libcloudph++: warm-rain cloud microphysics in C++

Sylwester Arabas

cloud-aerosol modelling team
Faculty of Physics, University of Warsaw

foss.igf.fuw.edu.pl

TU Delft, Jan. 15th 2015

Plan of the talk

- “HARMONIA” project: goals and the team
- libcloudph++: design choices and their rationale
- libcloudph++: Lagrangian “super-droplet” μ-physics
- libcloudph++ / DALES coupling

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Hanna Pawłowska, Piotr Smolarkiewicz & Wojtek Grabowski

develop a new LES tool for aerosol-cloud interactions research

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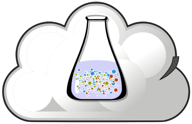

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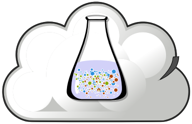

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- overseas:
  - prof. Piotr Smolarkiewicz @ ECMWF
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  - Dorota Jarecka @ NCAR (postdoc)

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why not to develop everything from scratch:

- have to wait 3 years before tackling scientific problems

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libmpdata++ & libcloudph++

project target

LES-type tool featuring:

- robust numerics (MPDATA)
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current "products" – C++ libraries

libmpdata++ parallel solvers for systems of transport equations

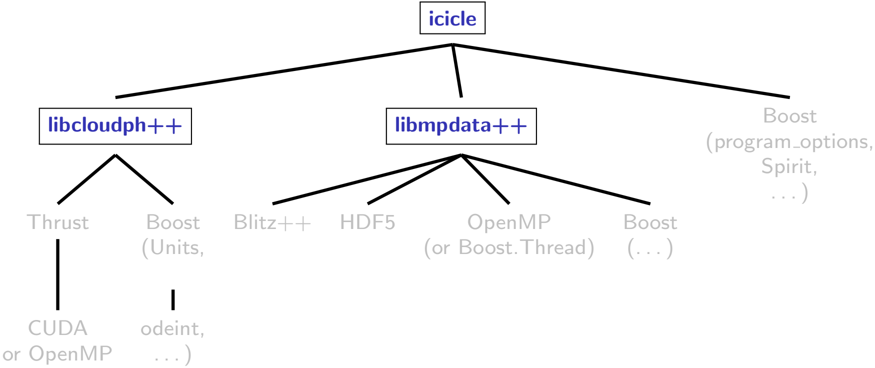
- `http://libmpdataxx.igf.fuw.edu.pl/`
- doi:10.5194/gmdd-7-8179-2014

libcloudph++ aerosol/cloud μ-physics algorithm collection

- `http://libcloudphxx.igf.fuw.edu.pl/`
- doi:10.5194/gmdd-7-8275-2014

a few words on first design choices

- structure the code into “standalone” libraries



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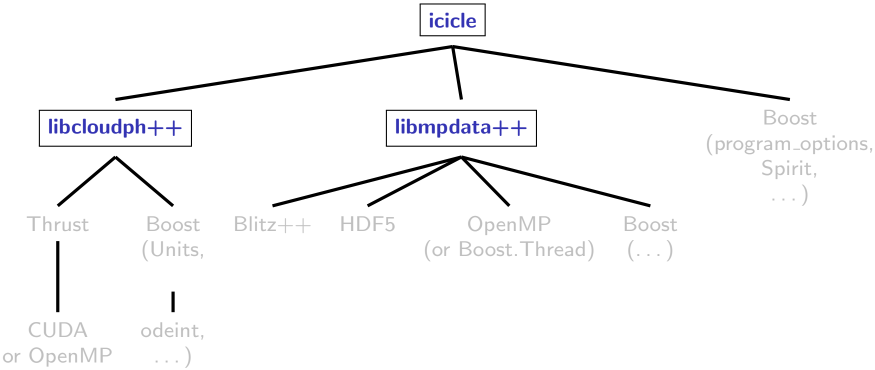

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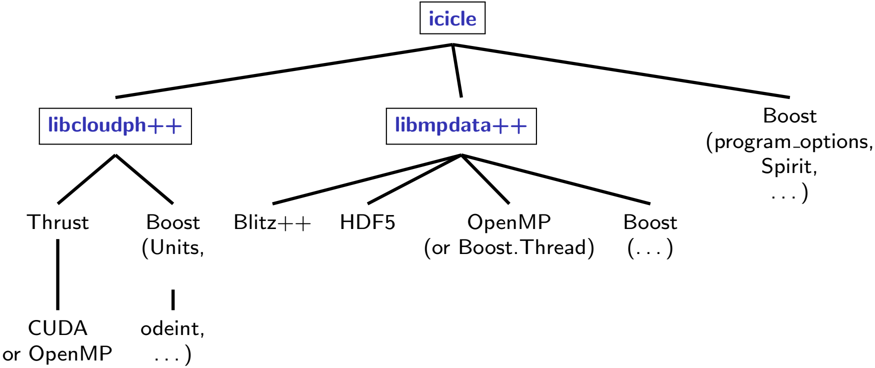

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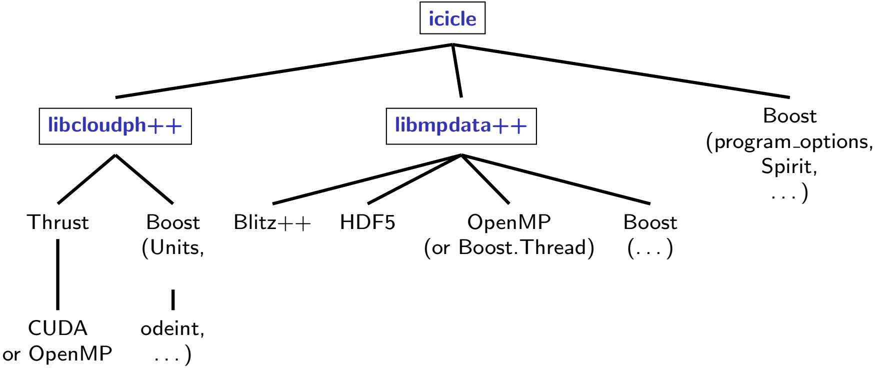
- leverage existing **reusable** software
  ⇝ save time, benefit from state-of-the-art components



libcloudph++ components

- single-moment bulk saturation-adjustment scheme
  with Kessler's coalescence

- double-moment bulk scheme with predicted supersaturation
  (Morrison & Grabowski 2007)

- particle-based scheme with Monte-Carlo coalescence
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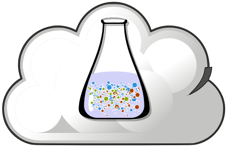

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- aqueous chemistry

- precipitation
- wet deposition
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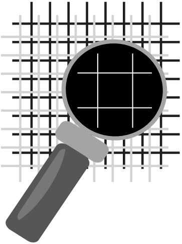
Eulerian vs. Lagrangian μ-physics



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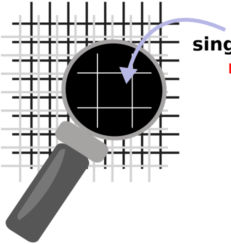

single-moment bulk

no influence of aerosol on cloud

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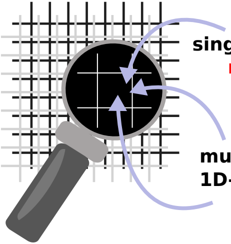

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multi-moment bulk, 1D-bin

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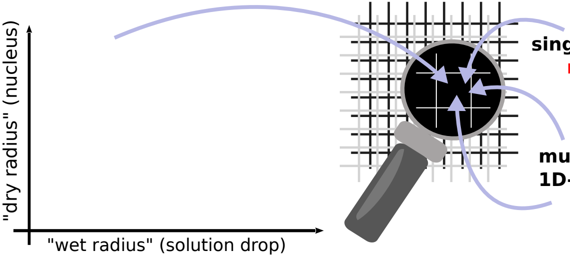

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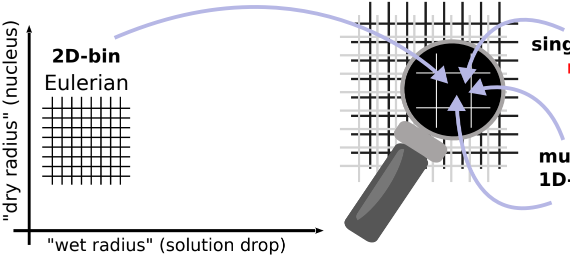

2D-bin

Eulerian

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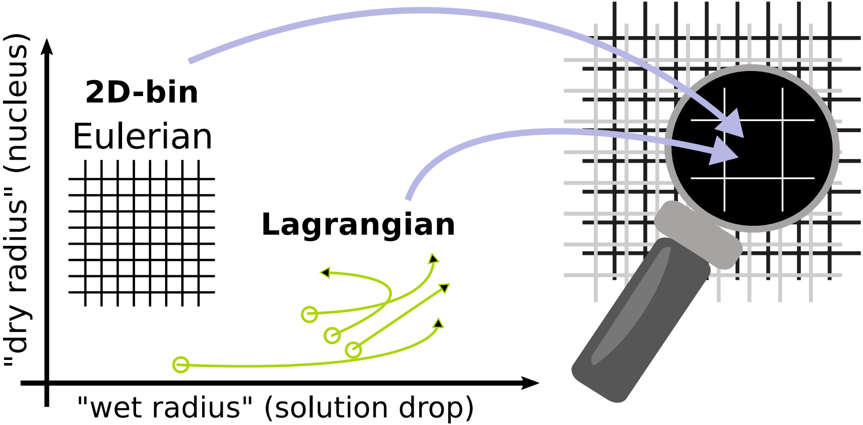
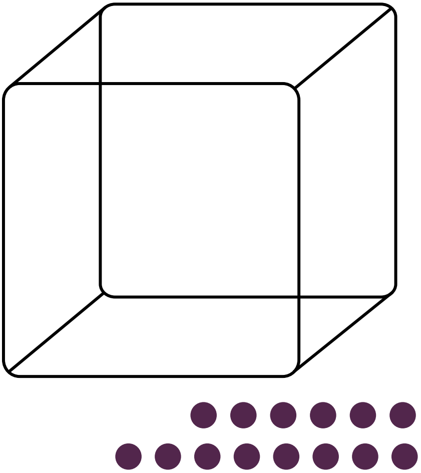


Lagrangian μ-physics: key concepts



The domain is populated with "information carriers" (alias computational particles, super droplets)

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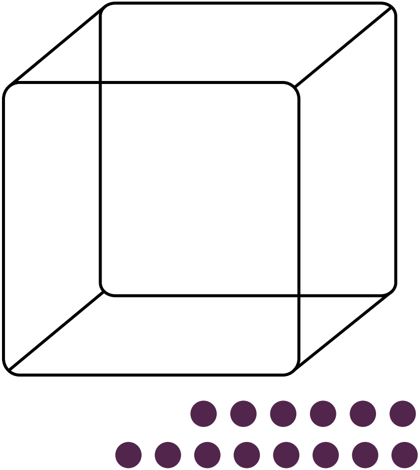

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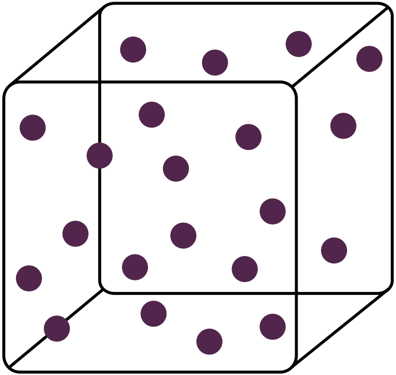

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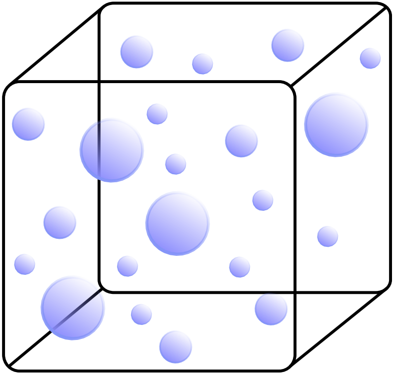

