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:

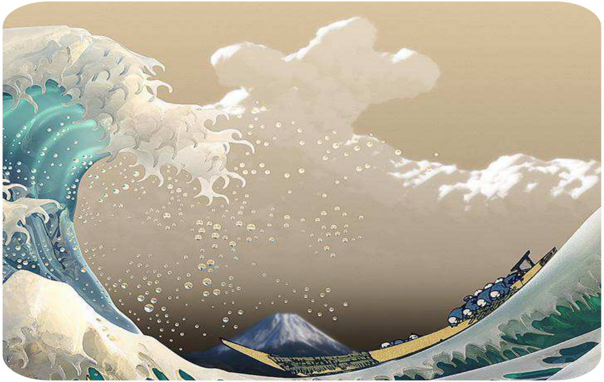
Department of Earth Sciences, University of Southern California, L.A., Sep 12th 2025

Aerosol-cloud interactions: a conceptual picture

Aerosol-cloud interactions: a conceptual picture

background image: vitsly / Hokusai

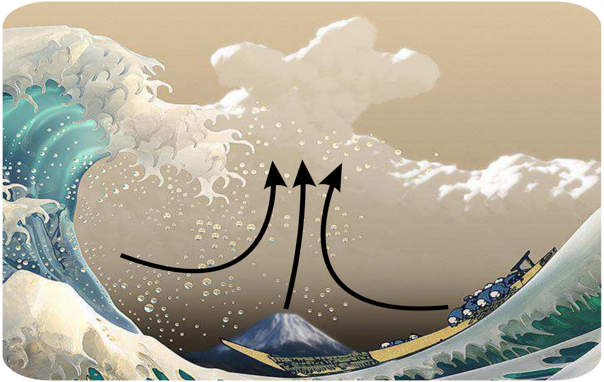
Aerosol-cloud interactions: a conceptual picture



background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

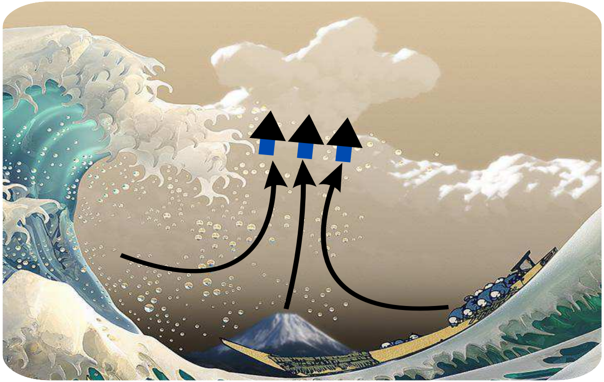
- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei



background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural
  and anthropogenic origin
  act as condensation/crystallisation nuclei
- droplets and ice particles grow through
  vapour condensation and deposition...



background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural
  and anthropogenic origin
  act as condensation/crystallisation nuclei
- droplets and ice particles grow through
  vapour condensation and deposition...
- ... and collisions-coalescence/aggregation

background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei
- droplets and ice particles grow through vapour condensation and deposition...
- ... and collisions-coalescence/aggregation
- aqueous chemical reactions alter droplet composition

background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei
- droplets and ice particles grow through vapour condensation and deposition...
- ... and collisions-coalescence/aggregation
- aqueous chemical reactions alter droplet composition
- water and ice precipitates (possibly breaking up into smaller particles) washing out sub-cloud aerosol

background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei
- droplets and ice particles grow through vapour condensation and deposition...
- ... and collisions-coalescence/aggregation
- aqueous chemical reactions alter droplet composition
- water and ice precipitates (possibly breaking up into smaller particles) washing out sub-cloud aerosol
- particles evaporating before reaching surface (with potentially altered size/composition) contribute to ambient aerosol

background image: vitsly / Hokusai

Aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei
- droplets and ice particles grow through vapour condensation and deposition...
- ... and collisions-coalescence/aggregation
- aqueous chemical reactions alter droplet composition
- water and ice precipitates (possibly breaking up into smaller particles) washing out sub-cloud aerosol
- particles evaporating before reaching surface (with potentially altered size/composition) contribute to ambient aerosol

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

background image: vitsly / Hokusai

Aerosol-cloud interactions: μ-physics models

JAMES | Journal of Advances in Modeling Earth Systems

COMMISSIONED MANUSCRIPT
10.1029/2019MS001689

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

Hugh Morrison[1], Marcus van Lier-Walqui[2], Ann M. Fridlind[3], Wojciech W. Grabowski[1], Jerry Y. Harrington[4], Corinna Hoose[5], Alexei Korolev[6], Matthew R. Kumjian[4], Jason A. Milbrandt[7], Hanna Pawlowska[8], Derek J. Posselt[9], Olivier P. Prat[10], Karly J. Reimel[4], Shin-Ichiro Shima[11], Bastiaan van Diedenhoven[2], and Lulin Xue[1]

Key Points:

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

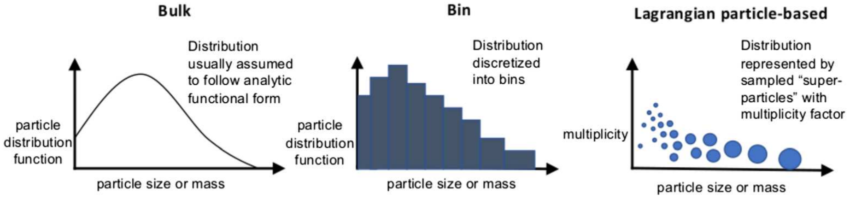


Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

Aerosol-cloud interactions: μ-physics models

well suited for two-way aerosol-cloud interactions!

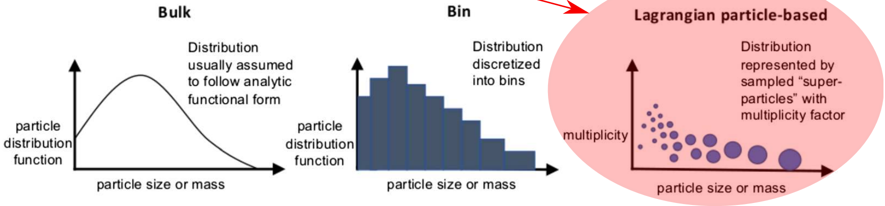
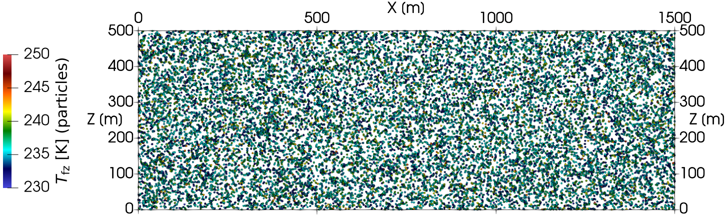


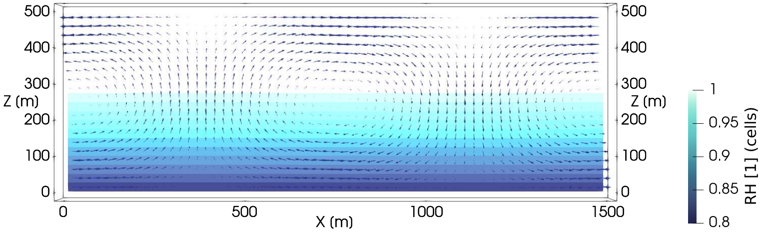
Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

Particle-based μ-physics + prescribed-flow: model state

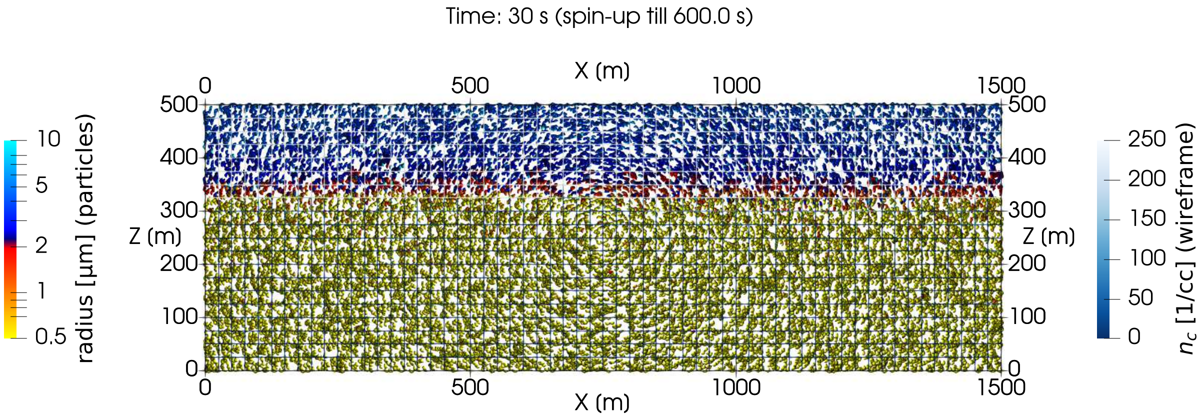
Lagrangian component



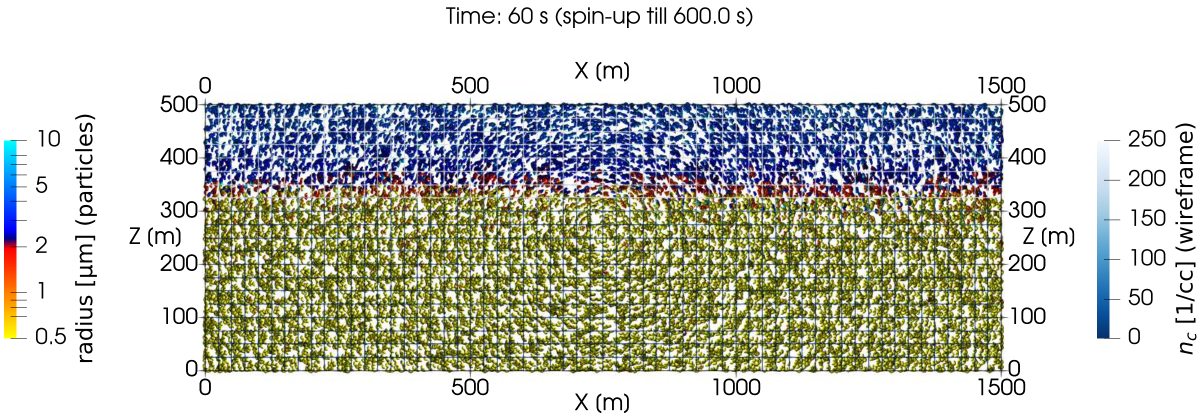
Eulerian component



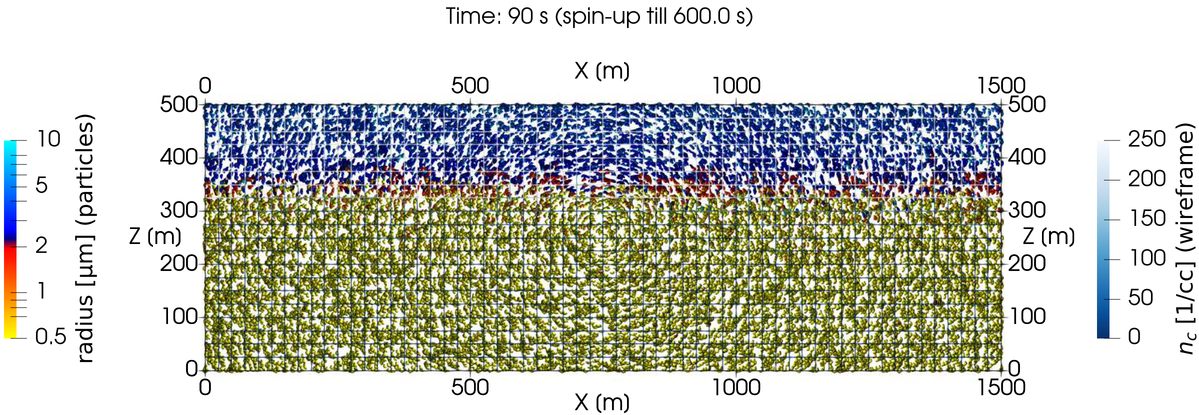
Particle-based μ-physics + prescribed-flow: spin-up



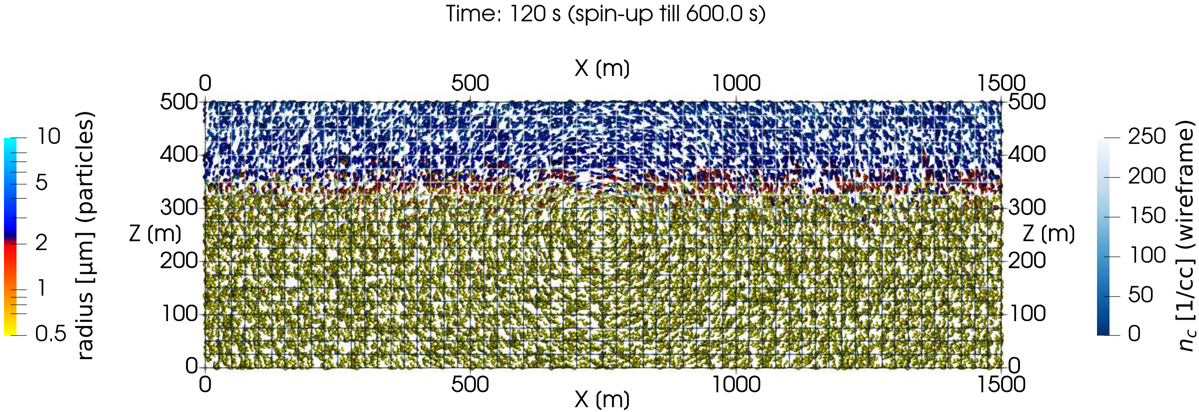
Particle-based μ-physics + prescribed-flow: spin-up



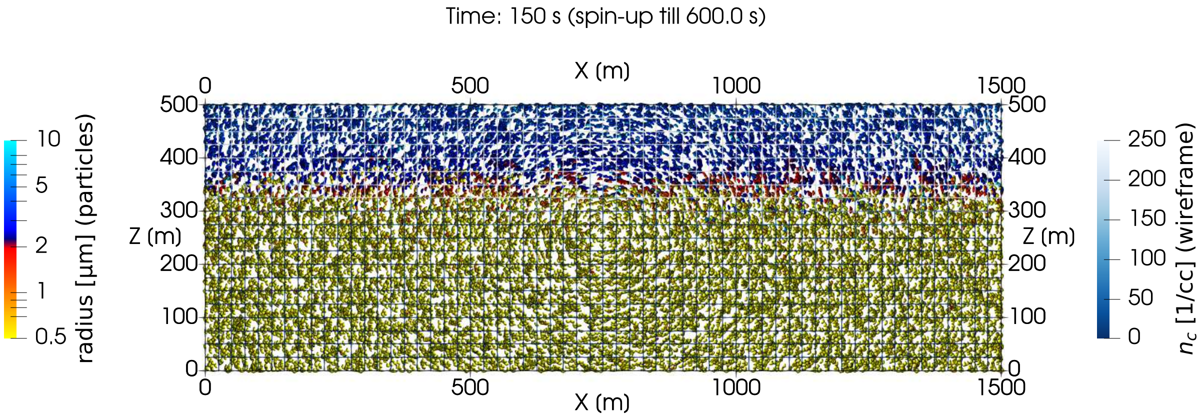
Particle-based μ-physics + prescribed-flow: spin-up



