On the design and Boost-based implementation of two new C++ libraries for atmospheric research

Sylwester Arabas

Faculty of Physics, University of Warsaw, Poland

C++Now, Aspen, Colorado, May 13 2015

few words about myself

- atmospheric cloud physicist (MSc, PhD, postdoc)

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  - developer of open-source C++ libraries

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- programmer

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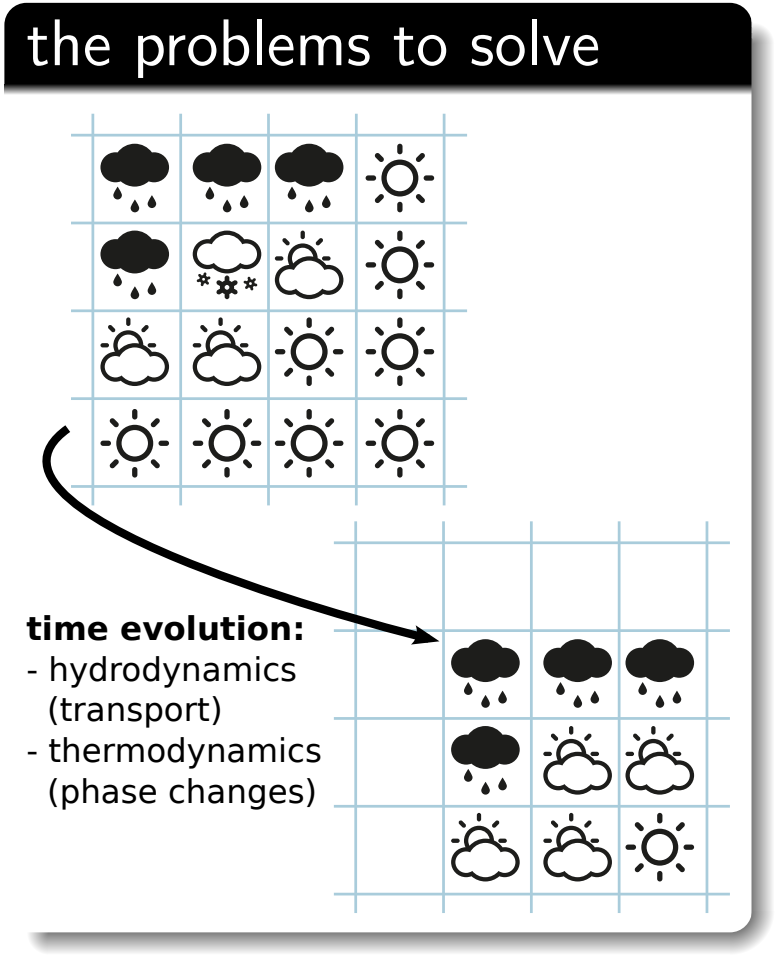

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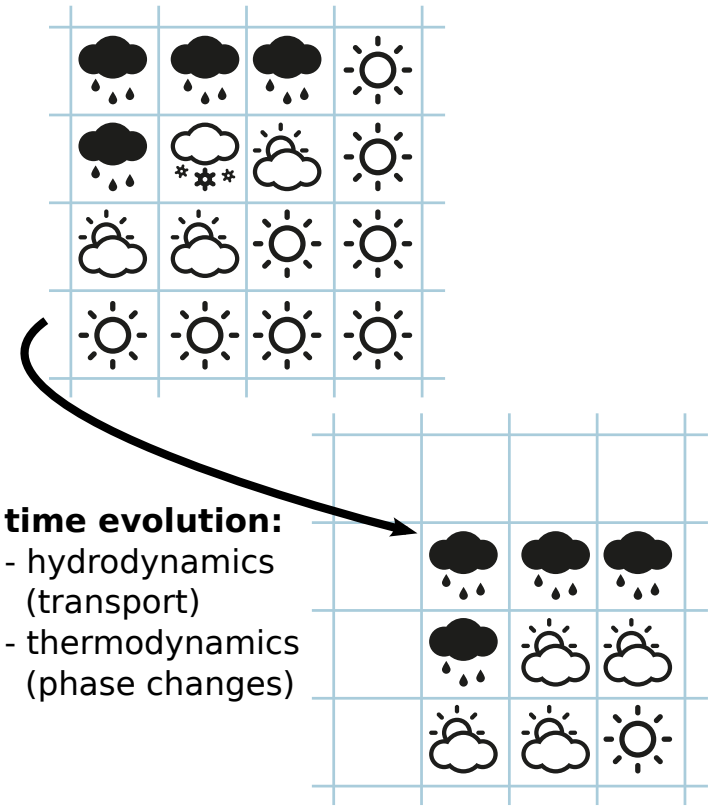
the problems with solving

Nature 467 (2010), doi:10.1038/467775a

the problems to solve



time evolution:
- hydrodynamics (transport)
- thermodynamics (phase changes)

scientific computing in atmospheric sciences

- we are all its users! (e.g., weather prediction)

scientific computing in atmospheric sciences

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- has very long tradition and notorious inertia
  - codes from 80-ties happen to be used till today,
  - it is not uncommon to hear of new codes written in Fortran 77

scientific computing in atmospheric sciences

- we are all its users! (e.g., weather prediction)
- has very long tradition and notorious inertia
  - codes from 80-ties happen to be used till today,
  - it is not uncommon to hear of new codes written in Fortran 77
- is mostly done by reseachers working in a publish-or-perish system in which it is hard to get credit for the time spent on embracing:
  - code reuse
  - unit testing
  - FOSS development model
  - modern coding techniques

scientific computing in atmospheric sciences

- in a longer perspective can benefit from the above through improved:
  - code readability and quality
  - software maintainability
  - result reproducibility

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... I don't have to convince you,
the point is we have convinced a funding agency!

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NATIONAL SCIENCE CENTRE
POLAND

- Title: **Aerosol processing by clouds - a multifaceted object-oriented numerical simulation framework**
- Duration: 3 years (till April 2016)
- Partners: ECMWF, Reading, UK & NCAR, Boulder, CO, US
- Budget: 1/4 M€

the team @ the University of Warsaw, Poland

Anna Zimniak | prof. Hanna Pawłowska | Anna Jaruga | Piotr Dziekan | Sylwester Arabas | Maciek Waruszewski

@ NCAR, Boulder, Colorado, USA

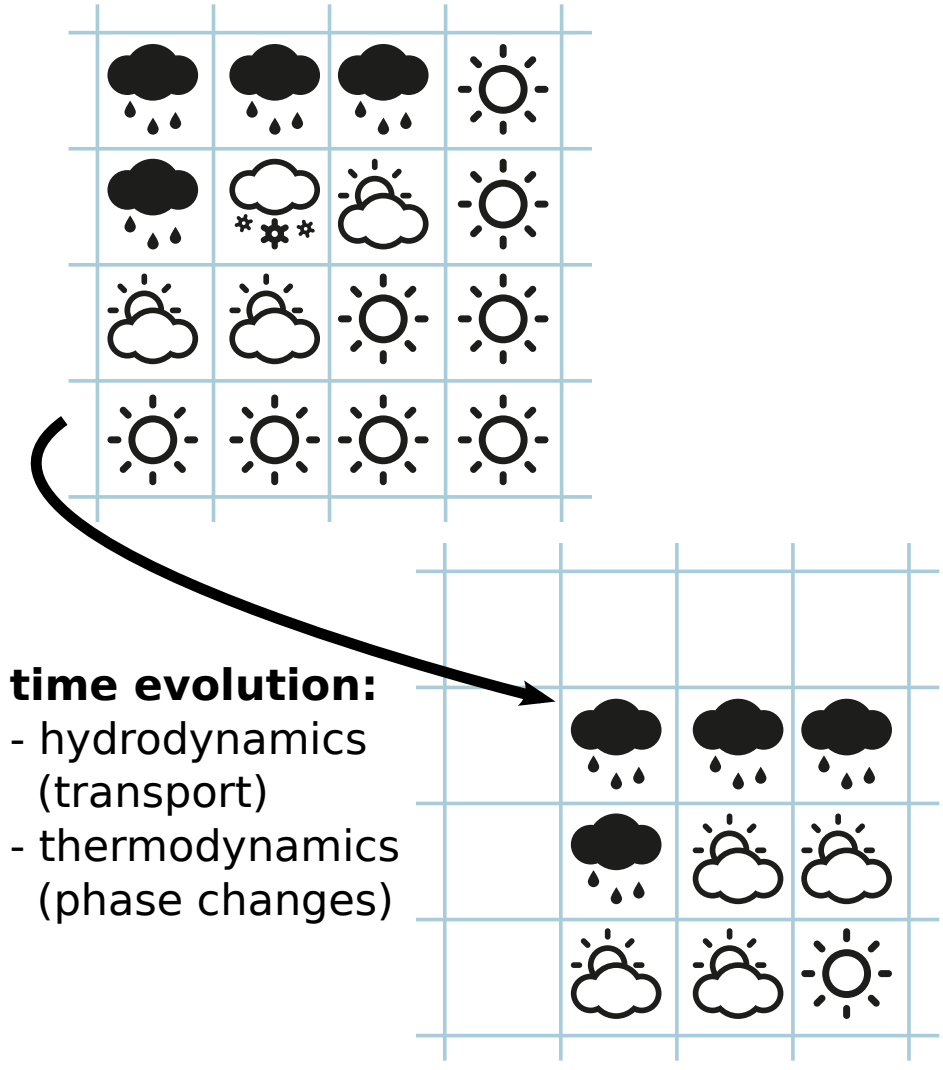
prof. Wojciech Grabowski

Dorota Jarecka

@ ECMWF, Reading, UK

prof. Piotr Smolarkiewicz

a C++ cloud-modelling hello world



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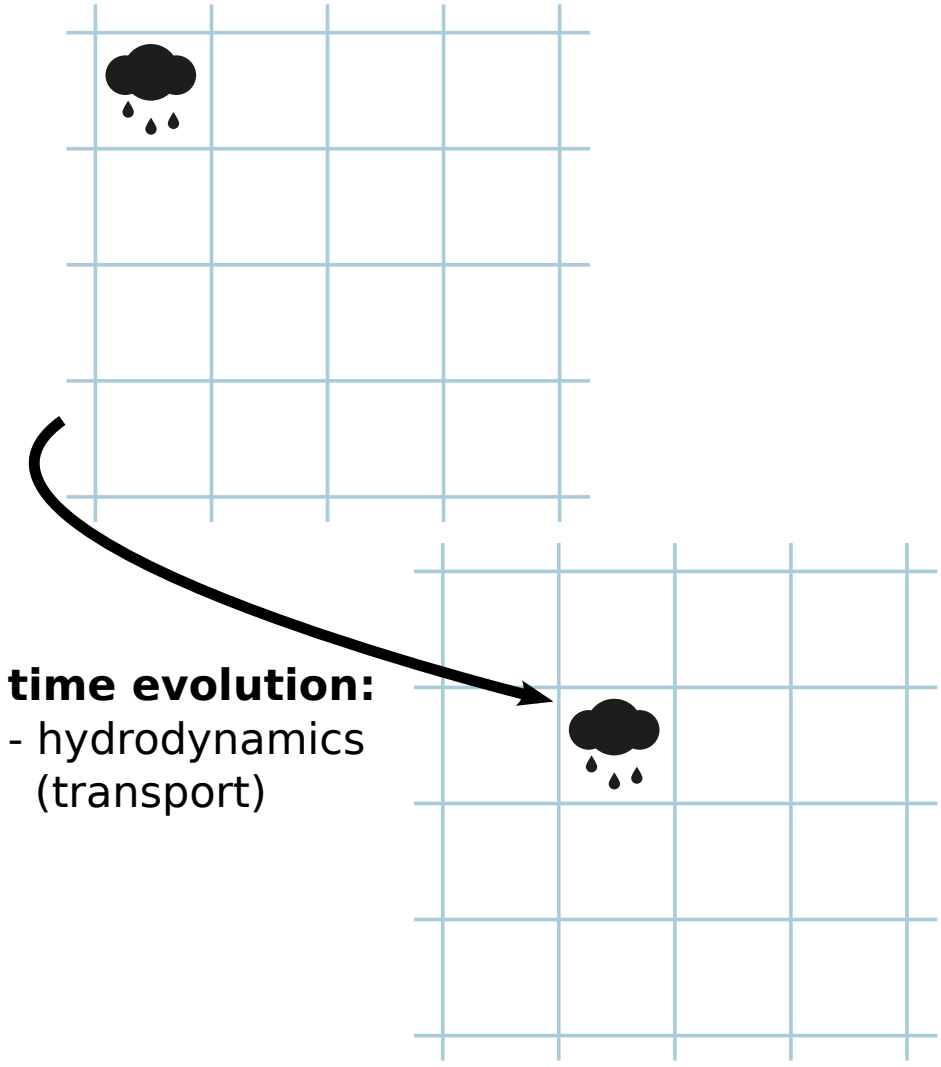

a C++ cloud-modelling hello world (non const-optimal, ...)

```
 1 #include <blitz/array.h>
 2
 3 const int n_dims = 2;
 4 using rng_t = blitz::Range;
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 6 using arr_t = blitz::Array<double, n_dims>;
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27 // integration
28 int main()
29 {
30   int nx = 4, nz = 4;         // domain size
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33   rng_t i(1, nx), j(1, nz);   // i,j indices
34   arr_t psi(nx+2);            // arrays (+halo)
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36   psi = 0;                    // initial cond.
37   psi(1,1) = 1;
38   std::cout << psi(i,j) << std::endl;
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#include <blitz/array.h>

const int n_dims = 2;
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```
$ clang++ hello.cpp
$ ./a.out
(0,3) x (0,3)
[ 1 0 0 0
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  0 0 0 0 ]
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```cpp

// integration
int main()
{
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42     tmp(i,j) = psi(i,j)
43       + 0                     // x term
44       + 0;                    // y term
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46     blitz::cycleArrays(psi, tmp);
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```cpp

// integration
int main()
{
  int nx = 4, nz = 4;         // domain size
  double C[2] = {.5, .5};     // wind vector

  rng_t i(1, nx), j(1, nz);   // i,j indices
  arr_t psi(nx+2), tmp(nz+2);// arrays (+halo)

  psi = 0;                    // initial cond.
  psi(1,1) = 1;
  std::cout << psi(i,j) << std::endl;

  for (int it=0; it<3; ++it) // time-stepping
  {
    tmp(i,j) = psi(i,j)
      + f<0>(psi, C, i, j)   // x term
      + 0;                   // y term

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    std::cout << psi(i,j) << std::endl;
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16
17 // array-valued dimension-independent function
18 template <int d, class arr_t>
19 auto f(arr_t psi, double *C, rng_t i, rng_t j)
20 {
21   return blitz::safeToReturn(
22     -C[d] * psi(      i,   j ) +  // outflow
23     +C[d] * psi(      i-1, j )    // inflow
24   );
25 }
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17 // array-valued dimension-indep
18 template <int d, class arr_t>
19 auto f(arr_t psi, double *C, rn
20 {
21   return blitz::safeToReturn(
22     -C[d] * psi(      i,   j )
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24   );
25 }
```

```
$ clang++ -std=c++14 hello.cpp
$ ./a.out
(0,3) x (0,3)
[ 1 0 0 0
  0 0 0 0
  0 0 0 0
  0 0 0 0 ]

(0,3) x (0,3)
[ 0.5 0 0 0
  0.5 0 0 0
  0 0 0 0
  0 0 0 0 ]

(0,3) x (0,3)
[ 0.25 0 0 0
  0.5 0 0 0
  0.25 0 0 0
  0 0 0 0 ]

(0,3) x (0,3)
[ 0.125 0 0 0
  0.375 0 0 0
  0.375 0 0 0
  0.125 0 0 0 ]
```

```
tion


4, nz = 4;          // domain size
2] = {.5, .5};     // wind vector

, nx), j(1, nz);   // i,j indices
(nx+2), tmp(nz+2);// arrays (+halo)

                    // initial cond.
= 1;
 << psi(i,j) << std::endl;

it=0; it<3; ++it) // time-stepping

) = psi(i,j)
>(psi, C, i, j)    // x term
                    // y term

cycleArrays(psi, tmp);

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const int n_dims = 2;
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// array-valued dimension-independent function
template <int d, class arr_t>
auto f(arr_t psi, double *C, rng_t i, rng_t j)
{
  return blitz::safeToReturn(
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int main()
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  int nx = 4, nz = 4;         // domain size
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  rng_t i(1, nx), j(1, nz);  // i,j indices
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    tmp(i,j) = psi(i,j)
      + f<0>(psi, C, i, j)   // x term
      + f<1>(psi, C, j, i);  // y term

    blitz::cycleArrays(psi, tmp);

    std::cout << psi(i,j) << std::endl;
  }
}
```

a C++ cloud-modelling hello world (non const-optimal, ...)

```cpp
#include <blitz/array.h>

const int n_dims = 2;
using rng_t = blitz::Range;
using idx_t = blitz::RectDomain<n_dims>;
using arr_t = blitz::Array<double, n_dims>;

// index permutations
template<int d> idx_t pi(rng_t i, rng_t j);

template<> idx_t pi<0> (rng_t i, rng_t j)
{ return idx_t({ i, j}); } // ~\_____ /~   !!!
                           // ./      \.
template<> idx_t pi<1> (rng_t j, rng_t i)
{ return idx_t({ i, j}); }

// array-valued dimension-independent function
template <int d, class arr_t>
auto f(arr_t psi, double *C, rng_t i, rng_t j)
{
  return blitz::safeToReturn(
    -C[d] * psi(pi<d>(i,   j)) +  // outflow
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11 template<> idx_t pi<0> (rng_t
12 { return idx_t({ i, j}); } //
13                             //
14 template<> idx_t pi<1> (rng_t
15 { return idx_t({ i, j}); }
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17 // array-valued dimension-indep
18 template <int d, class arr_t>
19 auto f(arr_t psi, double *C, r
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21   return blitz::safeToReturn(
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[ 0 0.5 0 0
  0.5 0 0 0
  0 0 0 0
  0 0 0 0 ]

(0,3) x (0,3)
[ 0 0 0.25 0
  0 0.5 0 0
  0.25 0 0 0
  0 0 0 0 ]

(0,3) x (0,3)
[ 0 0 0 0.125
  0 0 0.375 0
  0 0.375 0 0
  0.125 0 0 0 ]
```

```
tion


4, nz = 4;          // domain size
2] = {.5, .5};     // wind vector

, nx), j(1, nz);   // i,j indices
(nx+2), tmp(nz+2);// arrays (+halo)

                    // initial cond.
= 1;
 << psi(i,j) << std::endl;

it=0; it<3; ++it) // time-stepping

) = psi(i,j)
>(psi, C, i, j)    // x term
>(psi, C, j, i);   // y term

cycleArrays(psi, tmp);

ut << psi(i,j) << std::endl;
```

a cloud-modelling hello world: summary

OOP for "blackboard abstractions"

- multidimensional array containers

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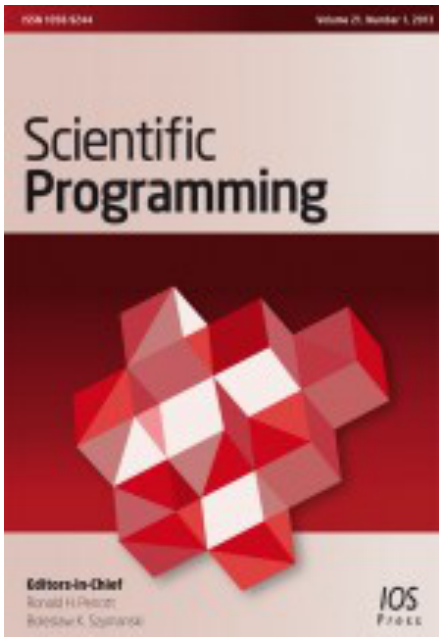

Formula translation in Blitz++, NumPy and modern Fortran: A case study of the language choice tradeoffs

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

[1]Institute of Geophysics, Faculty of Physics, University of Warsaw
[2]PyPy Team

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Online Date	Monday, March 24, 2014

plan of the talk

introduction

libmpdata++

libcloudph++

n-dim array containers

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n-dim array containers

libmpdata++

http://libmpdataxx.igf.fuw.edu.pl/

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- multiple dimensions

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libmpdata++: hello world

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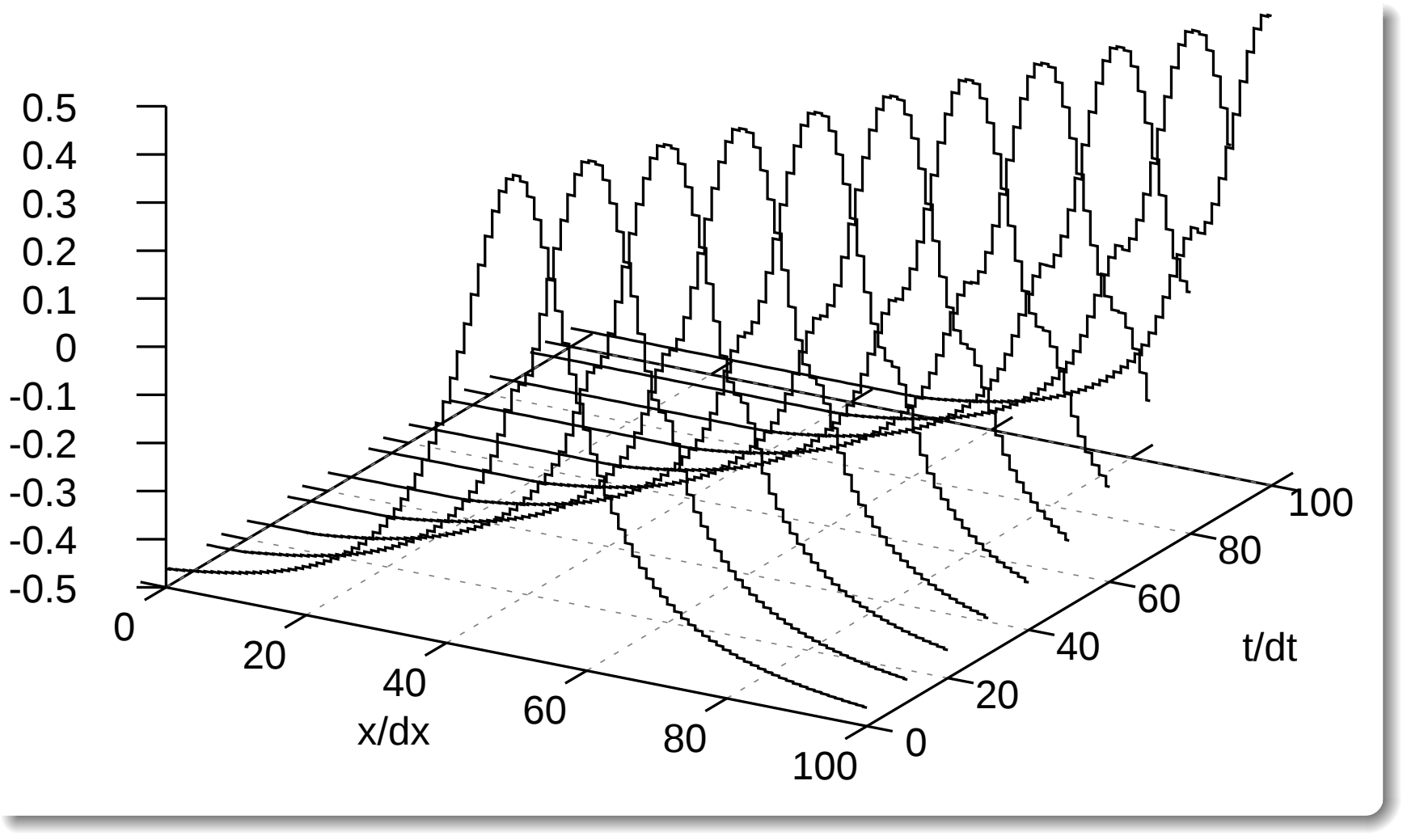


libmpdata++: hello world

hello.cpp 1/2

```
 1 #include <libmpdata++/solvers/mpdata.hpp>
 2 #include <libmpdata++/concurr/serial.hpp>
 3 #include <libmpdata++/output/gnuplot.hpp>
 4 using namespace libmpdataxx;
 5
 6 int main()
 7 {
 8   struct ct_params_t : ct_params_default_t // compile-time parameters
 9   {
10     using real_t = double;
11     enum { n_dims = 1 };
12     enum { n_eqns = 1 };
13     enum { opts = opts::fct };
14   };
15
16   using solver_t = output::gnuplot<        // solver & ouput choice
17     solvers::mpdata<ct_params_t>
18   >;
```

. . .

libmpdata++: hello world

hello.cpp 2/2

. . .

```
19
20    typename solver_t::rt_params_t p;          // run-time parameters
21    p.grid_size = { 101 };
22    p.outfreq = 10;
23
24    concurr::serial<                           // concurrency choice
25      solver_t,                                // solver defined above
26      bcond::open, bcond::open                 // left, right boundary cond.
27    > run(p);
28
29    blitz::firstIndex i;                       // initial condition
30    run.advectee() = -.5 + 1 / (
31      pow(0.1 * (i - (p.grid_size[0]-1)/2.), 2) + 1
32    );
33
34    run.advector() = .5;                       // Courant number
35    run.advance(100);                          // integration (100 timesteps)
36  }
```

libmpdata++: hello world

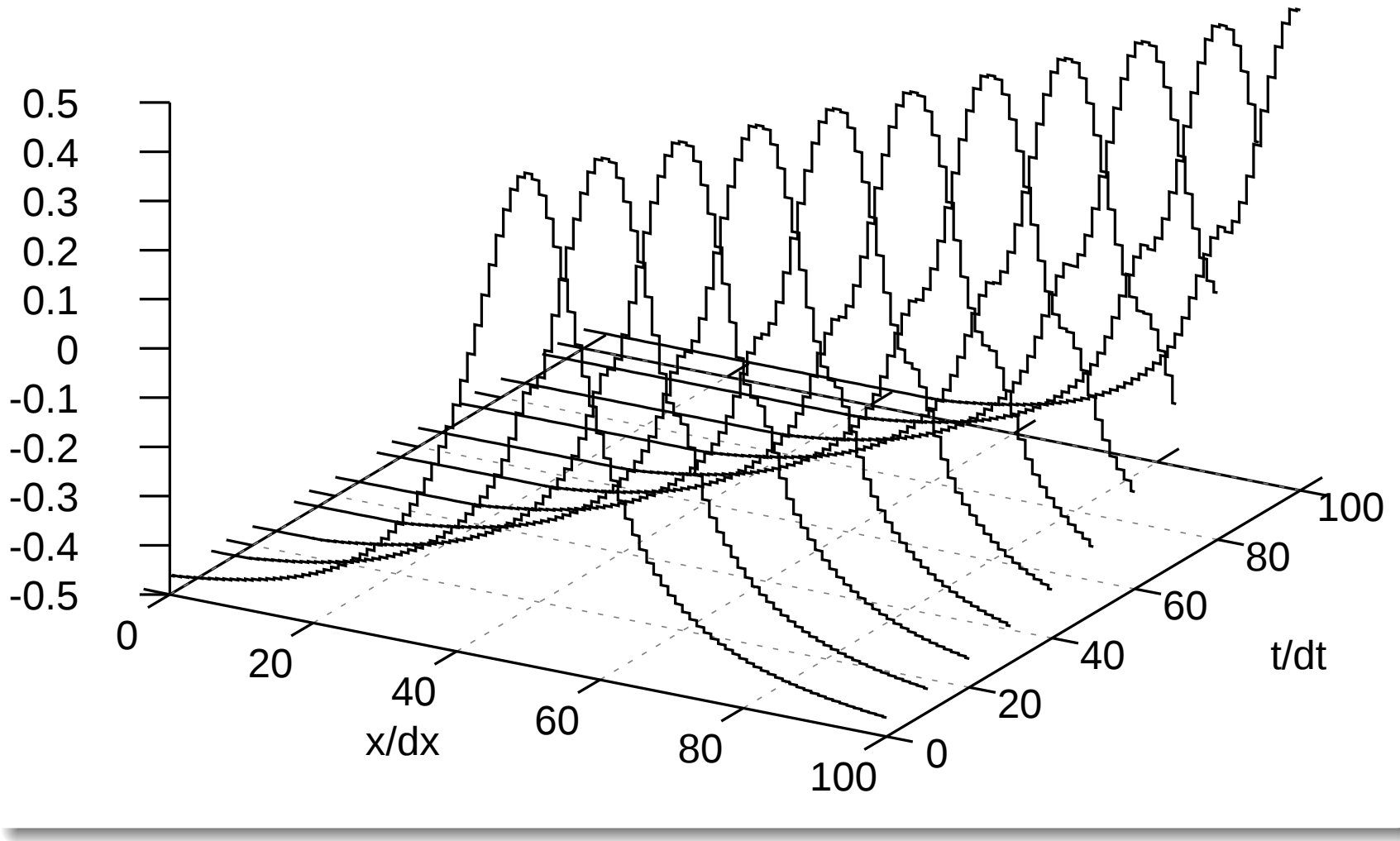
CMakeLists.txt

```
1 cmake_minimum_required(VERSION 3.0)
2 project(hello CXX)
3 find_package(libmpdata++)
4 set(CMAKE_CXX_FLAGS ${libmpdataxx_CXX_FLAGS_RELEASE})
5 add_executable(hello hello.cpp)
6 target_link_libraries(hello ${libmpdataxx_LIBRARIES})
```

```
$ cmake .
-- Configuring done
-- Generating done
-- Build files have been written to: ...
$ make
[100%] Building CXX object CMakeFiles/hello.dir/hello.cpp.o
Linking CXX executable hello
[100%] Built target hello
$ ./hello
 wall time: 0.0177881s user time: 0.02s system time: 0s
```

libmpdata++: hello world

out.svg



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homogeneous advection

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user/test code

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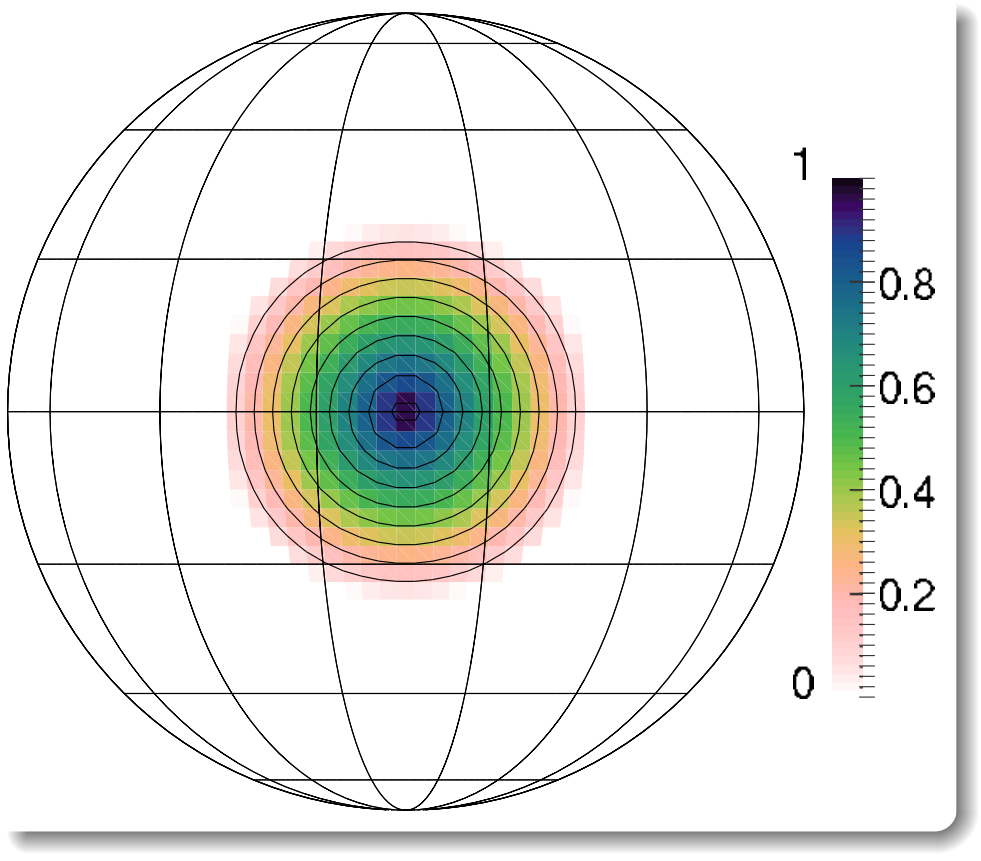

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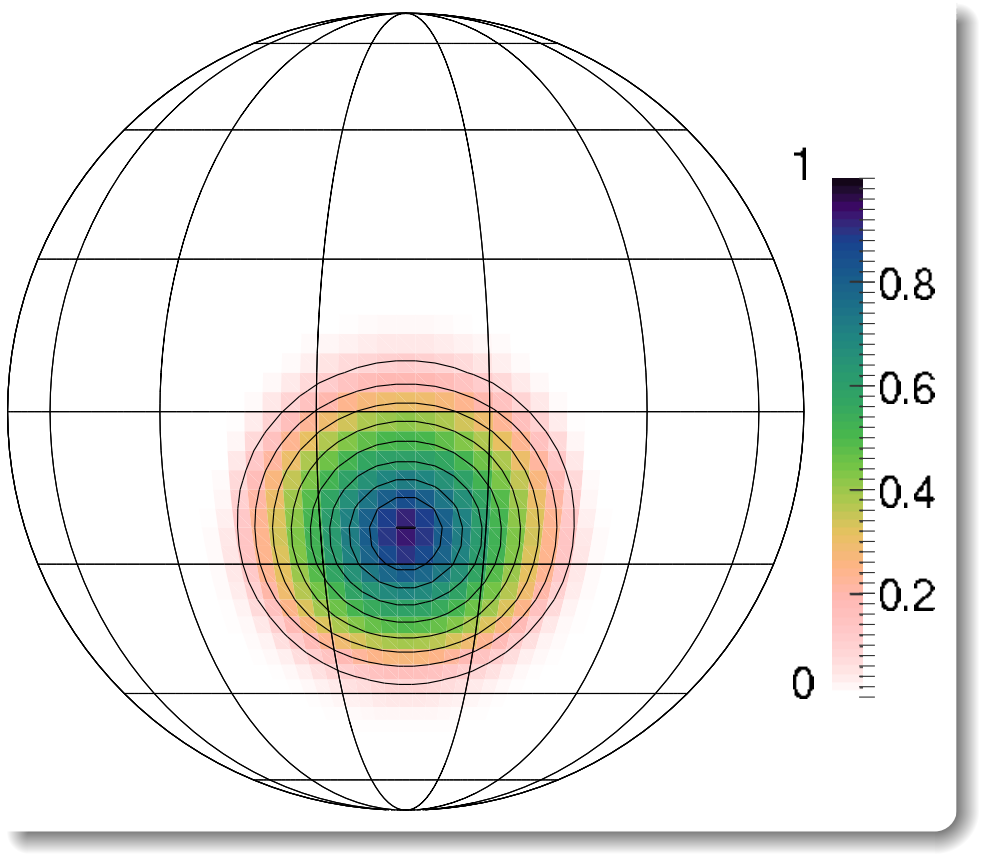

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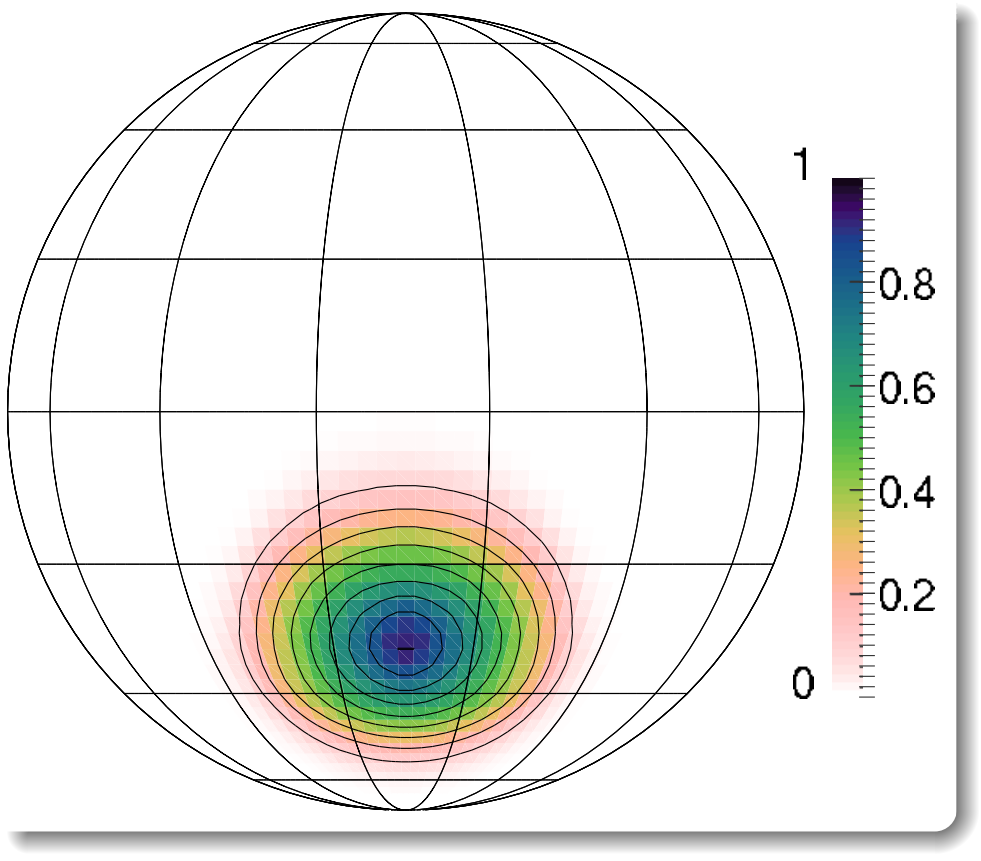

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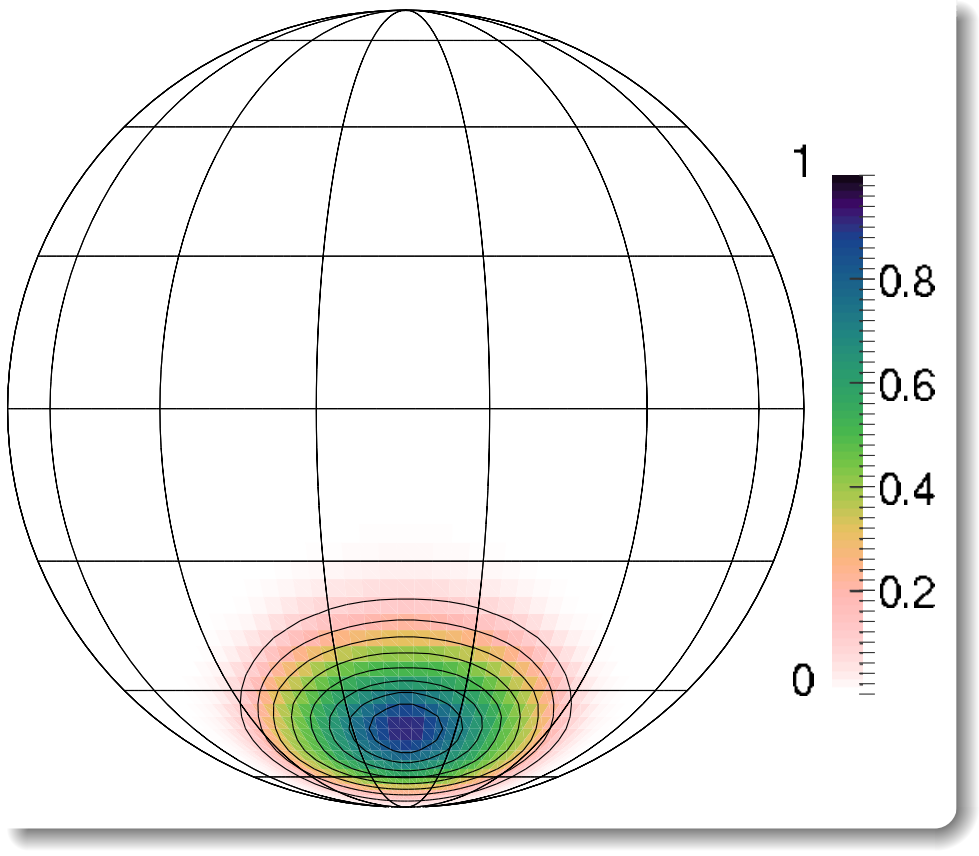

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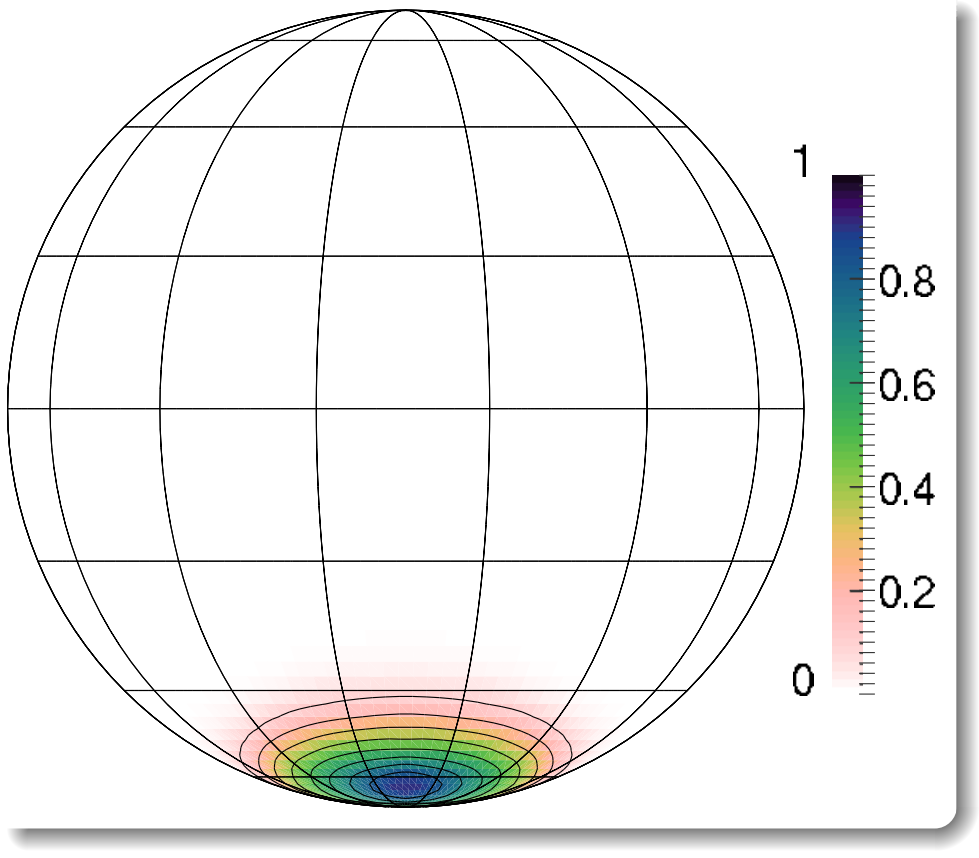

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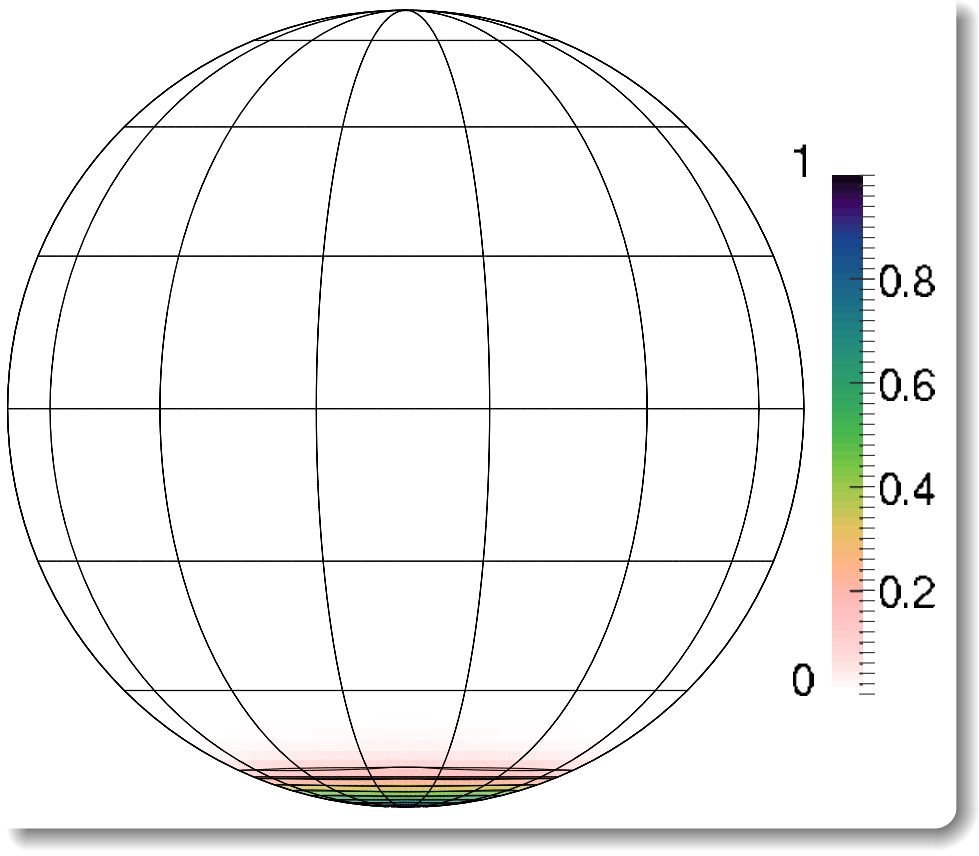

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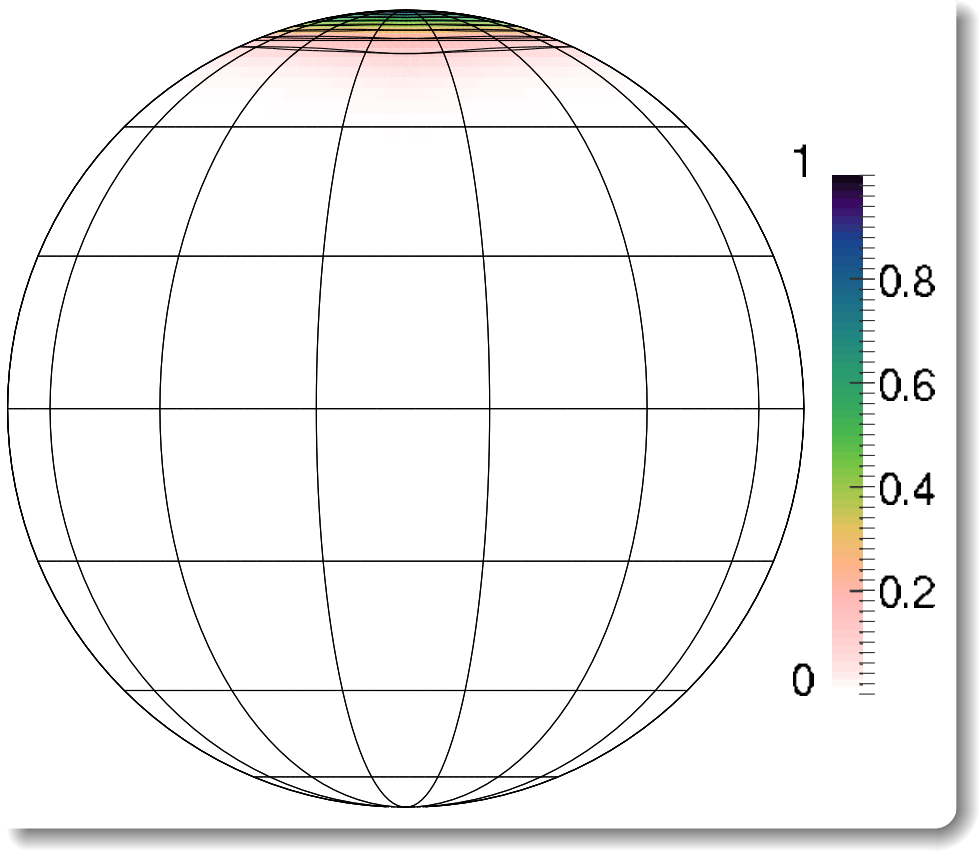

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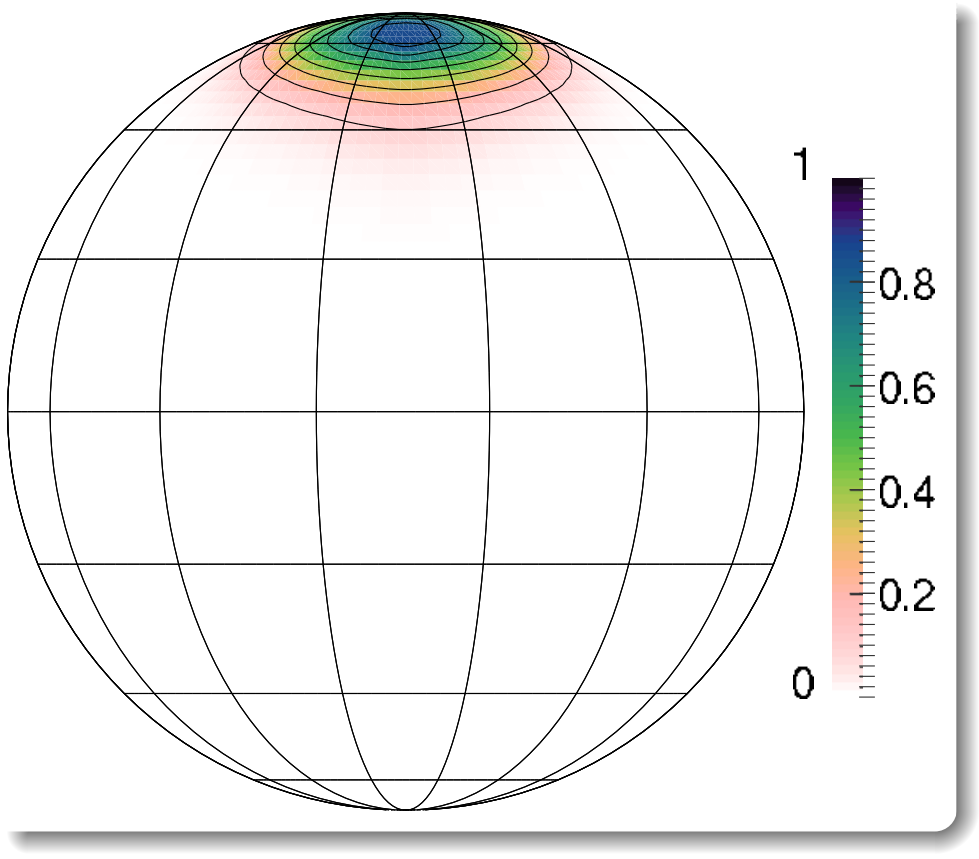

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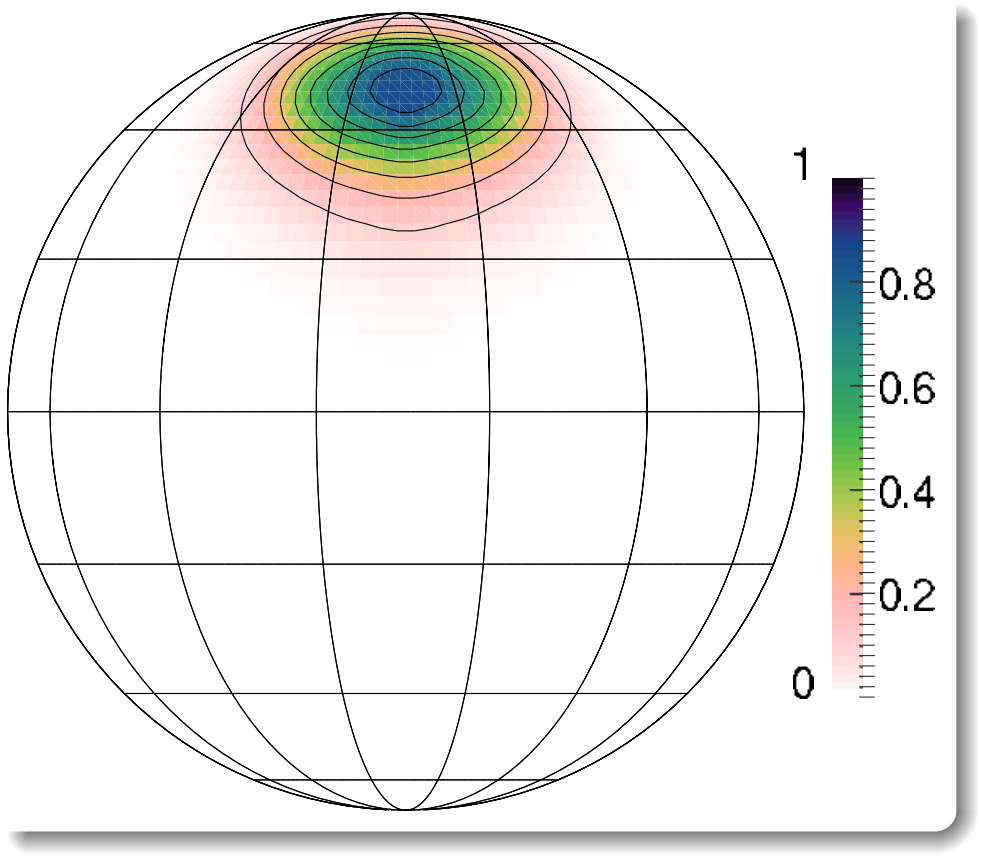

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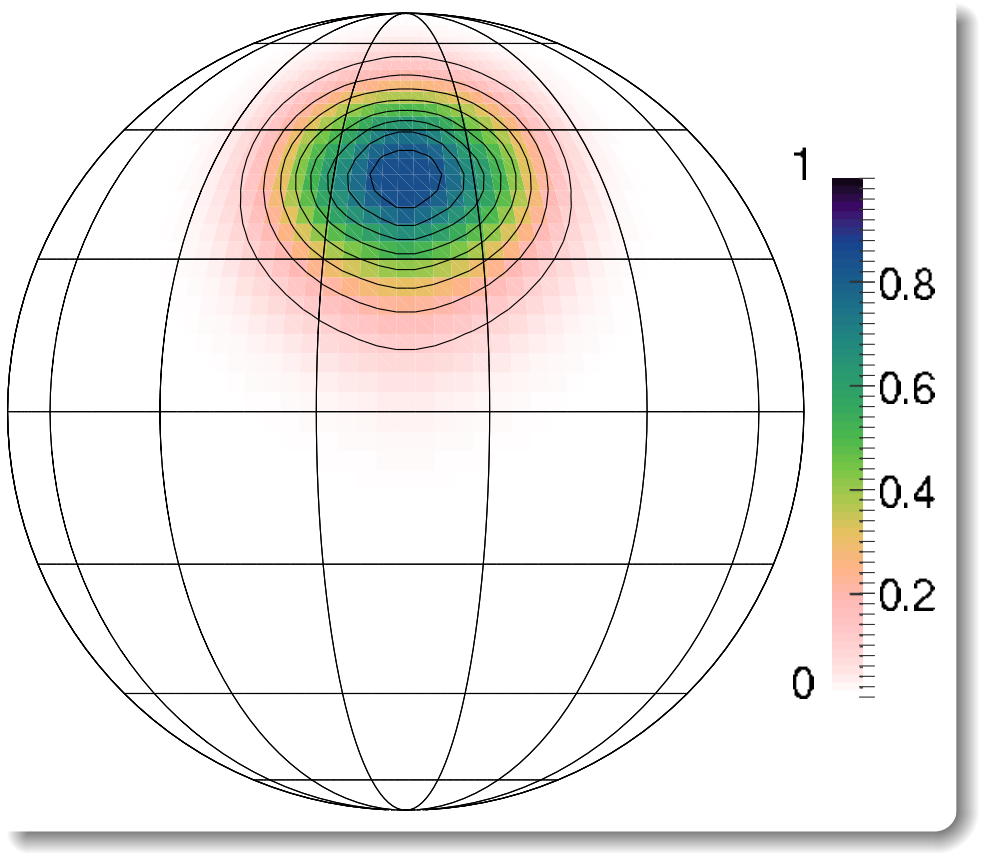

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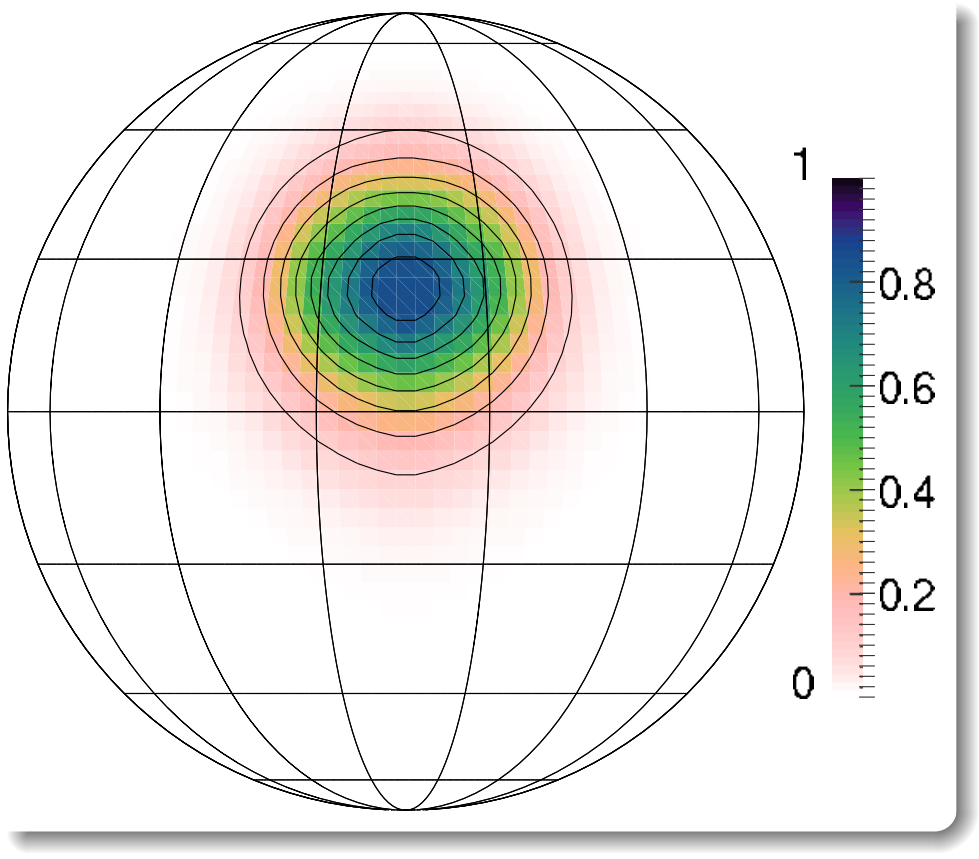

