/ OPENATMOS / PySDM

PySDM v3.0 (soon to be released):

summary of features, recent developments and perspectives

Sylwester Arabas (agh.edu.pl) & **PySDM contributors**

AGH EXCELLENCE INITIATIVE RESEARCH UNIVERSITY

CliMA group meeting, Caltech, Pasadena, Sep 9th 2025

particle-based μ-physics

aerosol-cloud-precipitation interactions: scales

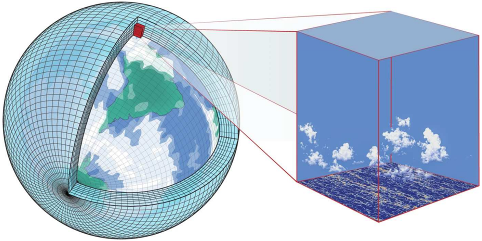
"Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain"

(photo: Yevgen Timashov / National Geographic)

aerosol-cloud-precipitation interactions: scales

“Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain”

(photo: Yevgen Timashov / National Geographic)



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

(fig. from Schneider et al. 2017)

aerosol-cloud-precipitation interactions: μ-physics models

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[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]

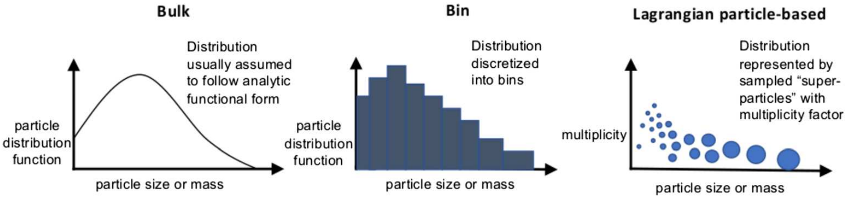
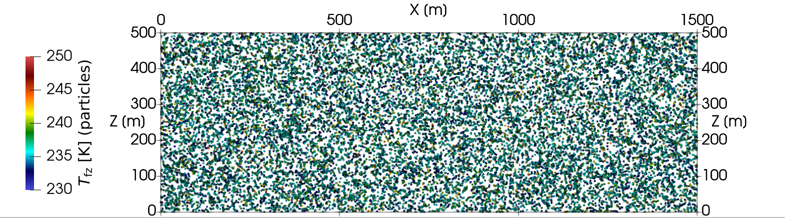


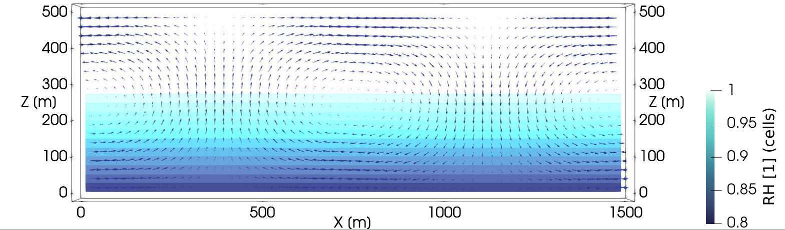
Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

