Super-droplet simulations with libcloudph++ and PySDM

Sylwester Arabas
Jagiellonian University

Jagiellonian University, Kraków, Poland

- founded in 1364 (ca. coeval with the Joseon dynasty)
- among 20 oldest surviving universities in the world
- ca. 40 000 students, 7000 staff (4000 acad.), 16 faculties
- offers double-degree Korean Studies with Keimyung Univ.

Jagiellonian University, Kraków, Poland

https://en.uj.edu.pl/en_GB/news

King Sejong Institute established at JU

28 March 2017 saw the official opening of King Sejong Institute at the Jagiellonian University – an institution aimed at promoting Korean language learning and fostering intercultural exchange between South Korea and Poland. The unit is part of a wider network of King Sejong institutes, operating in 174 locations in 58 countries.

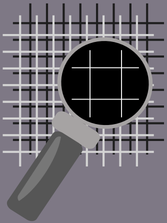
The opening ceremony, which was held in the historic building of Collegium Maius, featured the Rector of the Jagiellonian University Prof. Wojciech Nowak, the Ambassador of the Republic of Korea to Poland Choi Sung-joo, as well as the President of King Sejong Institute Foundation Song Hyang-keun, who came to Kraków from Korea specially to attend the event.

super-droplet simulations

rationale: aerosol-cloud interactions

"Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain"
(photo: Yevgen Timashov / National Geographic)

rationale: modelling aerosol-cloud interactions



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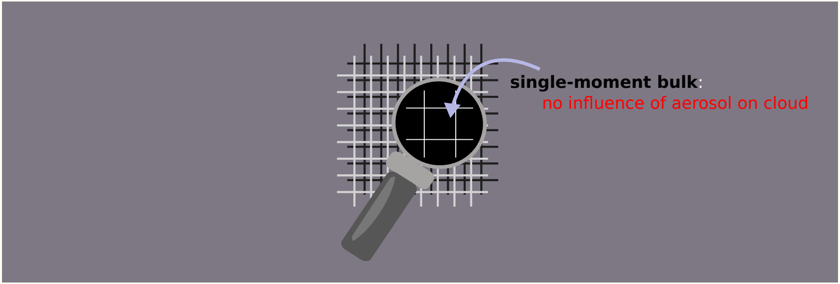

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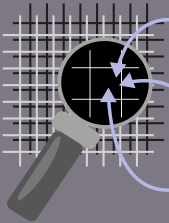

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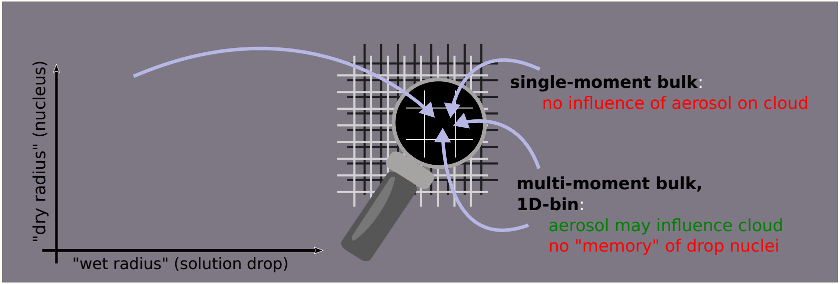

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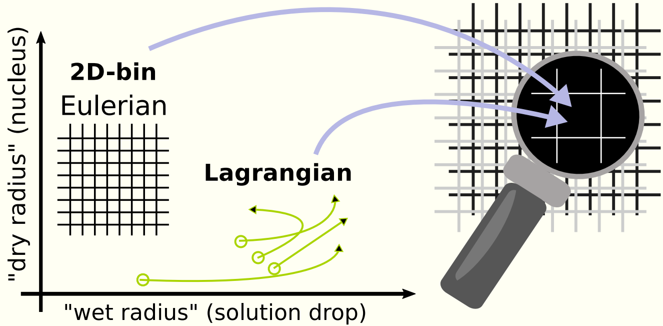

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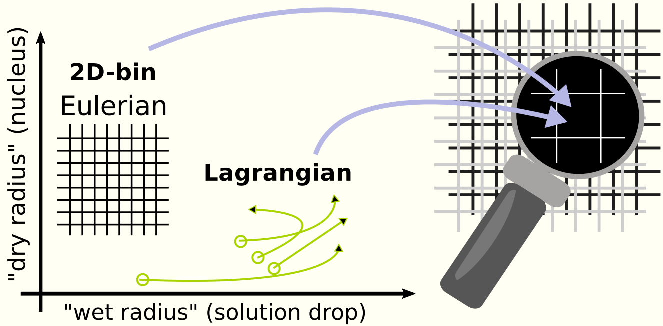

Lagrangian:

- parcel model
  $\rightsquigarrow$ moving-sectional schemes (40-ties onwards: Howell, Mordy, ...)

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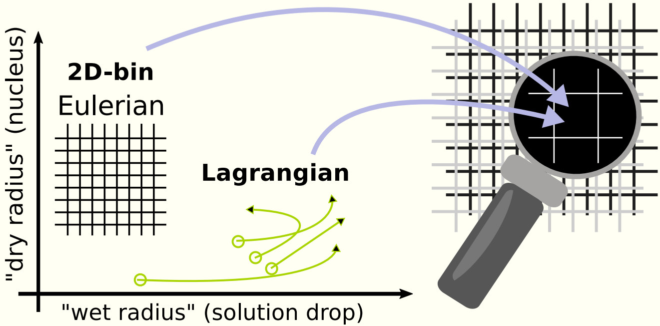


Lagrangian:

- parcel model
  ⇝ moving-sectional schemes (40-ties onwards: Howell, Mordy, . . .)
- LES + Lagrangian-in-space + coalescence
  ⇝ particle-based/super-droplet μ-physics (00-ties onwards: Andrejczuk et al., Shima et al., Noh & Raasch et al., Unterstrasser et al.. . .)

BAMS super-droplet review (Grabowski et al. ’19)

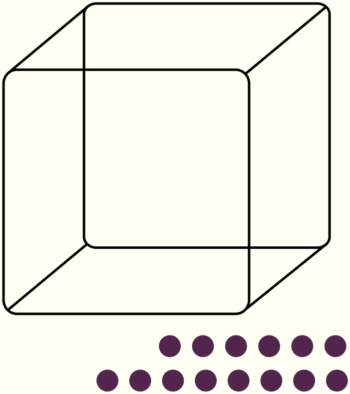
MODELING OF CLOUD MICROPHYSICS

Can We Do Better?

WOJCIECH W. GRABOWSKI, HUGH MORRISON, SHIN-ICHIRO SHIMA, GUSTAVO C. ABADE, PIOTR DZIEKAN, AND HANNA PAWLOWSKA

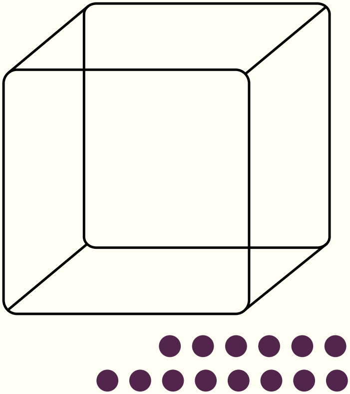
The Lagrangian particle-based approach is an emerging technique to model cloud microphysics and its coupling with dynamics, offering significant advantages over Eulerian approaches typically used in cloud models.

doi:10.1175/BAMS-D-18-0005.1



Domain randomly populated with "μ-physics information carriers" (super particles / super droplets)

particle-based μ-physics: key concepts



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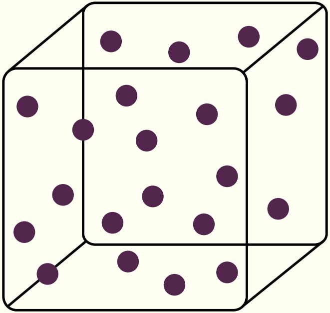

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carrier attributes:

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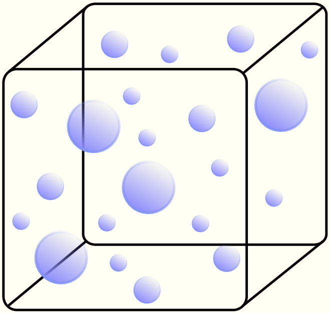

Domain randomly populated with "μ-physics information carriers" (super particles / super droplets)

carrier attributes:

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- wet radius

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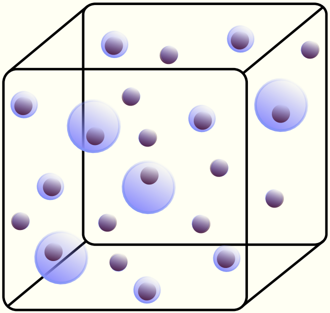

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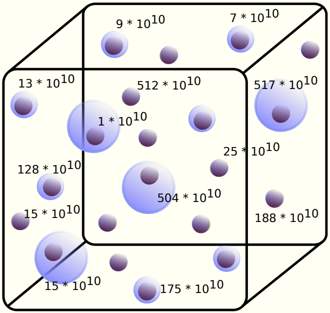

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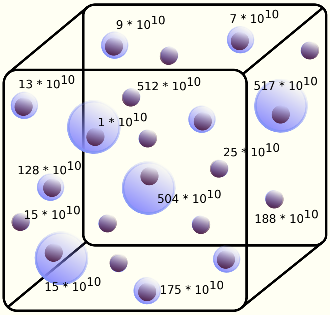

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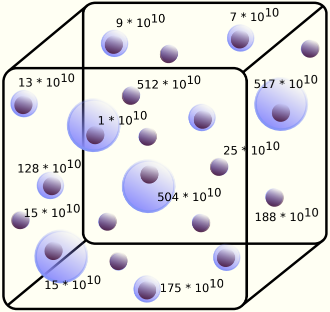

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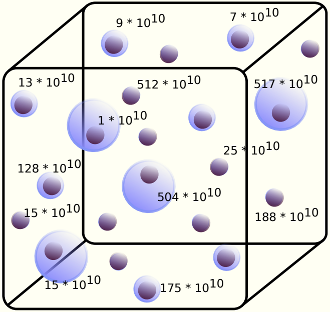

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advantage over Eulerian approach: adding attributes does not increase dimensionality (ice, chemistry, charge, isotopic composition, ...)