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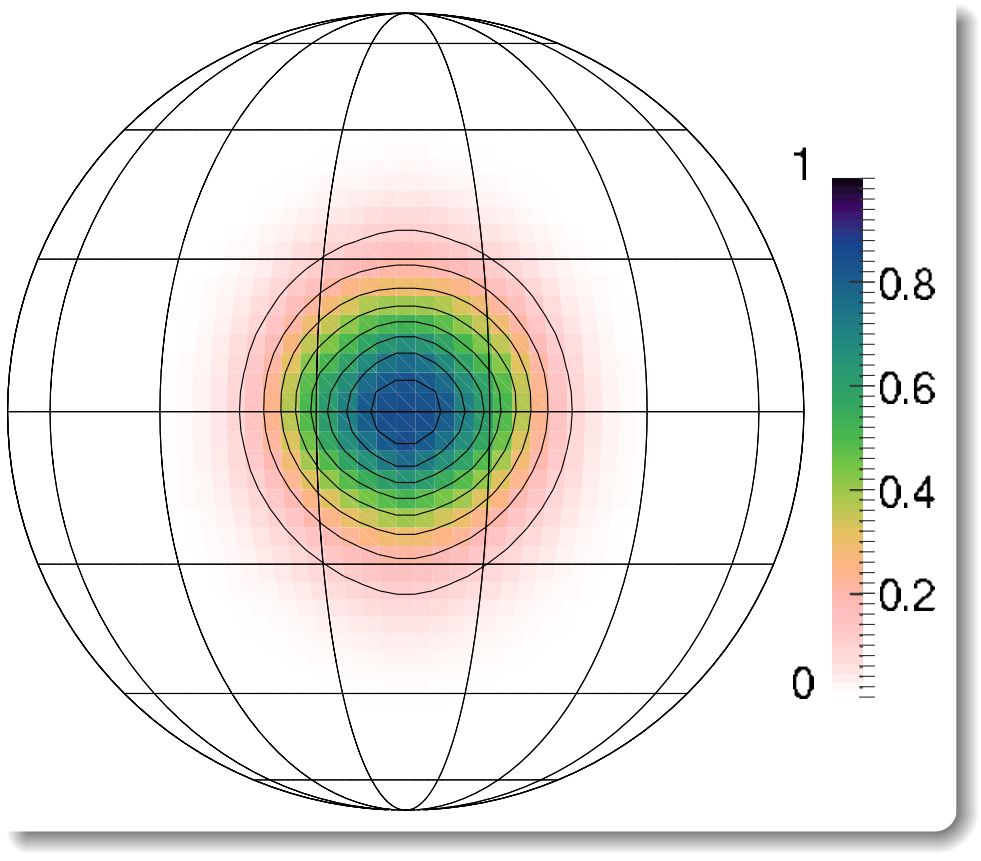

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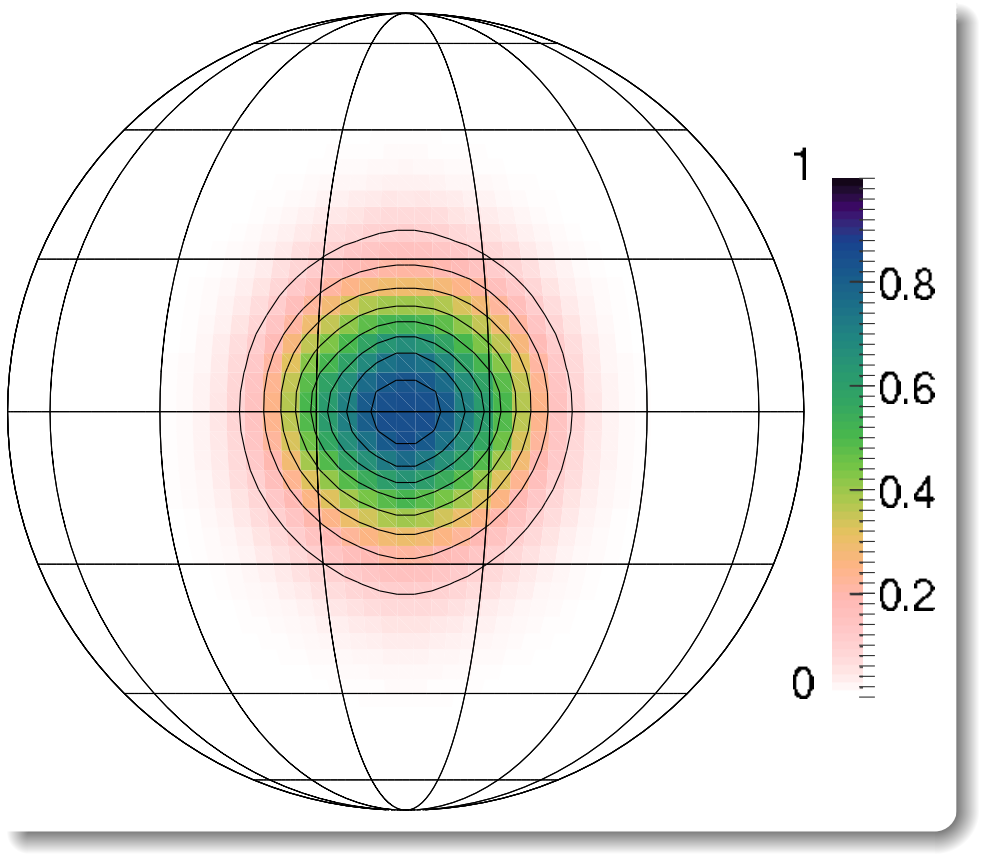

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- <100 lines of code with libmpdata++

`https://github.com/igfuw/libmpdataxx/tree/master/tests/paper_2015_GMD/5_over_the_pole_2d`

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homogeneous advection

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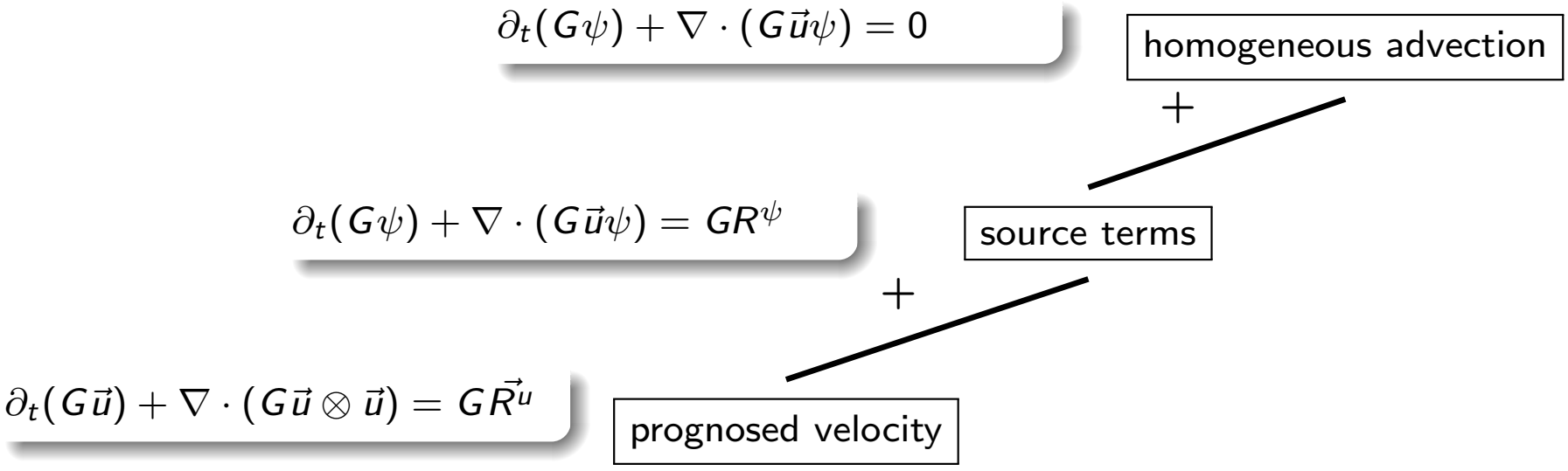
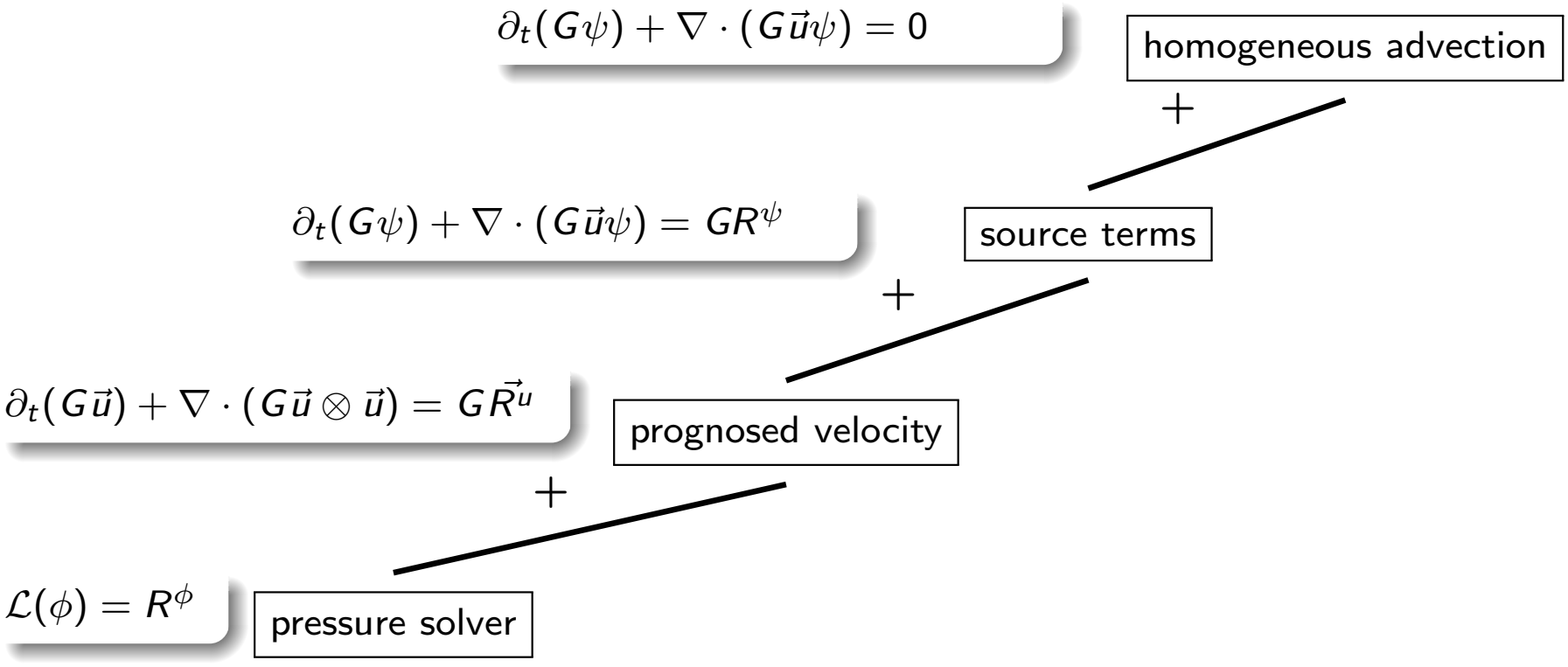
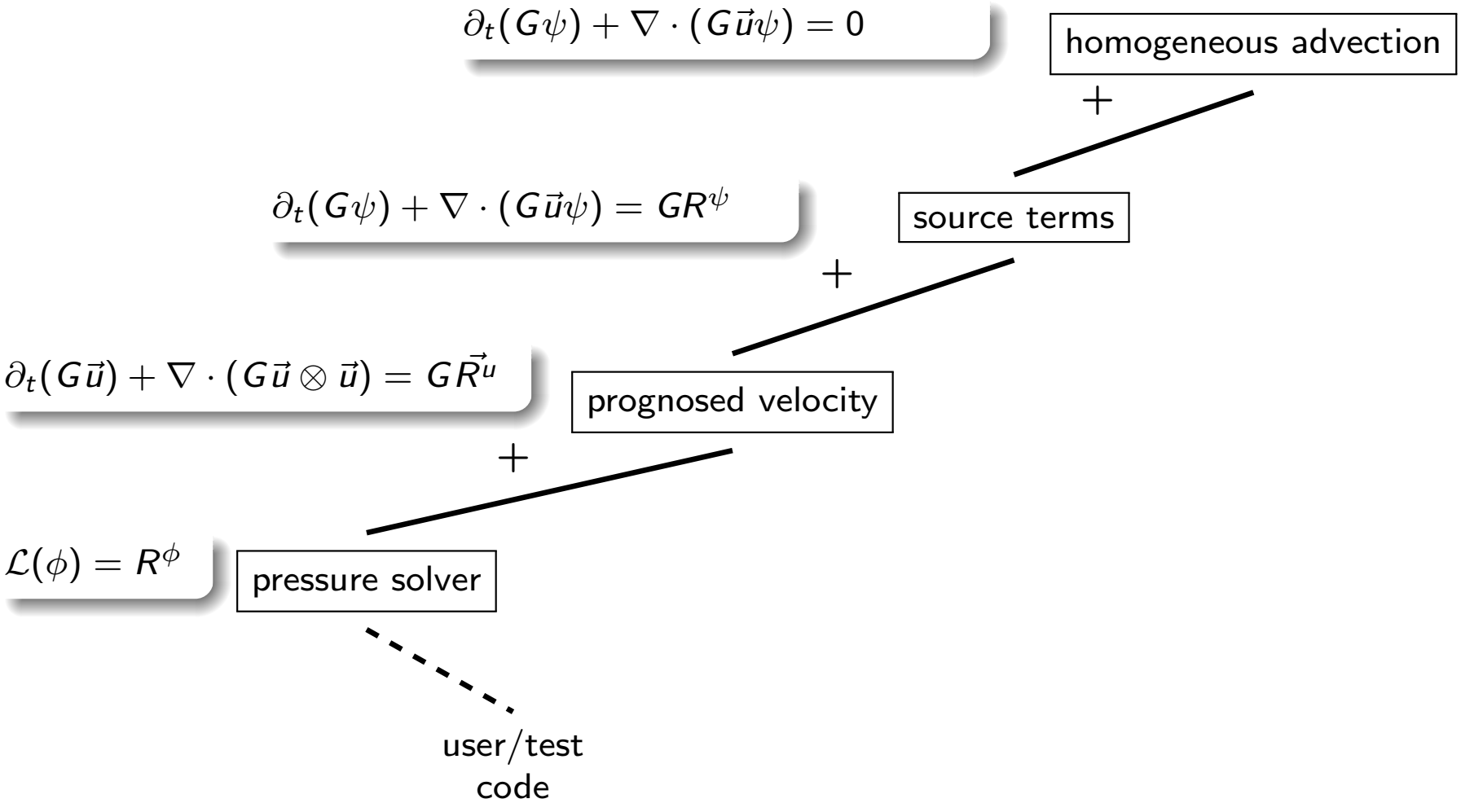


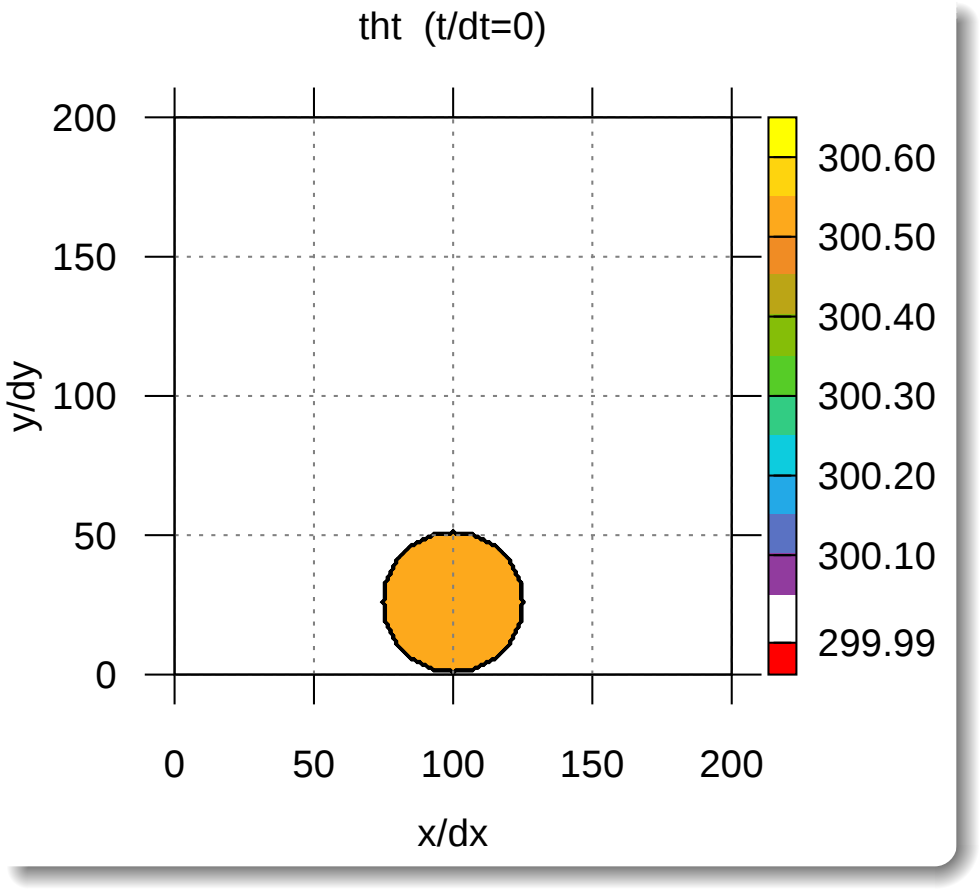
libmpdata++: solver/algorithm hierarchy



libmpdata++: solver/algorithm hierarchy

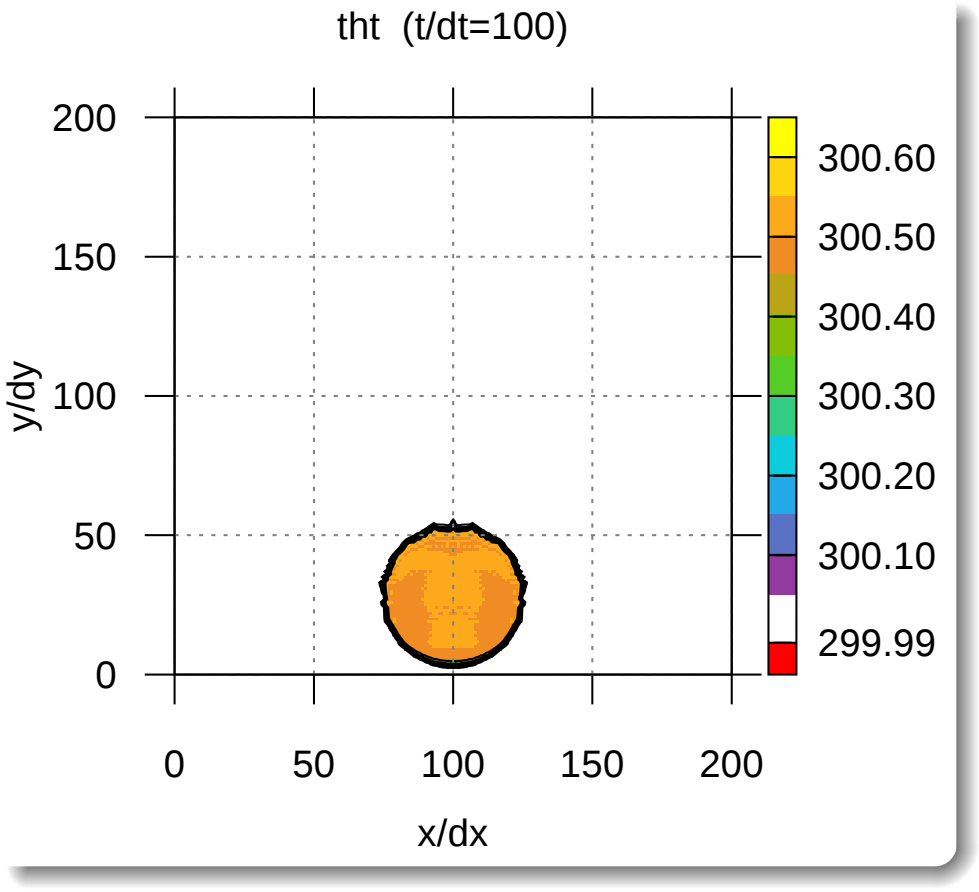


libmpdata++: 2D Boussinesq convection example



- reproduced experiment of Smolarkiewicz and Pudykiewicz, 1992

libmpdata++: 2D Boussinesq convection example



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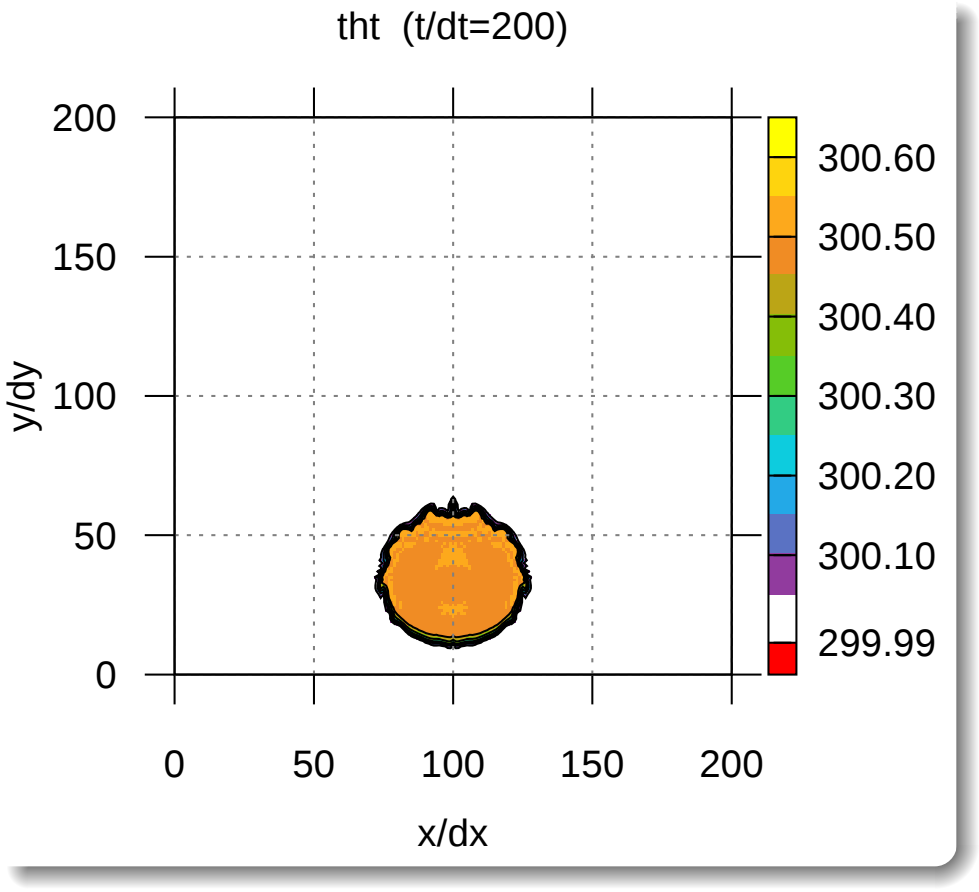

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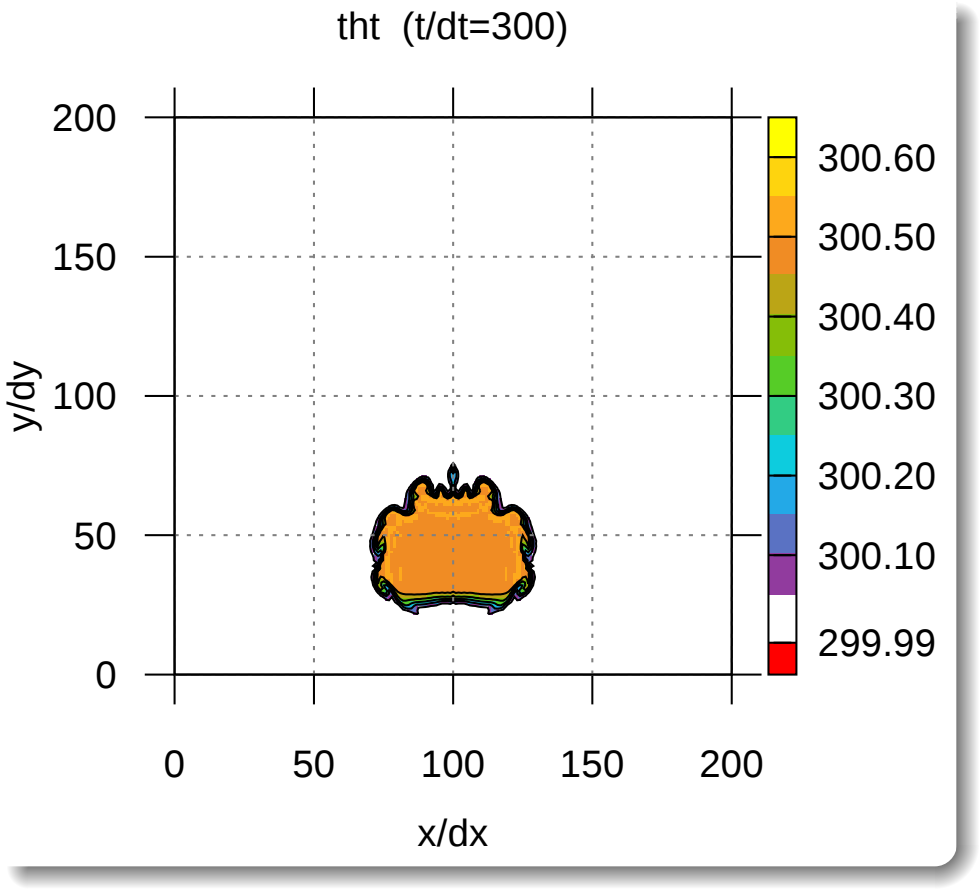
libmpdata++: 2D Boussinesq convection example



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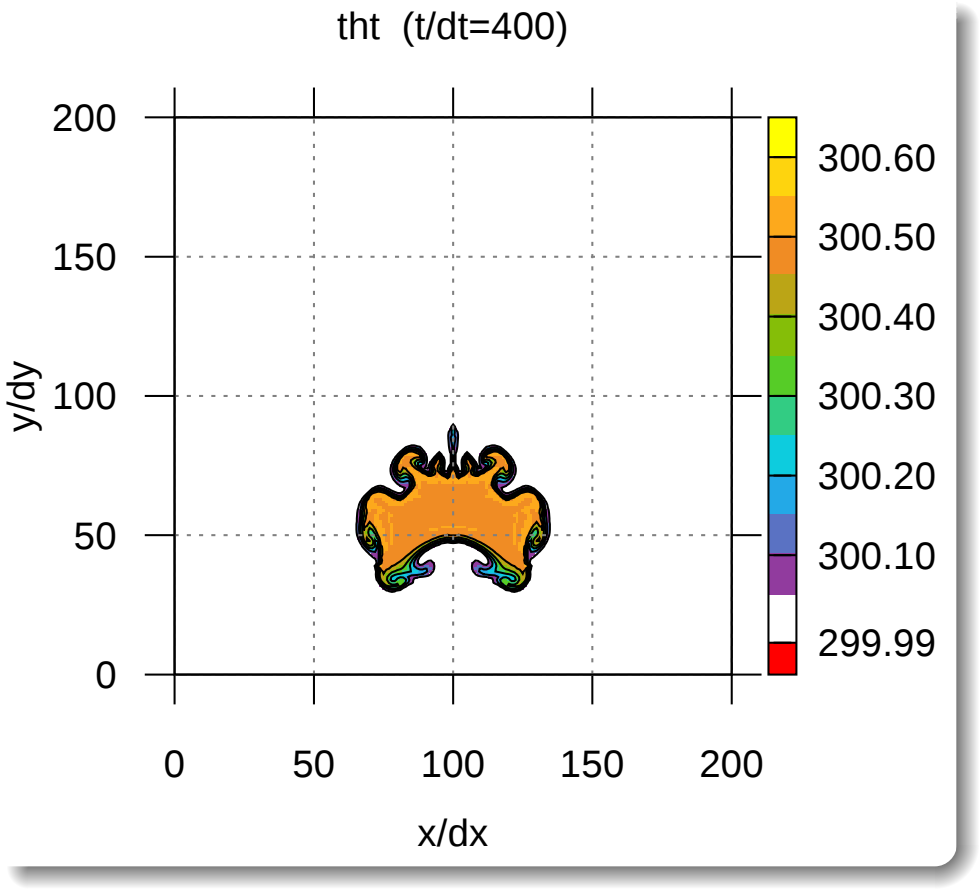

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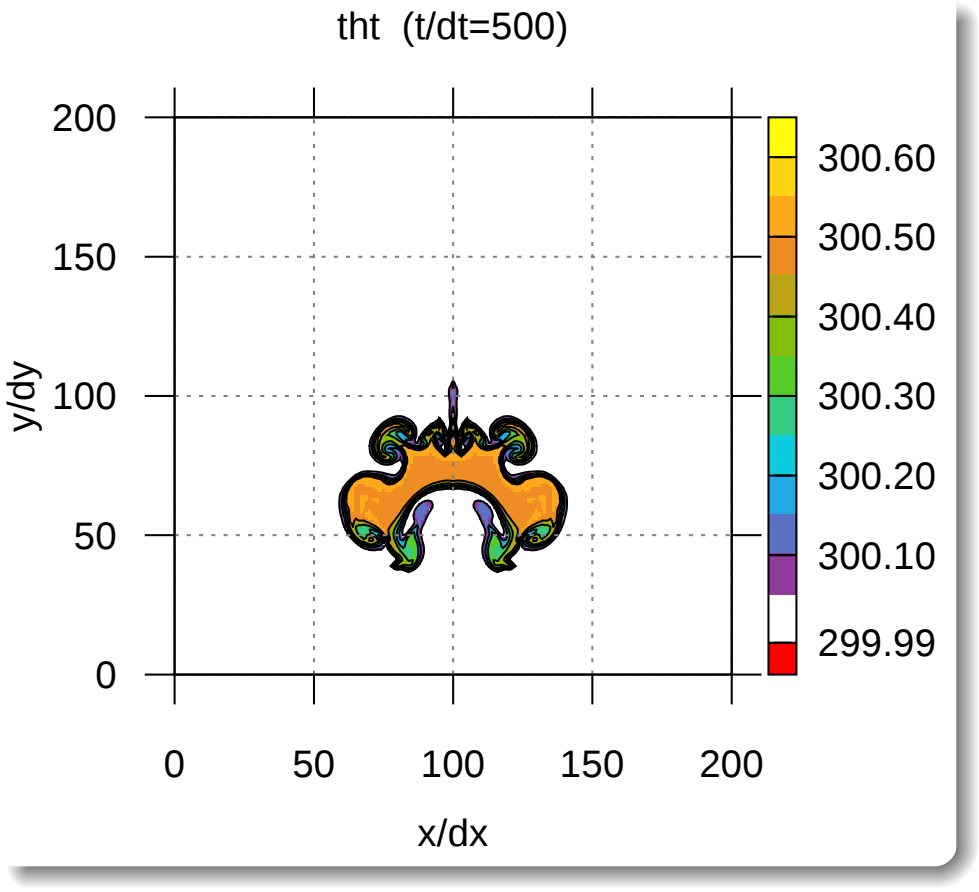

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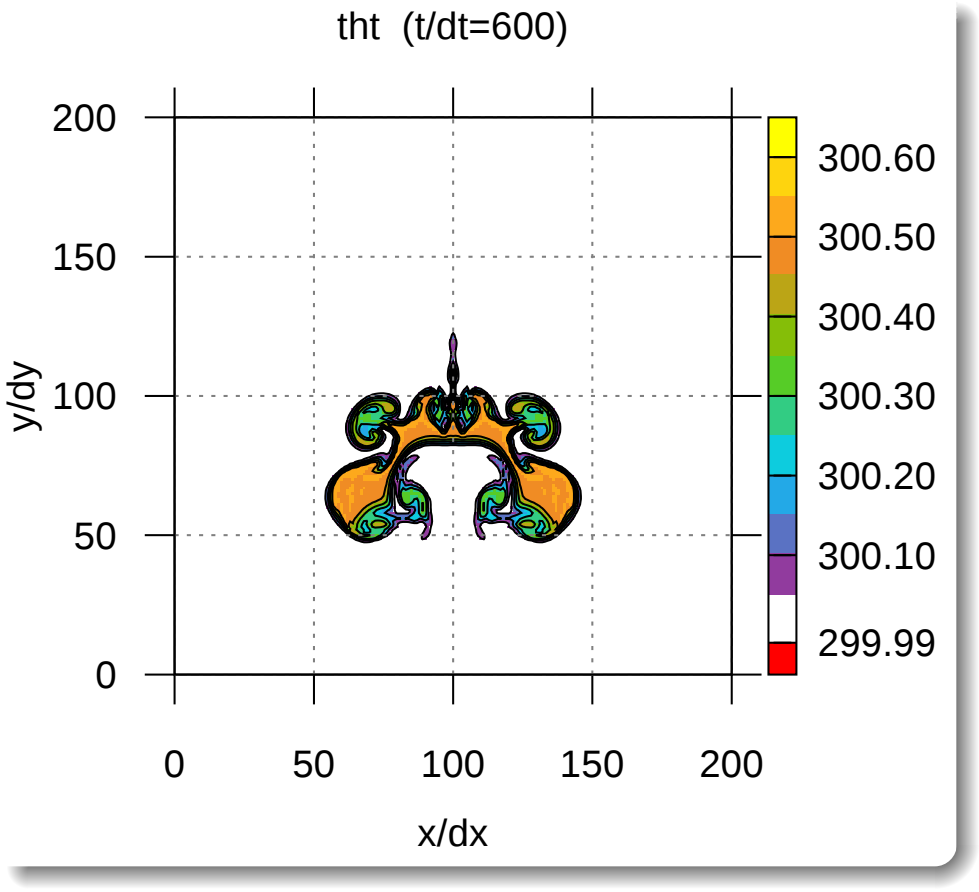
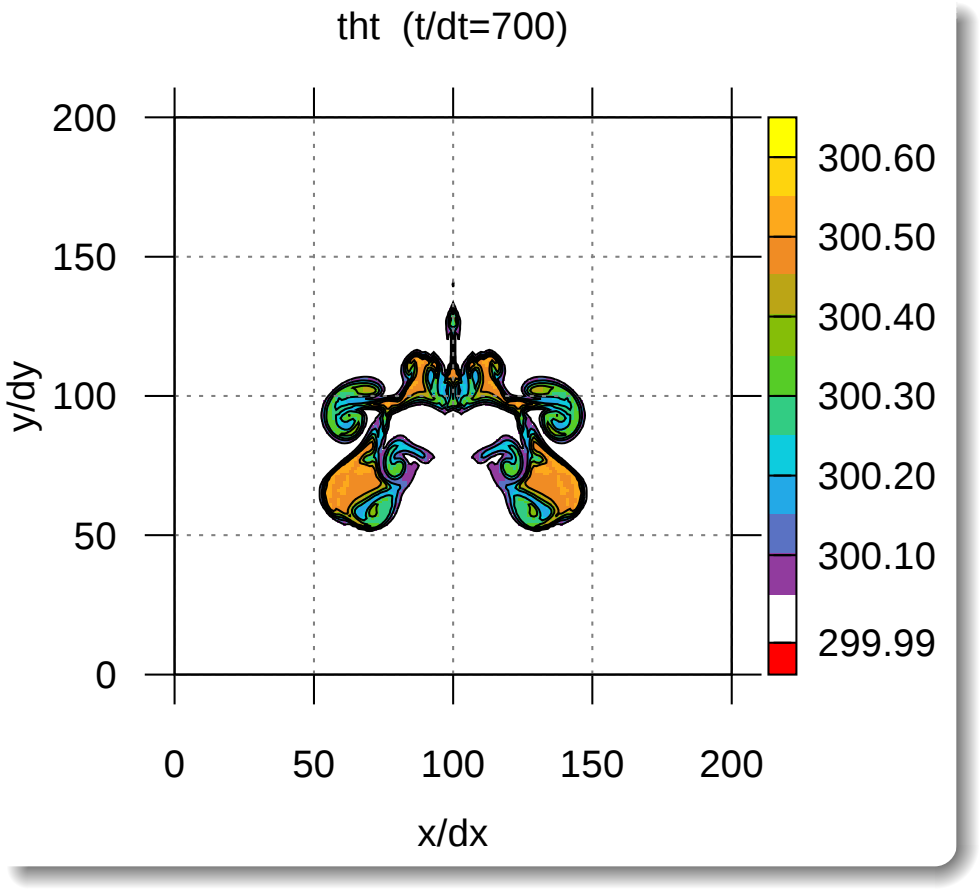
libmpdata++: 2D Boussinesq convection example



- reproduced experiment of Smolarkiewicz and Pudykiewicz, 1992

libmpdata++: 2D Boussinesq convection example



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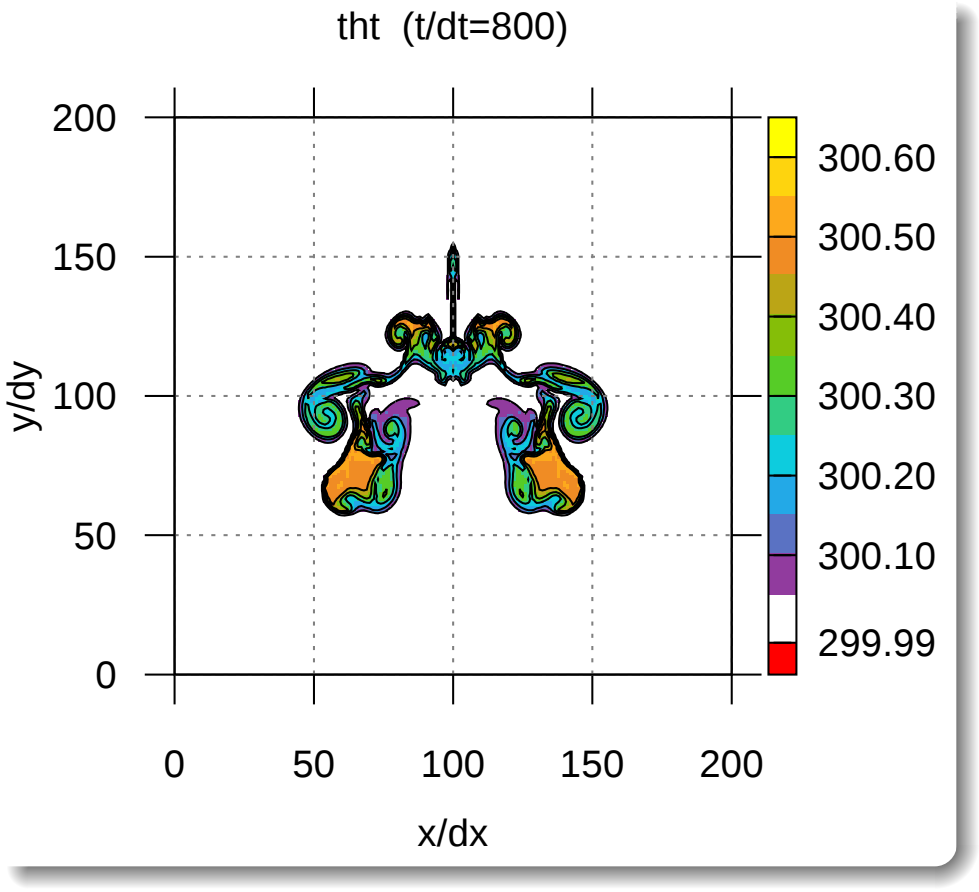
libmpdata++: 2D Boussinesq convection example



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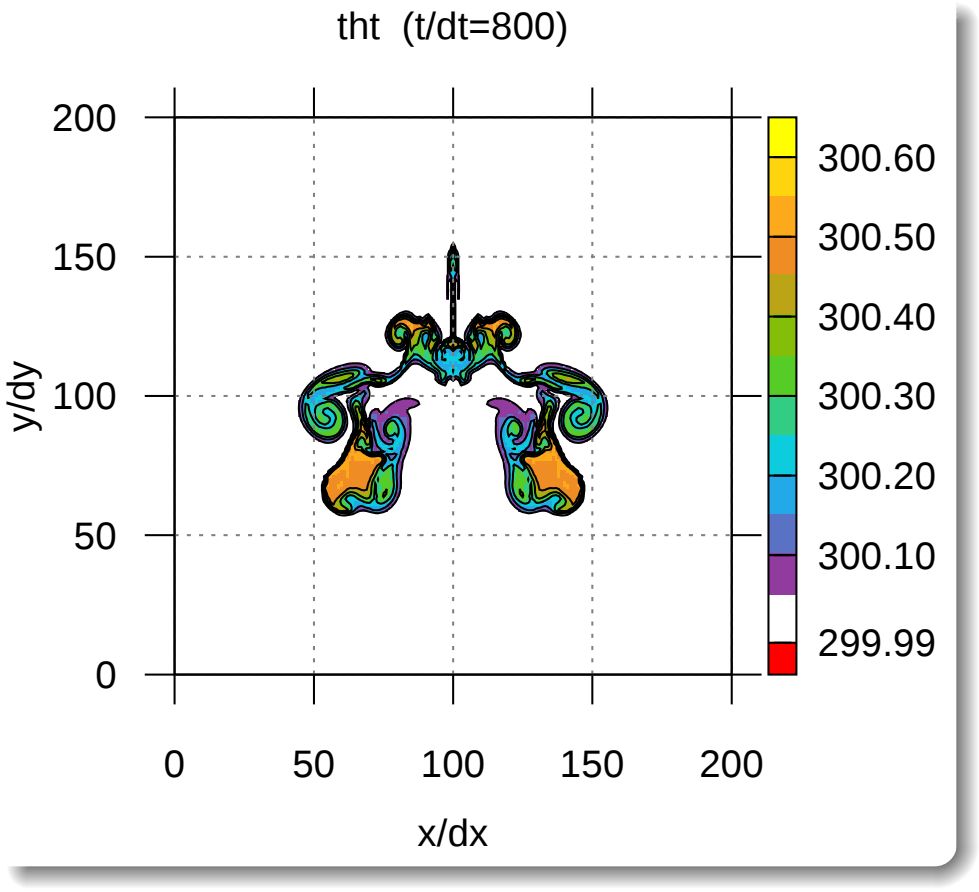

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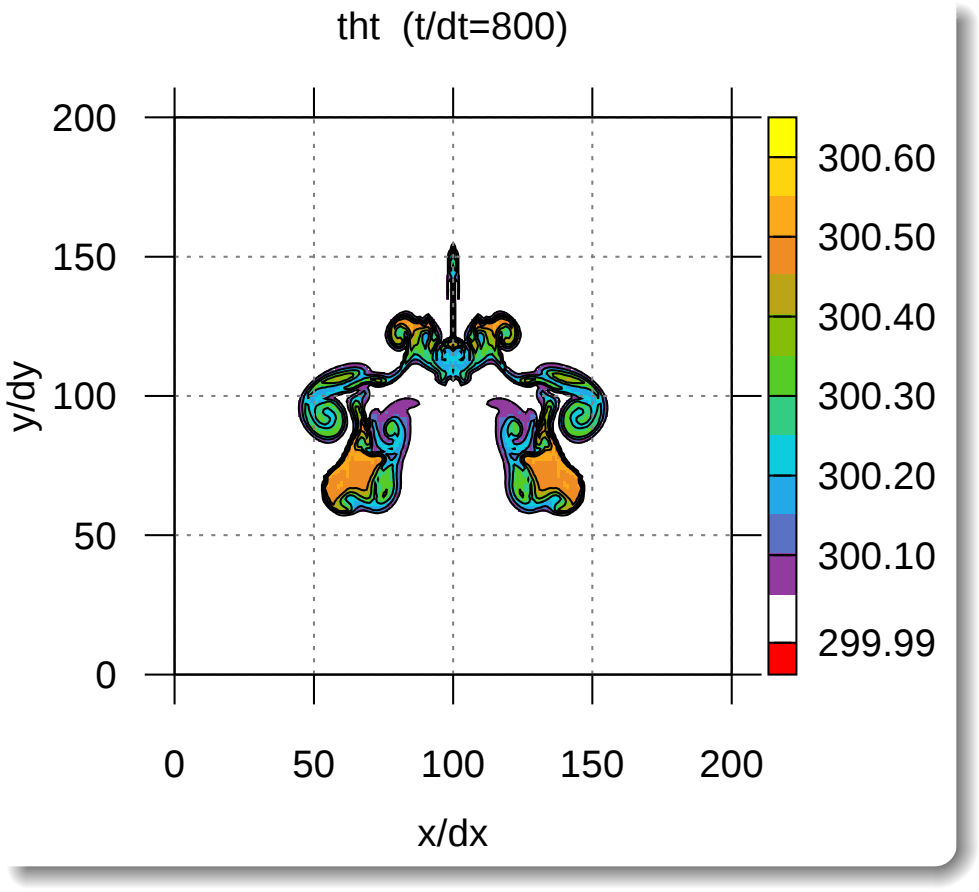
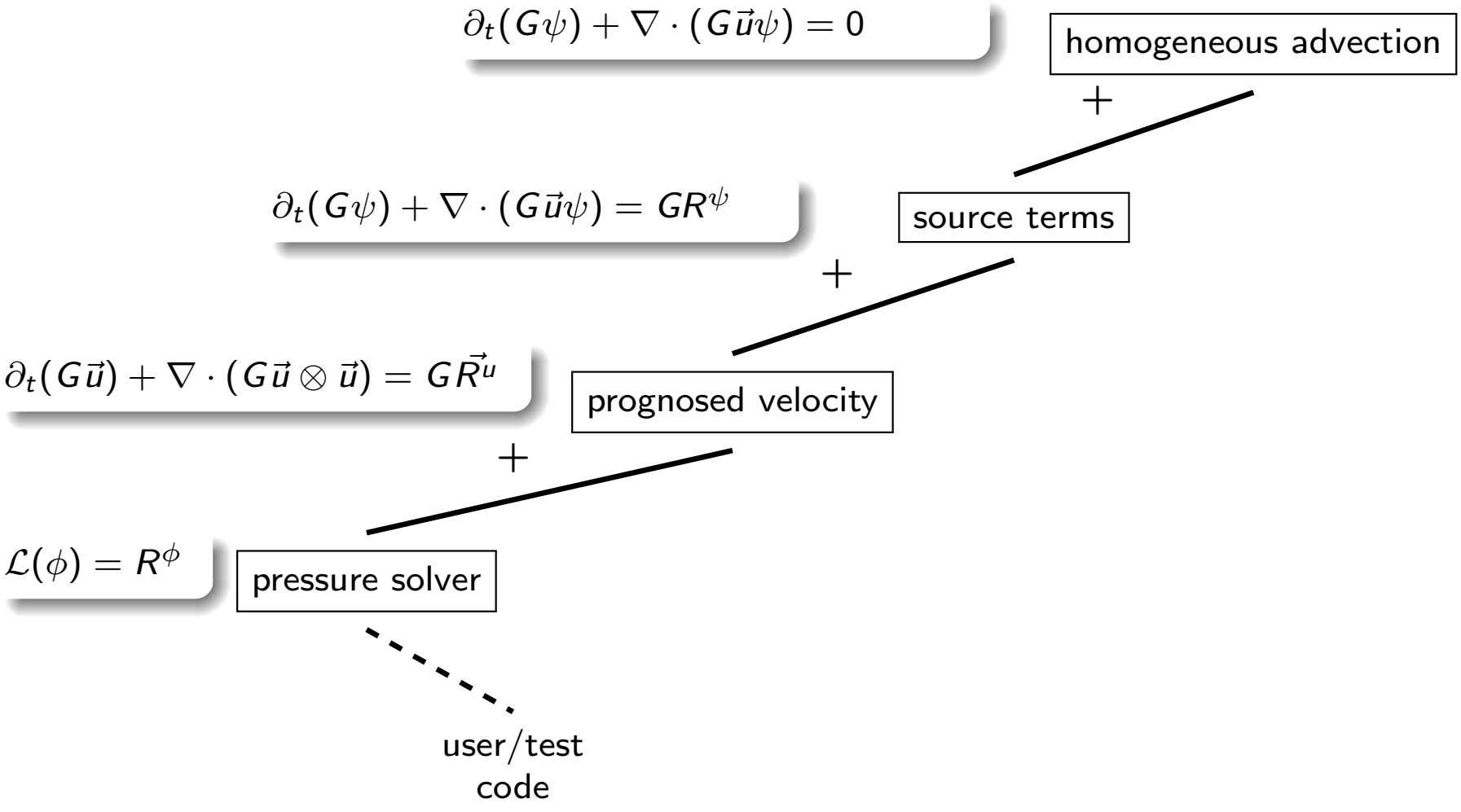


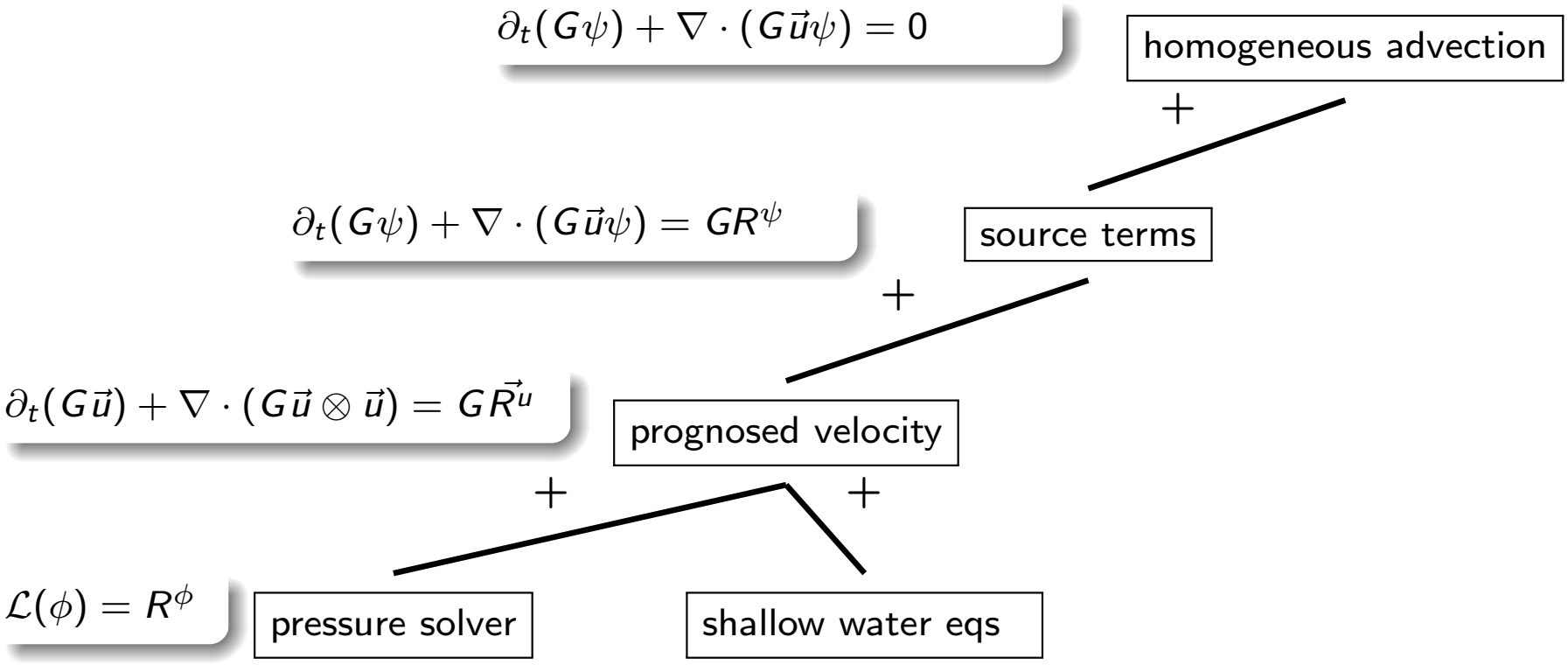
- reproduced experiment of Smolarkiewicz and Pudykiewicz, 1992
- <200 lines of code with libmpdata++

`https://github.com/igfuw/libmpdataxx/tree/master/tests/paper_2015_GMD/8_boussinesq_2d`

