What's new in libmpdata++ (towards the 2.0 release)

Sylwester Arabas
Faculty of Physics, University of Warsaw, Poland

seminar presented at the
Graduate School for Computational Studies, Hyogo University

Kōbe, Japan, September 7, 2015

let me introduce myself

alma mater (MSc/2008, PhD/2013, postdoc)

	est.	staff	students	
			BSc/MSc	PhD
University of Warsaw	1816	6000	55000	3000
Faculty of Physics	1816	300	1000	150
Institute of Geophysics	1948	30	20	20
Atmospheric Physics Division	1949	10	10	10

collaboration with Shima-san

2010: first contact thanks to Enomoto-san

2010: 4 weeks at JAMSTEC/Yokohama: RICO-SDM project

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2015 super-droplet workshop at the University of Warsaw

let me introduce our team

the team © the University of Warsaw, Poland

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the team @ the University of Warsaw, Poland

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1. what's libmpdata++
2. libmpdata++: a hello-world program
3. libmpdata++ 1.0: summary of features
4. libmpdata++ 2.0: new features under development
5. closing remarks

Plan of the talk

the generalised transport equation

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

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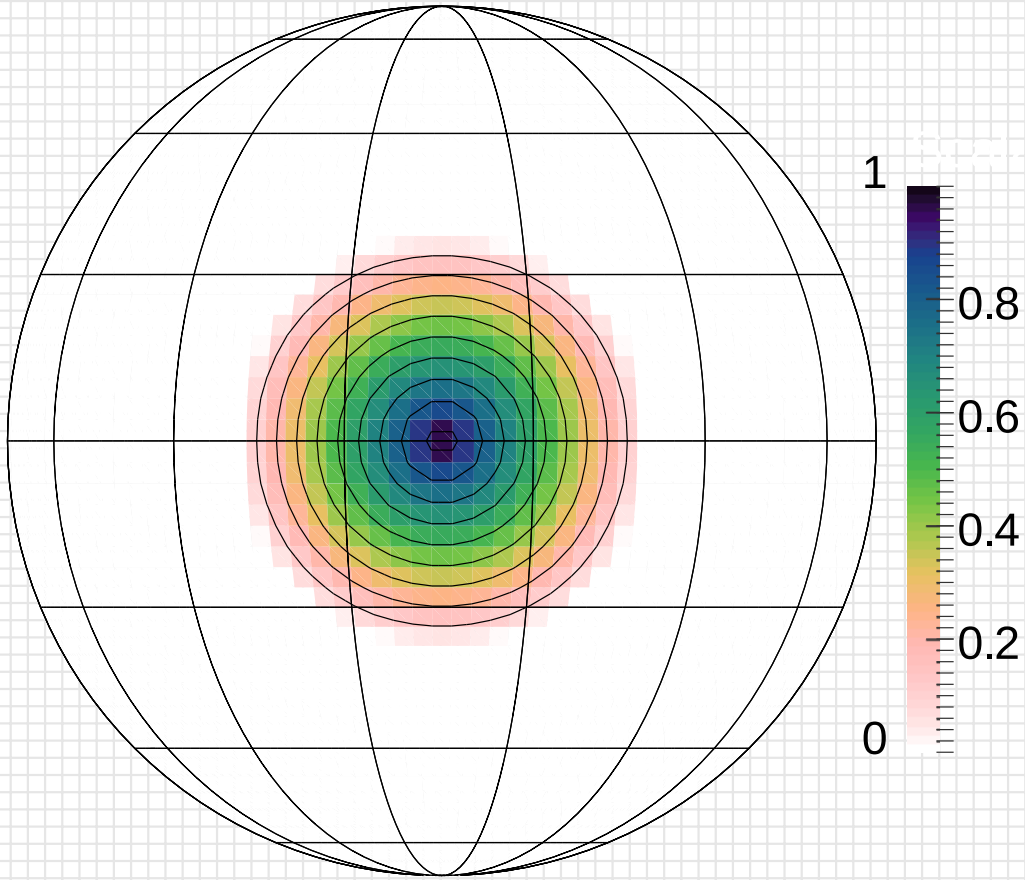

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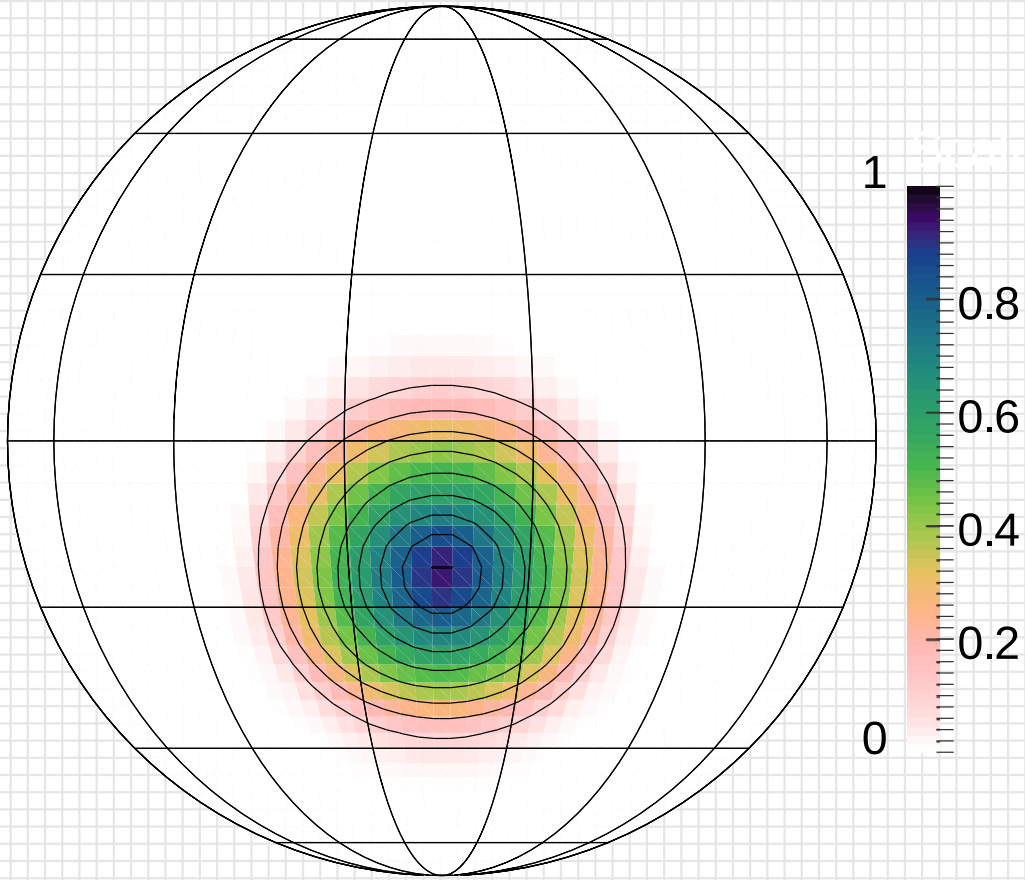

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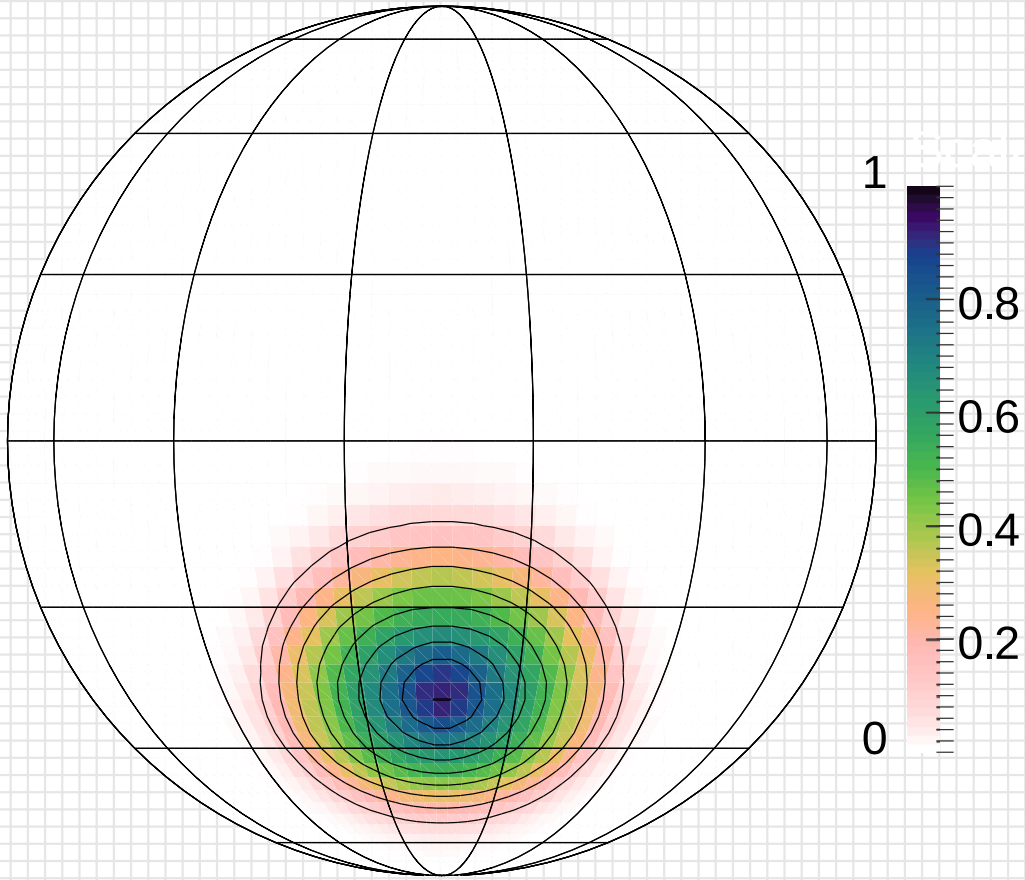

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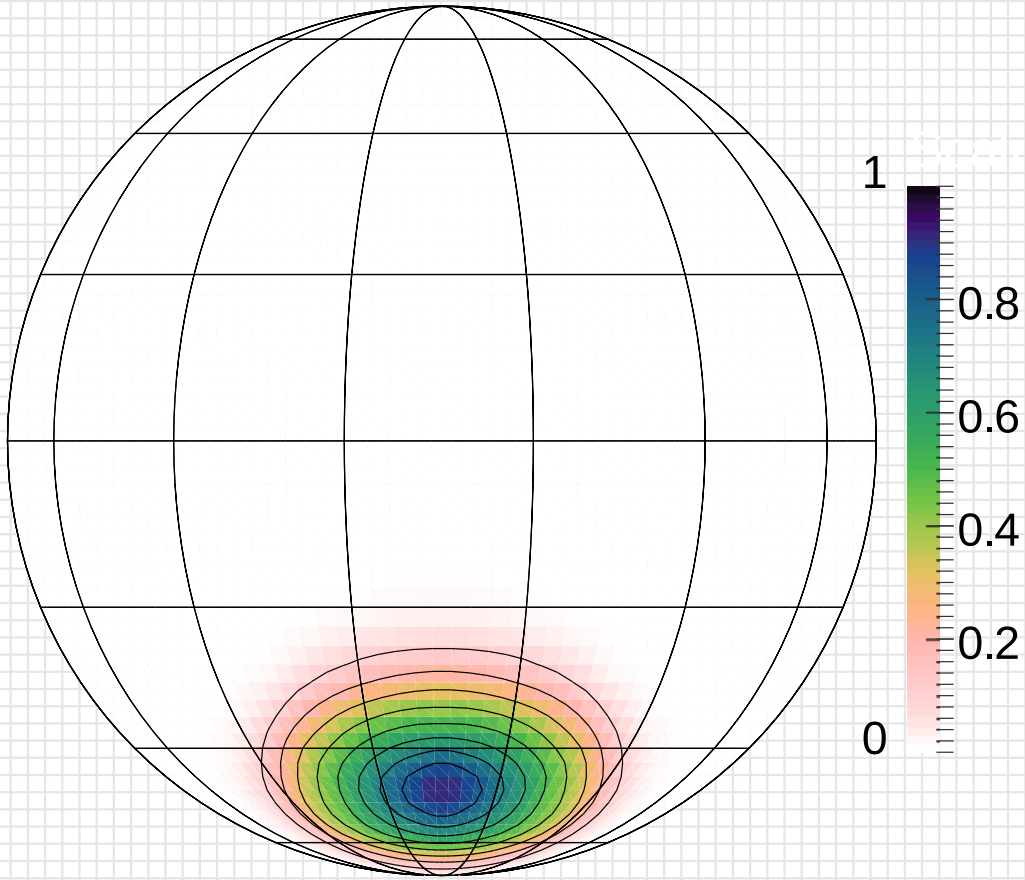

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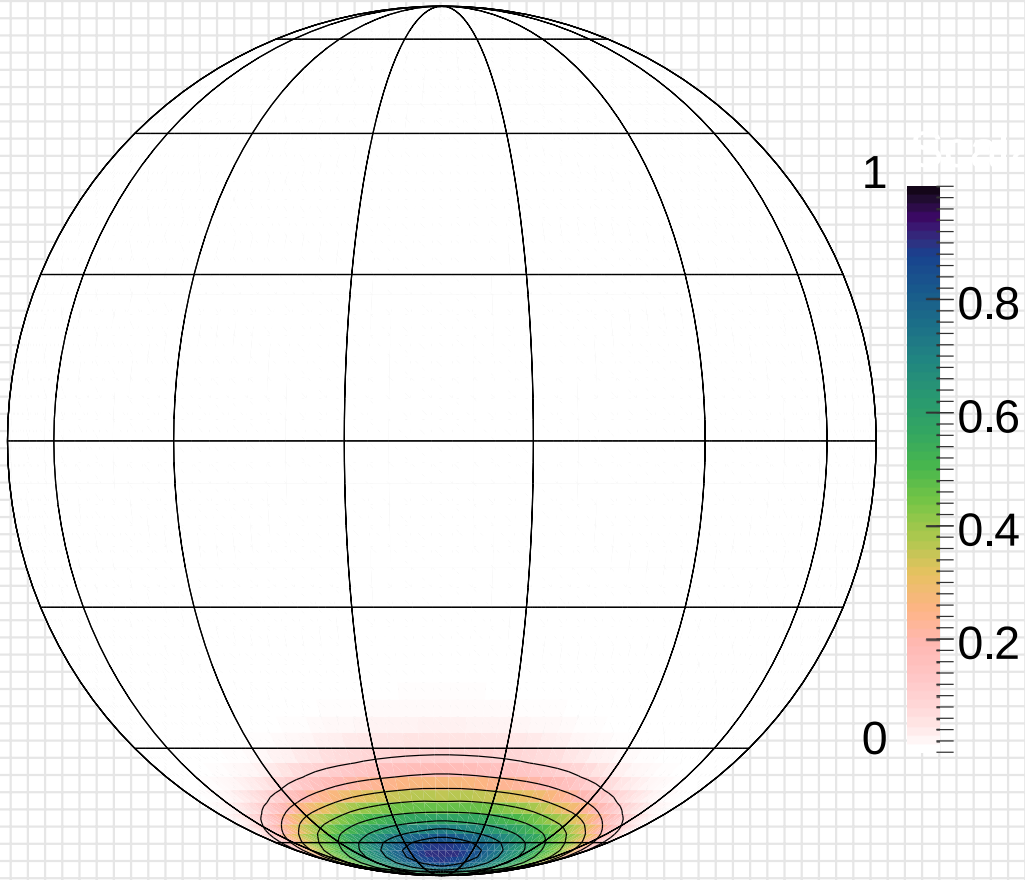

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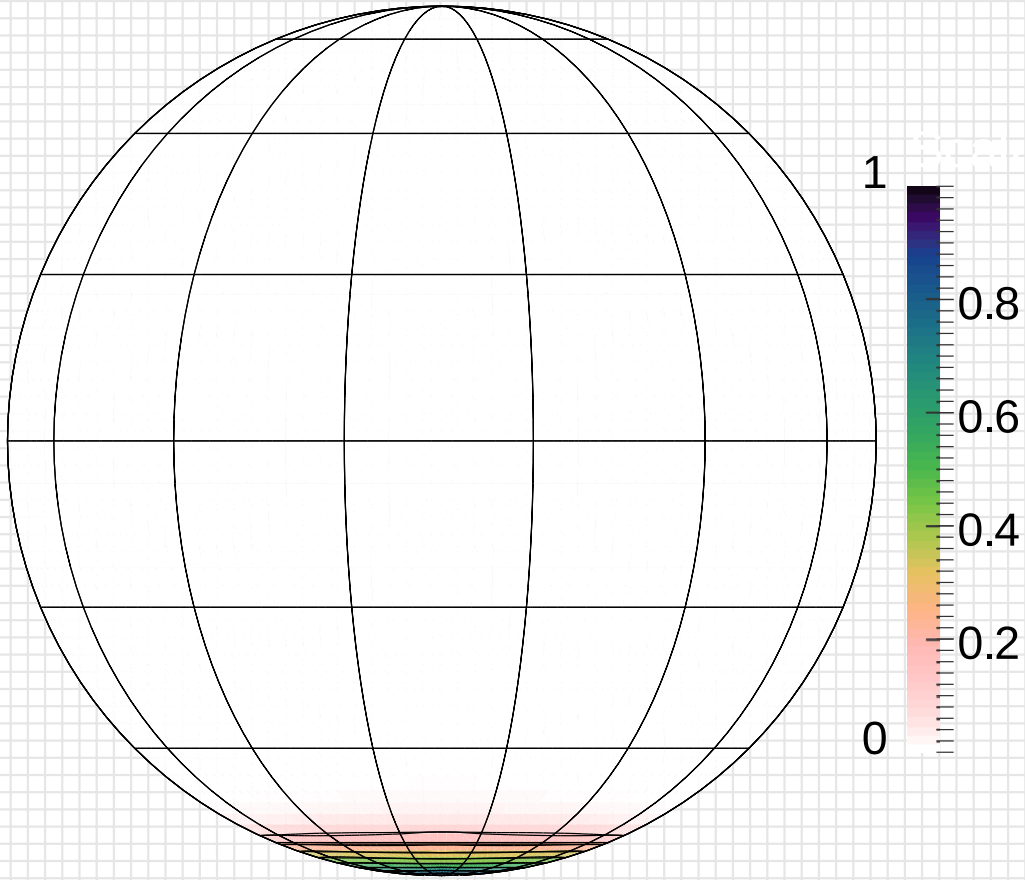

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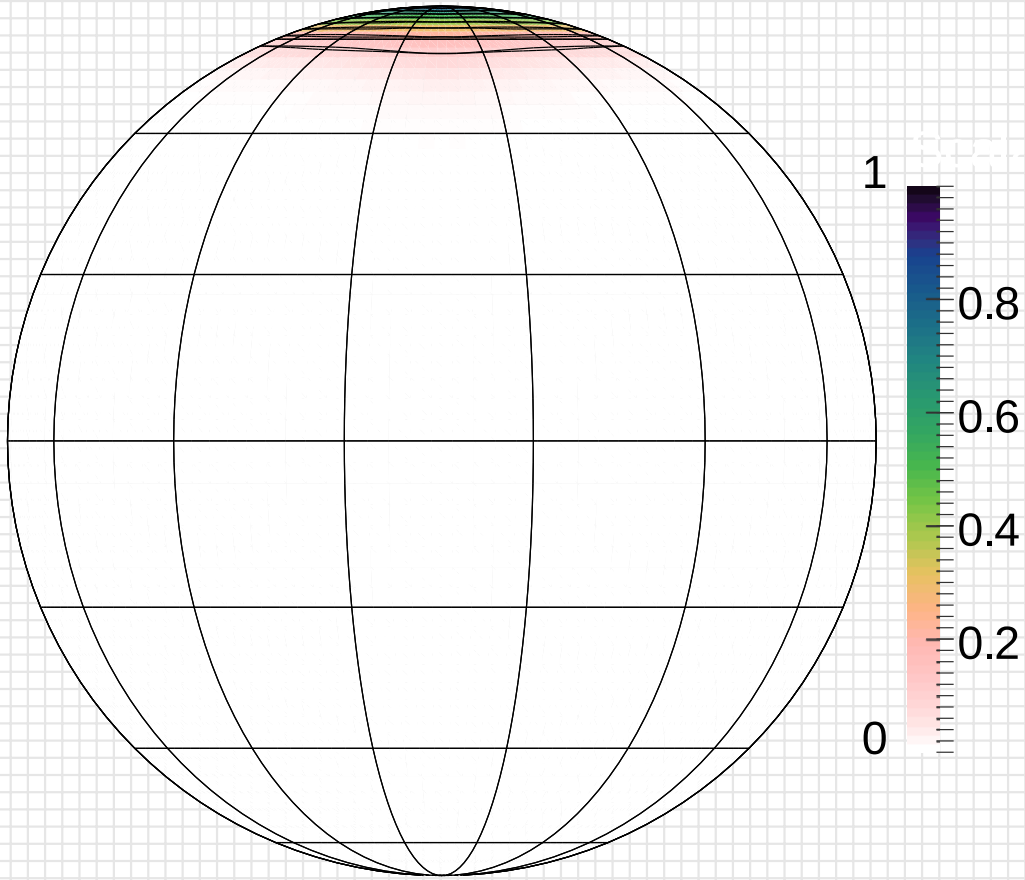

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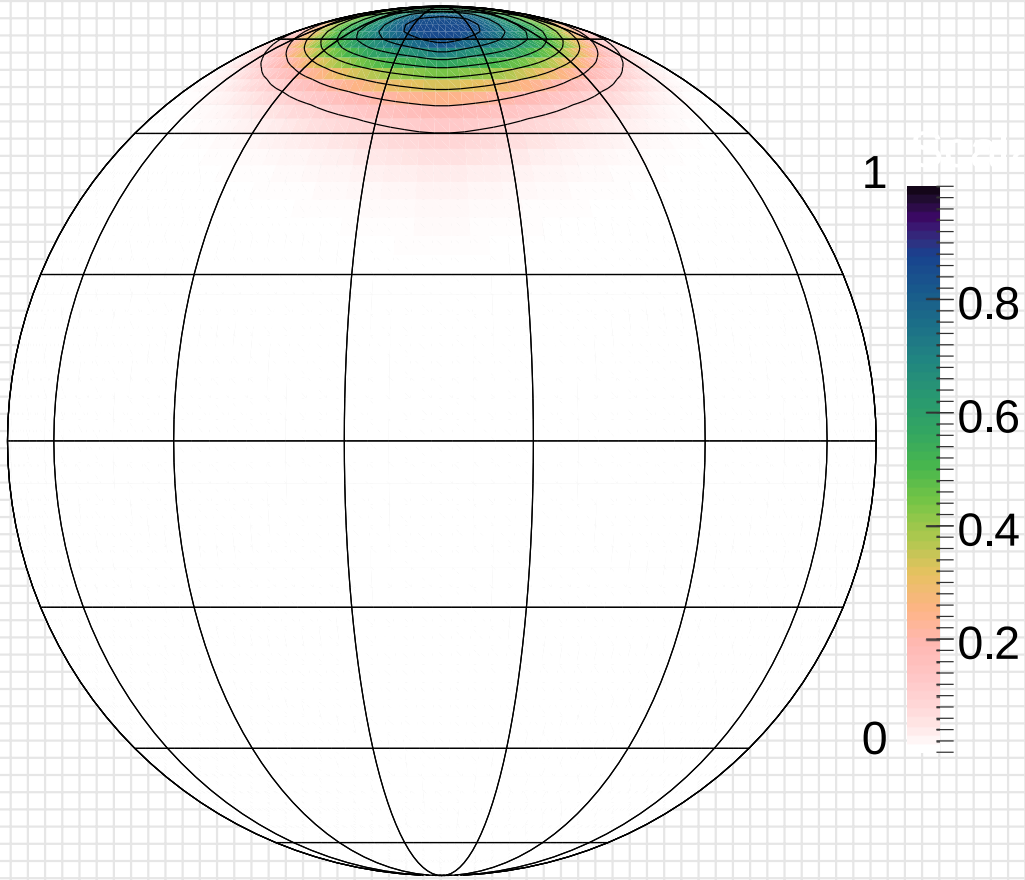

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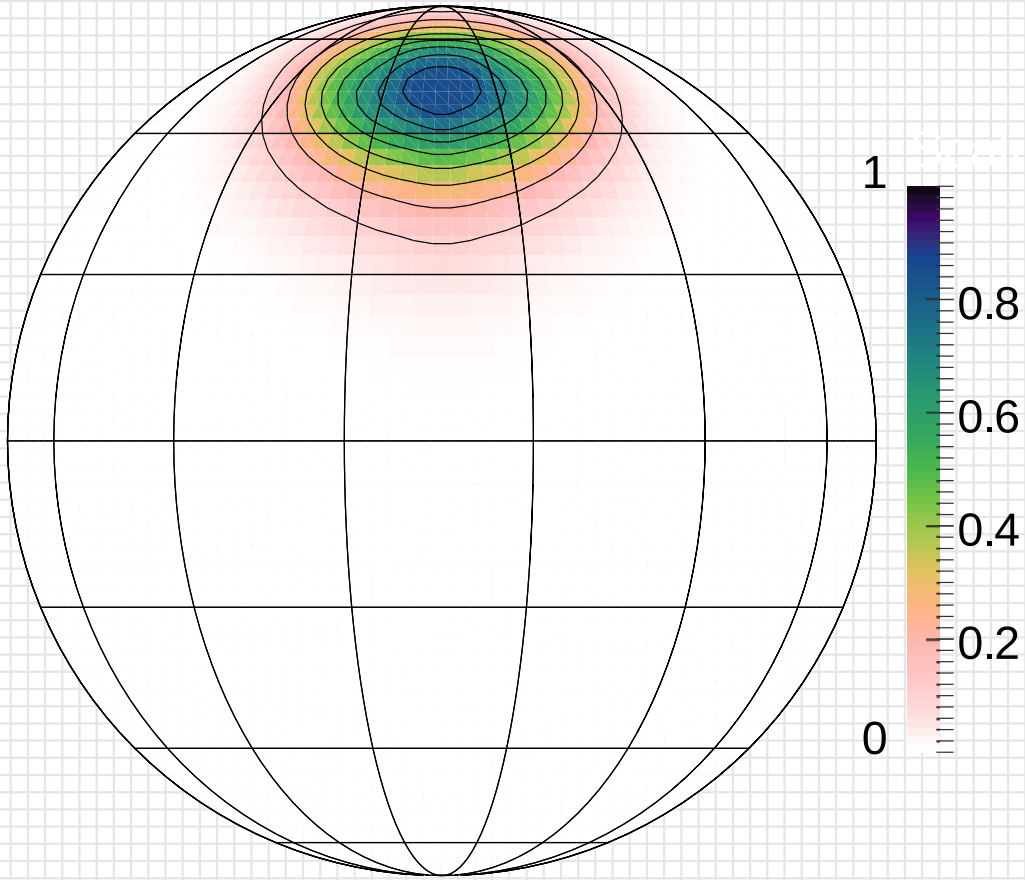

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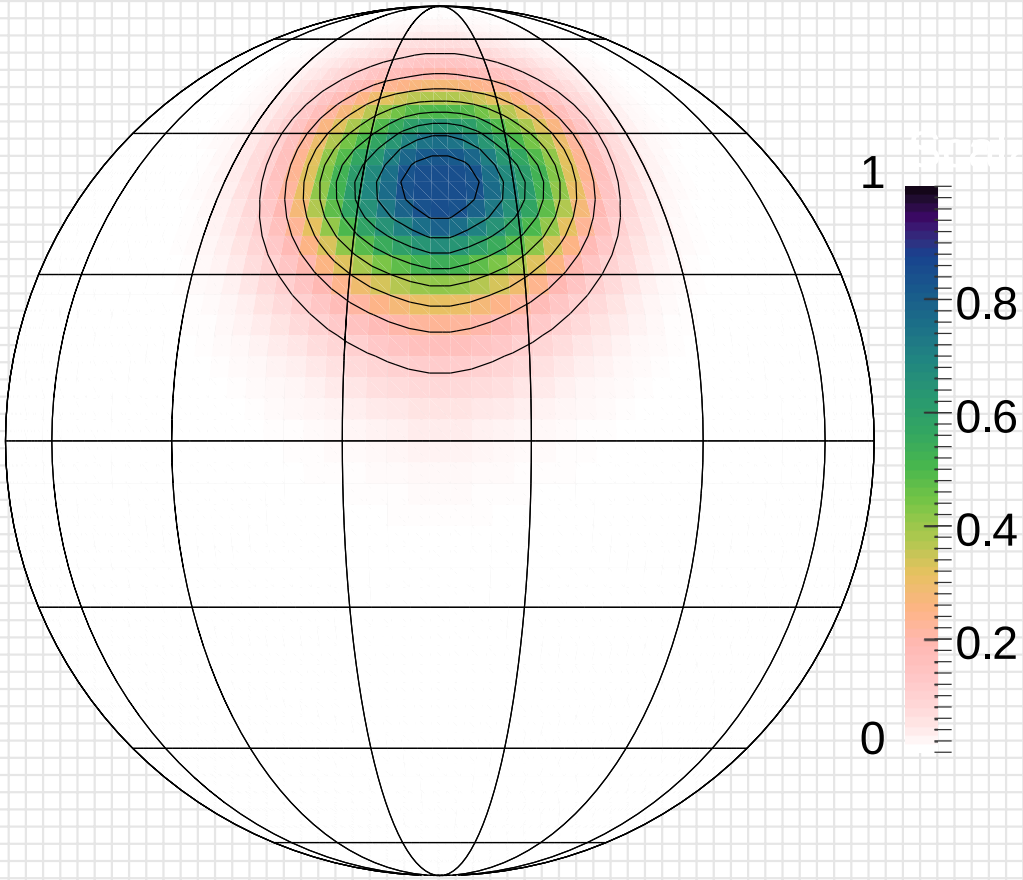

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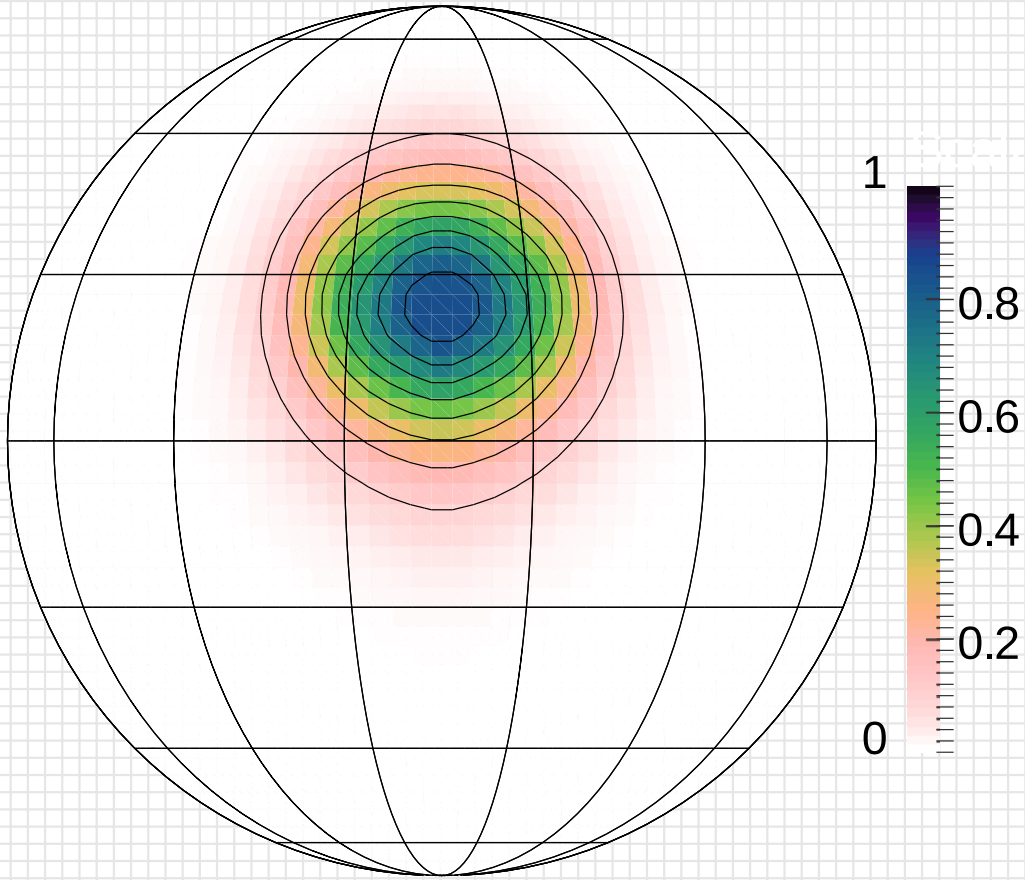

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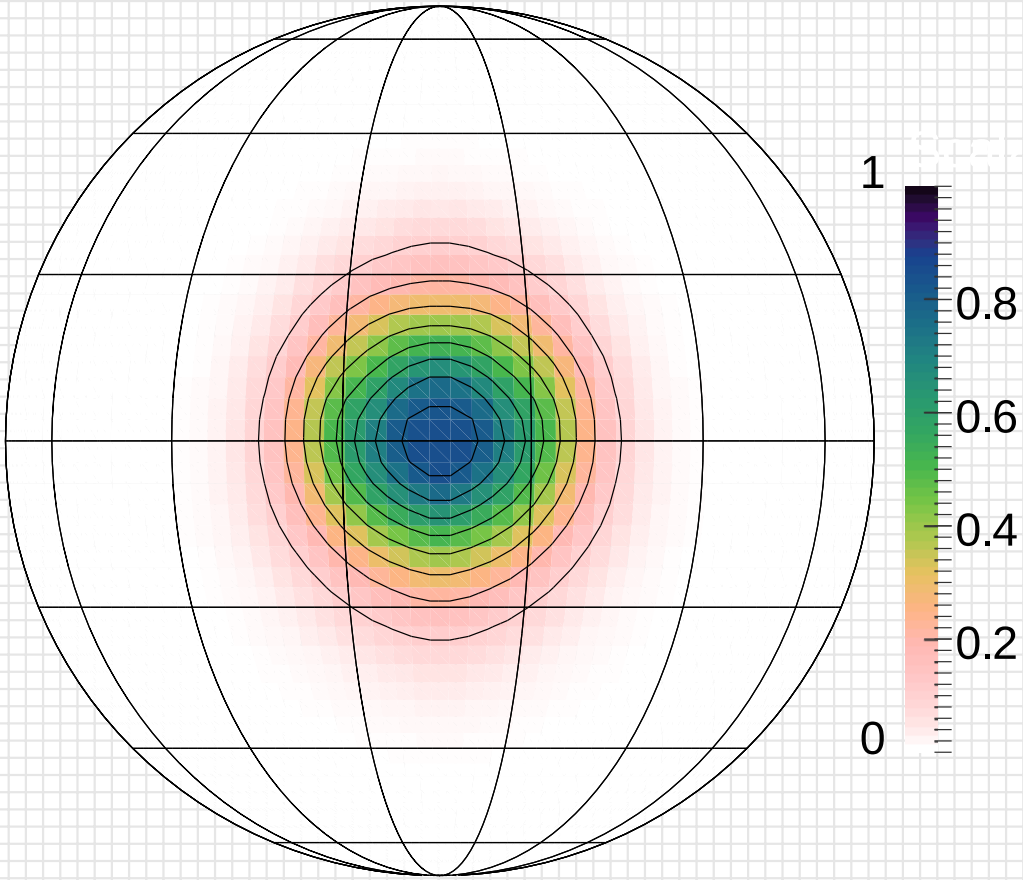

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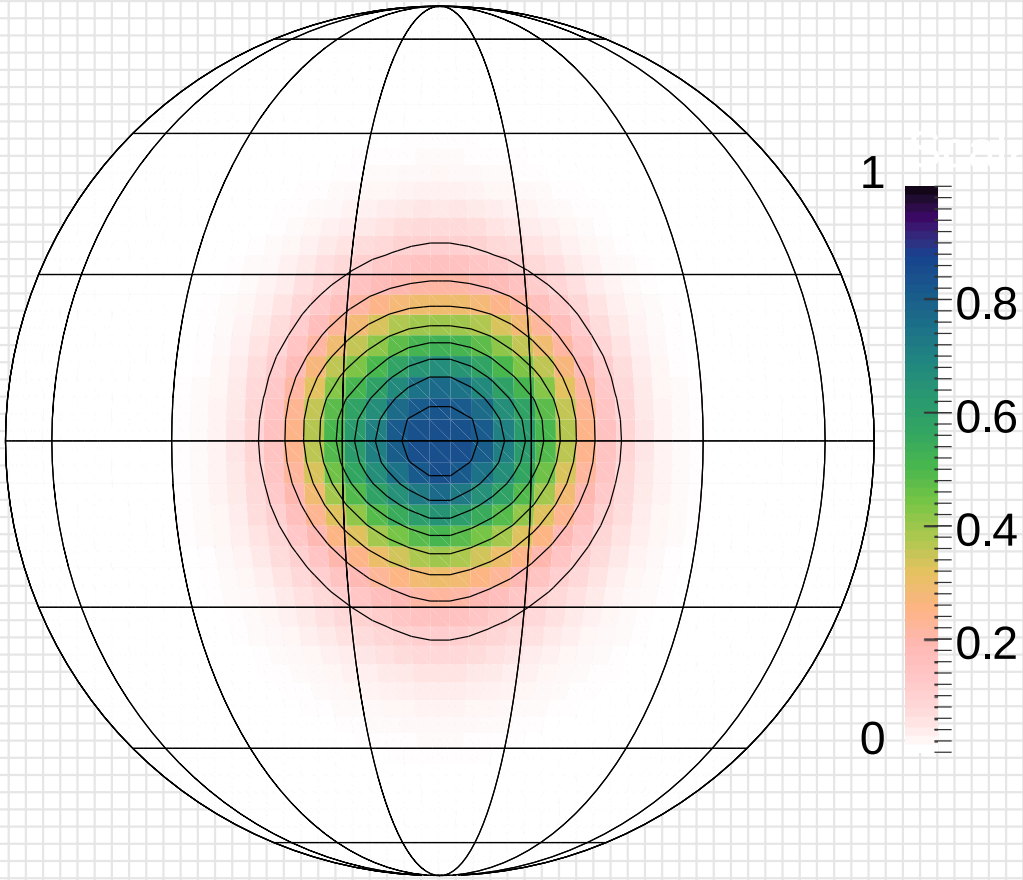

numerical integration using MPDATA

MPDATA (father: Piotr Smolarkiewicz)

Multi-dimensional Positive-Definite Advection Transport Algorithm

a family of robust schemes for solving transport problems

- the seminal MPDATA article (Smolarkiewicz, 1984): >600 citations
- Google Scholar: $\sim$ 700 research papers
- Google Books: $\sim$ 200 mentions in books

original single-file Fortran 77 implementation used till today

- unspecified license, no versioning
- e-mail distribution, copy-paste-modify reuse
- no unit/regression tests

libmpdata++: a new C++11 / Blitz++ based implementation

- an over order-of-magnitude lower number of lines of code
- comparable performance
- major improvement in reusability and maintainability

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researcher = user

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- **result correctness**
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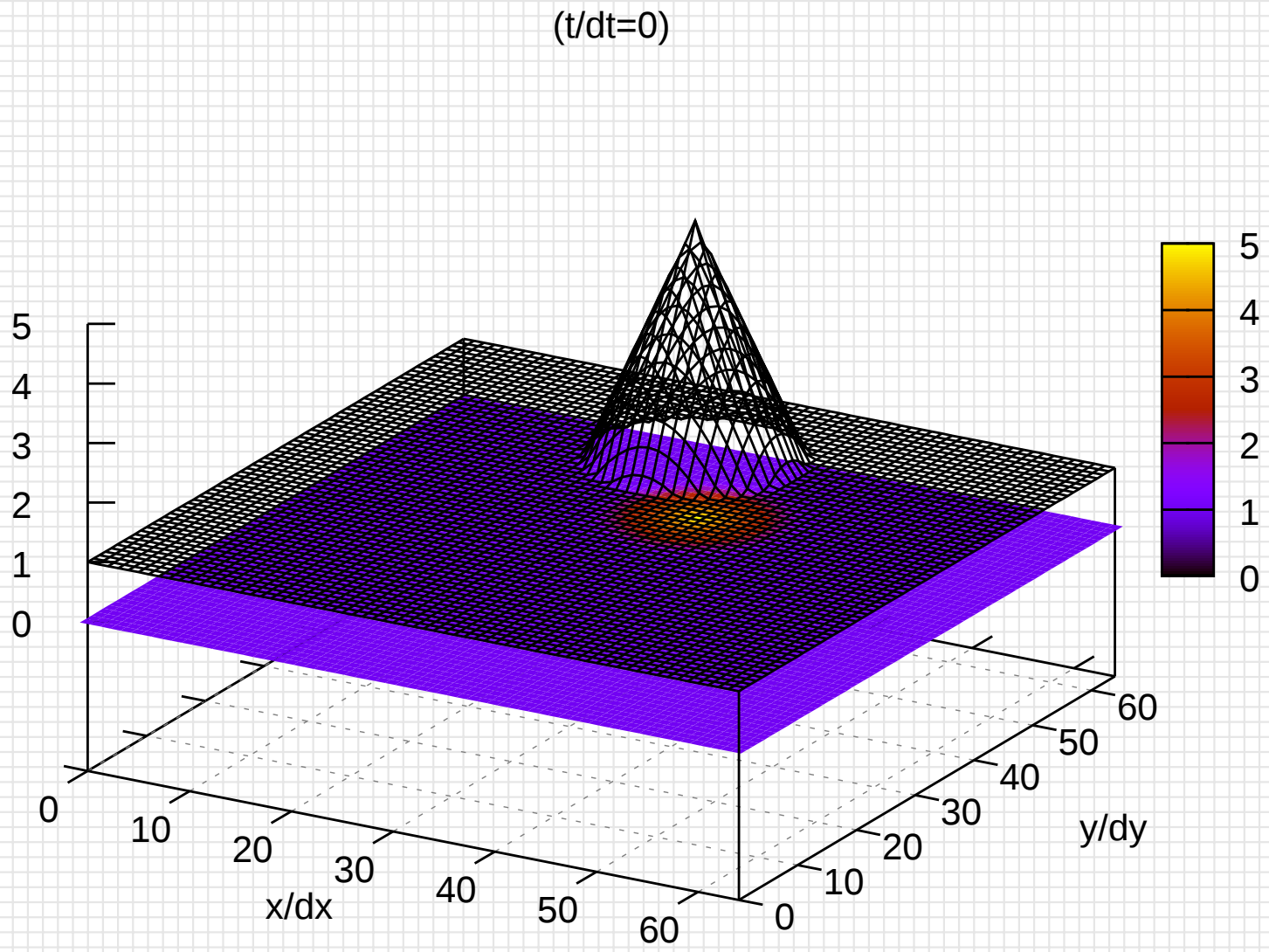

