

# On Particle-Based Modeling of Immersion Freezing

S. Arabas<sup>1,2</sup>, J.H. Curtis<sup>1</sup>, I. Silber<sup>3</sup>, A. Fridlind<sup>4</sup>, D.A Knopf<sup>5</sup> & N. Riemer<sup>1</sup>



atmos.illinois.edu



JAGIELLONIAN  
UNIVERSITY  
uj.edu.pl



met.psu.edu



giss.nasa.gov



stonybrook.edu

funding:



14<sup>th</sup> Symposium on Aerosol-Cloud-Climate Interactions / 102<sup>nd</sup> AMS Annual Meeting

virtual, Jan 27 2022

super-particles as a probabilistic alternative to bulk or bin  $\mu$ -physics

# JAMES

**Journal of Advances in  
Modeling Earth Systems**

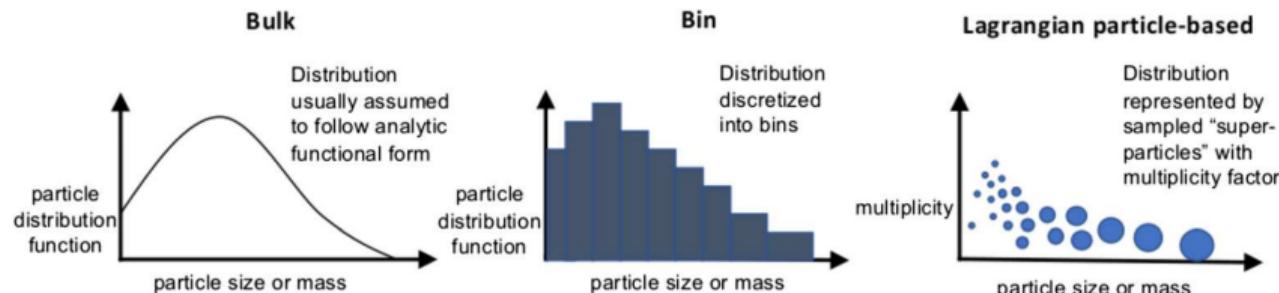
**COMMISSIONED  
MANUSCRIPT**  
10.1029/2019MS001689

### Key Points:

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

# Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

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



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

super-particles as a probabilistic alternative to bulk or bin  $\mu$ -physics

JAMES

**Journal of Advances in  
Modeling Earth Systems**

# COMMISSIONED MANUSCRIPT

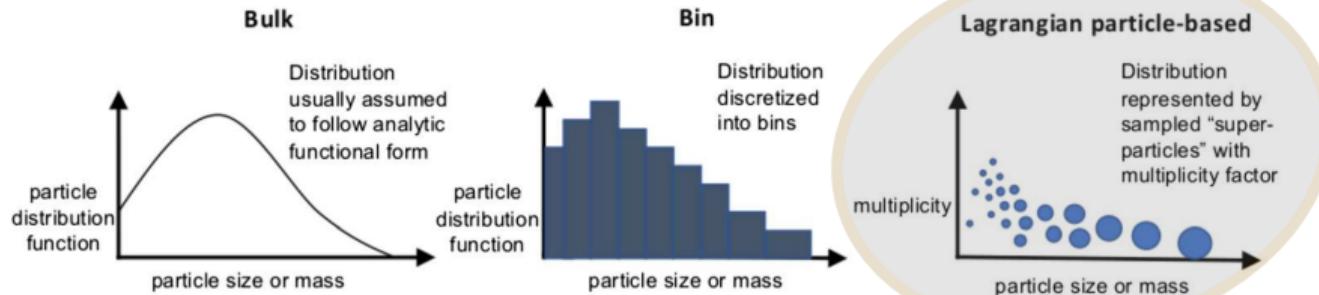
10.1029/2019MS001689

### Key Points:

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

## Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

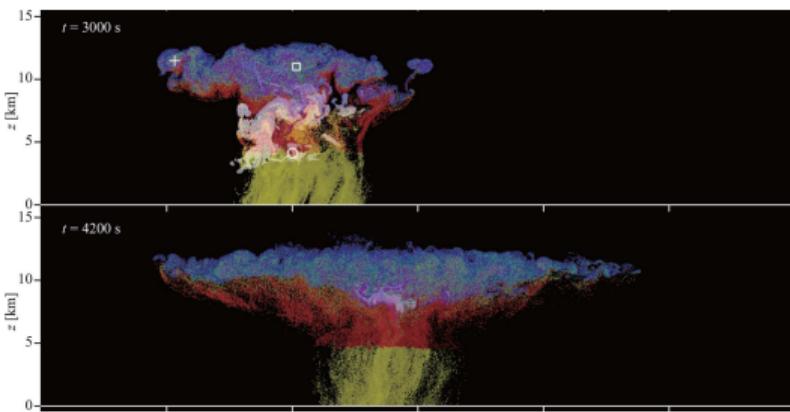
Hugh Morrison<sup>1</sup> , Marcus van Lier-Walqui<sup>2</sup> , Ann M. Fridlind<sup>3</sup> , Wojciech W. Grabowski<sup>1</sup> , Jerry Y. Harrington<sup>4</sup>, Corinna Hoose<sup>5</sup> , Alexei Korolev<sup>6</sup> , Matthew R. Kumjian<sup>4</sup> , Jason A. Milbrandt<sup>7</sup>, Hanna Pawlowska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



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

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

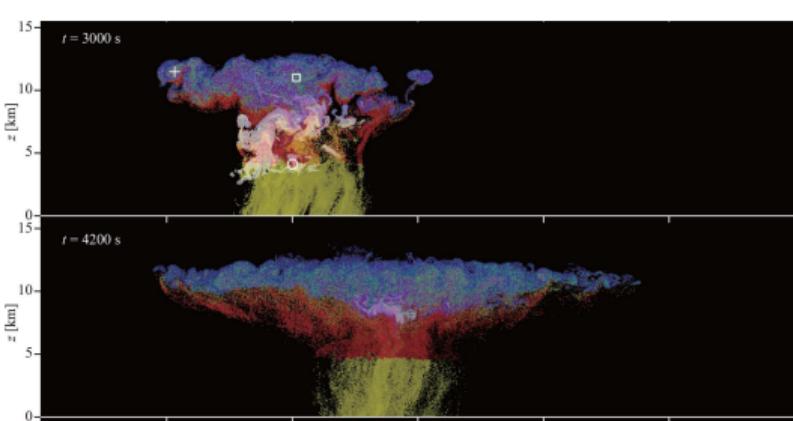
Predicting the morphology of ice particles in deep convection using the super-droplet method



**Figure 1.** Typical realization of CTRL cloud spatial structures at  $t = 2040, 2460, 3000, 4200$ , and  $5400\text{s}$ . 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, Sato, Hashimoto & Misumi 2020 (GMD):

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

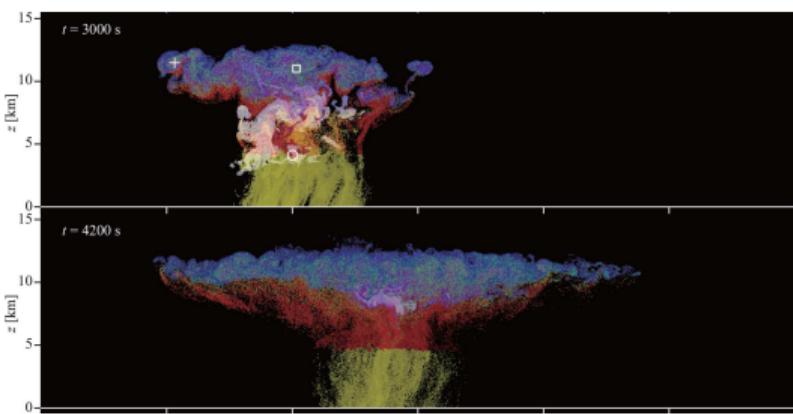


- ▶ Eulerian component: momentum, heat, moisture budget

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

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

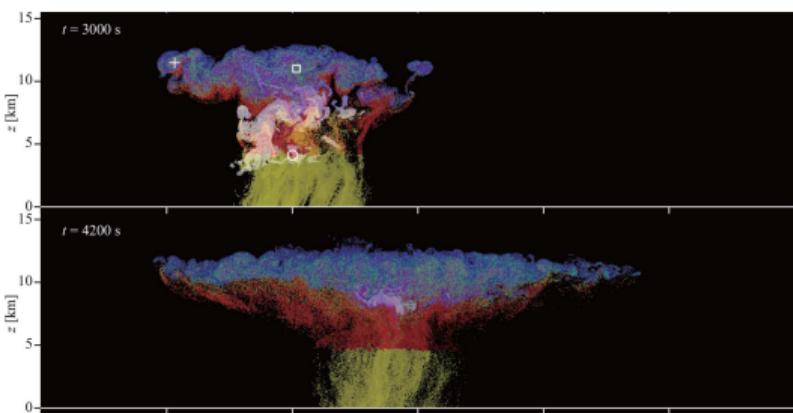


**Figure 1.** Typical realization of CTRL cloud spatial structures at  $t = 2040, 2460, 3000, 4200$ , and  $5400\text{ s}$ . The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate 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, Sato, Hashimoto & Misumi 2020 (GMD):

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

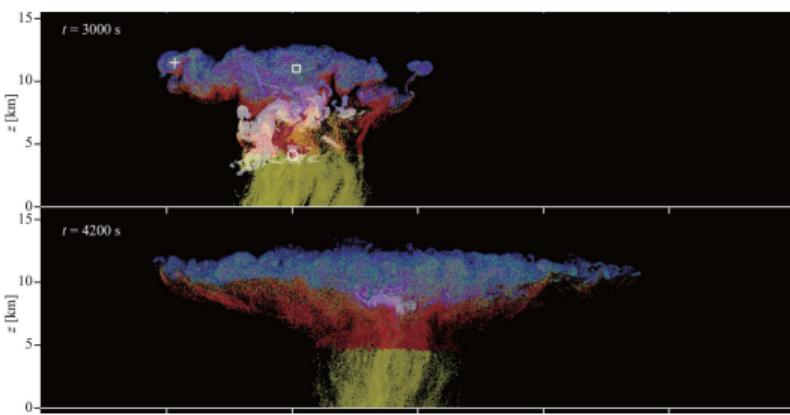


**Figure 1.** Typical realization of CTRL cloud spatial structures at  $t = 2040, 2460, 3000, 4200$ , and  $5400\text{ s}$ . The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate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

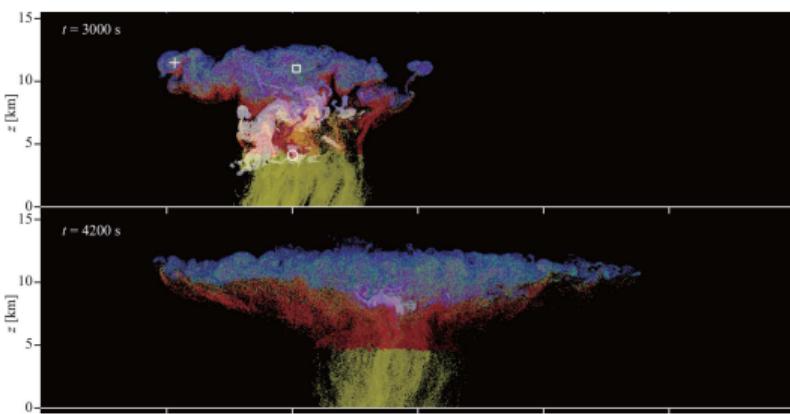


**Figure 1.** Typical realization of CTRL cloud spatial structures at  $t = 2040, 2460, 3000, 4200$ , and  $5400\text{ s}$ . The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate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

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  $5400\text{ s}$ . 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 with **monodisperse INP**

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

theory (in modern notation)

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

# 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  $r$ :

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

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

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

# 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  $r$ :

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

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

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

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

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

# 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  $r$ :

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

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

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

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

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

INAS:  $I(T) = n_s(T) = \exp(a \cdot (T - T_0^{\circ}C) + b)$

# 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  $r$ :

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

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

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

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

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

INAS:  $I(T) = n_s(T) = \exp(a \cdot (T - T_0^{\circ}C) + b)$

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

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

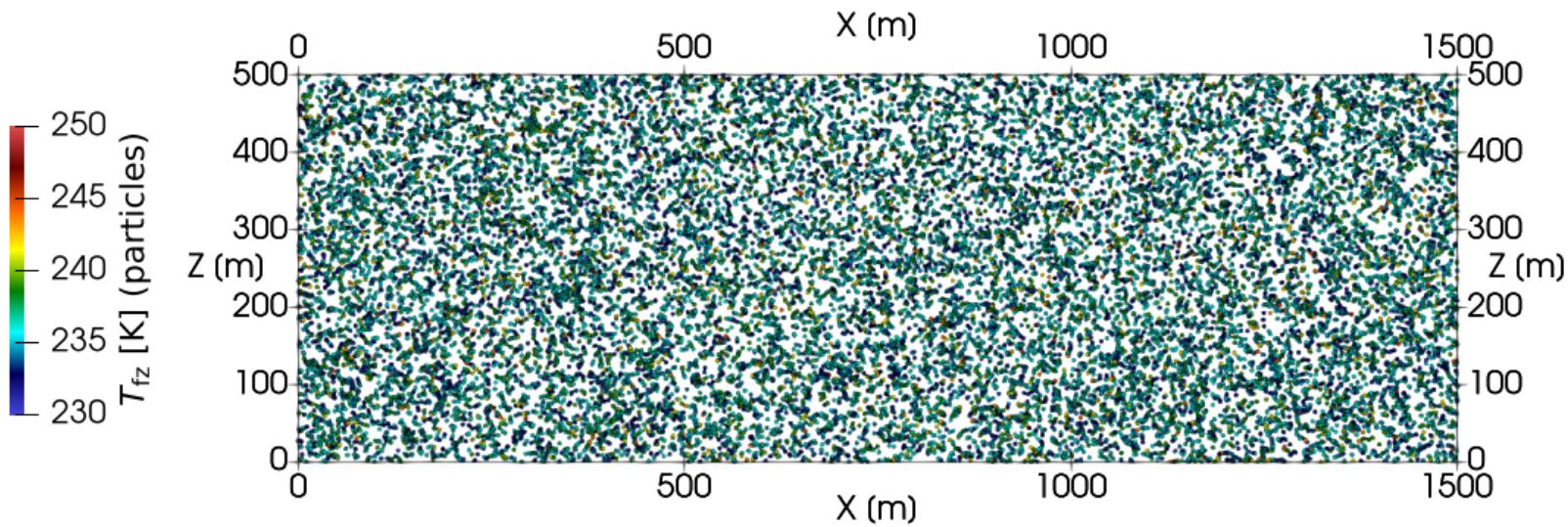
$$P(A, T_{\text{fz}}) = 1 - \exp(-A \cdot n_s(T_{\text{fz}}))$$

spectrum of  $T_{\text{fz}}$  even for monodisperse  $A$

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

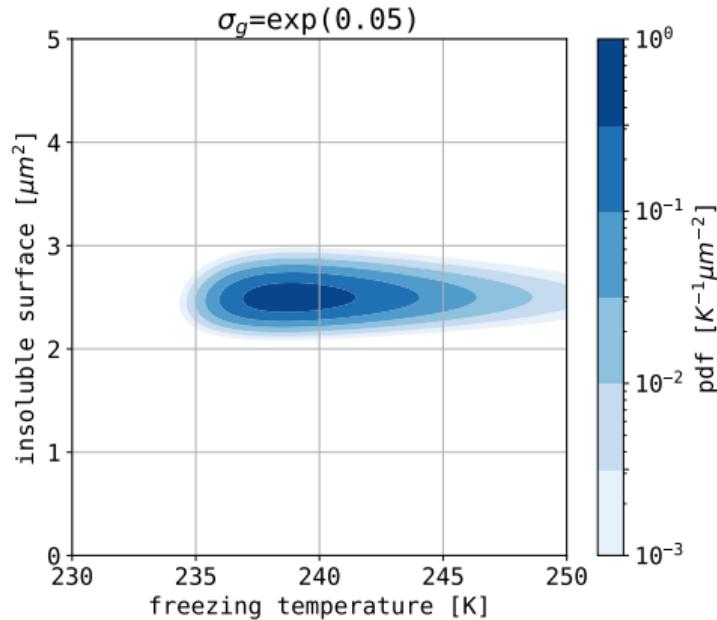
$$P(A, T_{\text{fz}}) = 1 - \exp(-A \cdot n_s(T_{\text{fz}}))$$

spectrum of  $T_{fz}$  even for monodisperse A



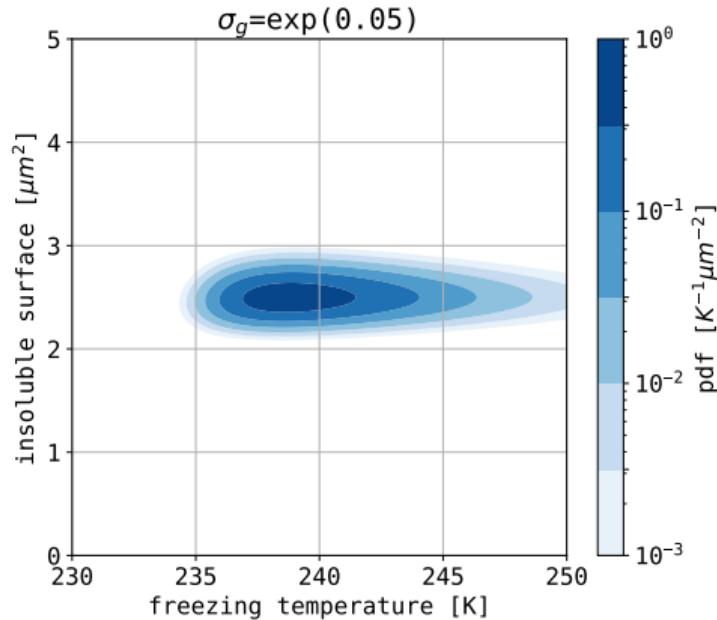
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)



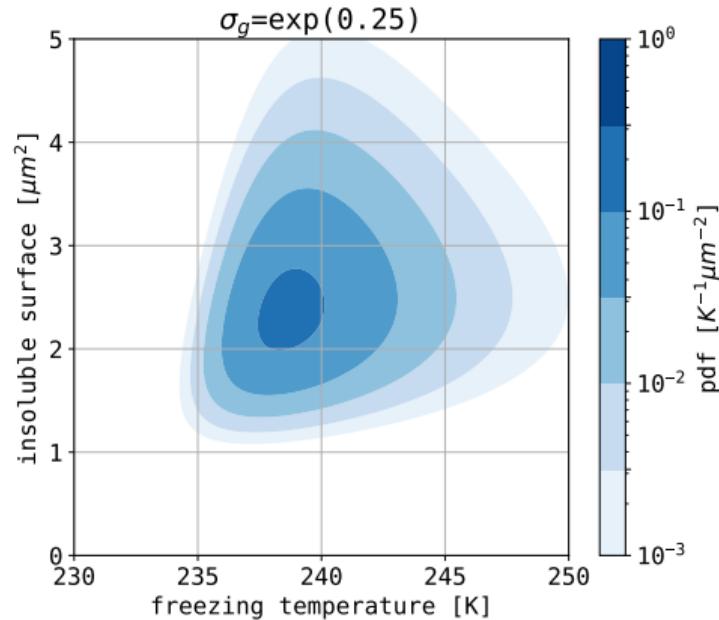
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)



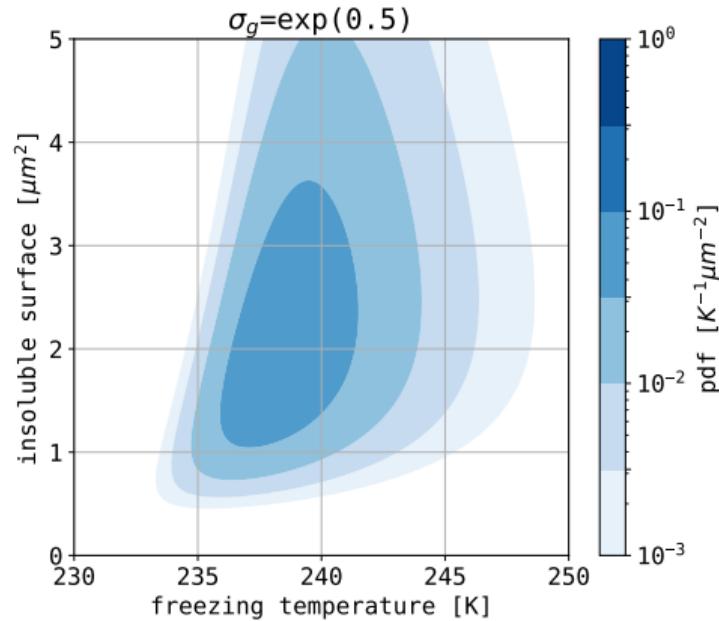
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)



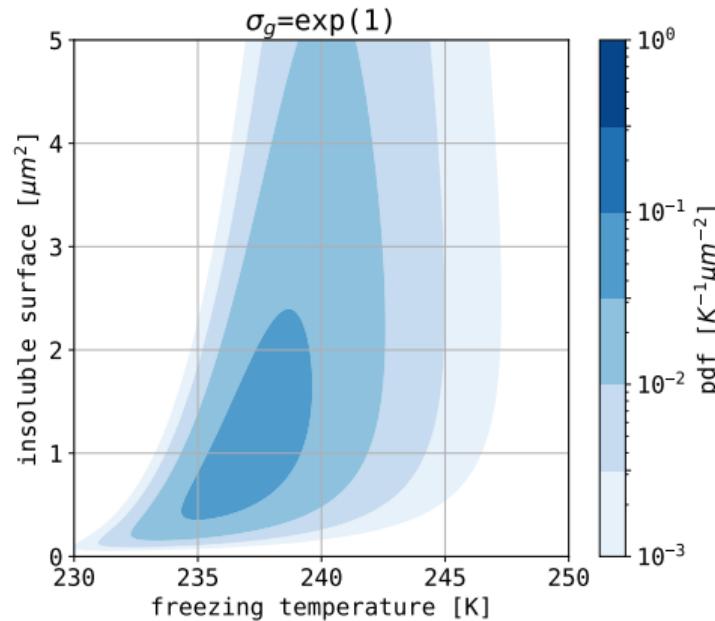
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)



