Introducing libmpdata++ and libcloudph++: reusable software for atmospheric modelling

Sylwester Arabas

cloud-aerosol modelling team @ University of Warsaw
`foss.igf.fuw.edu.pl`

NCAR, Sep. 4th 2014

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aim: developing tools for studying aerosol-cloud interactions

aerosol-cloud interactions: a conceptual picture

aerosol-cloud interactions: a conceptual picture

background image: vitsly.ru / Hokusai

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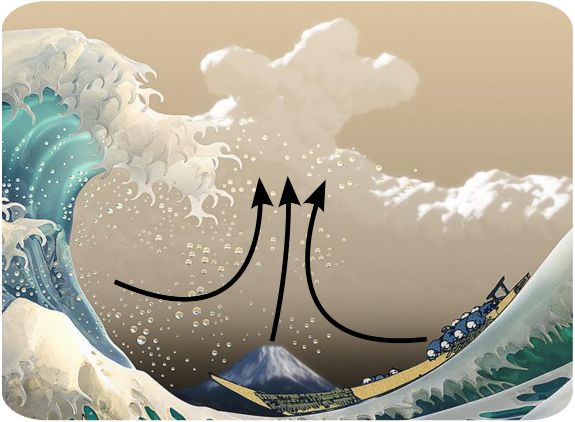
aerosol-cloud interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation nuclei



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- cloud droplets grow by water vapour condensation
- rain drops form through collisions of cloud droplets
- aqueous chemical reactions irreversibly modify the drop composition
- rain drops precipitate washing out aerosol
- rain drops evaporate into aerosol particles of potentially altered size and/or composition (collisions, chemistry)

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aim: developing tools for studying aerosol-cloud interactions

- novel cloud/aerosol microphysics models,
- state-of-the-art numerical schemes,
- modern coding techniques
  ⇝ priorities: researchers' productivity and result reproducibility

free & open-source C++ libraries developed at our group

libmpdata++ / arXiv:1407.1309 / accepted for GMDD

libmpdata++ 0.1: a library of parallel MPDATA solvers
for systems of generalised transport equations

Anna Jaruga[1], Sylwester Arabas[1], Dorota Jarecka[1,2], Hanna Pawlowska[1], Piotr K. Smolarkiewicz[*3], and Maciej Waruszewski[1]

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libcloudph++ 0.2: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

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libmpdata++: 1D advection / hello world

$$\partial_t(G\psi) + \nabla \cdot (G\vec{u}\psi) = GR$$

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Smolarkiewicz's MPDATA scheme

- sign-preserving
- non-oscillatory
- small implicit diffusion

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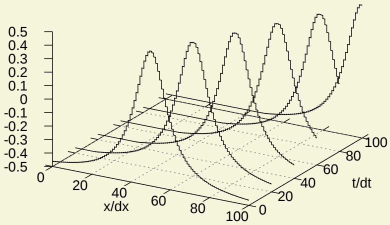
a "hello-world" example



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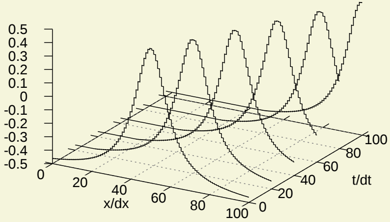
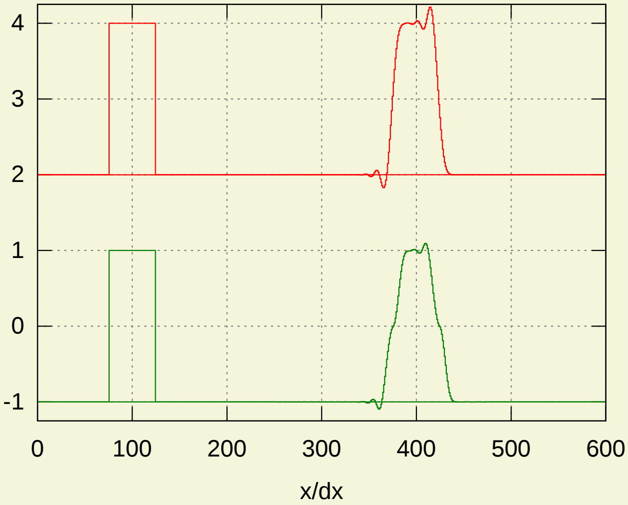



```cpp
#include <libmpdata++/solvers/mpdata.hpp>
#include <libmpdata++/concurr/serial.hpp>
#include <libmpdata++/output/gnuplot.hpp>

using namespace libmpdataxx;
using namespace blitz::tensor;

int main()
{
  // compile-time parameters
  struct ct_params_t : ct_params_default_t
  {
    using real_t = double;
    enum { n_dims = 1 };
    enum { n_eqns = 1 };
  };

  // solver choice
  using slv_t = solvers::mpdata<ct_params_t>;

  // output choice
  using slv_out_t = output::gnuplot<slv_t>;

  // concurency choice + boundary conditions
  using run_t = concurr::serial<slv_out_t,
    bcond::open, bcond::open>;

  // run-time parameters
  typename slv_out_t::rt_params_t p;
  int nx = 101, nt = 100;
  ct_params_t::real_t dx = 0.1;
  p.grid_size = { nx };
  p.outfreq = 20;

  run_t run(p);                  // instantiation
  run.advectee() =               // initial cond.
    -.5 + 1 / (pow(dx*(i - (nx-1)/2.), 2) + 1);
  run.advector() = .5;           // Courant number
  run.advance(nt);               // integration
}
```

libmpdata++: implemented MPDATA flavours

basic 2-pass MPDATA + "abs" trick for var-sign signals



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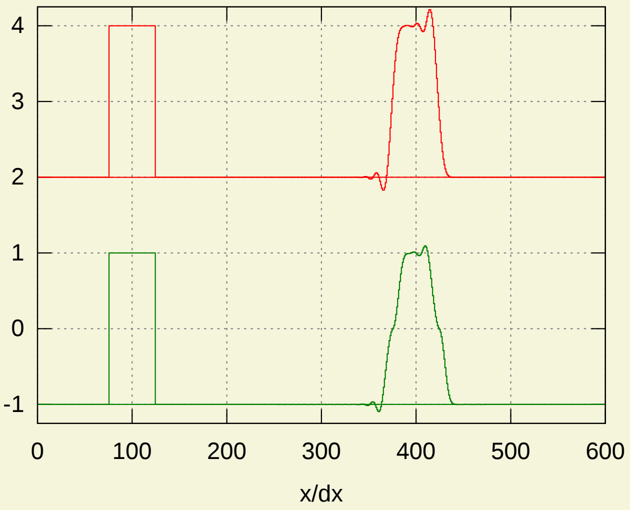

$$\frac{\psi_a-\psi_b}{\psi_a+\psi_b} \approx \frac{|\psi_a|-|\psi_b|}{|\psi_a|+|\psi_b|}$$

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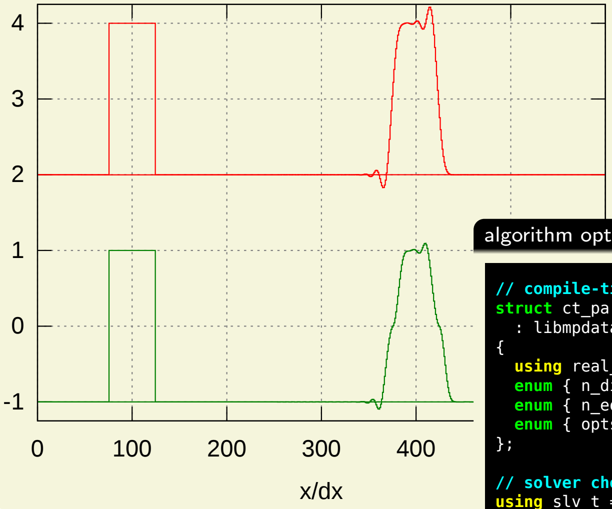


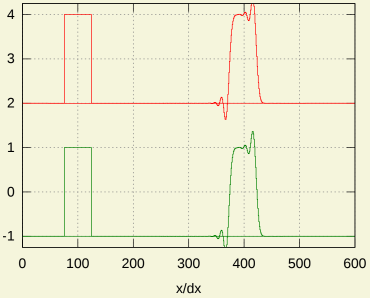
$$\frac{\psi_a - \psi_b}{\psi_a + \psi_b} \approx \frac{|\psi_a| - |\psi_b|}{|\psi_a| + |\psi_b|}$$

algorithm option as a compile-time parameter

```
// compile-time parameters
struct ct_params_t
  : libmpdataxx::ct_params_default_t
{
  using real_t = double;
  enum { n_dims = 1 };
  enum { n_eqns = 2 };
  enum { opts = opts::abs };
};

// solver choice
using slv_t = solvers::mpdata<ct_params_t>;
```

infinite-gauge option ("iga")



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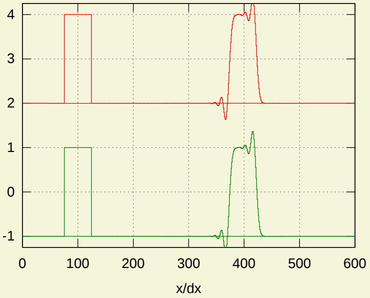
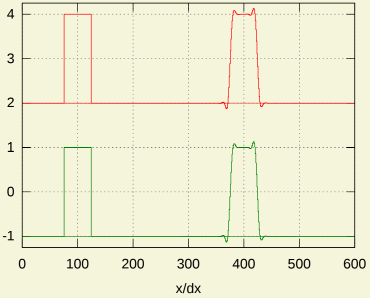


iga + 3rd-order-accurate variant ("tot")



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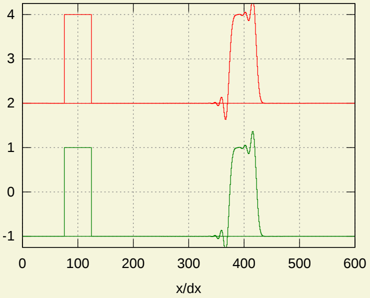

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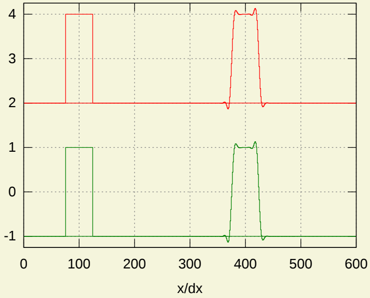

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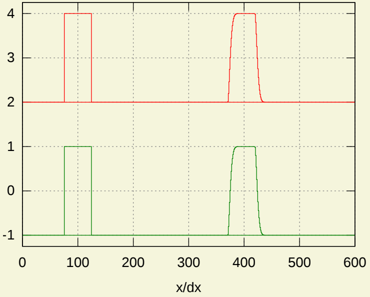

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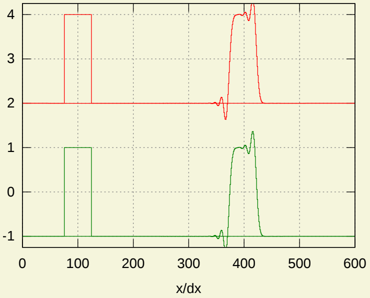

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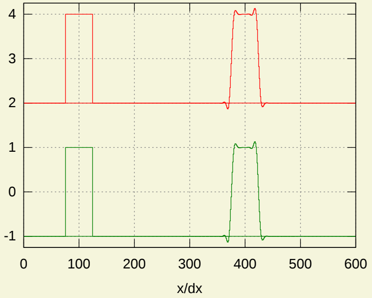

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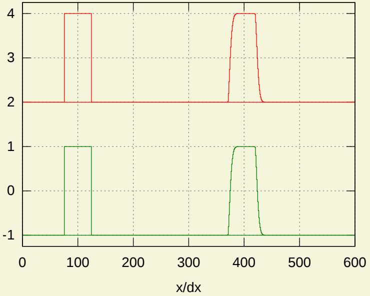

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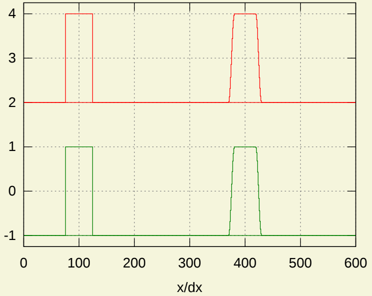
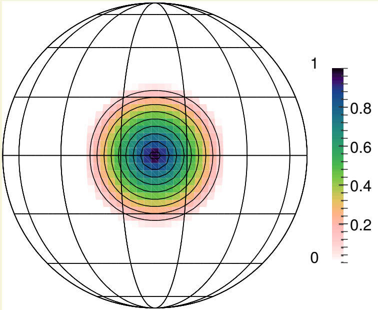
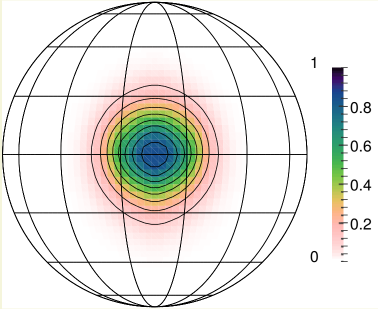


libmpdata++: 2D advection on a sphere

$t = 0$
cone-shaped signal (128×64)
over-the-pole advection



$t/\Delta t = 5120$ (one revolution)
3-pass FCT MPDATA
with third-order terms



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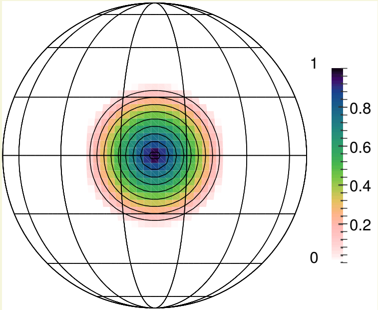

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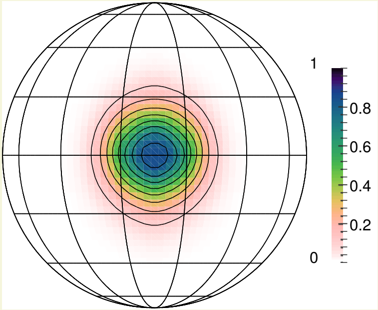

- reproduced experiment of Williamson and Rasch, 1989

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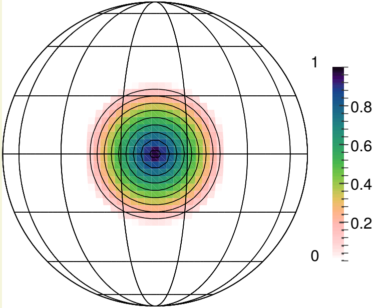

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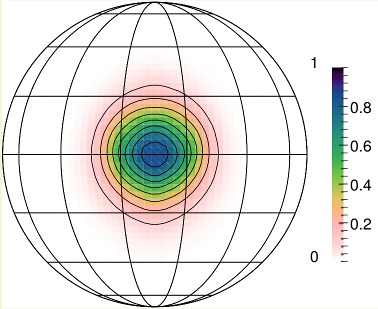

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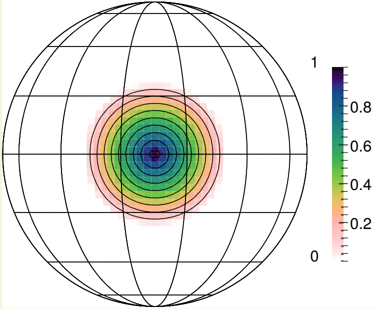

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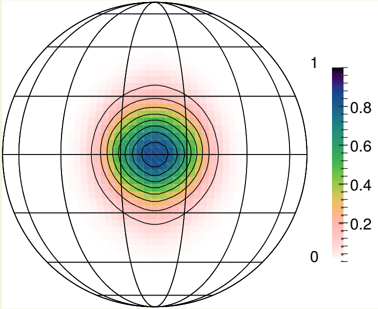