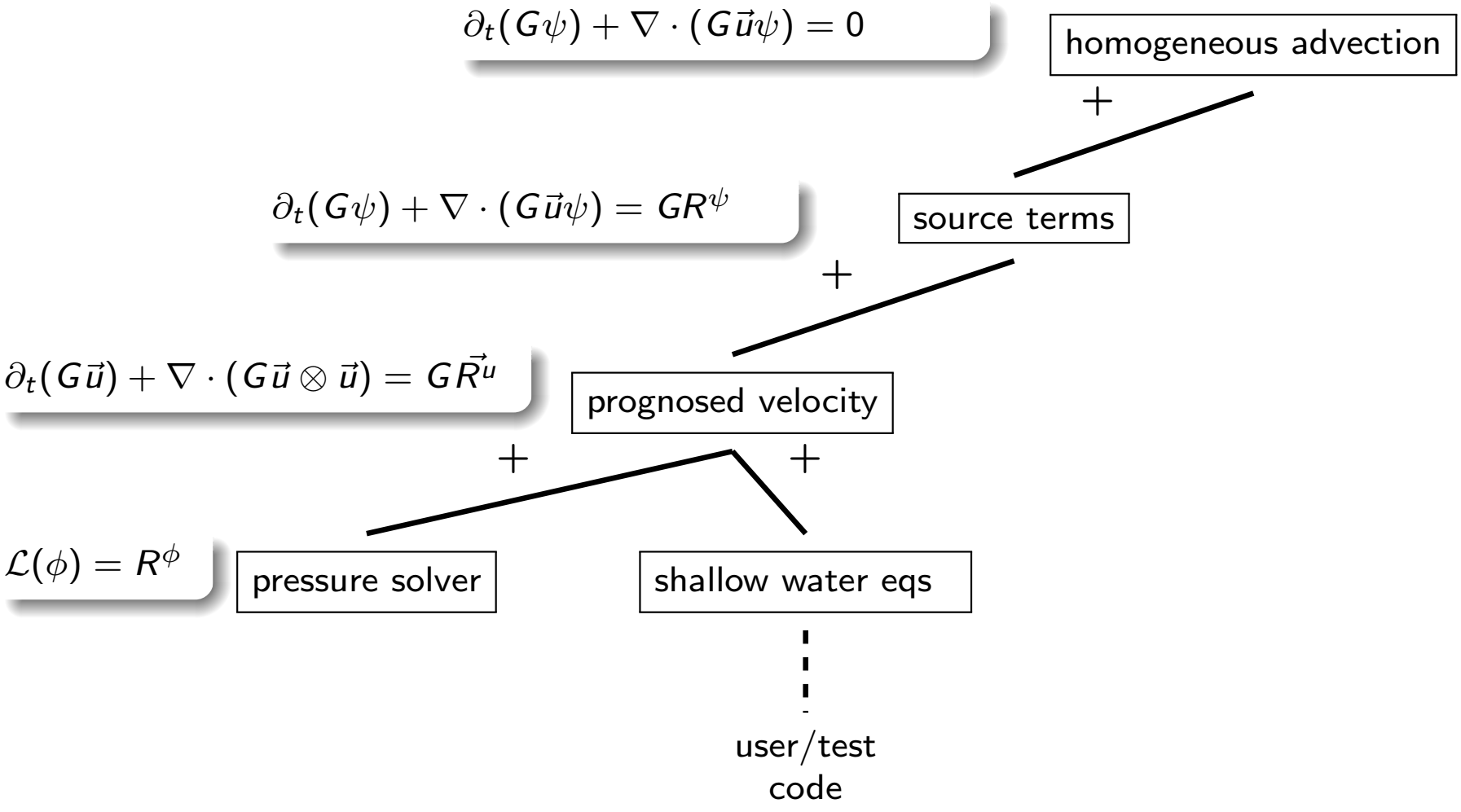
libmpdata++: solver/algorithm hierarchy



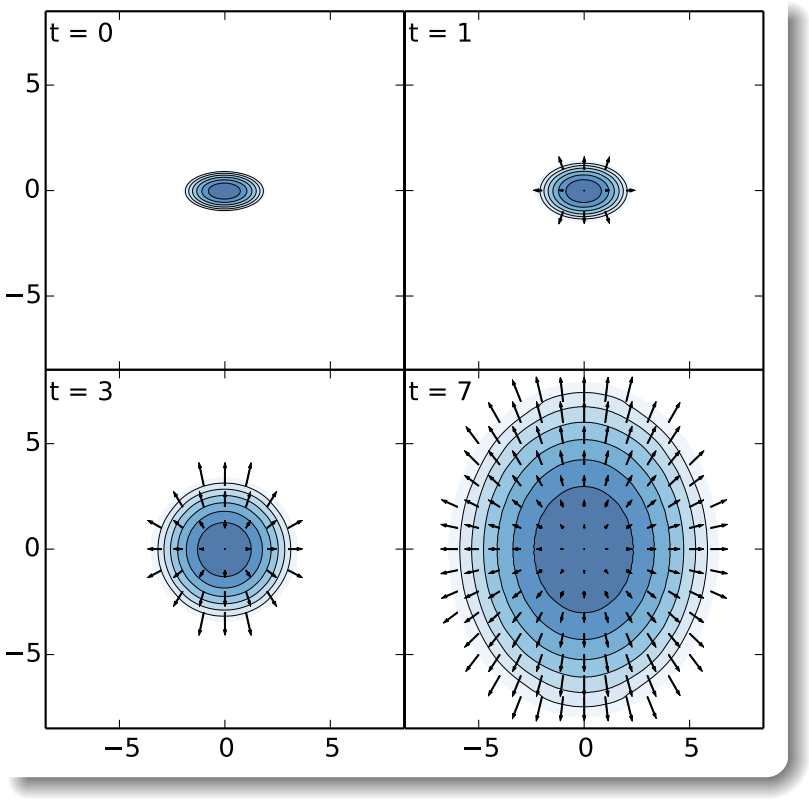
libmpdata++: solver/algorithm hierarchy



libmpdata++: solver/algorithm hierarchy

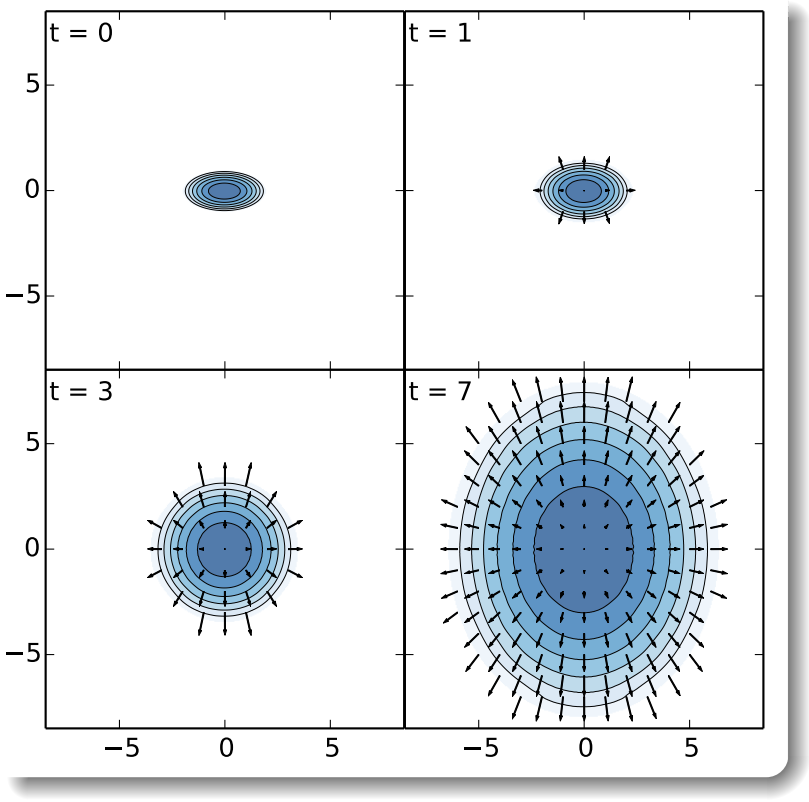


libmpdata++: 3D shallow-water system example



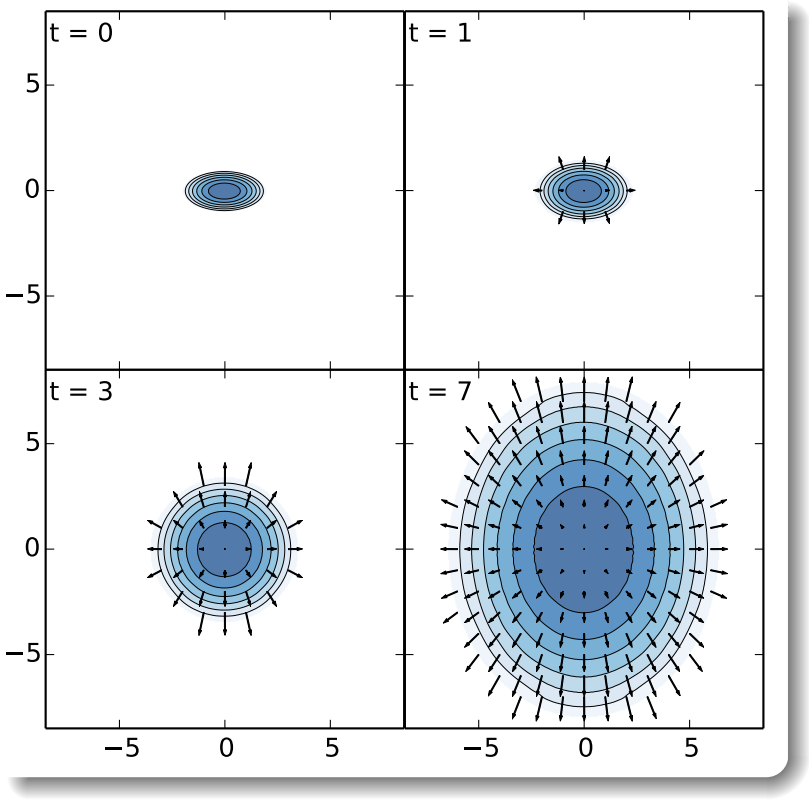
- inspired by 2D experiment of Schär and Smolarkiewicz, 1996

libmpdata++: 3D shallow-water system example



- inspired by 2D experiment of Schär and Smolarkiewicz, 1996
- example and original analytic solution by Dorota Jarecka / NCAR (Jarecka, Jaruga & Smolarkiewicz 2015, J. Comp. Phys. 289)

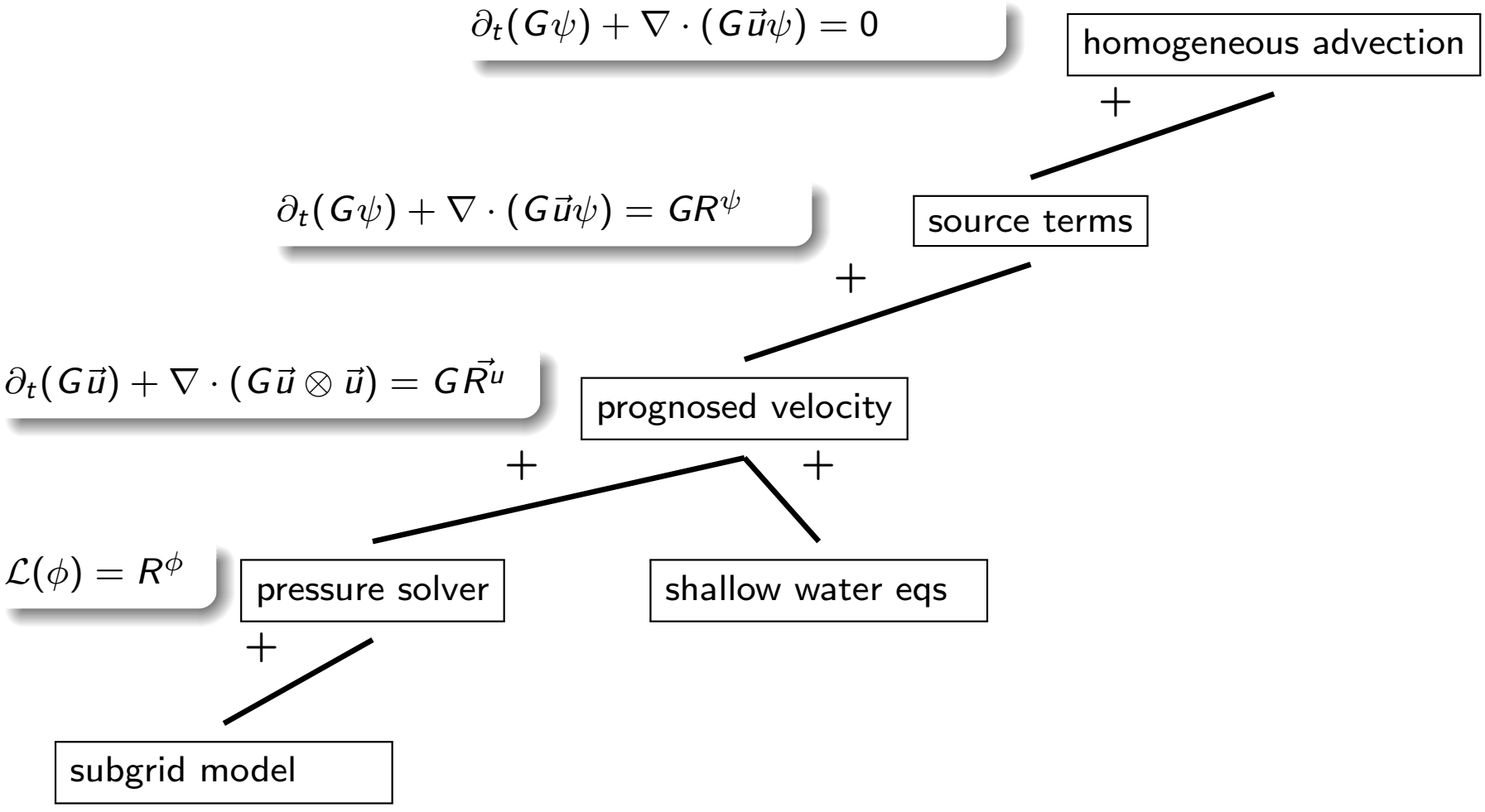
libmpdata++: 3D shallow-water system example



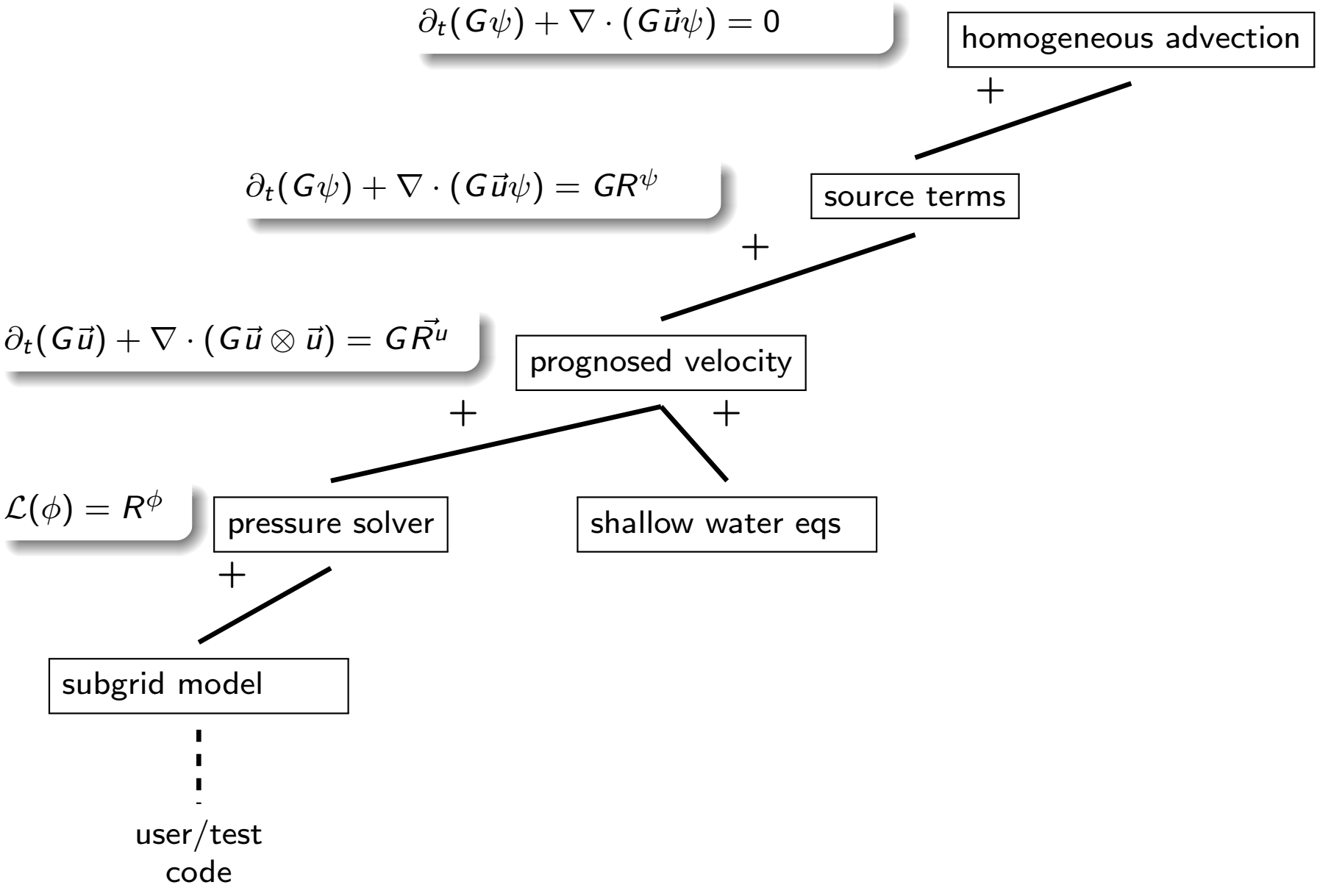
- inspired by 2D experiment of Schär and Smolarkiewicz, 1996
- example and original analytic solution by Dorota Jarecka / NCAR (Jarecka, Jaruga & Smolarkiewicz 2015, J. Comp. Phys. 289)
- <120 lines of code with libmpdata++

`https://github.com/igfuw/shallow-water-elliptic-drop/tree/master/numerical`

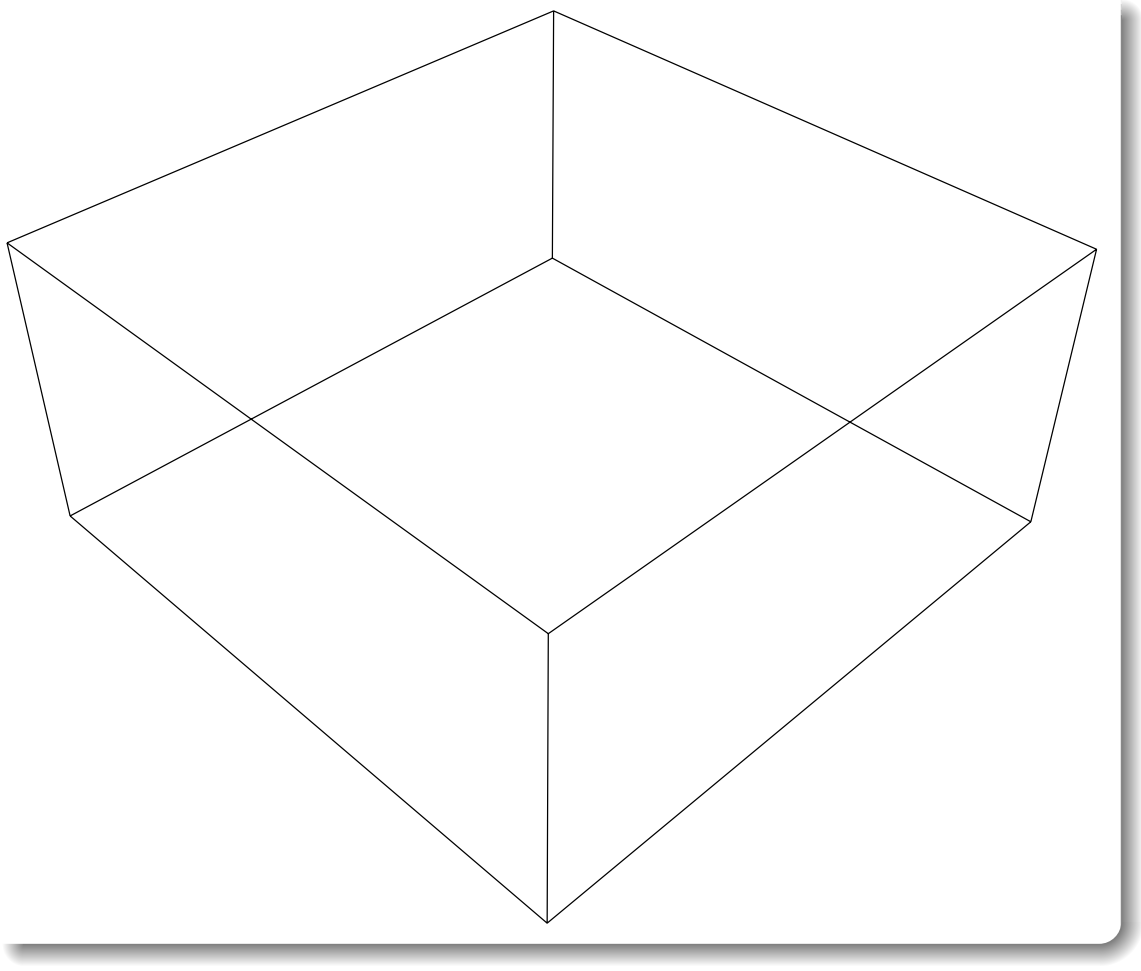
libmpdata++: solver/algorithm hierarchy



libmpdata++: solver/algorithm hierarchy

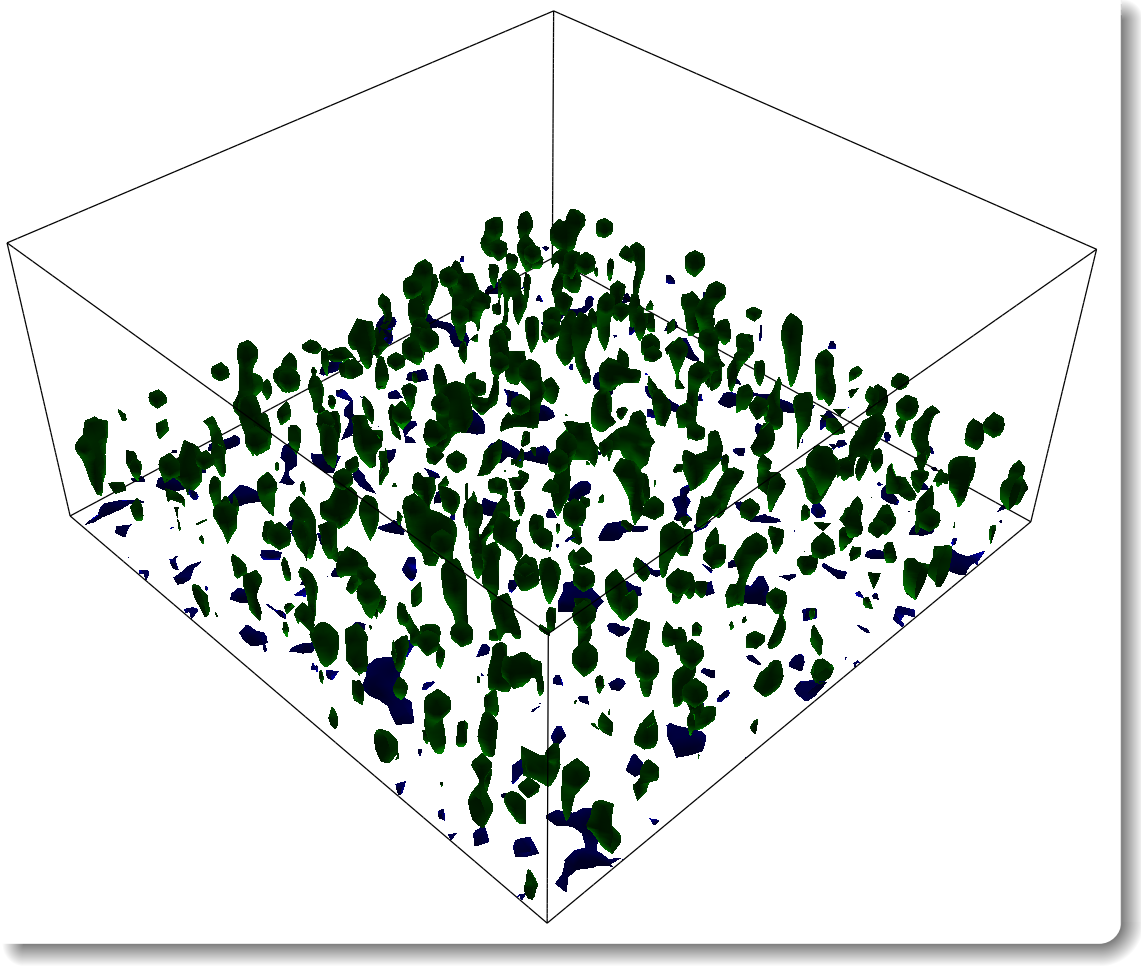


libmpdata++: convective boundary layer example



- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



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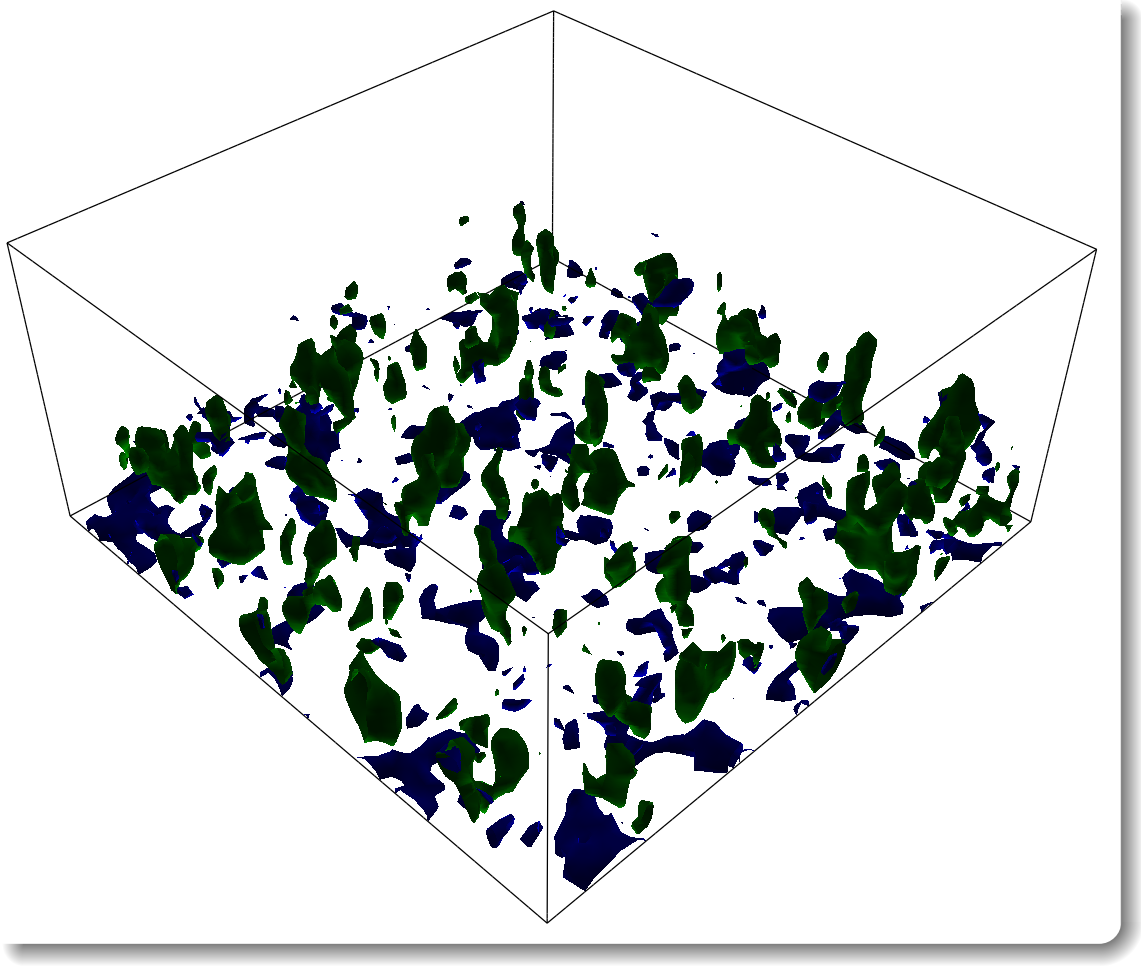
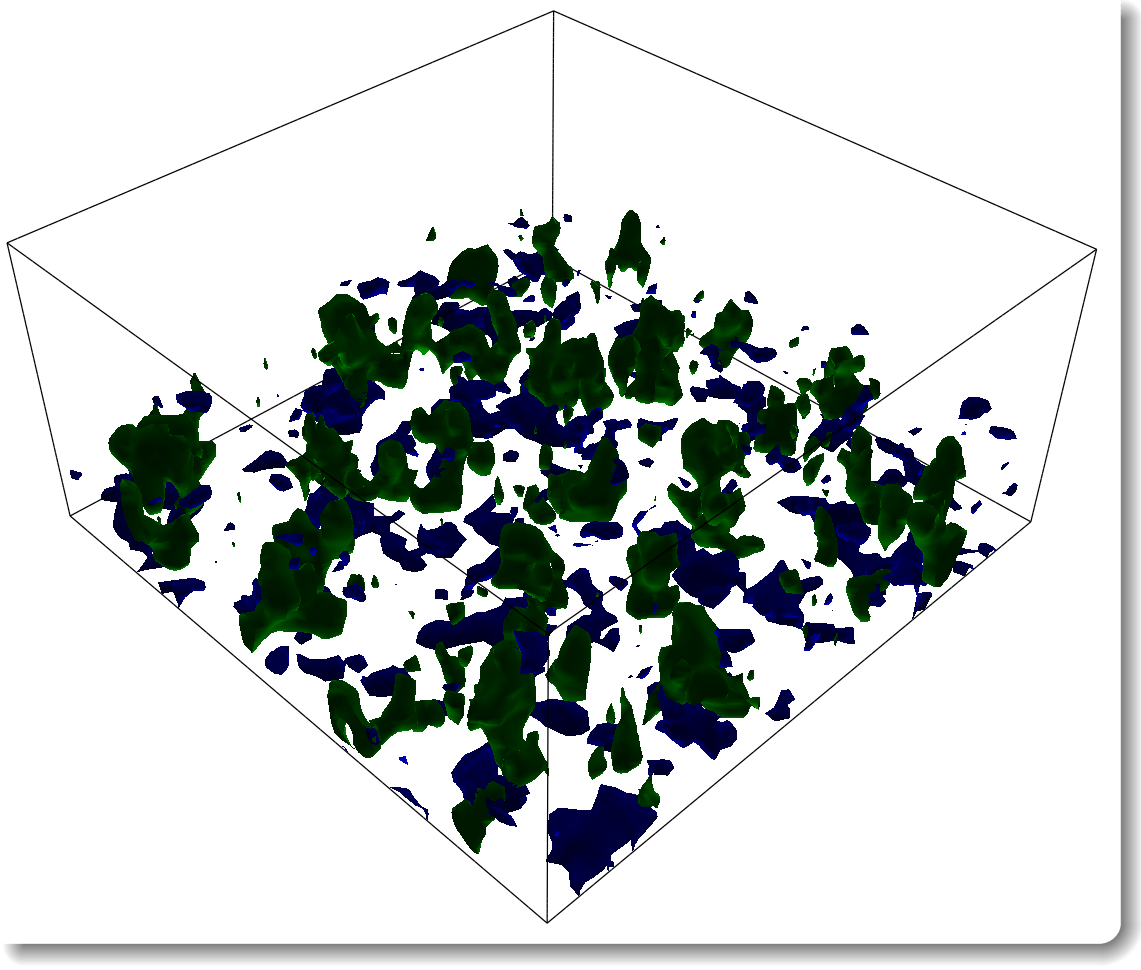


- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



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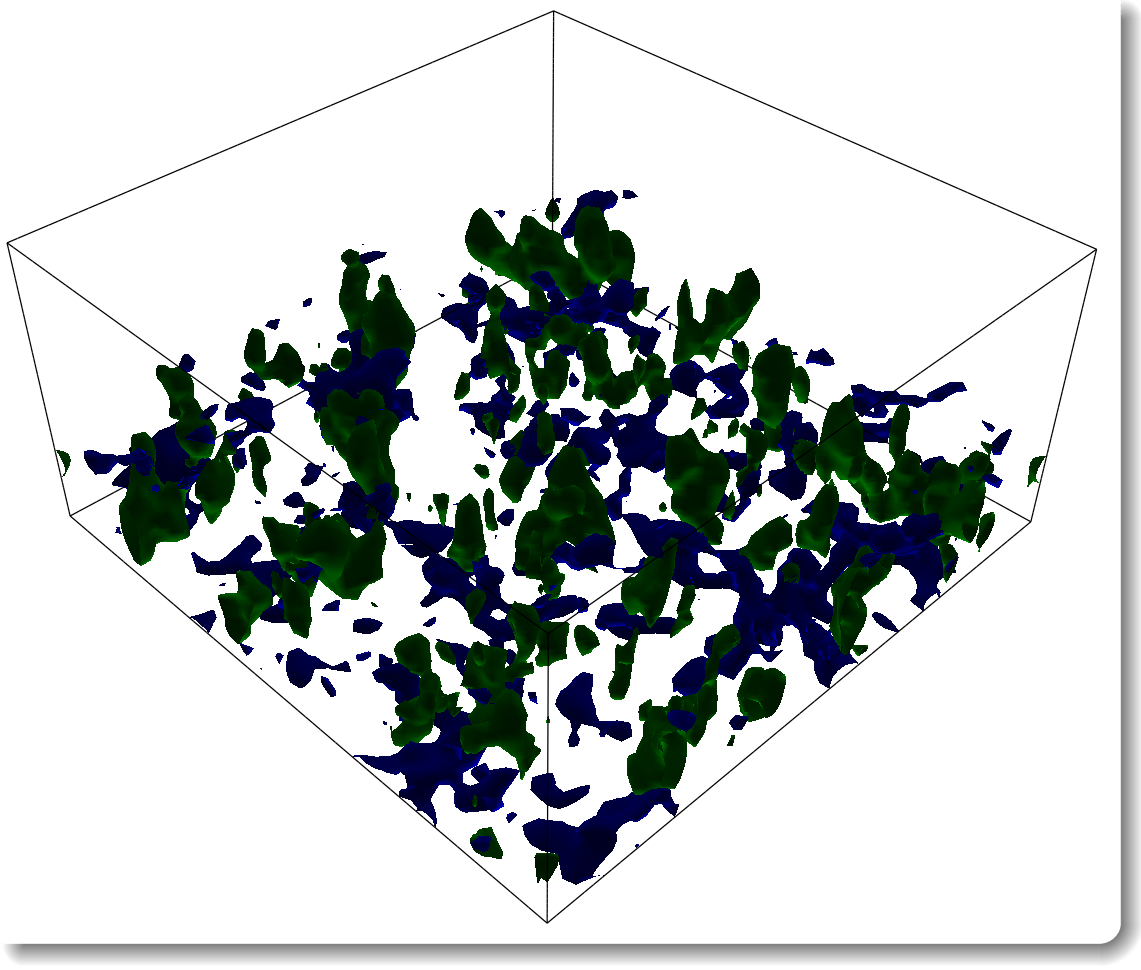
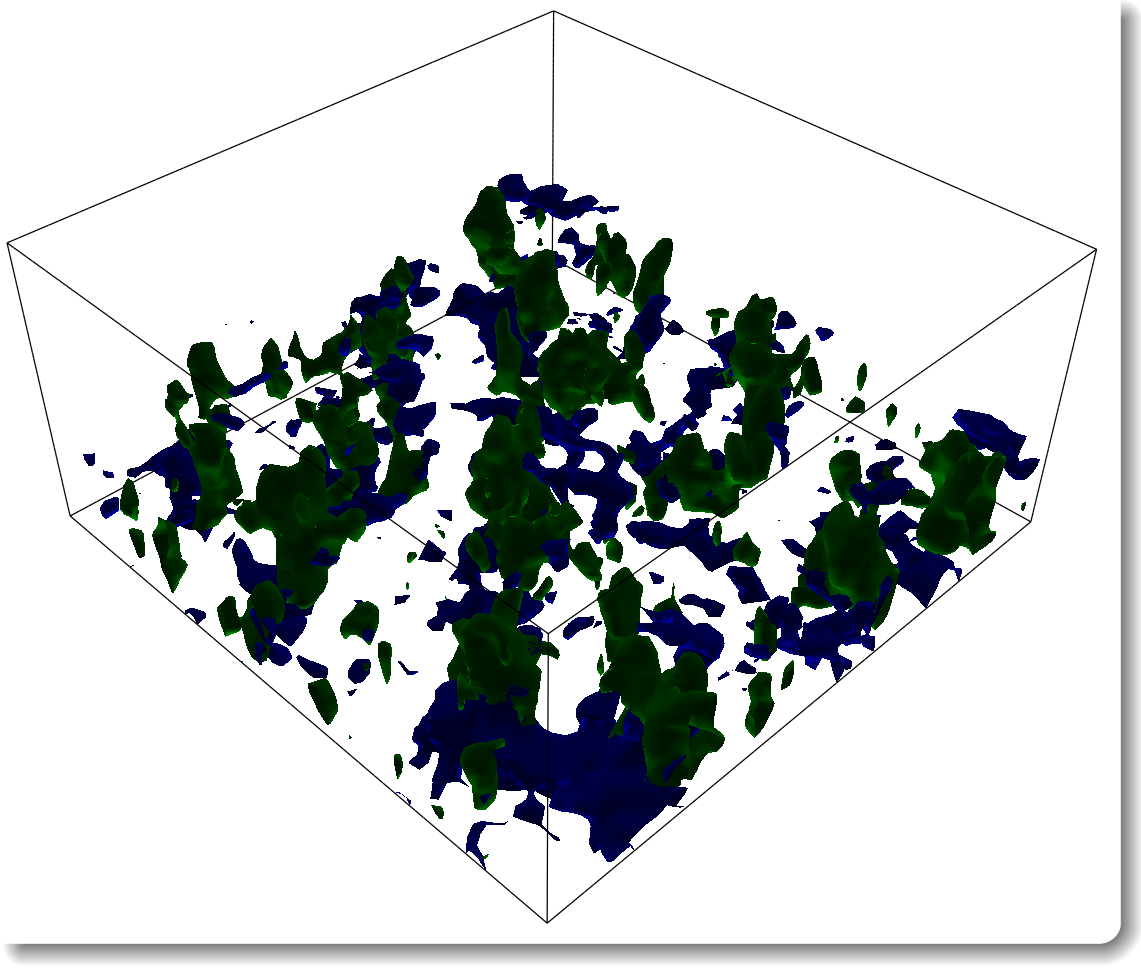


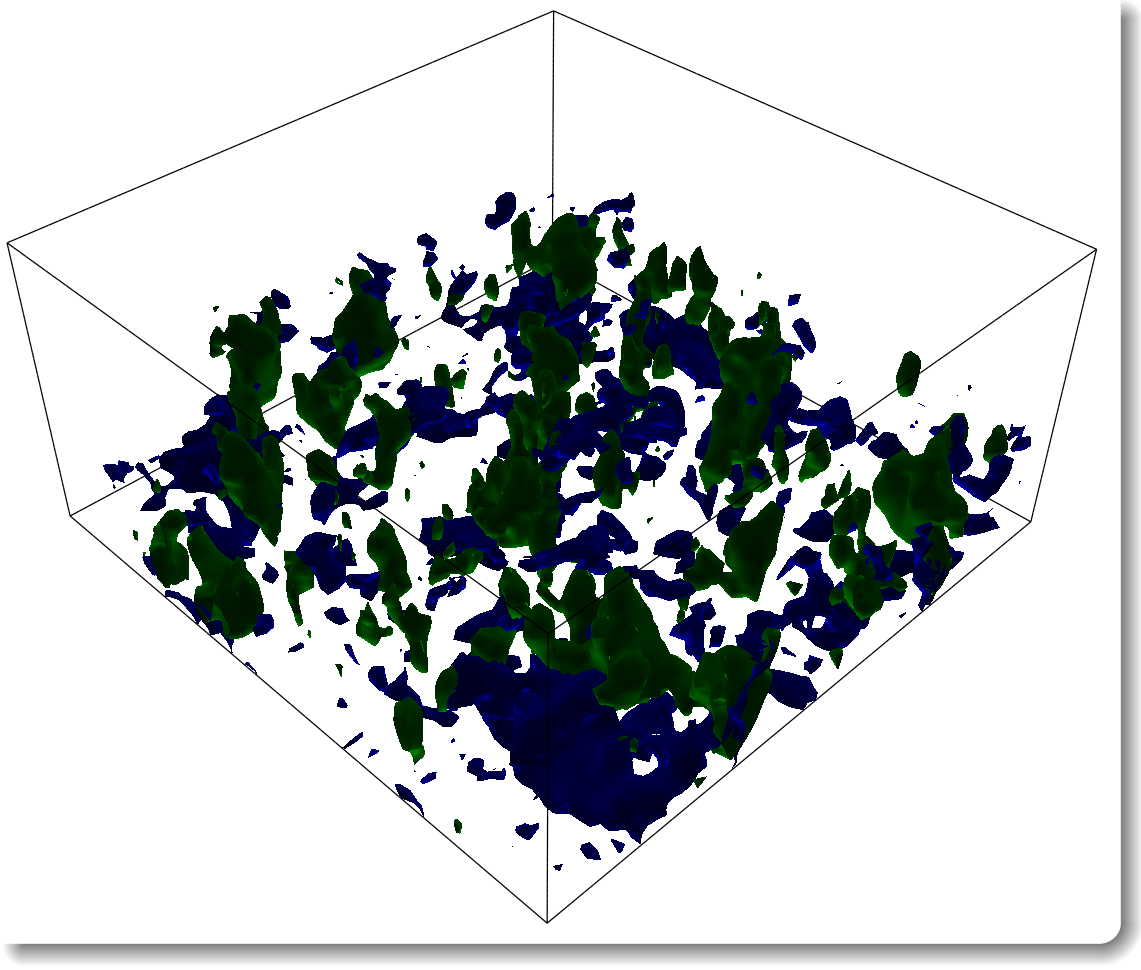
- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



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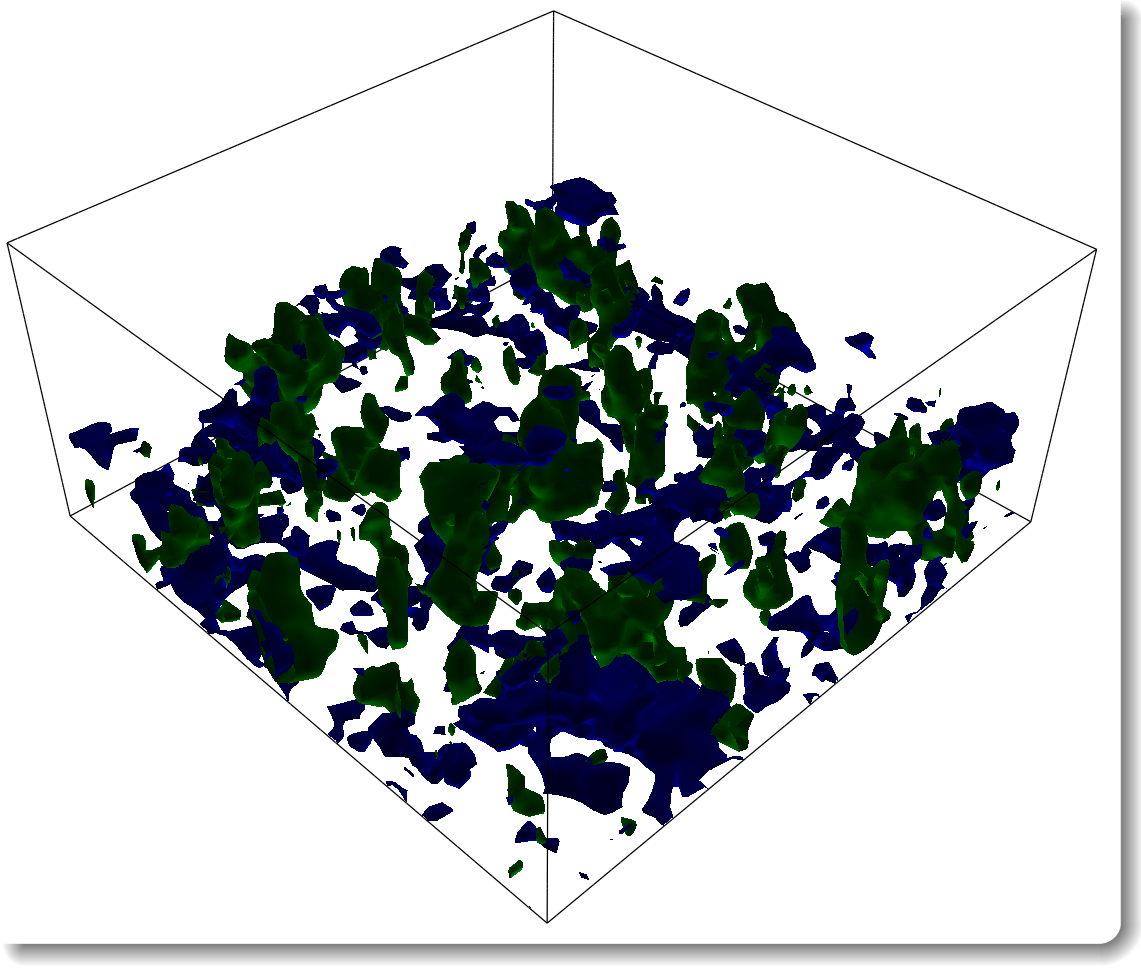
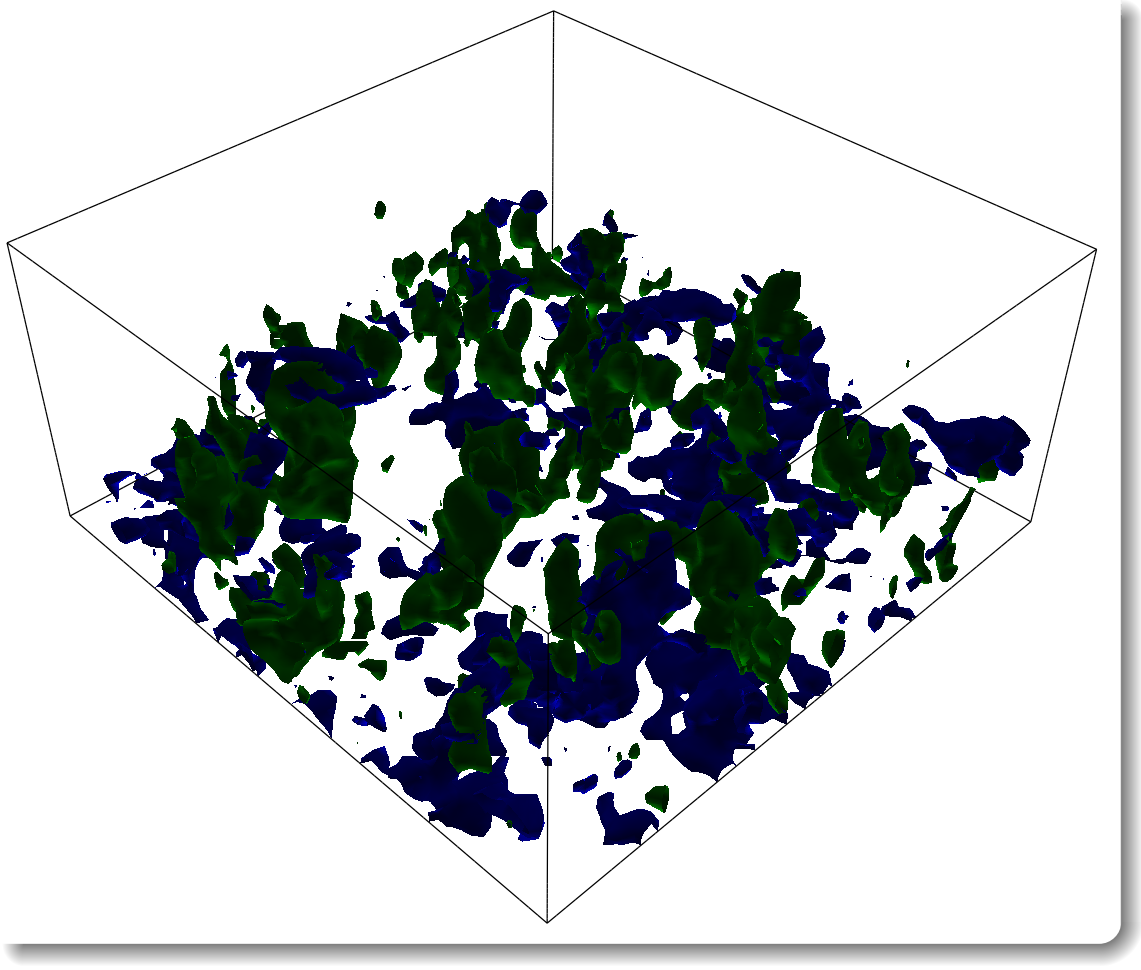


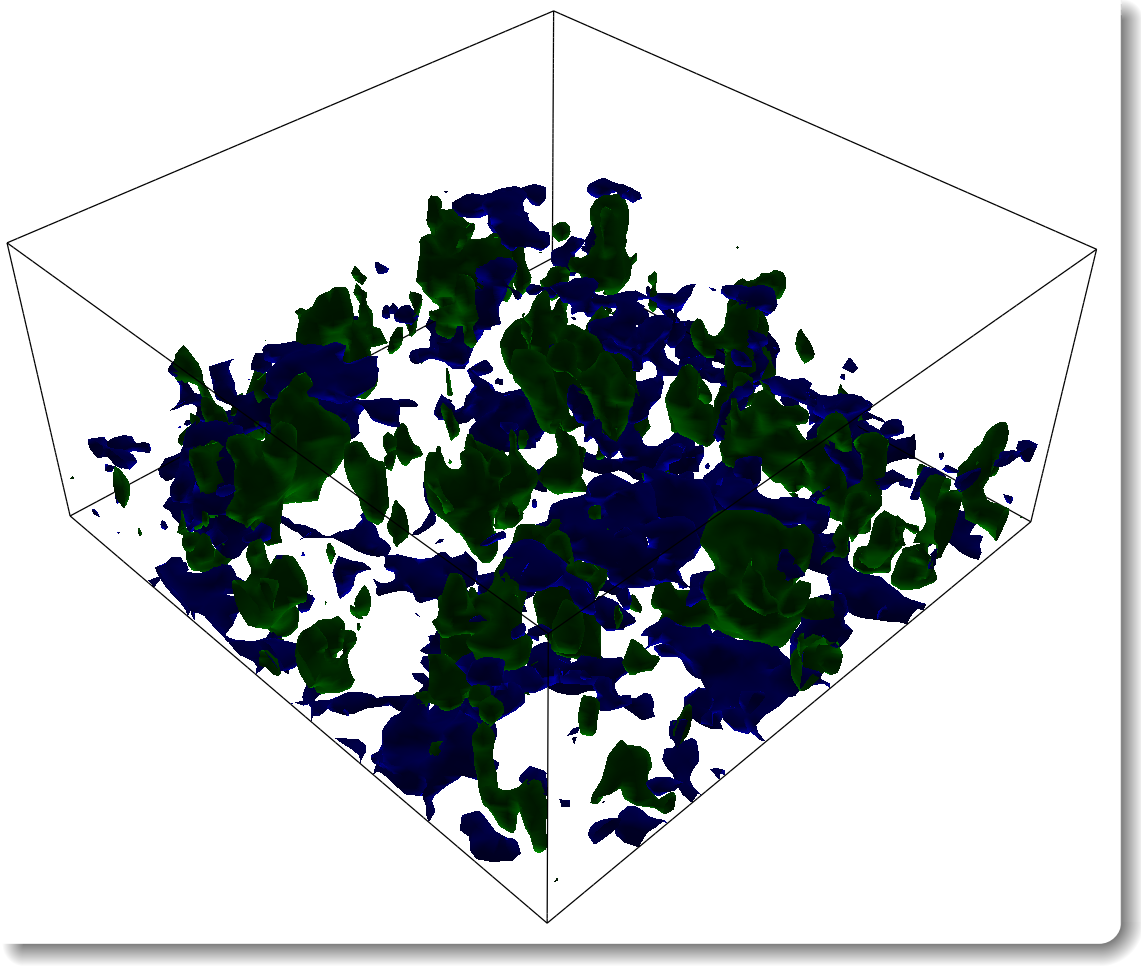
- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



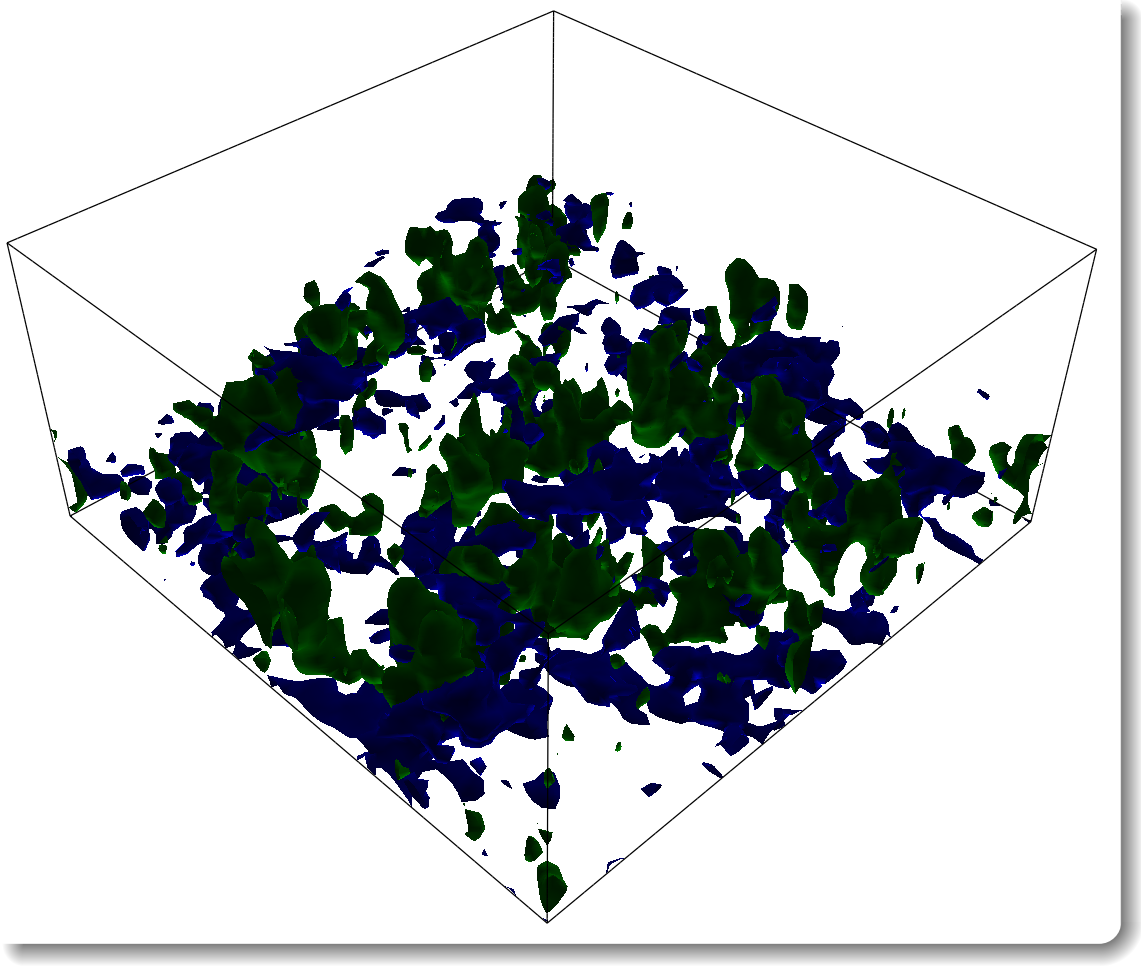
- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



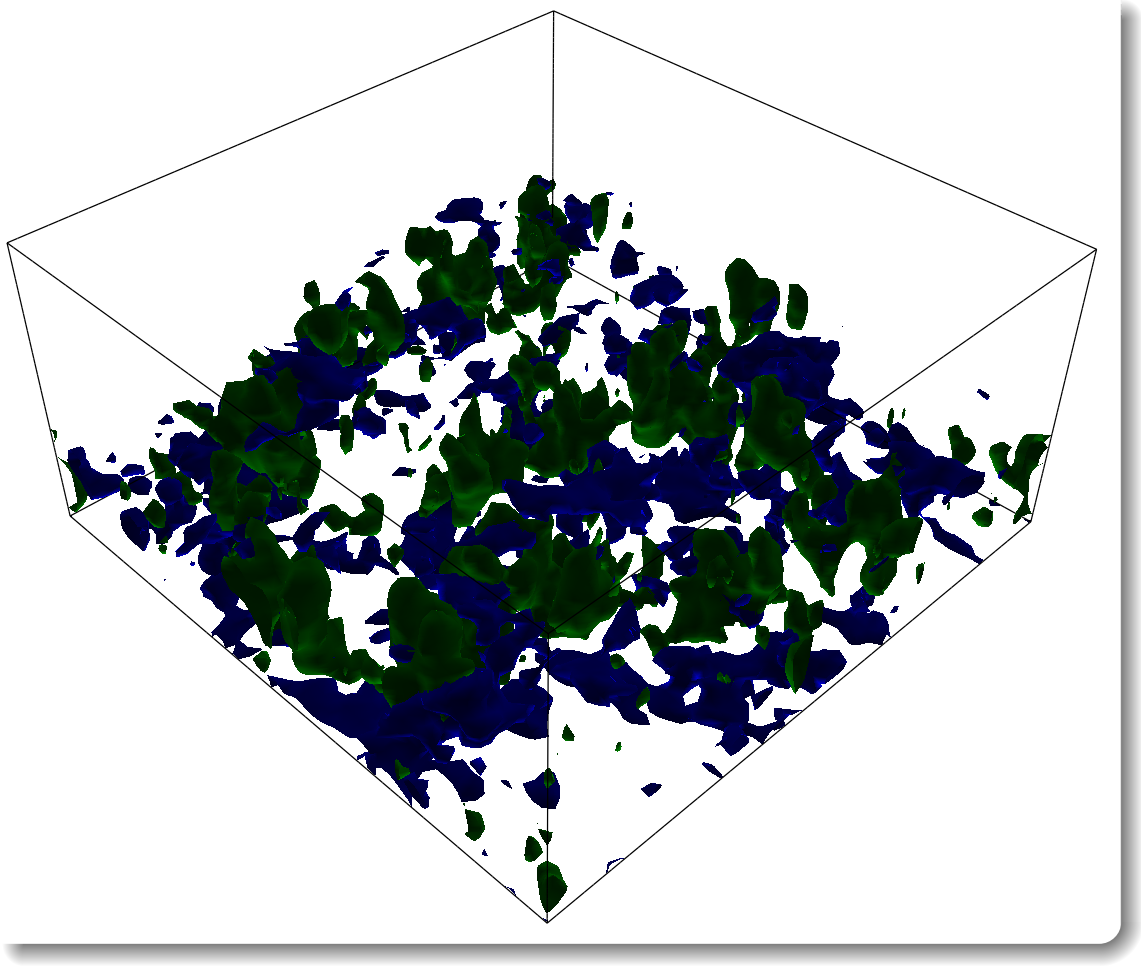
- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



- setup following Margolin et al., 1999

libmpdata++: convective boundary layer example



- setup following Margolin et al., 1999
- <250 lines of code with libmpdata++

Jaruga et al 2015

Geosci. Model Dev., 8, 1005–1032, 2015
www.geosci-model-dev.net/8/1005/2015/
doi:10.5194/gmd-8-1005-2015

Geoscientific Model Development
Open Access

libmpdata++ 1.0: a library of parallel MPDATA solvers for systems of generalised transport equations

A. Jaruga[1], S. Arabas[1], D. Jarecka[1,2], H. Pawlowska[1], P. K. Smolarkiewicz[3], and M. Waruszewski[1]

[1]Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[2]National Center for Atmospheric Research, Boulder, CO, USA
[3]European Centre for Medium-Range Weather Forecasts, Reading, UK

libmpdata++: documentation

Jaruga et al 2015

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[1]Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[2]National Center for Atmospheric Research, Boulder, CO, USA
[3]European Centre for Medium-Range Weather Forecasts, Reading, UK

Geosci. Model Dev. policy (doi: 10.5194/gmd-6-1233-2013)

- *"paper must be accompanied by the code, or means of accessing the code, for the purpose of peer-review"*
- *"we strongly encourage referees to compile the code, and run test cases supplied by the authors"*

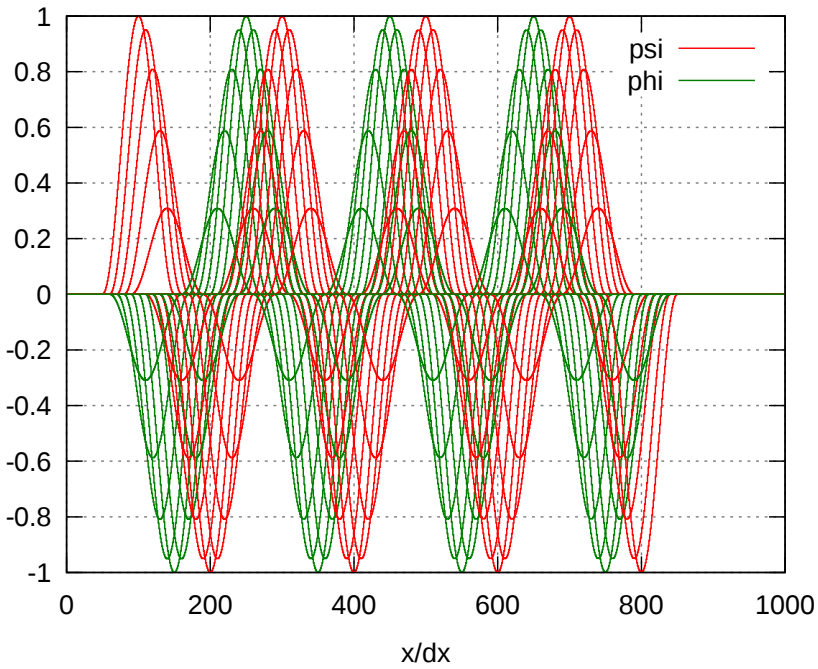


Figure 15. Simulation results of the example presented in Sect. 4.3. Abscissa marks the spatial dimension and ordinate represents the oscillator amplitude. The oscillator state is plotted every 20 time steps.