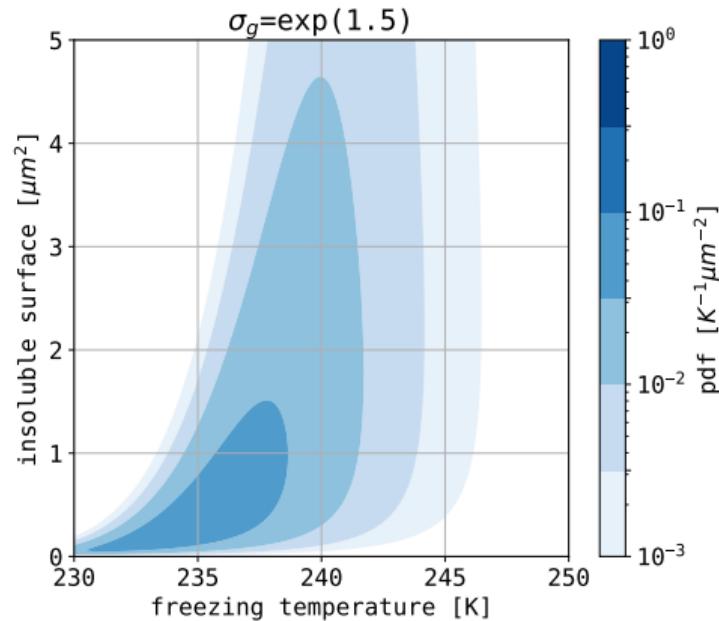
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)



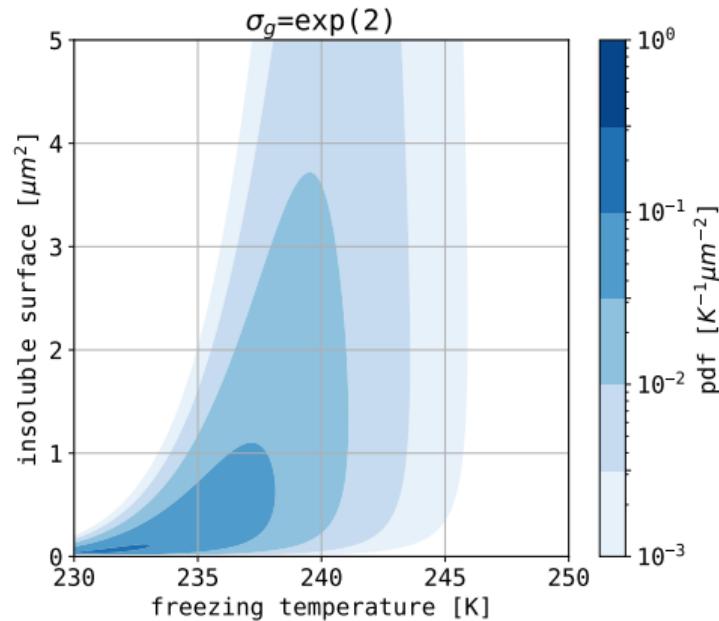
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)



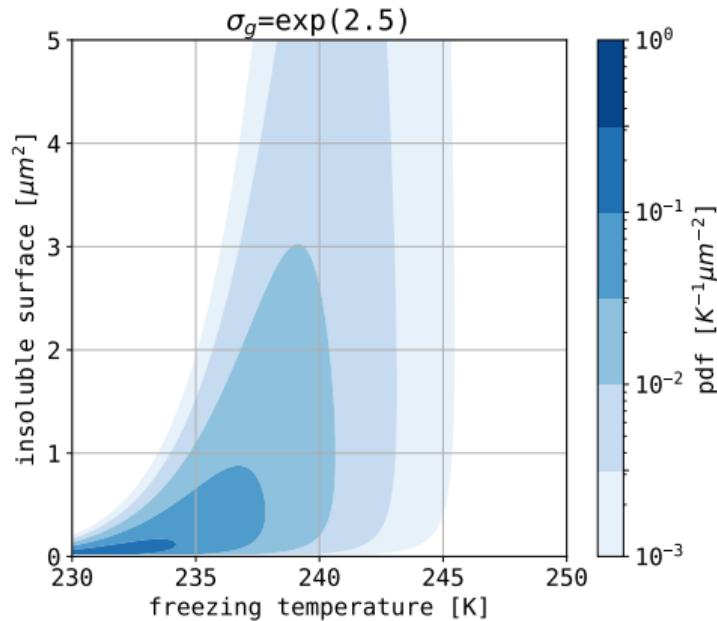
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)



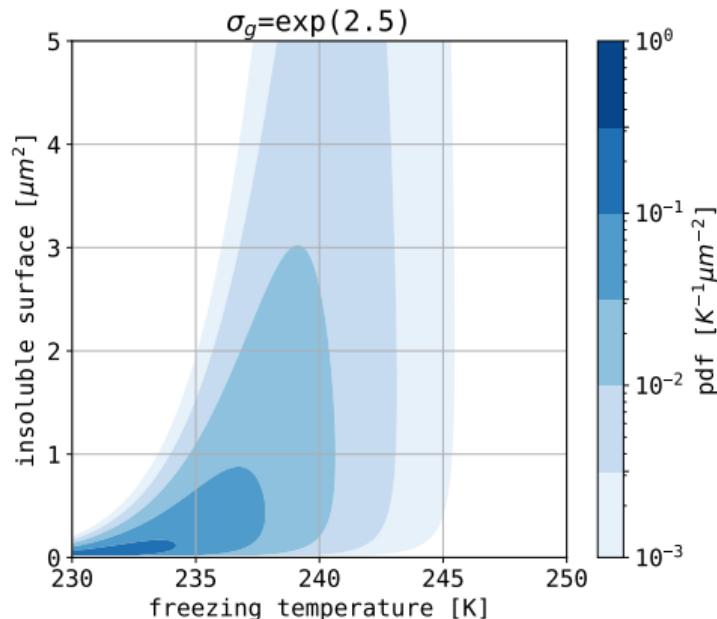
freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)

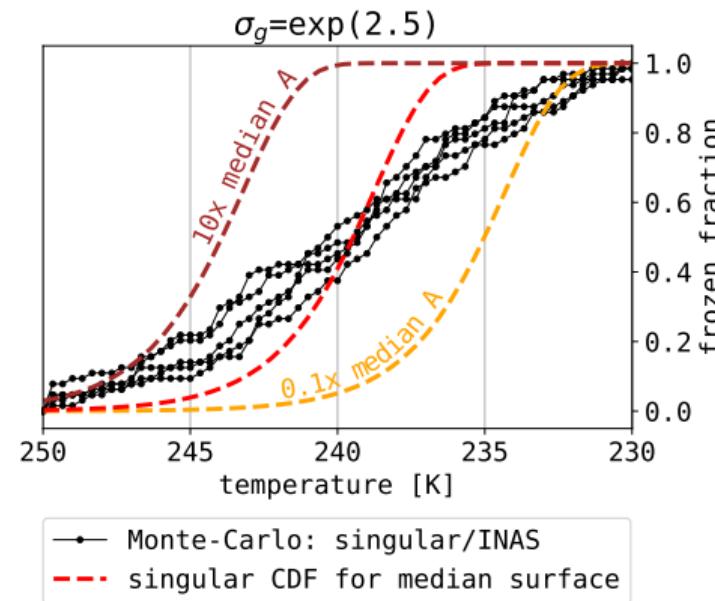


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)

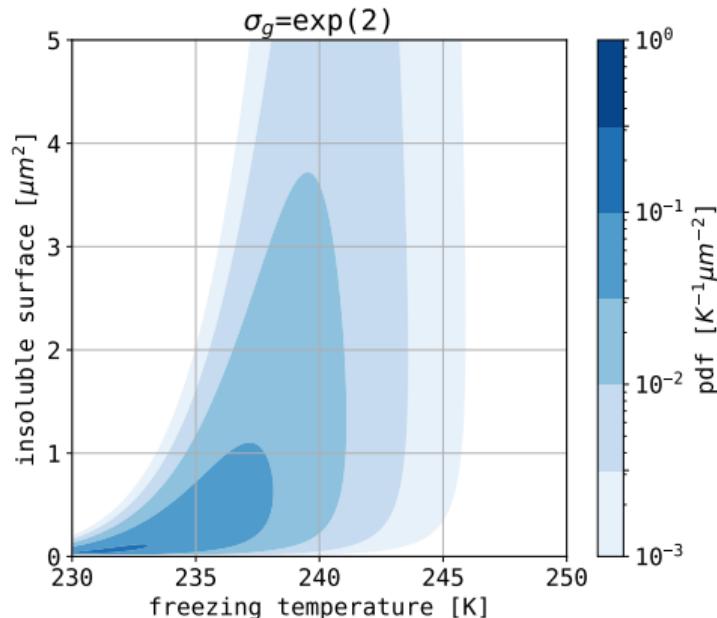


box model (or single grid cell)

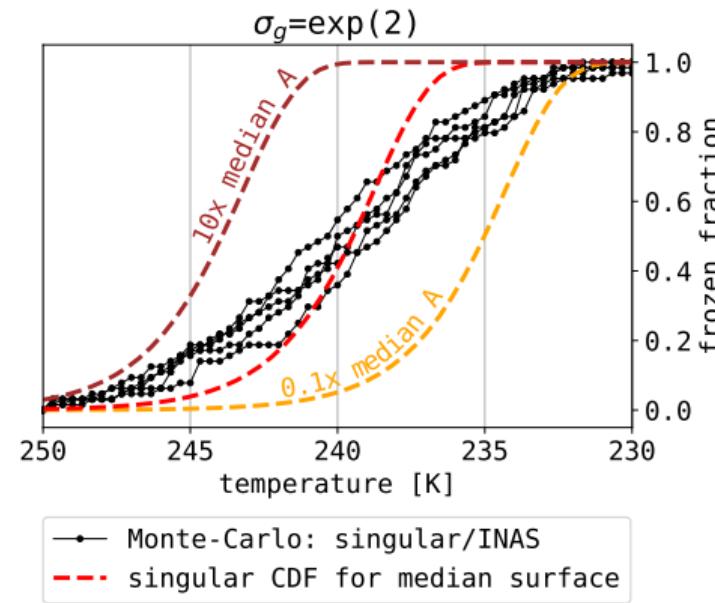


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)

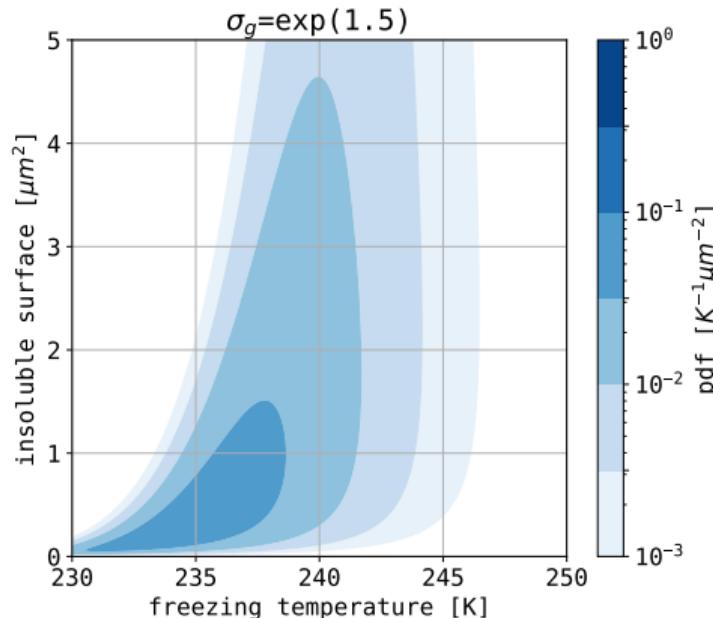


box model (or single grid cell)

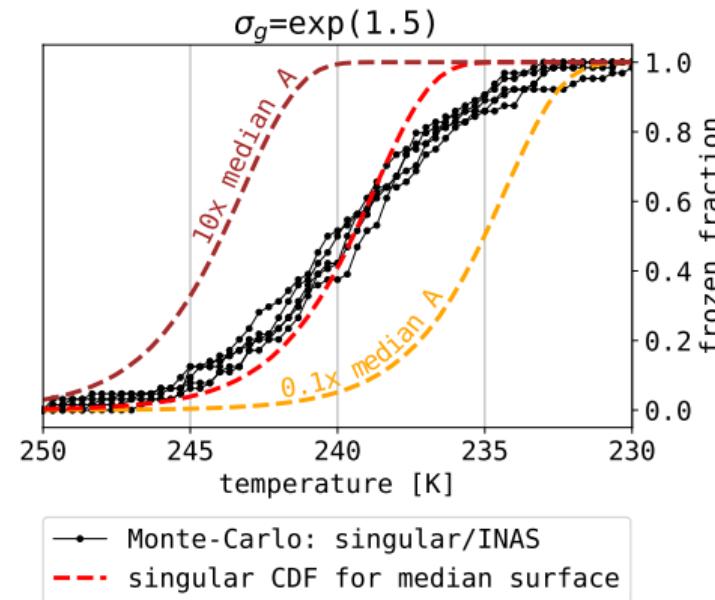


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

### INAS P( $T_{fz}$ ,A) sampling (A lognormal)

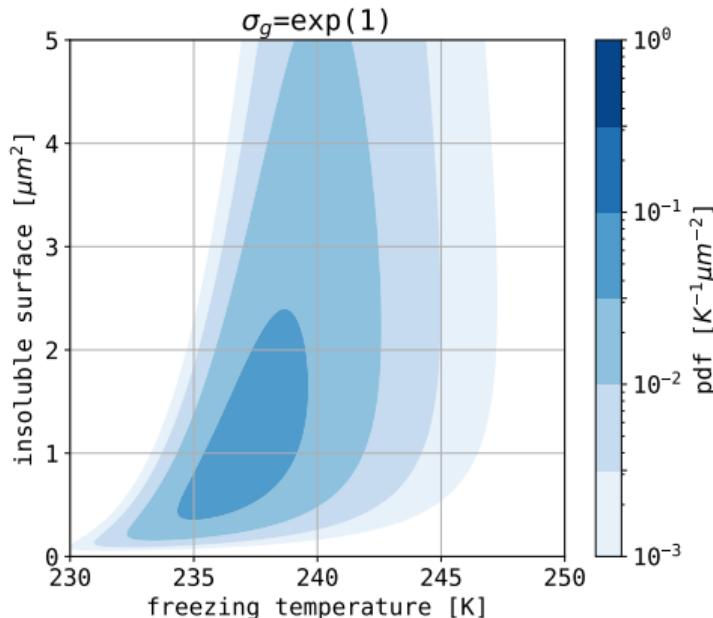


box model (or single grid cell)

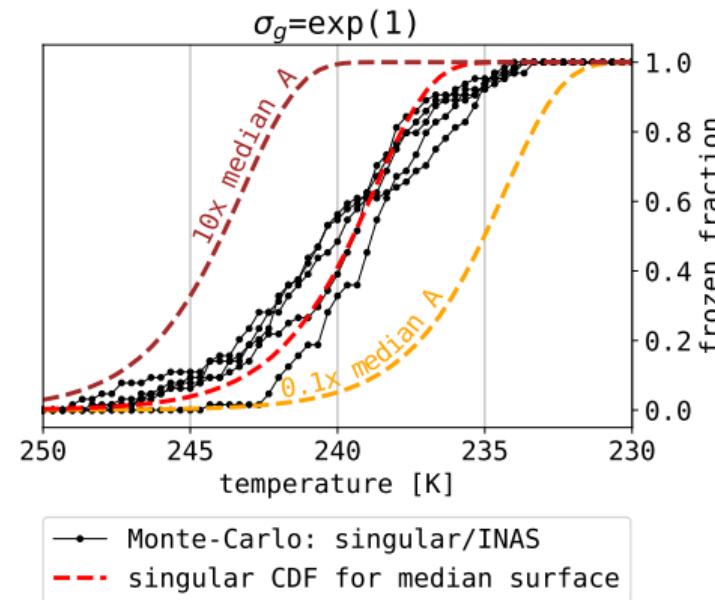


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)

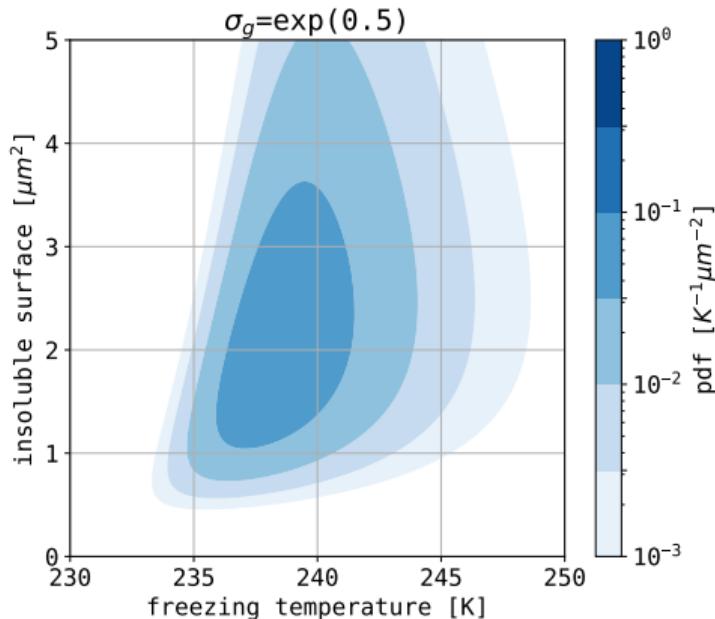


box model (or single grid cell)

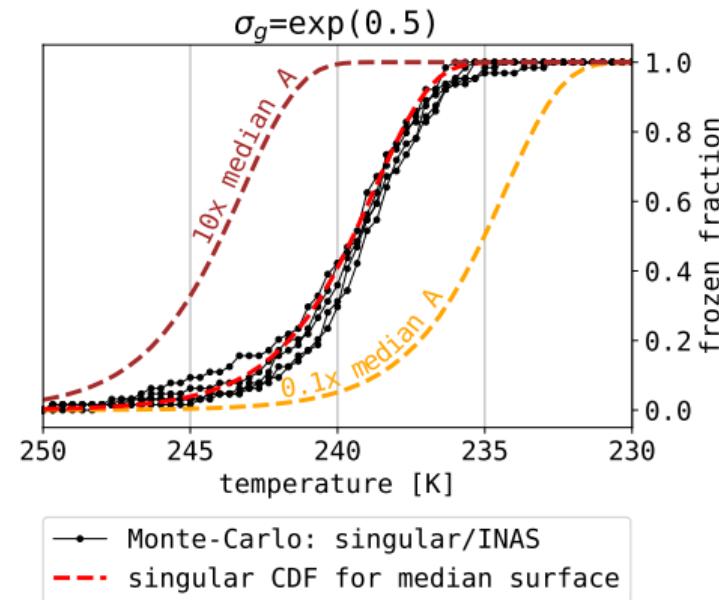


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)

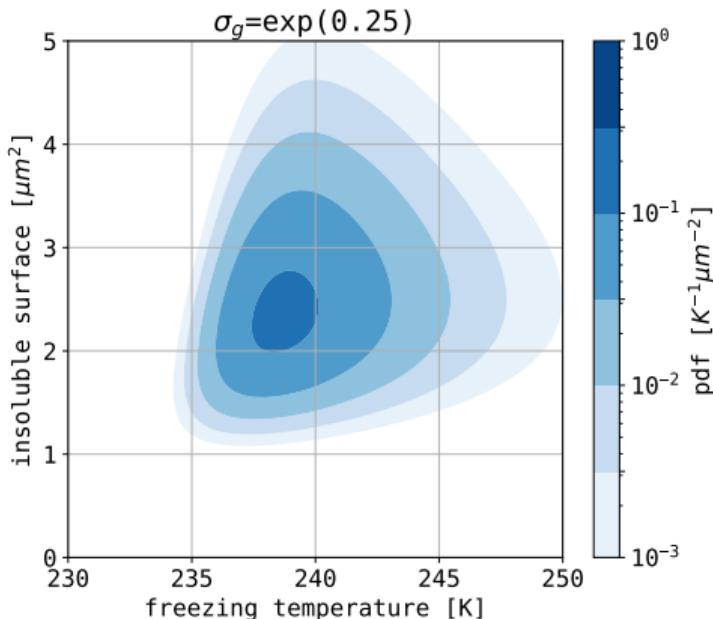


box model (or single grid cell)

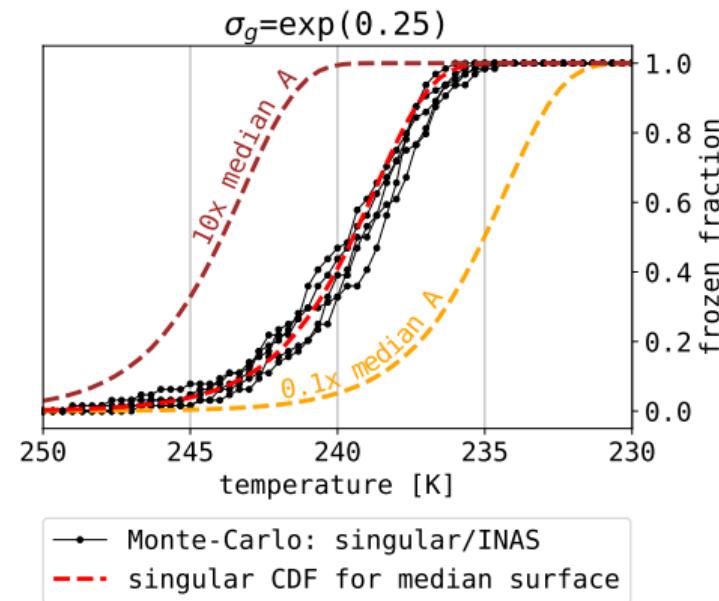


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

INAS P( $T_{fz}$ ,A) sampling (A lognormal)

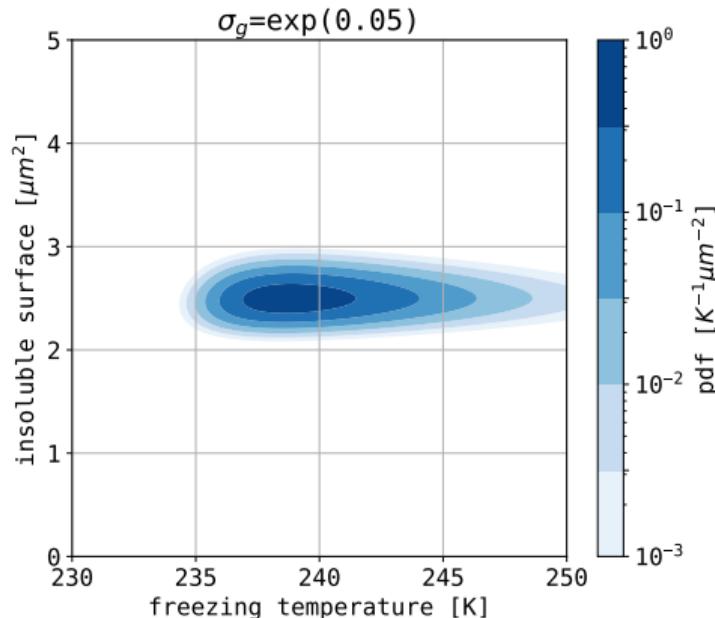


box model (or single grid cell)

