libmpdata++: library of parallel MPDATA-based solvers built with emphasis on maintainability

Maciej Waruszewski

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

EULAG Workshop 2014, 21th Oct. 2014

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aim: developing tools for studying aerosol-cloud interactions

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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
  $\rightsquigarrow$ priorities: researchers' productivity and result reproducibility

aerosol-cloud interactions: a conceptual picture



- aerosol activation
- condensation

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- collisions between droplets
- chemical reactions in droplets

aerosol-cloud interactions: a conceptual picture

- aerosol activation
- condensation

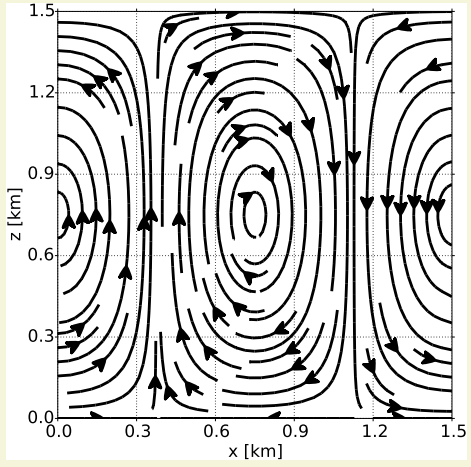
- collisions between droplets
- chemical reactions in droplets

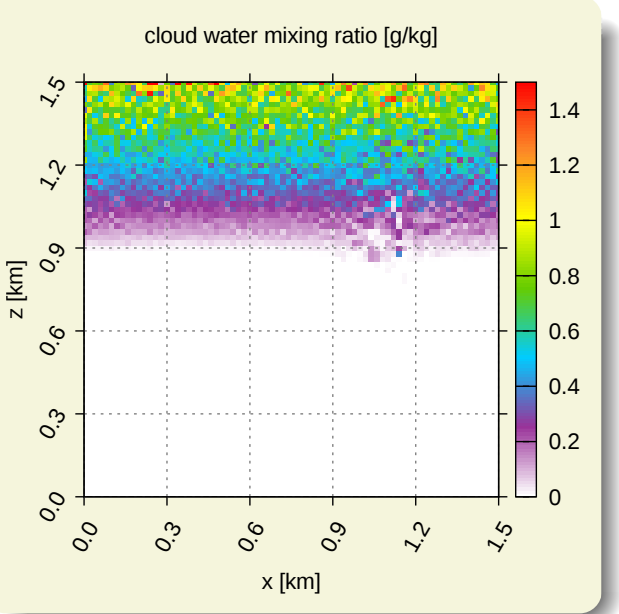
- precipitation
- wet deposition
- droplet evaporation

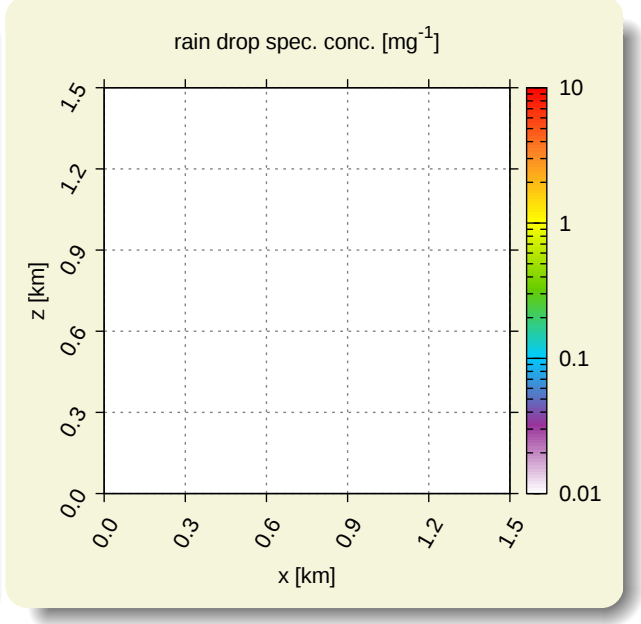
example: VOCALS-inspired aerosol processing set-up

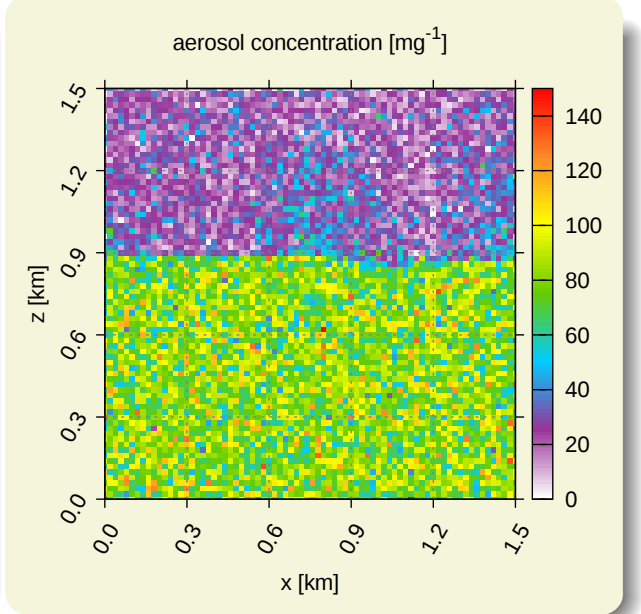
- 2D prescribed flow
- advection: MPDATA (2-pass FCT)
- μ-physics: Super Droplets

single-eddy velocity field









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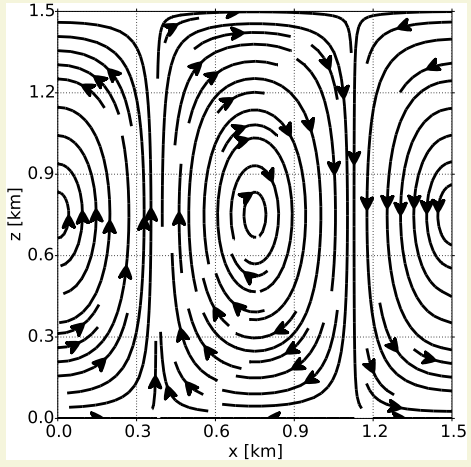

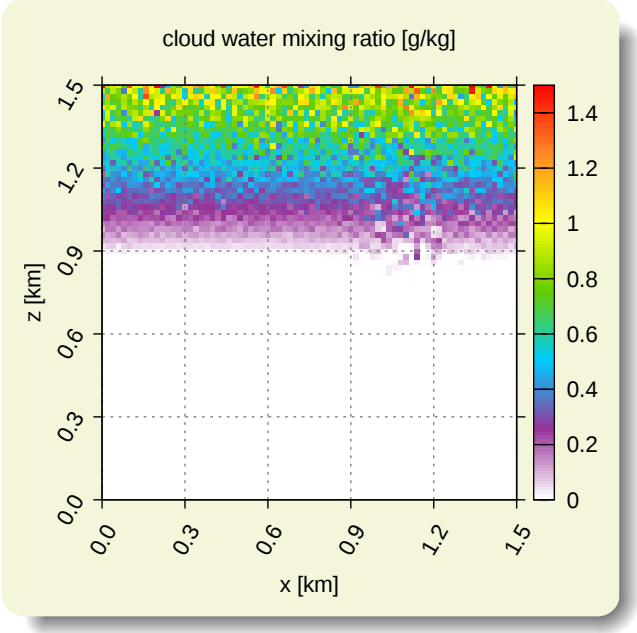

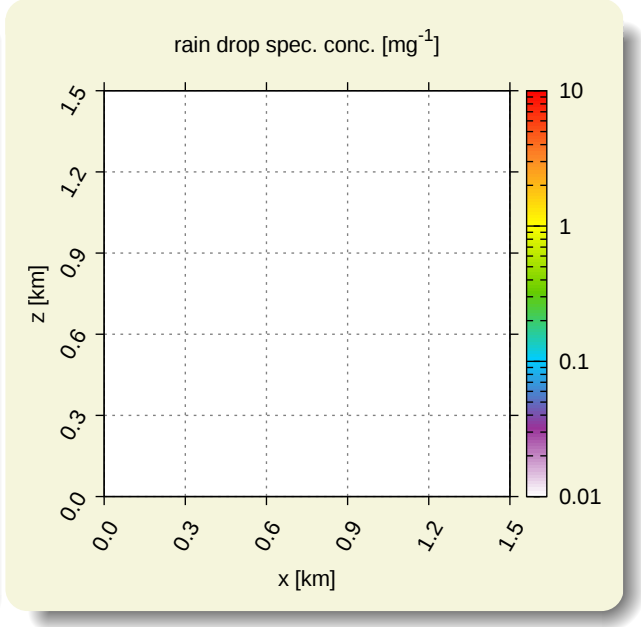

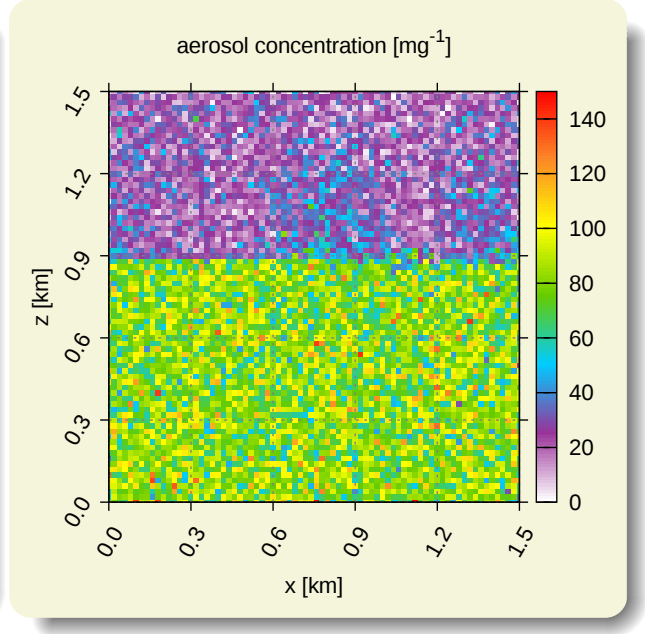

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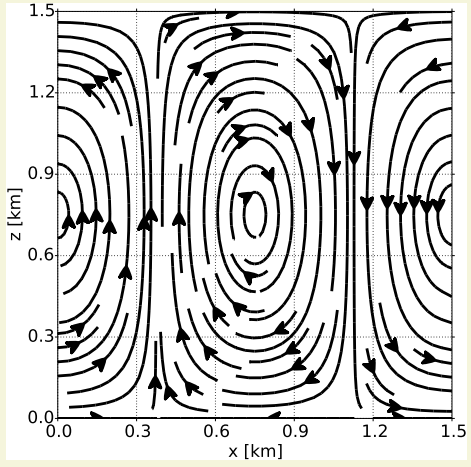

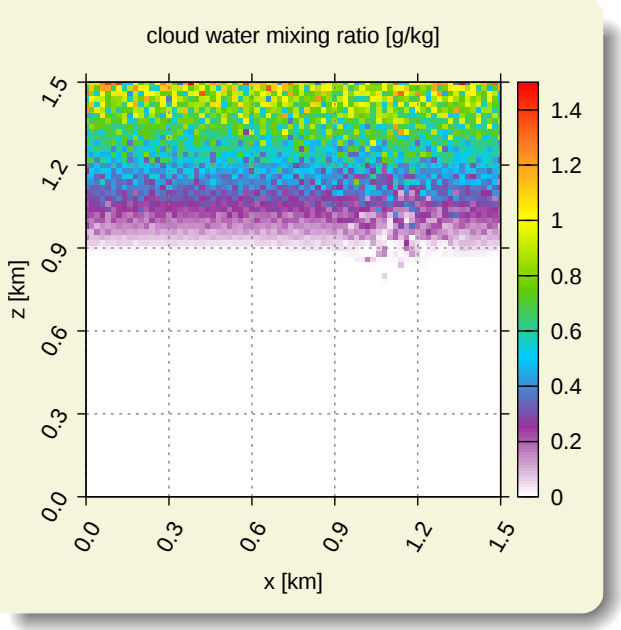

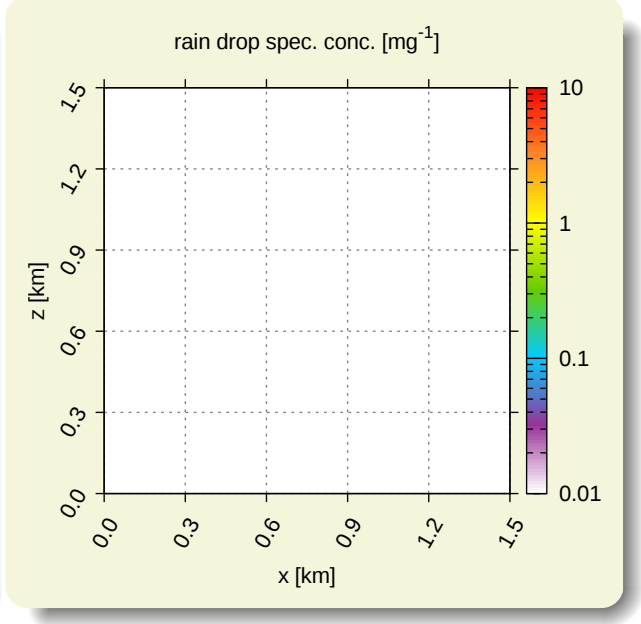

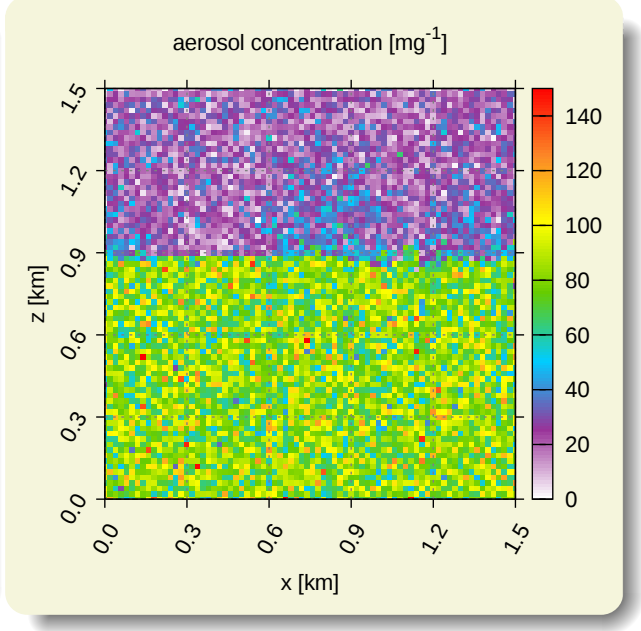

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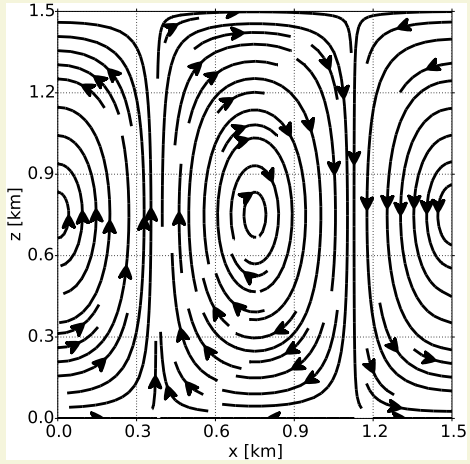

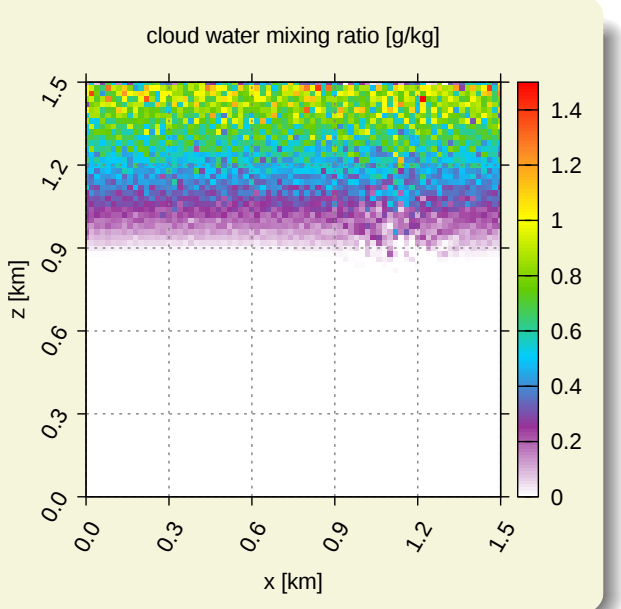

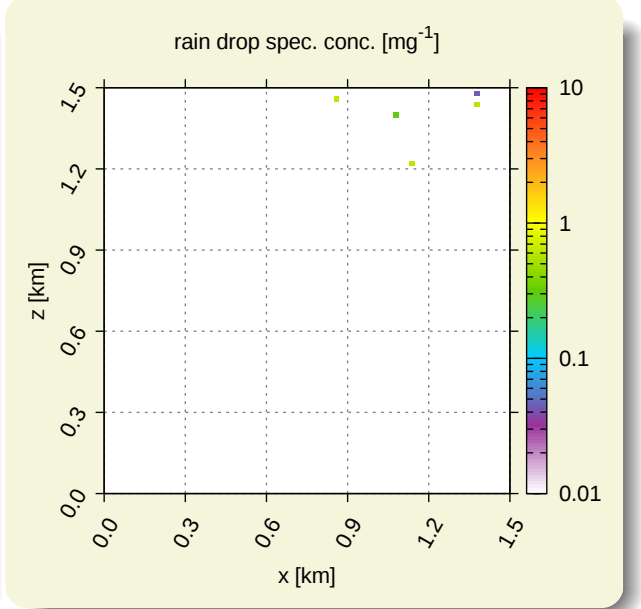

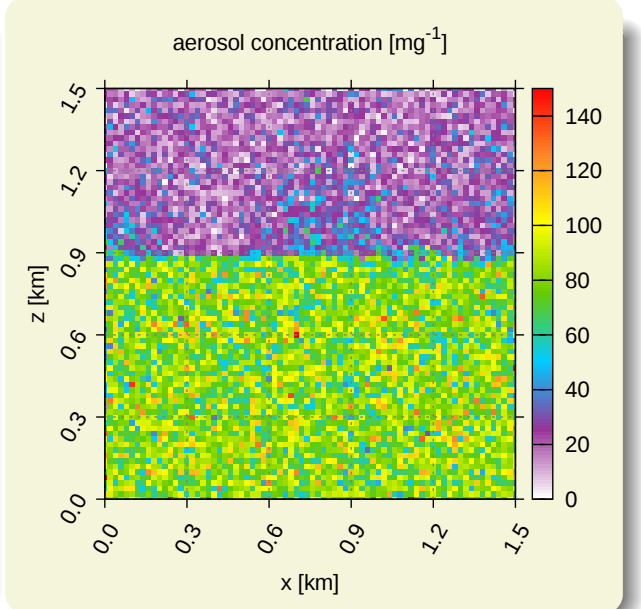

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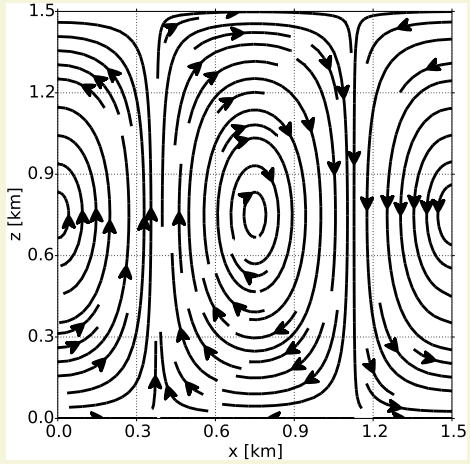

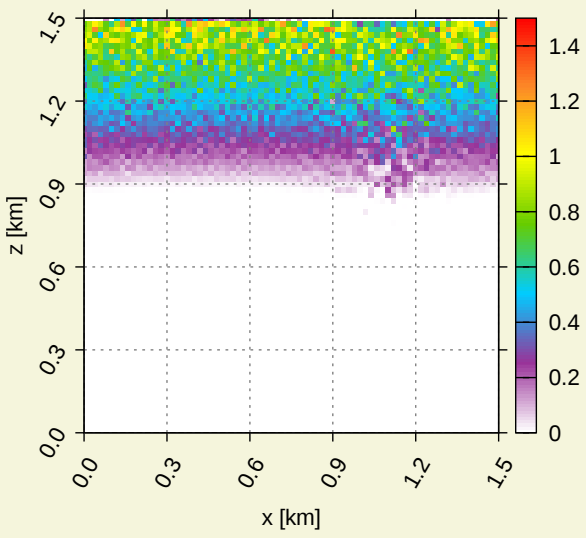

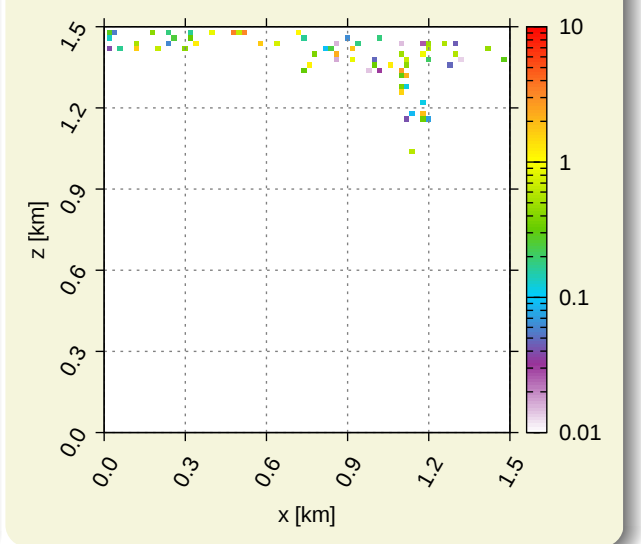

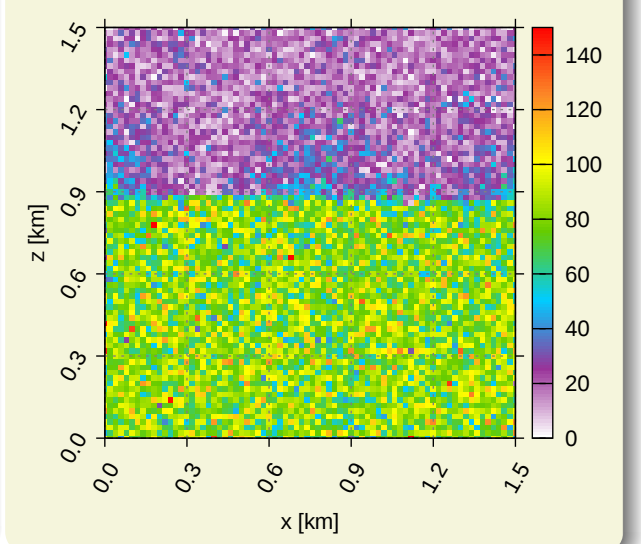

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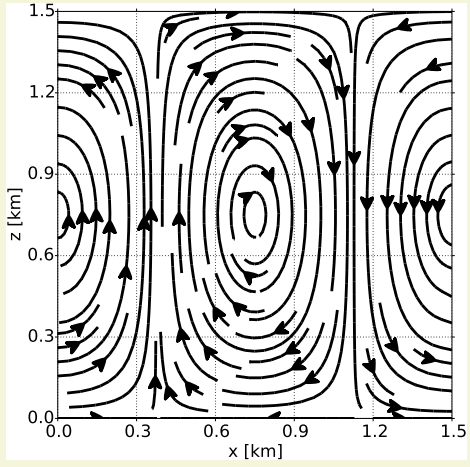

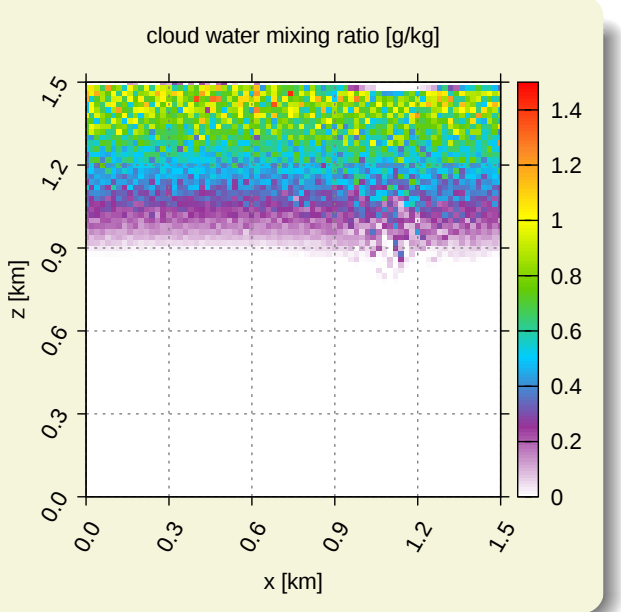

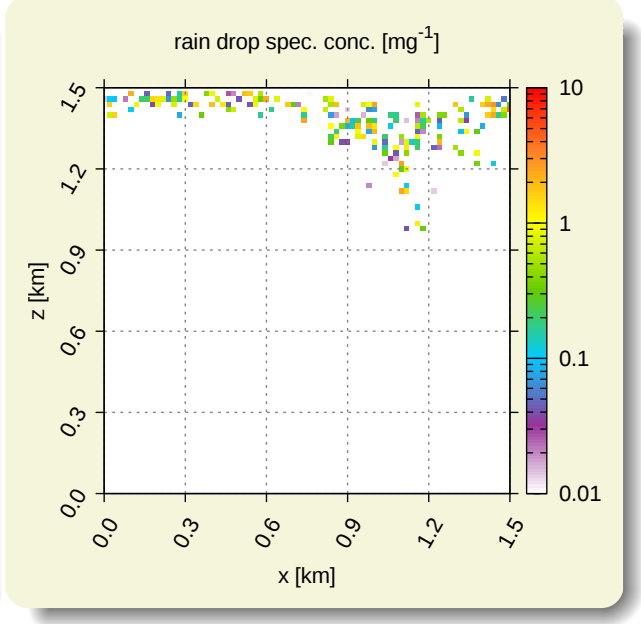

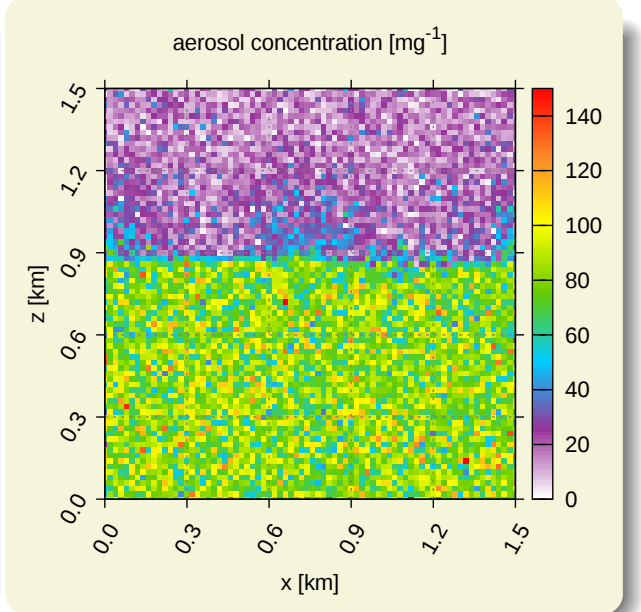

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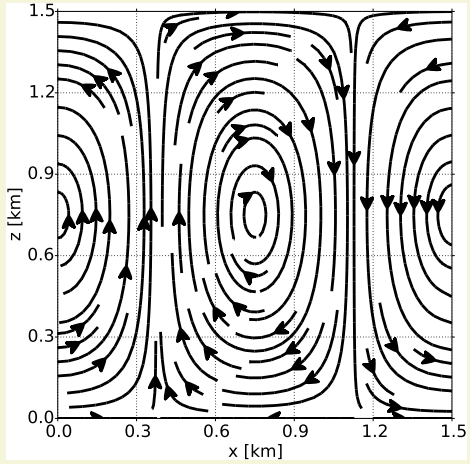