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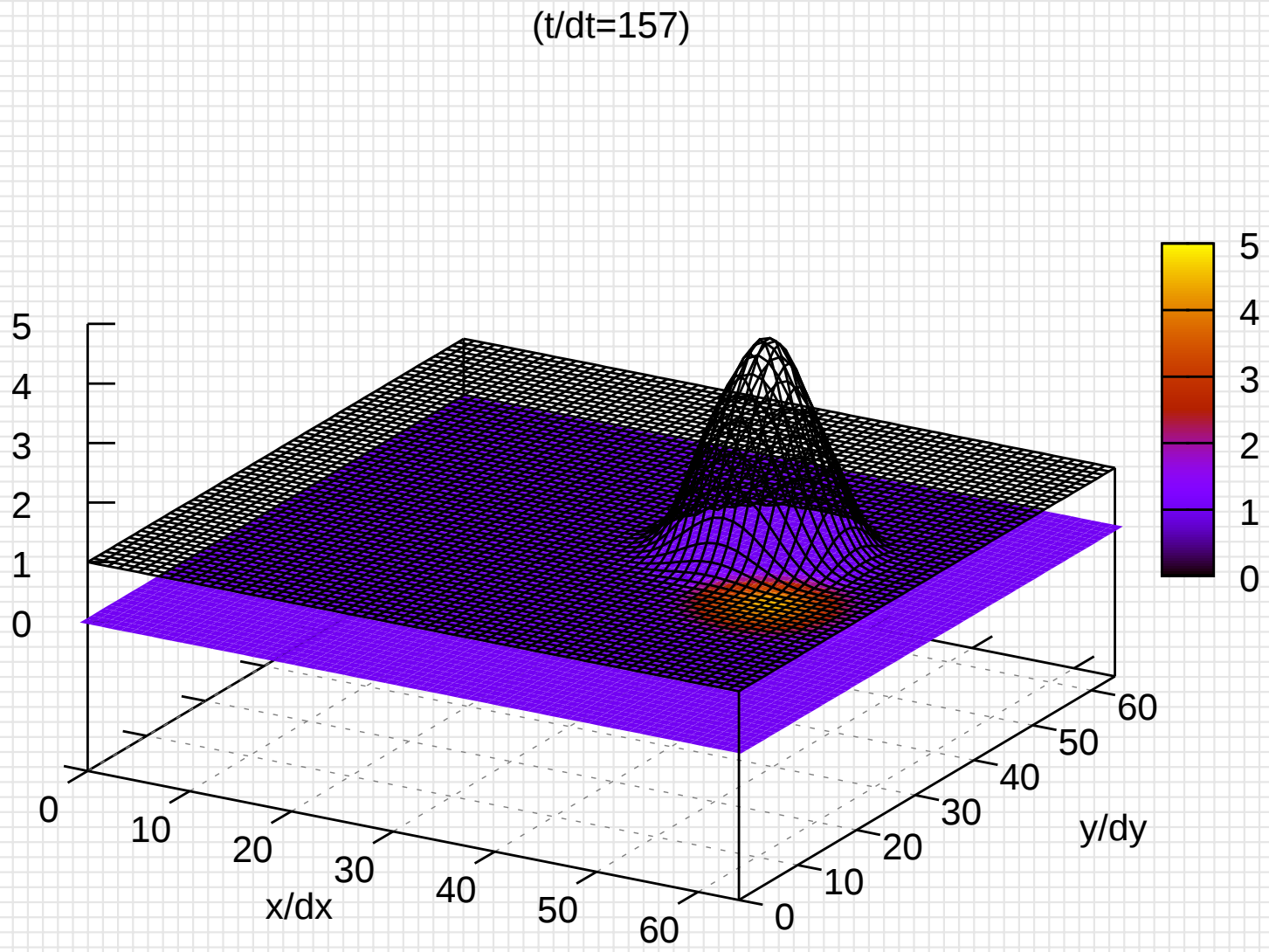

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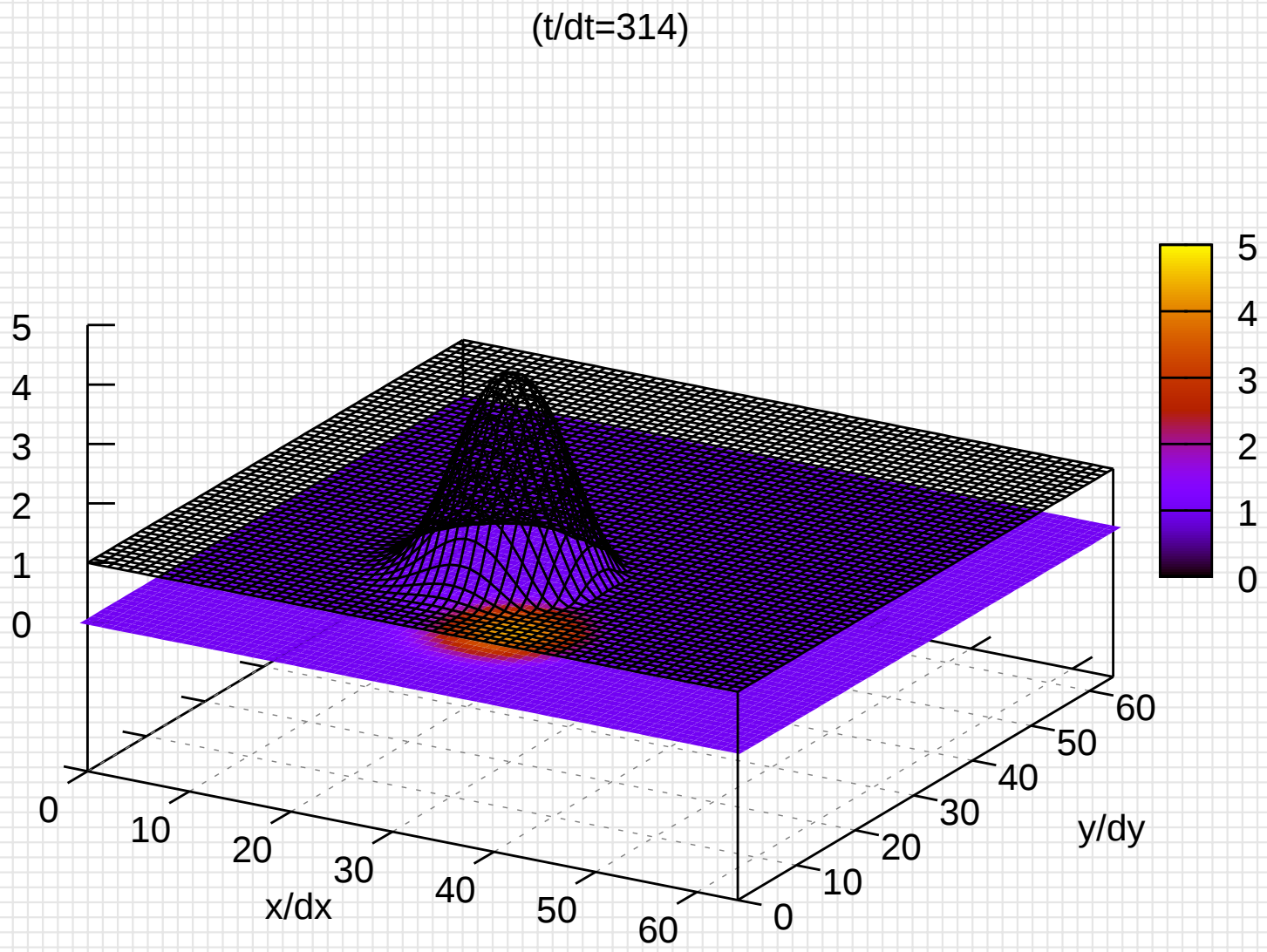

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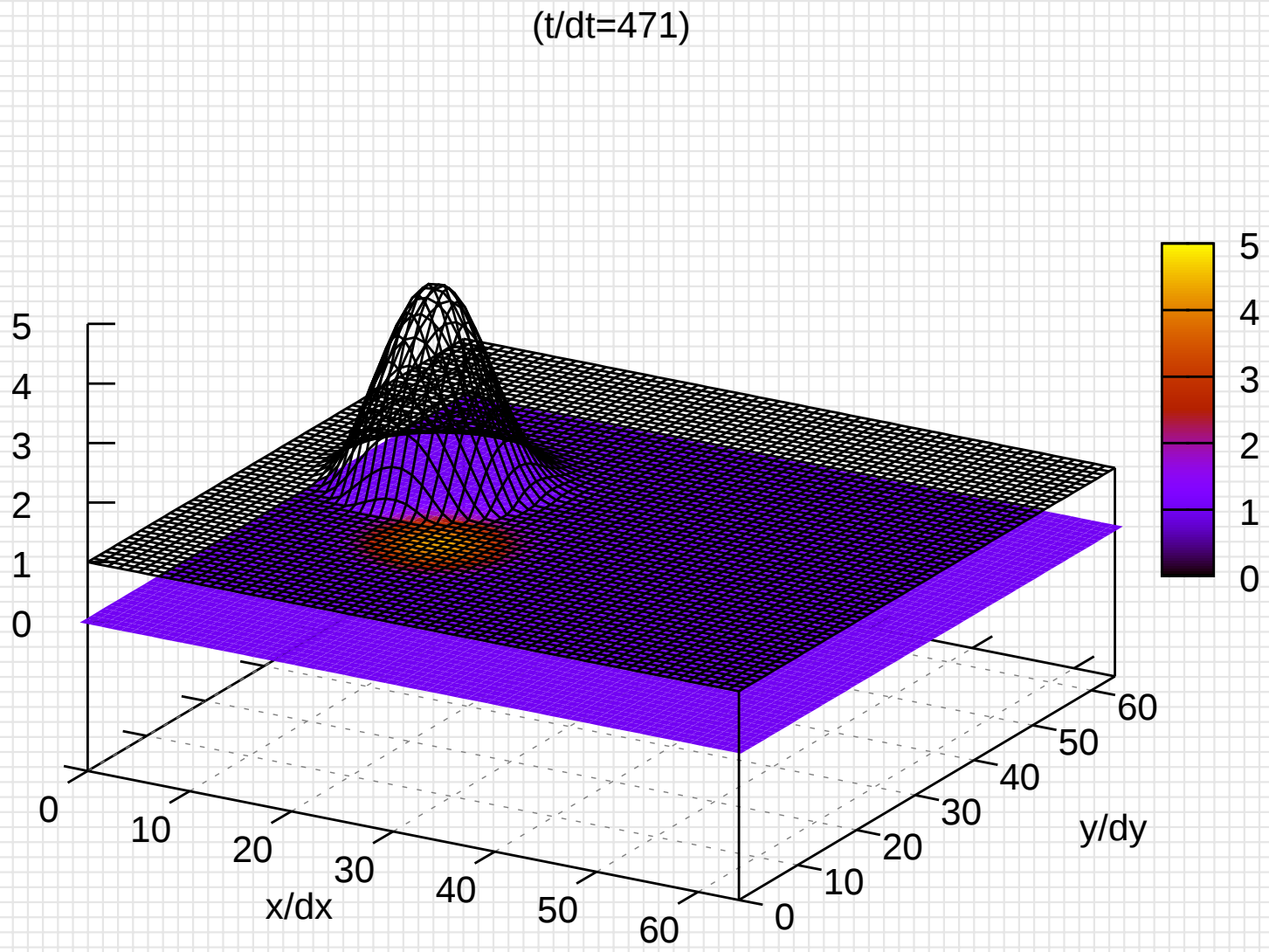

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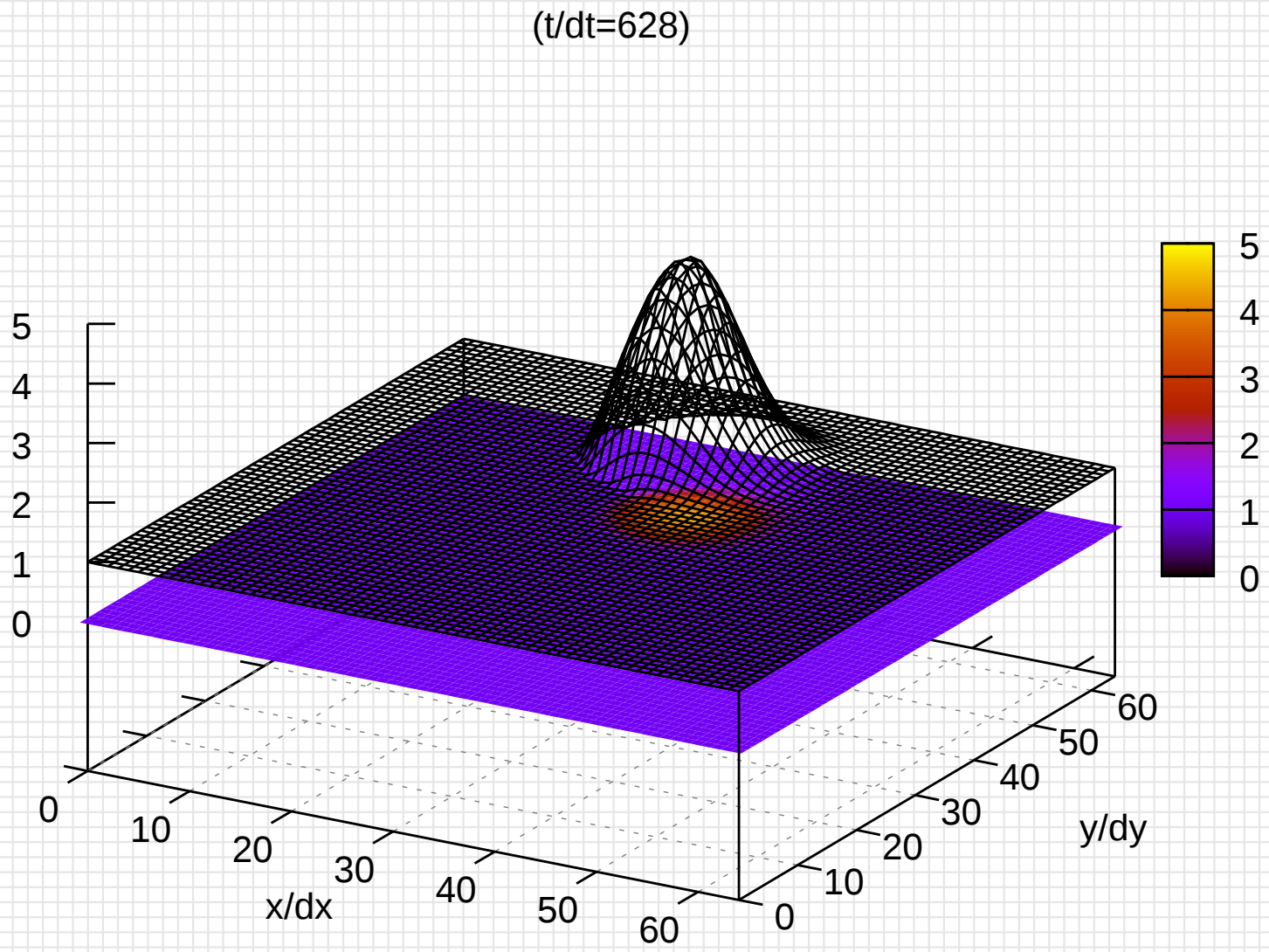

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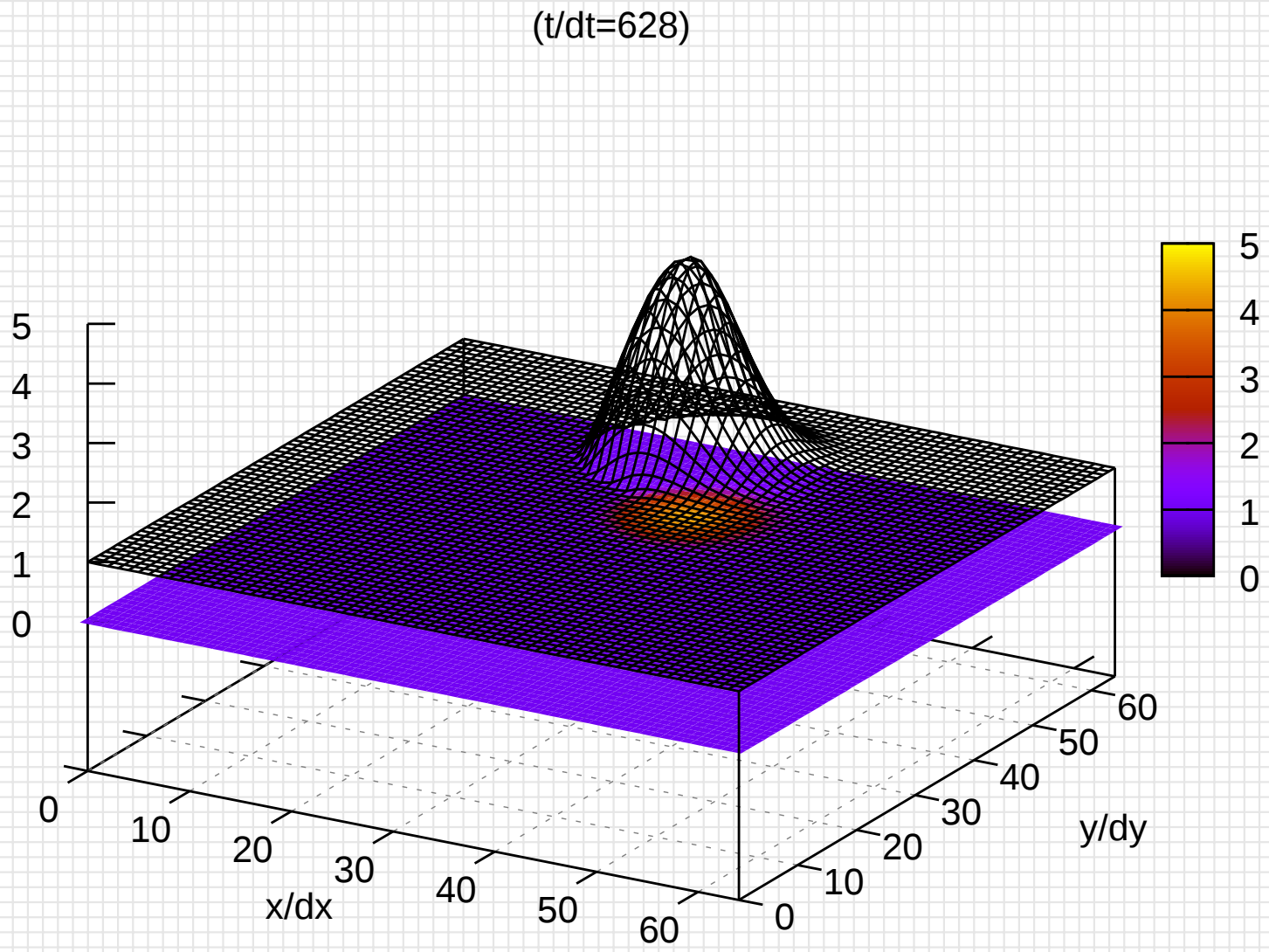

64 LOC using libmpdata++

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

int main()
{
  namespace lmpdt = libmpdataxx;
  const int nx=64, ny=64, nt = 628;

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

  // solver choice
  using run_t = lmpdt::output::gnuplot< lmpdt::solvers::mpdata< ct_params_t >>;

  // runtime parameters
  typename run_t::rt_params_t p;
  p.grid_size = {nx+1, ny+1};
  p.outfreq = nt/4;
  p.gnuplot_output = "out_%s_%d.svg";
  p.gnuplot_with = "lines";
  p.gnuplot_cbrange = p.gnuplot_zrange = "[0:5]";

  // sharedmem concurency and boundary condition choice
  lmpdt::concurr::serial<
    run_t,
    lmpdt::bcond::open, lmpdt::bcond::open, // x-left, x-right
    lmpdt::bcond::open, lmpdt::bcond::open  // y-left, y-right
  > run(p);
```

```
35
36   // initial condition
37   {
38     using namespace blitz::tensor;
39     auto psi = run.advectee();
40
41     const double
42       dt = .1, dx = 1, dy = 1, omega = .1,
43       h = 4., h0 = 1, r = .15 * nx * dx,
44       x0 = .5 * nx * dx, y0 = .75 * ny * dy,
45       xc = .5 * nx * dx, yc = .50 * ny * dy;
46
47     // cone shape cut at h0
48     psi = blitz::pow(i * dx - x0, 2) +
49           blitz::pow(j * dy - y0, 2);
50
51     psi = h0 + where(
52       psi - pow(r, 2) <= 0,                 // if
53       h - blitz::sqrt(psi / pow(r/h,2)),    // then
54       0.                                    // else
55     );
56
57     // constant-angular-velocity rotational field
58     run.advector(0) =  omega * (j * dy - yc) * dt/dx;
59     run.advector(1) = -omega * (i * dx - xc) * dt/dy;
60   }
61
62   // time stepping
63   run.advance(nt);
64 }
```

```
35
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37   {
38     using namespace blitz::tensor;
39     auto psi = run.advectee();
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60   }
61
62   // time stepping
63   run.advance(nt);
64 }
```
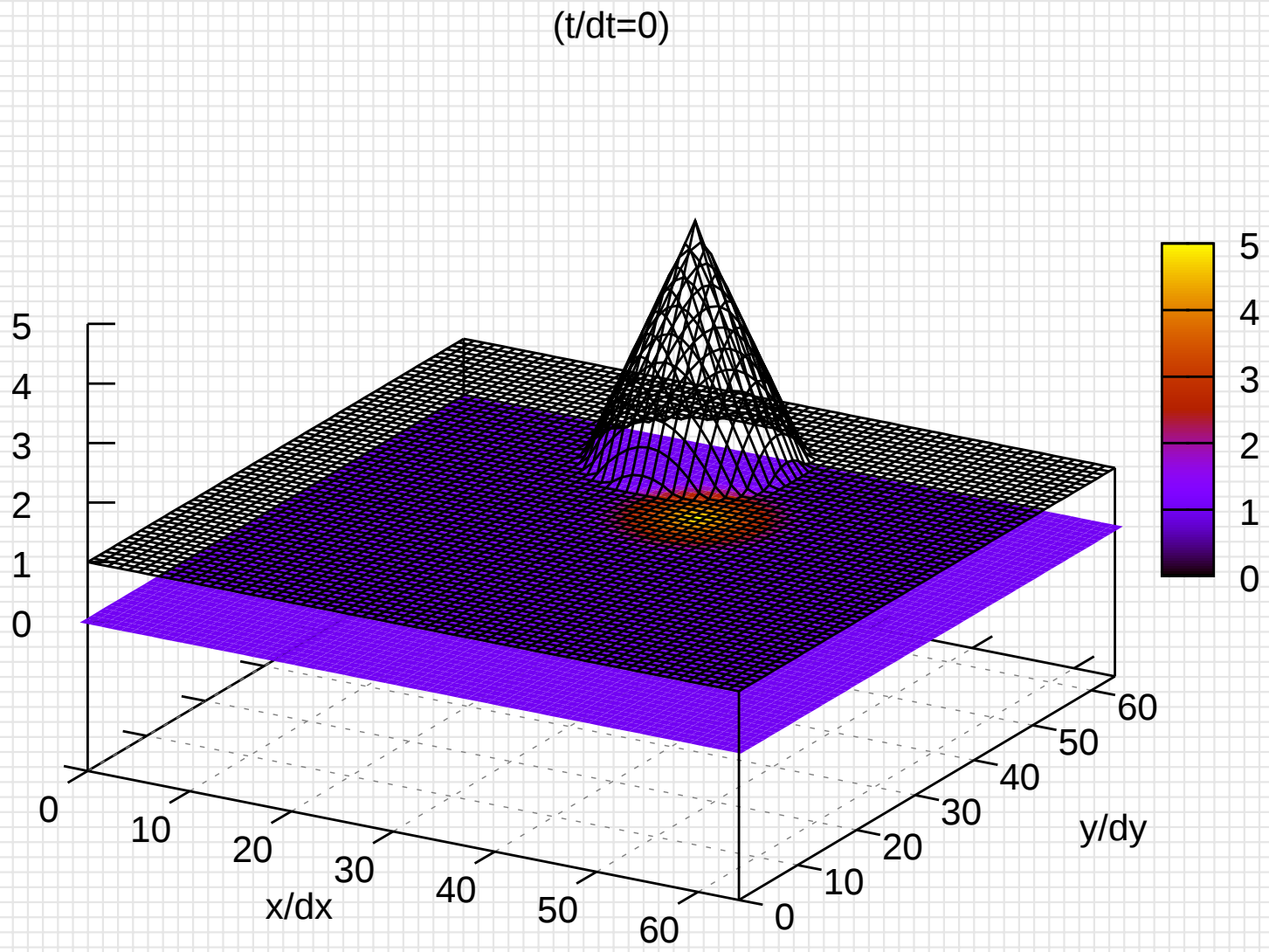

CMakeLists.txt

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

libmpdata++: rotating cone test



64 LOC using libmpdata++

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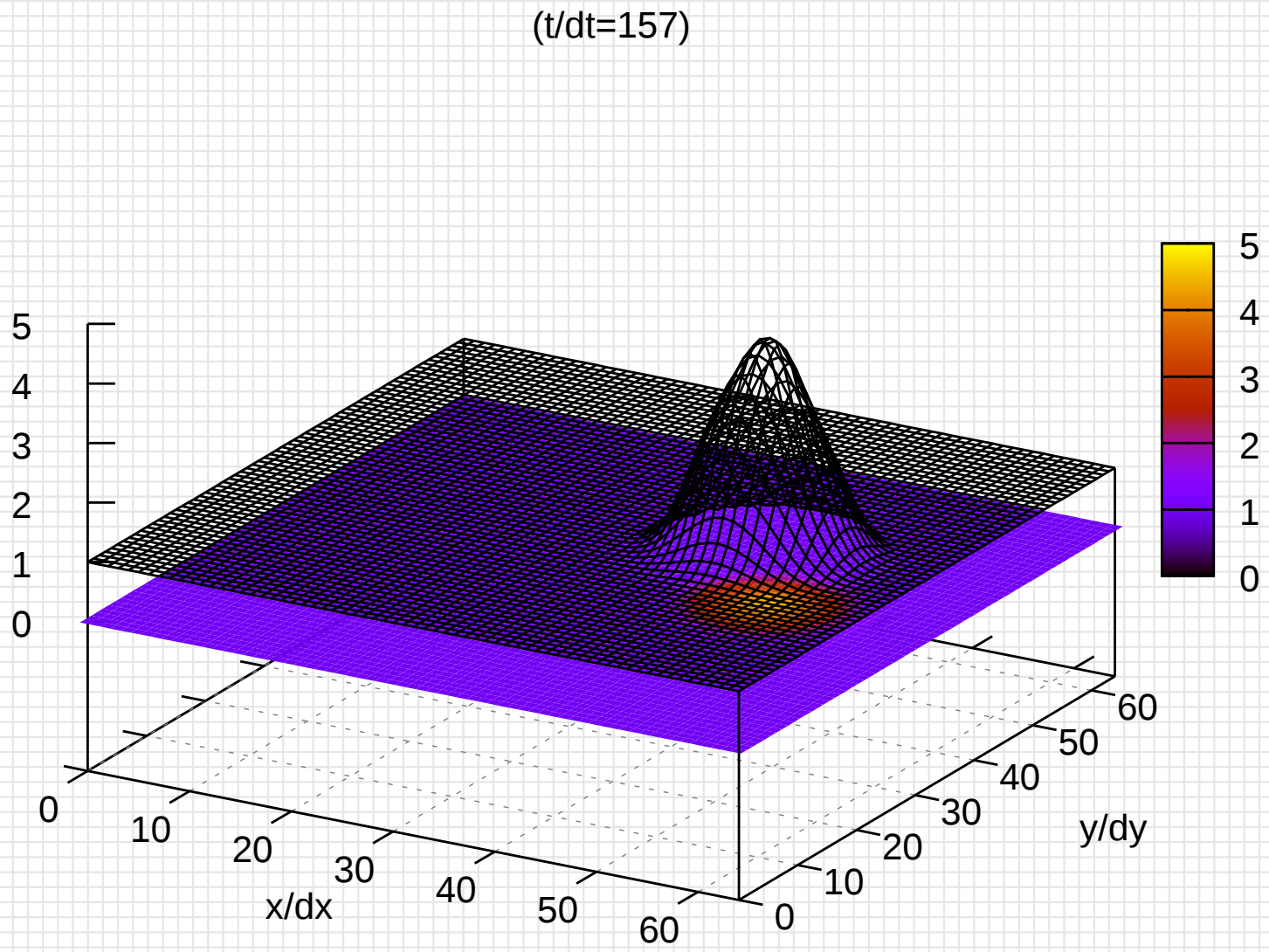

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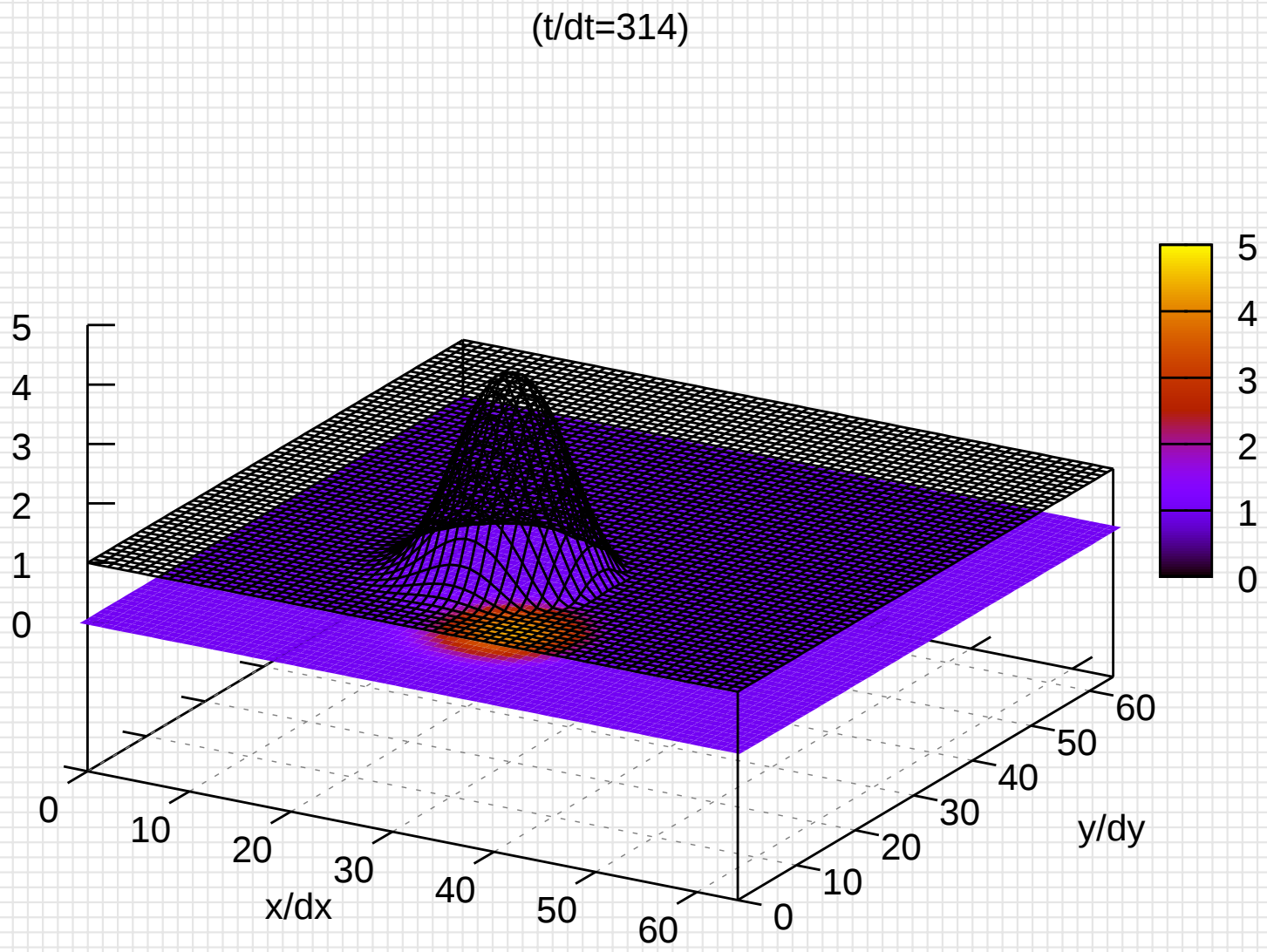

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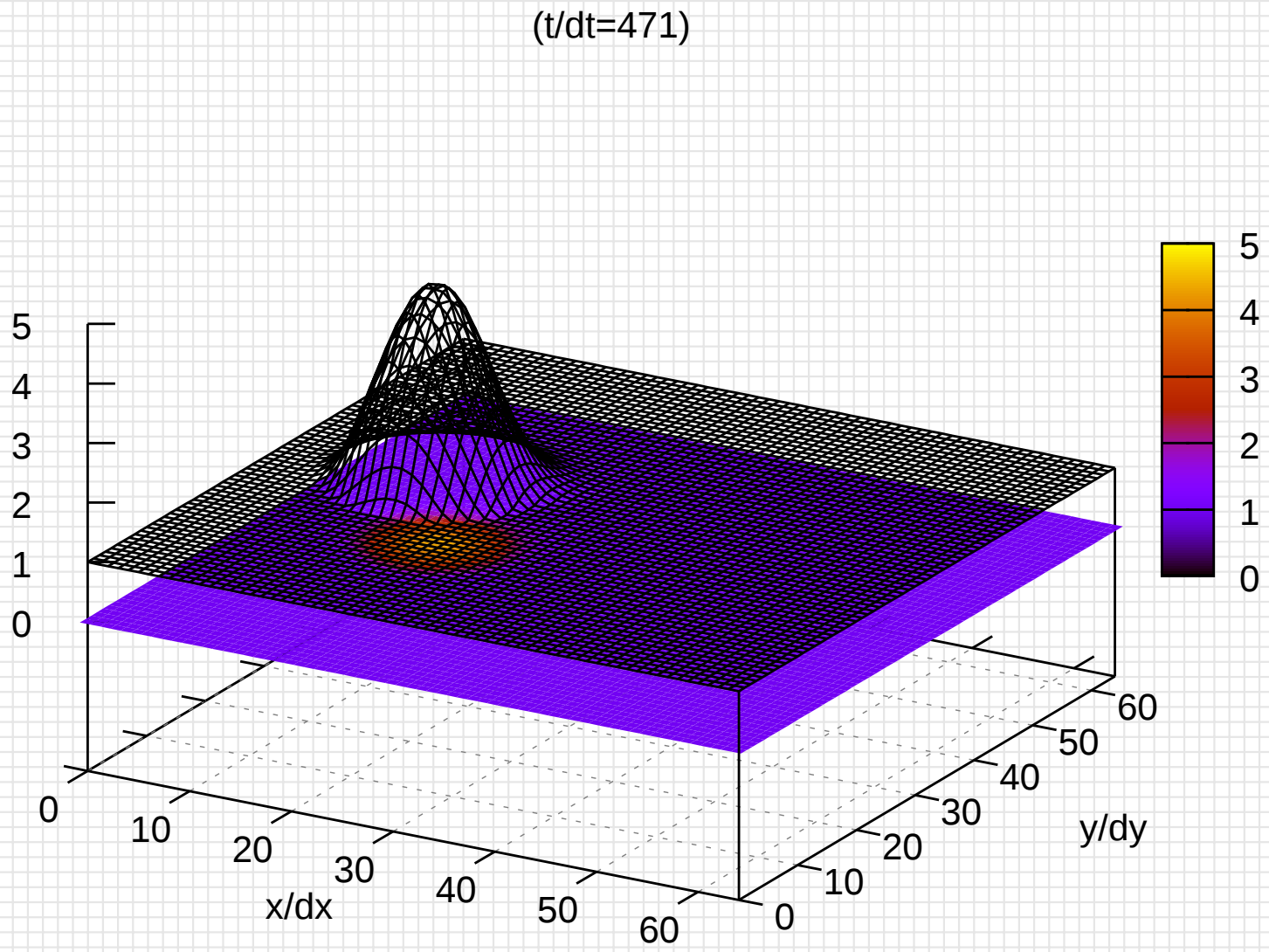

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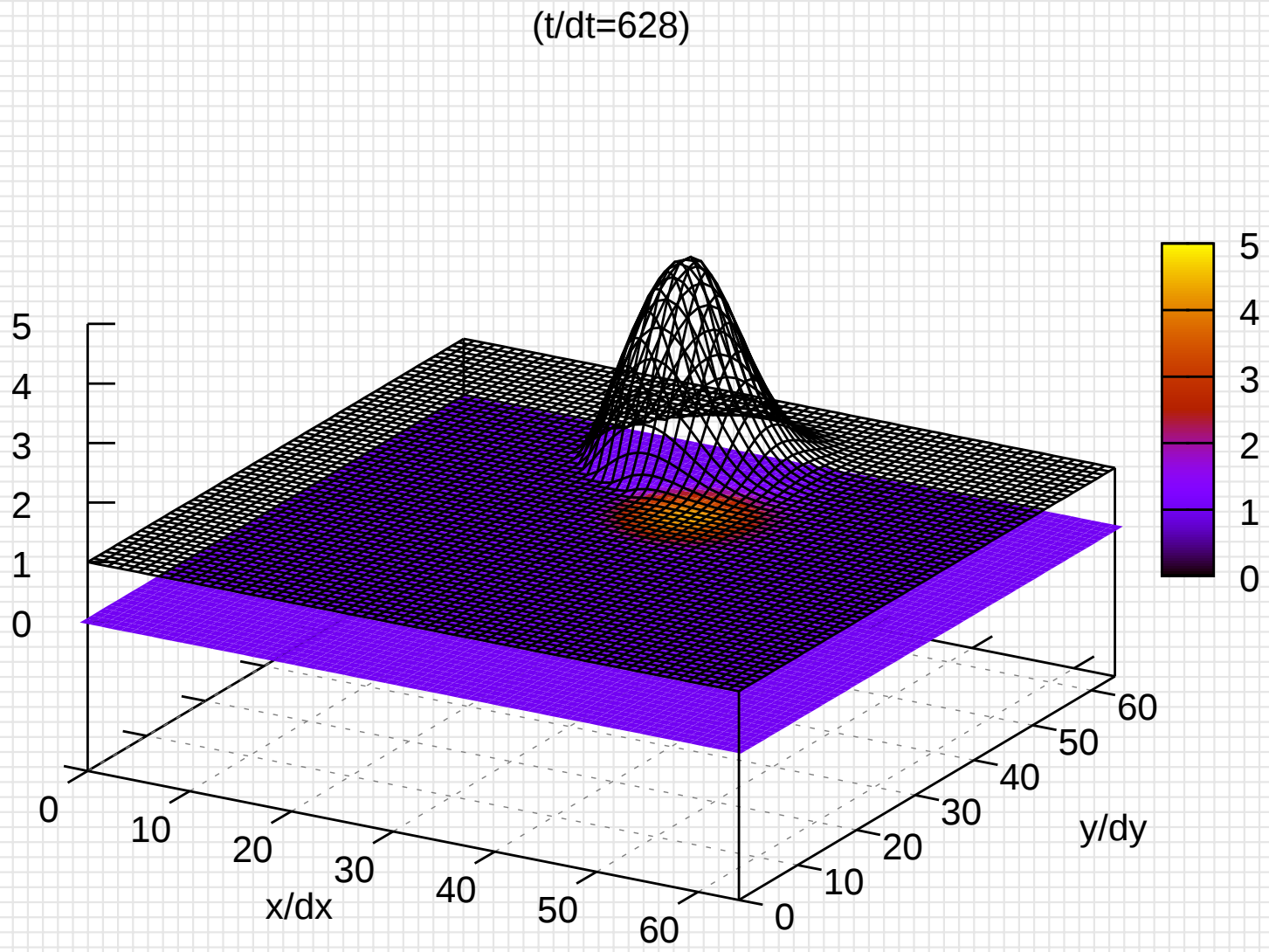

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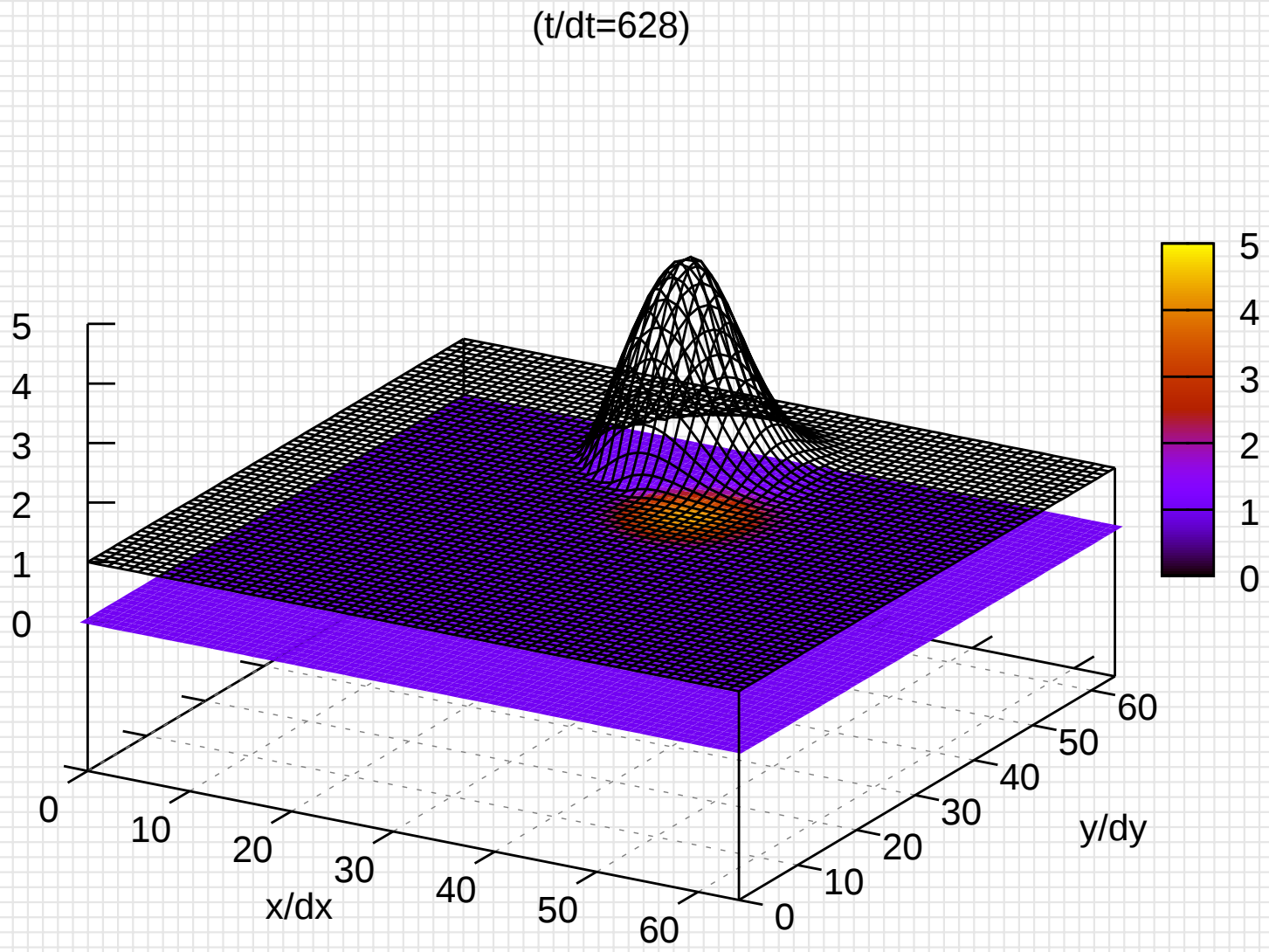


64 LOC using libmpdata++

with multi-threading ⇝ also 64 LOC!

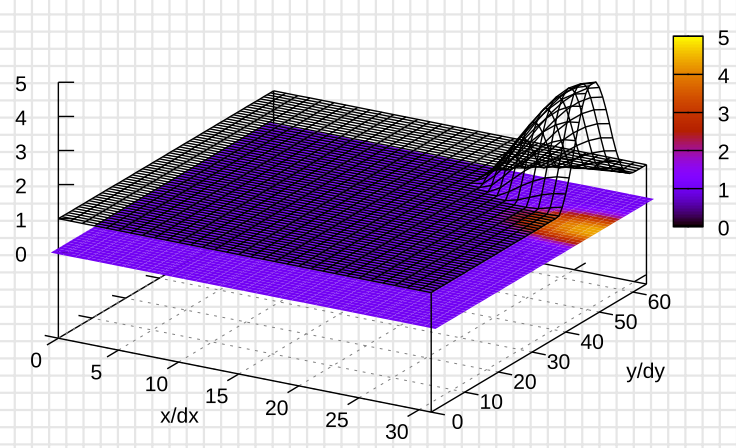
```
2c2
< #include <libmpdata++/concurr/serial.hpp>
---
> #include <libmpdata++/concurr/threads.hpp>
30c30
<   lmpdt::concurr::serial<
---
>   lmpdt::concurr::threads<
```

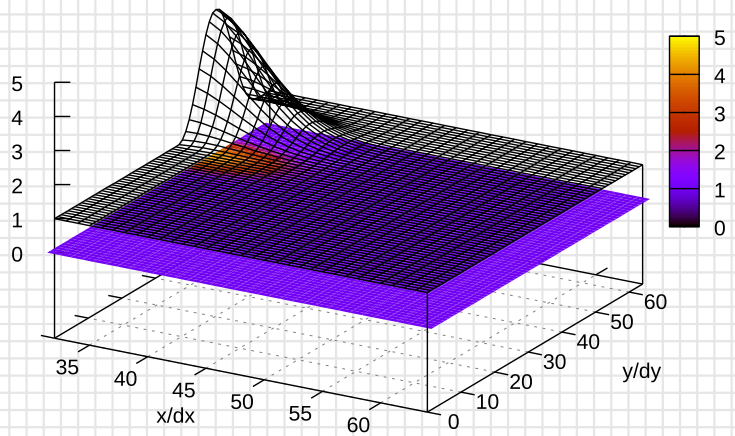
```
$ top
...
  PID USER      PR  NI    S  %CPU %MEM nTH     TIME+ COMMAND
21031 slayoo    20   0    R  73.7  0.1   4   0:01.68 hello_worl  90%
...
```

MPI + threads $\rightsquigarrow$ also 64 LOC!!! (recompilation only)