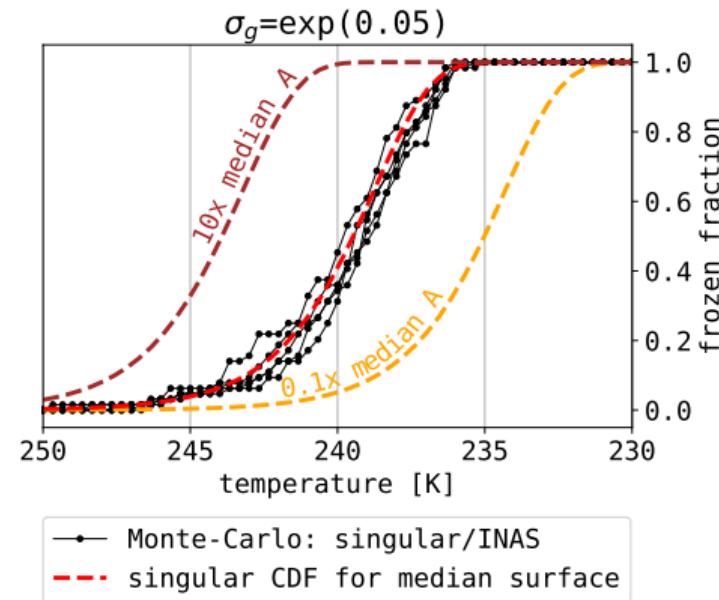


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

## INAS P( $T_{fz}$ ,A) sampling (A lognormal)

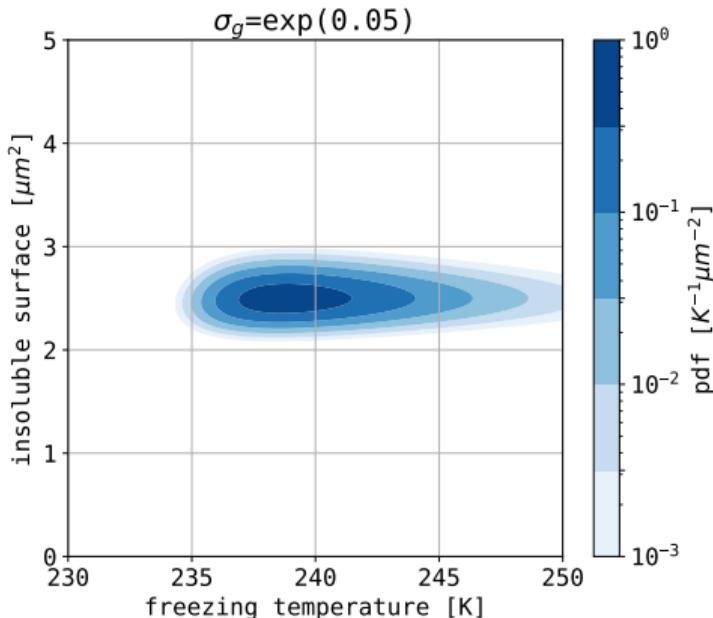


box model (or single grid cell)

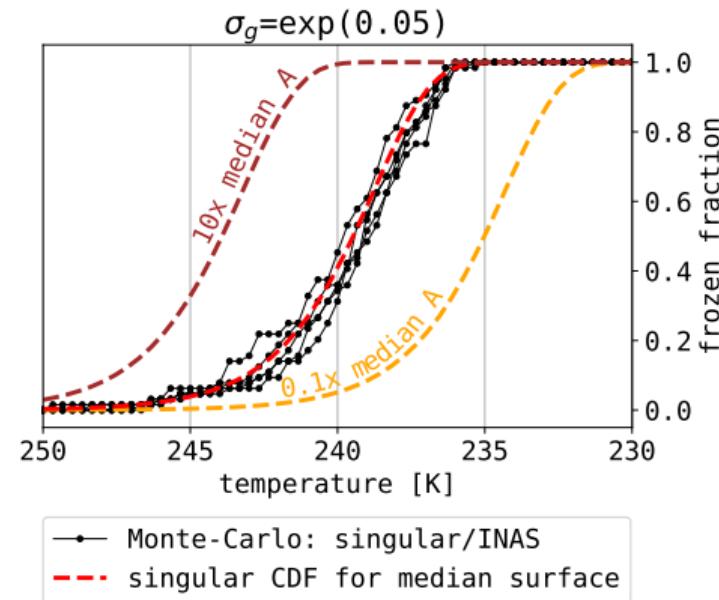


freezing temperature  $T_{\text{fz}}$  as a super-particle attribute: initialisation

INAS P( $T_{fz}$ ,A) sampling (A lognormal)



box model (or single grid cell)



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

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

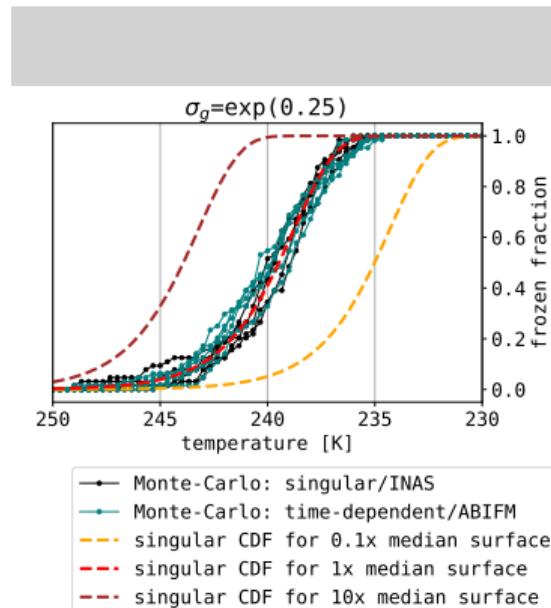
**singular:** INAS  $T_{fz}$  as attribute; initialisation by random sampling from  $P(T_{fz}, A)$  with lognormal  $A$  ( $A$  is not an attribute, initialisation only); freezing if  $T(t) < T_{fz}(t = 0)$

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

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

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

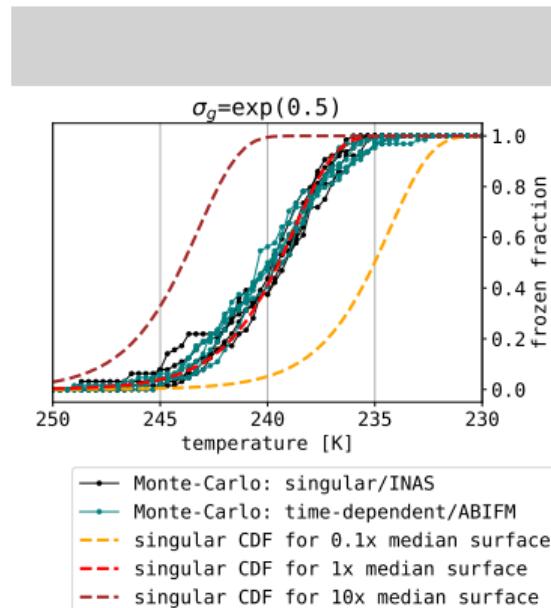
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

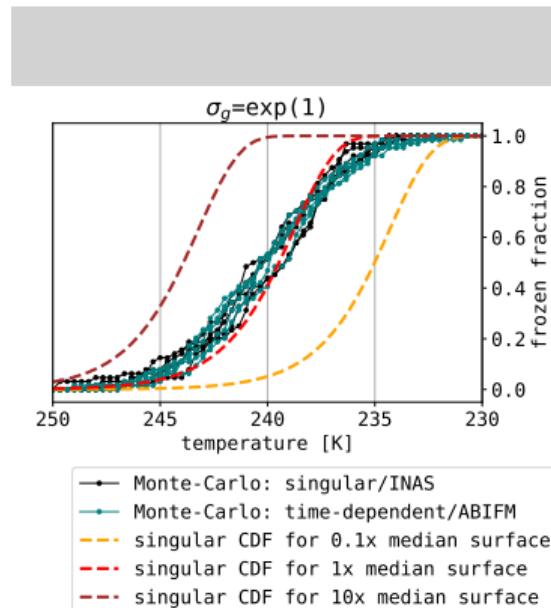
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

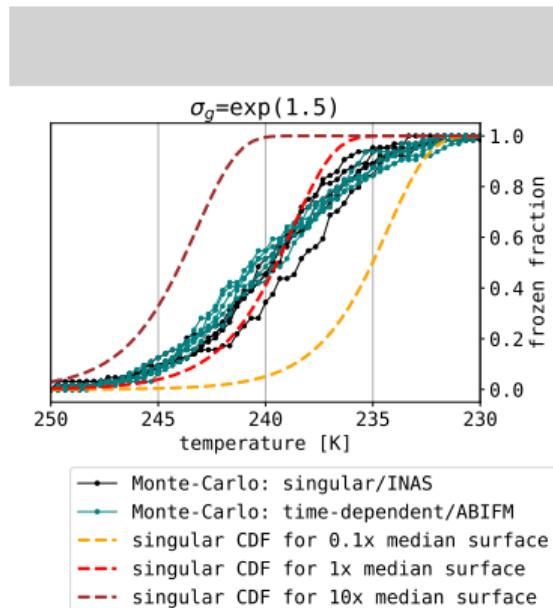
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

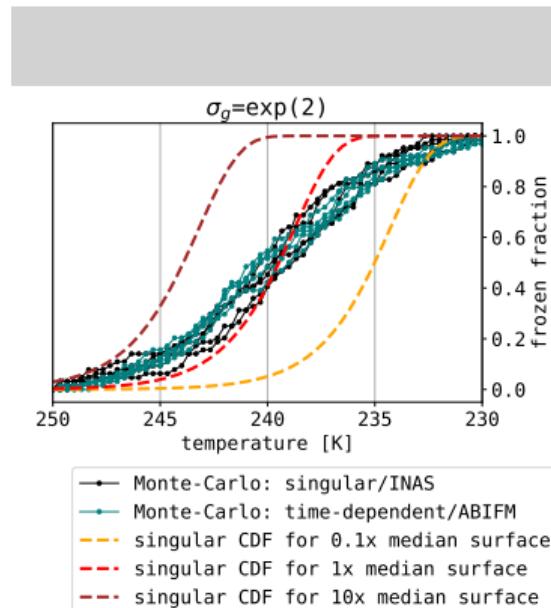
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

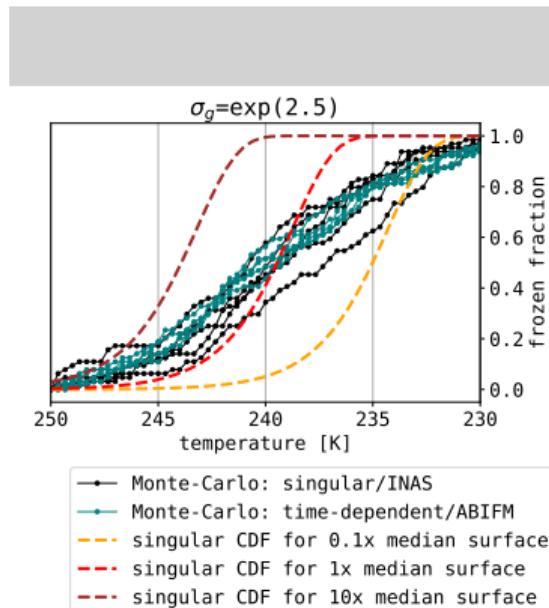
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

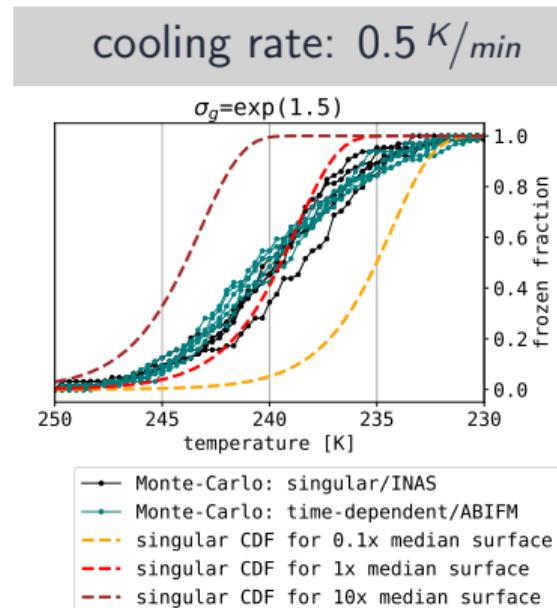
**time-dependent:**  $A$  as attribute (randomly sampled from the same lognormal)  
 Monte-Carlo freezing trigger using  $P(J_{\text{het}}(T(t)))$



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

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

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

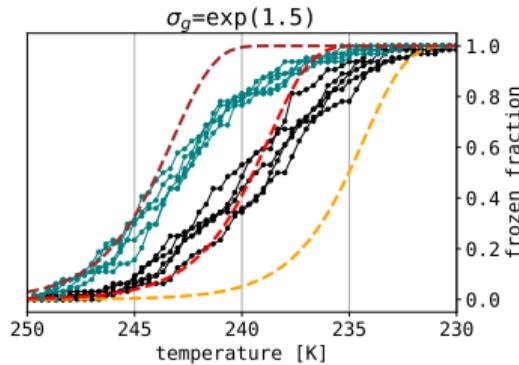


# particle-based freezing: singular (Shima et al.) / time-dependent (this work)

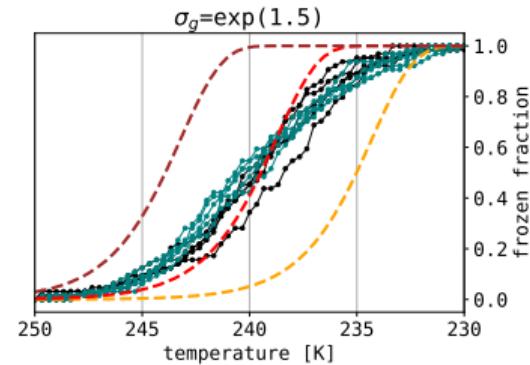
**singular:** INAS  $T_{fz}$  as attribute; initialisation by random sampling from  $P(T_{fz}, A)$  with lognormal  $A$  ( $A$  is not an attribute, initialisation only); freezing if  $T(t) < T_{fz}(t = 0)$

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

cooling rate:  $0.1 \text{ K/min}$



cooling rate:  $0.5 \text{ K/min}$



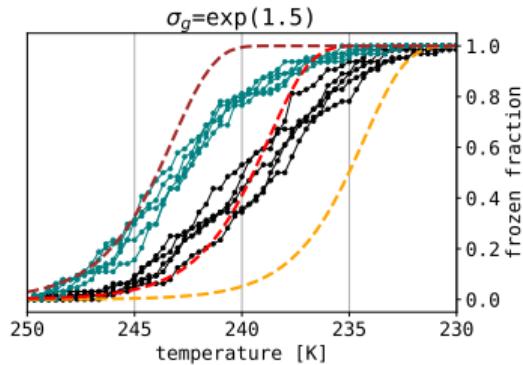
- Monte-Carlo: singular/INAS
- Monte-Carlo: time-dependent/ABIFM
- singular CDF for  $0.1x$  median surface
- - singular CDF for  $1x$  median surface
- - - singular CDF for  $10x$  median surface

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

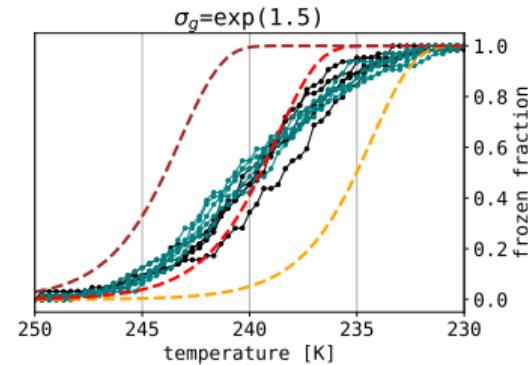
**singular:** INAS  $T_{fz}$  as attribute; initialisation by random sampling from  $P(T_{fz}, A)$  with lognormal  $A$  ( $A$  is not an attribute, initialisation only); freezing if  $T(t) < T_{fz}(t = 0)$

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

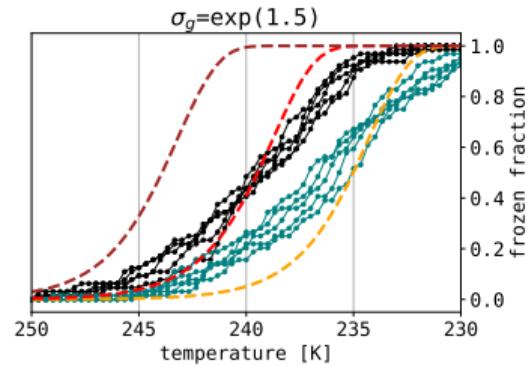
cooling rate:  $0.1 \text{ K/min}$



cooling rate:  $0.5 \text{ K/min}$



cooling rate:  $2.5 \text{ K/min}$



# 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  $r$ :

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

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

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

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

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

INAS:  $I(T) = n_s(T) = \exp(a \cdot (T - T_0{}^\circ C) + b)$

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

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

theory (in modern notation)

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

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

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

Poisson counting process with rate  $r$ :

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

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

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

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

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

INAS:  $I(T) = n_s(T) = \exp(a \cdot (T - T_0^\circ C) + b)$

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

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

theory (in modern notation)

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

Poisson counting process with rate  $r$ :

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

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

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

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

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

INAS:  $I(T) = n_s(T) = \exp(a \cdot (T - T_0{}^\circ C) + b)$

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

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

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

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

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  $r$ :

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

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

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

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

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

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

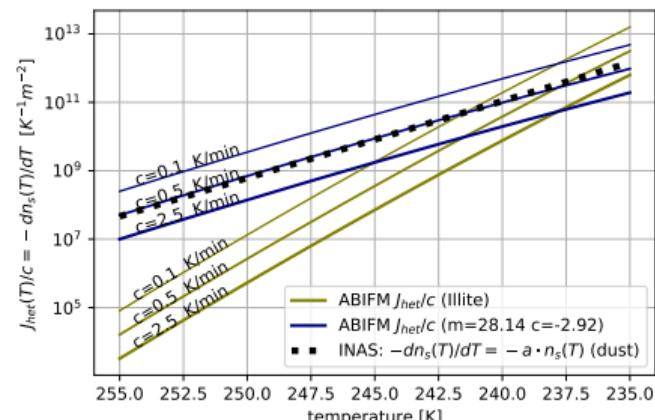
experimental  $n_s(T)$  fits: e.g., Niemand et al. 2012

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

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

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

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



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

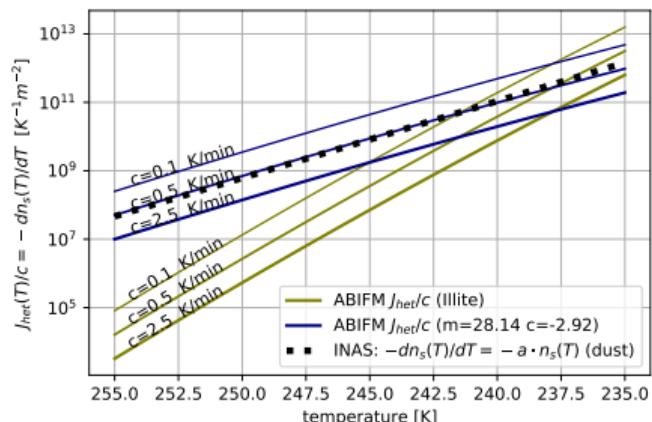
for a constant cooling rate  $c = dT/dt$ :

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

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

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

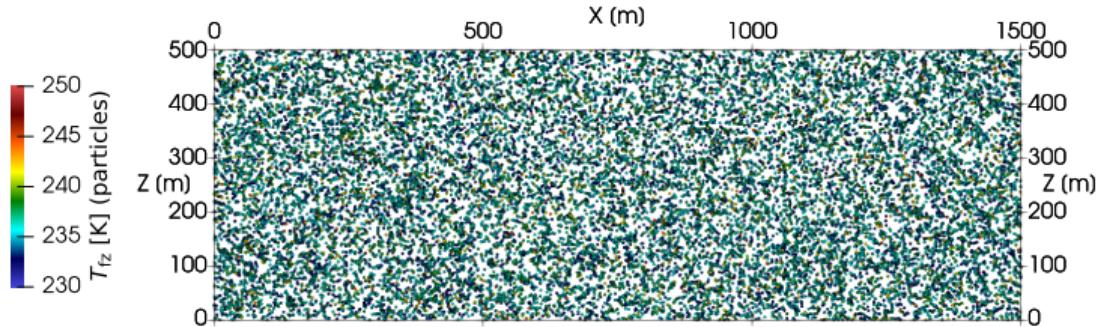
## Houston, we have a problem



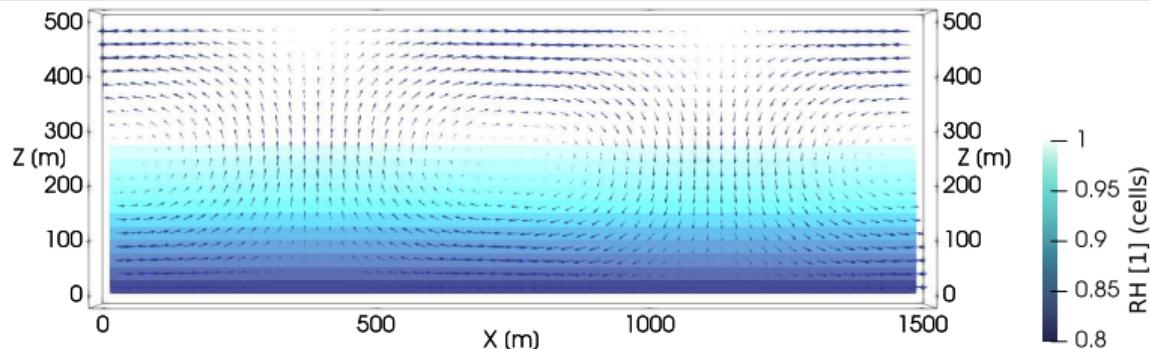
addressed in the modified singular model of Vali '94 (also: Murray et al. '11)  
but the singular ansatz limitation of sampling  $T_{\text{fz}}$  at  $t=0$  remains

# particle-based $\mu$ -physics + prescribed-flow test (aka KiD-2D)<sup>a,b,c,d,e</sup>

Lagrangian component (PySDM)