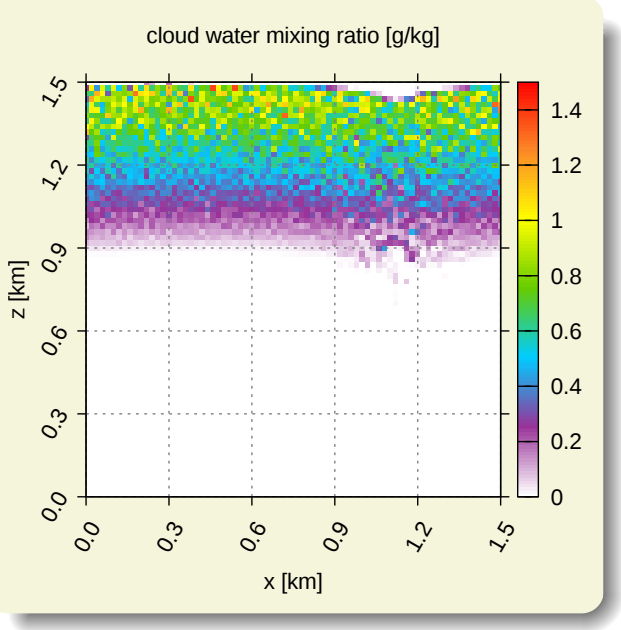

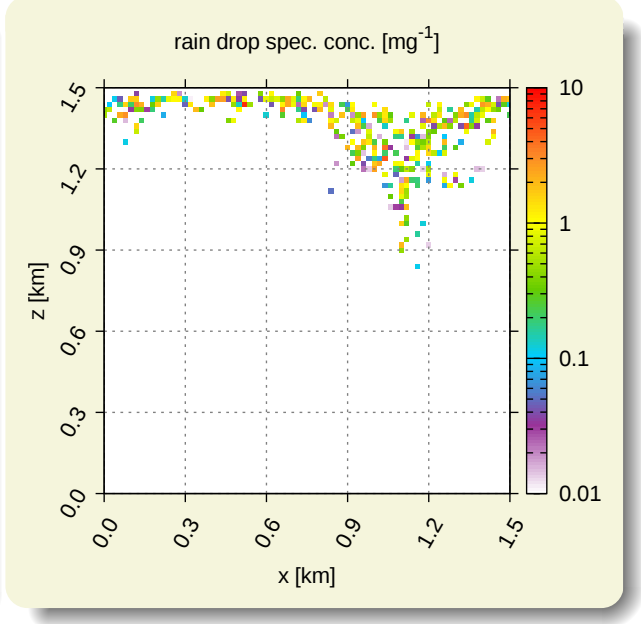

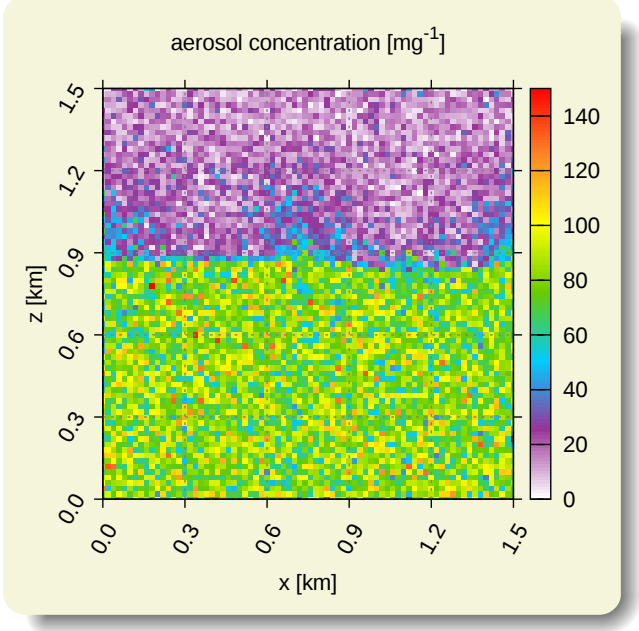

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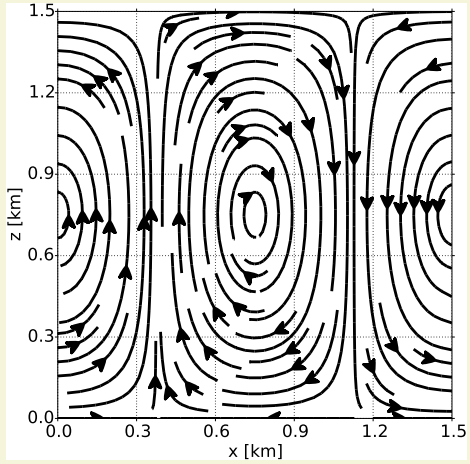

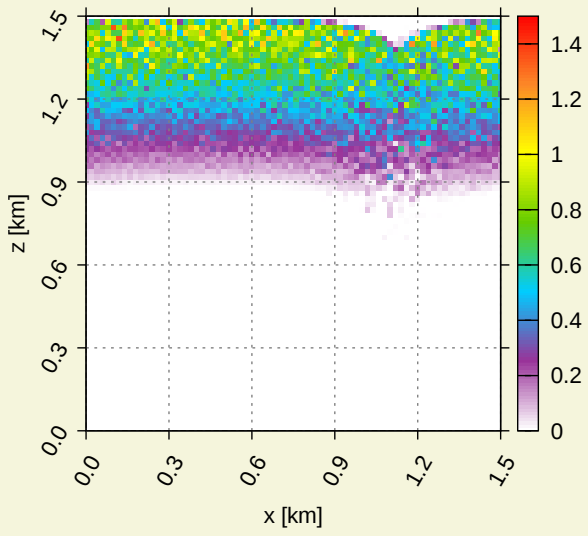

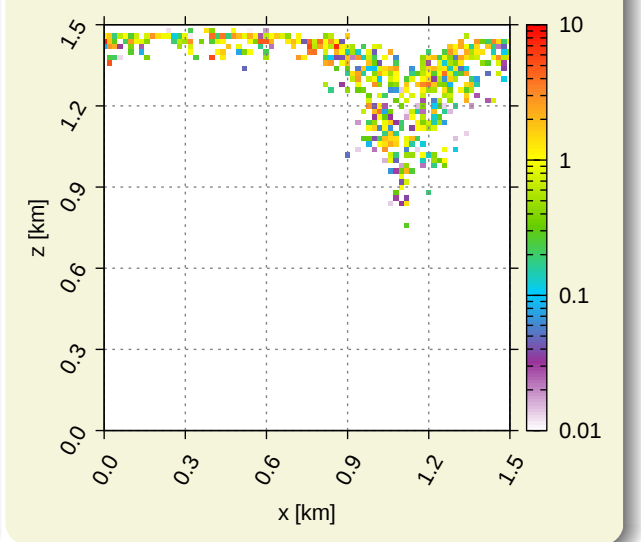

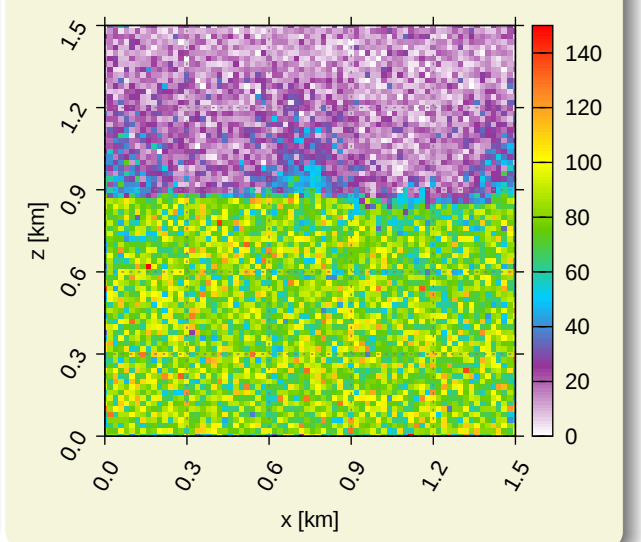

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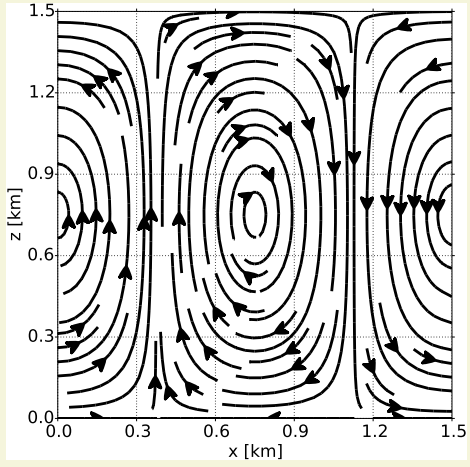

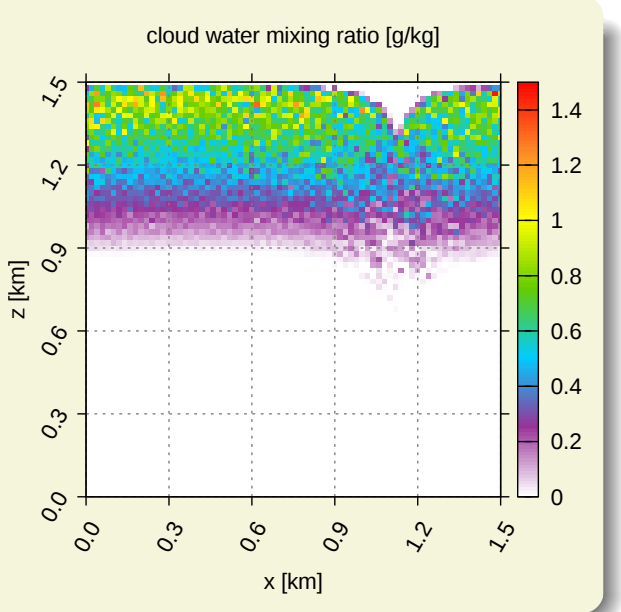

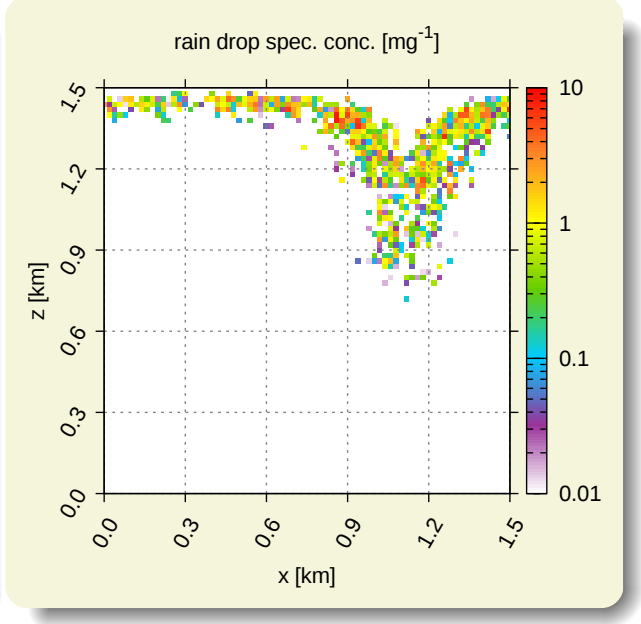

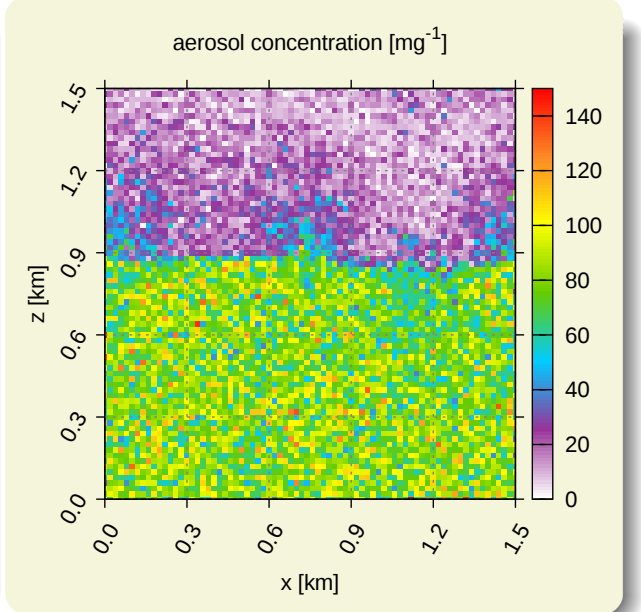

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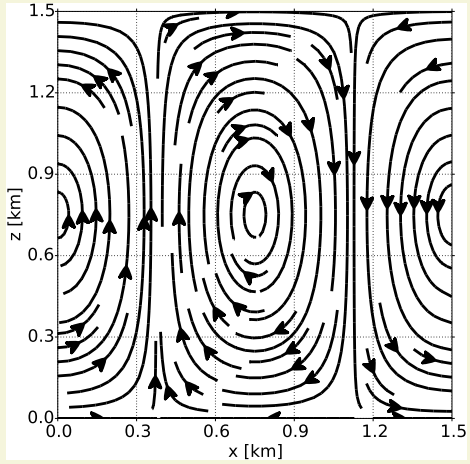

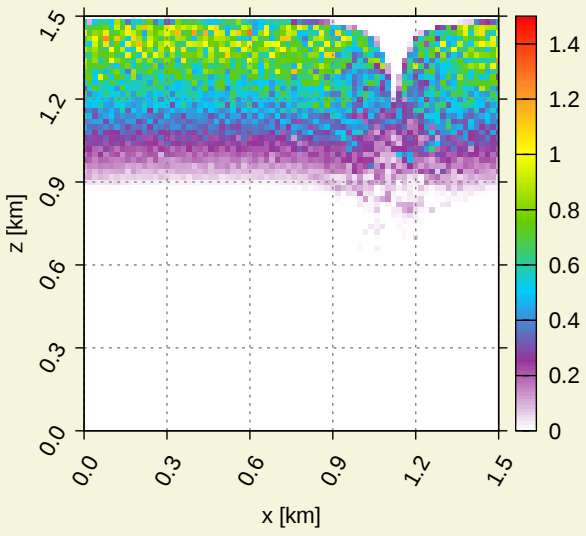

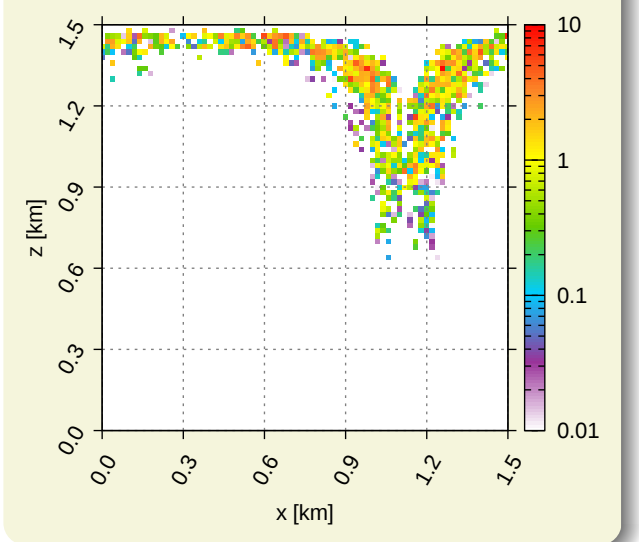

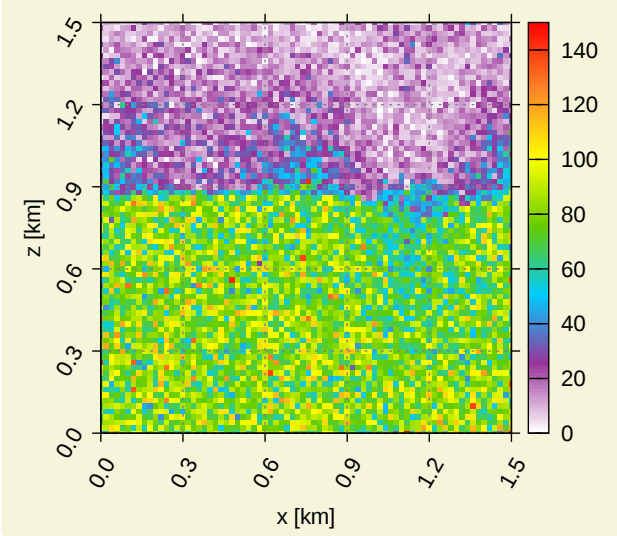

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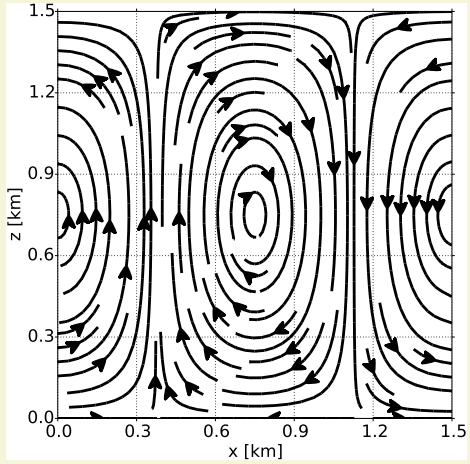

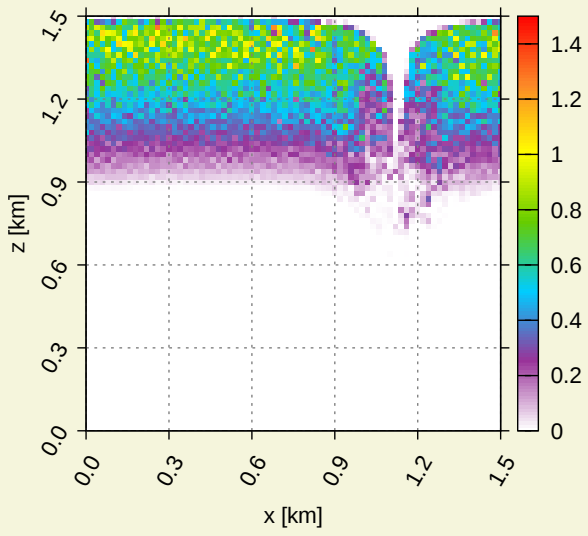

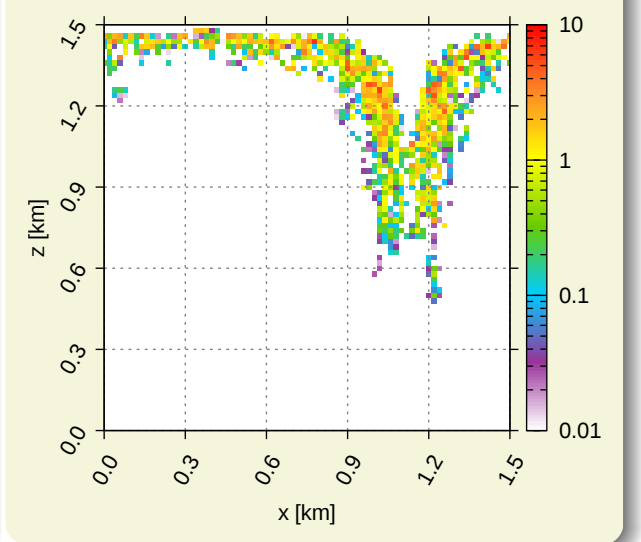

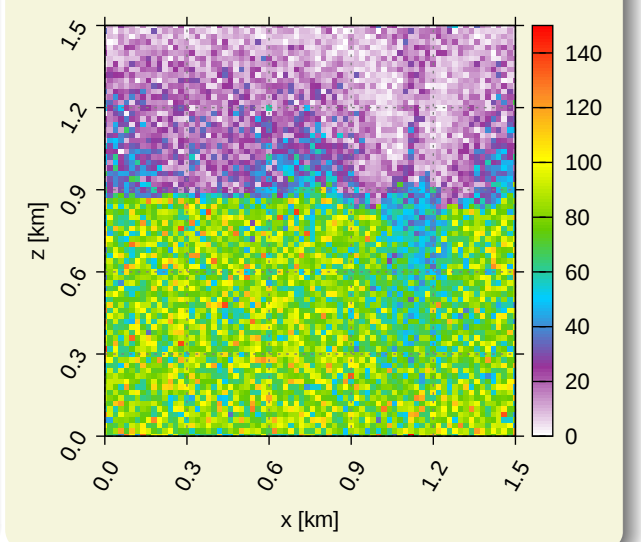

free & open-source C++ libraries developed at our group

libmpdata++ / arXiv:1407.1309 / under review in 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]

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

libcloudph++ / arXiv:1310.1905 / under review in GMDD

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

Sylwester Arabas[1], Anna Jaruga[1], Hanna Pawlowska[1], Wojciech W. Grabowski*[2]

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

Sylwester Arabas[1], Anna Jaruga[1], Hanna Pawlowska[1], Wojciech W. Grabowski[*2]

[1]Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[2]National Center for Atmospheric Research (NCAR), Boulder, Colorado, USA

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

libmpdata++ / arXiv:1407.1309 / under review in 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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free & open source C++ library of parallel MPDATA solvers

library

- set of reusable components (solvers, output, concurency)
- well-defined interface (documented in the paper)

key features

- variety of MPDATA-based solvers in 1D, 2D & 3D
- rich set of algorithm options
- shared-memory parallelisation using OpenMP or Boost.Thread
- built-in HDF5/XDMF output
- implemented using Blitz++ (multi-array expression templates)
- ...

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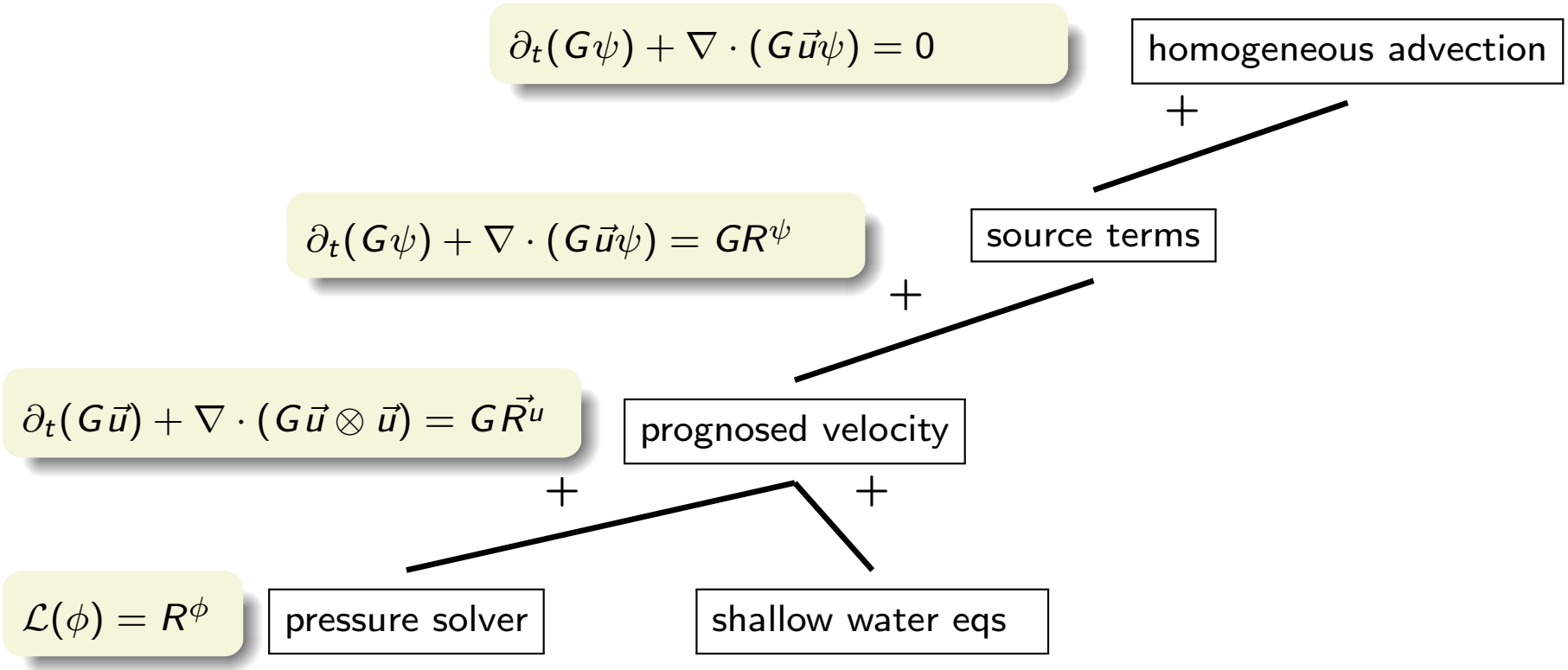

building blocks of libmpdata++

$$\partial_t(G\psi) + \nabla \cdot (G\vec{u}\psi) = 0$$

homogeneous advection

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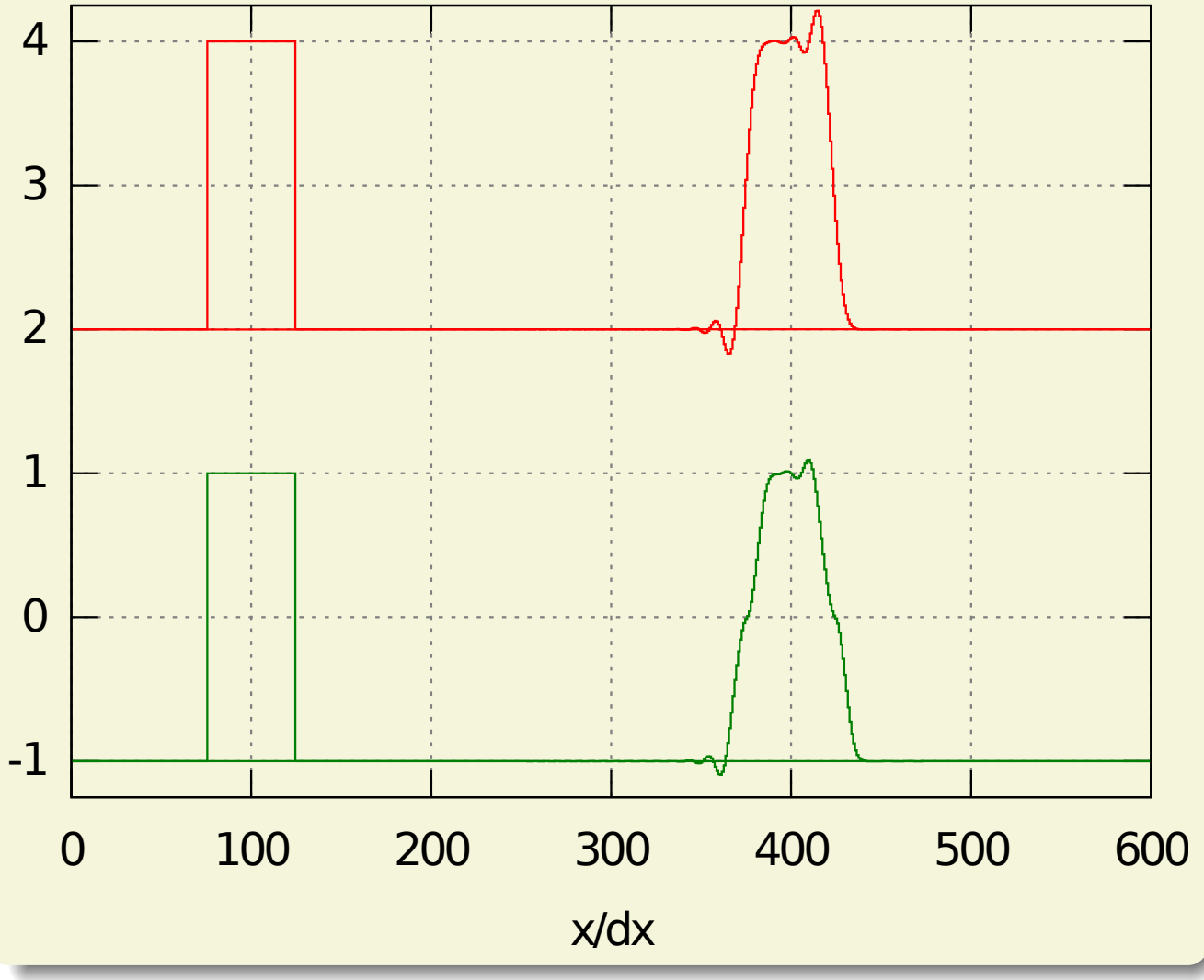
user/test code

example: implemented MPDATA flavours

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



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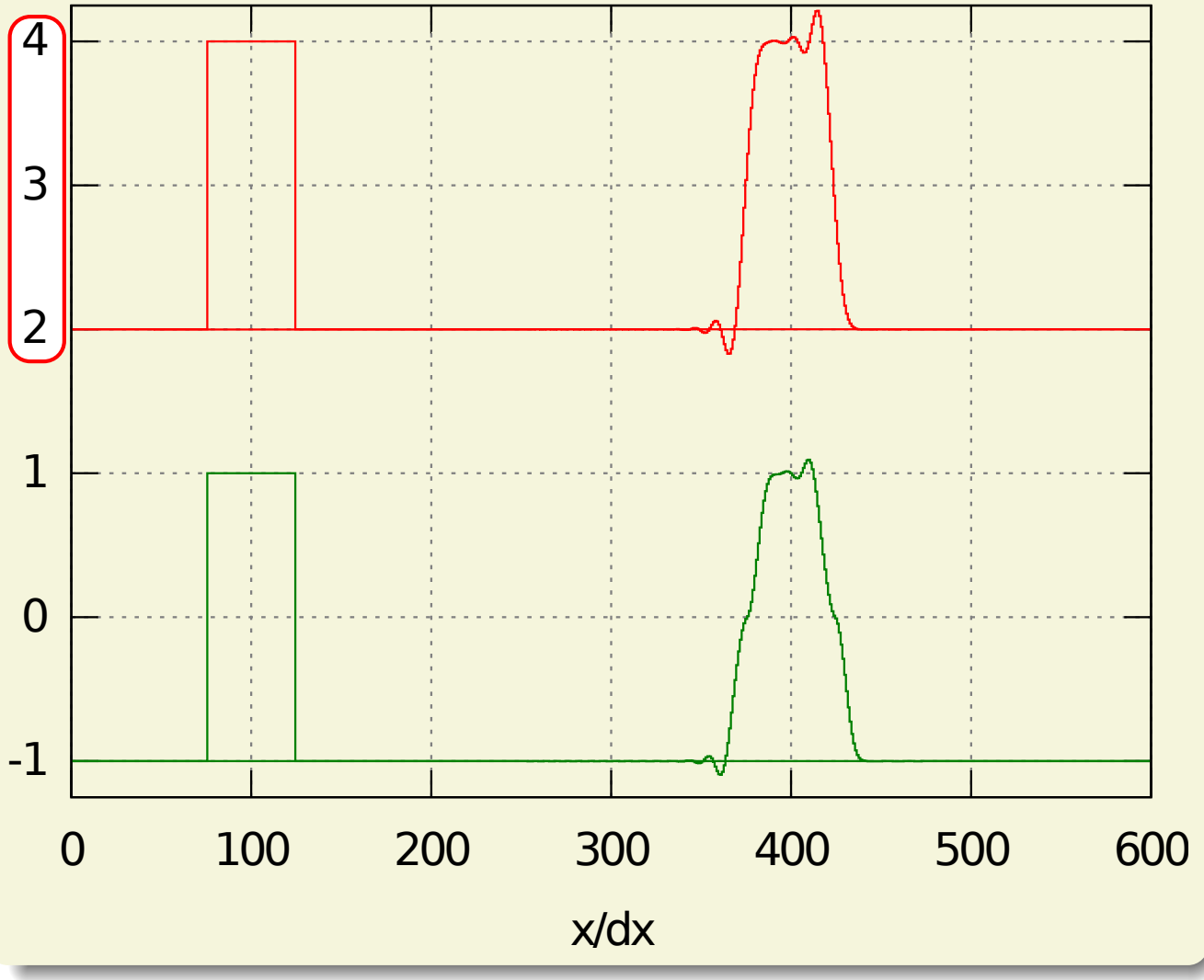