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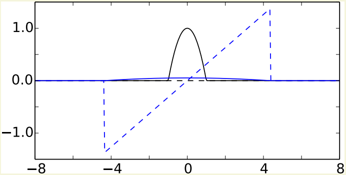
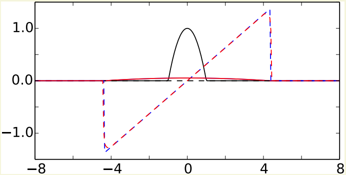
- example developed by Maciej Waruszewski / U. Warsaw

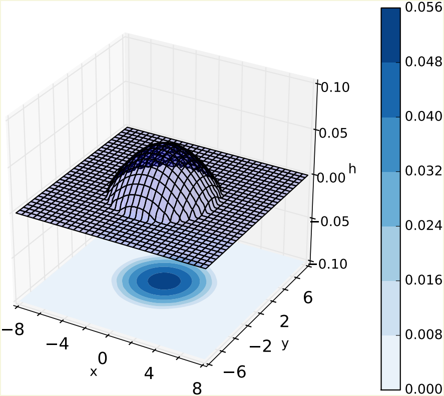
libmpdata++: 2D (3D) shallow-water system

black: initial; blue: analytic; red: MPDATA





initial condition



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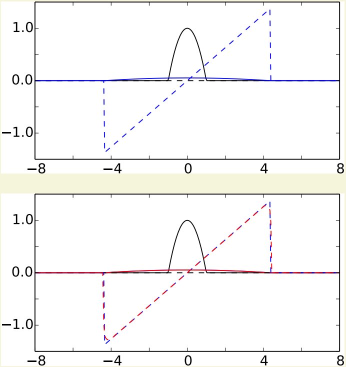

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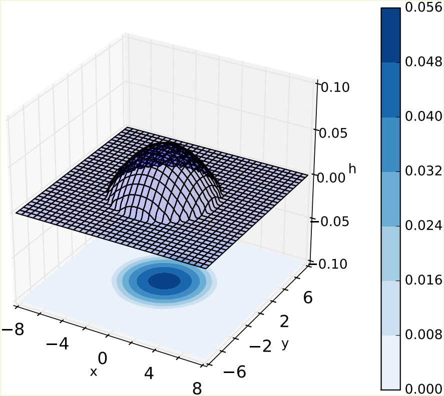

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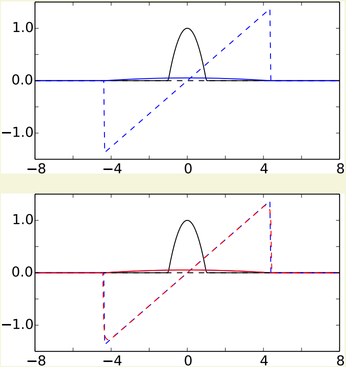

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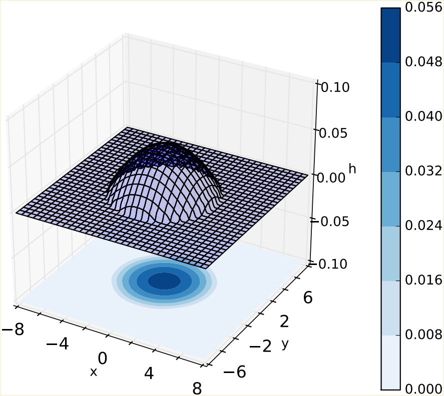

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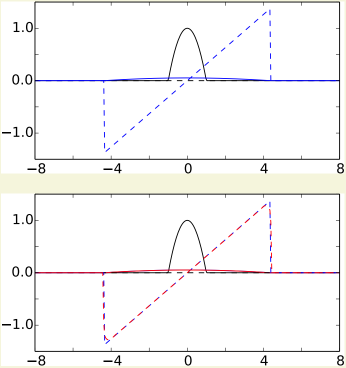

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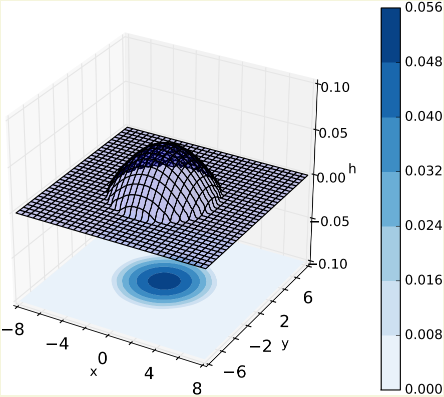

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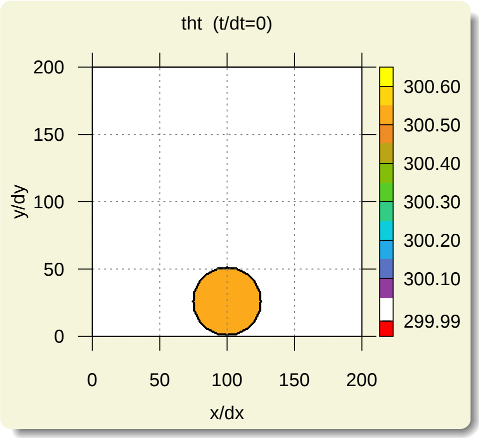

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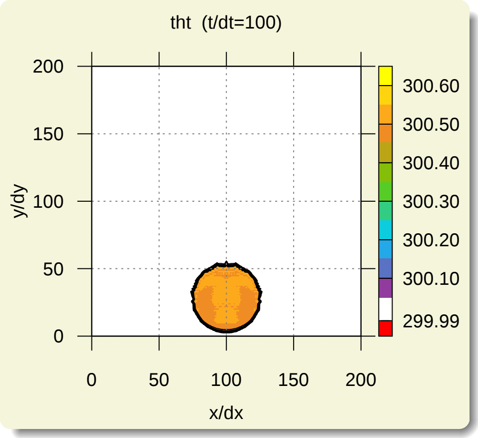

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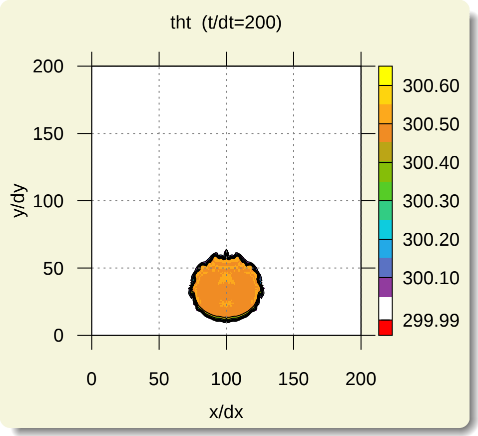

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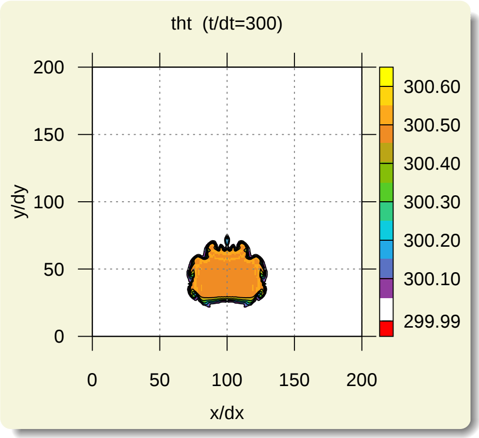

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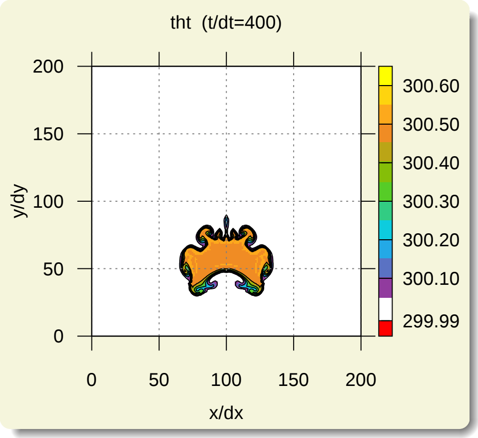

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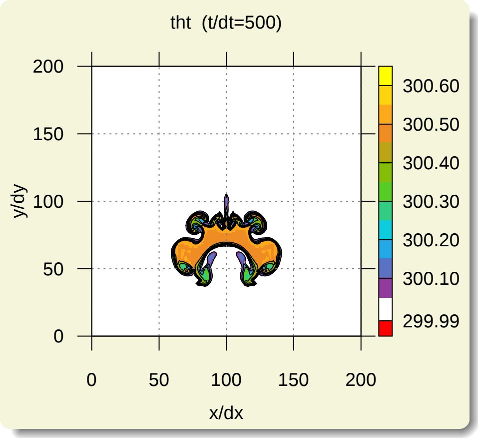

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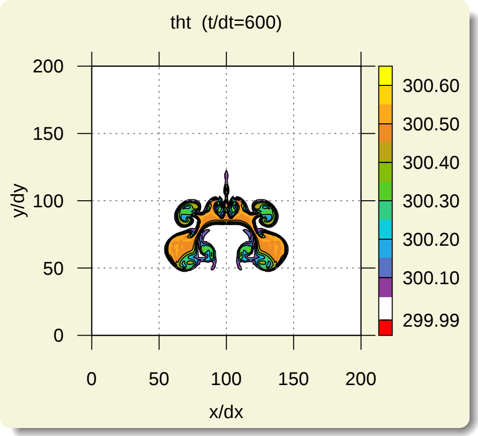

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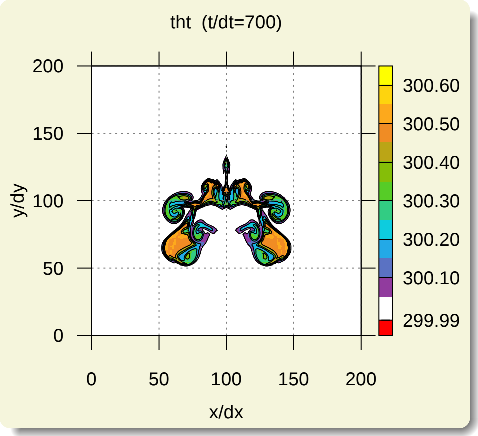

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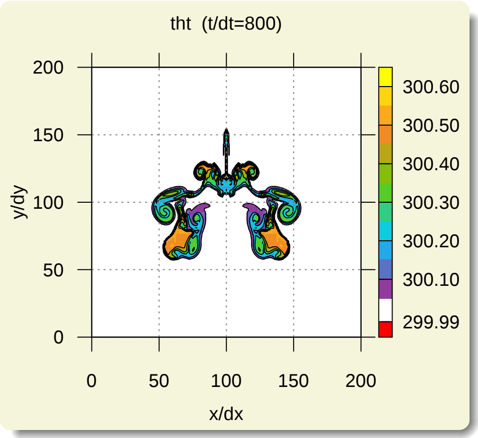

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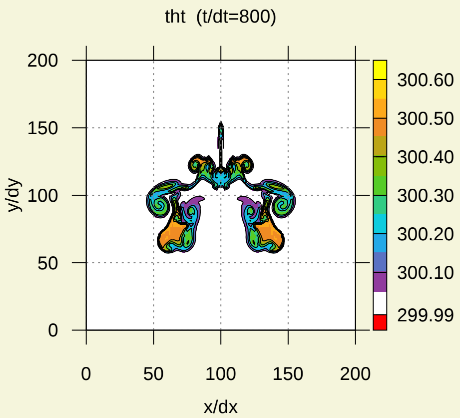

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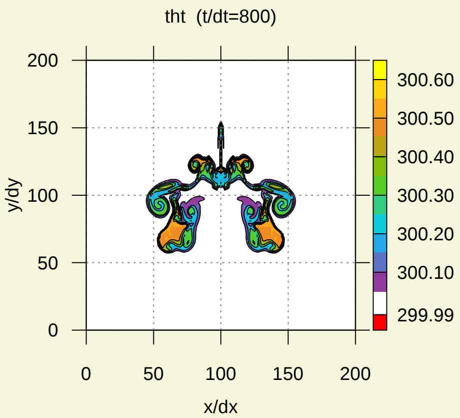

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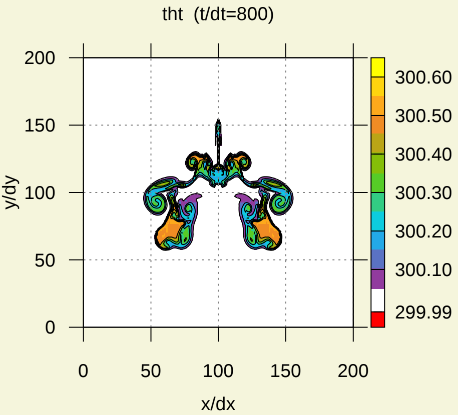

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libmpdata++: summary & some technicalities

free & open source C++ library of parallel MPDATA solvers

key features:

- reusable – API documented in the paper; out-of-tree setups
- rich set of MPDATA flavours (incl. FCT, infinite-gauge, ...)
- 1D, 2D & 3D integration; optional coordinate transformation
- four types of solvers:
- implemented using Blitz++ (no loops, expression templates)
- built-in HDF5/XDMF output
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libmpdata++ / arXiv:1407.1309 / accepted for GMDD

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[1]Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[2]National Center for Atmospheric Research, Boulder, Colorado, USA
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libcloudph++ / arXiv:1310.1905 / submitted to GMDD

libcloudph++ 0.2: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

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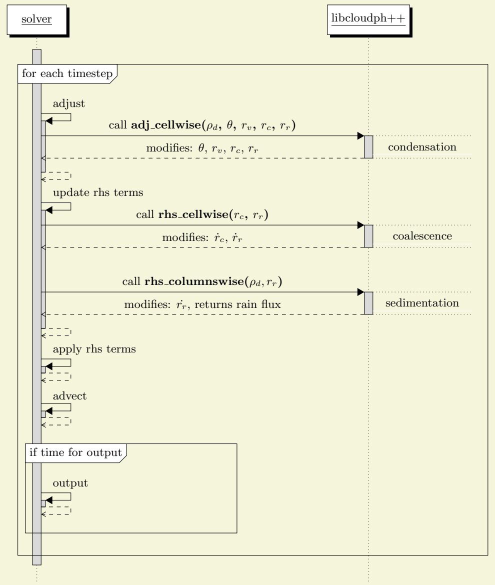
libcloudph++: reusable μ-physics

sequence diagram



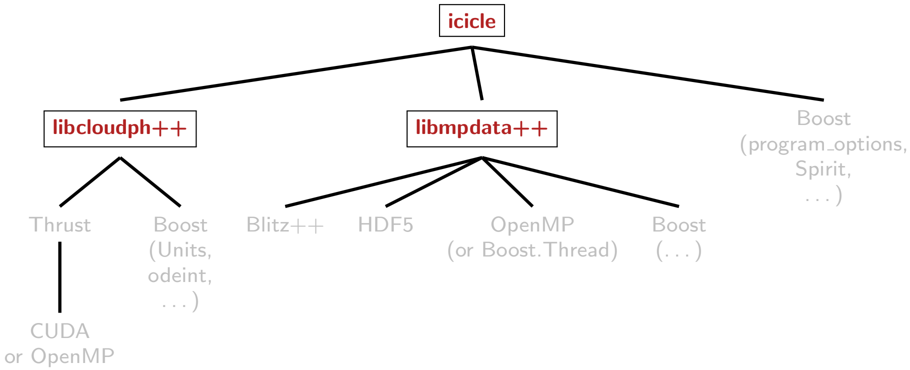
programming interface

```
template<typename real_t>
struct opts_t
{
  bool
    acti = true, // activation
    cond = true, // condensation
    acnv = true, // autoconversion
    accr = true, // accretion
    sedi = true; // sedimentation

  // RH limit for activation
  real_t RH_max = 44;

  // aerosol spectrum
  struct lognormal_mode_t
  {
    real_t
      mean_rd,   // [m]
      sdev_rd,   // [1]
      N_stp,     // [m-3] @STP
      chem_b;    // [1]
  };
  std::vector<lognormal_mode_t> dry_distros;
};
```

libcloudph++: example coupling with libmpdata++



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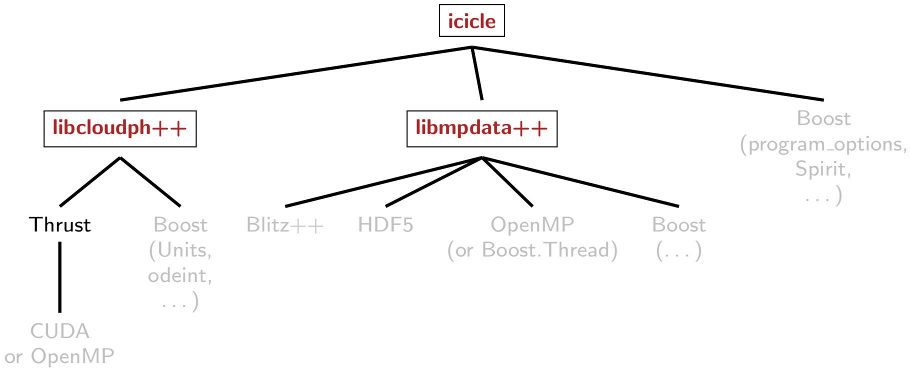