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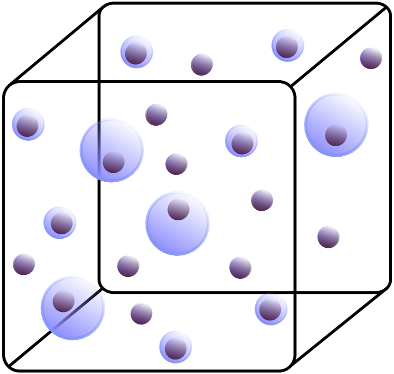

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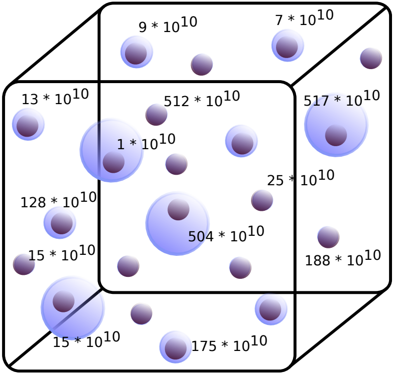

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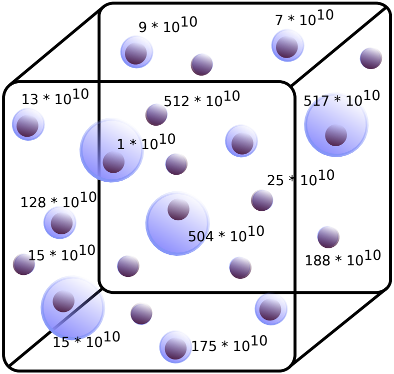

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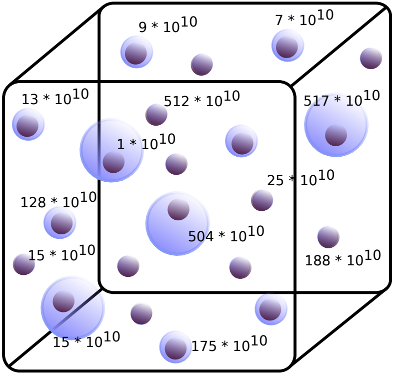

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transport does not incur numerical diffusion!

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	collisional growth
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- recent examples in context of precipitating clouds:
  - Shima et al. 2009, QJ
  - Andrejczuk et al. 2010, JGR
  - Riechelmann et al. 2012, NJP

Monte-Carlo coalescence scheme (Shima et al. 2009)

- for all n super-droplets in a grid box of volume ΔV in timestep Δt

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where r – drop radii, $E(r_i, r_j)$ – collection efficiency, v – drop velocities

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- extensive parameters summed ($\rightsquigarrow$ conserved), intensive averaged

Monte-Carlo coalescence scheme (Shima et al. 2009)

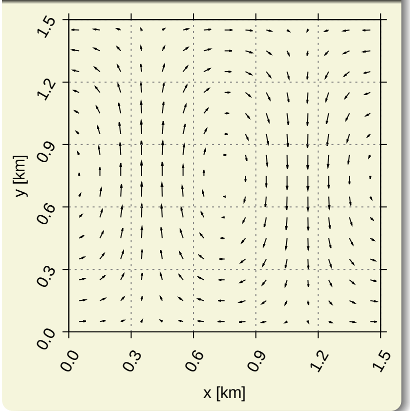
- for all n super-droplets in a grid box of volume ΔV in timestep Δt
- each representing ξ real particles (aerosol/cloud/drizzle/rain)
- the probability of coalescence of i-th and j-th super-droplets is:

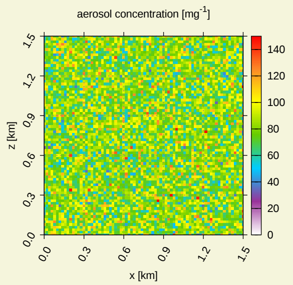
$$P_{ij} = max(\xi_i, \xi_j) \cdot \underbrace{E(r_i, r_j) \cdot \pi(r_i + r_j)^2 \cdot |v_i - v_j|}_{\text{coalescence kernel}} \cdot \frac{\Delta t}{\Delta V} \cdot \frac{n \cdot (n-1)}{2} / \left[\frac{n}{2}\right]$$

  where r – drop radii, $E(r_i, r_j)$ – collection efficiency, v – drop velocities
- coalescence takes place once in a number of timesteps (def. by P_{ij})
- all min(ξ_i,ξ_j) droplets coalesce
  $\rightsquigarrow$ there's always a "bin" of the right size to store the collided particles
- collisions triggered by comparing a uniform random number with P_{ij}
- extensive parameters summed ($\rightsquigarrow$ conserved), intensive averaged
- [n/2] random non-overlapping (i,j) pairs examined instead of all (i,j) pairs
  cost: $O(n^2) \rightsquigarrow O(n)$, probability upscaled by $\frac{n \cdot (n-1)}{2} / \left[\frac{n}{2}\right]$

libcloudph++: VOCALS-inspired aerosol processing set-up

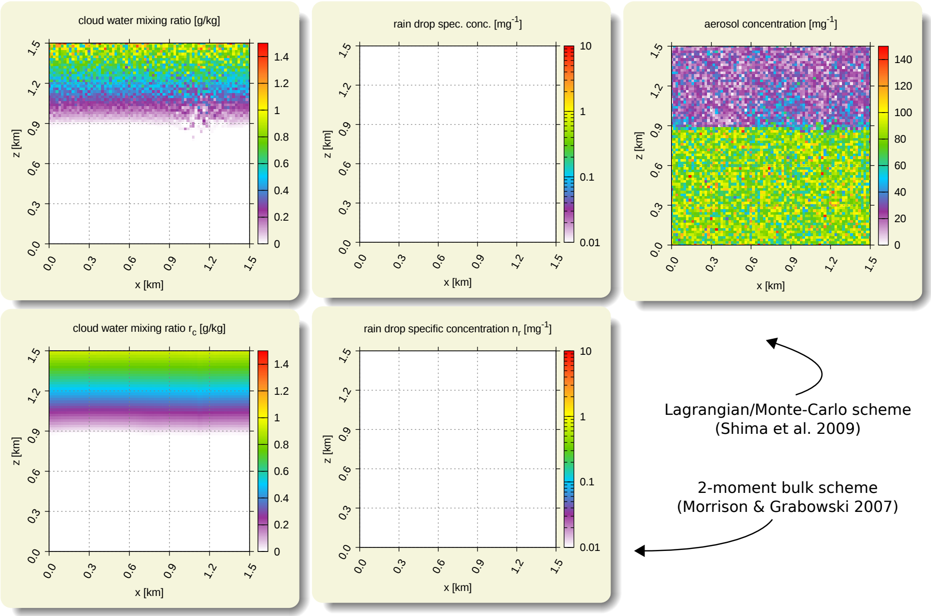
single-eddy velocity field





- set-up: Grabowski & Lebo (ICMW 2012)
- 2D prescribed flow
- advection: libmpdata++ (2-pass FCT)
- μ-physics: libcloudph++

libcloudph++: VOCALS-inspired aerosol processing set-up



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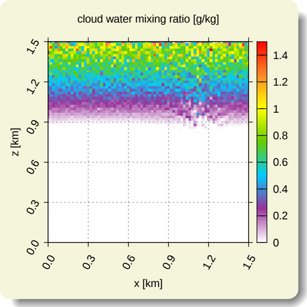

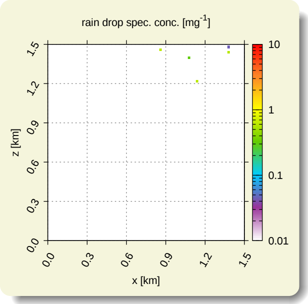

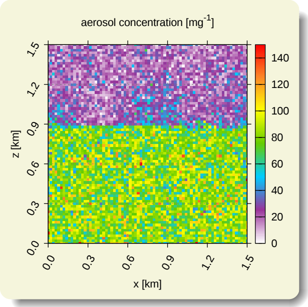

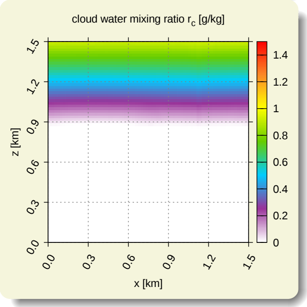

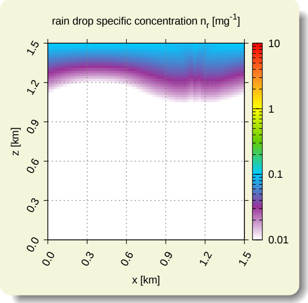

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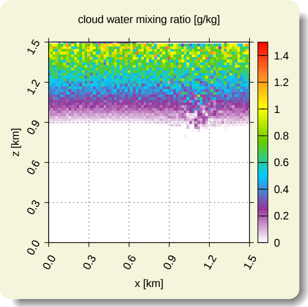

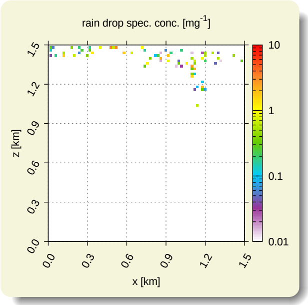

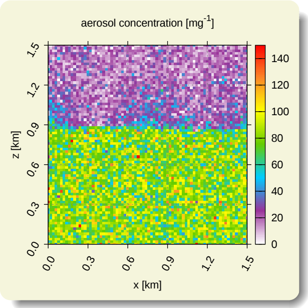

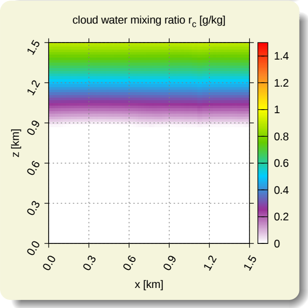

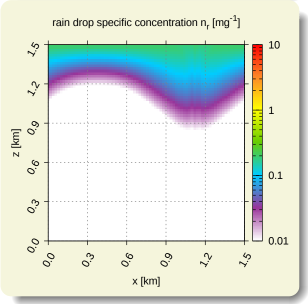

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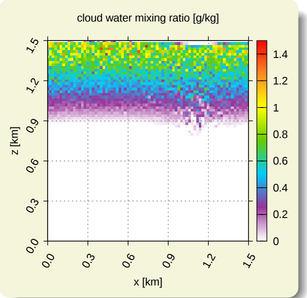

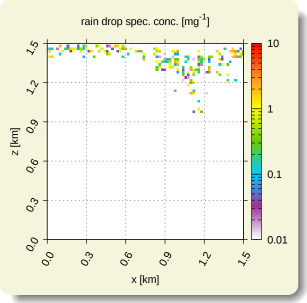

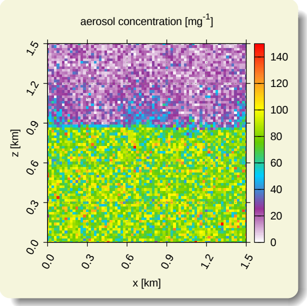

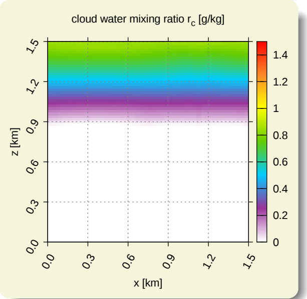

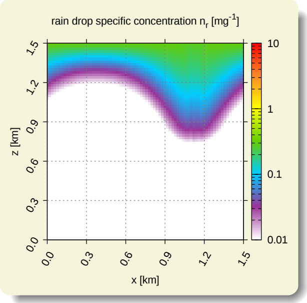

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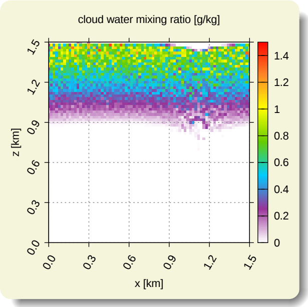
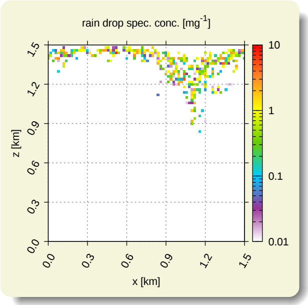
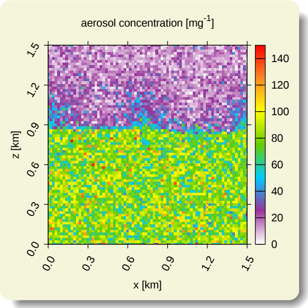
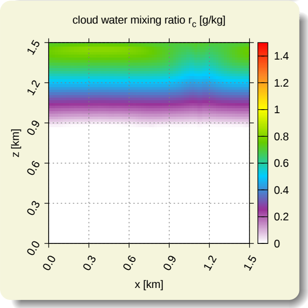
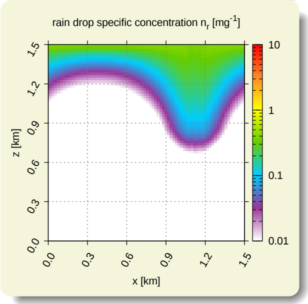

cloud water mixing ratio [g/kg]


rain drop spec. conc. [mg^{-1}]


aerosol concentration [mg^{-1}]


cloud water mixing ratio r_c [g/kg]


rain drop specific concentration n_r [mg^{-1}]