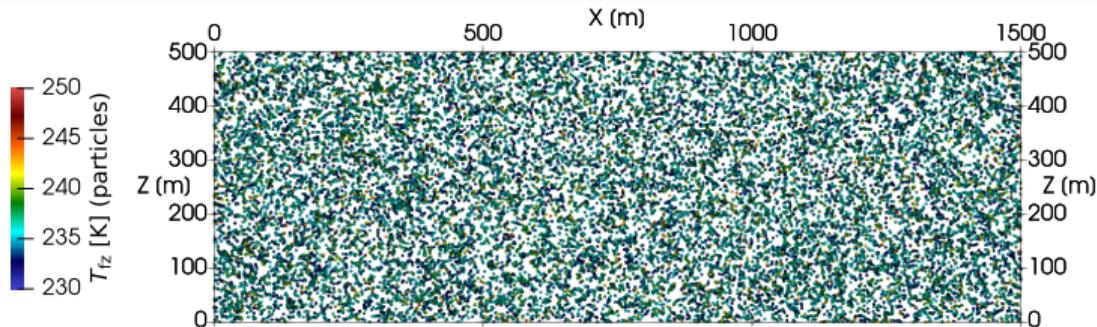
Eulerian component (PyMPDATA)



- 
- <sup>a</sup>concept: Gedzelman & Arnold '93
  - <sup>b</sup>stratiform: Morrison & Grabowski '07
  - <sup>c</sup>particle-based: Arabas et al. '15
  - <sup>d</sup>KiD-2D: [github.com/BShipway/KiD](https://github.com/BShipway/KiD)
  - <sup>e</sup>here: SHEBA case (Fridlind et al. '12)

# particle-based $\mu$ -physics + prescribed-flow test (aka KiD-2D)<sup>a,b,c,d,e</sup>

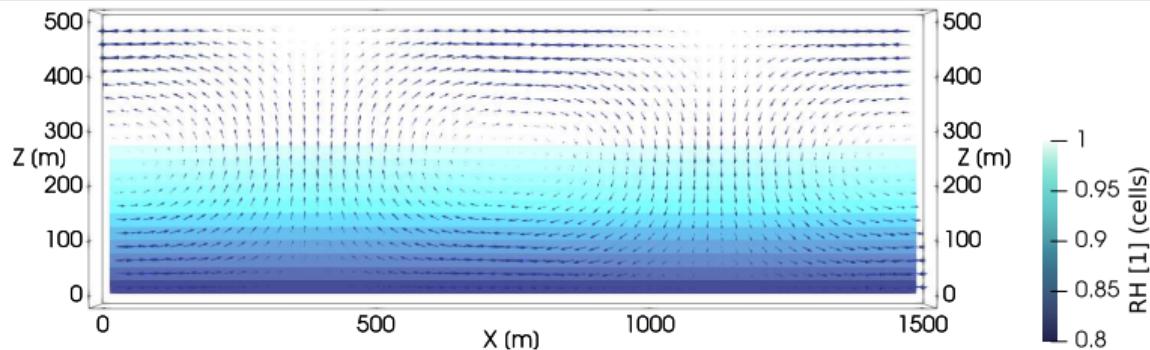
Lagrangian component (PySDM)



PySDM & PyMPDATA  
(Bartman et al. 2022)

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

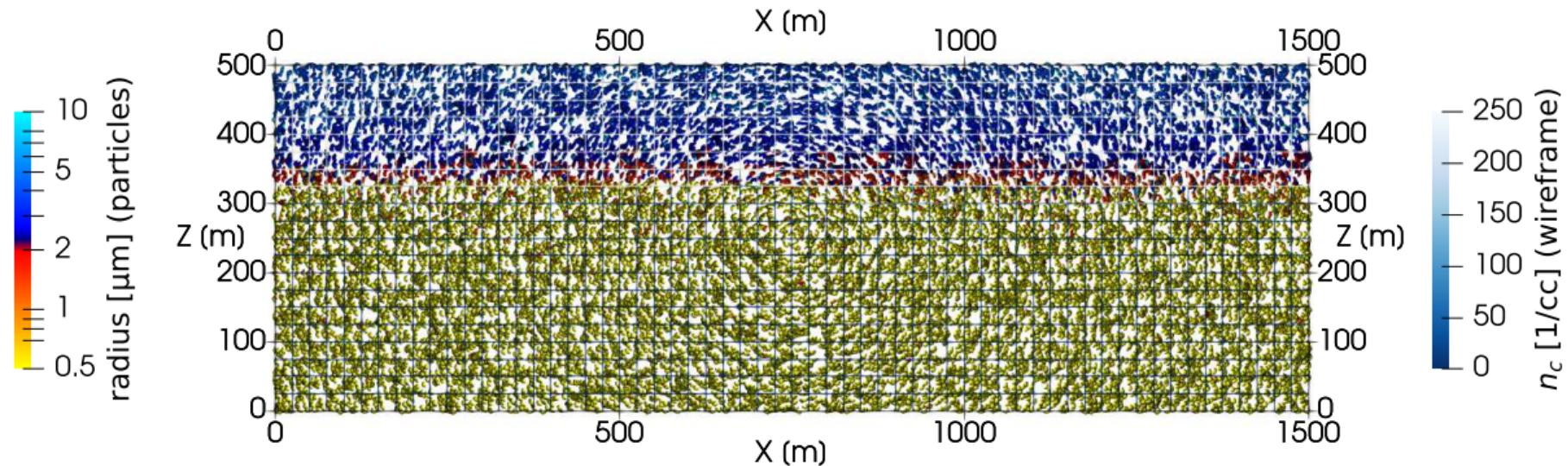
Eulerian component (PyMPDATA)



- 
- <sup>a</sup>concept: Gedzelman & Arnold '93
  - <sup>b</sup>stratiform: Morrison & Grabowski '07
  - <sup>c</sup>particle-based: Arabas et al. '15
  - <sup>d</sup>KiD-2D: [github.com/BShipway/KiD](https://github.com/BShipway/KiD)
  - <sup>e</sup>here: SHEBA case (Fridlind et al. '12)

## particle-based $\mu$ -physics + prescribed-flow test

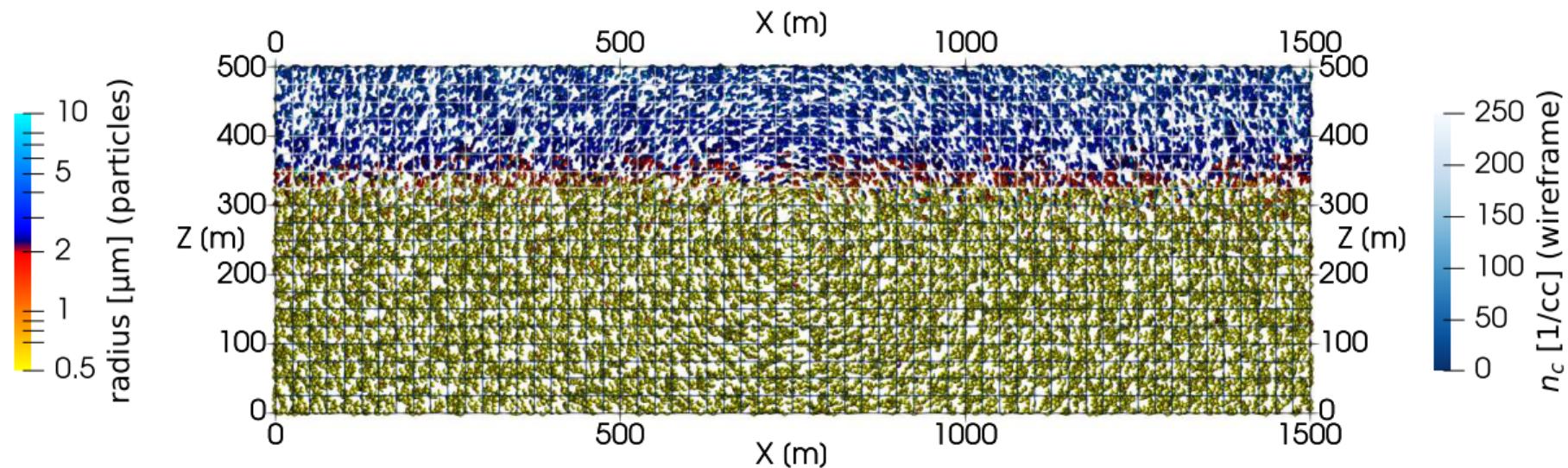
Time: 30 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

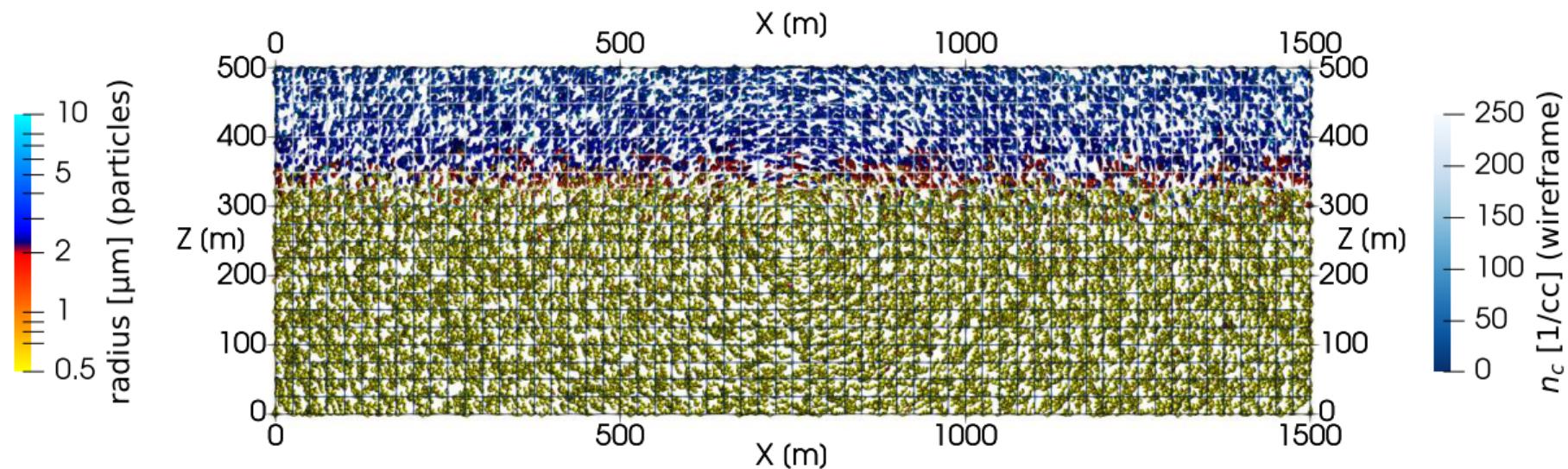
Time: 60 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

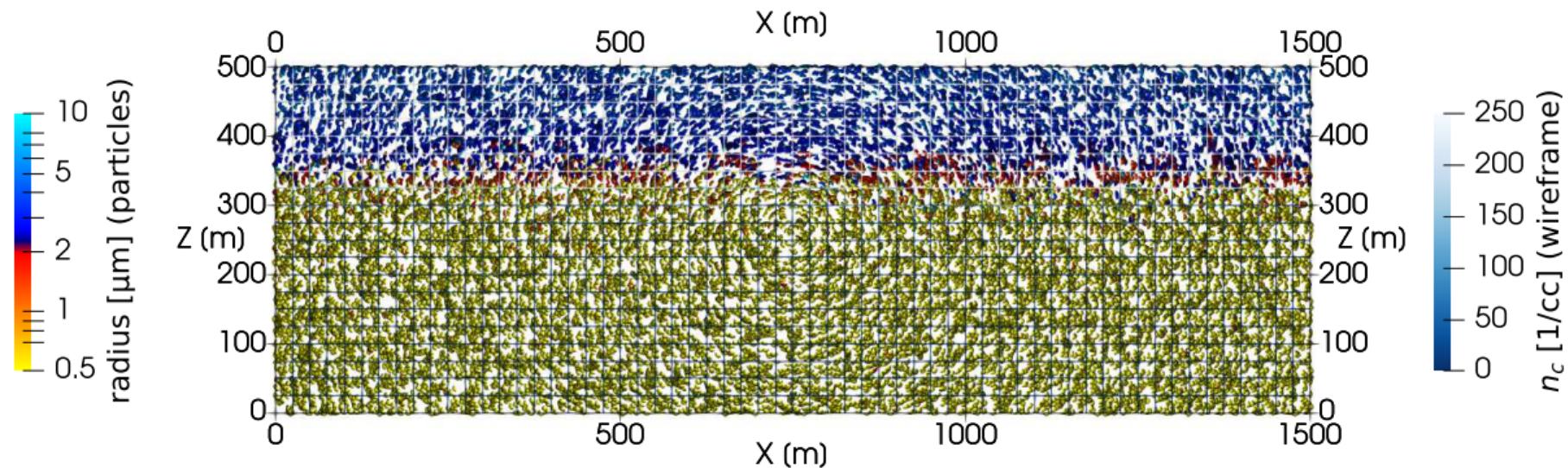
Time: 90 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

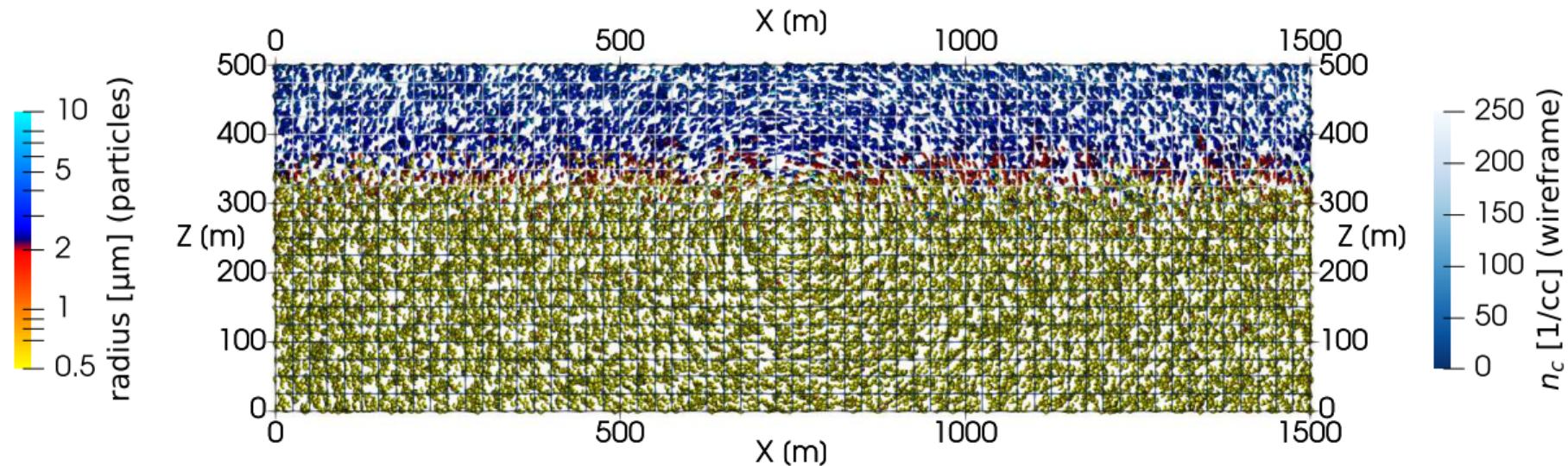
Time: 120 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

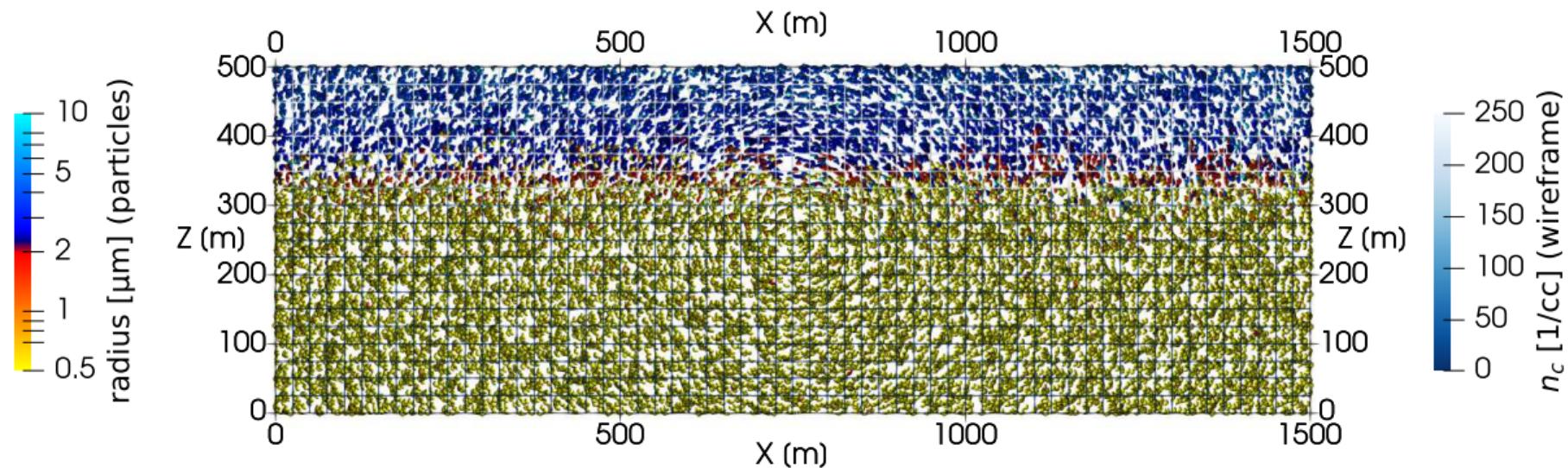
Time: 150 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

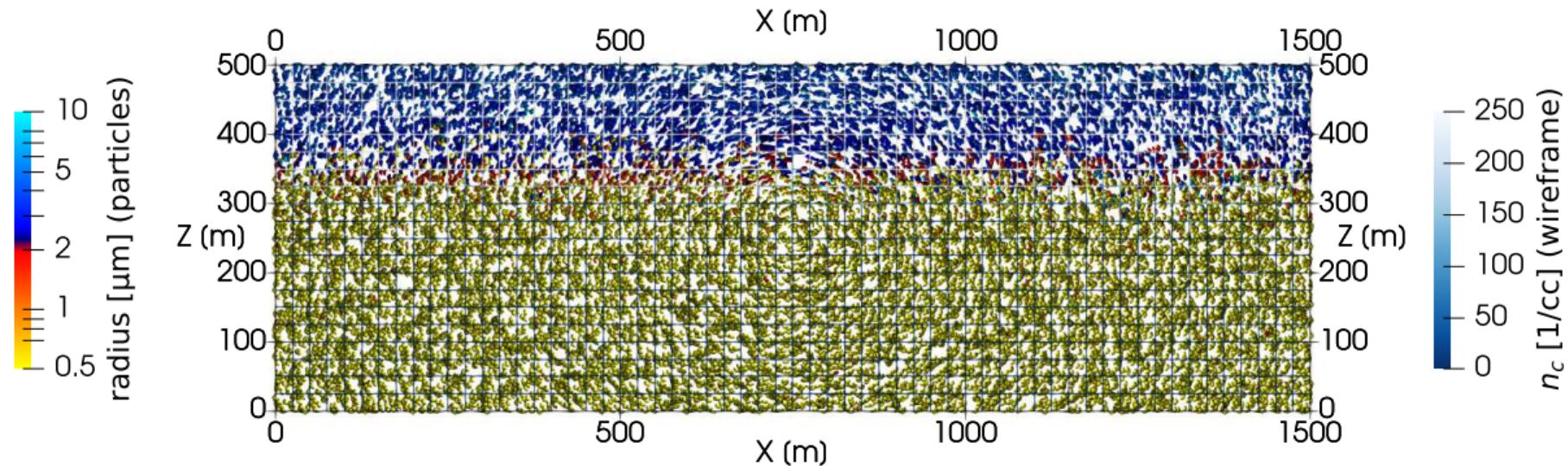
Time: 180 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

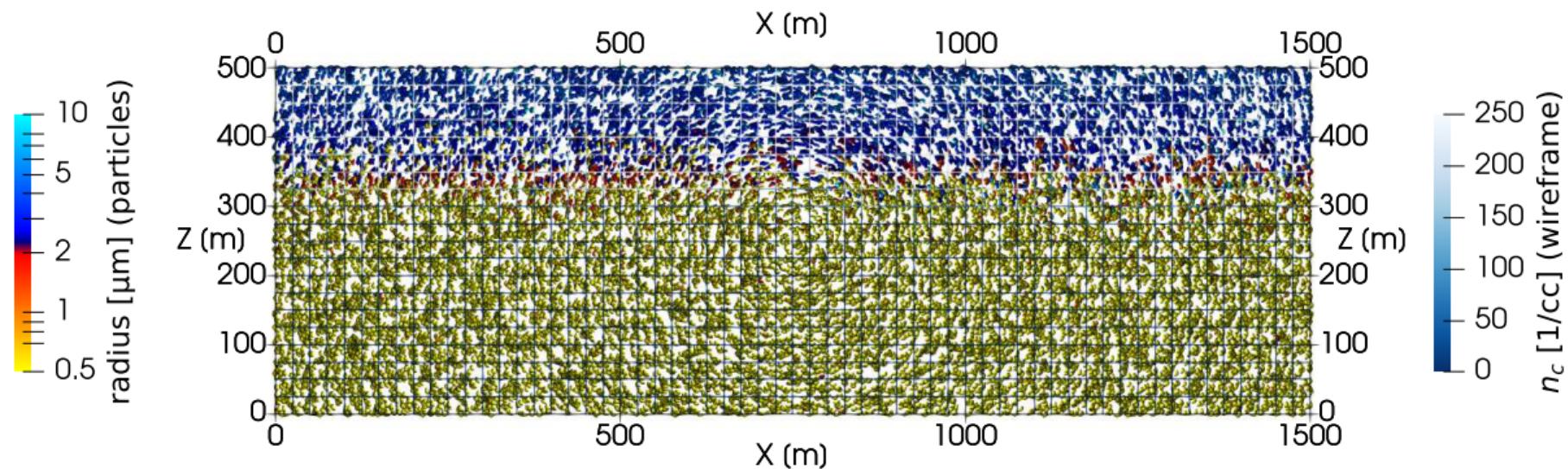
Time: 210 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