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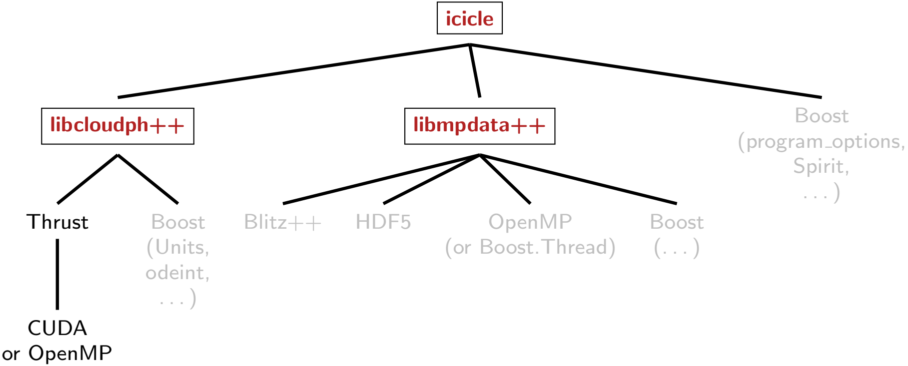

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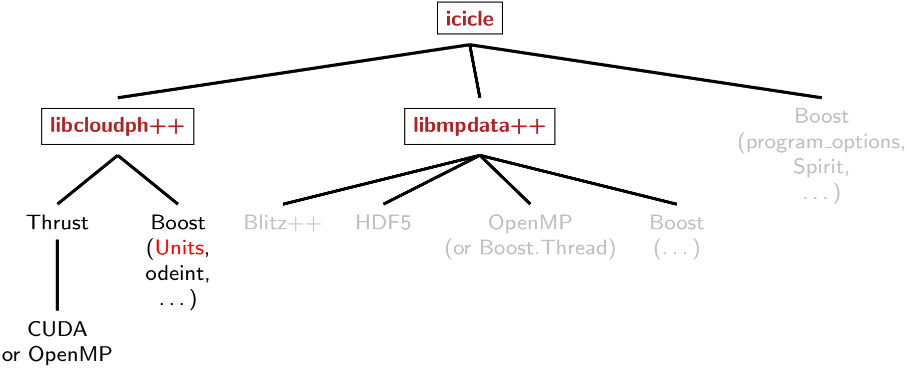

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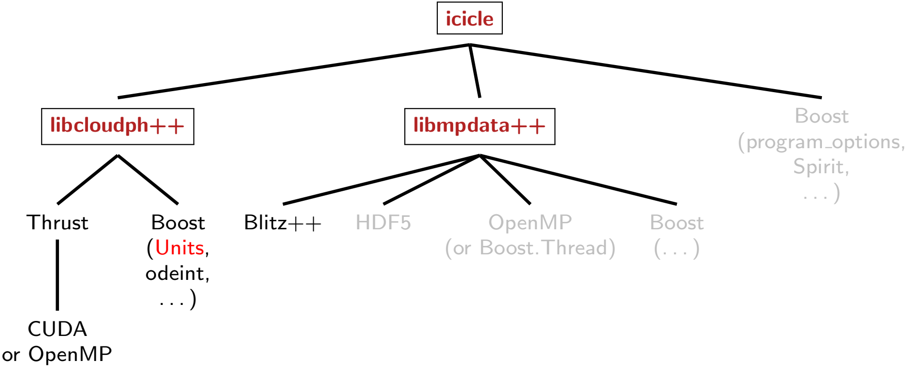

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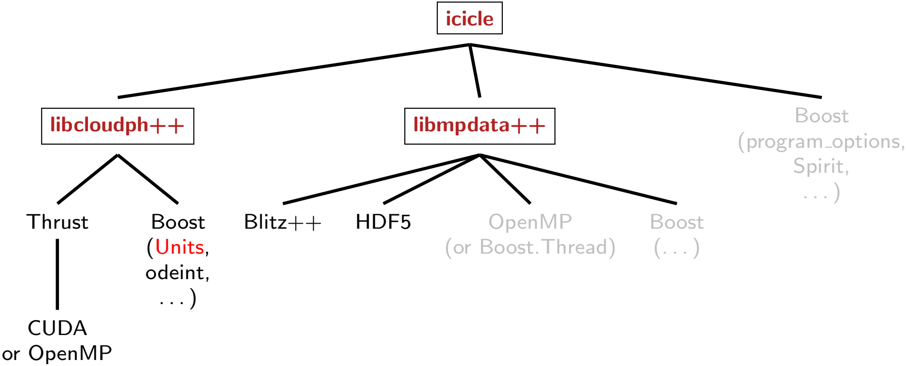

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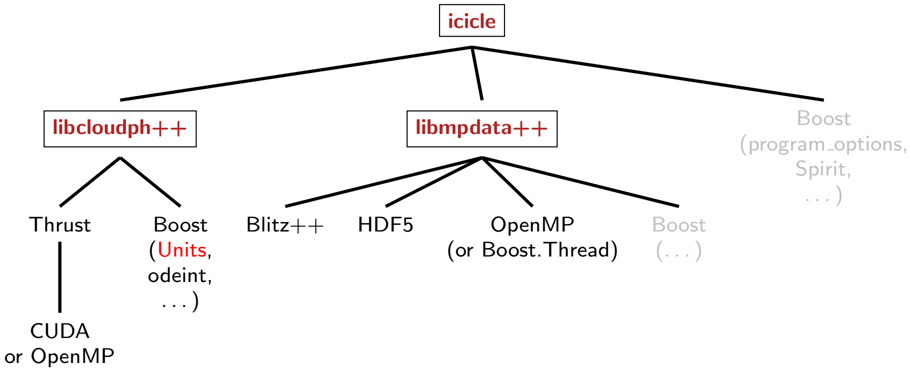

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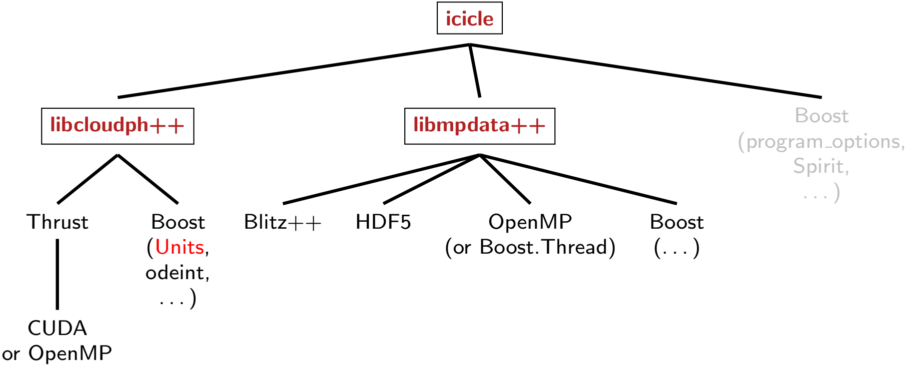

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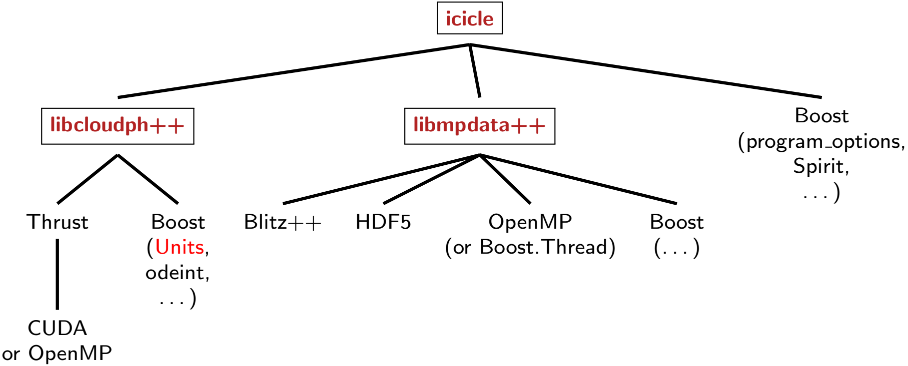
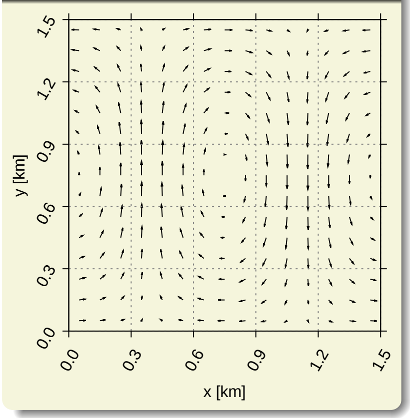
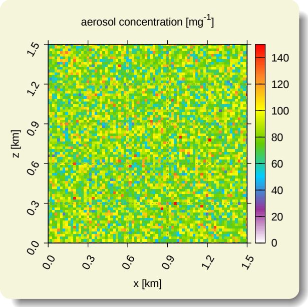


libcloudph++: VOCALS-inspired aerosol processing set-up

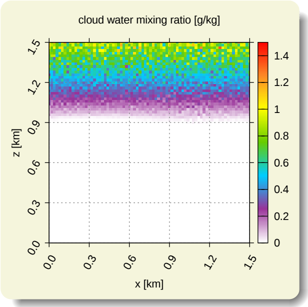
single-eddy velocity field

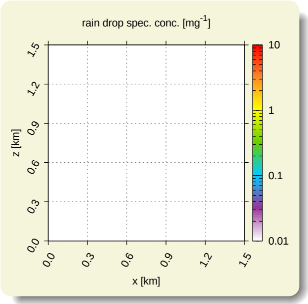


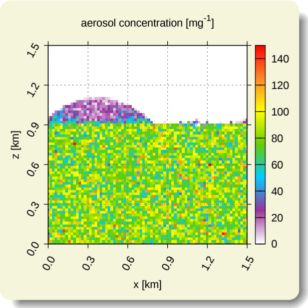


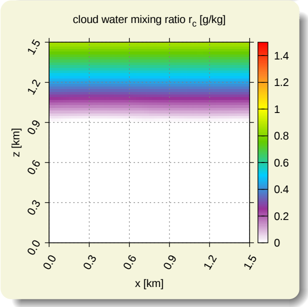
- set-up: Grabowski & Lebo (ICMW 2012)
- 2D prescribed flow
- advection: libmpdata++ (2-pass FCT)
- μ-physics: libcloudph++

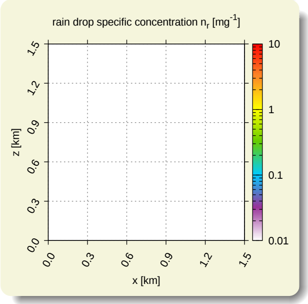
libcloudph++: VOCALS-inspired aerosol processing set-up
x











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

2-moment bulk scheme
(Morrison & Grabowski 2007)

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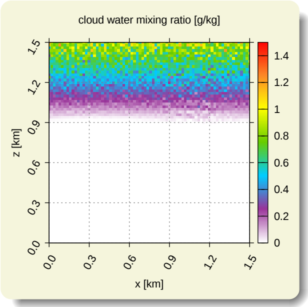
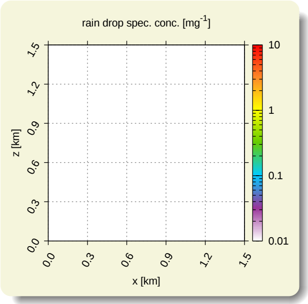
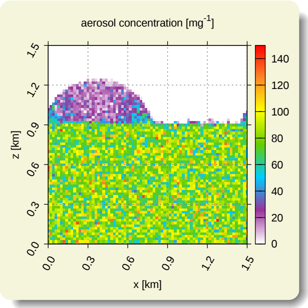
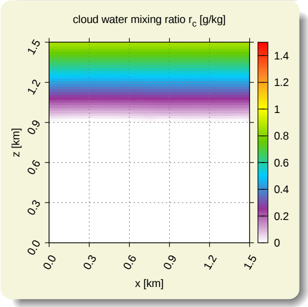
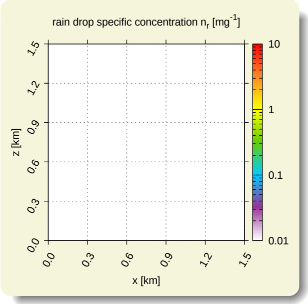
x x











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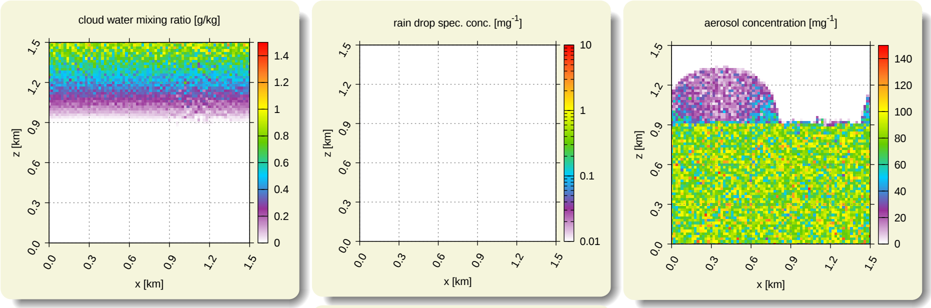

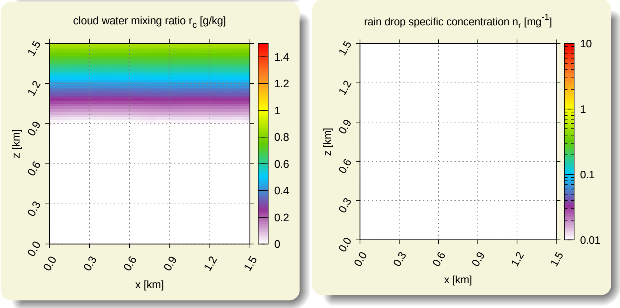

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libcloudph++: VOCALS-inspired aerosol processing set-up