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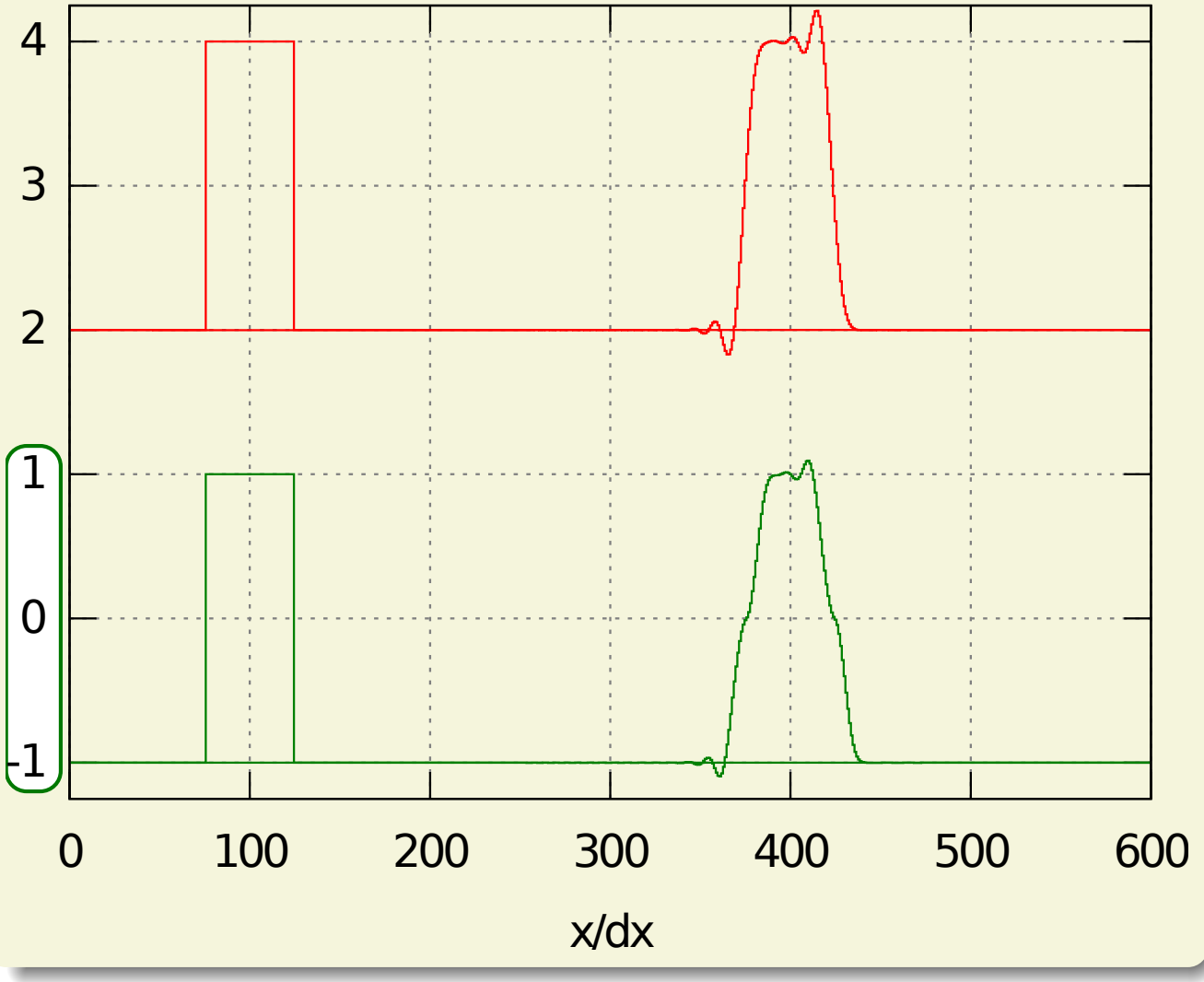

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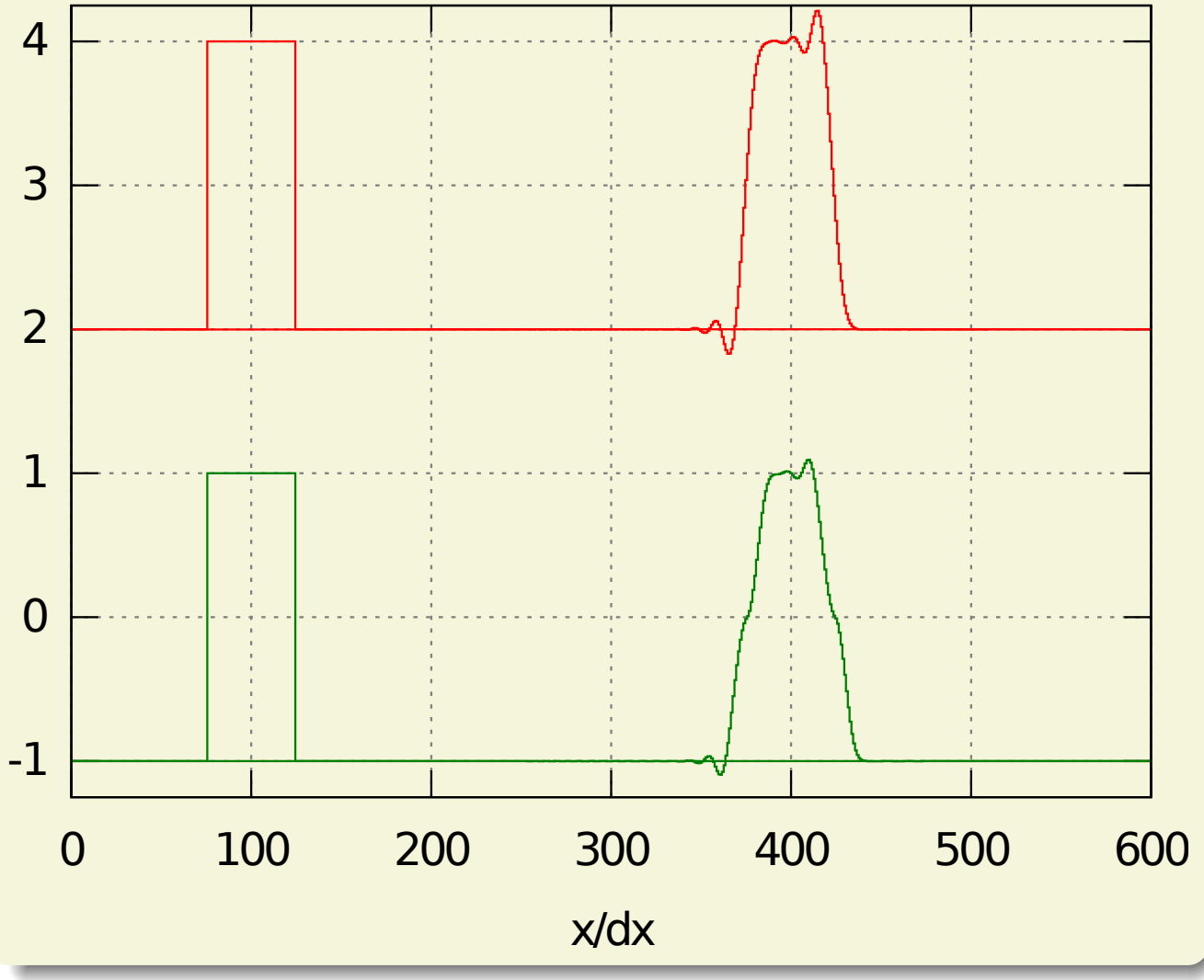

$$\frac{\psi_a - \psi_b}{\psi_a + \psi_b} \approx \frac{|\psi_a| - |\psi_b|}{|\psi_a| + |\psi_b|}$$

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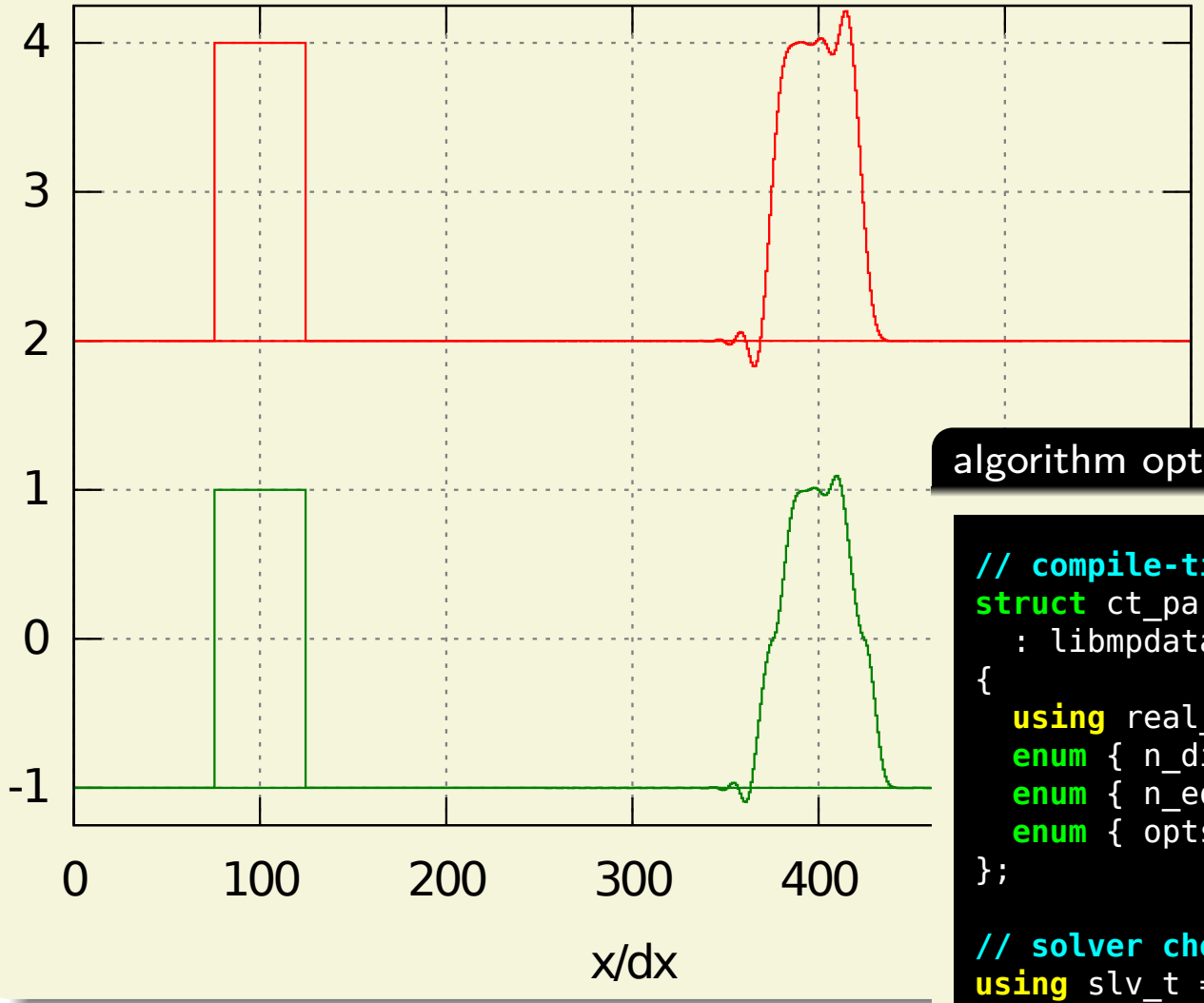