Eulerian / PDE	Lagrangian / ODE

particle-based μ-physics: coupling with the host model

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advection of heat	particle transport by the flow
advection of moisture	

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	collisional growth
	sedimentation

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$\partial_t(\rho_d r) + \nabla \cdot (\vec{v}\rho_d r) = \rho_d \dot{r}$	$\dot{r} = \sum\limits_{\text{particles} \in \Delta V} \ldots$
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challenges:

- scalability (cost vs. number of particles),
- super-particles "conservation" (coalescence!)

libcloudph++

libcloudph++: summary & some technicalities

key features (as of v1.0):

- three schemes (all written from scratch):
  - 1-moment: Kessler
  - 2-moment: Morrison & Grabowski 2008
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- Lagrangian scheme optionally GPU-resident (via Thrust)
- compact code (500 / 1000 / 4500 LOC)
- written using Boost.units – compile-time dimensional analysis
- reusable:
  - design: no assumptions on dimensionality or dyn-core type
  - documentation: API described in the paper/manual
  - legal/practical matters: open source, GPL, hosted on github

Geosci. Model Dev., 8, 1677-1707, 2015

https://doi.org/10.5194/gmd-8-1677-2015

Model description paper | 09 Jun 2015

libcloudph++ 1.0: a single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

S. Arabas[1], A. Jaruga[1], H. Pawlowska[1], and W. W. Grabowski[2]

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[2]National Center for Atmospheric Research (NCAR), Boulder, CO, USA

libcloudph++: example simulation (Arabas et al. 2015)

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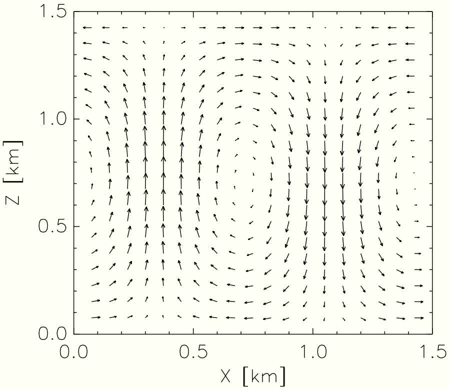

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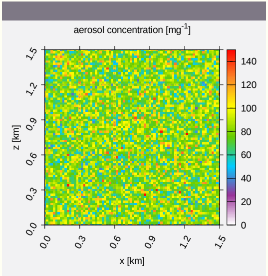

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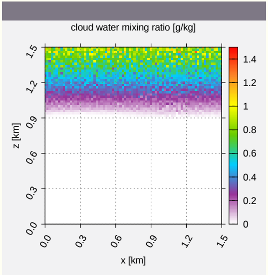

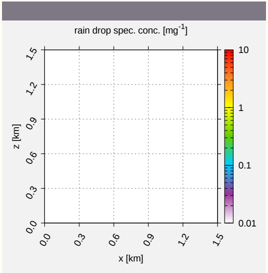

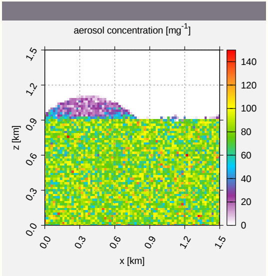

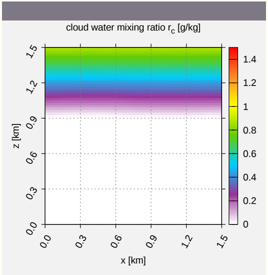

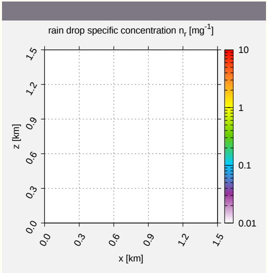

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(Shima et al. 2009)

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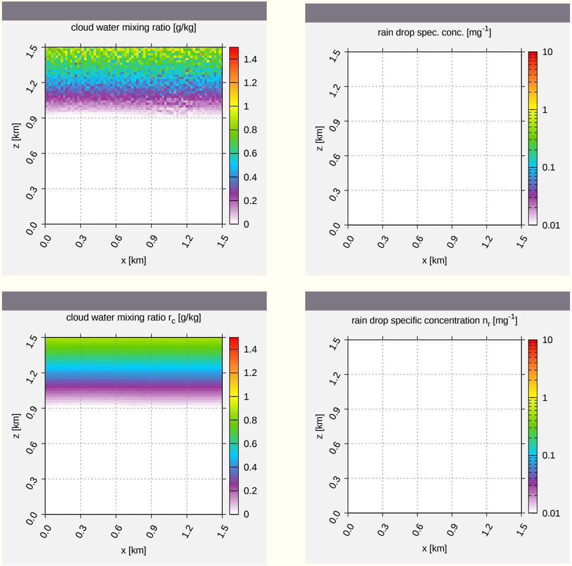

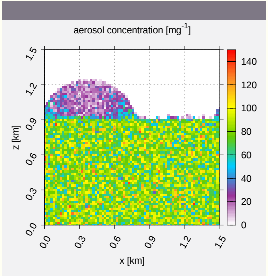

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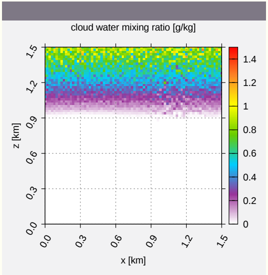

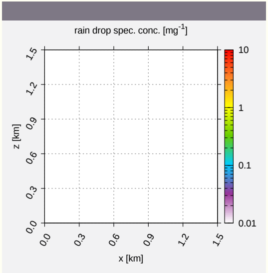

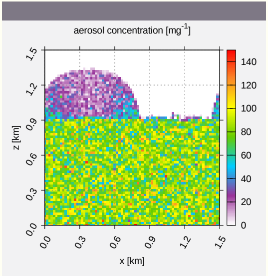

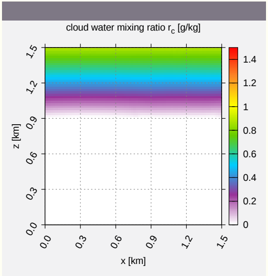

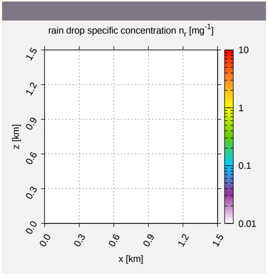

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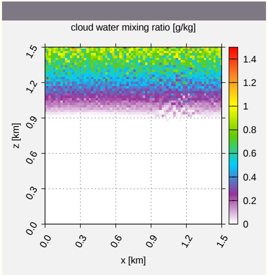

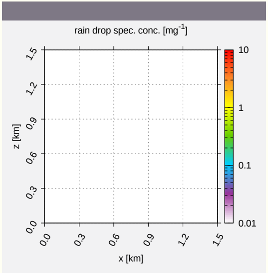

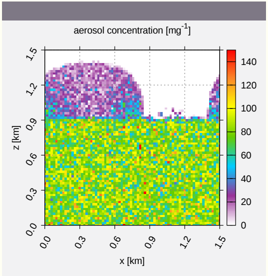

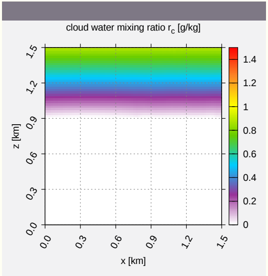

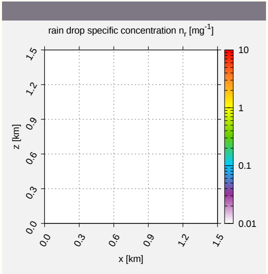

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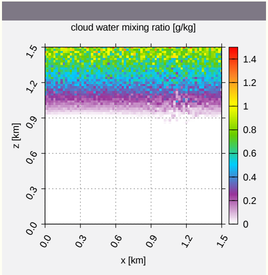

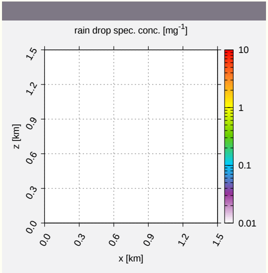

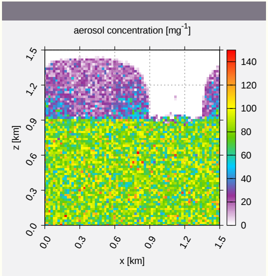

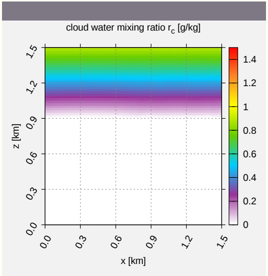

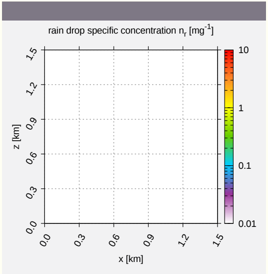

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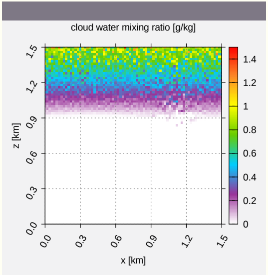

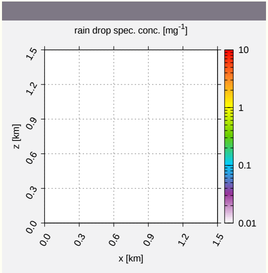

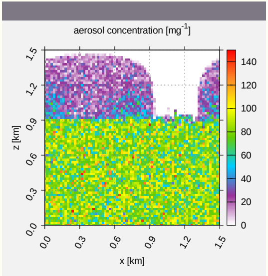

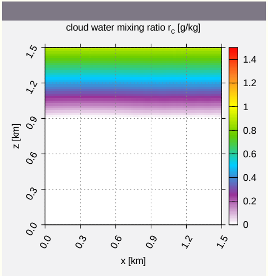

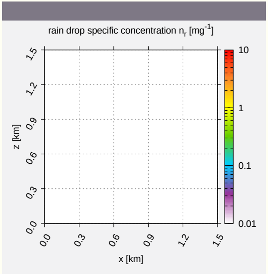

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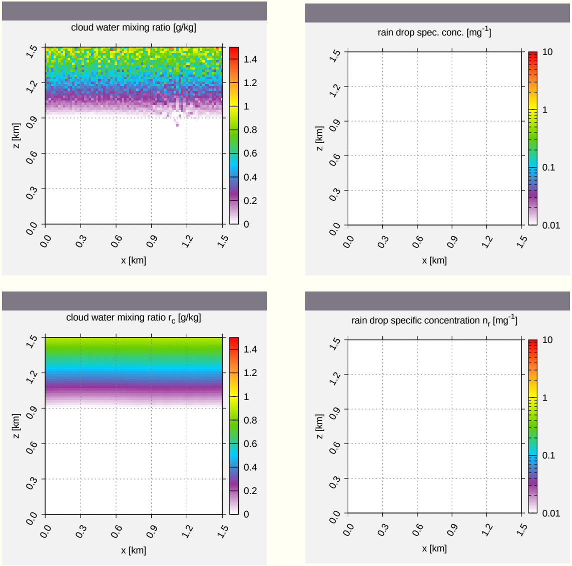