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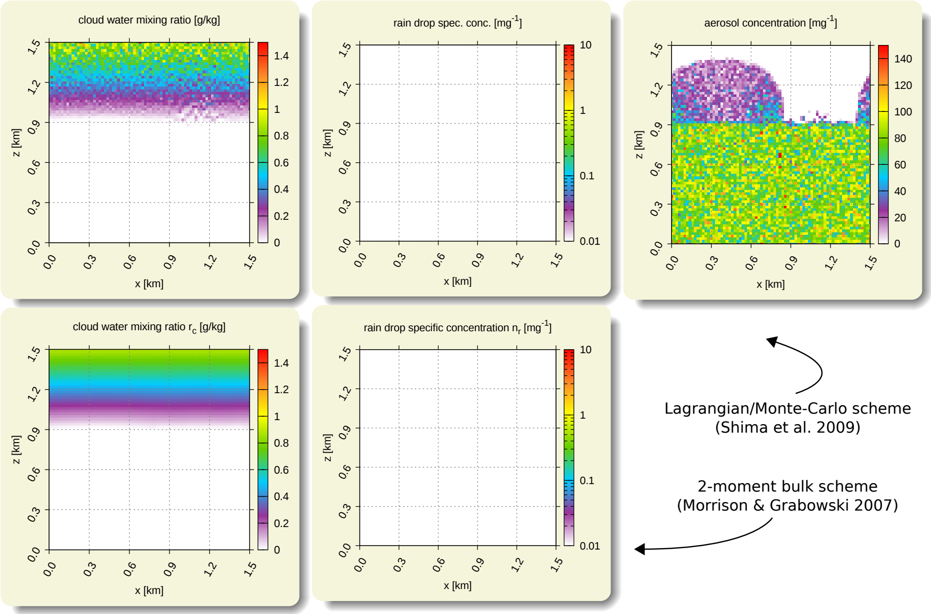

libcloudph++: VOCALS-inspired aerosol processing set-up

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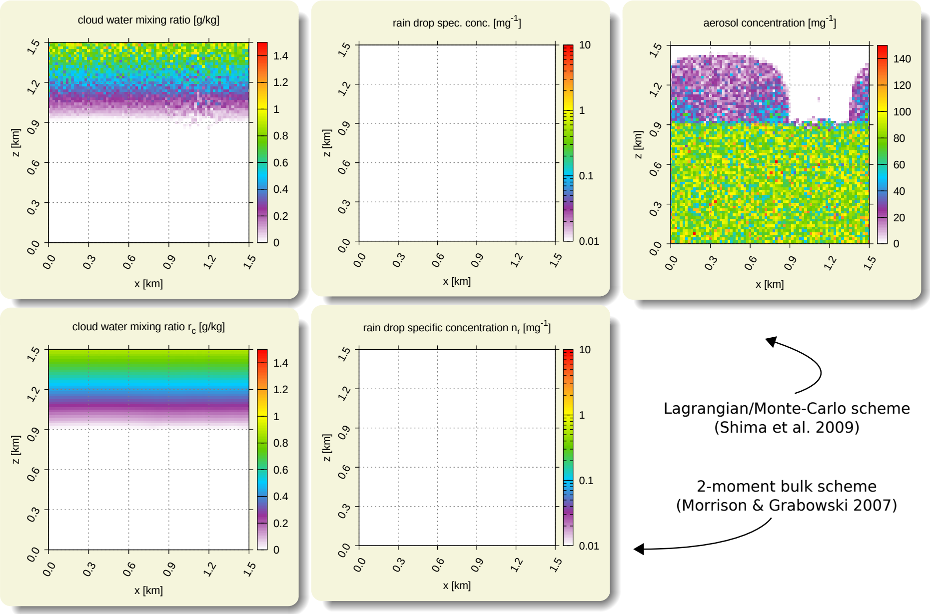

libcloudph++: VOCALS-inspired aerosol processing set-up

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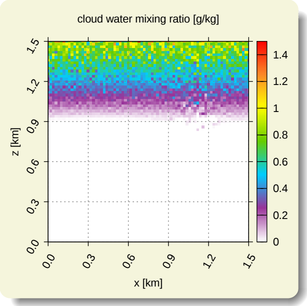

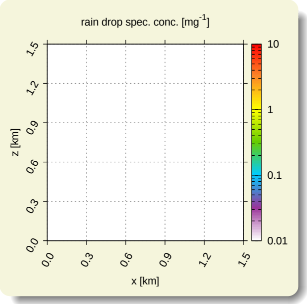

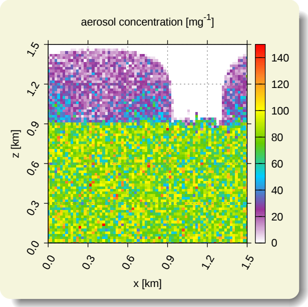

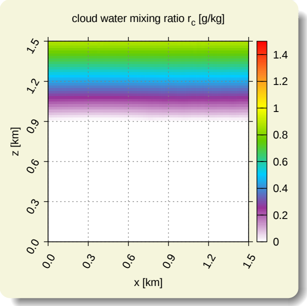

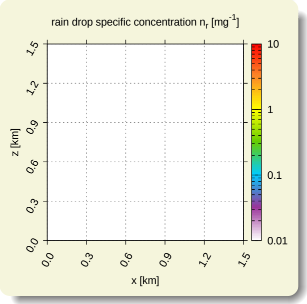

Lagrangian/Monte-Carlo scheme
(Shima et al. 2009)

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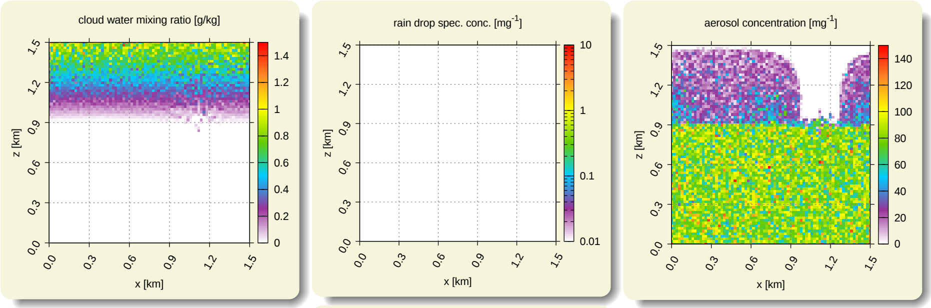

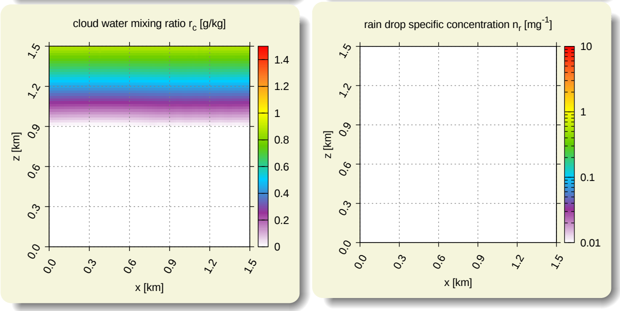

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libcloudph++: VOCALS-inspired aerosol processing set-up

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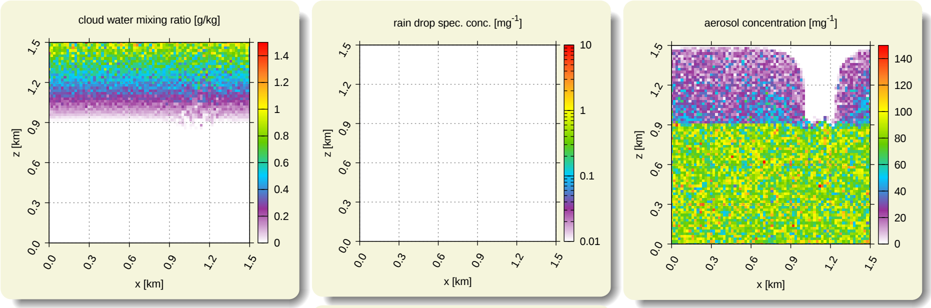

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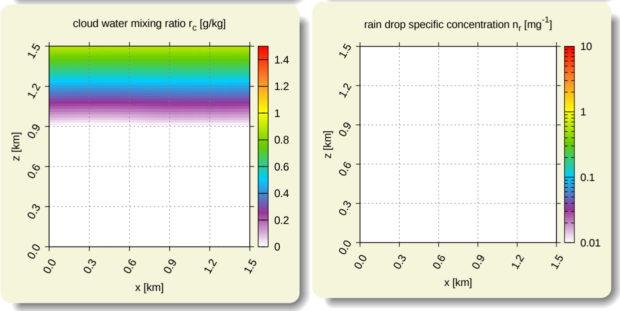

libcloudph++: VOCALS-inspired aerosol processing set-up

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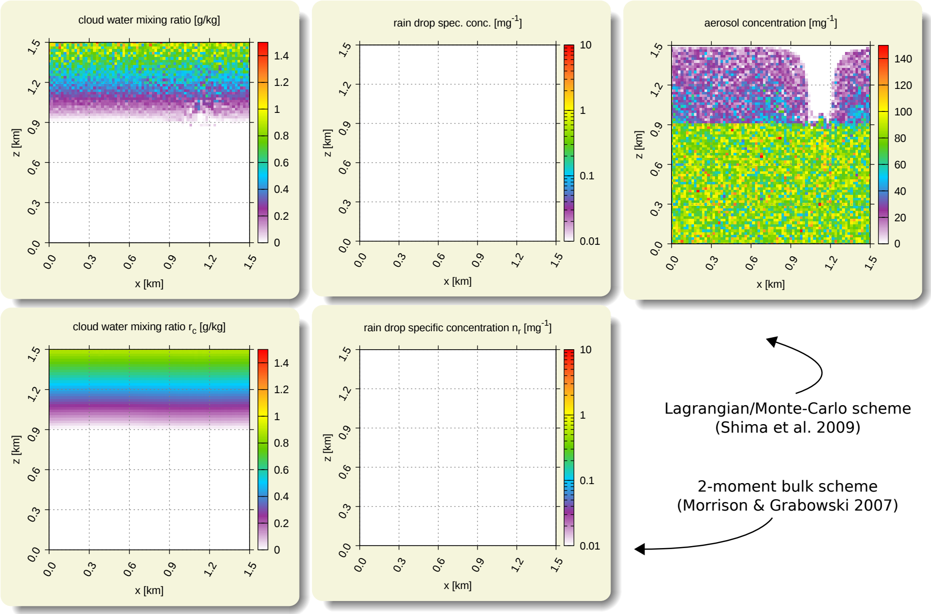

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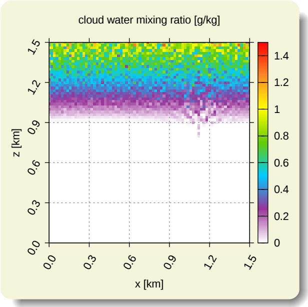

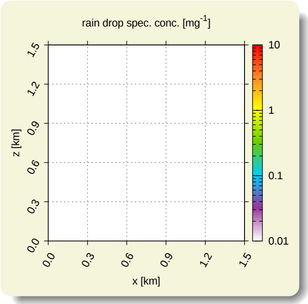

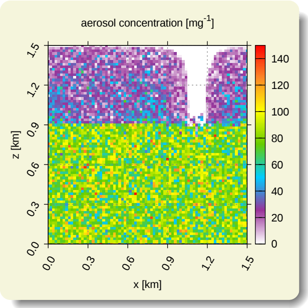

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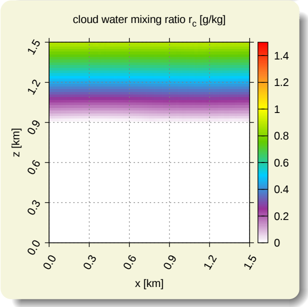
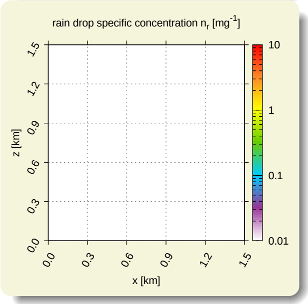
(Shima et al. 2009)





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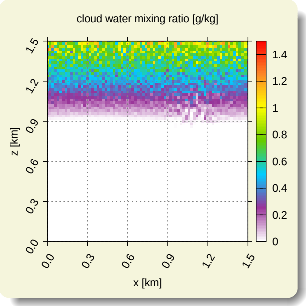

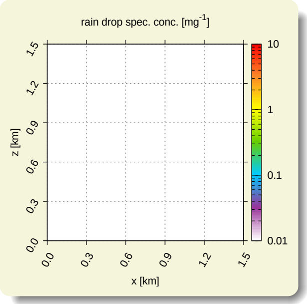

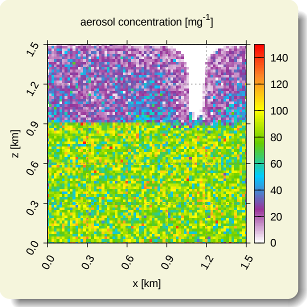

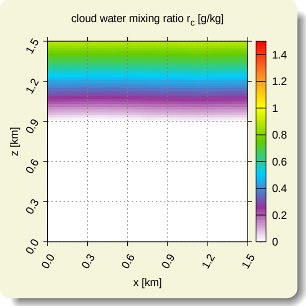

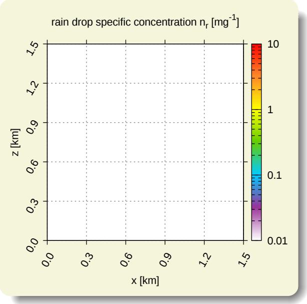

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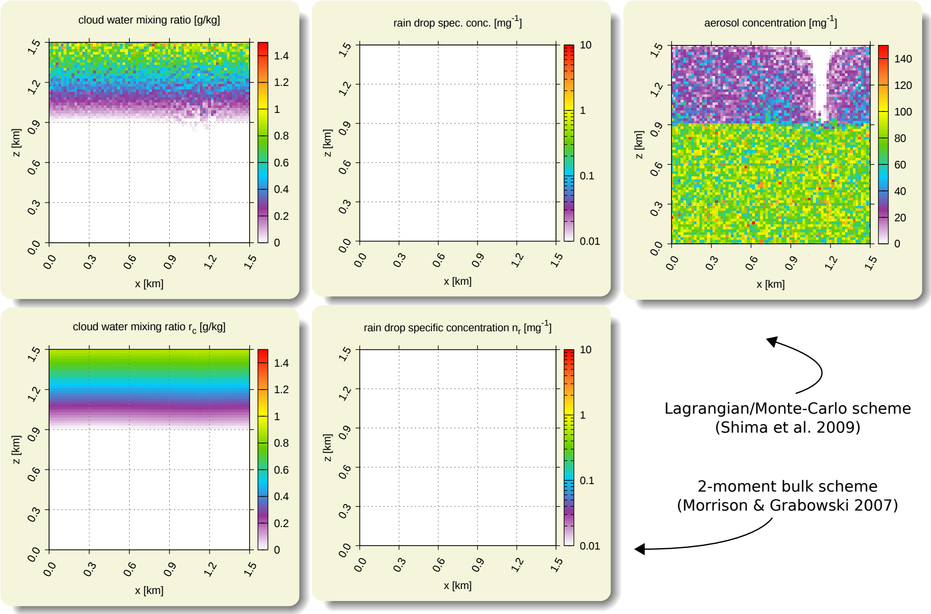

libcloudph++: VOCALS-inspired aerosol processing set-up

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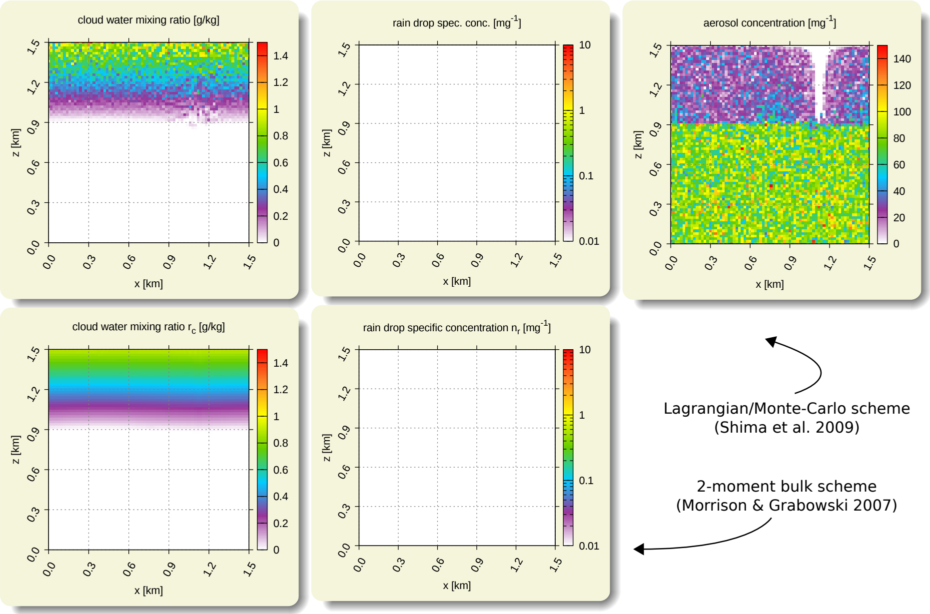