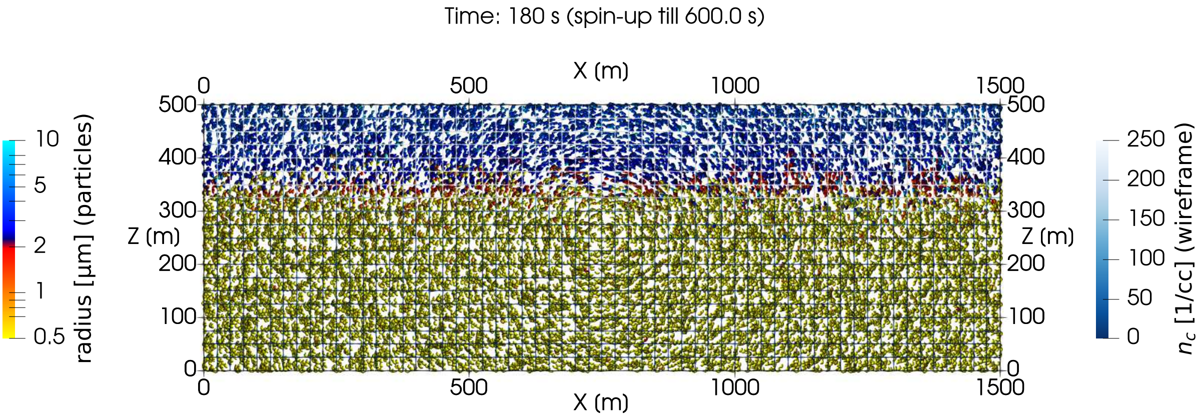
Particle-based μ-physics + prescribed-flow: spin-up



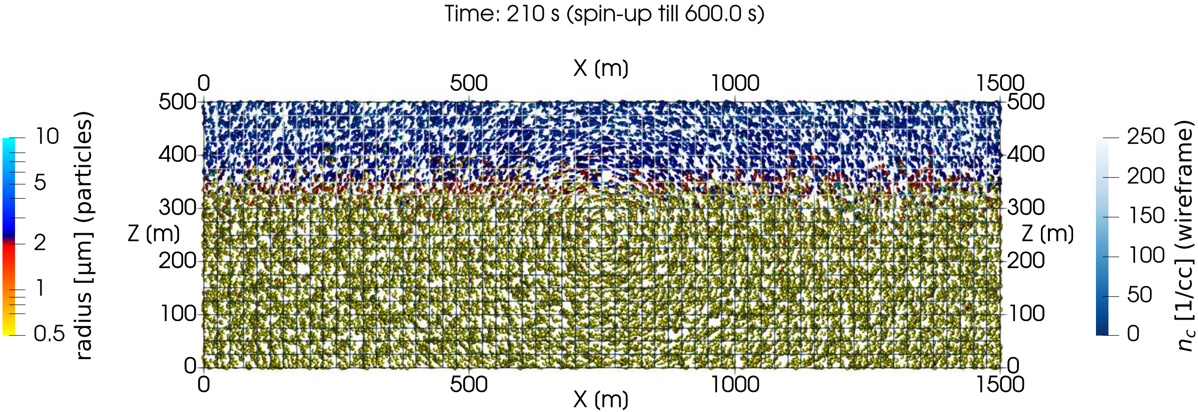
Particle-based μ-physics + prescribed-flow: spin-up



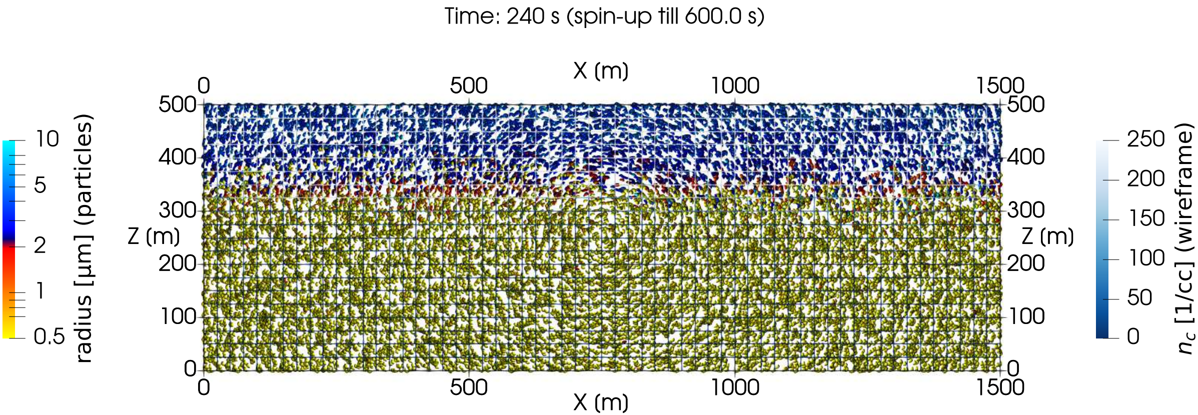
Particle-based μ-physics + prescribed-flow: spin-up



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

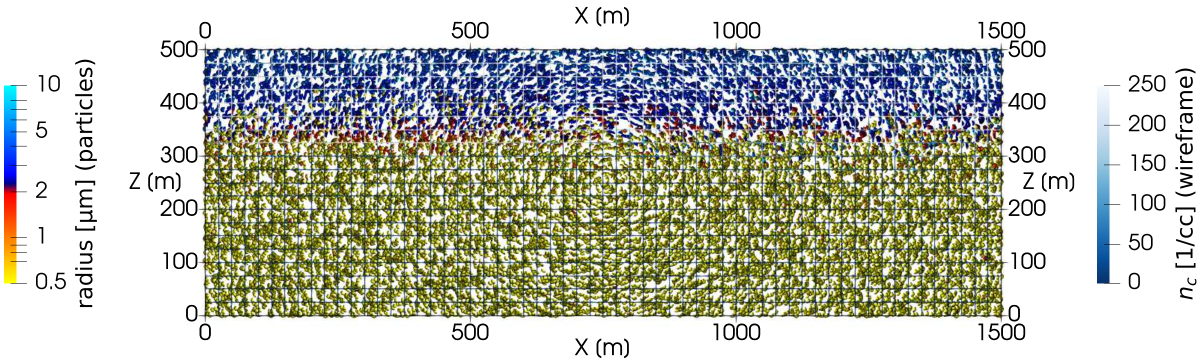


Particle-based μ-physics + prescribed-flow: spin-up

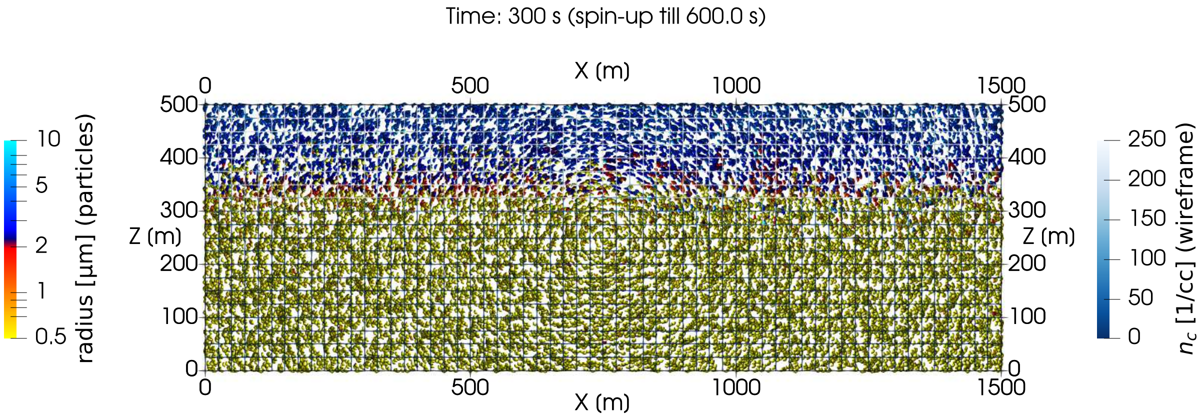


Particle-based μ-physics + prescribed-flow: spin-up

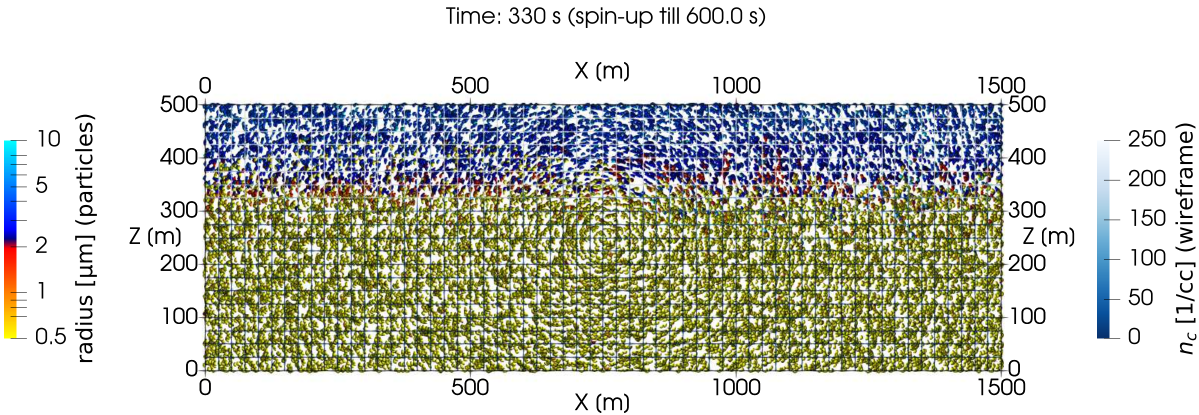
Time: 270 s (spin-up till 600.0 s)



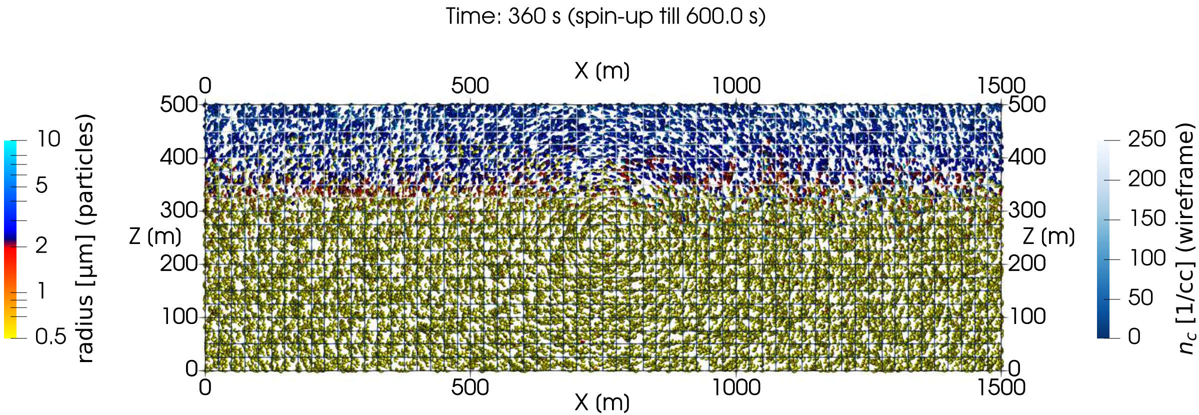
Particle-based μ-physics + prescribed-flow: spin-up



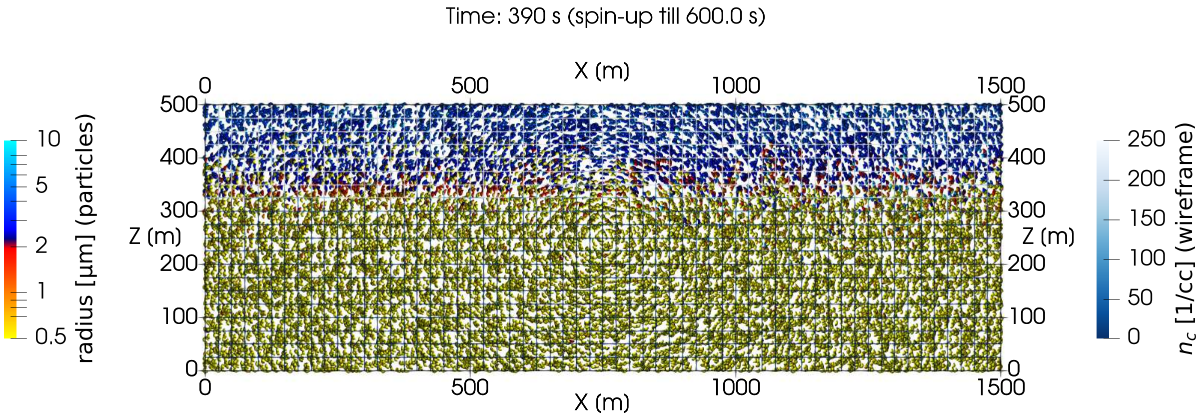
Particle-based μ-physics + prescribed-flow: spin-up



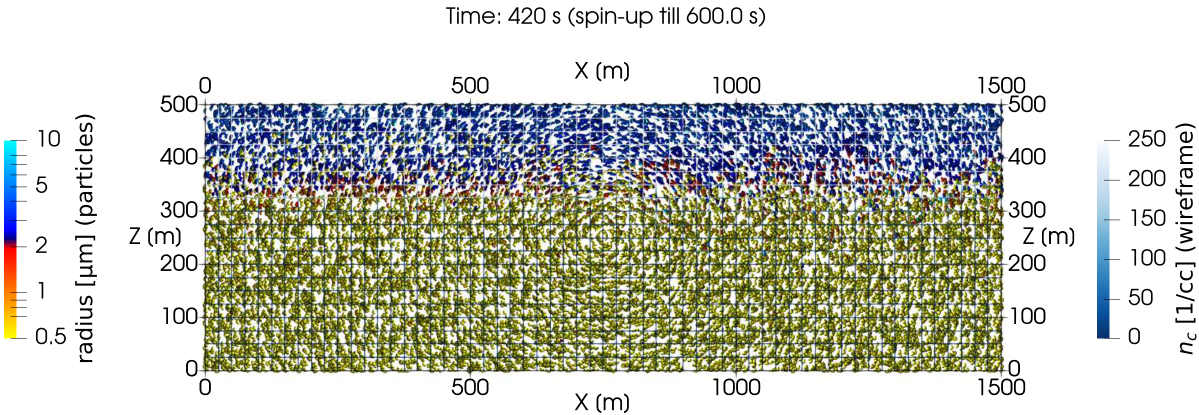
Particle-based μ-physics + prescribed-flow: spin-up



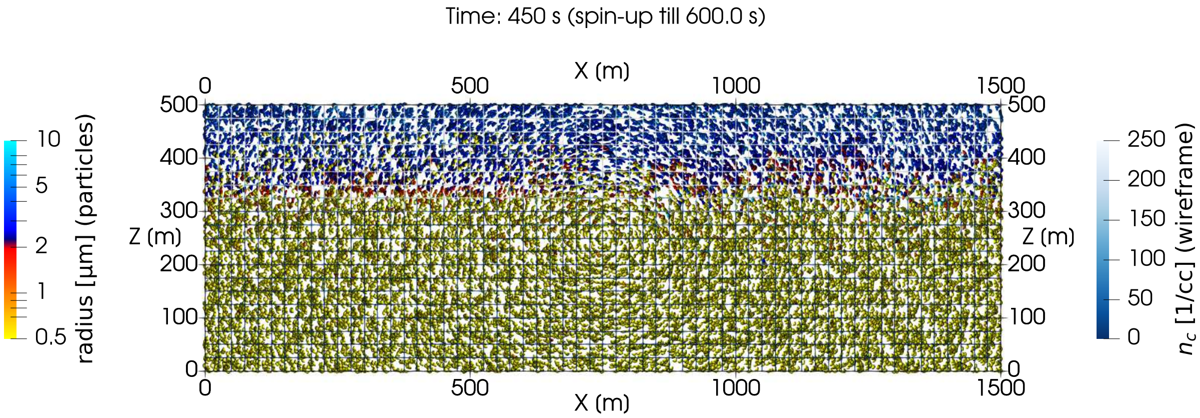
Particle-based μ-physics + prescribed-flow: spin-up