(partial differential equation) system (16) leads to the following system of coupled implicit algebraic equations:

$$\psi_i^{n+1} = \psi_i^* + 0.5\ \Delta t\ \omega\ \phi_i^{n+1},$$
$$\phi_i^{n+1} = \phi_i^* - 0.5\ \Delta t\ \omega\ \psi_i^{n+1}, \tag{17}$$

where ψ_i^* and ϕ_i^* stand for

```
#include <libmpdata++/solvers/mpdata_rhs.hpp>

template <class ct_params_t>
struct coupled_harmosc : public
  libmpdataxx::solvers::mpdata_rhs<ct_params_t>
{ // aliases
  using parent_t =
    libmpdataxx::solvers::mpdata_rhs<ct_params_t>;
  using ix = typename ct_params_t::ix;
  // member fields
  typename ct_params_t::real_t omega;

  // method called by mpdata_rhs
  void update_rhs(
    libmpdataxx::arrvec_t<
      typename parent_t::arr_t
    > &rhs,
    const typename parent_t::real_t &dt,
    const int &at
  ) {
    parent_t::update_rhs(rhs, dt, at);

    // just to shorten code
    const auto &psi = this->state(ix::psi);
    const auto &phi = this->state(ix::phi);
    const auto &i = this->i;

    switch (at)
    { // explicit solution for R^{n}
      // (note: with trapez used only at t=0)
      case (0):
      rhs.at(ix::psi)(i) += omega * phi(i);
      rhs.at(ix::phi)(i) -= omega * psi(i);
      break;
```

plan of the talk

introduction

libmpdata++

libcloudph++

n-dim array containers

plan of the talk

introduction

libmpdata++

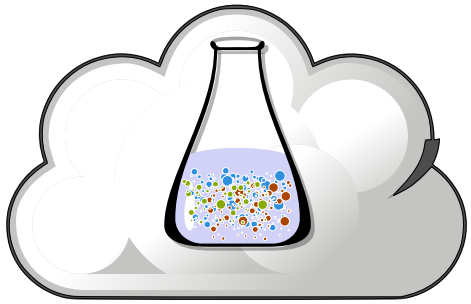
libcloudph++

n-dim array containers

libcloudph++

http://libcloudphxx.igf.fuw.edu.pl/

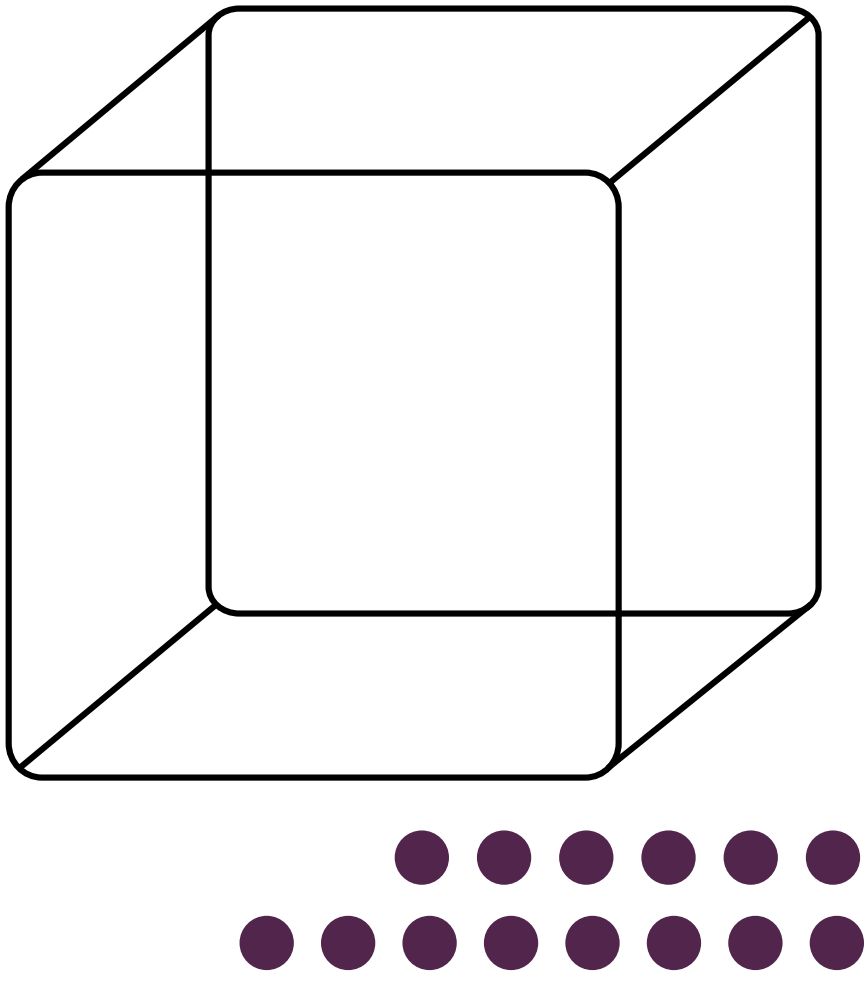
- droplet formation
- condensation



- collisional growth
- aqueous chemistry

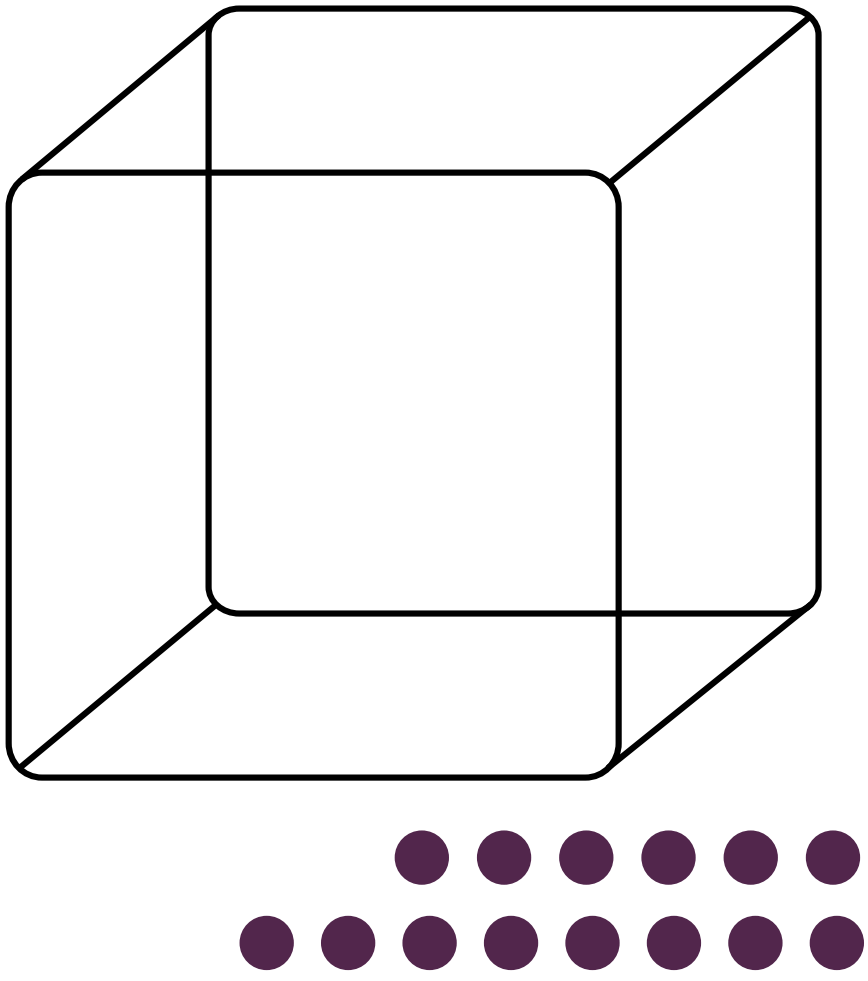
- precipitation
- evaporation

libcloudph++: particle-based Monte-Carlo algorithm



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

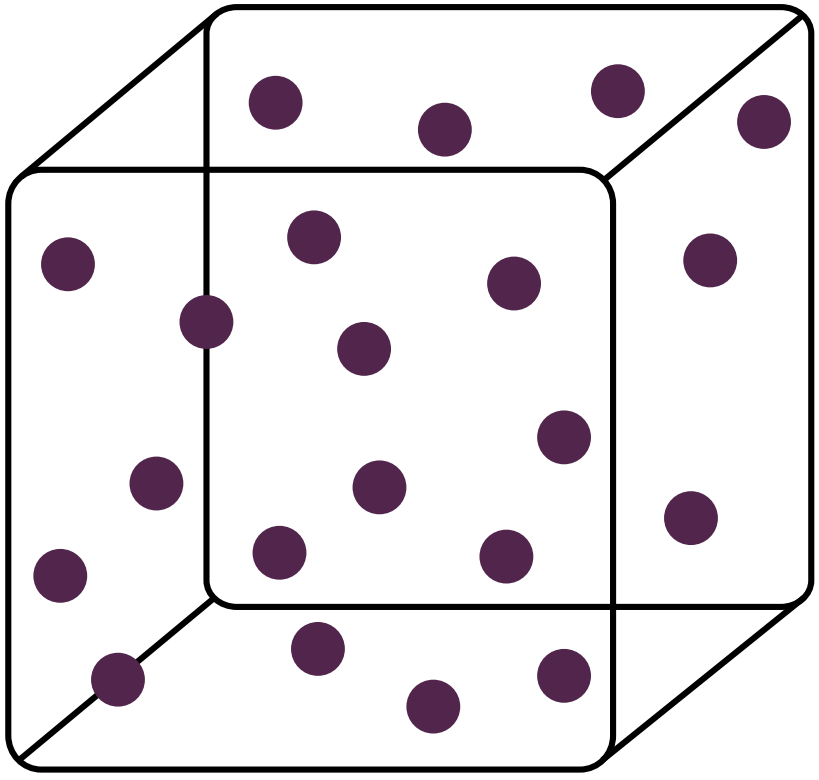
libcloudph++: particle-based Monte-Carlo algorithm



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

attributes:

libcloudph++: particle-based Monte-Carlo algorithm

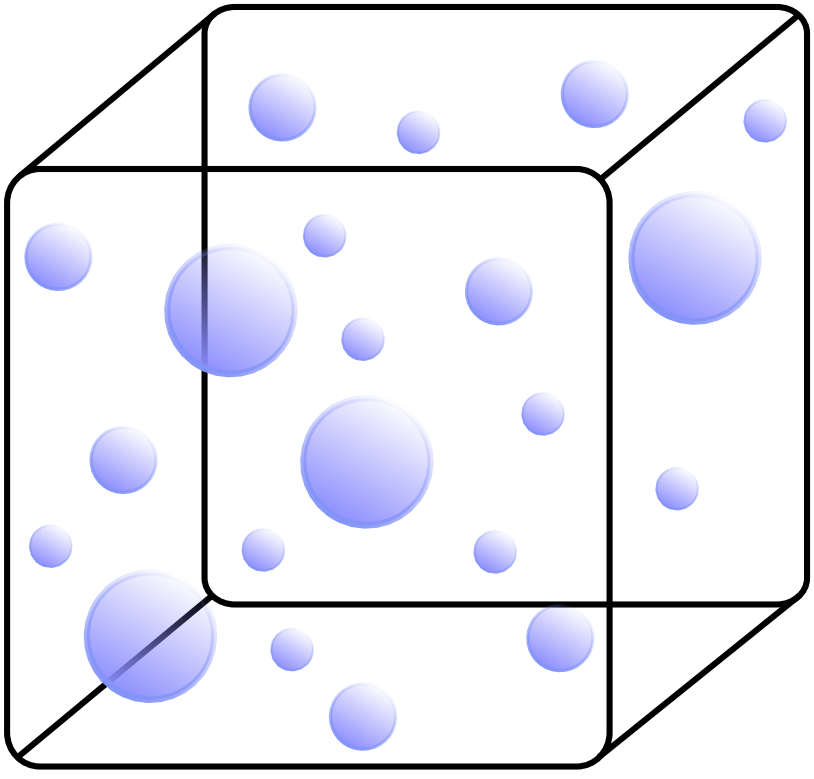


The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

- spatial coords

libcloudph++: particle-based Monte-Carlo algorithm

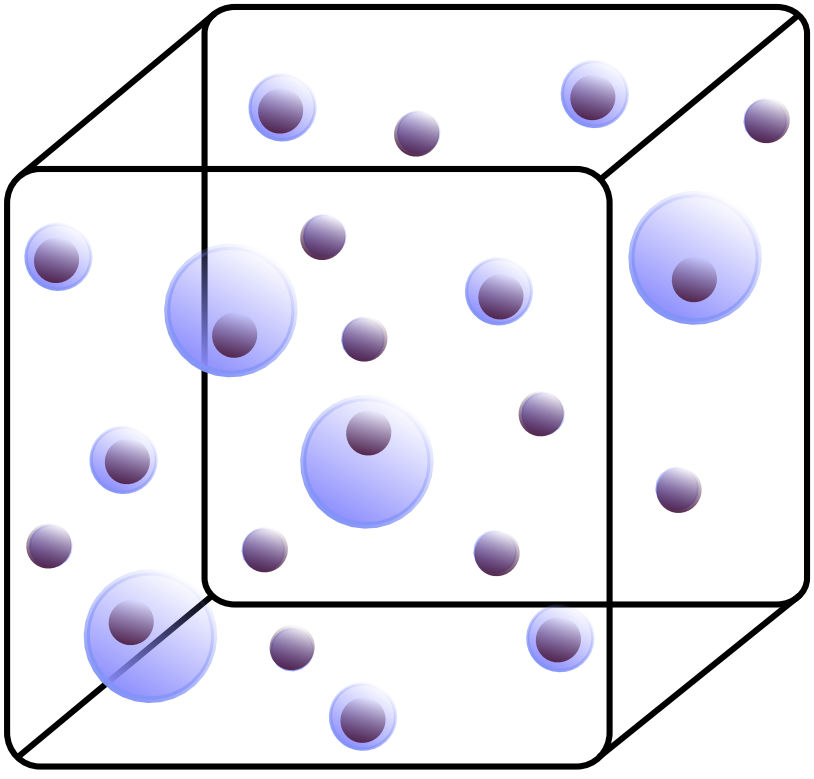


The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

- spatial coords
- wet radius

libcloudph++: particle-based Monte-Carlo algorithm

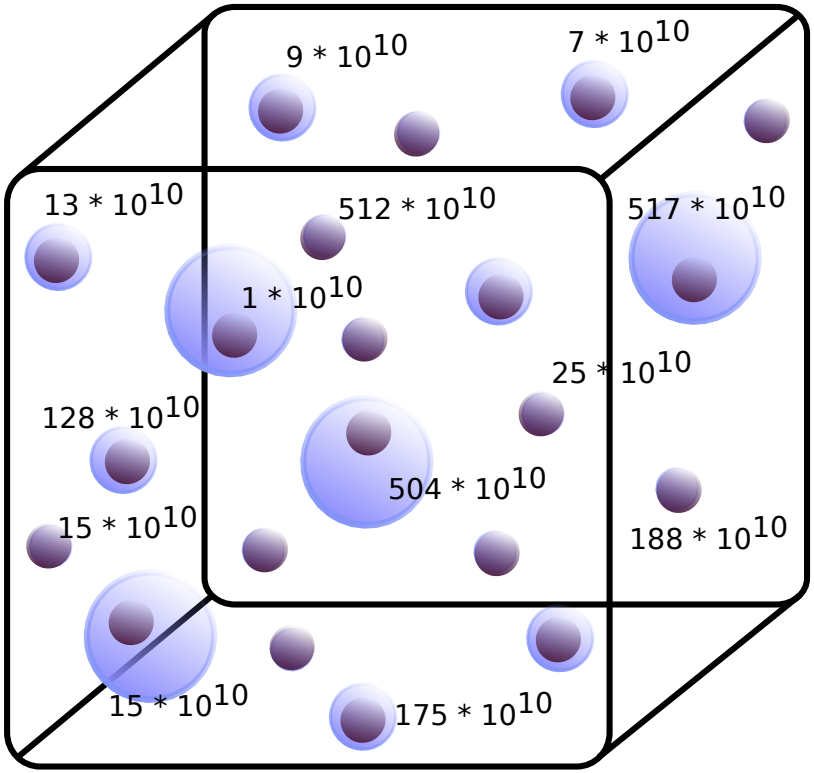


The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

- spatial coords
- wet radius
- dry radius

libcloudph++: particle-based Monte-Carlo algorithm

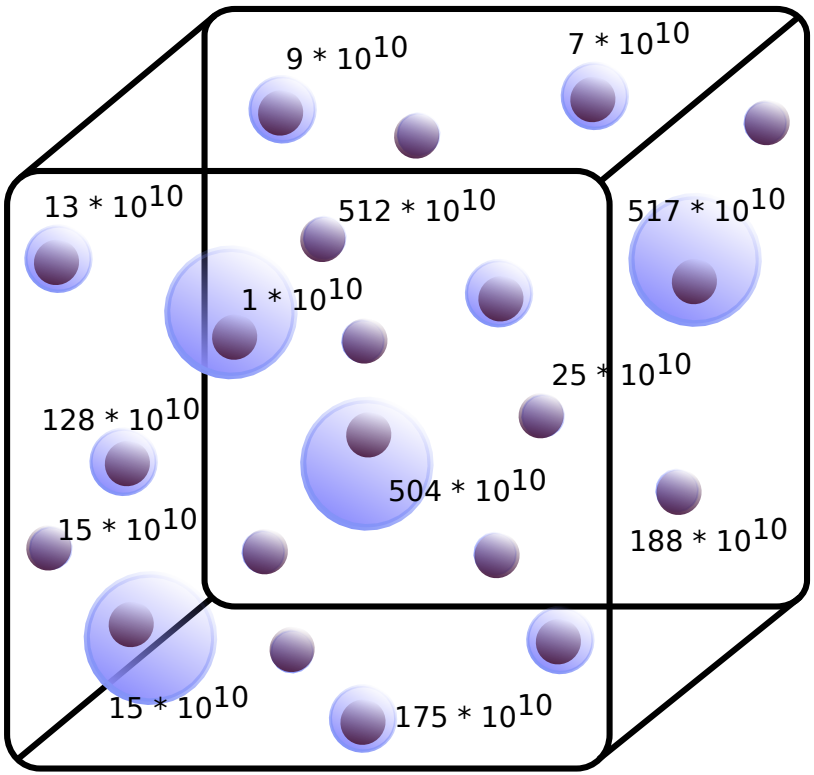


The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

- spatial coords
- wet radius
- dry radius
- multiplicity

libcloudph++: particle-based Monte-Carlo algorithm

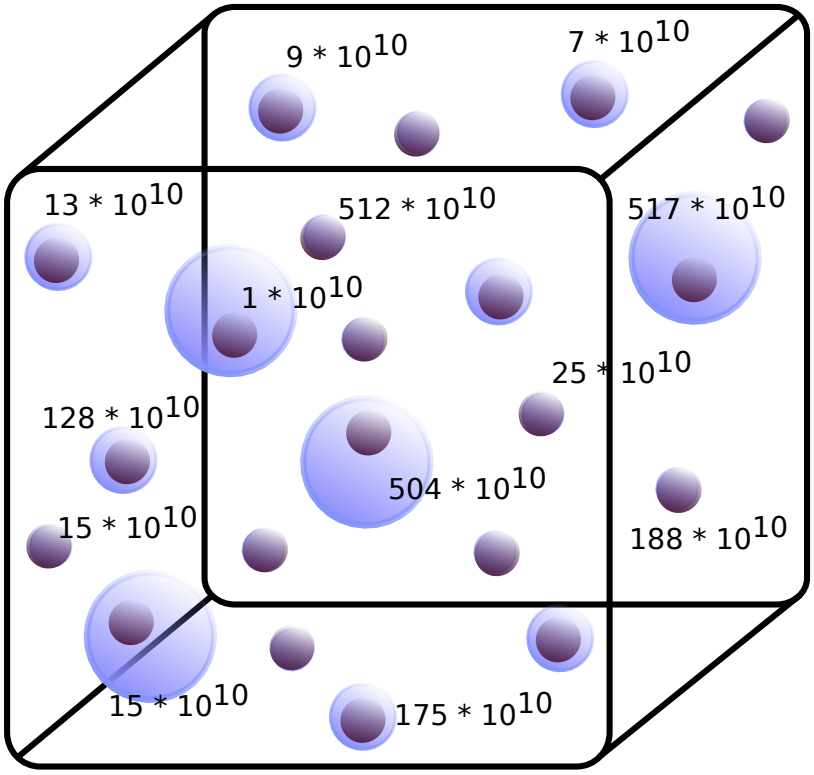


The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

- spatial coords
- wet radius
- dry radius
- multiplicity
- ...

libcloudph++: particle-based Monte-Carlo algorithm



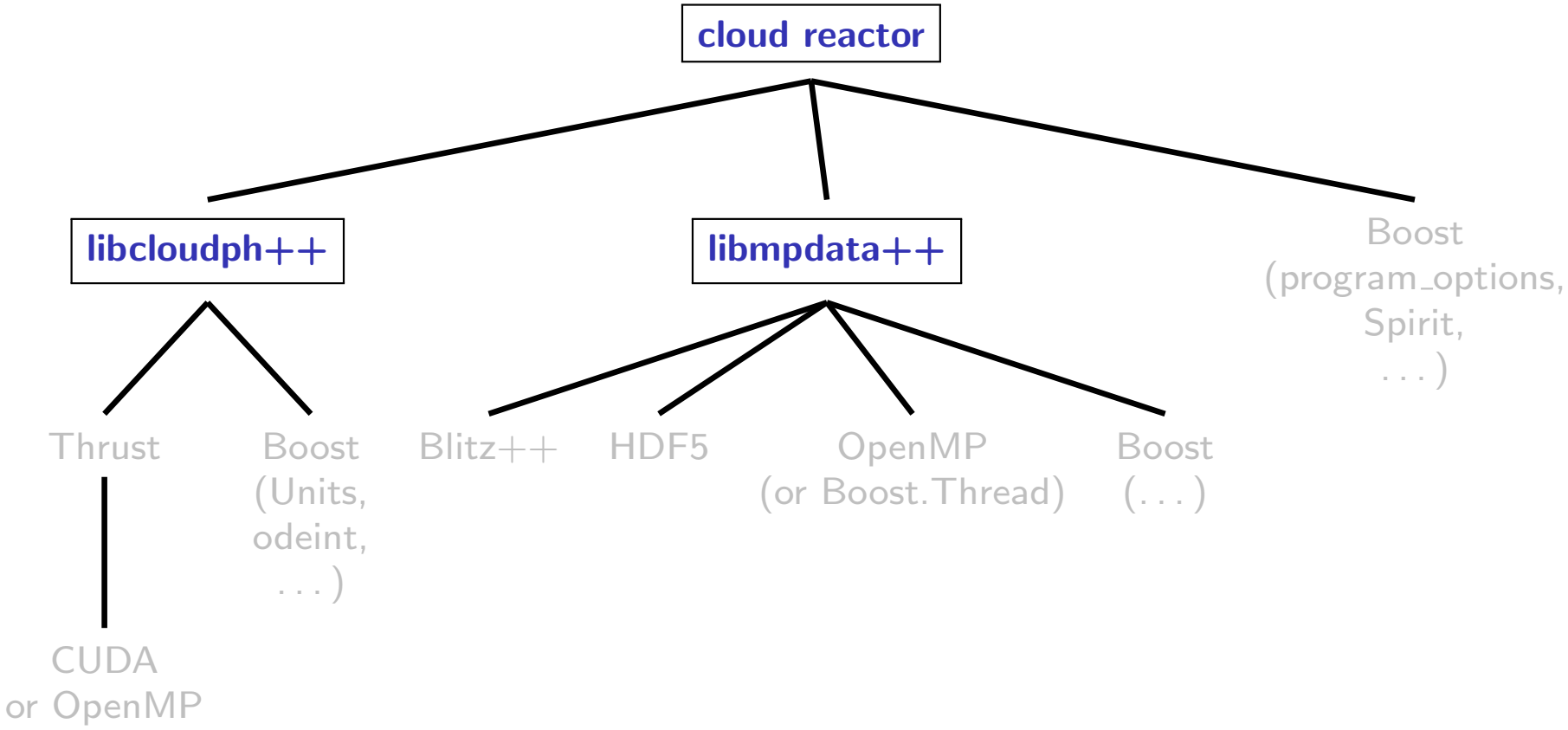
The domain is populated with "information carriers" (alias computational particles, super droplets)

attributes:

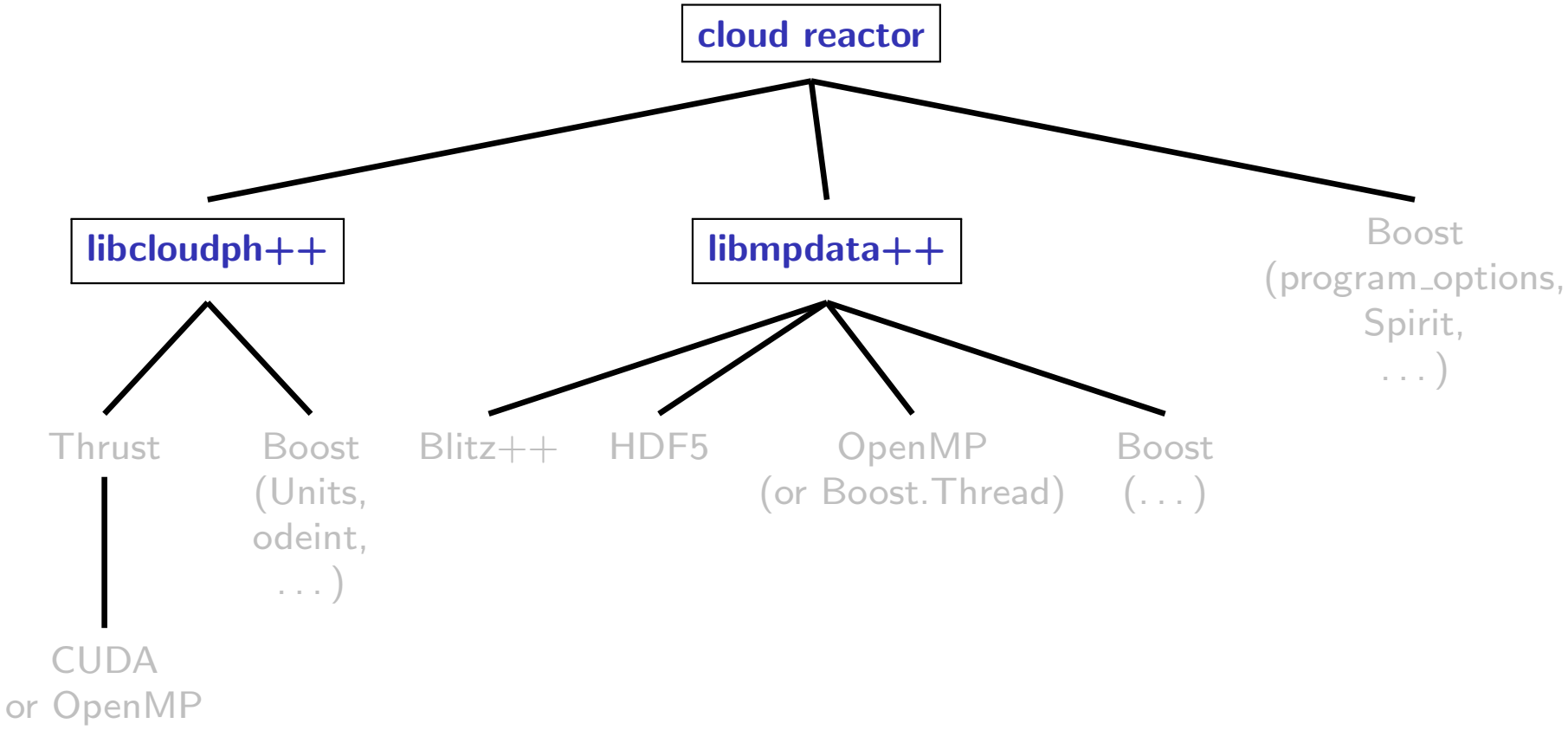
- spatial coords
- wet radius
- dry radius
- multiplicity
- ...

transport does not incur numerical diffusion!

libcloudph++: some design choices



libcloudph++: some design choices



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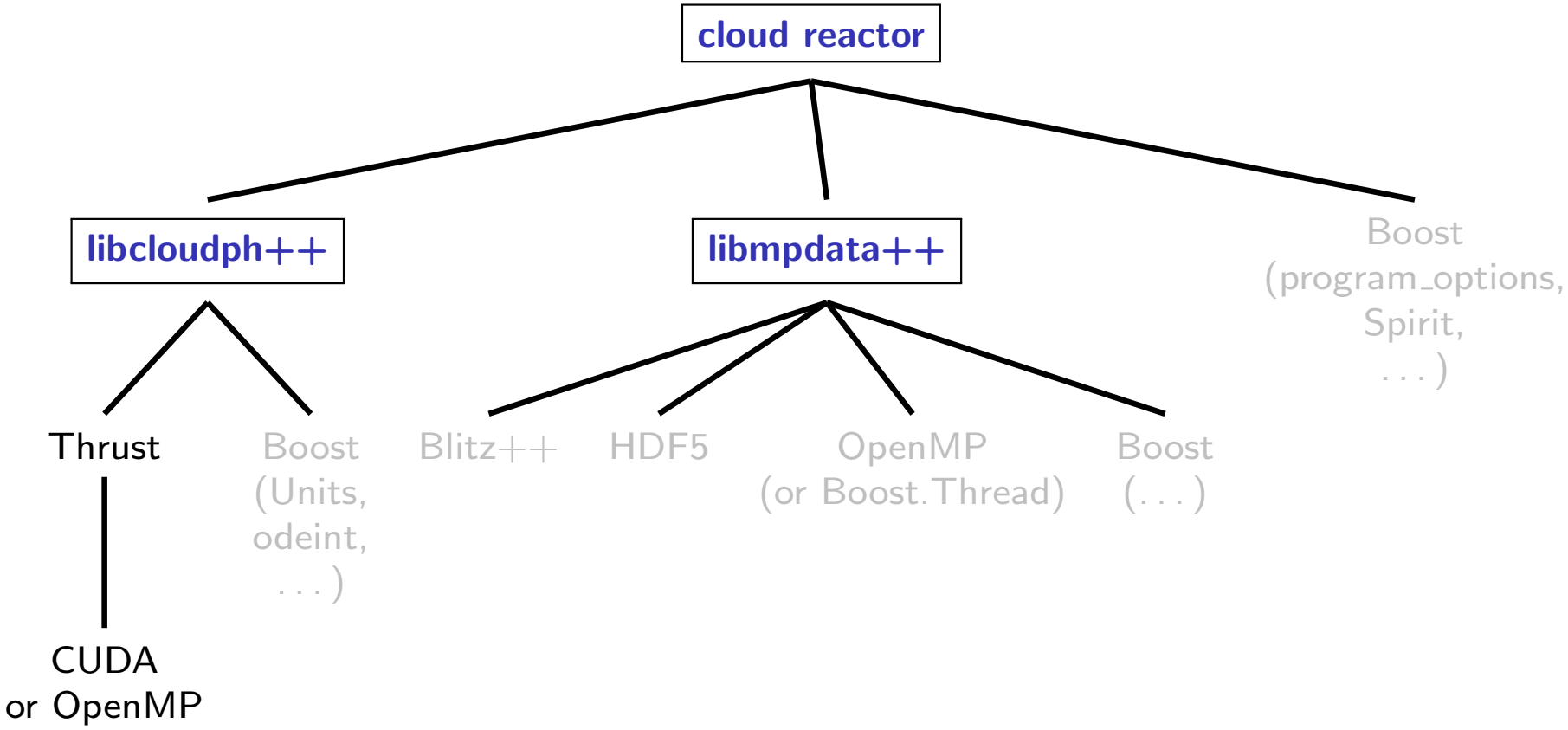
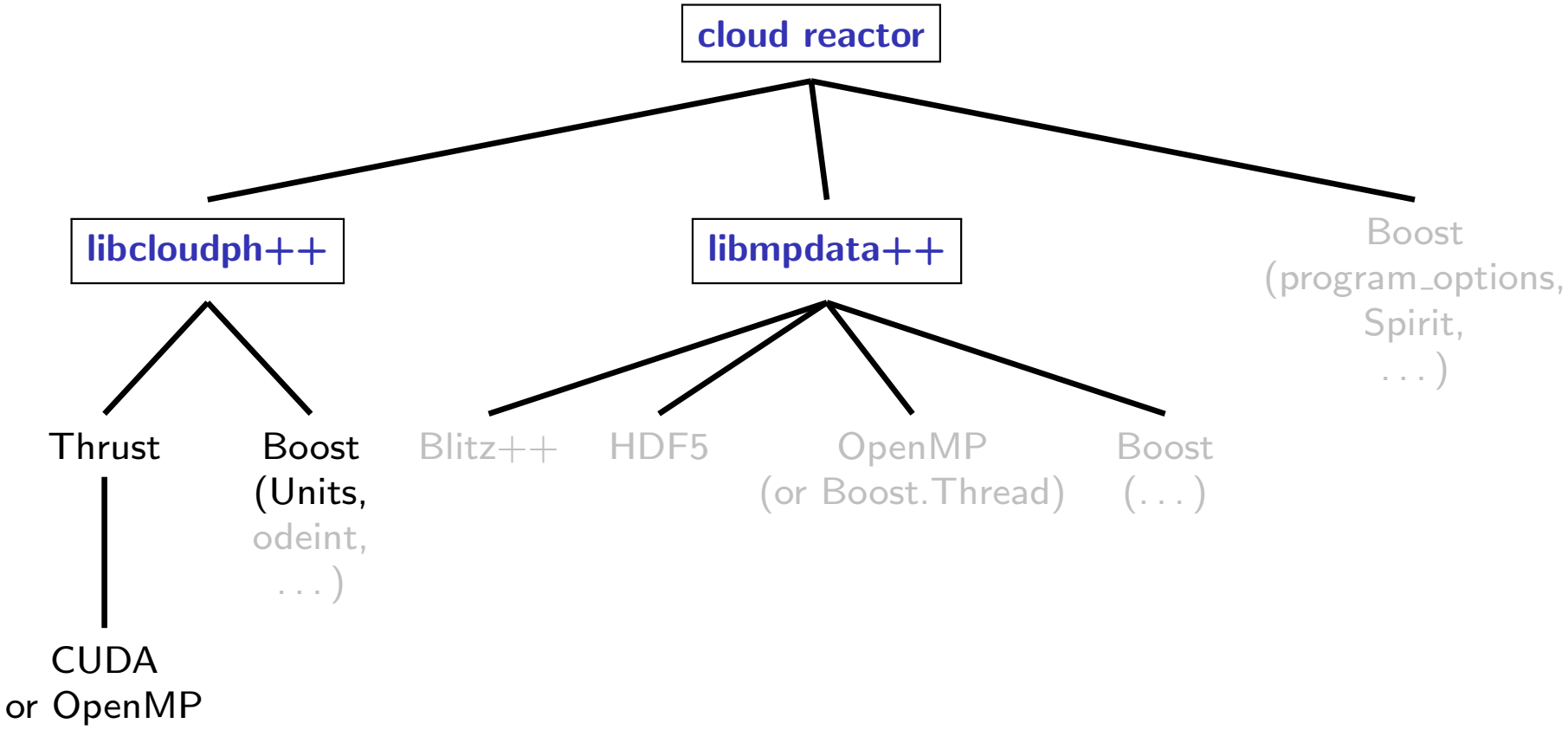
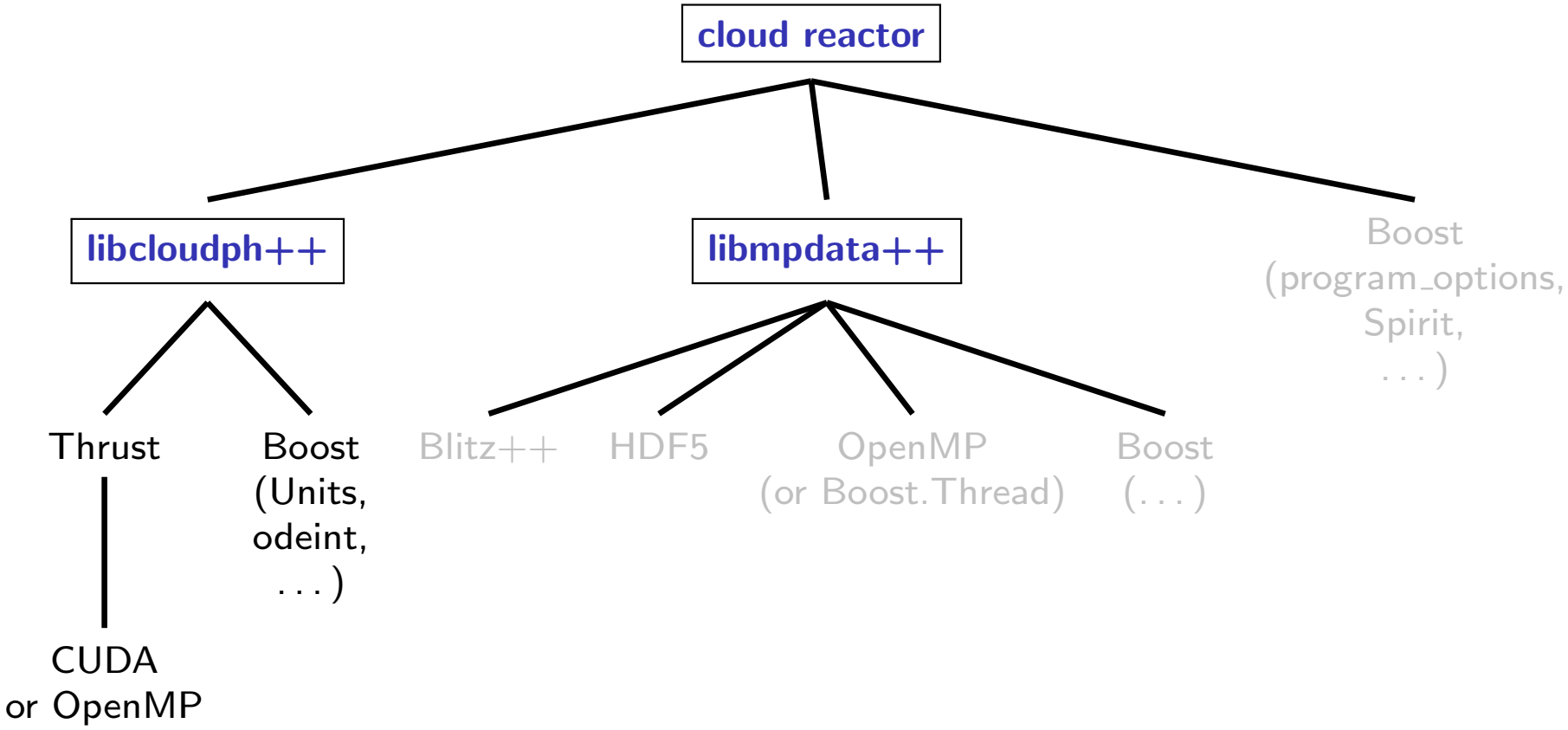


libcloudph++: some design choices



libcloudph++: some design choices



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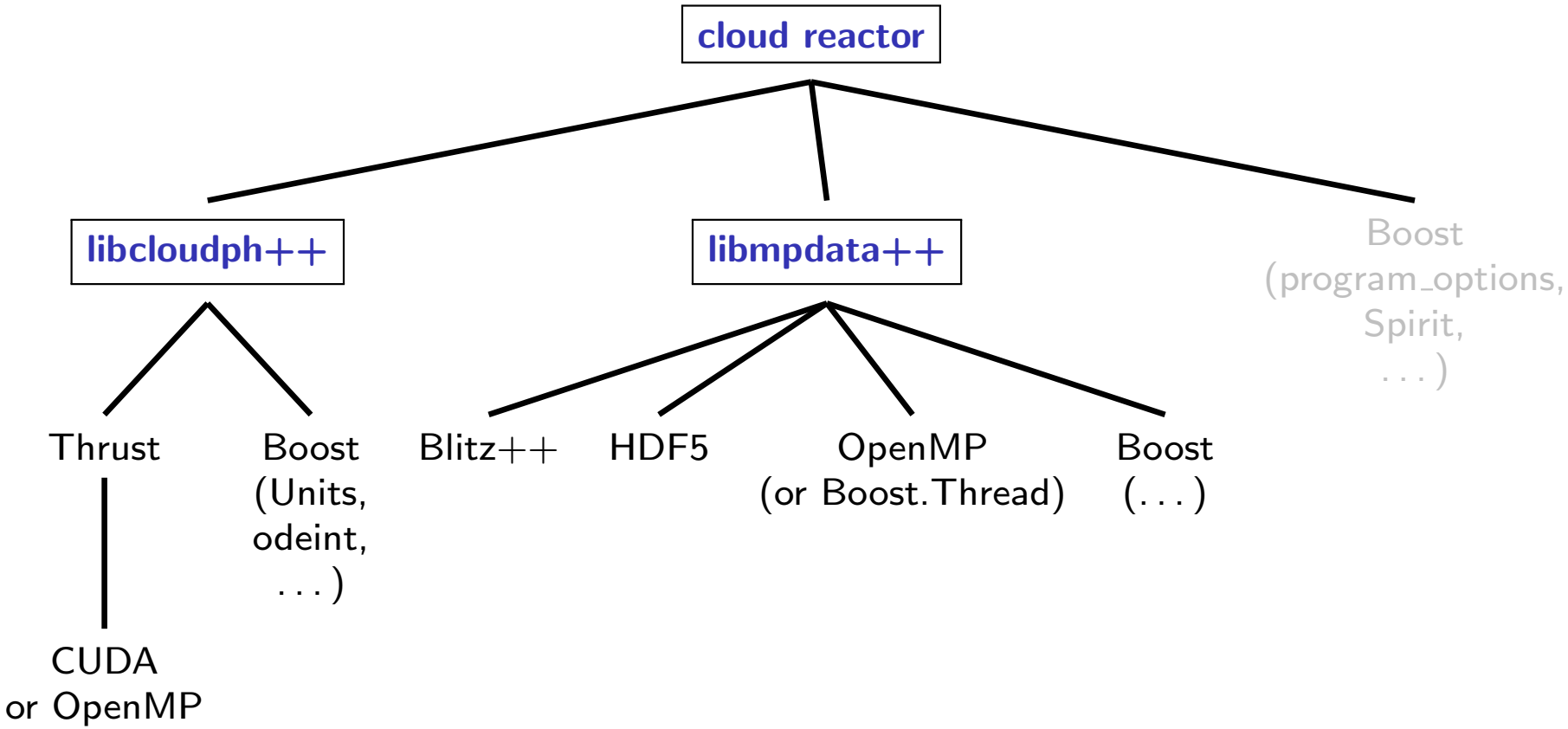
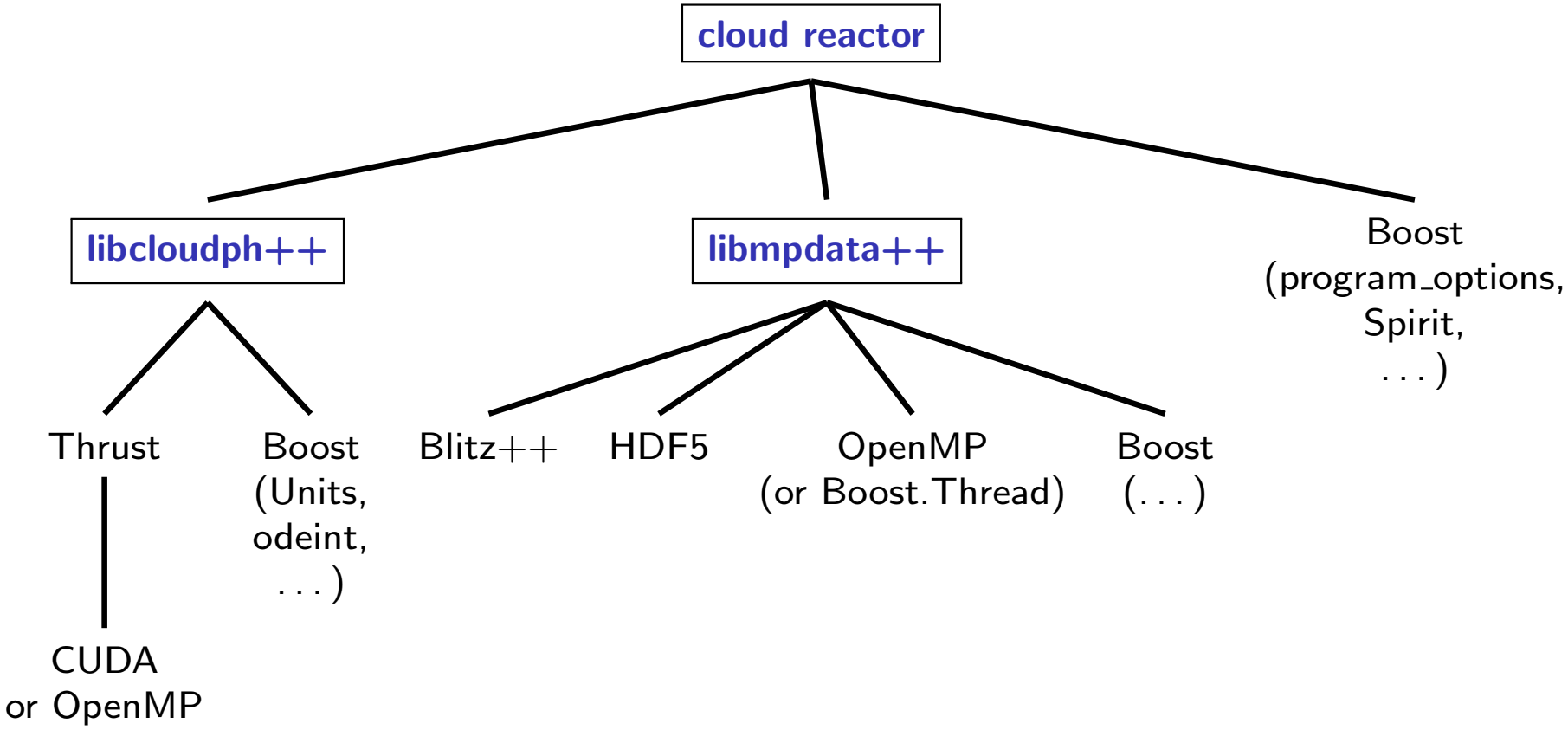
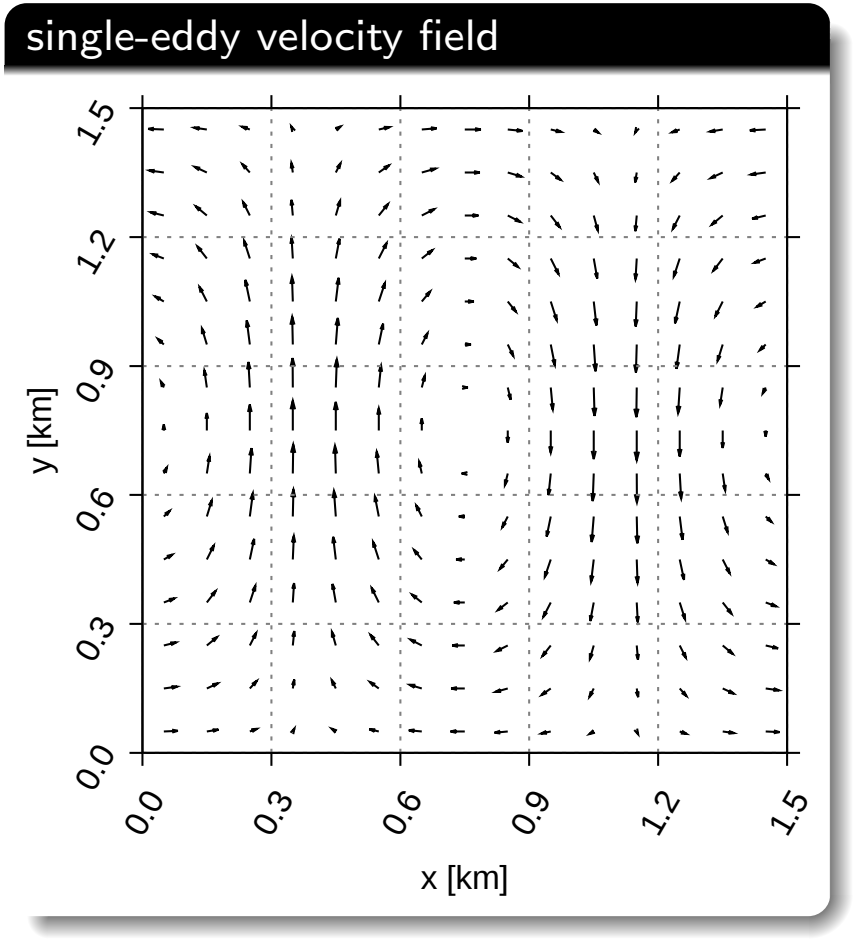


libcloudph++: some design choices



libcloudph++: example 2D prescribed-flow simulation



libcloudph++: example 2D prescribed-flow simulation

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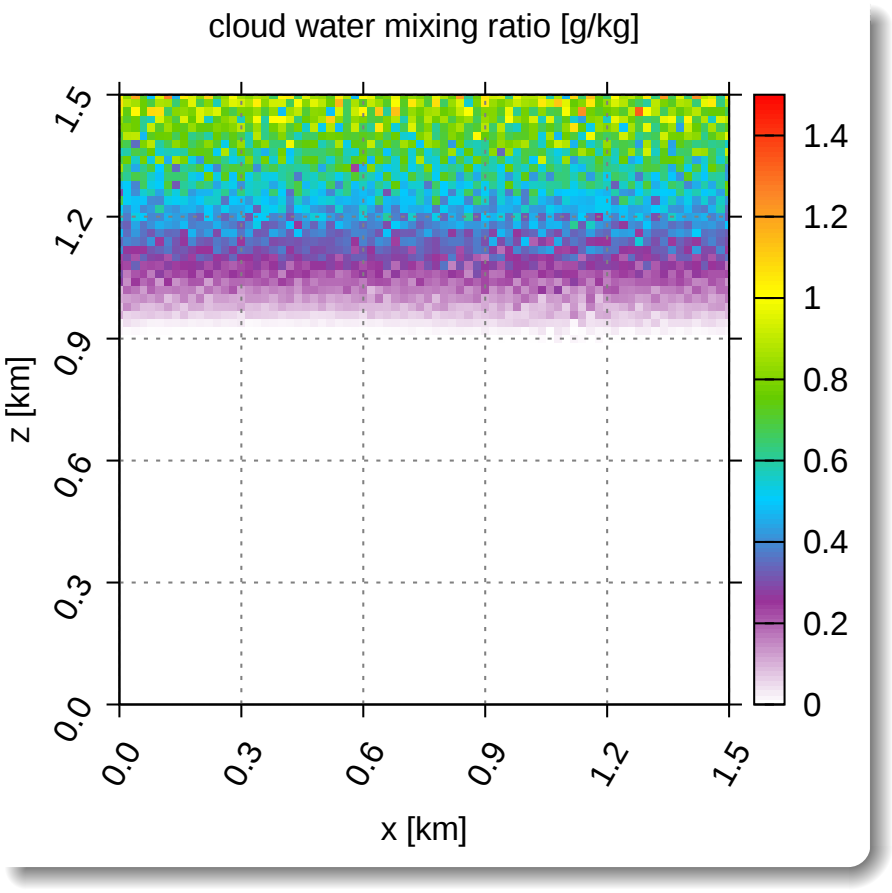

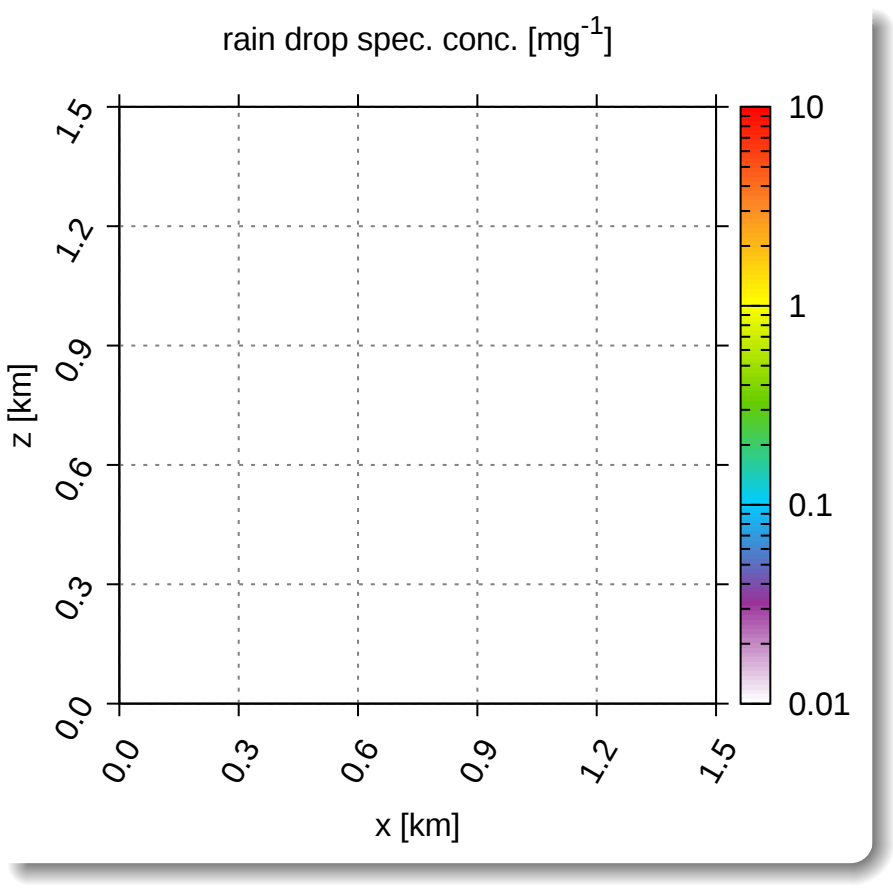

libcloudph++: example 2D prescribed-flow simulation

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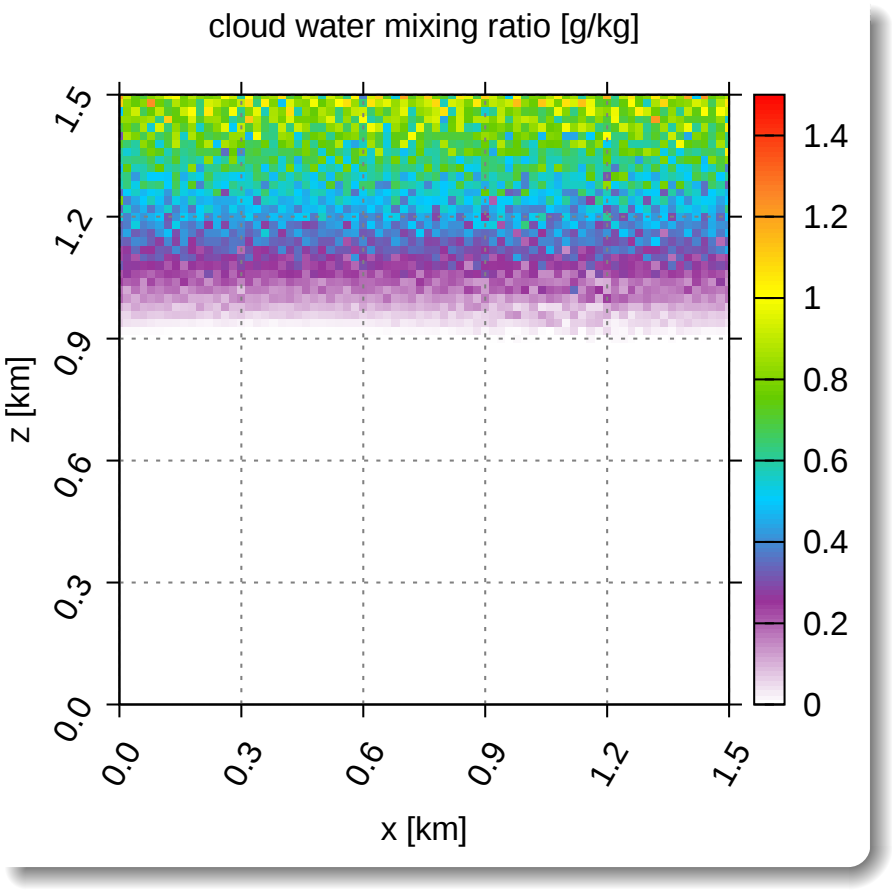