```
$ cmake . -DCMAKE_CXX_COMPILER=mpic++
$ make
$ OMP_NUM_THREADS=2 mpirun -np 2 ./hello_world
```

```
$ top
...
  PID USER      PR  NI    S  %CPU %MEM nTH     TIME+ COMMAND
19640 slayoo    20   0    R  65.5  0.3   2   0:00.92 hello_worl  98%
19641 slayoo    20   0    R  64.0  0.3   2   0:00.91 hello_worl  99%
...
```





Plan of the talk

1. what's libmpdata++
2. libmpdata++: a hello-world program
3. libmpdata++ 1.0: summary of features
4. libmpdata++ 2.0: new features under development
5. closing remarks

Plan of the talk

libmpdata++ 1.0: from hello-world to real-world problems

- support for integration in 1D, 2D & 3D
- support for multiple transported fields
- numerous MPDATA options implemented:
  - non-oscillatory option
  - flux-corrected transport option
  - infinite-gauge option (for sign-preserving fields)
  - third-order terms
- coordinate transformations
- open, cyclic, polar & rigid boundary conditions
- source-term handling
- shallow-water and Boussinesq dynamics

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Geoscientific Model Development
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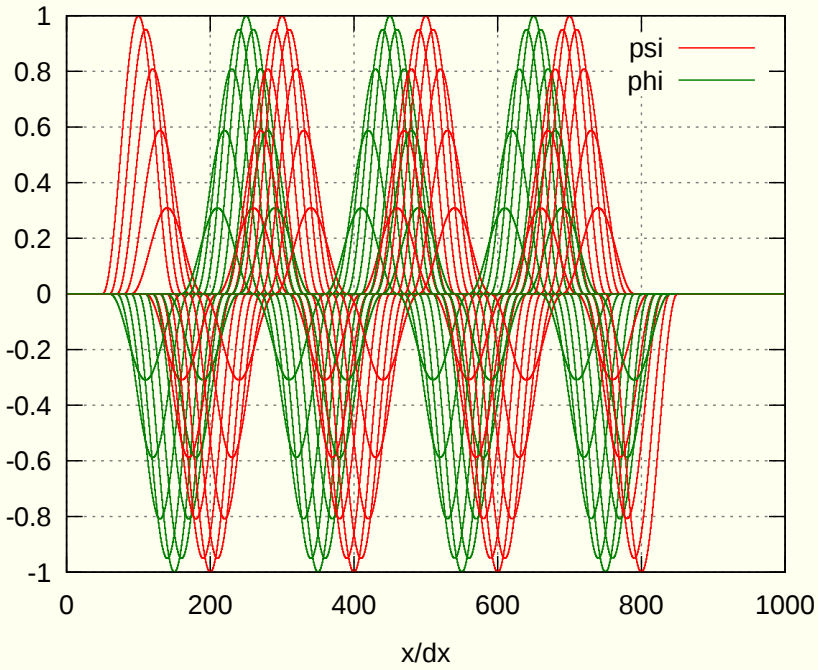

Figure 15. Simulation results of the example presented in Sect. 4.3. Abscissa marks the spatial dimension and ordinate represents the oscillator amplitude. The oscillator state is plotted every 20 time steps.

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

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