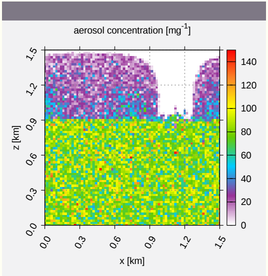

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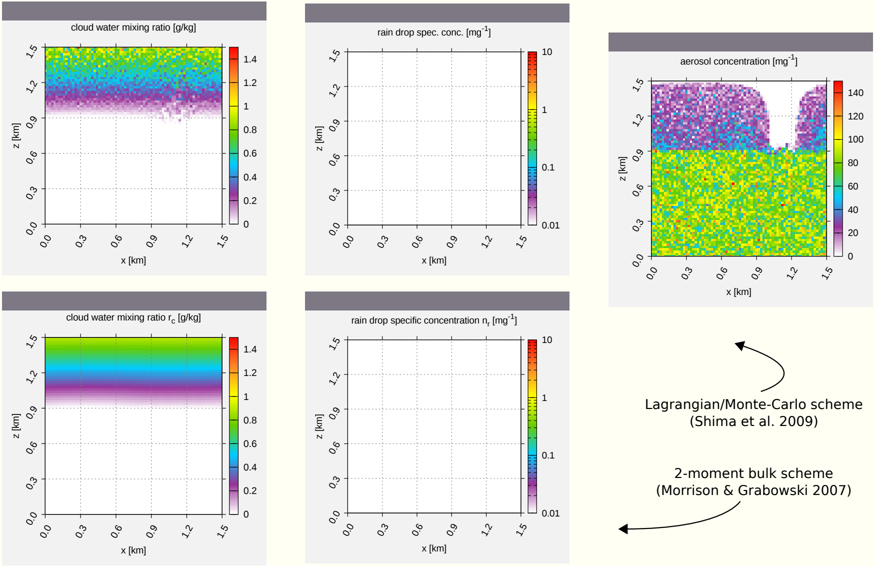

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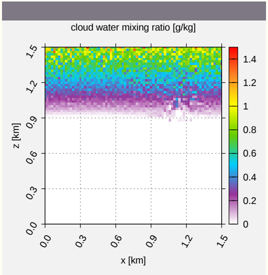

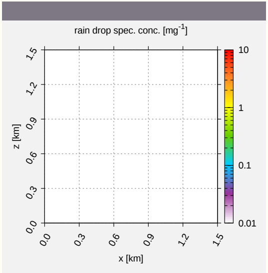

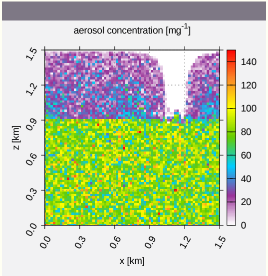

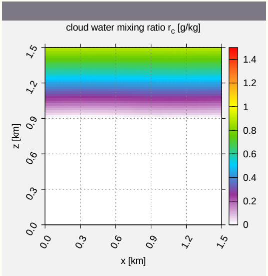

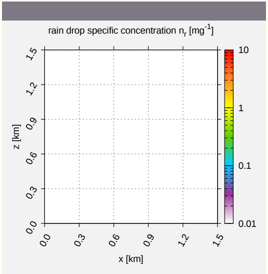

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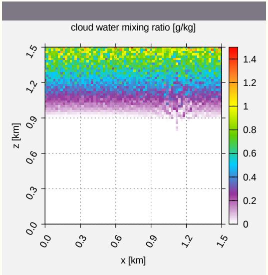

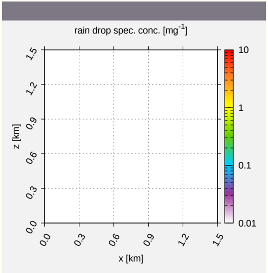

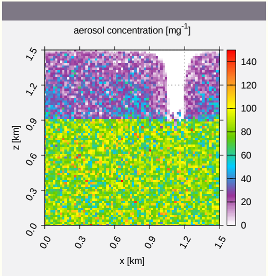

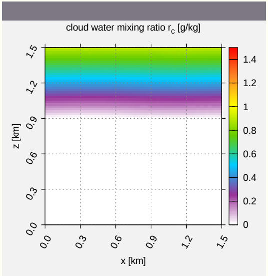

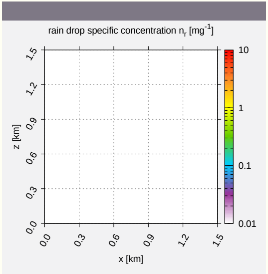

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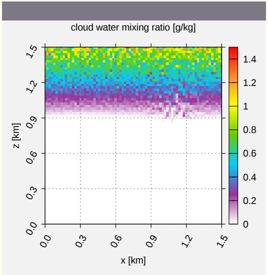

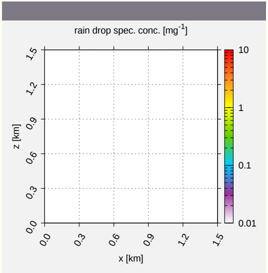

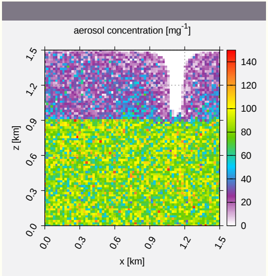

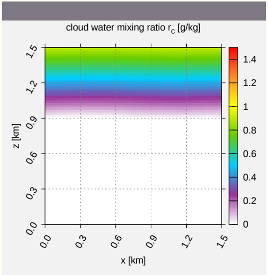

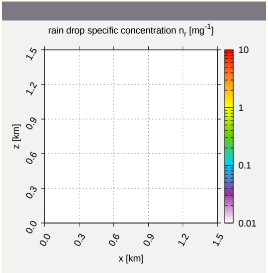

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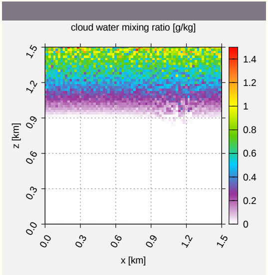

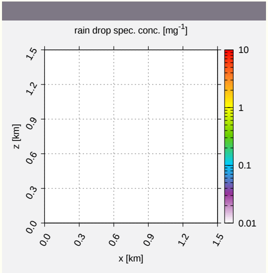

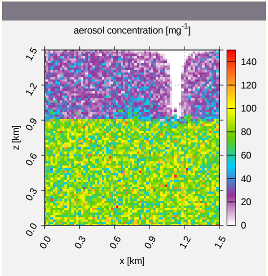

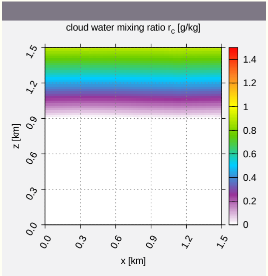

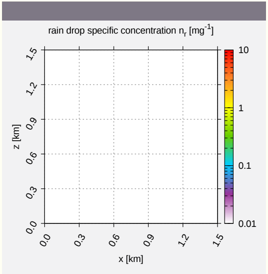

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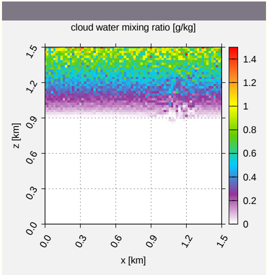

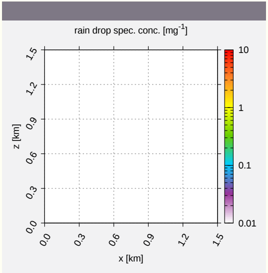

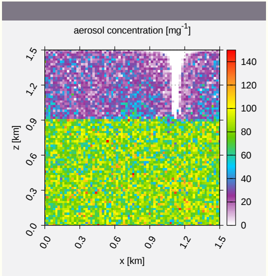

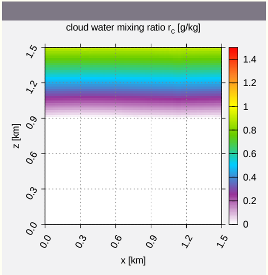

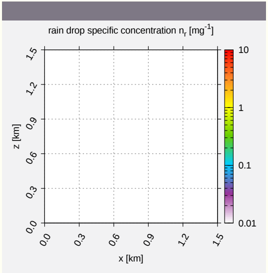

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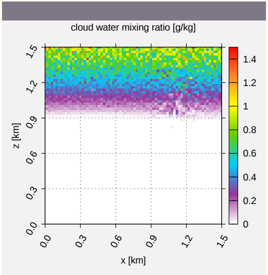

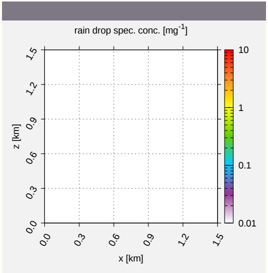

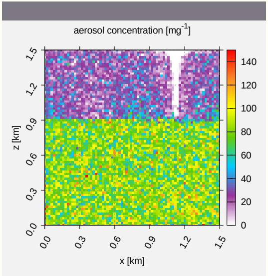

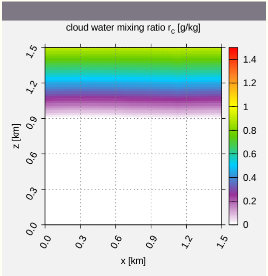

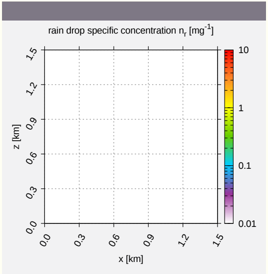

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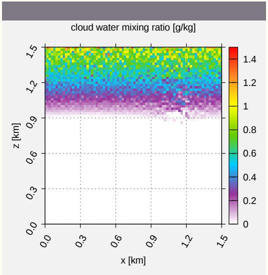

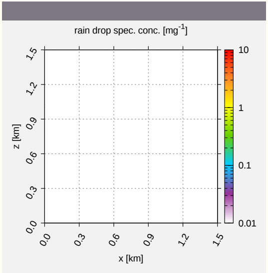

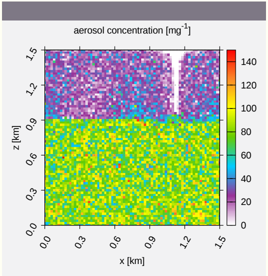

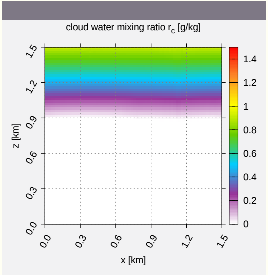

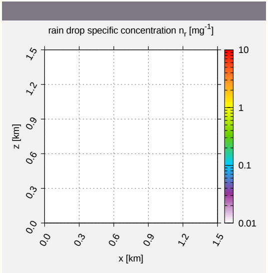

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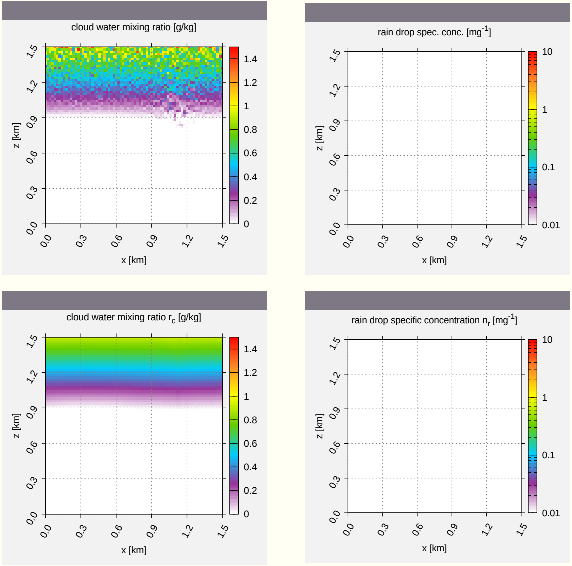