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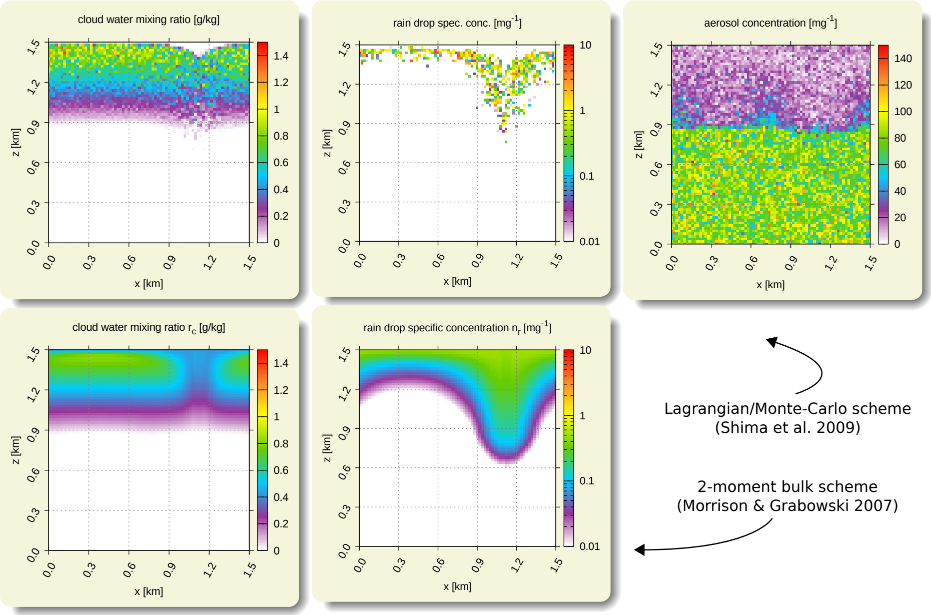

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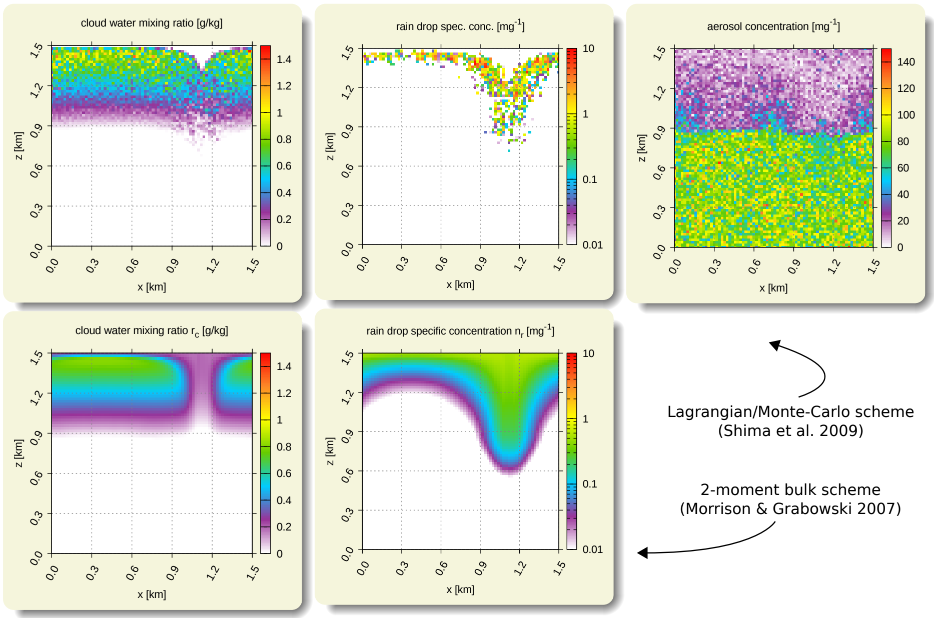

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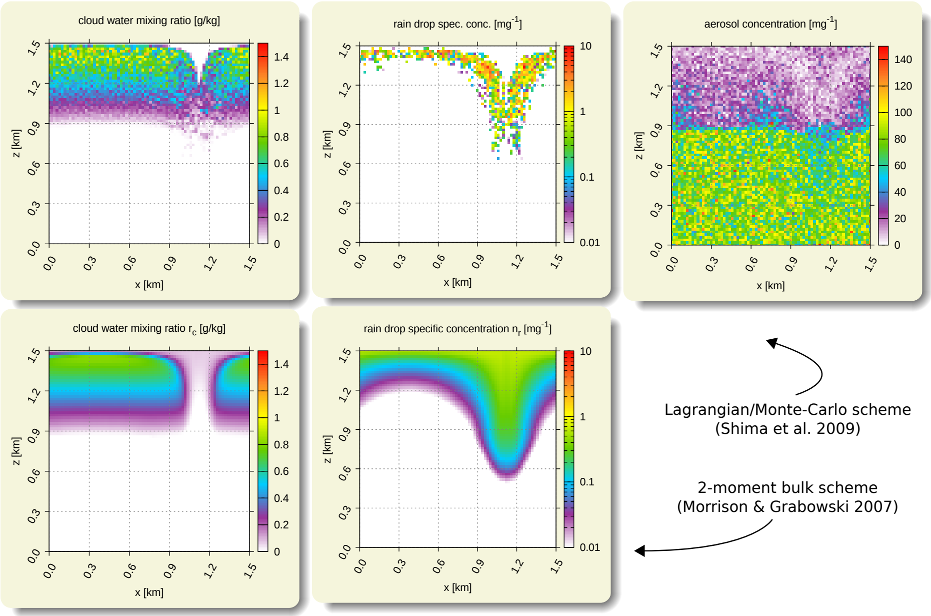

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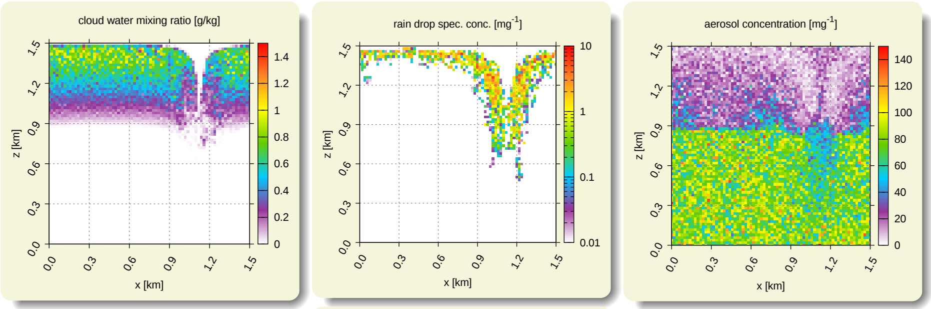

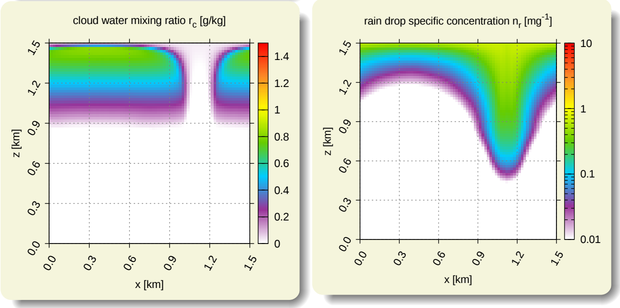

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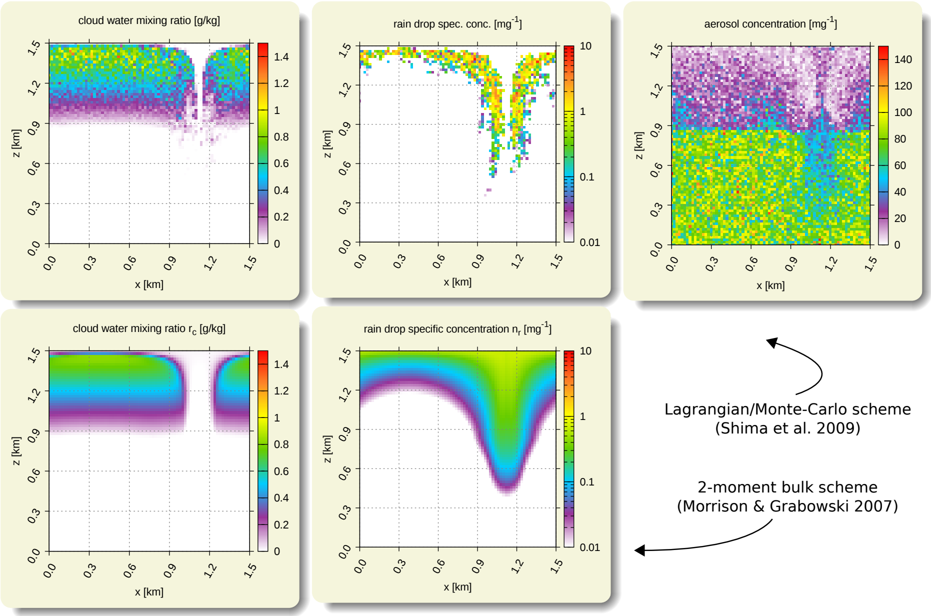

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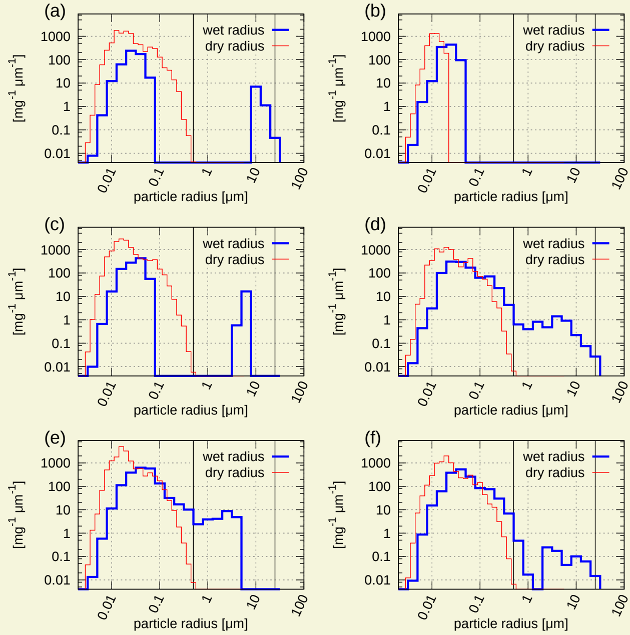
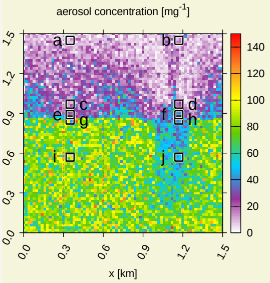
2×2 cell particle-derived spectra





libcloudph++: summary & some technicalities

key features:

- three schemes (all written from scratch):
    - 1-moment: Kessler
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- 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

Plan of the talk

- “HARMONIA” project: goals and the team
- libcloudph++: design choices and their rationale
- libcloudph++: Lagrangian “super-droplet” μ-physics
- libcloudph++ / DALES coupling