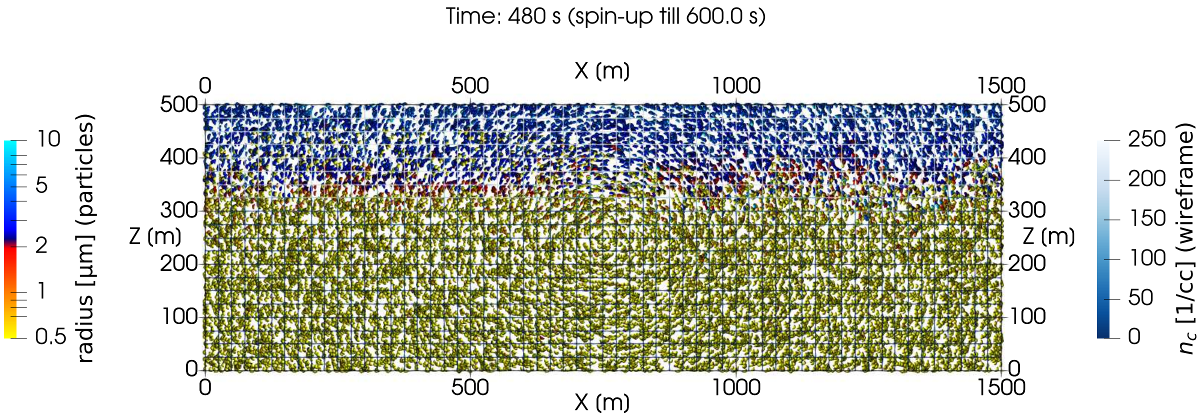
Particle-based μ-physics + prescribed-flow: spin-up



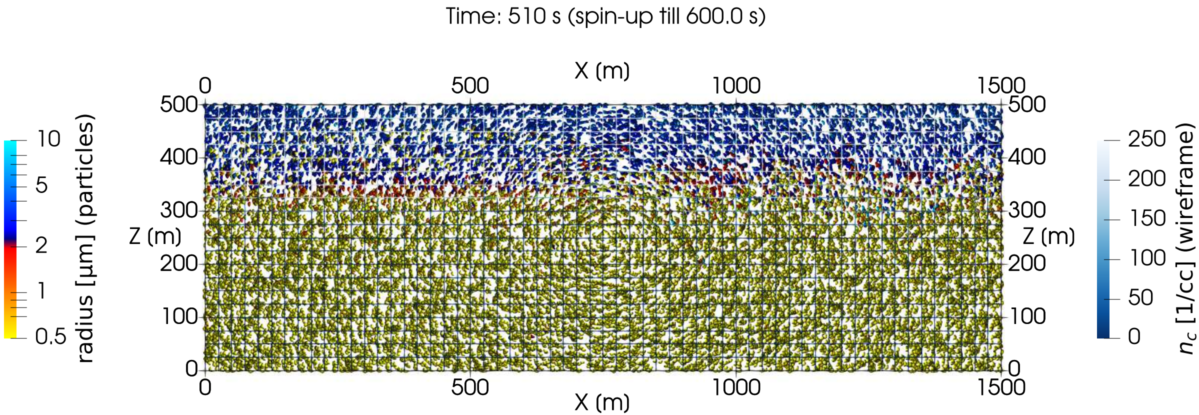
Particle-based μ-physics + prescribed-flow: spin-up



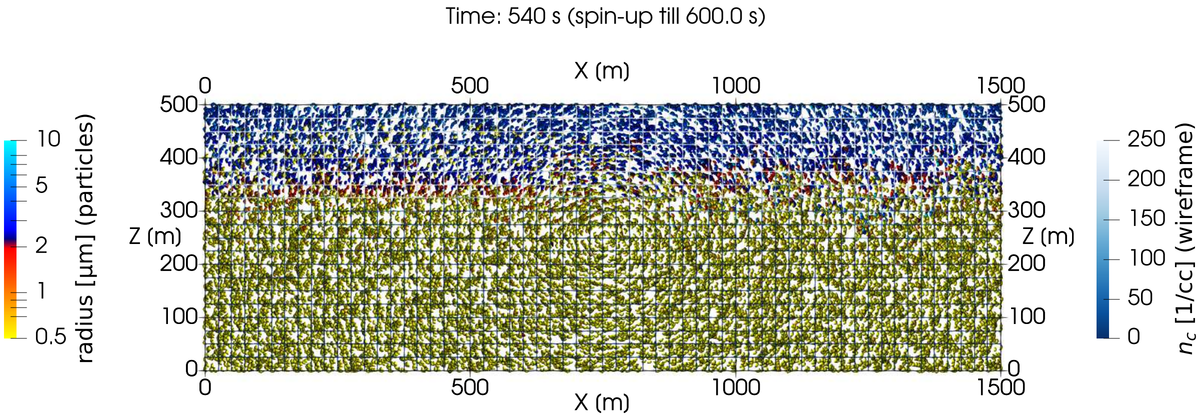
Particle-based μ-physics + prescribed-flow: spin-up



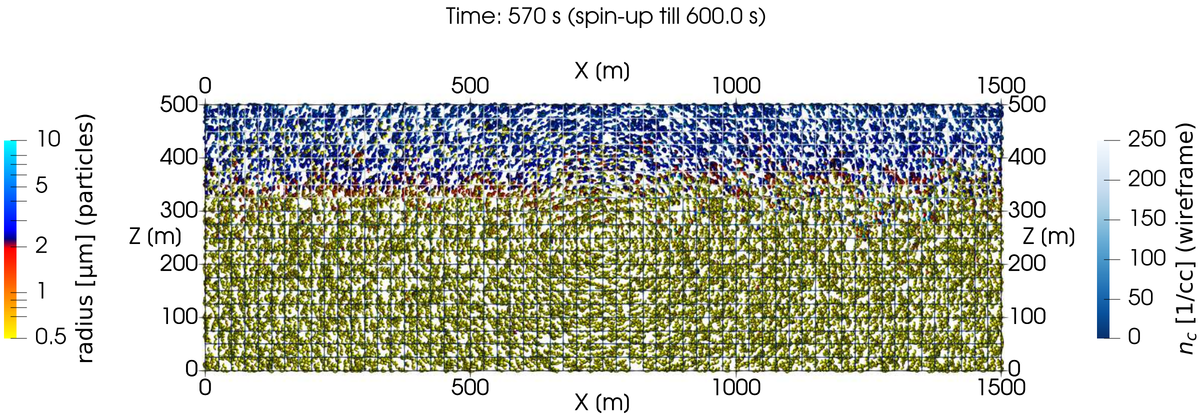
Particle-based μ-physics + prescribed-flow: spin-up



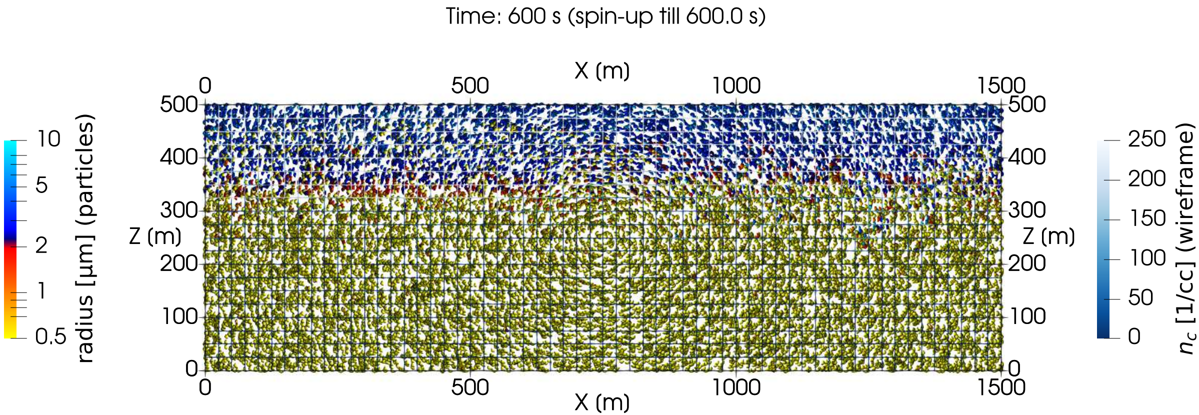
Particle-based μ-physics + prescribed-flow: spin-up



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



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



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

Predicting the morphology of ice particles in deep convection using the super-droplet method

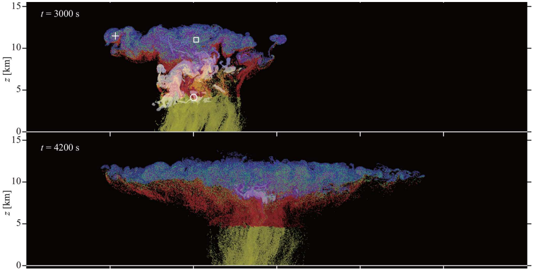


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic 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

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

Predicting the morphology of ice particles in deep convection using the super-droplet method

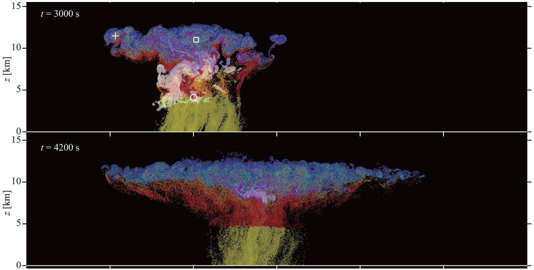


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

- Eulerian component: momentum, heat, moisture budget

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

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

Predicting the morphology of ice particles in deep convection using the super-droplet method

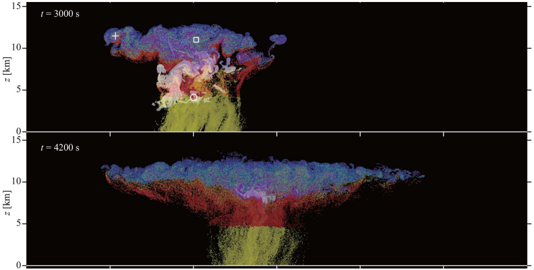


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

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

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

Shima, Sato, Hashimoto & Misumi 2020 (GMD):
Predicting the morphology of ice particles in deep convection using the super-droplet method

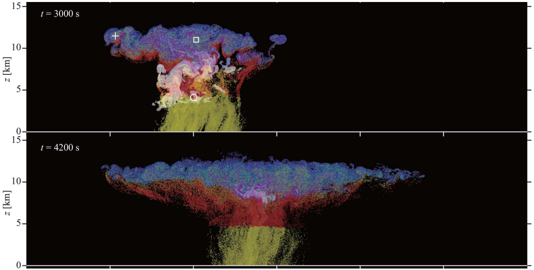


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

- Eulerian component: momentum, heat, moisture budget
- Lagrangian component: super particles representing aerosol, water droplets, ice particles (porous spheroids)
- particle-resolved processes:
  — advection and sedimentation
  — homogeneous and immersion freezing (singular)
  — melting
  — condensation and evaporation (incl. CCN [de]activation)
  — deposition and sublimation
  — collisions (coalescence, riming, aggregation, washout)

Shima, Sato, Hashimoto & Misumi 2020 (GMD):
Predicting the morphology of ice particles in deep convection using the super-droplet method

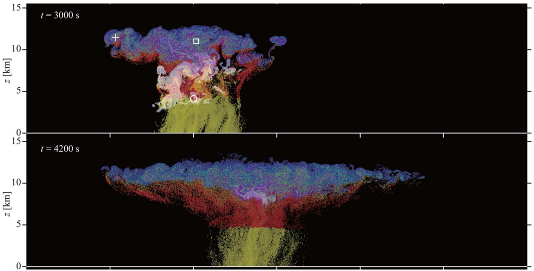


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

- Eulerian component: momentum, heat, moisture budget
- Lagrangian component: super particles representing aerosol, water droplets, ice particles (porous spheroids)
- particle-resolved processes:
  — advection and sedimentation
  — homogeneous and immersion freezing (singular)
  — melting
  — condensation and evaporation (incl. CCN [de]activation)
  — deposition and sublimation
  — collisions (coalescence, riming, aggregation, washout)
- 2D Cb test case

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

Shima, Sato, Hashimoto & Misumi 2020 (GMD):
Predicting the morphology of ice particles in deep convection using the super-droplet method

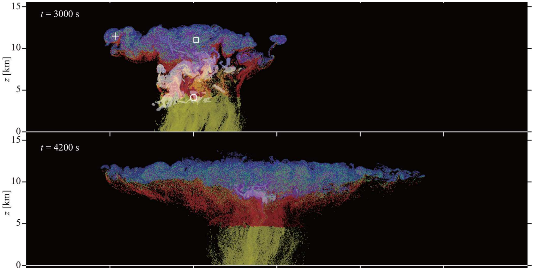
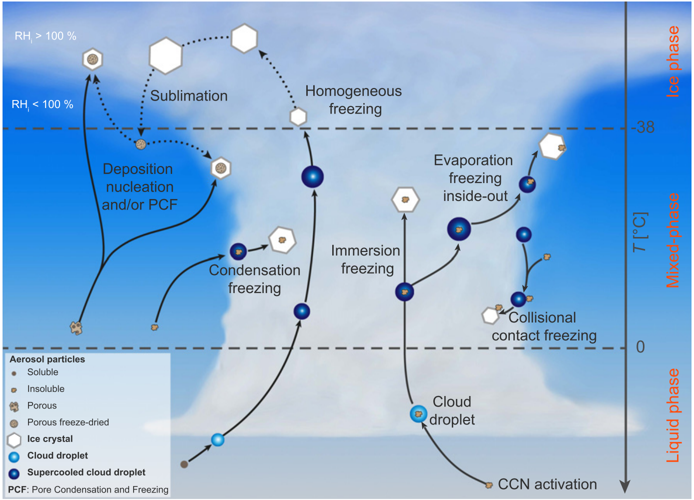


Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic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

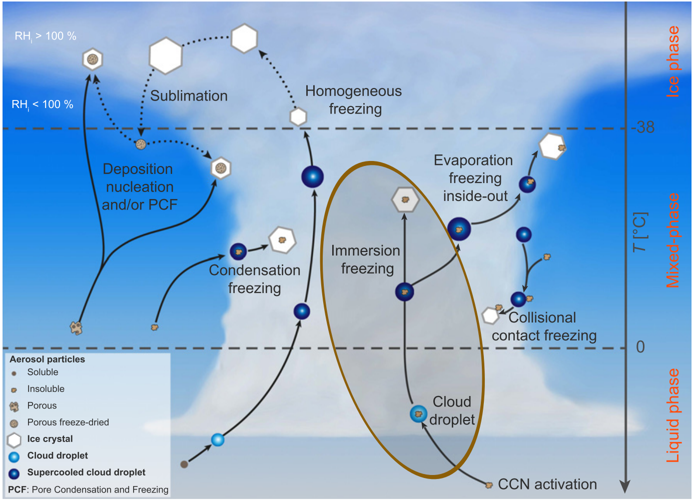
- Eulerian component: momentum, heat, moisture budget
- Lagrangian component: super particles representing aerosol, water droplets, ice particles (porous spheroids)
- particle-resolved processes:
  — advection and sedimentation
  — homogeneous and immersion freezing (singular)
  — melting
  — condensation and evaporation (incl. CCN [de]activation)
  — deposition and sublimation
  — collisions (coalescence, riming, aggregation, washout)
- 2D Cb test case