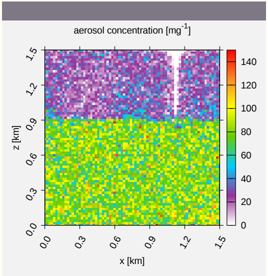

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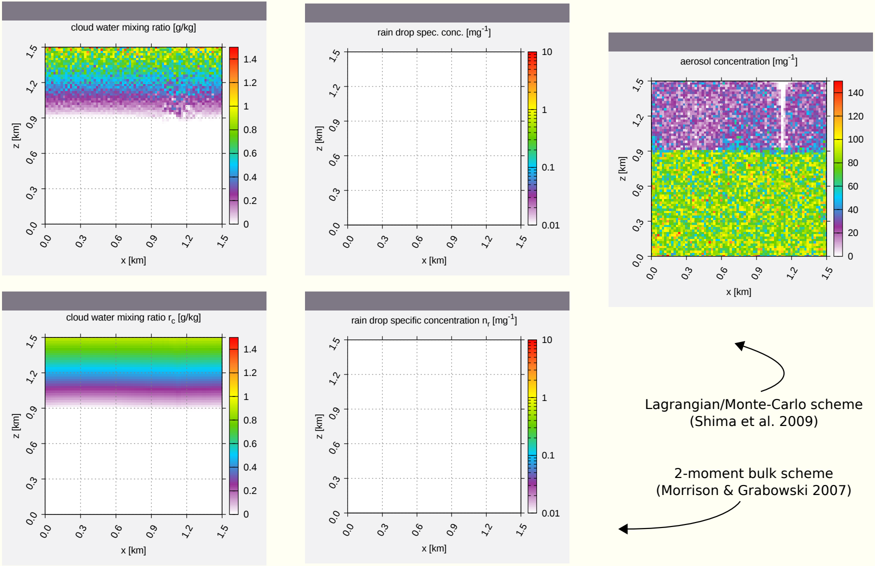

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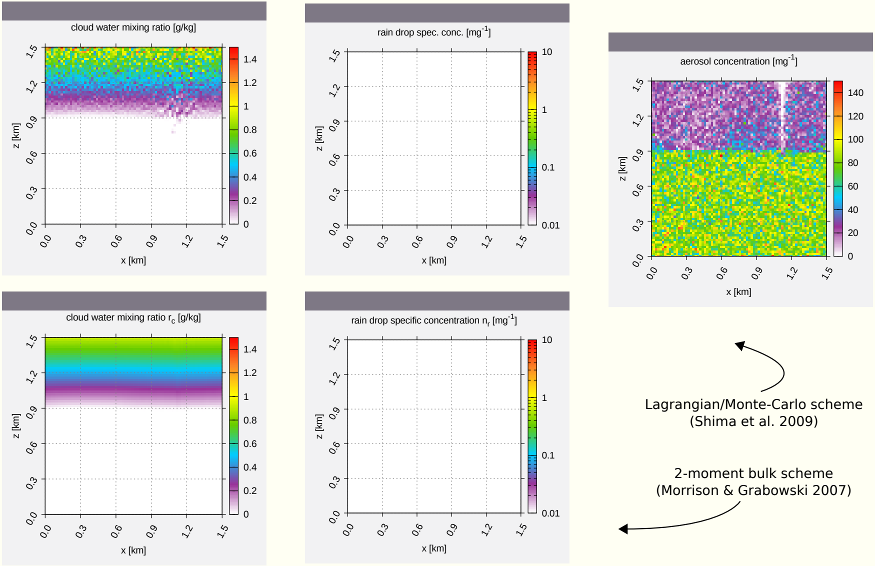

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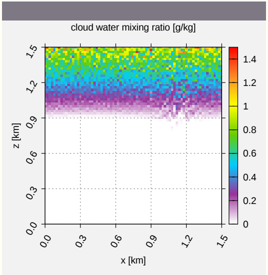

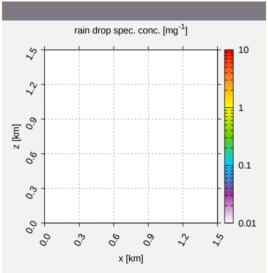

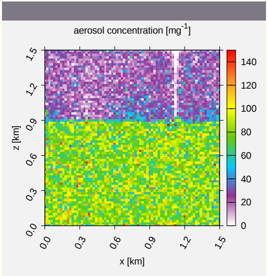

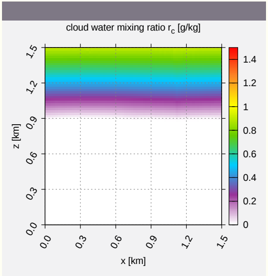

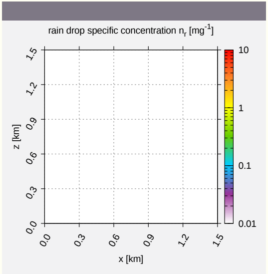

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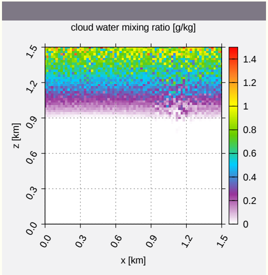

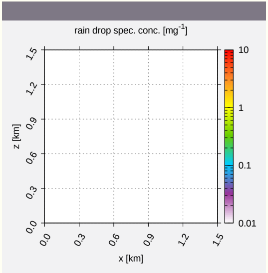

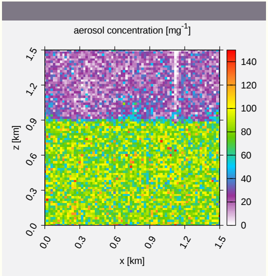

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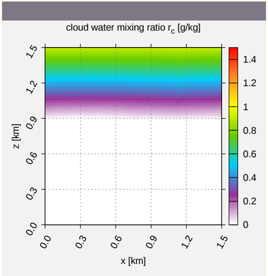

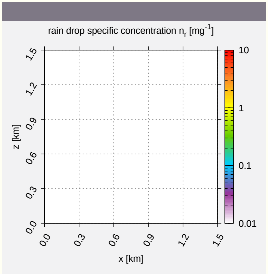

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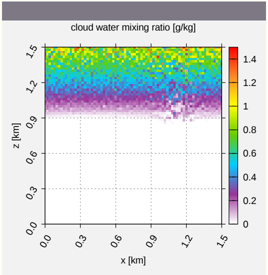

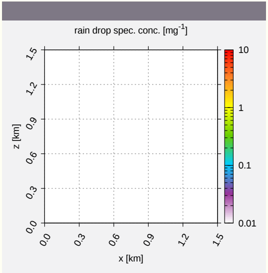

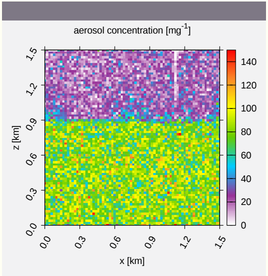

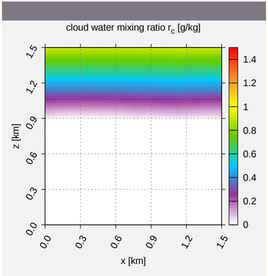

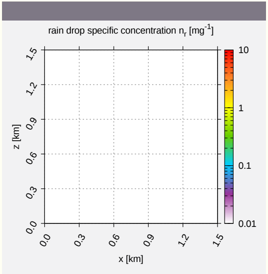

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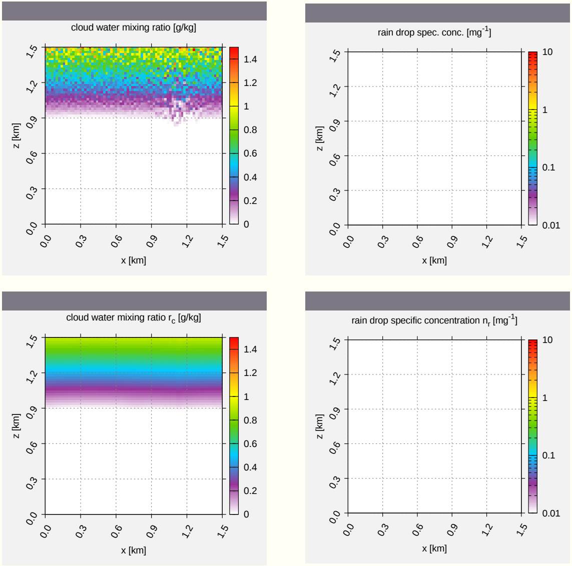

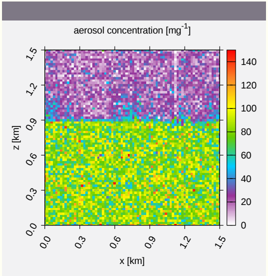

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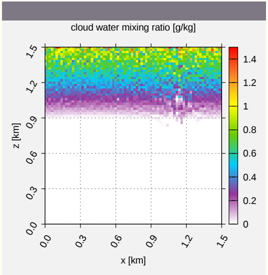

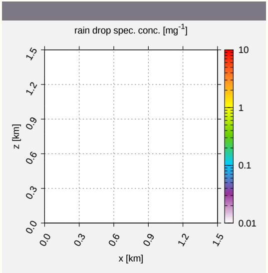

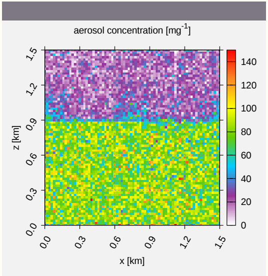

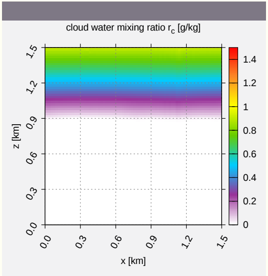

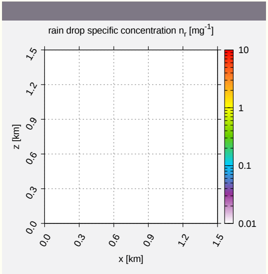

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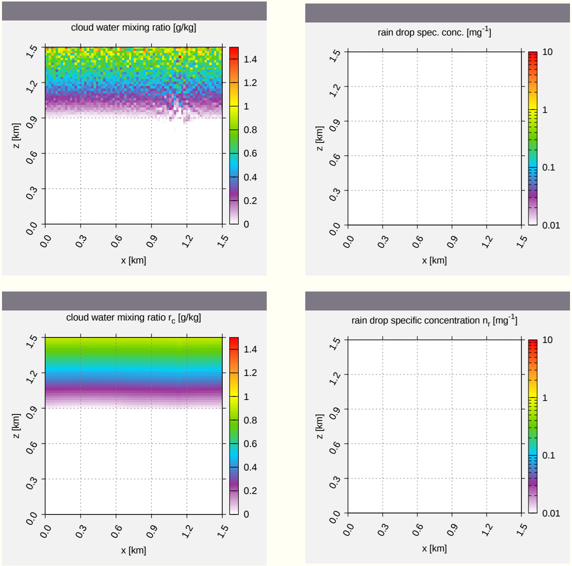