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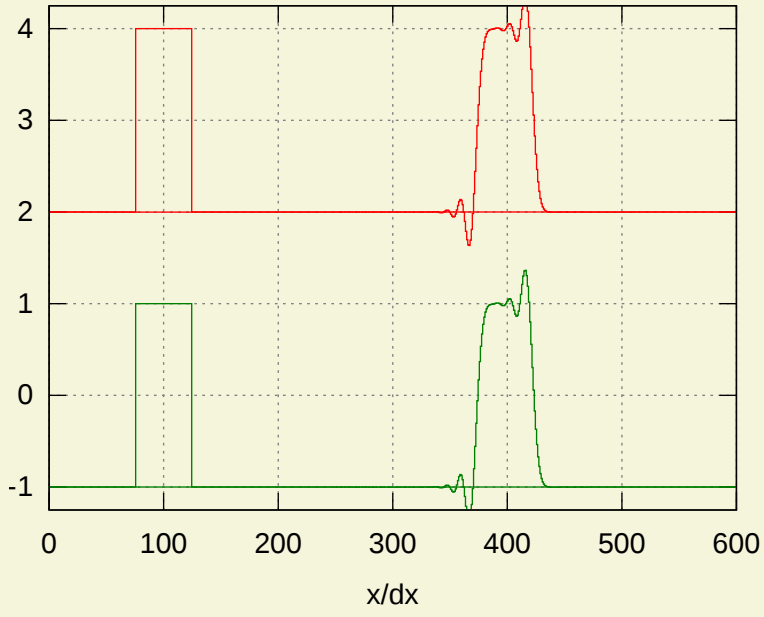
algorithm option as a compile-time parameter

```
// 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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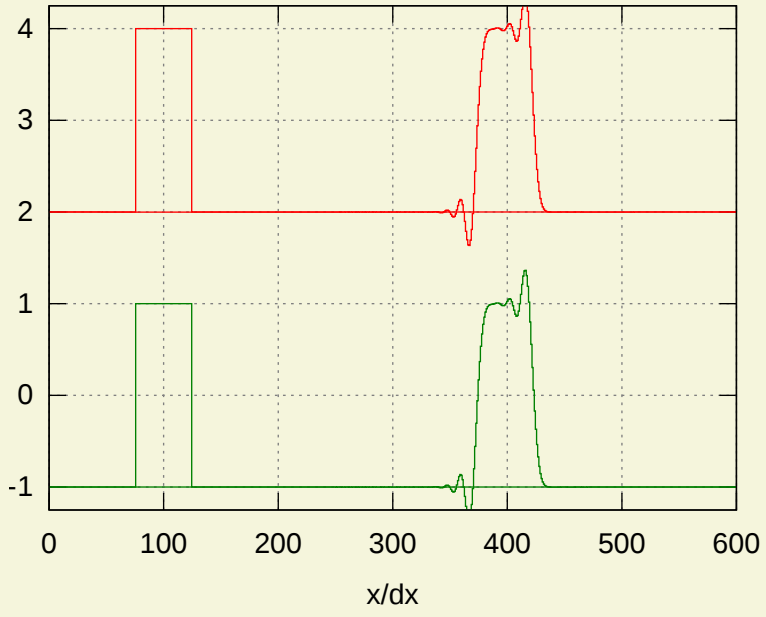
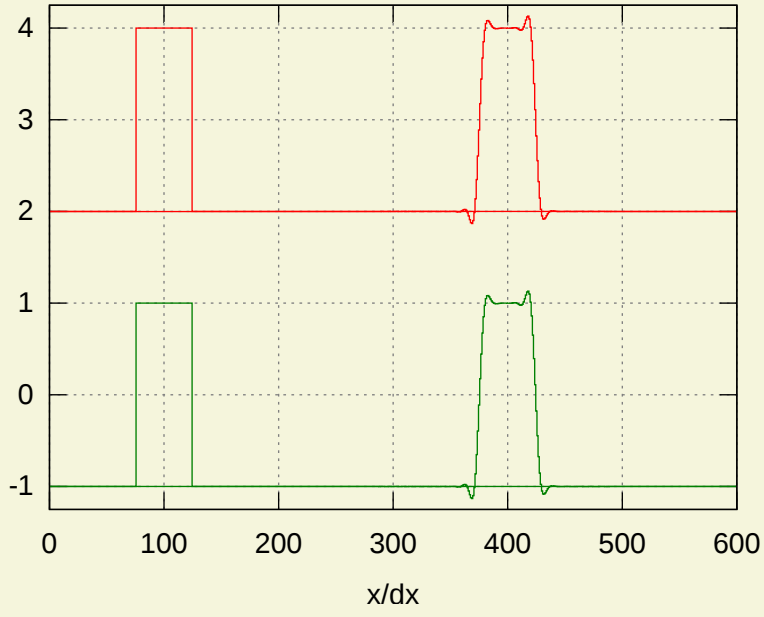


iga + 3rd-order-accurate variant ("tot")



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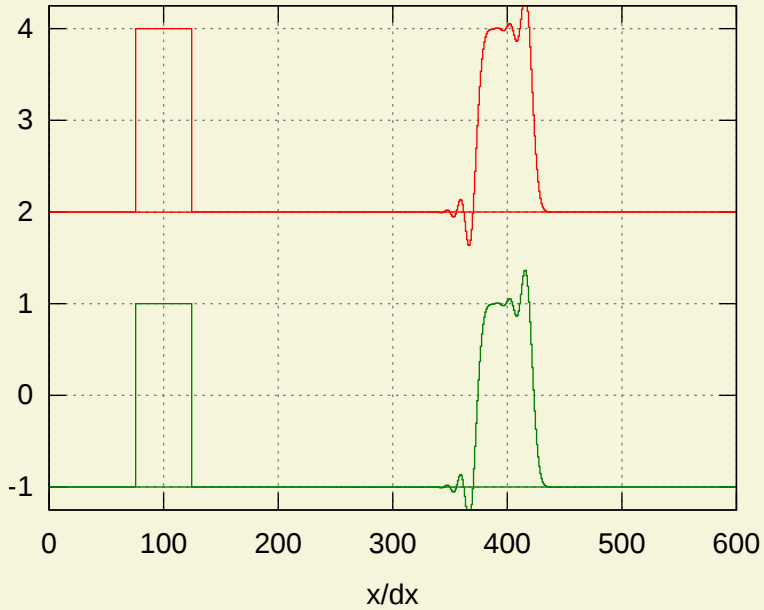

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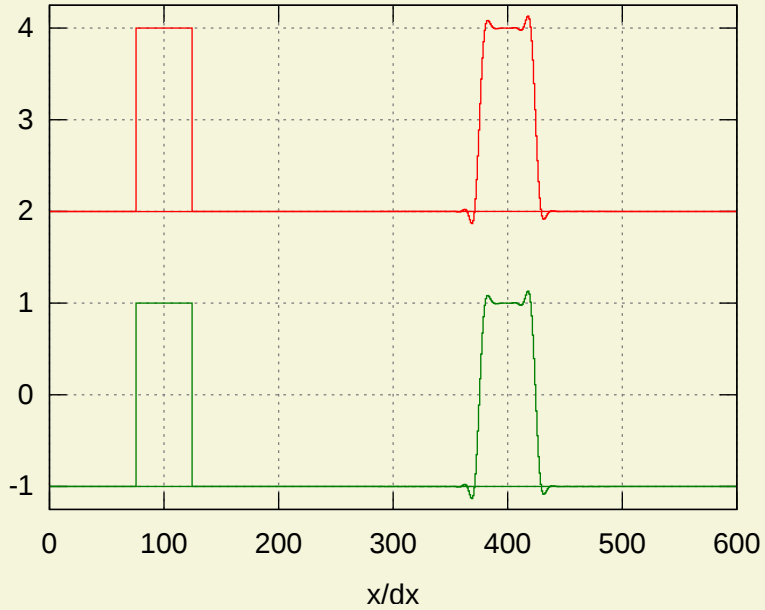

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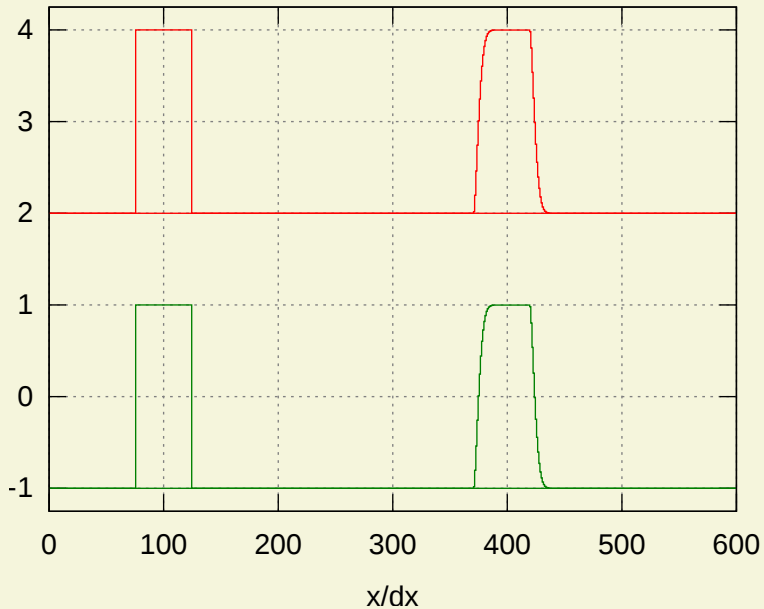

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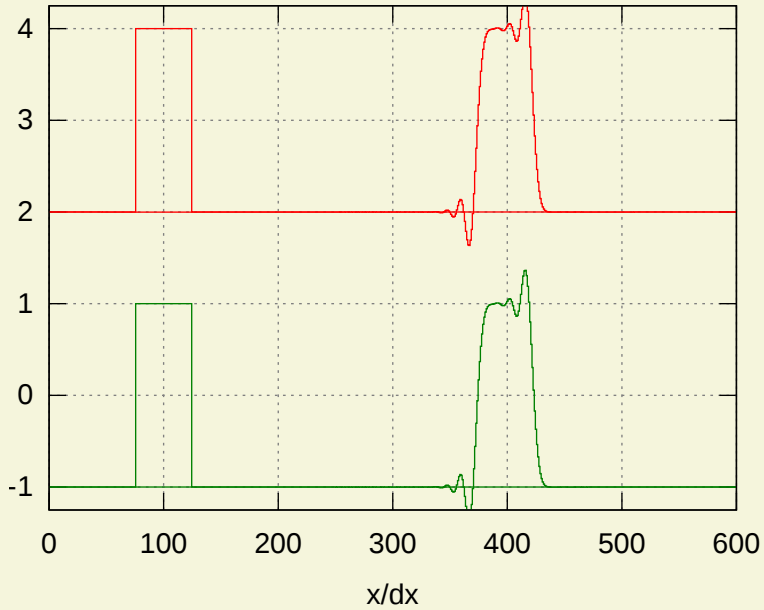

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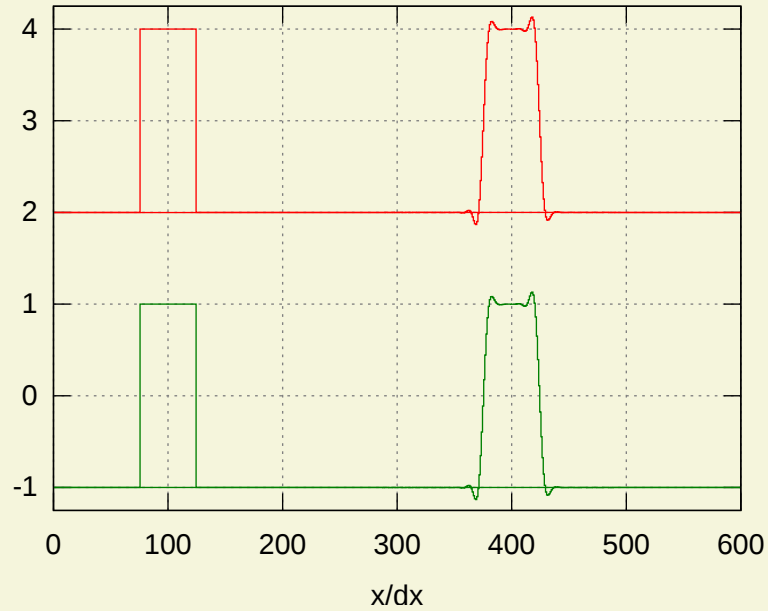

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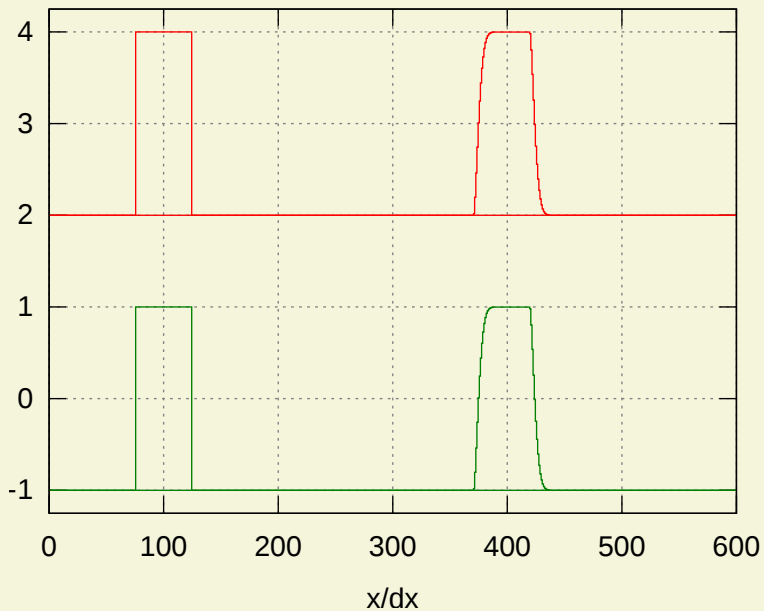

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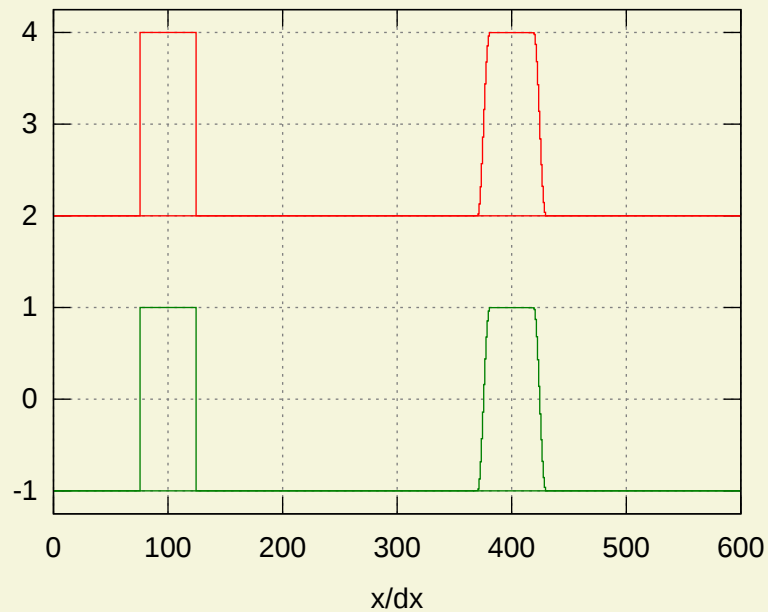

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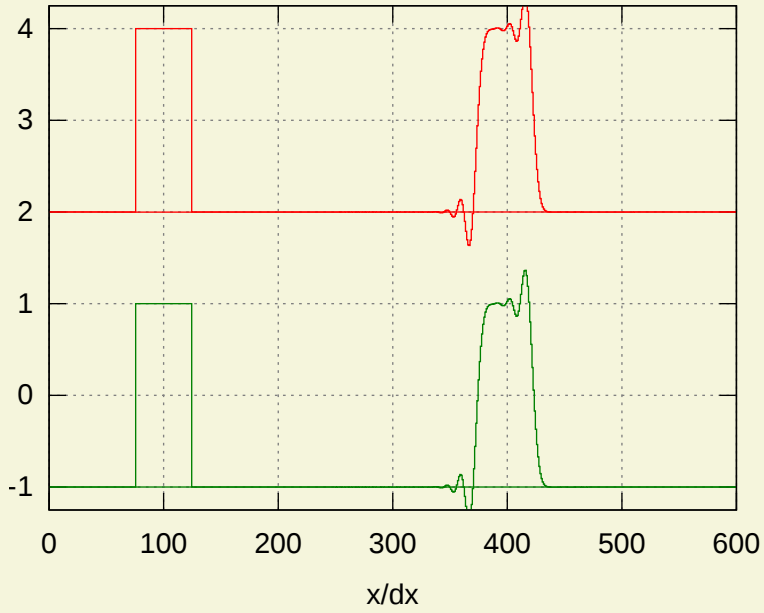

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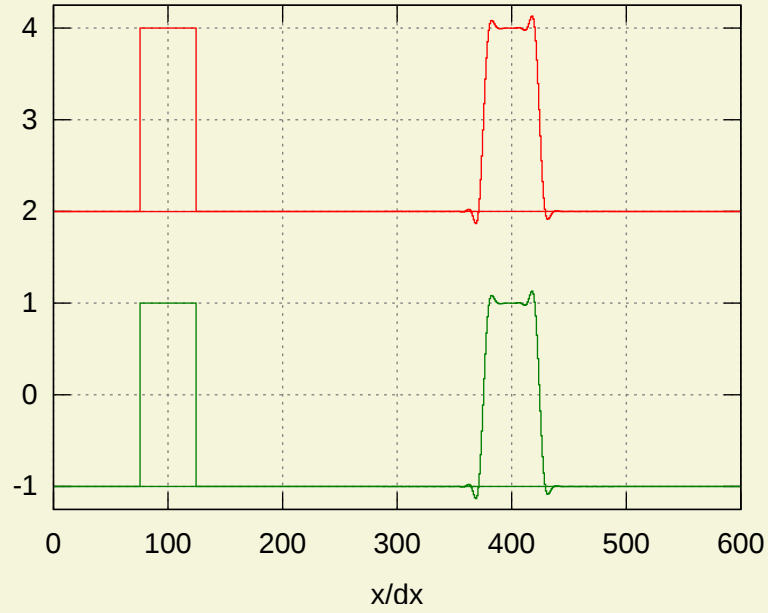

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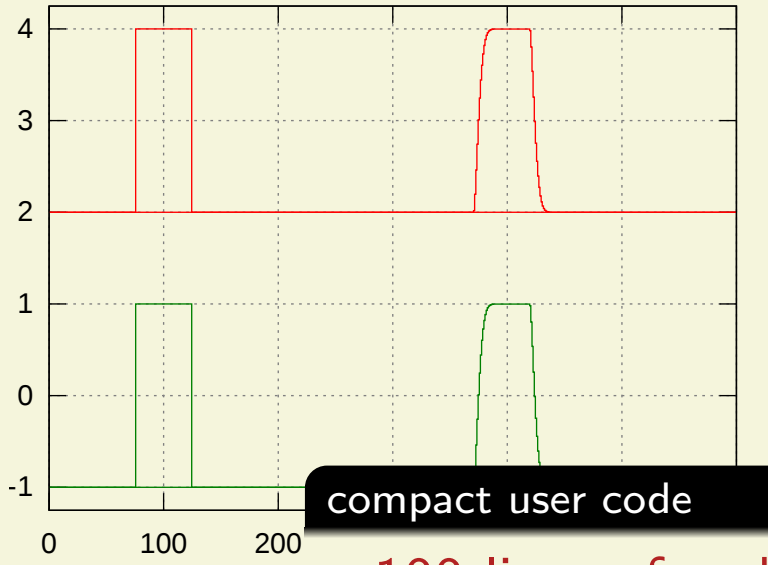

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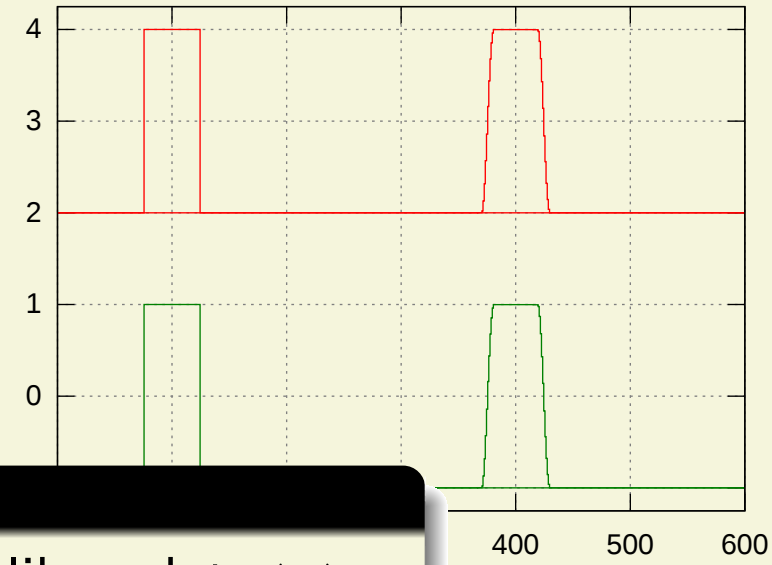