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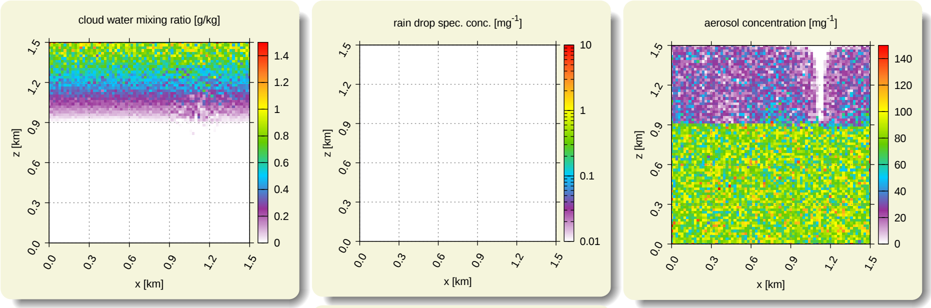

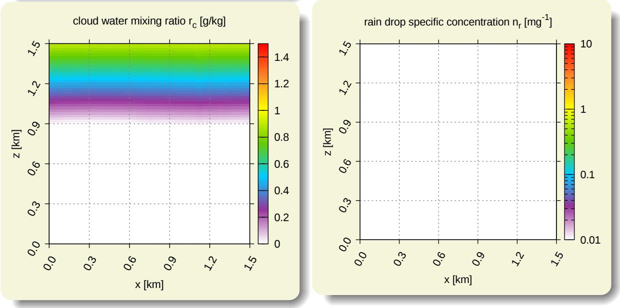

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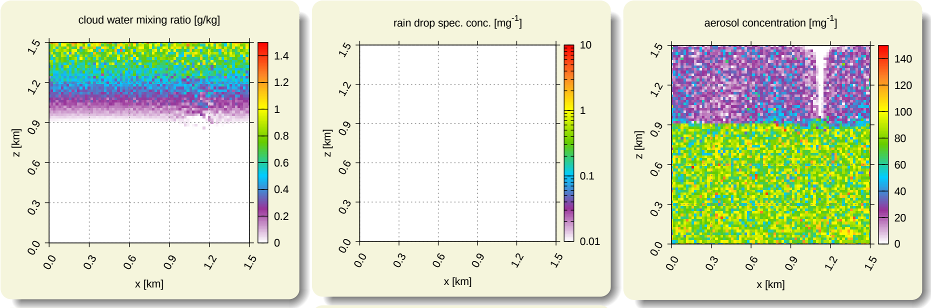

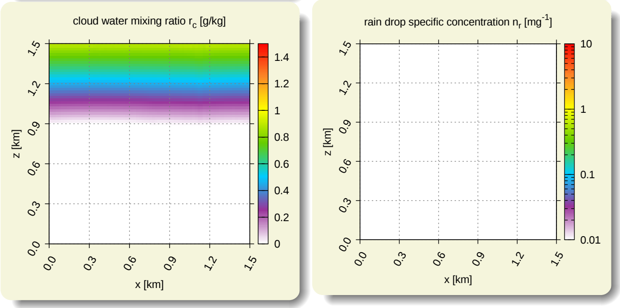

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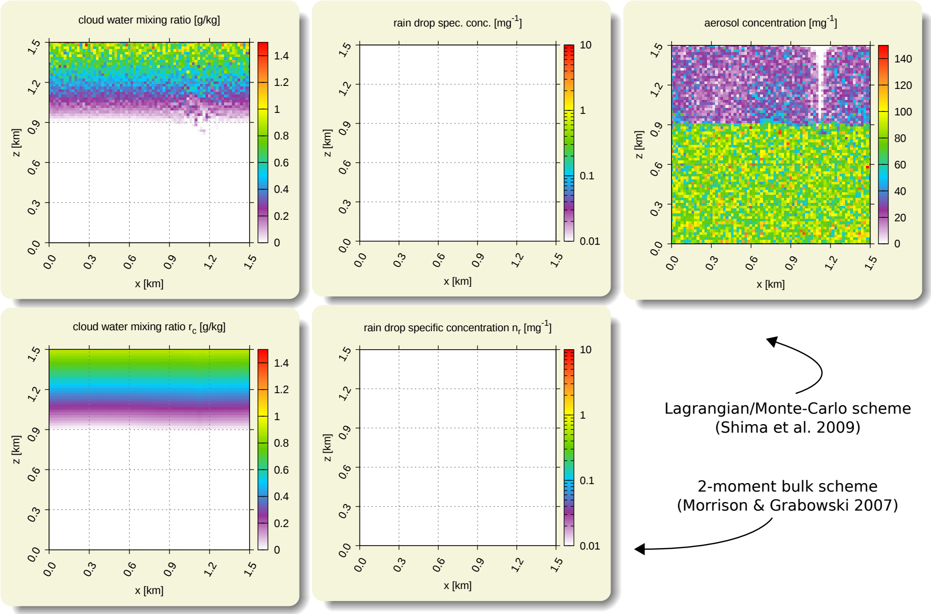

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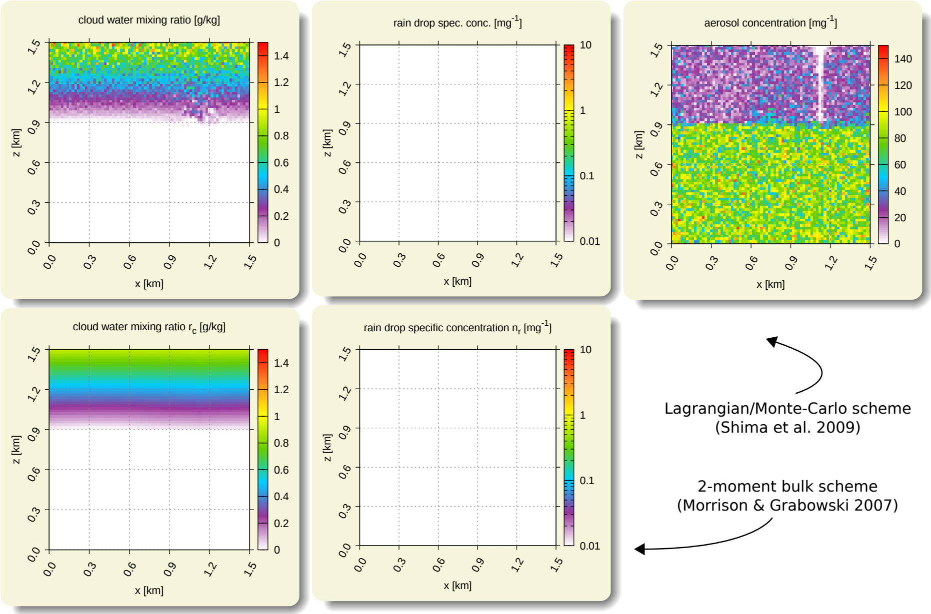

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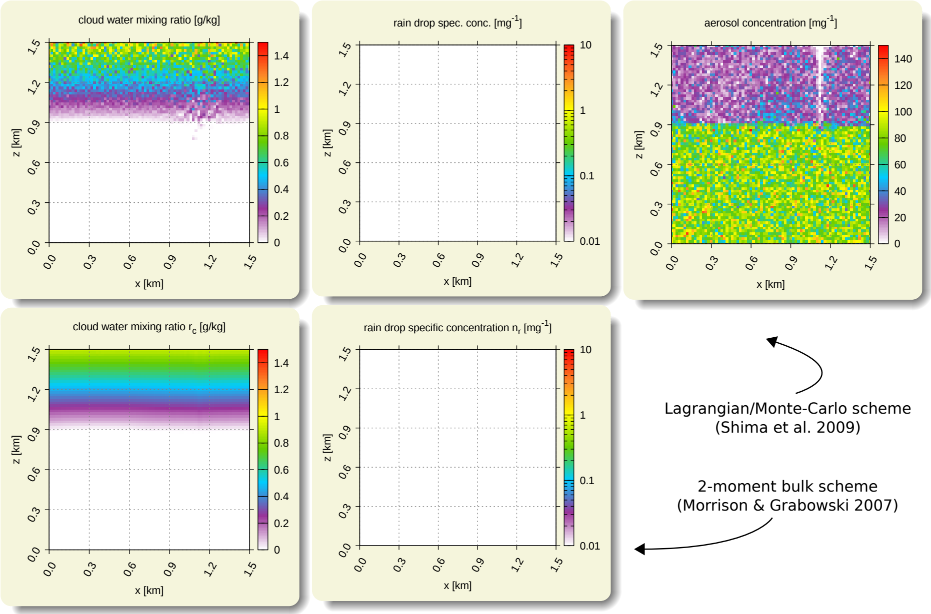

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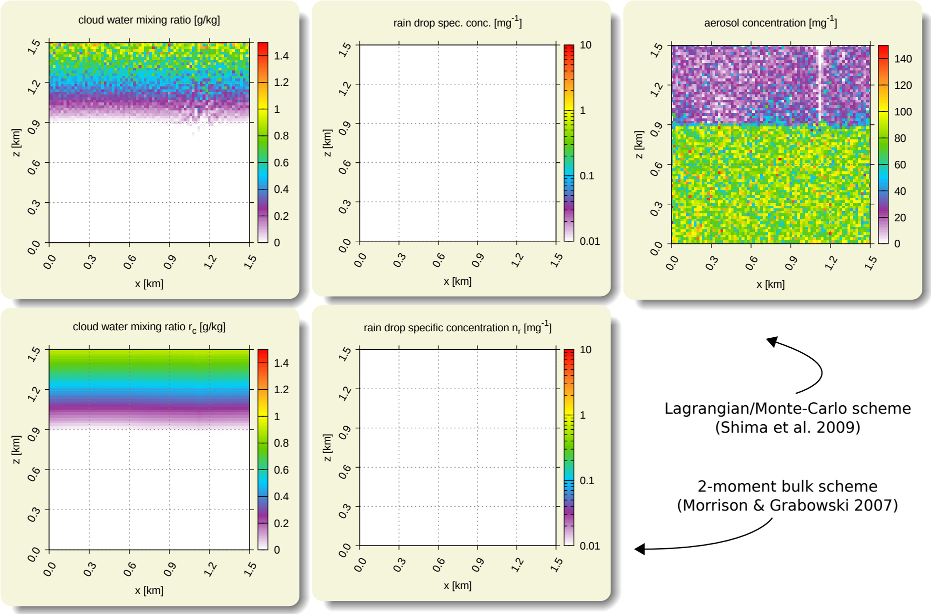

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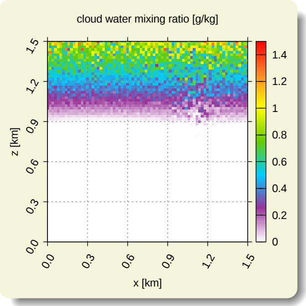

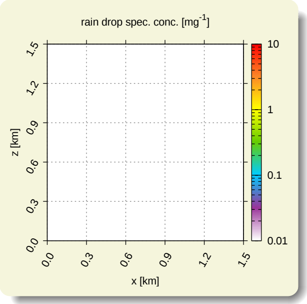

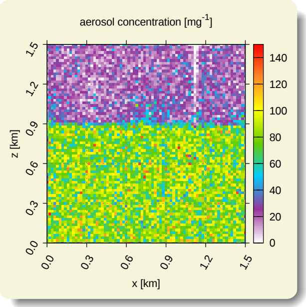

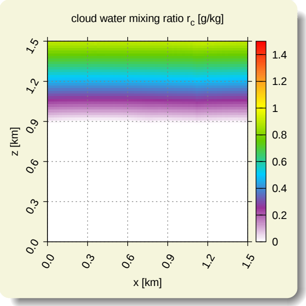

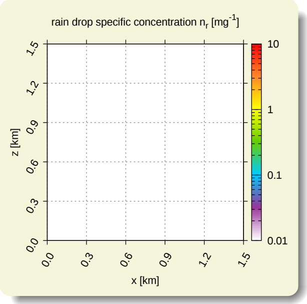

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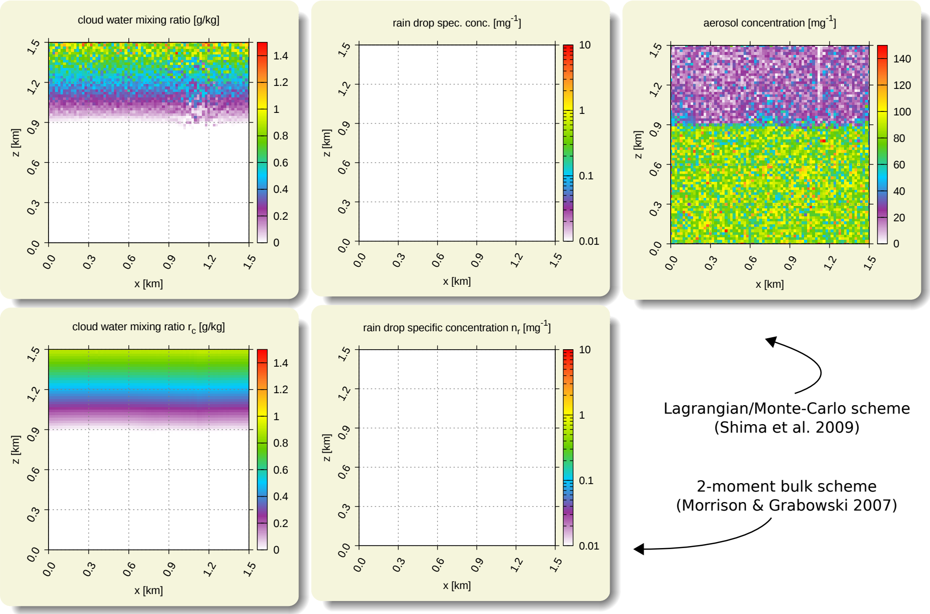

libcloudph++: VOCALS-inspired aerosol processing set-up

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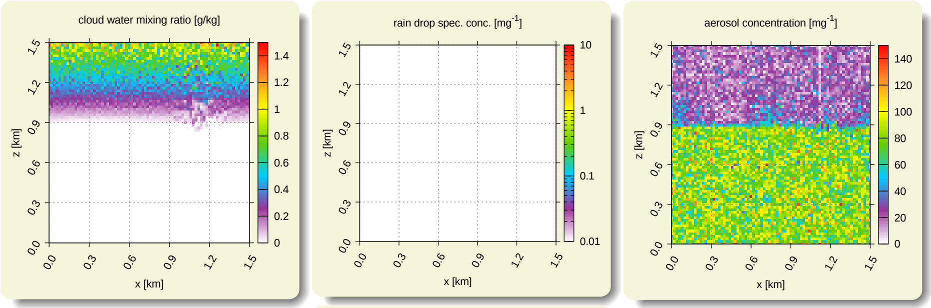