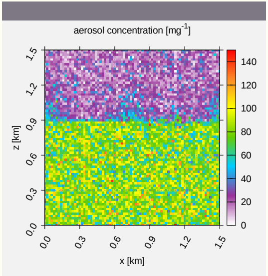

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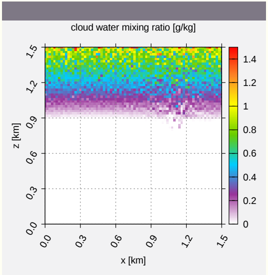

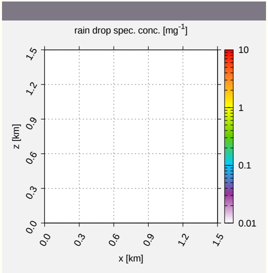

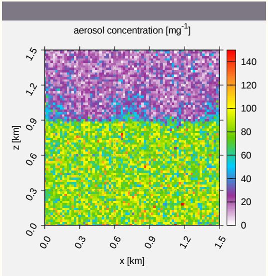

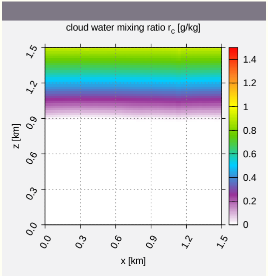

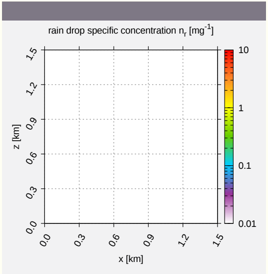

Lagrangian/Monte-Carlo scheme
(Shima et al. 2009)

2-moment bulk scheme
(Morrison & Grabowski 2007)

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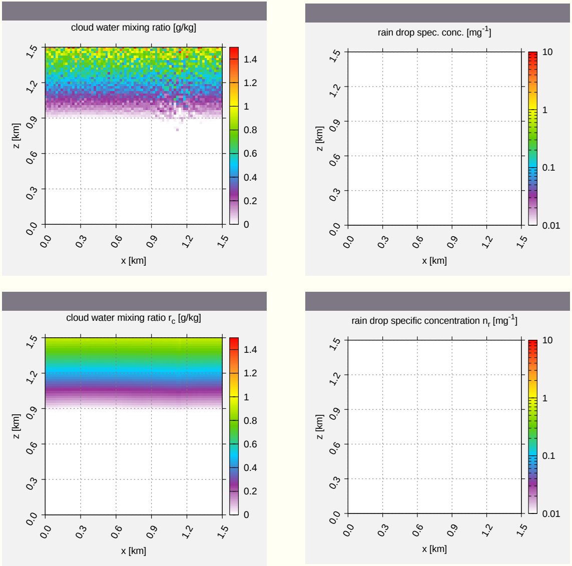
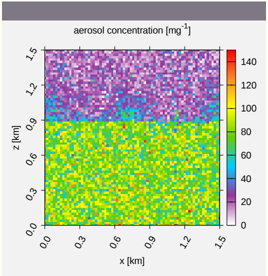
libcloudph++: example simulation (Arabas et al. 2015)





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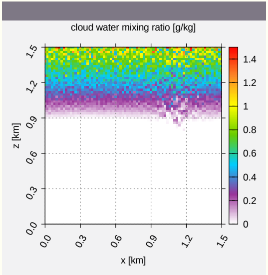

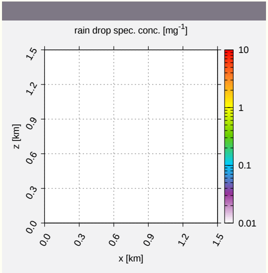

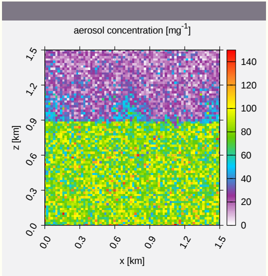

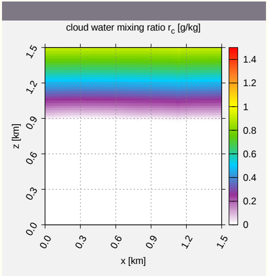

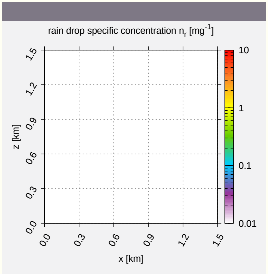

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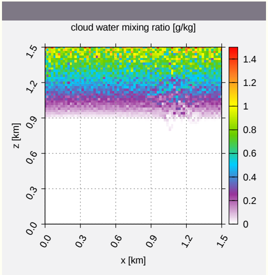

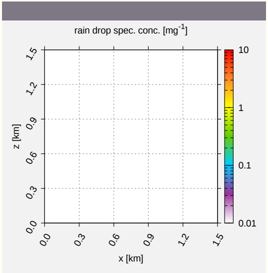

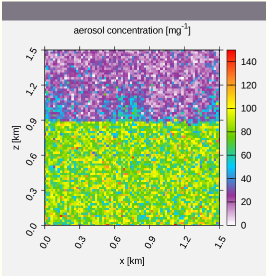

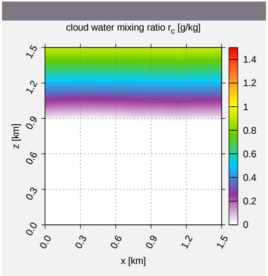

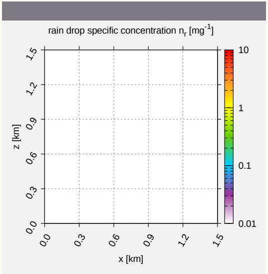

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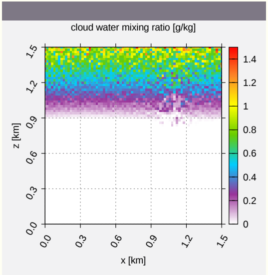

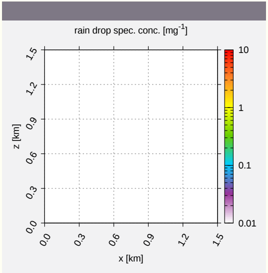

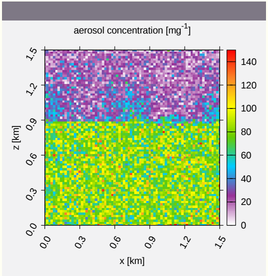

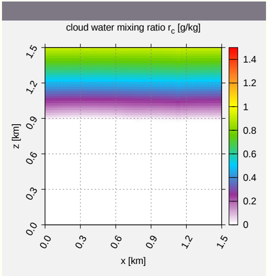

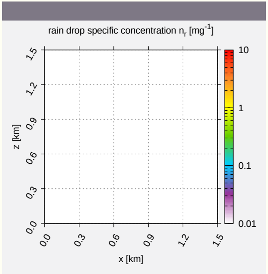

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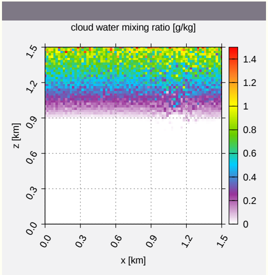

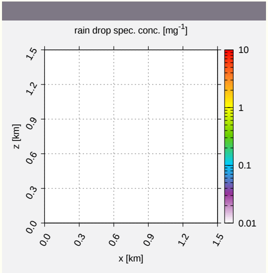

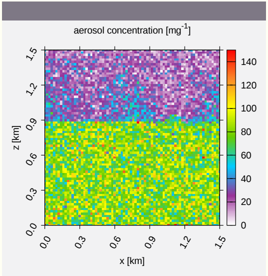

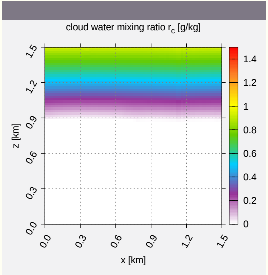

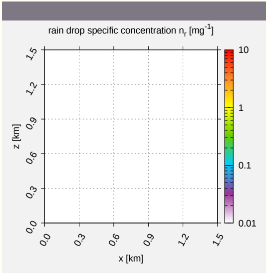

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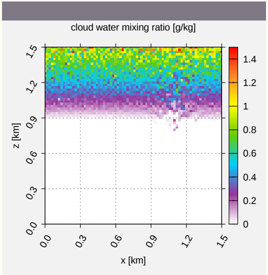

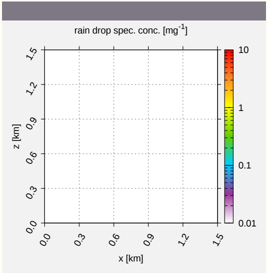

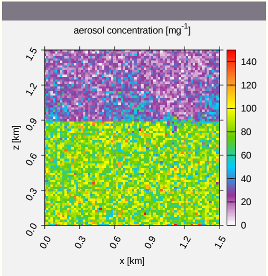

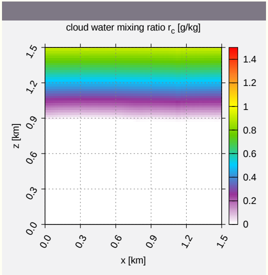

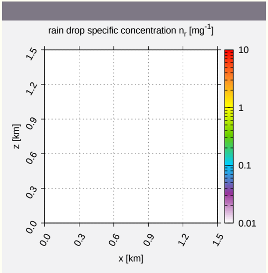

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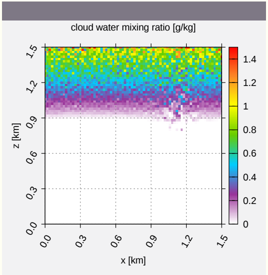

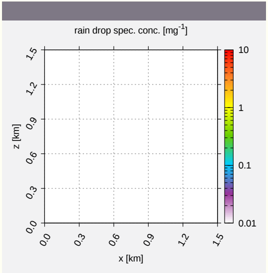

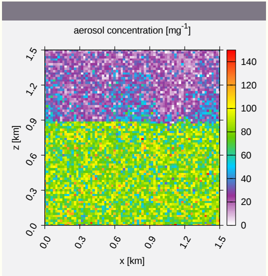

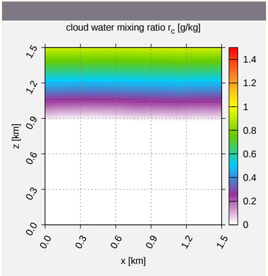

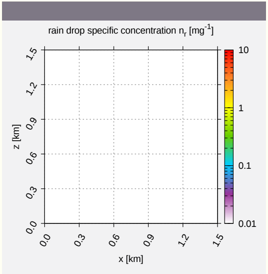

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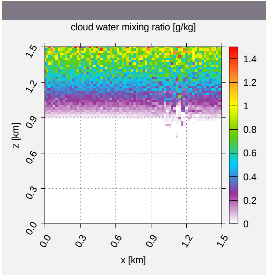