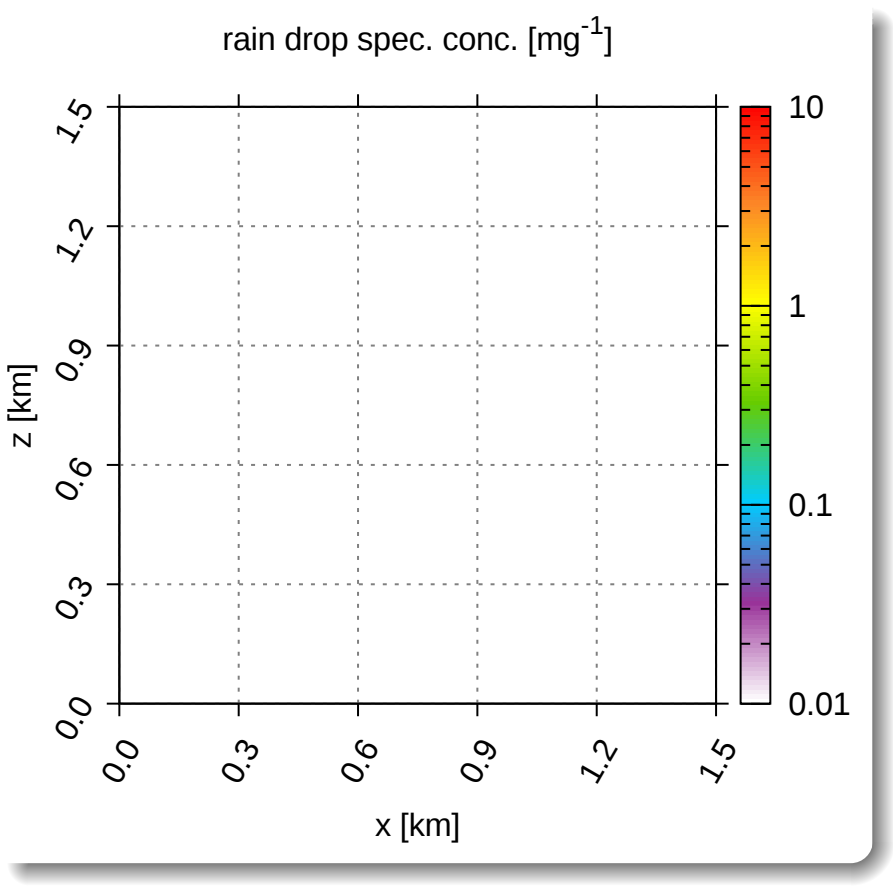

libcloudph++: example 2D prescribed-flow simulation

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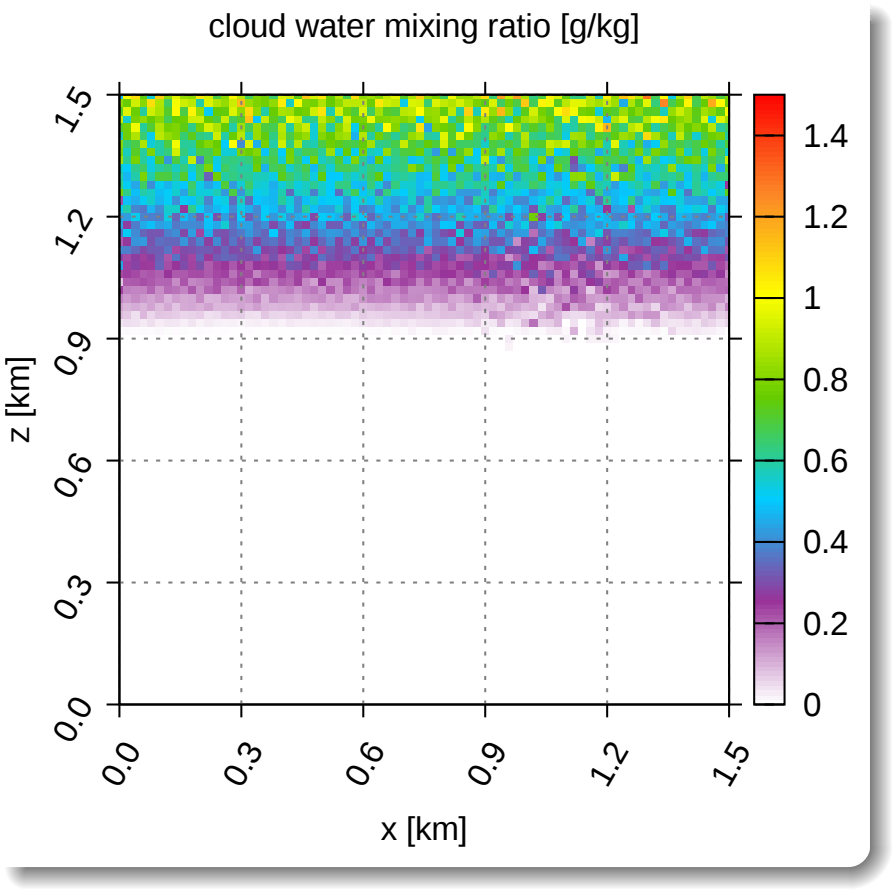

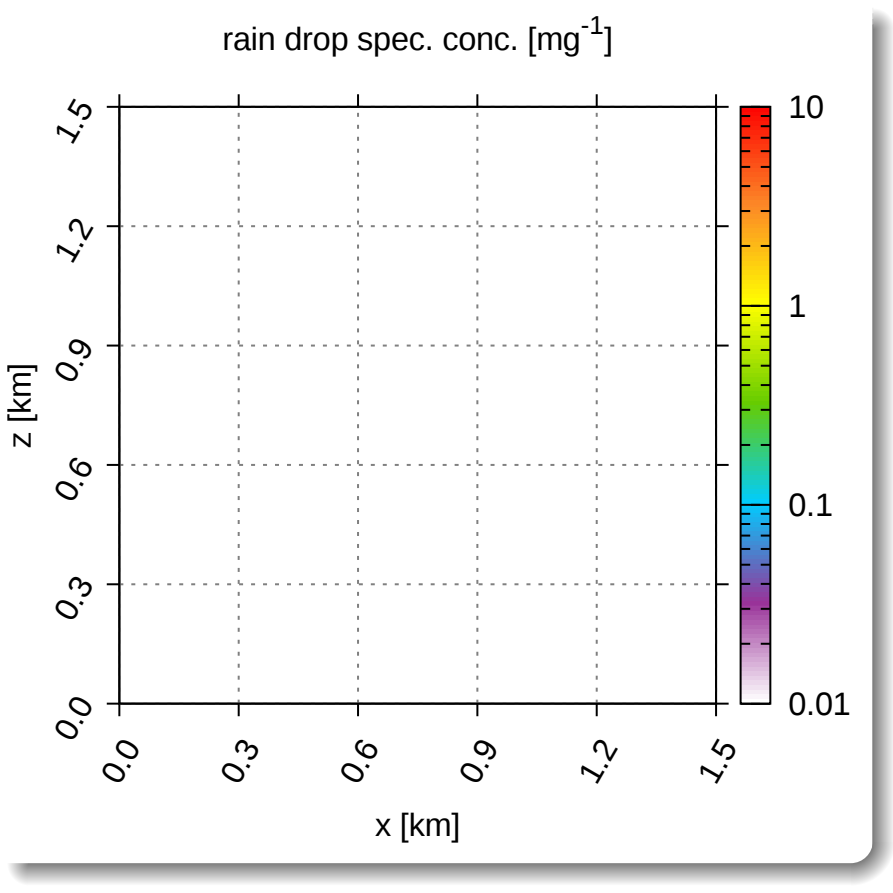

libcloudph++: example 2D prescribed-flow simulation

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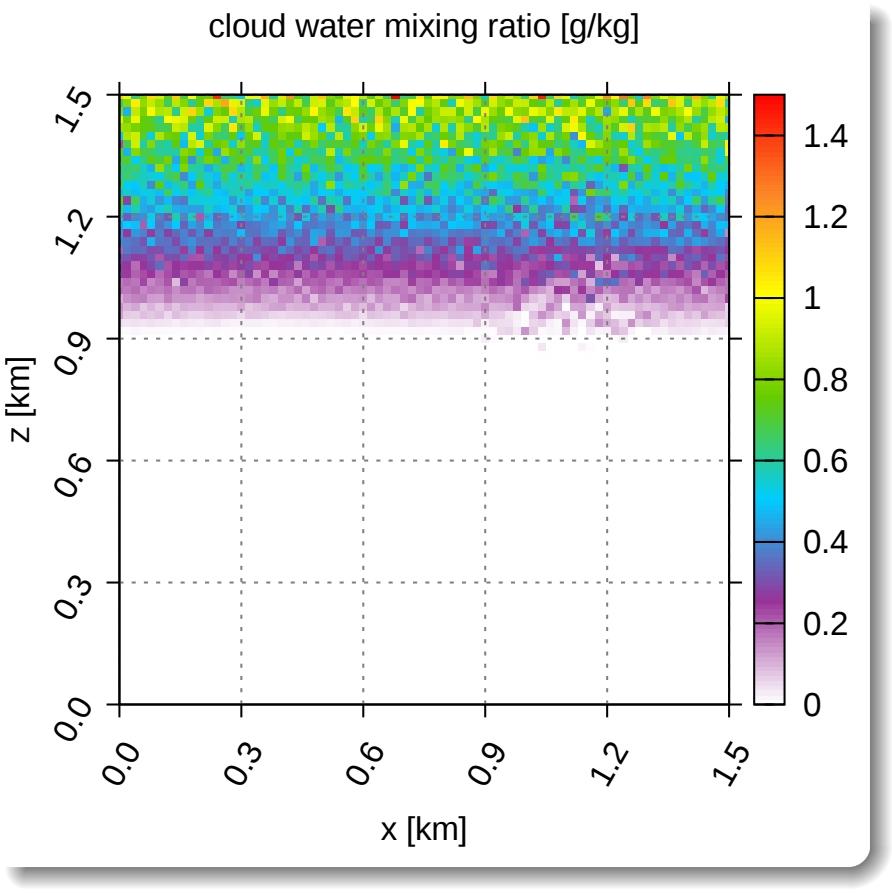

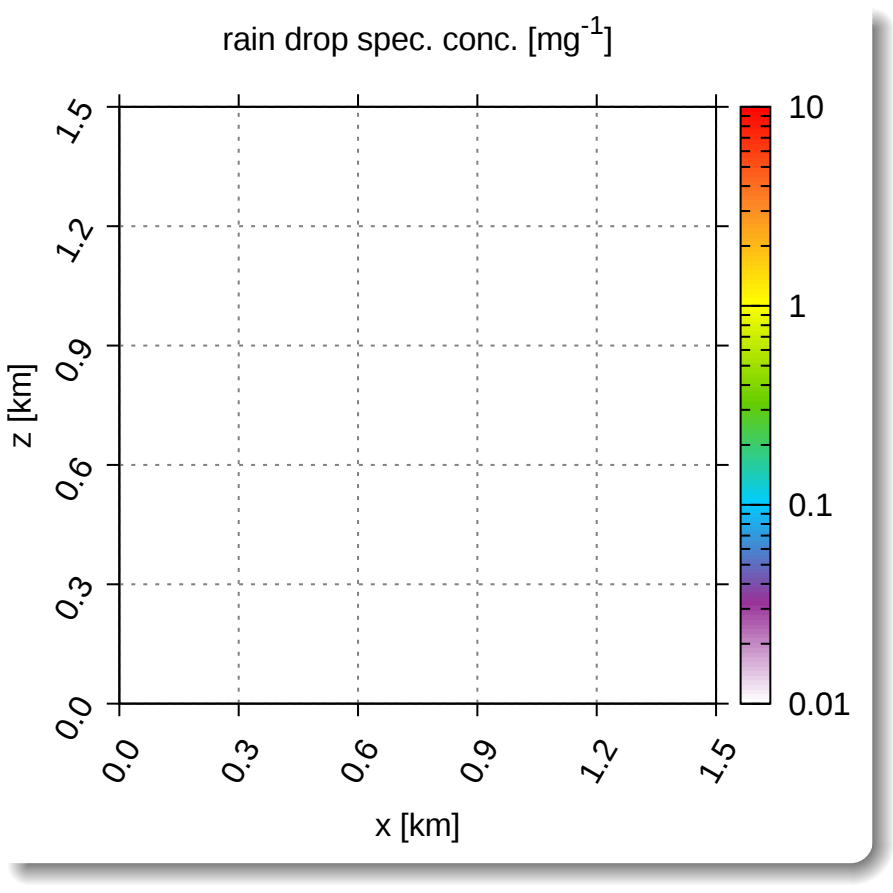

libcloudph++: example 2D prescribed-flow simulation

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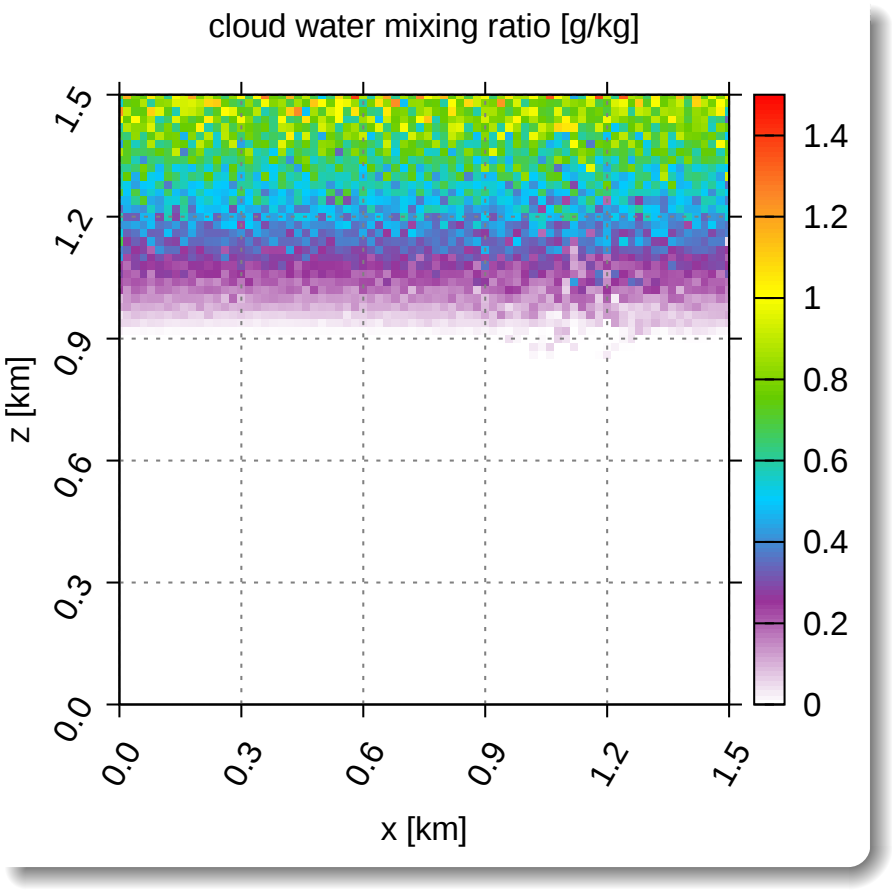

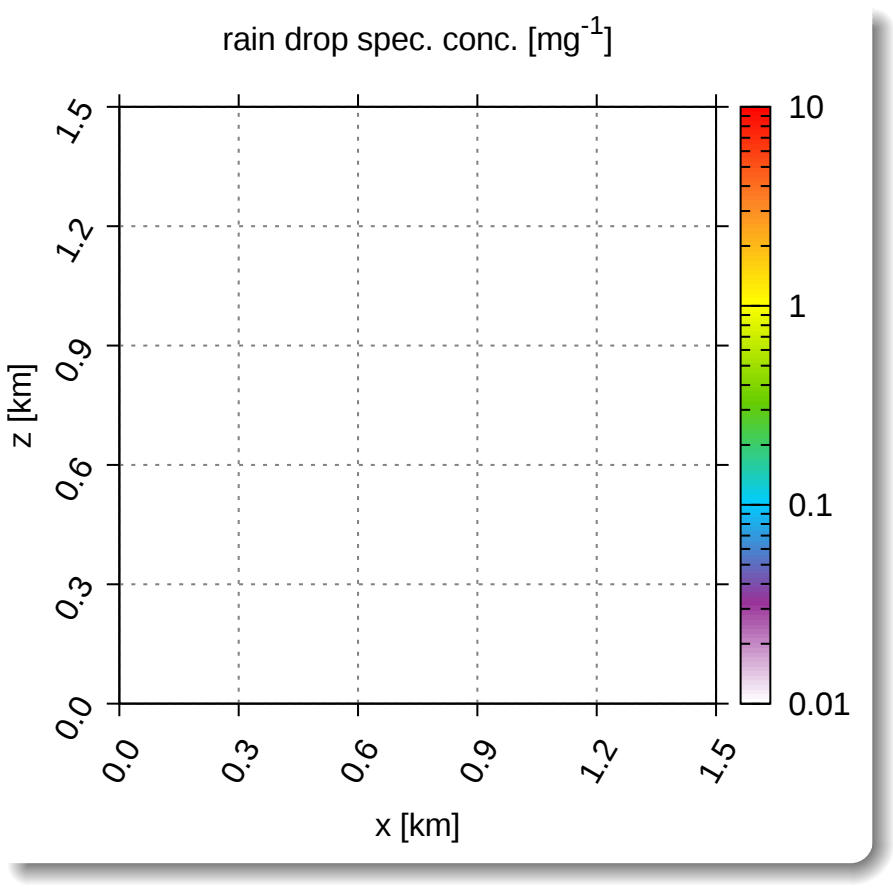

libcloudph++: example 2D prescribed-flow simulation
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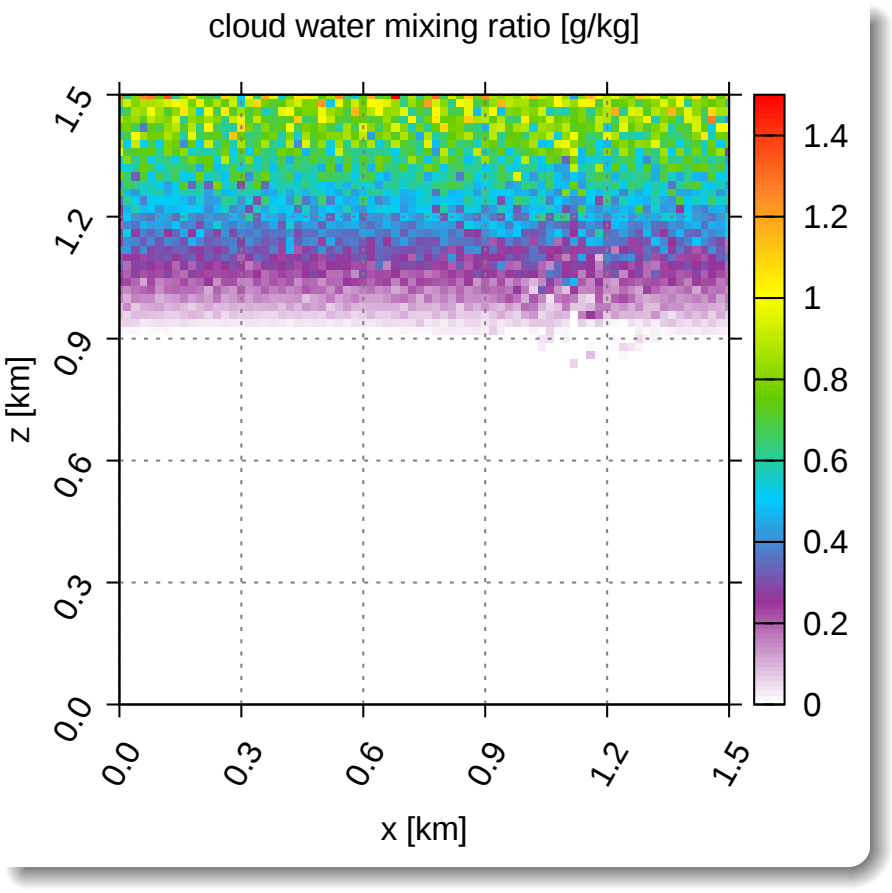

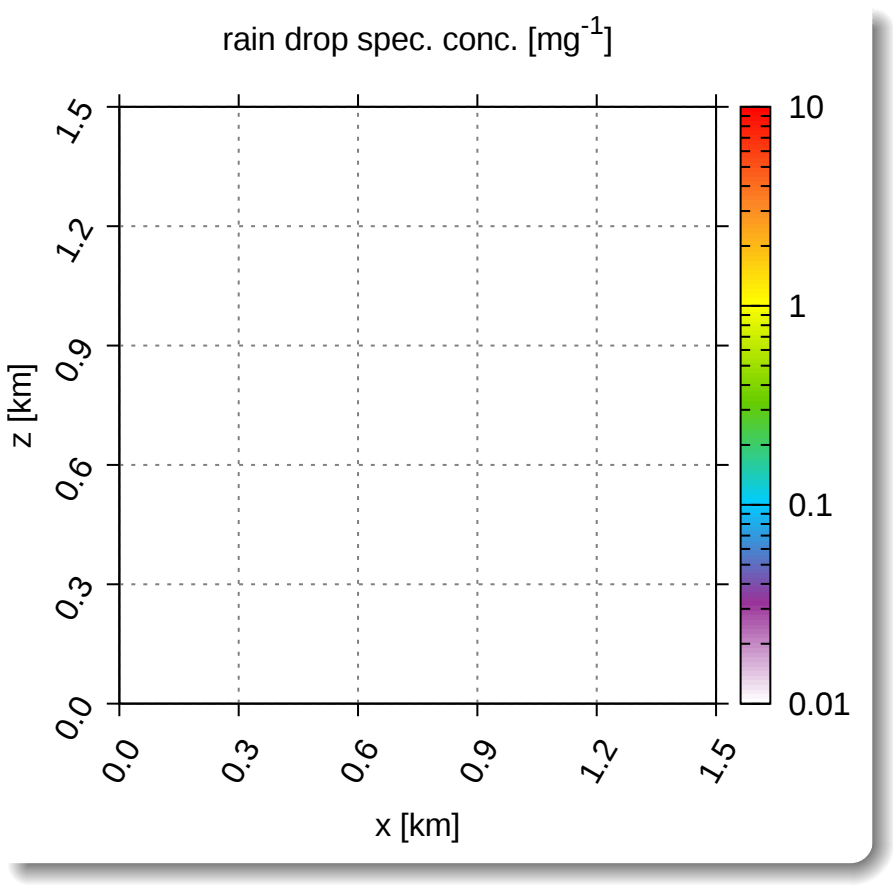

libcloudph++: example 2D prescribed-flow simulation
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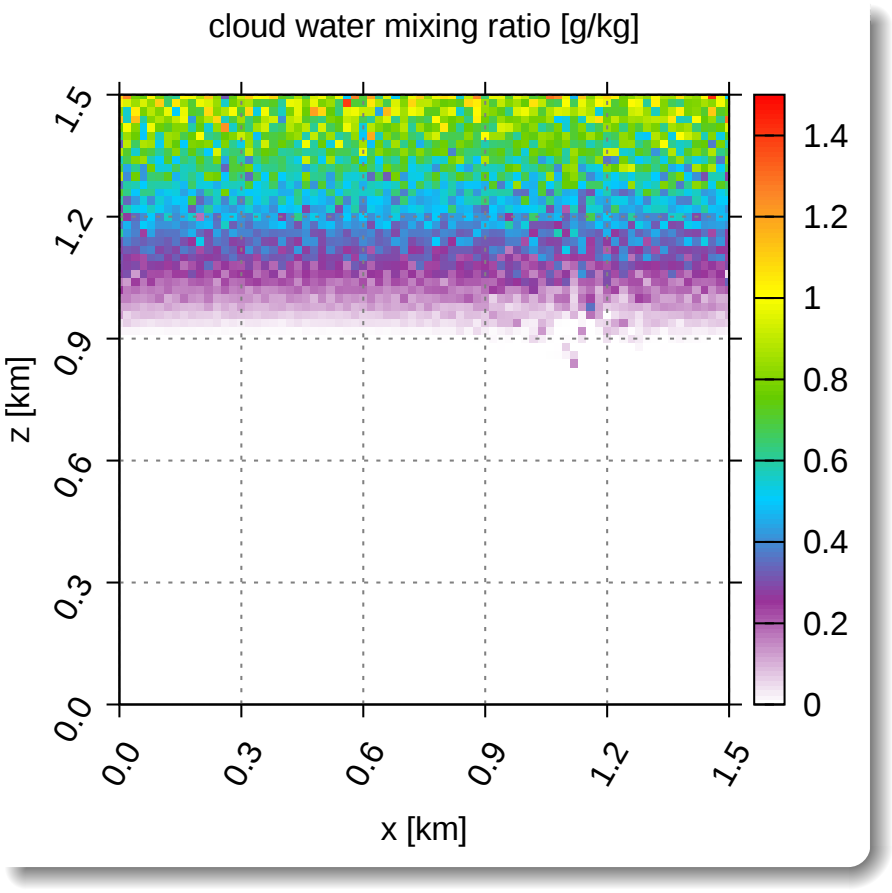

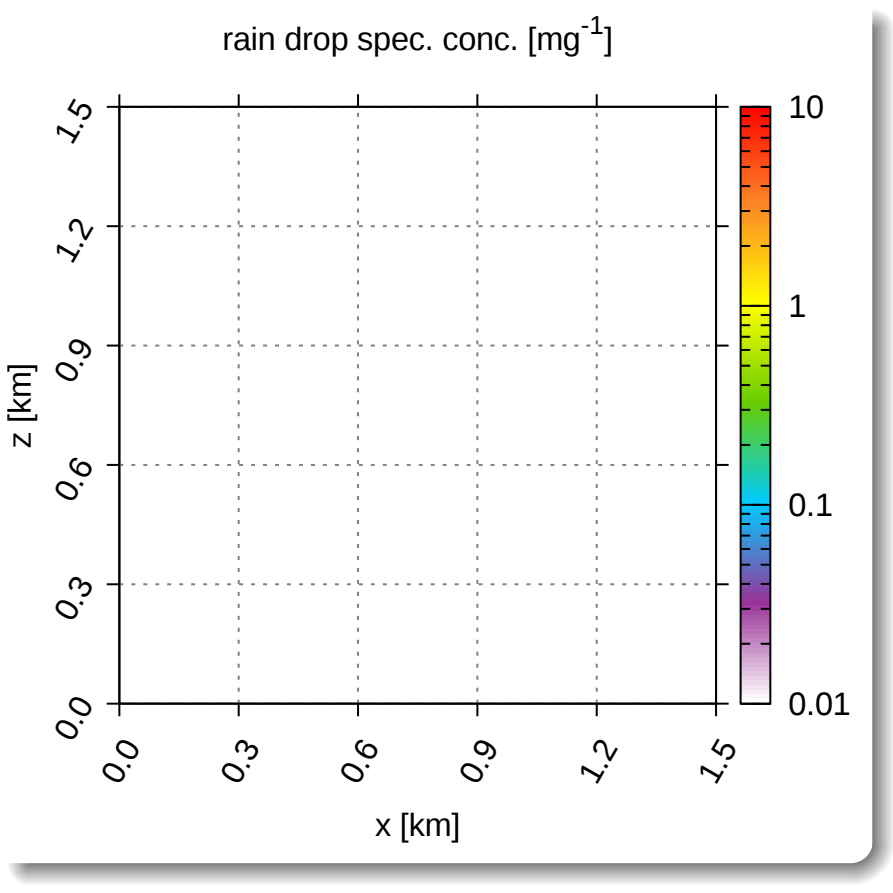

libcloudph++: example 2D prescribed-flow simulation
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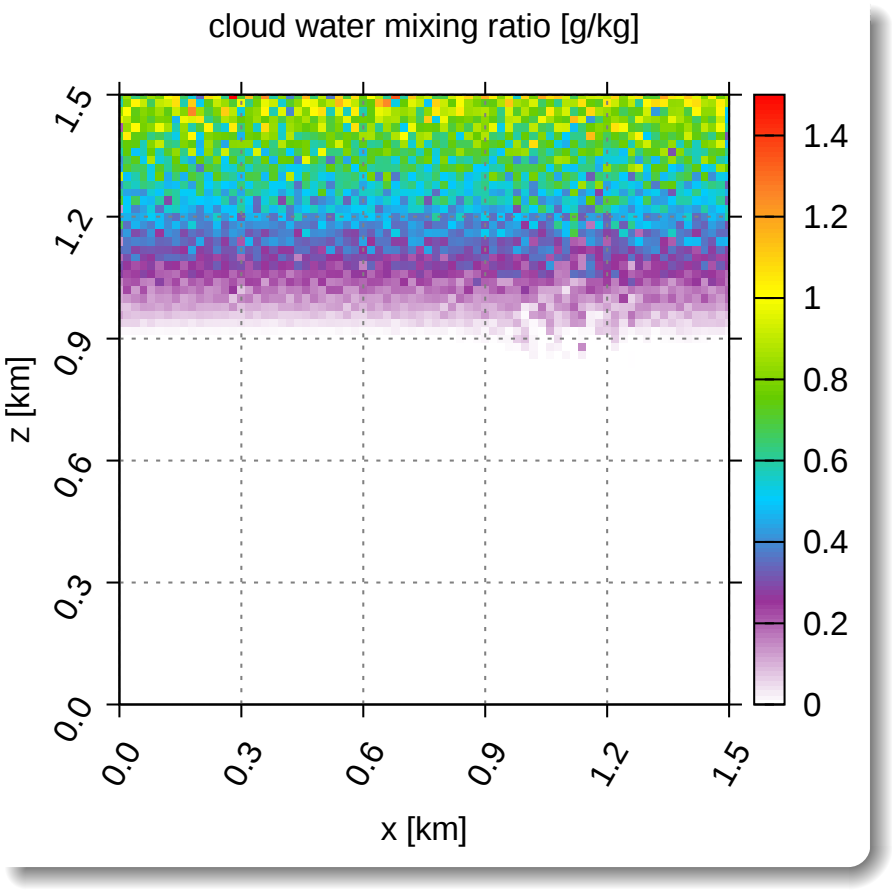

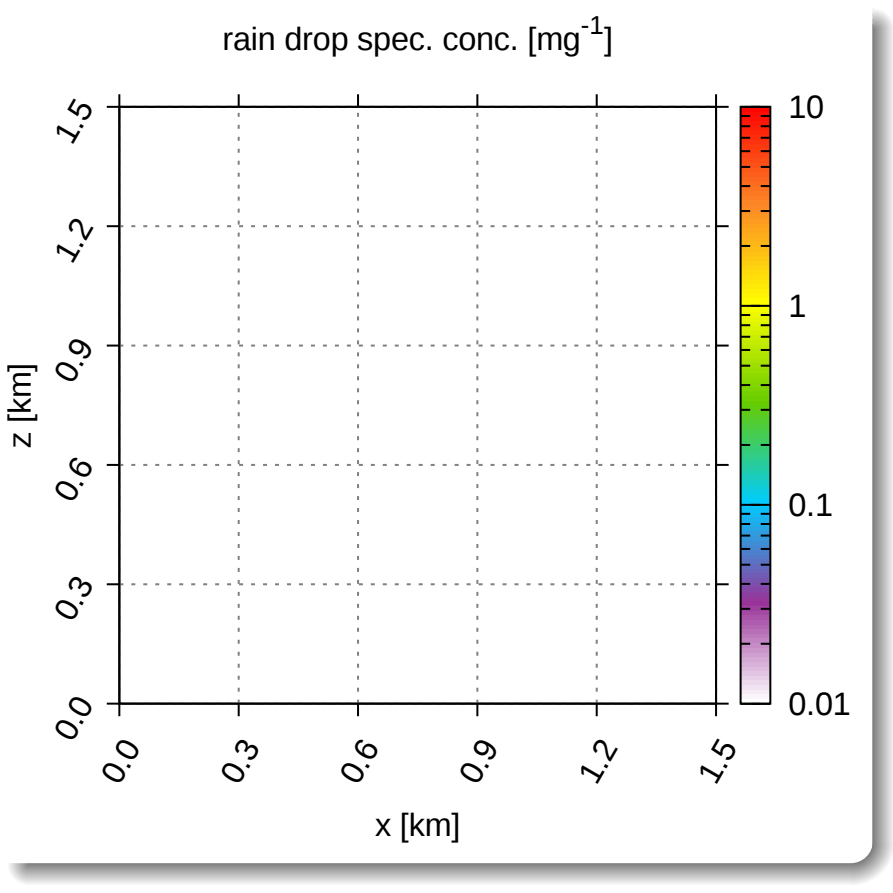

libcloudph++: example 2D prescribed-flow simulation

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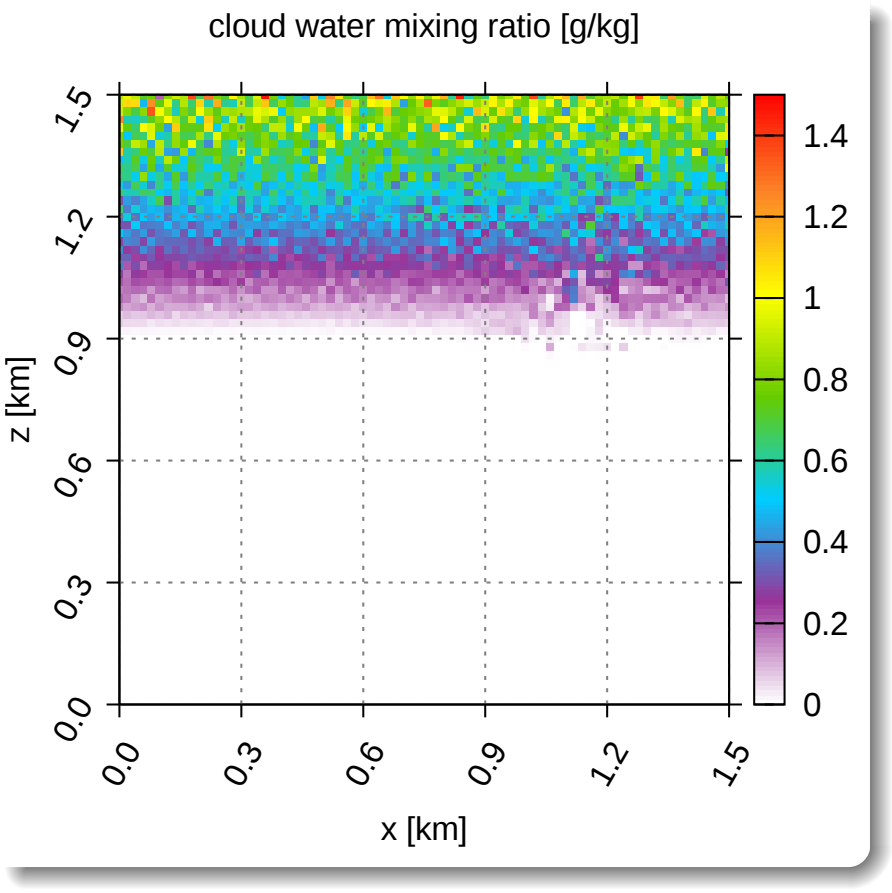

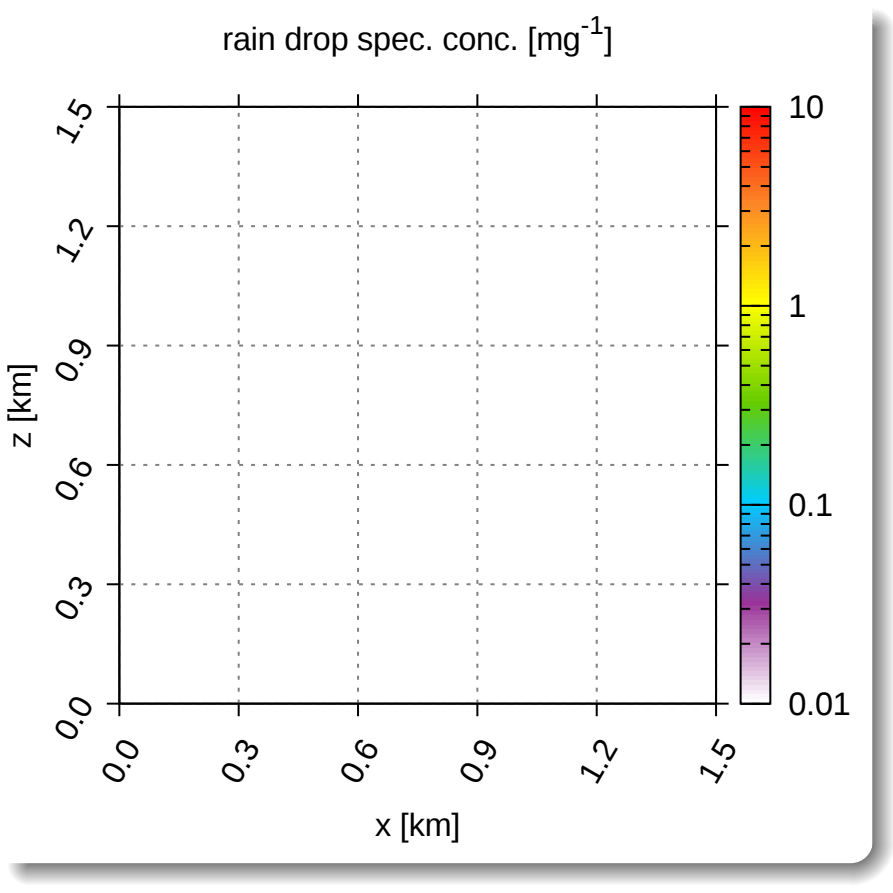

libcloudph++: example 2D prescribed-flow simulation

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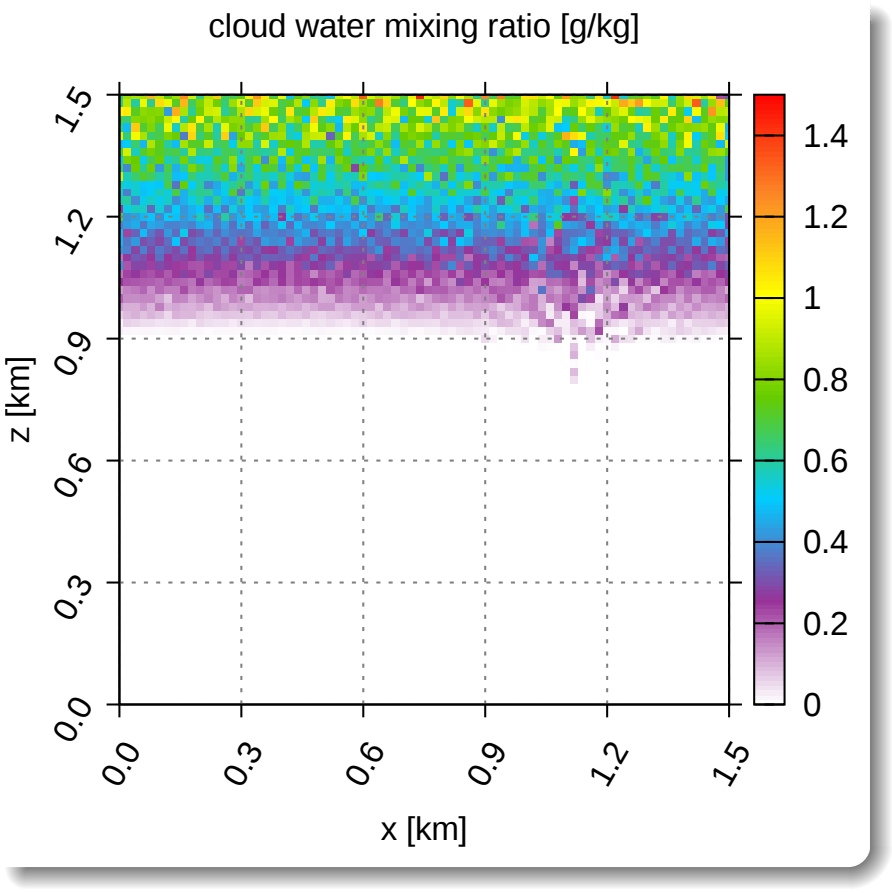

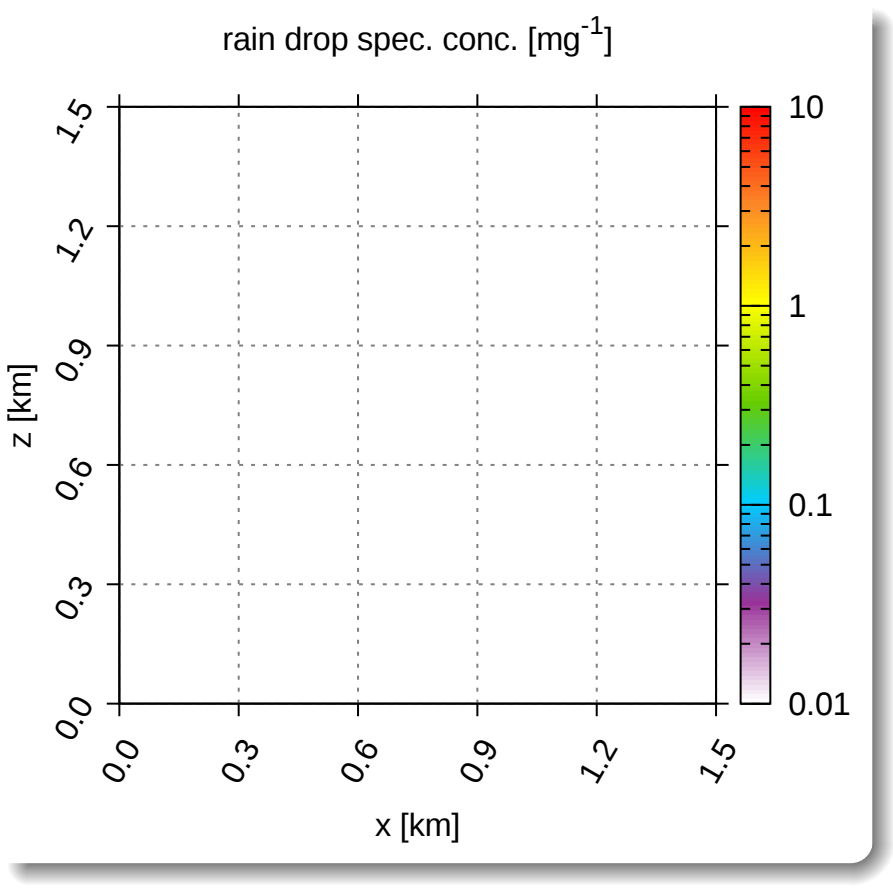

libcloudph++: example 2D prescribed-flow simulation
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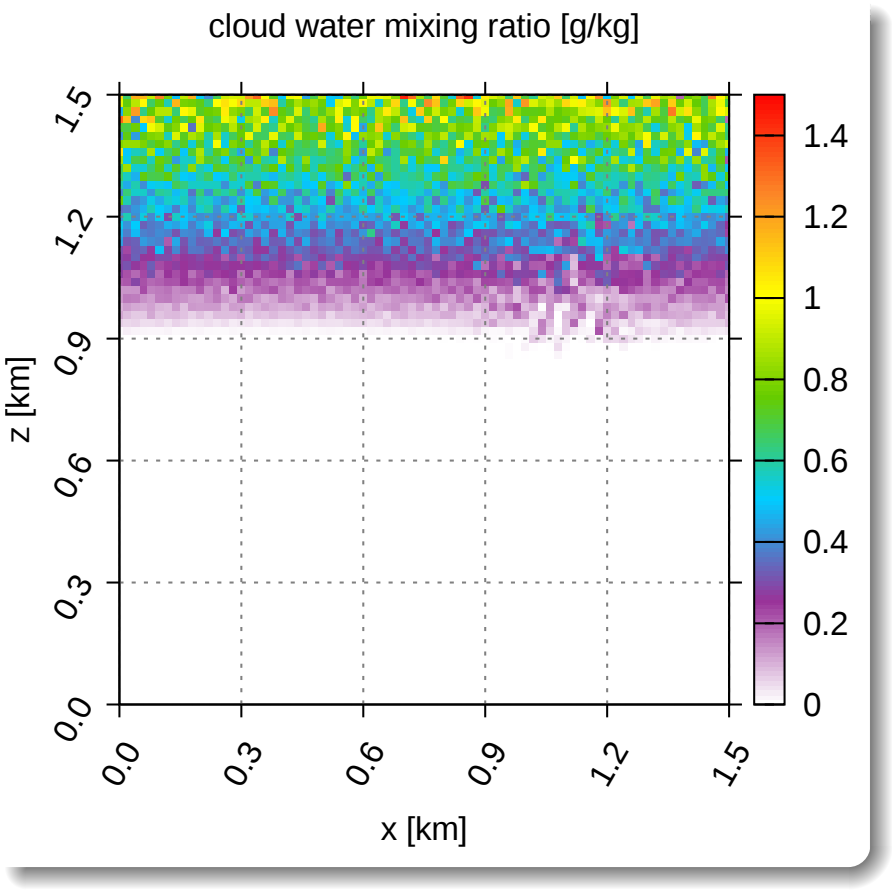

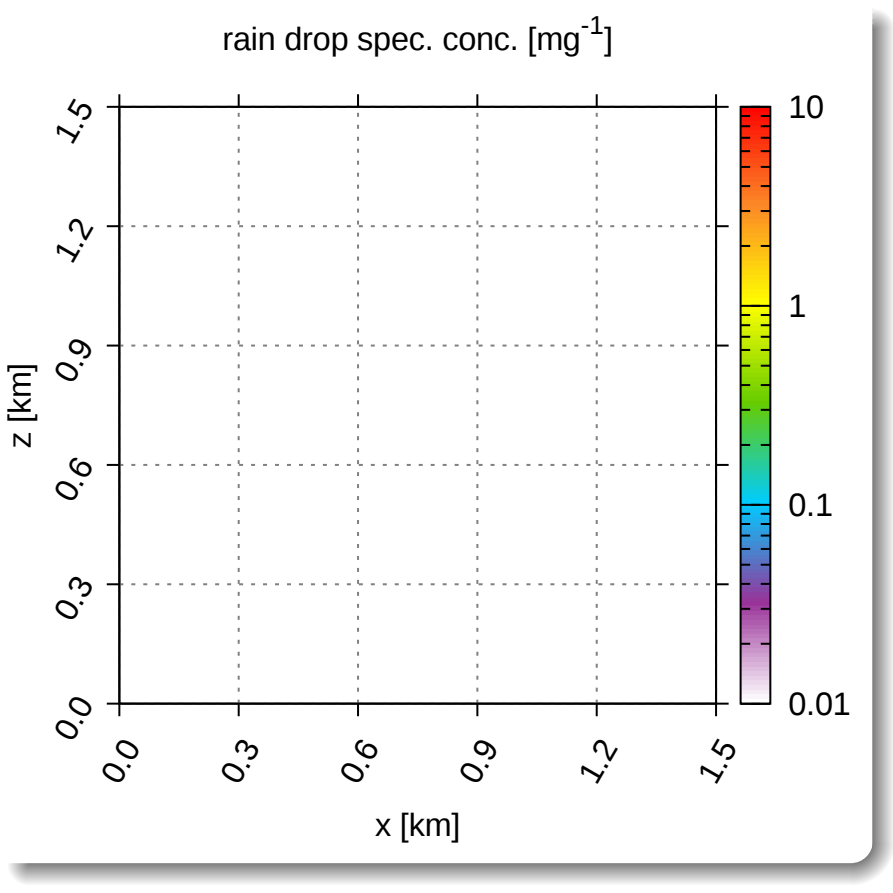

libcloudph++: example 2D prescribed-flow simulation
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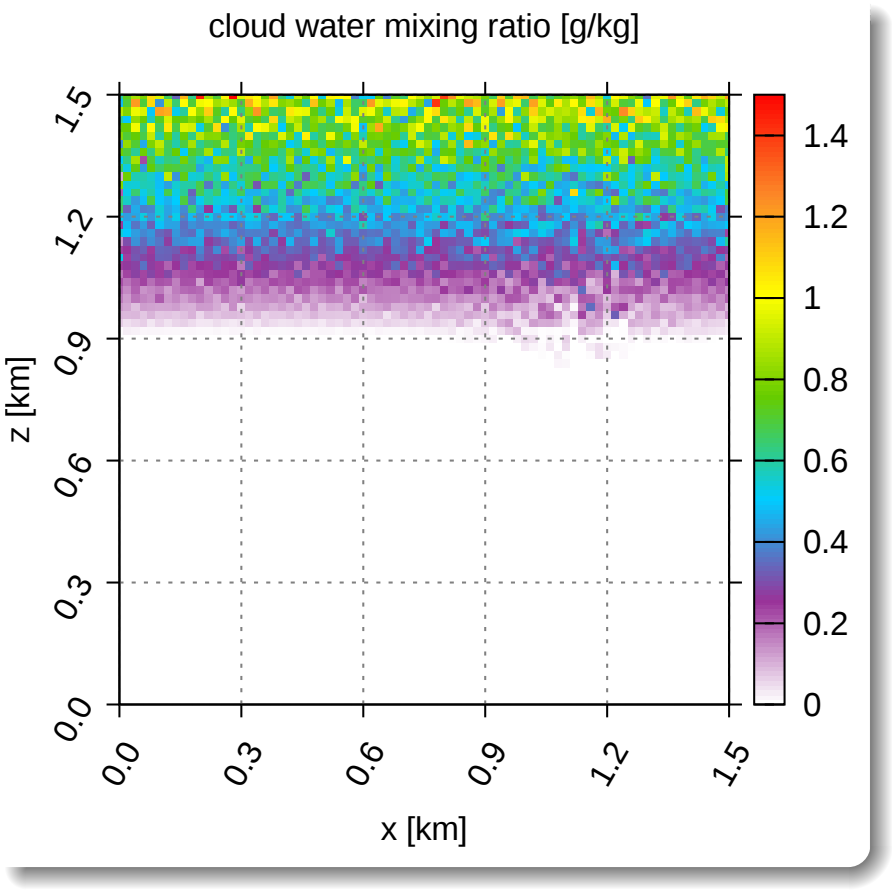

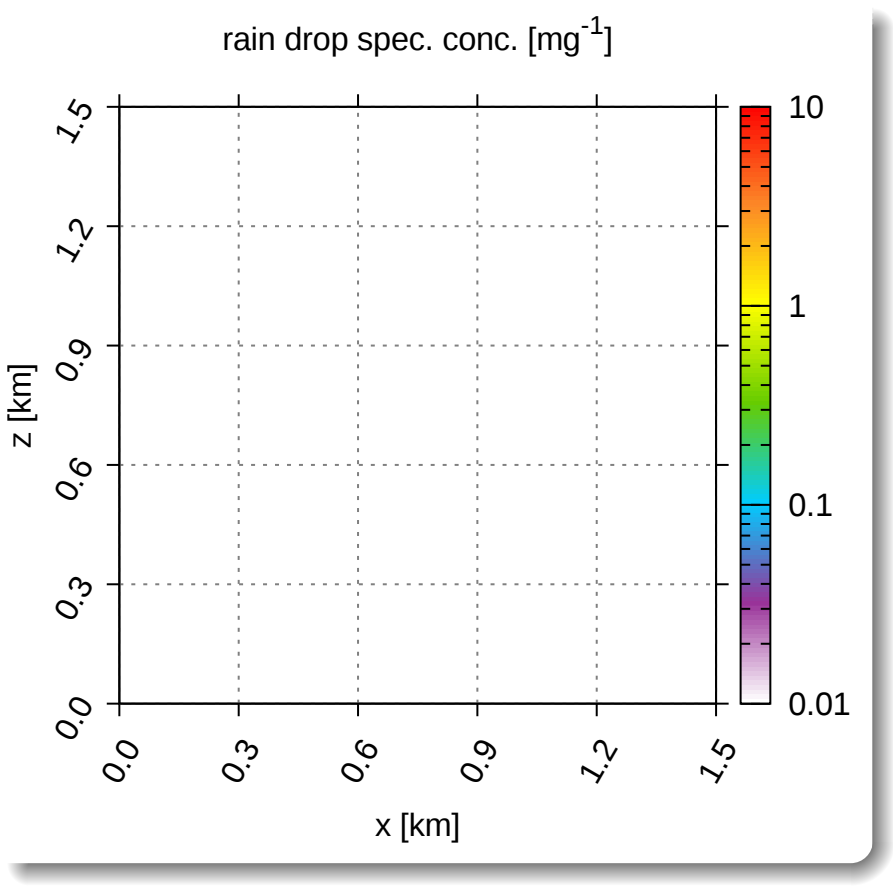

libcloudph++: example 2D prescribed-flow simulation
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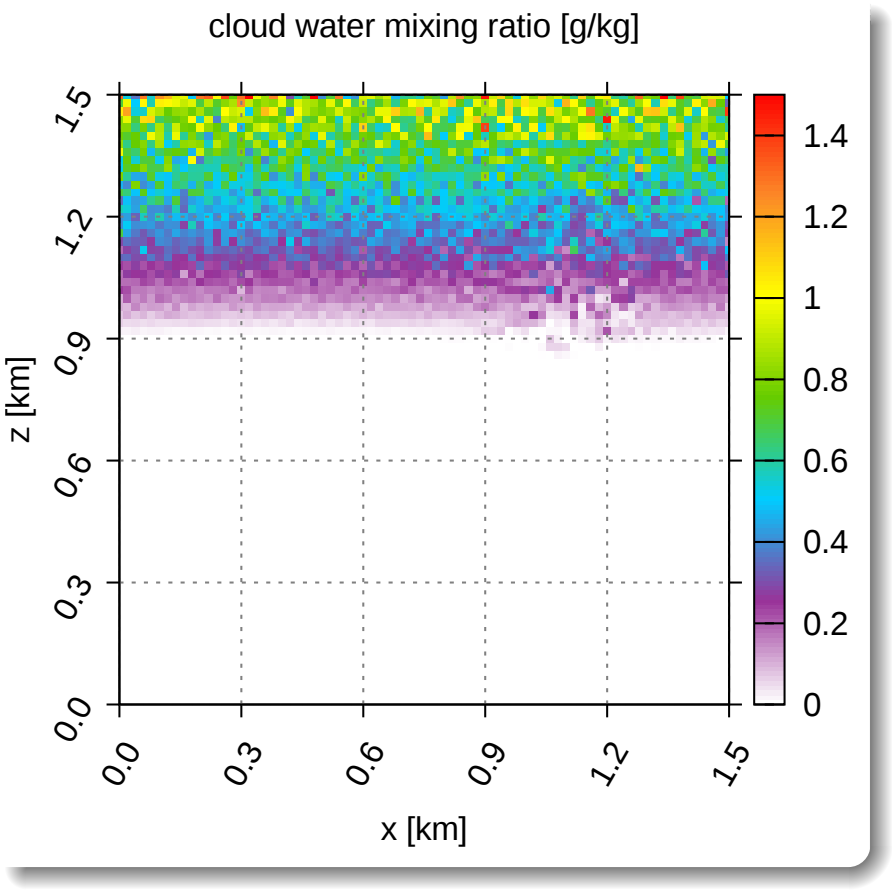

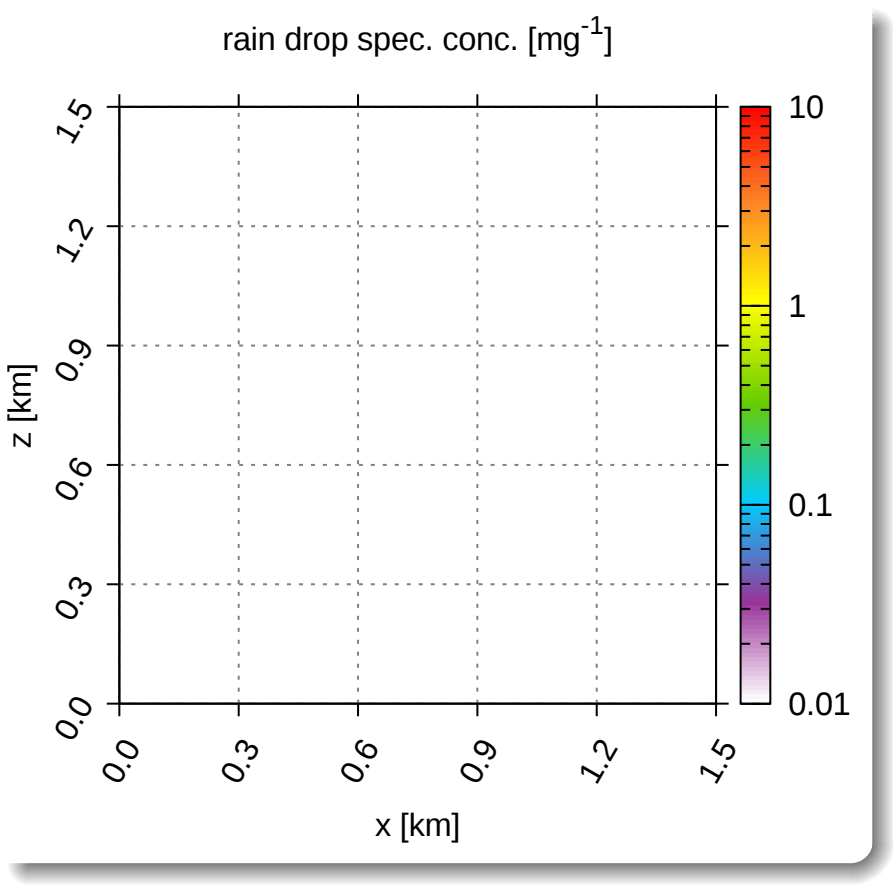

libcloudph++: example 2D prescribed-flow simulation
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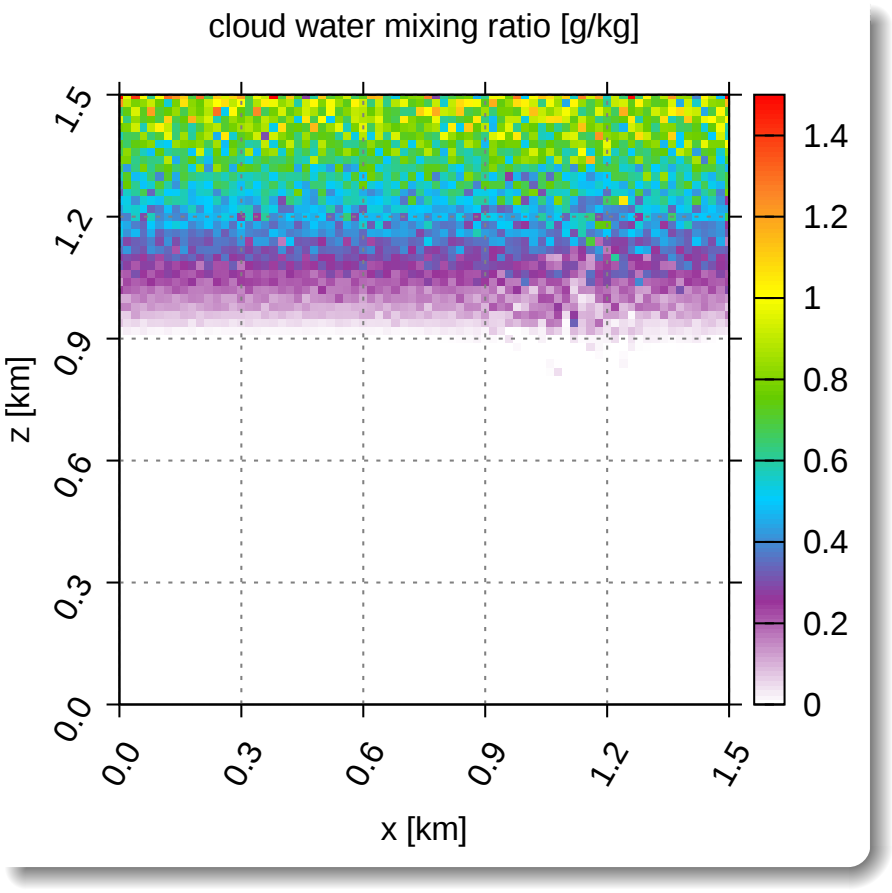