```
#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);
```

libmpdata++ 1.0: solver/algorithm hierarchy

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

homogeneous advection

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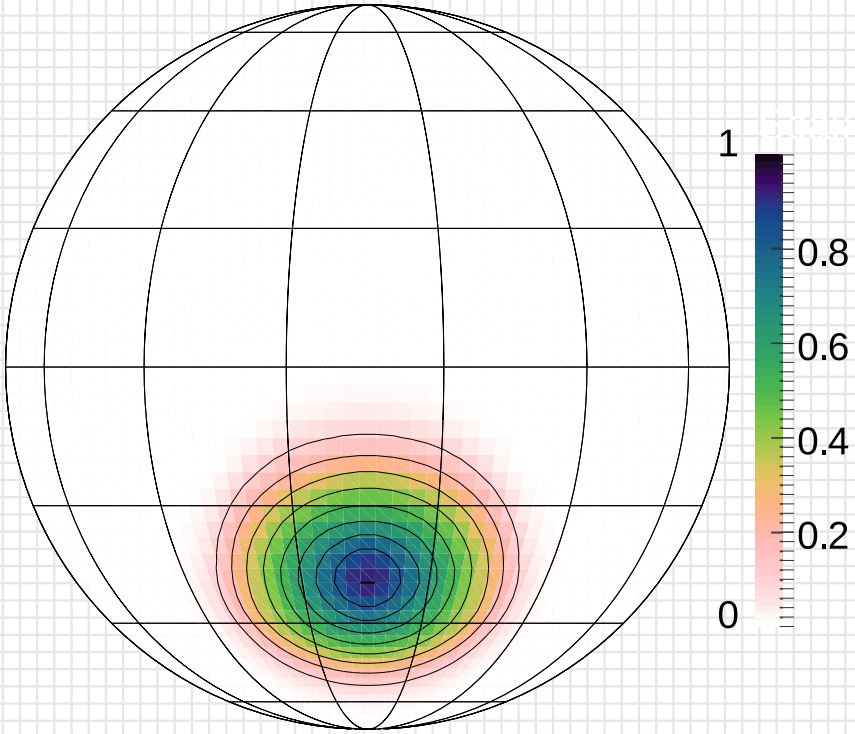
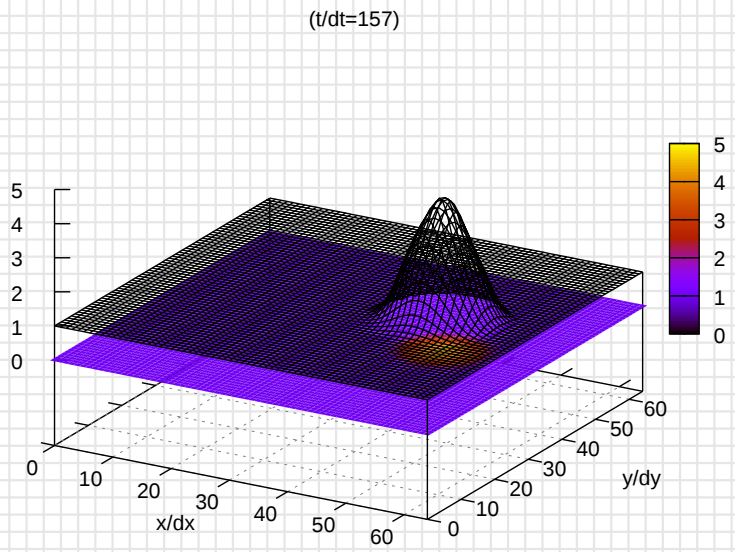
$$\partial_t(G\psi) + \nabla \cdot (G\vec{u}\psi) = 0$$

homogeneous advection

user/test code





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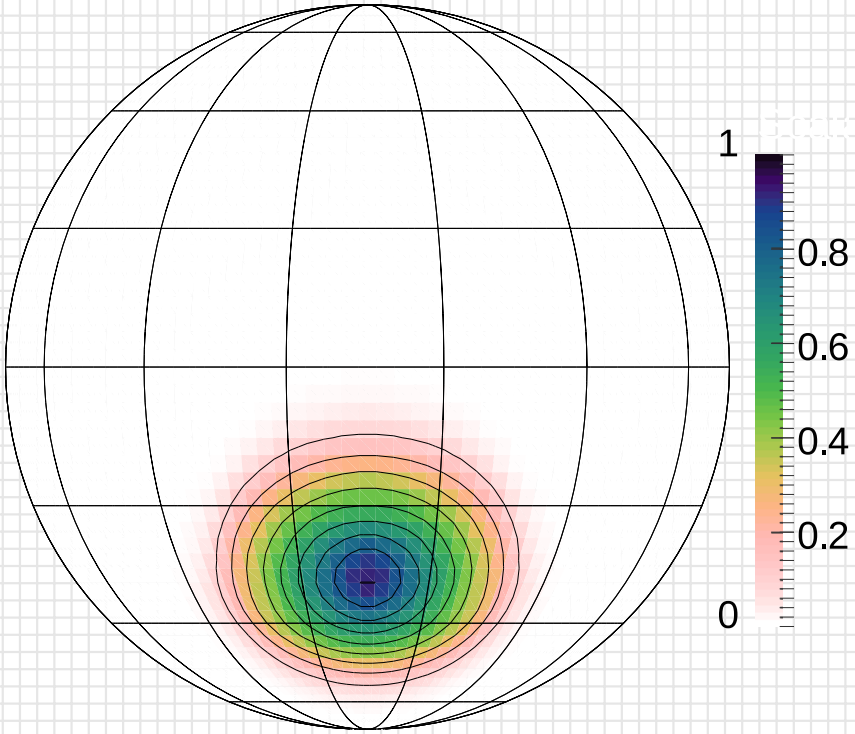
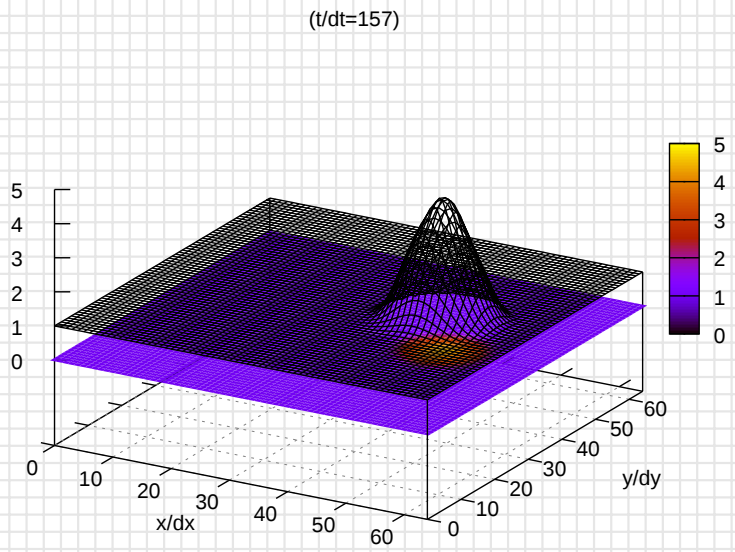
$$\partial_t(G\psi) + \nabla \cdot (G\vec{u}\psi) = 0$$

homogeneous advection

user/test code





libmpdata++ 1.0: solver/algorithm hierarchy

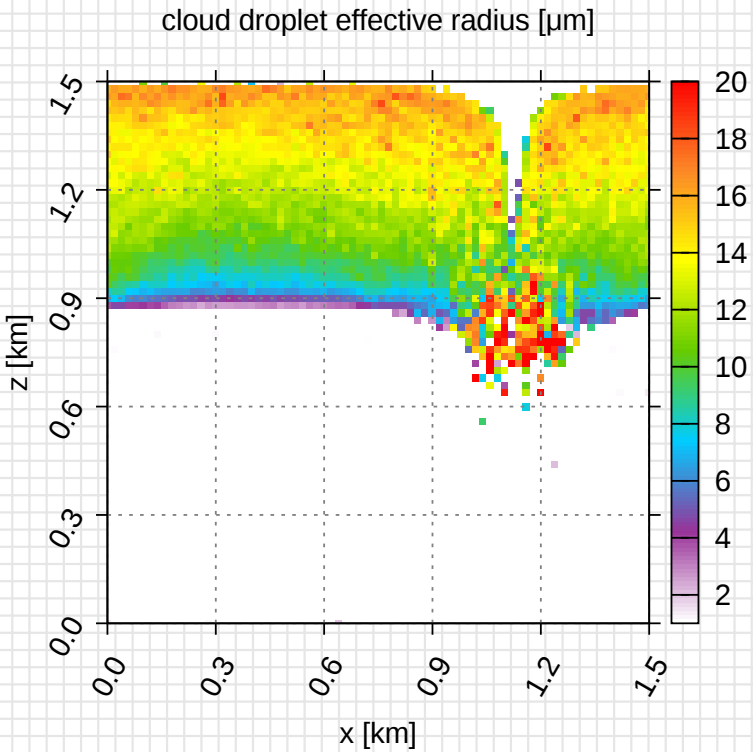
$$\partial_t(G\psi) + \nabla \cdot (G\vec{u}\psi) = 0$$

homogeneous advection

+

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

source terms



libmpdata++ 1.0: solver/algorithm hierarchy

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

homogeneous advection

+

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

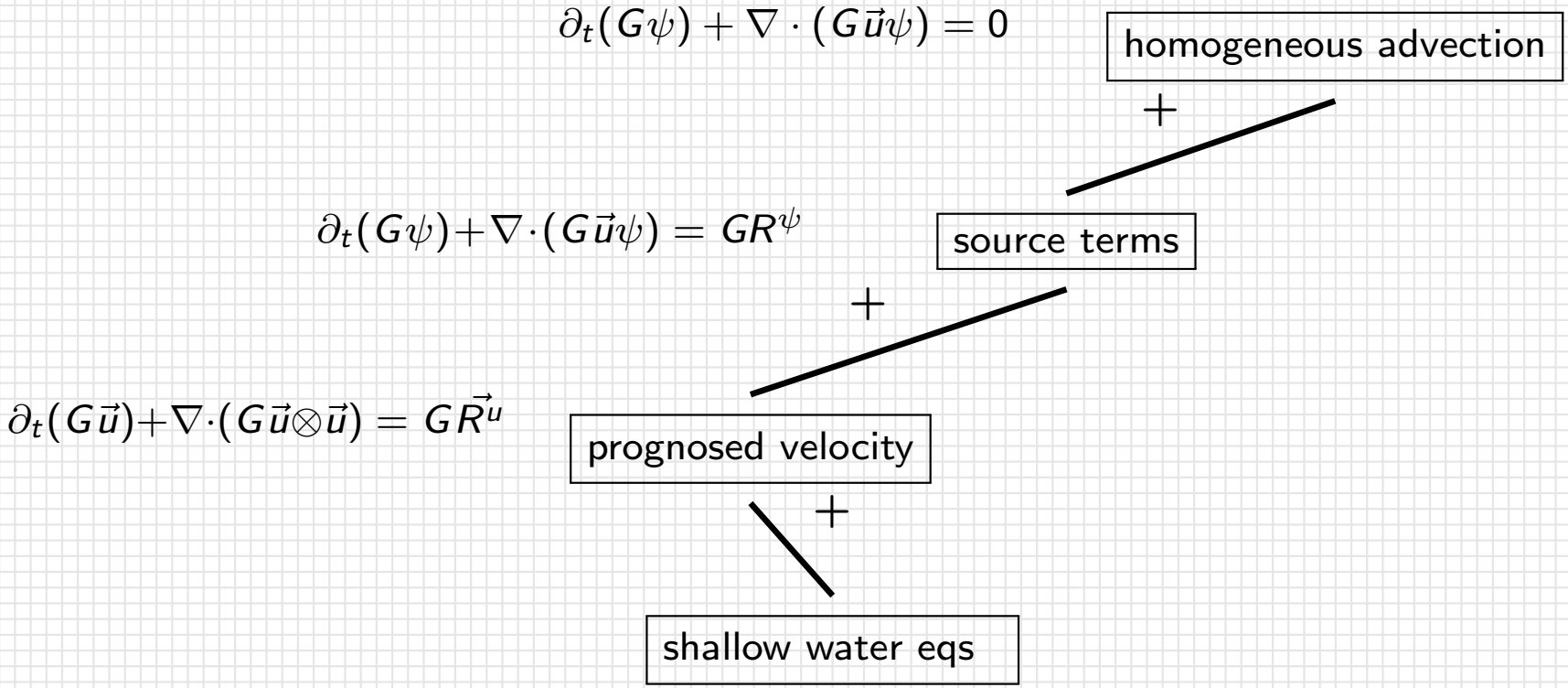
source terms

+

$$\partial_t(G\vec{u}) + \nabla \cdot (G\vec{u} \otimes \vec{u}) = G\vec{R}^{u}$$

prognosed velocity

libmpdata++ 1.0: solver/algorithm hierarchy



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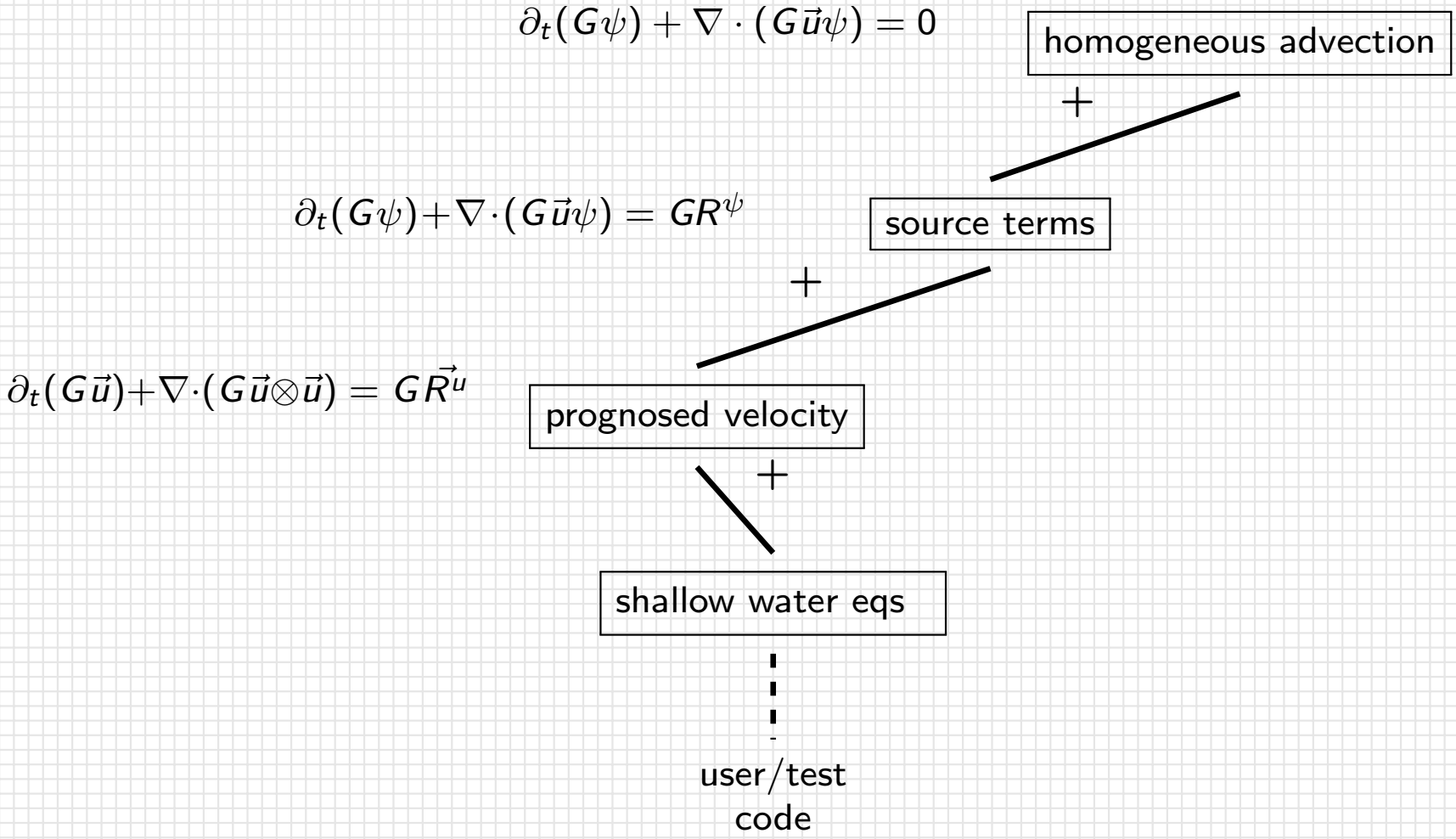
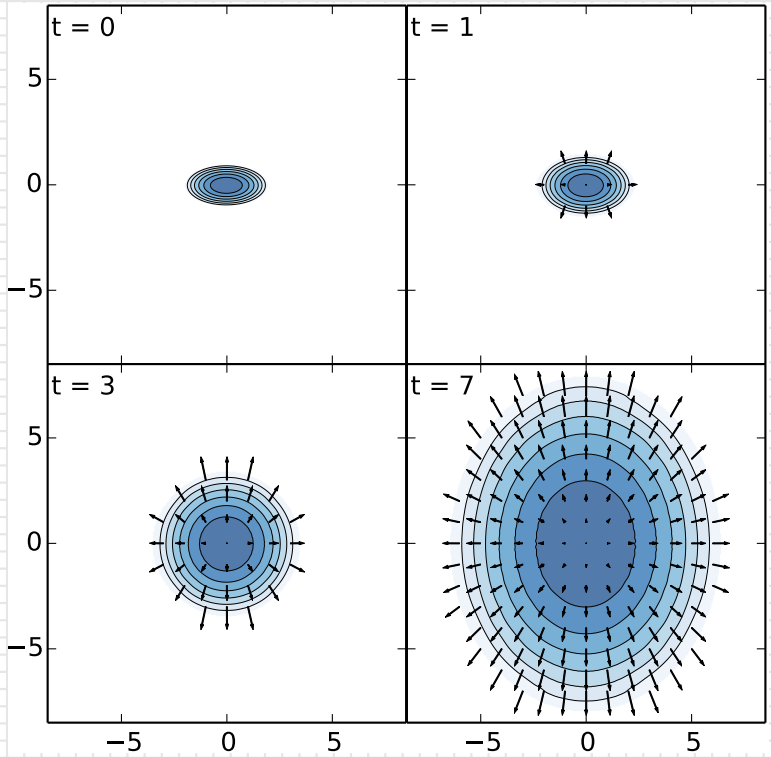


libmpdata++: 3D shallow-water system example



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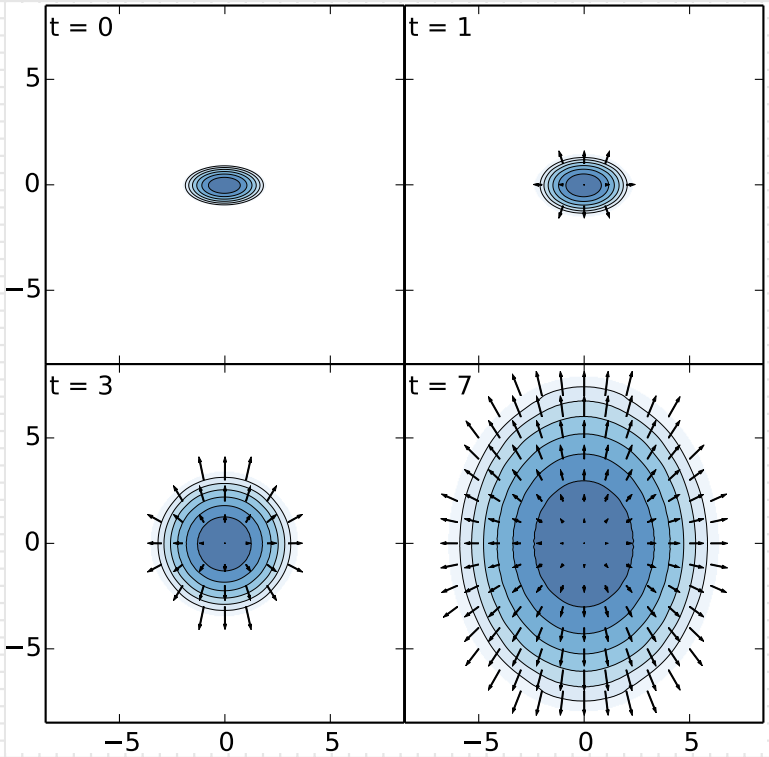

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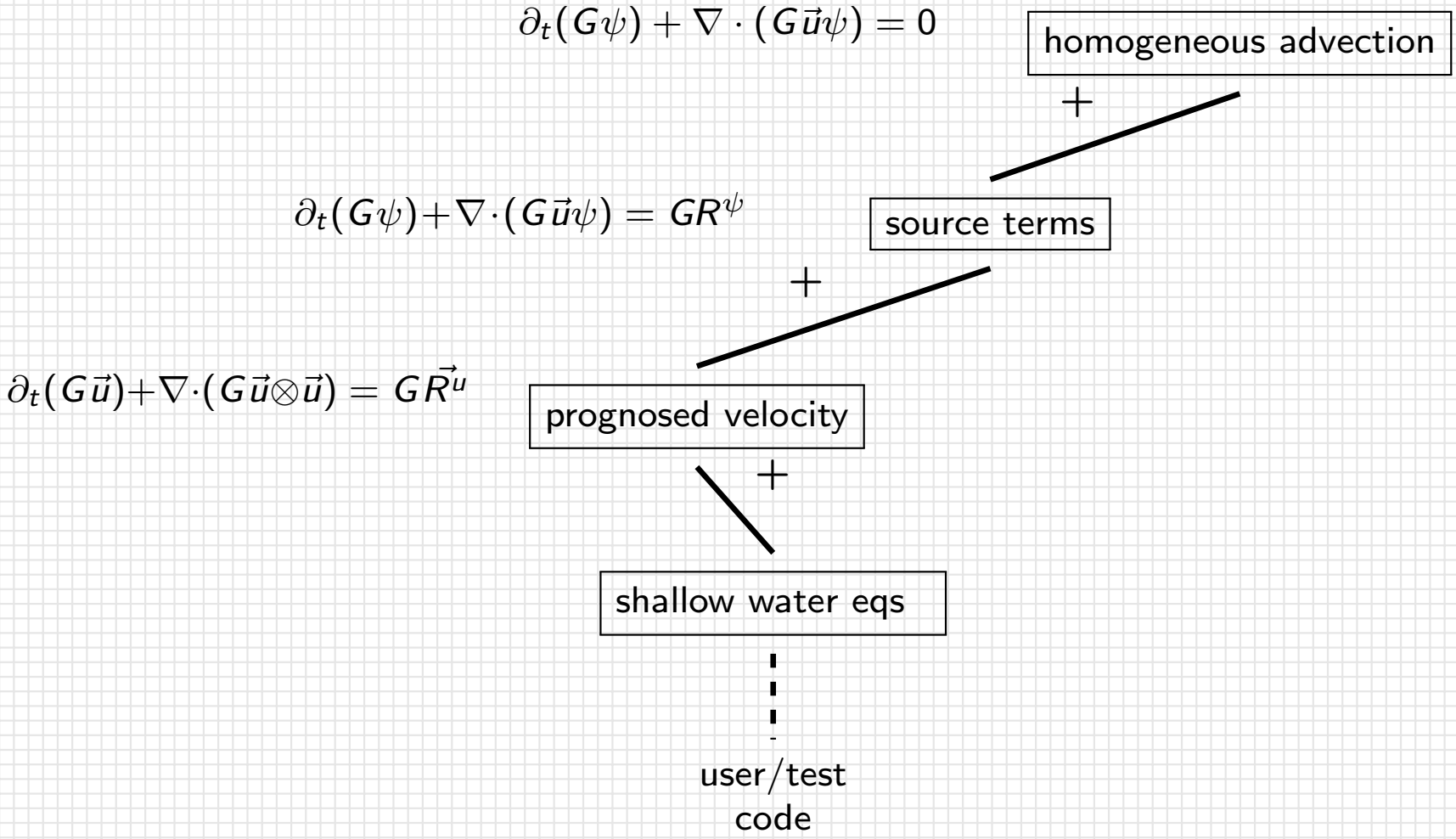

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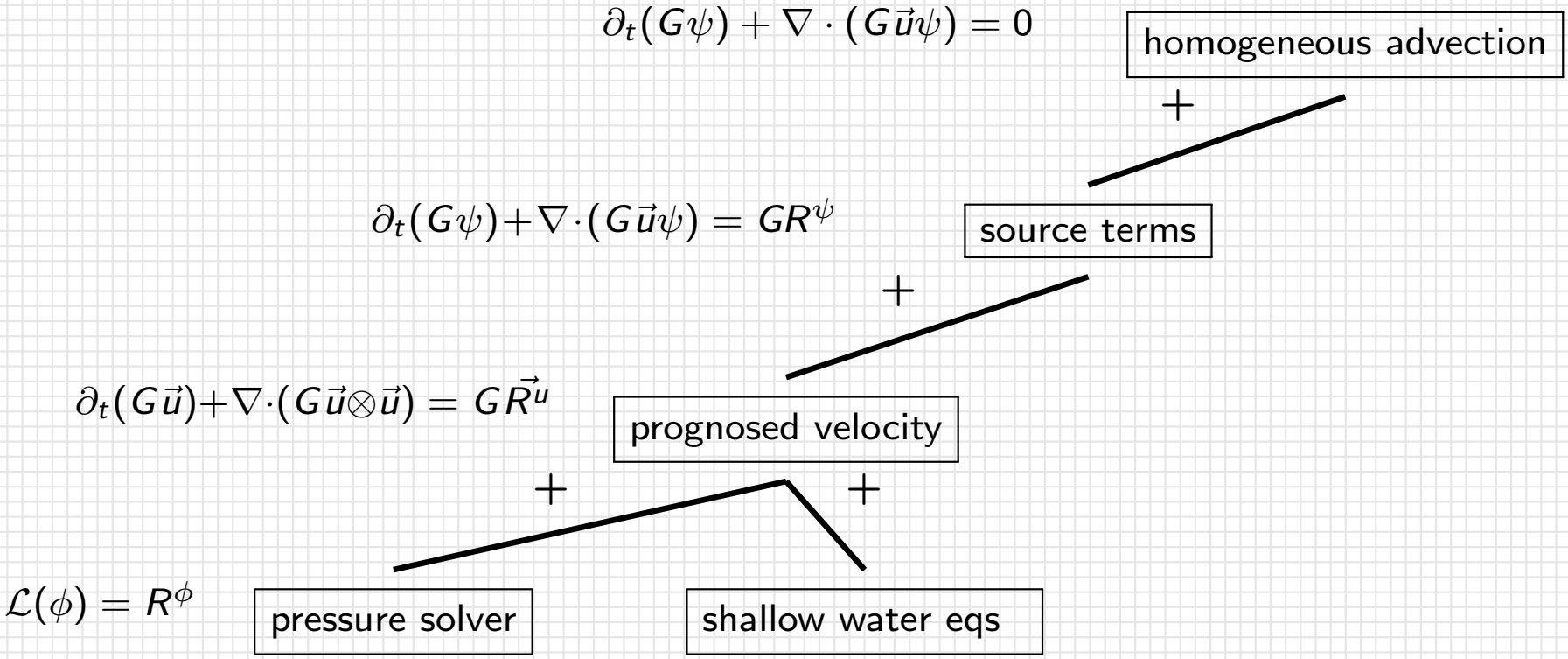

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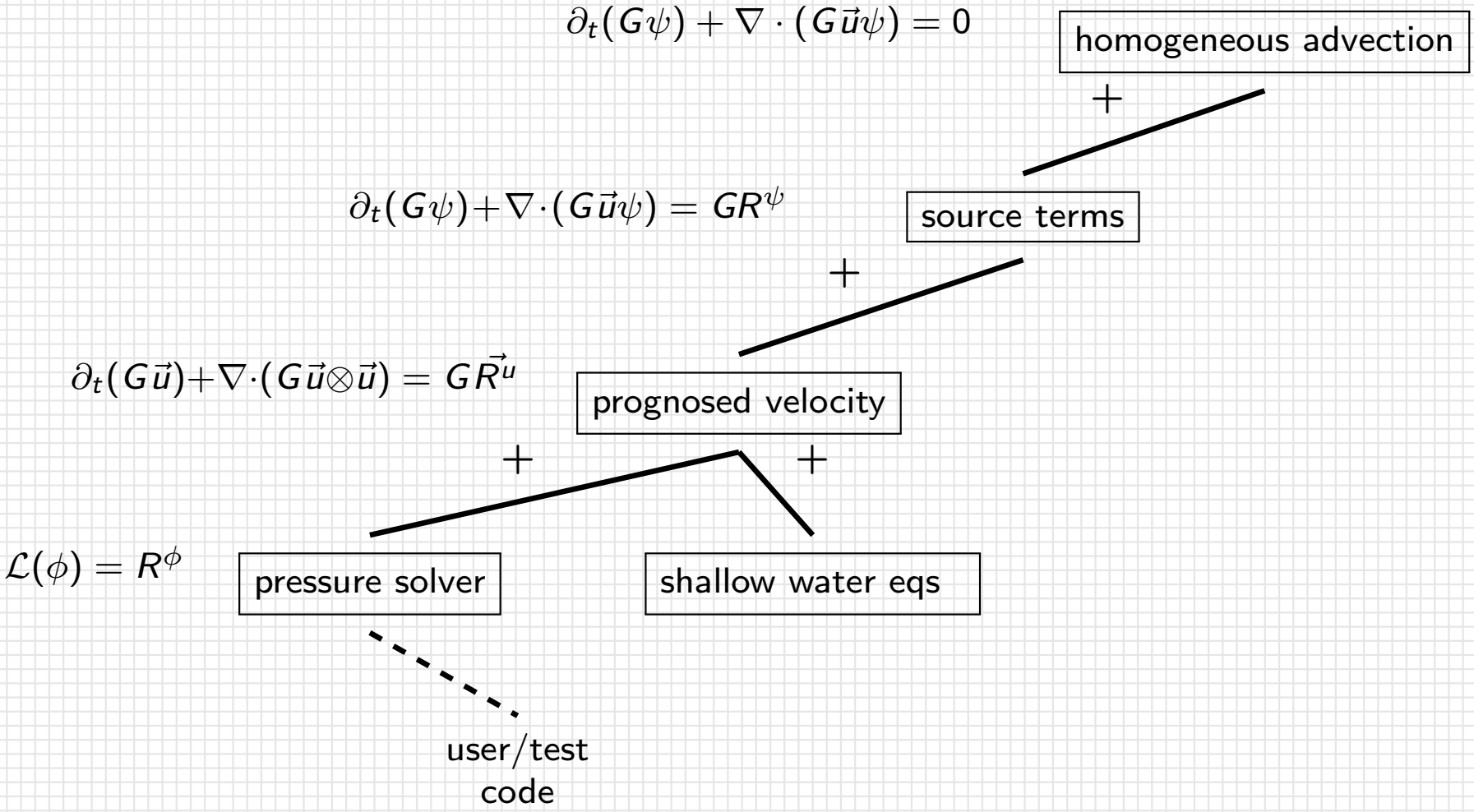
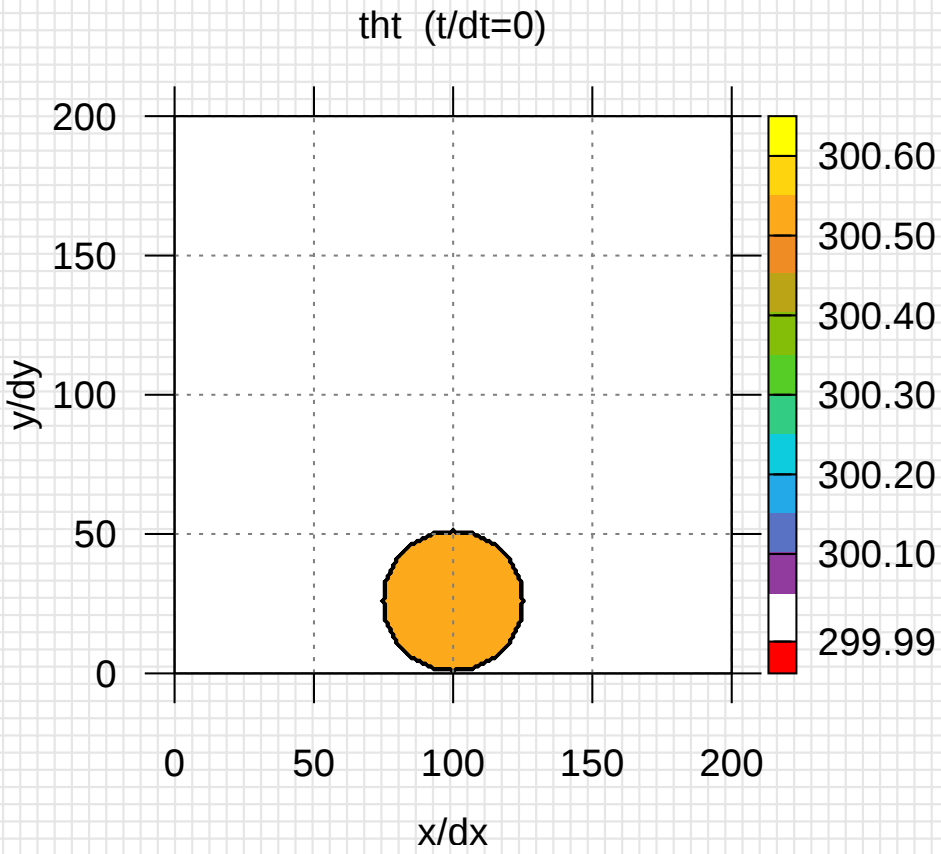