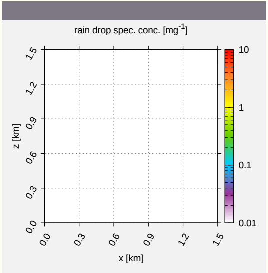

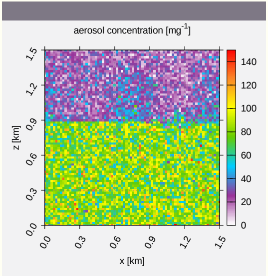

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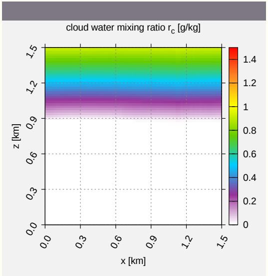

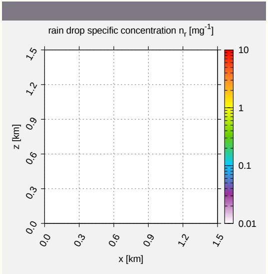

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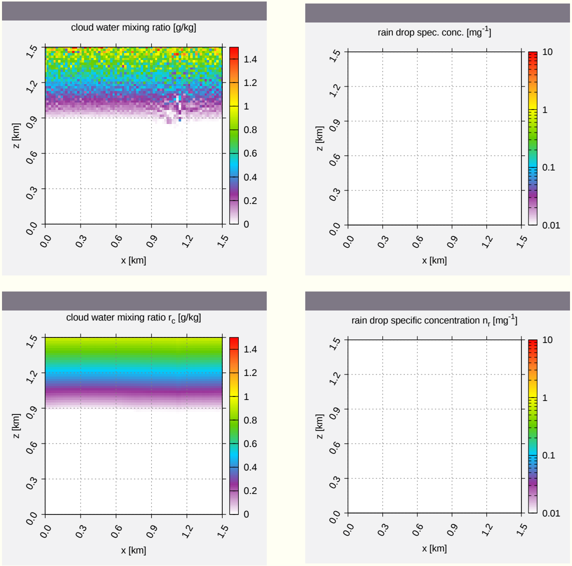

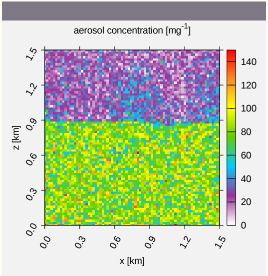

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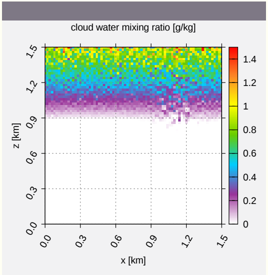

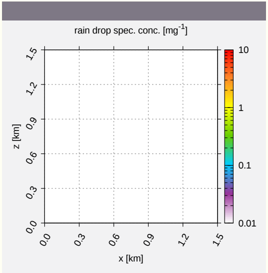

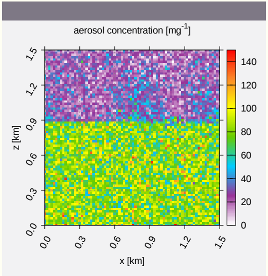

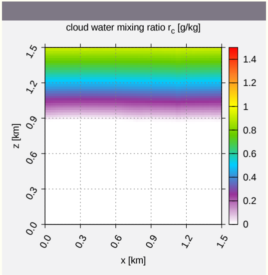

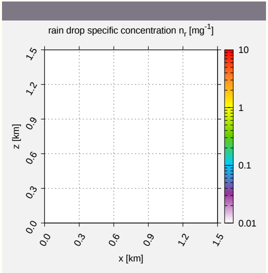

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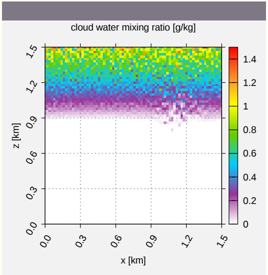

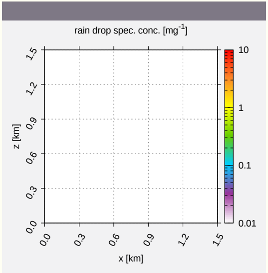

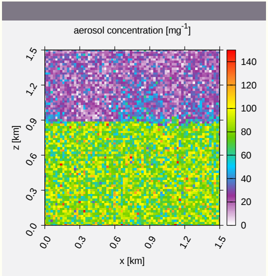

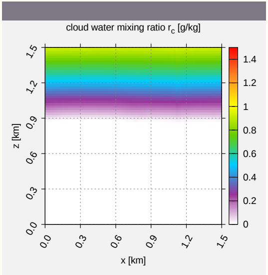

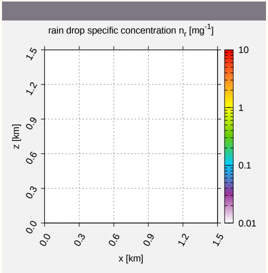

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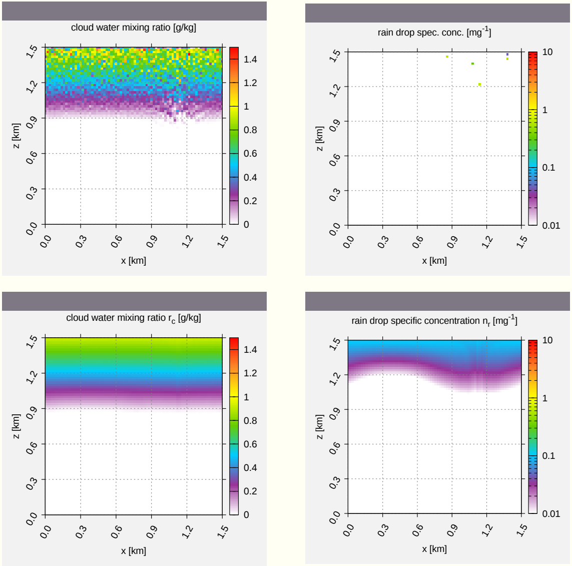

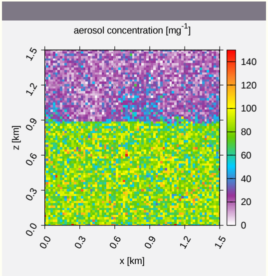

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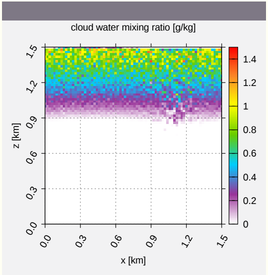

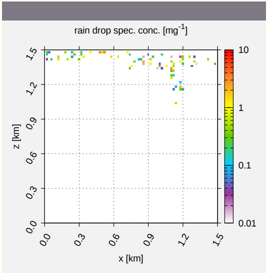

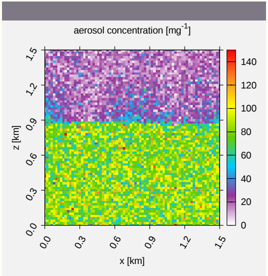

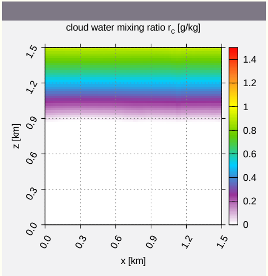

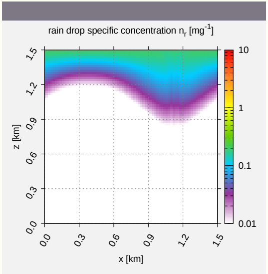

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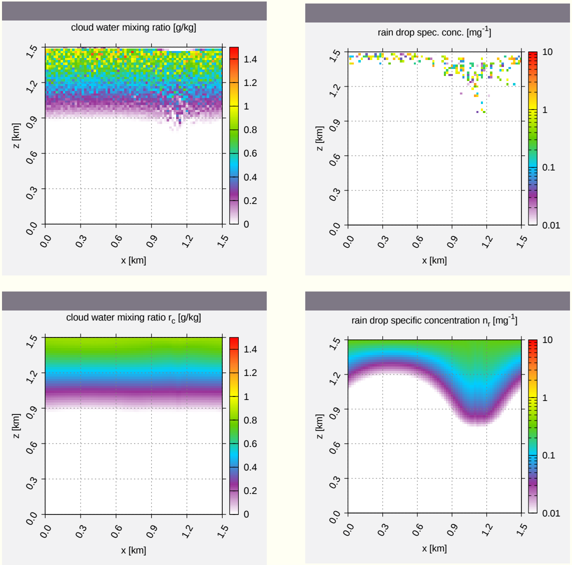

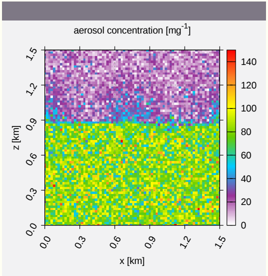

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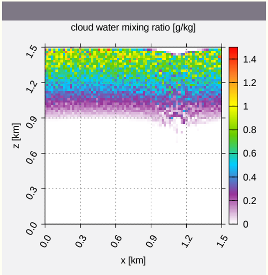

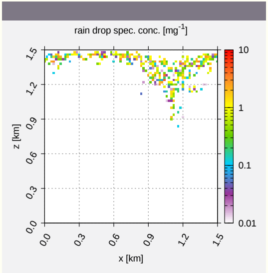

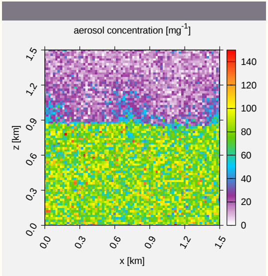

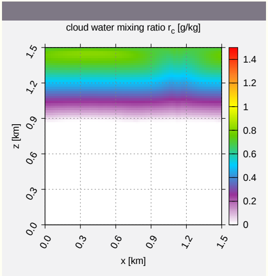

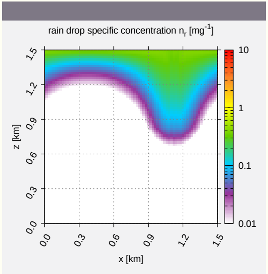

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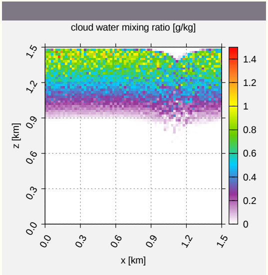
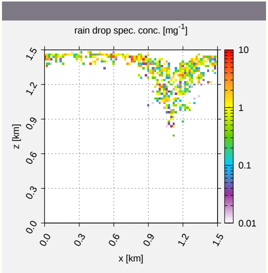
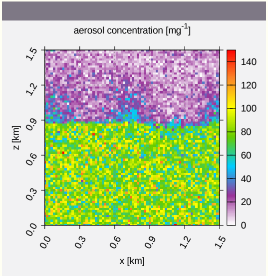
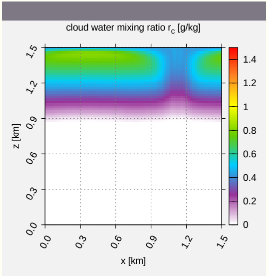
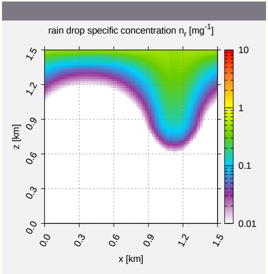