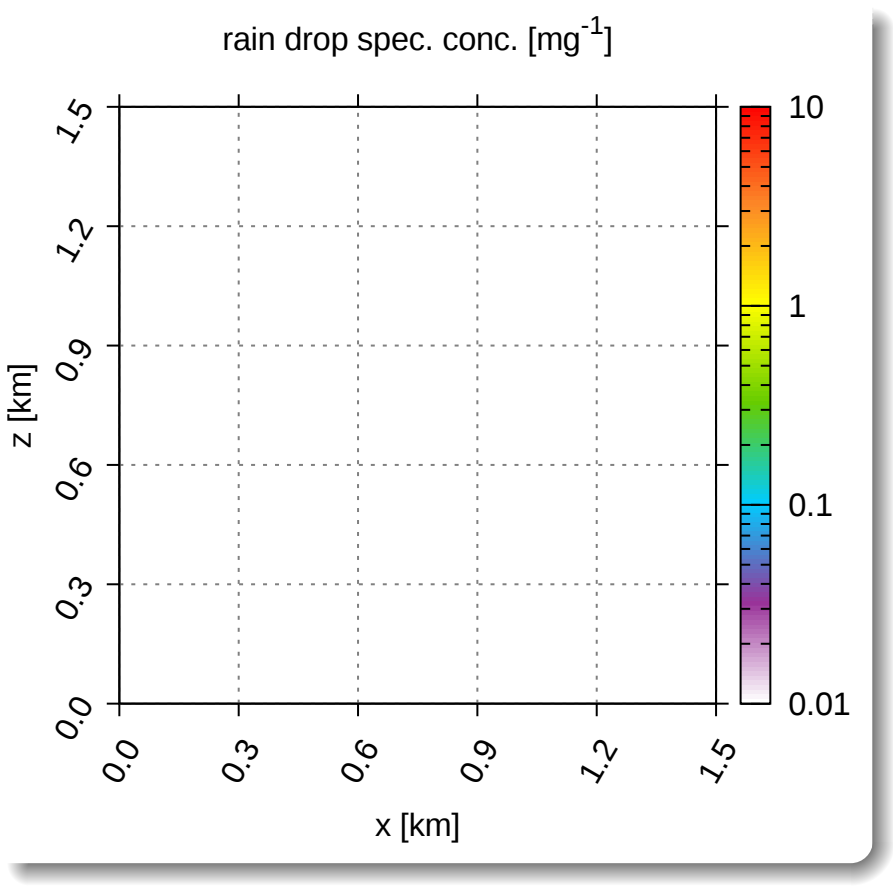

libcloudph++: example 2D prescribed-flow simulation

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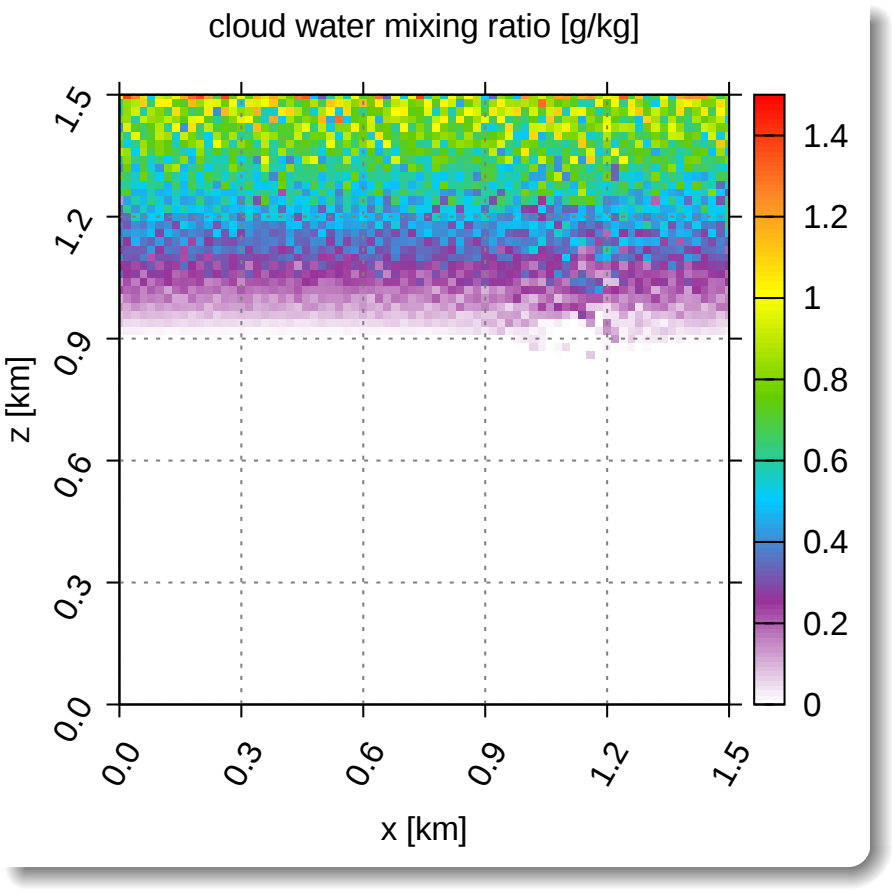

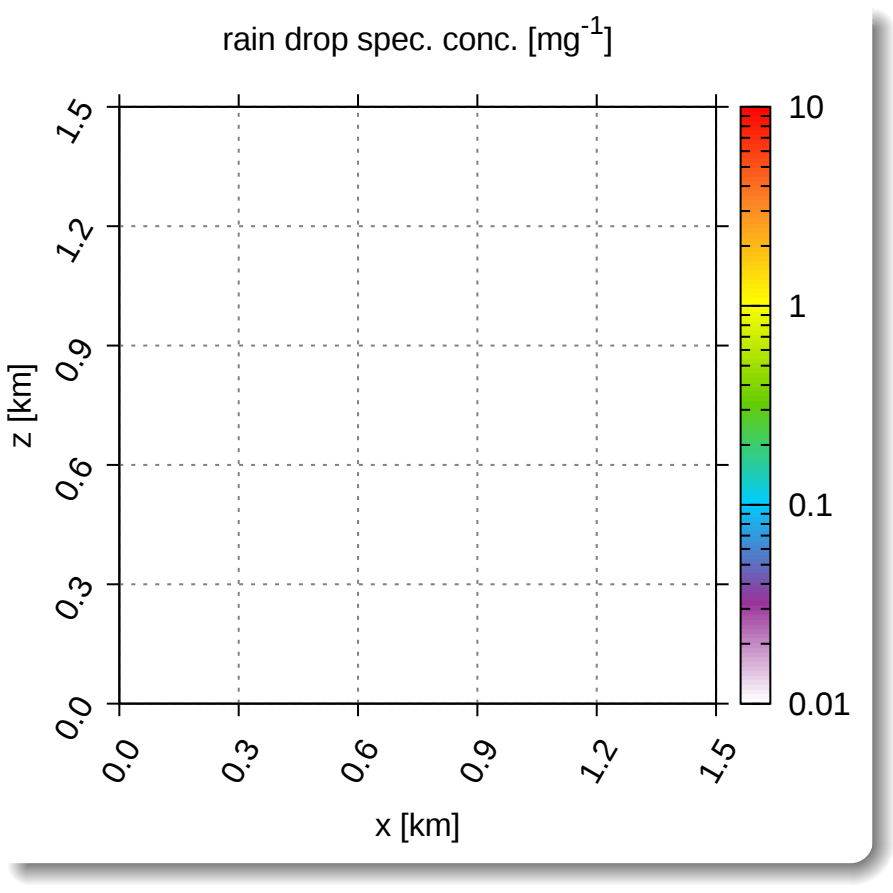

libcloudph++: example 2D prescribed-flow simulation

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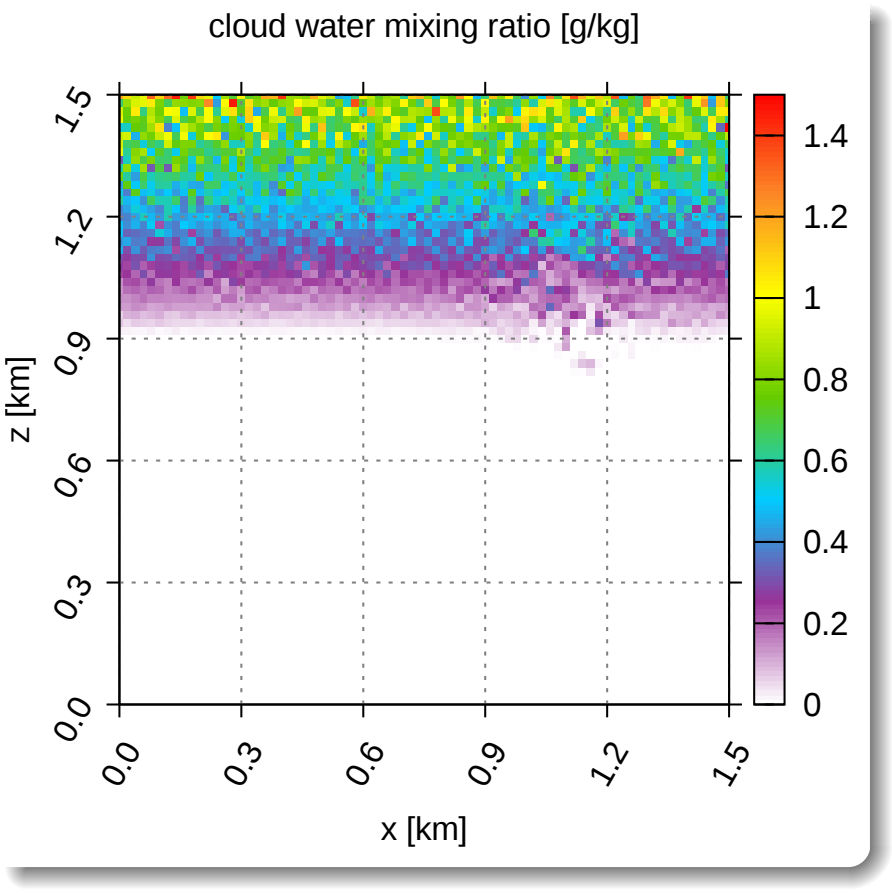

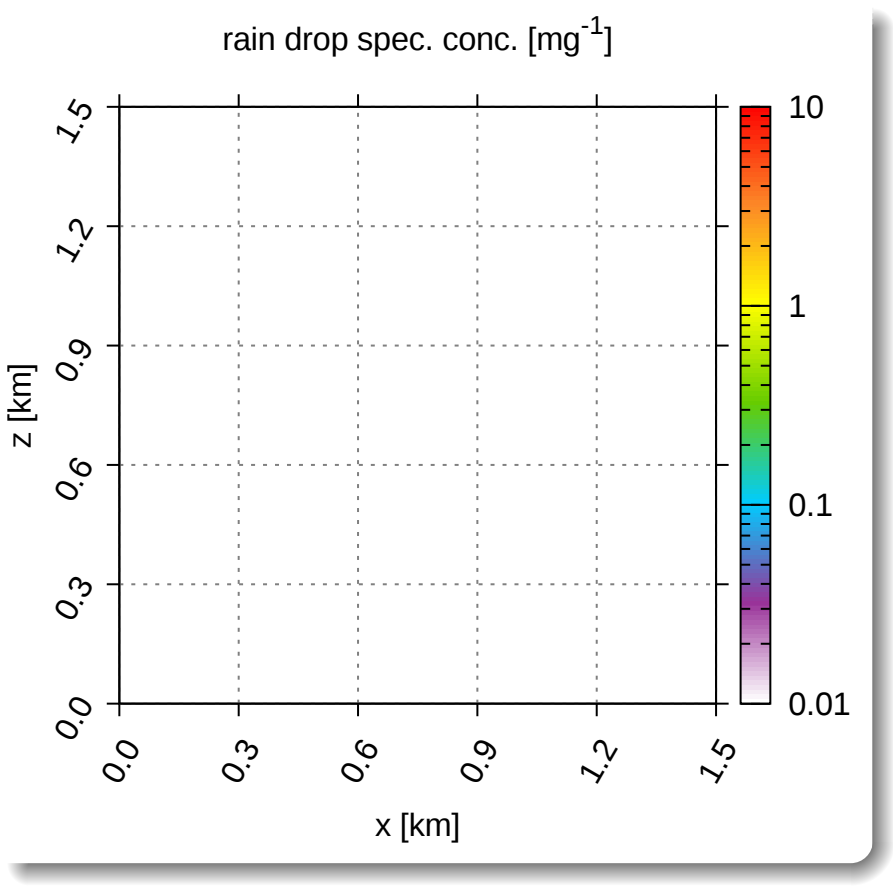

libcloudph++: example 2D prescribed-flow simulation

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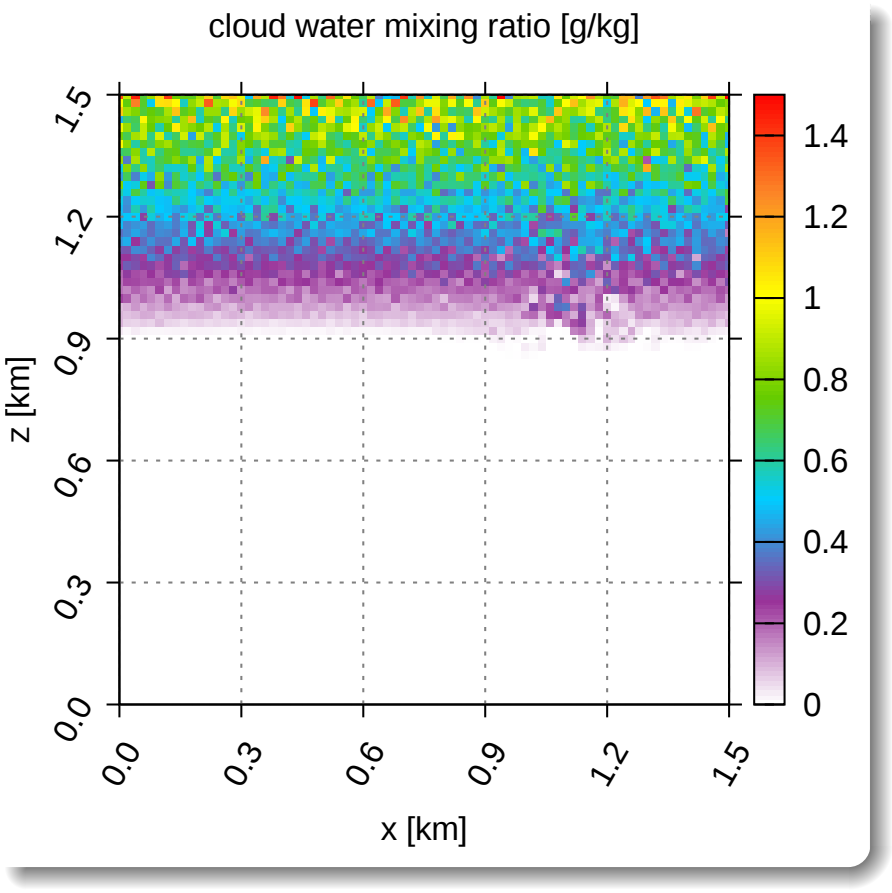

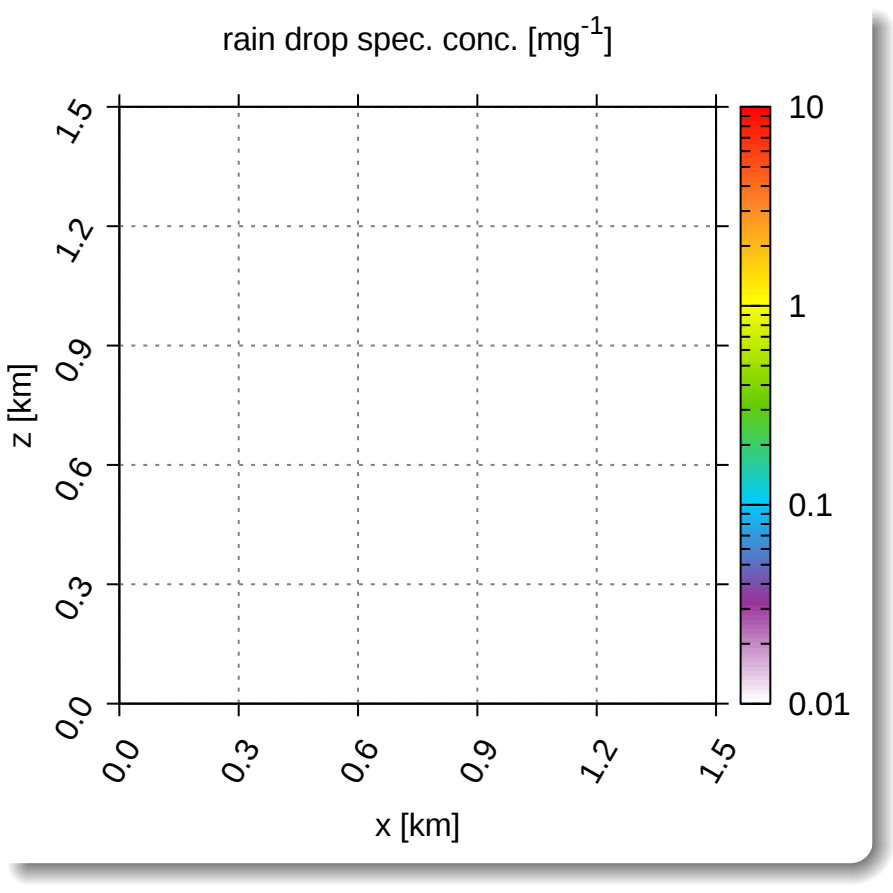

libcloudph++: example 2D prescribed-flow simulation

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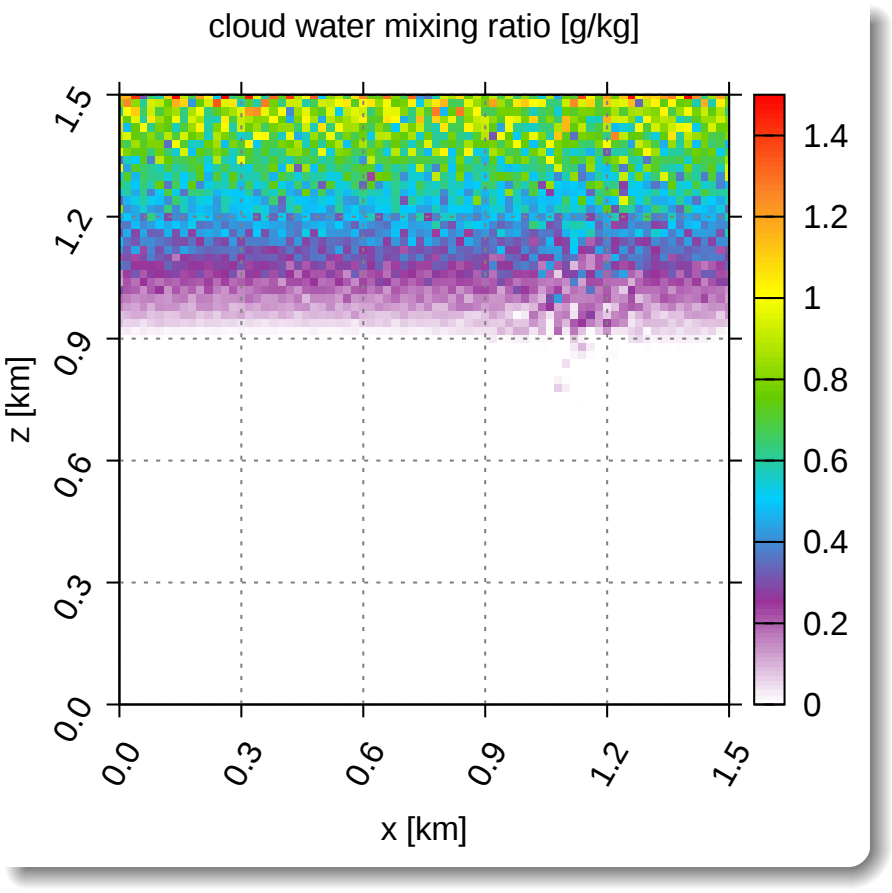

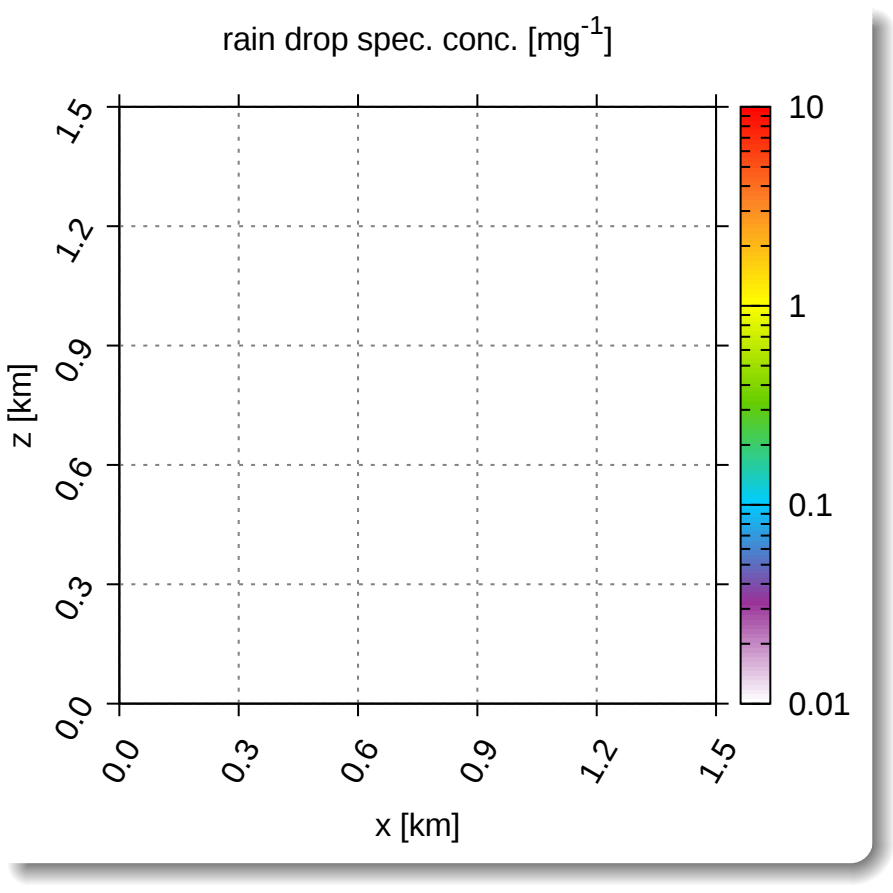

libcloudph++: example 2D prescribed-flow simulation
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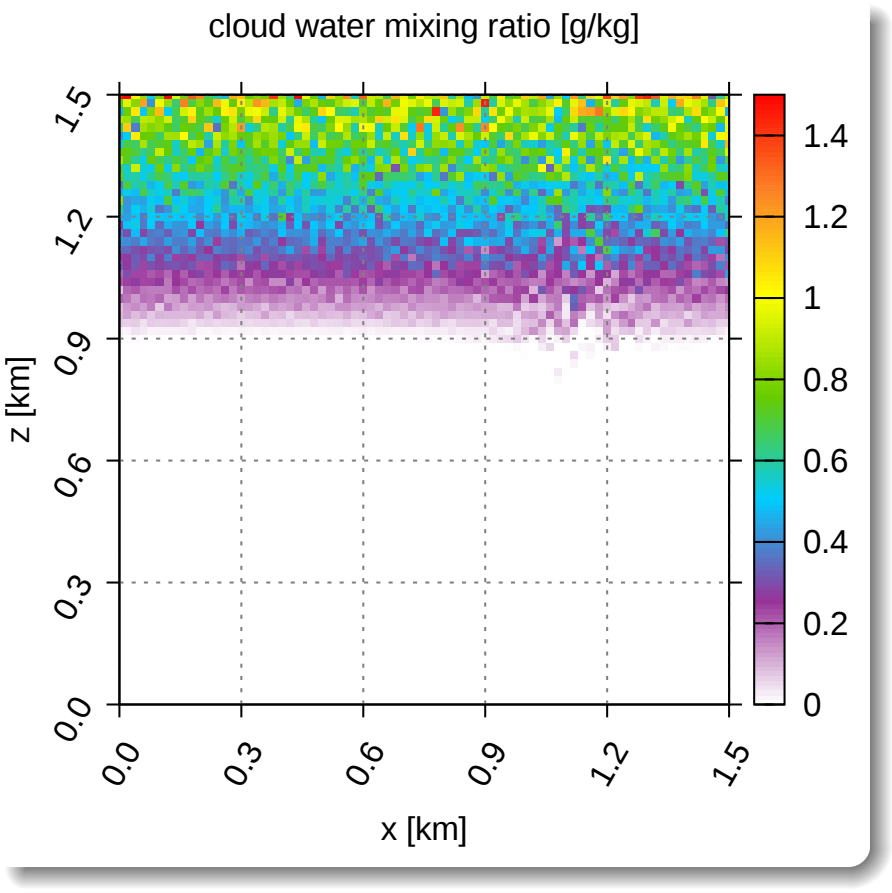

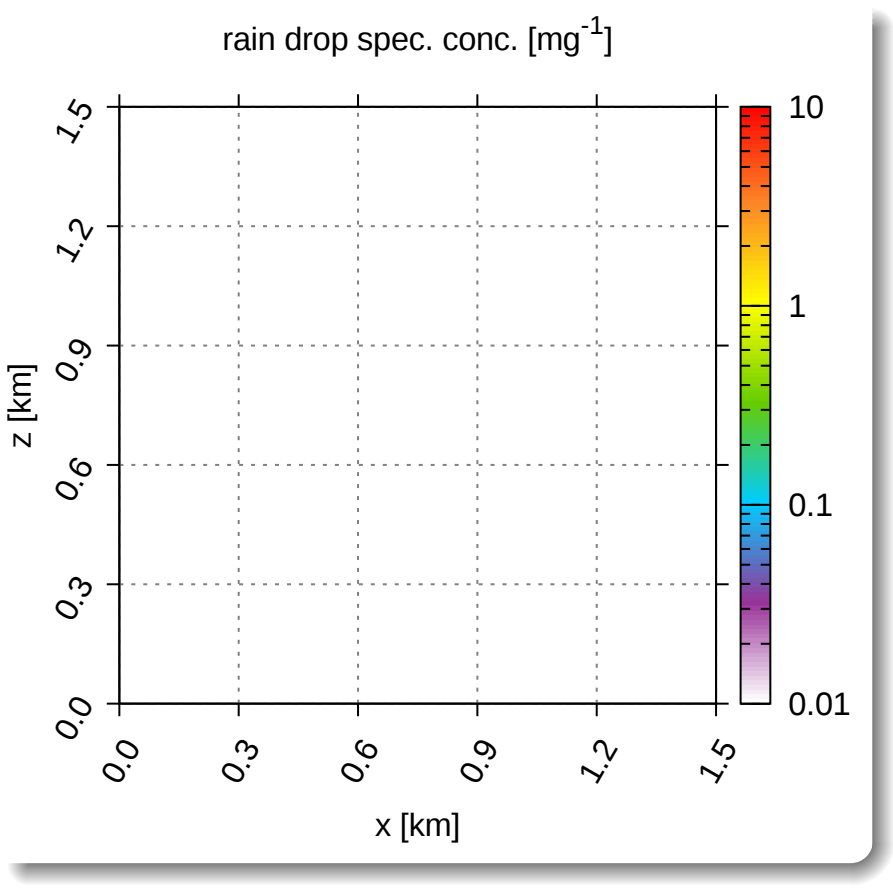

libcloudph++: example 2D prescribed-flow simulation
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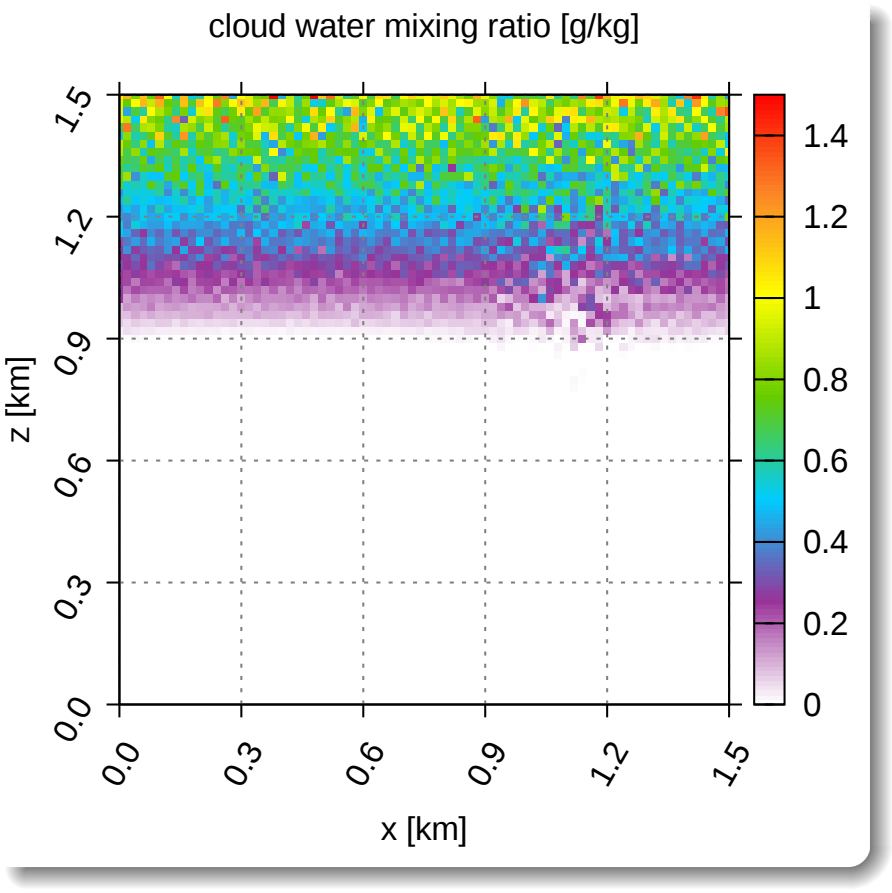

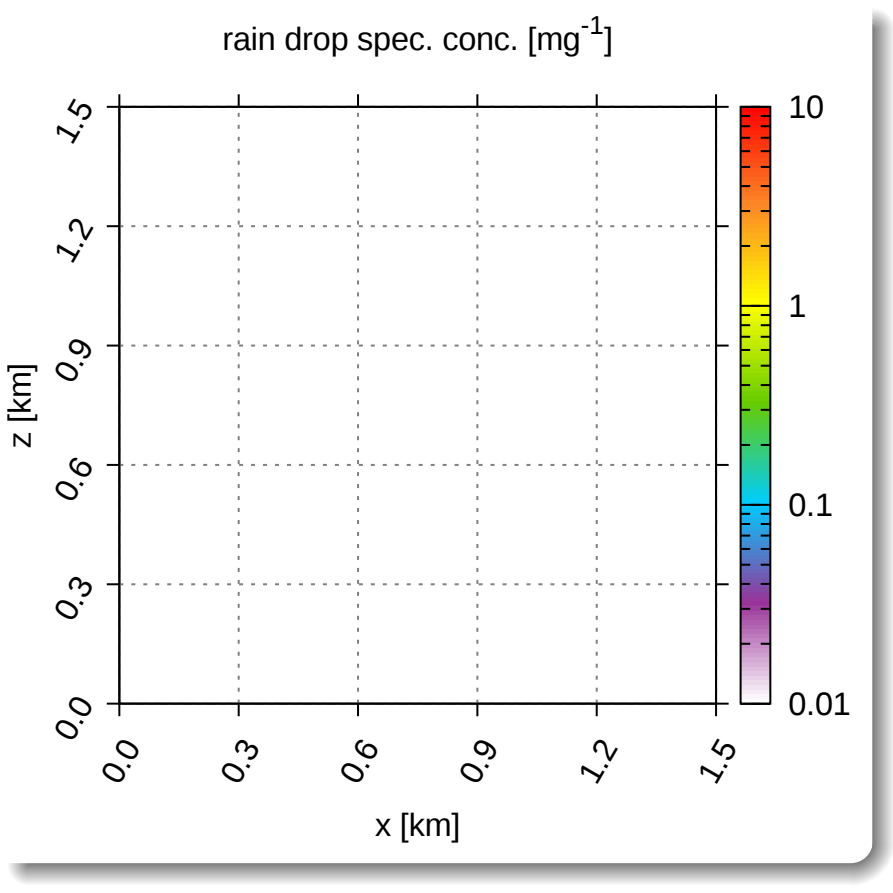

libcloudph++: example 2D prescribed-flow simulation

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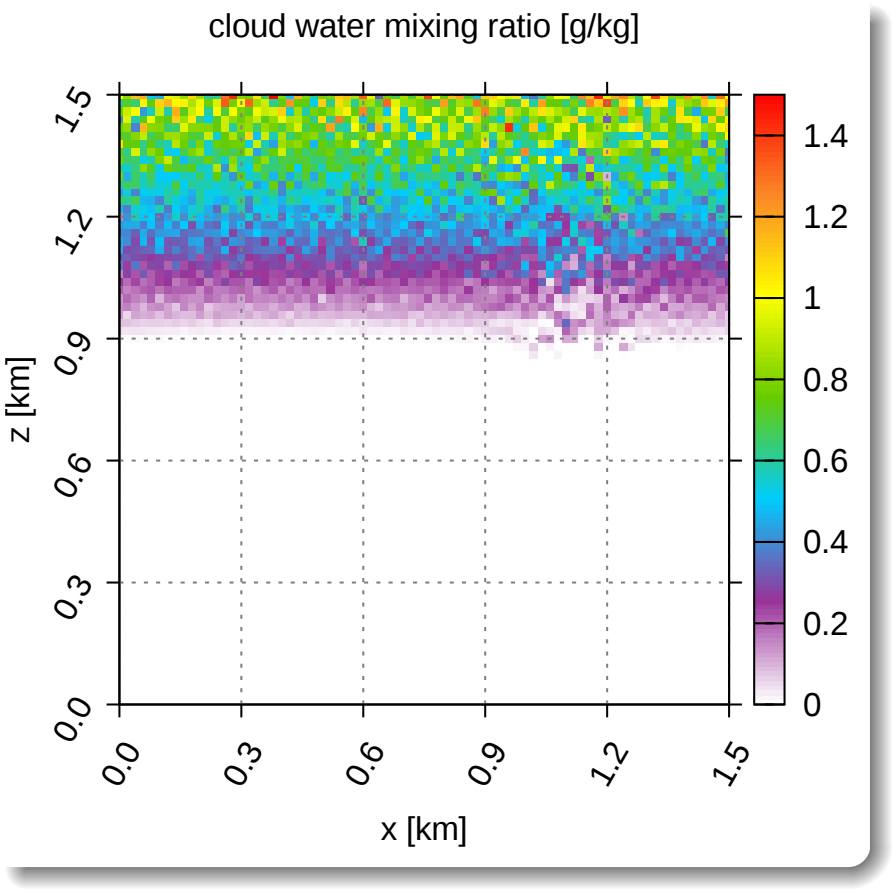
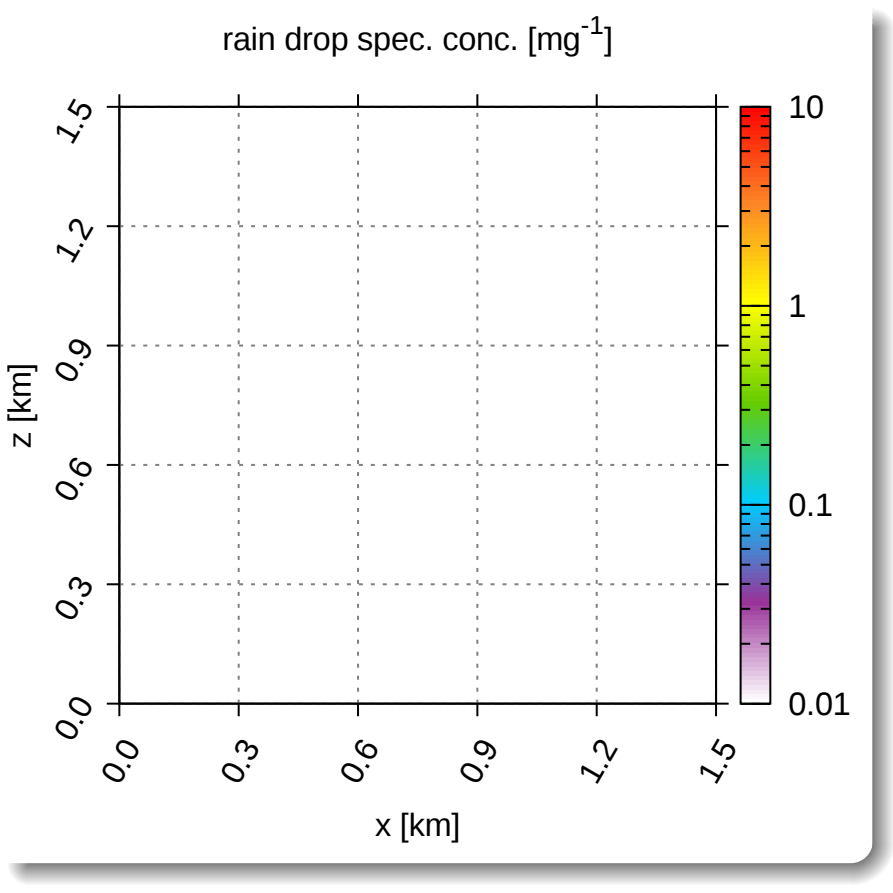
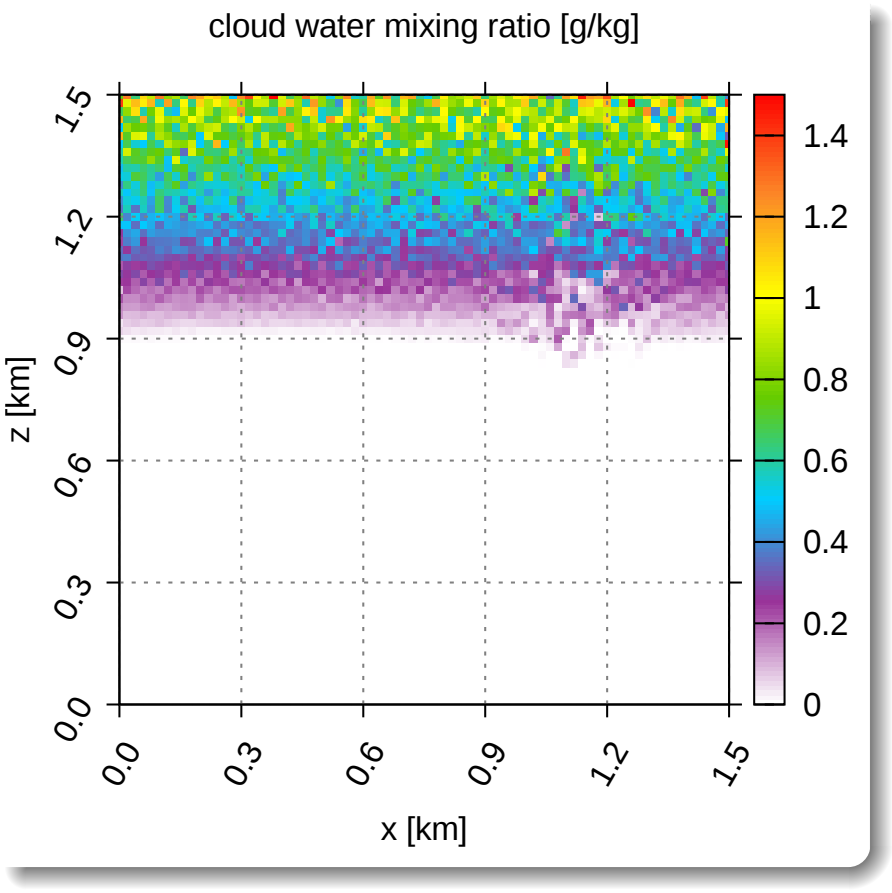
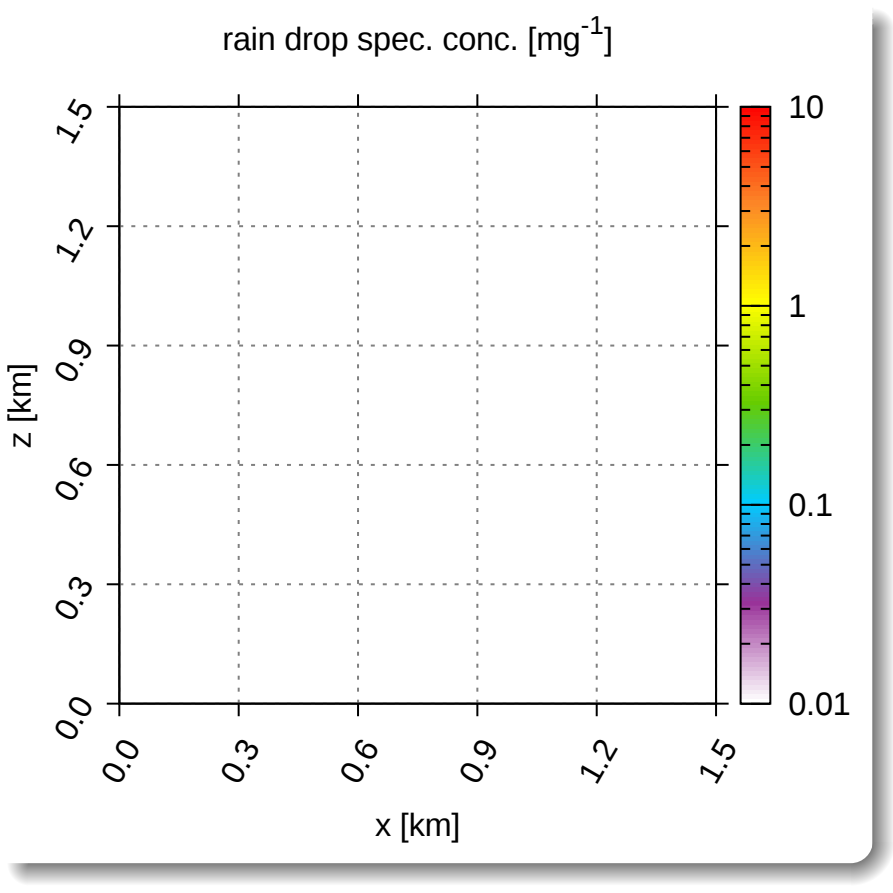




libcloudph++: example 2D prescribed-flow simulation





libcloudph++: example 2D prescribed-flow simulation
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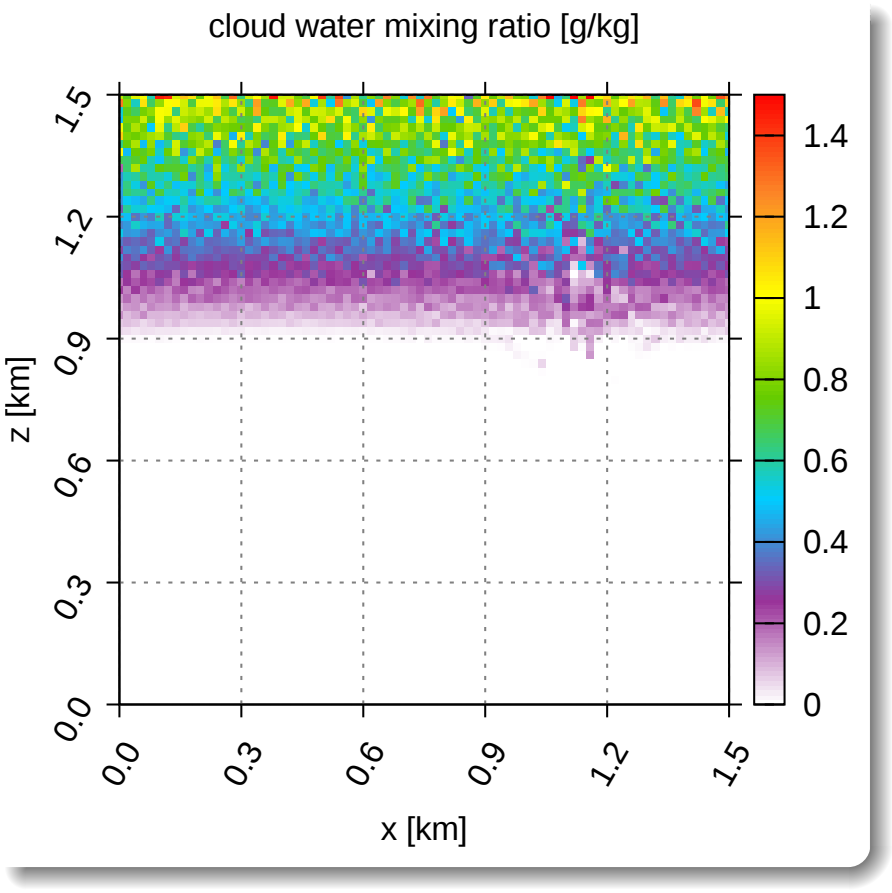

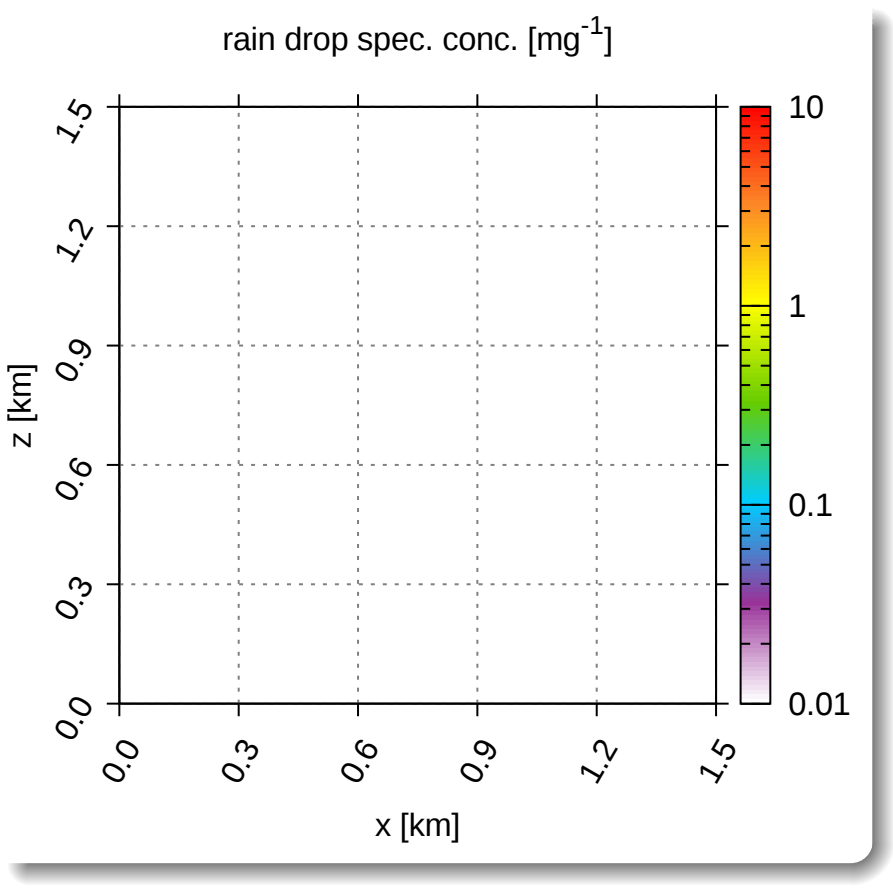

libcloudph++: example 2D prescribed-flow simulation

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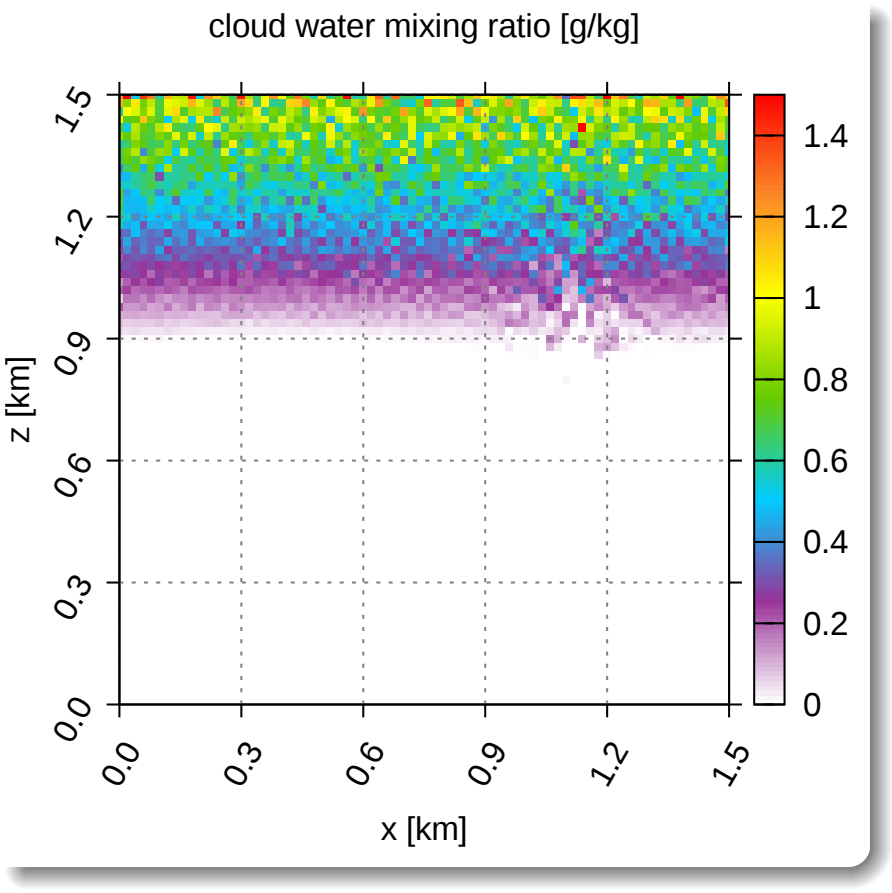

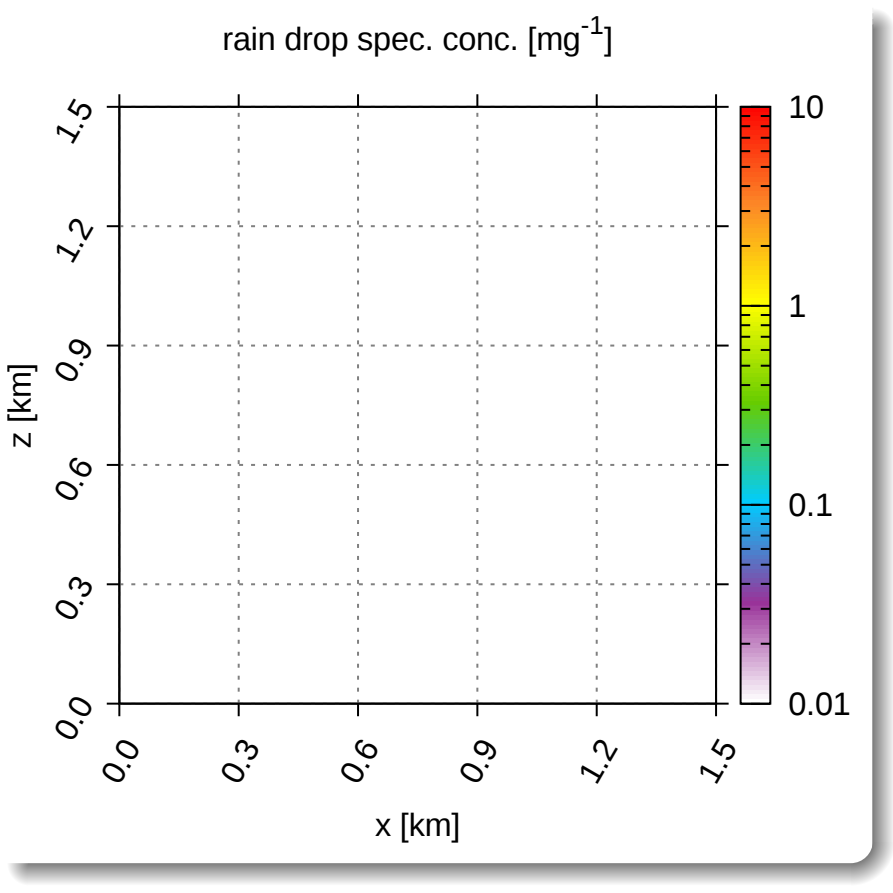

libcloudph++: example 2D prescribed-flow simulation

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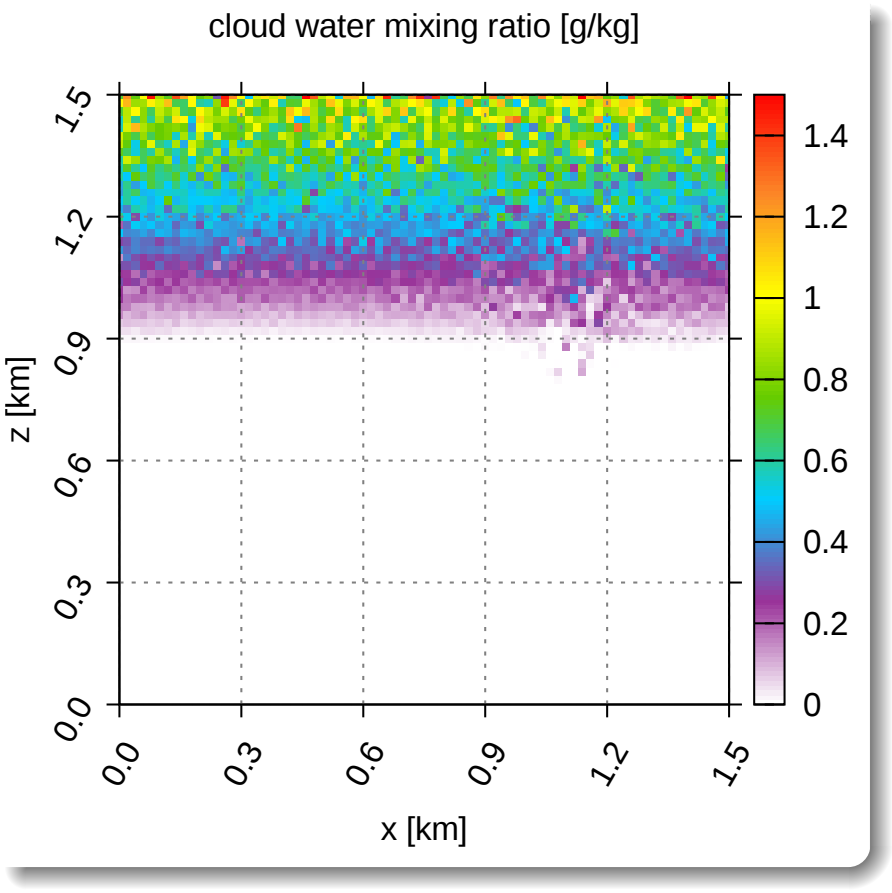

