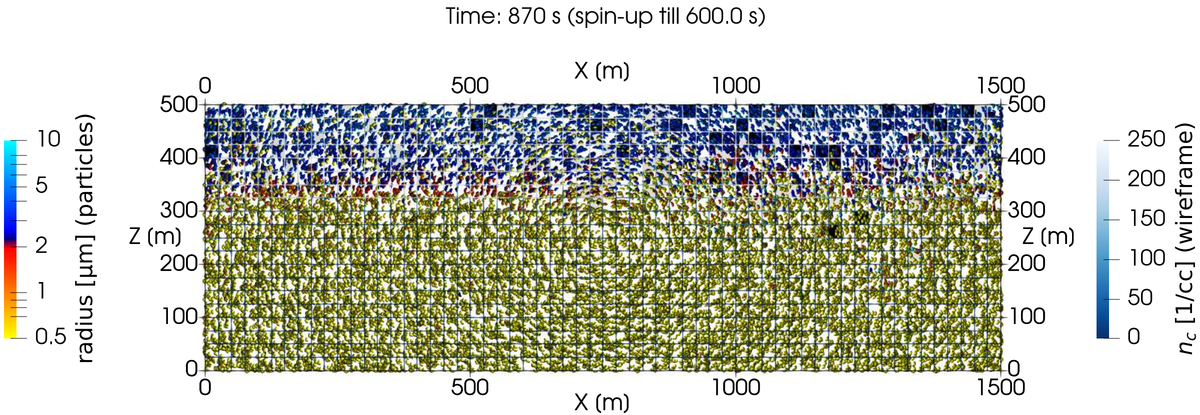

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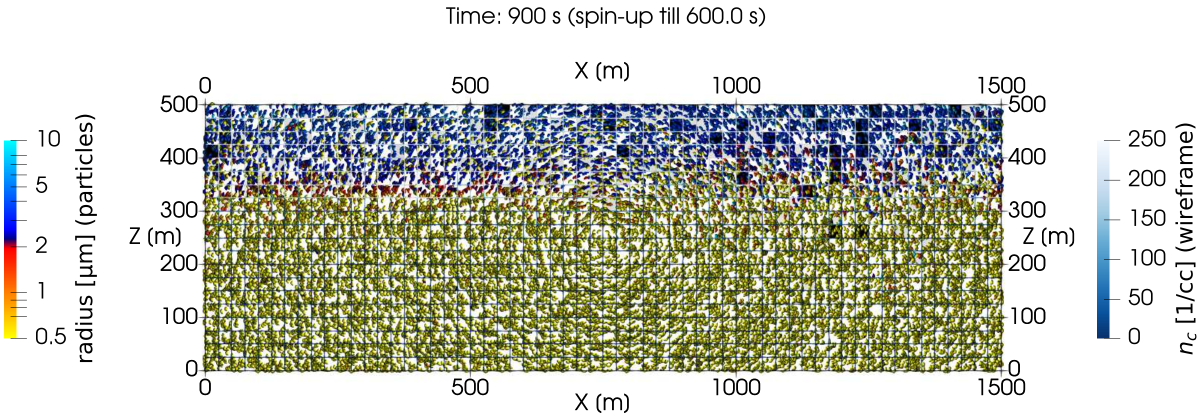