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`

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`

Immersion freezing: bacteria and the Olympics

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

The unstable ice nucleation properties of Snomax® bacterial particles

Michael Polen[1], Emily Lawlis[1], and Ryan C. Sullivan[1]

[1]Center for Atmospheric Particle Studies, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA

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: bacteria and the Olympics

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

The unstable ice nucleation properties of Snomax® bacterial particles

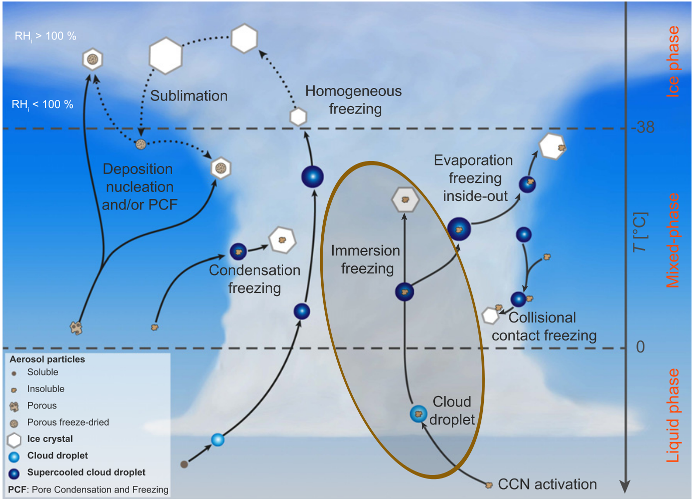
Michael Polen[1], Emily Lawlis[1], and Ryan C. Sullivan[1]

[1]Center for Atmospheric Particle Studies, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA

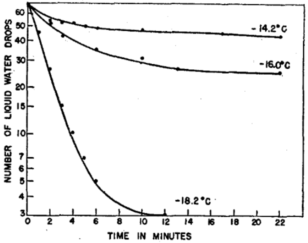
Abstract Snomax® is often used as a surrogate for biological ice nucleating particles (INPs) and has recently been proposed as an INP standard for evaluating ice nucleation methods. We have found the immersion freezing properties of Snomax particles to be substantially unstable, observing a loss of ice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

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

Immersion freezing and other ice crystal formation pathways in clouds



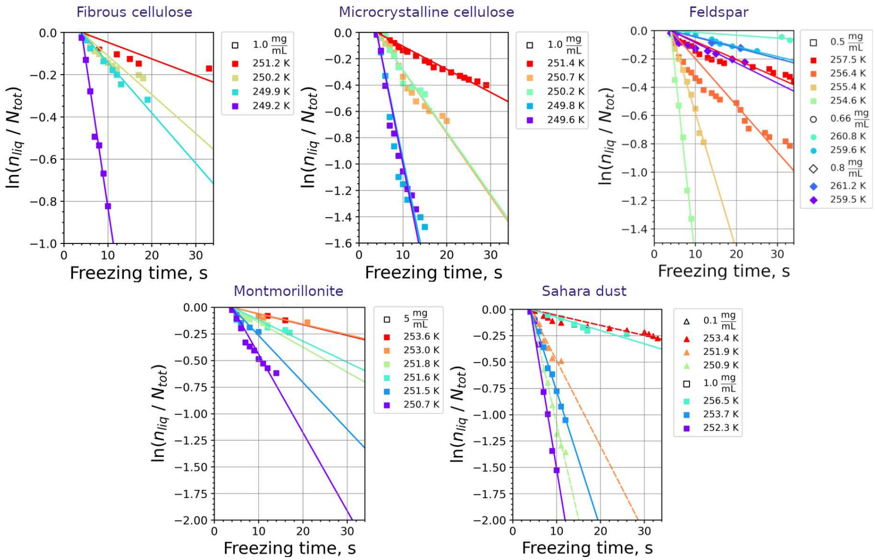
Vonnegut 1948 (J. Colloid Sci.)



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

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

Szakáll et al. 2021, ACP 21: isothermal experiments



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:

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

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

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

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:

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

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

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

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

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

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:

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

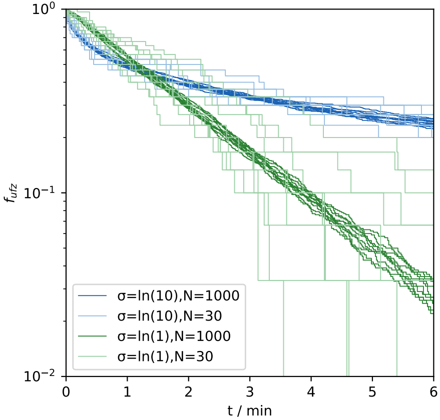
$$P(\text{one or more events in time t}) = 1 - P^*(k=0, t)$$

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

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

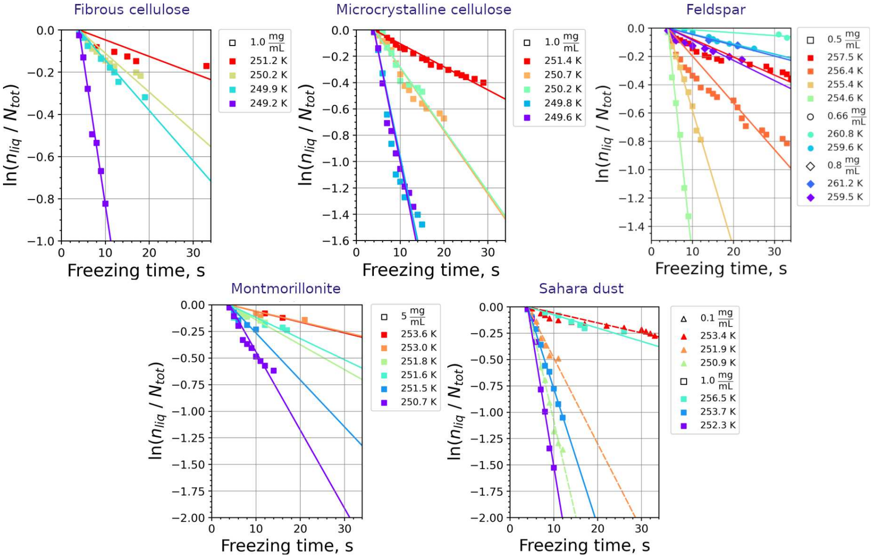
$$\ln\left(1-P(A,t)\right) = \underbrace{-A\int_0^t J_{\text{het}}(T(t'))\,dt'}$$

Monte Carlo: const J_{het}, lognormal A



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

Szakáll et al. 2021, ACP 21: isothermal experiments



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:

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

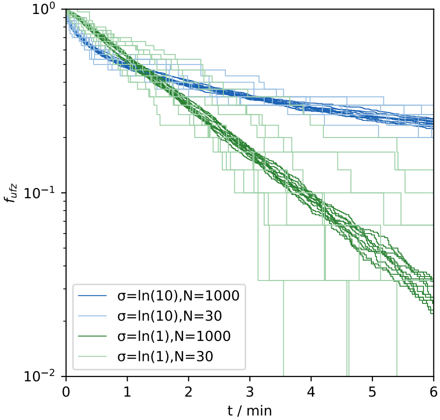
$$P(\text{one or more events in time t}) = 1 - P^*(k=0, t)$$

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

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

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

Monte Carlo: const J_{het}, lognormal A



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

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:

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

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

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

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

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

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

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:

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

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

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

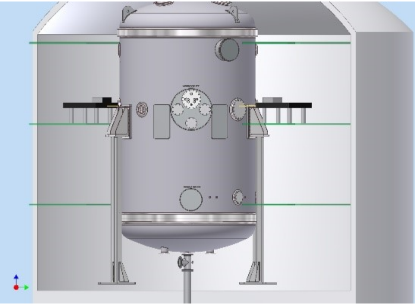
introducing $J_{\text{het}}(T)$, $T(t)$ and INP surface A:

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

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

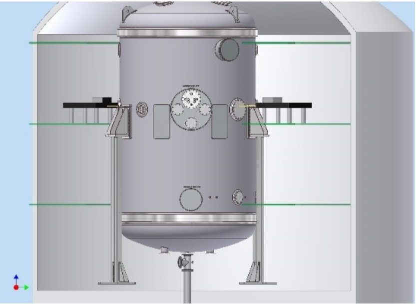
experimental $n_s(T)$ fits: e.g., Niemand et al. 2012

AIDA @ KIT



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

AIDA @ KIT



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

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

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:

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

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

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

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

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:

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

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

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

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

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

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 $c = dT/dt$:

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

$J_{\rm het}$ or $n_{\rm s}$?

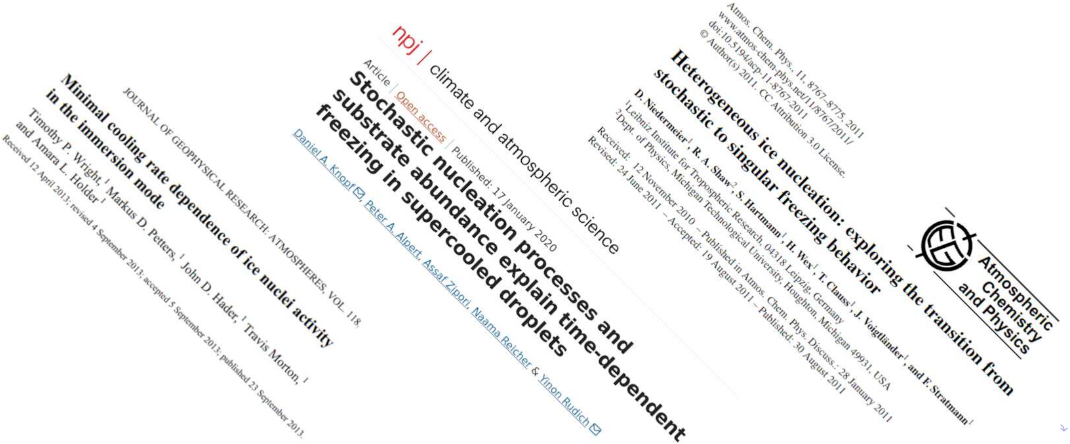
Vali 2014 (ACP)

"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"

J_{het} or n_s ?

Vali 2014 (ACP)

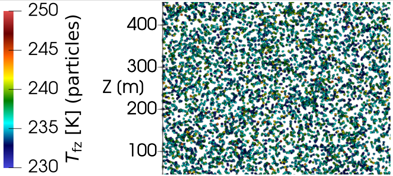
"Interpretations of the experimental results face considerable difficulties … two separate ways of interpreting the same observations; one assigned primacy to time the other emphasized the temperature-dependent impacts of the impurities … dichotomy – the stochastic and singular models"



Particle-based freezing: singular (Shima et al.)

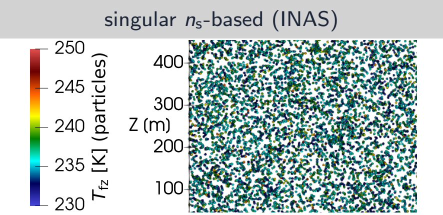
singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\text{fz}})$ with lognormal A
freezing if $T_{\text{ambient}}(t) < T_{\text{fz}}|_{\text{sampled at } t=0}$

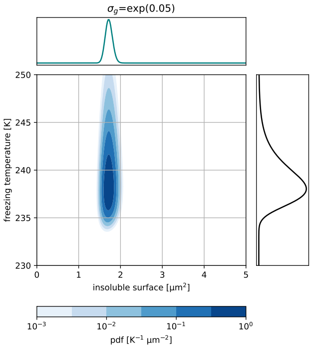
singular n_s-based (INAS)



Particle-based freezing: singular (Shima et al.)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ }t=0}$

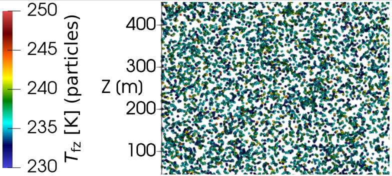


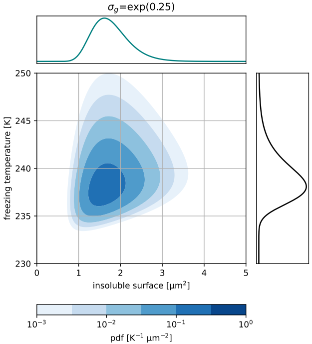


Particle-based freezing: singular (Shima et al.)

singular: INAS $T_{\mathbf{fz}}$ **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ } t=0}$

singular n_s-based (INAS)

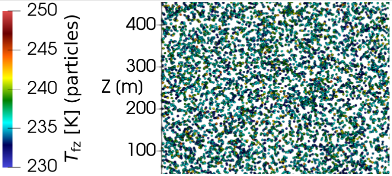


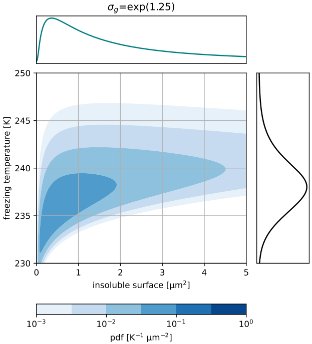


Particle-based freezing: singular (Shima et al.)

singular: INAS $T_{\mathbf{fz}}$ **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at}\ t=0}$

singular n_s-based (INAS)

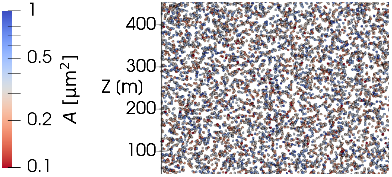




Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular:	INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}\|_{\text{sampled at } t=0}$
time-dependent:	A **as attribute** (randomly sampled from the same lognormal) Monte-Carlo freezing trigger using $P(A \cdot J_{\mathrm{het}}(T_{\mathrm{ambient}}(t)))$

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

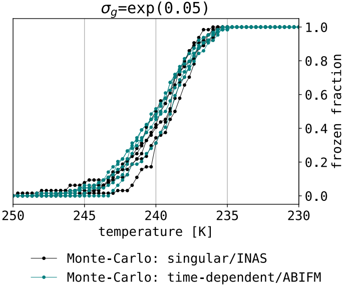


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS $T_{\mathbf{fz}}$ **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ }t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\mathrm{het}}(T_{\mathrm{ambient}}(t)))$

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

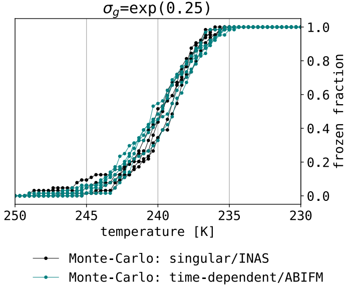


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\mathrm{het}}(T_{\mathrm{ambient}}(t)))$

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

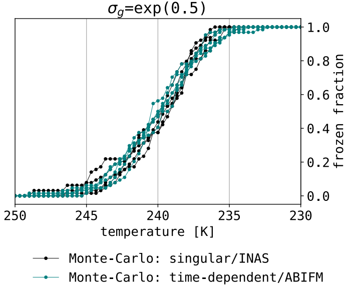


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\text{fz}})$ with lognormal A
freezing if $T_{\text{ambient}}(t) < T_{\text{fz}}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\text{het}}(T_{\text{ambient}}(t)))$

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

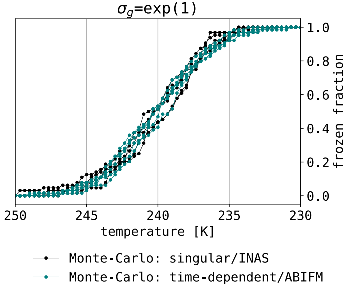


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS $T_{\rm fz}$ **as attribute**; initialisation by random sampling from $P(A, T_{\rm fz})$ with lognormal A
freezing if $T_{\rm ambient}(t) < T_{\rm fz}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\rm het}(T_{\rm ambient}(t)))$