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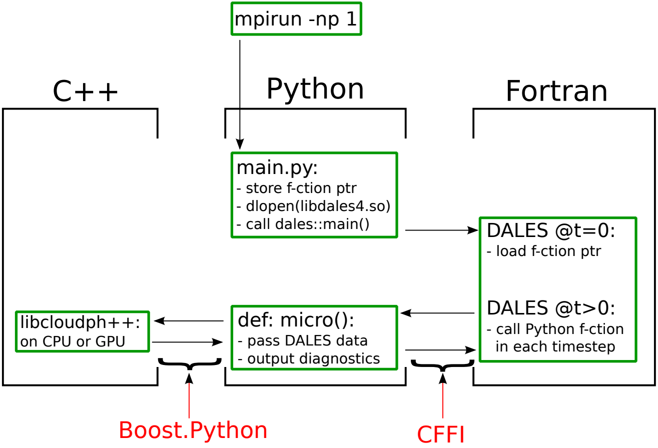


mpirun -np 1

C++

Python

Fortran

main.py:
- store f-ction ptr
- dlopen(libdales4.so)
- call dales::main()

DALES @t=0:
- load f-ction ptr

DALES @t>0:
- call Python f-ction in each timestep

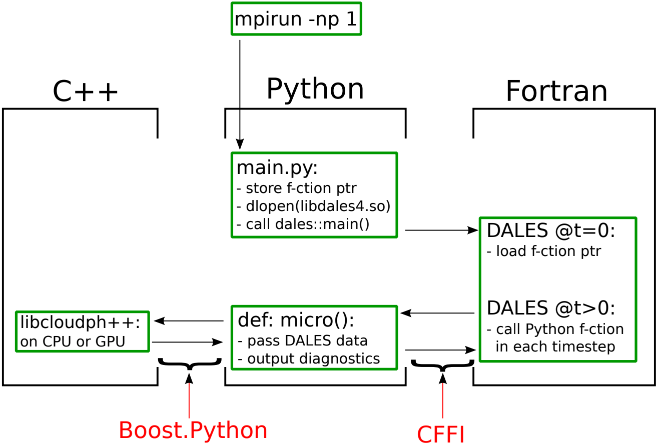
libcloudph++: on CPU or GPU

def: micro():
- pass DALES data
- output diagnostics

Boost.Python

CFFI

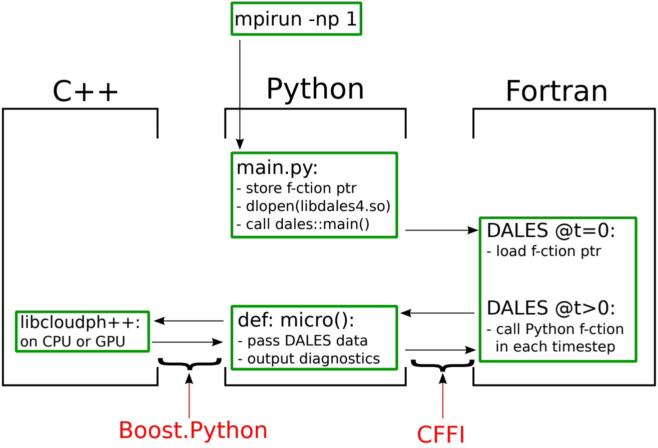
DALES/libcloudph++ coupling: technicalities



rationale:

- minimal changes to DALES
- no changes to libcloudph++
- interfacing C++ & Fortran from Python using pre-existing packages

DALES/libcloudph++ coupling: technicalities



acknowledgement:

- the Python-Fortran coupling concept & code by Dorota Jarecka

DALES/libcloudph++ coupling: "physics"

libcloudph++/Lagrangian:

- $q_v(t; x, y, z)$
- $\theta_d(t; x, y, z) = \left({}^{p_0}/_{p_d}\right)^{R_d/c_{pd}}$
- $\rho_d(z)$ or $\rho_d(t; z) = \frac{p_d}{R_d T}$
- $\rho\vec{u}(t; x, y, z)$
- supersaturation allowed ($q_v \neq q_s$)

DALES/bulk:

- $q_t(t; x, y, z) = q_v + q_l$
- $\theta_l(t; x, y, z) = \theta - q_l \frac{L}{c_{pd}}$
- $\rho_b(z)$ & $\rho(t; z)/\pi(t; z)$
- $\vec{u}(t; x, y, z)$
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- $\rho_d(z) = \rho_d\left(\pi\big|_{t=0}\,,\ \bar{q}_t\big|_{t=0}\,,\ \bar{\theta}_l\big|_{t=0}\right)$
- $q_v = q_t - \overbrace{\sum_{i\in cell} \frac{{}^4\!/_3\ \pi\ n_i\ r_i^3 \rho_w}{\Delta v\ \ \rho_d}}^{q_l}$ ⇝ no $q_v = q_s$ assumption
- $\theta_d = \underbrace{\left(\theta_l + \frac{q_t - q_v}{\pi}\,\frac{L}{c_{pd}}\right)}_{\theta} \cdot \left(1 + q_v\,\frac{R_v}{R_v}\right)^{R_d/c_{pd}}$
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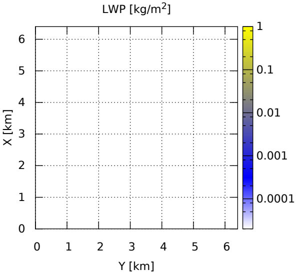
DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

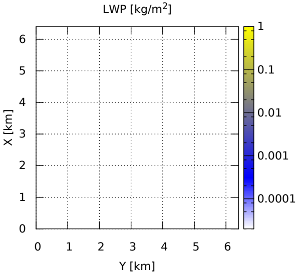
DALES (BOMEX, bulk μ-physics, t=17m)

LWP [kg/m^2]

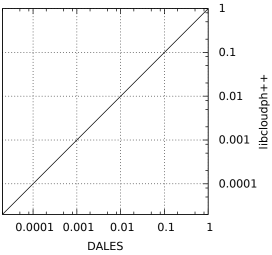


off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

LWP [kg/m^2]

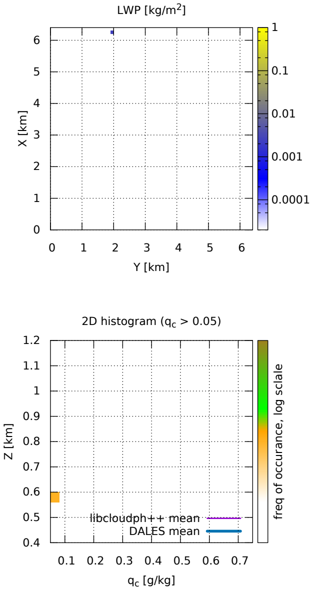


LWP [kg/m^2] (scatter plot)

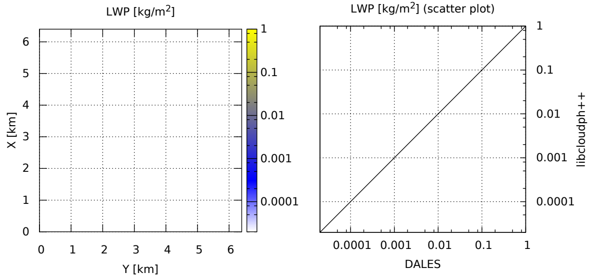


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=18m)

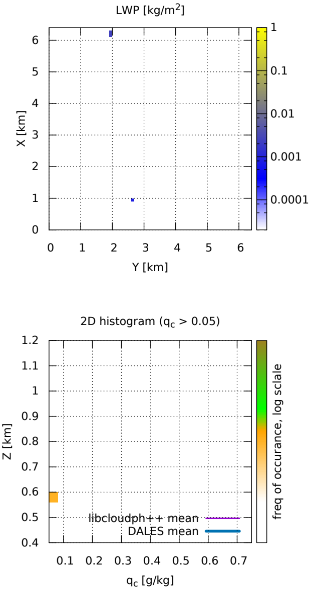


off-line libclouph++ Lagrangian/Monte-Carlo μ-physics on a GPU

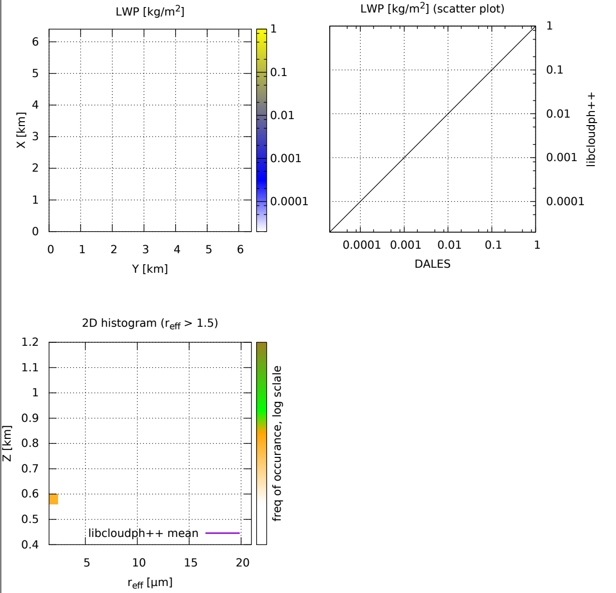


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=19m)

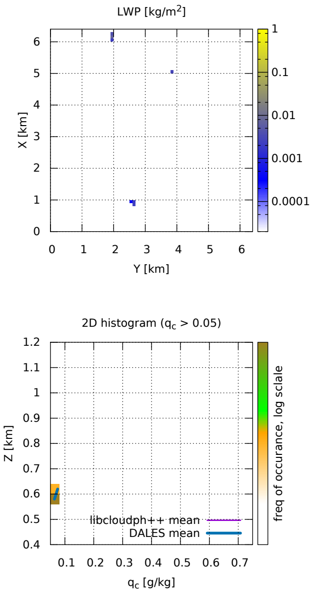


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

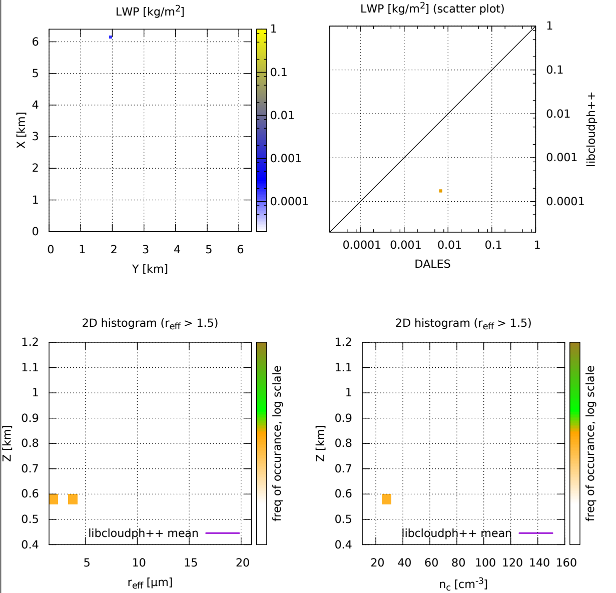


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=20m)

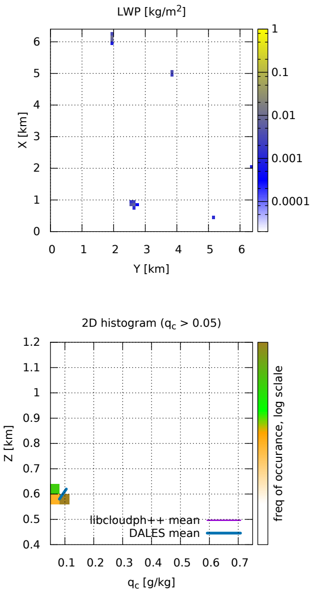


off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

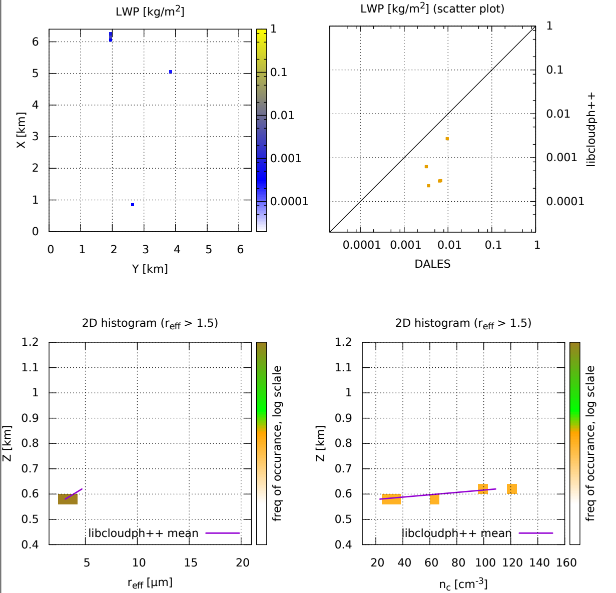


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=21m)