particle-based μ-physics simulation: model state

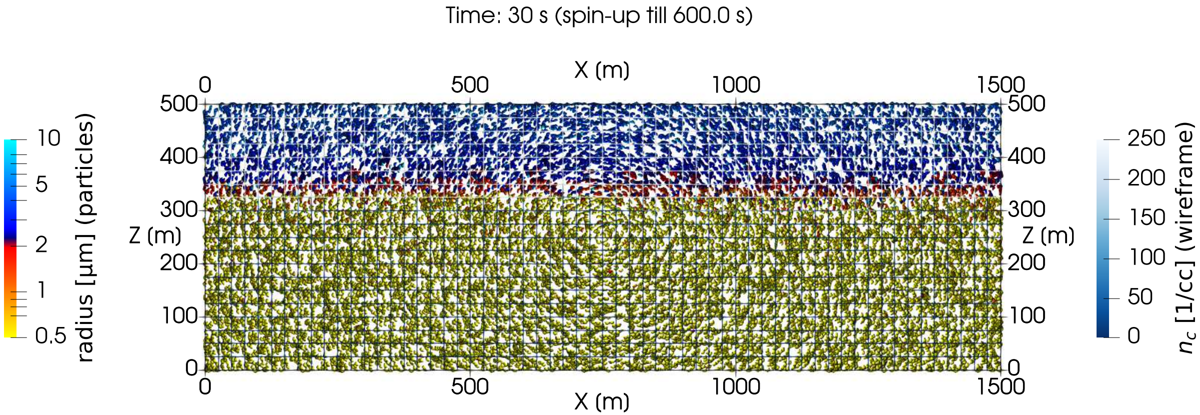
Lagrangian component



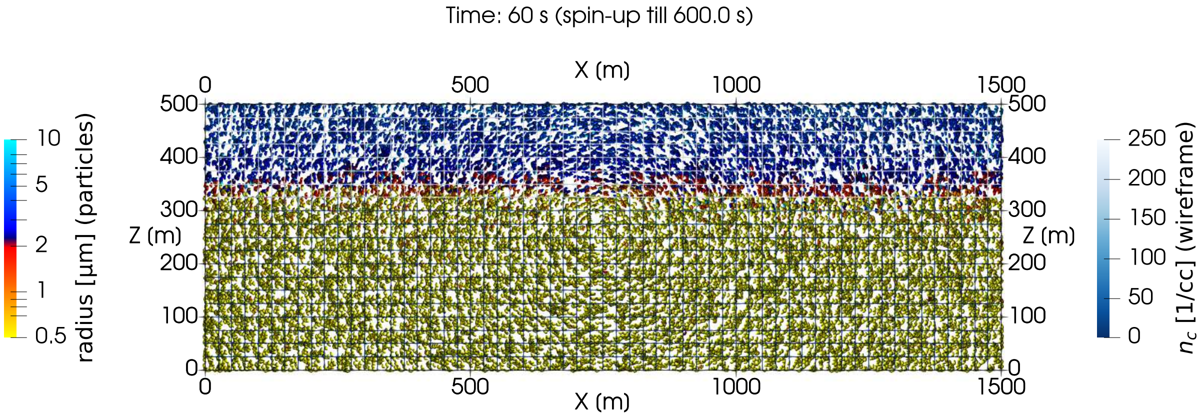
Eulerian component



particle-based μ-physics simulation: hello-world



particle-based μ-physics simulation: hello-world



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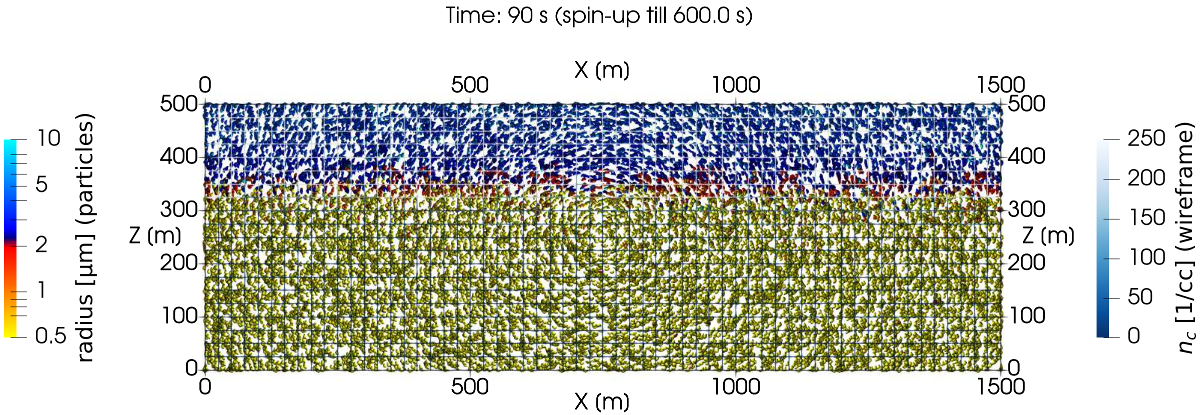
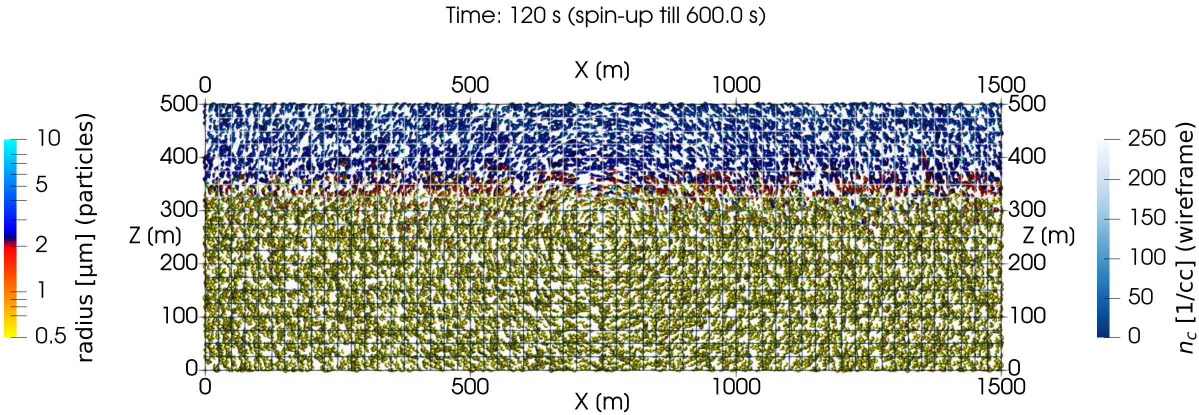
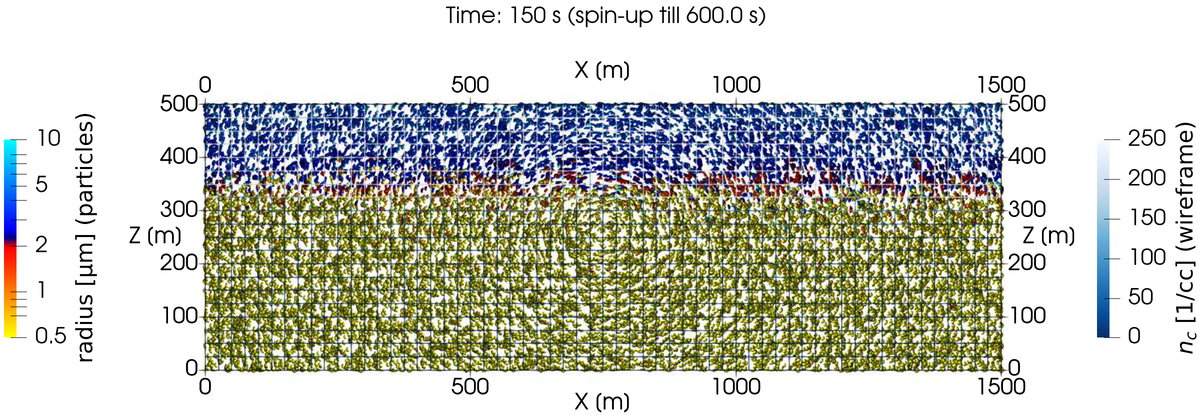


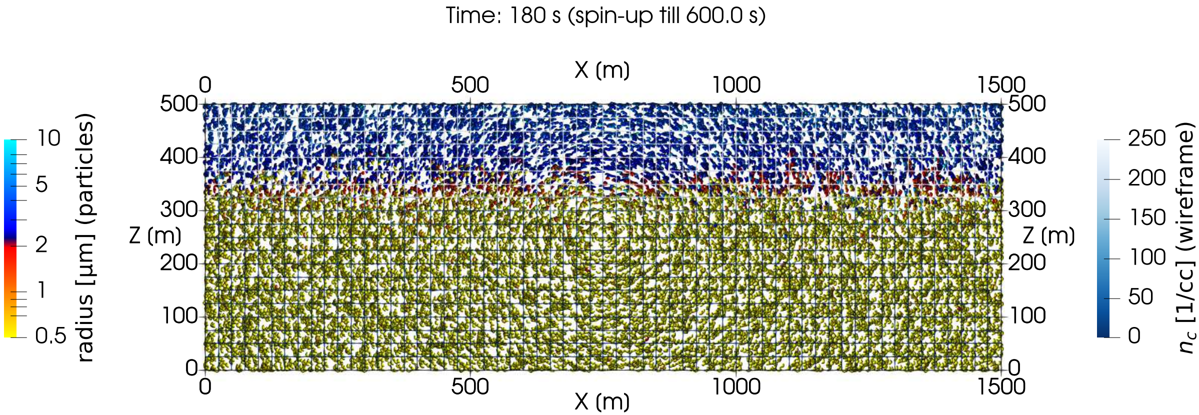
particle-based μ-physics simulation: hello-world



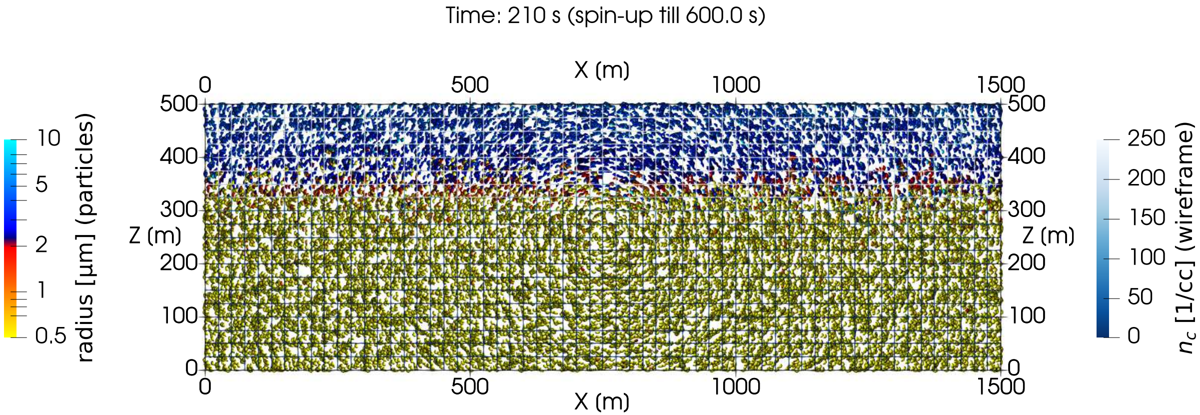
particle-based μ-physics simulation: hello-world



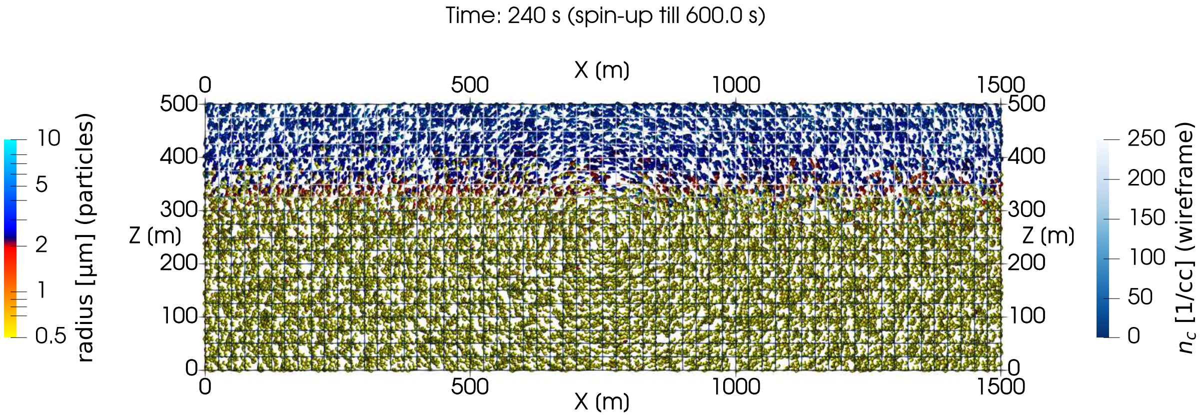
particle-based μ-physics simulation: hello-world