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

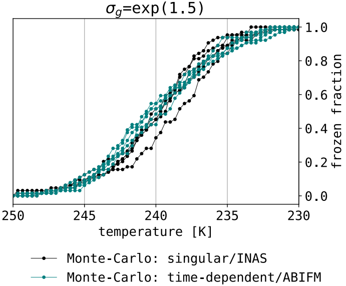


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{fz})$ with lognormal A
freezing if $T_{ambient}(t) < T_{fz}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{het}(T_{ambient}(t)))$

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

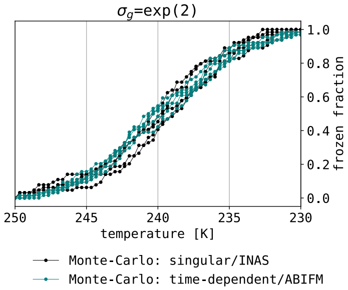


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ }t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\mathrm{het}}(T_{\mathrm{ambient}}(t)))$

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

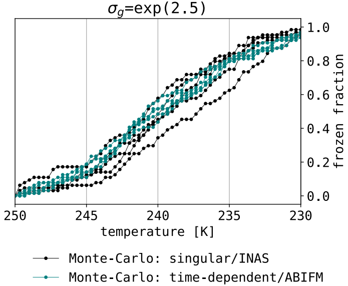


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{\mathrm{fz}})$ with lognormal A
freezing if $T_{\mathrm{ambient}}(t) < T_{\mathrm{fz}}|_{\mathrm{sampled\ at\ }t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{\mathrm{het}}(T_{\mathrm{ambient}}(t)))$

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

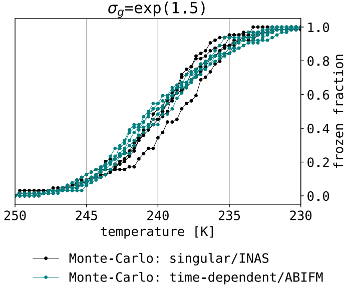


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{fz})$ with lognormal A
freezing if $T_{ambient}(t) < T_{fz}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{het}(T_{ambient}(t)))$

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

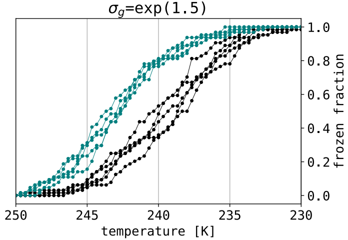


Particle-based freezing: singular (Shima et al.) / time-dependent (this work)

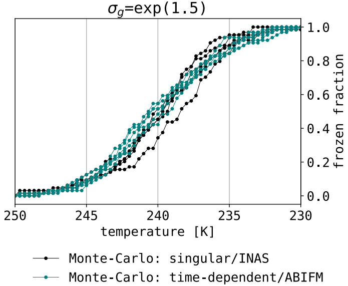
singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{fz})$ with lognormal A
freezing if $T_{ambient}(t) < T_{fz}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{het}(T_{ambient}(t)))$

cooling rate: $0.1\ {}^{K}/_{min}$



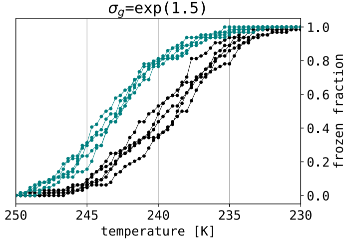
AIDA cooling rate: $0.5\ {}^{K}/_{min}$



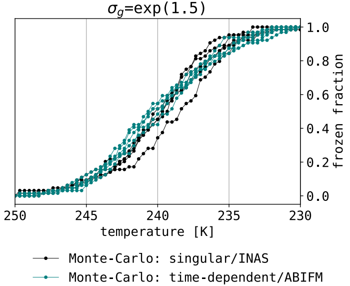
singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(A, T_{fz})$ with lognormal A
freezing if $T_{ambient}(t) < T_{fz}|_{\text{sampled at } t=0}$

time-dependent: A **as attribute** (randomly sampled from the same lognormal)
Monte-Carlo freezing trigger using $P(A \cdot J_{het}(T_{ambient}(t)))$

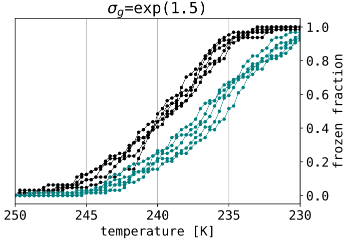
cooling rate: 0.1 $^{K}/_{min}$



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



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



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:

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

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

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

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

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

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 $c = dT/dt$:

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

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:

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

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

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

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

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

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 $c = dT/dt$:

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

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

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:

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

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

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

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

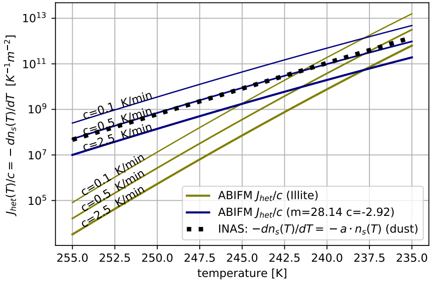
experimental $n_s(T)$ fits: e.g., Niemand et al. 2012

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

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

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

experimental fits: INAS n_s (Niemand et al. '12)
ABIFM J_{het} (Knopf & Alpert '13)



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:

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

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

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

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

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

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

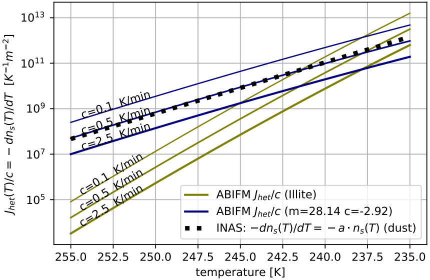
experimental $n_s(T)$ fits: e.g., Niemand et al. 2012

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

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

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

experimental fits: INAS n_s (Niemand et al. '12)
ABIFM J_{het} (Knopf & Alpert '13)



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

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

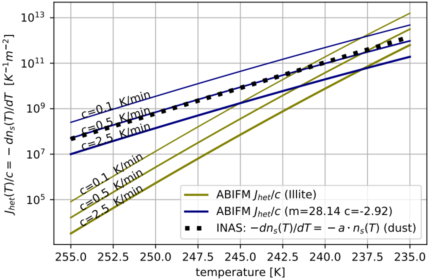
Is it a problem?

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

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

$$-\frac{1}{c}J_{\mathrm{het}}(T) = \frac{dn_{\mathrm{s}}(T)}{dT} = a \cdot n_{\mathrm{s}}(T)$$

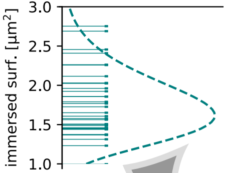
experimental fits: INAS n_{s} (Niemand et al. '12)
ABIFM J_{het} (Knopf & Alpert '13)



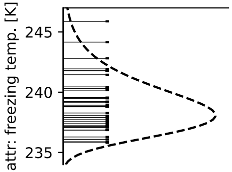
cf. Vali & Stansbury '66; modified singular model (Vali '94, Murray et al. '11)
but the singular ansatz limitation of sampling T_{fz} at t=0 remains

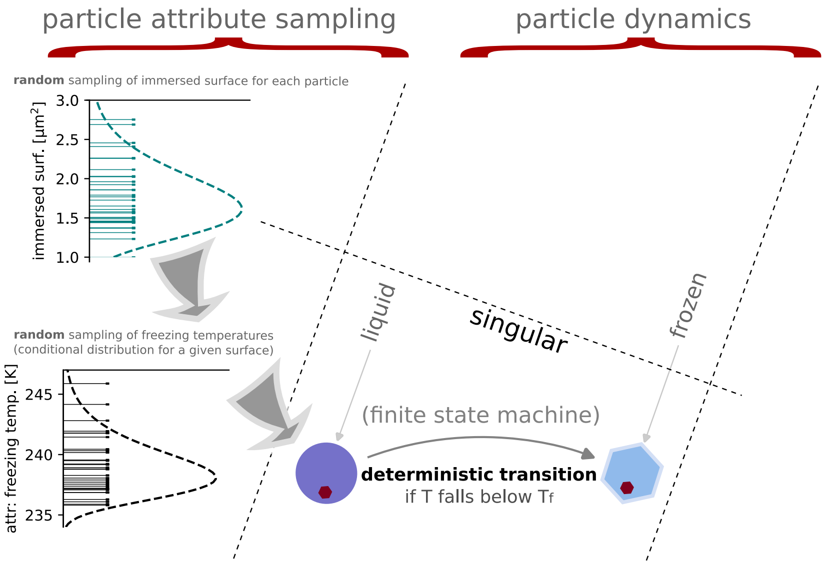
particle attribute sampling

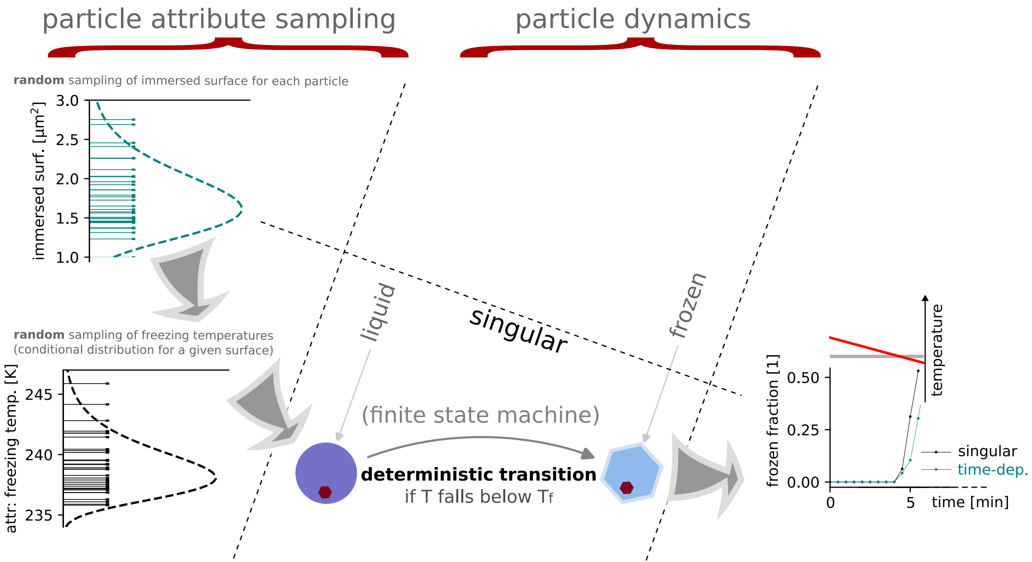
random sampling of immersed surface for each particle

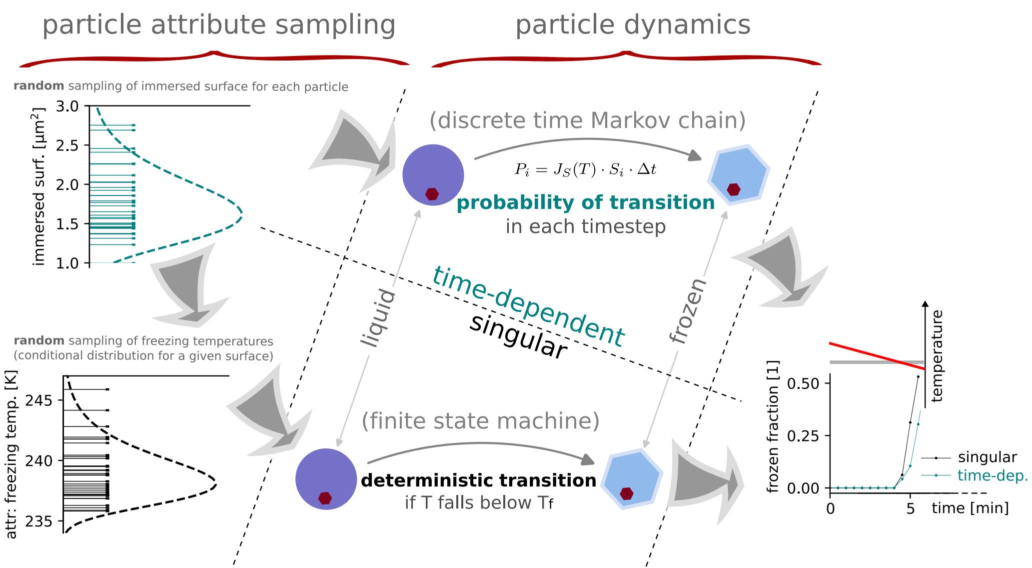


random sampling of freezing temperatures
(conditional distribution for a given surface)



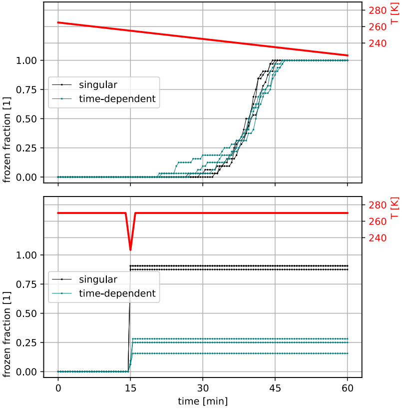

particle attribute sampling
particle dynamics
random sampling of immersed surface for each particle
immersed surf. [μm²]
3.0
2.5
2.0
1.5
1.0
random sampling of freezing temperatures
(conditional distribution for a given surface)
attr: freezing temp. [K]
245
240
235
liquid
singular
frozen
(finite state machine)
deterministic transition
if T falls below Tf


particle attribute sampling
particle dynamics
random sampling of immersed surface for each particle
immersed surf. [μm²]
3.0
2.5
2.0
1.5
1.0
random sampling of freezing temperatures
(conditional distribution for a given surface)
attr: freezing temp. [K]
245
240
235
liquid
singular
frozen
(finite state machine)
deterministic transition
if T falls below Tf
frozen fraction [1]
0.50
0.25
0.00
0
5
time [min]
temperature
singular
time-dep.

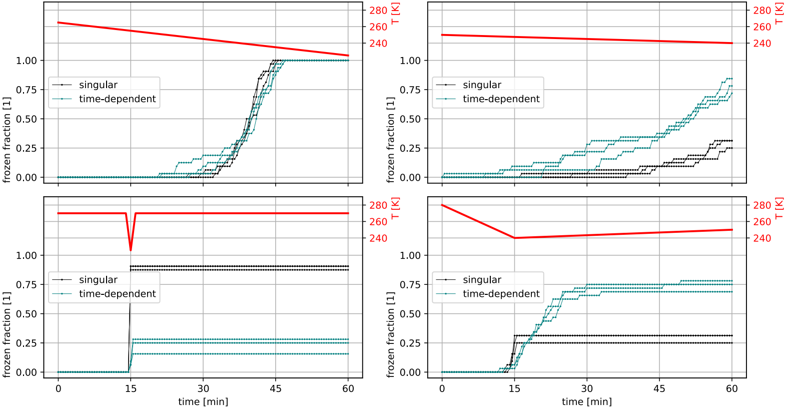


particle attribute sampling
particle dynamics
random sampling of immersed surface for each particle
immersed surf. [μm²]
3.0
2.5
2.0
1.5
1.0
random sampling of freezing temperatures
(conditional distribution for a given surface)
attr: freezing temp. [K]
245
240
235
(discrete time Markov chain)
$P_i = J_S(T) \cdot S_i \cdot \Delta t$
probability of transition
in each timestep
time-dependent
singular
liquid
frozen
(finite state machine)
deterministic transition
if T falls below Tf
temperature
frozen fraction [1]
0.50
0.25
0.00
0
5
time [min]
singular
time-dep.