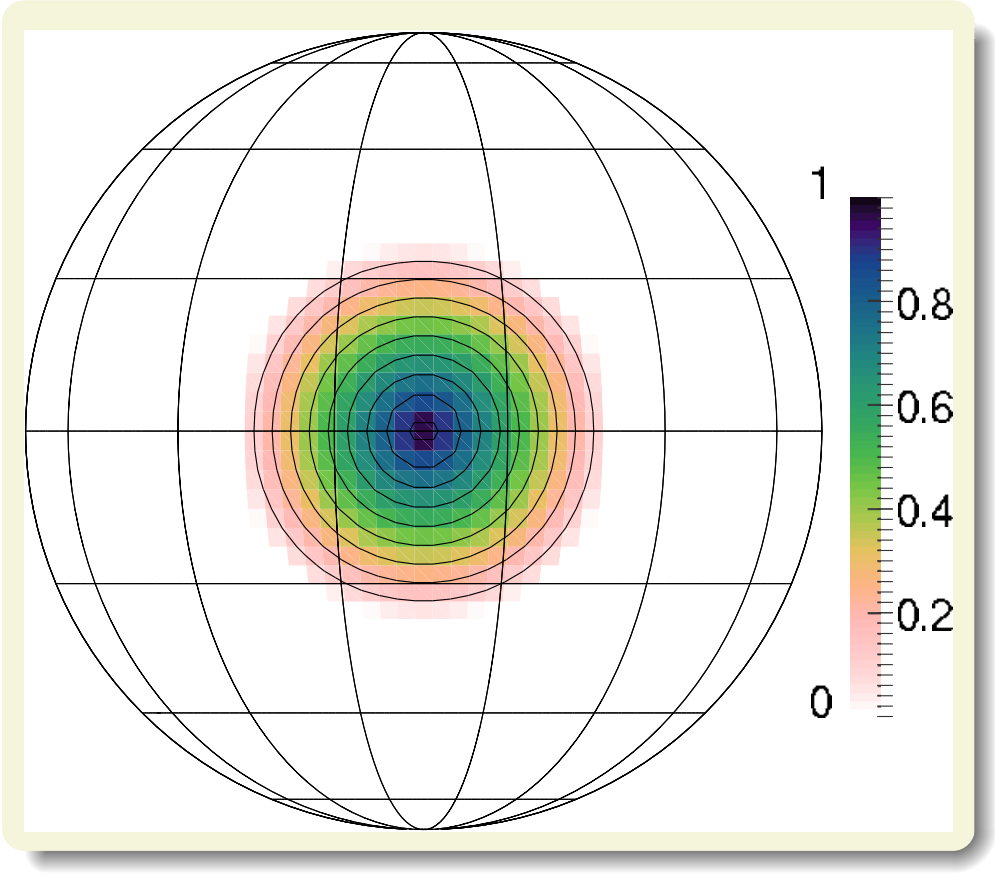


compact user code

<100 lines of code with libmpdata++

example: 2D advection on a sphere



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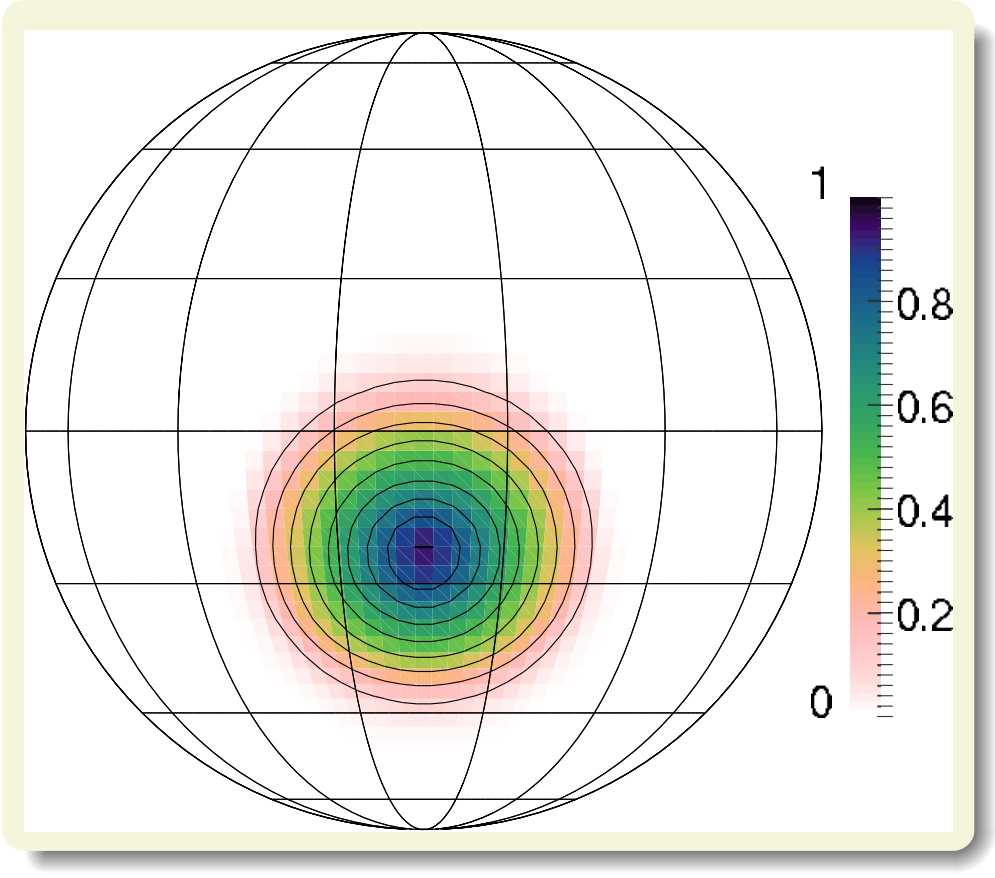

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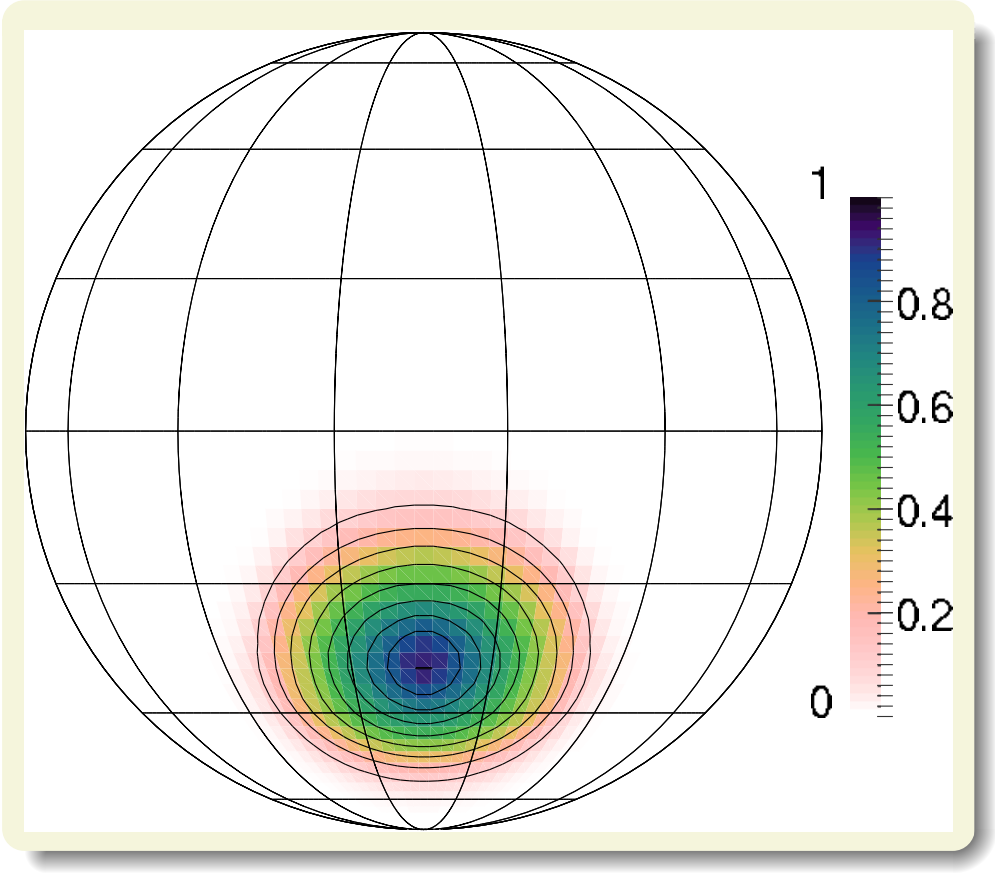

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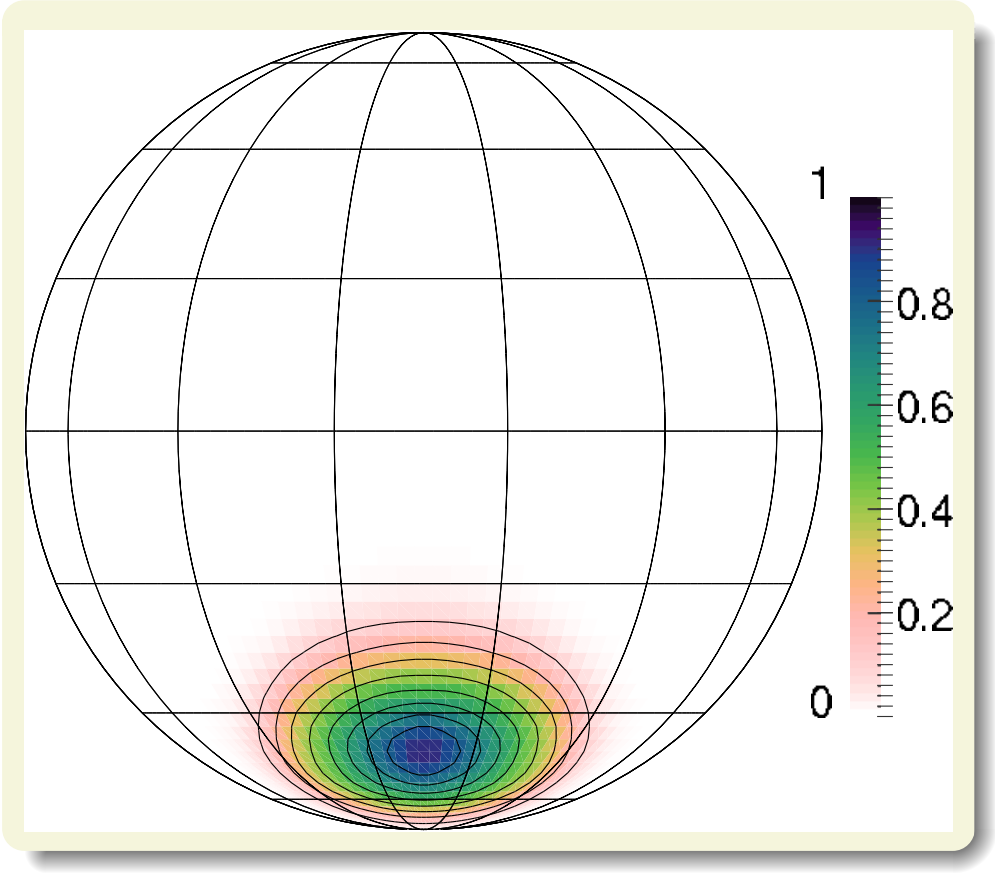

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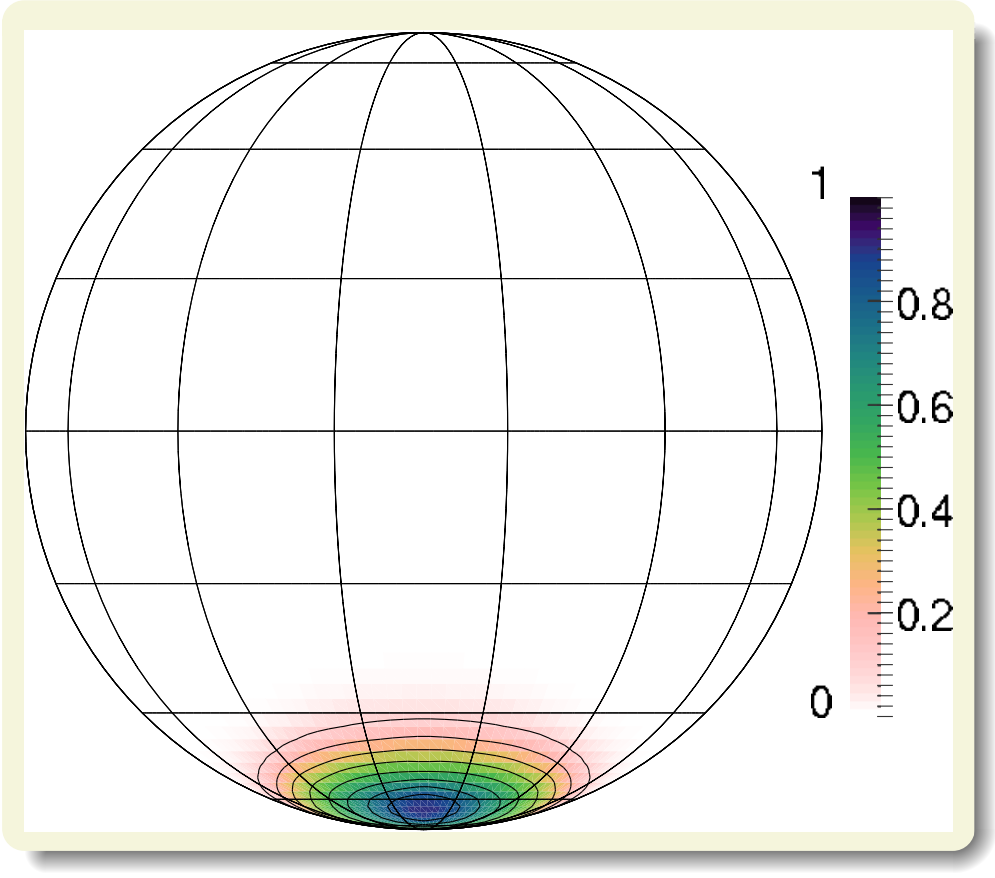

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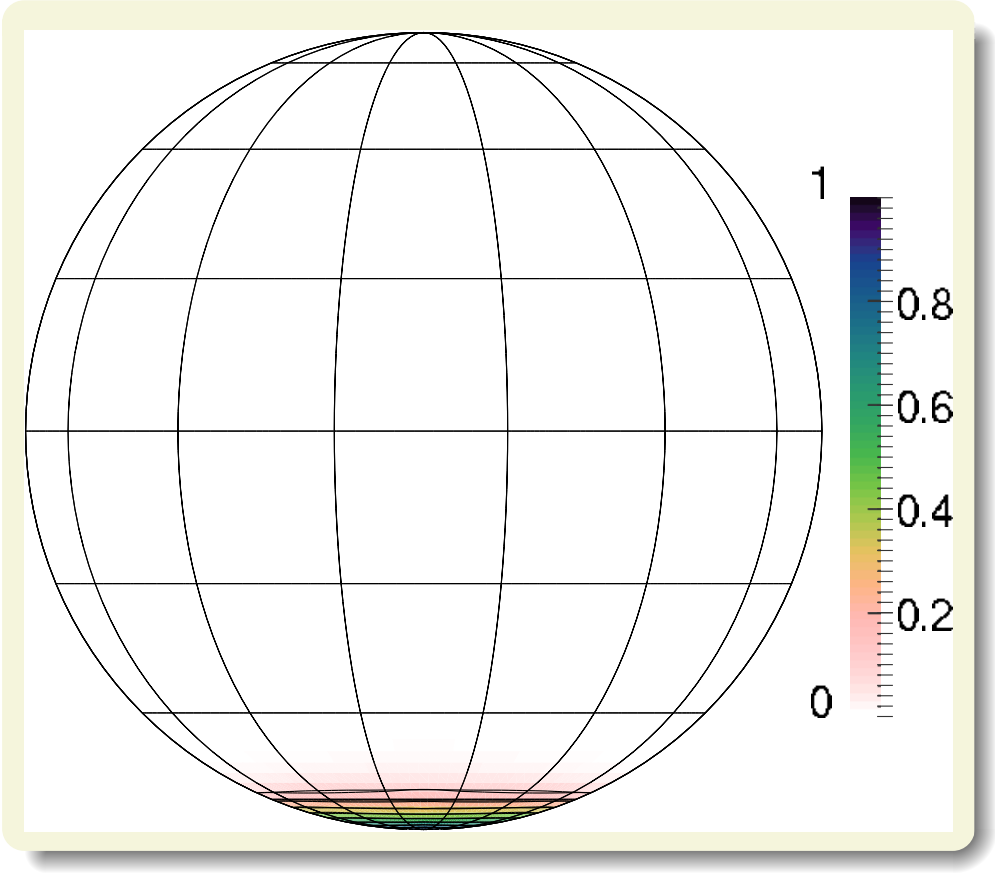

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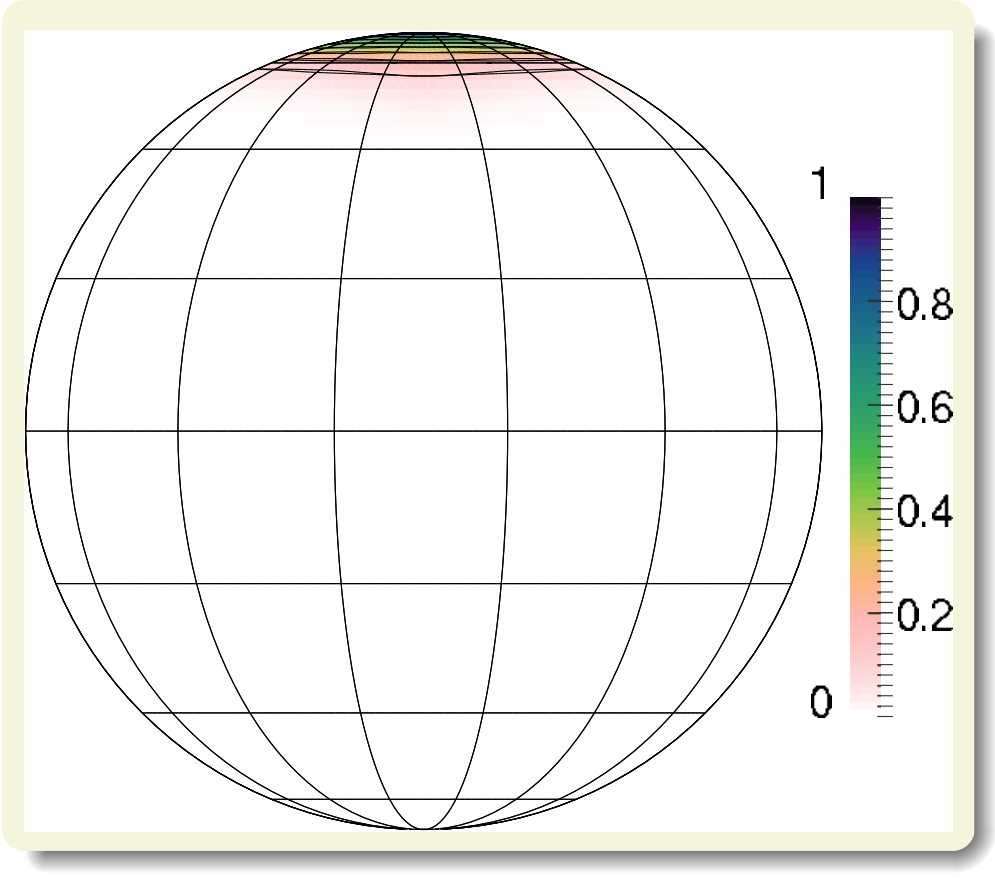

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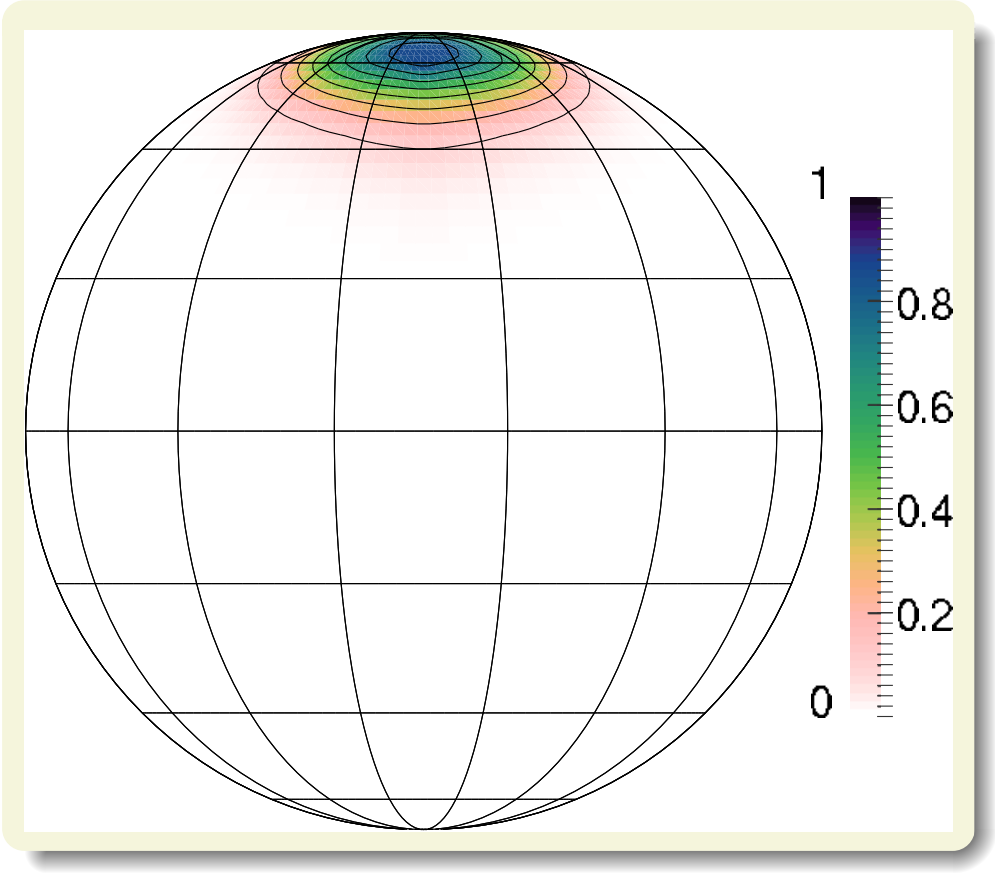

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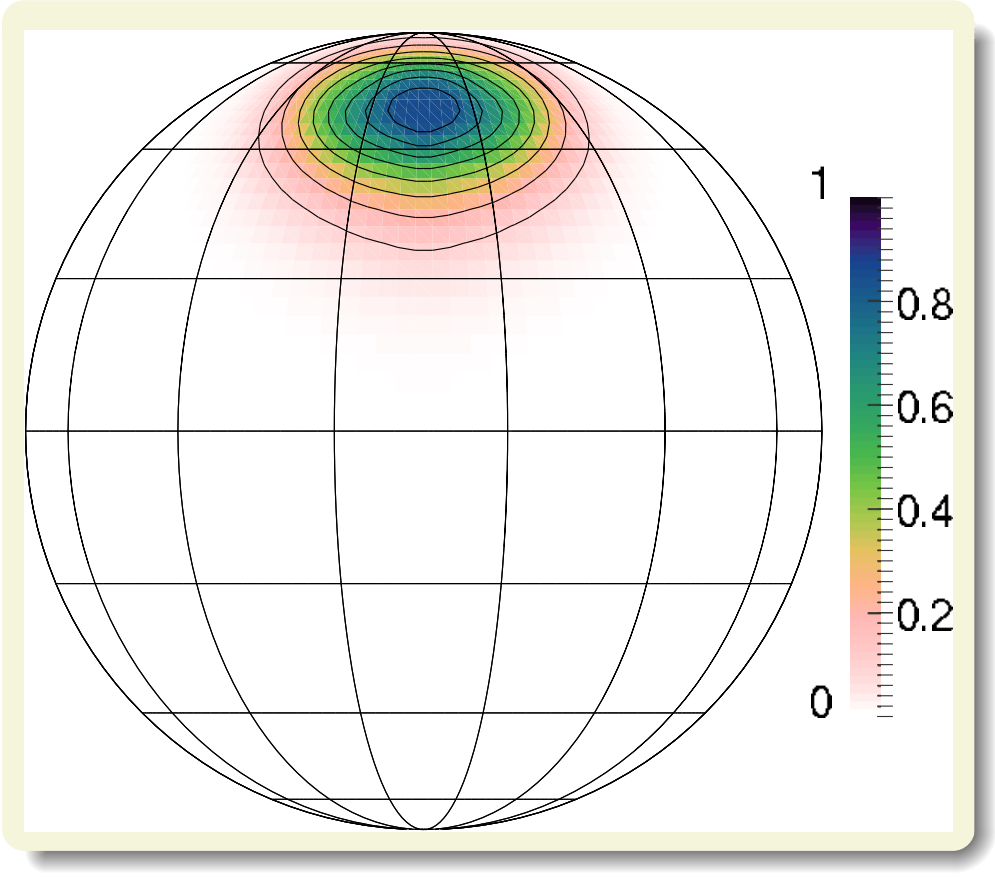

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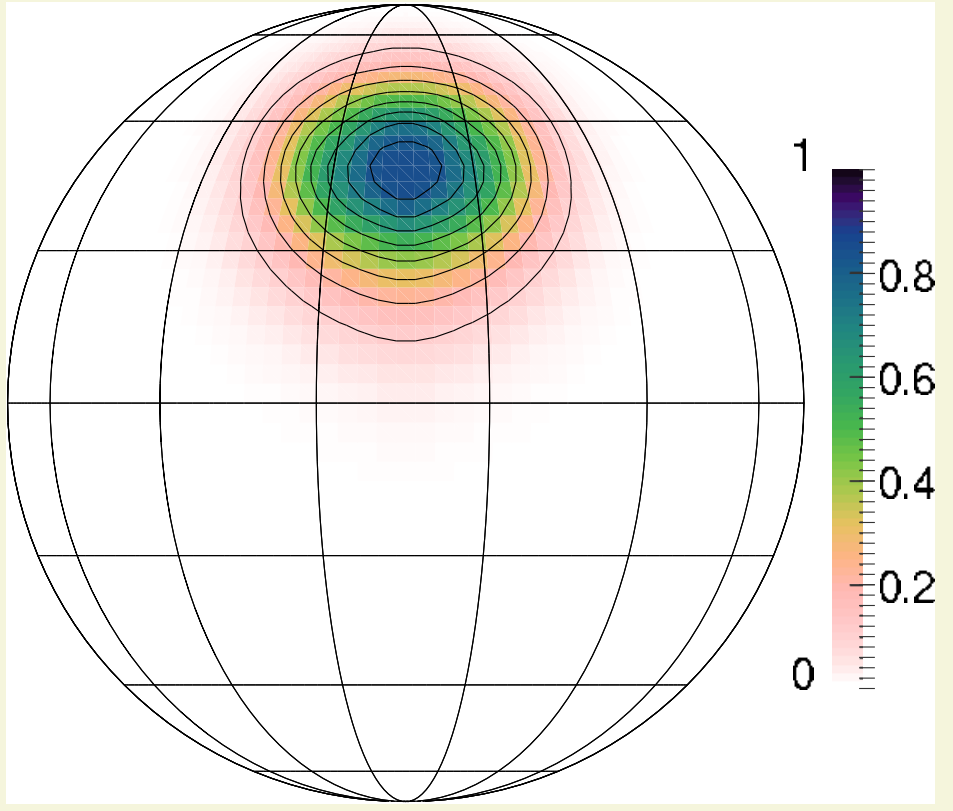

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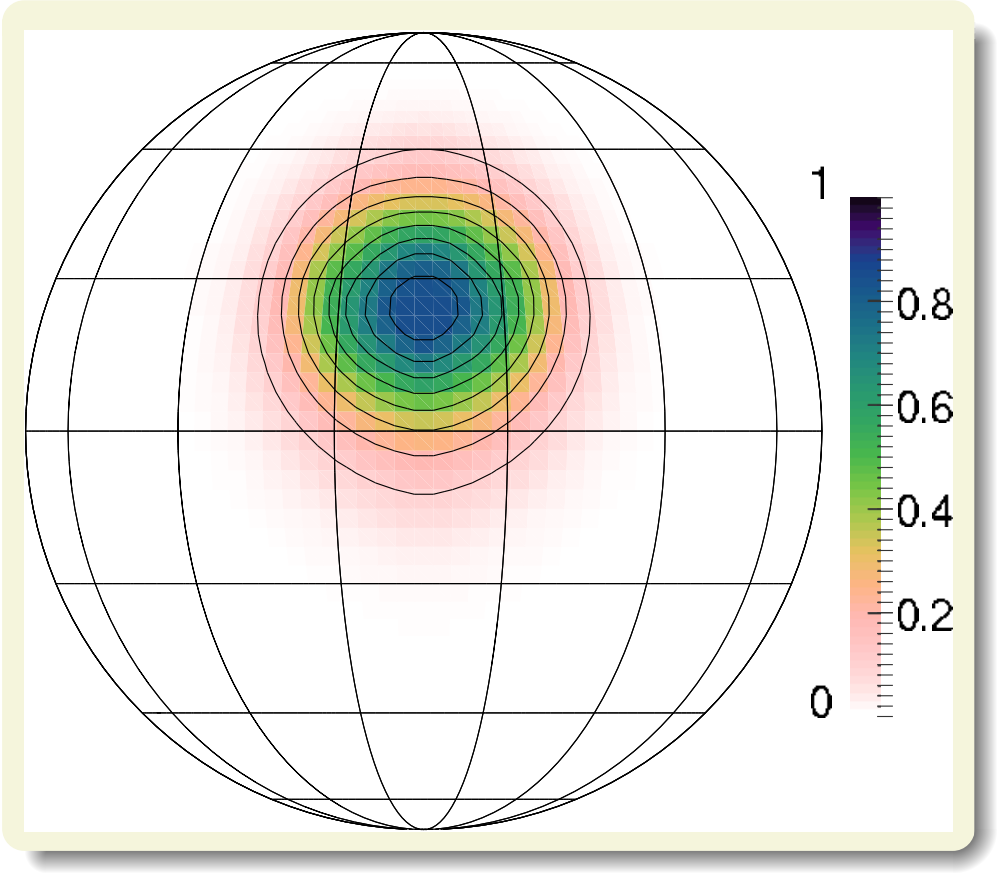

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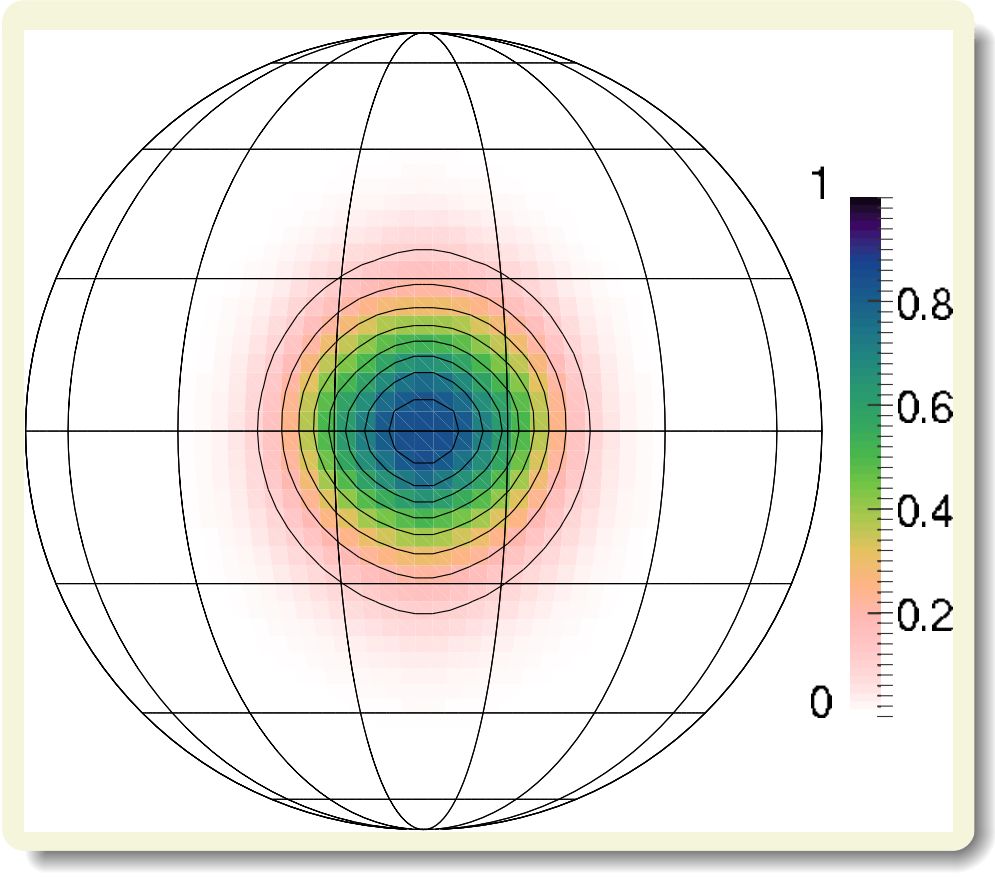

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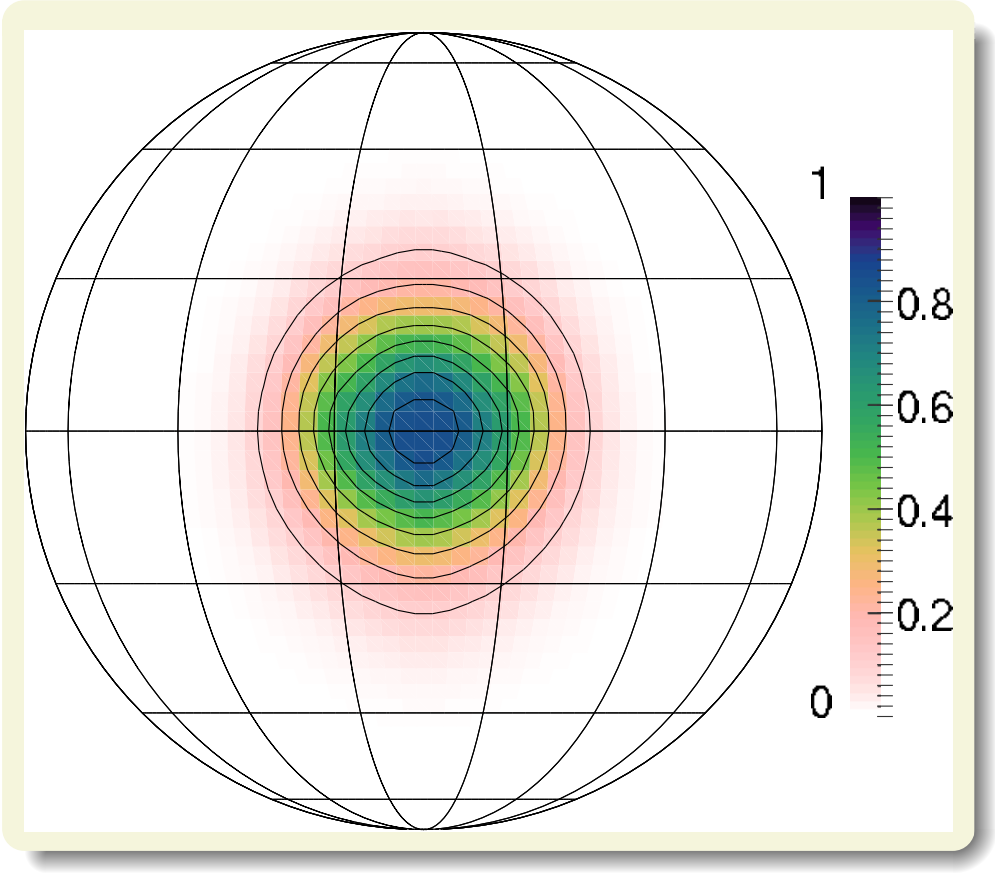

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+

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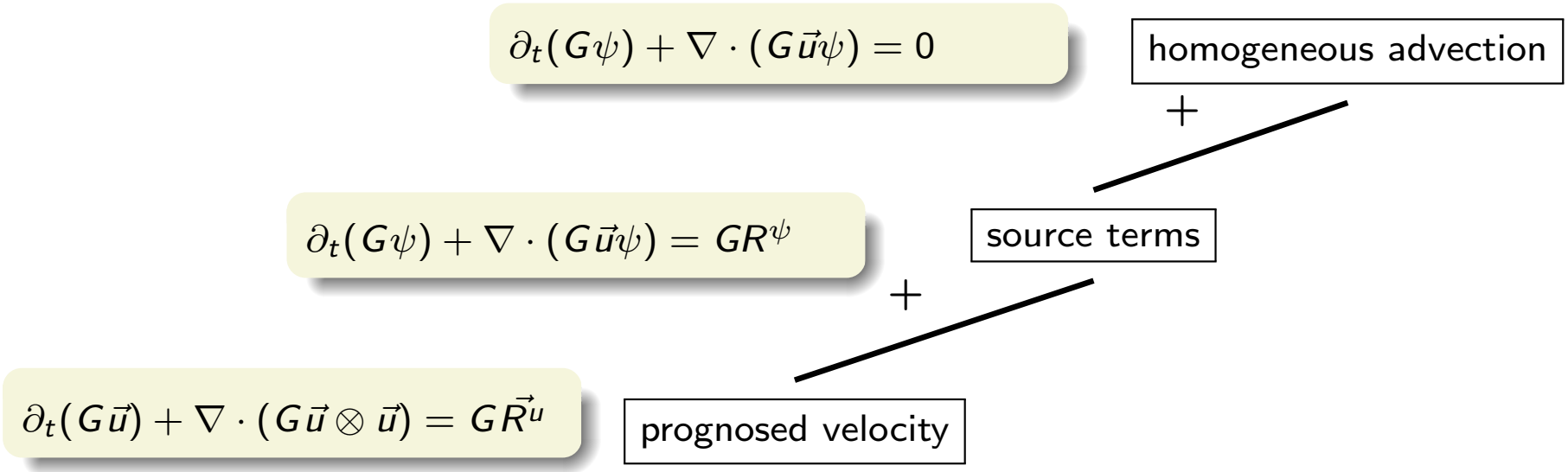