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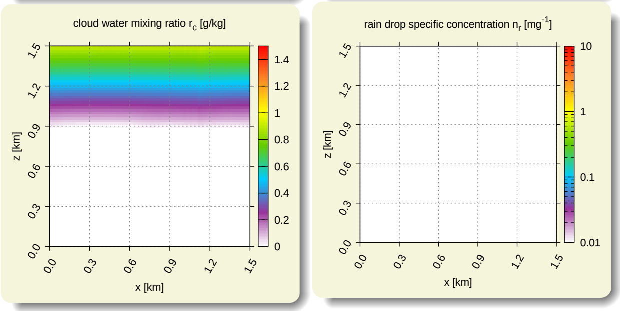

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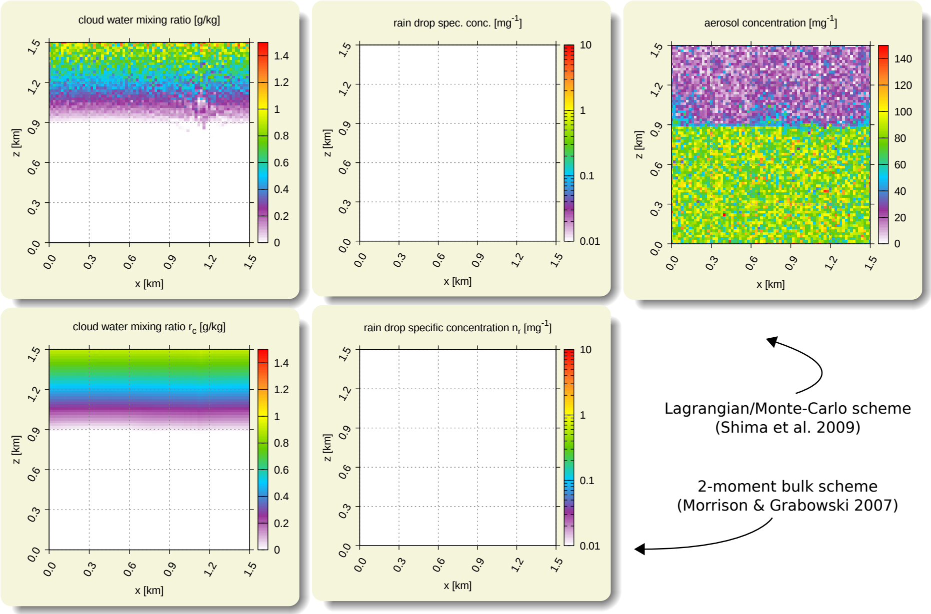

libcloudph++: VOCALS-inspired aerosol processing set-up

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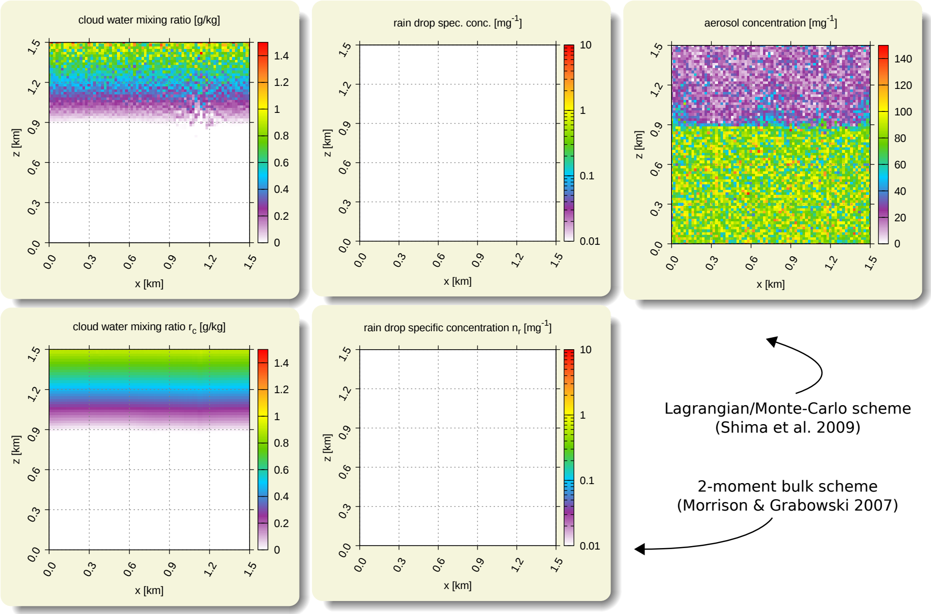

libcloudph++: VOCALS-inspired aerosol processing set-up

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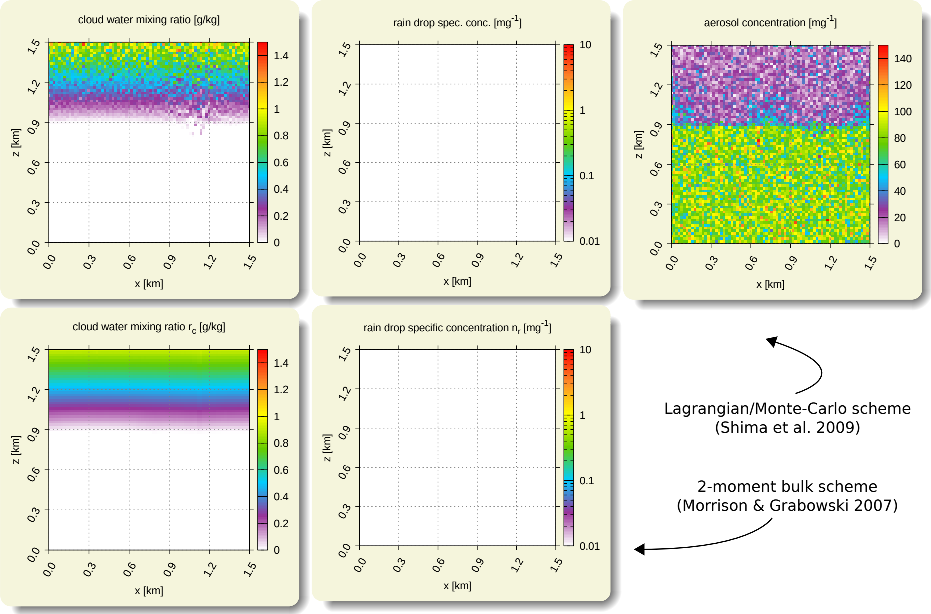

libcloudph++: VOCALS-inspired aerosol processing set-up

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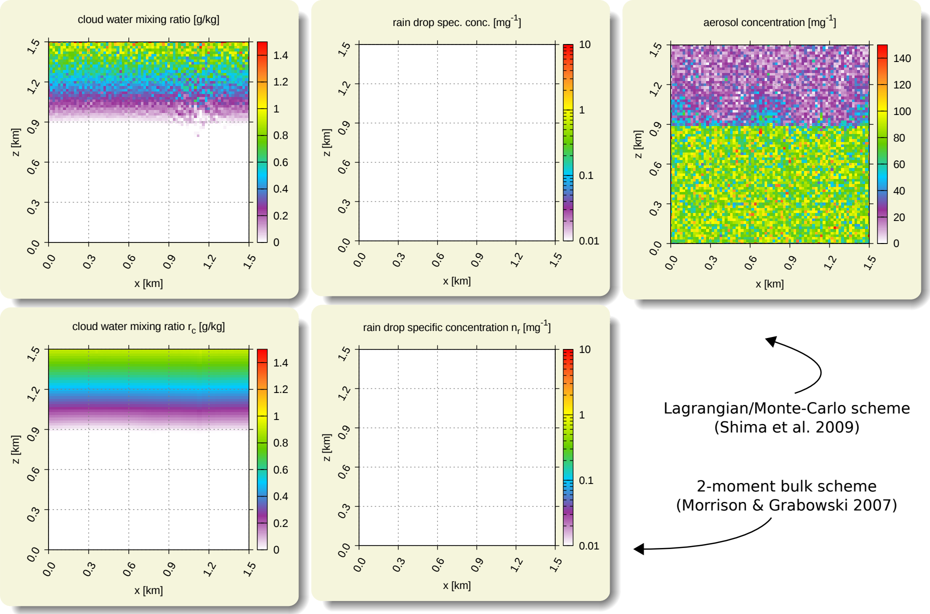

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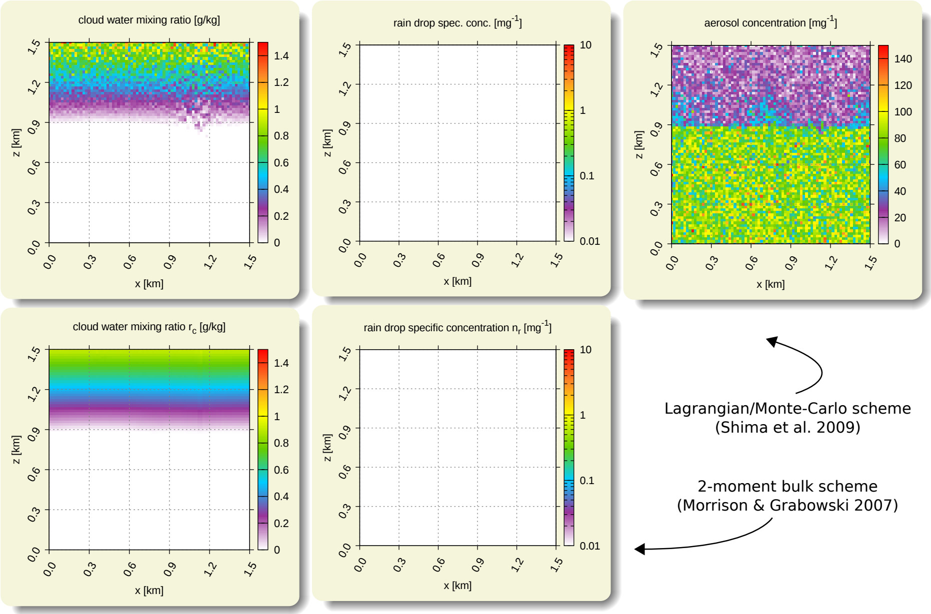

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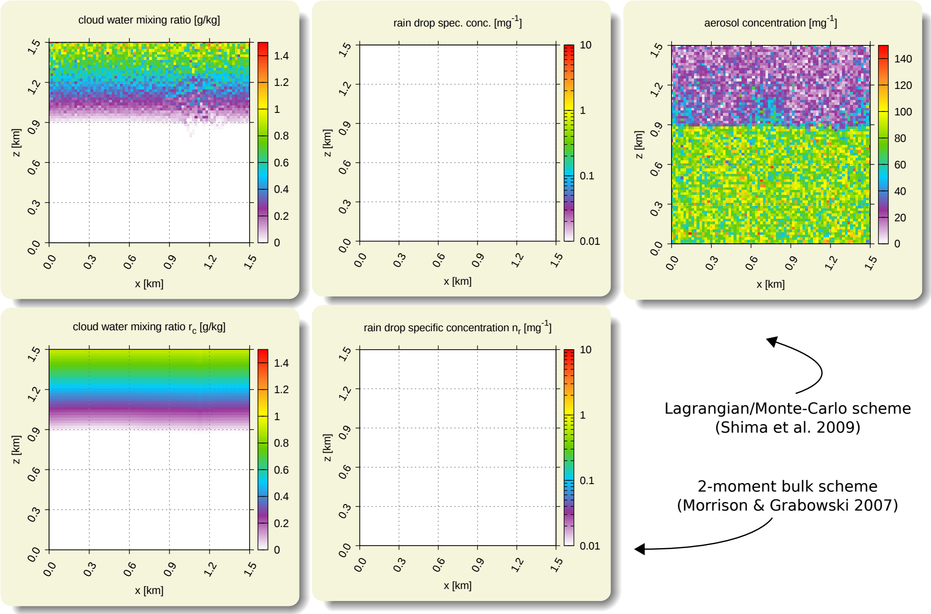

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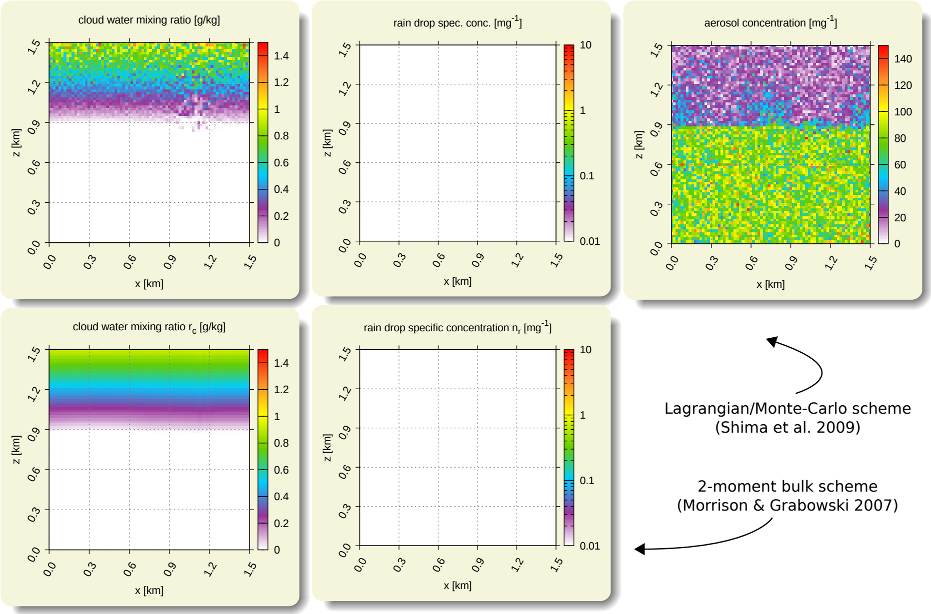

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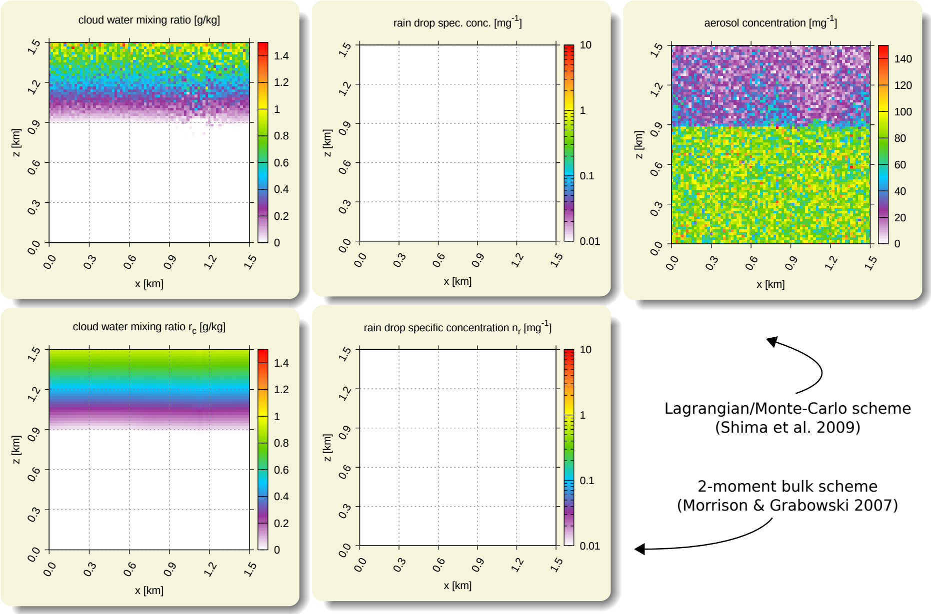