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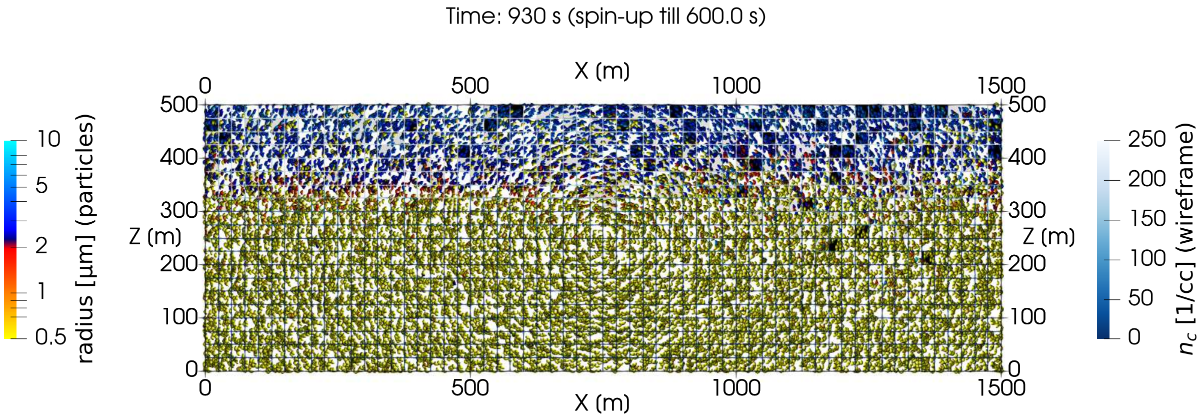

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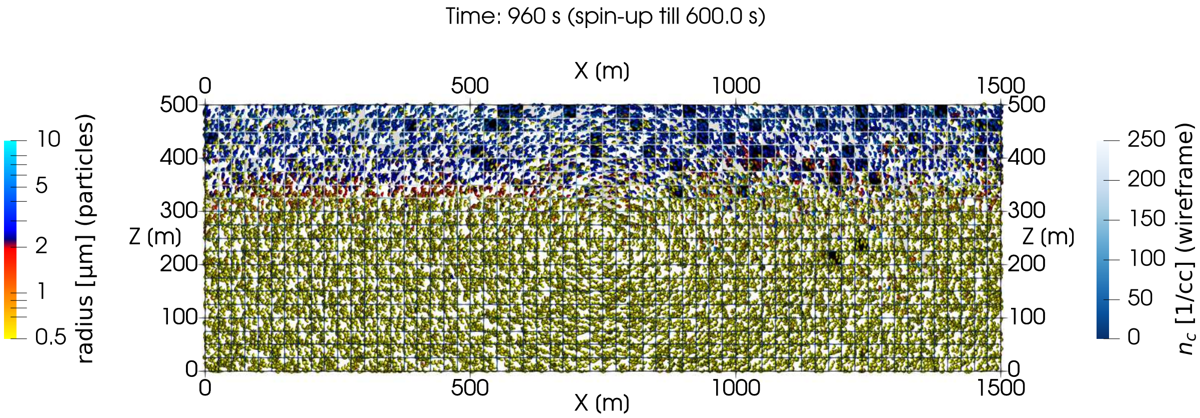

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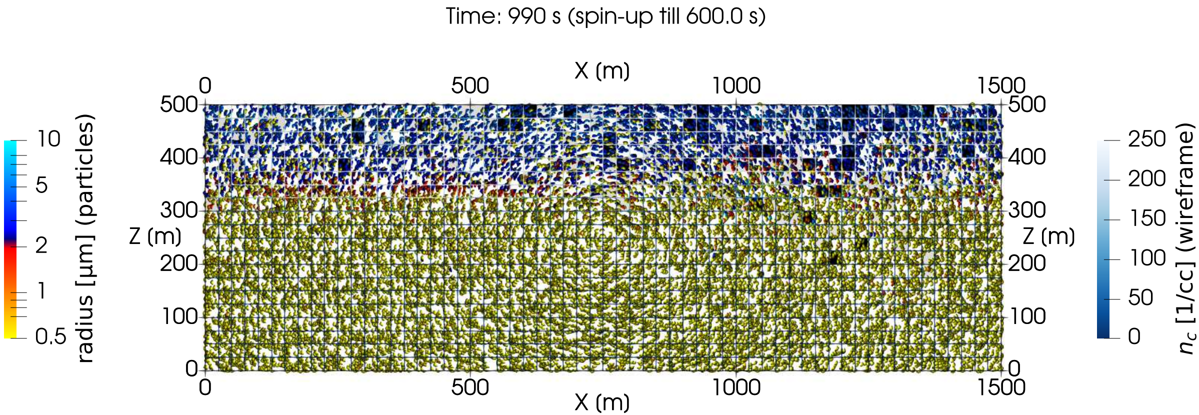