source terms

building blocks of libmpdata++



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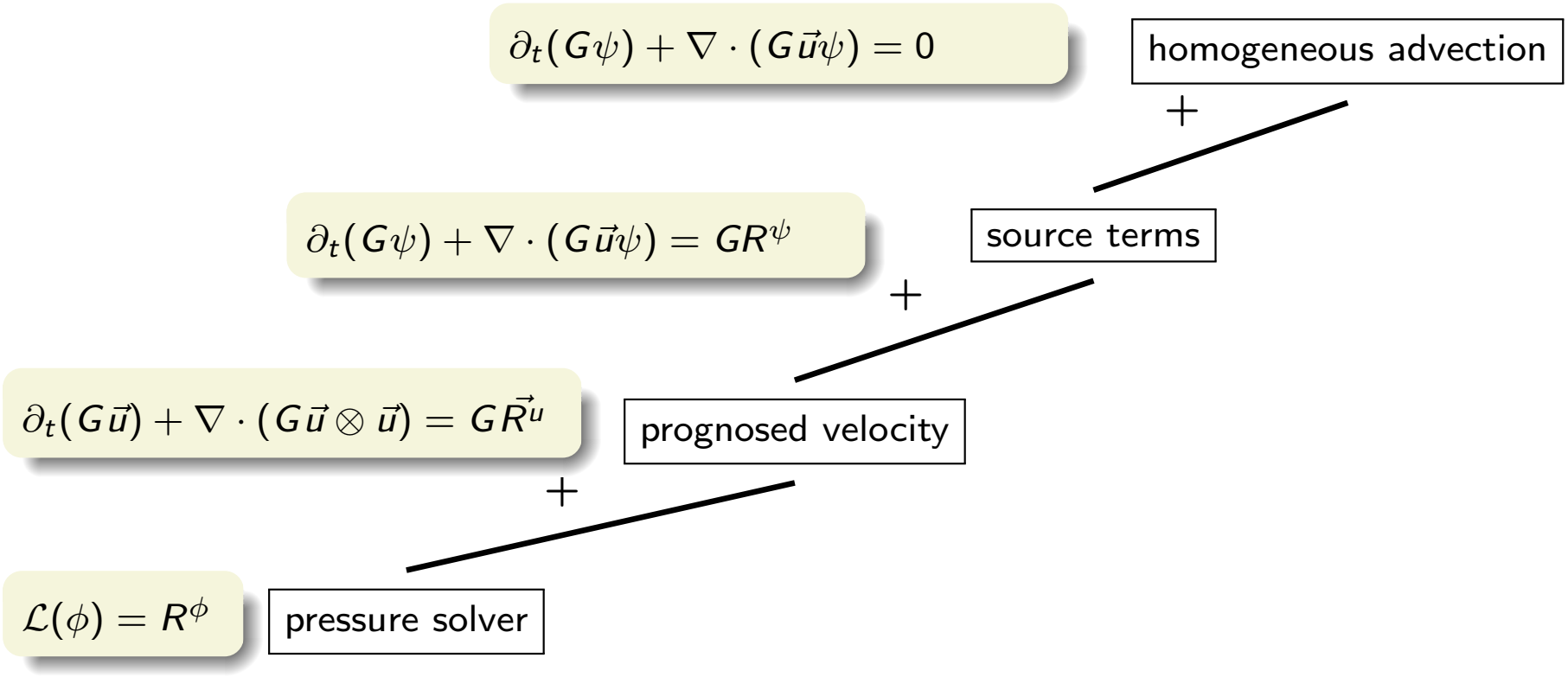

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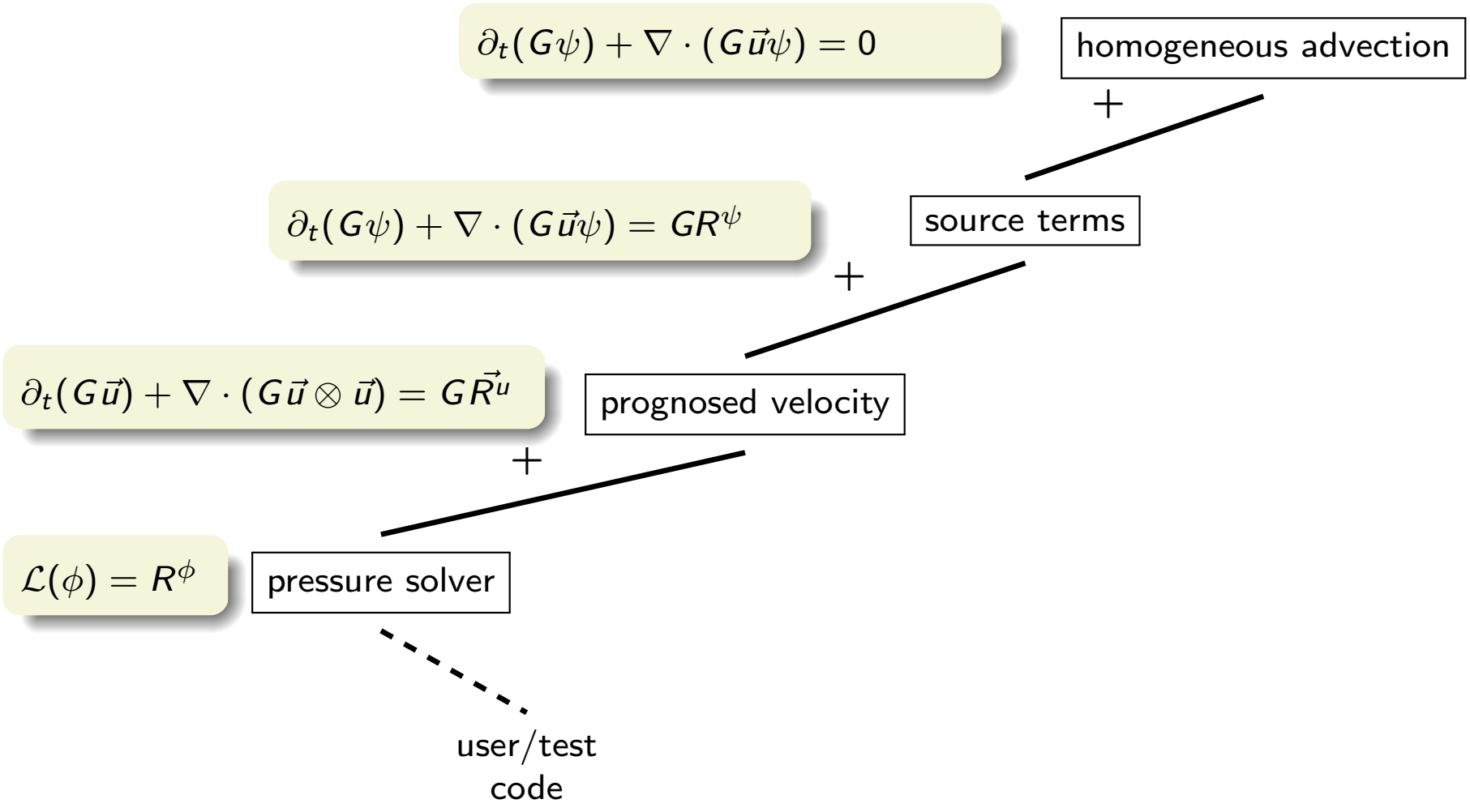

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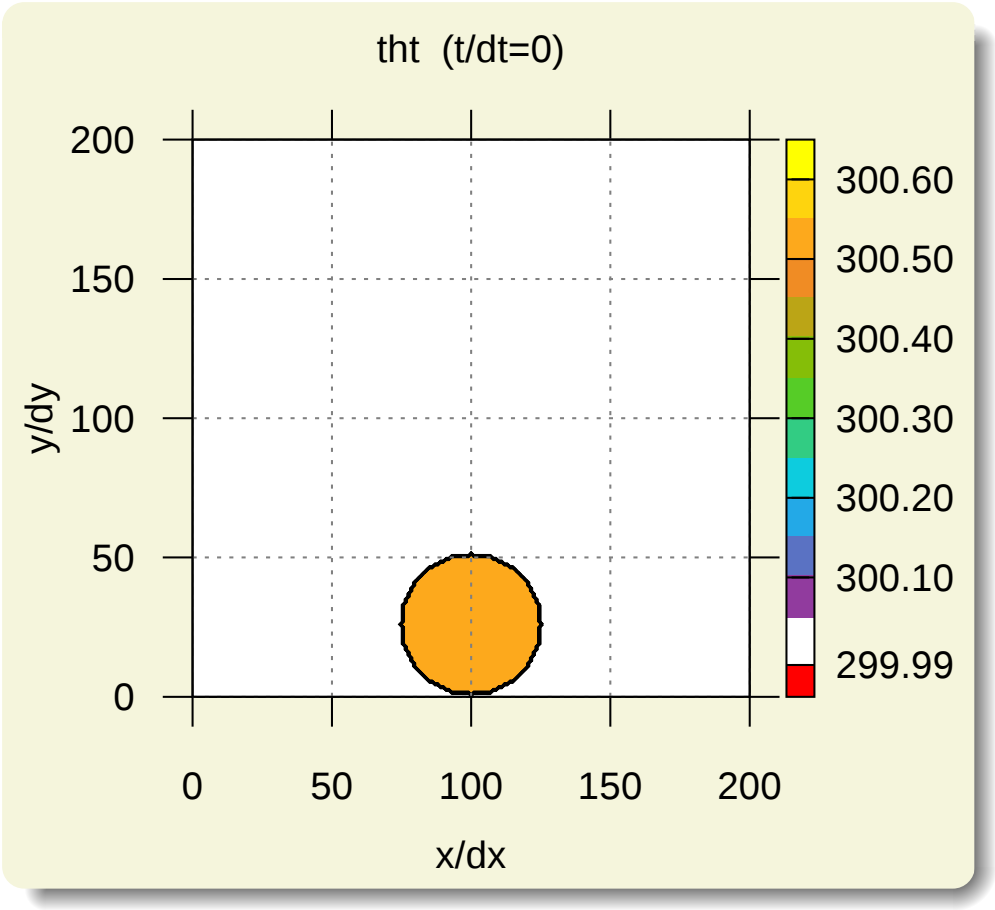

- reproduced experiment of Smolarkiewicz and Pudykiewicz, 1992

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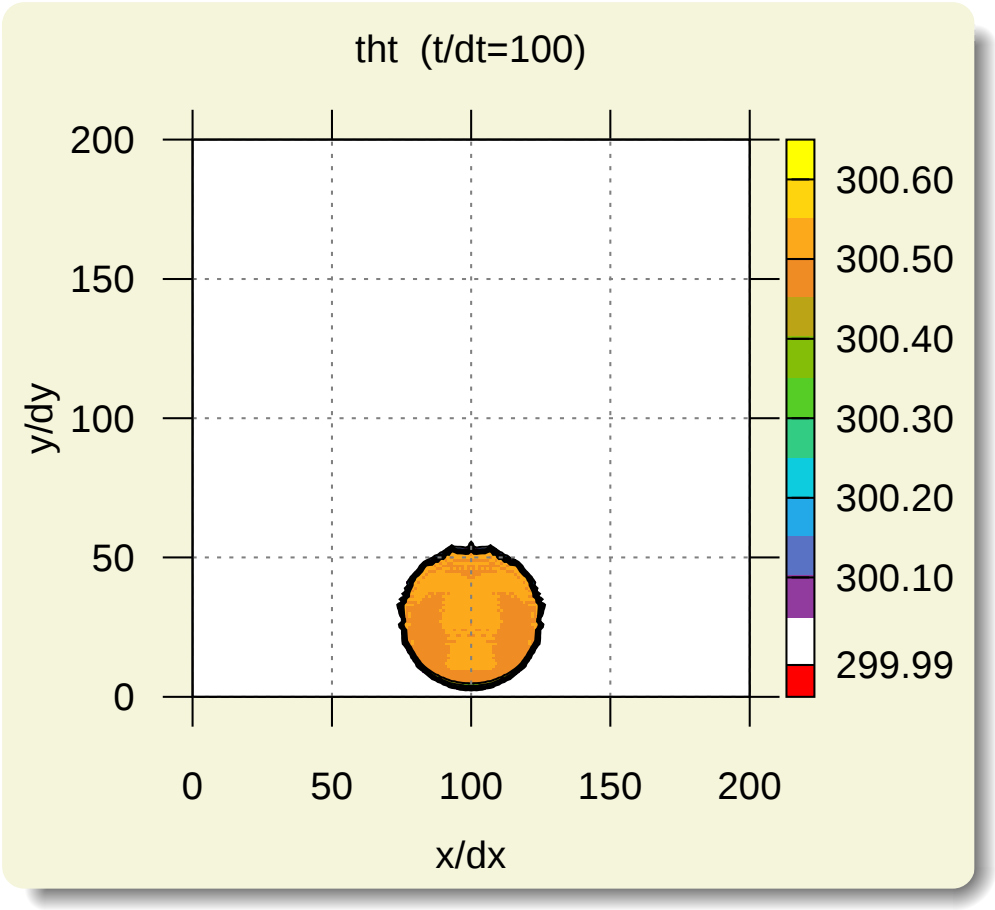

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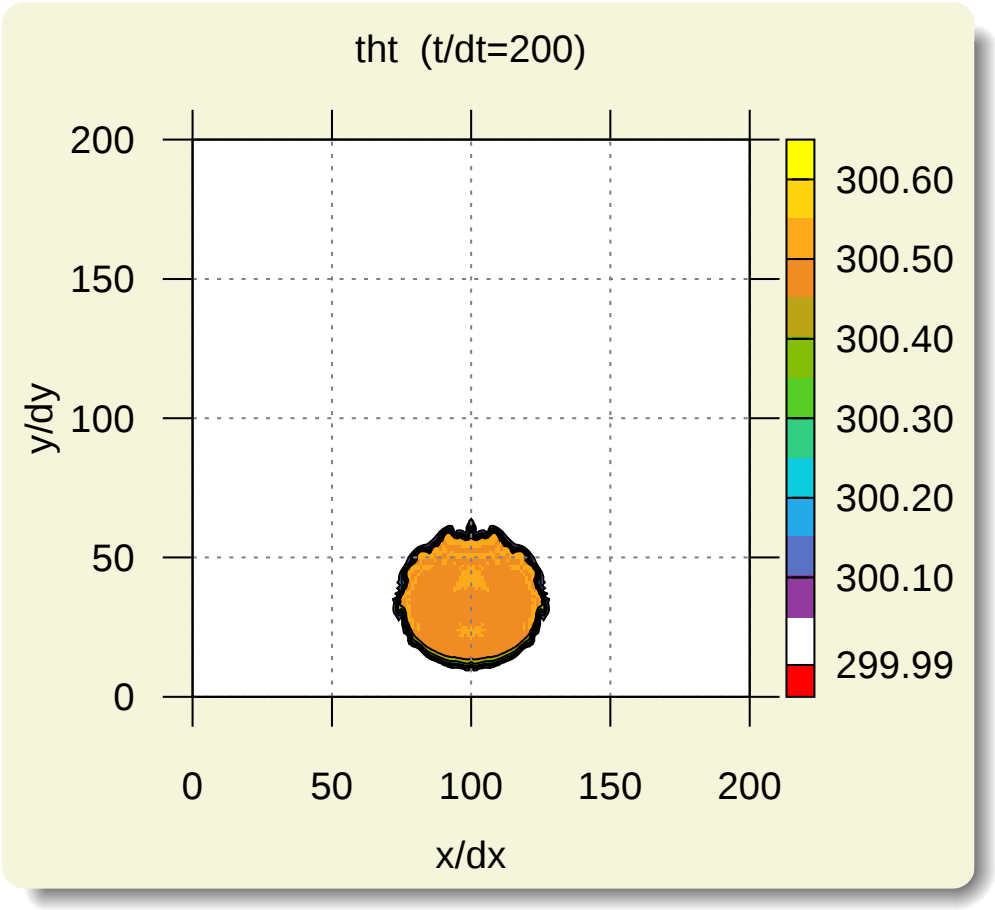

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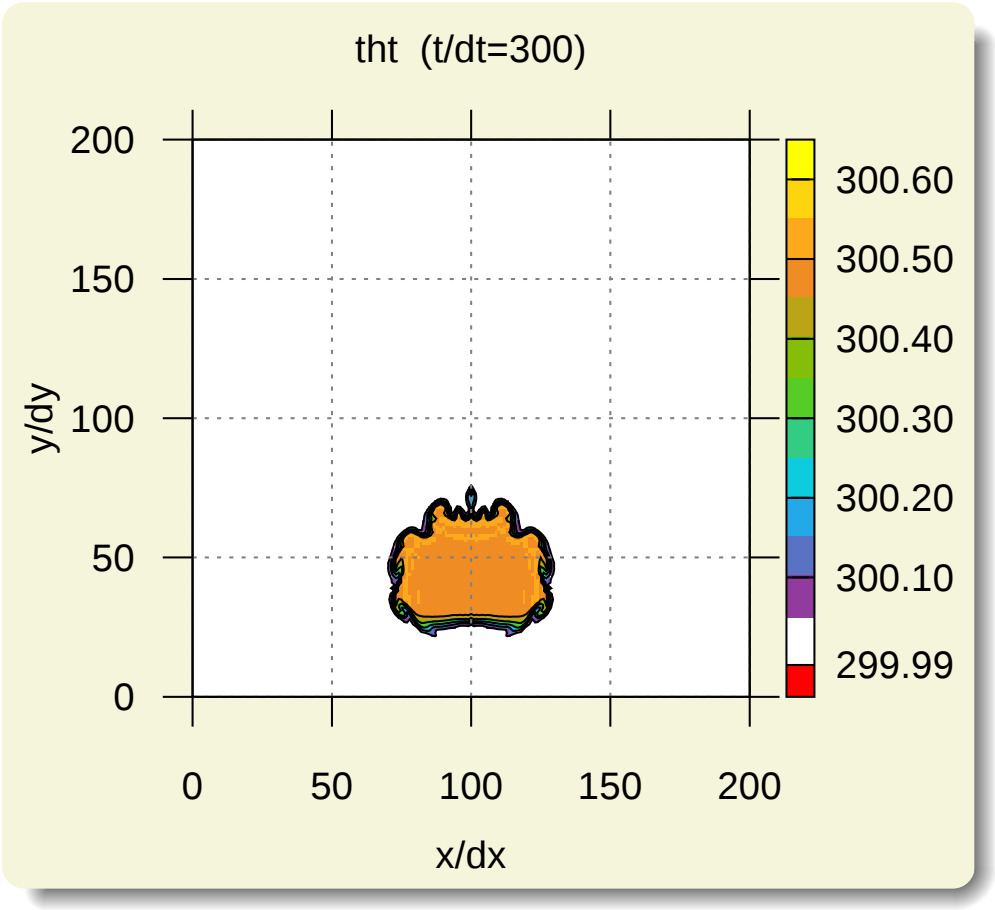

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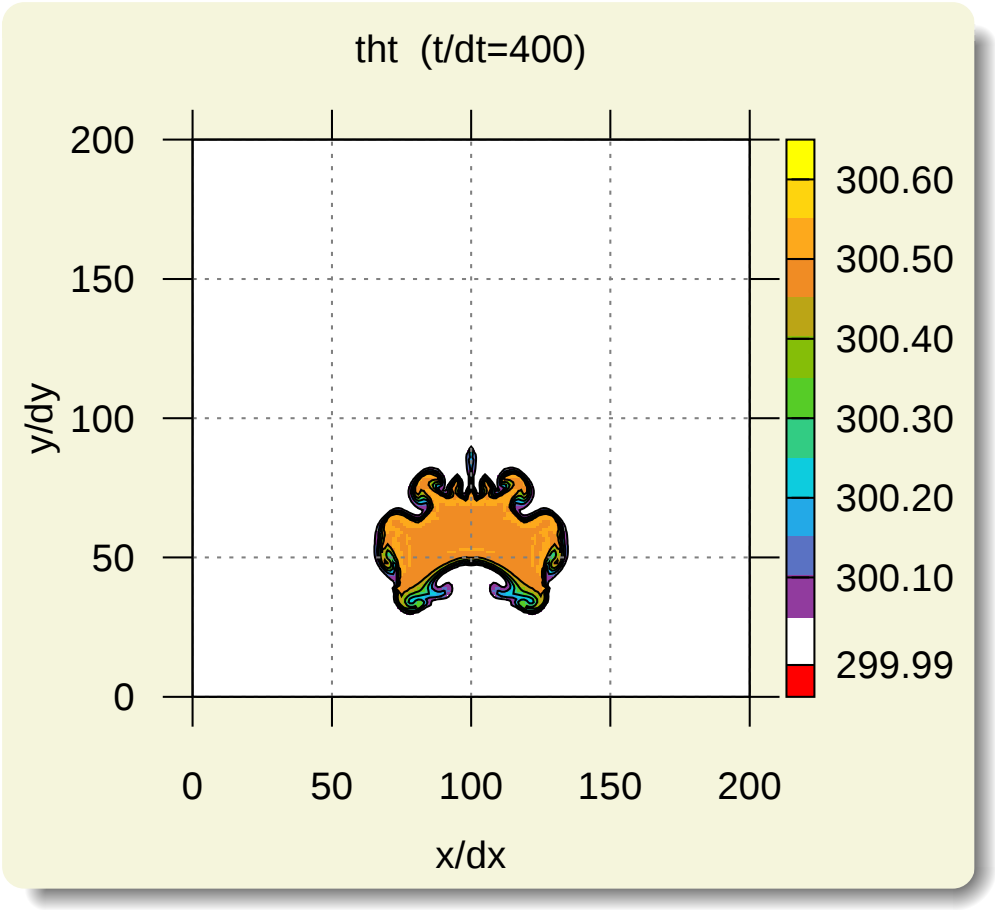
example: 2D Boussinesq convection



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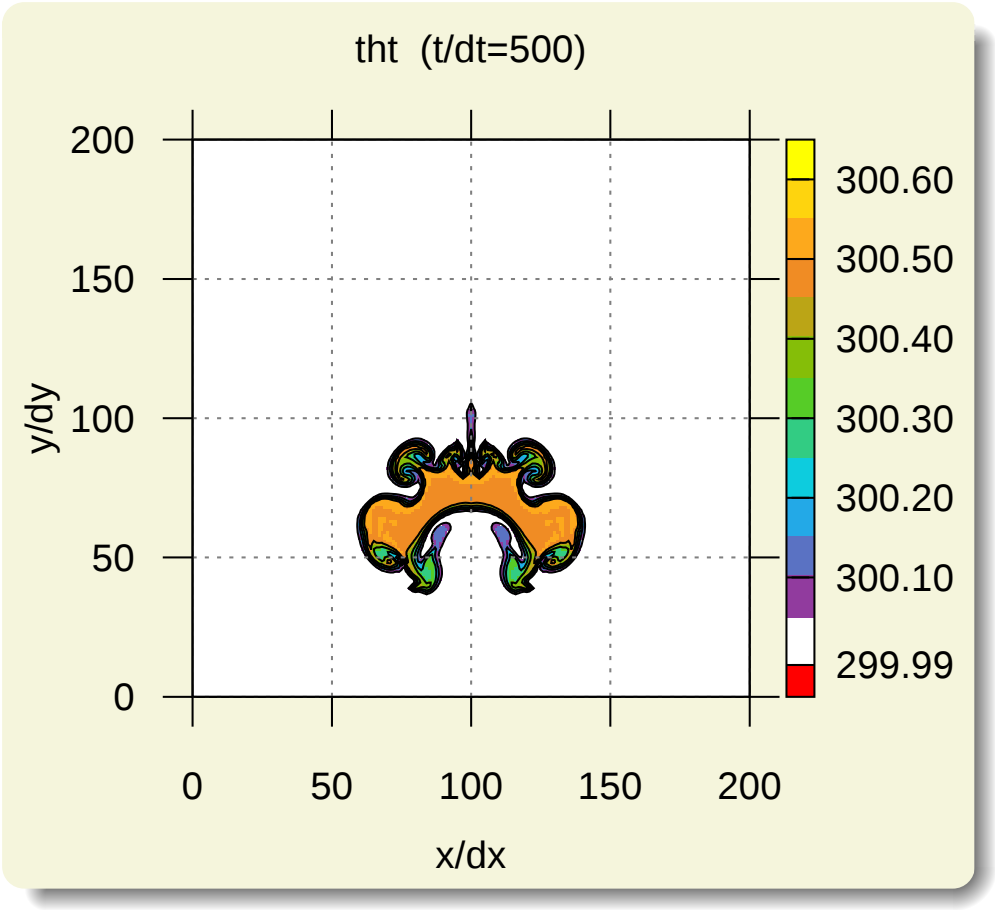

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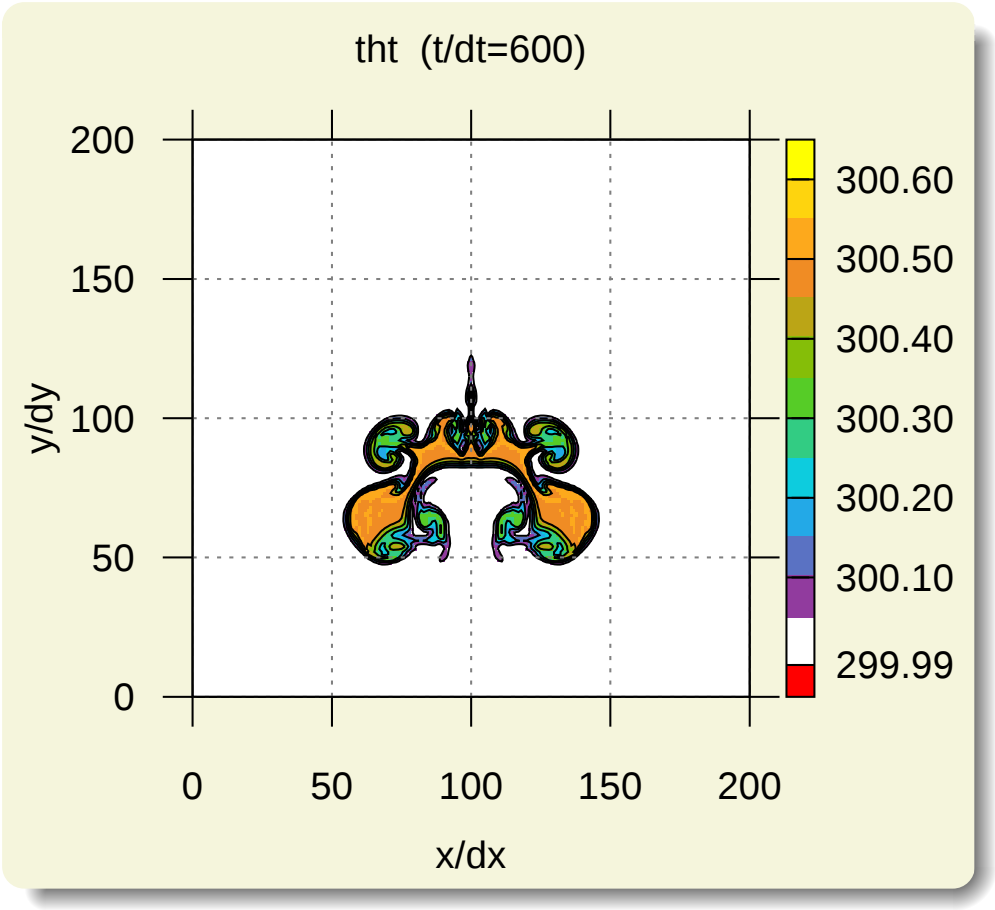

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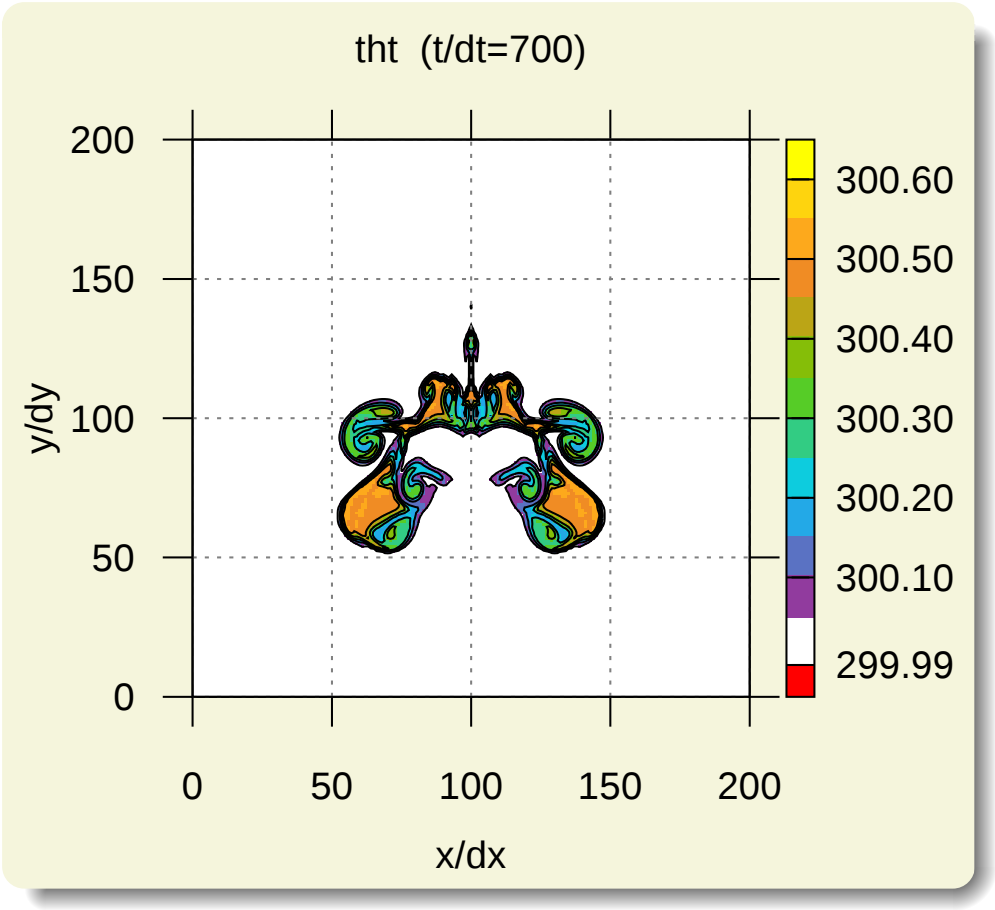

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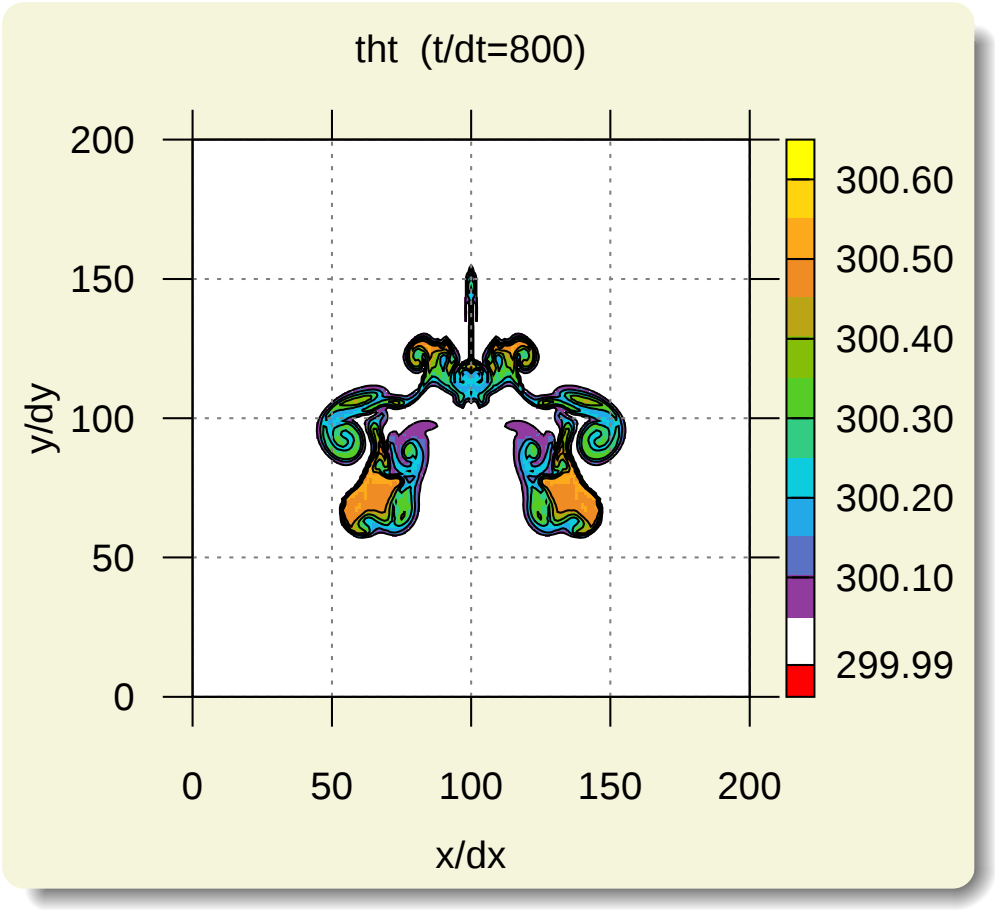

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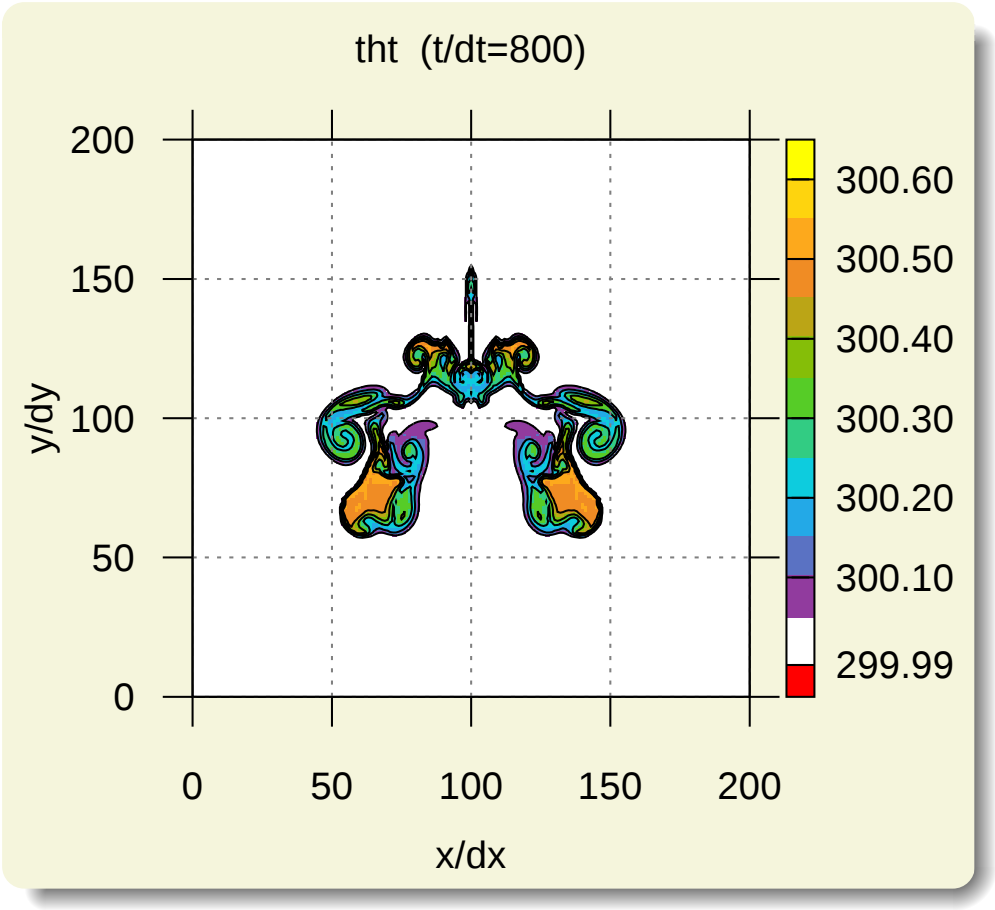

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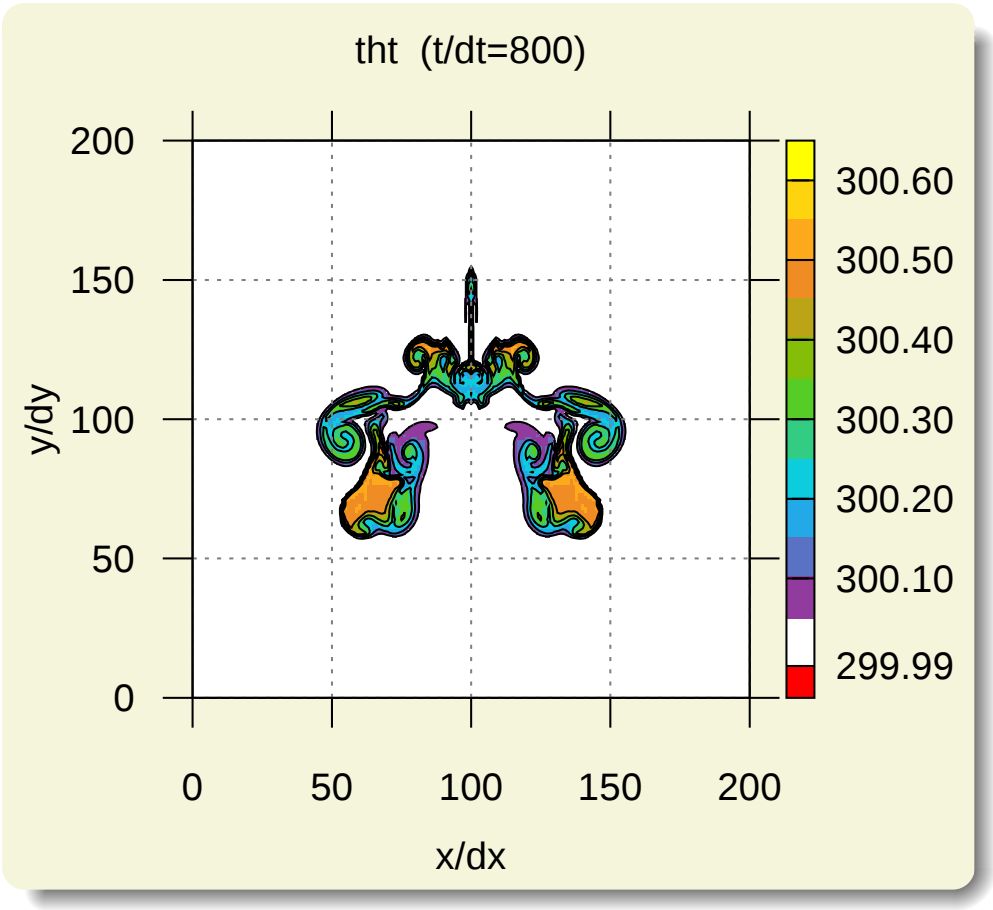