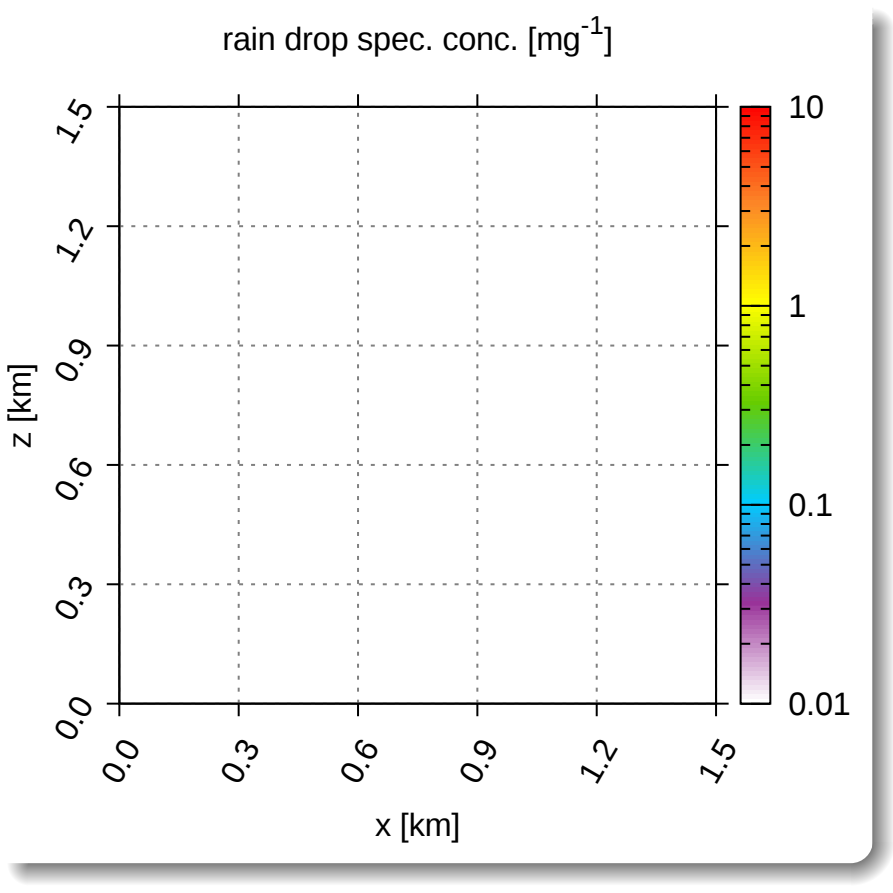

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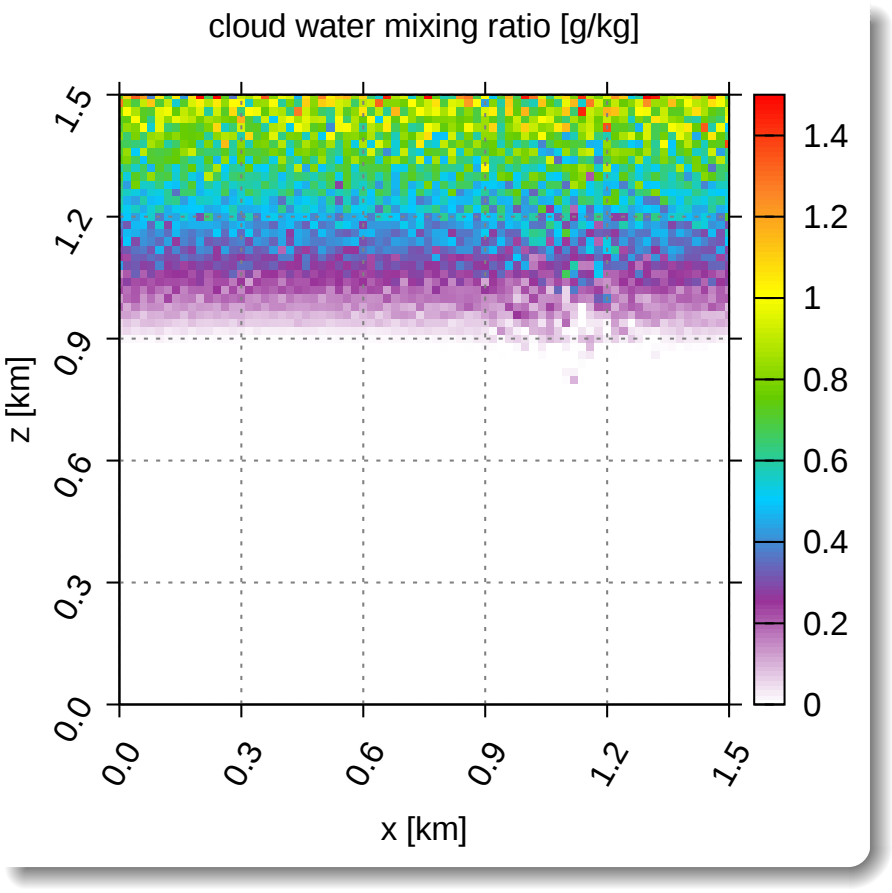

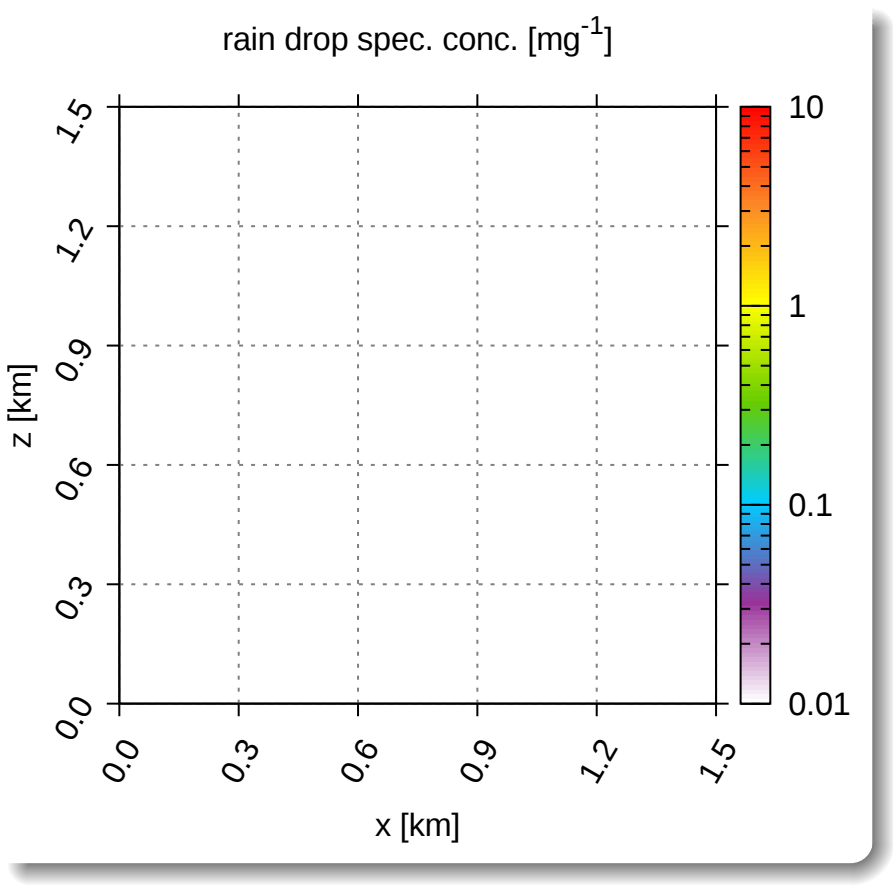

libcloudph++: example 2D prescribed-flow simulation

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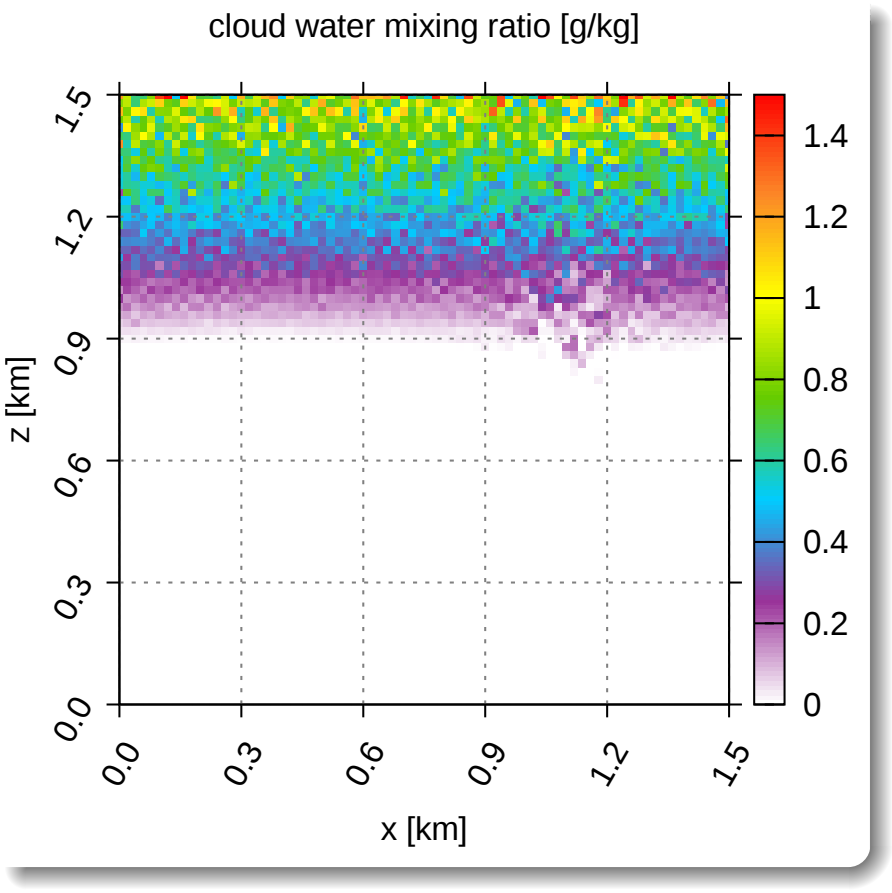

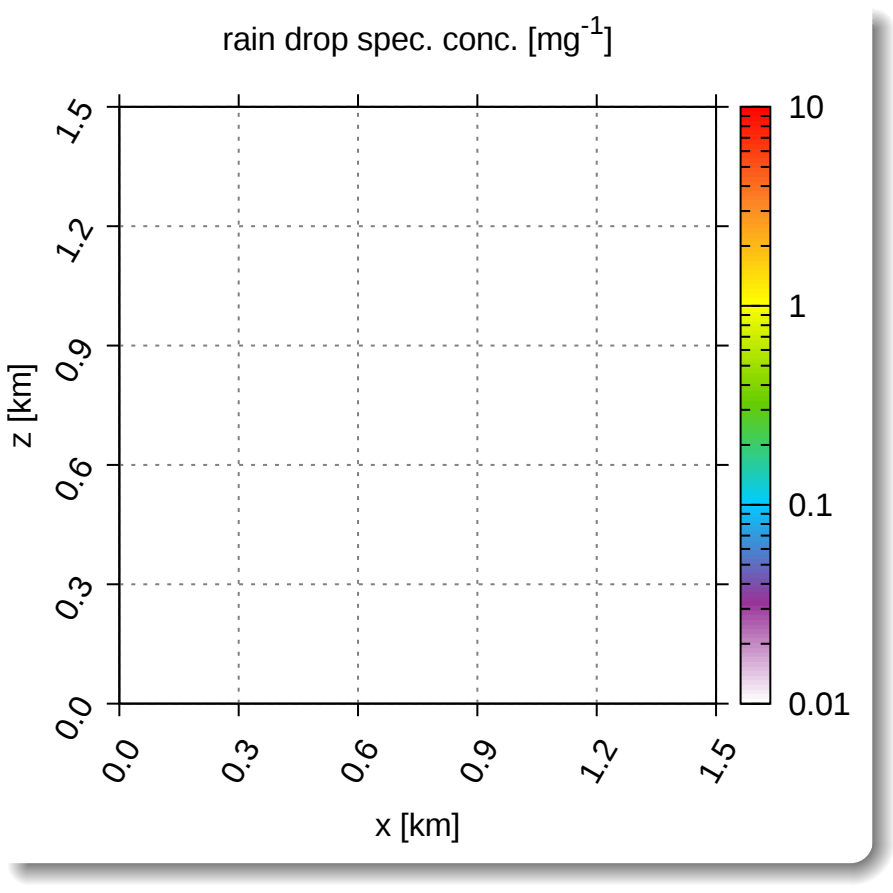

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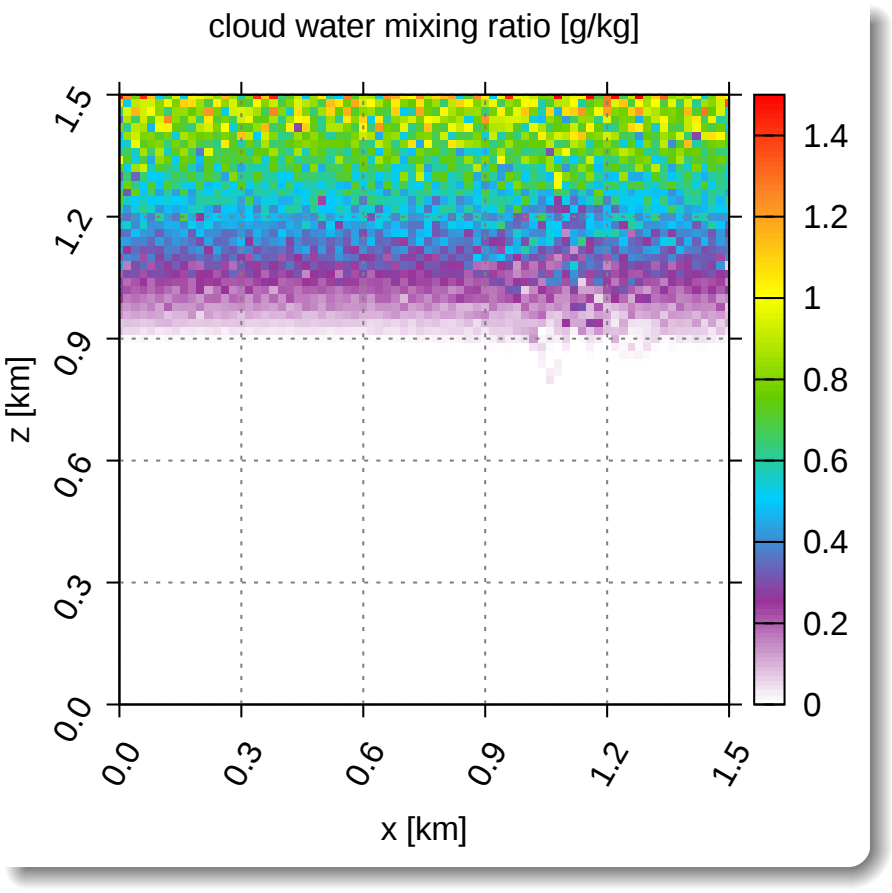

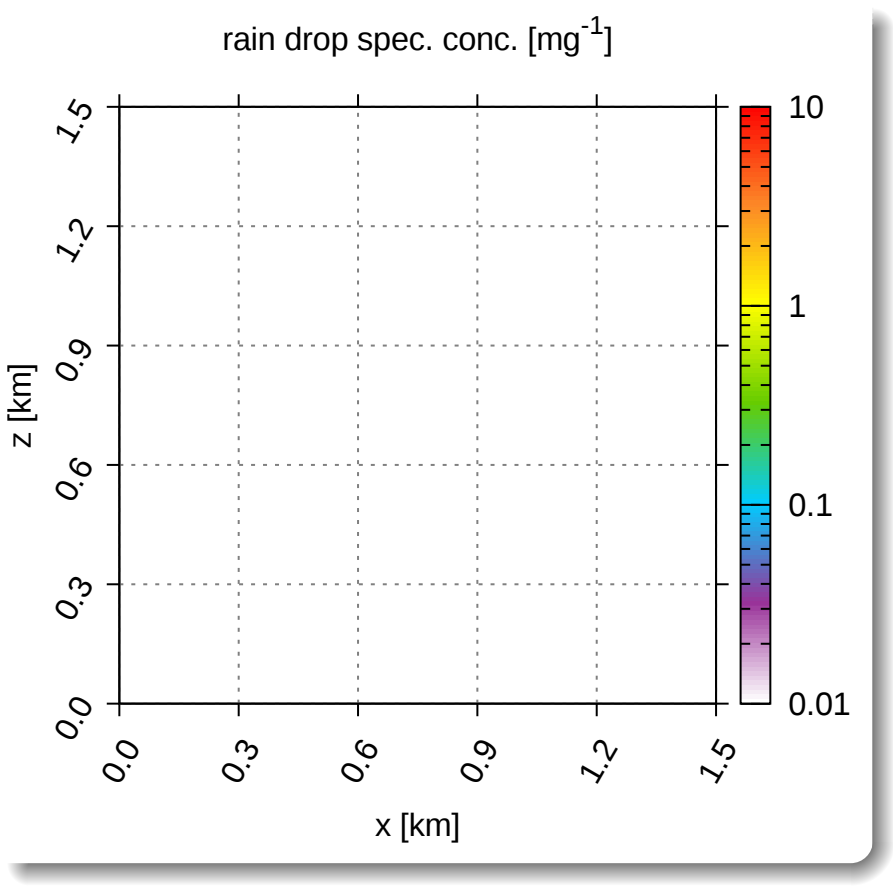

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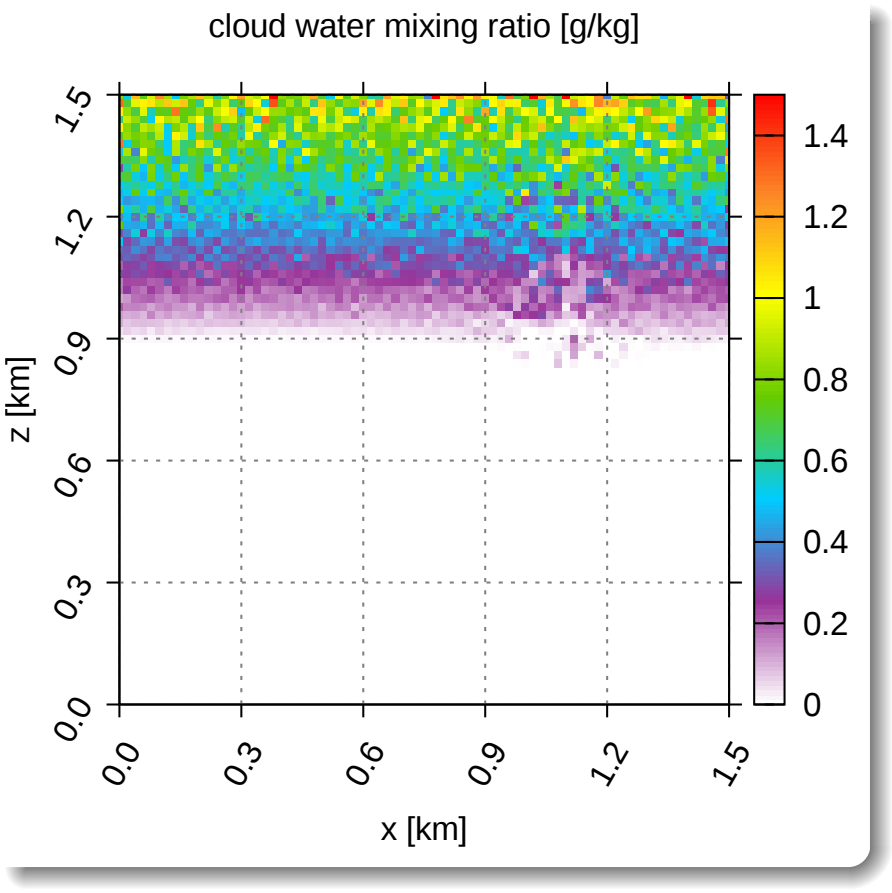

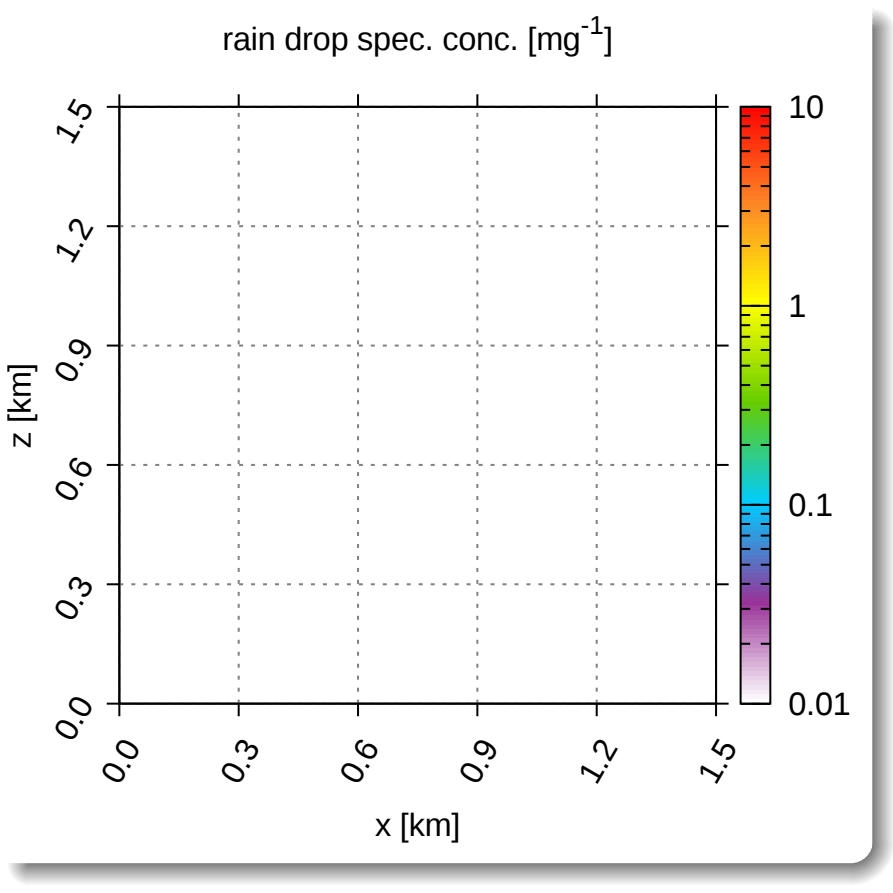

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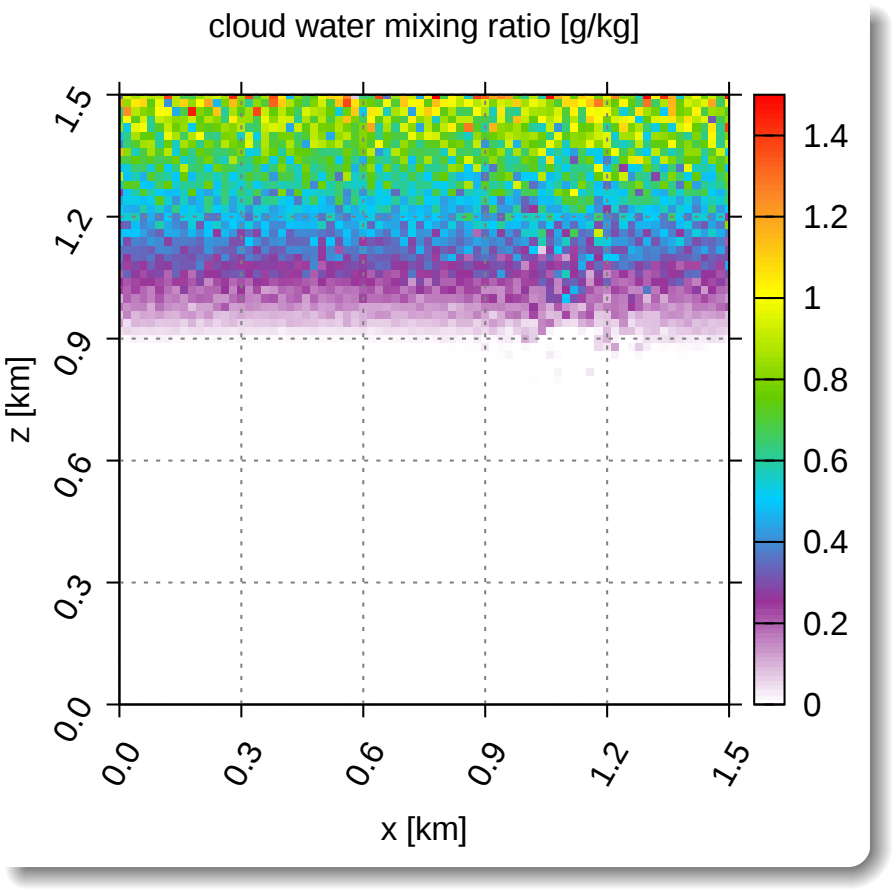

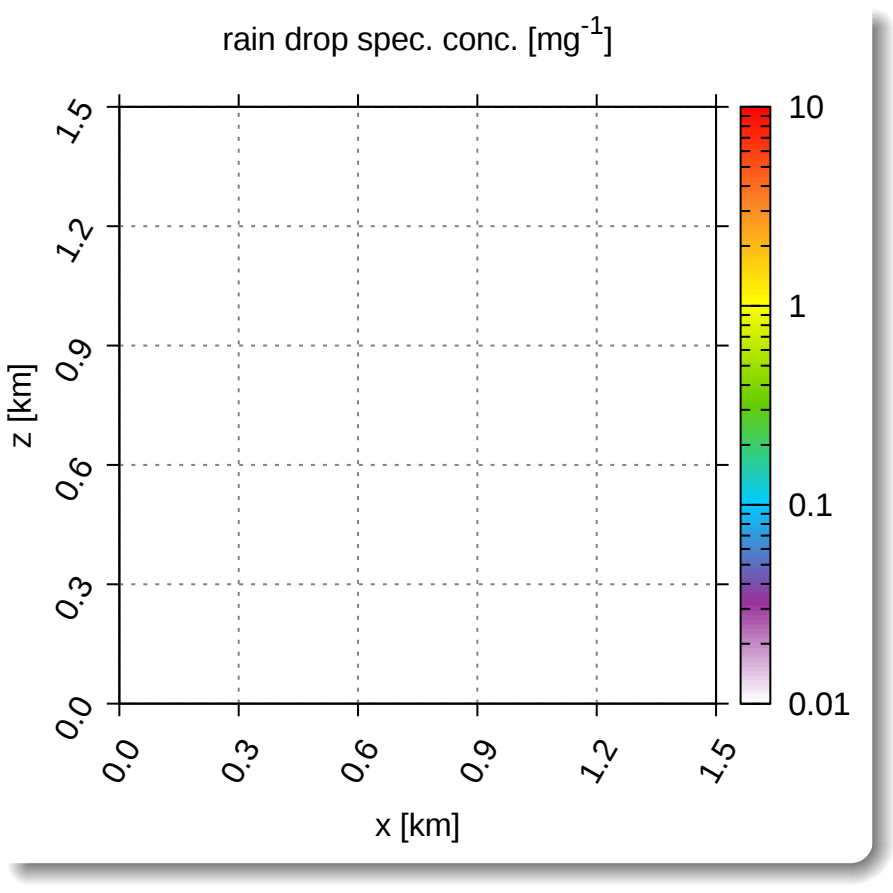

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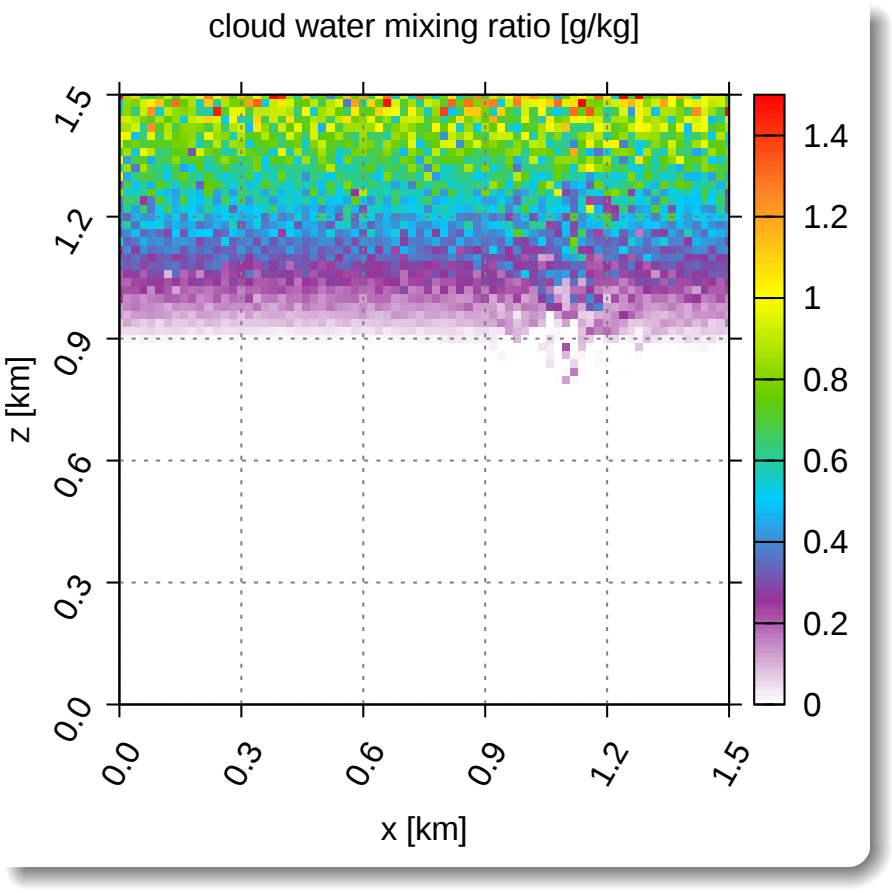

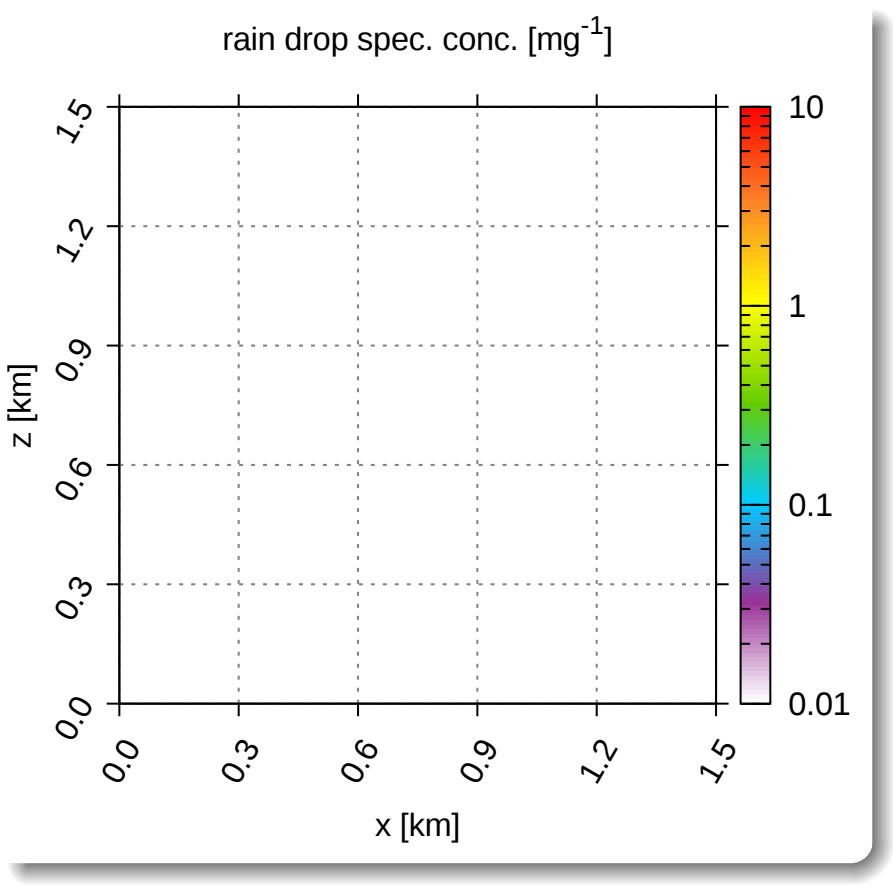

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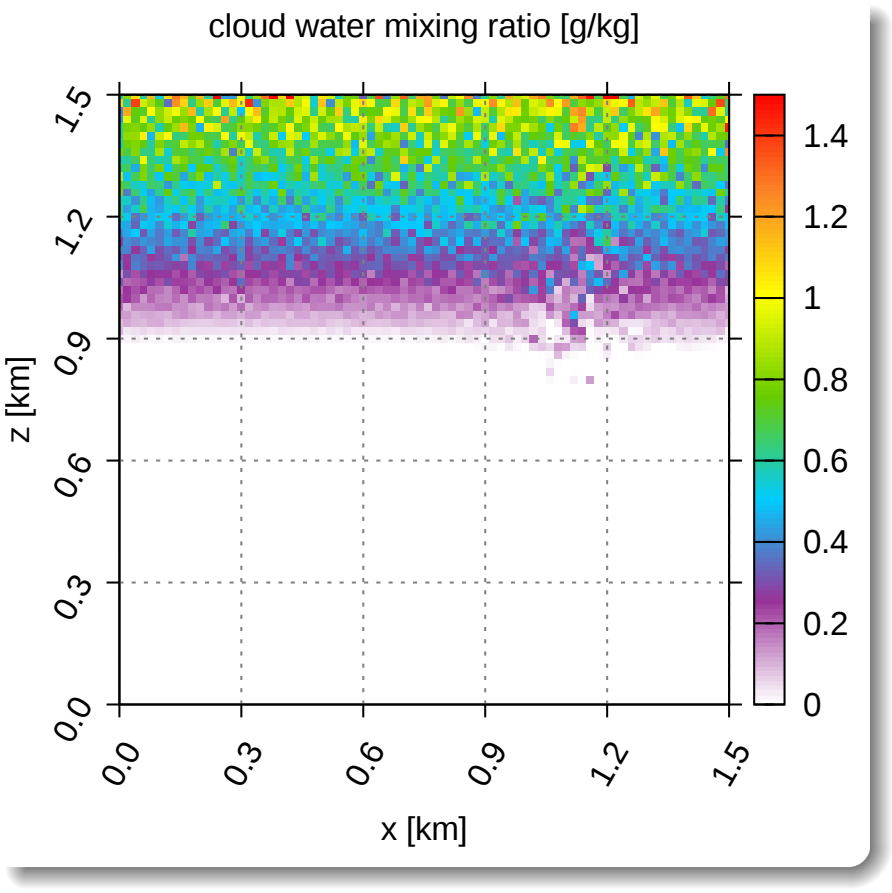

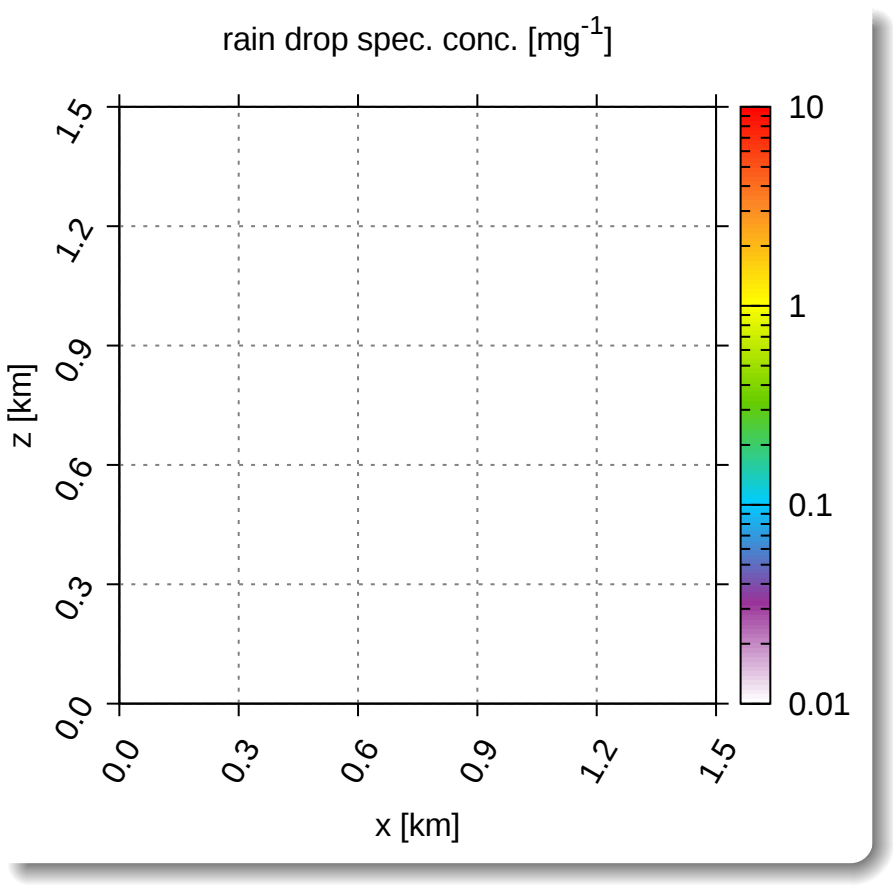

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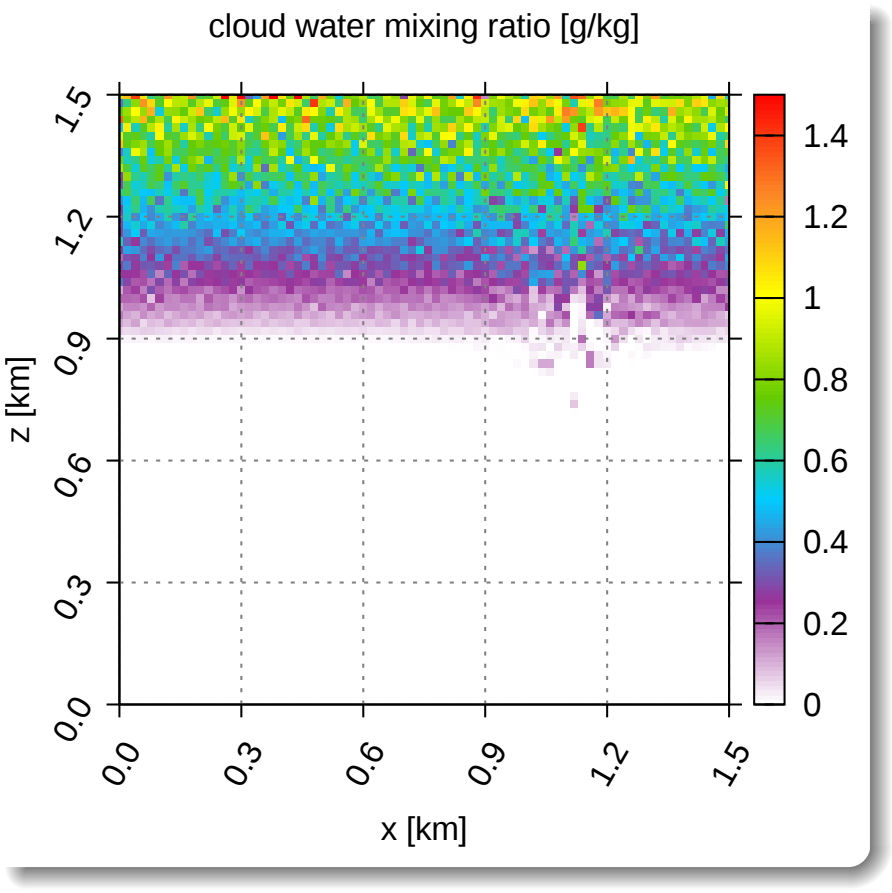

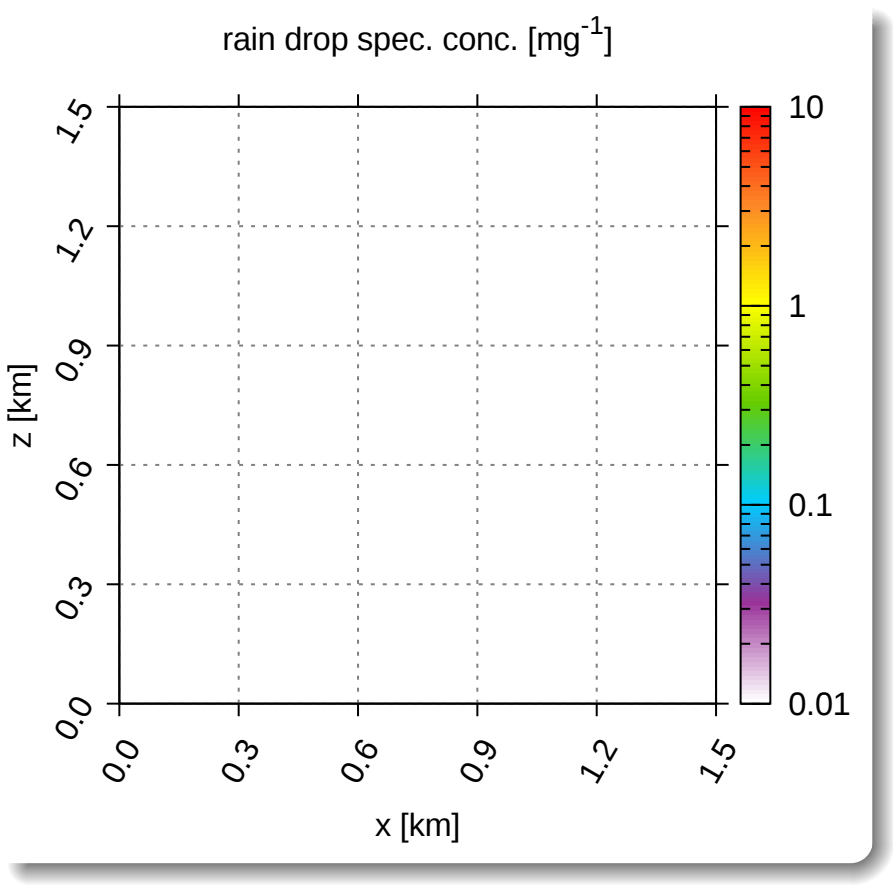

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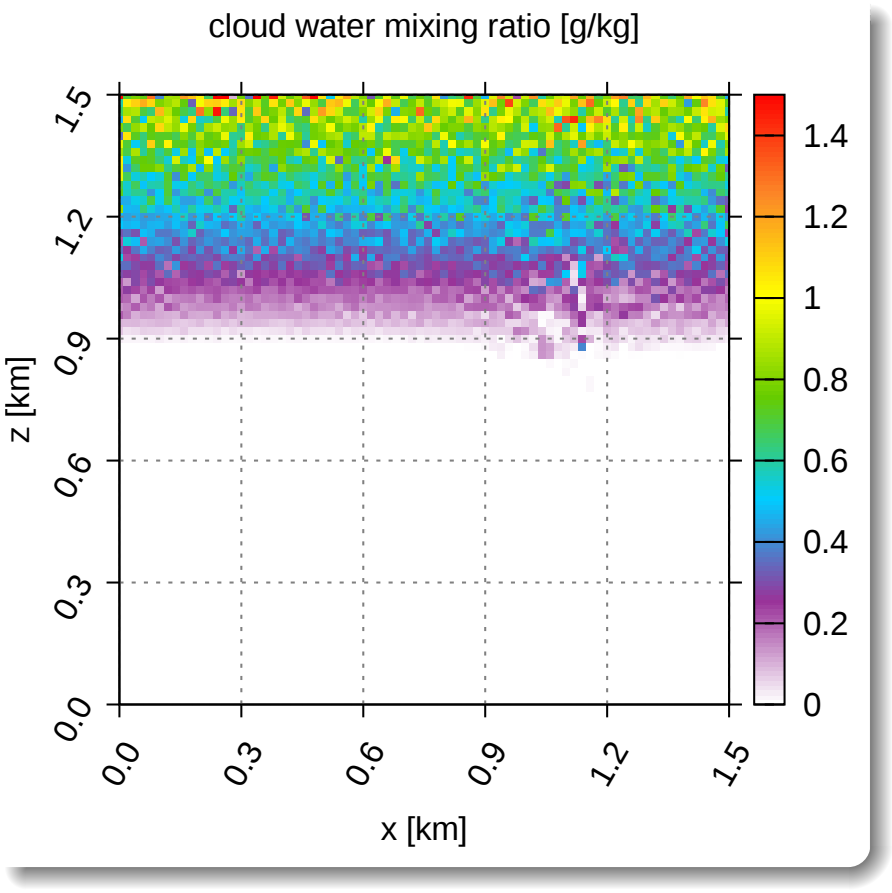

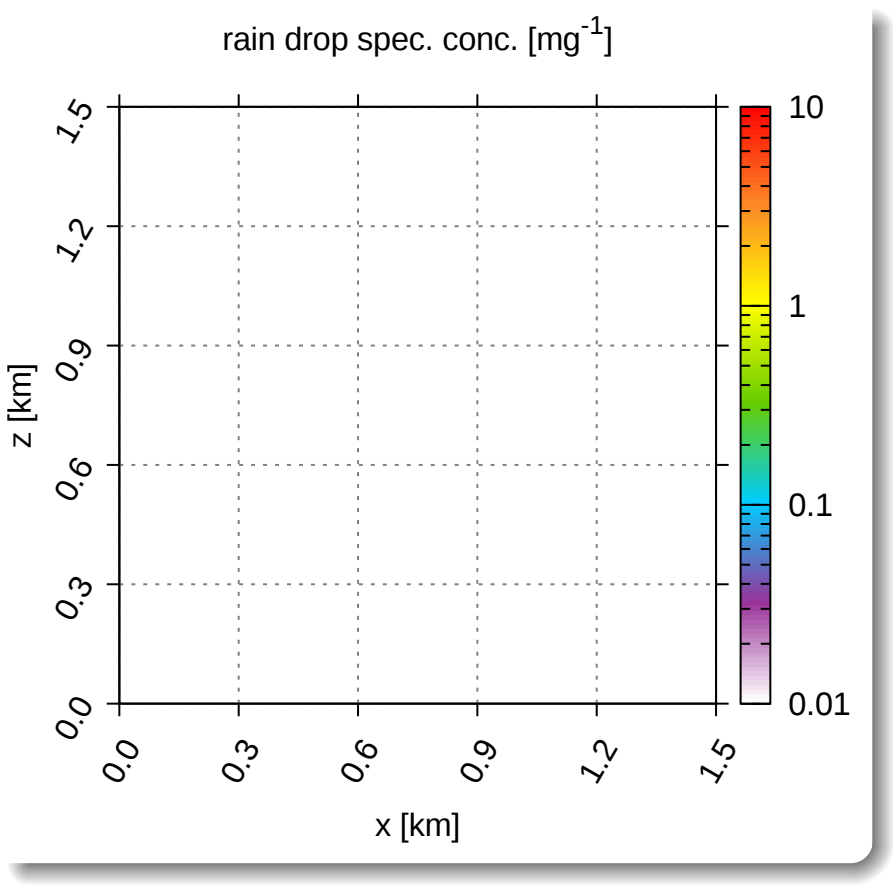

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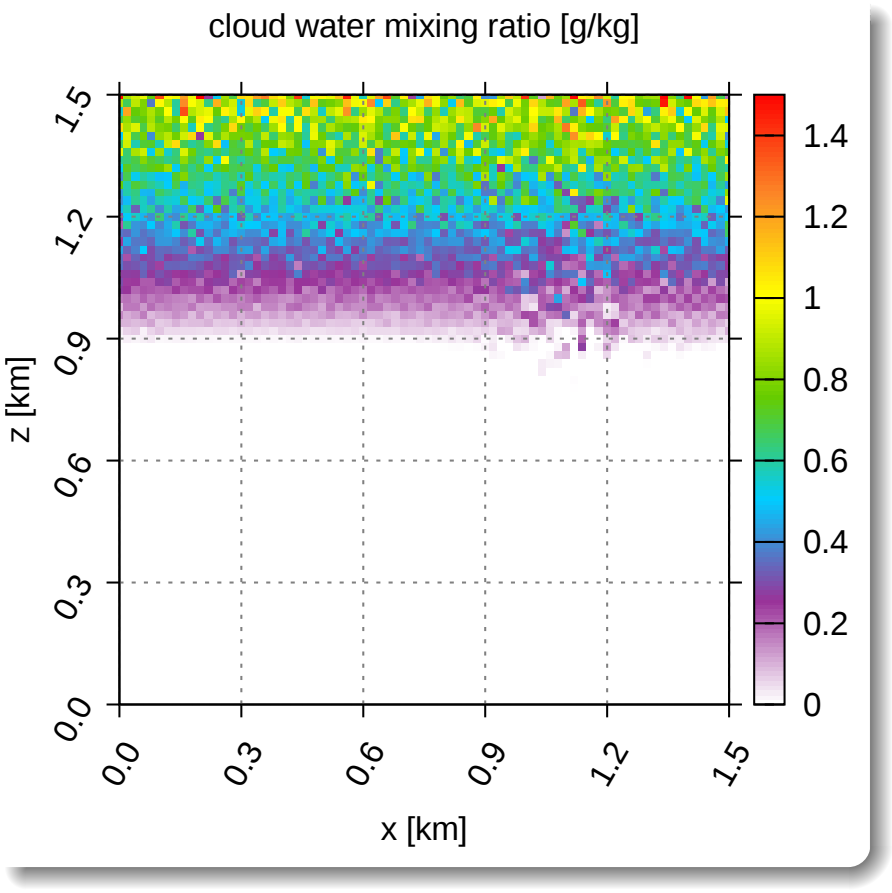

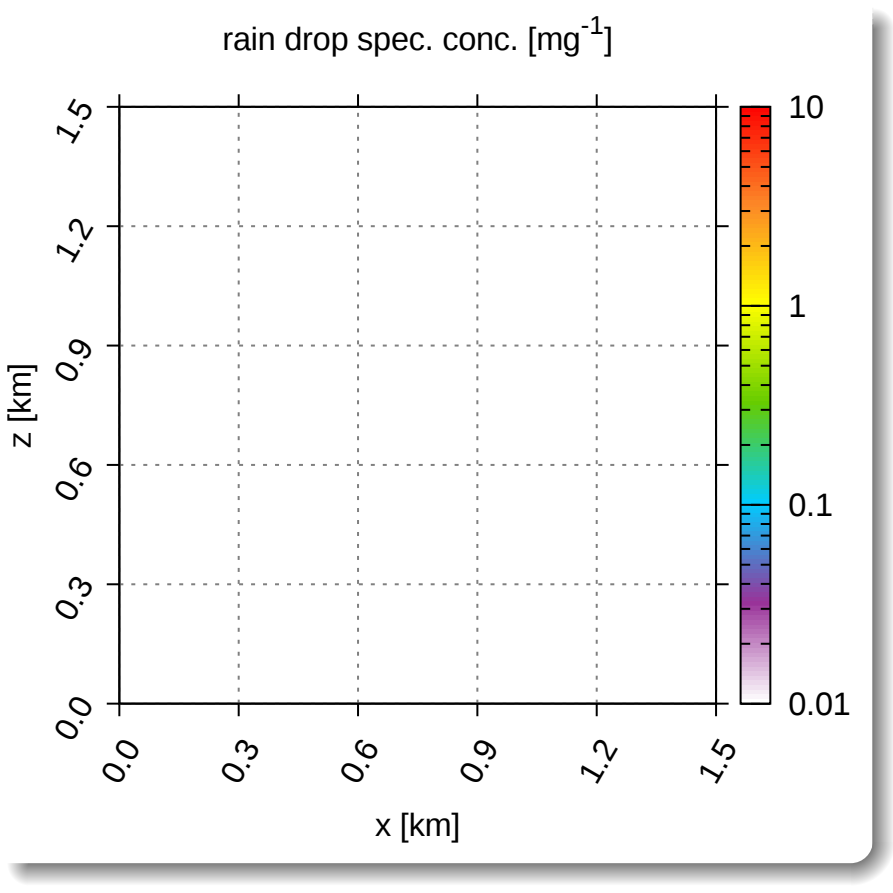

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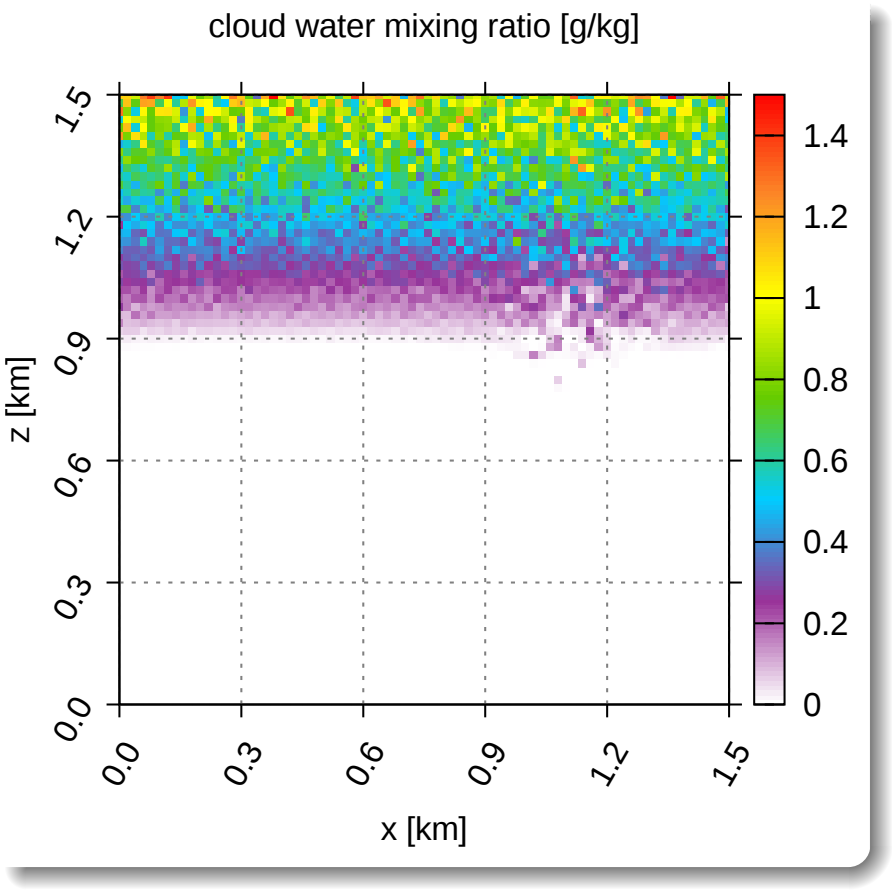