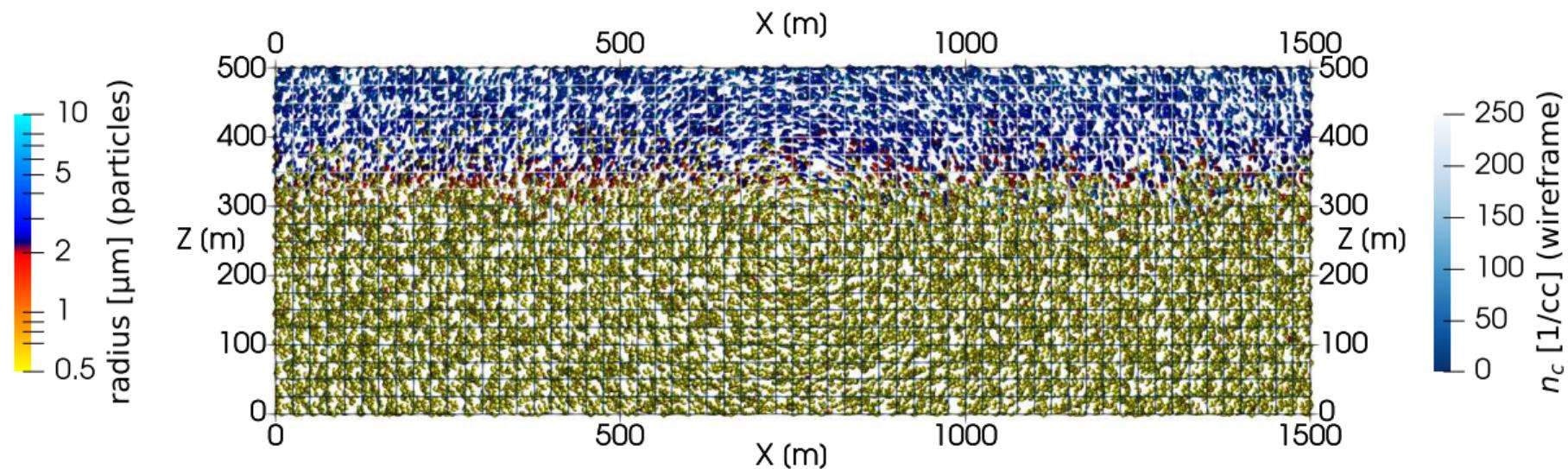
Time: 240 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

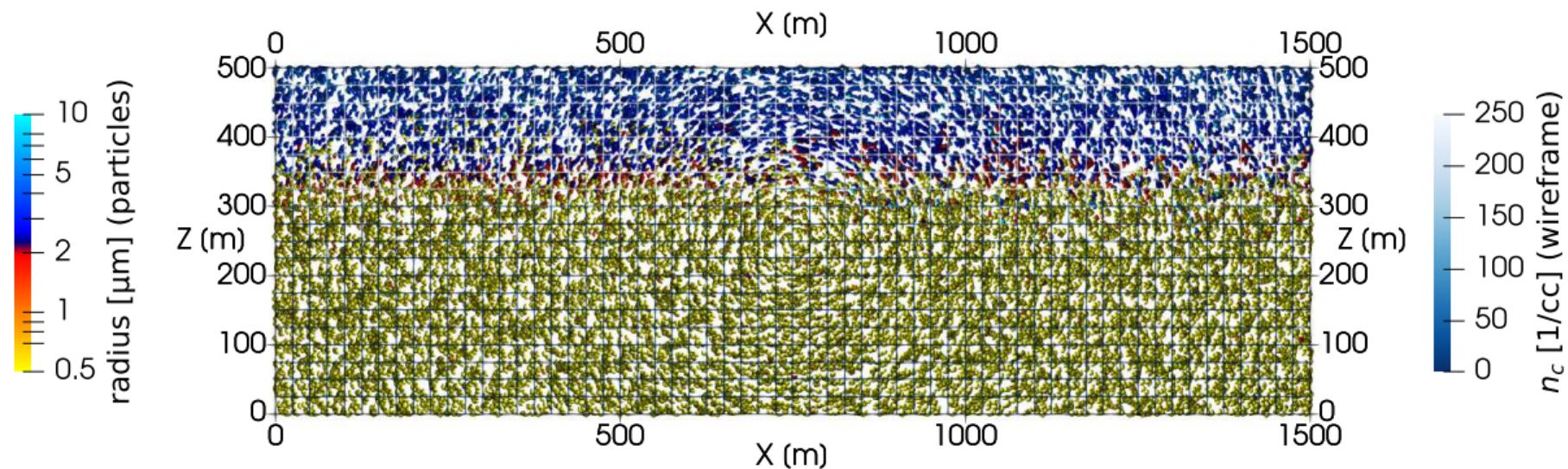
Time: 270 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

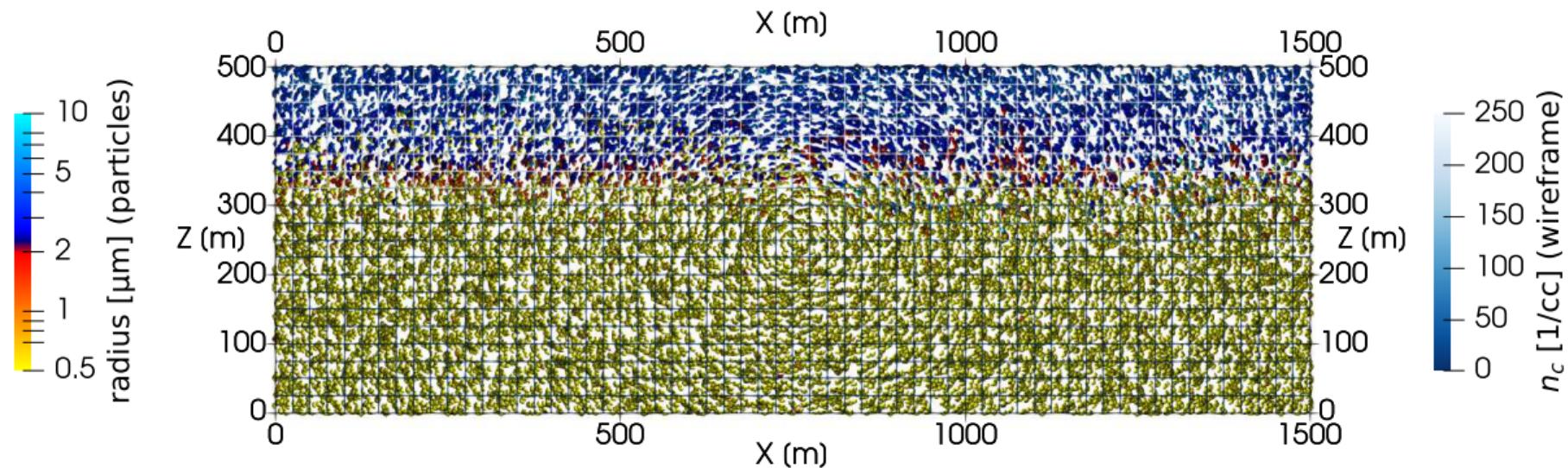
Time: 300 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

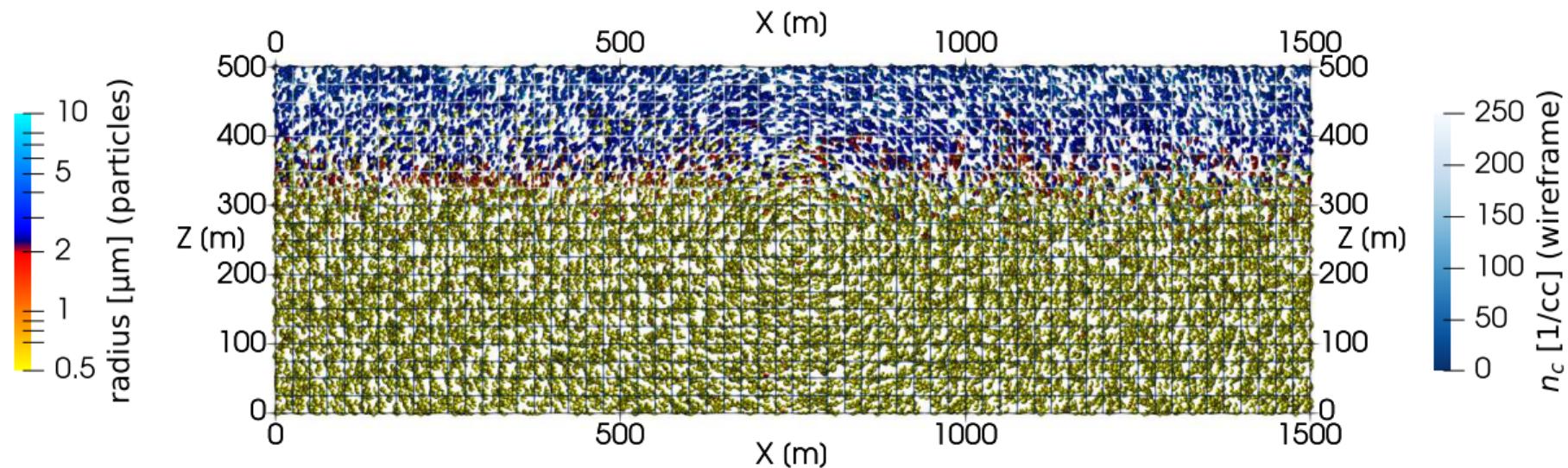
Time: 330 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

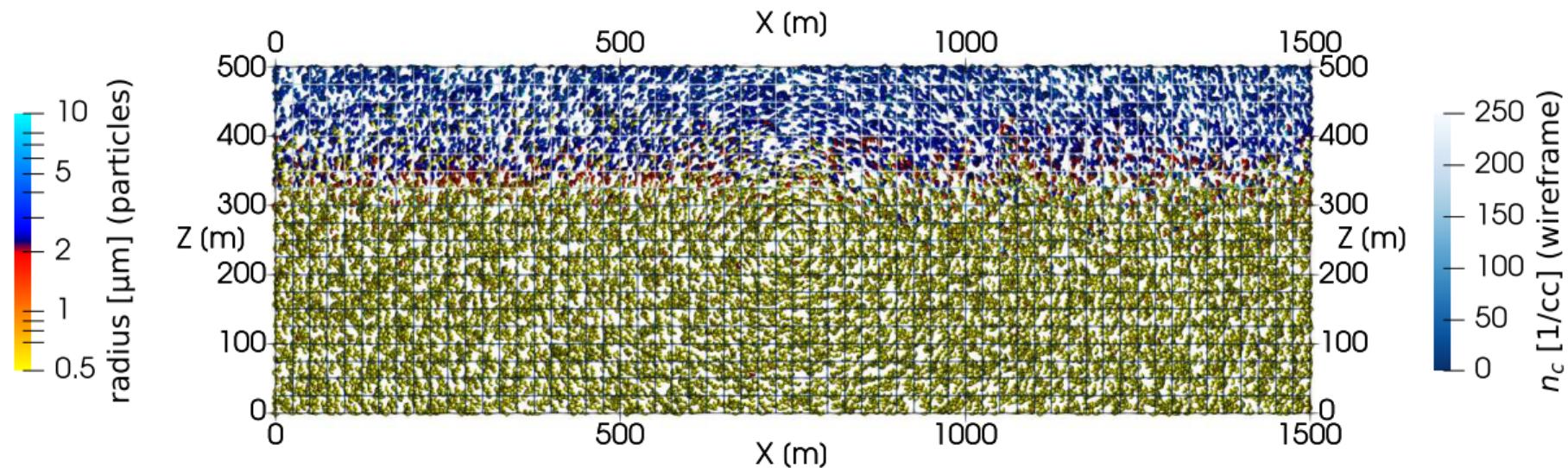
Time: 360 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

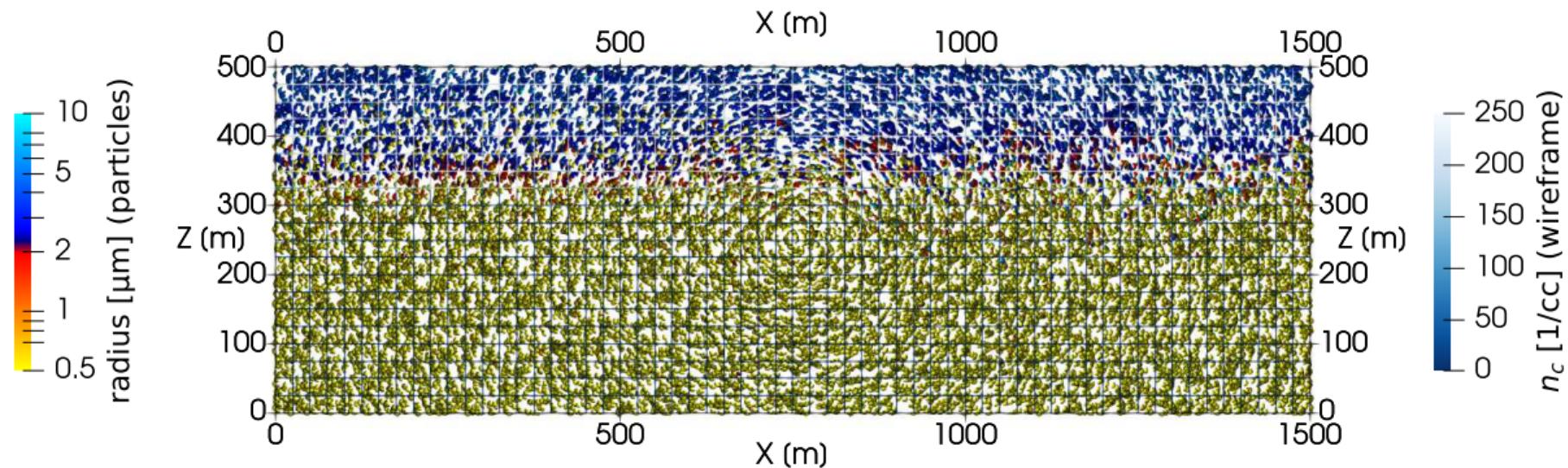
Time: 390 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

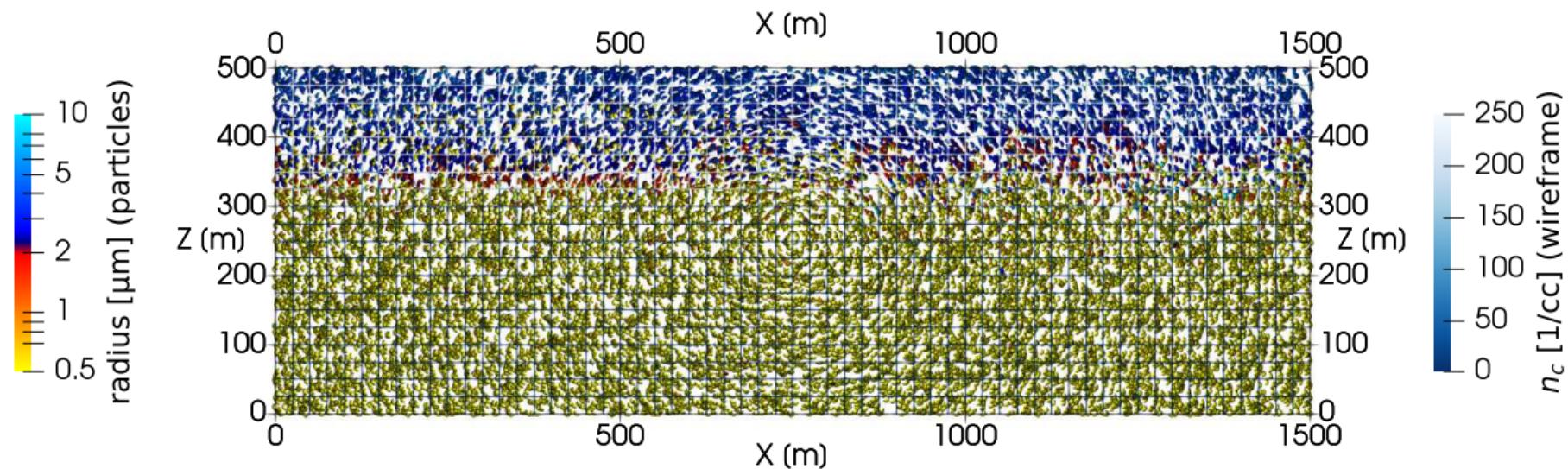
Time: 420 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

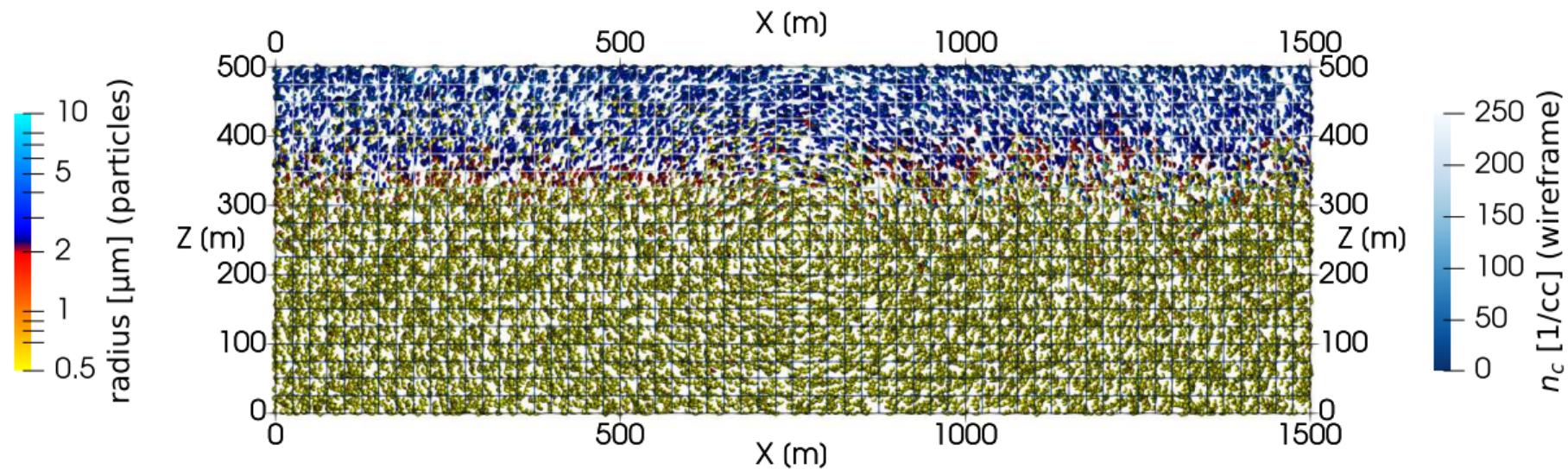
Time: 450 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

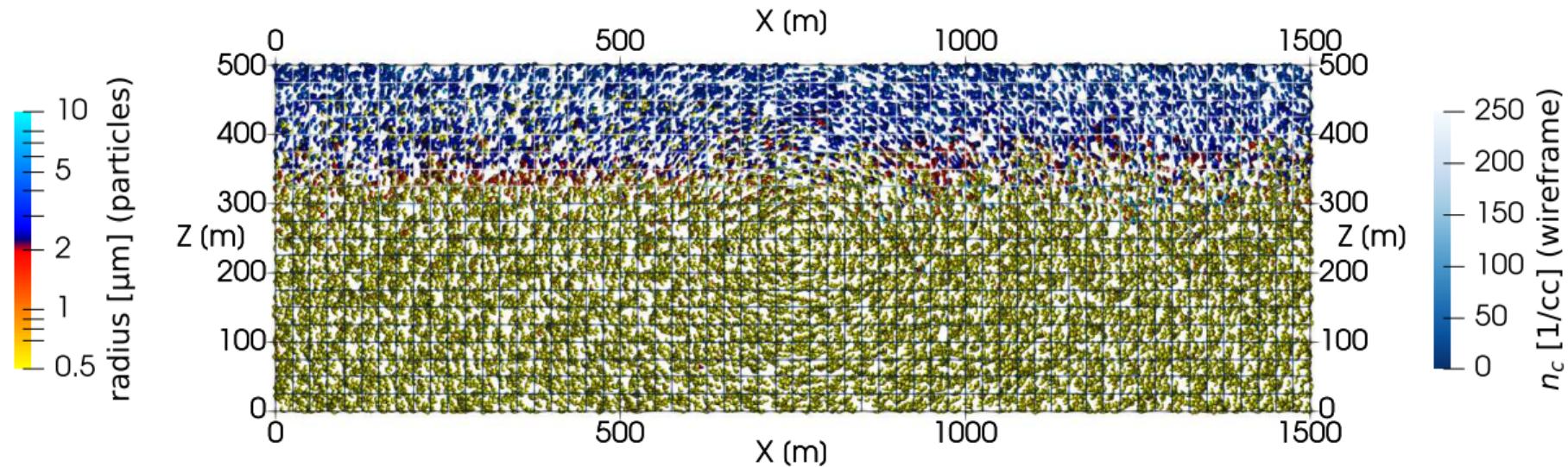
Time: 480 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

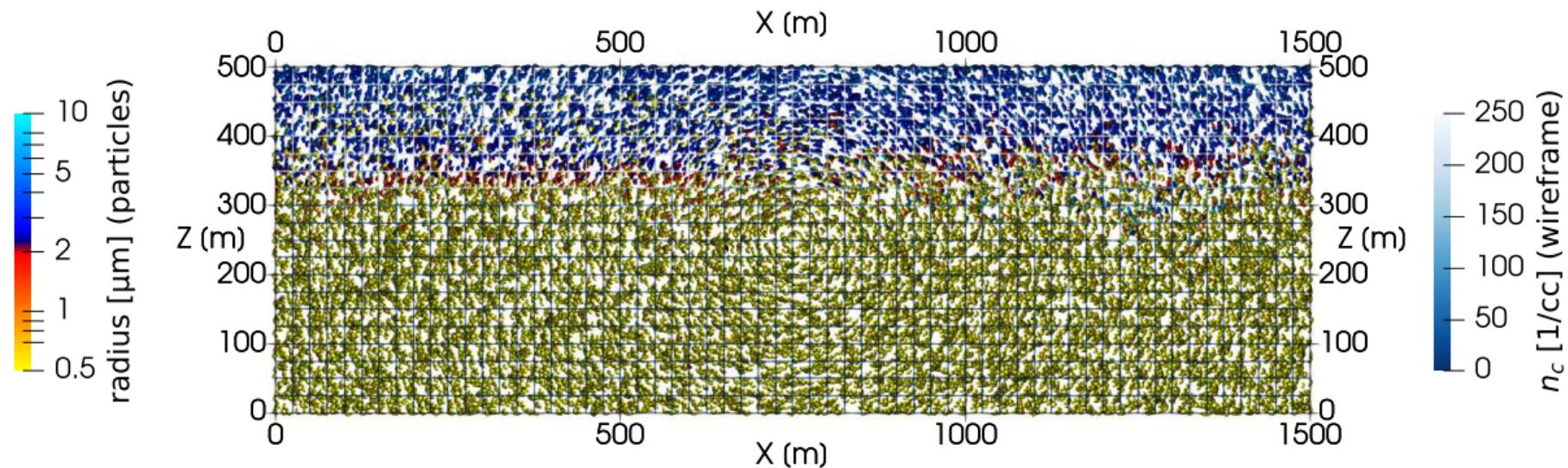
Time: 510 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