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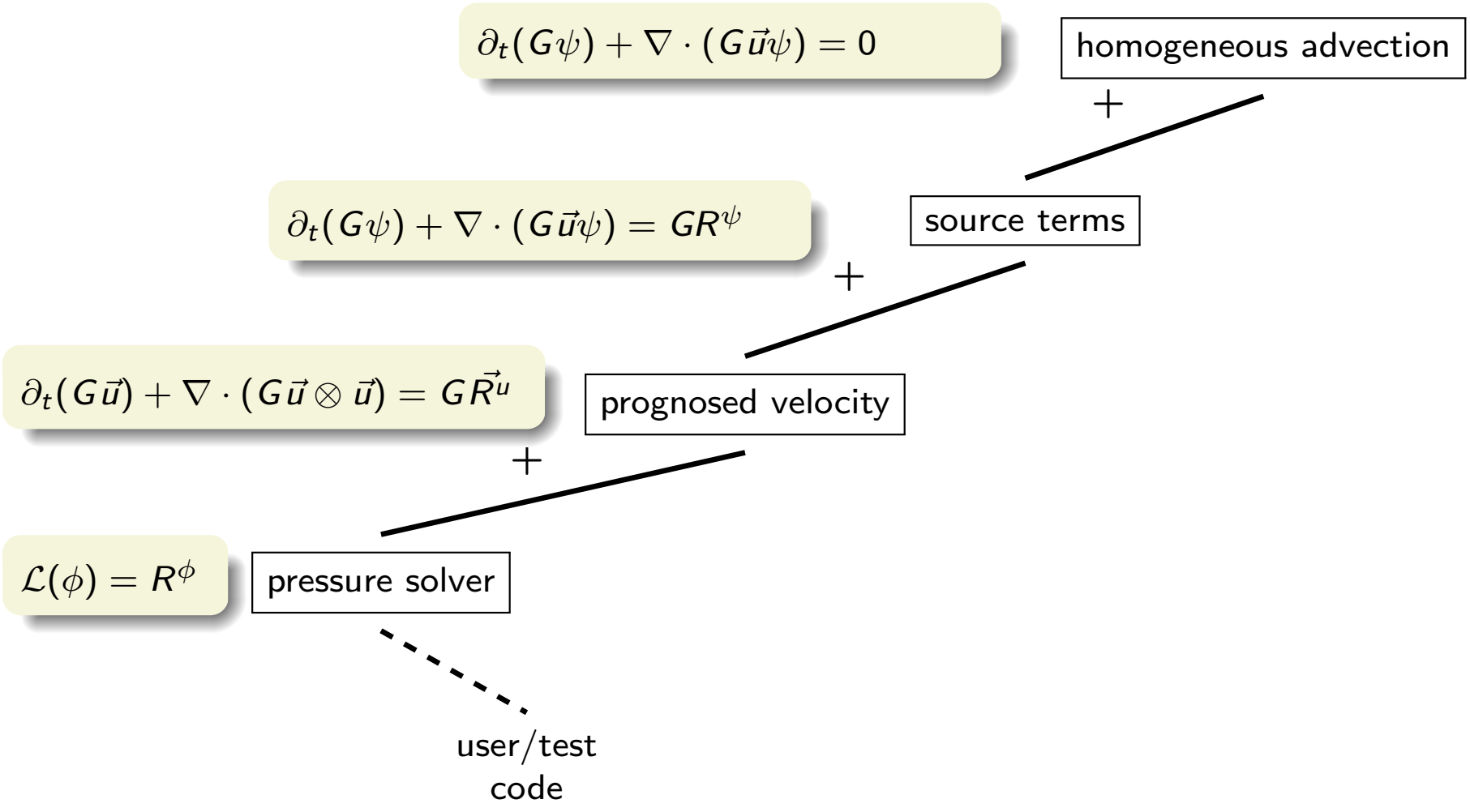
- <200 lines of code with libmpdata++
  (using built-in elliptic pressure solver)

building blocks of libmpdata++



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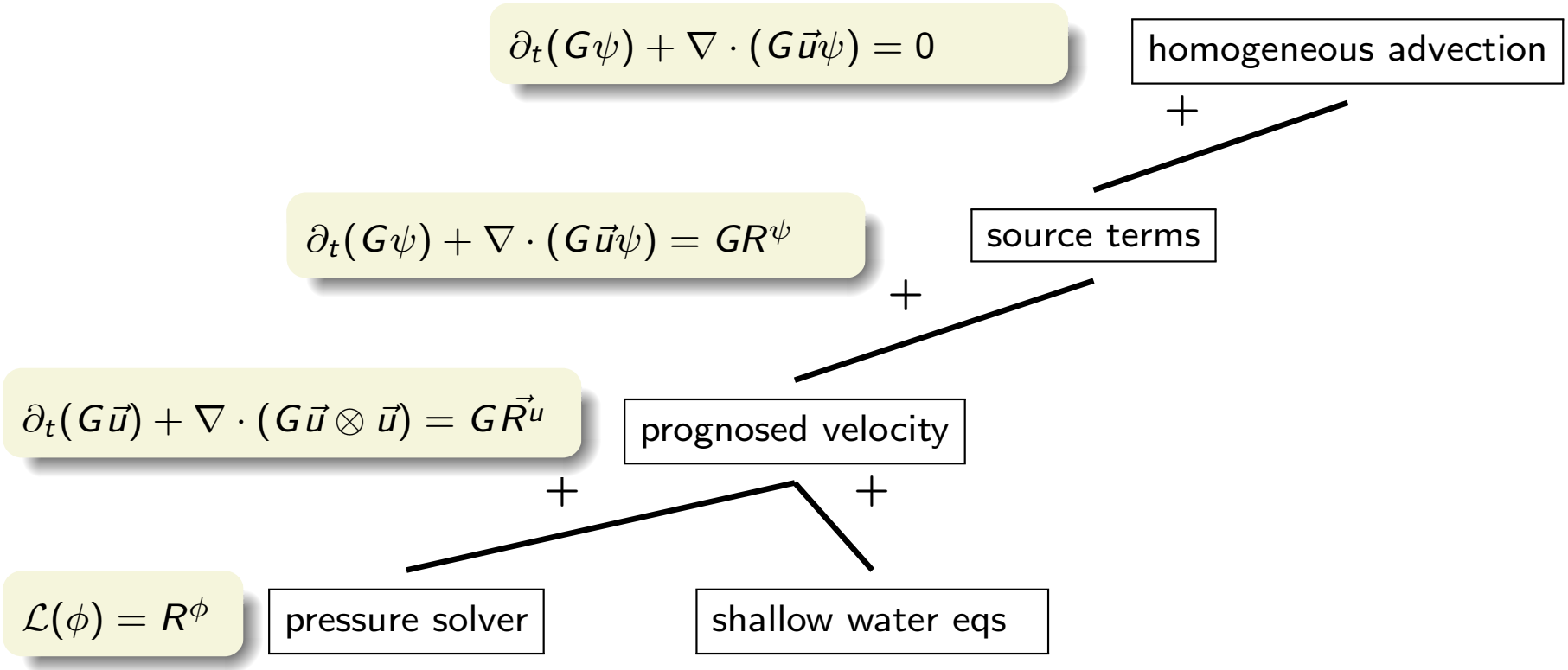

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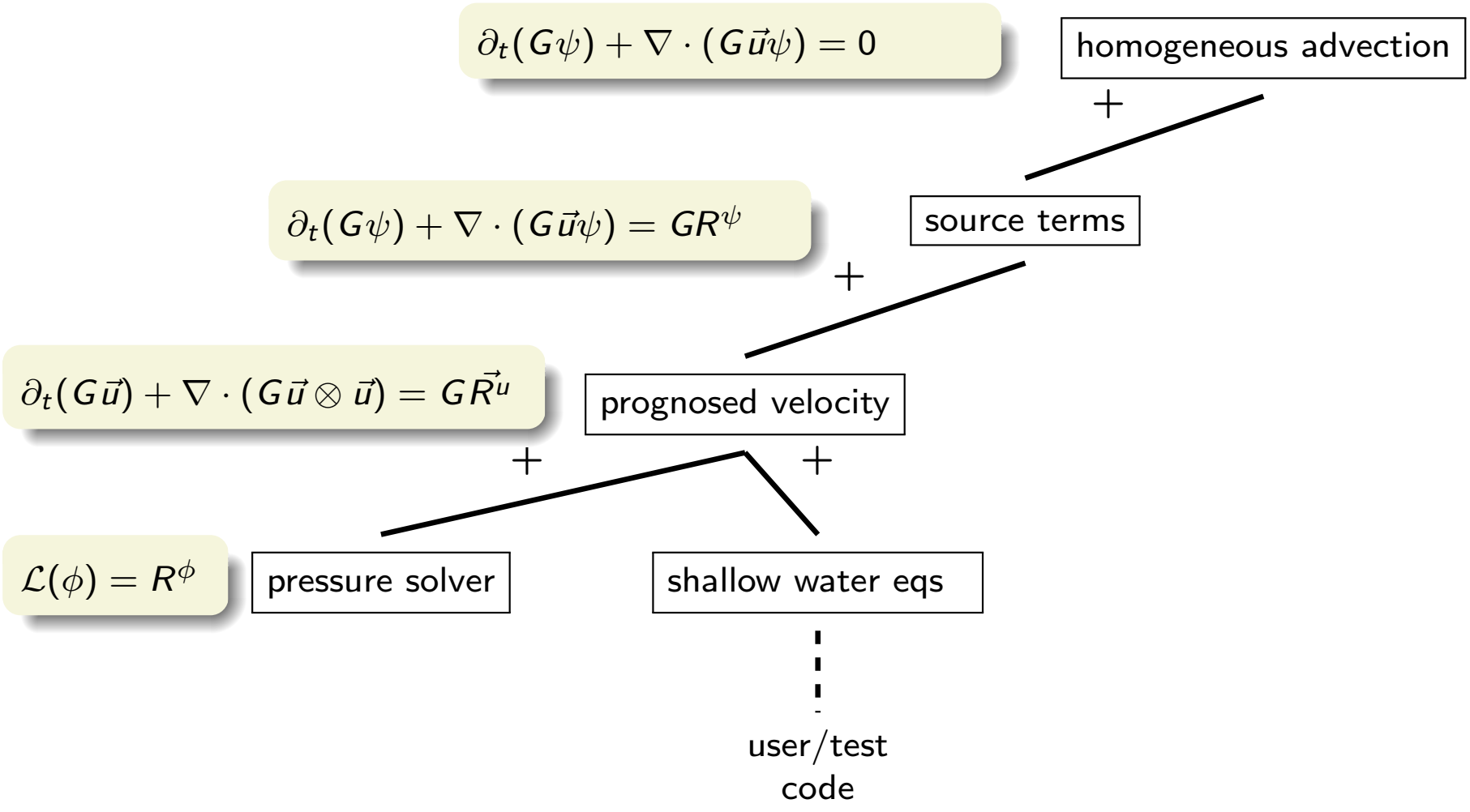
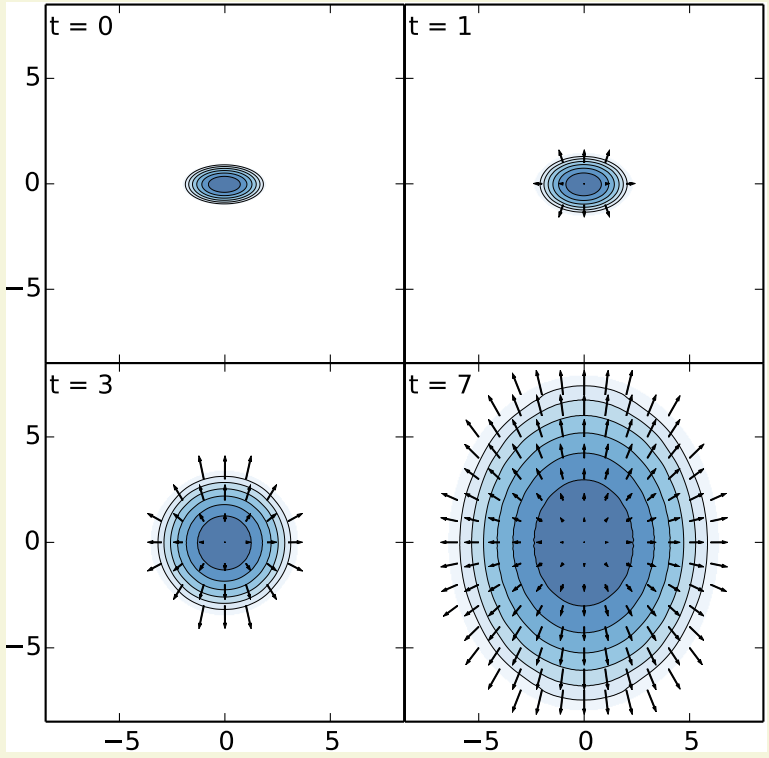


example: spreading drop of shallow water in 3D



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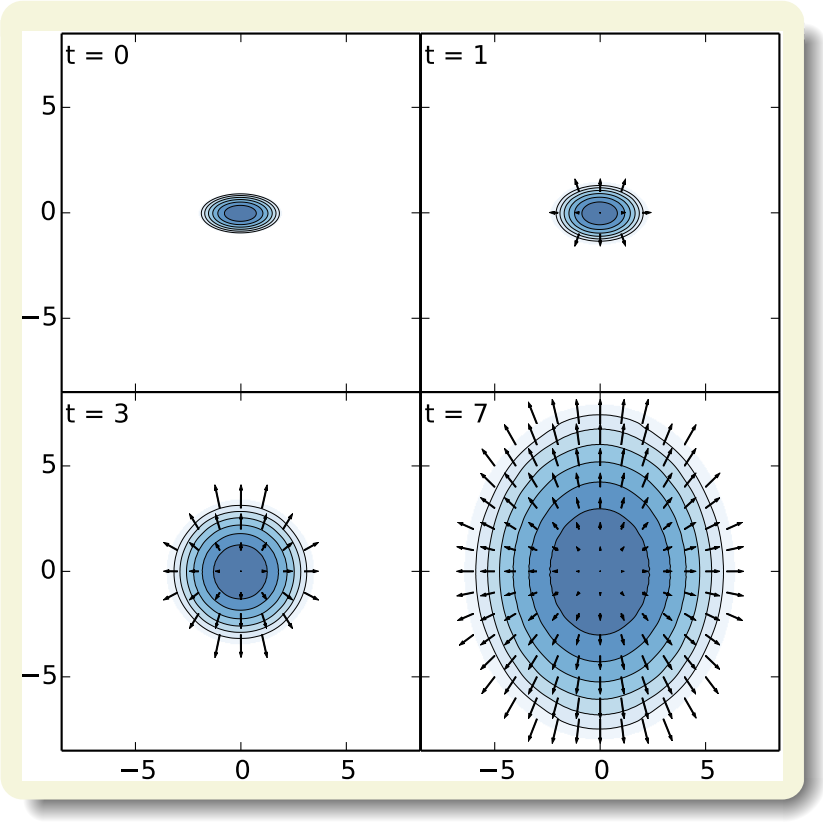

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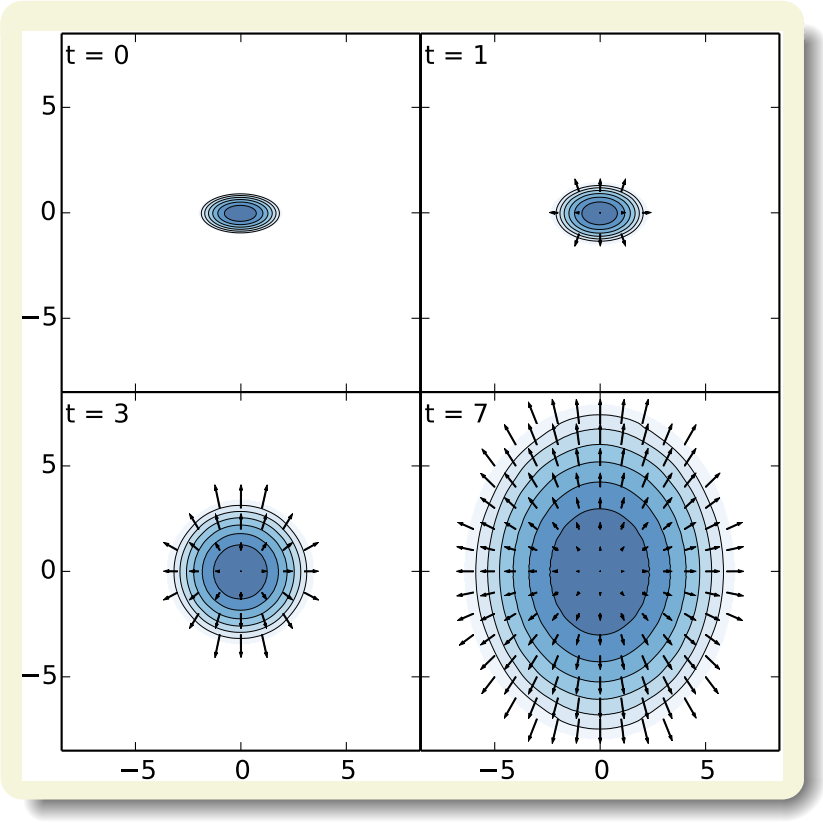

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- <120 lines of code with libmpdata++

summary of design choices for maintainability

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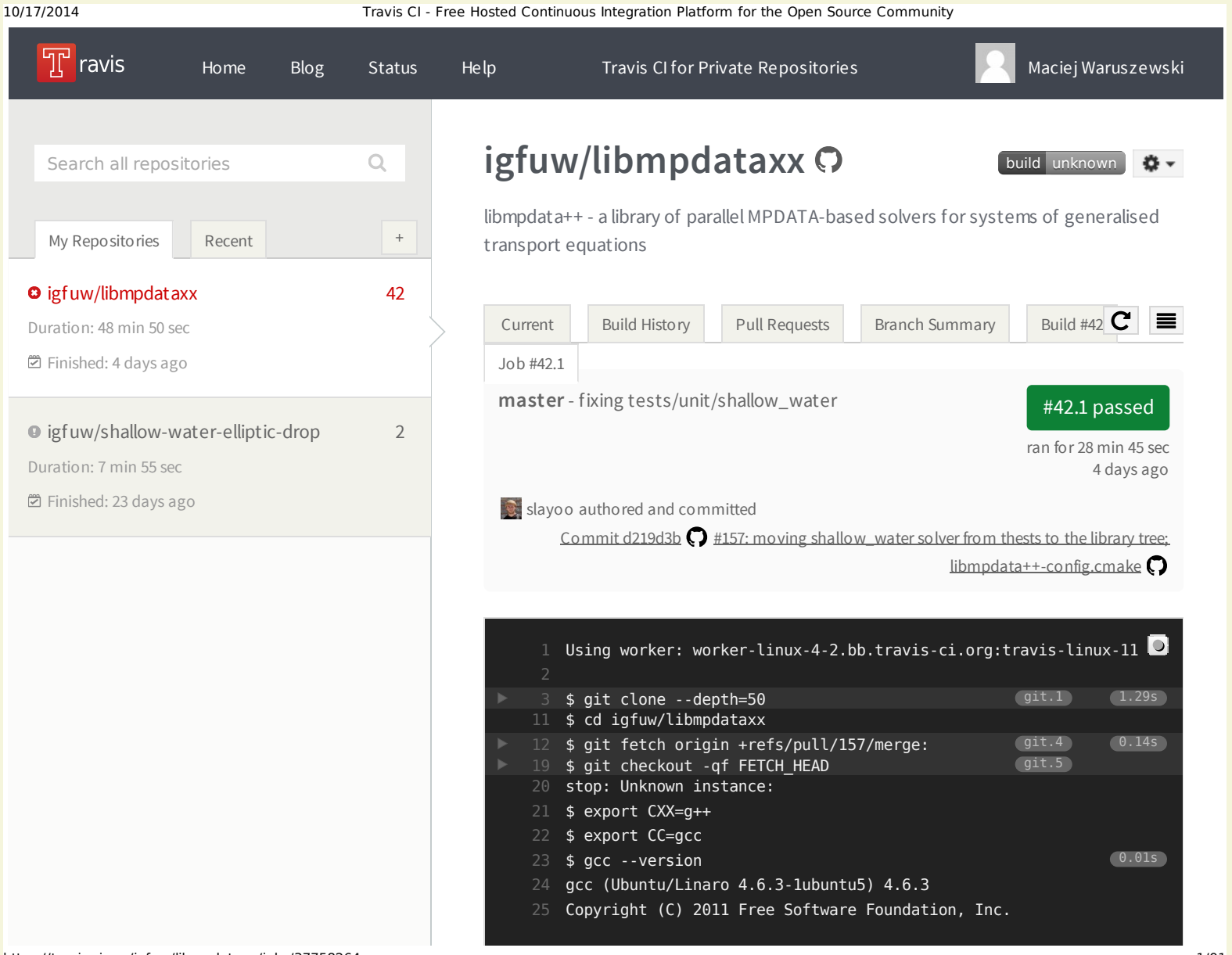
- automated builds and testing after changes

summary of design choices for maintainability

Travis CI



ongoing work

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- distributed memory parallelisation (Boost.MPI)

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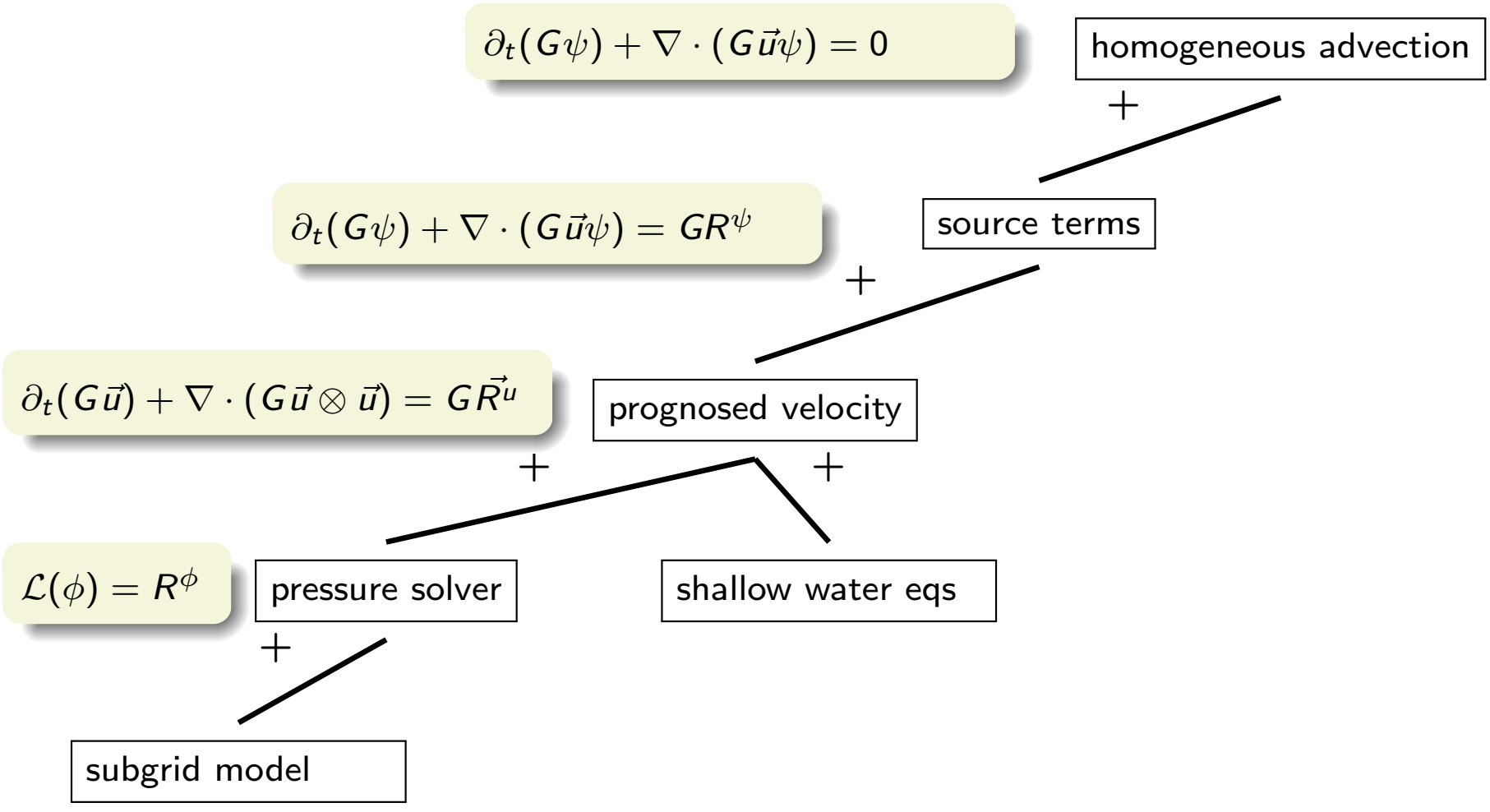
- complex geometries using immersed boundary method

building blocks of libmpdata++



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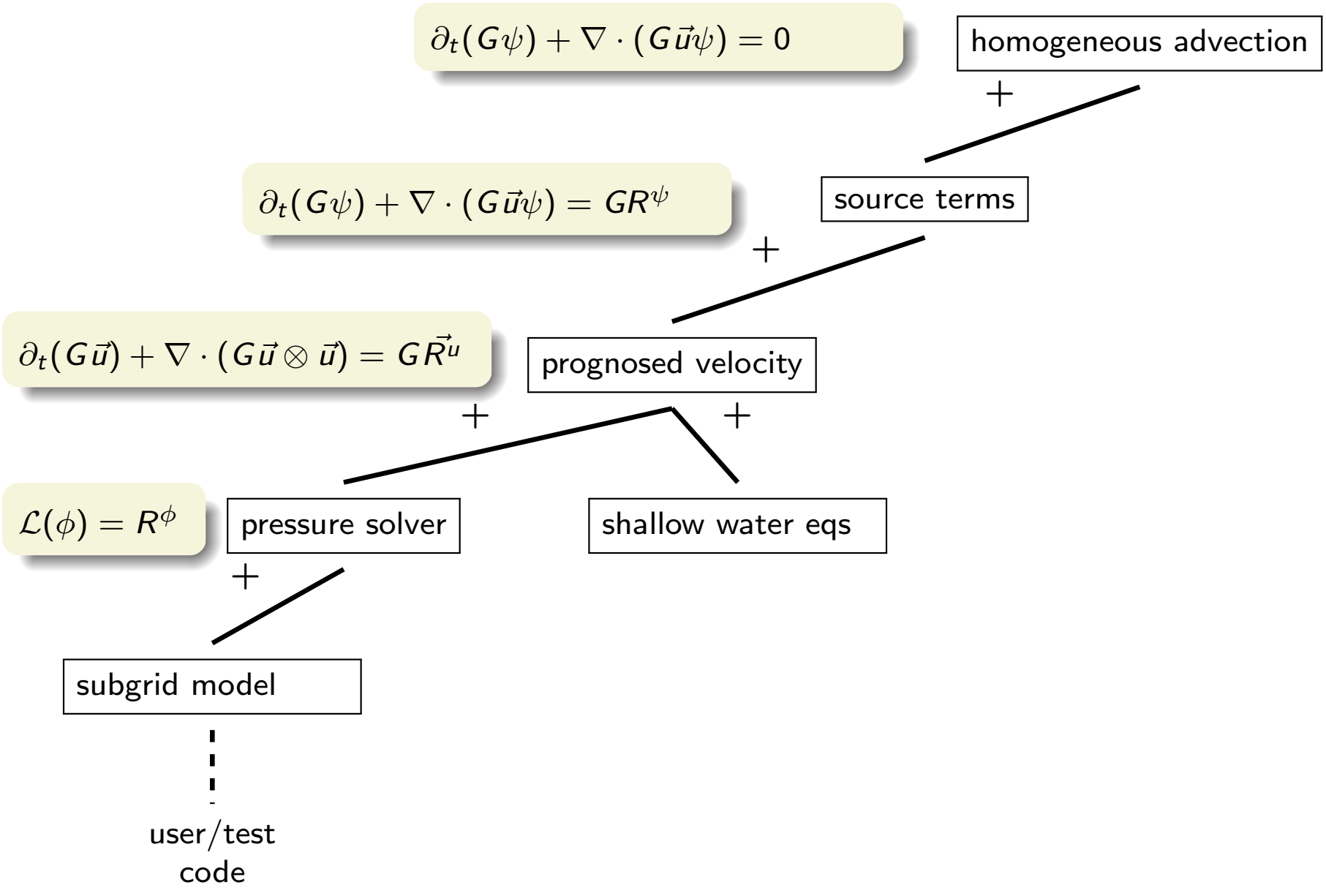