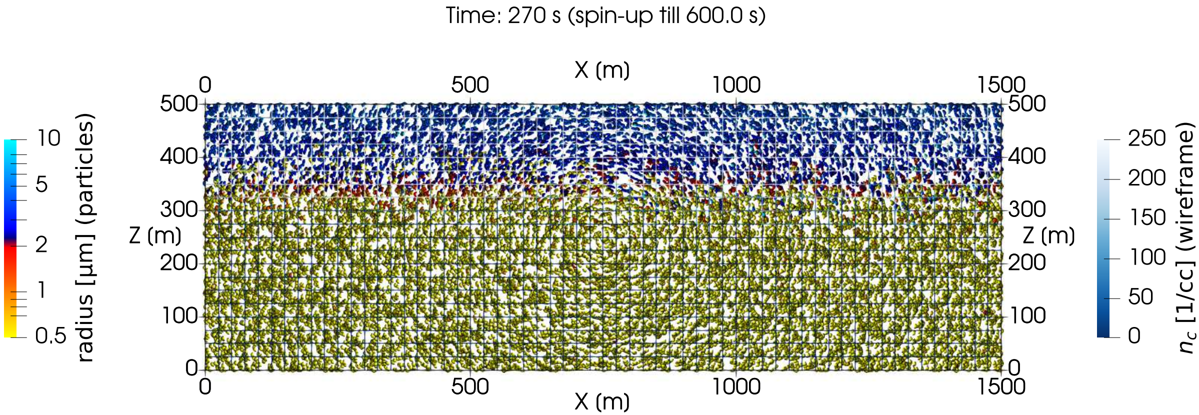
particle-based μ-physics simulation: hello-world



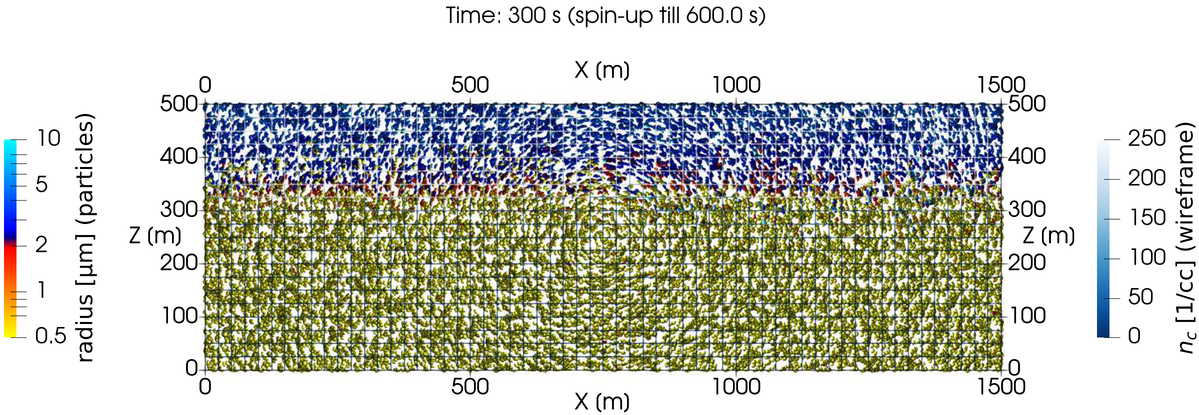
particle-based μ-physics simulation: hello-world



particle-based μ-physics simulation: hello-world



particle-based μ-physics simulation: hello-world



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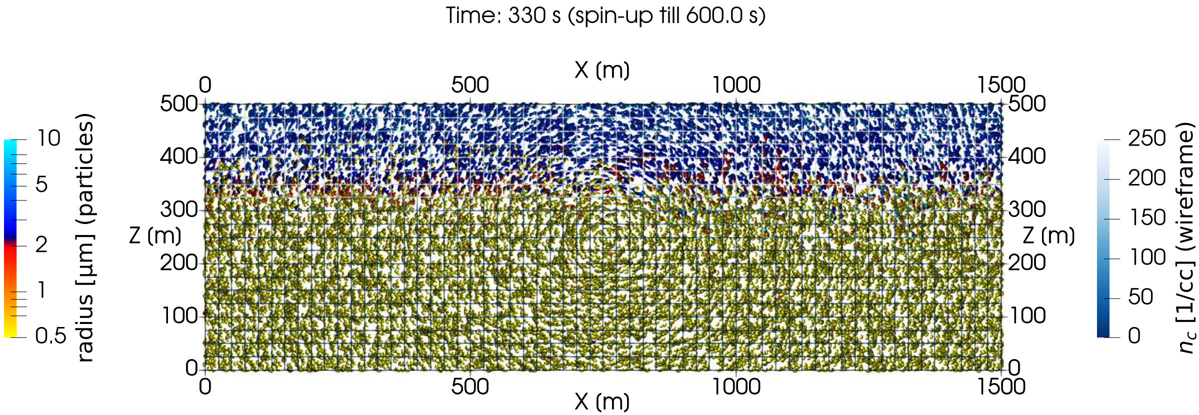

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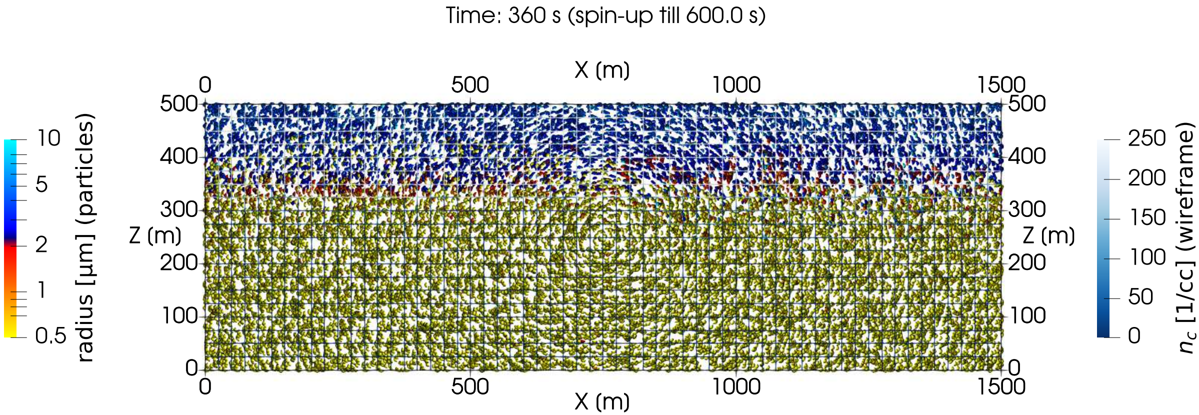
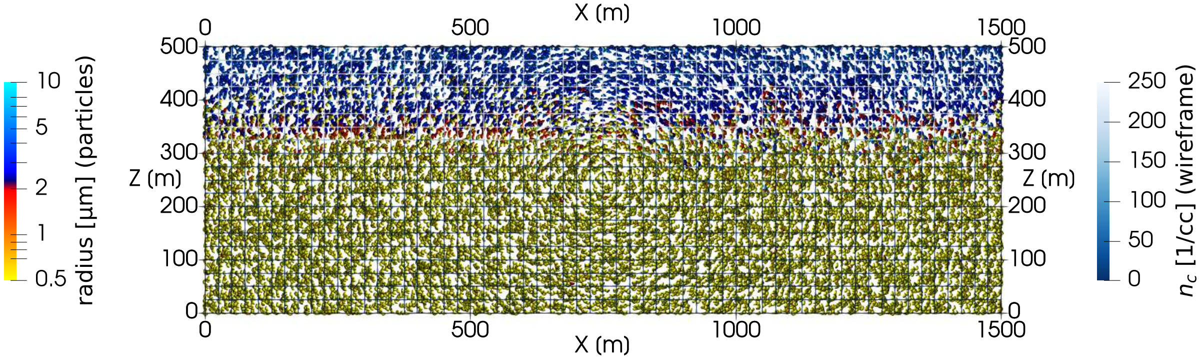
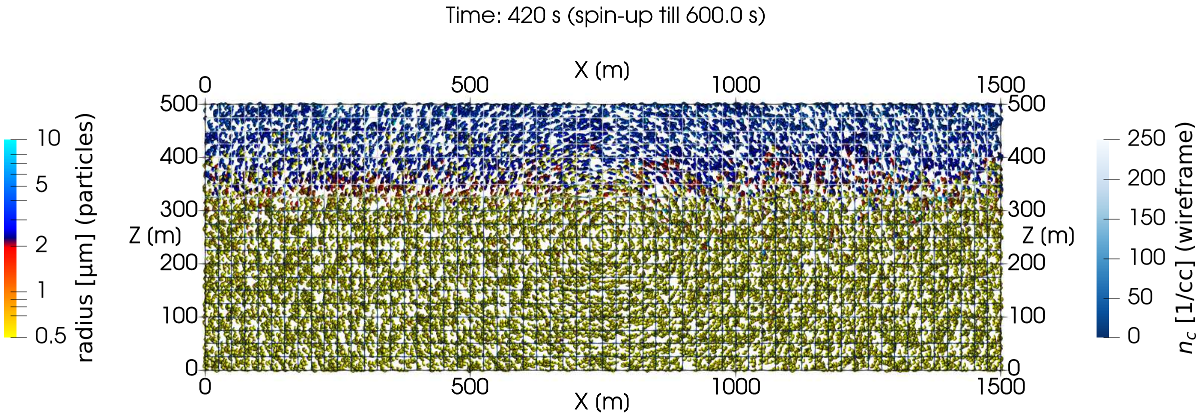