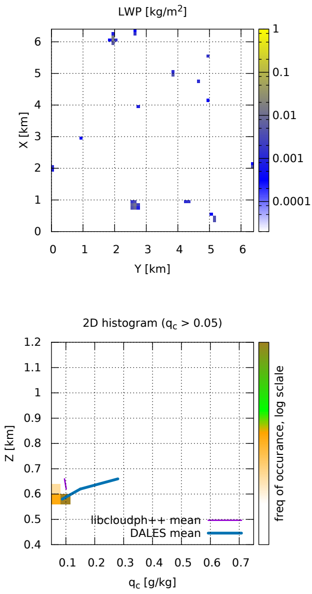


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

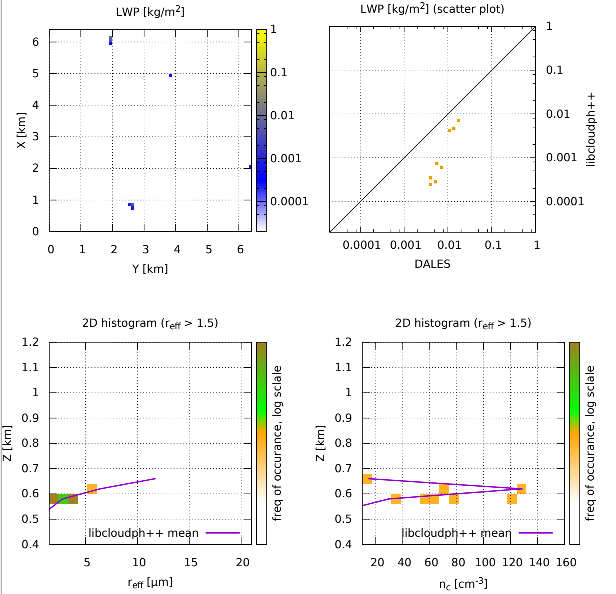


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=22m)

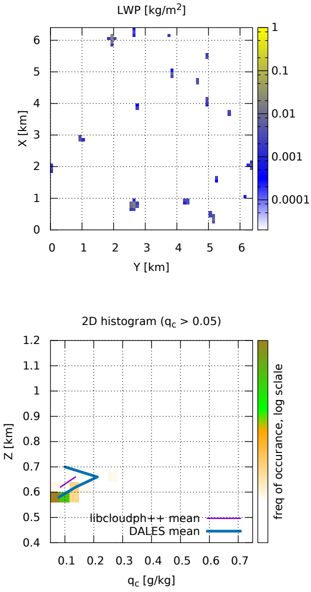


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

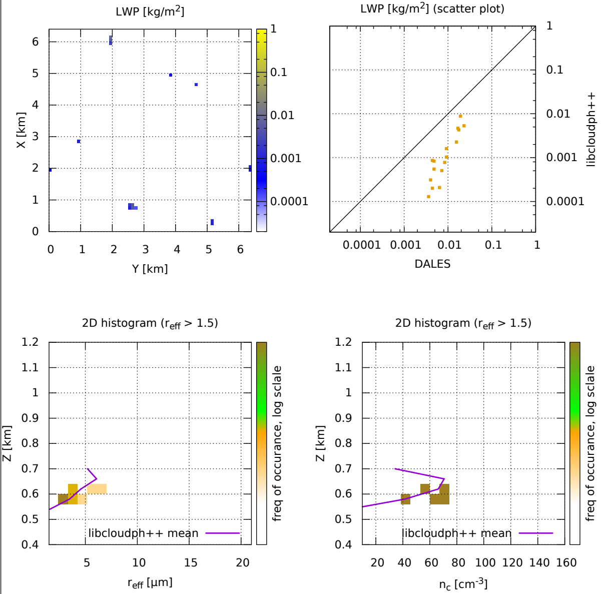


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=23m)

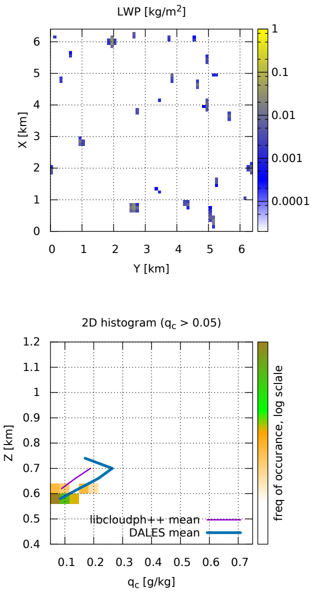


off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

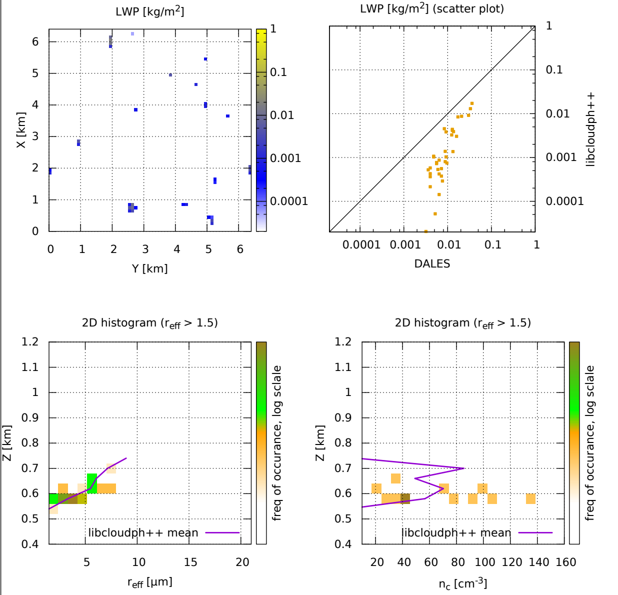


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=24m)

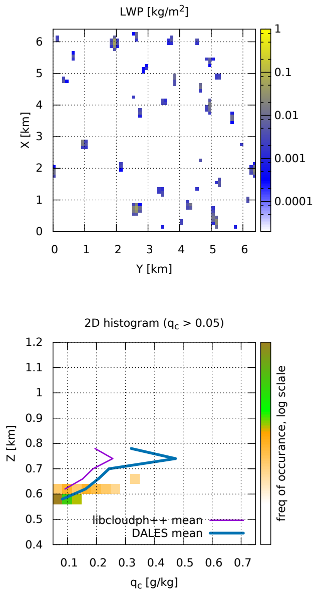


off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

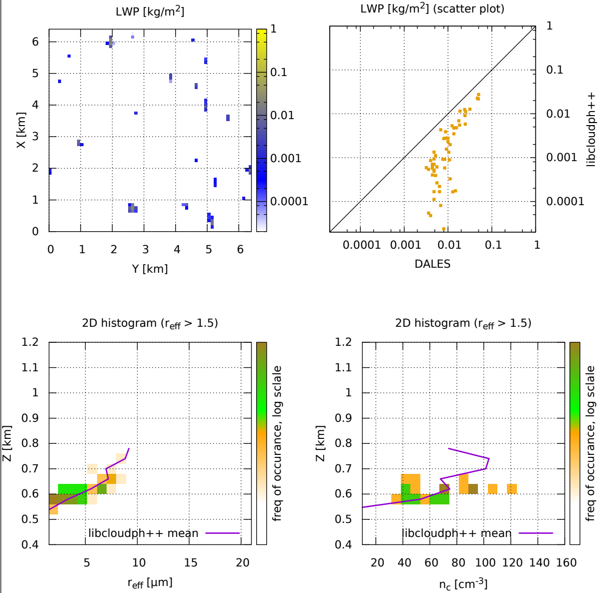


DALES/libcloudph++: proof-of-concept test ($\mathrm{dt}_{\mathrm{adv}}$=20s, $\mathrm{dt}_{\mathrm{cond}}$=0.5s, dz=40m, 10 SD/cell)

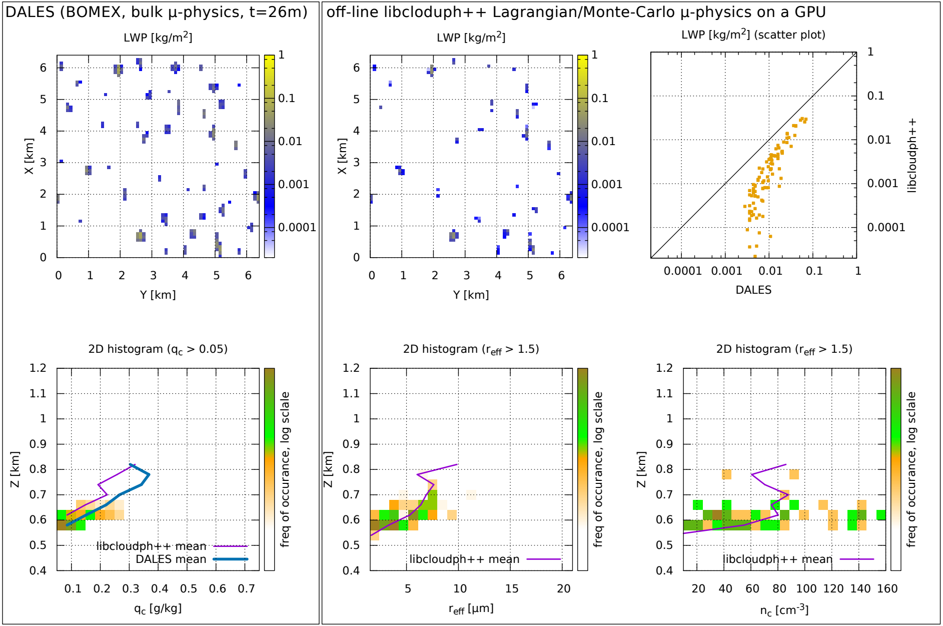
DALES (BOMEX, bulk μ-physics, t=25m)



off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU



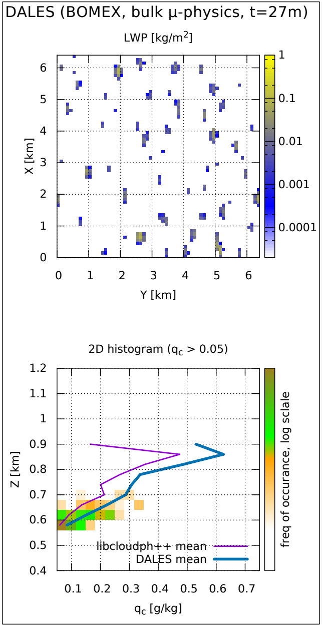
DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)



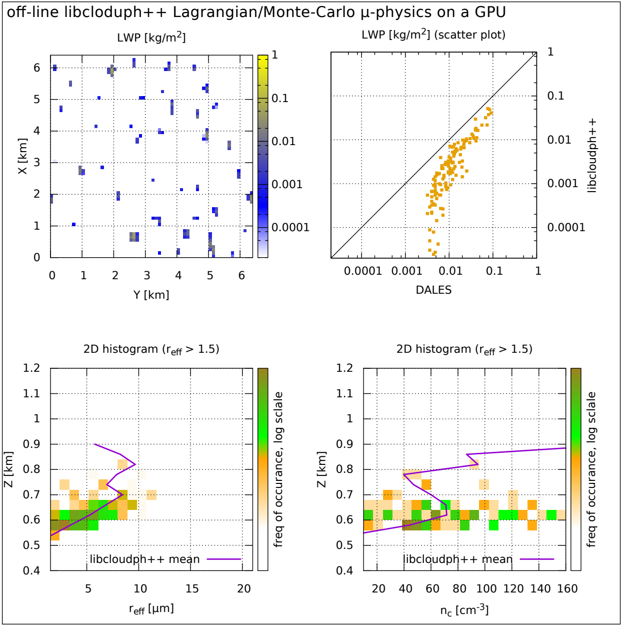
DALES (BOMEX, bulk μ-physics, t=26m)

off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

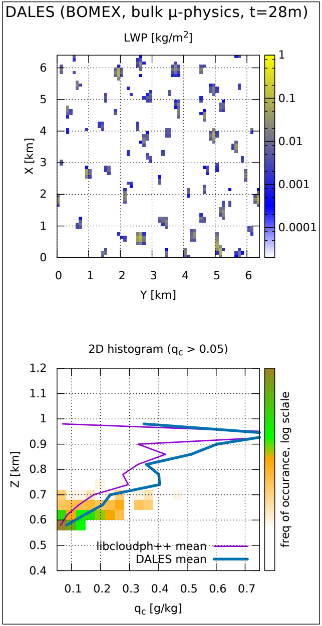


DALES (BOMEX, bulk μ-physics, t=27m)

