Lagrangian Particle-Based Microphysics In Cloud Simulation: Progress & Prospects

W.W. Grabowski, S. Arabas, K.K. Chandrakar, P. Dziekan, F. Hoffmann, E. de Jong, H. Morrison, S. Shima, A. Seifert, S. Unterstrasser













@ucar.edu





Background

LPBM – Lagrangian Particle-Based Microphysics models track the evolution (snigle- and many-particle physiochemical processes) and transport of notional particles, and are an alternative to Eulerian bulk or bin methods

Model developments

drop breakup

CM1-SDM/balloon-borne obs

Validation

Laboratory experiments of particle growth (tied to crystal morphology via vapor deposition density) are combined with **LES+LPBM** simulations to examine sources of microphysical variability in cirrus. Cirrus case from ARM Ice Cryo-Encapsulation by Balloon (ICE-Ball) campaign. Variability is dominated by particles' thermodynamic histories (see Fig. 4), however, diversity in crystal morphology notably increases spatial variability of mean particle size and density.

Applications

References

@dlr.de

cirrus & contrail studies

In [16], LES of natural and contrail cirri were carried out. Scenarios where contrails were surrounded by later forming natural cirrus were investigated. An important question was to understand whether contrails (as an anthropogenic cloud) would remain distinguishable from natural cirrus when sampled in in-situ measurement campaigns. The analyses benefited from the use of LPBM (no numerical diffusion in space, freely evolving ice crystal size distributions, inexpensive tagging of origin).

[1] S. Azimi, A. Jaruga, E. de Jong, S. Arabas, and T. Schneider.

Training warm-rain bulk microphysics schemes using super-droplet simulations. JAMES (in press), 2024.

[2] K. Chandrakar, H. Morrison, J. Harrington, G. Pokrifka, and N. Magee.

What controls crystal diversity and microphysical variability in cirrus clouds?*Geophys. Res. Lett.*, 51, 2024.

 [3] K. Chandrakar, H. Morrison, and M. Witte.
 Evolution of droplet size distributions during the transition of an ultraclean stratocumulus cloud system to open cell structure: An les investigation using lagrangian microphysics.
 Geophys. Res. Lett., 2022.

Collisional breakup poses a challenge to **LPBM** in terms of comp. scaling, as the fragments produced in collisions may have many different sizes. In [4], a Monte-Carlo scheme is proposed that avoids creating new superdroplets, respecting the physical probability of coalescence/breakup and the fragment size distribution.



Fig. 1: Sample comparison of drop spectra with and without breakup in a single-column (KiD/**PySDM**) kinematic framework

habit prediction/ventilation

Being able to track the history of individual representative particles, **LPBMs** are well suited to tackle ice habits. Taking into account a habit dependent ventilation improves the physics of cirrus clouds [17].



Fig. 4:(a) Selected ice particle trajectories sampled at 15 s intervals (trajectory length > 900 m). Evolution of the ice particle size distributions (b-c) with particle age after nucleation (τ_l). Color bars: probability; squares: mean values; black lines: running mean; red lines: 90th percentile; and blue lines: 10th percentile. See [2]

Π chamber

A model intercomparison study is underway within the framework of the ICCP International Cloud Modeling Workshop, including comparison of **LPBM** simulations with holographic particle size spectrometry inside the MTU Π chamber.



Fig. 6: L: snapshot of a contrail becoming surrounded by natural cirrus (extinction coefficient plotted); R: ice crystal size distribution of such a dual-origin ice cloud

marine cloud brightening

LPBM have been used to support assessment of marine cloud brightening as a viable climate engineering approach (through increasing the reflectance of clouds by artificially increasing the aerosol and hence droplet concentration). **LES+LPBM** setup allows simulating: the sprayers that disperse seawater droplets, evaporation of droplets to sea salt aerosols that are lifted to the cloud layer, [4] E. de Jong, J. Mackay, O. Bulenok, A. Jaruga, and S. Arabas.

Breakups are complicated: an efficient representation of collisional breakup in the superdroplet method. *Geosci. Model Dev.*, 16.

[5] P. Dziekan, J. B. Jensen, W. W. Grabowski, and H. Pawlowska.

Impact of giant sea salt aerosol particles on precipitation in marine cumuli and stratocumuli: Lagrangian cloud model simulations.

- J. Atmos. Sci., 2021.
- [6] P. Dziekan, M. Waruszewski, and H. Pawlowska.
 University of warsaw lagrangian cloud model (uwlcm)
 1.0: a modern large-eddy simulation tool for warm cloud modeling with lagrangian microphysics. *Geosi. Model Dev.*, (6), 2019.
- 7] P. Dziekan and P. Żmijewski.
 University of warsaw lagrangian cloud model (uwlcm)
 2.0: adaptation of a mixed eulerian–lagrangian numerical model for heterogeneous computing clusters.
 Geosci. Model Dev., 15(11), 2022.
- [8] F. Hoffmann and G. Feingold.
 Entrainment and mixing in stratocumulus: Effects of a new explicit subgrid-scale scheme for large-eddy simulations with particle-based microphysics.
 J. Atmos. Sci., 2019.
- [9] F. Hoffmann and G. Feingold.