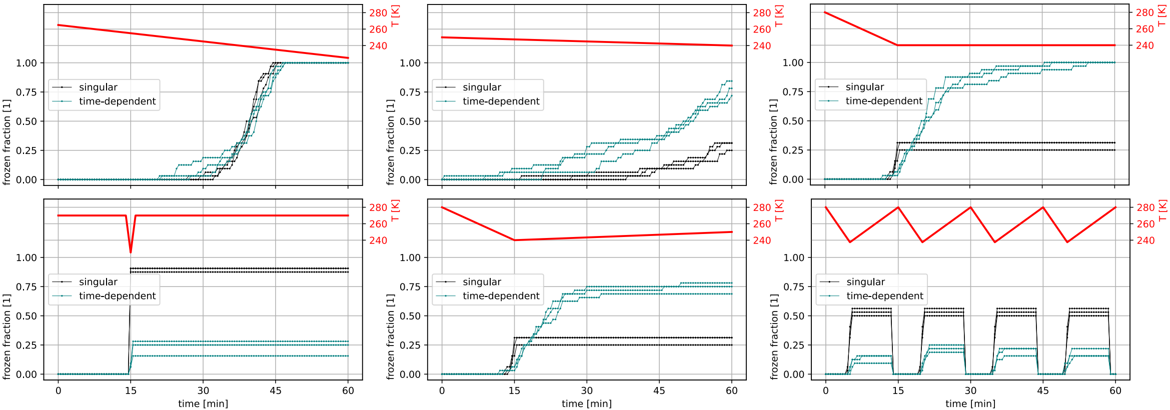
Testing different cooling-rate profiles in a box model



Testing different cooling-rate profiles in a box model

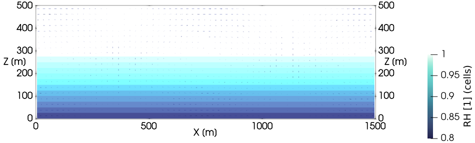


Testing different cooling-rate profiles in a box model



Testing three flow regimes and two immersion freezing representations

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

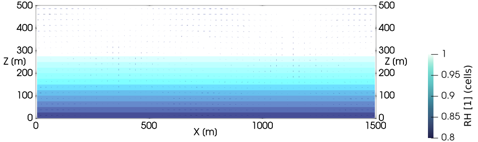


$w_{max} \approx 1$ m/s

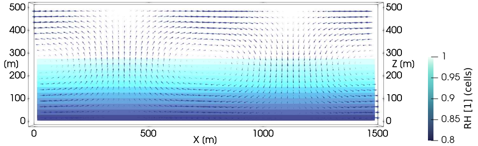
$w_{max} \approx 3$ m/s

Testing three flow regimes and two immersion freezing representations

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



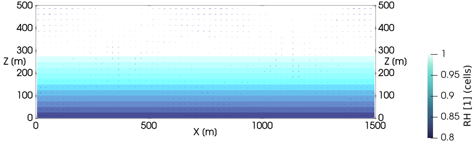
$w_{max} \approx 1$ m/s



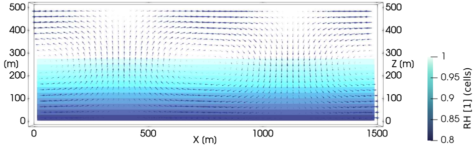
$w_{max} \approx 3$ m/s

Testing three flow regimes and two immersion freezing representations

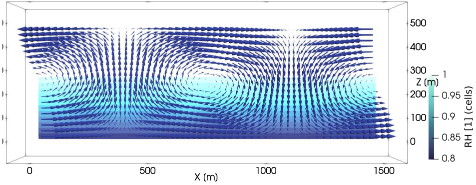
$w_{max} \approx 1/3$ m/s



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

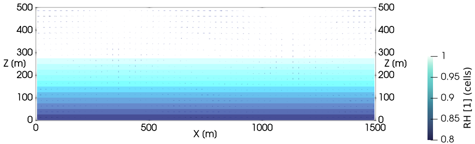


$w_{max} \approx 3$ m/s

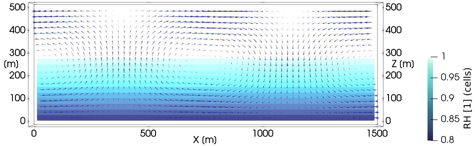


Testing three flow regimes and two immersion freezing representations

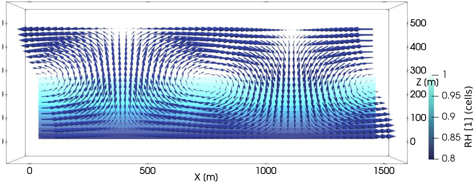
$w_{max} \approx 1/3$ m/s



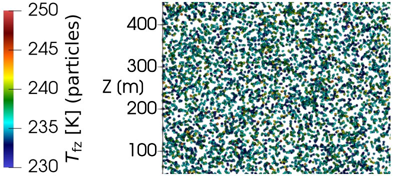
$w_{max} \approx 1$ m/s



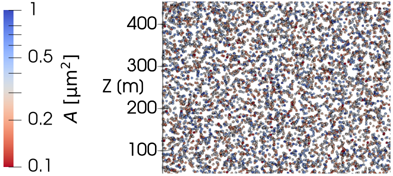
$w_{max} \approx 3$ m/s



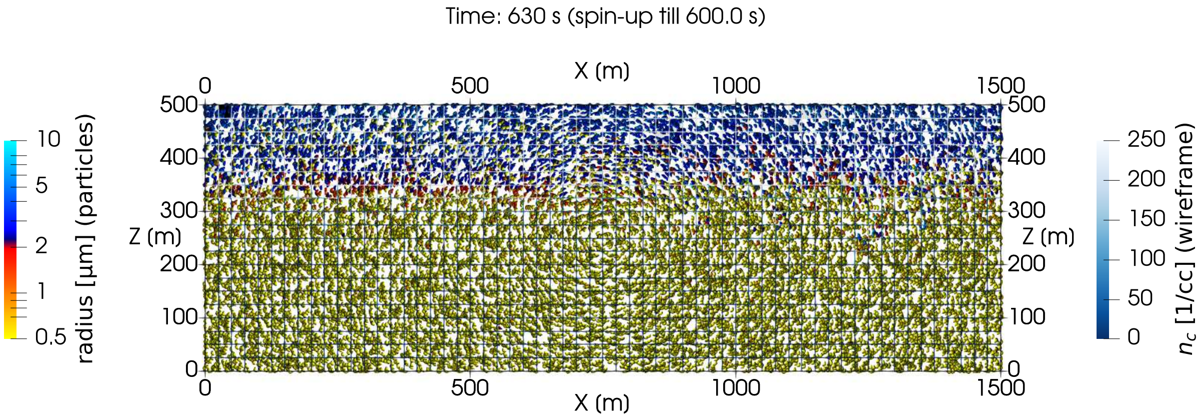
singular (INAS)



time-dependent (J_{het})



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

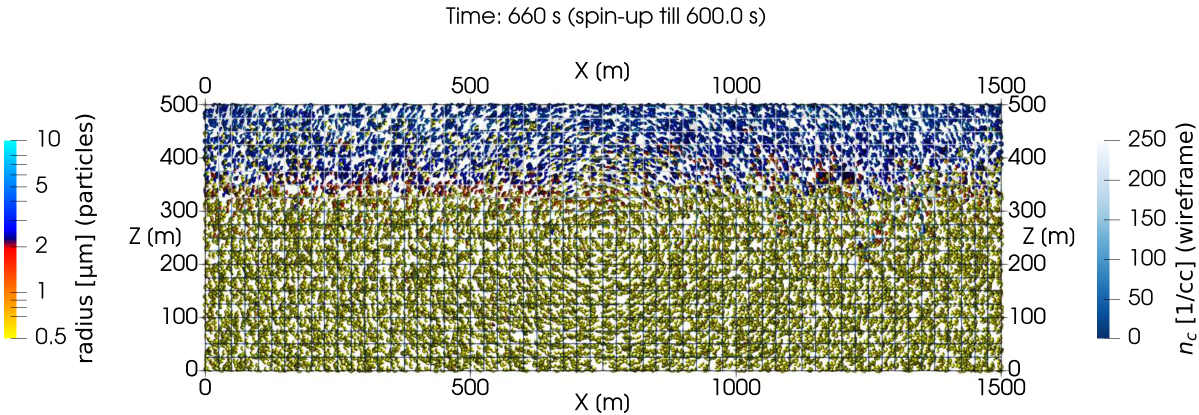


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

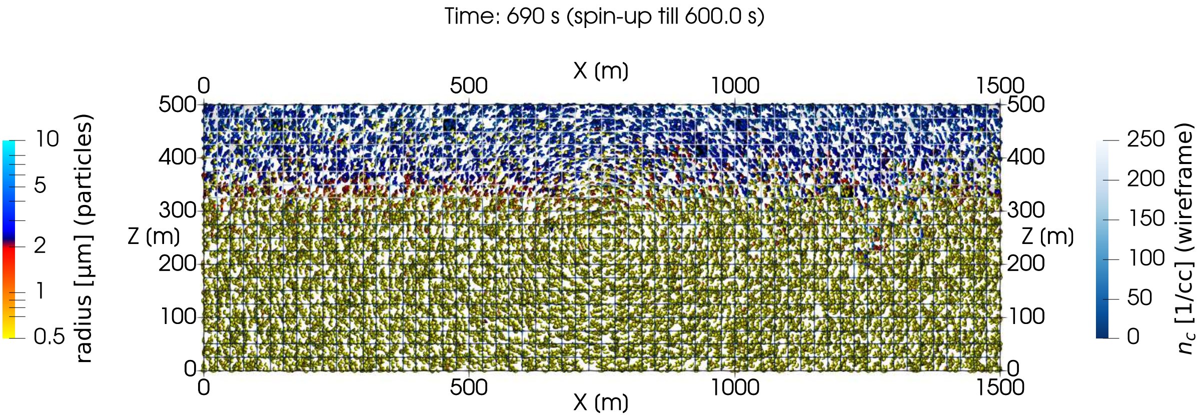


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

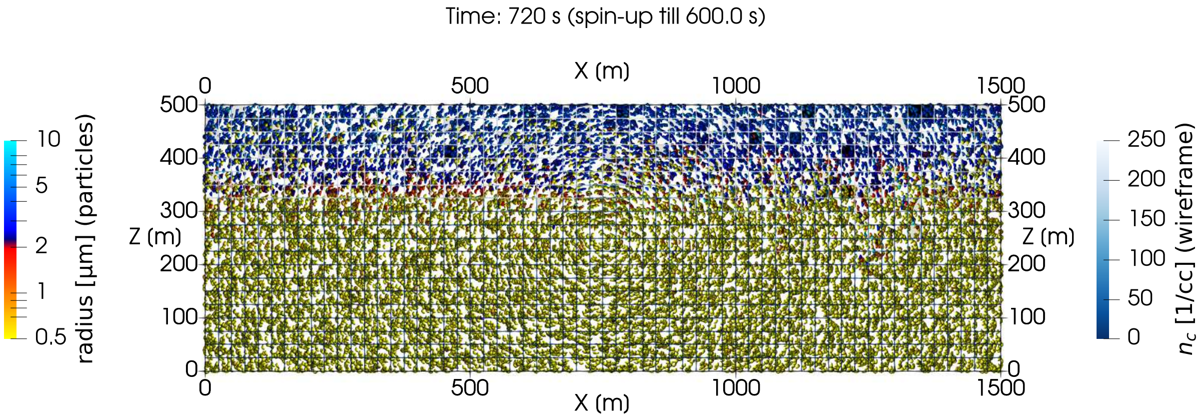


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\mathrm{aer}} = 300/cc$ (two-mode lognormal) $N_{\mathrm{INP}} = 150/L$ (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