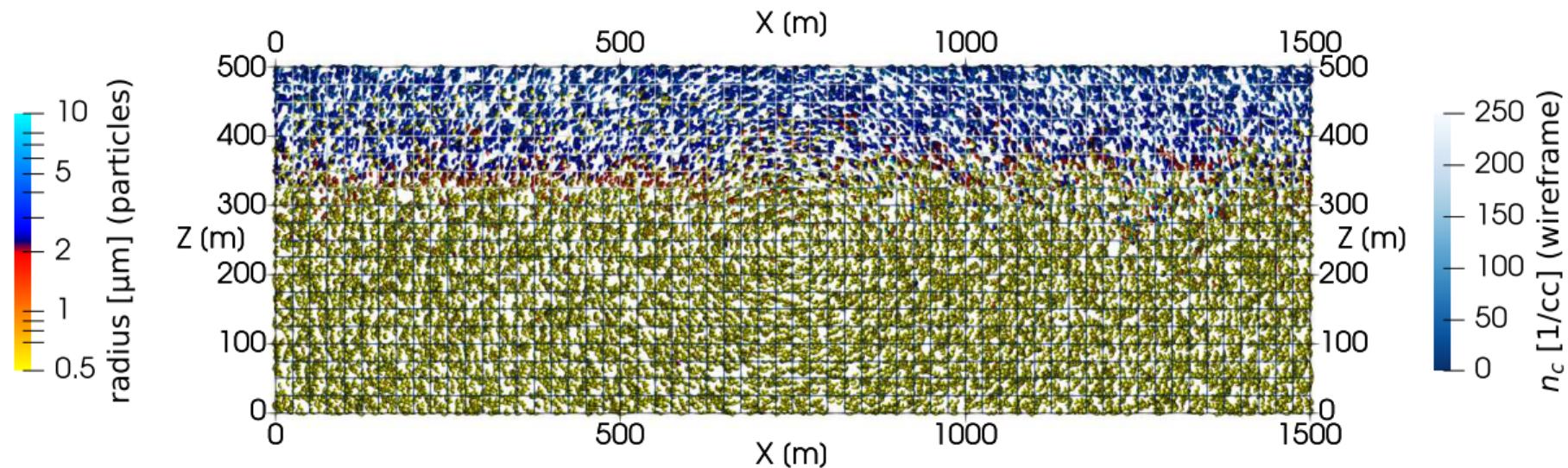
Time: 540 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

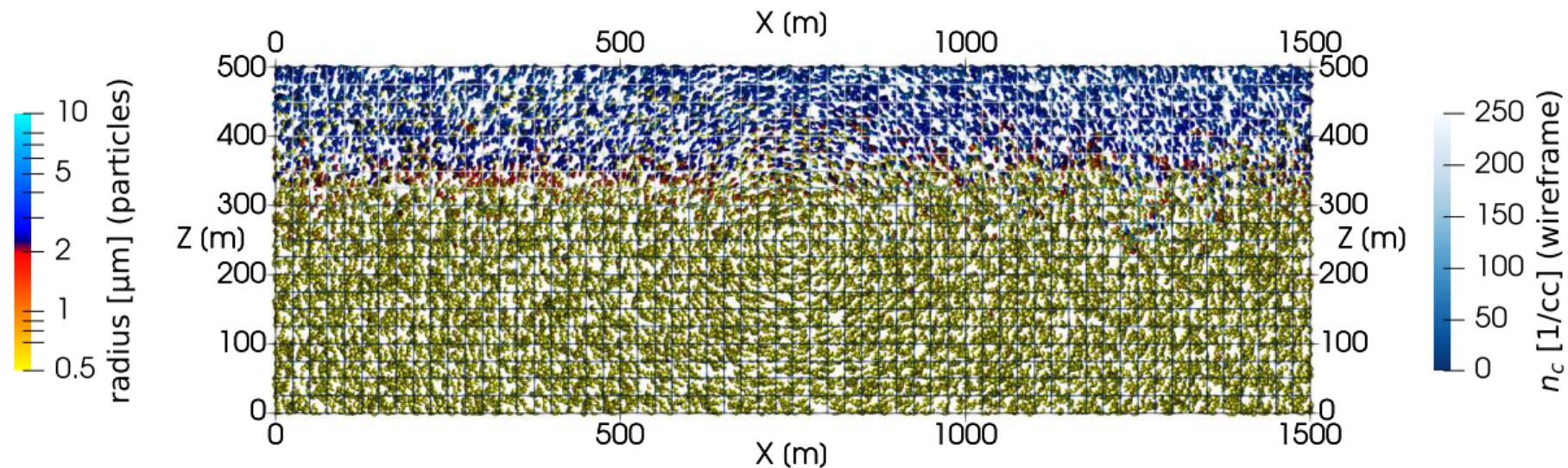
Time: 570 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

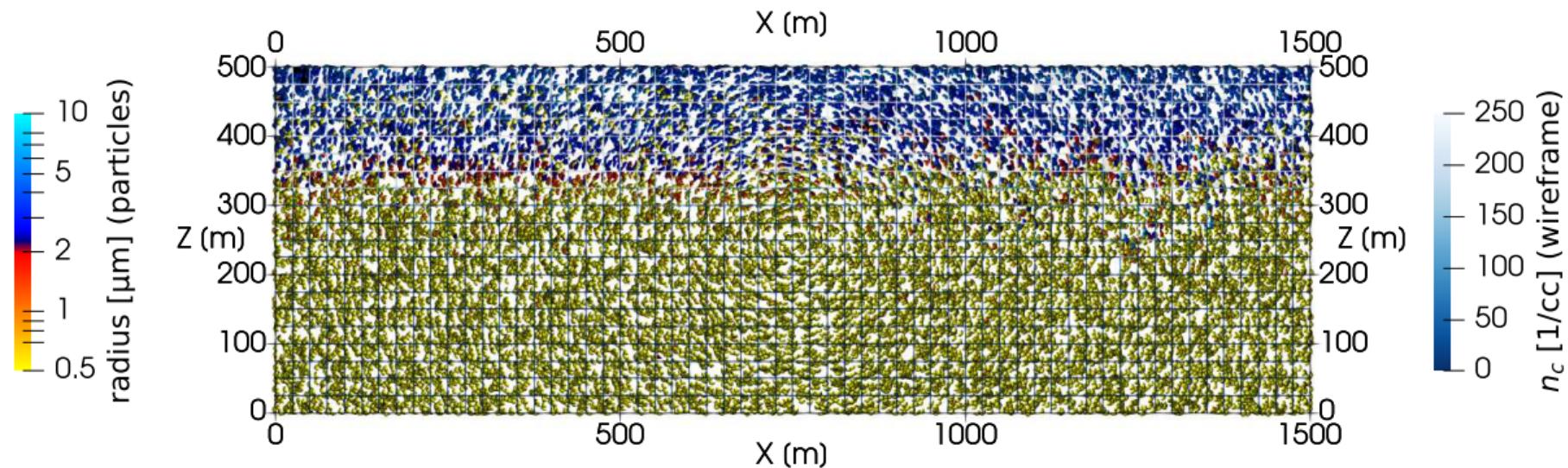
Time: 600 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

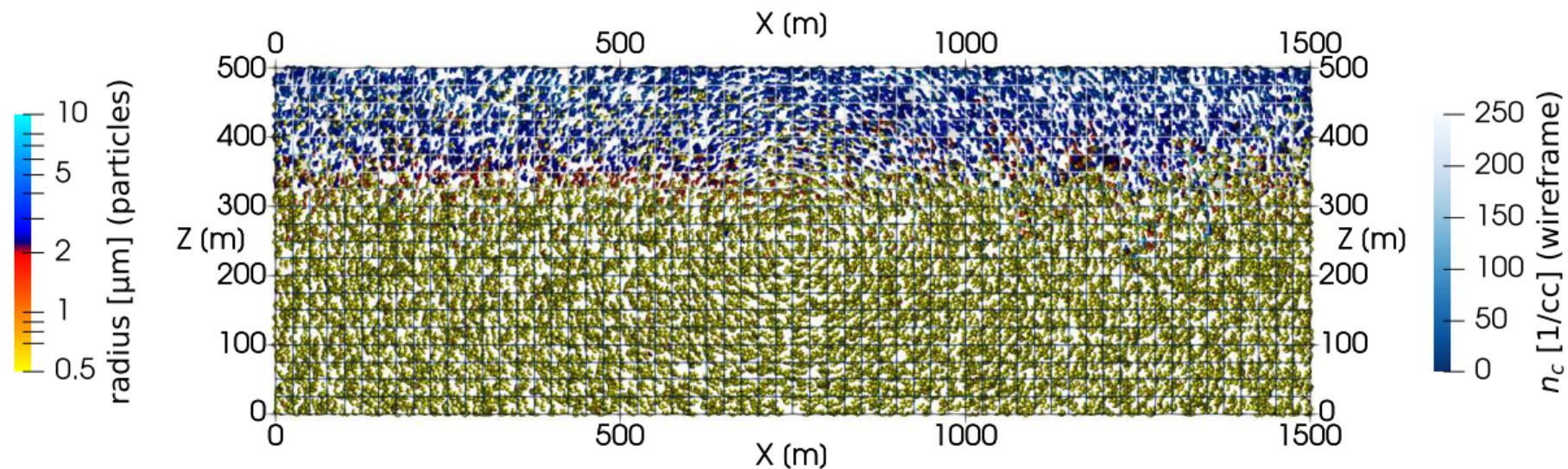
Time: 630 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

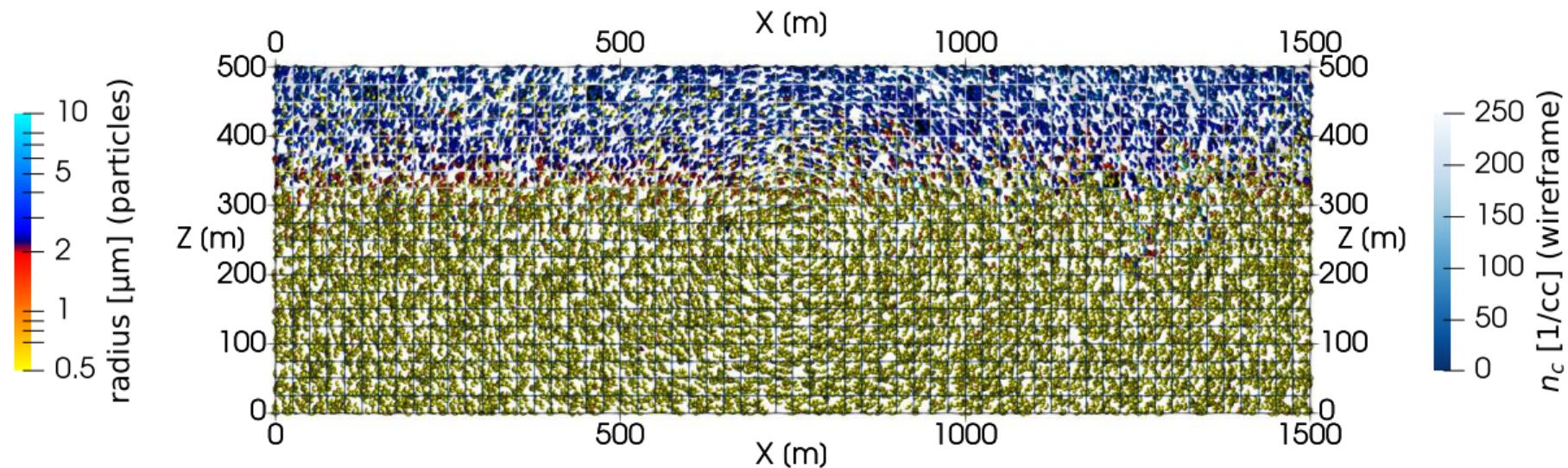
Time: 660 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

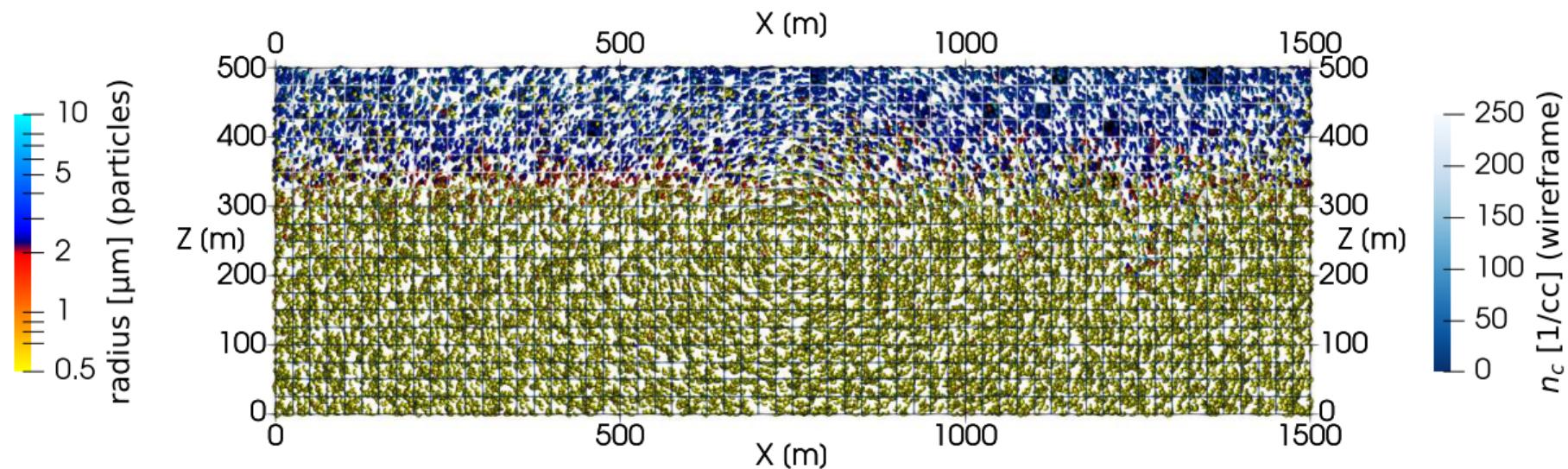
Time: 690 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

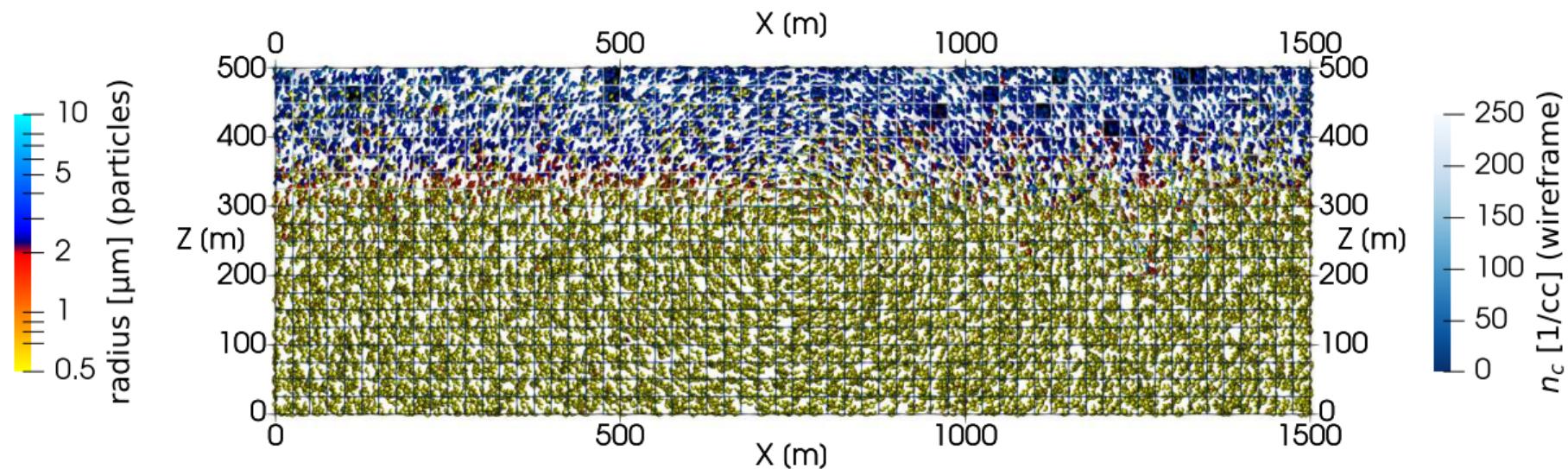
Time: 720 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

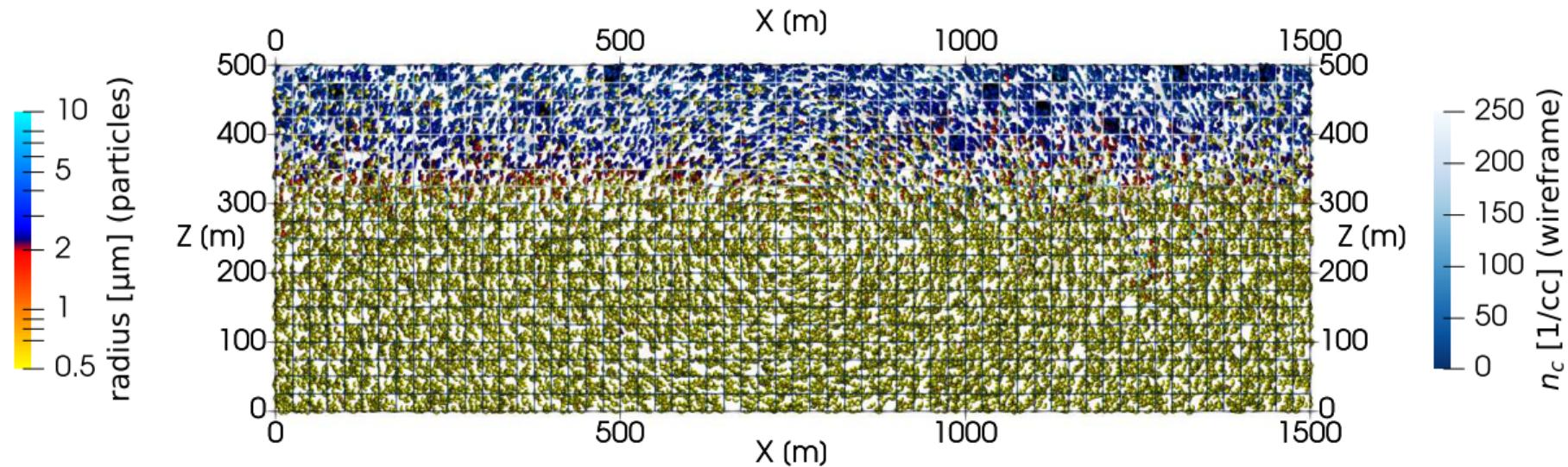
Time: 750 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

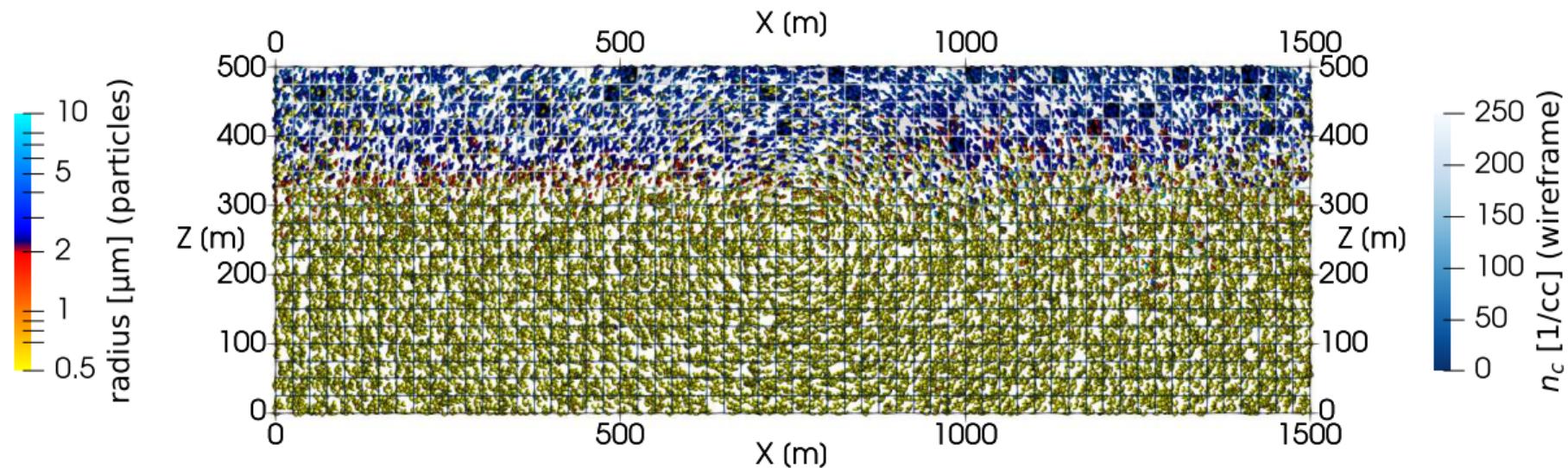
Time: 780 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

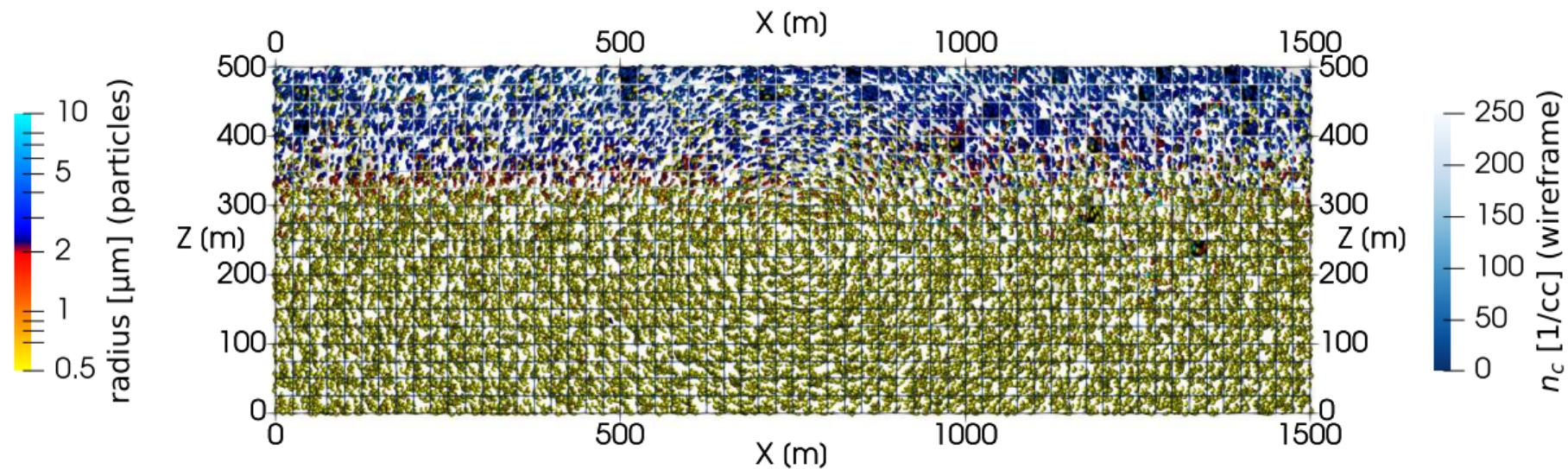
Time: 810 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