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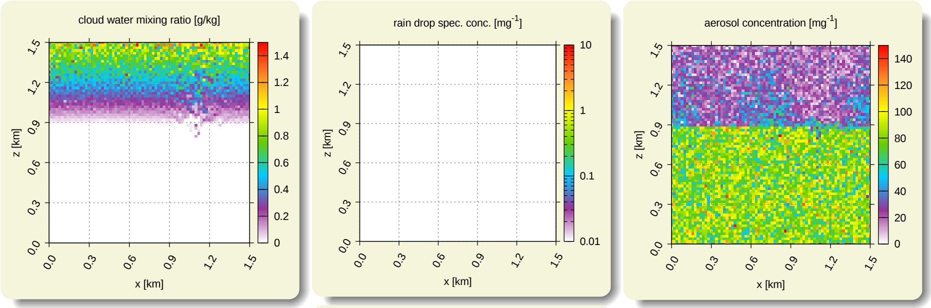

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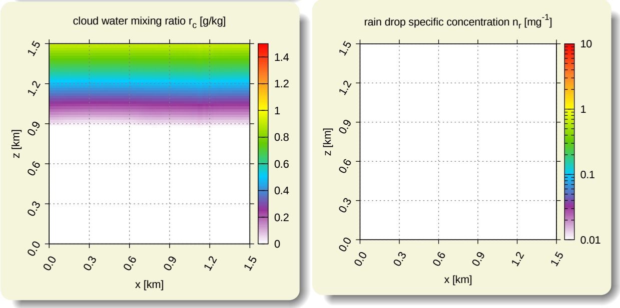

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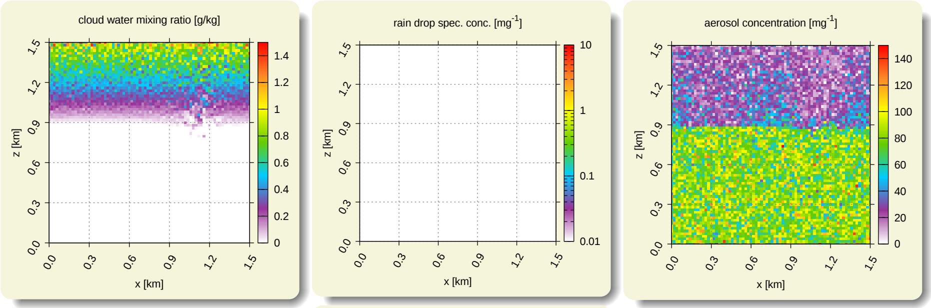

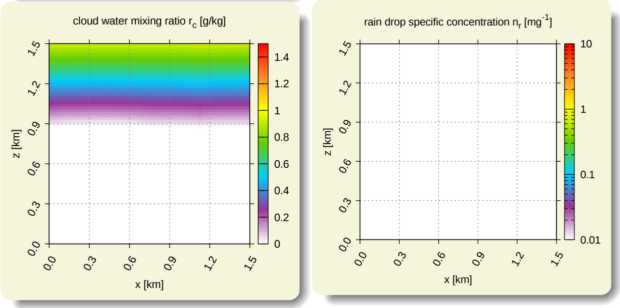

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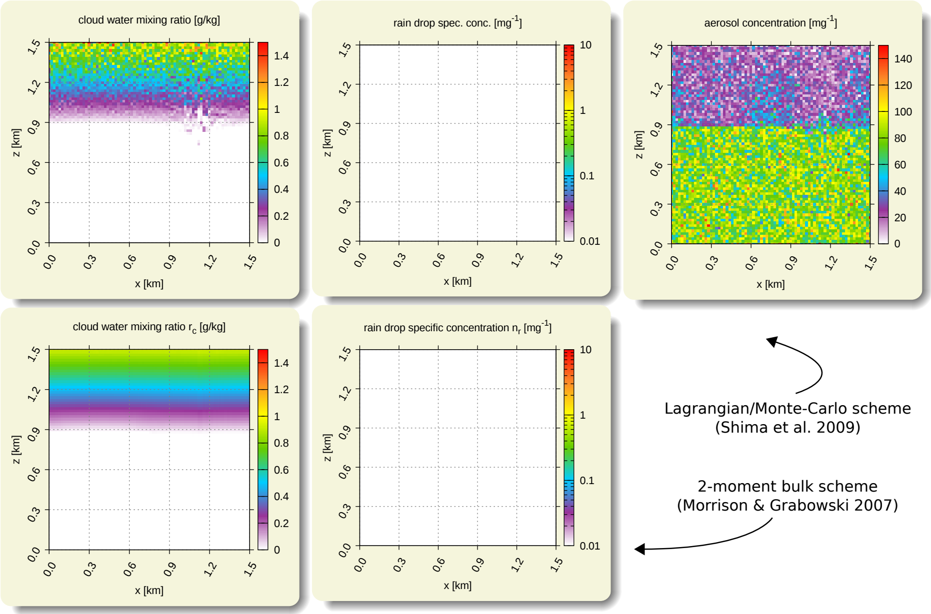

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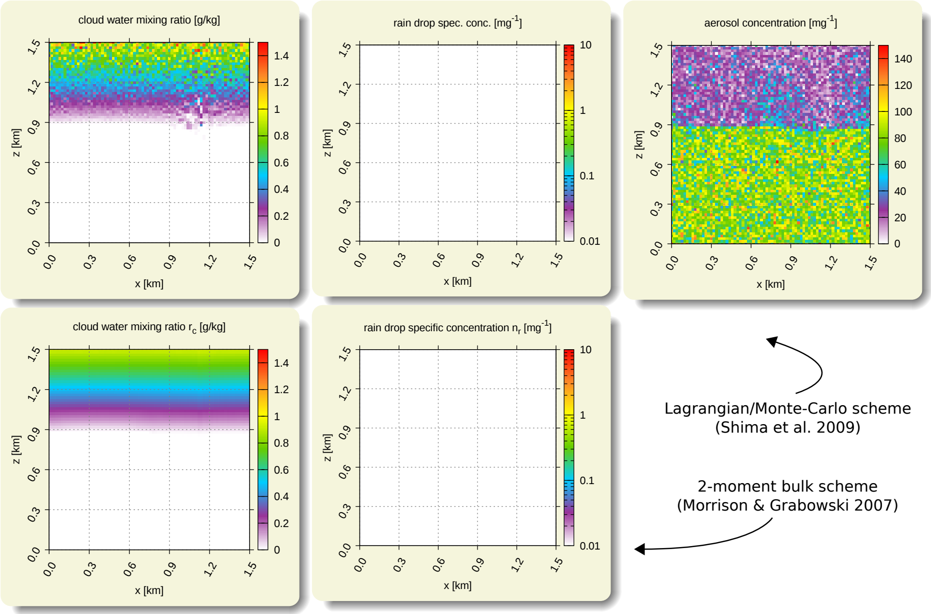

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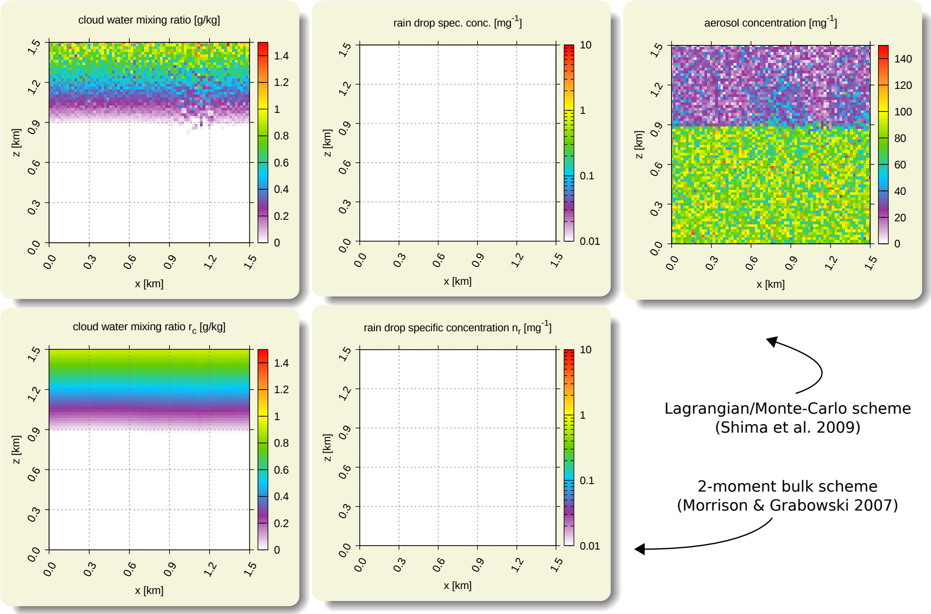

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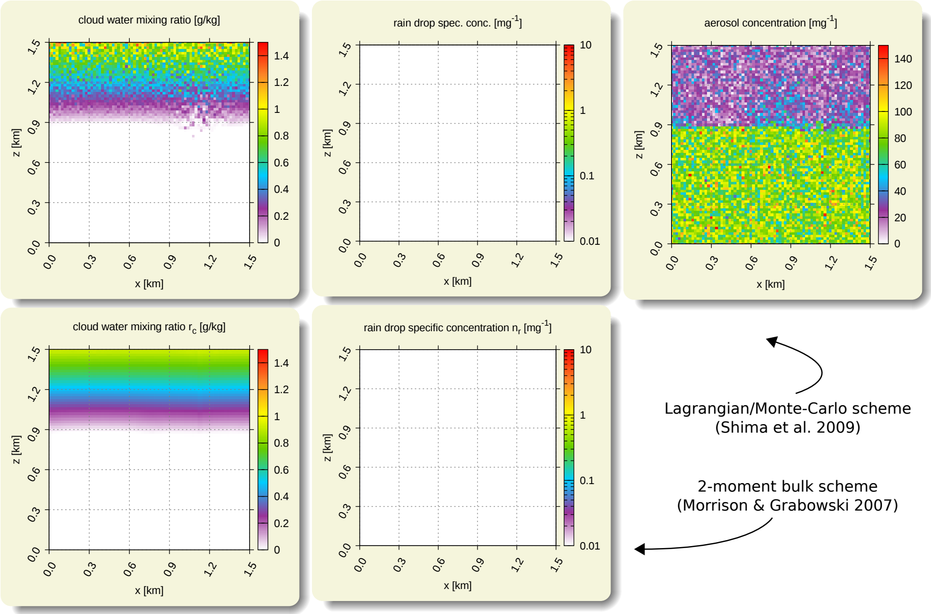

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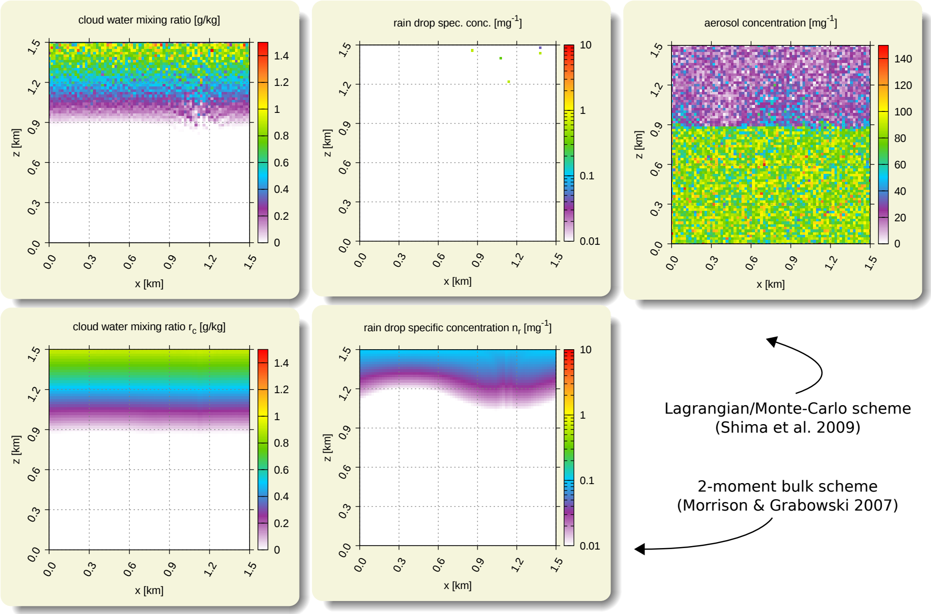

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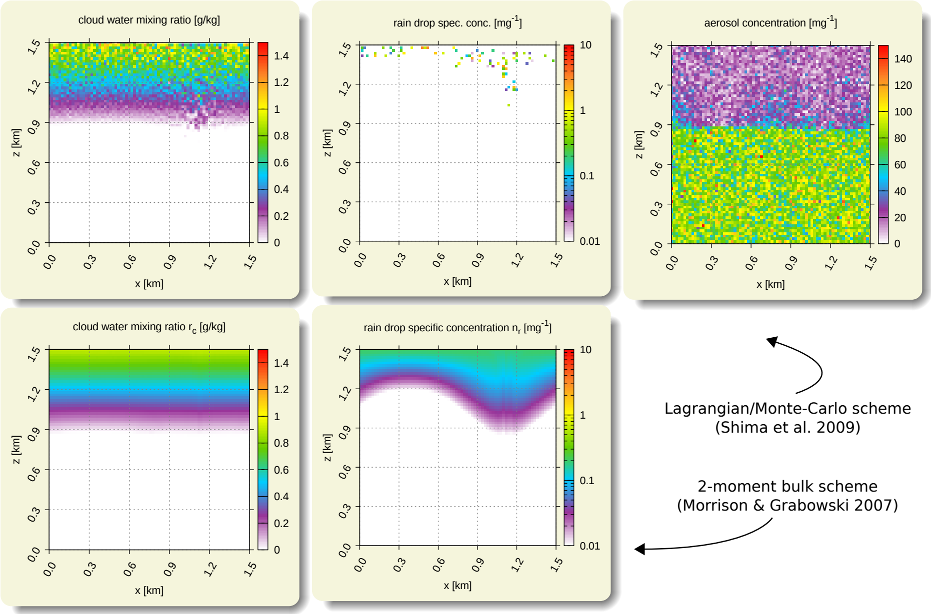