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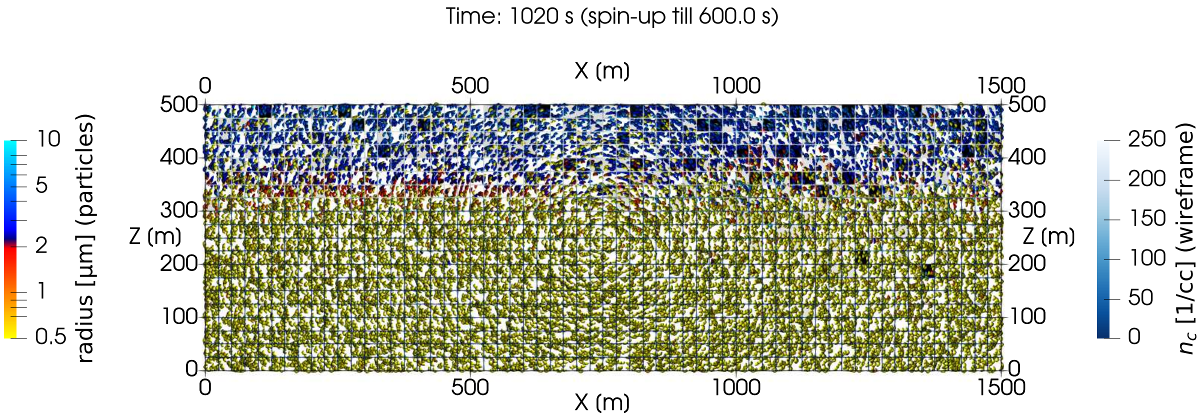
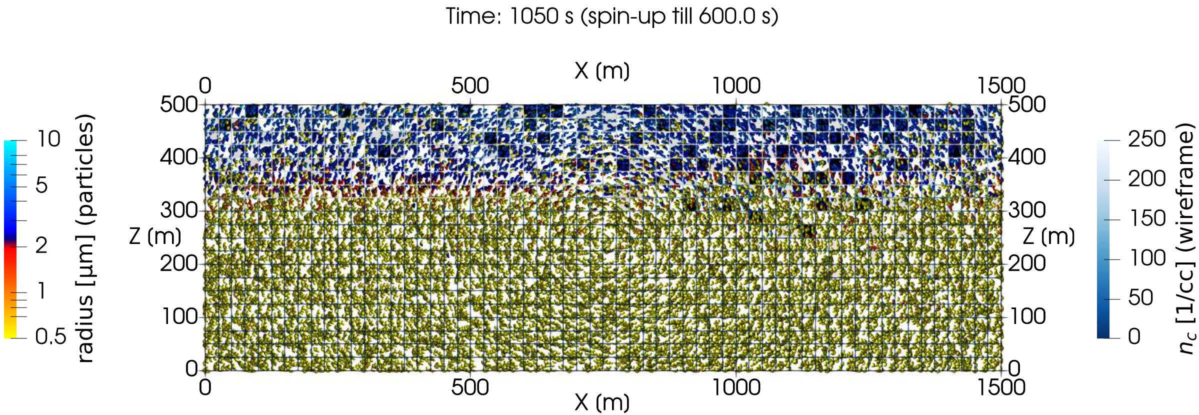


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{aer} = 300/cc$ (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: glaciation