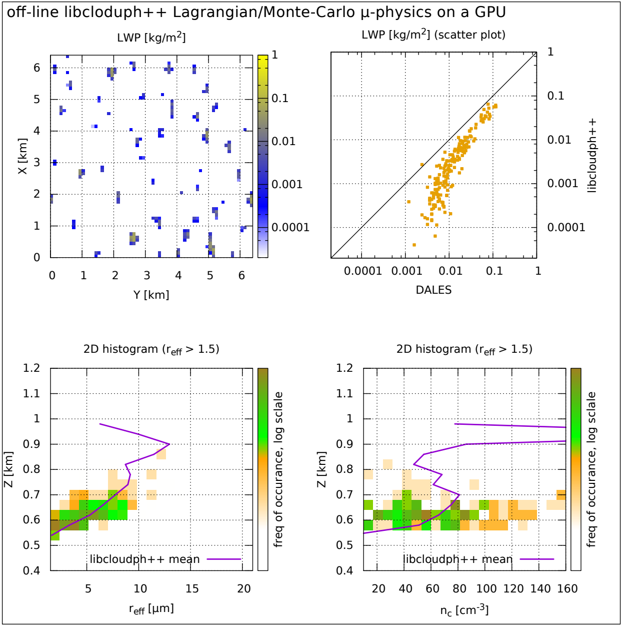


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)



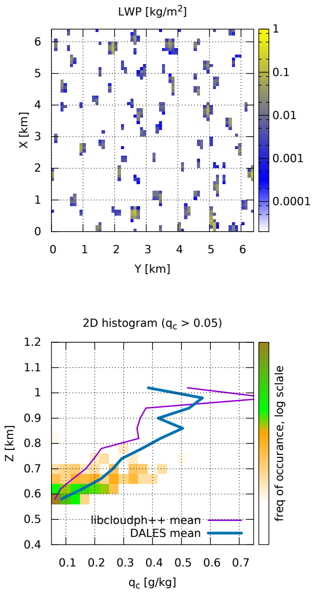
DALES (BOMEX, bulk μ-physics, t=28m)



off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

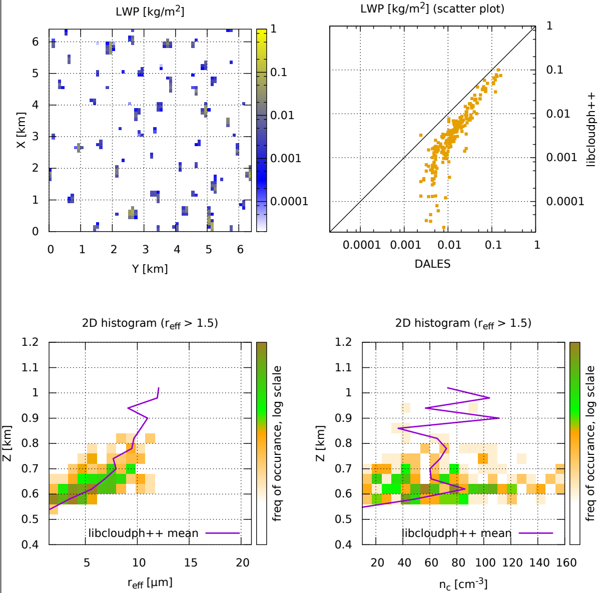
DALES (BOMEX, bulk μ-physics, t=29m)



LWP [kg/m^2]

2D histogram (q_c > 0.05)

off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU



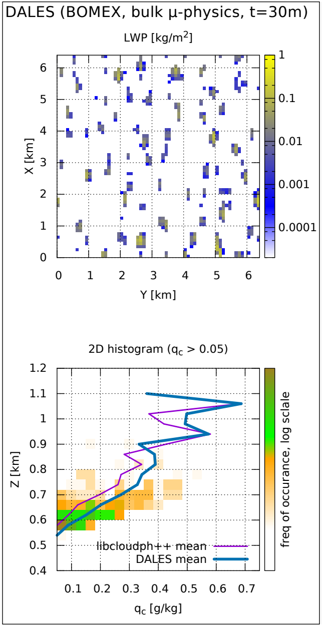
LWP [kg/m^2]

LWP [kg/m^2] (scatter plot)

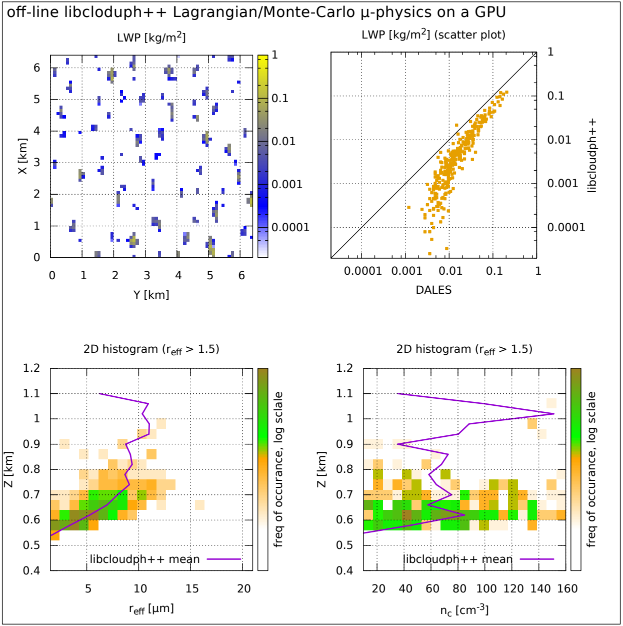
2D histogram (r_{eff} > 1.5)

2D histogram (r_{eff} > 1.5)

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)



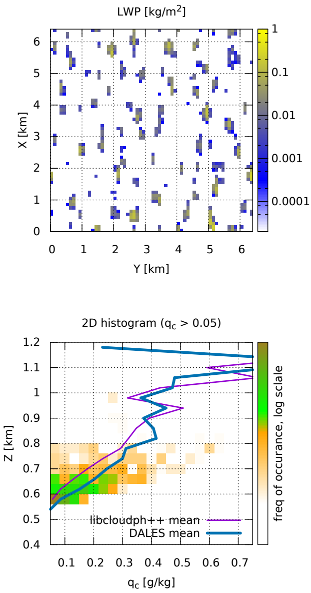
DALES (BOMEX, bulk μ-physics, t=30m)



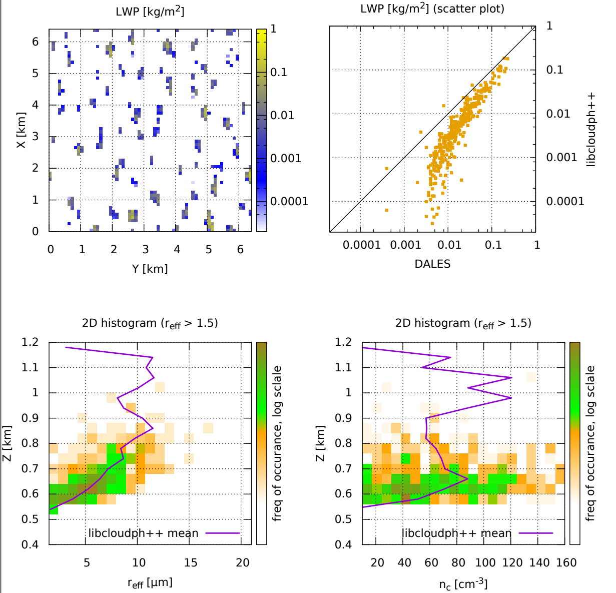
off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

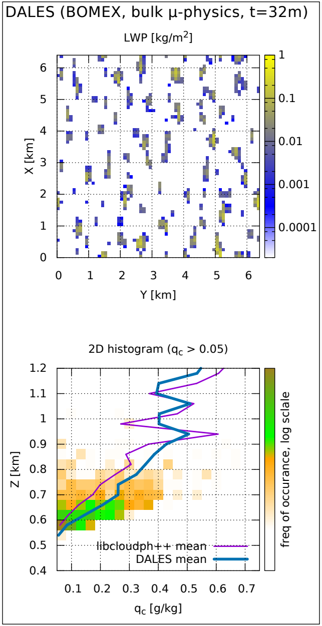
DALES (BOMEX, bulk μ-physics, t=31m)



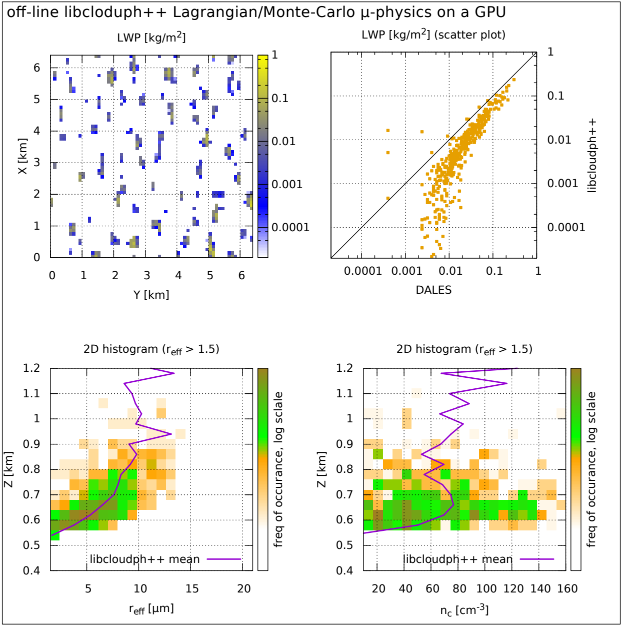
off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU



DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)



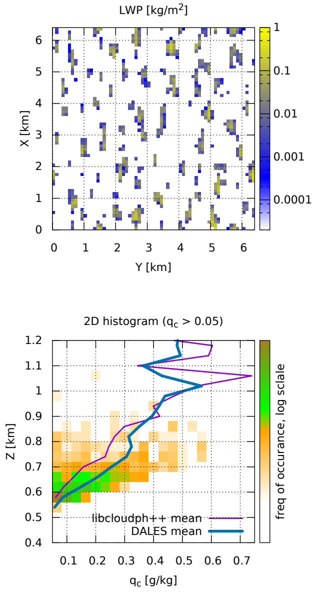
DALES (BOMEX, bulk μ-physics, t=32m)



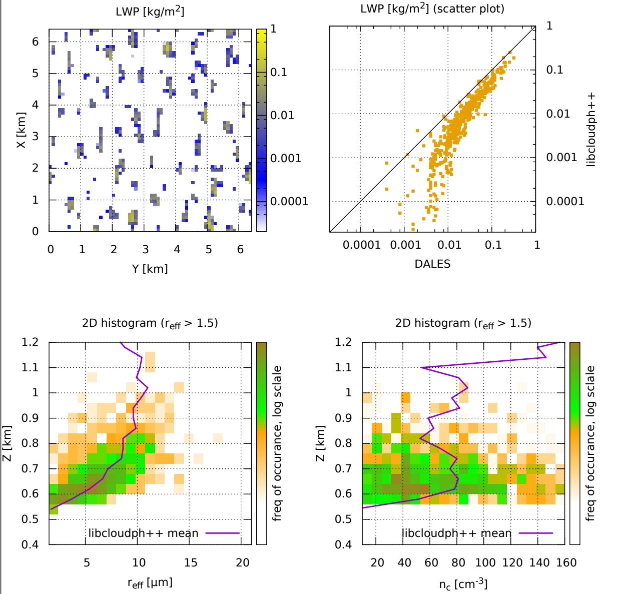
off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