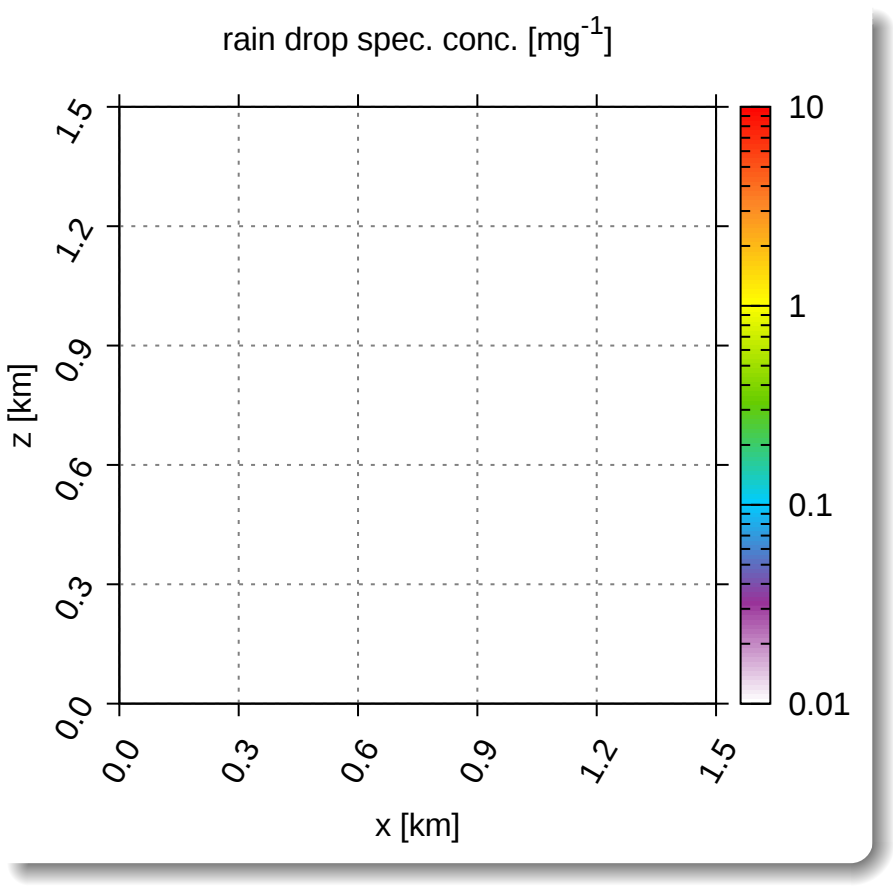

libcloudph++: example 2D prescribed-flow simulation

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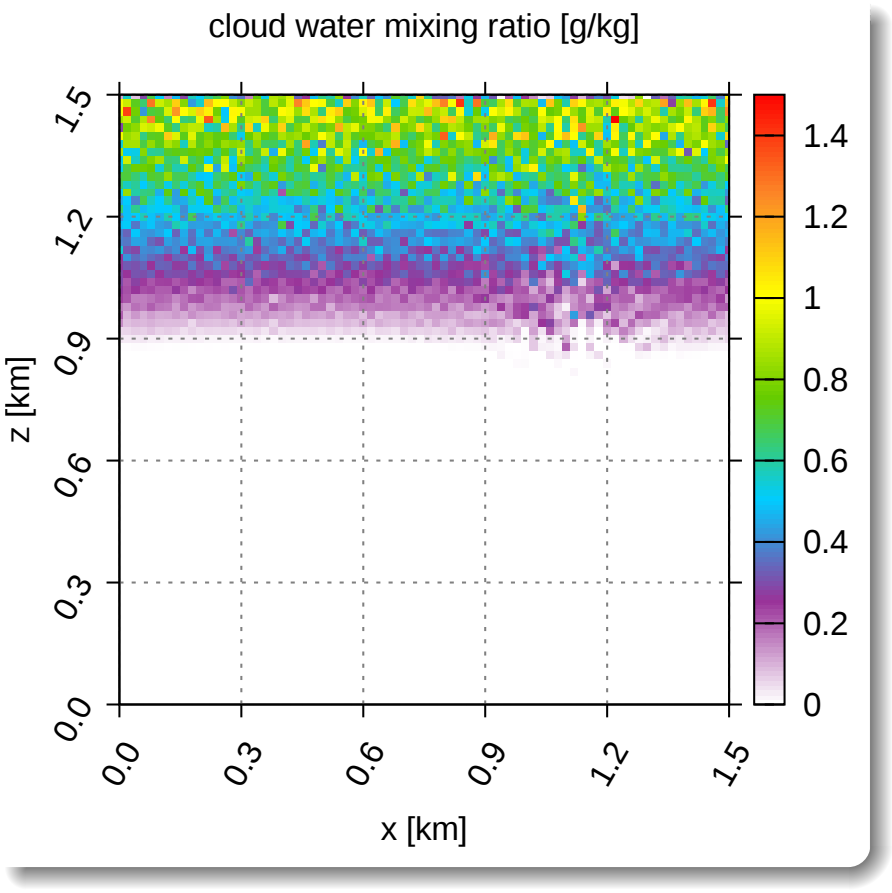
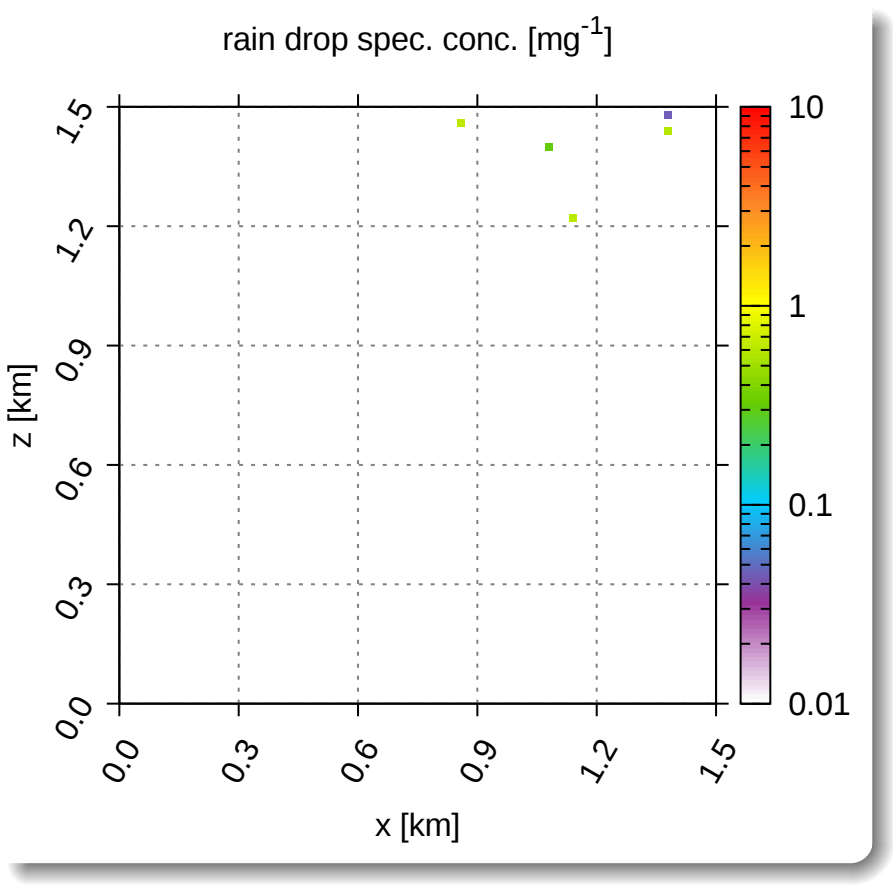
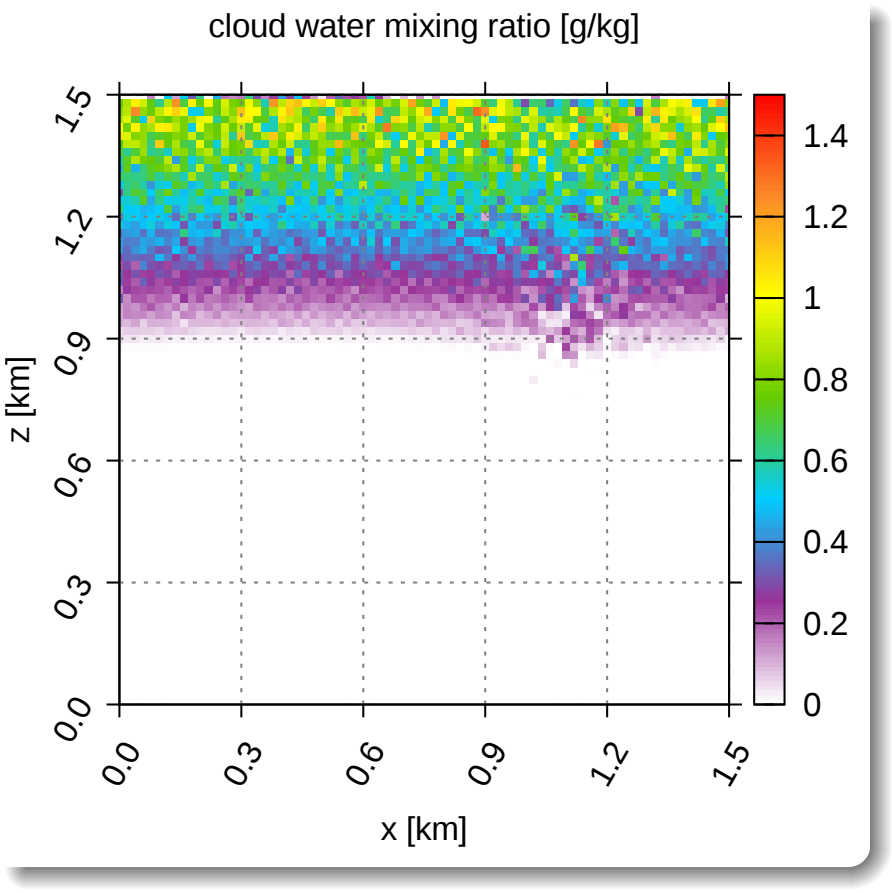
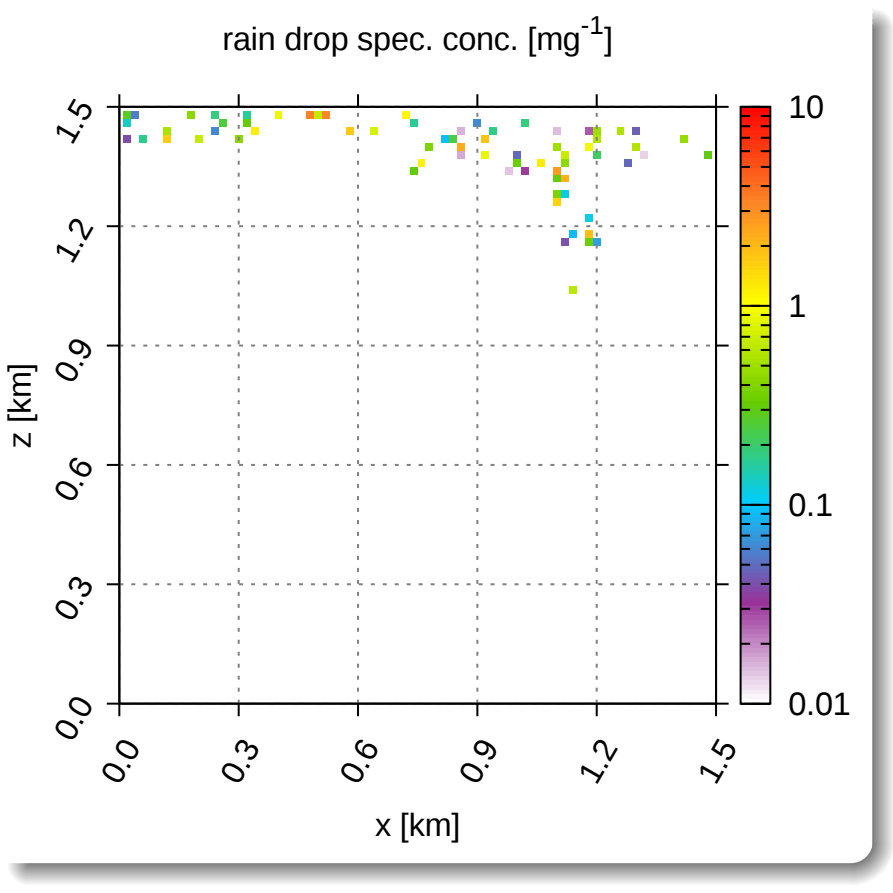




libcloudph++: example 2D prescribed-flow simulation





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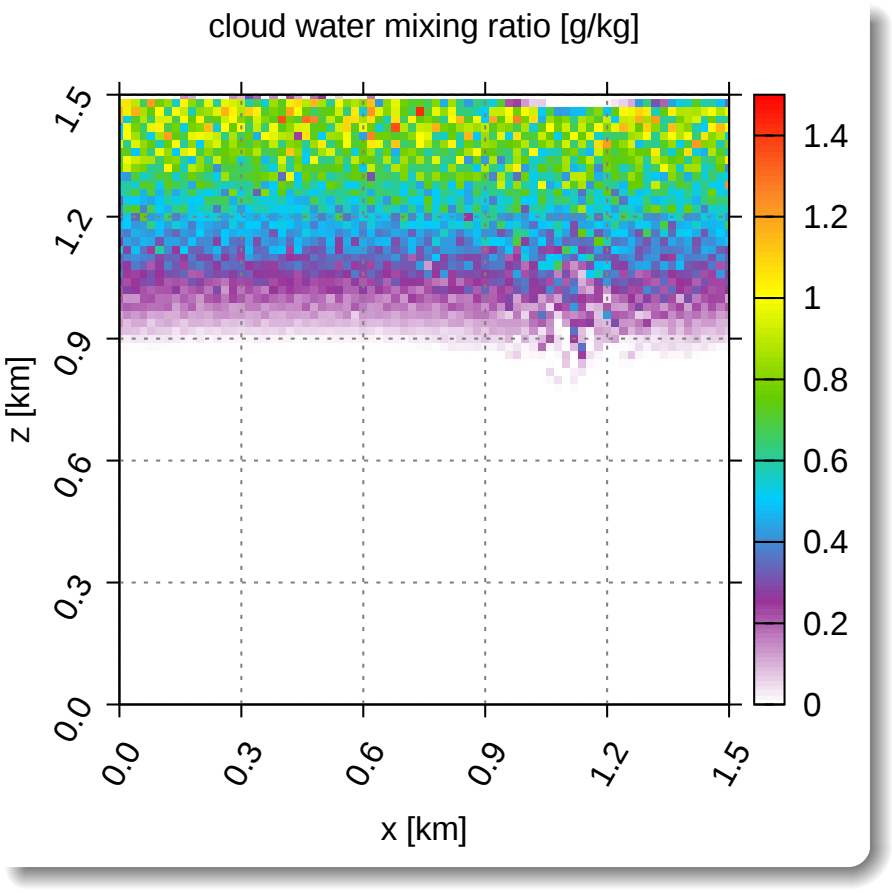

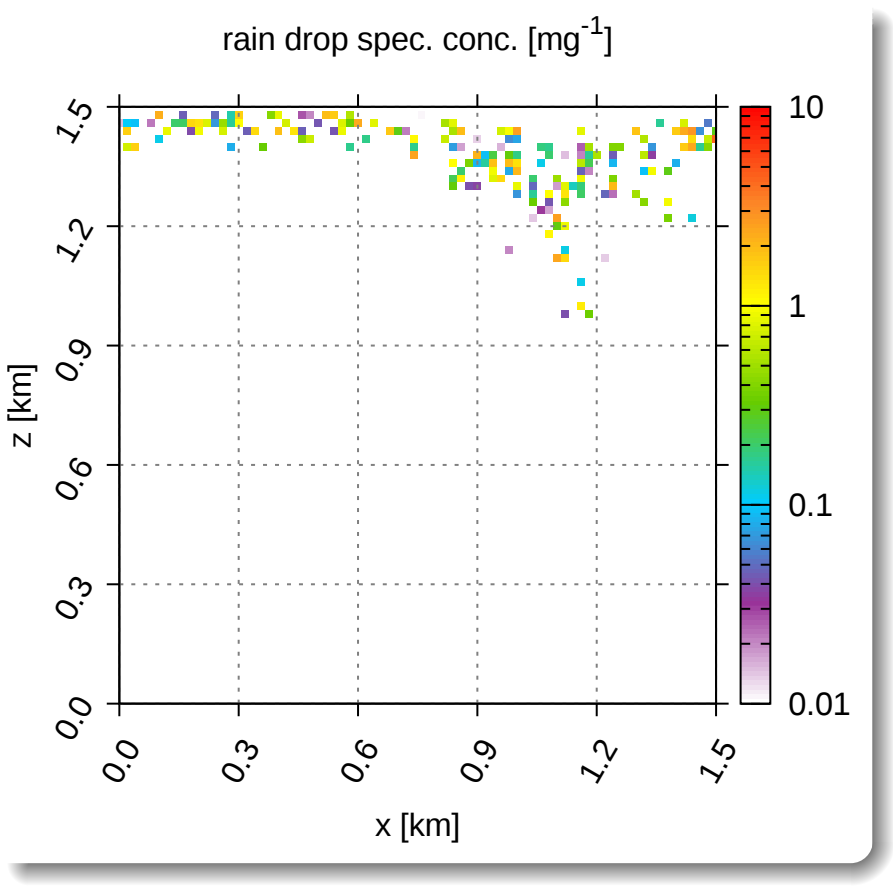

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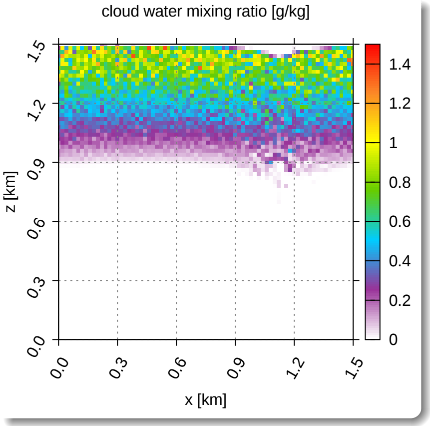

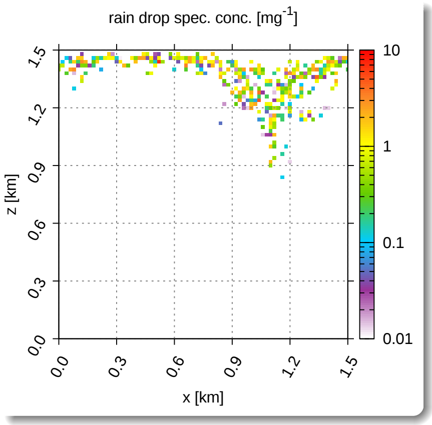

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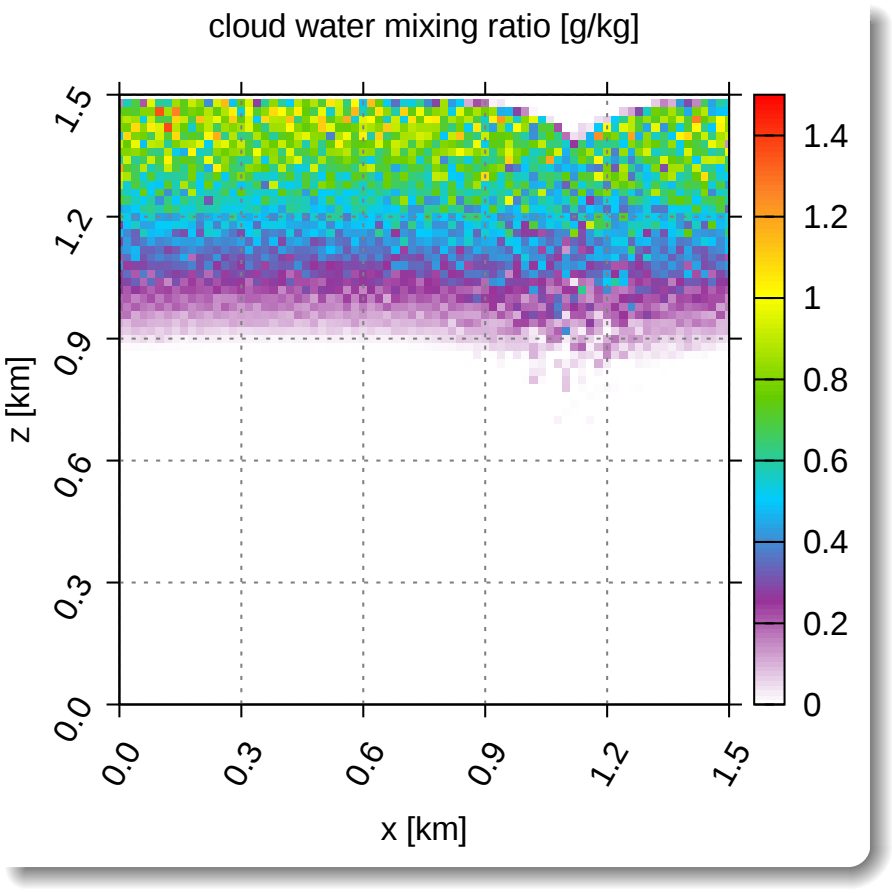

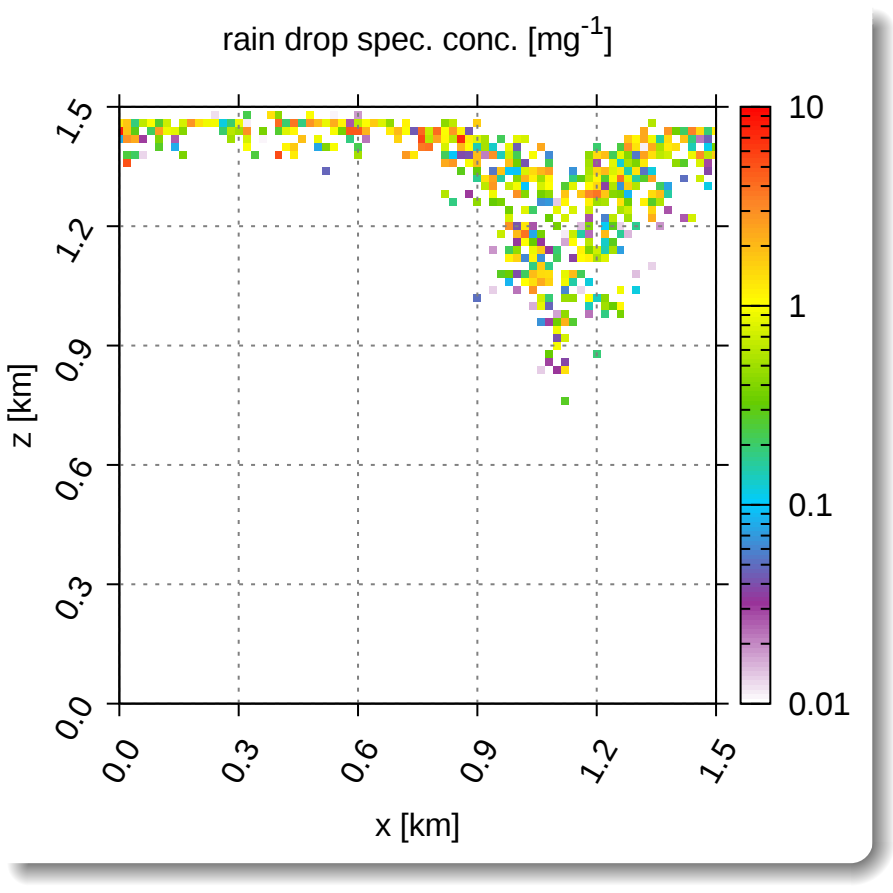

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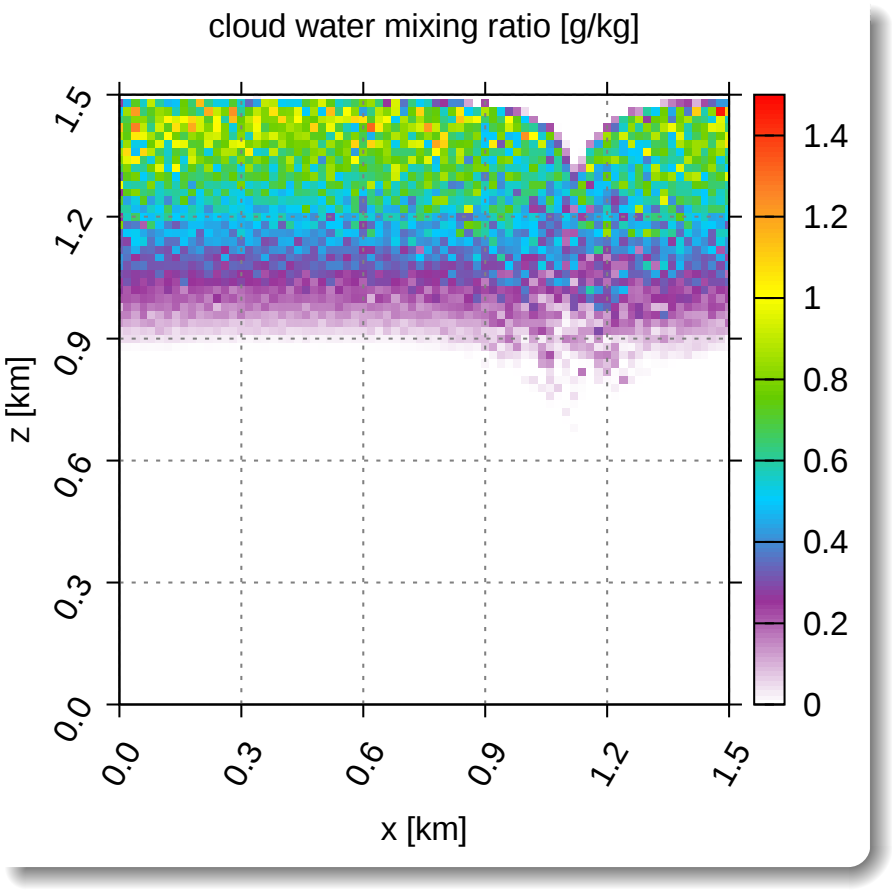

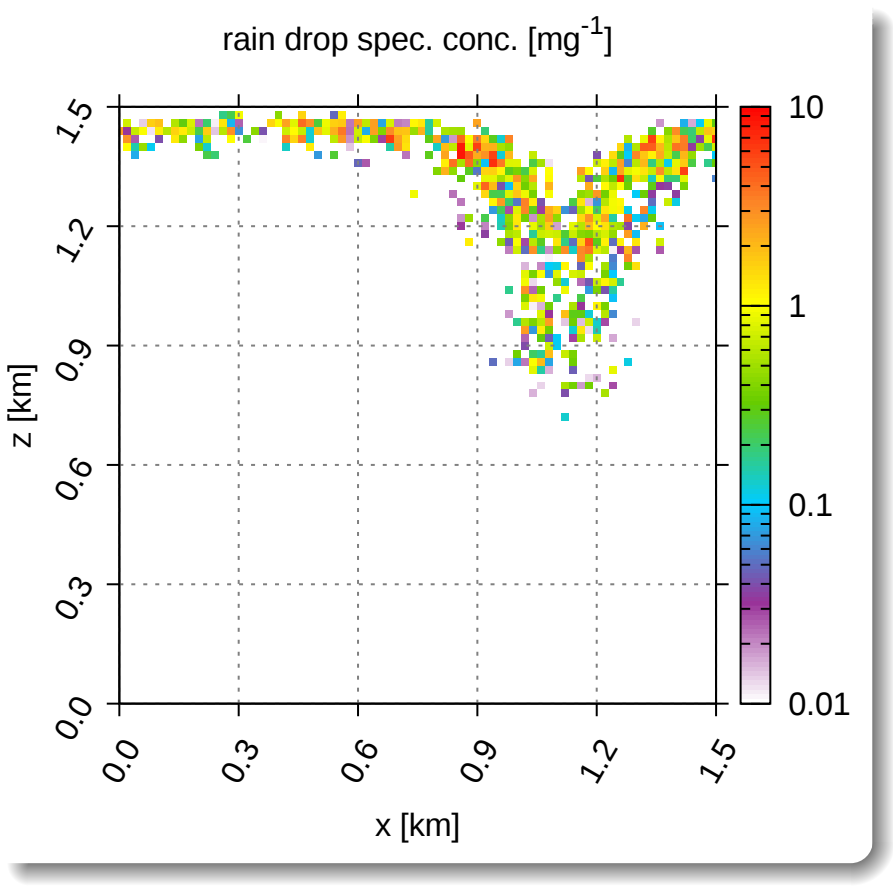

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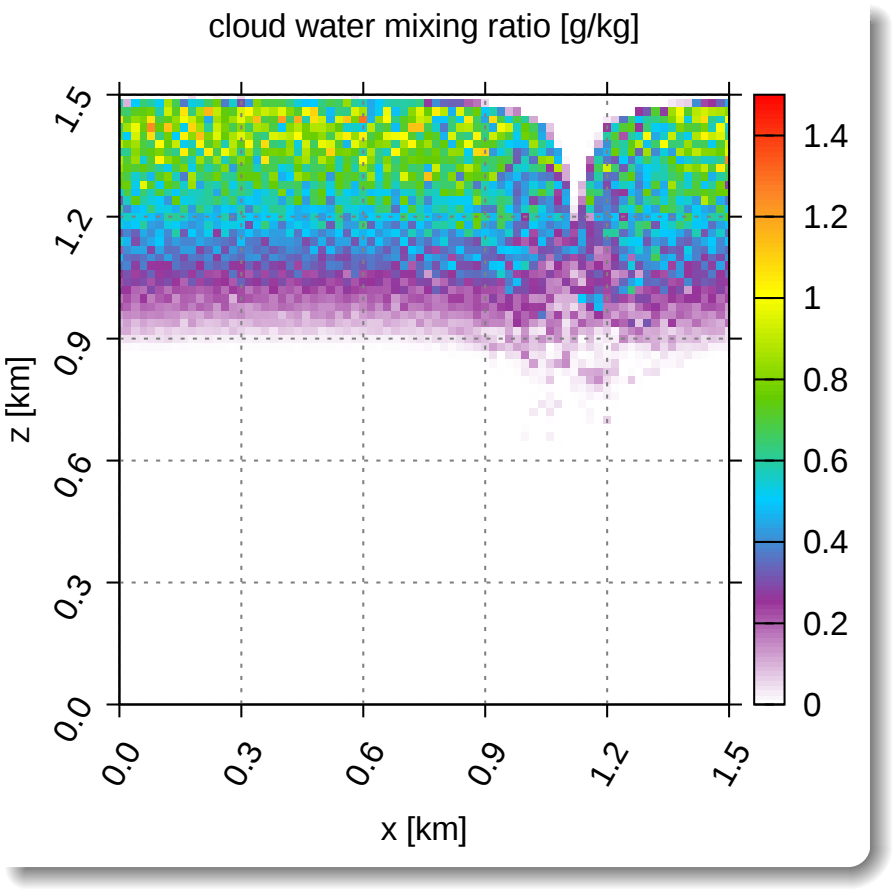

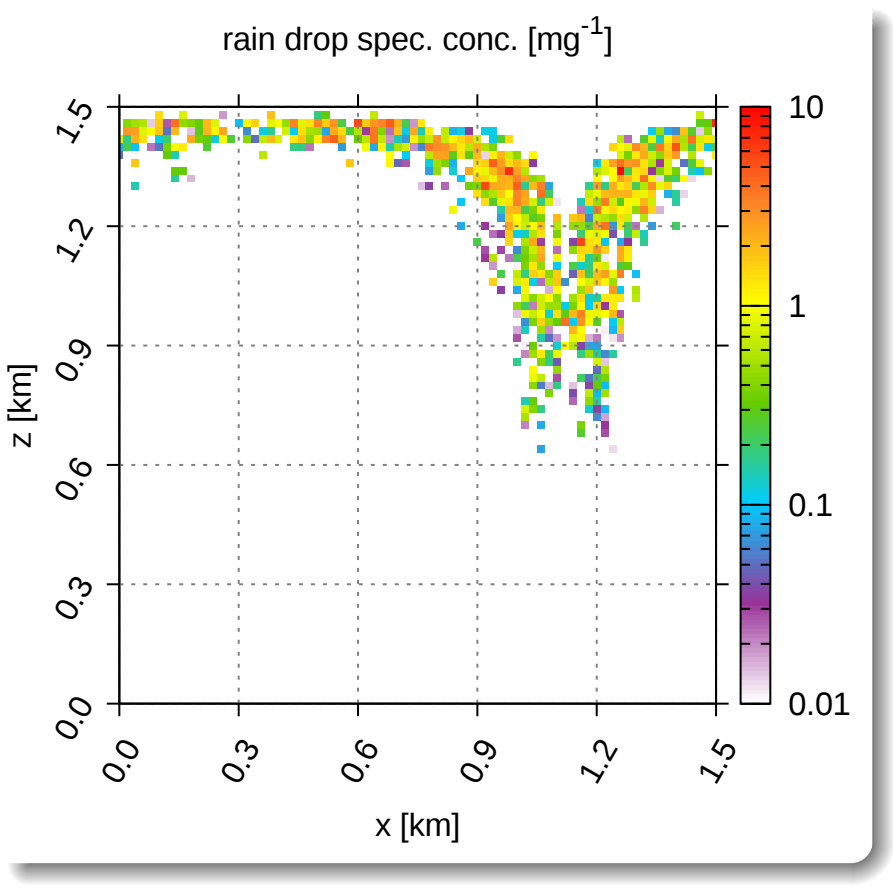

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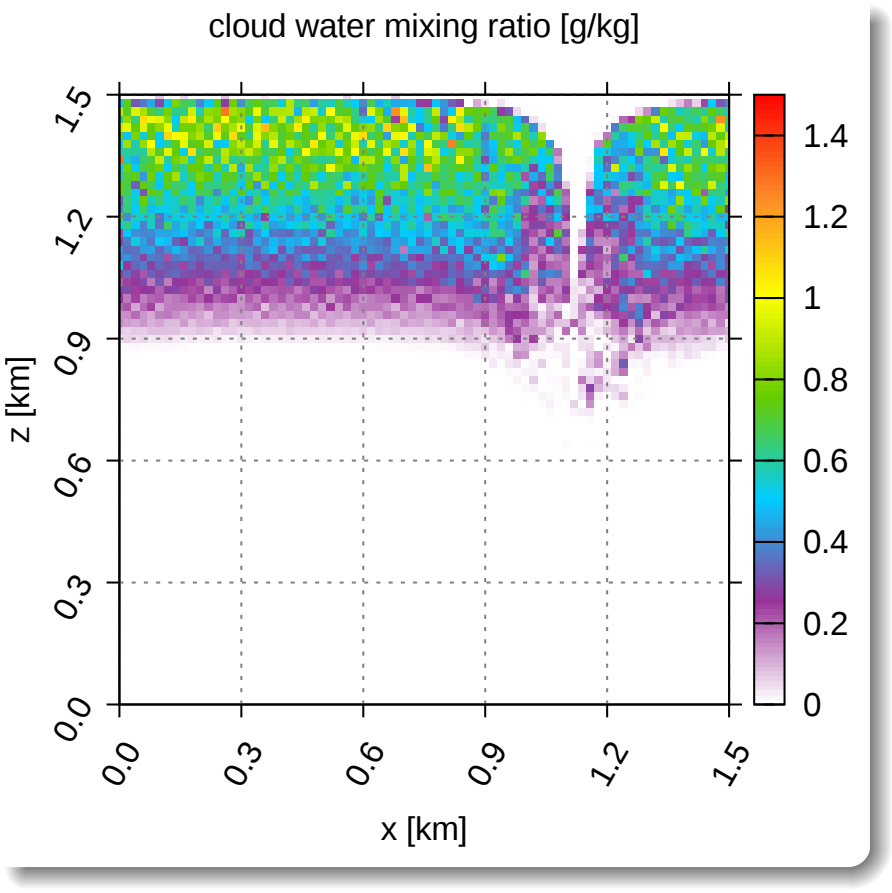

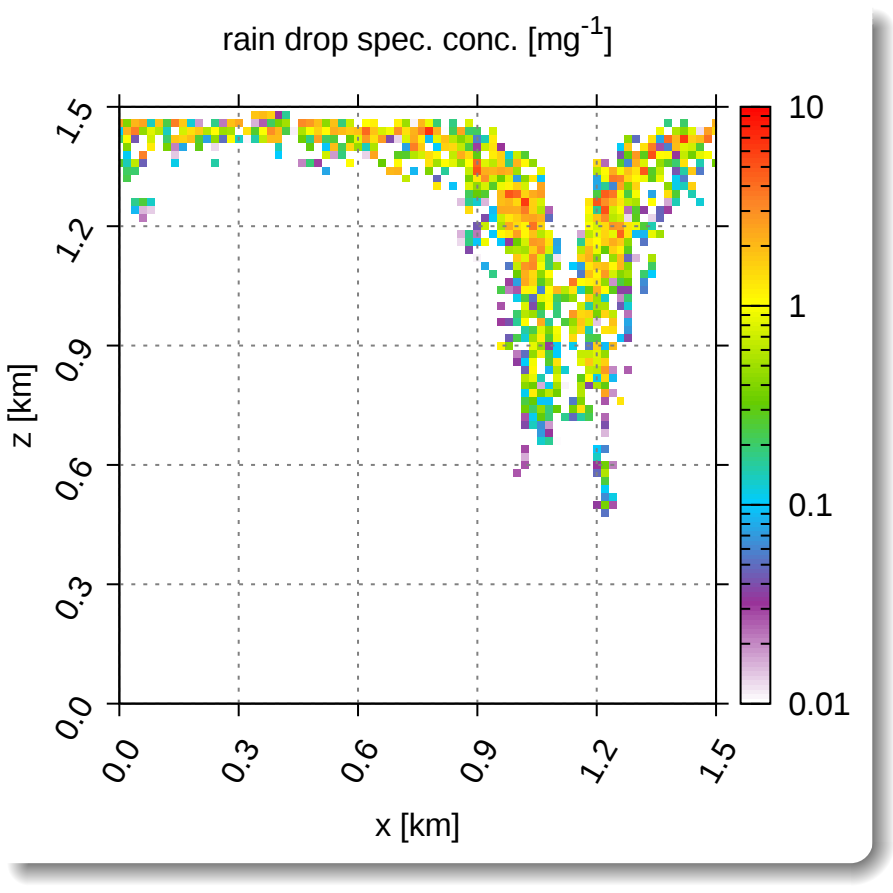

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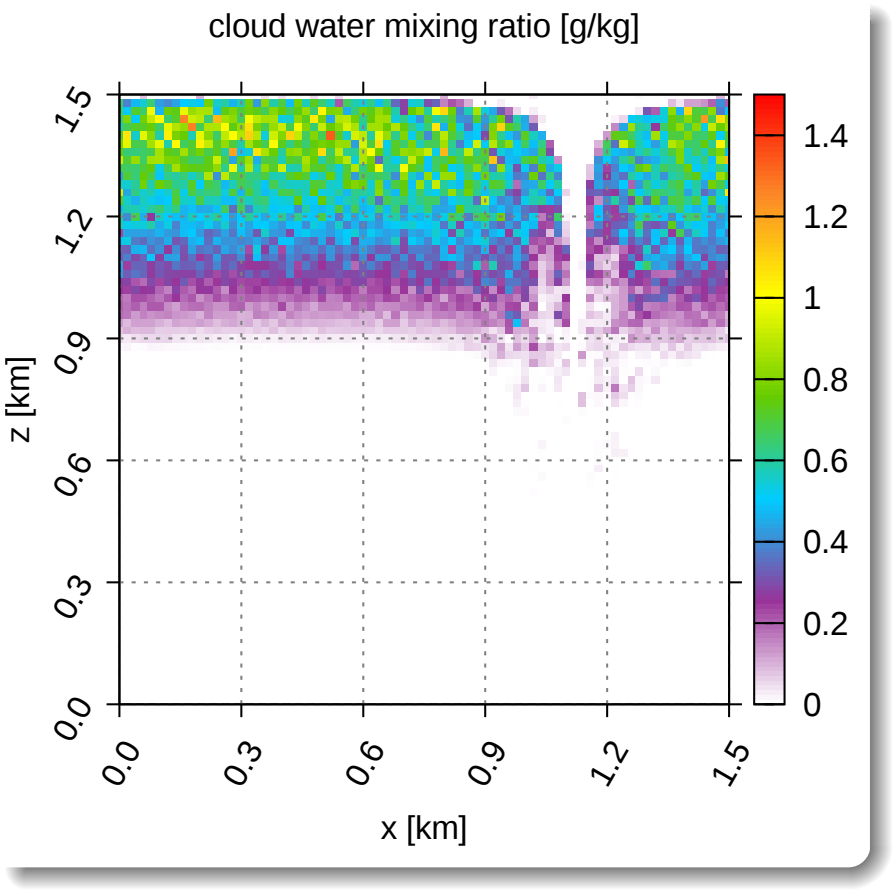

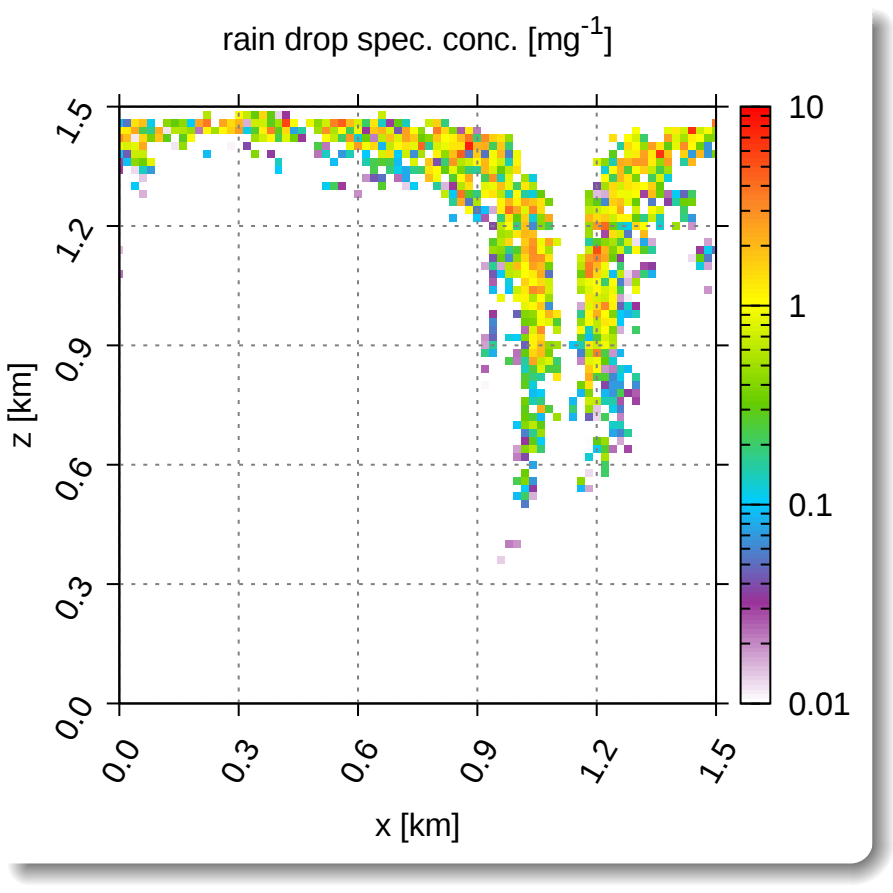

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www.geosci-model-dev-discuss.net/7/8275/2014/
doi:10.5194/gmdd-7-8275-2014

Geoscientific Model Development
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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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[2]National Center for Atmospheric Research (NCAR), Boulder, Colorado, USA
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and H. Pawlowska (hanna.pawlowska@igf.fuw.edu.pl)

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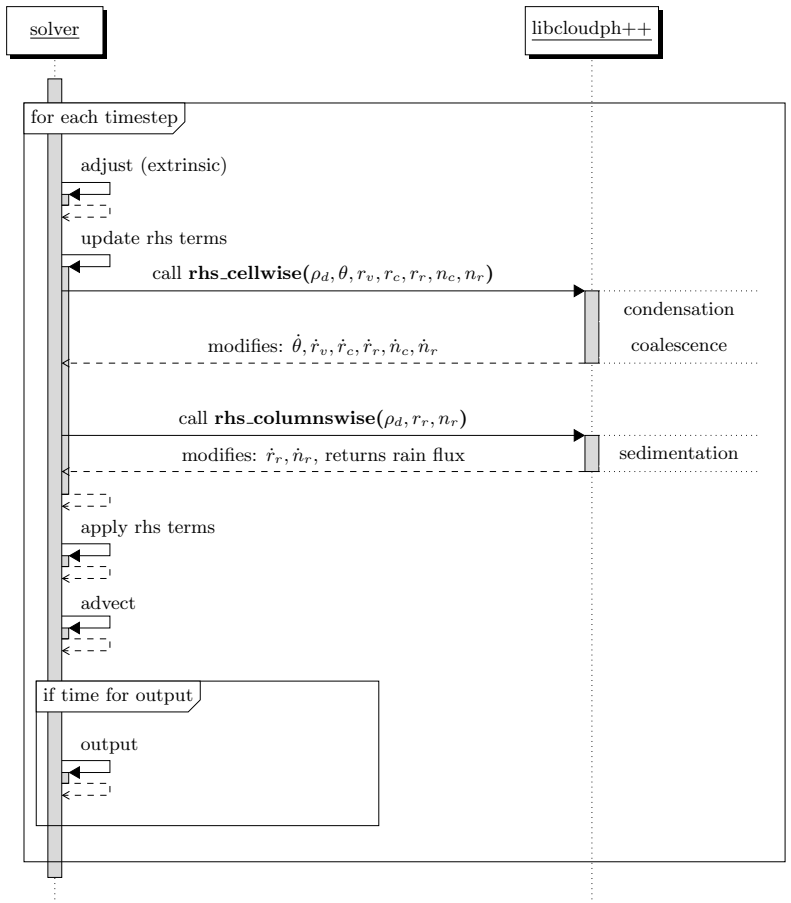
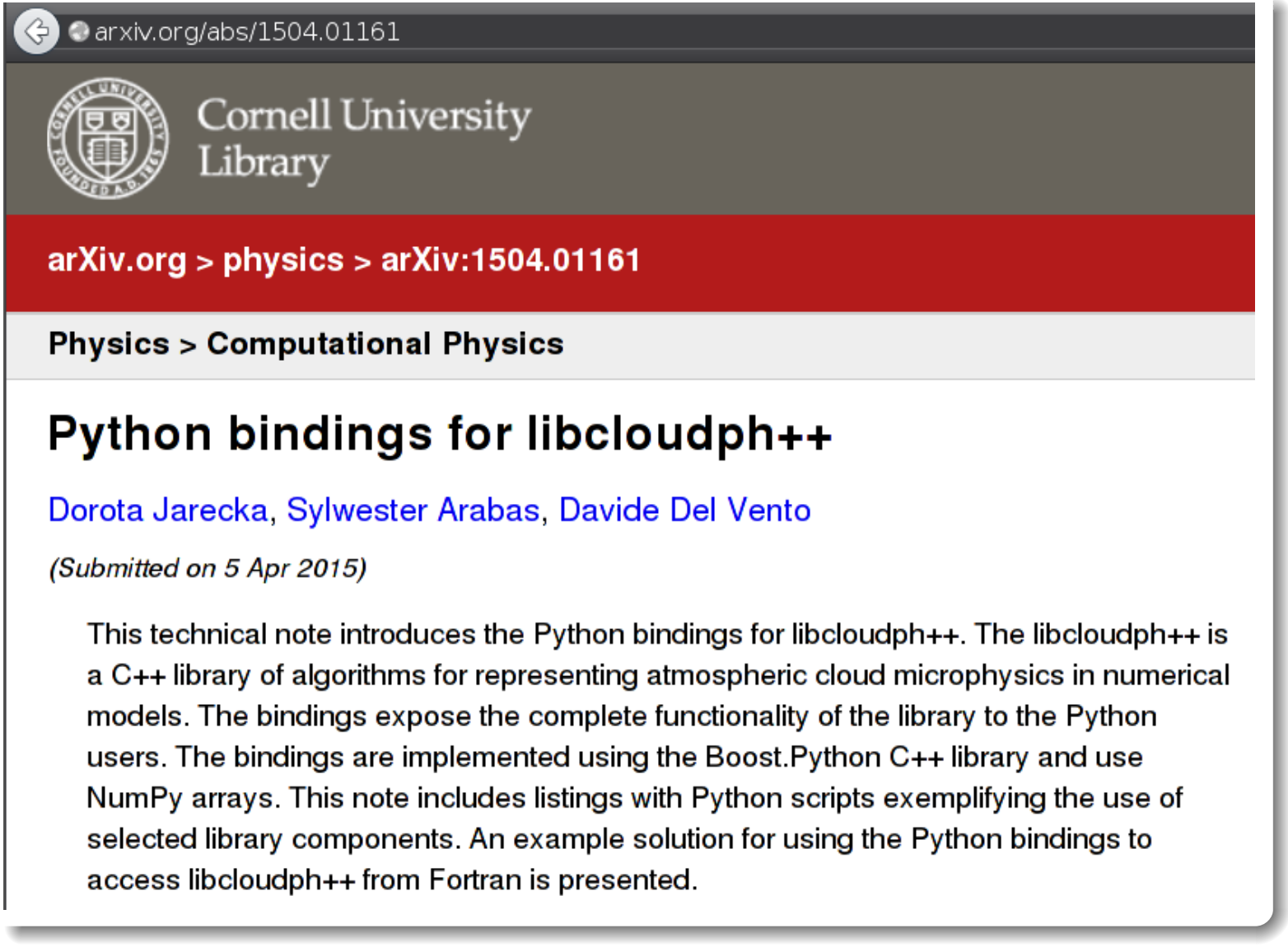


Figure 5. Sequence diagram of *libcloudph++* API calls for the double-moment bulk scheme and a prototype transport equation solver. Diagram discussed in Sect. 4.2.2. See also caption of Fig. 2 for description or diagram elements.

GMDD
7, 8275–8360, 2014



http://arxiv.org/abs/1504.01161

libcloudph++: Python bindings

C++

Python

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C++

- numerically-intensive algorithms
- concurrency, CPU/GPU

Python

libcloudph++: Python bindings

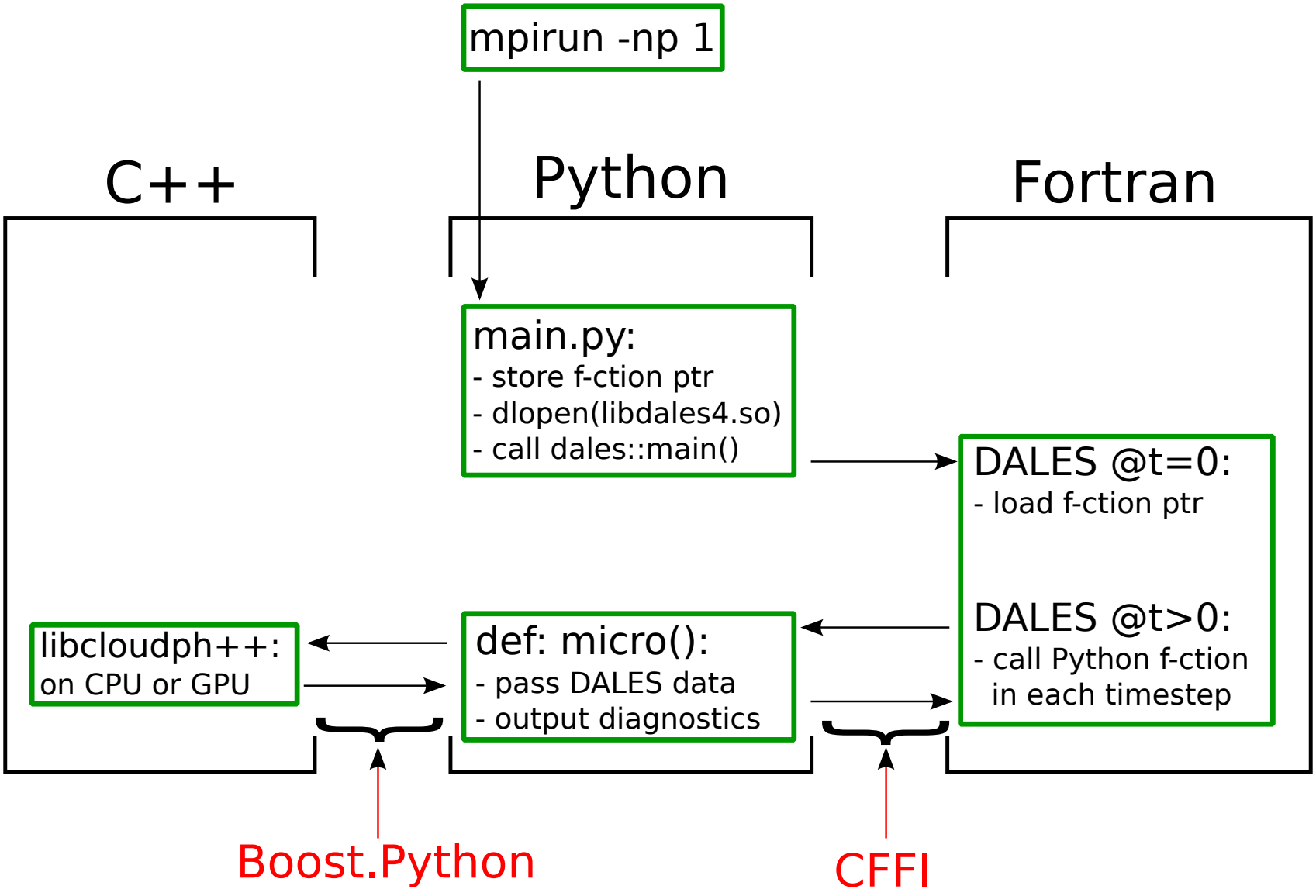
C++

- numerically-intensive algorithms
- concurrency, CPU/GPU

Python

- rapid-development of new features
- interfacing with other languages

libcloudph++: accessing from Fortran via Python



plan of the talk

introduction

libmpdata++

libcloudph++

n-dim array containers

plan of the talk

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n-dim array containers

C++ 3D array containers (cloud modeller's perspective)

- `blitz::Array<real_t, 3>`
- `Eigen::Tensor<real_t, 3>`
- `arma::Cube<real_t>`
- `boost::multi_array<real_t, 3>`
- `std::valarray<real_t>` & `std::gslice`
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no NumPy-like de-facto standard

$\rightsquigarrow$ interoperability with libraries through C pointers

Blitz++

cons

pros

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- SIMD support
- convenient debug mode
- built-in iostream i/o
- **well-suited API! . . .**

C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

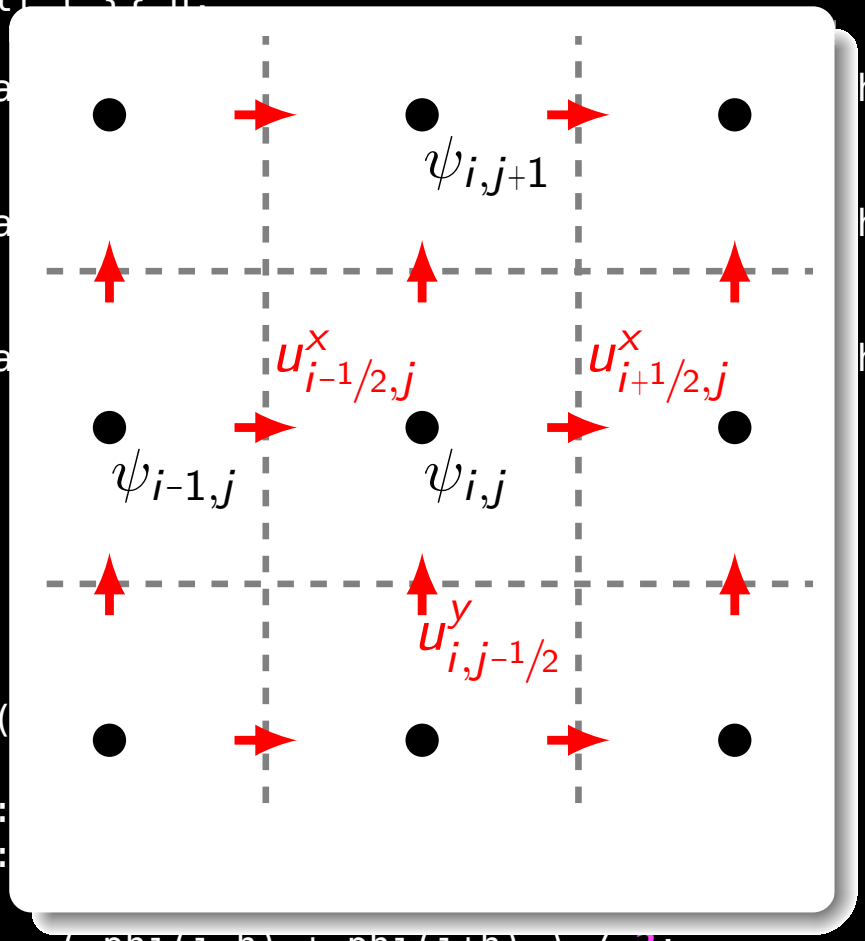
Blitz++ API: **overloadable OO index arithmetics**

```
 1 #include <blitz/array.h>
 2
 3 struct hlf_t {} h;
 4
 5 blitz::Range operator+( const blitz::Range &i, hlf_t &)
 6 { return i;  }
 7
 8 blitz::Range operator-( const blitz::Range &i, hlf_t &)
 9 { return i-1; }
10
11 blitz::Range operator^( const blitz::Range &r, hlf_t &n)
12 {
13   return blitz::Range(
14     (r - n).first(),
15     (r + n).last()
16   );
17 }
18
19 int main()
20 {
21   blitz::Range i(0,10);
22   blitz::Array<float, 1> psi(i), phi(i^h);
23
24   psi(i) = ( phi(i-h) + phi(i+h) ) / 2;
25 }
```

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **overloadable OO index arithmetics**

```
 1 #include <blitz/array.h>
 2
 3 struct hlf_t {} h;
 4
 5 blitz::Ra                                                    hlf_t &)
 6 { return
 7
 8 blitz::Ra                                                    hlf_t &)
 9 { return
10
11 blitz::Ra                                                    hlf_t &n)
12 {
13   return
14     (r -
15     (r +
16   );
17 }
18
19 int main(
20 {
21   blitz::
22   blitz::
23
24   psi(i) = ( phi(i-h) + phi(i+h) ) / 2;
25 }
```



C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **multi-dim. index with single obj.**

```
 1 #include <blitz/array.h>
 2
 3 int main()
 4 {
 5   blitz::Range i(0,9), j(0,9), k(0,9);
 6
 7   blitz::Array<int, 3> psi(i,j,k);
 8
 9   std::cerr << psi(i,j,k);
10
11   blitz::RectDomain<3> ijk({i,j,k});
12
13   std::cerr << psi(ijk);
14 }
```

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: multi-dim. index with single obj.

```
 1 #include <blitz/array.h>
 2
 3 int main()
 4 {
 5   blitz::Range i(0,9), j(0,9), k(0,9);
 6
 7   blitz::Array<int, 3> psi(i,j,k);
 8
 9   std::cerr << psi(i,j,k);
10
11   blitz::RectDomain<3> ijk({i,j,k});
12
13   std::cerr << psi(ijk);
14 }
```

index permutations!

C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **tensor notation**

```
 1 #include <blitz/array.h>
 2
 3 int main()
 4 {
 5   blitz::Array<float,2> psi(4,4);
 6   {
 7     using namespace blitz::tensor;
 8     psi = sqrt(i*i + j*j);
 9   }
10   std::cout << psi;
11 }
```

C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **array-valued functions**

```
 1 //#define BZ_THREADSAFE // to enable access locks for ref counting
 2 #include <blitz/array.h>
 3
 4 enum { opt_sin, opt_cos };
 5
 6 template <int opt, typename T>
 7 auto func(T &a, typename std::enable_if<opt == opt_sin>::type* = 0)
 8 {
 9   return safeToReturn(pow(sin(a), 2)); // keeps ref count
10 }
11
12 template <int opt, typename T>
13 auto func(T &a, typename std::enable_if<(opt == opt_cos)>::type* = 0)
14 {
15   return safeToReturn(pow(cos(a), 2)); // keeps ref count
16 }
17
18 int main()
19 {
20   blitz::Array<float, 1> psi(1000);
21   {
22     using namespace blitz::tensor;
23     psi = i / 20.;
24   }
25   psi = func<opt_sin>(psi) + func<opt_cos>(psi);
26   std::cout << psi;
27 }
```

C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **elemental functors**

```
 1 #include <blitz/array.h>
 2
 3 struct func
 4 {
 5   float a = .25, b = .1;
 6
 7   float operator()(float x) const
 8   {
 9     return a * x + b;
10   }
11
12   // to make it accept Blitz arrays as arguments
13   BZ_DECLARE_FUNCTOR(func);
14 };
15
16 int main()
17 {
18   blitz::Array<float, 1> psi(10), x(10);
19
20   x = blitz::tensor::i;
21
22   psi = func()(x);
23 }
```

C++ 3D array containers (cloud modeller's perspective)

C++ 3D array containers (cloud modeller's perspective)

Blitz++ API: **ternary op. & reductions**

```
 1 #include <blitz/array.h>
 2
 3 int main()
 4 {
 5   blitz::Array<float, 2> psi(5,5);
 6   {
 7     using namespace blitz::tensor;
 8     psi = sqrt((i*i) + (j*j));
 9   }
10
11   // ternary operator
12   psi = where(psi>3, 0, psi);
13
14   // partial reduction
15   {
16     using namespace blitz::tensor;
17     auto xpr = sum(psi, j); // delayed eval!
18   }
19 }
```

last slide

last slide

- C++ does constitute a viable alternative to Fortran for maintainable code and reproducible results in cloud-modelling

last slide

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- multi-dimensional C++ array containers:
  - Is there an alternative to Blitz++?

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- thank you for your attention!