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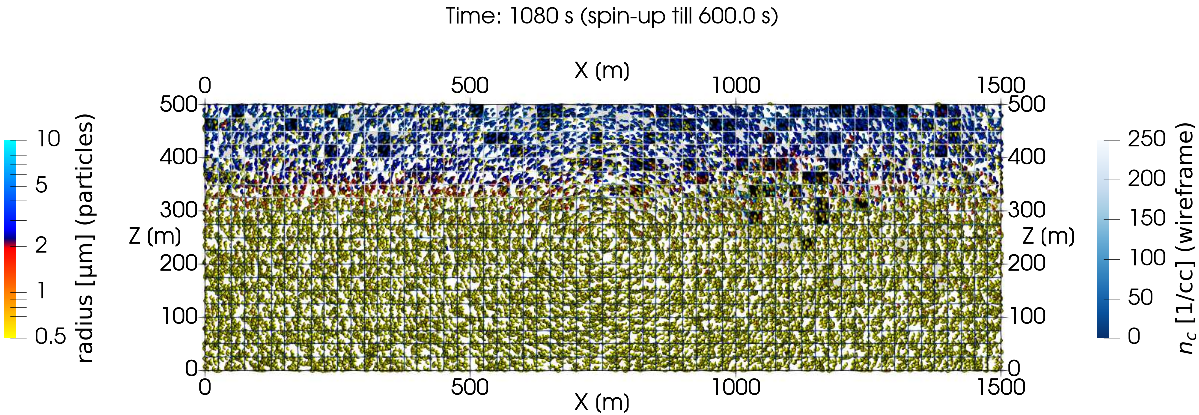

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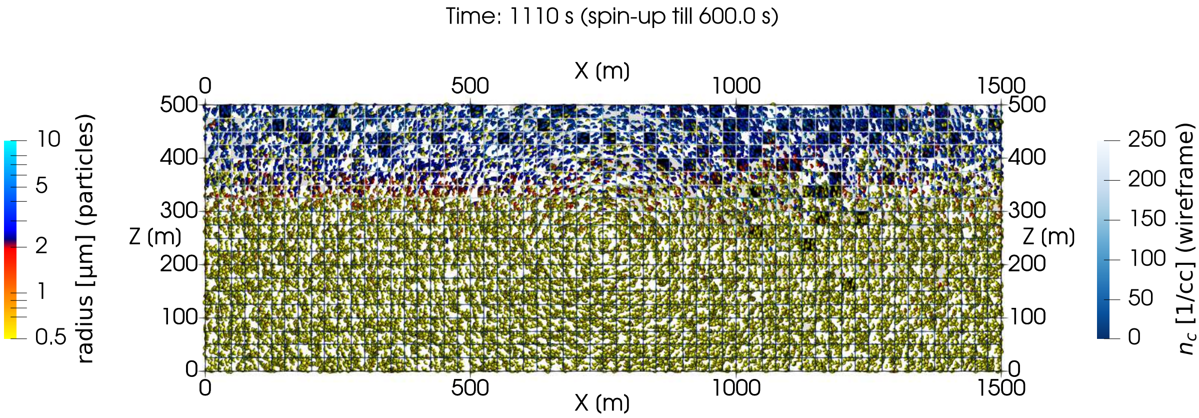