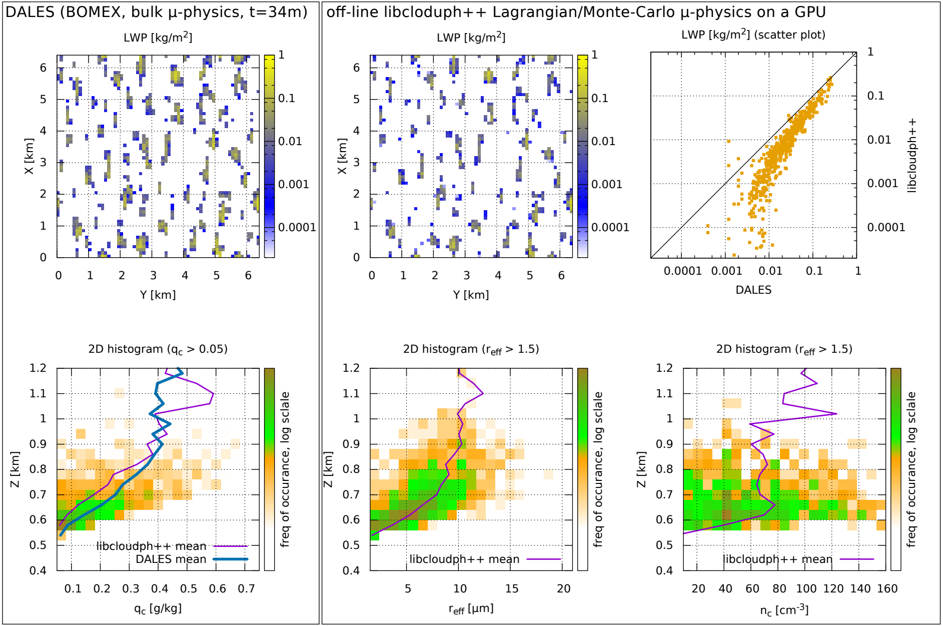
DALES (BOMEX, bulk μ-physics, t=33m)



off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU



DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

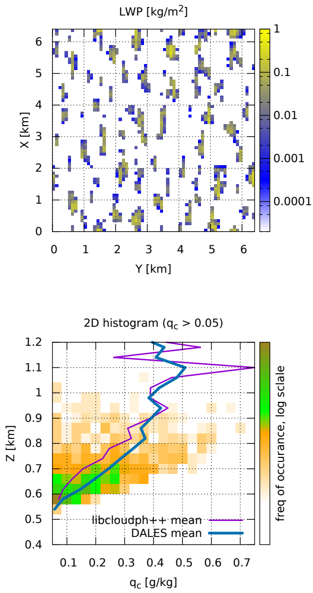


DALES (BOMEX, bulk μ-physics, t=34m)

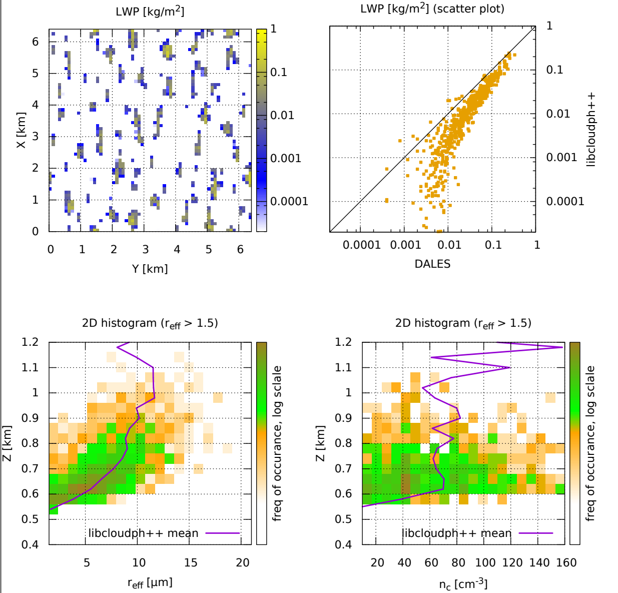
off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

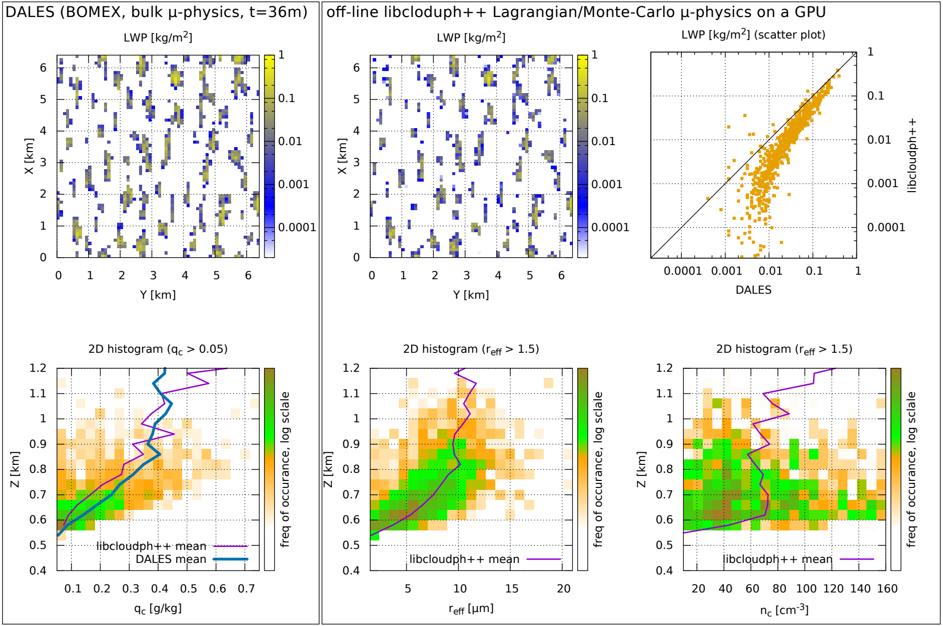
DALES (BOMEX, bulk μ-physics, t=35m)



off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU



DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)



DALES (BOMEX, bulk μ-physics, t=36m)

off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

LWP [kg/m^2]

LWP [kg/m^2]

LWP [kg/m^2] (scatter plot)

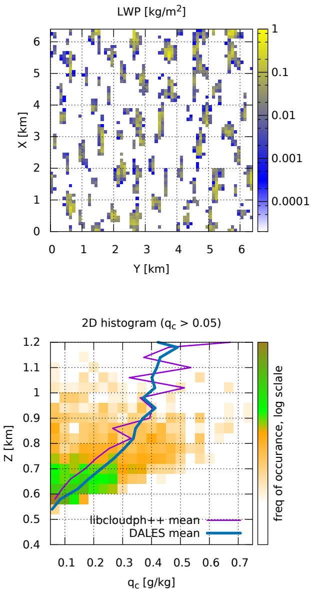
2D histogram (q_c > 0.05)

2D histogram (r_{eff} > 1.5)

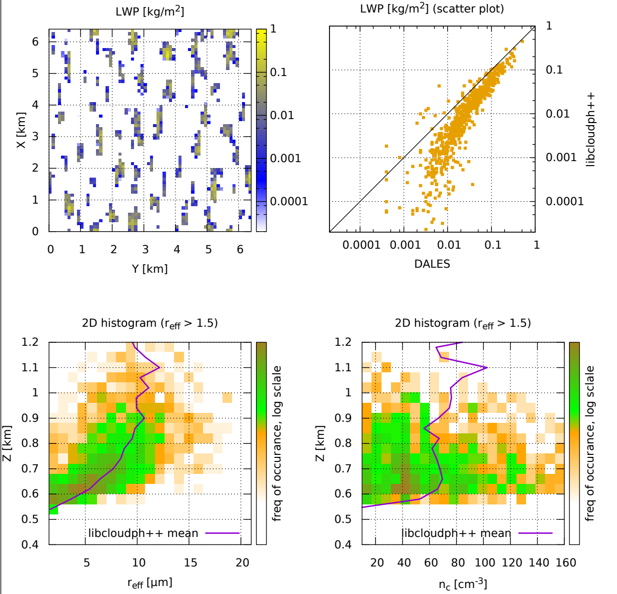
2D histogram (r_{eff} > 1.5)

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=37m)

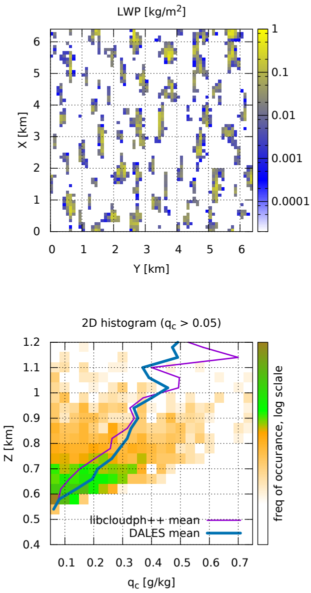


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

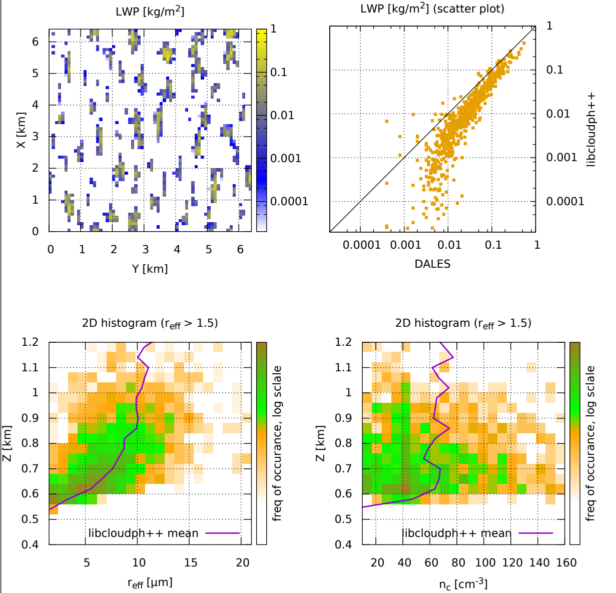


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=38m)

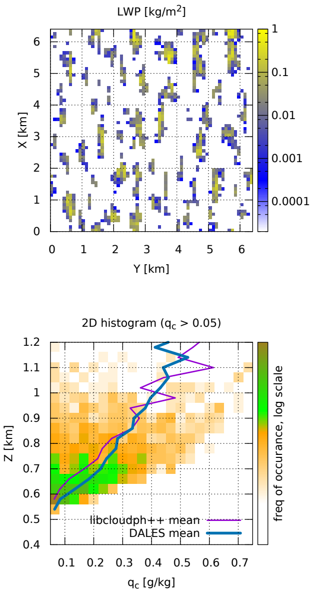


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

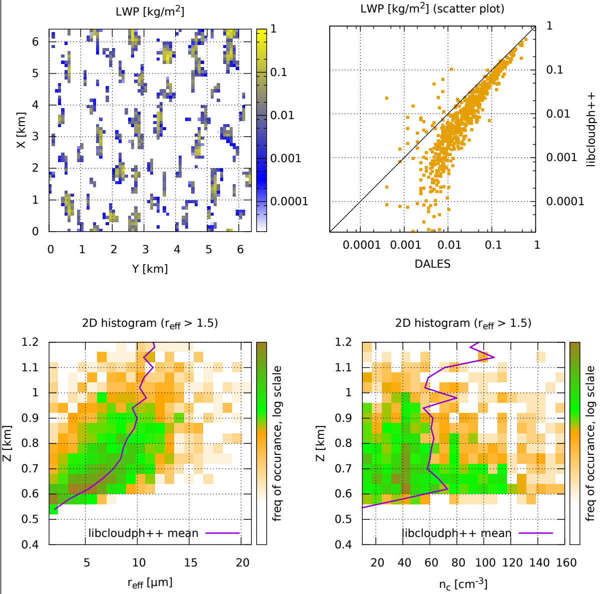


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

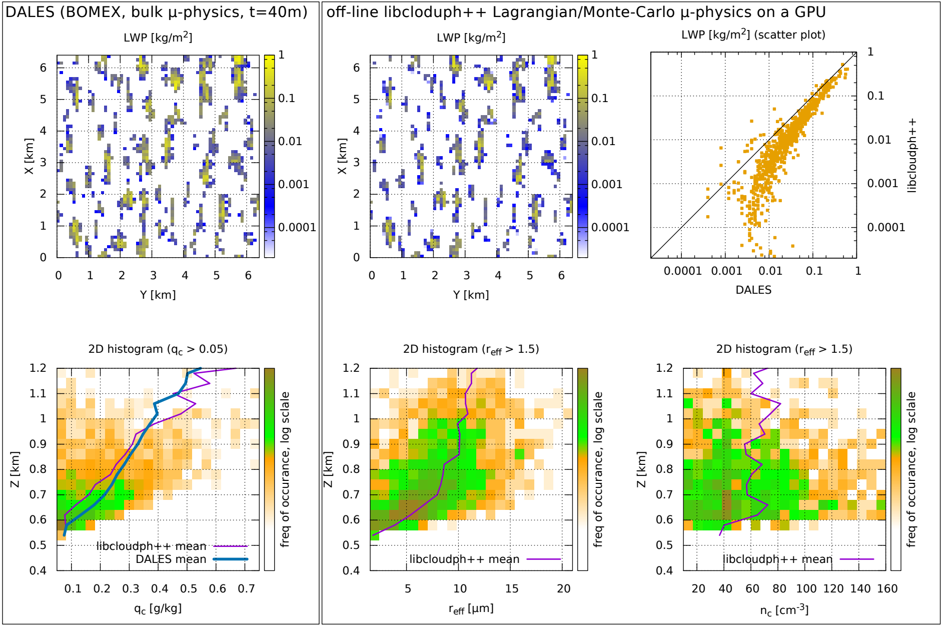
DALES (BOMEX, bulk μ-physics, t=39m)