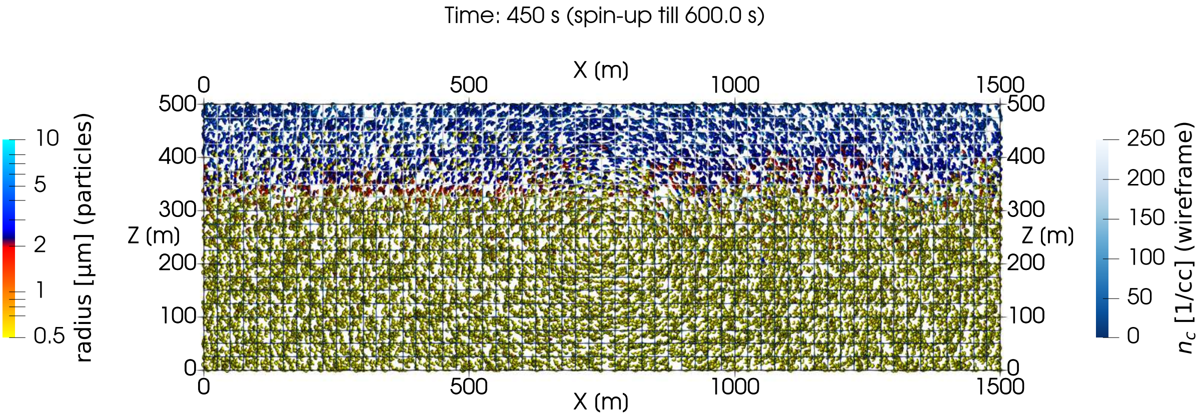
particle-based μ-physics simulation: hello-world

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



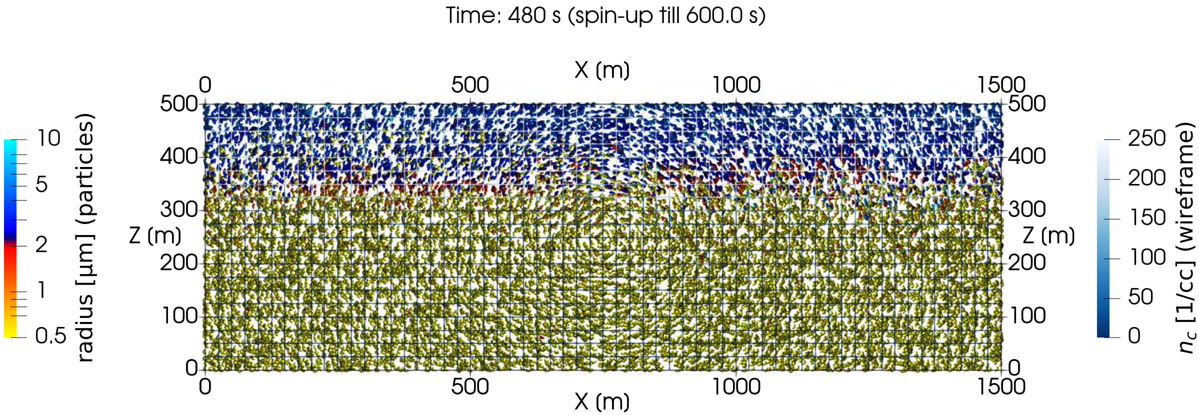
particle-based μ-physics simulation: hello-world



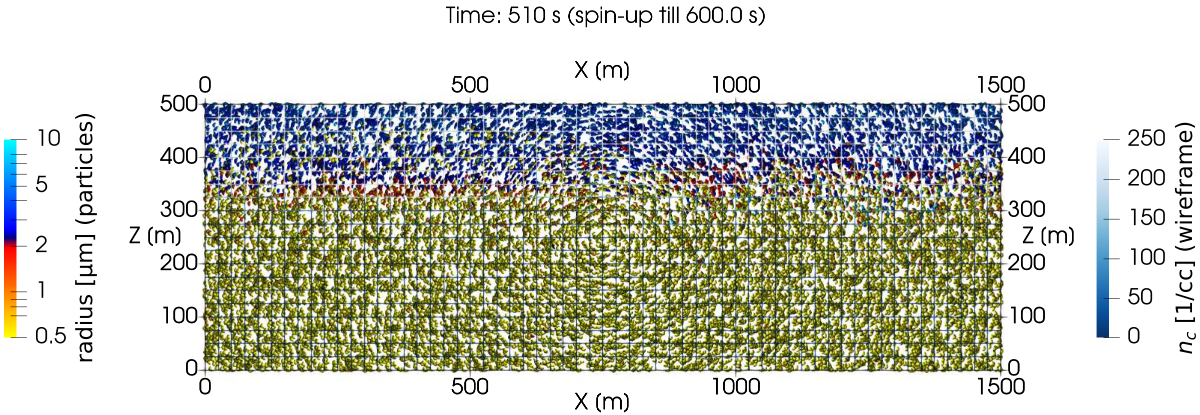


Time: 450 s (spin-up till 600.0 s)
X (m)
0
500
1000
1500
Z (m)
500
400
300
200
100
0
radius [μm] (particles)
10
5
2
1
0.5
n_c [1/cc] (wireframe)
250
200
150
100
50
0

particle-based μ-physics simulation: hello-world



particle-based μ-physics simulation: hello-world



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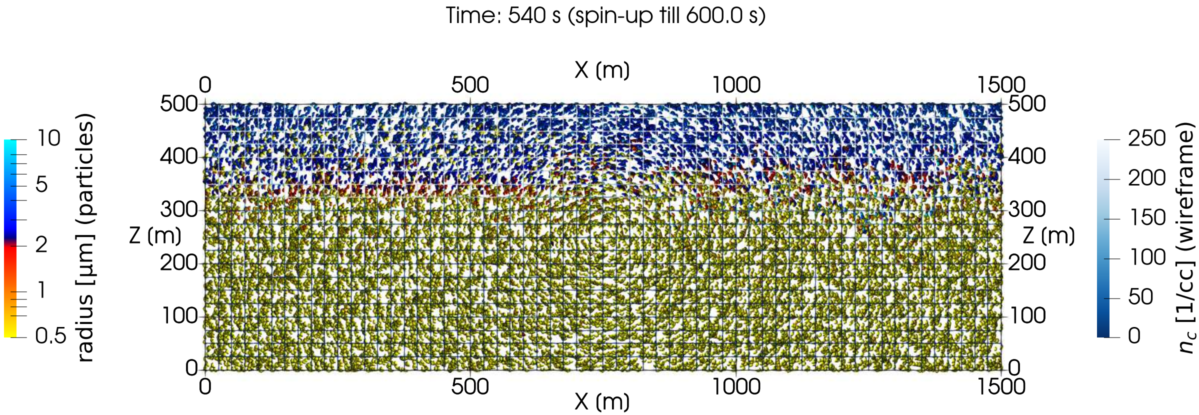