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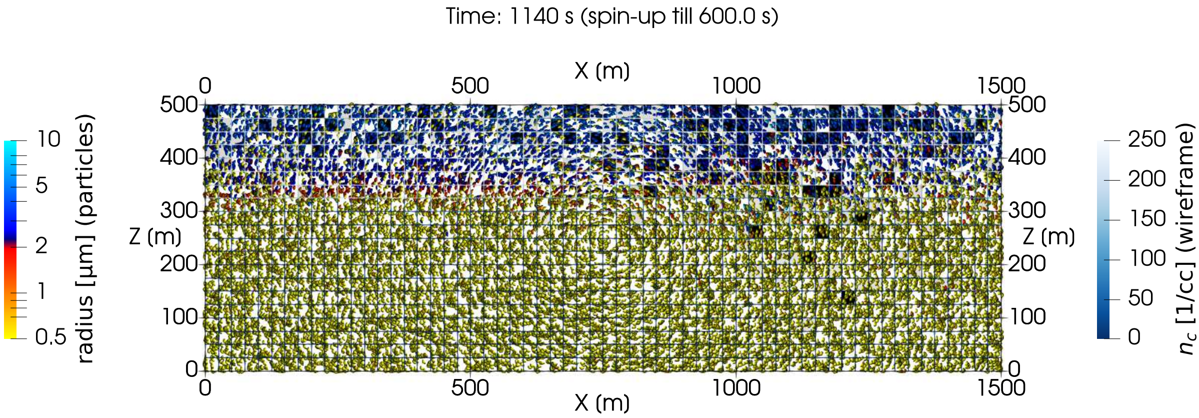

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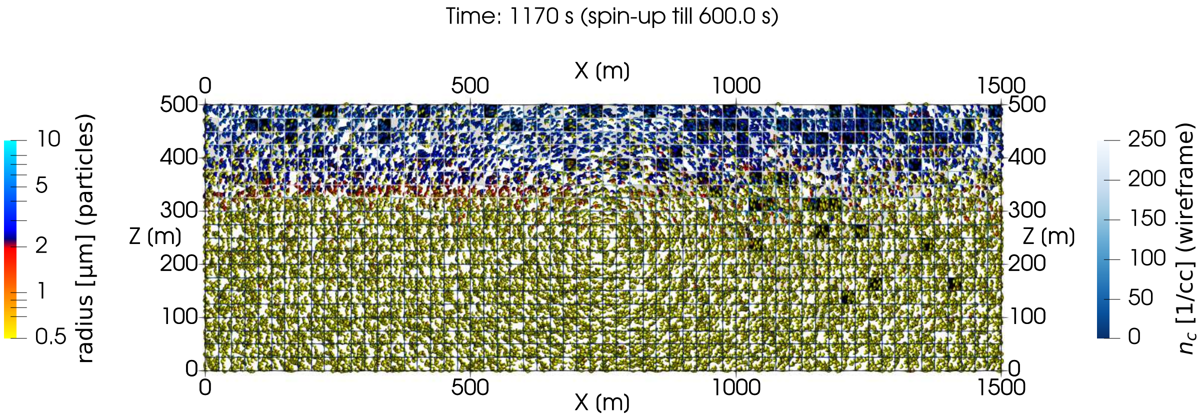

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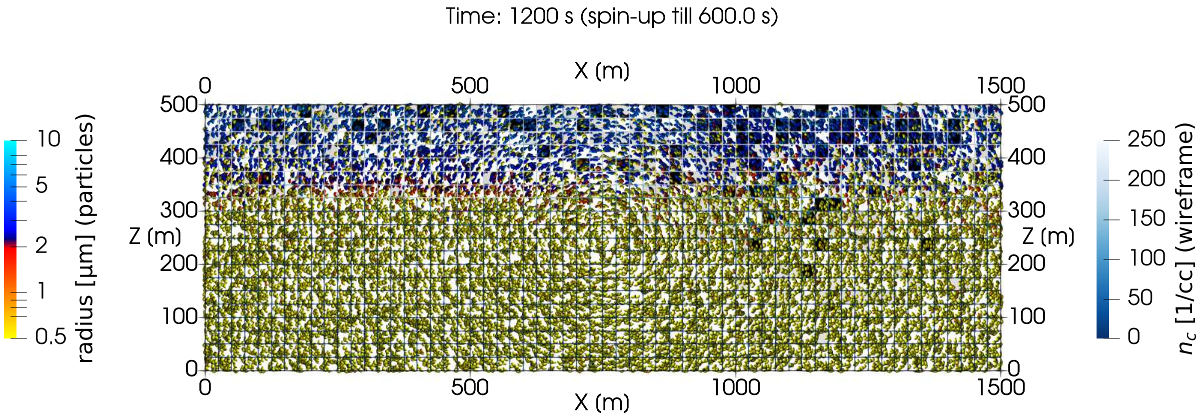