Cloud microphysical implications for marine cloud brightening: The importance of the seeded particle size distribution.



Fig. 2: Data evidence that columns experience stronger ventilation than spheres or plates. Solid lines: parameterization for LPBM that include habit prediction

performance optimizations

Optimizations discussed in [11] led to an **LPBM** module for **SCALE-SDM** with computational cost comparable to a 2-mom. bulk method (see Fig. 3). A 2m grid-length shallow cloud LES in a $\sim 10 \text{ km}^2$ domain is used for performance evaluation; depicts path to turbulence and microphysics studies over wide range of scales.

Monte-Carlo vs. deterministic collisions

In [12], three methods for drop coalescence in LPBM are compared: deterministic average impact method (AIM), Monte-Carlo (SDM), deterministic SDM (dSDM). Results highlight the critical role of statistical fluctuations ("lucky drops") in driving rain formation in warm clouds.



Fig. 5:Warm rain in LES of a Cu con cloud

is substantially delayed using dSDM (red and blue lines, thick lines are mean and thin lines are $\pm \sigma$) versus SDM (black lines)

Fig. 8: Scaling of the time

to complete a time step

of **LPBM** LES

CPU+GPU cluster

4000

<u>2</u> 3000

2000

1000

t_{CPU&GPU}

on a

where they activate; **[9]** addressed the optimal size distribution of sprayed particles; **[10]** their transport to the clouds (Fig. 7).



Fig. 7: Sprayed particle plume (yellow) is lifted to the clouds (white), where some of the sprayed aerosols activate (magenta).

marine stratocumulus

Recent LES+LPBM marine Sc studies: [6] assessed the impact of LES vs.
iLES, whereas [8] applied Linear Eddy
Model for subgrid RH; [5] found giant
CCNs significantly increase precipitation;
[3] studied the transition to open-cell;
[18] investigated the grid convergence and a comparison with 2-moment.

machine learning

Particle-based models are used for simulations to provide training data for machine learning models: **[13, 14, 15, 1]**

J. Atmos. Sci., 78(10), 2021.

- [10] J. Kainz and F. Hoffmann.
 - High-resolution simulations of aerosol spraying in the great barrier reef: A marine cloud brightening study. In *104th AMS Annual Meeting*. 2024.
- T. Matsushima, S. Nishizawa, and S. Shima.
 Overcoming computational challenges to realize meterto submeter-scale resolution in cloud simulations using the super-droplet method.
 Geosci. Model Dev., 16.
- [12] H. Morrison, K. Chandrakar, S.-I. Shima, P. Dziekan, and W. Grabowski.
 - Impacts of stochastic coalescence variability on warm rain initiation using lagrangian microphysics in box and large-eddy simulations.
- J. Atmos. Sci., 81(6), 2024
- [13] A. Seifert and S. Rasp.
 - Potential and limitations of machine learning for modeling warm-rain cloud microphysical processes. JAMES, 12(12), 2020.
- [14] A. Seifert and C. Siewert.
- An ML-based P3-like multimodal two-moment ice microphysics in the ICON model. *Authorea Preprints*, 2024.
- [15] S. Sharma and D. Greenberg.
 Superdropnet: a stable and accurate machine learning proxy for droplet-based cloud microphysics.
 arXiv preprint 2402.18354, 2024.
- [16] S. Unterstrasser, K. Gierens, I. Sölch, and M. Wirth. Numerical simulations of homogeneously nucleated natural cirrus and contrail-cirrus. part 2: Interaction on



Fig. 3: Total simulation time (circles, triangles) and tracer advection and SD tracking time (squares) for bulk, bin, pre- (SDMorig) and post-optimization (SDM-new)

CPU + GPU + MPI

In [7], the performance of hybrid MPI+threading+GPU mode of operation of **UWLCM** is explored, see Fig. 8. On 40 nodes, wall time of CPU+GPU **LPBM** is twice that of CPU-only bulk.

Open Source LPBM Software

- McSnow: aims at understanding precipitation formation via mixed-phase processes https://gitlab.dkrz.de/mcsnow/mcsnow
 PySDM: tutorial notebooks based on 30+ papers
- https://github.com/open-atmos/PySDM
 SCALE-SDM: mixed-phase LES+SDM https://github.com/Shima-Lab
 UWLCM: hybrid MPI+CPU+GPU LES https://github.com/igfuw/UWLCM

local scale.

Meteorol. Z., 26, 2017.

 [17] J.-N. Welss, C. Siewert, and A. Seifert.
 Explicit habit-prediction in the Lagrangian super-particle ice microphysics model McSnow. *JAMES*, 16(4):e2023MS003805, 2024.

[18] C. Yin, S.-I. Shima, L. Xue, and C. Lu. Simulation of marine stratocumulus using the super-droplet method: Numerical convergence and comparison to a double-moment bulk scheme using scale-sdm 5.2.6-2.3.1. *Geosi. Model Dev.*, (in press), 2024.

GMD/ACP Special Issue

Particle-based methods for simulating atmospheric aerosol and clouds https://gmd.copernicus.org/articles/ special_issue1164.html