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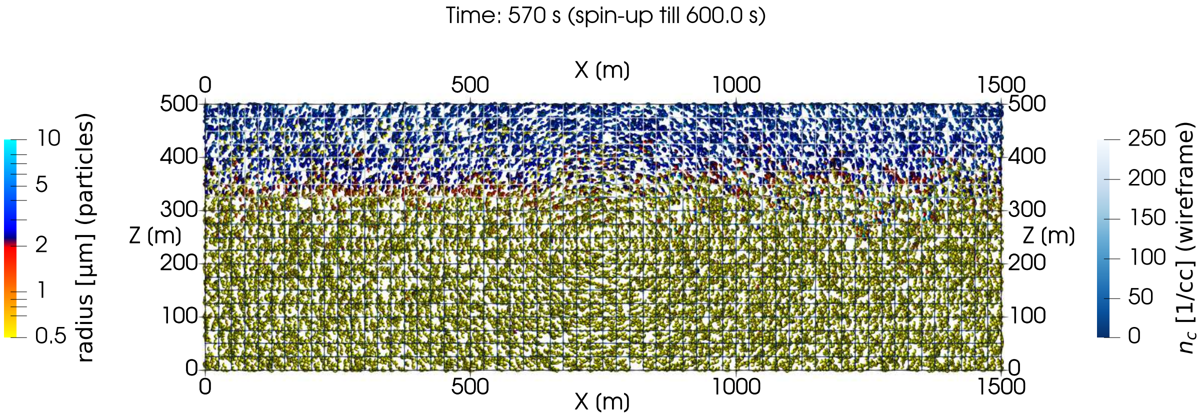

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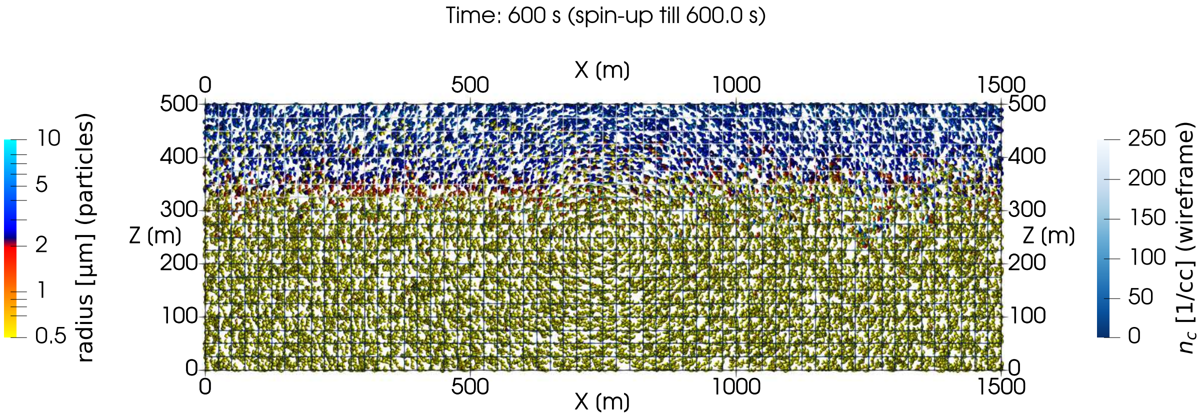

particle-based μ-physics: early works (3D)

JOURNAL OF THE ATMOSPHERIC SCIENCES

A Numerical Experiment on Stochastic Condensation Theory

TERRY L. CLARK AND W. D. HALL

National Center for Atmospheric Research,[1] *Boulder, CO 80307*

(Manuscript received 30 August 1978, in final form 20 November 1978)

ABSTRACT

A three-dimensional numerical model is used to study the effect of small-scale supersaturation fluctuations on the evolving droplet distribution in the first 150 m above cloud base. The primary purpose of this research is to determine whether the irreversible coupling between the thermodynamics and dynamics due to finite phase relaxation time scales τ_S is sufficient to produce significant small-scale horizontal variations in supersaturation. Thus, the paper is concerned only with this internal source for thermodynamic variability. All other source terms, such as the downgradient flux of the variance of thermodynamic fields, have purposely been neglected.

Lagrangian particle experiments were run in parallel with the basic Eulerian model. The purpose of these experiments is to relax some of the microphysical parameterization assumptions with respect to assumed distribution shape and as a result add credibility to the results of distribution broadening.

Eulerian vs. Lagrangian microphysics: a (probabilistic) breakthrough

pre-2009:

,,advantage of the full-moving size structure is that core particle material is preserved during growth … second advantage … it eliminates numerical diffusion … [but] nucleation, coagulation … cause problems … the full-moving structure is not used in three-dimensional models"[a]

,,the use of a fixed grid allows for an easy implementation of collision processes, which is not possible for a moving grid (Lagrangian) approach"[b]

[a] Jacobson 2005: Fundamentals of Atmospheric Modeling

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

Eulerian vs. Lagrangian microphysics: a (probabilistic) breakthrough

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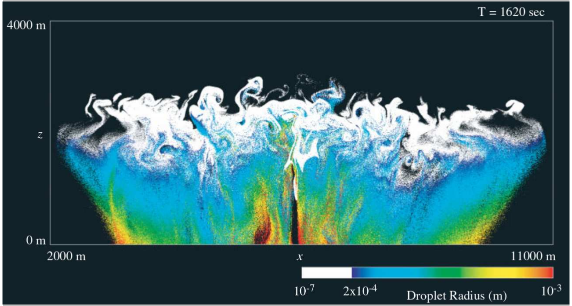
,,the use of a fixed grid allows for an easy implementation of collision processes, which is not possible for a moving grid (Lagrangian) approach"[b]

Shima 2009: Monte-Carlo particle-based collision scheme "SDM" for cloud simulations



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

[a] Jacobson 2005: Fundamentals of Atmospheric Modeling

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

PySDM: idea & demo

100% python™, open, Colab-executable super-droplet pkg

100% python™, open, Colab-executable super-droplet pkg

PySDM

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

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

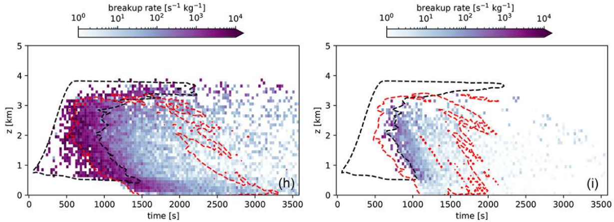
Geoscientific
Model Development
Open Access

Development and technical paper

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

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

[1]Department of Mechanical and Civil Engineering, California Institute of Technology, Pasadena, CA, USA
[2]Scripps Institution of Oceanography, San Diego, CA, USA
[3]Faculty of Mathematics and Computer Science, Jagiellonian University, Kraków, Poland
[4]Department of Environmental Science and Engineering, California Institute of Technology, Pasadena, CA, USA
[5]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Kraków, Poland
[a]formerly at: Department of Environmental Science and Engineering, California Institute of Technology, Pasadena, CA, USA
[b]formerly at: Department of Atmospheric Sciences, University of Illinois Urbana-Champaign, Urbana, IL, USA
[c]formerly at: Faculty of Mathematics and Computer Science, Jagiellonian University, Kraków, Poland



de Jong et al. 2023 (Geosci. Model Dev. DOI:10.5194/gmd-16-4193-2023)

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

Emily de Jong et al.

Code and data availability

Implementation of this breakup algorithm in the SDM is available at https://doi.org/10.5281/zenodo.7851352 (Arabas et al., 2023a). The simulations presented in this work (and all necessary input information) are available in the folder "deJong_Mackay_2022" at https://doi.org/10.5281/zenodo.7851288 (Arabas et al., 2023b). The notebooks in this folder reproduce all results and figures presented in this study, with no external datasets required. The scripts run the relevant model configuration in a matter of minutes and plot the resulting output. All results presented in this paper can be reproduced by one of two means: (1) downloading and installing "PySDM" and "PySDM-examples" (e.g., using "pip install") and running the notebooks locally or (2) accessing the PySDM-examples repository online and running the examples notebooks in the folder "deJong_Mackay_2022" on Google Colab. These codes, PySDM and PySDM-examples, are continuously under development at https://github.com/atmos-cloud-sim-uj/PySDM and https://github.com/atmos-cloud-sim-uj/PySDM-examples (last access: 21 April 2023) and are further documented in a software publication (de Jong et al., 2023).