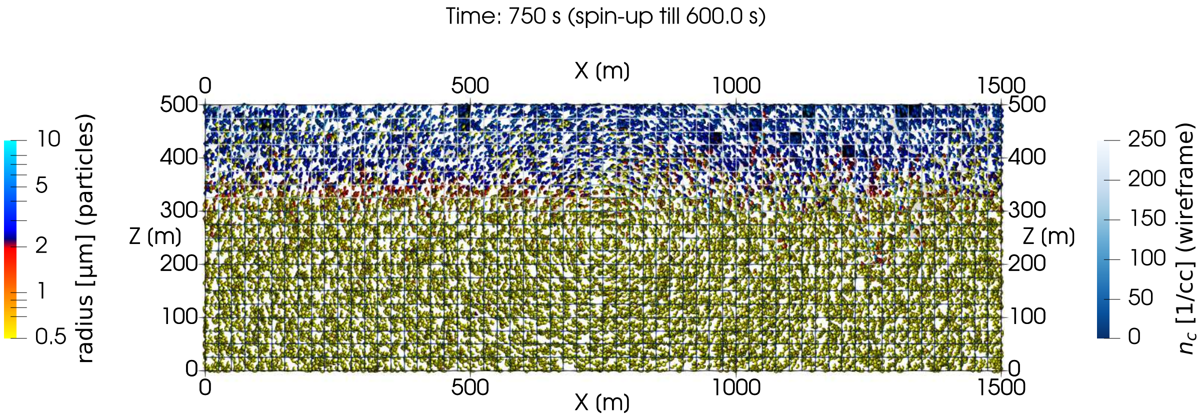


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

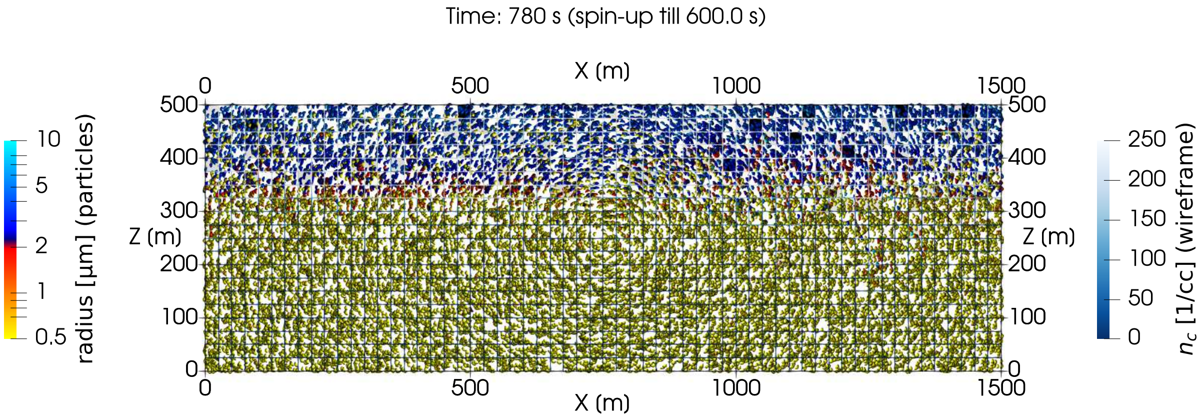


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

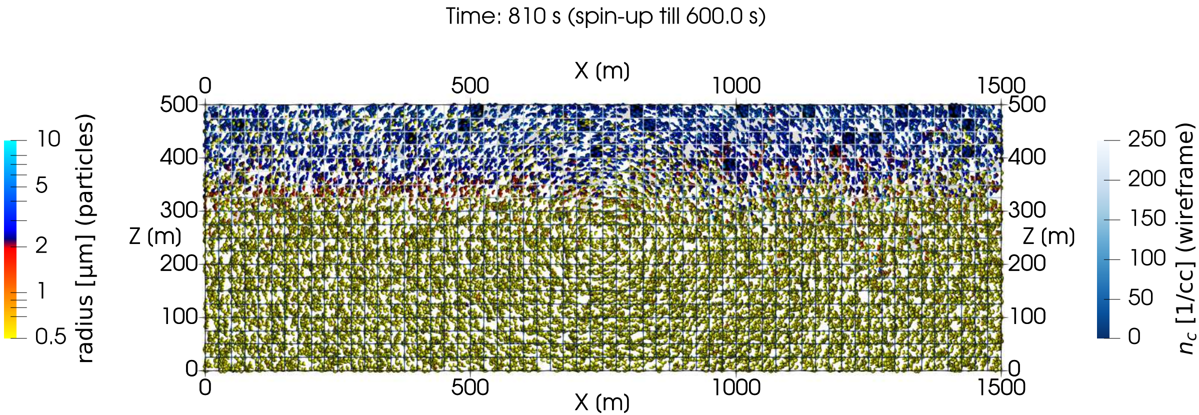


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

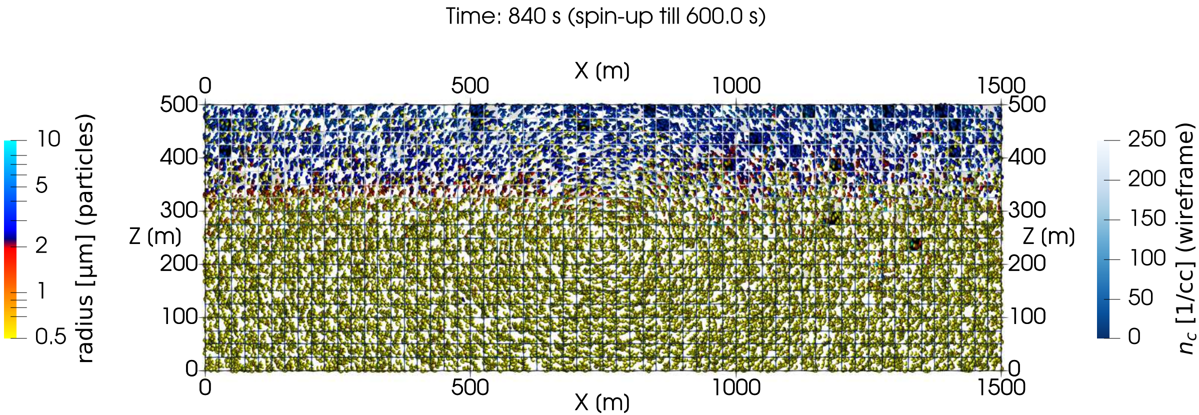


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{aer} = 300/cc$ (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

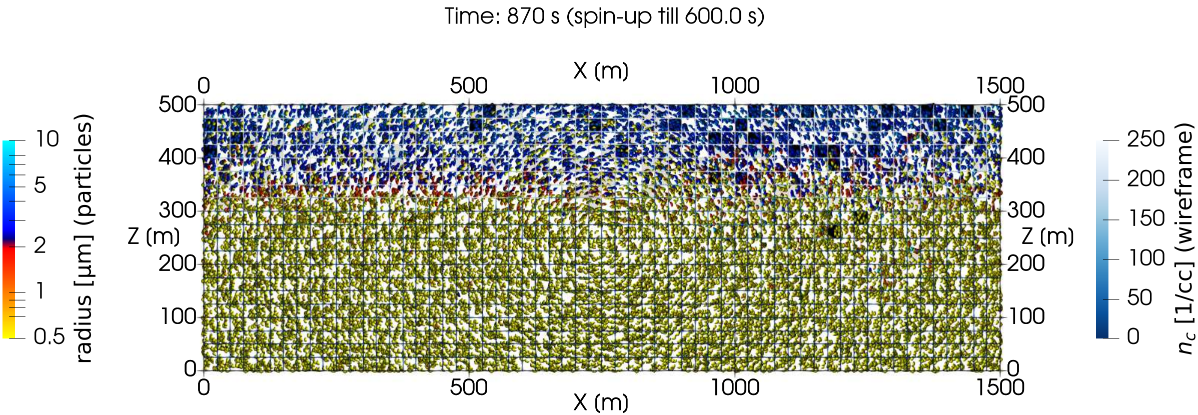


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

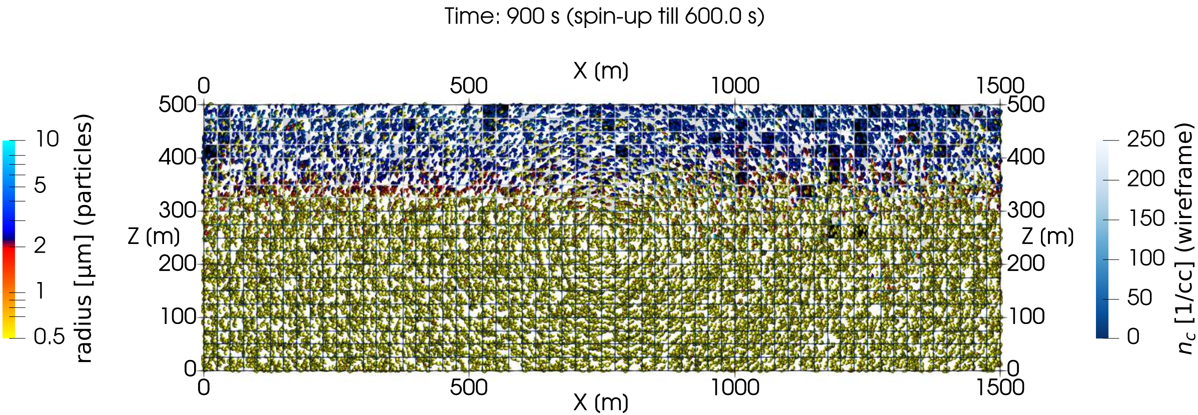


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

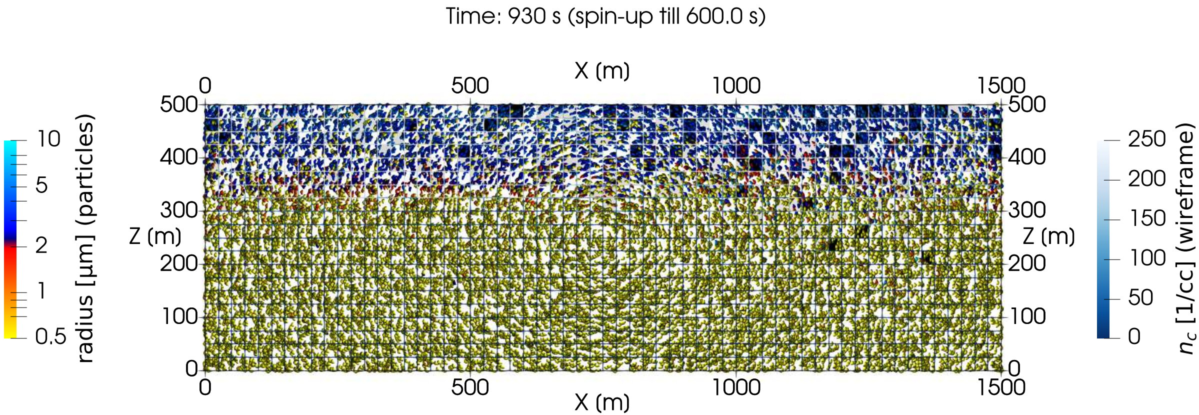


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\mathrm{aer}} = 300/cc$ (two-mode lognormal) $N_{\mathrm{INP}} = 150/L$ (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

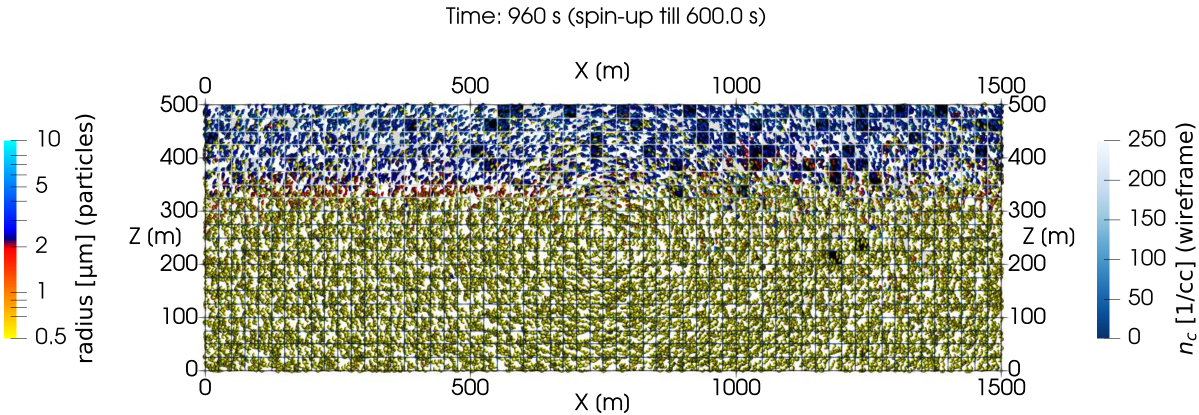


16+16 super-particles/cell for INP-rich + INP-free particles

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

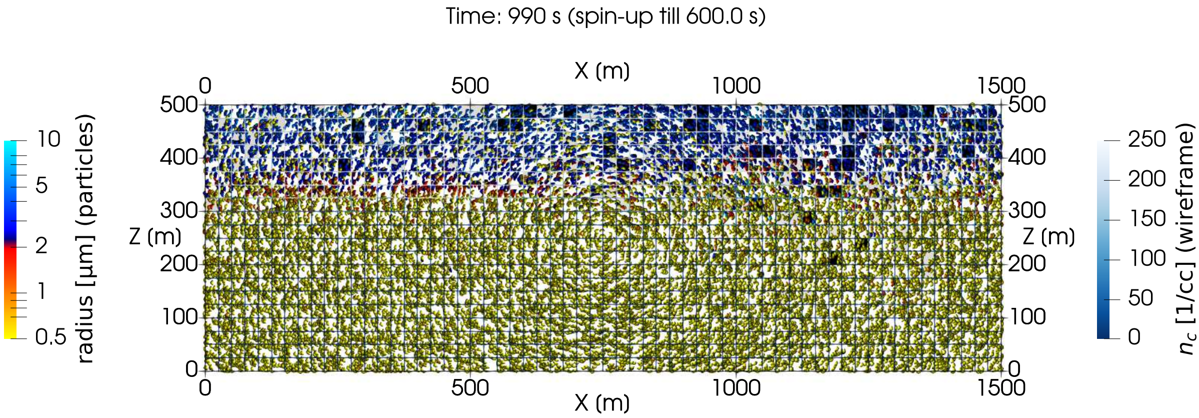
spin-up = freezing off; subsequently frozen particles act as tracers

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



16+16 super-particles/cell for INP-rich + INP-free particles
$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

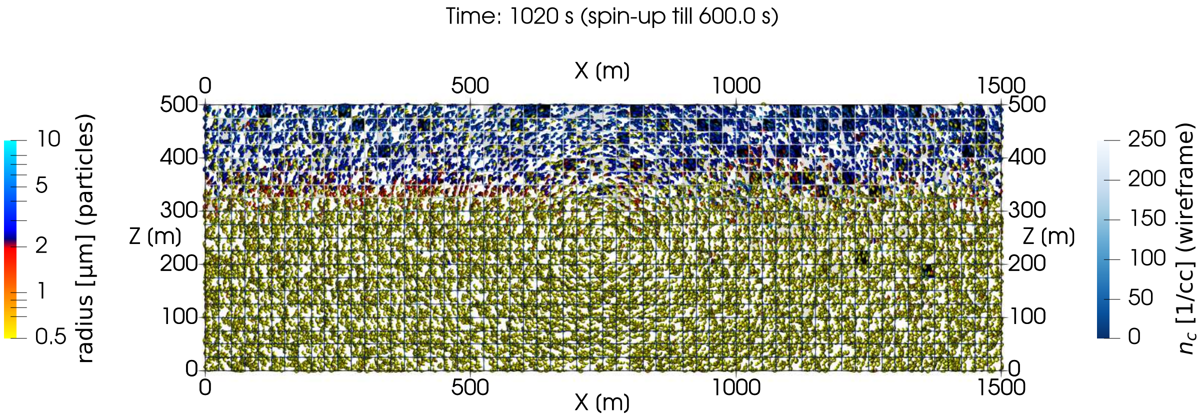


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

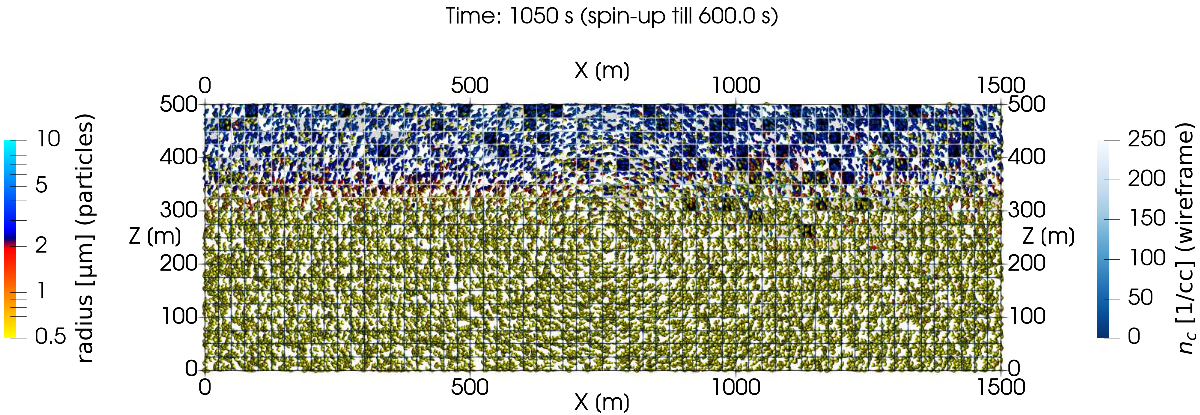


16+16 super-particles/cell for INP-rich + INP-free particles

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

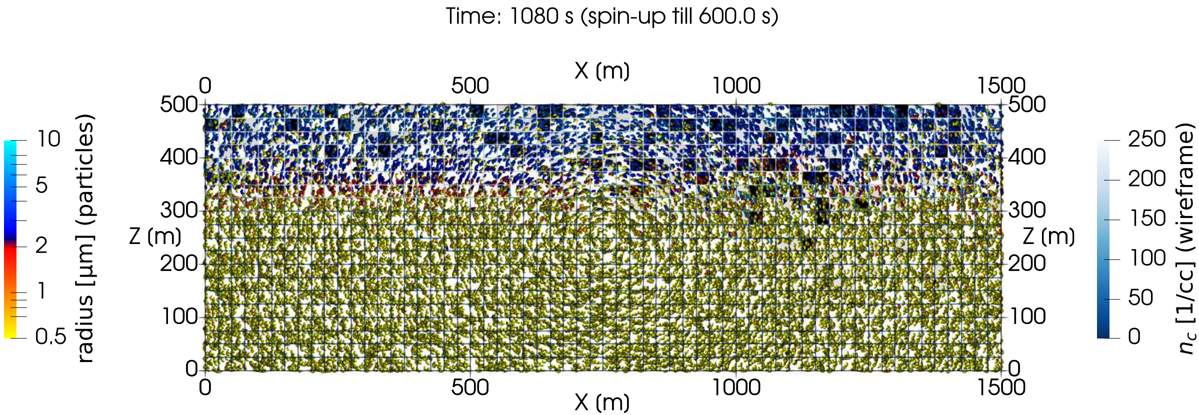
spin-up = freezing off; subsequently frozen particles act as tracers