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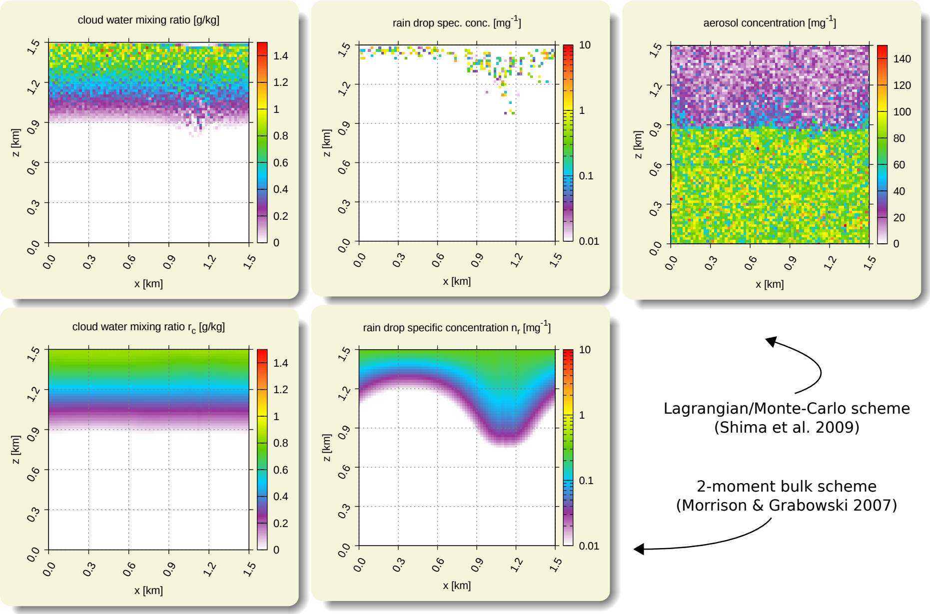

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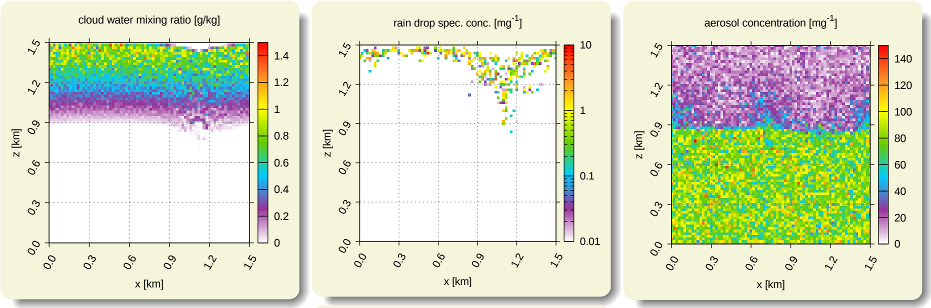

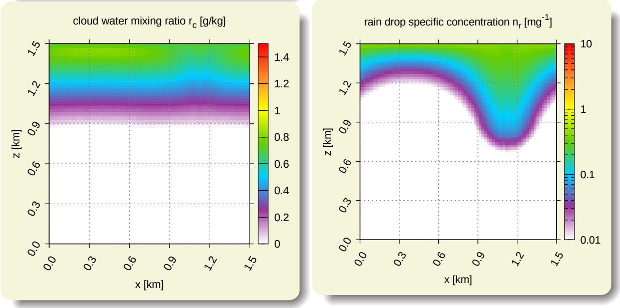

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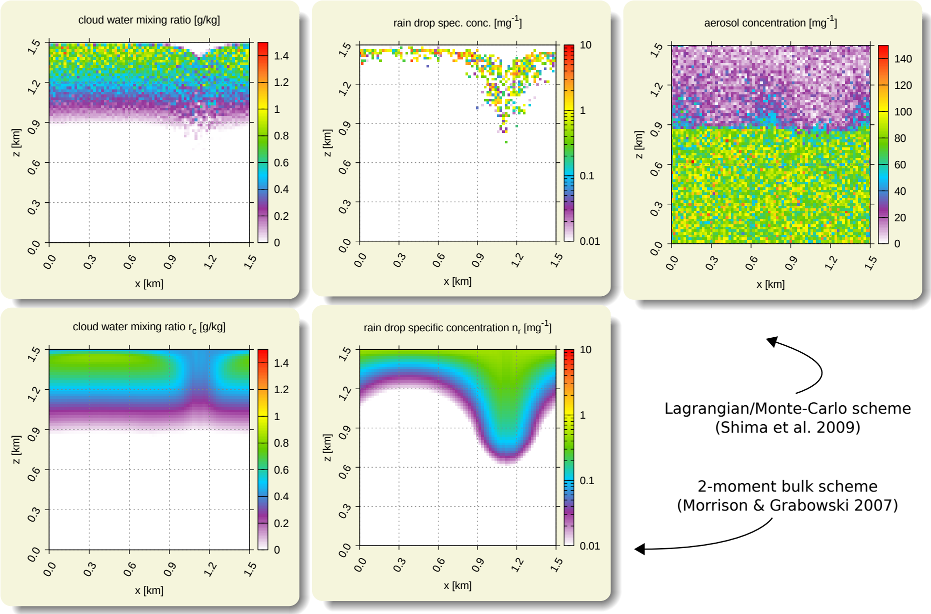

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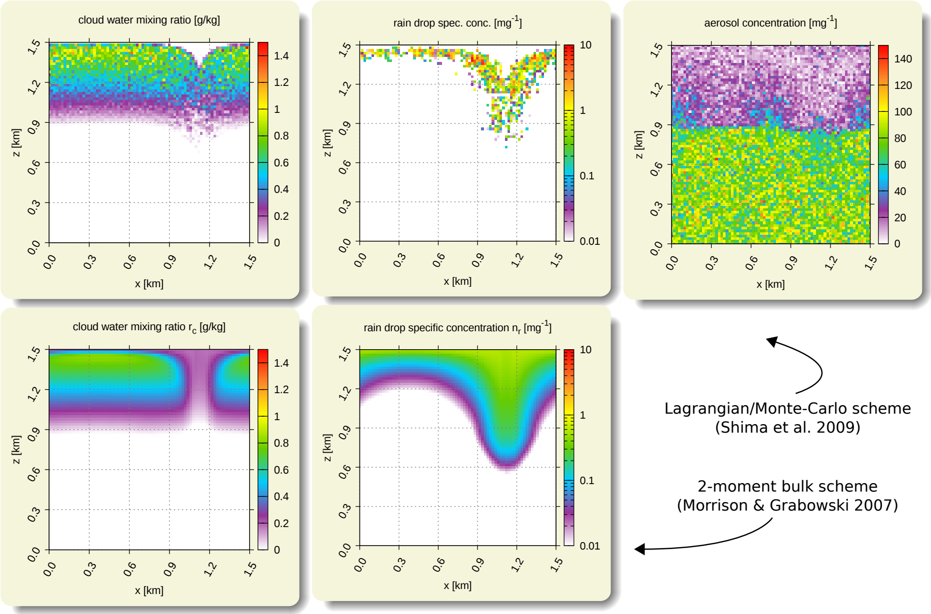

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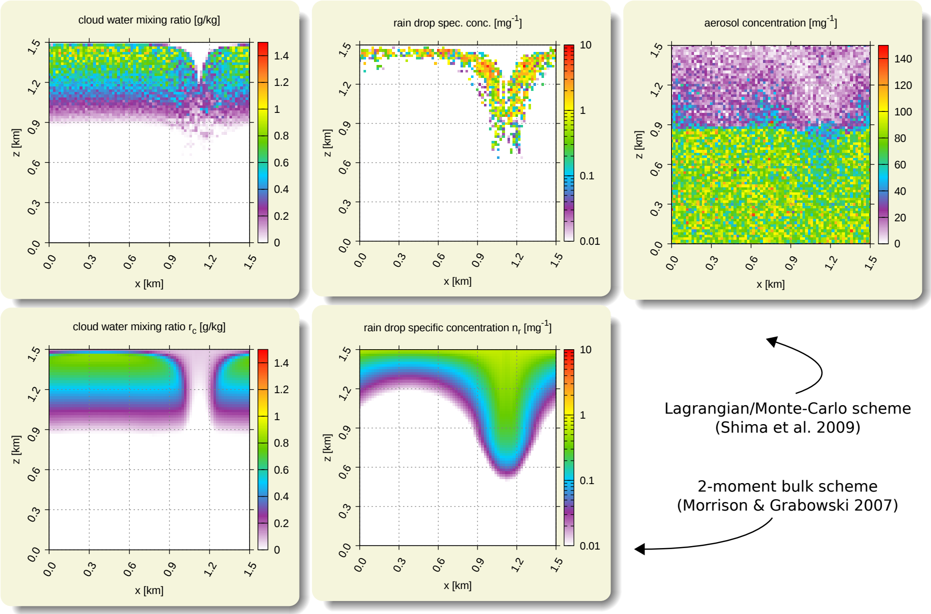

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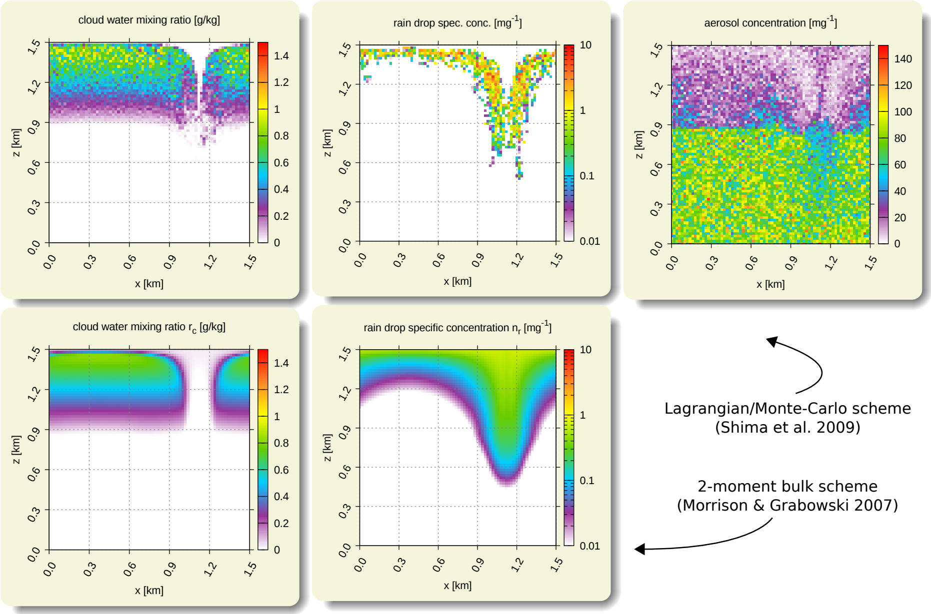
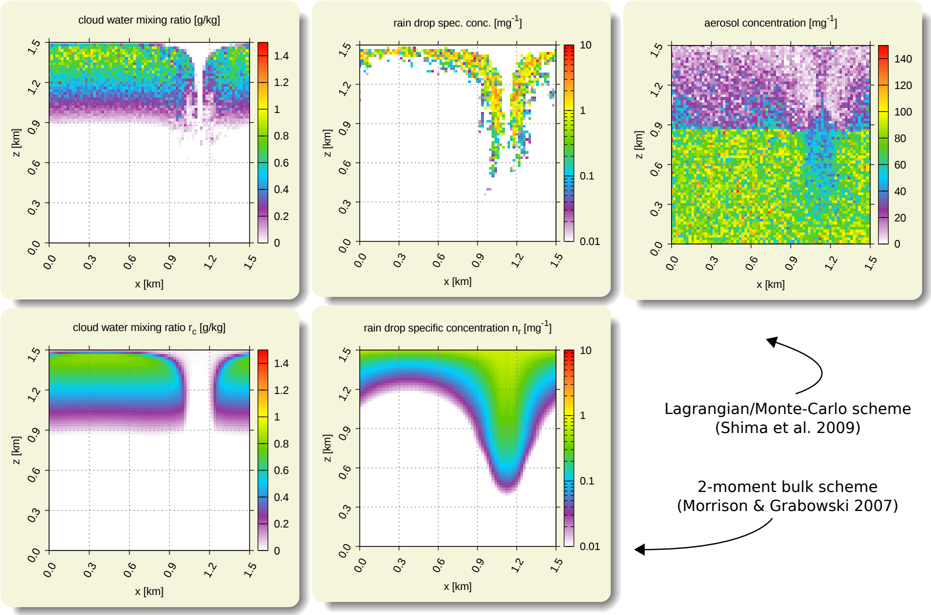
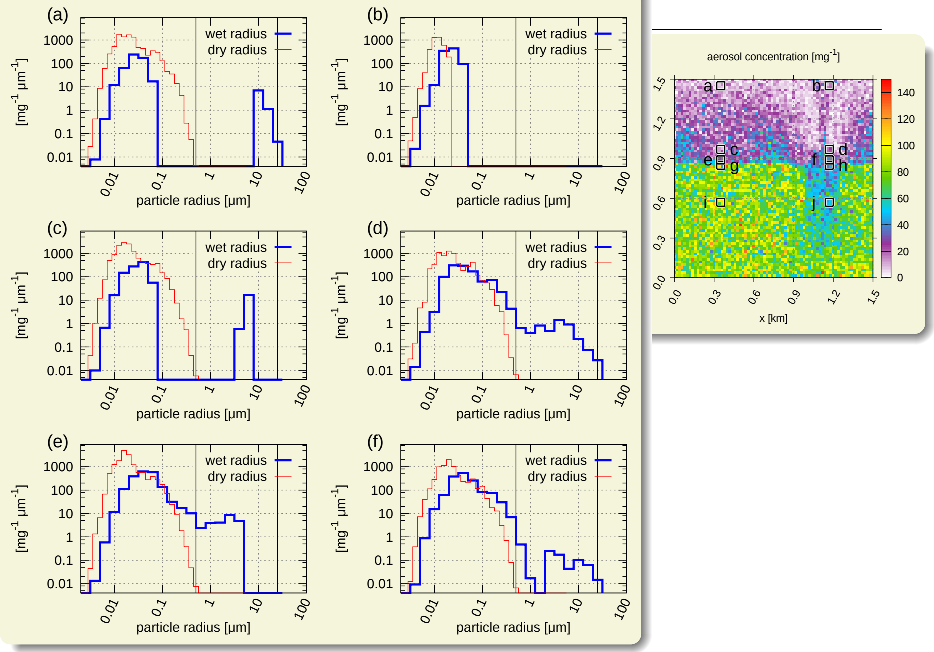


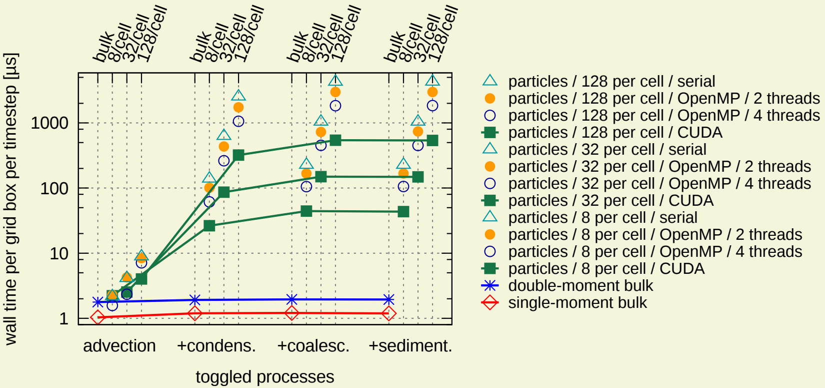
libcloudph++: VOCALS-inspired aerosol processing set-up



2×2 cell particle-derived spectra



libcloudph++: GPU-resident option for Lagrangian scheme



implemented using Thrust: OpenMP/GPU choice with no code modif.

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free & open source C++ library of algorithms for cloud μ-physics

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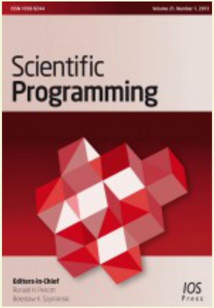
MPDATA in C++, Fortran and Python



Formula translation in Blitz++, NumPy and modern Fortran: A case study of the language choice tradeoffs

Sylwester Arabas[1], Dorota Jarecka[1], Anna Jaruga[1], Maciej Fijałkowski[2]

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Journal	Scientific Programming
DOI	10.3233/SPR-140379
Online Date	Monday, March 24, 2014