PySDM: smoke tests

main

PySDM / tests / smoke_tests / box / dejong_and_mackay_et_al_2023 / **test_fig_7.py**

Code | Blame | 192 lines (172 loc) · 6.12 KB

```python
class TestFig7:
    def test_fig_7a(backend_class, plot=False):

        # assert
        for datum_x in data_x.values():
            np.testing.assert_array_equal(data_x["initial"], datum_x)

        peaks_expected = {
            "initial": (30, 0.017),
            "n_f = 1": (1600, 0.015),
            "n_f = 4": (500, 0.01),
            "n_f = 16": (200, 0.0075),
        }

        for lbl, x_y in peaks_expected.items():
            print(lbl)
            peak = np.argmax(data_y[lbl][0])
            np.testing.assert_approx_equal(data_x[lbl][peak], x_y[0], significant=1)
            np.testing.assert_approx_equal(
                data_y[lbl][0][peak] * settings.rho, x_y[1], significant=1
            )
```

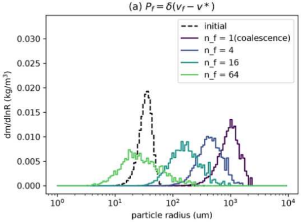


Figure 7. Sensitivity to fragmentation function of PSDs

open-atmos-jupyter-utils 1.3.0

```
pip install open-atmos-jupyter-utils
```

Latest version

Released: Feb 2, 2025

utility routines used in PySDM, PyMPDATA and PyPartMC examples and tests

Navigation

Project description

Release history

Download files

Verified details

These details have been verified by PyPI

Project links

Homepage

Documentation

Source

Tracker

Maintainers

AgnieszkaZaba

slayoo

Project description

open-atmos-jupyter-utils

License GPL v3 | Pylint no status | pypi package 1.3.0 | jupyter-utils code repository

Functions and Examples

- `show_plot()` - a drop-in replacement for matplotlib.pyplot.show() that displays figures inline as SVG vector graphics. The function also provides a download widget that allows users to download the figure as PDF or SVG. On Google Colab, the widget triggers a Google Drive download. Example:
  render on GitHub | launch binder | Open in Colab
- `show_anim(plot_func: typing.Callable, frame_range: typing.Iterable)` - a replacement for matplotlib.animation.FuncAnimation that displays inline animations in GIF format (which is compatible with GitHub rendering). It also provides a download widget to save the animation as a GIF file, with Colab support for Google Drive download. Example:
  render on GitHub | launch binder | Open in Colab
- `notebook_vars(notebook: pathlib.Path, plot: bool)` - a function that executes notebook code and returns a dictionary of variables present in the notebook. This is particularly useful for setting up automated tests using pytest fixtures without any modification to the original notebooks. The `plot` flag controls if `show_plot()` calls within the notebook should be run or not. Example:
  view on GitHub
- `pip_install_on_colab('package_a', 'package_b', ...)` - a function that automates the installation of Python packages in Colab environments via pip (and ldconfig for system libraries). This ensures smooth setup for notebooks running on Colab.

b06464d PySDM / tests / smoke_tests / parcel_d / jensen_and_nugent_2017 / **test_fig_6.py** Top

Code Blame 80 lines (65 loc) · 2.58 KB Raw

```
@pytest.fixture(scope="session", name="variables")
def variables_fixture():
    return notebook_vars(
        file=Path(Jensen_and_Nugent_2017.__file__).parent / "Fig_6.ipynb", plot=PLOT
    )
[redacted]

class TestFig6:
[redacted]
    @staticmethod
    @pytest.mark.parametrize("drop_id", range(int(0.77 * N_SD), N_SD))
    def test_radii(variables, drop_id):
        """checks that the largest aerosol activate and still grow upon descent"""
        # arrange
        cb_idx = find_cloud_base_index(variables["output"]["products"])
        ma_idx = find_max_alt_index(variables["output"]["products"])

        radii = variables["output"]["attributes"]["radius"][drop_id]
        r1 = radii[0]
        r2 = radii[cb_idx]
        r3 = radii[ma_idx]

        assert r1 < r2 < r3
```

PySDM: units and unit tests

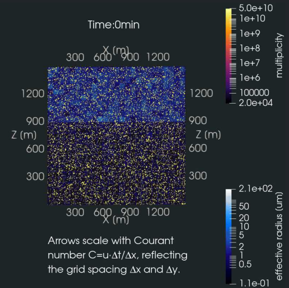
Files ↑	Tracked lines	Covered	Partial	Missed	Coverage %
attributes	551	502	0	49	91.11%
backends	3619	3235	0	384	89.39%
dynamics	1229	1074	0	155	87.39%
environments	273	223	0	50	81.68%
exporters	286	75	0	211	26.22%
impl	204	199	0	5	97.55%
initialisation	375	355	0	20	94.67%
physics	1985	1701	0	284	85.69%
products	1279	1062	0	217	83.03%
__init__.py	11	9	0	2	81.82%
builder.py	89	80	0	9	89.89%
formulae.py	206	203	0	3	98.54%
particulator.py	159	147	0	12	92.45%
Subtotal	10266	8865	0	1401	

PySDM: docs & example gallery

PySDM Documentation

What is PySDM?

PySDM is a package for simulating the dynamics of population of particles undergoing diffusional and collisional growth (and breakage). The package features a Pythonic high-performance (multi-threaded CPU & CUDA GPU) implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth (Shima et al. 2009), hence the name. It is intended to serve as a building block for simulation systems modelling fluid flows involving a dispersed phase, with PySDM being responsible for representation of the dispersed phase. Currently, the development is focused on atmospheric cloud physics applications, in particular on modelling the dynamics of particles immersed in moist air using the particle-based (a.k.a. super-droplet) approach to represent aerosol/cloud/rain microphysics. The key goal of PySDM is to enable rapid development and independent reproducibility of simulations in cloud microphysics while being free from the two-language barrier commonly separating prototype and high-performance research code. PySDM ships with a set of examples reproducing results from literature and serving as tutorials. The animation shown here depicts a flow-coupled simulation in which the flow is resolved using PySDM's sibling project: PyMPDATA. The examples include also single-column setups (with PyMPDATA used for advection) as well as adiabatic cloud parcel model setups (with PySDM alone sufficient to constitute a microphysics-resolving cloud parcel model in Python).



Jupyter notebook setting up and running the above PySDM simulation and generating the visualisation using Paraview

Literature Reference	Cond/Evap	Collisions	Isotopes	Breakup	Transport	Chemistry	Freezing	Comments/keywords
no-environment								
Pierchala et al. 2022			x					theoretical curves for a lab experiment
0D box environment								
Shima et al. 2009		x						Golovin kernel example
Berry 1967		x						Several different kernels
Bieli et al. 2022		x		x				
de Jong et al. 2023		x		x				
Alpert & Knopf 2016							x	
0D parcel environment								
Kreidenweis et al. 2003	x					x		"Hoppel" gap
Jaruga & Pawlowska 2018	x					x		"Hoppel" gap
Lowe et al. 2019	x							surfactants
Yang et al. 2018	x							ripening (depending on the definition)
Graf et al. 2019	x		x					
Grabowski and Pawlowska 2023	x							ripening (not named so in the paper)
Arabas and Shima 2017	x							monodisperse, activation/deactivation cycle
Abdul-Razzak & Ghan 2000	x							parcel vs. activation parameterisation
1D single-column kinematic env.								
Shipway & Hill 2012	x	x			x			KiD 1D
deJong et al. 2023 (figures 6-8)	x	x		x	x			
2D prescribed-flow environment								
Arabas et al. 2015	x	x			x			includes GUI
Arabas et al. 2023 (figure 11)	x	x			x		x	Paraview script example

PySDM: features & team

uj.edu.pl clima.caltech.edu climas.illinois.edu agh.edu.pl uni-mainz.de uw.edu.pl columbia.edu washington.edu ucdavis.edu

Piotr Bartman & SA @uj.edu.pl code architecture, CPU & GPU backends, parcel & KiD env. . . .
Emily de Jong @caltech.edu collisional breakup, . . .

uj.edu.pl clima.caltech.edu climas.illinois.edu agh.edu.pl uni-mainz.de uw.edu.pl columbia.edu washington.edu ucdavis.edu

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Clare Singer @caltech.edu, @columbia.edu surfactants, aerosol attribute sampling. . .