off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU



DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

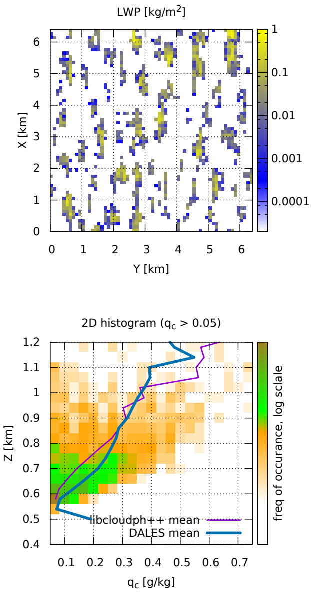


DALES (BOMEX, bulk μ-physics, t=40m)

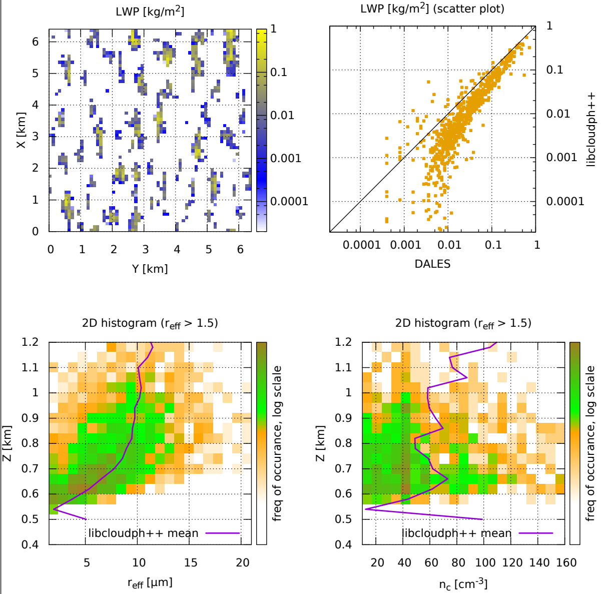
off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=41m)

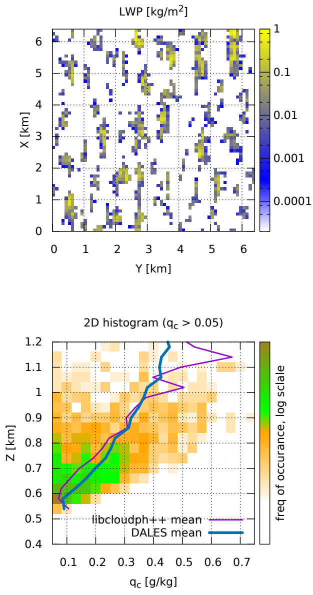


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

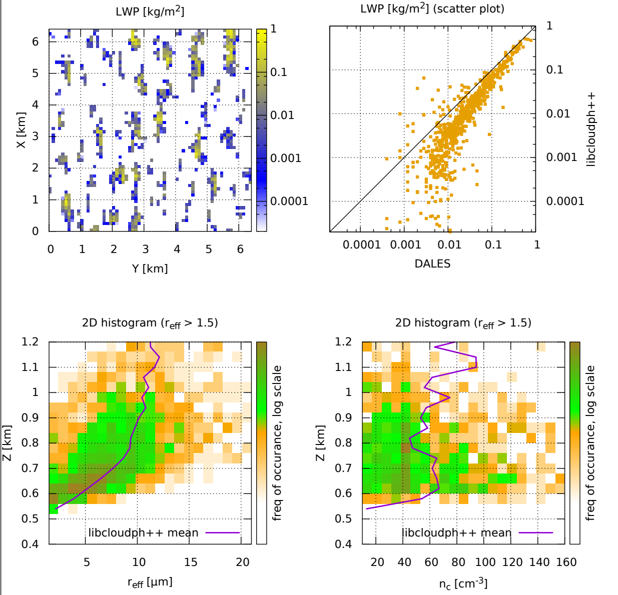


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=42m)

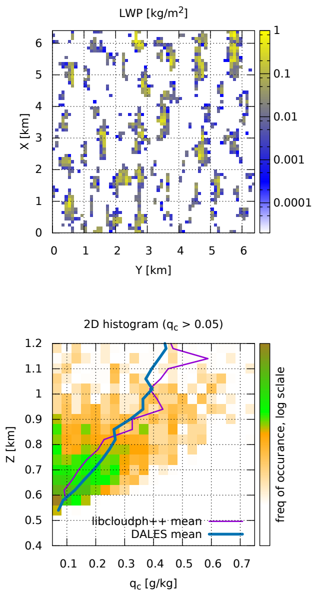


off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU

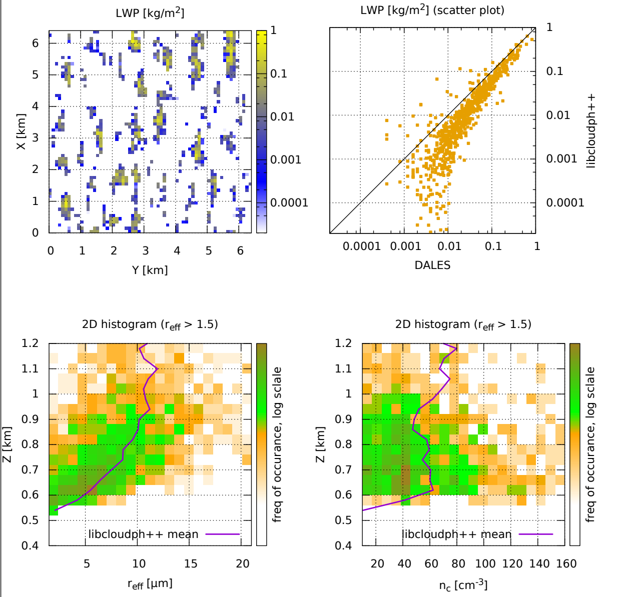


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=43m)



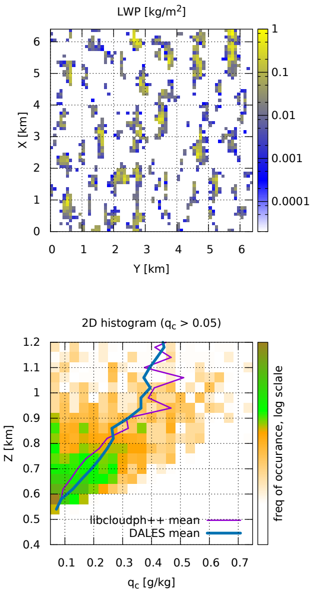
off-line libcloduph++ Lagrangian/Monte-Carlo μ-physics on a GPU



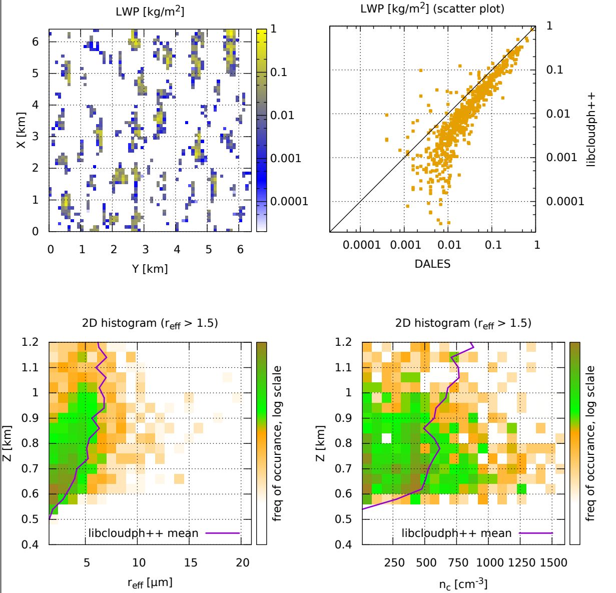
Let's see what happens if we multiply aerosol concentration by a factor of 10...

DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk µ-physics, t=43m)

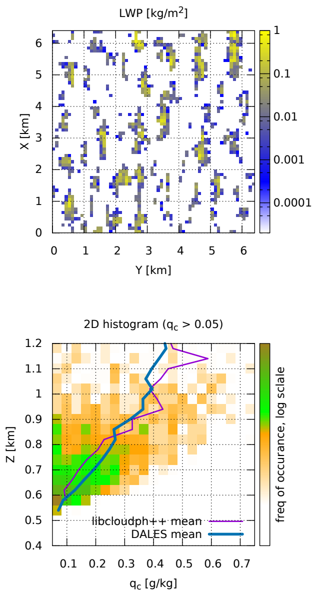


off-line libcloduph++ Lagrangian/Monte-Carlo µ-physics on a GPU

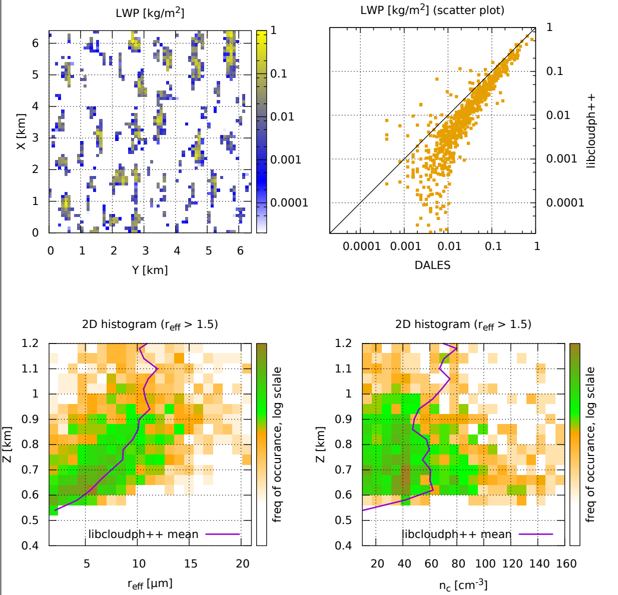


DALES/libcloudph++: proof-of-concept test (dt_{adv}=20s, dt_{cond}=0.5s, dz=40m, 10 SD/cell)

DALES (BOMEX, bulk μ-physics, t=43m)



off-line libcloudph++ Lagrangian/Monte-Carlo μ-physics on a GPU



DALES/libcloudph++ coupling: summary

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- proof-of-concept off-line simulations done

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- proof-of-concept off-line simulations done
- challenge to the reusability of libcloudph++:

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- current libcloudph++ limitations:
  - only geometric collisions, no breakup
  - explicit supersaturation scheme
  - no distributed-memory parallelisation
  - no aerosol sources

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