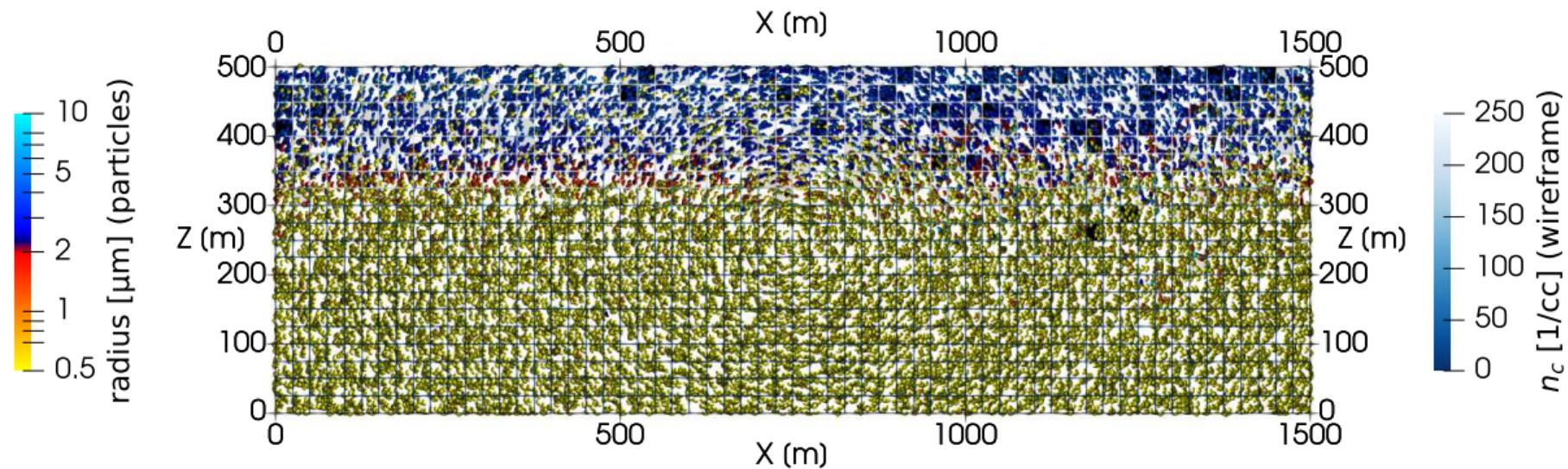
Time: 840 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

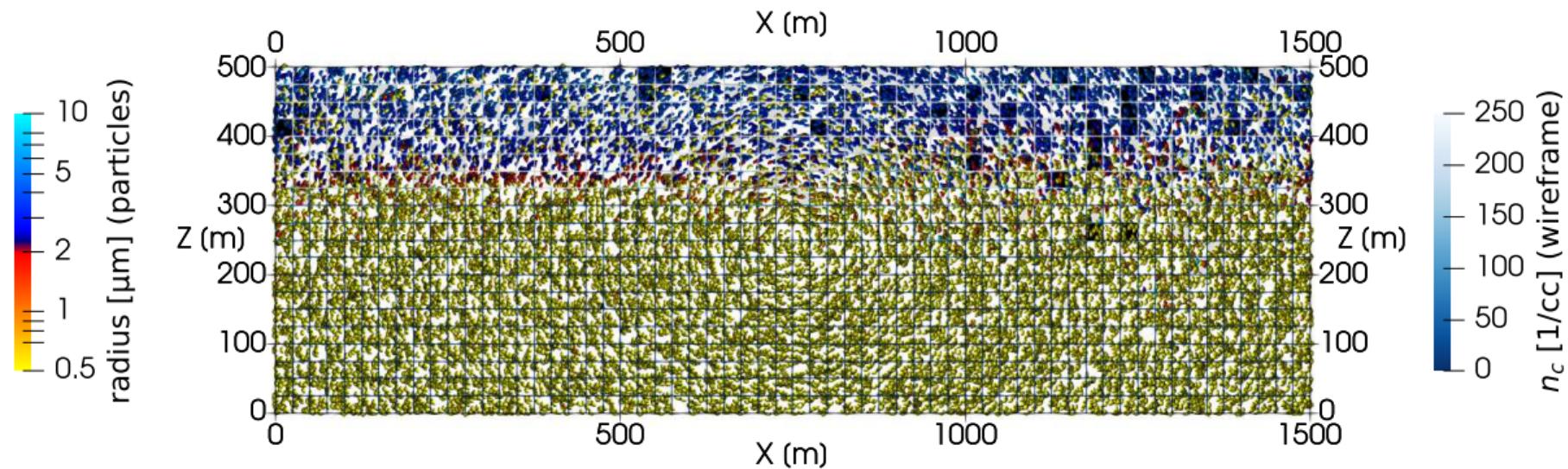
Time: 870 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

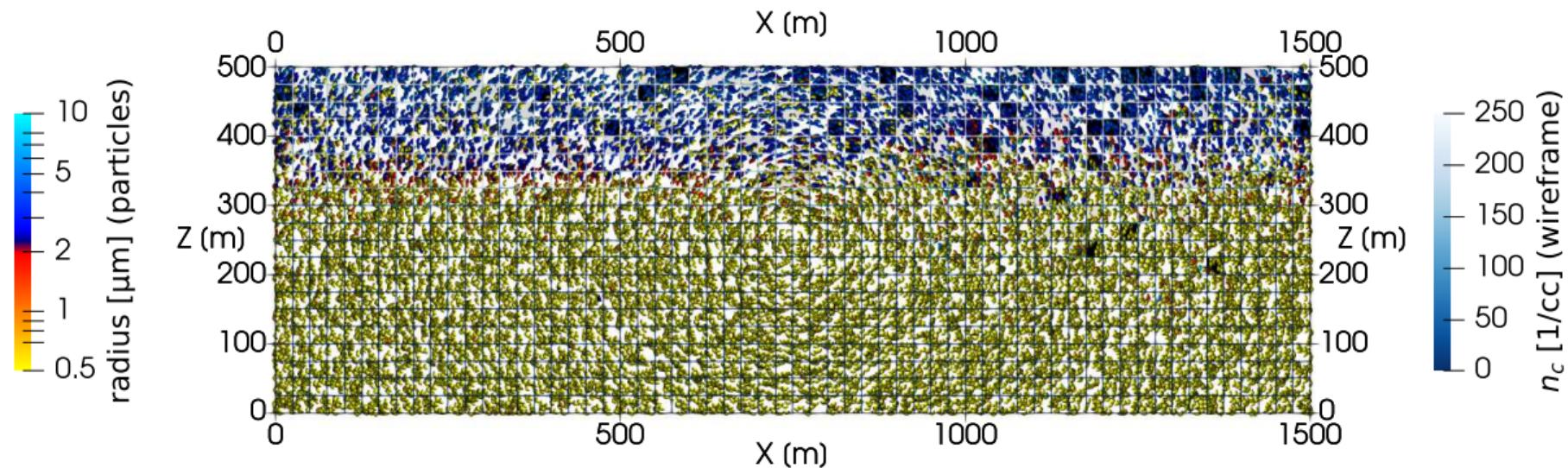
Time: 900 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

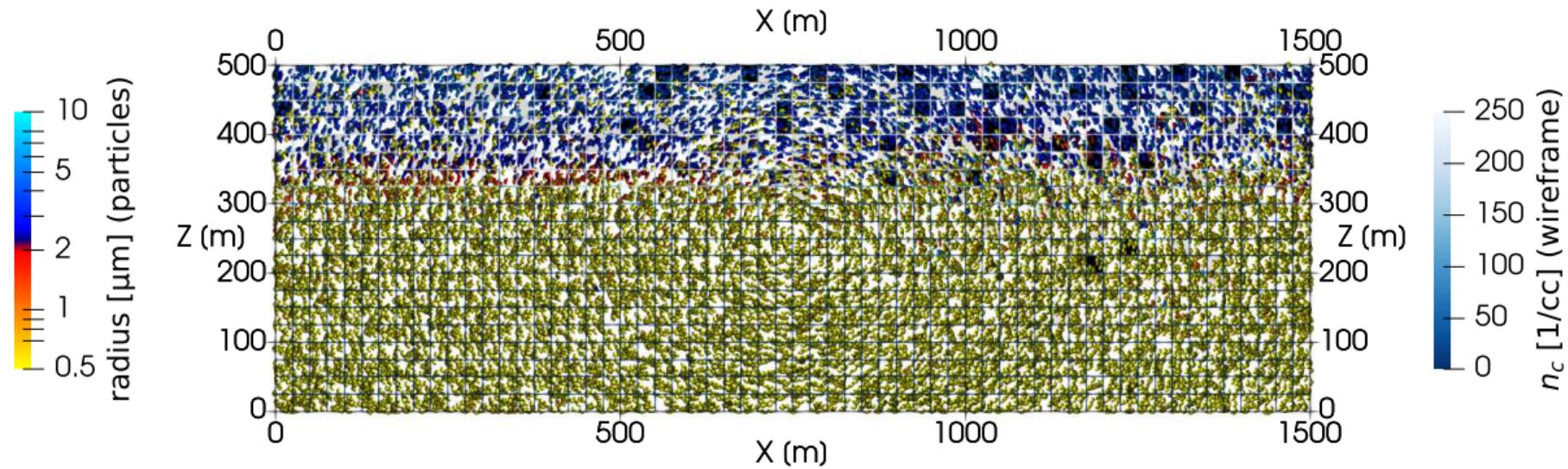
Time: 930 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

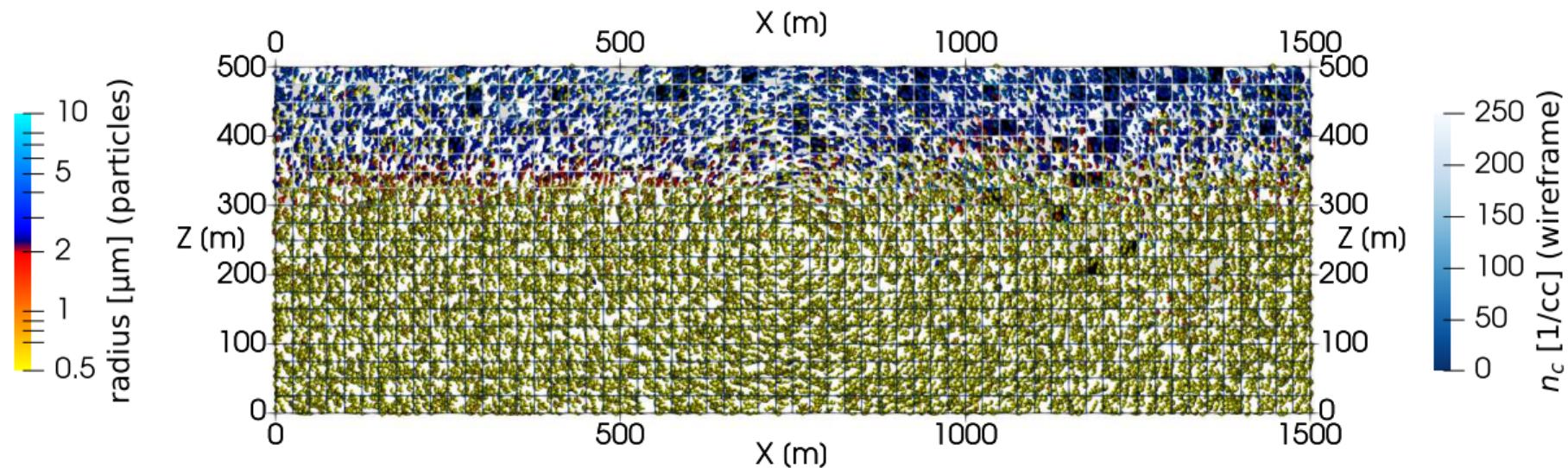
Time: 960 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

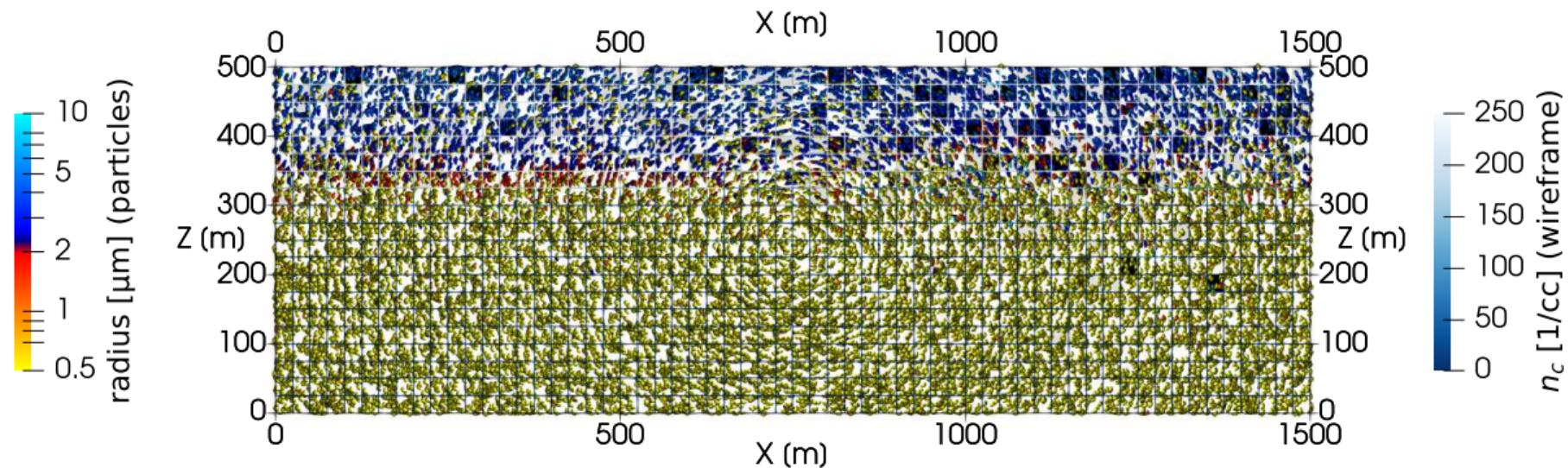
Time: 990 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

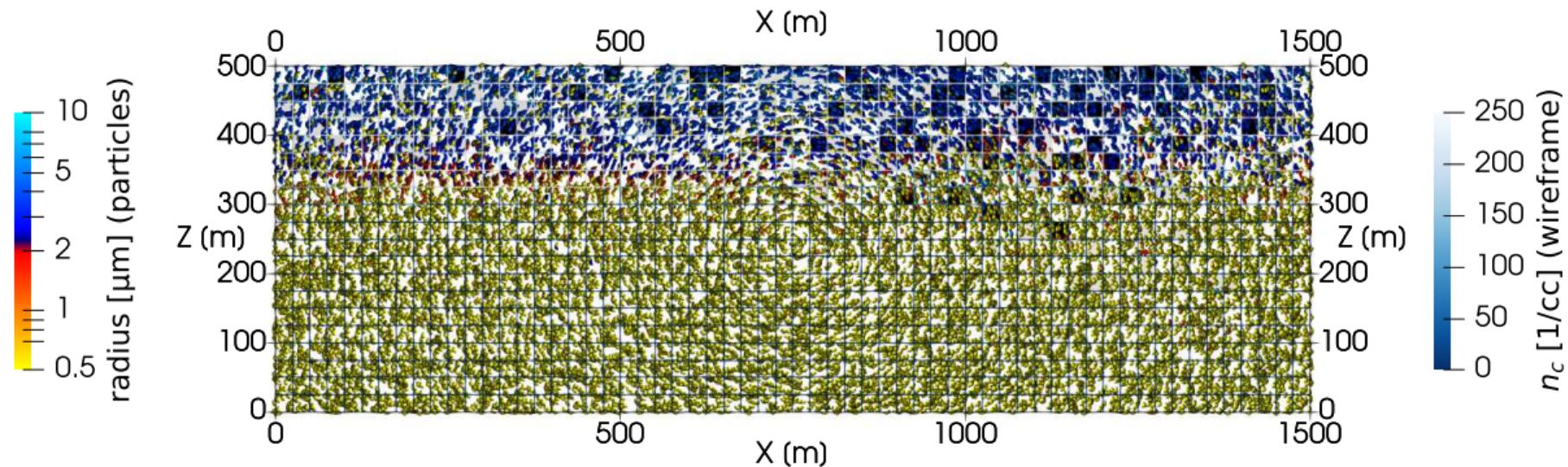
Time: 1020 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

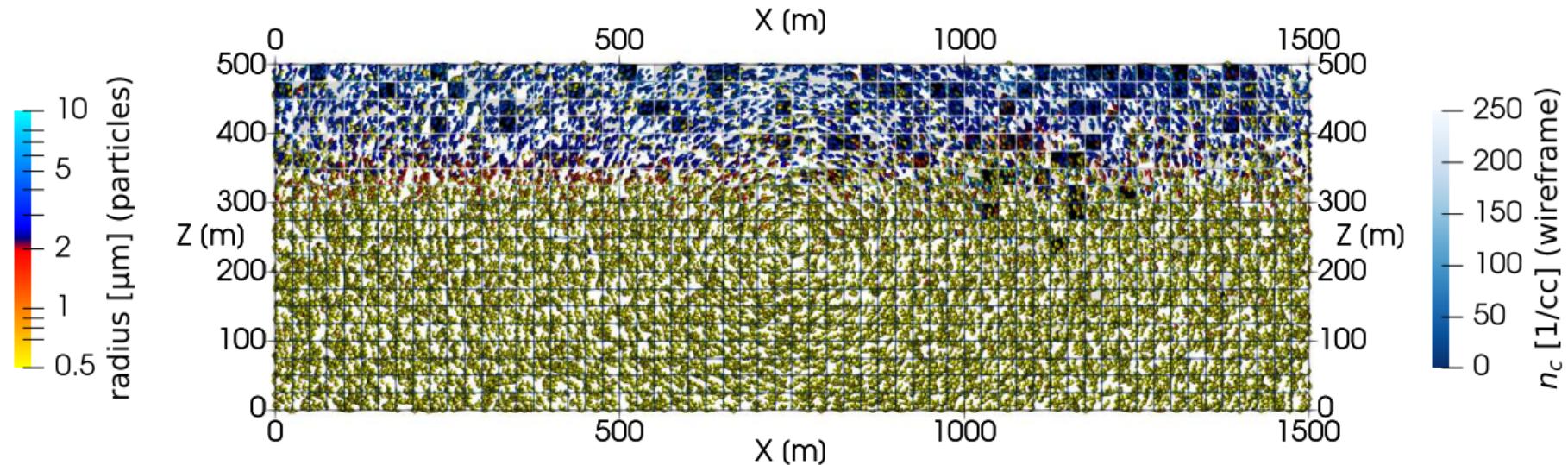
Time: 1050 s (spin-up till 600.0 s)



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

## particle-based $\mu$ -physics + prescribed-flow test

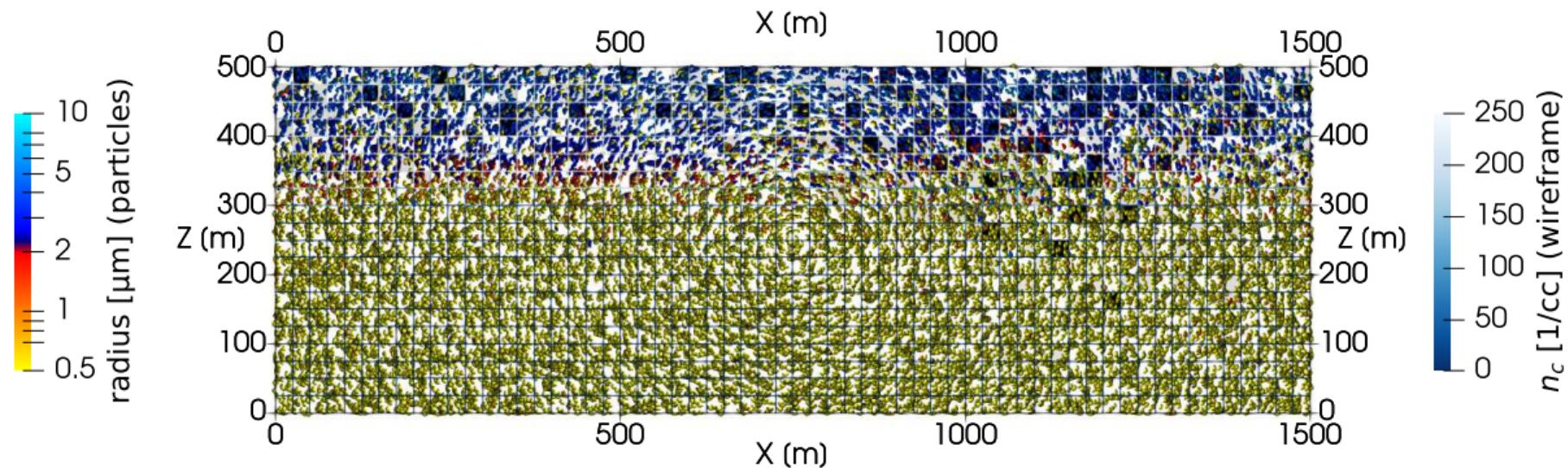
Time: 1080 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

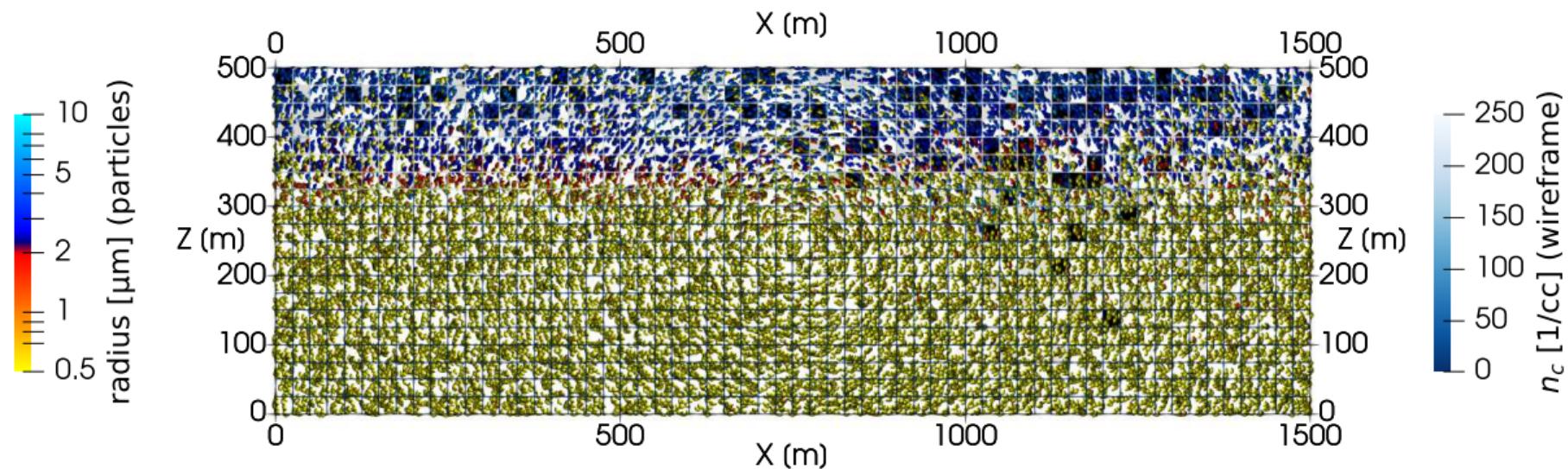
Time: 1110 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