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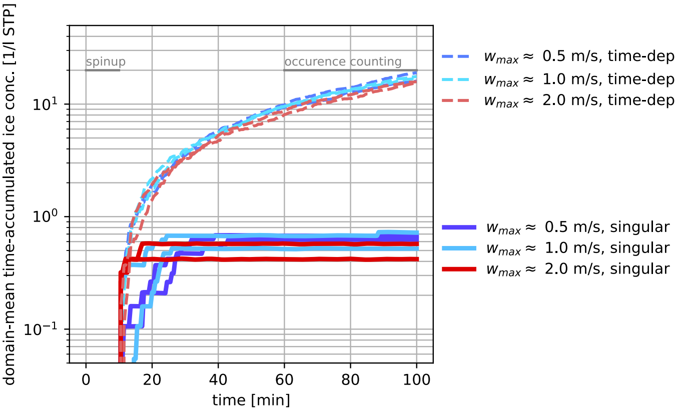
Testing three flow regimes and two immersion freezing representations



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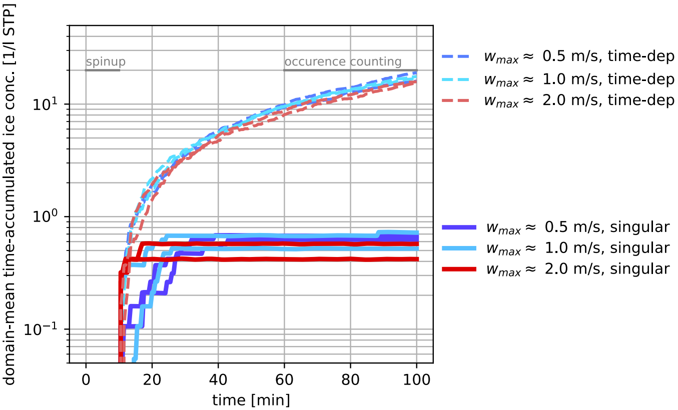