libmpdata++: 2D Boussinesq convection example



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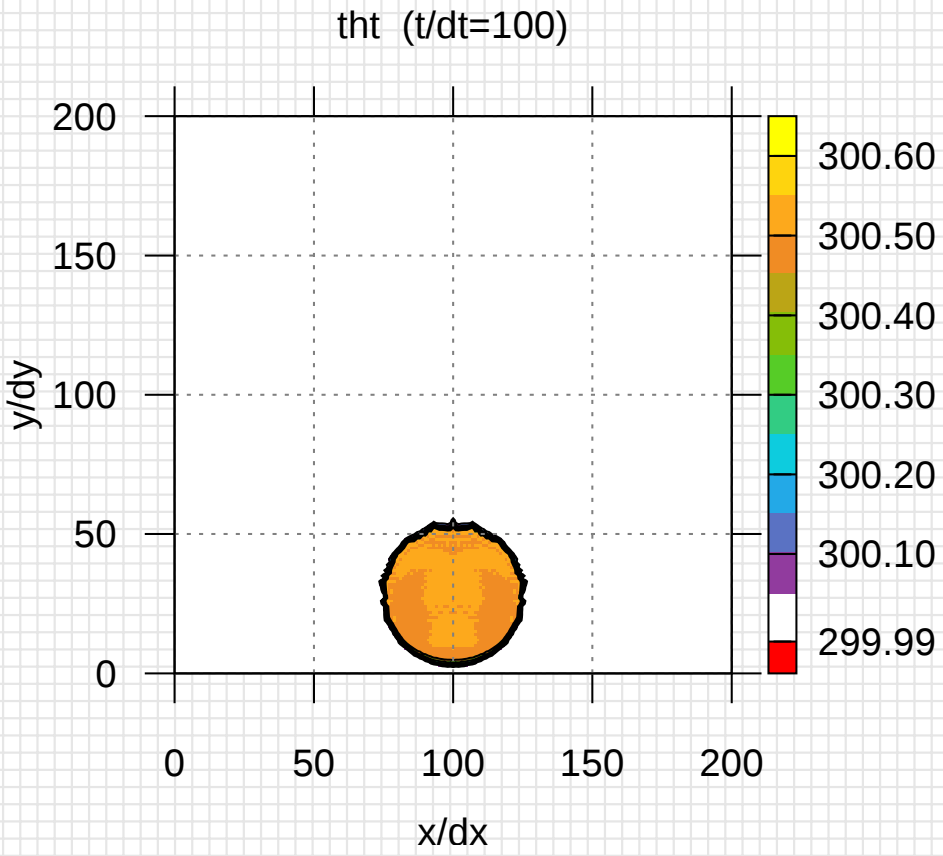

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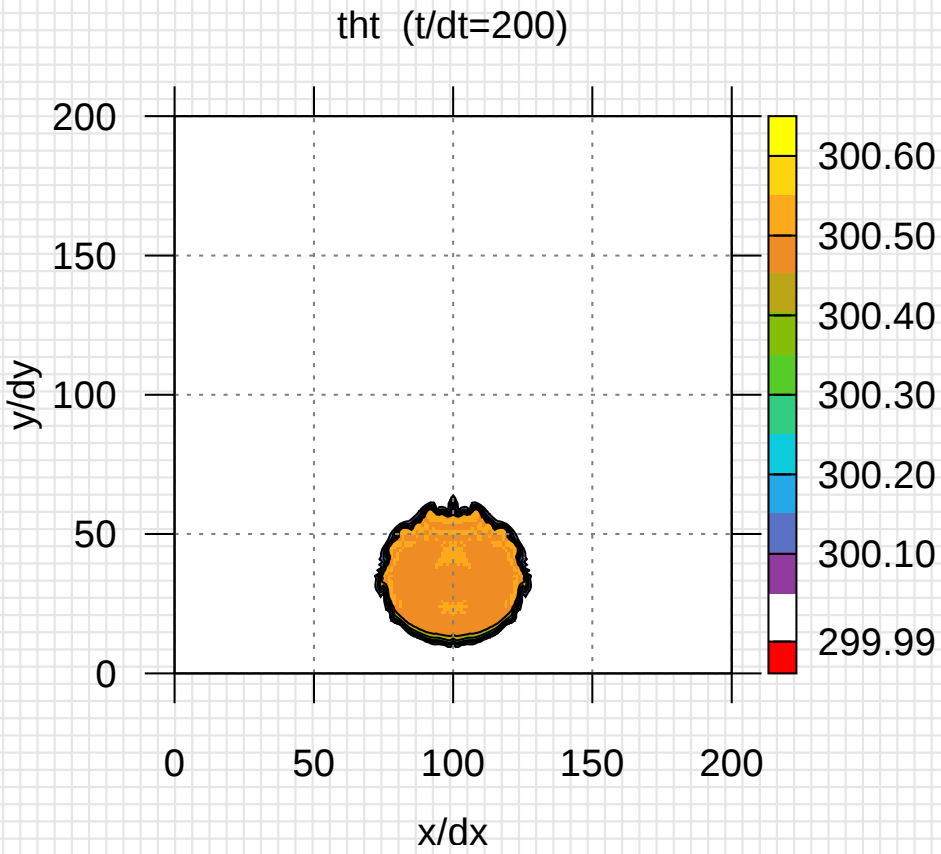

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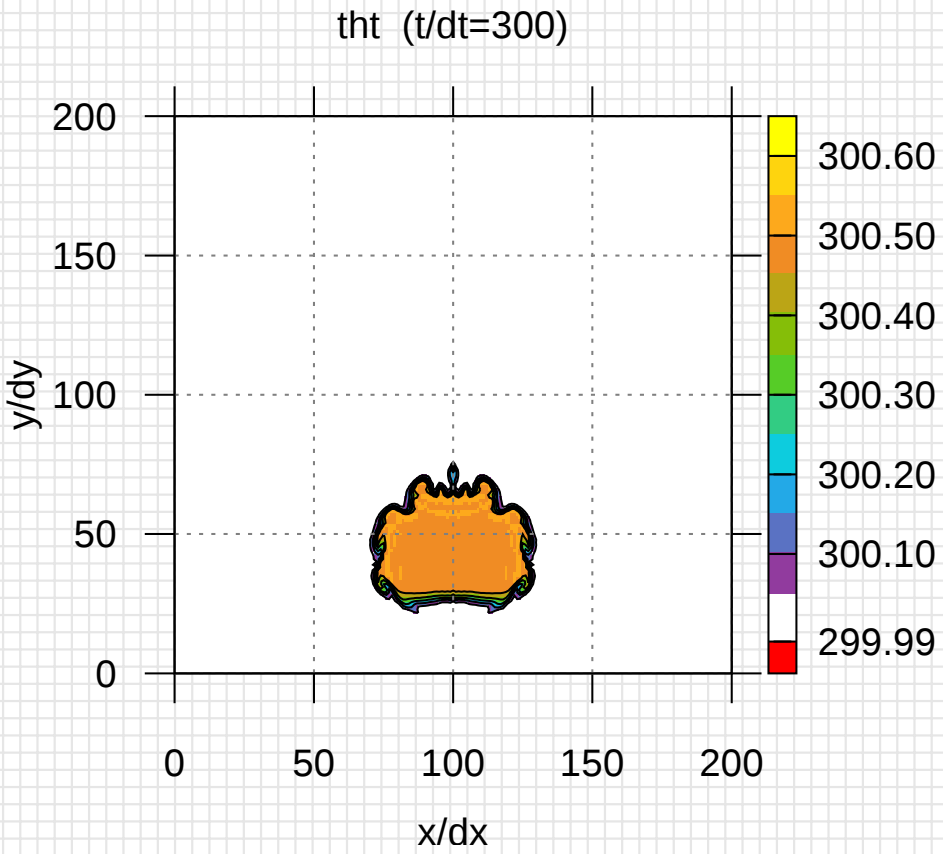

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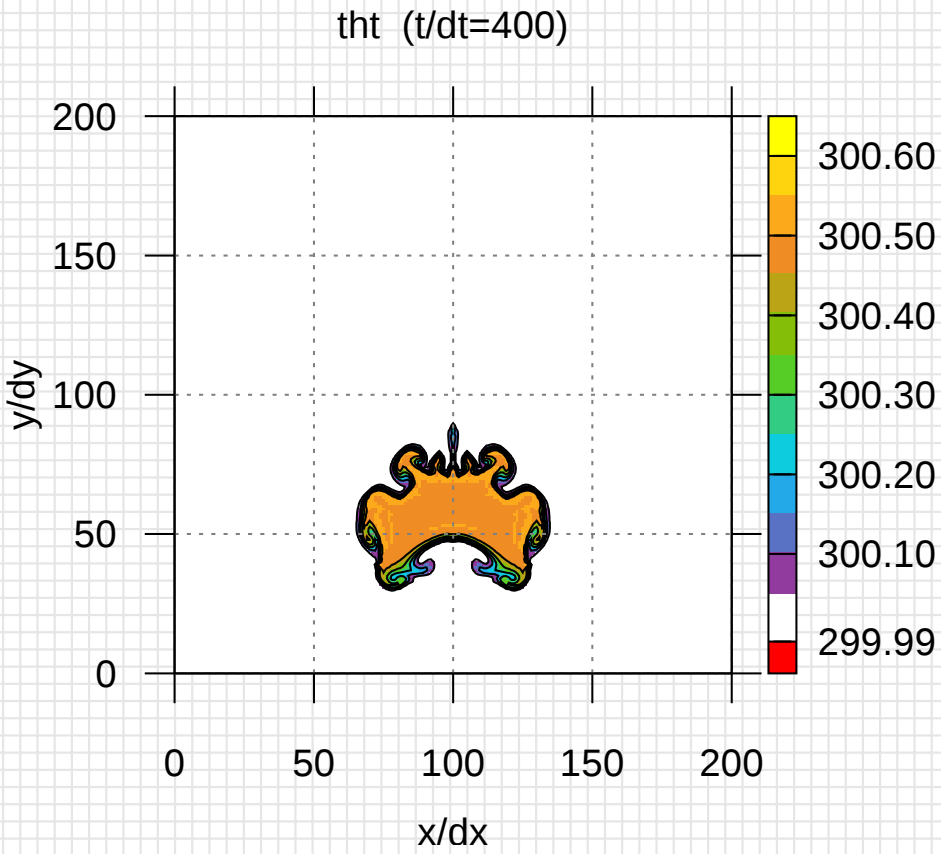

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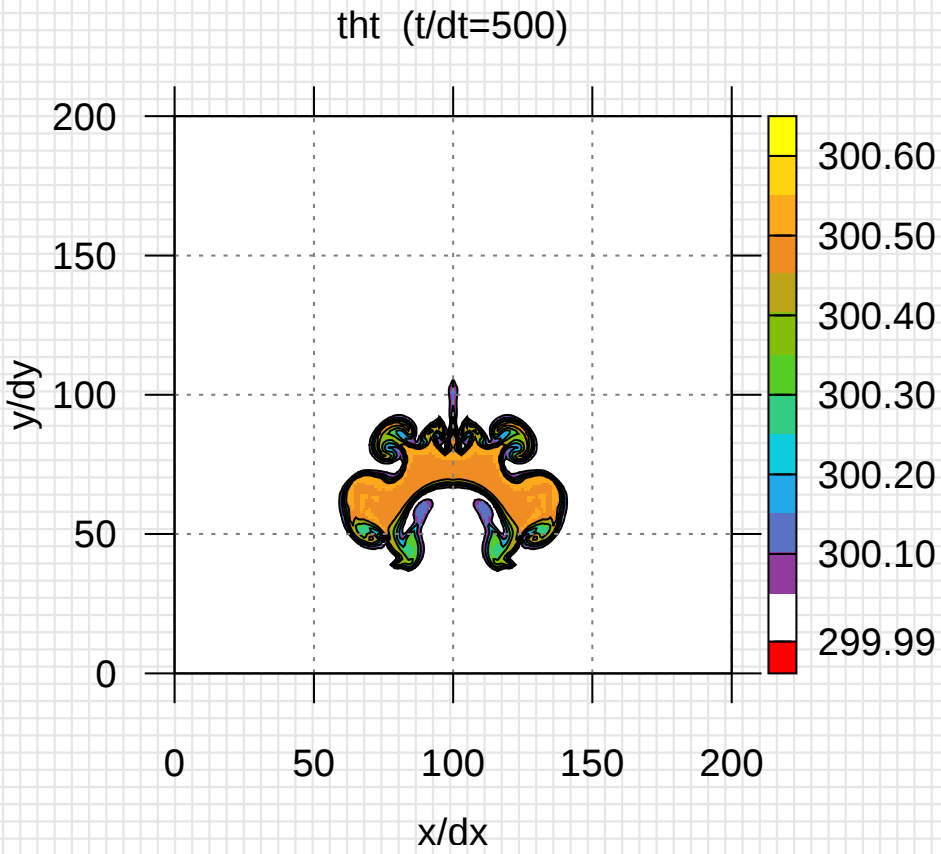

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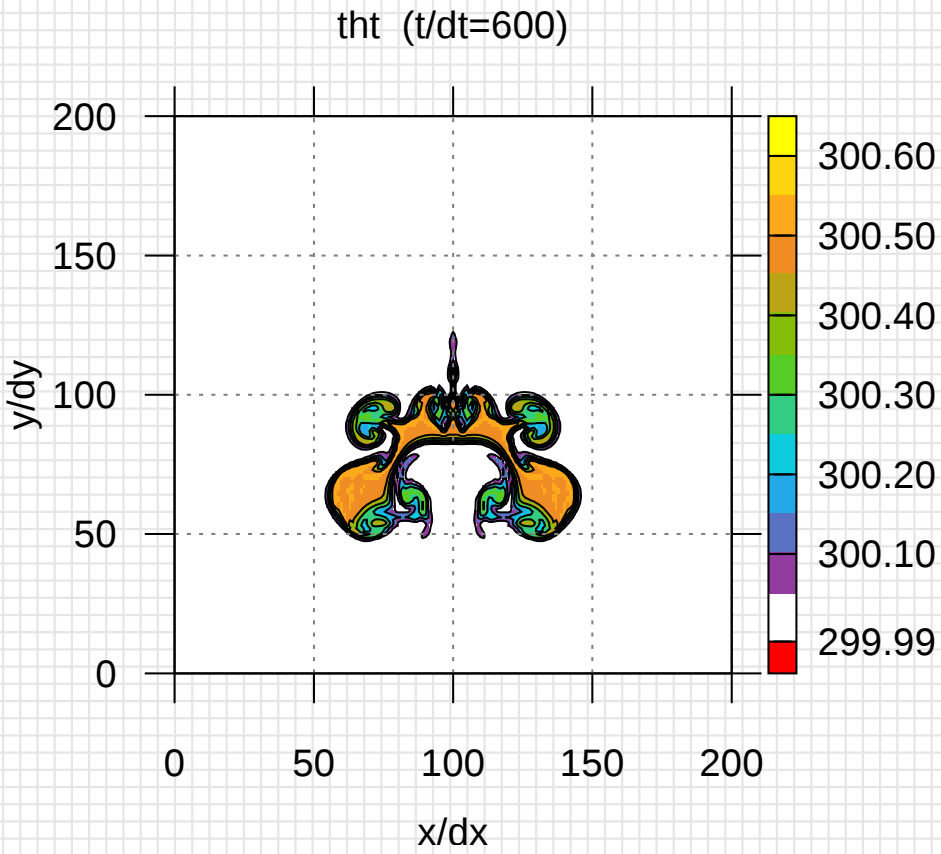

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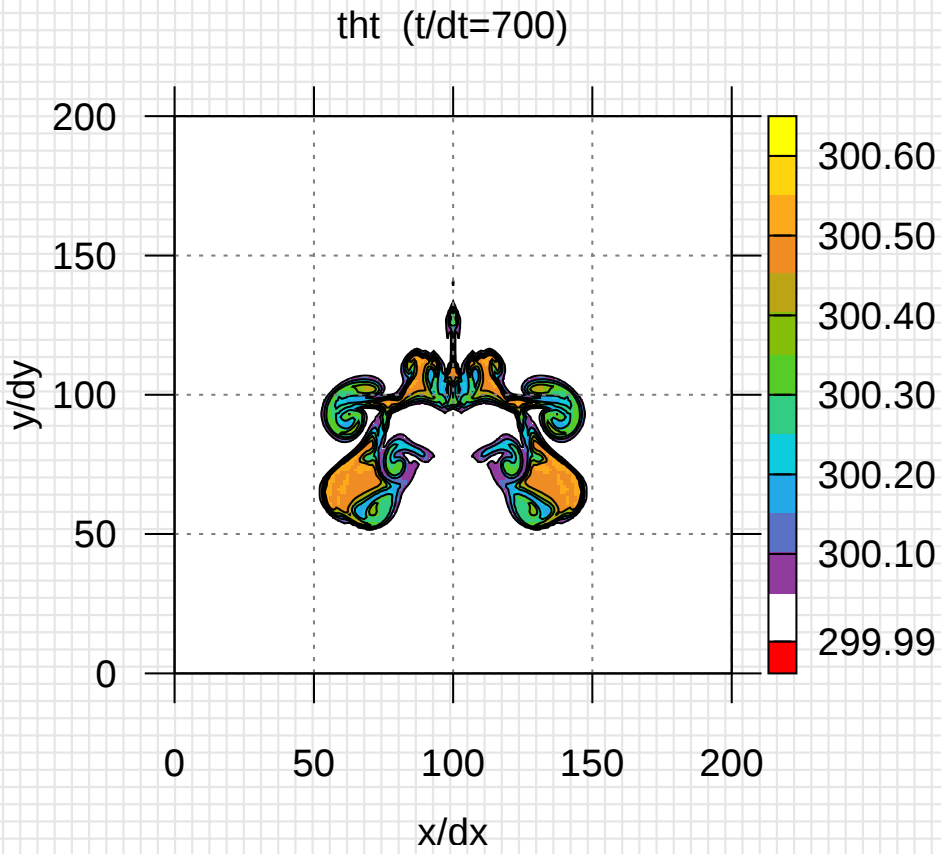

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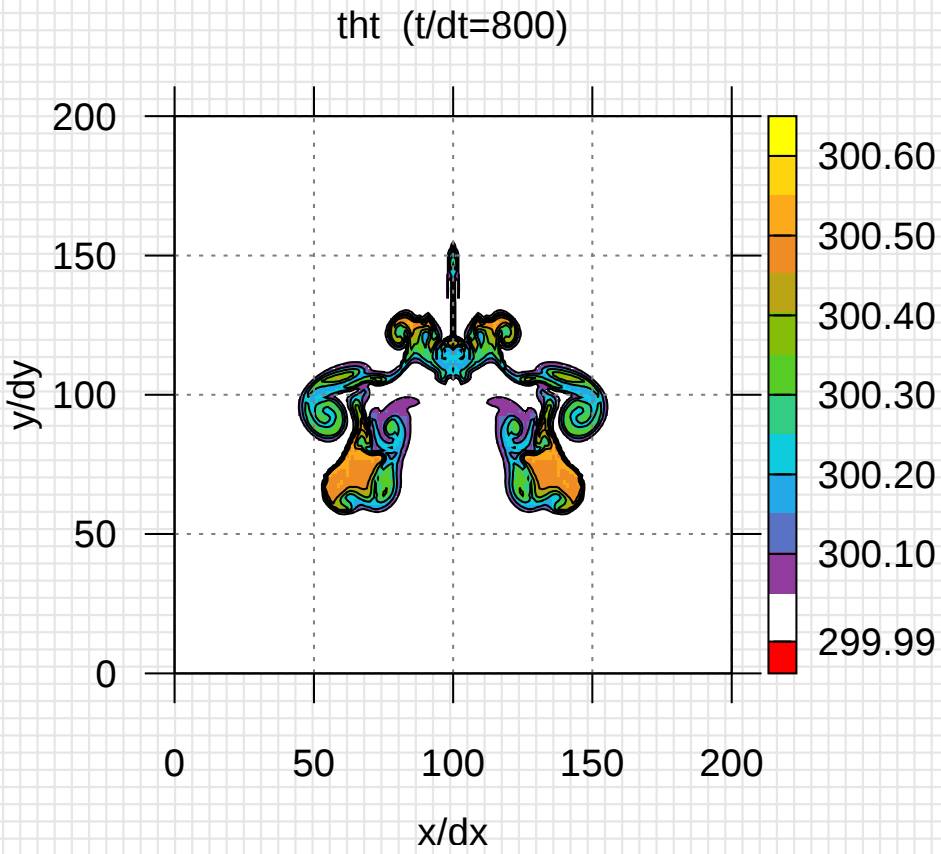

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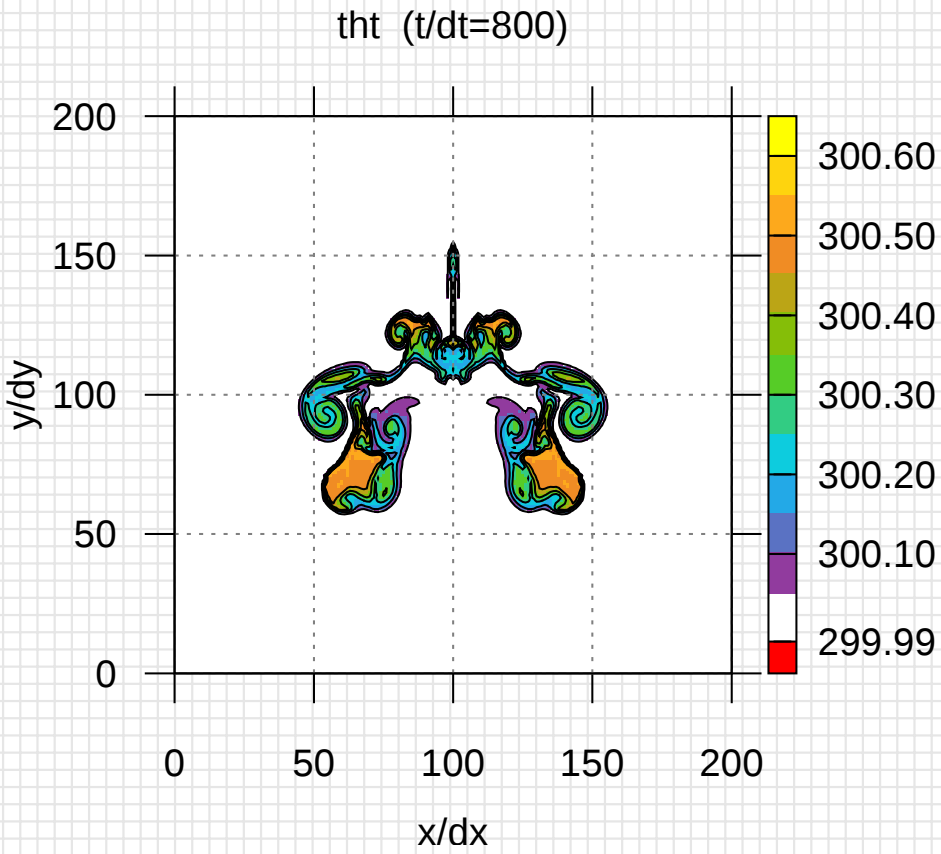

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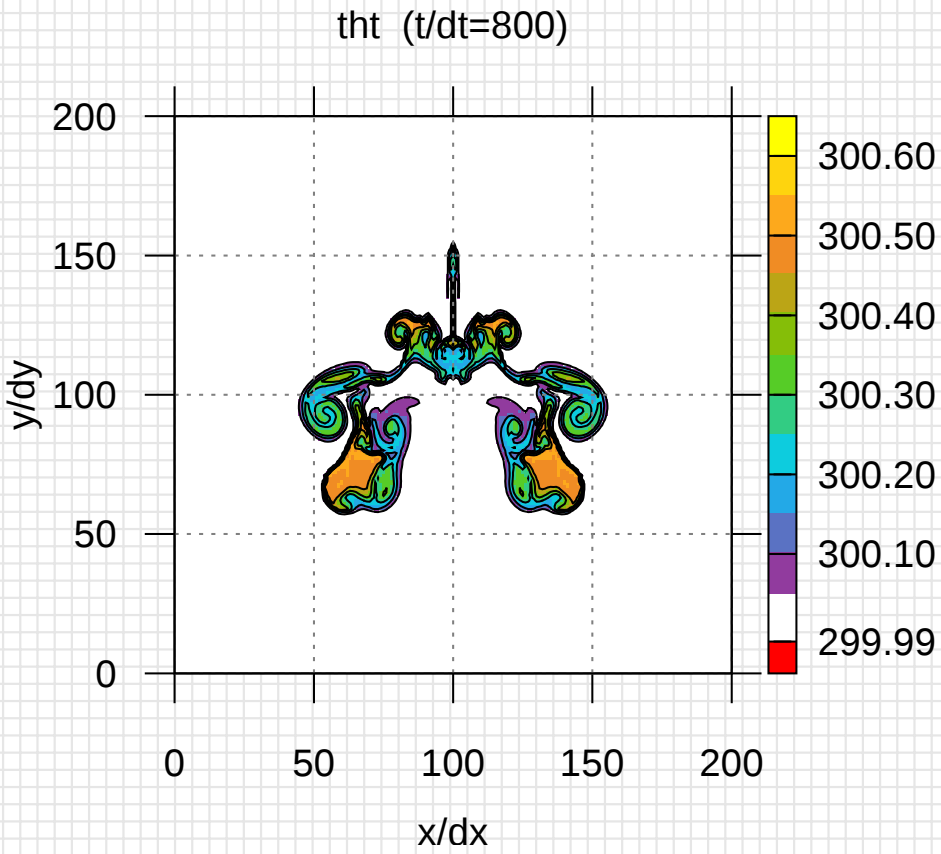

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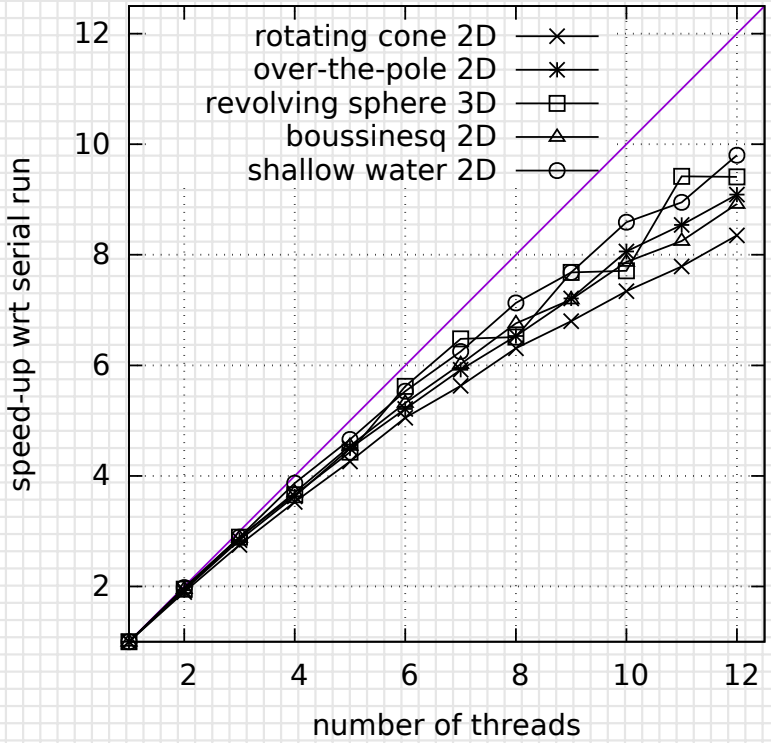

libmpdata++ / F77 CPU-time ratios

(3D, homogeneous advection, serial)

grid	ratio
59^3	4.8
$(2\times59)^3$	2.0
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Analysis performed by Maciek Waruszewski, computational time granted by the Center for Cooperative Work on Computational Science of the University of Hyogo

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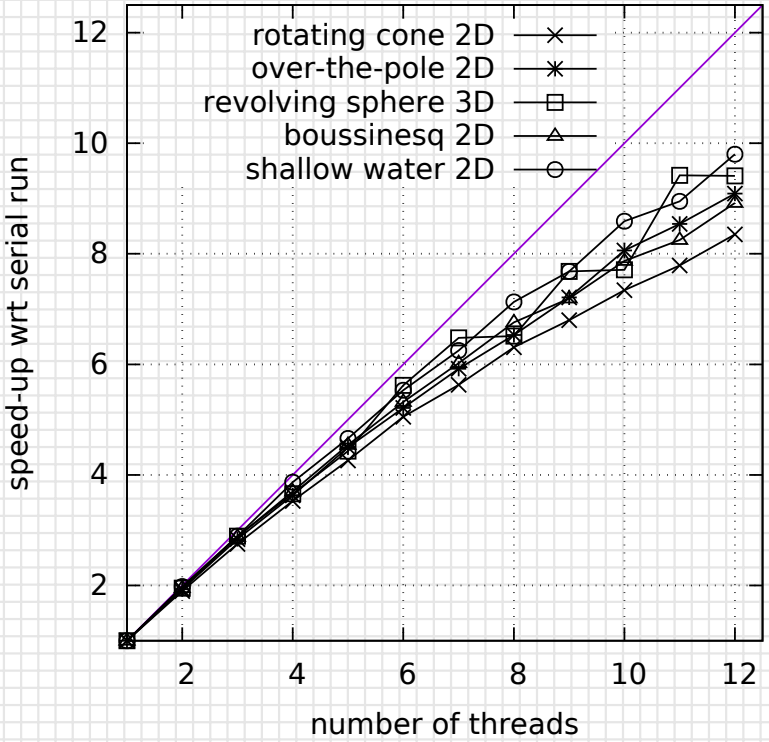

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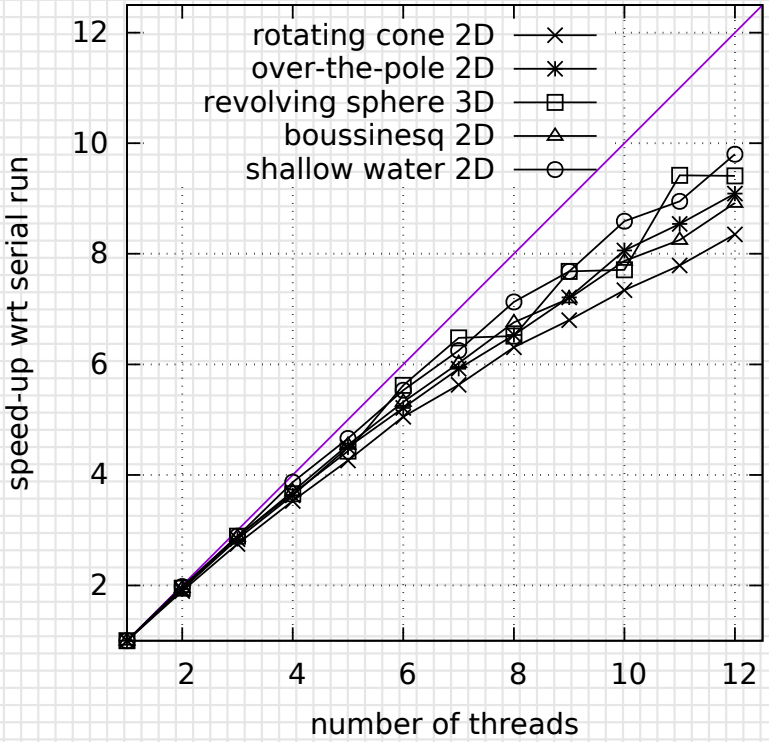

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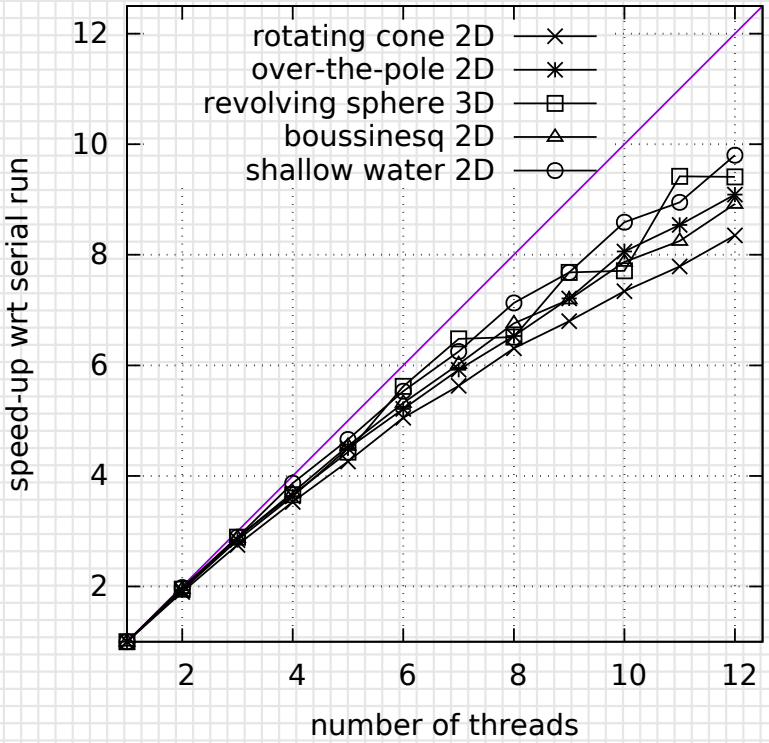

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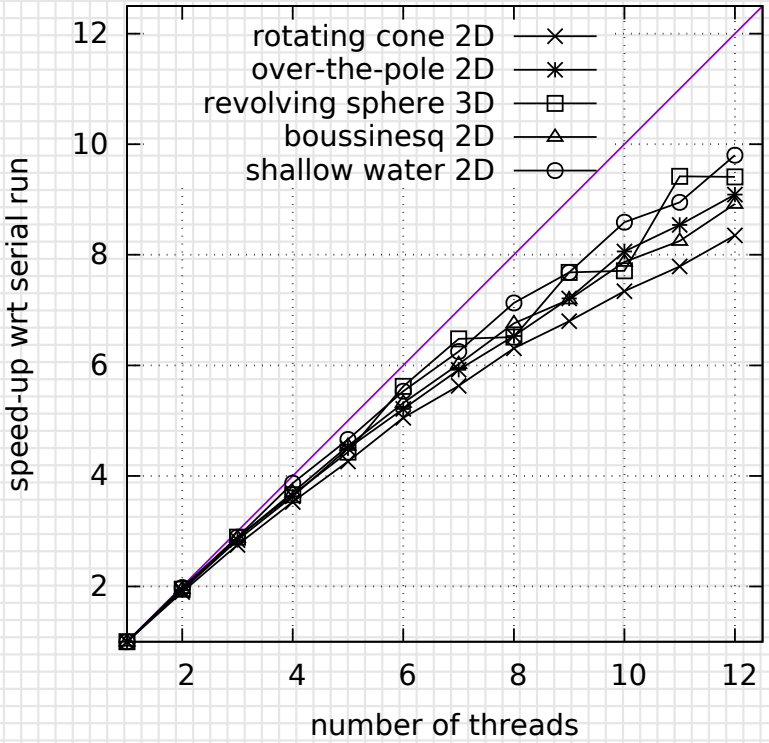

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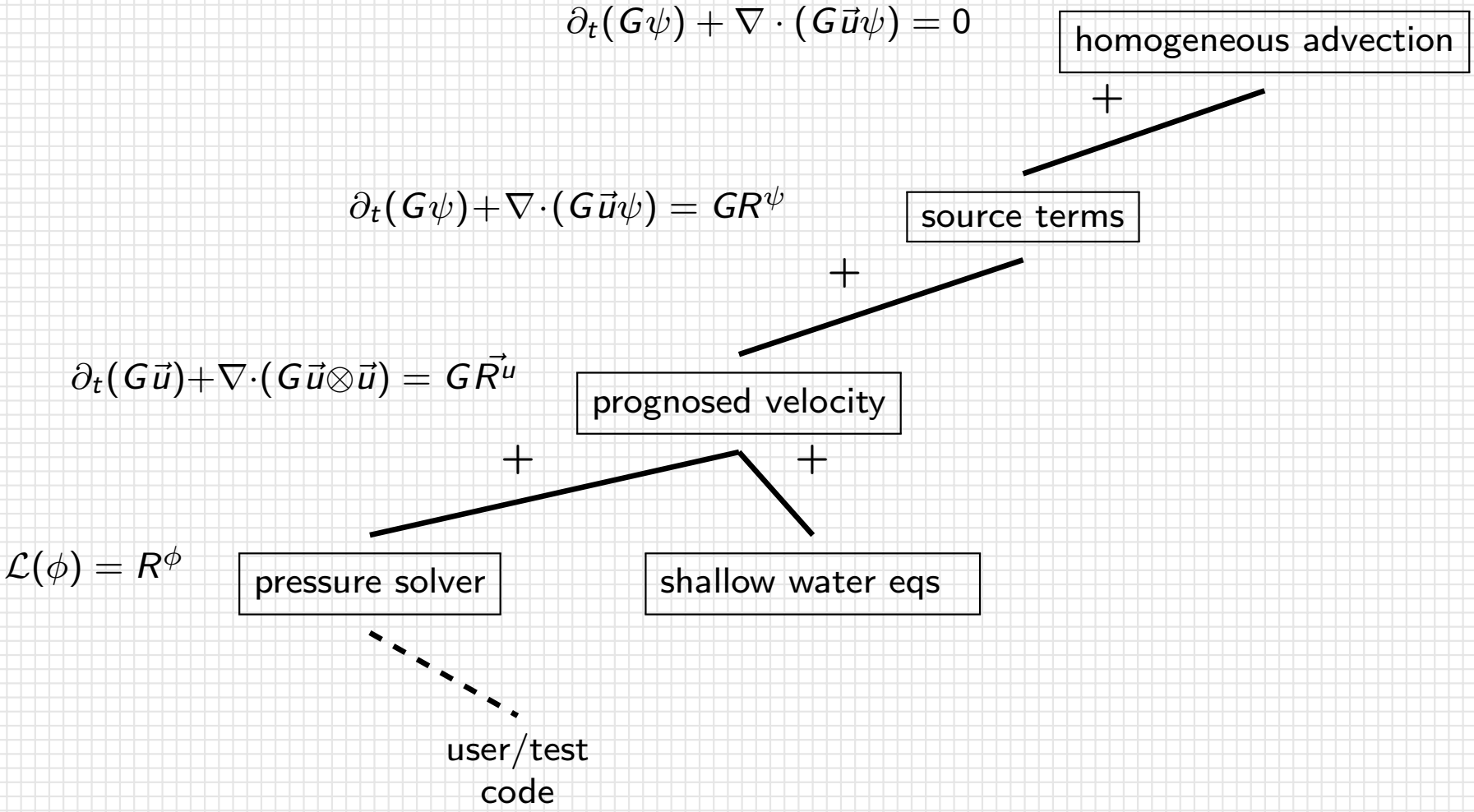