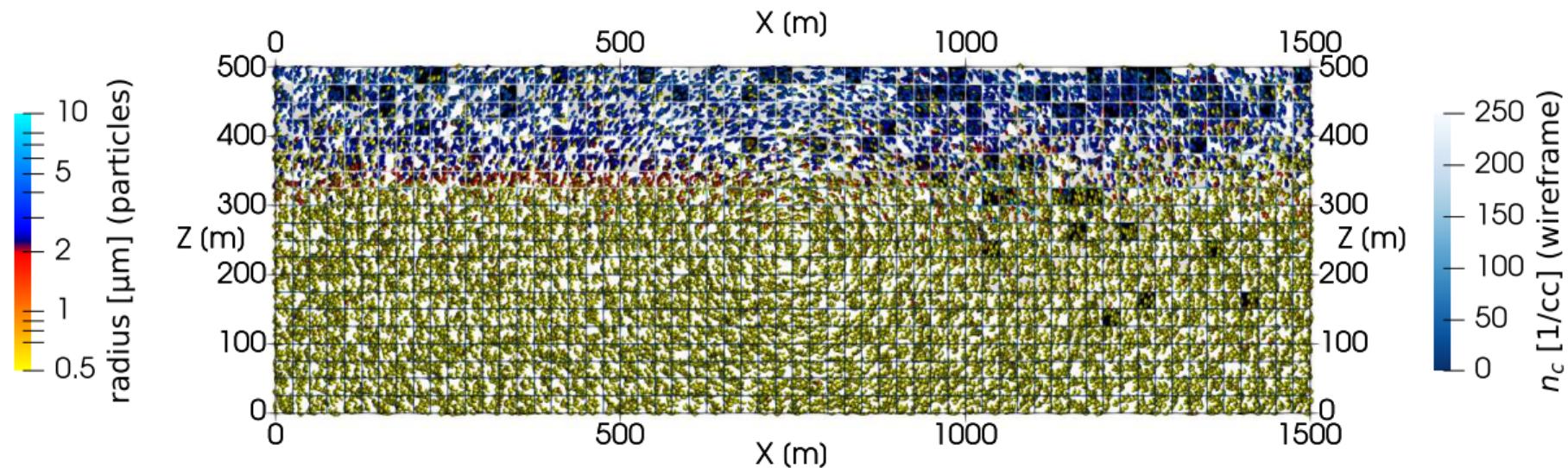
Time: 1140 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

## particle-based $\mu$ -physics + prescribed-flow test

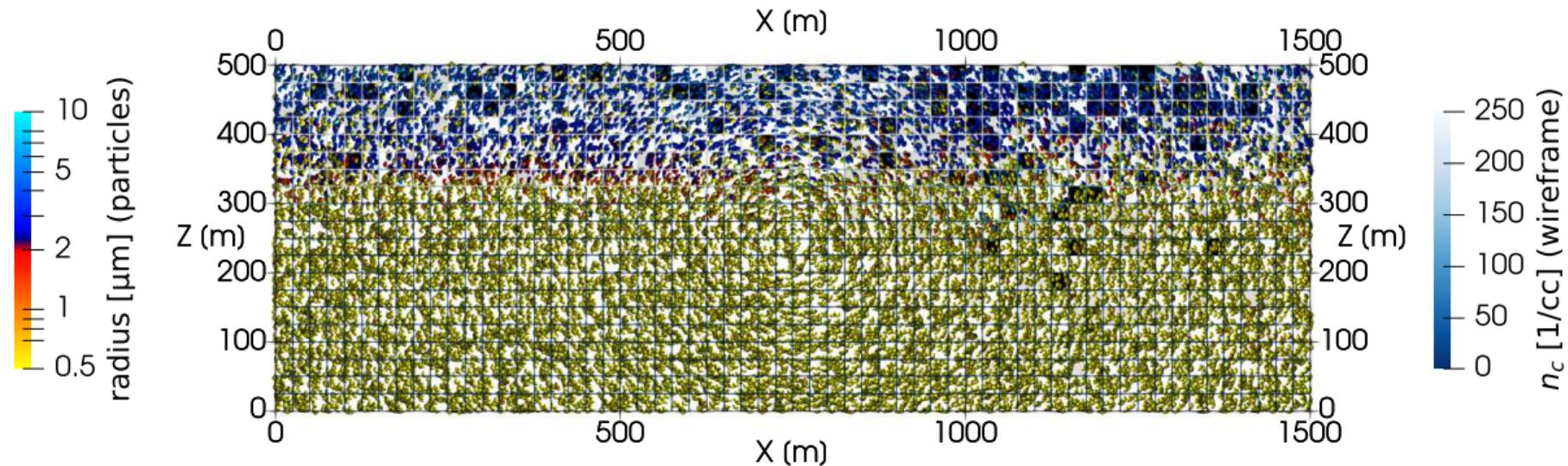
Time: 1170 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

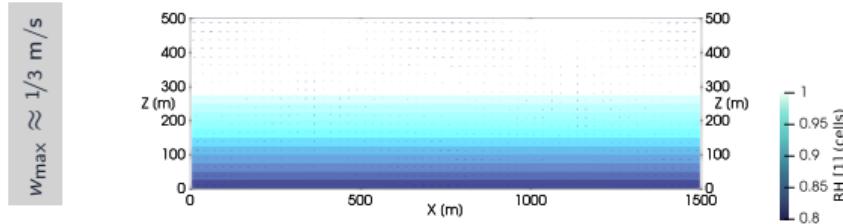
## particle-based $\mu$ -physics + prescribed-flow test

Time: 1200 s (spin-up till 600.0 s)



16+16 super-particles/cell for INP-rich + INP-free particles  
 $N_{\text{aer}} = 300/\text{cc}$  (two-mode lognormal)     $N_{\text{INP}} = 150/L$  (lognormal,  $D_g = 0.74 \mu\text{m}$ ,  $\sigma_g = 2.55$ )

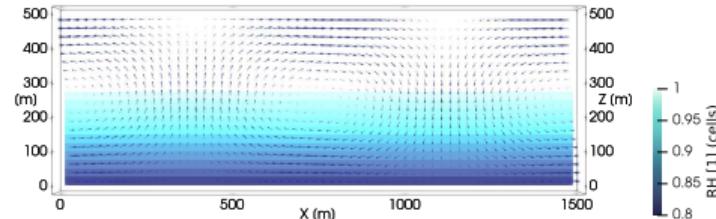
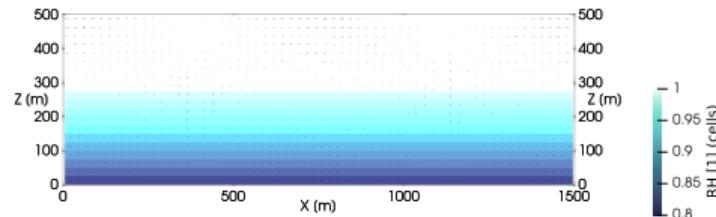
testing three flow regimes and two immersion freezing representations



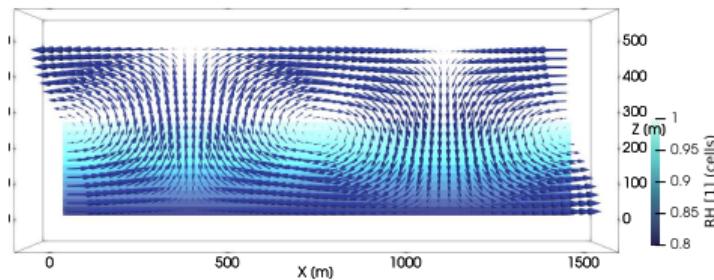
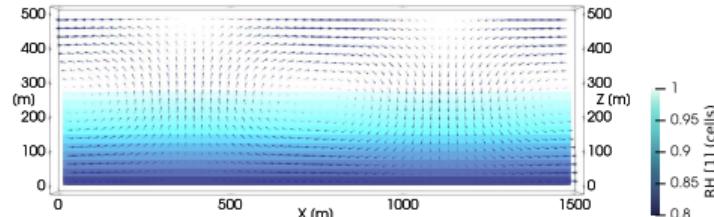
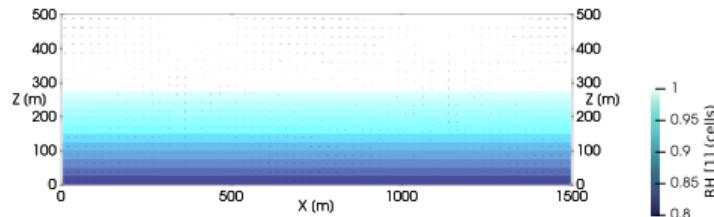
$$w_{\max} \approx 3 \text{ m/s}$$

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

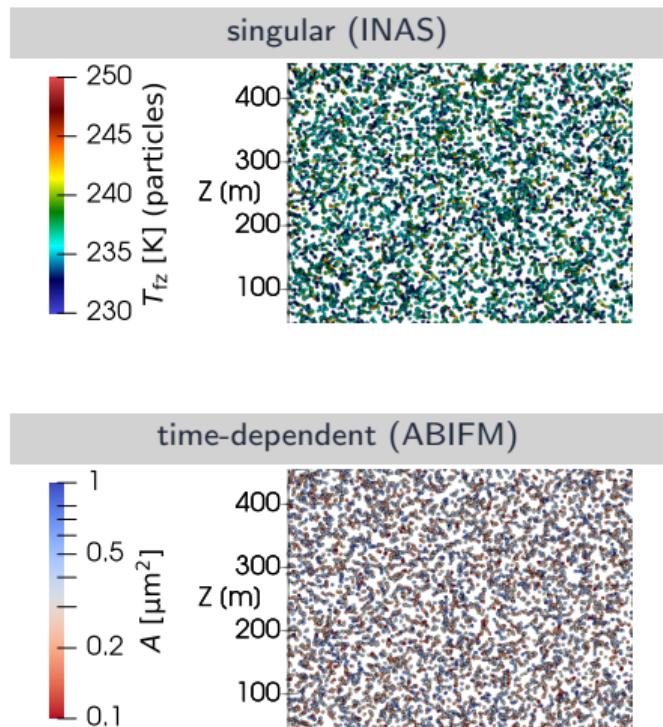
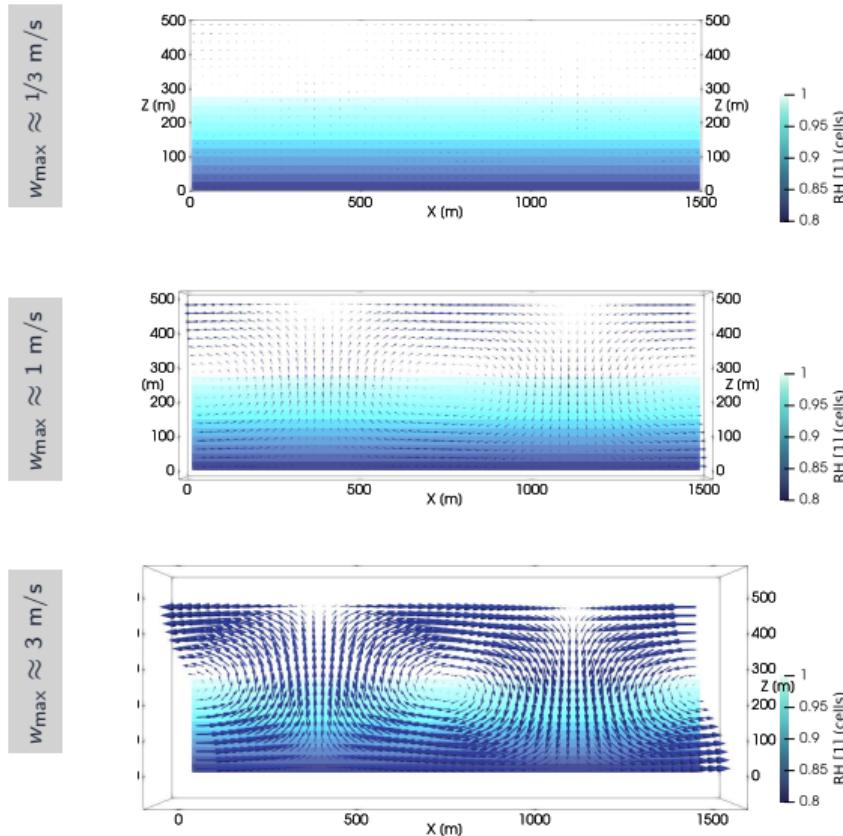
testing three flow regimes and two immersion freezing representations



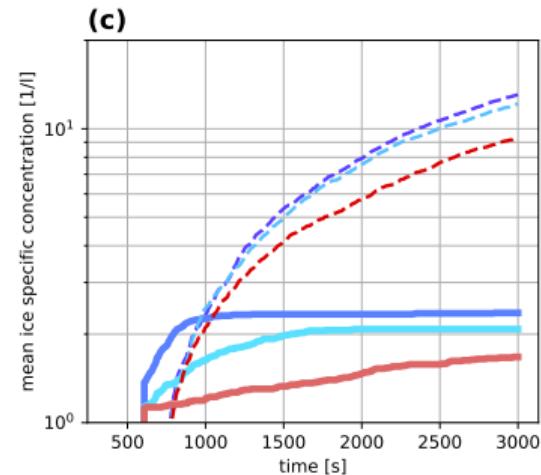
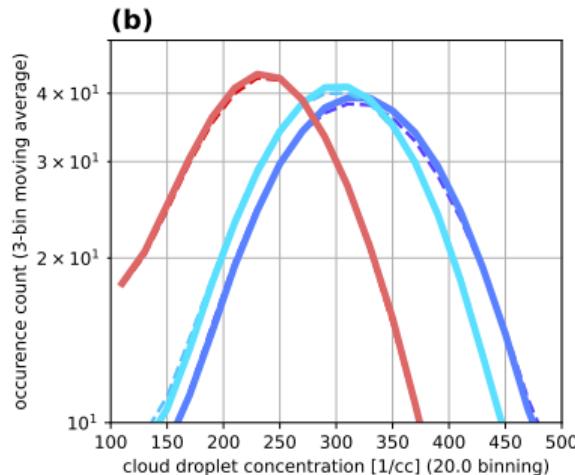
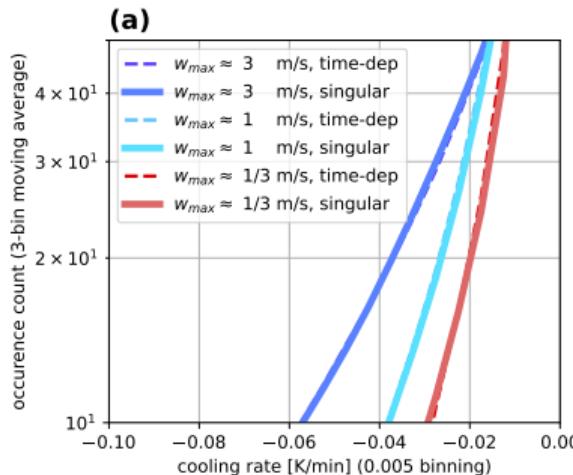
testing three flow regimes and two immersion freezing representations



testing three flow regimes and two immersion freezing representations

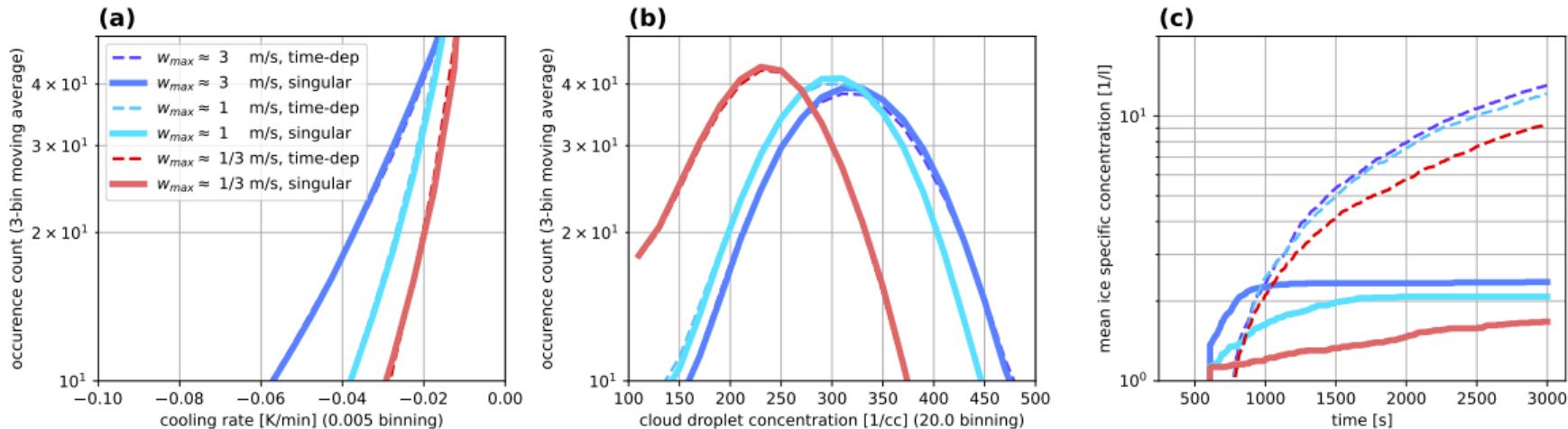


testing three flow regimes and two immersion freezing representations



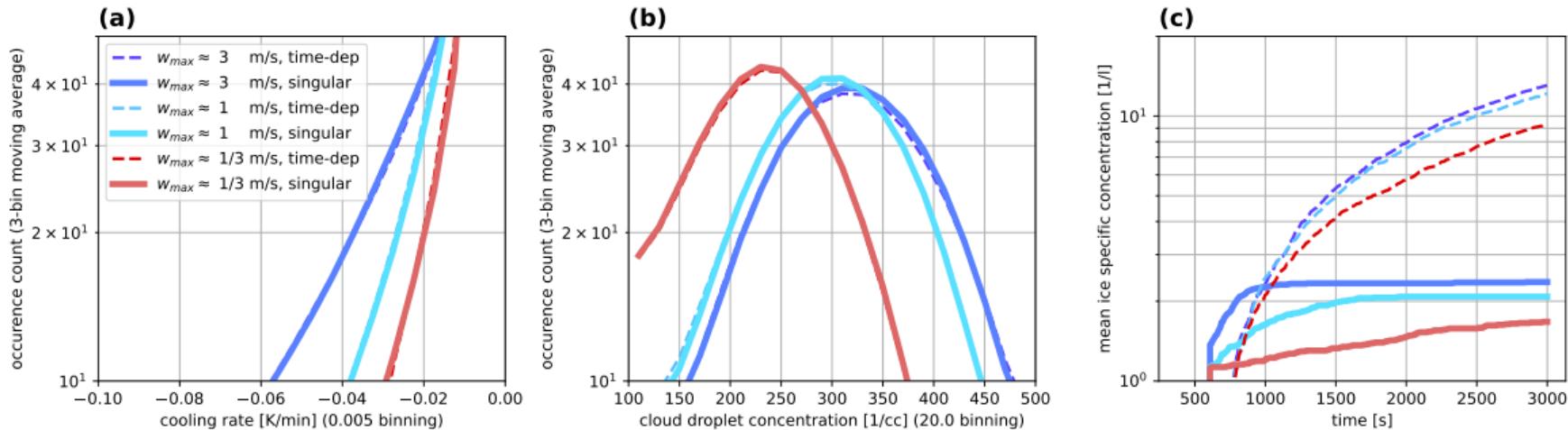
- range of cooling rates in simple flow (far from  $c \sim 1$  K/min for AIDA as in Niemand et al. 2012)

testing three flow regimes and two immersion freezing representations



- range of cooling rates in simple flow (far from  $c \sim 1 \text{ K/min}$  for AIDA as in Niemand et al. 2012)
  - singular vs. time-dependent markedly different (consistent with box model for  $c \ll 1 \text{ K/min}$ )

testing three flow regimes and two immersion freezing representations



- ▶ range of cooling rates in simple flow (far from  $c \sim 1$  K/min for AIDA as in Niemand et al. 2012)
  - ▶ singular vs. time-dependent markedly different (consistent with box model for  $c \ll 1$  K/min)
  - ▶ CPU time trade off: time dependent ca. 3-4 times costlier

- 
- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models  
(Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
  - ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models  
(Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ this study: **ABIFM-based time-dependent particle-based immersion freezing**

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ this study: **ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ this study: **ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir
- ▶ next steps: leverage particle-resolved representation to simulate diverse INP populations

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ **this study: ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir
- ▶ next steps: leverage particle-resolved representation to simulate diverse INP populations



- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ **this study: ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir
- ▶ next steps: leverage particle-resolved representation to simulate diverse INP populations



DOE ASR grant no.  
DE-SC0021034

project hosted at:  
**ILLINOIS**

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ **this study: ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir
- ▶ next steps: leverage particle-resolved representation to simulate diverse INP populations



DOE ASR grant no.  
DE-SC0021034

project hosted at:  
**ILLINOIS**

open python™ code:  
`@atmos-cloud-sim-uj`

- ▶ emergence of comprehensive mixed-phase particle-based aerosol/cloud/precip  $\mu$ -physics models (Shima et al.; McSnow by Brdar, Siewert, Seifert et al.; Sölch, Kärcher, Unterstrasser et al. @DLR)
- ▶ probabilistic particle-based methods apt for stochastic processes: nucleation, collisions, breakup,...
- ▶ **this study: ABIFM-based time-dependent particle-based immersion freezing**
  - ▶ box examples: role of INP size spectral width (same for time-dependent and singular)
  - ▶ box & 2D: cooling rate hardcoded in INAS fits  $\rightsquigarrow$  limited robustness to different flow regimes
  - ▶ particle-based schemes (both singular and time-dependent) resolve INP reservoir
- ▶ next steps: leverage particle-resolved representation to simulate diverse INP populations



DOE ASR grant no.  
DE-SC0021034

project hosted at:  
**ILLINOIS**

open  python™ code:  
o/atmos-cloud-sim-uj

 Thank you  
for your attention!