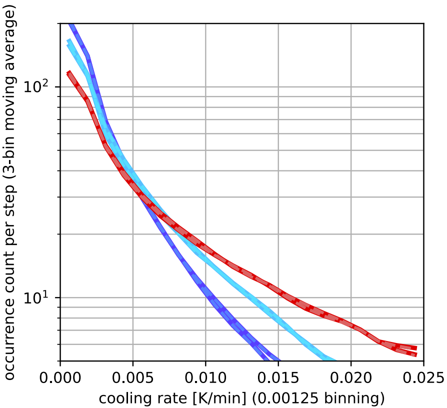

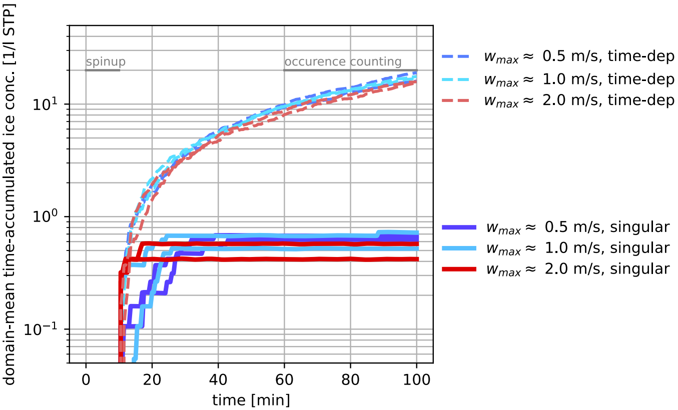

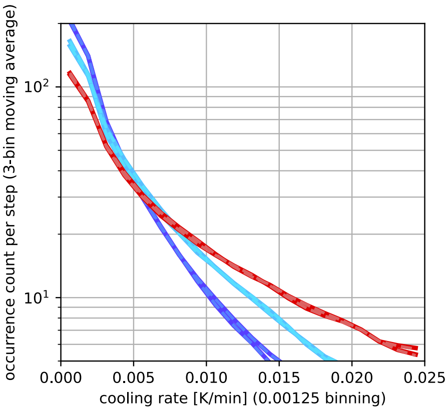

- range of cooling rates in simple flow (far from 0.5 K/min for AIDA as in Niemand et al. 2012)

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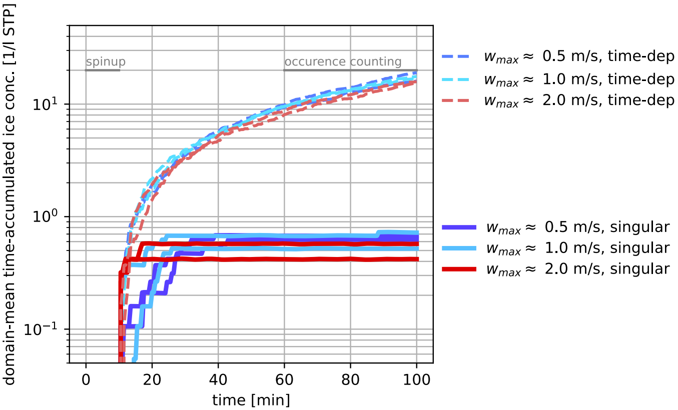

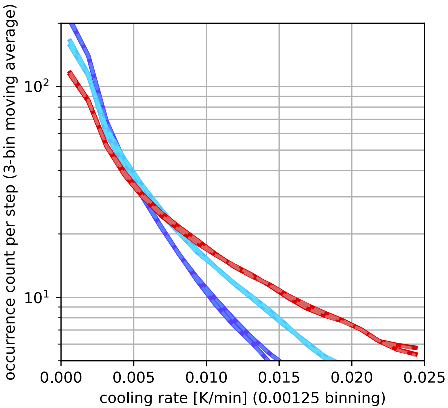

- range of cooling rates in simple flow (far from 0.5 K/min for AIDA as in Niemand et al. 2012)
- **only time-dependent scheme robust across flow regimes** (consistent with box model & theory)

https://en.wikipedia.org/wiki/Draft:Super_Droplet_Method

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Draft:Super Droplet Method

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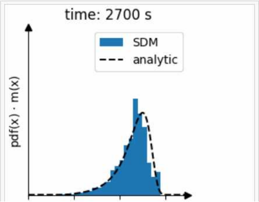
In mathematical modeling of aerosols, clouds and precipitation, **Super Droplet Method (SDM)** is a Monte-Carlo approach for representing collisions and coalescence of particles in atmospheric fluid dynamics simulations. The method and its name was introduced in a 2007 arXiv e-print by Shin-ichiro Shima et al.[1] (preceded by a 2006 patent application[2] and followed by 2008 RIMS Kôkyûroku[3] and 2009 QJRMS[4] papers).

SDM algorithm is a probabilistic alternative to the deterministic model of the process embodied in the Smoluchowski coagulation equations. Among the key characteristics of SDM is that it is not subject to the "curse of dimensionality" that hampers application of other methods when multiple particle attributes need to be resolved in a simulation[7]. The algorithm is embarrassingly parallel, has linear time complexity, constant state vector size (number conservation of simulated particles during collisions)



(thanks to Emma Ware and Clara Bailey for help)

聞いてくれておおきに!

Thank you for your attention!

https://doi.org/10.1029/2024MS004770
(Arabas et al. 2025, JAMES)

https://en.wikipedia.org/wiki/Draft:Super_Droplet_Method
(feedback & contributions most welcome!)

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