Plan of the talk

1. what's libmpdata++
2. libmpdata++: a hello-world program
3. libmpdata++ 1.0: summary of features
4. libmpdata++ 2.0: new features under development
5. closing remarks

Plan of the talk

libmpdata++ 1.0: solver/algorithm hierarchy



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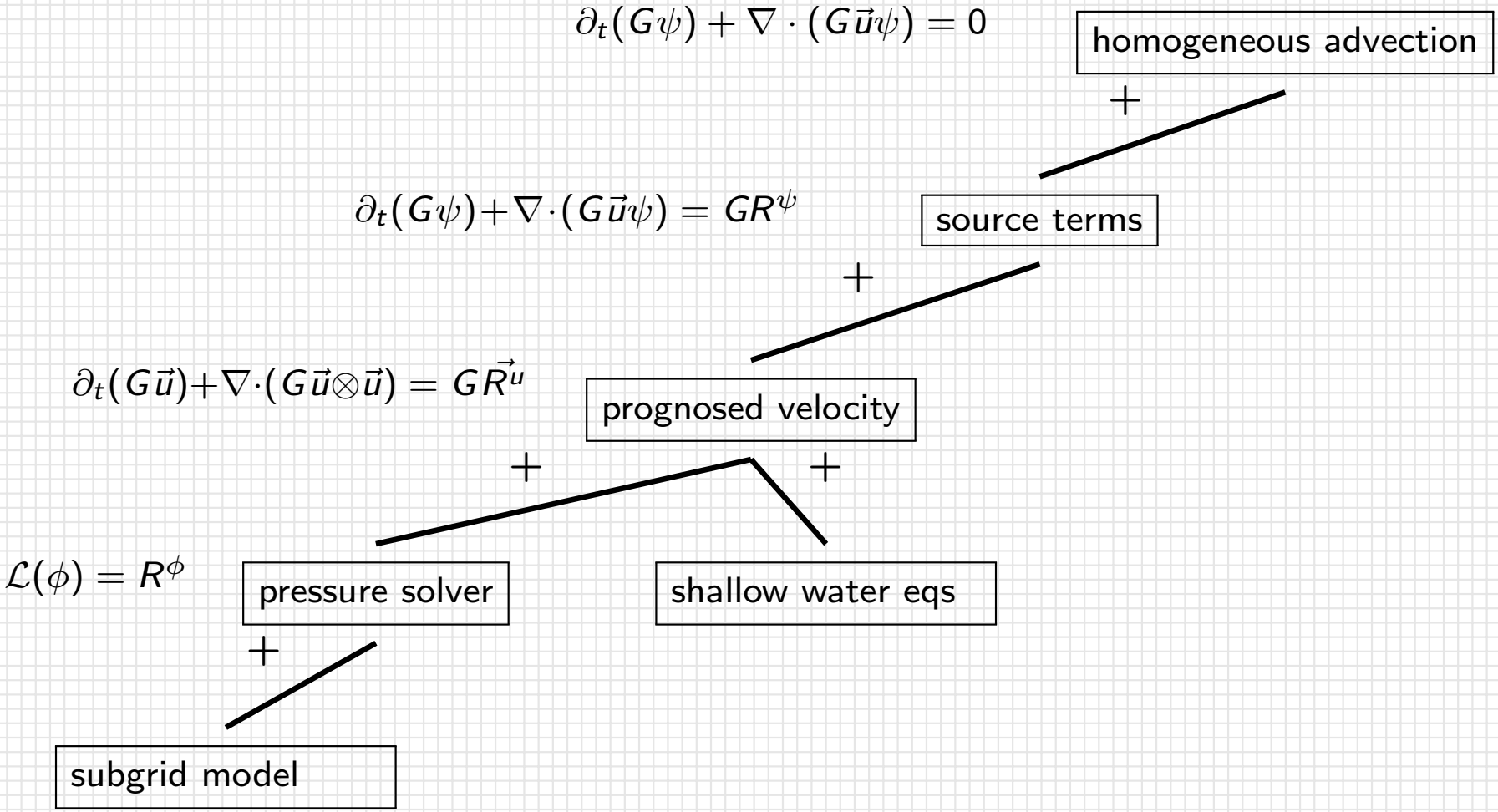

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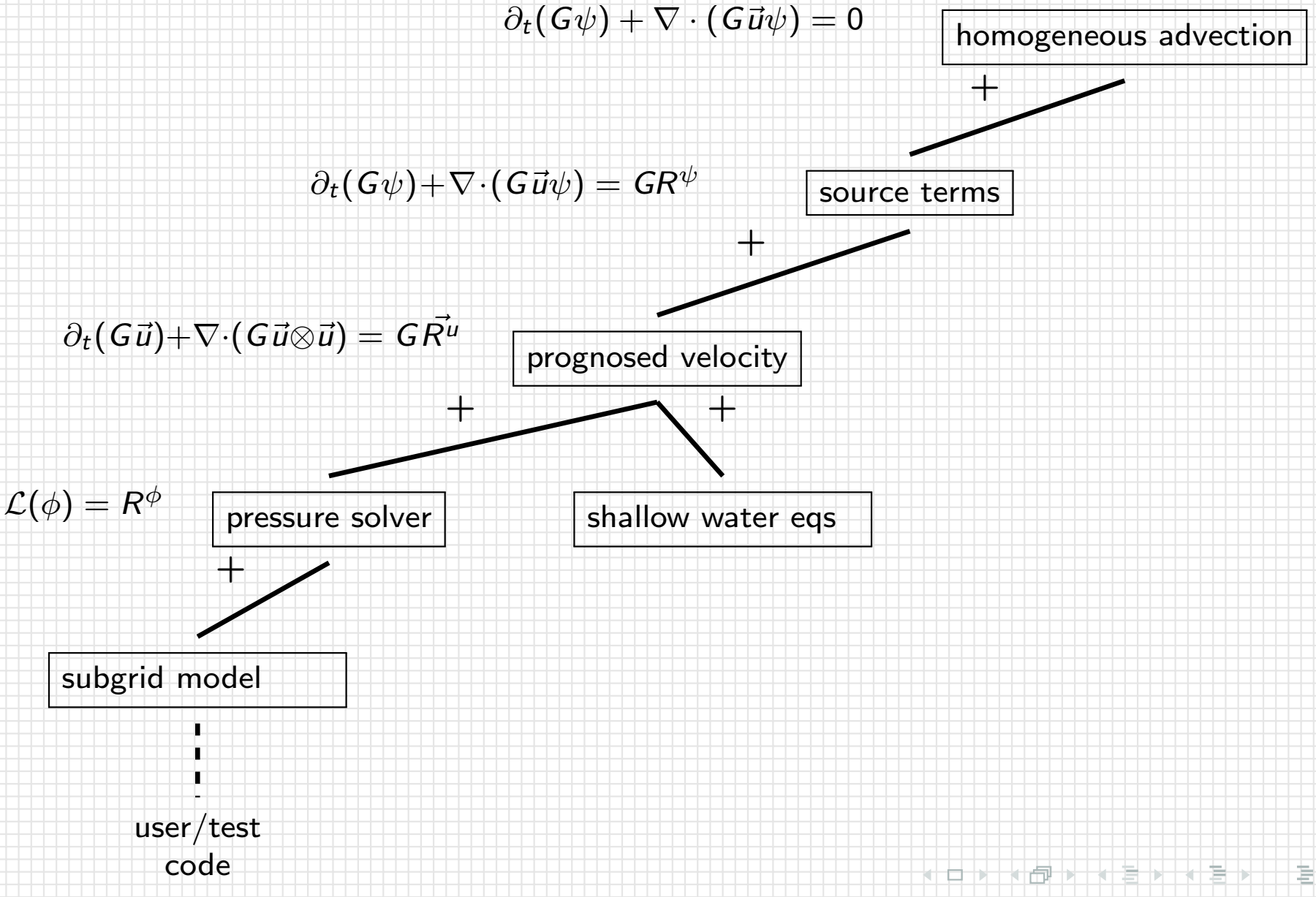

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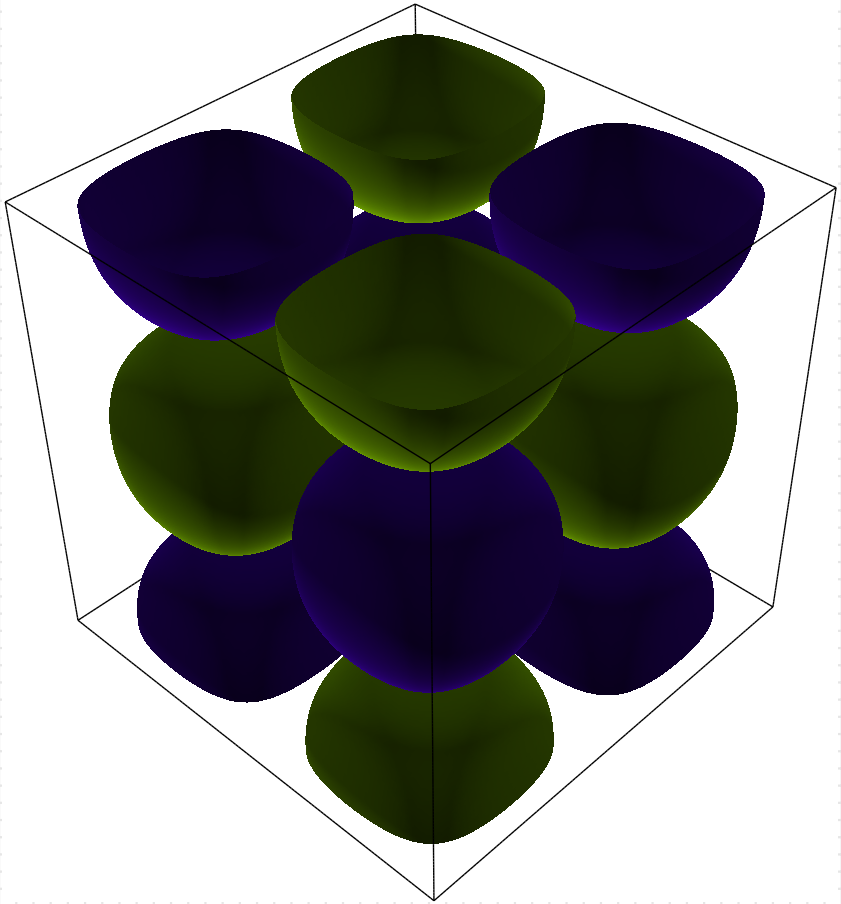

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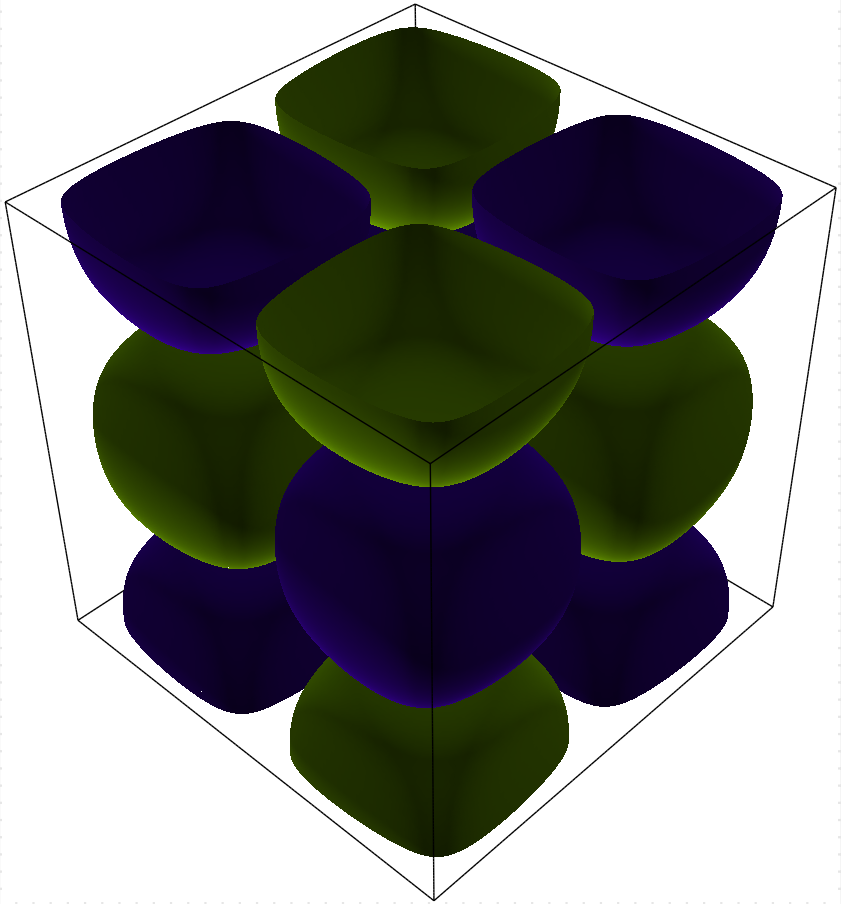

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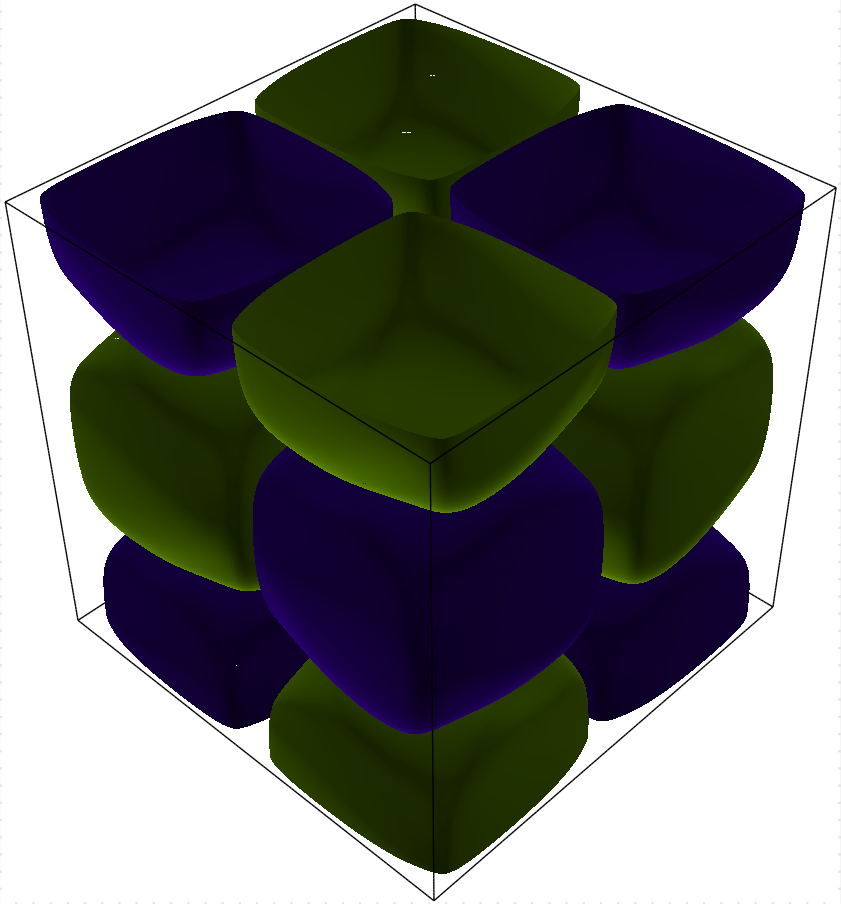

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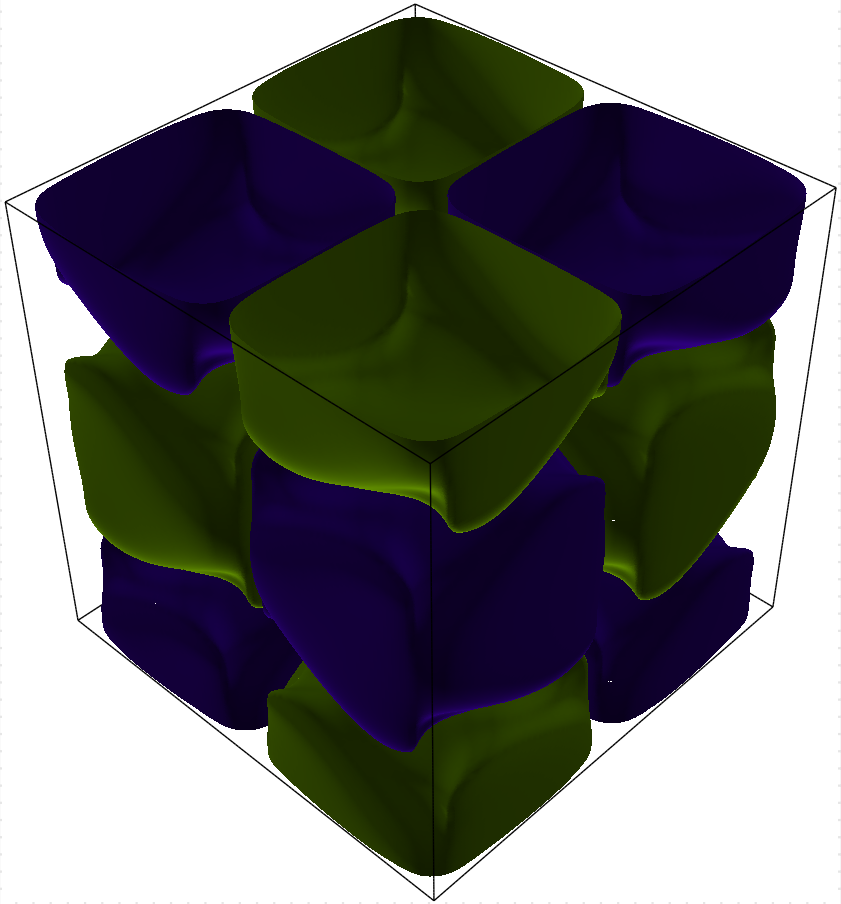

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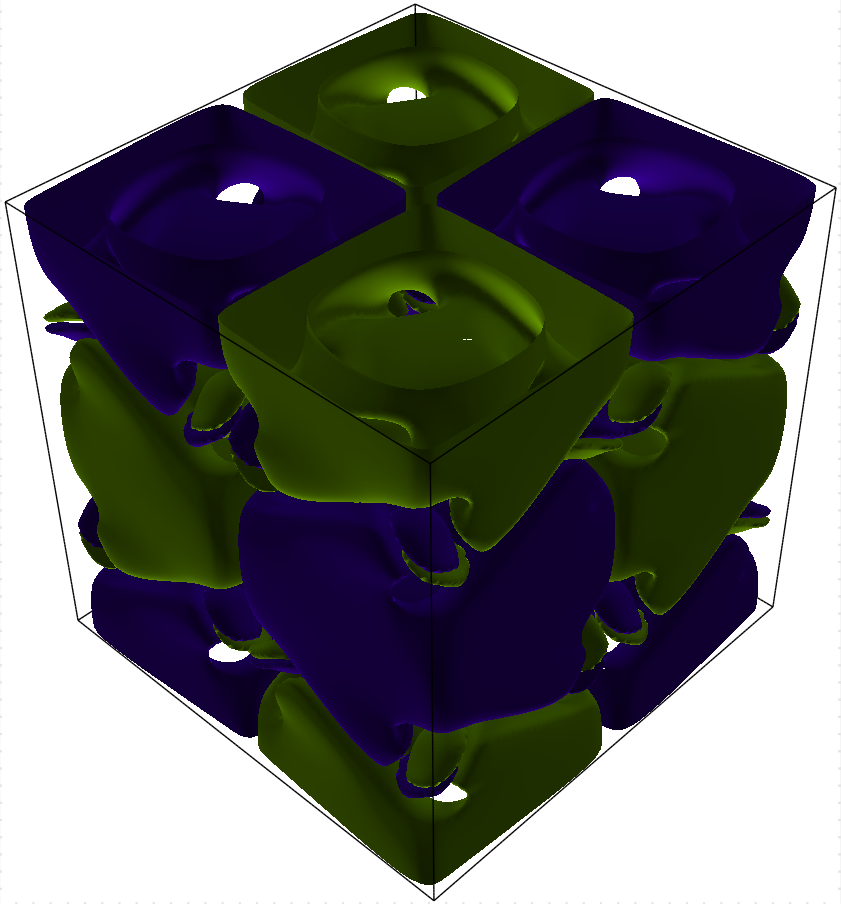

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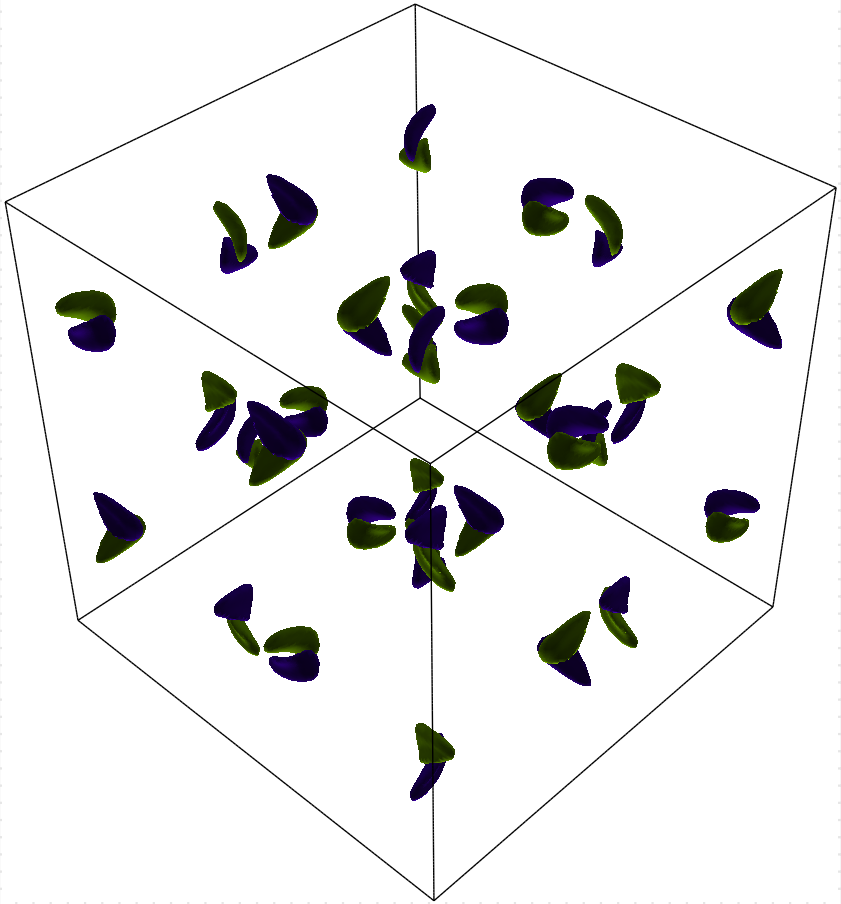

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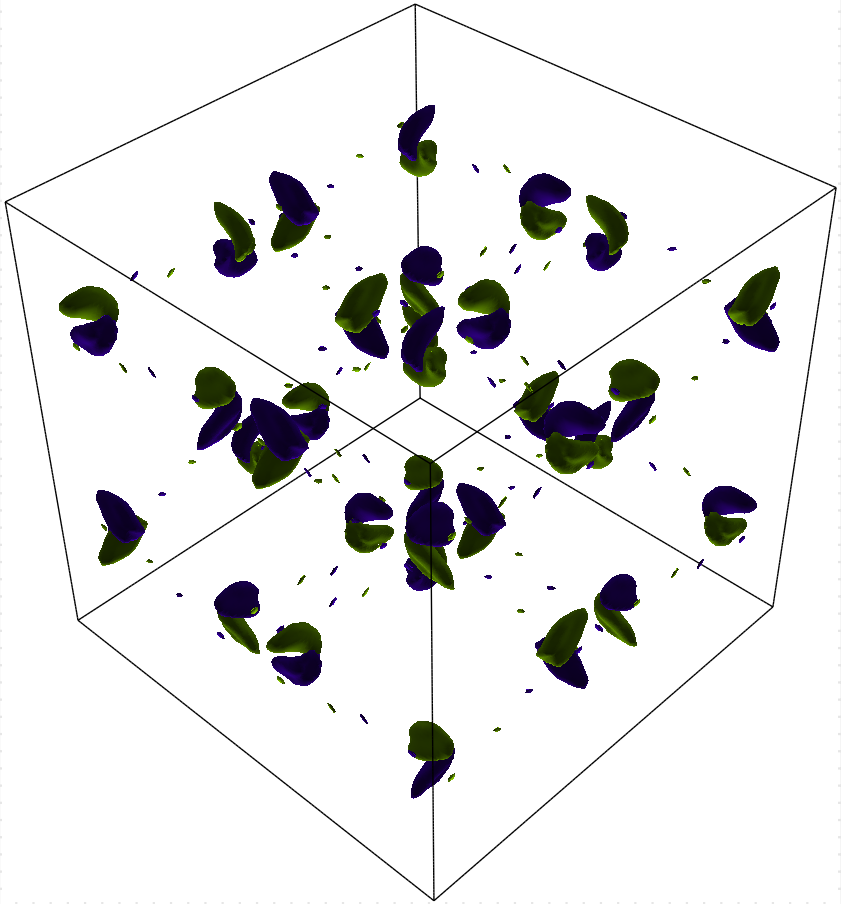

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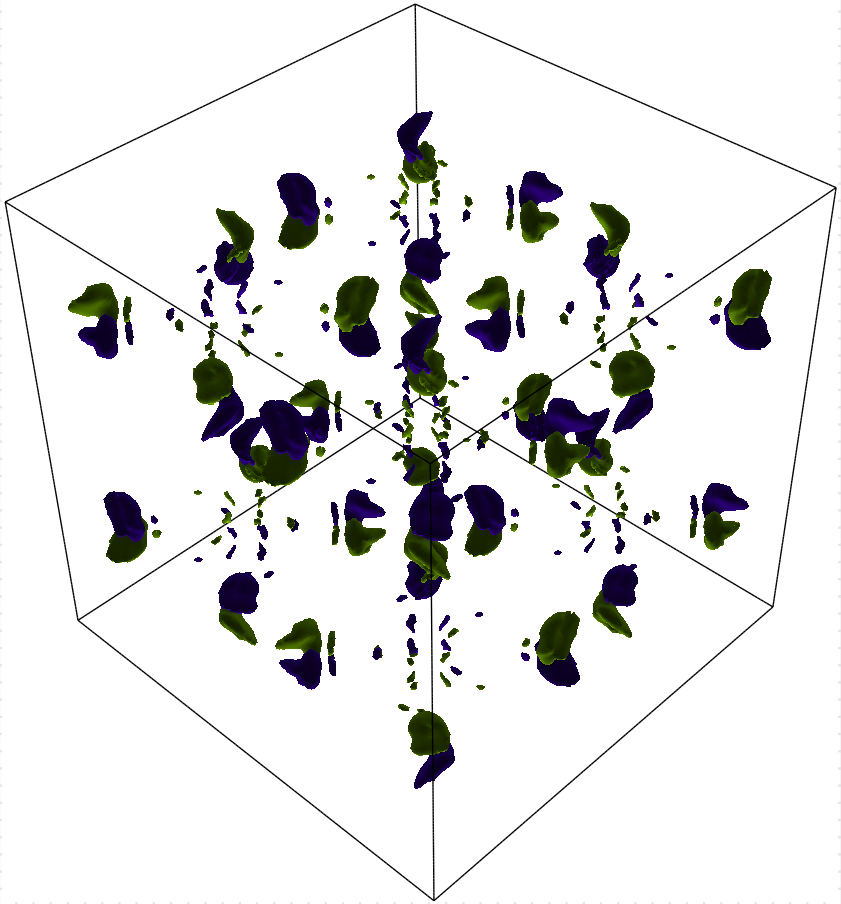

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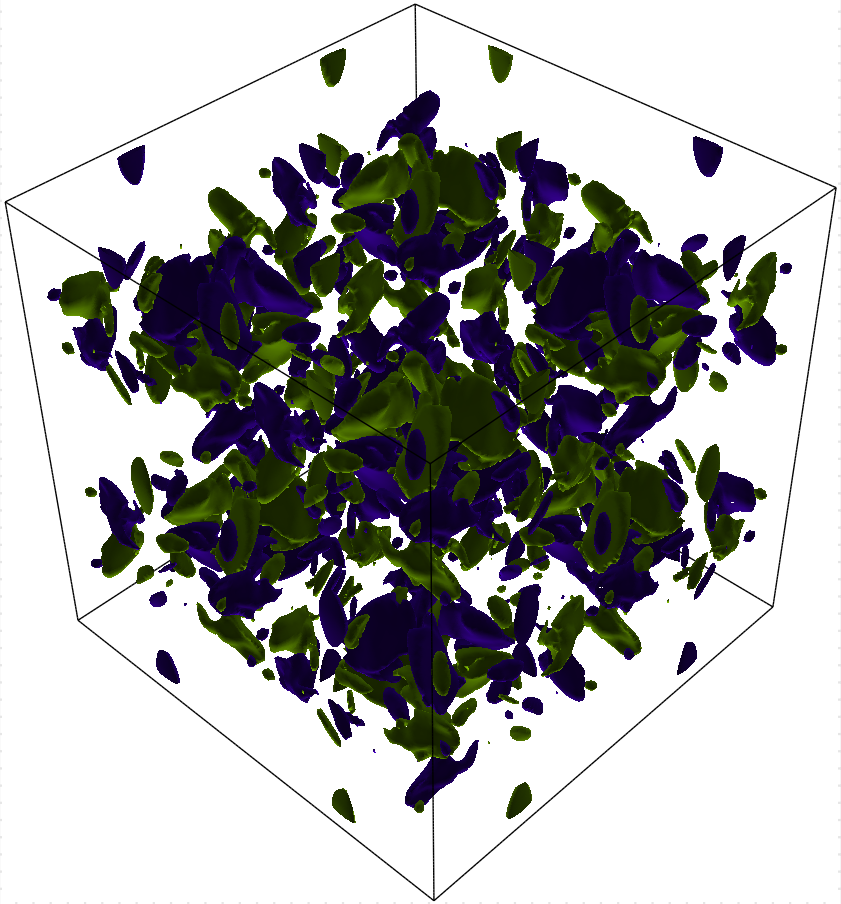

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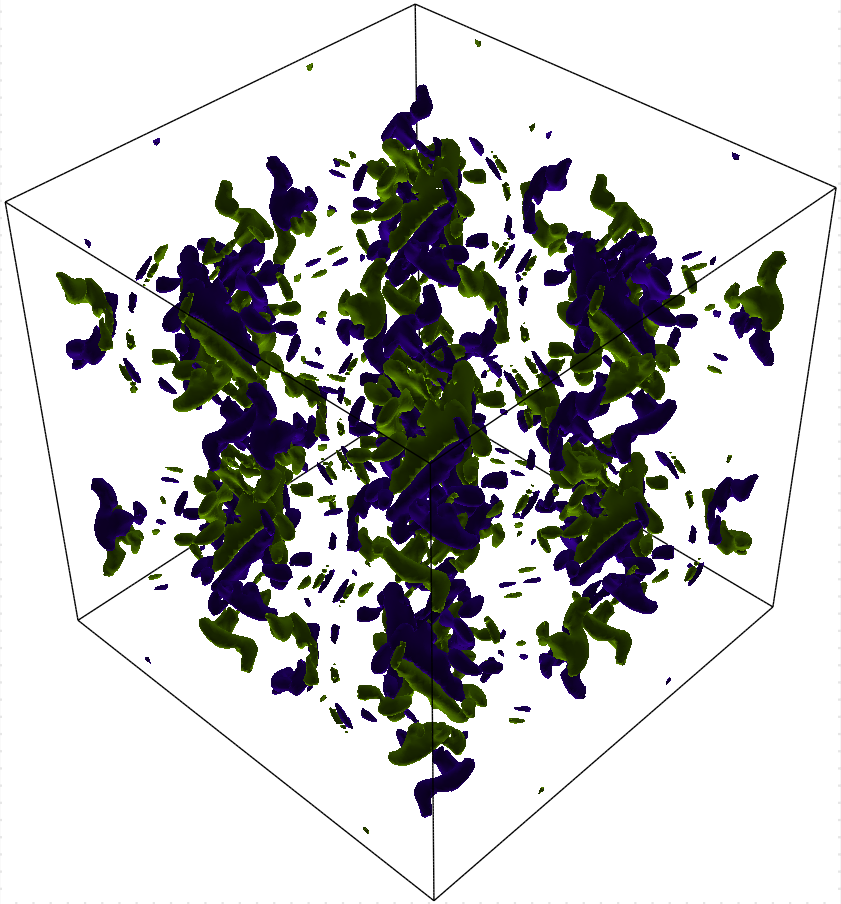

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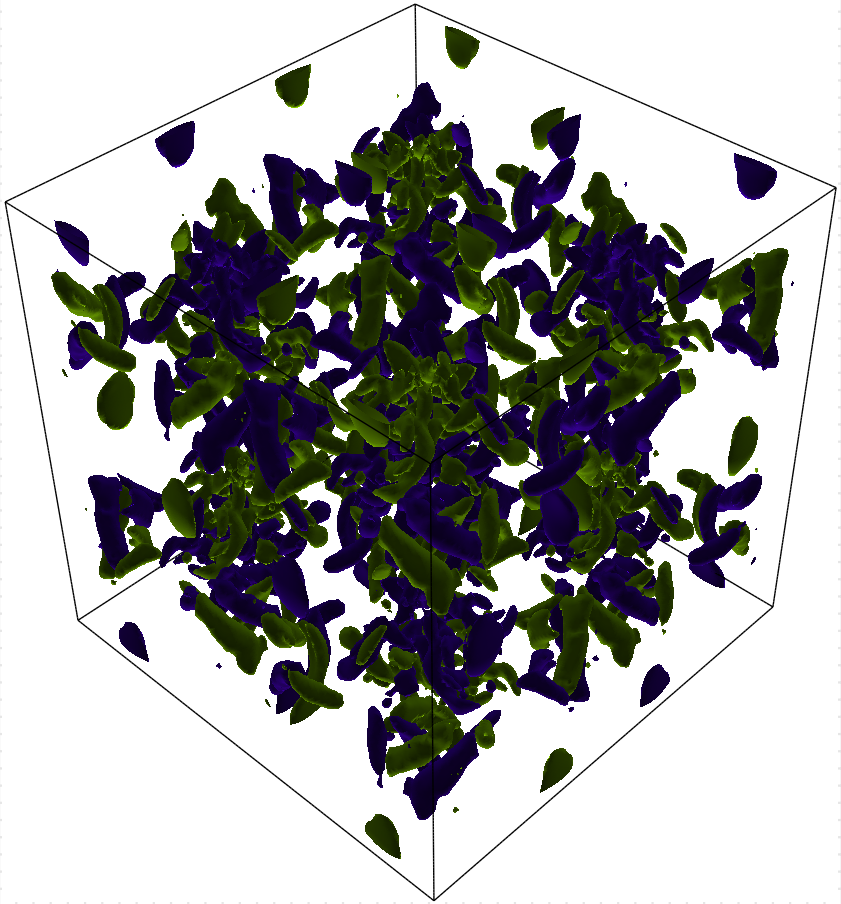

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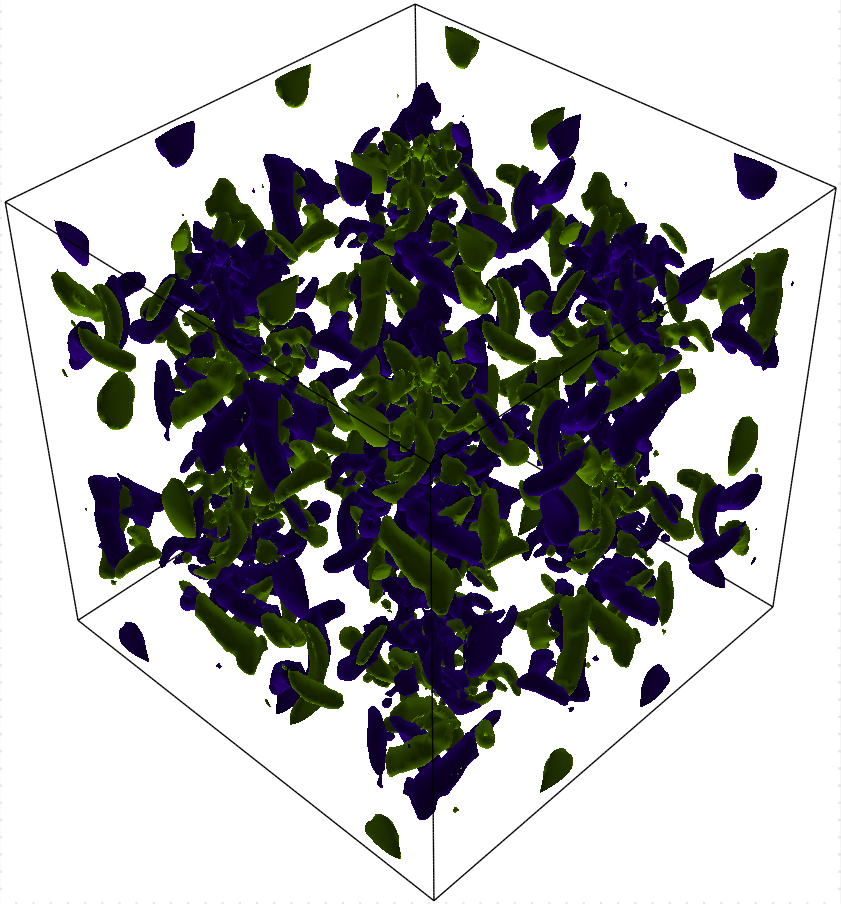

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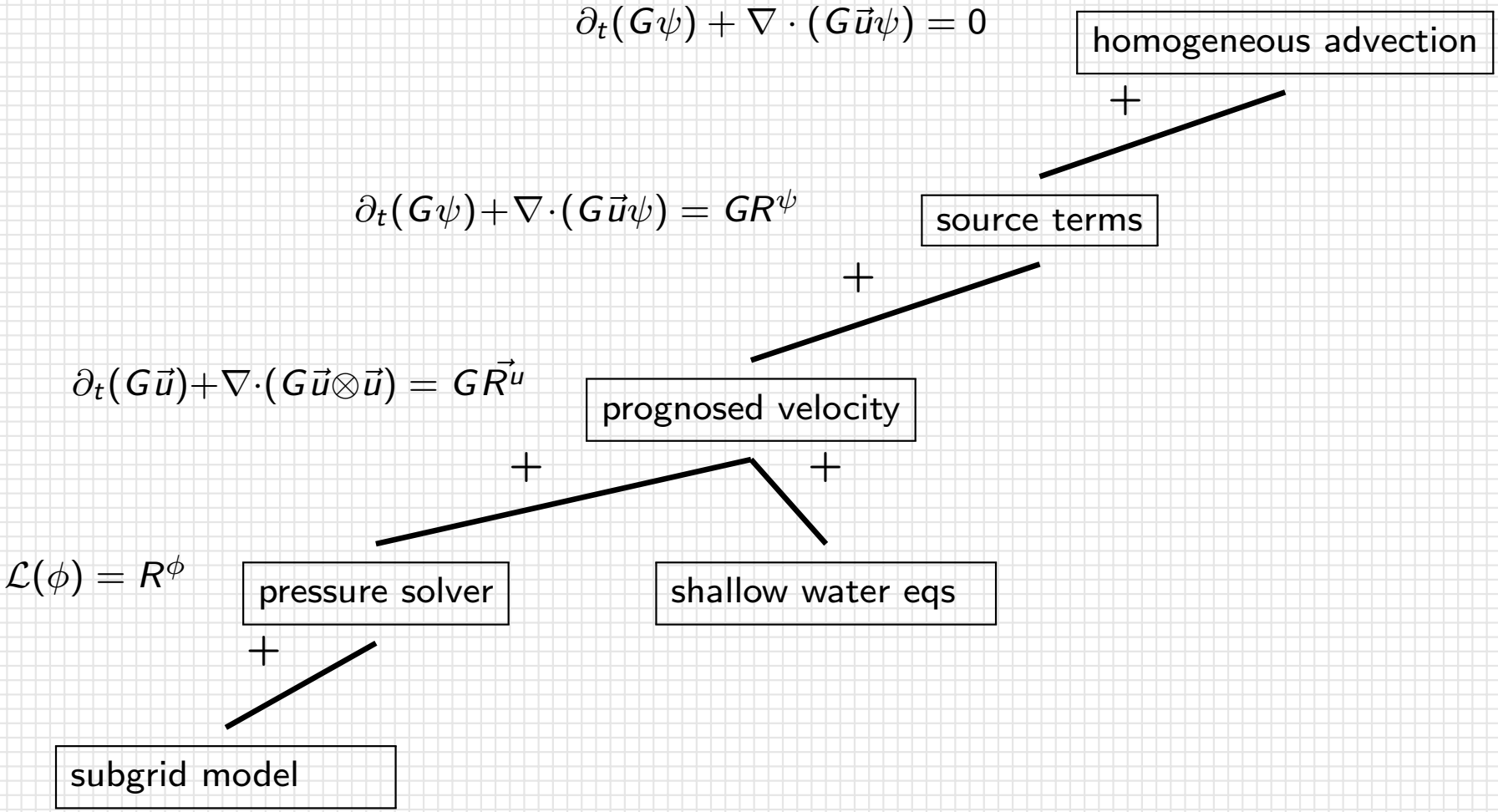

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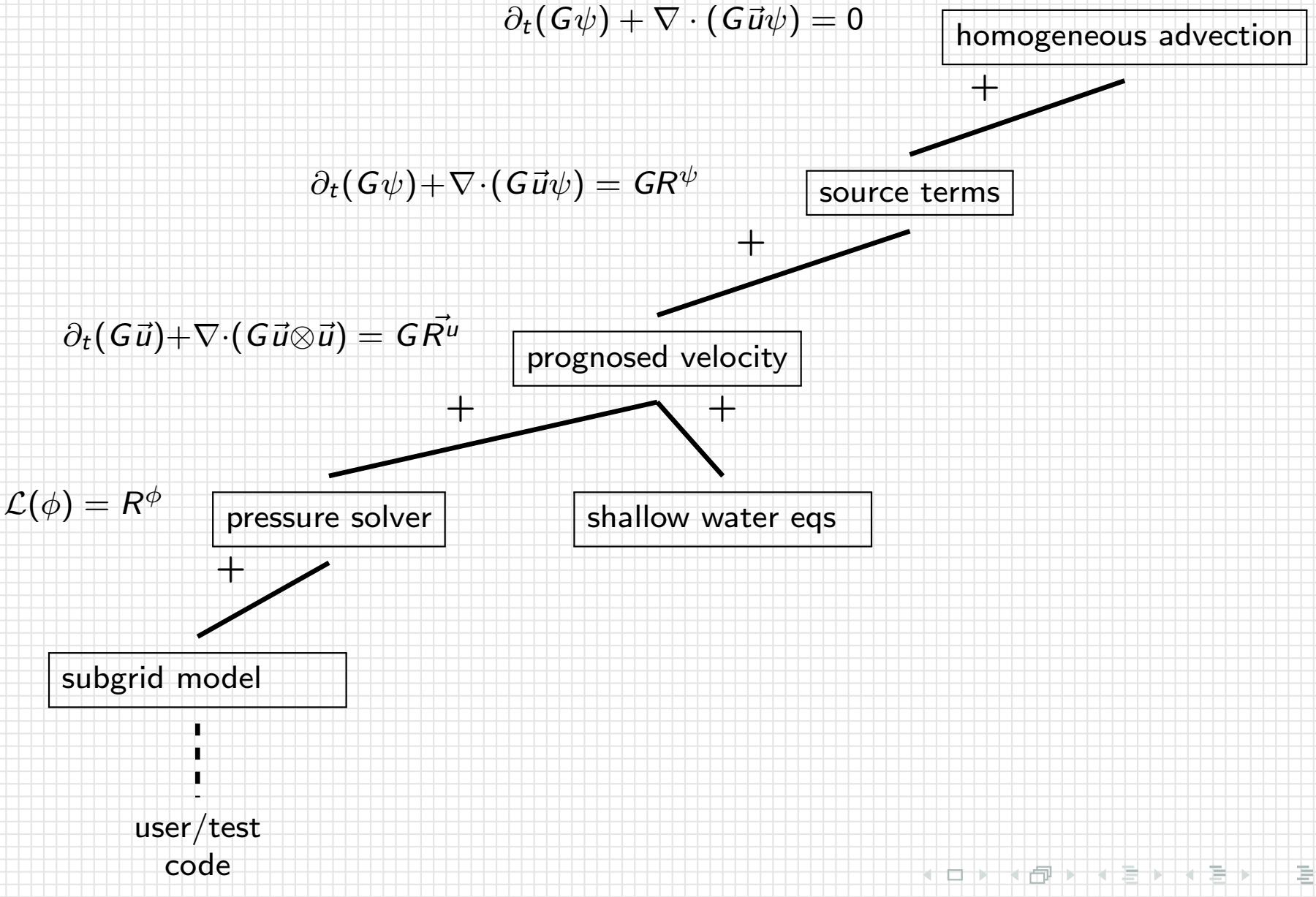
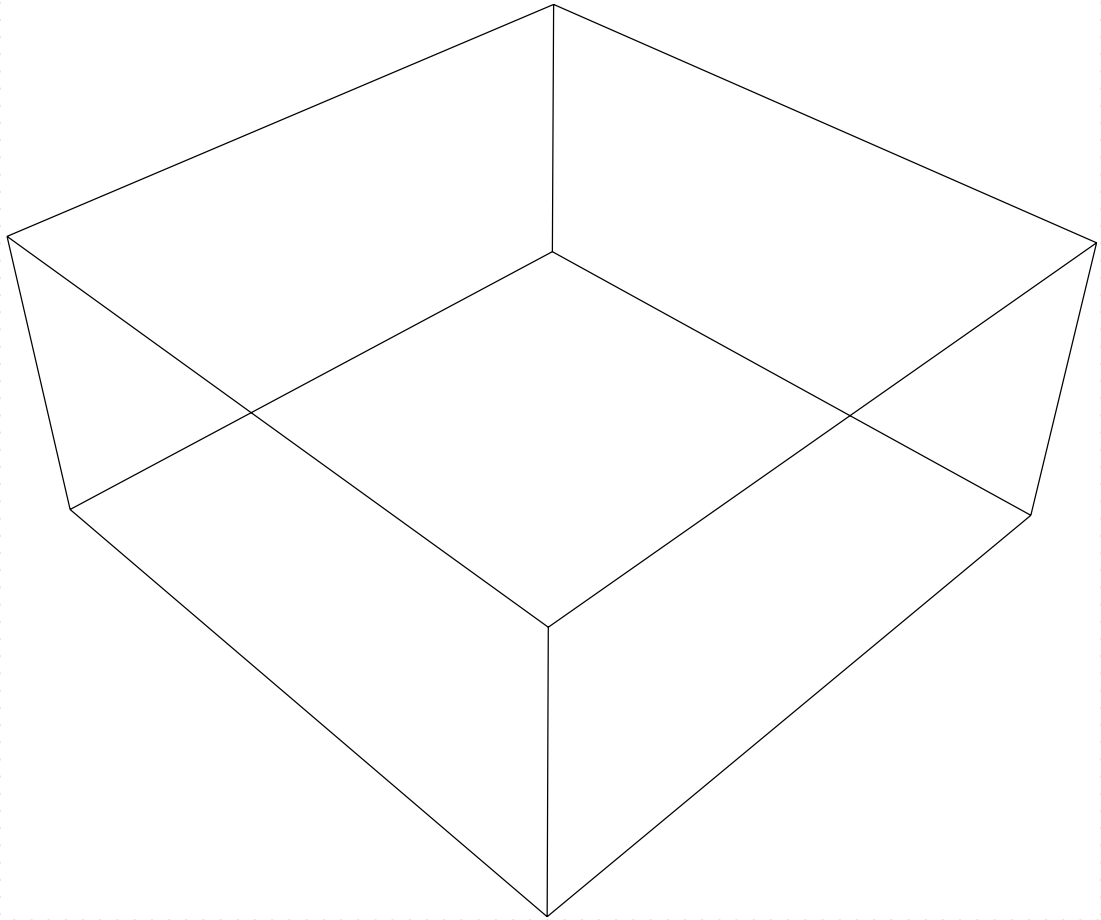


libmpdata++ 2.0: convective boundary layer example