Lagrangian/Monte-Carlo scheme
(Shima et al. 2009)





2-moment bulk scheme
(Morrison & Grabowski 2007)

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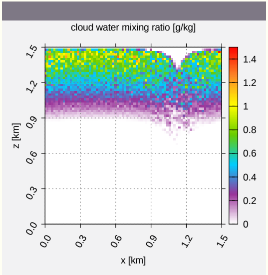

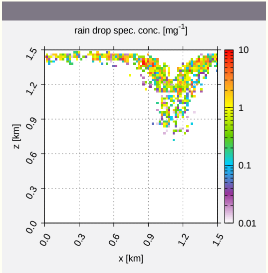

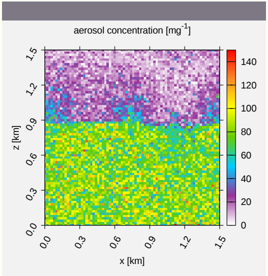

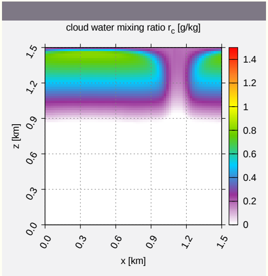

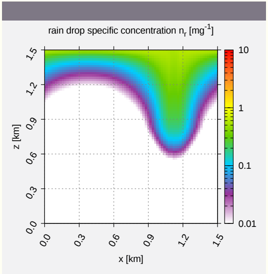

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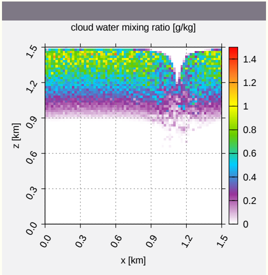

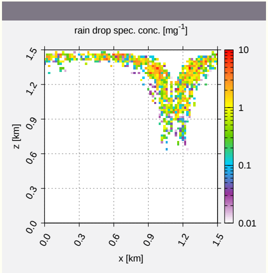

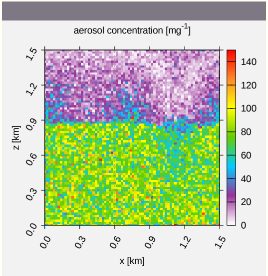

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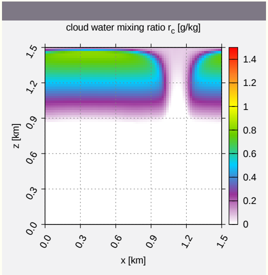

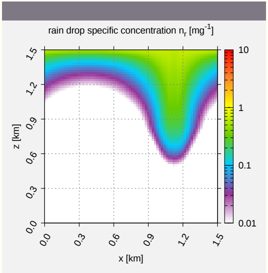

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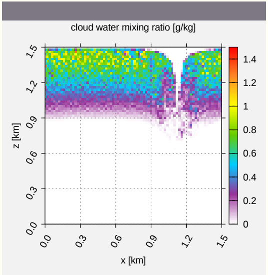

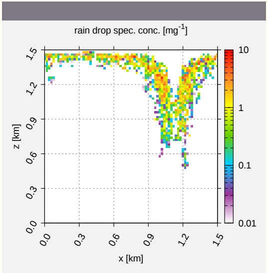

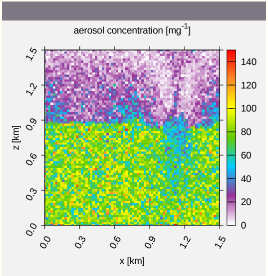

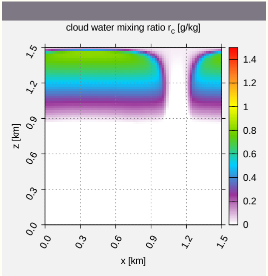

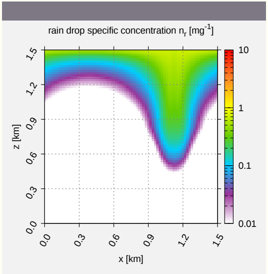

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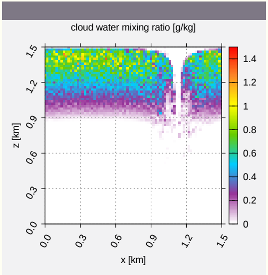

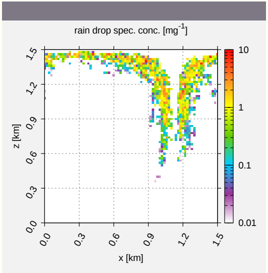

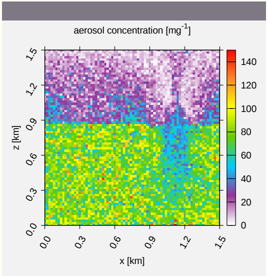

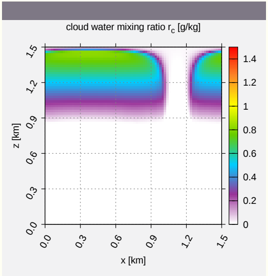

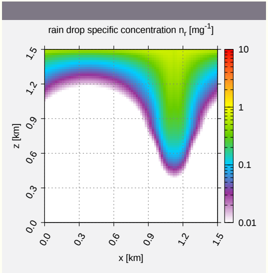

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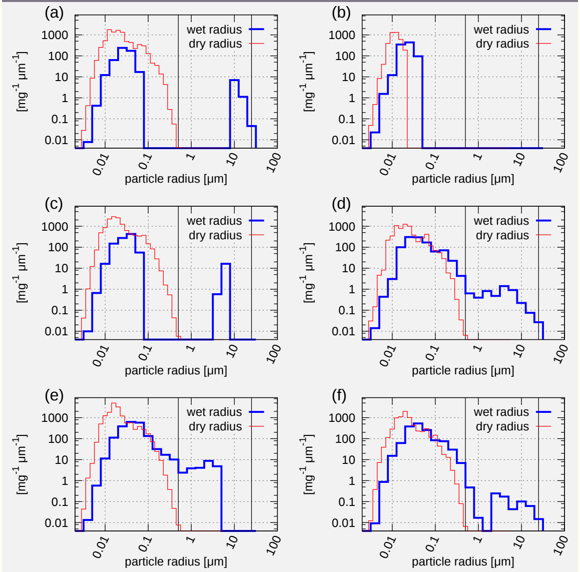
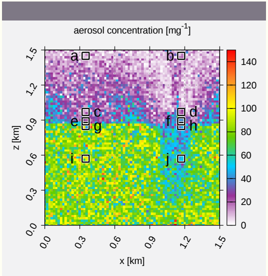
libcloudph++: example simulation (Arabas et al. 2015)

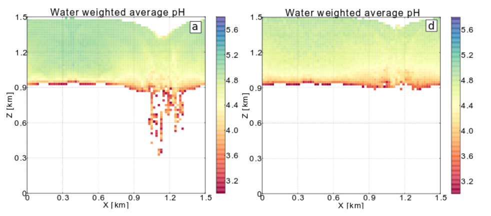
2×2 cell particle-derived spectra





libcloudph++ 2.0: Jaruga and Pawlowska 2018, GMD

Hoppel-gap resolving aqueous chemistry in particle-based μ-physics



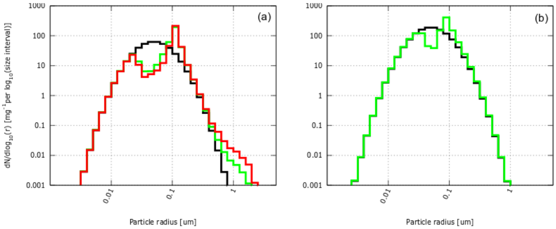


Figure 6. The size distributions of dry radii for the base case **(a)** and case3 **(b)**. The initial dry radius size distribution is marked in black, the final dry radius size distribution from grid cells with $r_c > 0.01\,\mathrm{g\,kg^{-1}}$ in green, and from grid cells with $r_r > 0.01\,\mathrm{g\,kg^{-1}}$ in red. See Tables 2 and 3 for a definition of simulation set-ups.

UWLCM: LES with libcloudph++ μ-physics

Dziekan, Waruszewski and Pawlowska 2019

Geosci. Model Dev., 12, 2587–2606, 2019
https://doi.org/10.5194/gmd-12-2587-2019

GMD | Articles | Volume 12, issue 6

Article | Assets | Peer review | Metrics | Related articles

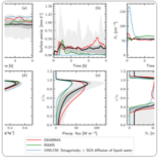
Model description paper

01 Jul 2019

University of Warsaw Lagrangian Cloud Model (UWLCM) 1.0: a modern large-eddy simulation tool for warm cloud modeling with Lagrangian microphysics

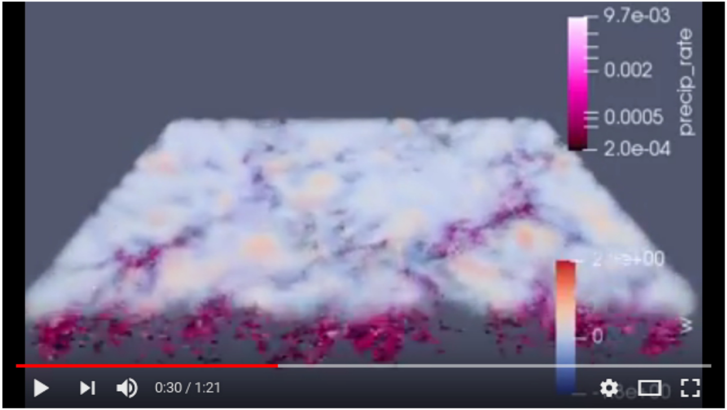
Piotr Dziekan, Maciej Waruszewski, and Hanna Pawlowska
Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland

Correspondence: Piotr Dziekan (pdziekan@fuw.edu.pl)



Received: 07 Nov 2018 – Discussion started: 04 Feb 2019 – Revised: 03 Jun 2019 – Accepted: 07 Jun 2019 – Published: 01 Jul 2019

UWLCM - DYCOMS example



`https://www.youtube.com/watch?v=BEidkhpw-MA`

libcloudph++: summary

references

- **Arabas, Jaruga, Pawlowska & Grabowski 2015** (GMD): *"libcloudph++ 1.0: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics..."*
- **Dziekan & Pawlowska 2017** (ACP): *"Stochastic coalescence in Lagrangian cloud microphysics"*
- **Grabowski, Dziekan & Pawlowska 2018** (GMD): *"Lagrangian condensation microphysics with Twomey CCN activation"*
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highlights

- GPU-resident (or multi-threaded) microphysics in C++
- Hoppel-gap resolving aqueous chemistry
- used for representing cloud μ-physics in the UWLCM LES

news: postdoc offer @ University of Warsaw (UWLCM)

met-jobs@lists.reading.ac.uk
August 2019
Message 15

Periods | Index: Date Thread Subject Author | Date: | Thread: | List Info

[Met-jobs] Postdoc position at the Institute of Geophysics, University of Warsaw

From	Gustavo Abade <Gustavo.Abade@fuw.edu.pl>
To	Met Jobs <met-jobs@lists.reading.ac.uk>
Date	Tue, 06 Aug 2019 16:03:32 +0200

Dear colleagues,

The cloud-modeling group at the Institute of Geophysics, Faculty of Physics, University of Warsaw, invites applications for a full-time postdoctoral position. The post holder is expected to join our team for 24 months. The successful candidate will work on the project entitled "Turbulent dynamics and microphysics in a Stochastic Lagrangian Cloud Model" funded by the Polish National Science Centre. The project investigates by numerical simulations the role of turbulence in the microphysical processes that shape the droplet spectrum in convective clouds. The candidate should be ready to start not later than January 2020.