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Clare Singer @caltech.edu, @columbia.edu surfactants, aerosol attribute sampling. . .
Isabella Dula, Ania Jaruga @caltech.edu ARG paper simulatios reproduced. . .

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Emily de Jong @caltech.edu collisional breakup, . . .
Clare Singer @caltech.edu, @columbia.edu surfactants, aerosol attribute sampling. . .
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Immersion Freezing in Particle-Based Aerosol-Cloud Microphysics: A Probabilistic Perspective on Singular and Time-Dependent Models

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

10.1029/2024MS004770

JAMES 17(4), 2025

nucleation rate (prognostic)

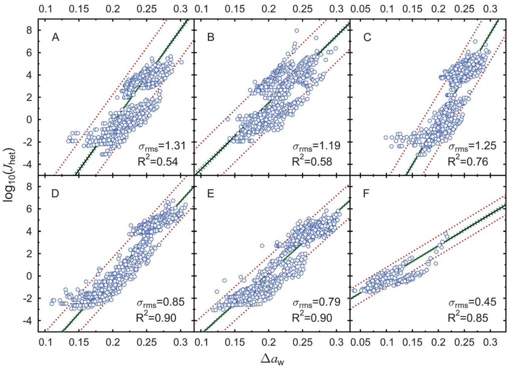


Fig. 3 The decadal log of the heterogeneous ice nucleation rate coefficients, $\log_{10}(J_{het})$, are shown as a function of Δa_w for individually analysed freezing events, initiated by the different IN types investigated in this study and previous work.[41,43,57,66,73,75,78,95] $\text{Log}_{10}(J_{het})$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

Knopf & Alpert '13

nuclation site density (diagnostic)

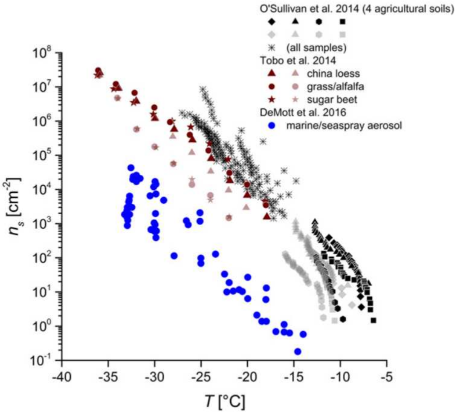
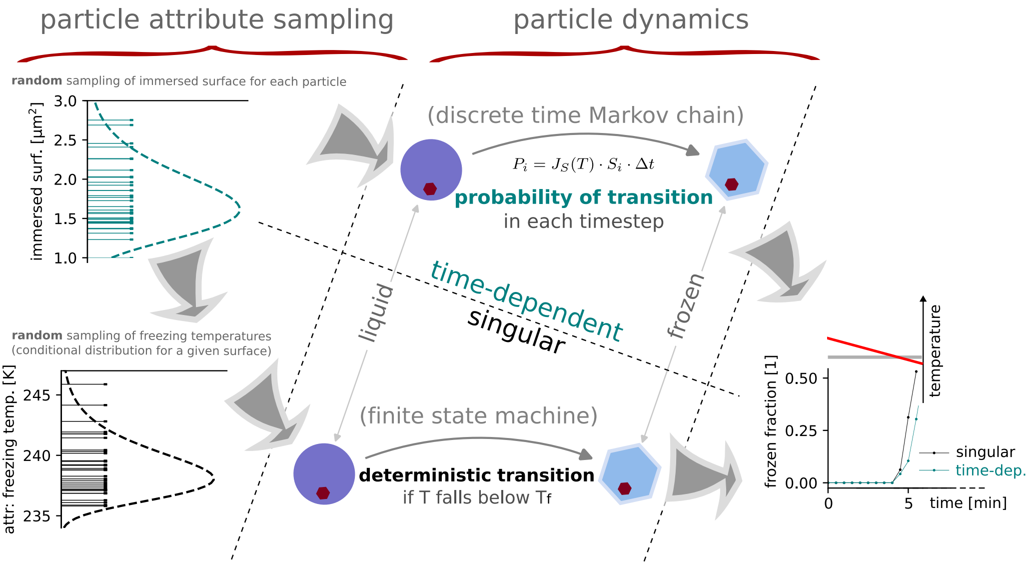
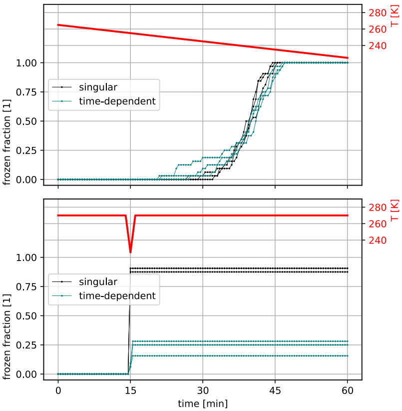


FIG. 1-6. Ice nucleation active site densities n_s as a function of temperature for H_2O_2 (hydrogen peroxide) treated (lighter-shaded symbols) and untreated (dark symbols) agricultural soil dusts in comparison to the n_s of marine aerosol. Differences between various black symbols are for organic content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

Kanji et al. '17


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
liquid
frozen
time-dependent
singular
(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.

Arabas et al. '25 (JAMES)



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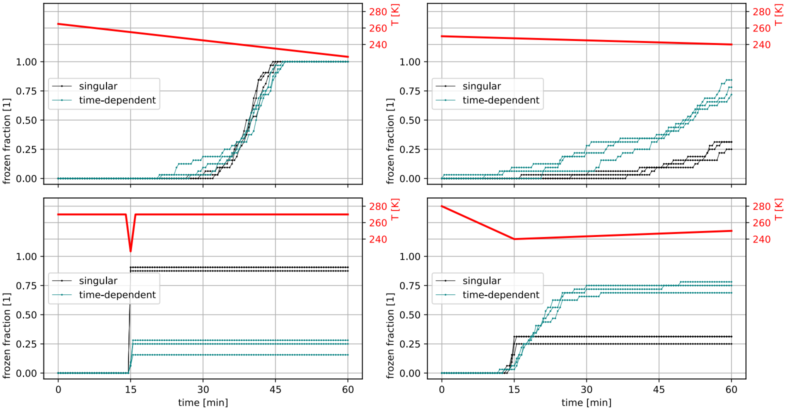

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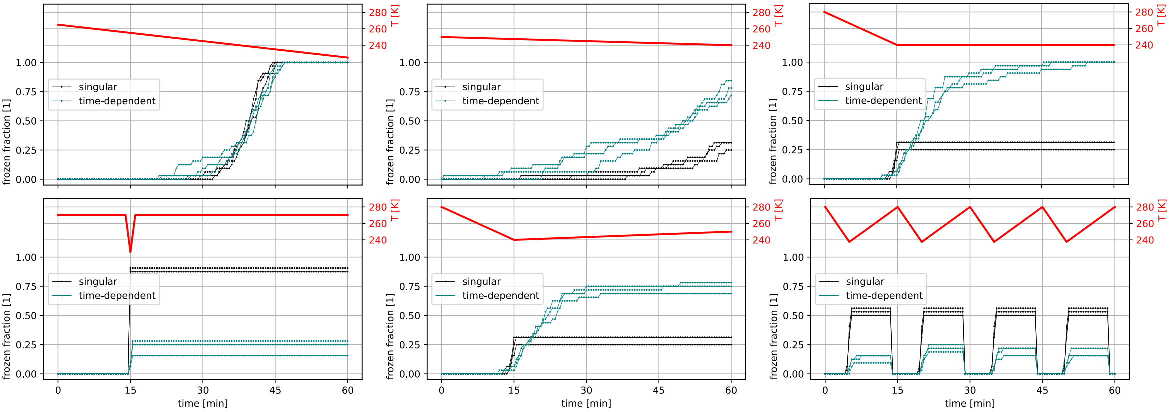

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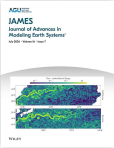

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This article also appears in:
The CliMA Earth System Model