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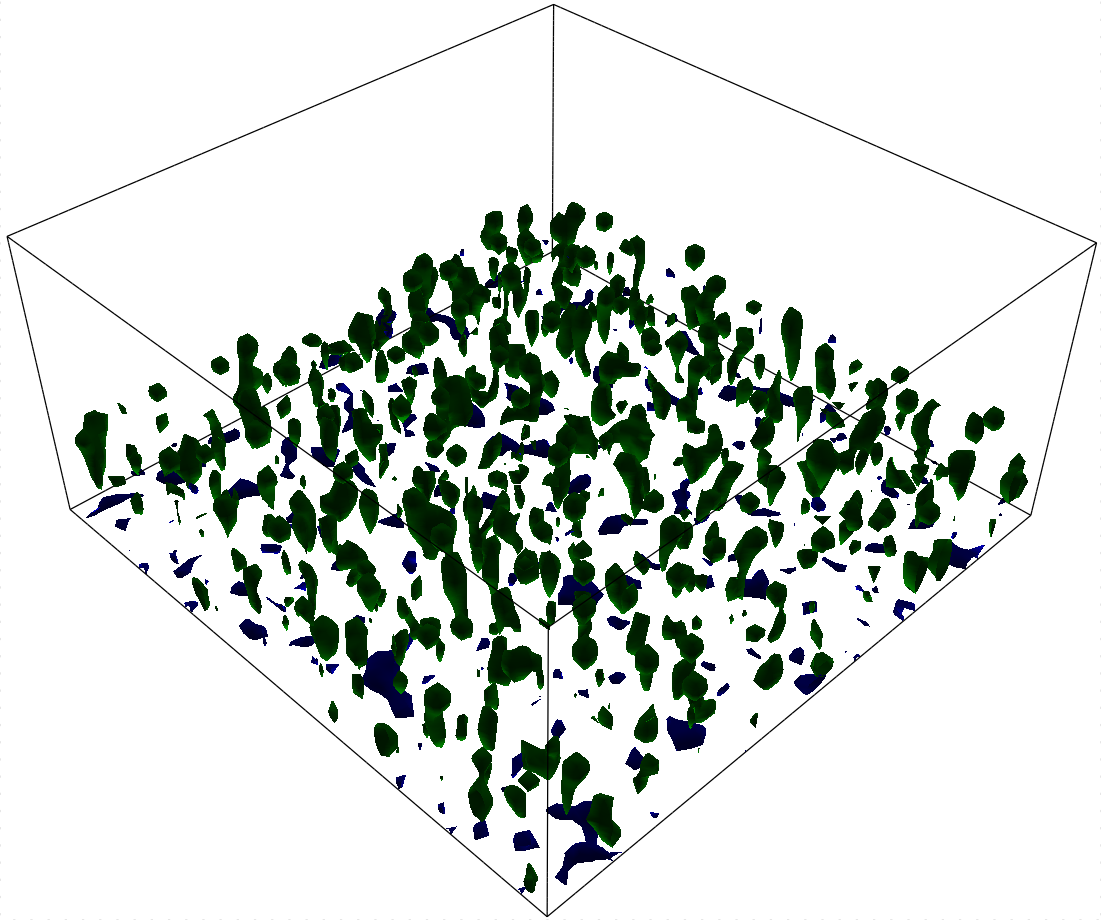

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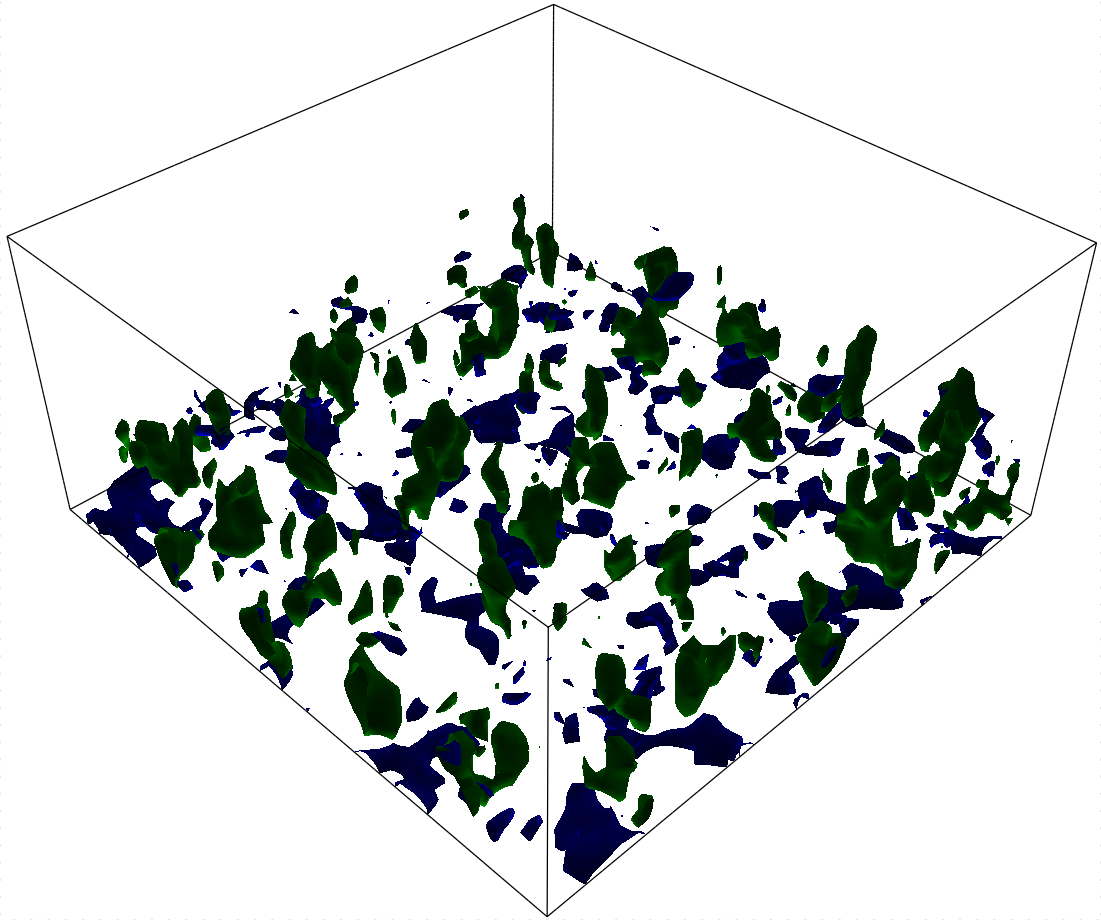

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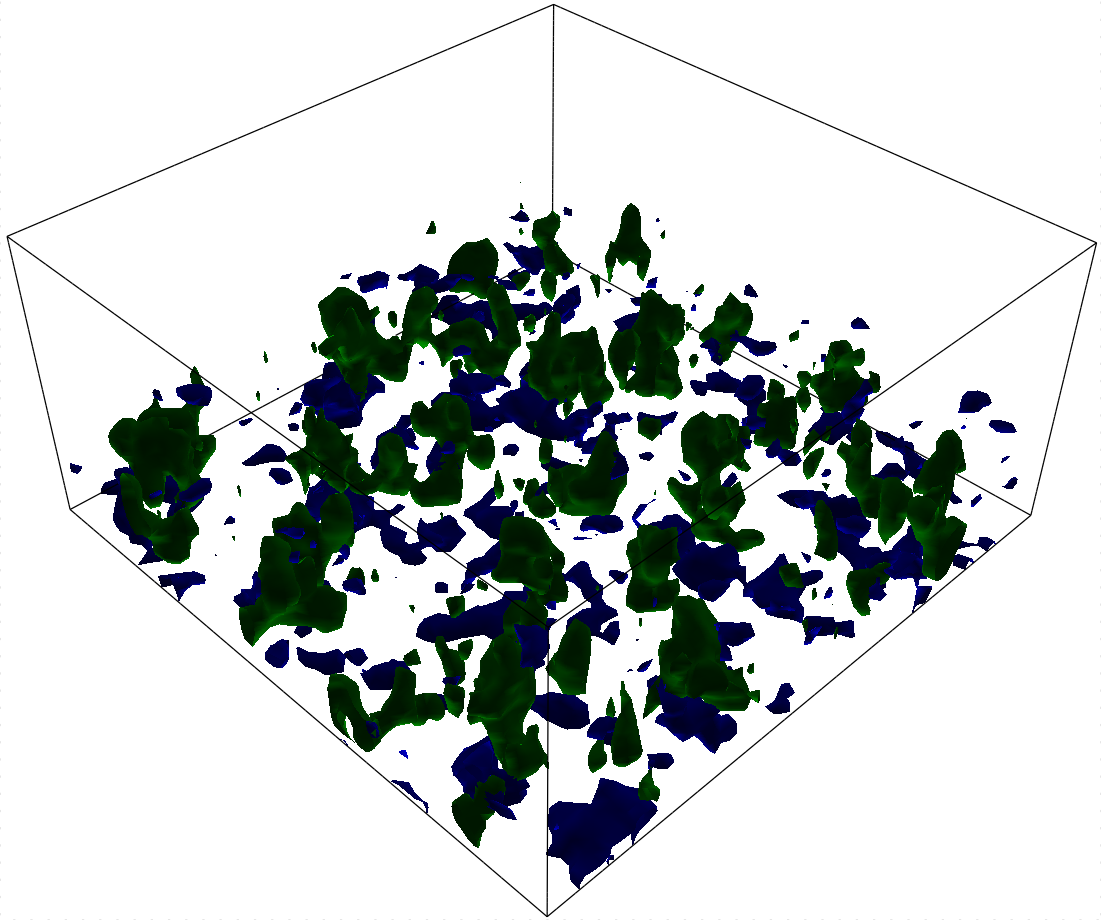

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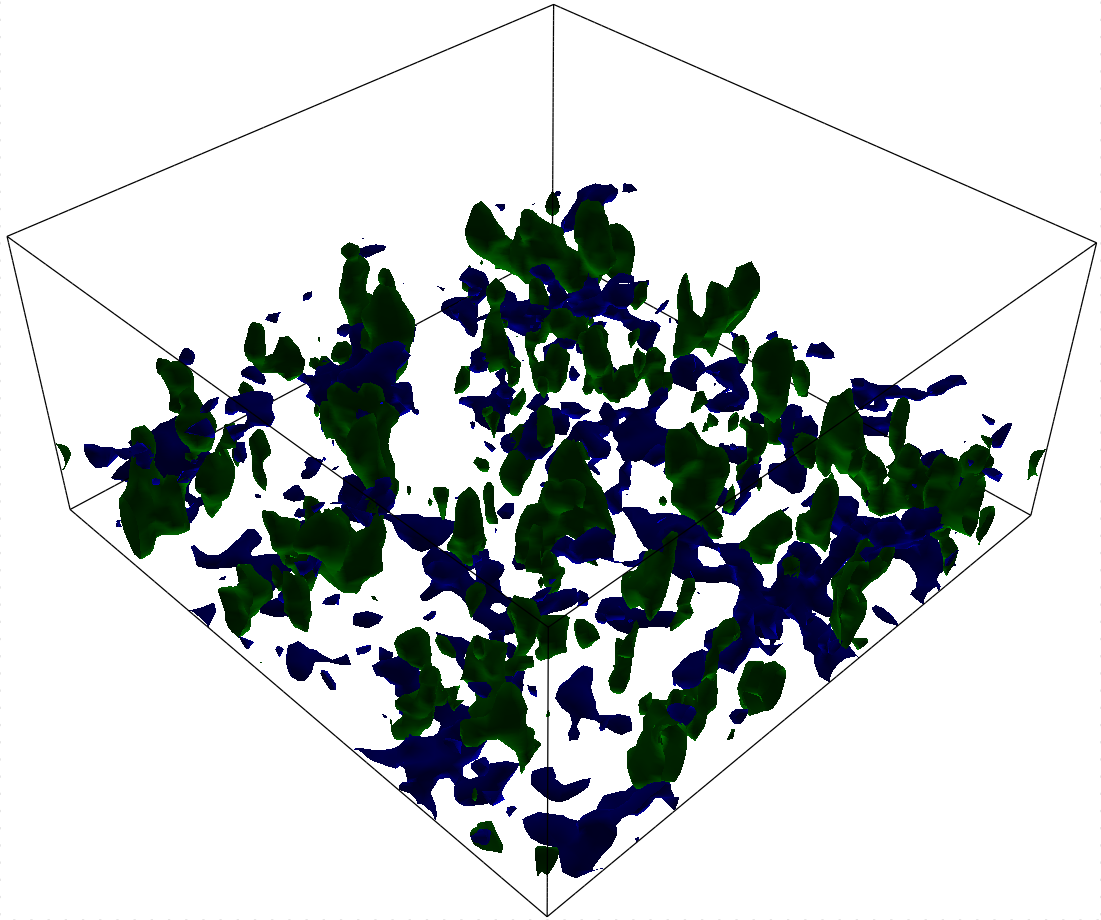

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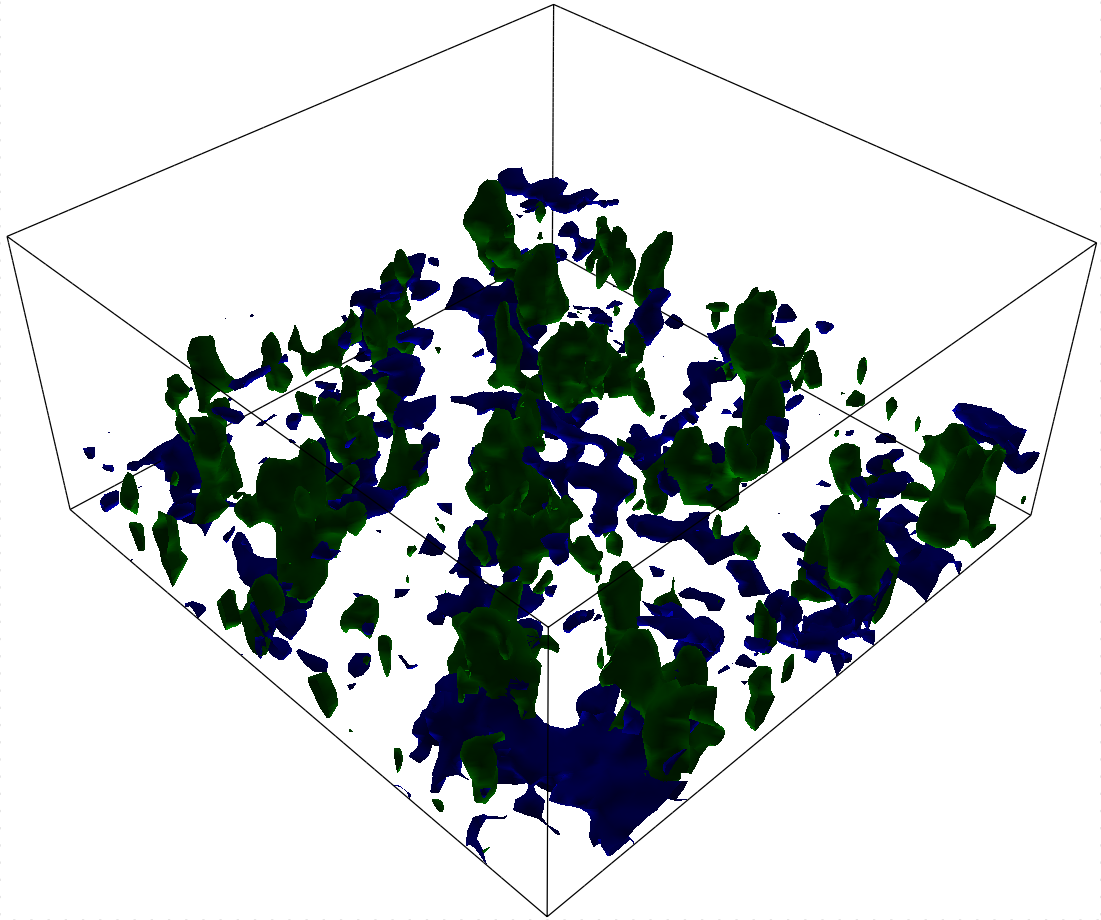

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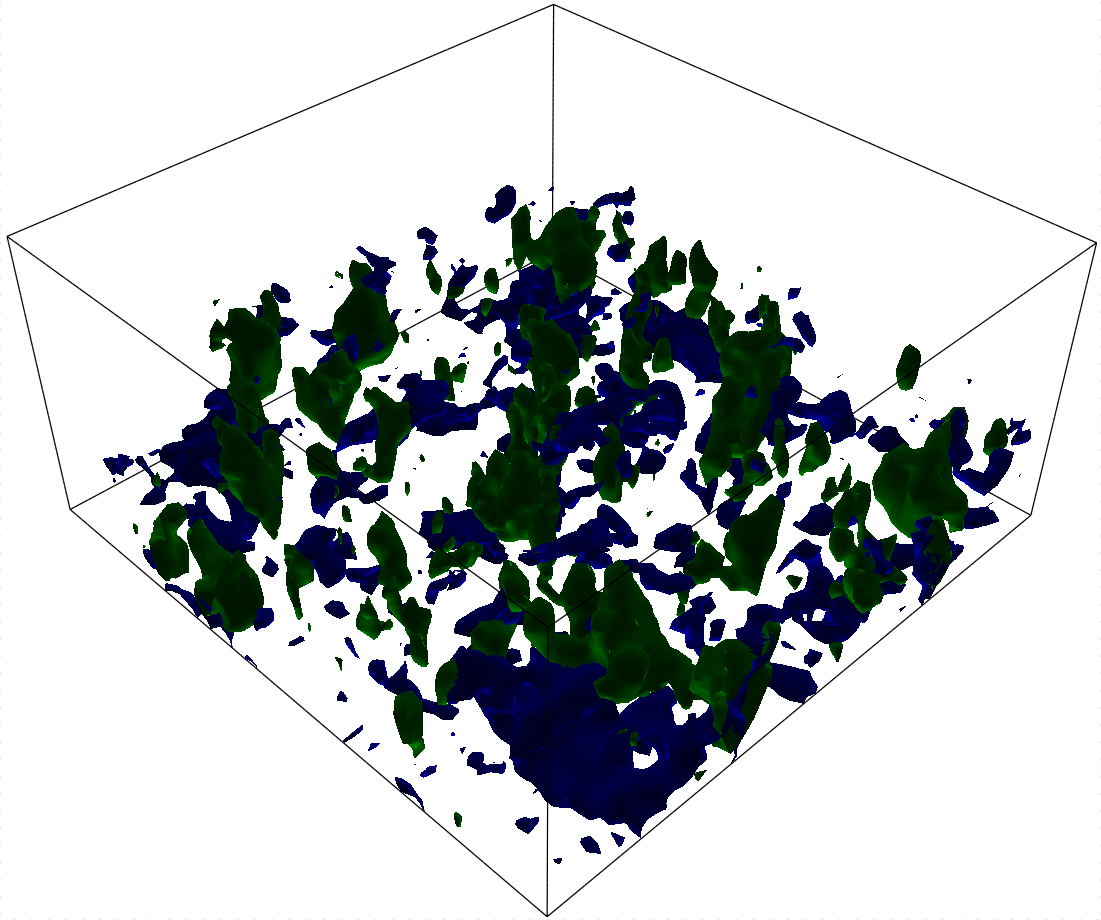

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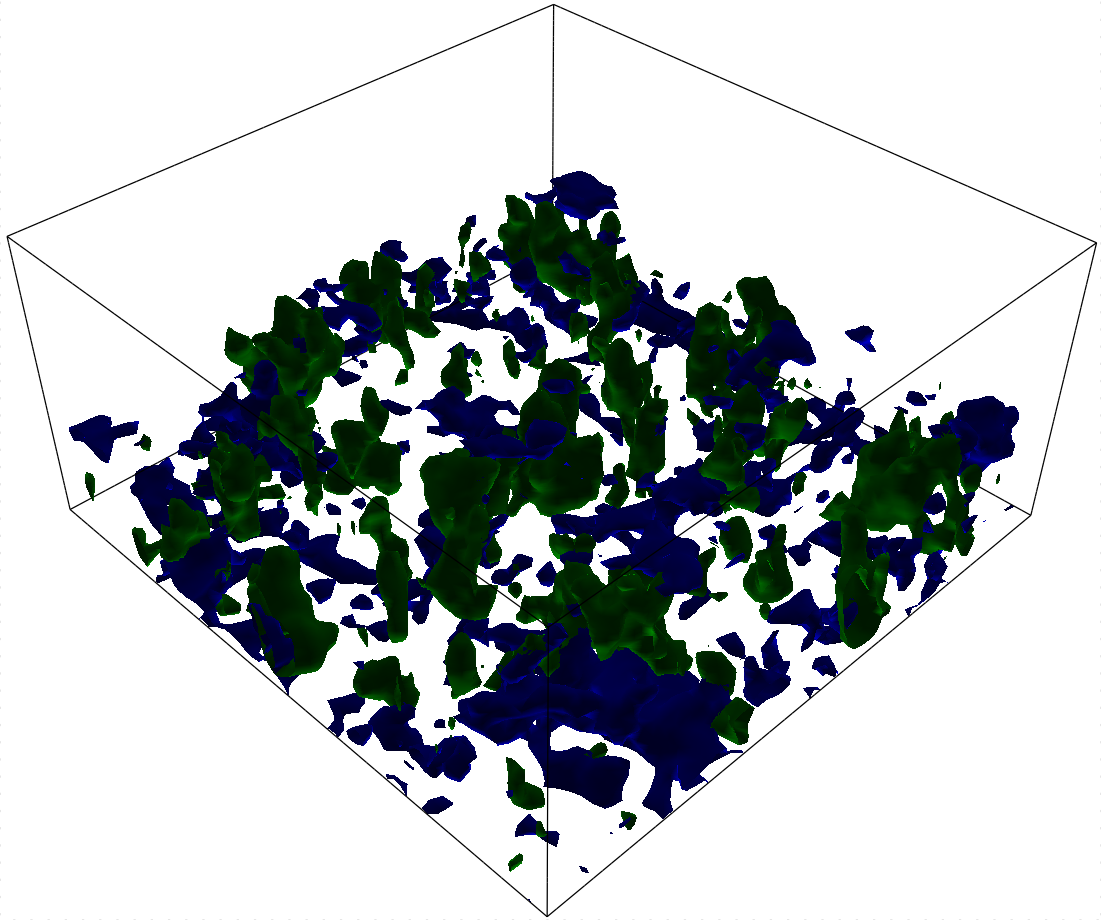

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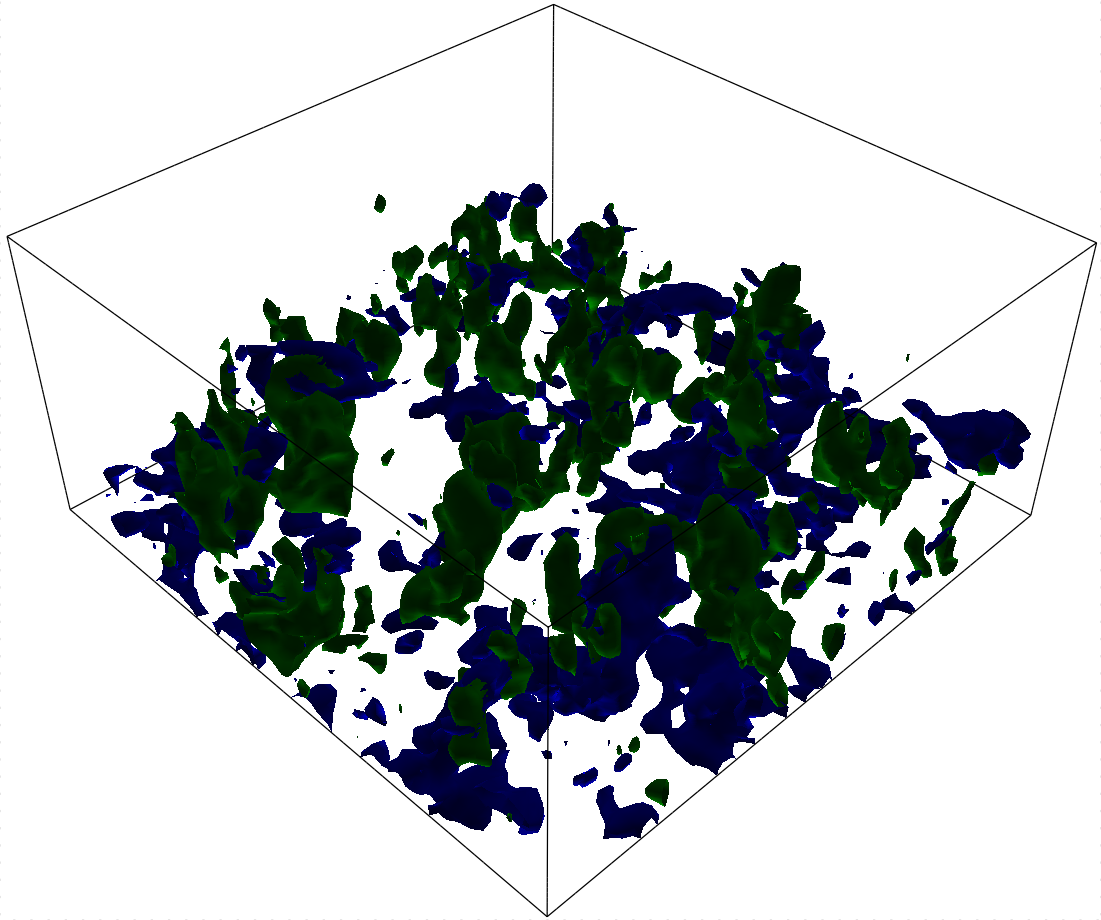

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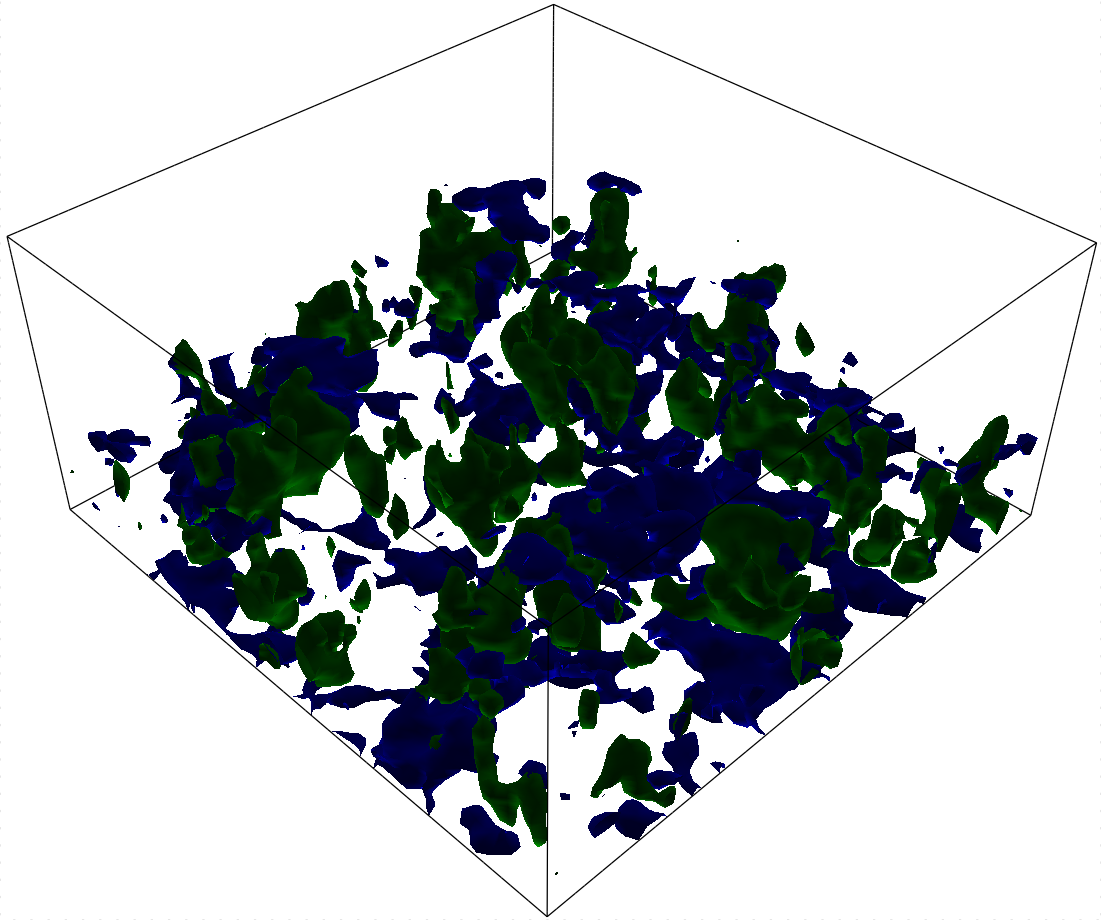

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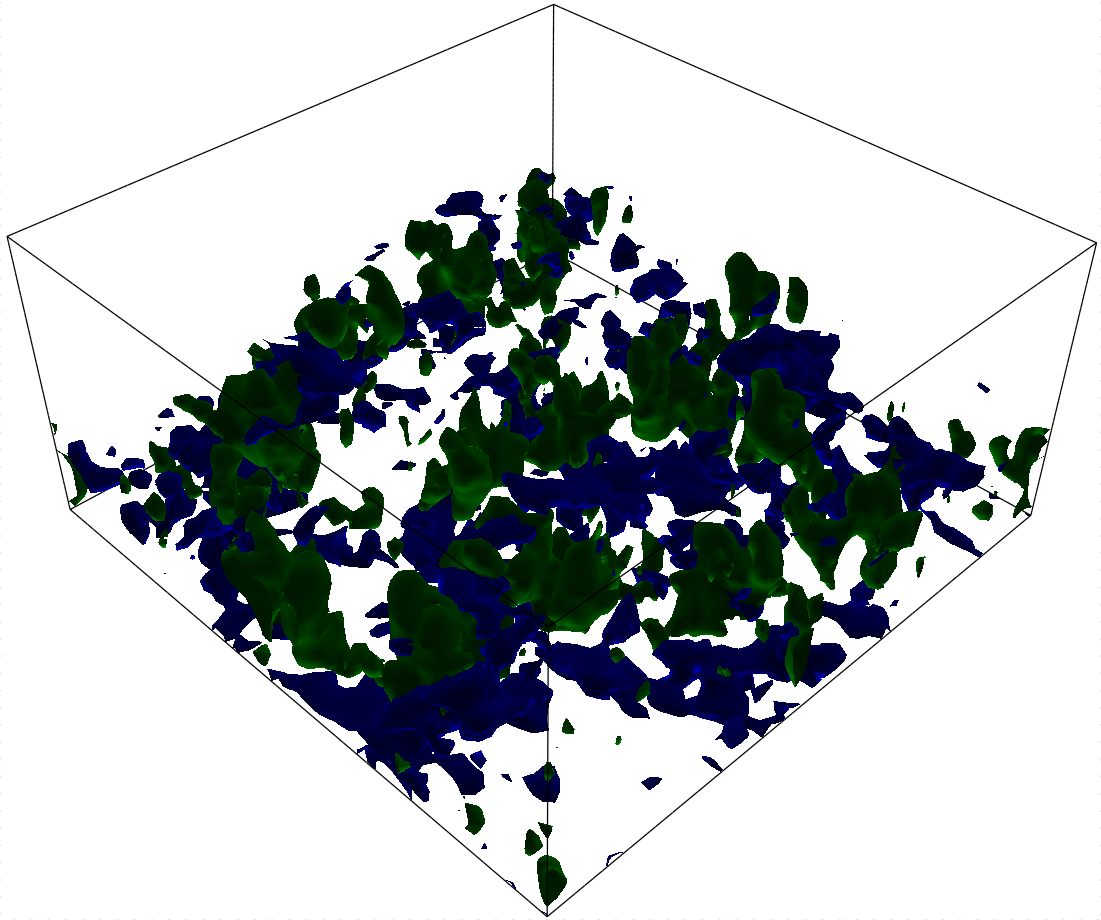

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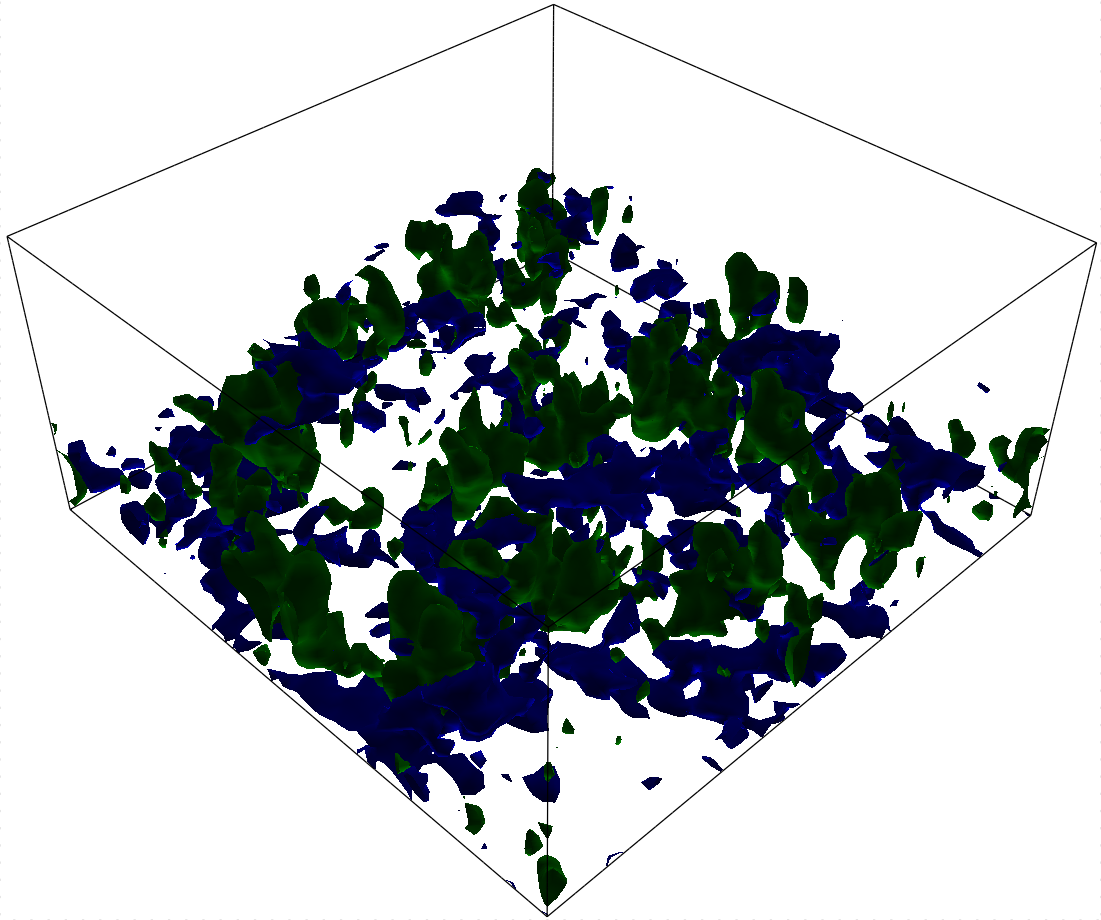

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libmpdata++ 2.0: summary of features under development

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coded by
Maciej Waruszewski

libmpdata++ 2.0: summary of features under development

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- implicit treatment of absorbers
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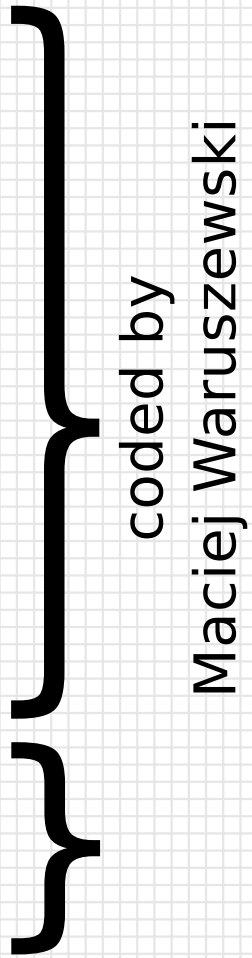

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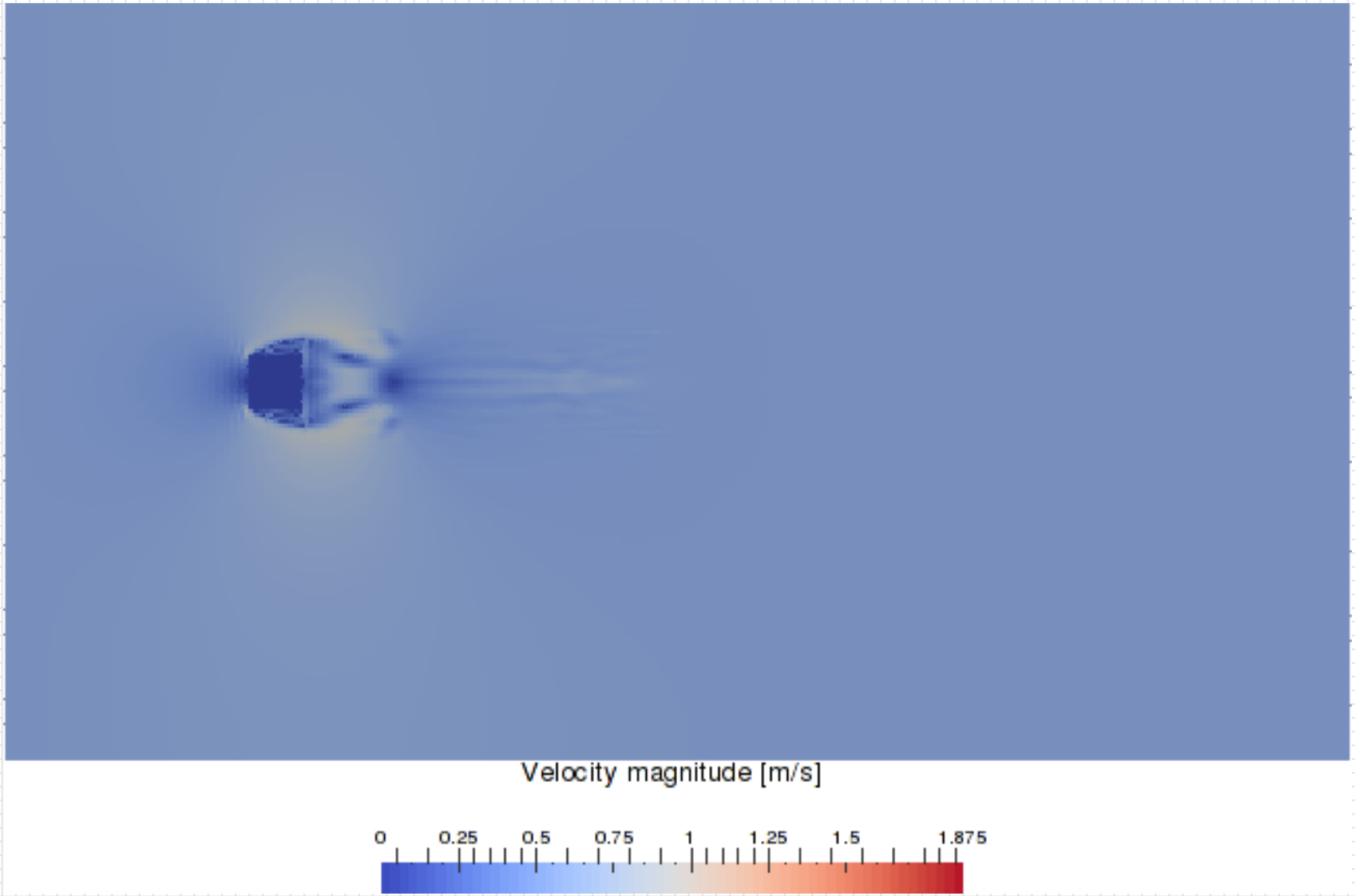

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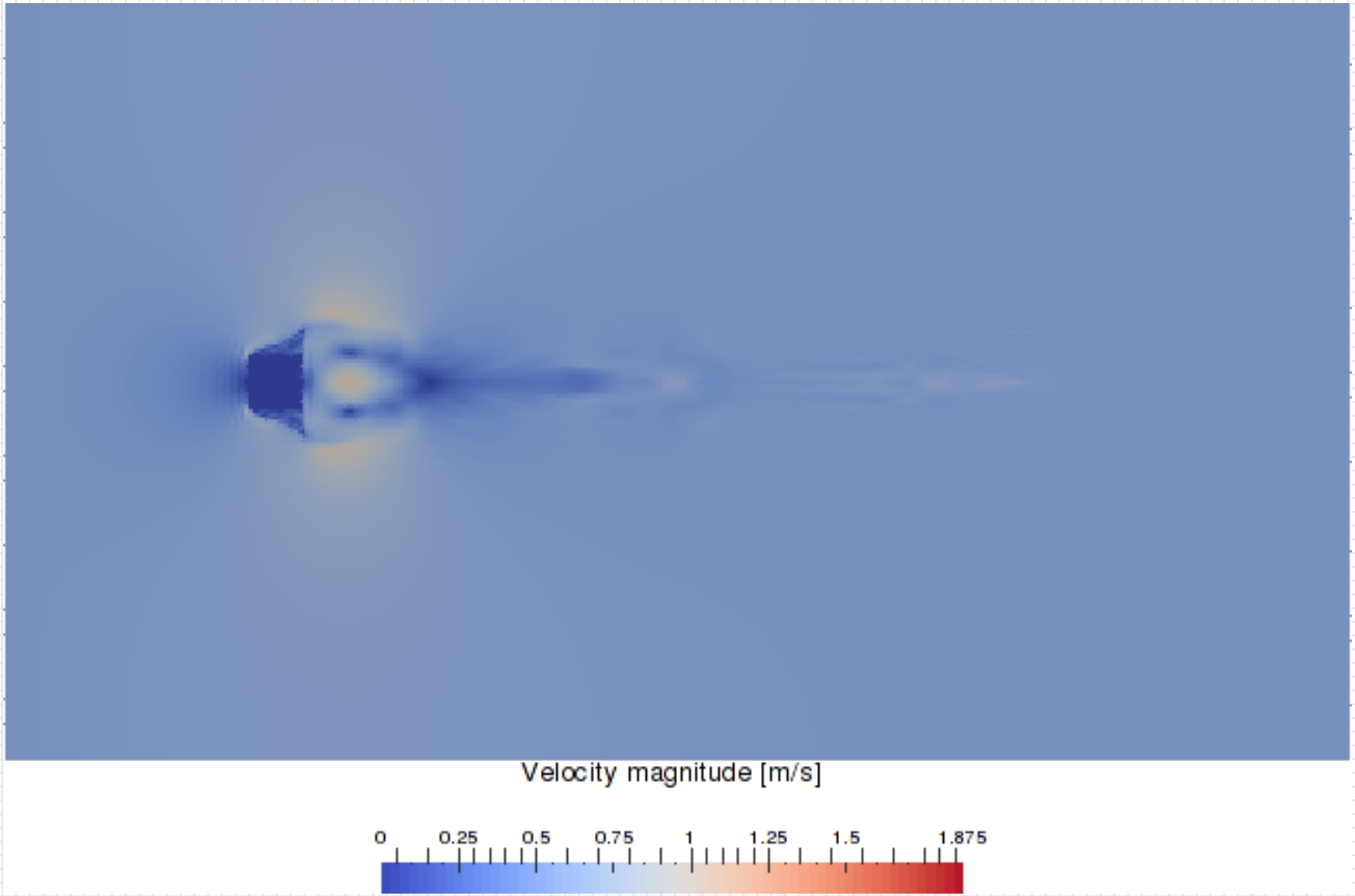

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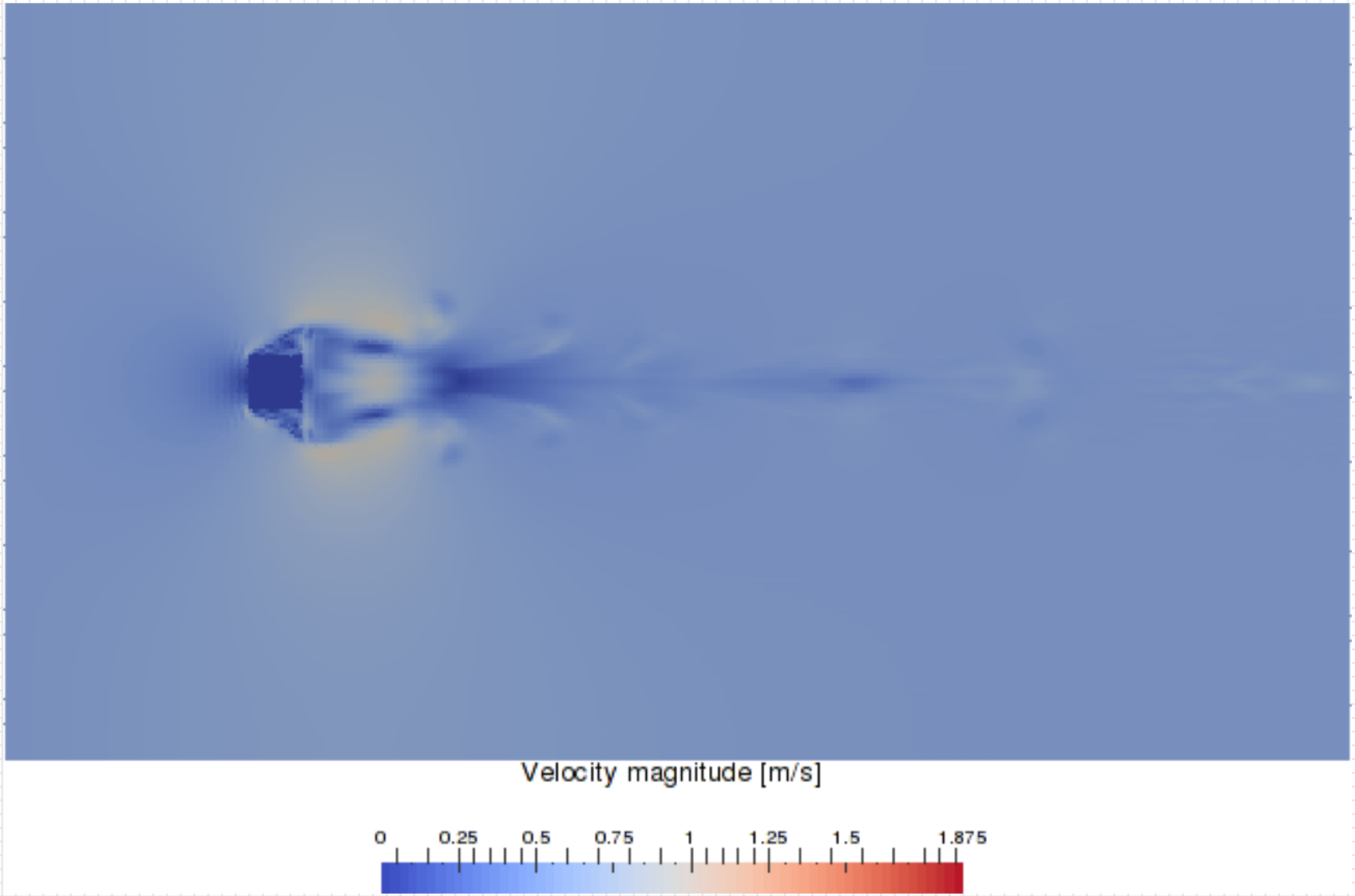

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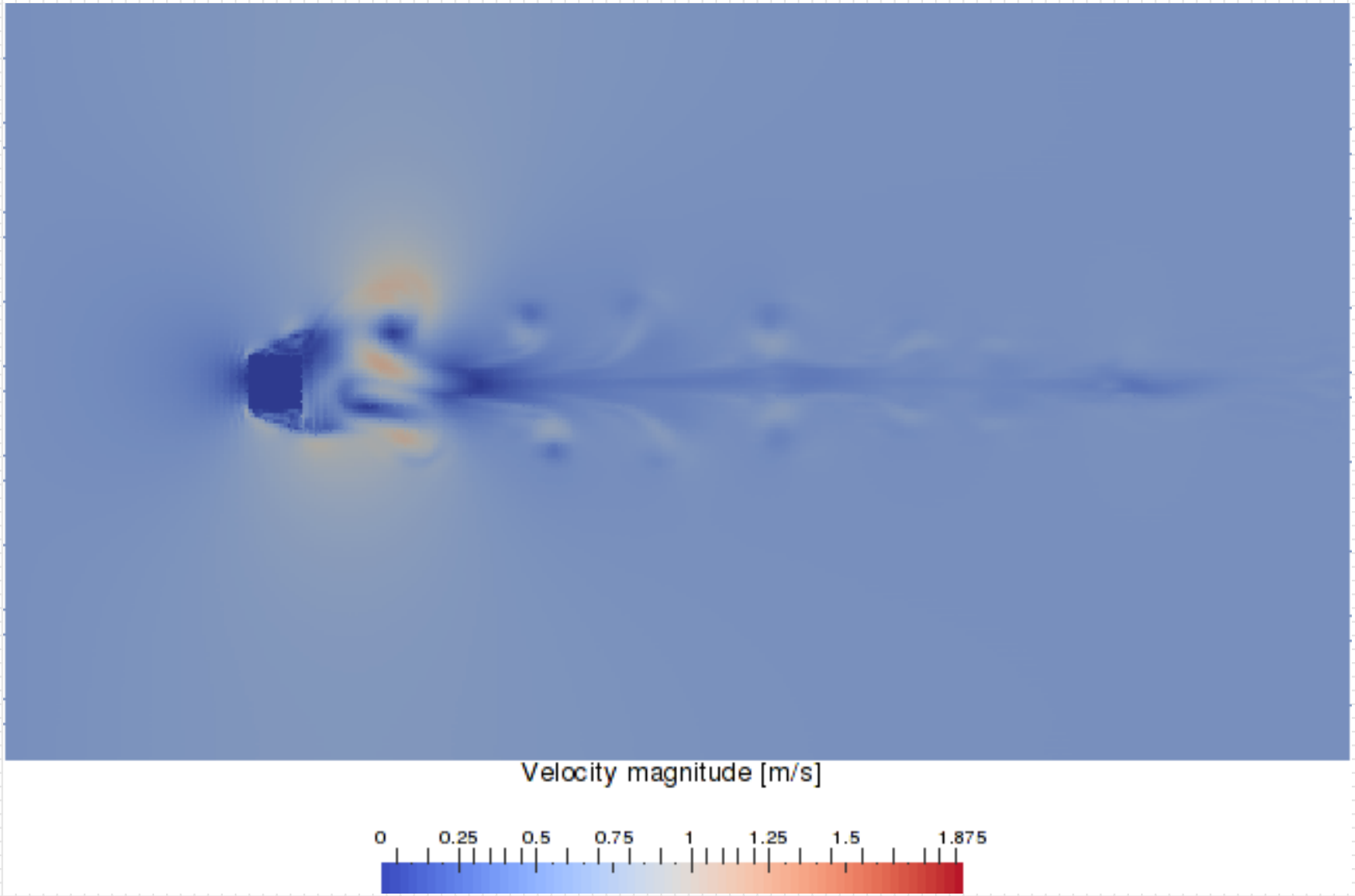

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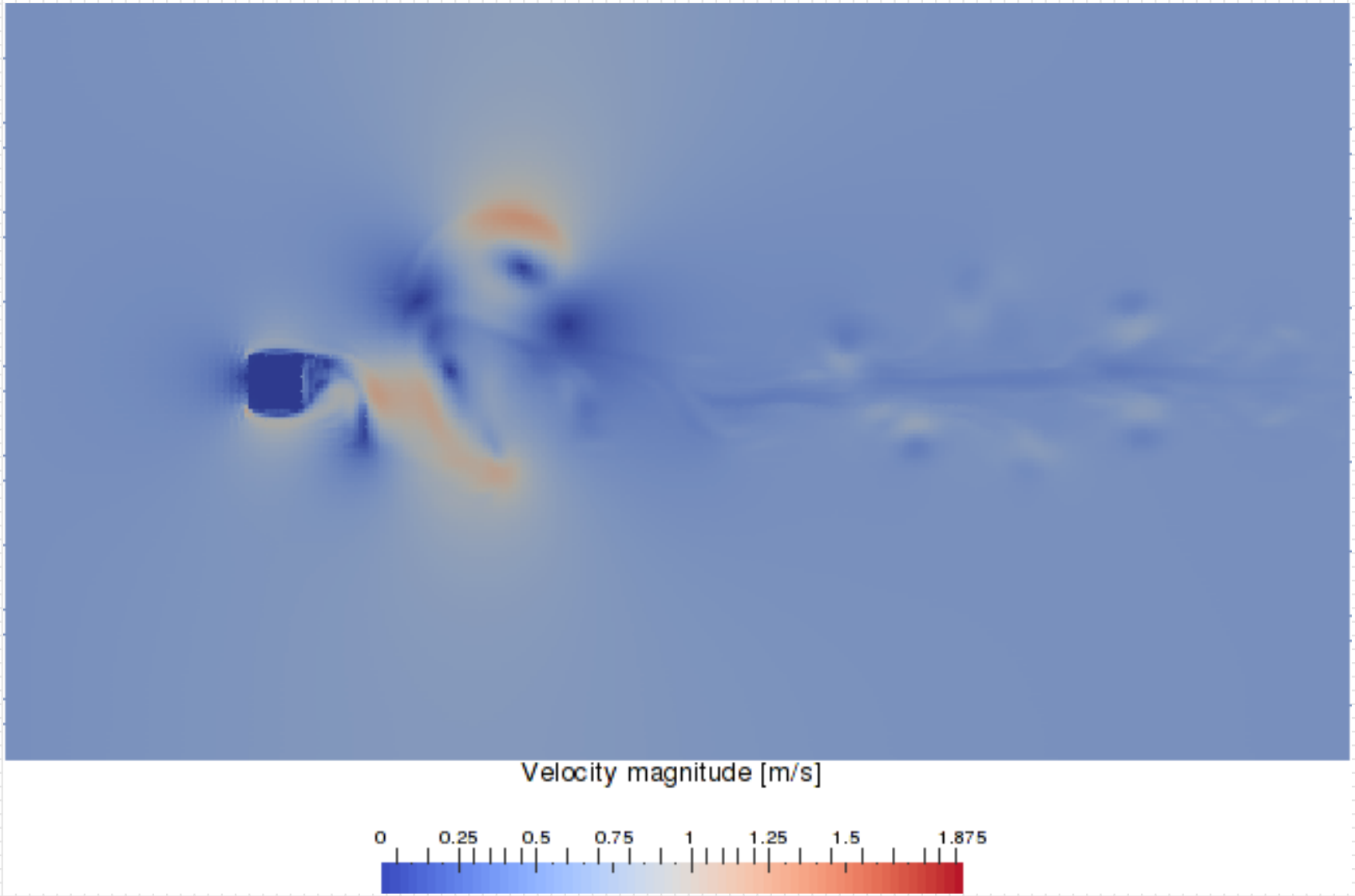