Applications are due on 30 September 2019.

For further details visit:

https://www.igf.fuw.edu.pl/en/articles/oferty-pracy-i-stypendia-f/oferta-pracy-post-doc-w-insty-q2019-08-06/

open-source projects @ IGFUW

https://github.com/igfuw

cloud modelling group at IGFUW

Cloud-microphysics modelling group at the Institute of Geophysics, Faculty of Physics, University of Warsaw, Poland

Warsaw, Poland   http://foss.igf.fuw.edu.pl/

Repositories 17   Packages   People   Projects

Pinned repositories

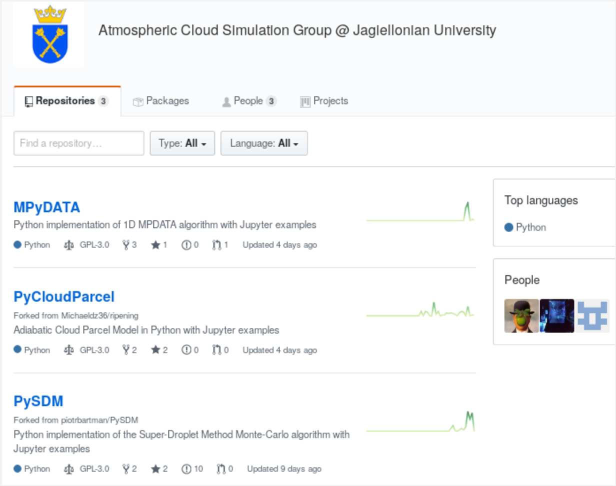
libcloudphxx
libcloudphysics++ - a library of algorithms for representing cloud microphysics in numerical models
C++ ★ 9 15

libmpdataxx
libmpdata++ - a library of parallel MPDATA-based solvers for systems of generalised transport equations
C++ ★ 9 12

UWLCM
University of Warsaw Lagrangian Cloud Model
C++ ★ 1 6

open-source projects @ atmos-cloud-sim-uj

https://github.com/atmos-cloud-sim-uj



PySDM

SDM: Monte-Carlo scheme of Shima et al. 2009

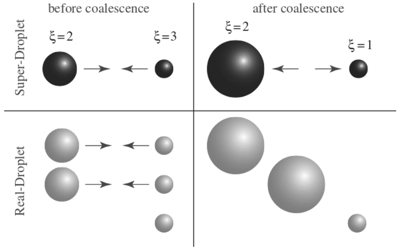
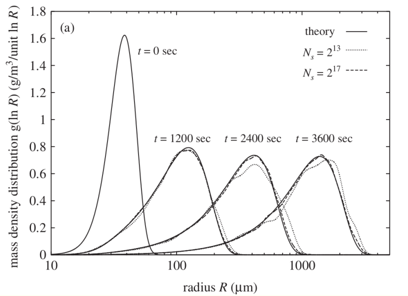
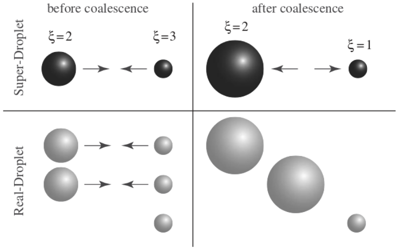


Figure 1. Schematic view of the coalescence of super-droplets. Two super-droplets with multiplicity 2 and 3 undergo coalescence (upper left panel). This represents the coalescence of two droplet pairs (lower panels). As a result, the super-droplet with multiplicity 2 becomes larger and the multiplicity of the other super-droplet decreases 3 → 1 (upper right panel).





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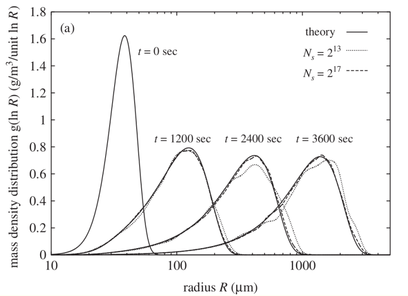

PySDM: high-performance Python implementation of SDM

motivation: journal/scientific method requirements

new 2019 GMD journal policy, doi:10.5194/gmd-12-2215-2019

motivation: journal/scientific method requirements

new 2019 GMD journal policy, doi:10.5194/gmd-12-2215-2019

- *„everything required to run the experiment must be provided, apart from the model itself"*

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- *„ensure that there is no manual processing of the data: models are run by a script, and all pre- and post-processing is scripted"*

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- *„It is the opinion of the GMD editors that if the code is not ready, then neither is the manuscript"*
- *„During the review process, the ease of model download, compilation, and running of test cases may be assessed"*

PySDM: aims

Explore tools from the Python ecosystem to simultaneously address:

- code readibility $\rightsquigarrow$ maintainability
- performance (incl. ability to leverage modern hardware)
- automation (incl. analysis and figure generation)
- dissemination (incl. ease of setting up the environment)

acceleration with Numba (JIT, multi-threading)

Numba

Numba makes Python code fast

Numba is an open source JIT compiler that translates a subset of Python and NumPy code into fast machine code.

https://numba.pydata.org/

PySDM/SDM/backends/numba.py

```
@staticmethod
@numba.njit(void(float64[:], float64[:], int64[:], int64), parallel=NUMBA_PARALLEL)
def sum_pair(data_out, data_in, idx, length):
    for i in prange(length // 2):
        data_out[i] = data_in[idx[2 * i]] + data_in[idx[2 * i + 1]]
```

acceleration with ThrustRTC and CURandRTC (GPU)

https://github.com/thrust/ (C++)
https://fynv.github.io/ (Python/C++/C#/Java)

PySDM/SDM/backends/thrustRTC.py

```
@staticmethod
def sum_pair(data_out, data_in, idx, length):
    perm_in = trtc.DVPermutation(data_in, idx)

    loop = trtc.For(['arr_in', 'arr_out'], "i", "arr_out[i] = arr_in[2 * i] + arr_in[2 * i + 1];")

    loop.launch_n(length // 2, [perm_in, data_out])
```

Pythran: ahead-of-time compilation, OpenMP

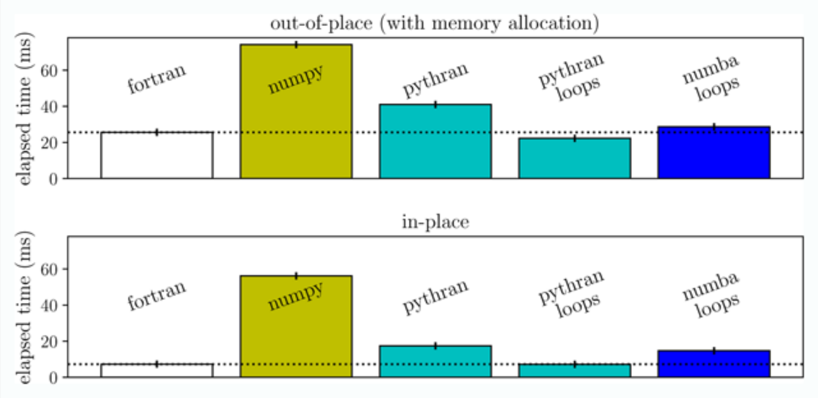
https://pythran.readthedocs.io/

PySDM/SDM/backends/pythran.py

```python
# pythran export sum_pair(float64[:], float64[:], int64[:], int)
def sum_pair(data_out, data_in, idx, length):
    # omp parallel for
    for i in range(length // 2):
        data_out[i] = data_in[idx[2 * i]] + data_in[idx[2 * i + 1]]
```

Pythran vs. Numba vs. Fortran ...

Mohanan et al. 2019, doi:10.5334/jors.238



demo (github.com/atmos-cloud-sim-uj/PySDM)

README.md

PySDM

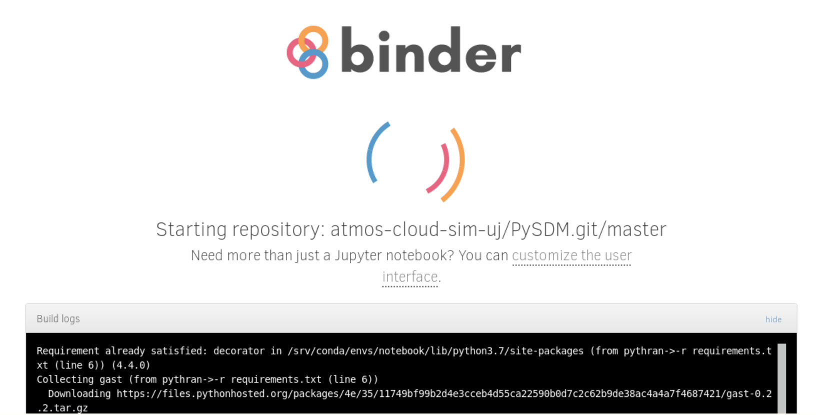
Python implementation of the Super-Droplet Method Monte-Carlo algorithm
Jupyter notebook examples.

build passing coverage 54%

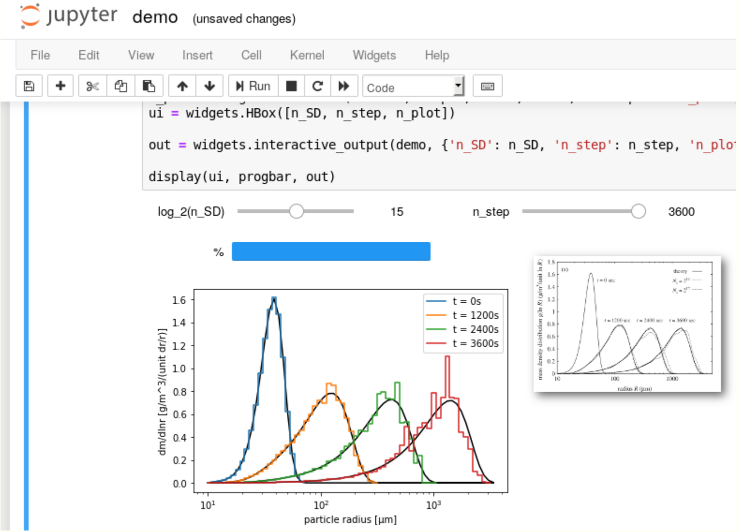
Demo:

- Shima et al. 2009 Fig 2 launch binder render nbviewer

demo (mybinder.org)



demo (ipywidgets)



고맙습니다

Thank you for your attention!

funding acknowledgement:
Foundation for Polish Science / European Union