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



16+16 super-particles/cell for INP-rich + INP-free particles
$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

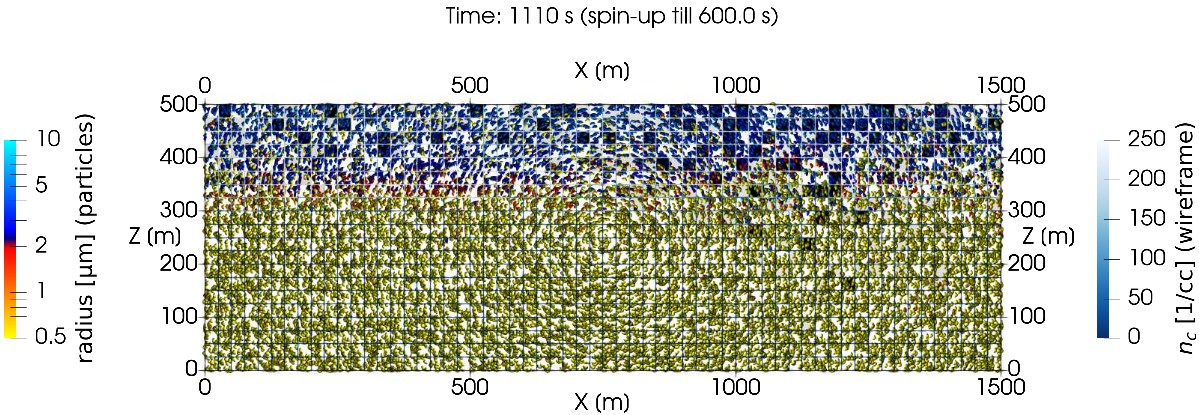


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

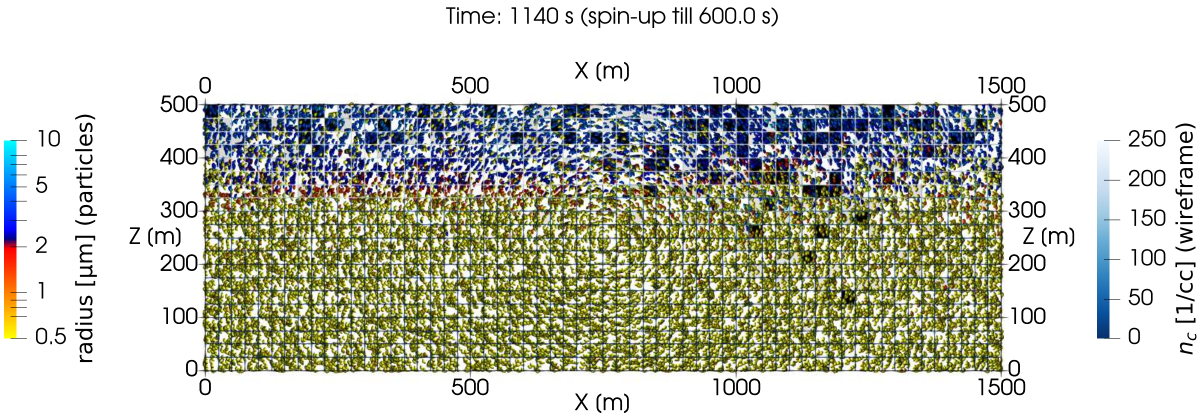


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{aer} = 300/cc$ (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

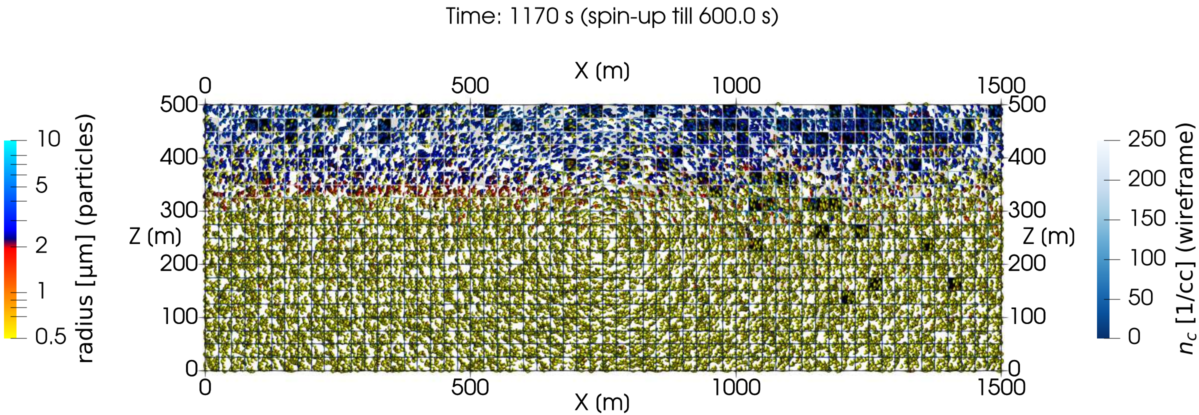


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

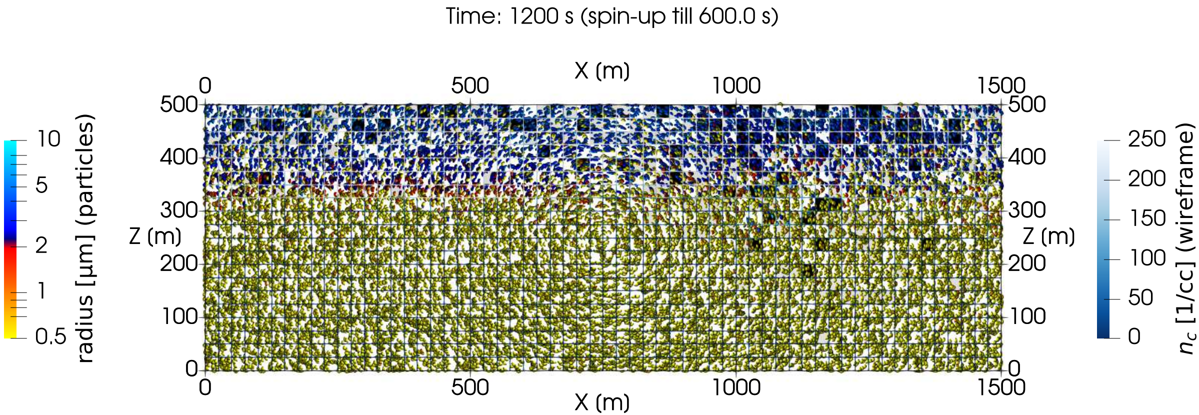


16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (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

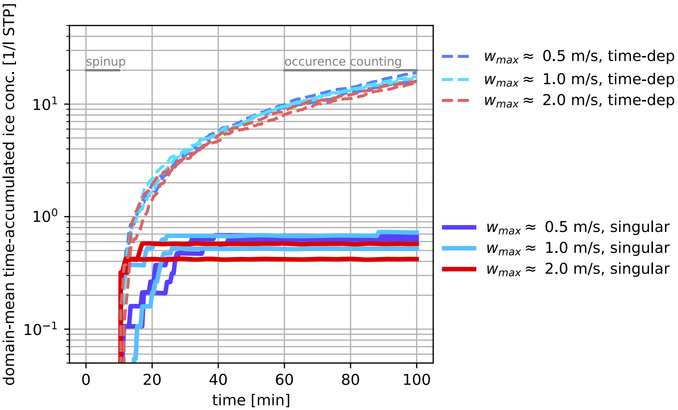


16+16 super-particles/cell for INP-rich + INP-free particles

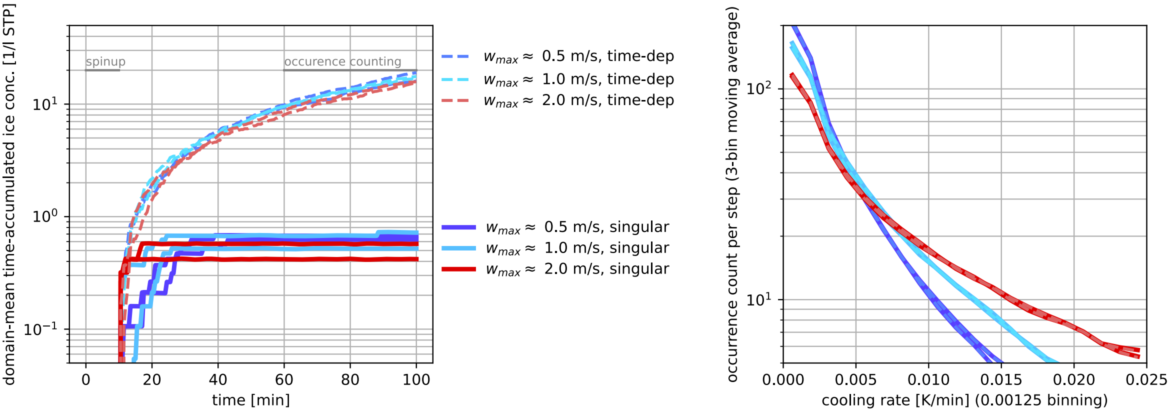
$N_{\text{aer}} = 300/cc$ (two-mode lognormal) $N_{\text{INP}} = 150/L$ (lognormal, $D_g = 0.74$ μm, $\sigma_g = 2.55$)

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

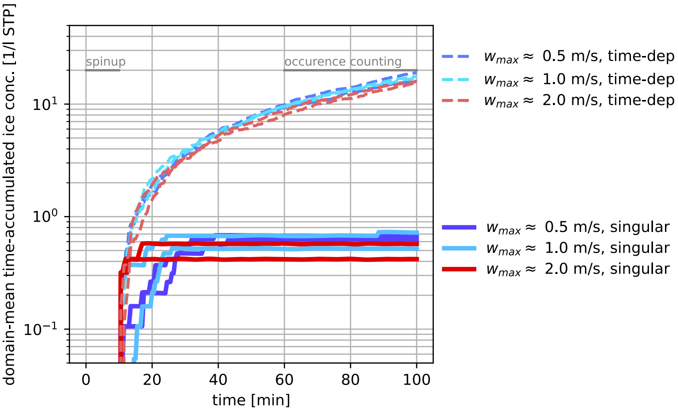
Testing three flow regimes and two immersion freezing representations

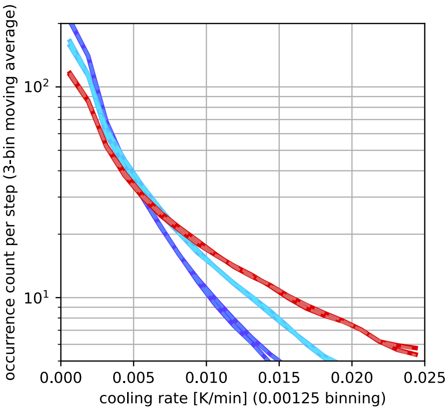


Testing three flow regimes and two immersion freezing representations



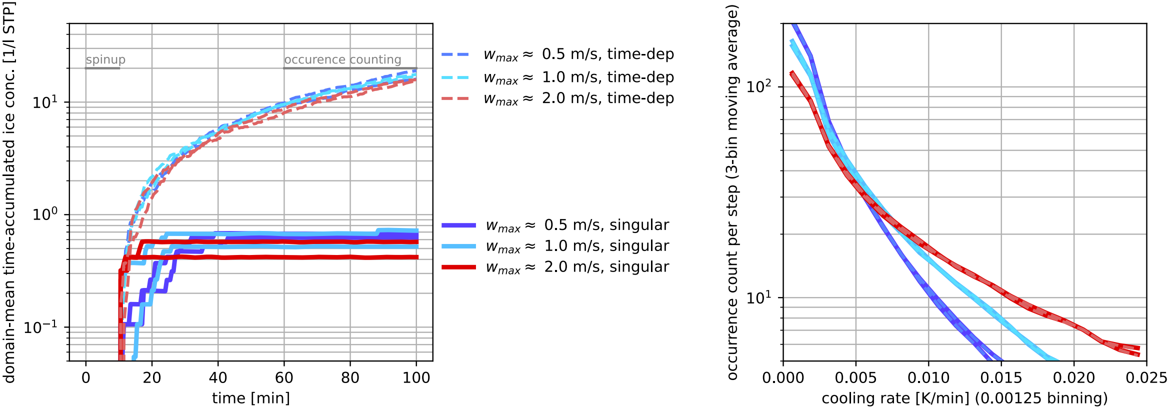
Testing three flow regimes and two immersion freezing representations





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

Testing three flow regimes and two immersion freezing representations



- 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)

100% python™ open-source code:

/ OPENATMOS / PySDM

J_{het} or n_s ?

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"

Knopf & Alpert '13

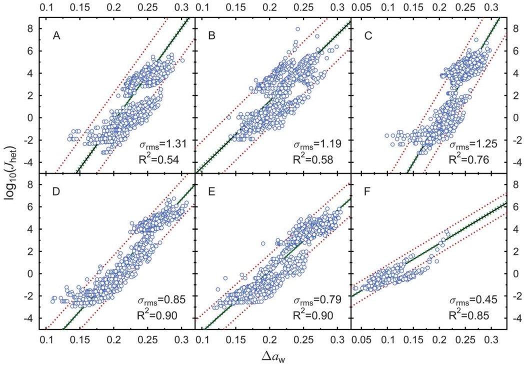


Fig. 3 The decadal log of the heterogeneous ice nucleation rate coefficients, $\log_{10}(J_{het})$, are shown as a function of Δa_w for individually analysed freezing events, initiated by the different IN types investigated in this study and previous work.[41,43,57,66,73,75,78,95] $\text{Log}_{10}(J_{het})$ 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

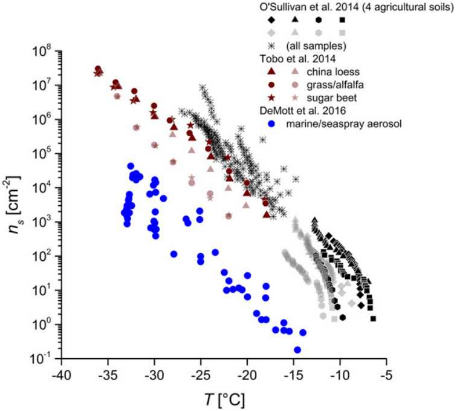


FIG. 1-6. Ice nucleation active site densities n_s as a function of temperature for H_2O_2 (hydrogen peroxide) treated (lighter-shaded symbols) and untreated (dark symbols) agricultural soil dusts in comparison to the n_s of marine aerosol. Differences between various black symbols are for organic content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

J_{het} or n_s ?

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"

stochastic or deterministic?

J_{het} or n_s ?

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"

stochastic or deterministic?

DeMott 1990 (J. Appl. Meteorol.)

"If one takes the standard definition of the "threshold temperature" for ice fomation: 1 particle in 10^4 producing an ice crystal, then this temperature (assuming all particles are immersed in drops) can be predicted from [a power law versus temperature]"

J_{het} or n_s ?

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"

stochastic or deterministic?

DeMott 1990 (J. Appl. Meteorol.)

"If one takes the standard definition of the "threshold temperature" for ice fomation: 1 particle in 10^4 producing an ice crystal, then this temperature (assuming all particles are immersed in drops) can be predicted from [a power law versus temperature]"

common underlying Poissonian model

Thank you for your attention!

JAMES | Journal of Advances in Modeling Earth Systems

AGU ADVANCING EARTH AND SPACE SCIENCES

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

vol 17(4), Apr 2025

sylwester.arabas@agh.edu.pl