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

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

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

Abstract

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

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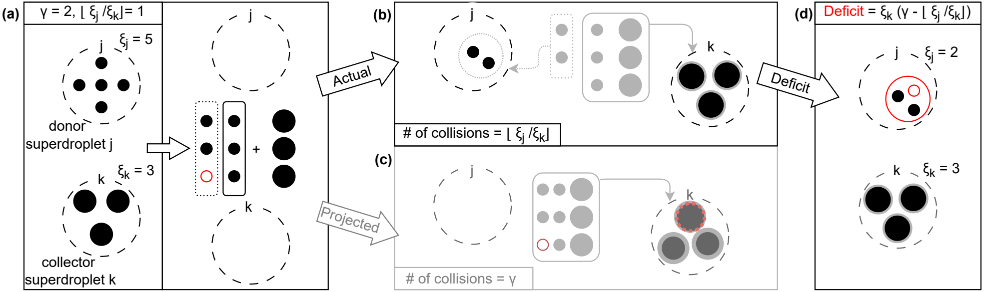
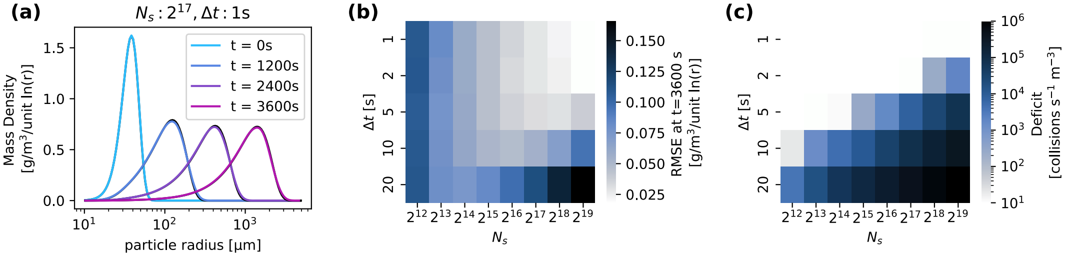
Emma Ware @agh.edu.pl (@ucdavis.edu) SDM adaptivity, spectral sampling, ...

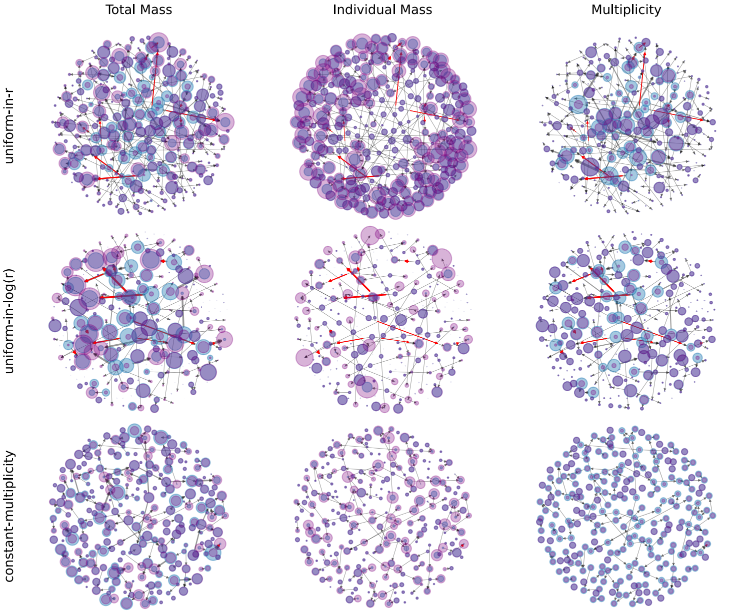
Ware et al. 2025 (arXiv:2509.05536)

Ware, Bartman-Szwarc, Igel & Arabas '25 (arXiv)



SDM colision deficit in a Safranov-Golovin kernel test case




Total Mass
Individual Mass
Multiplicity
uniform-in-r
uniform-in-log(r)
constant-multiplicity

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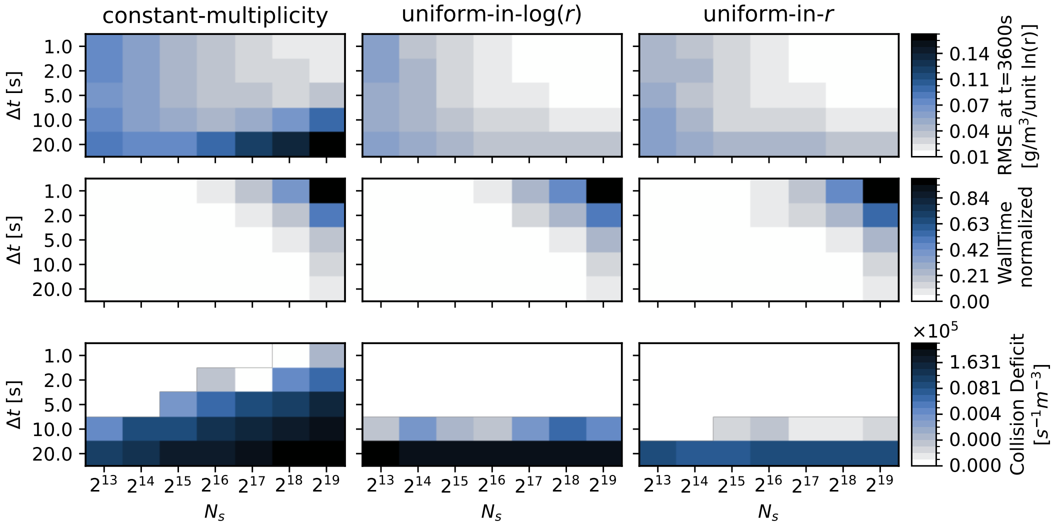

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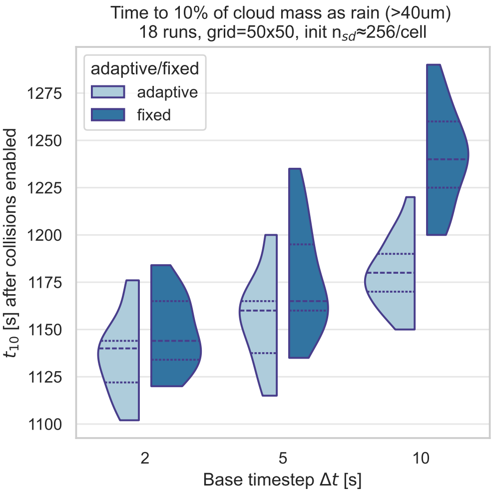

arXiv > physics > arXiv:2509.05536

Physics > Atmospheric and Oceanic Physics

[Submitted on 5 Sep 2025]

Adaptive time-stepping for the Super-Droplet Method Monte Carlo collision-coalescence scheme

Emma Ware, Piotr Bartman-Szwarc, Adele L. Igel, Sylwester Arabas

We present an analysis of an adaptive time-stepping scheme for the Super-Droplet Method (SDM), a Monte Carlo algorithm for simulating particle coagulation. SDM represents cloud droplets as weighted superdroplets, enabling high-fidelity representations of microphysical processes such as collision-coalescence. However, the algorithm can undercount collisions when the expected number of events is not realizable given the superdroplet configuration, introducing a biased error referred here as the collision deficit. While SDM exhibits statistical spread inherent to Monte Carlo schemes, the deficit is a systematic underestimation of collision events. This error can be addressed with adaptive time-stepping, which dynamically adjusts simulation time steps to eliminate this deficit. We analyze the behavior of the deficit across a wide range of timesteps, superdroplet counts, and initialization strategies, and explore trade-offs between accuracy and efficiency. Using the classical Safranov-Golovin test case, we show that the deficit increases with timestep and superdroplet count, and that adaptive time-stepping effectively removes the associated error without significant cost. We test a smooth continuum of initial distributions with extrema representing two different initialization methods, and find that while the deficit is sensitive to the choice of attribute-space sampling strategies, adaptive time-stepping substantially reduces the difference, allowing for users to choose initialization methods optimized for other processes. We also propose a method of visualization, capturing both the attribute sampling, droplet interactions over multiple timesteps, and the deficit using network connectivity graphs. In 2-D flow-coupled simulations, we find the deficit can have a stronger effect on convergence than previously shown, with uncorrected deficit delaying the onset of precipitation.

thanks!

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