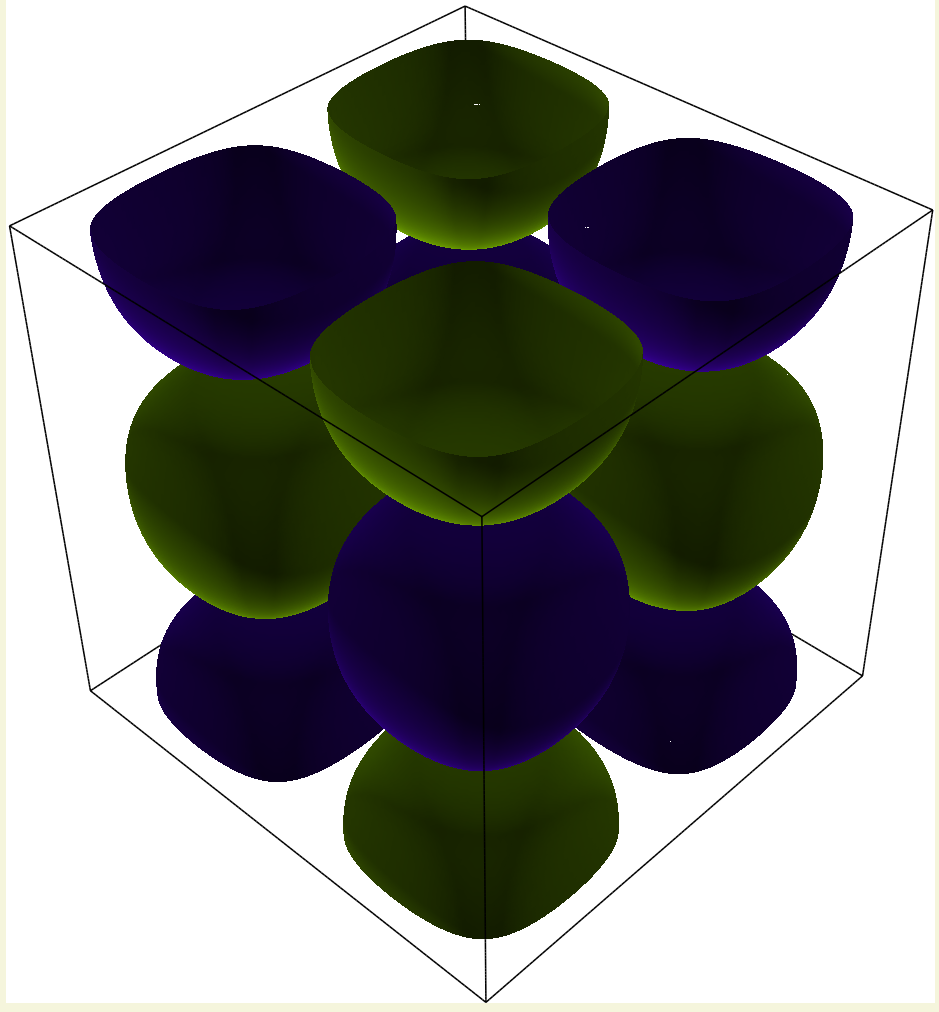


example: Taylor-Green vortex at Re = 800



- inspired by spectral calculations of Brachet et al., 1983

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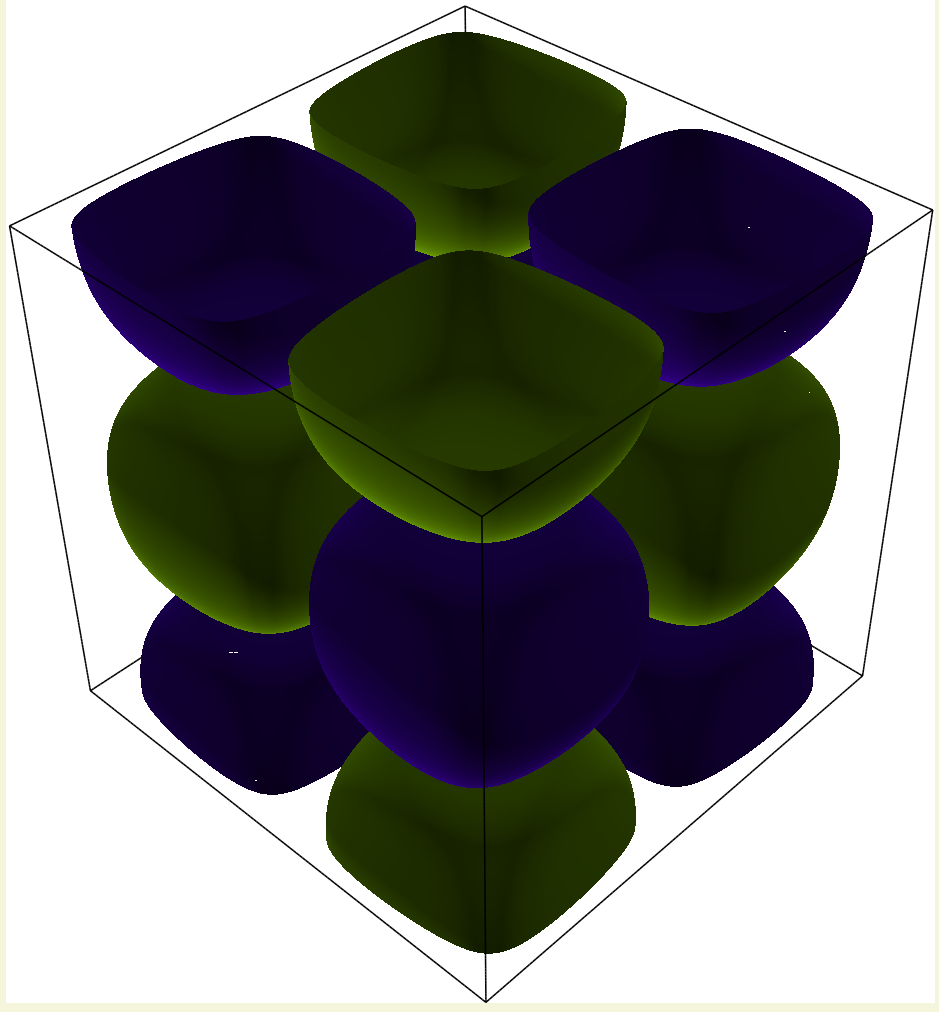

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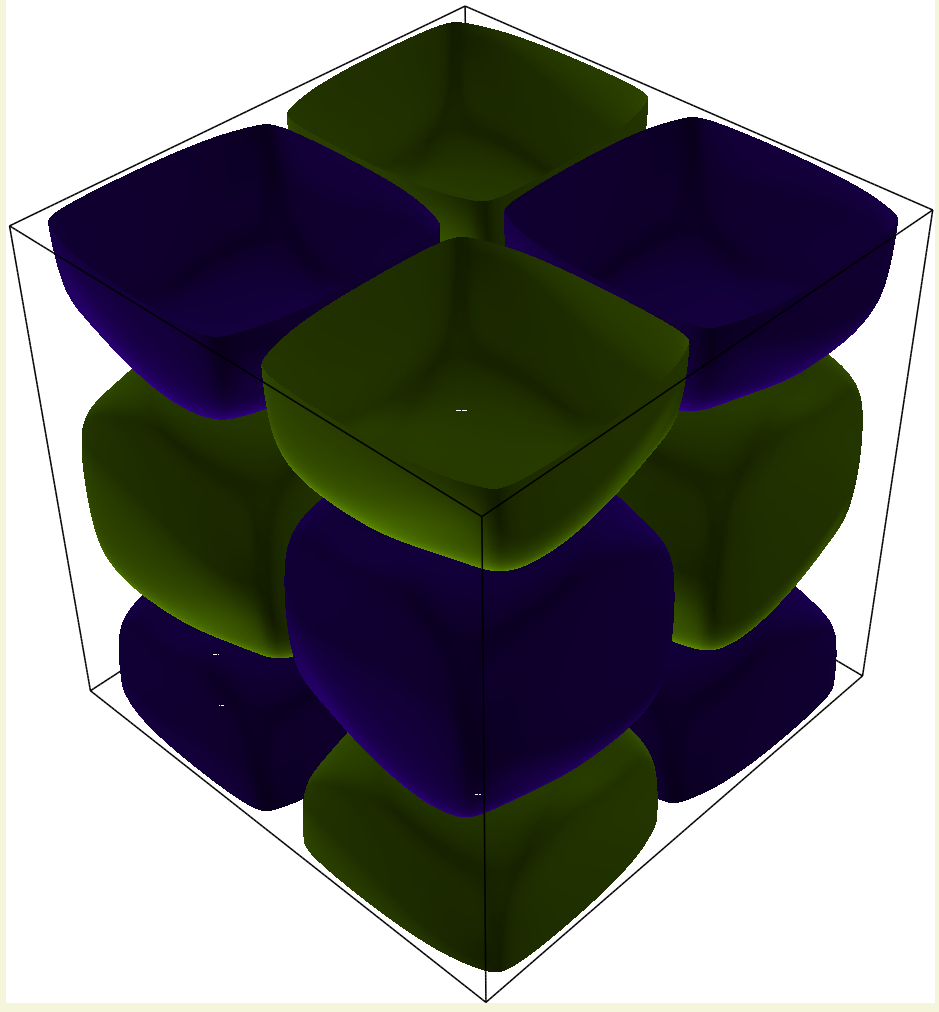

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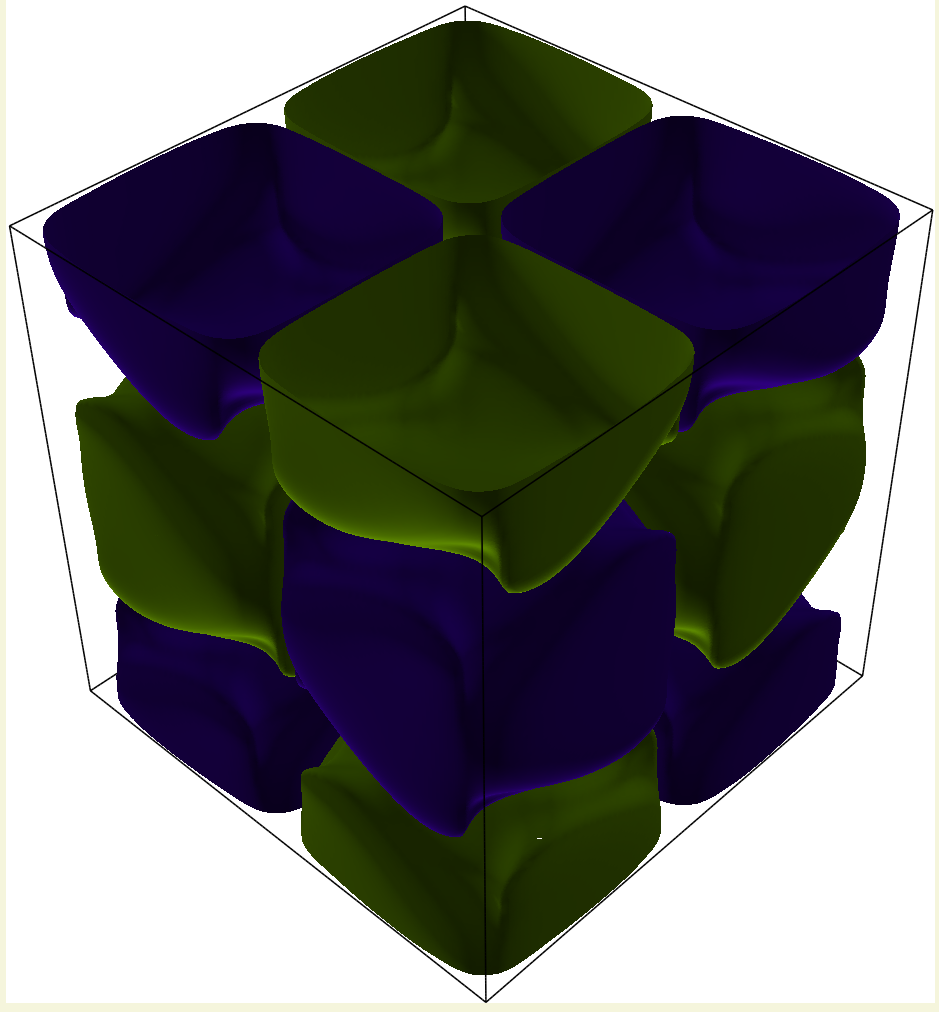

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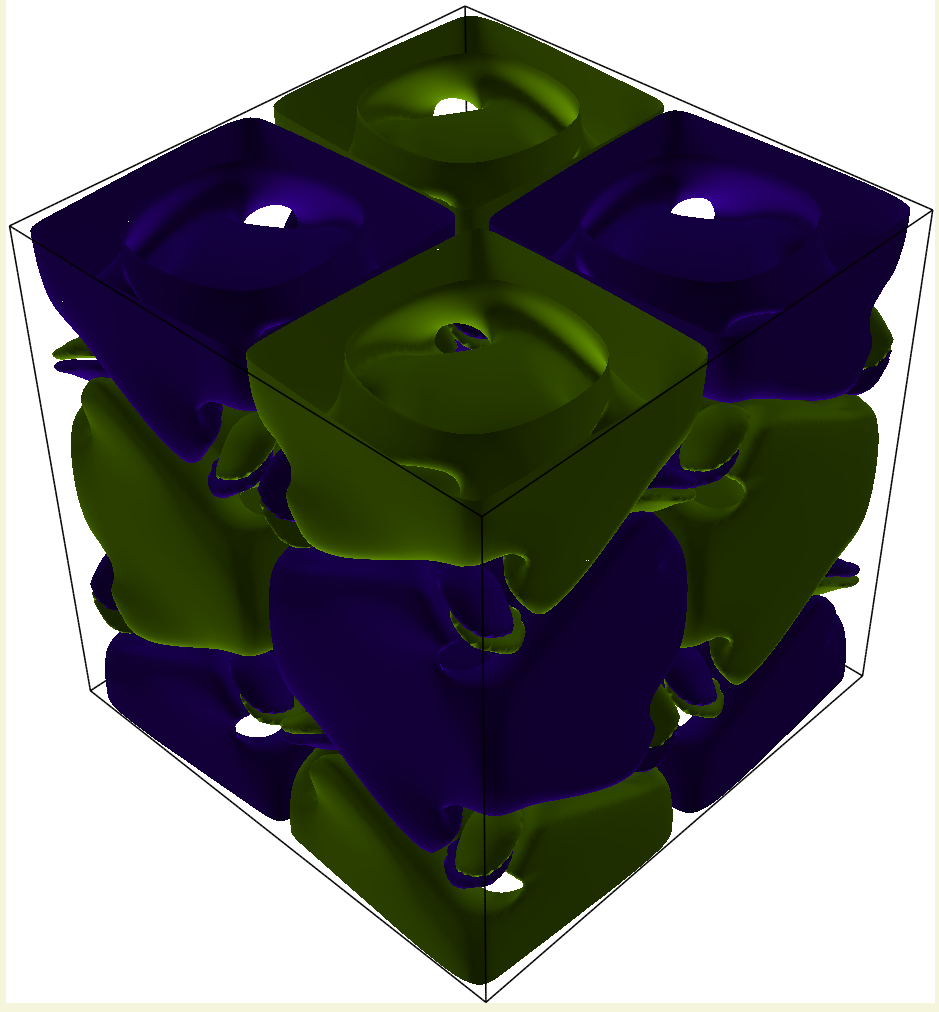

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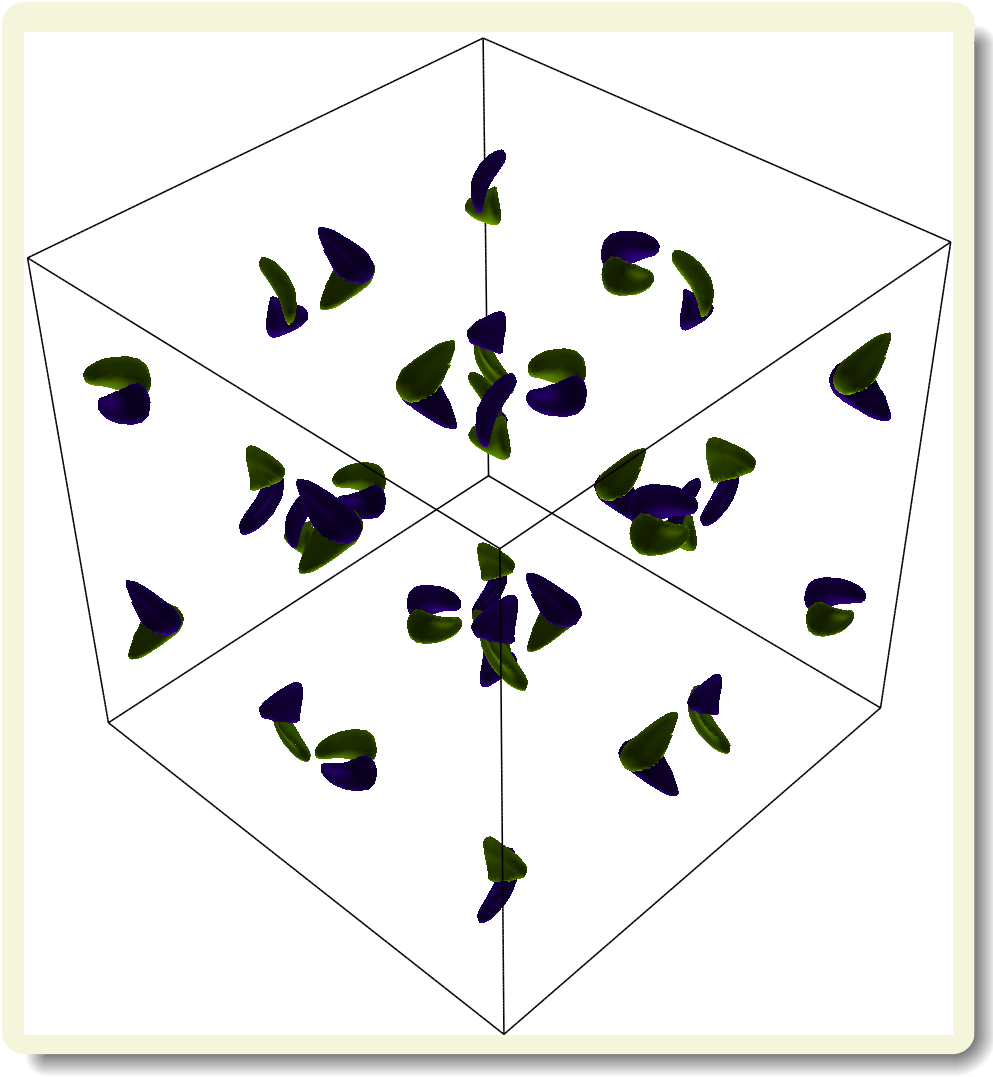

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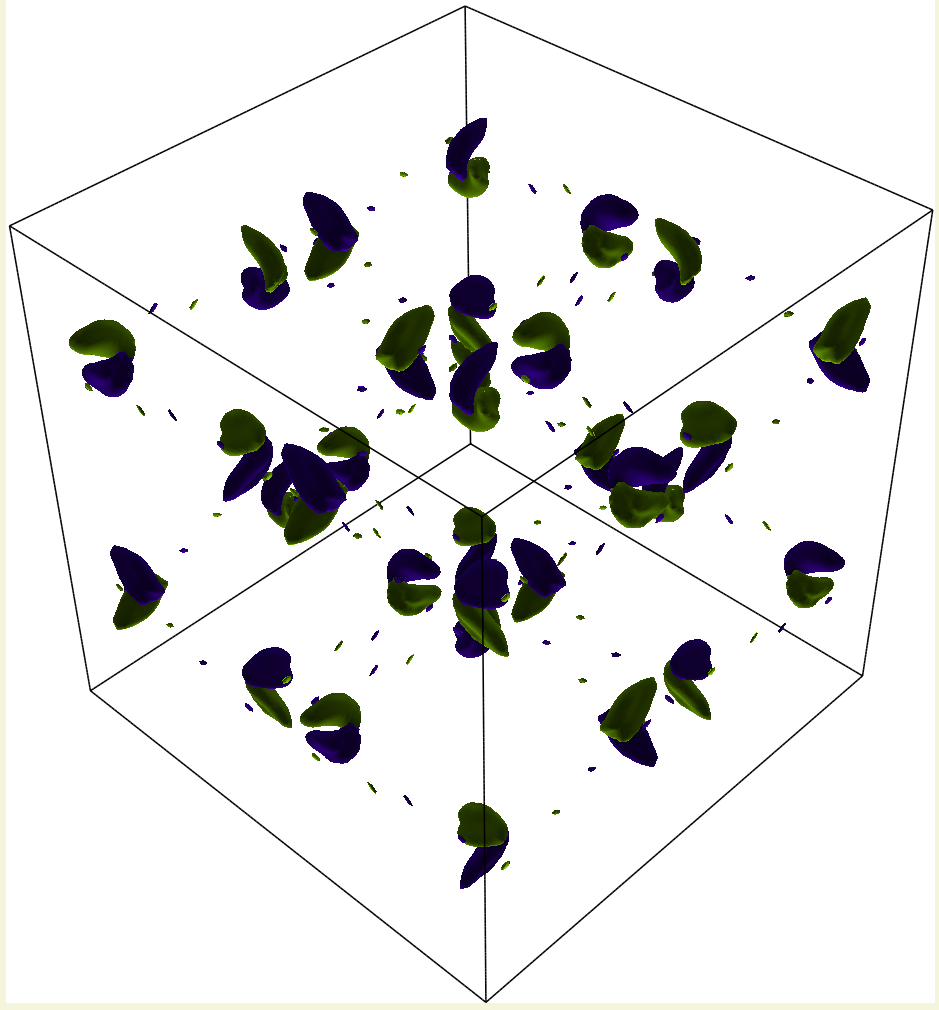

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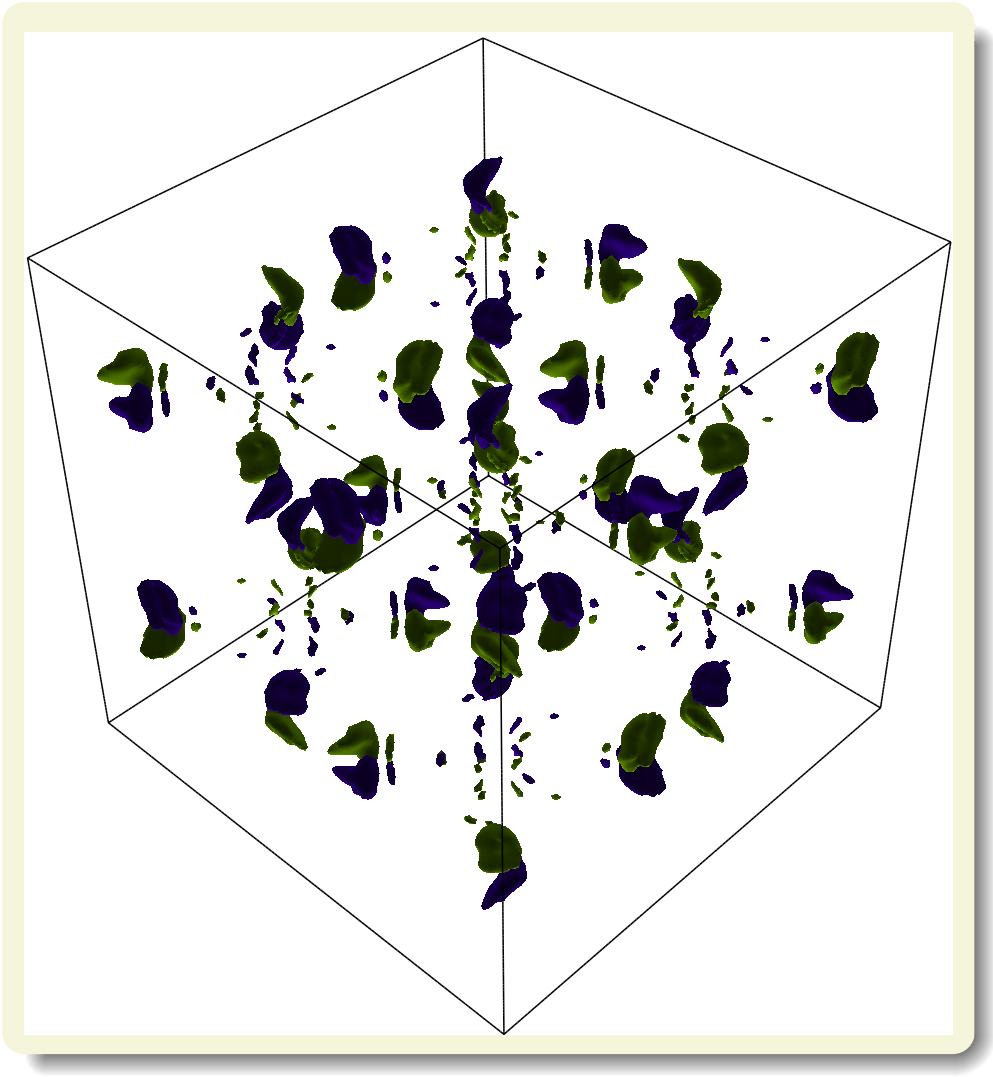

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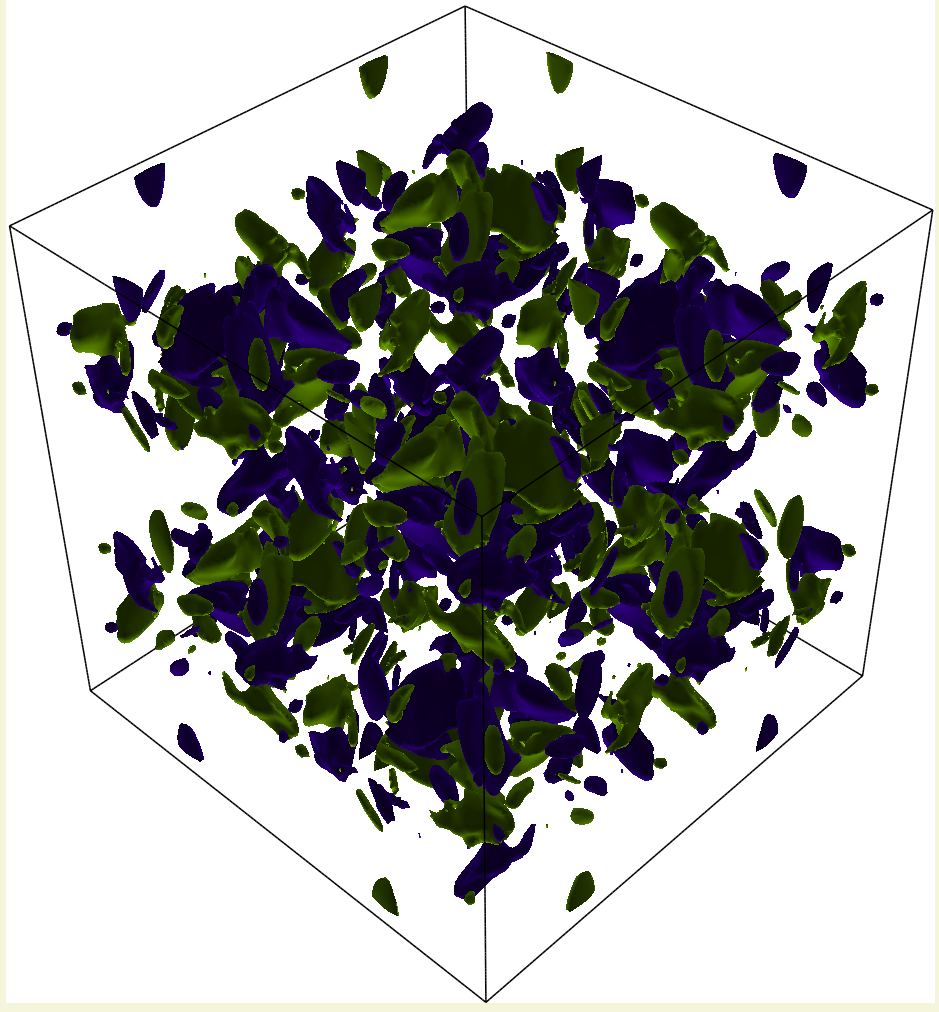

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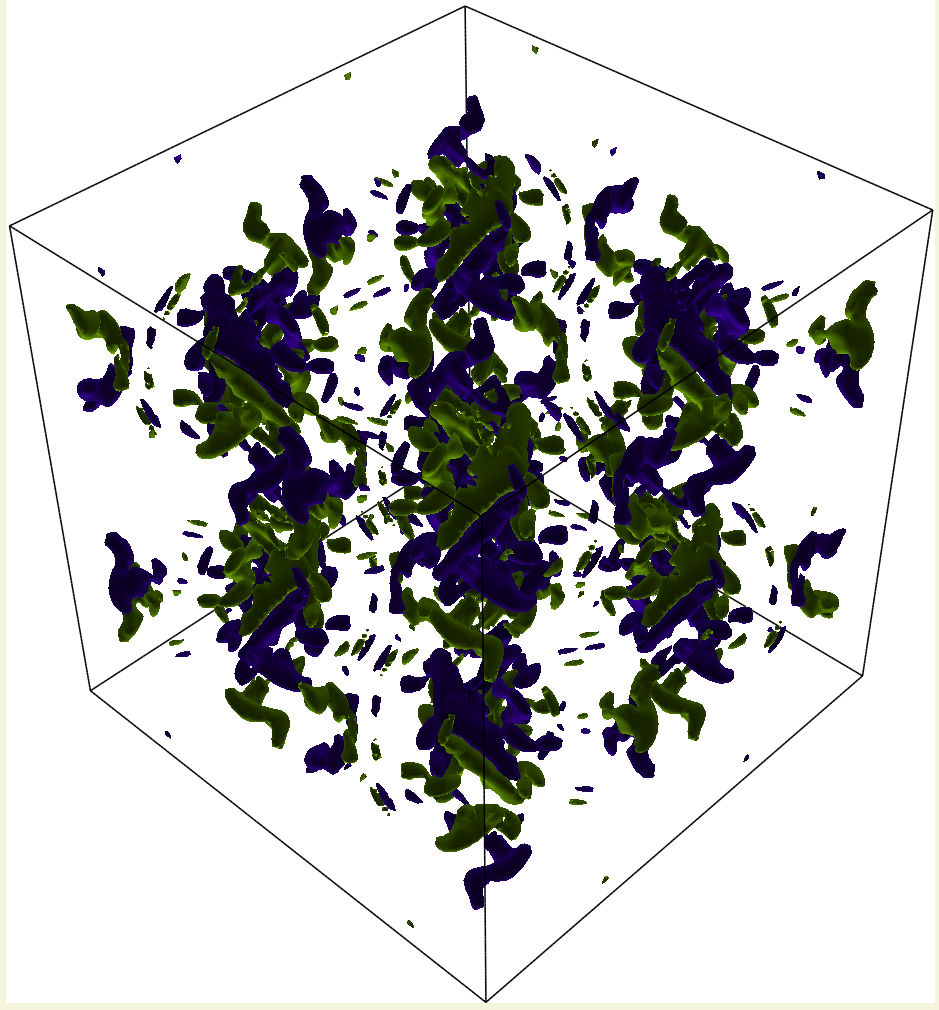

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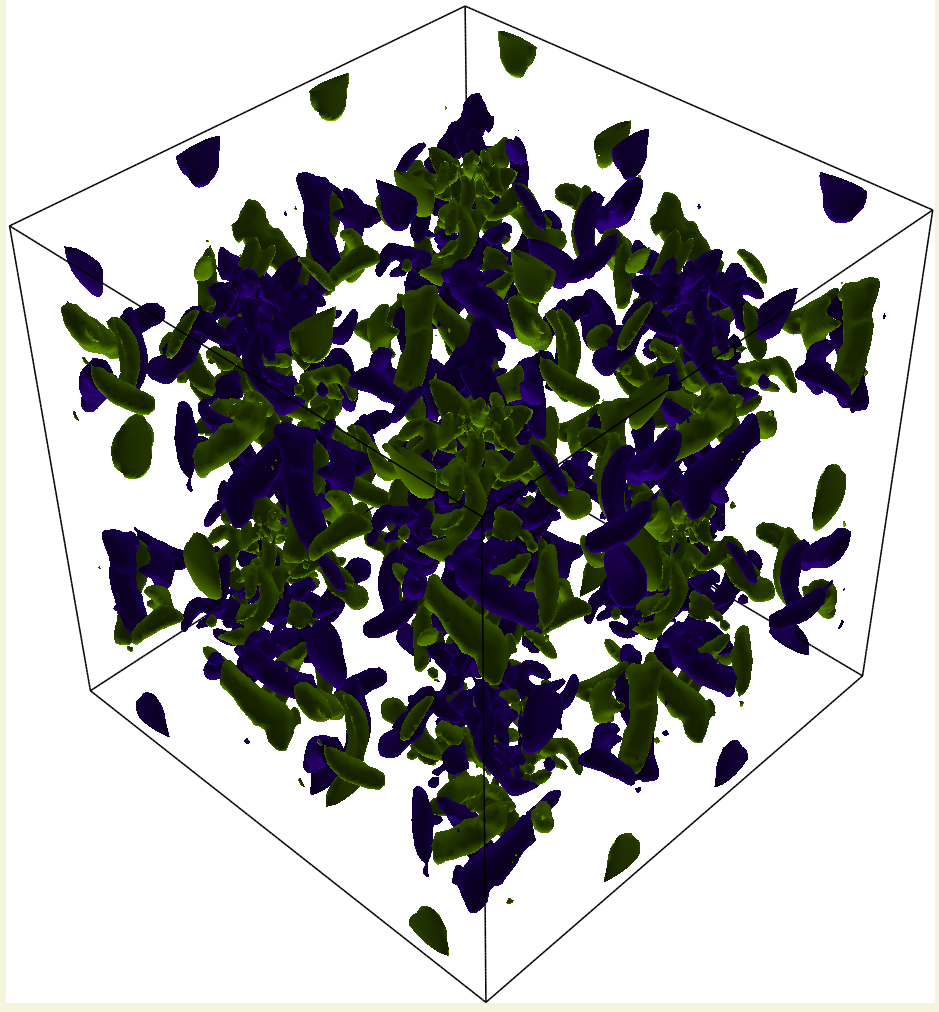

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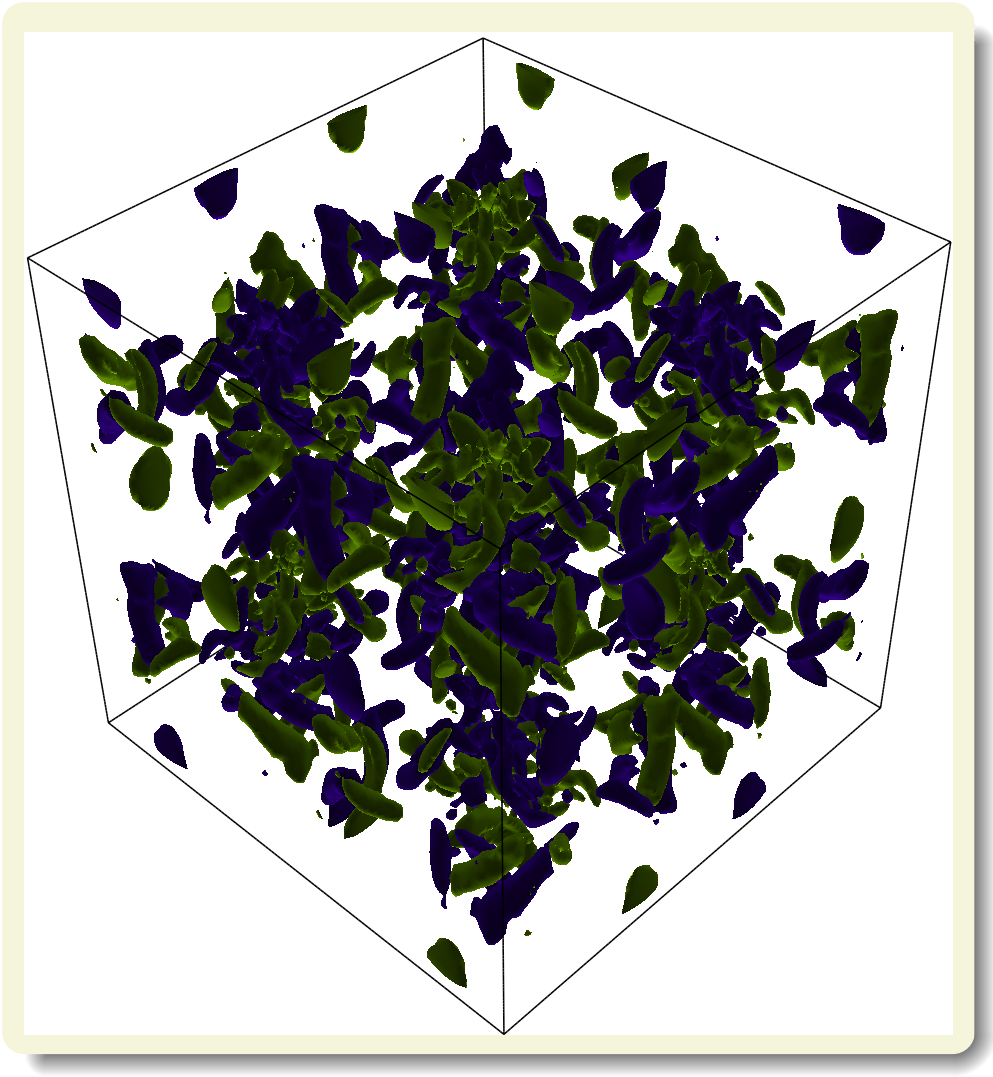

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acknowledgements:

- Development of libmpdata++ and libcloudph++ have been supported by Poland's National Science Centre (decision no. 2012/06/M/ST10/00434)