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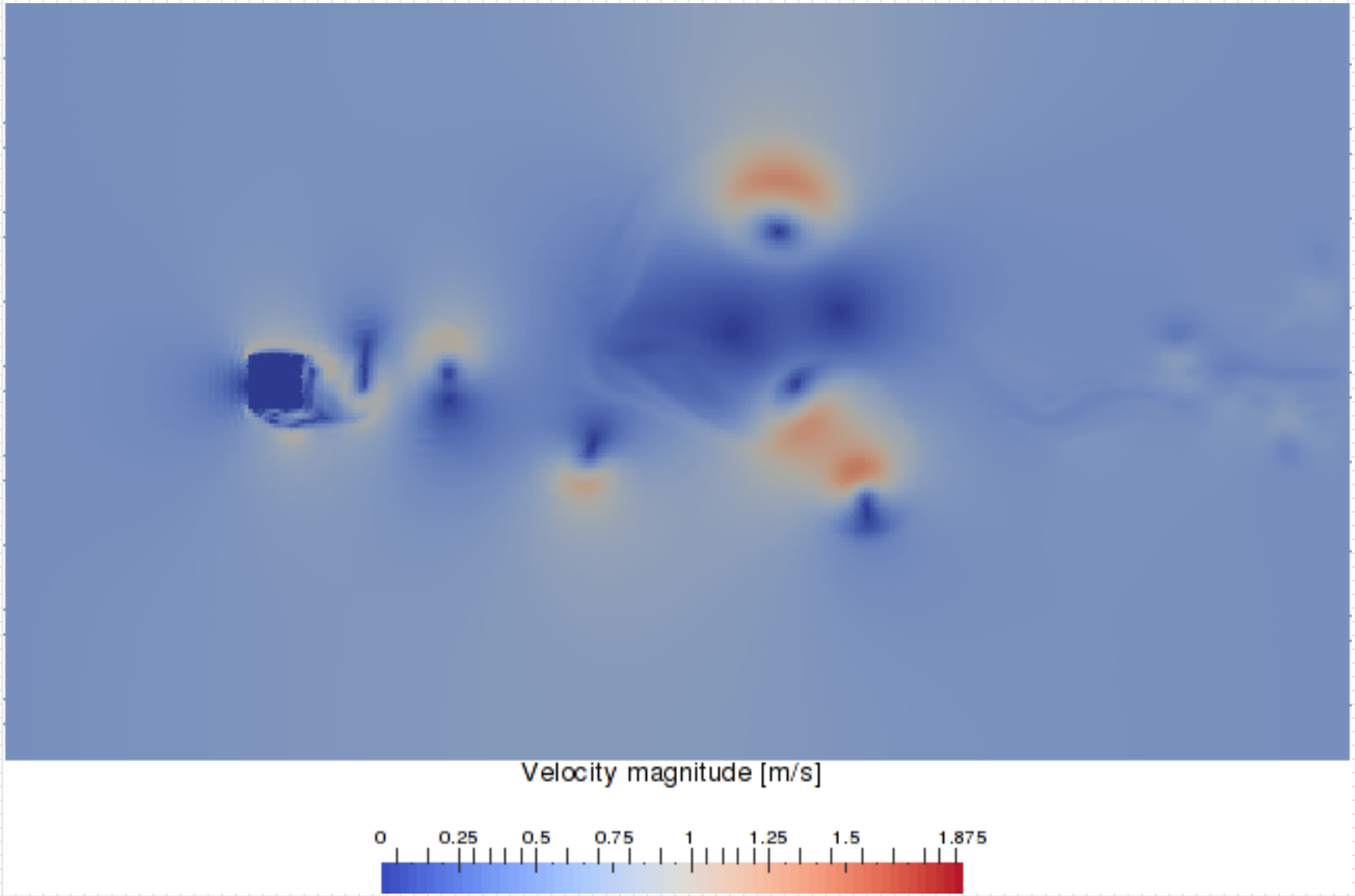

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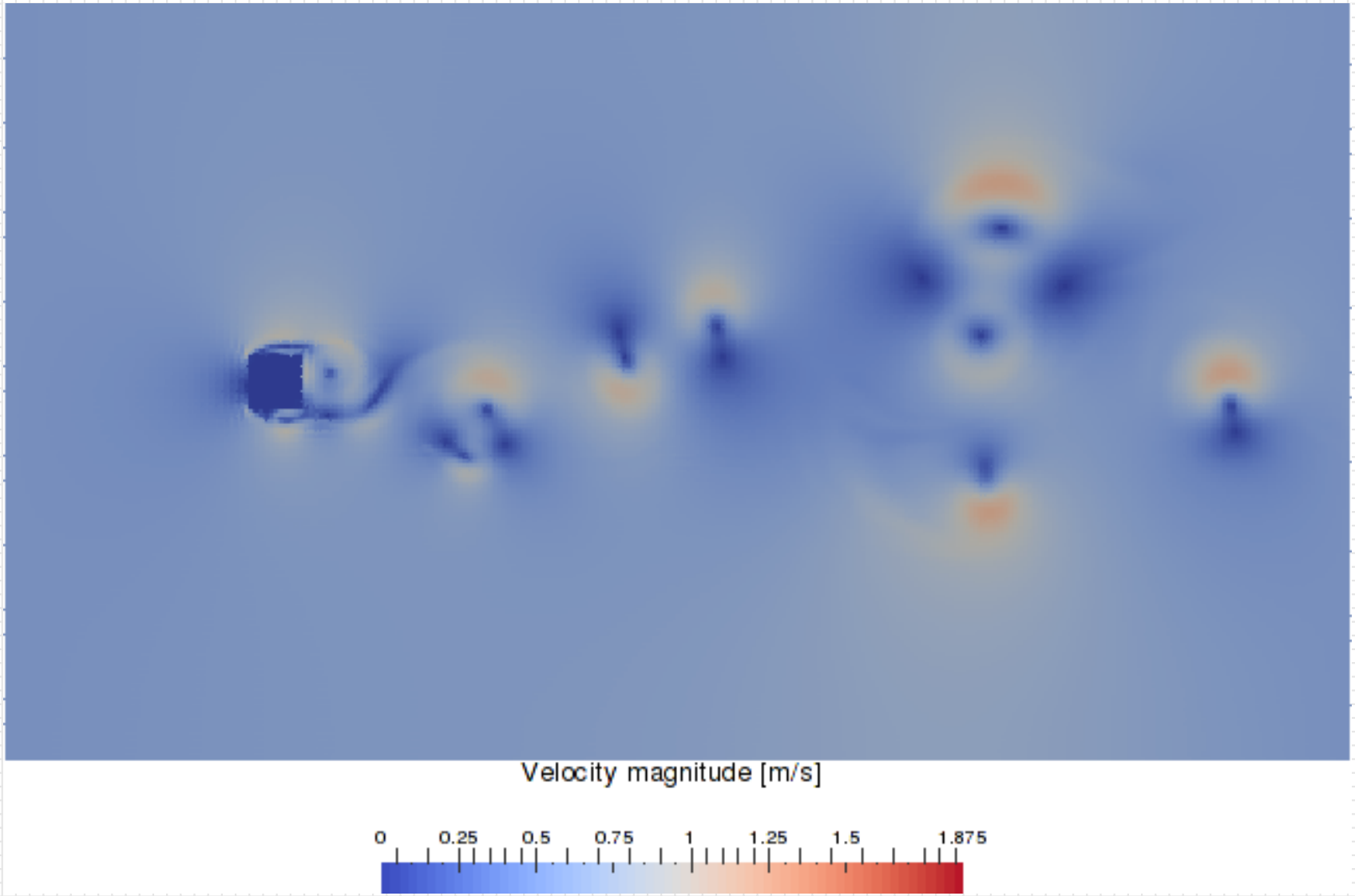

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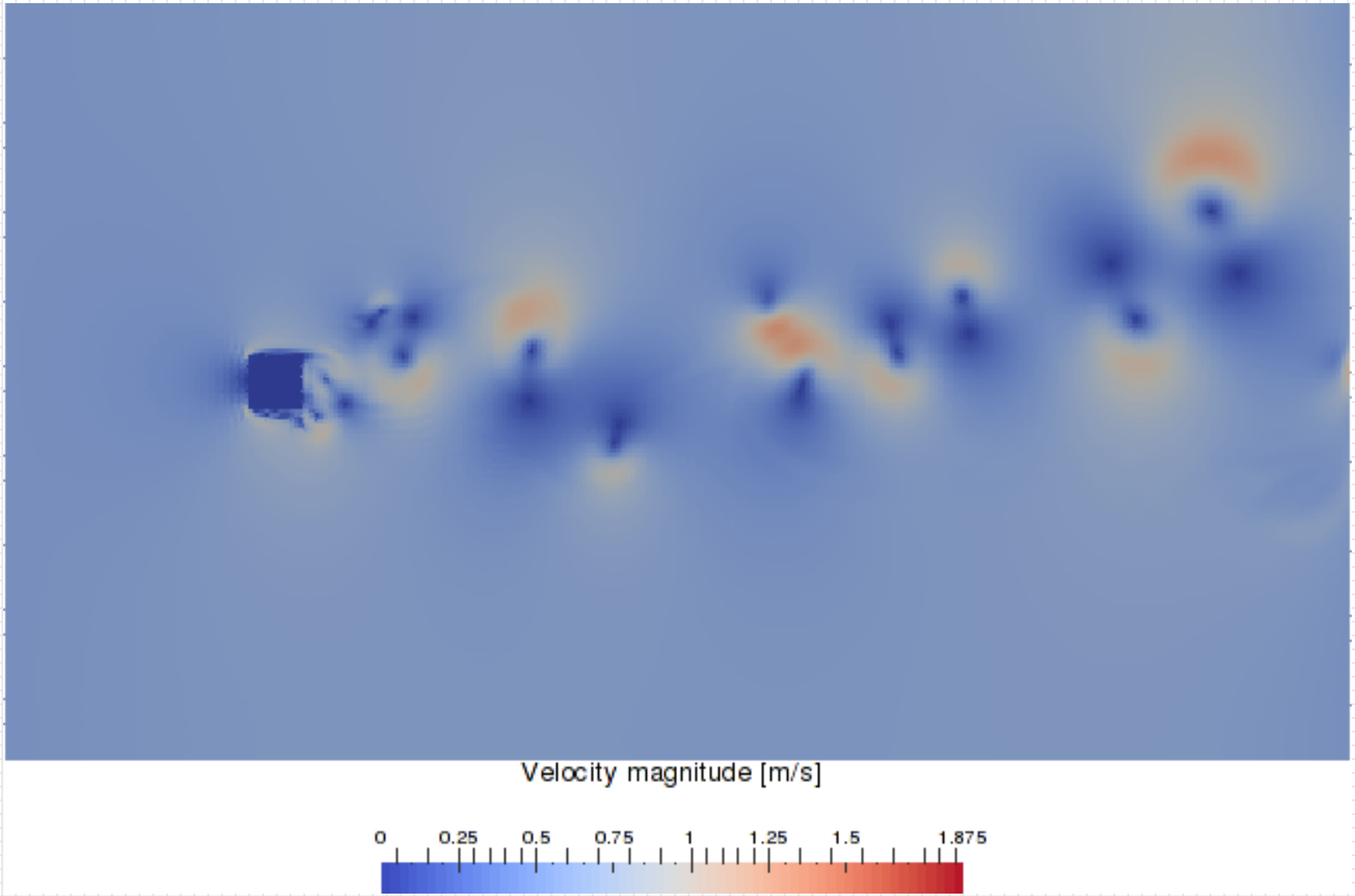

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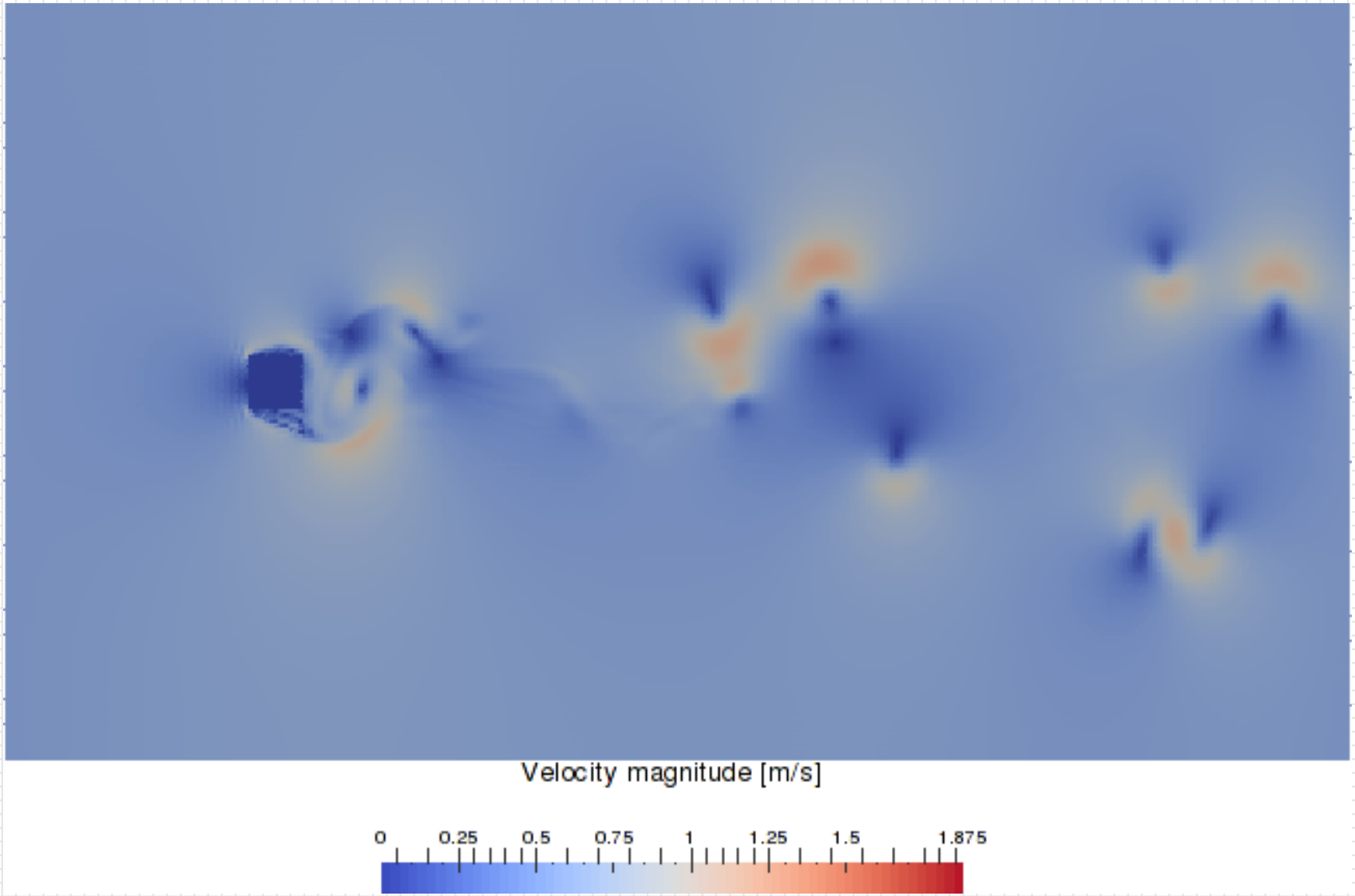

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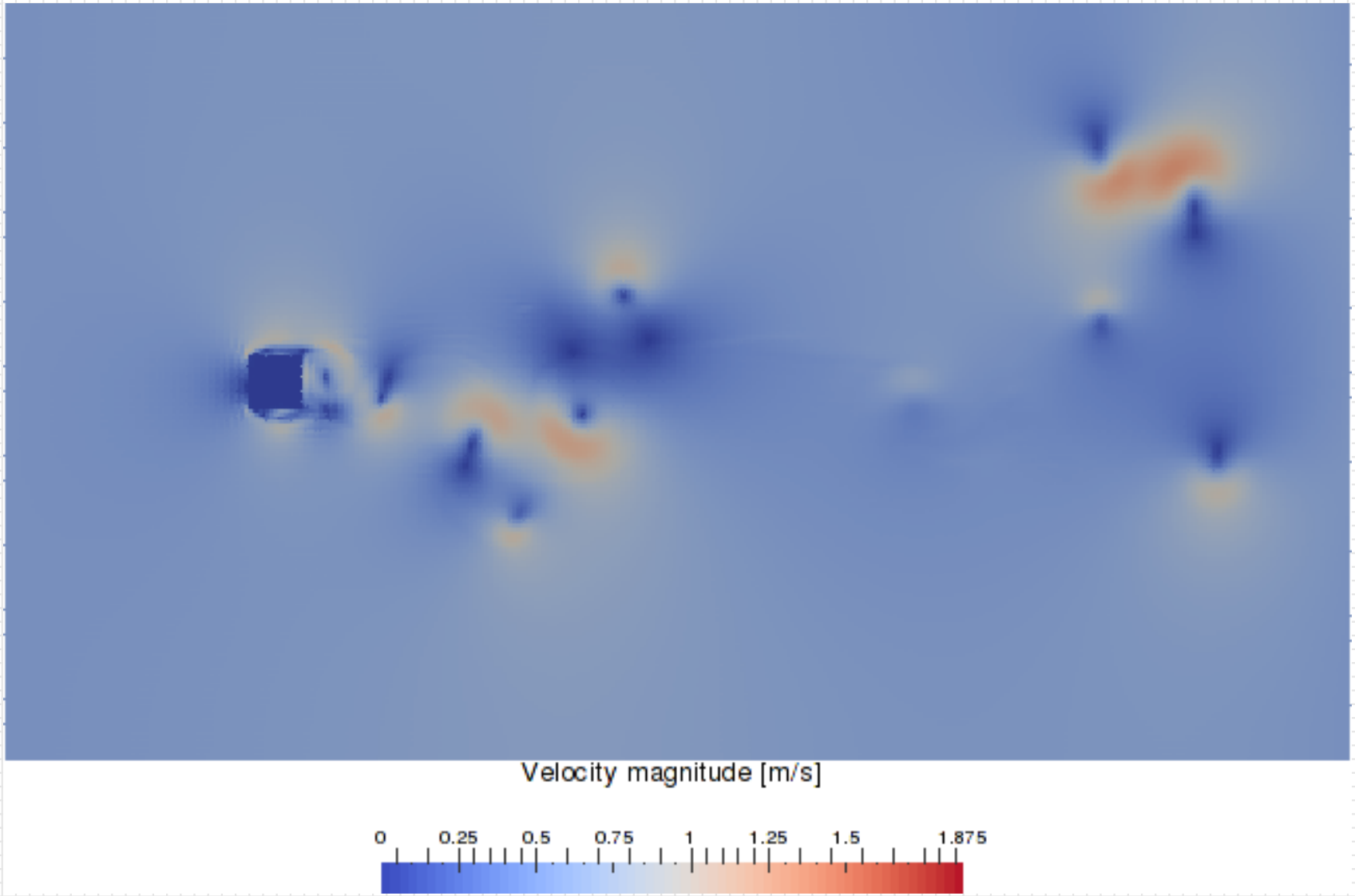

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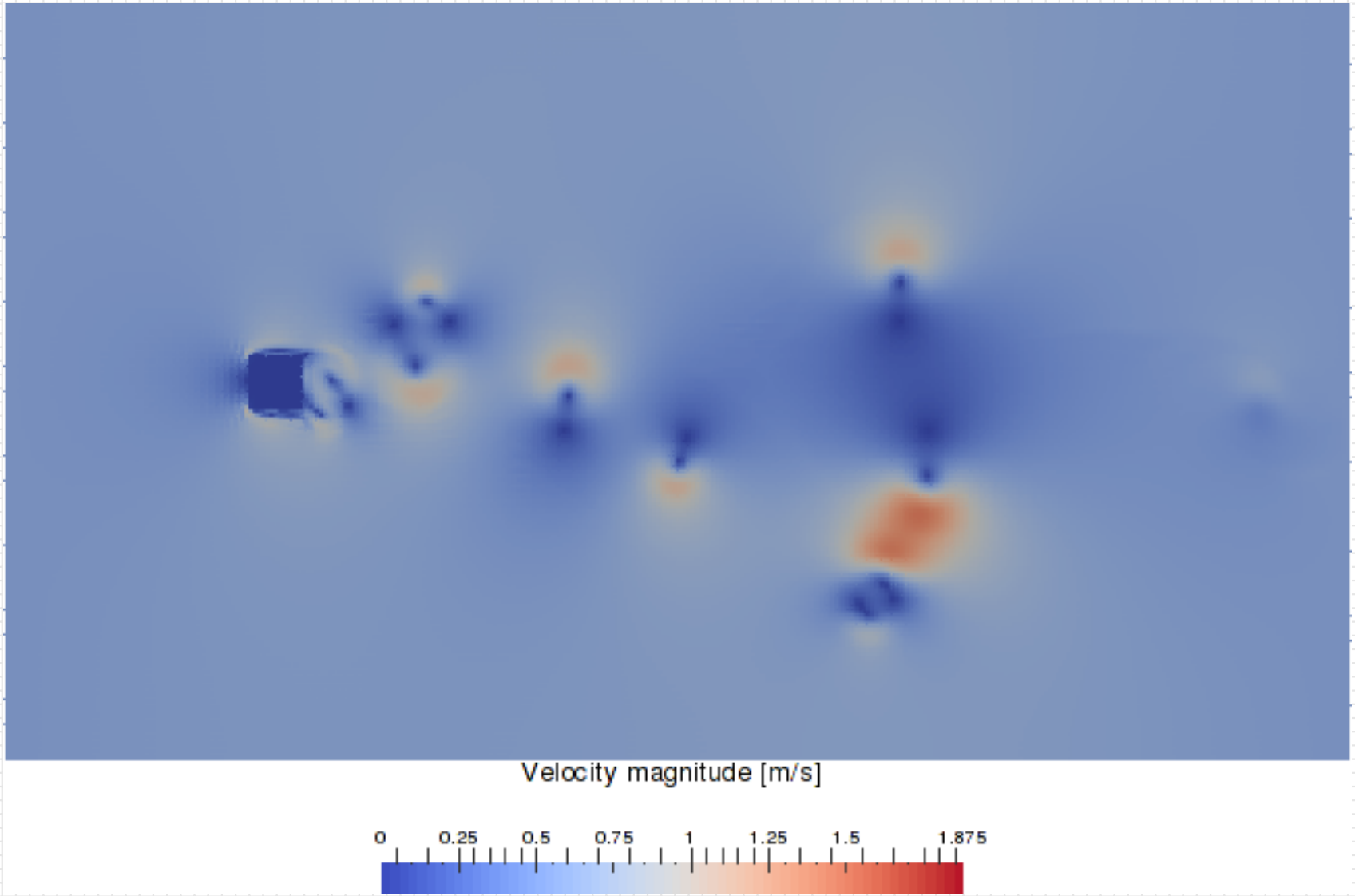

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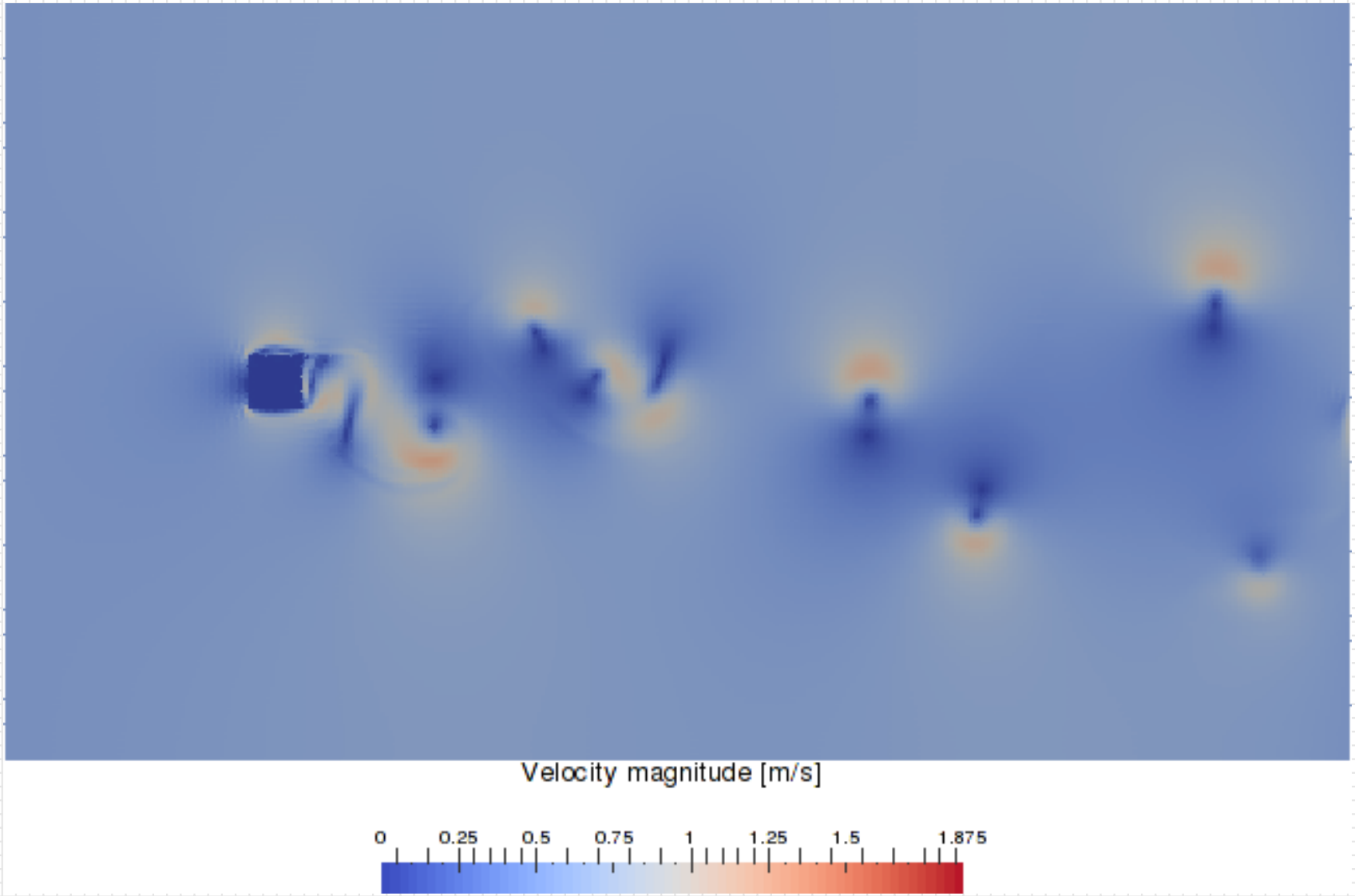

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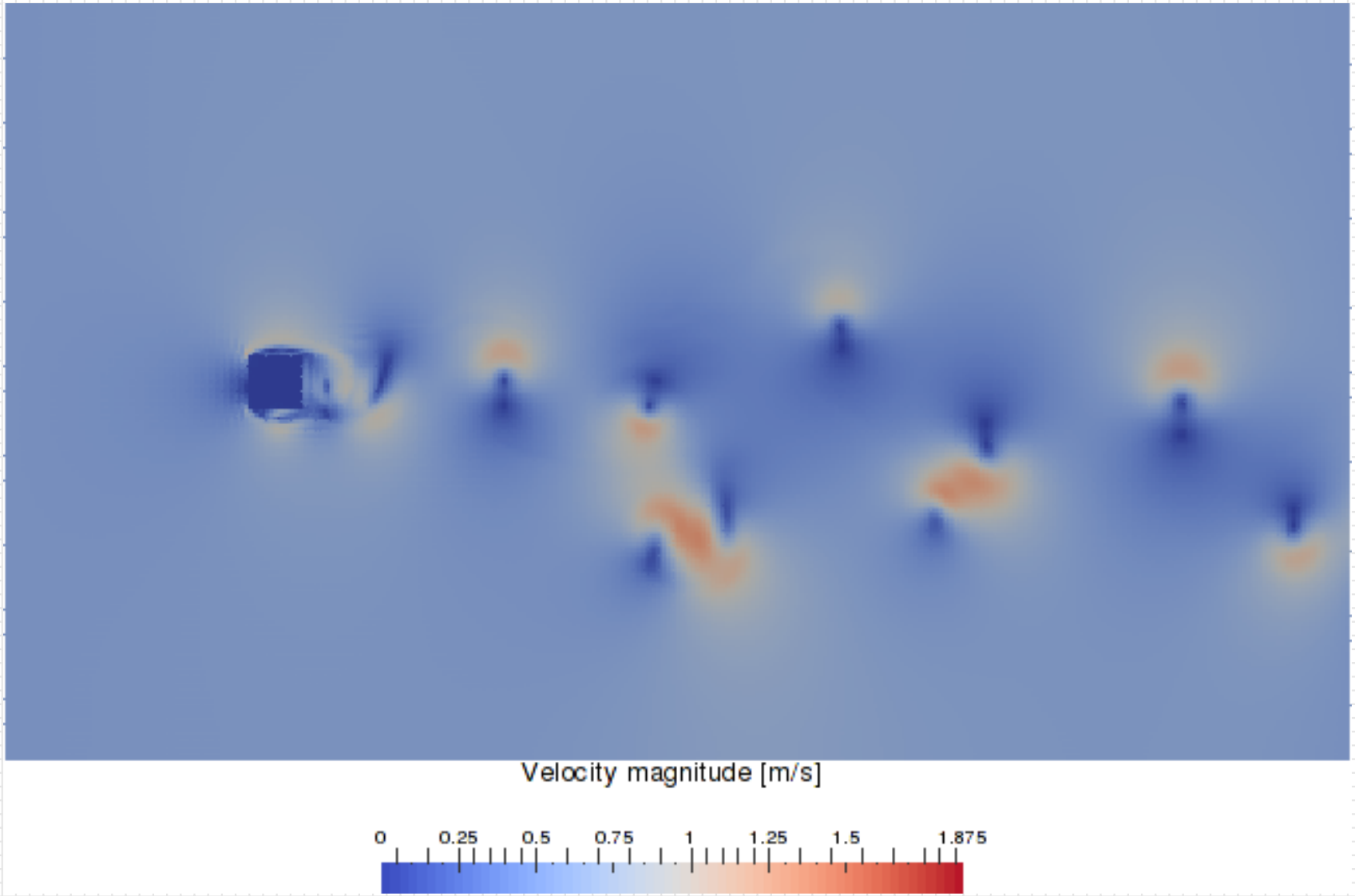

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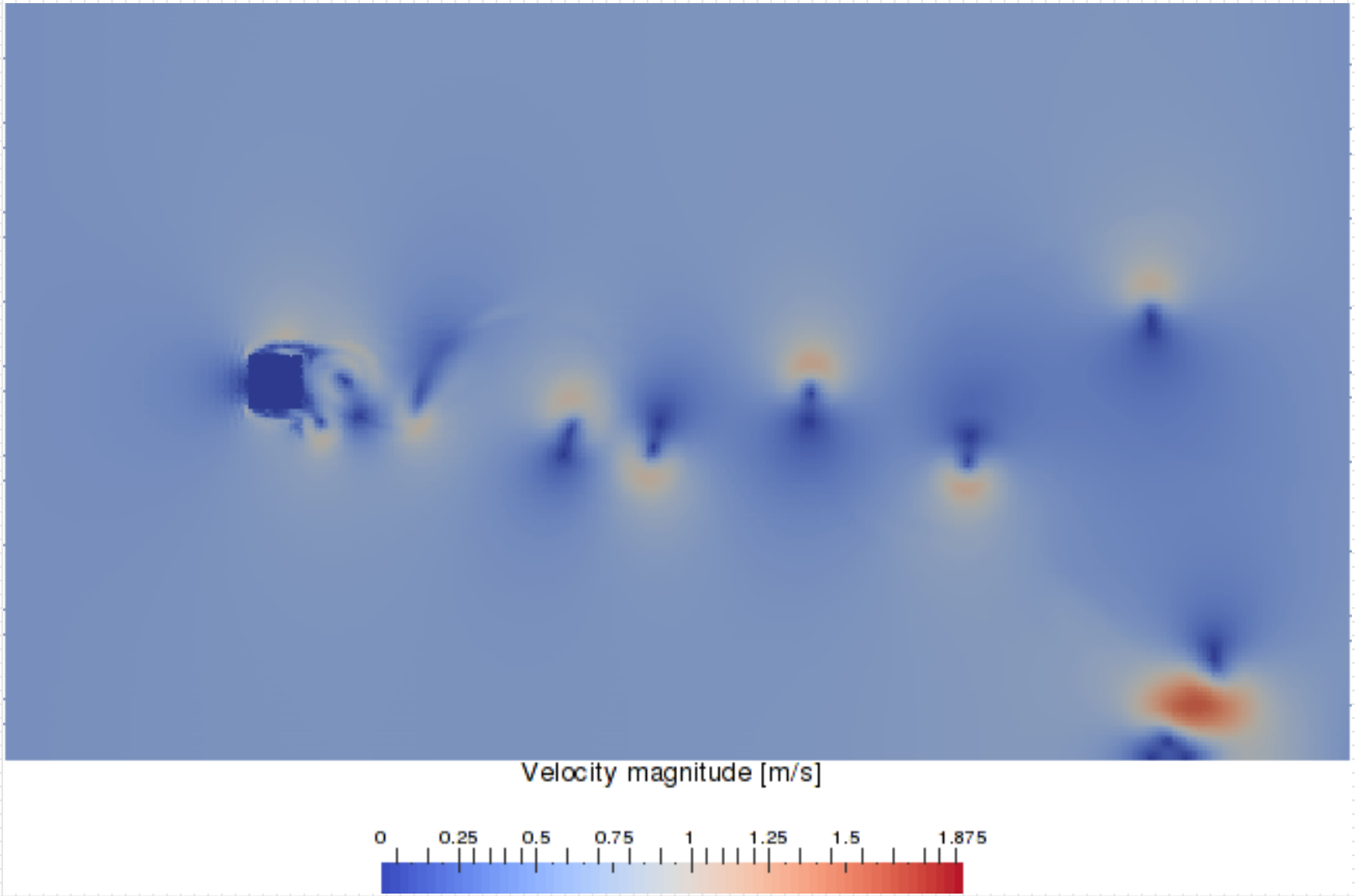

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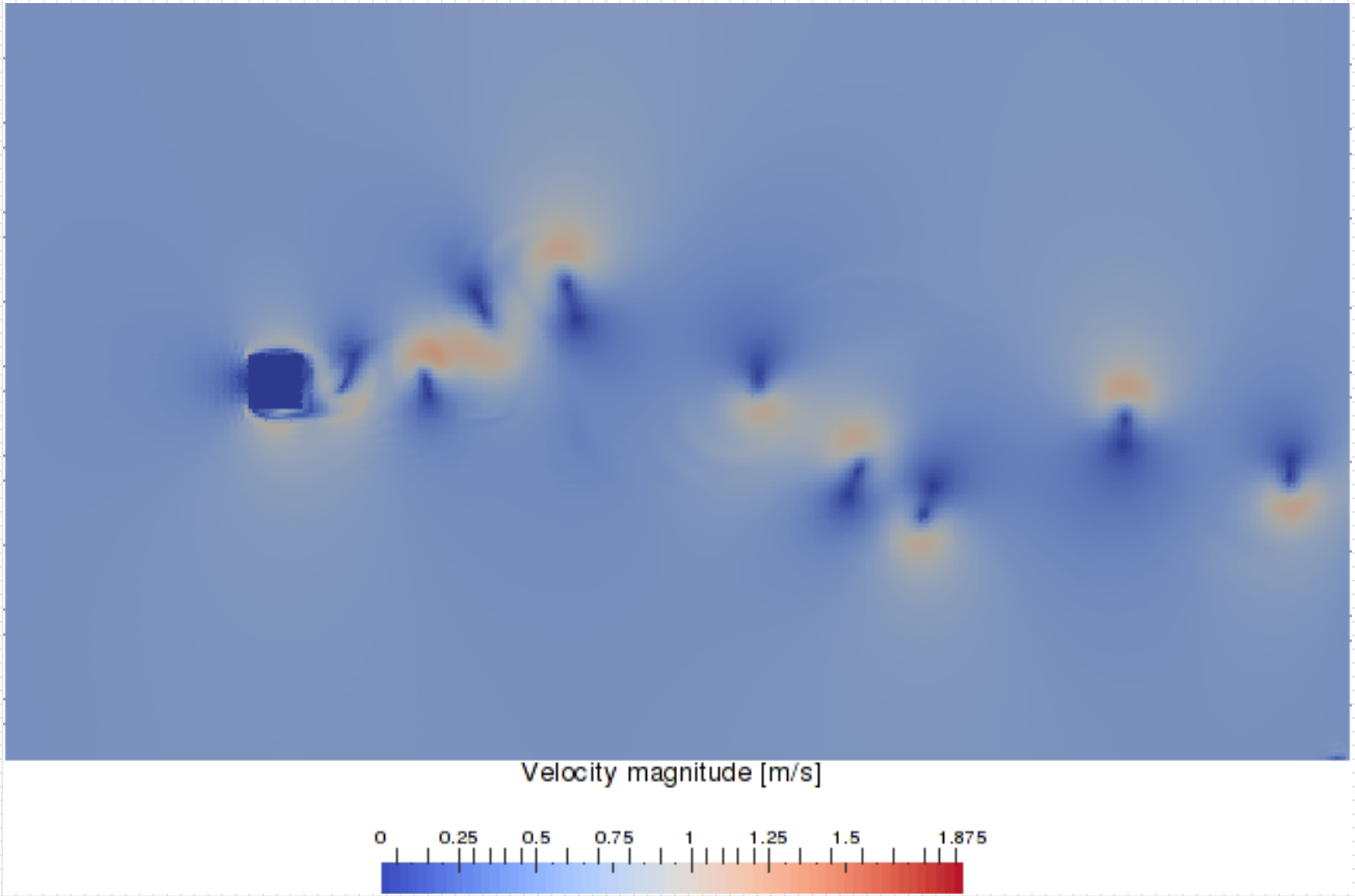

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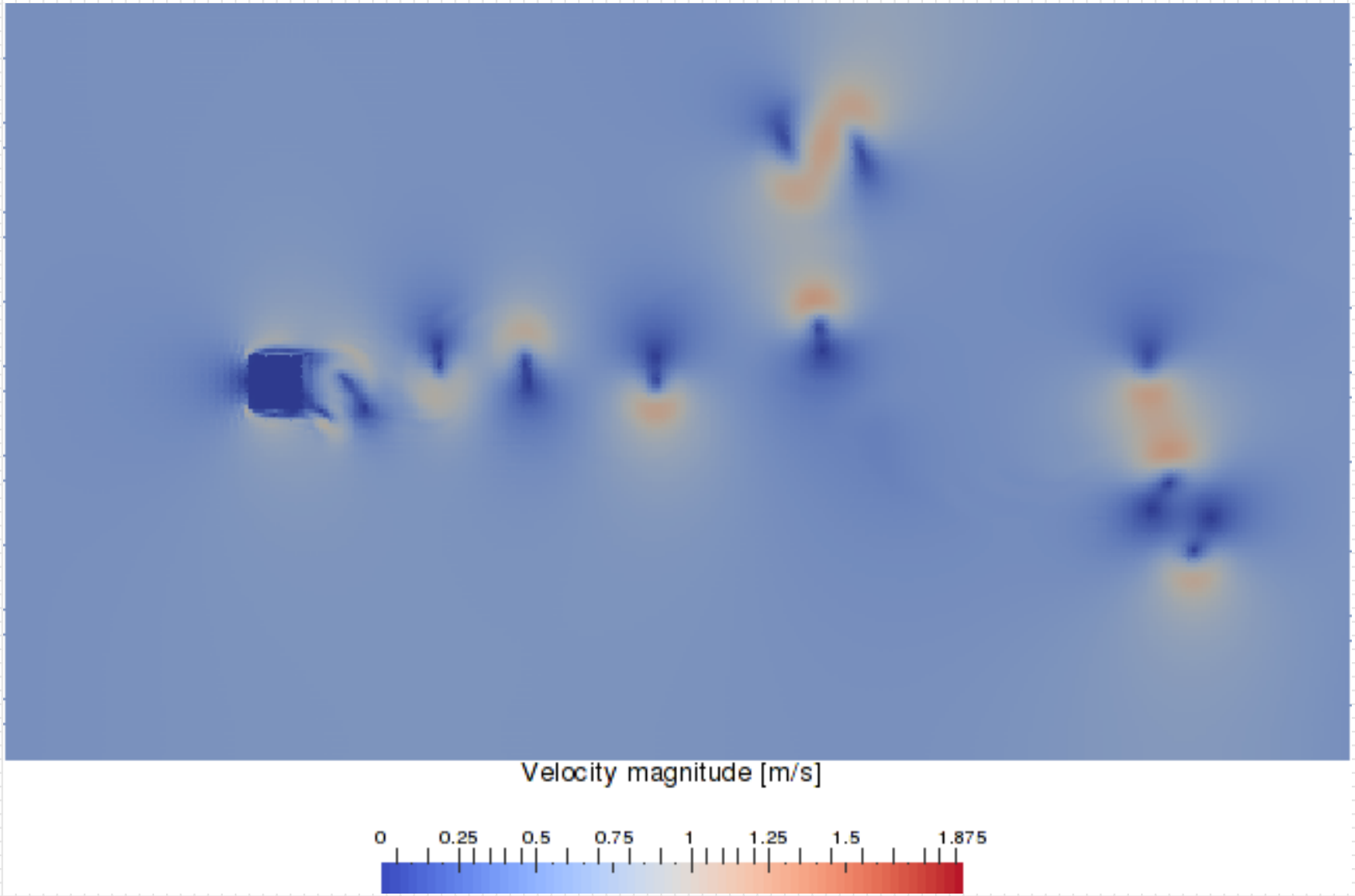

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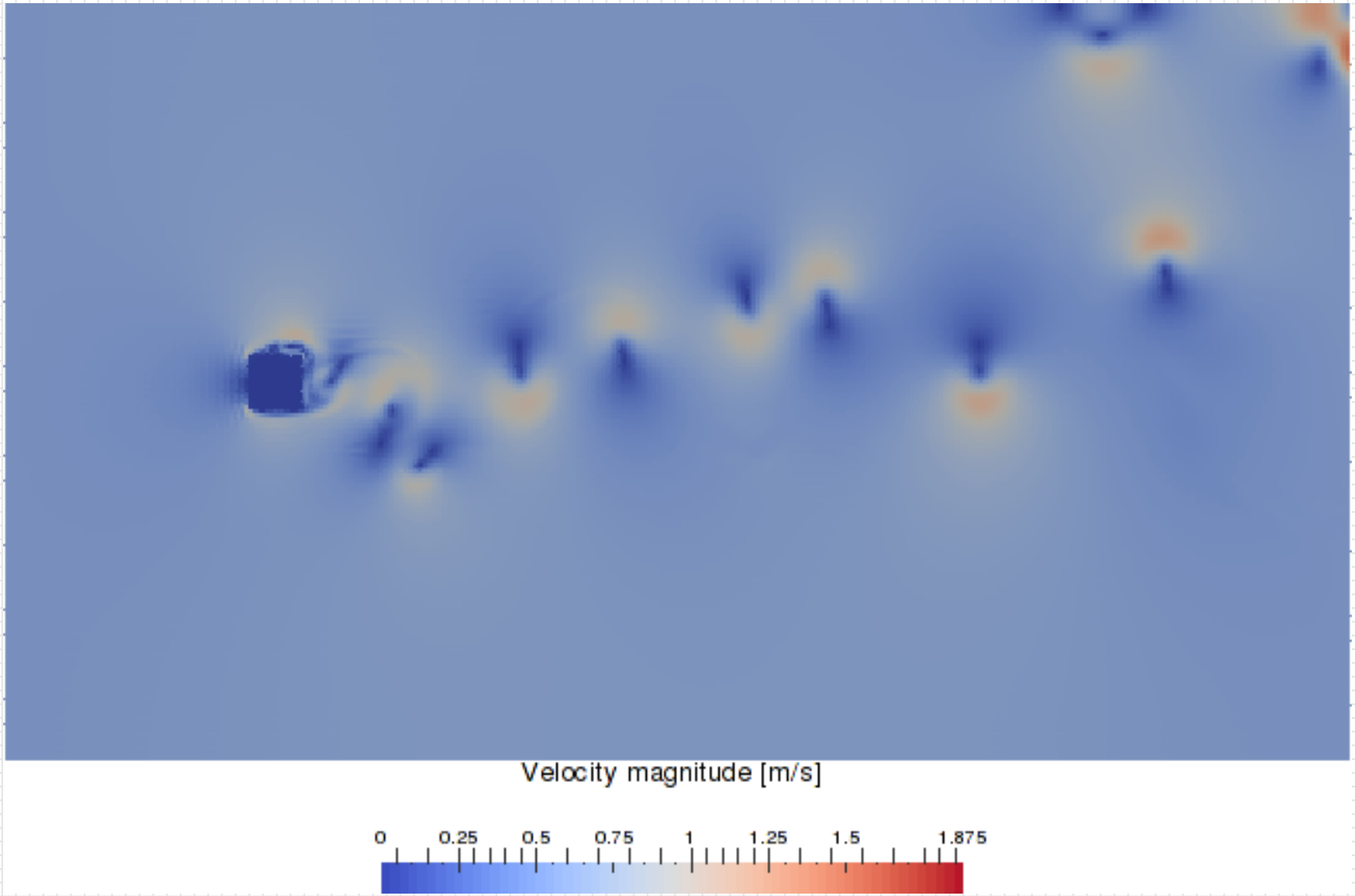

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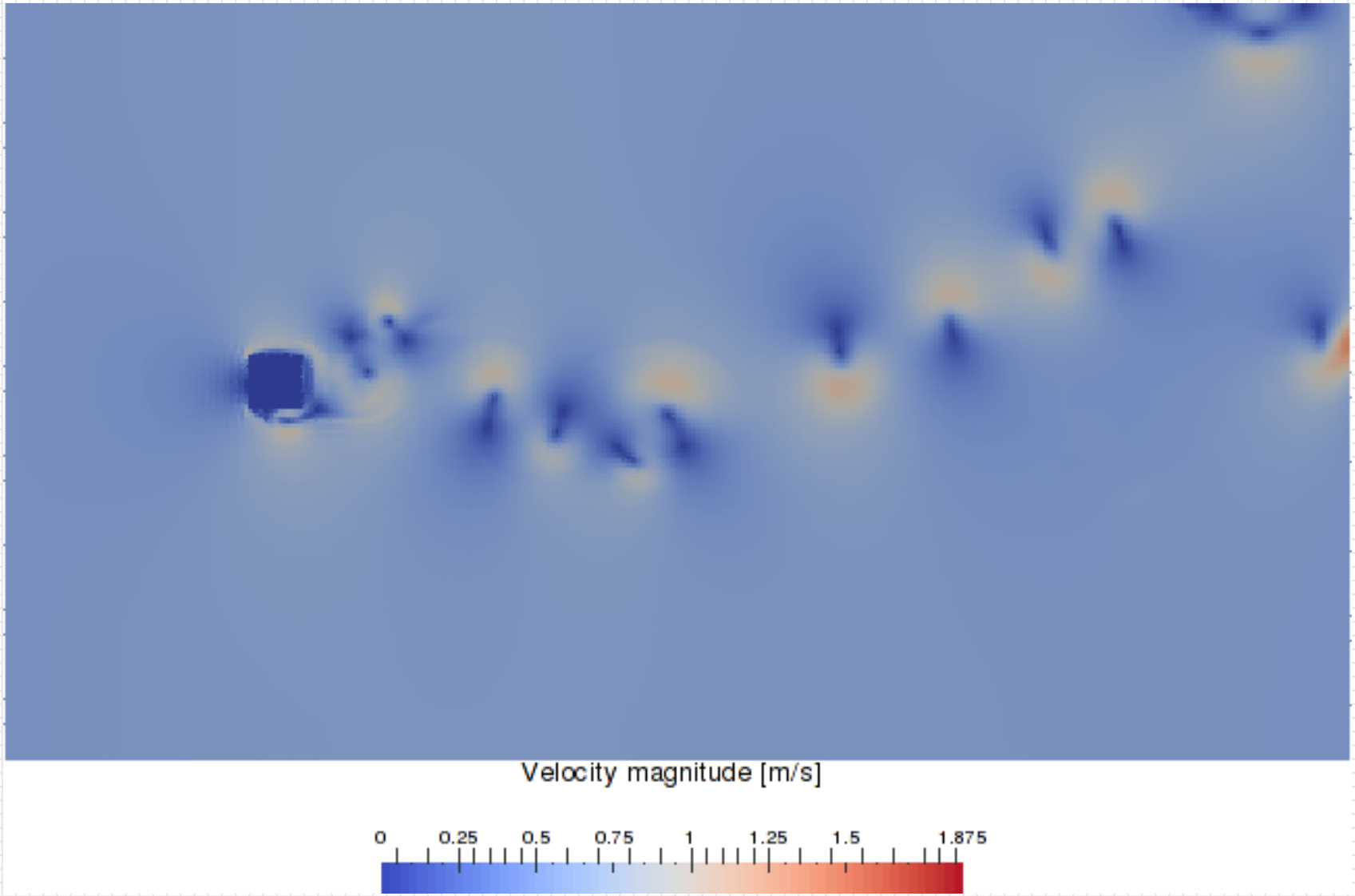

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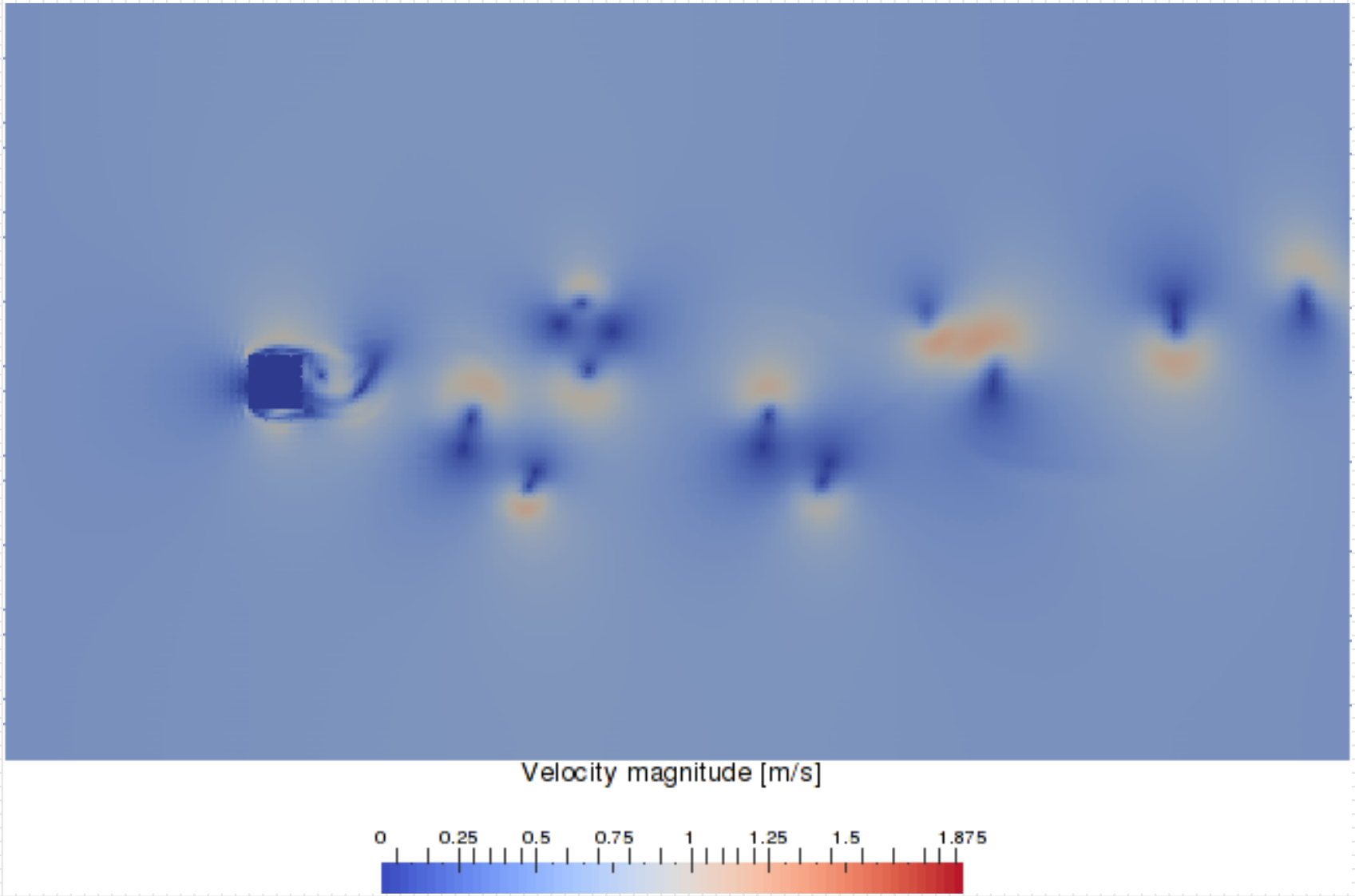

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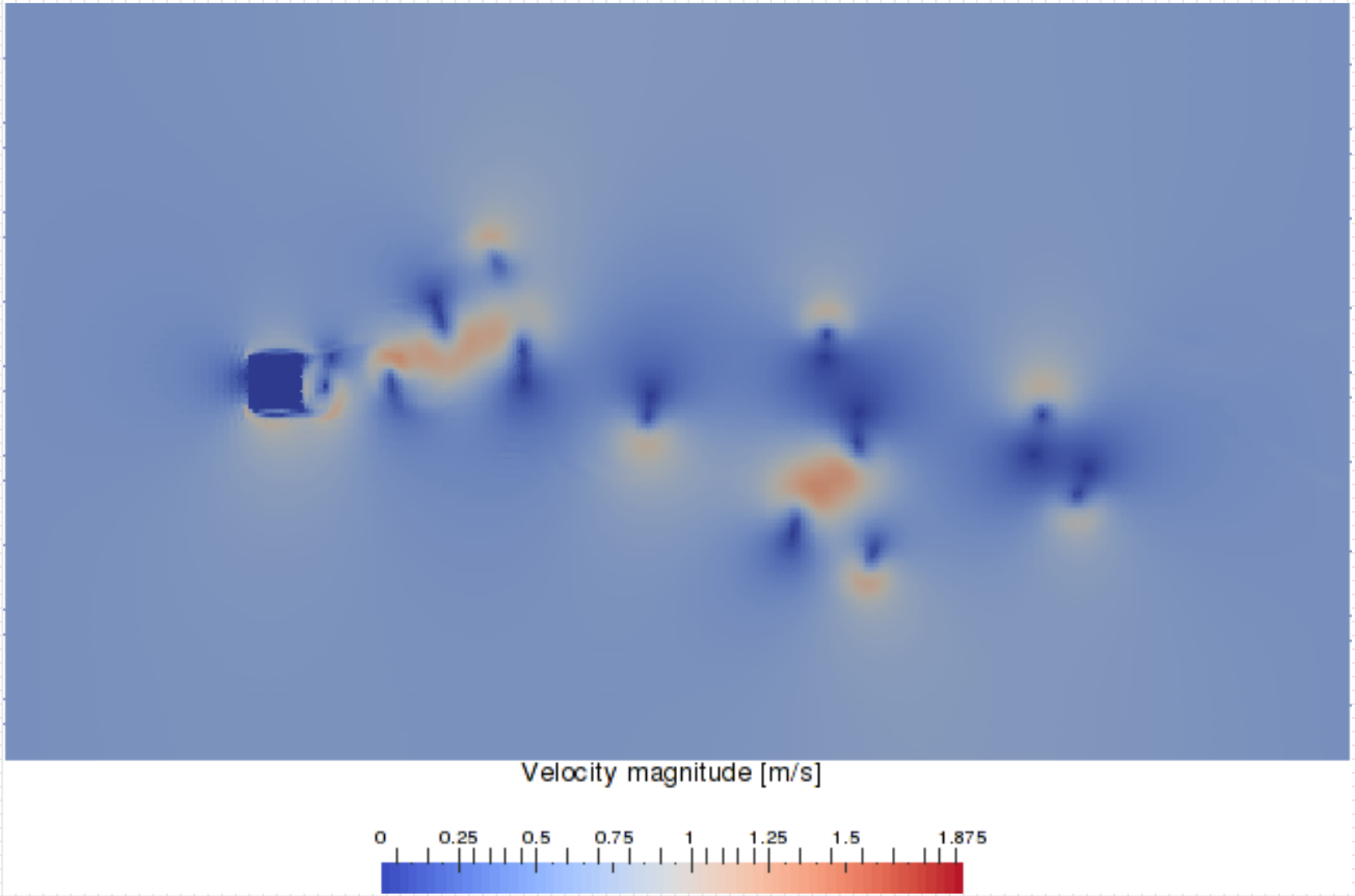

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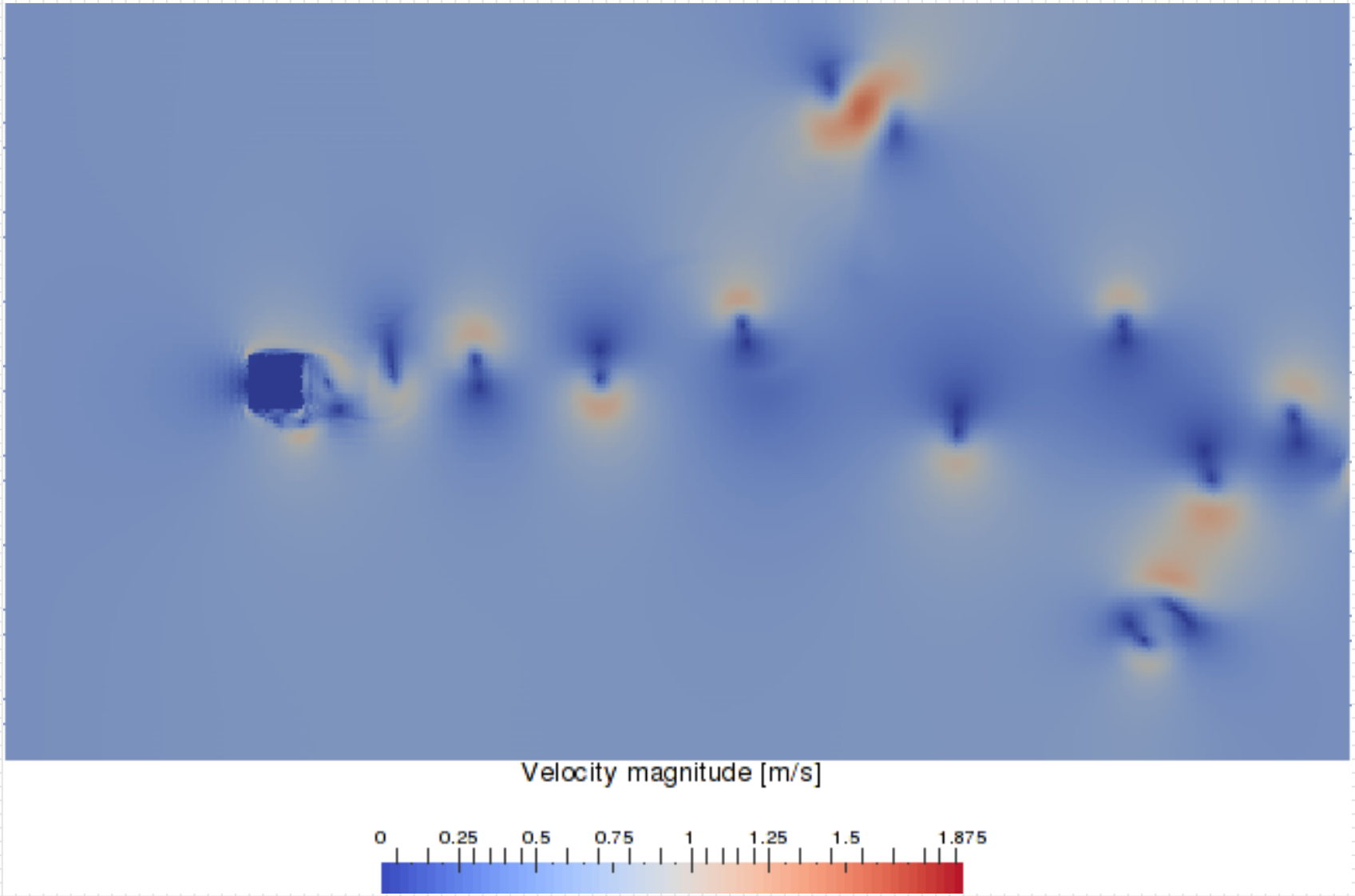

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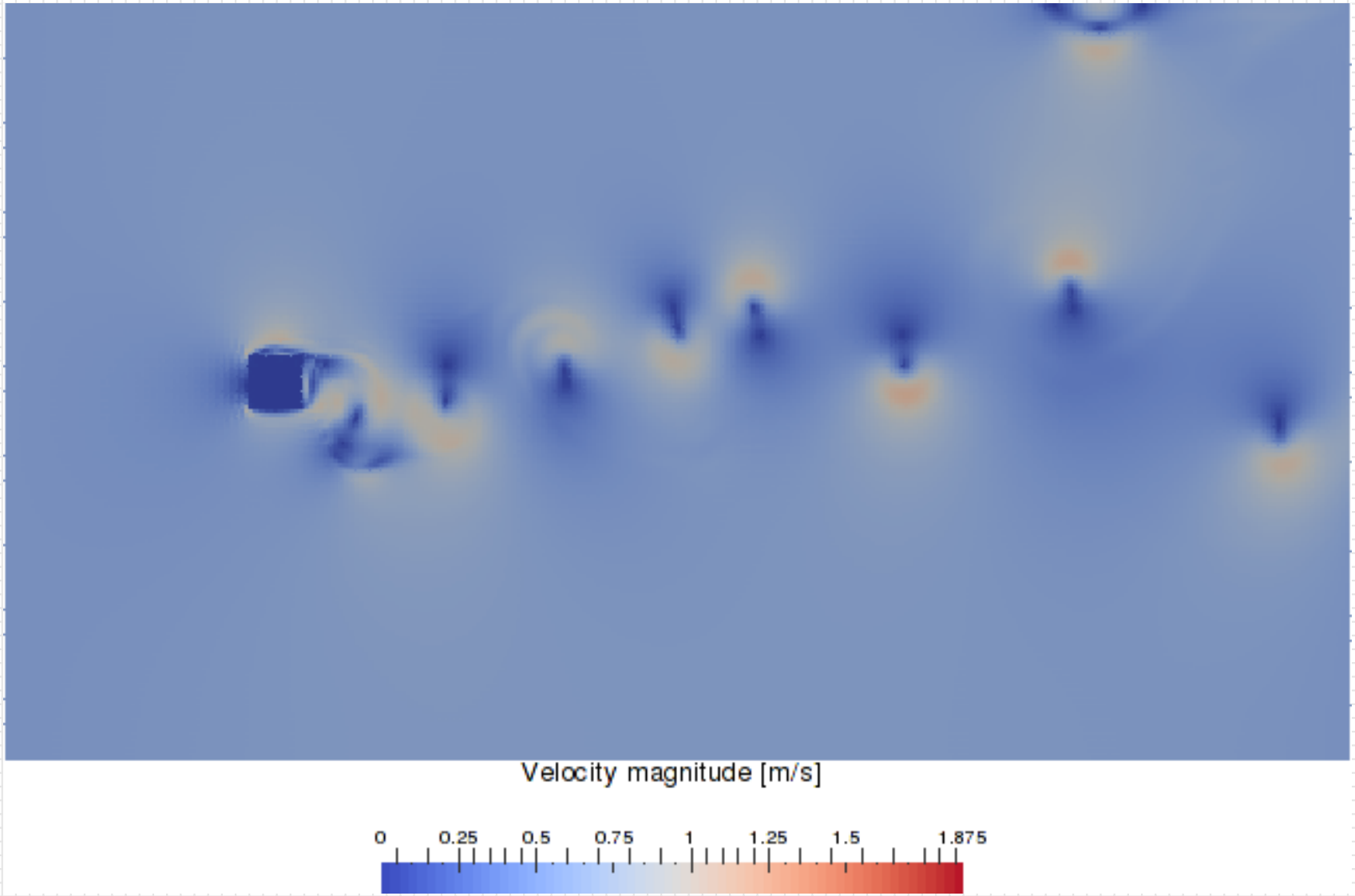

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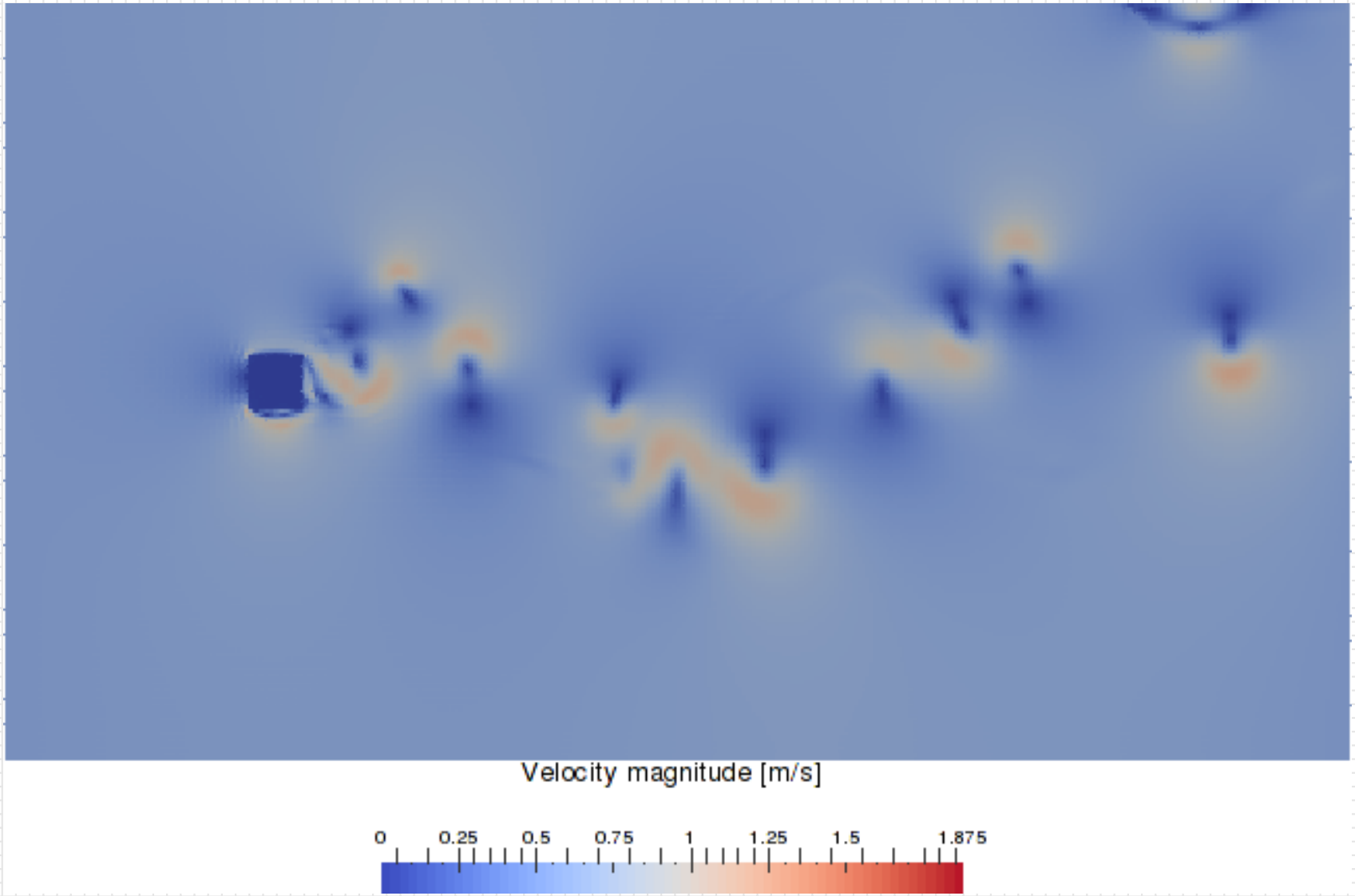

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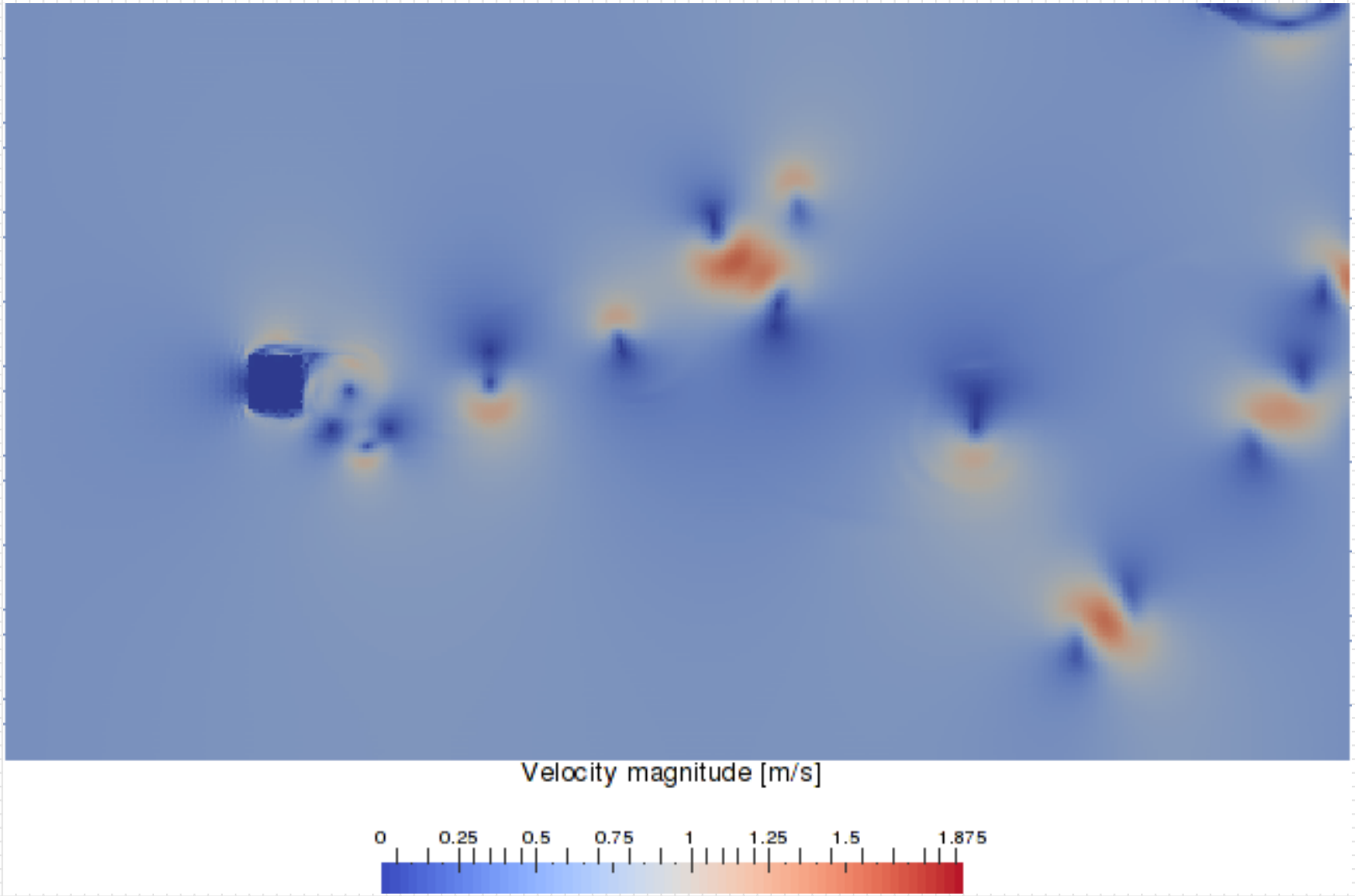

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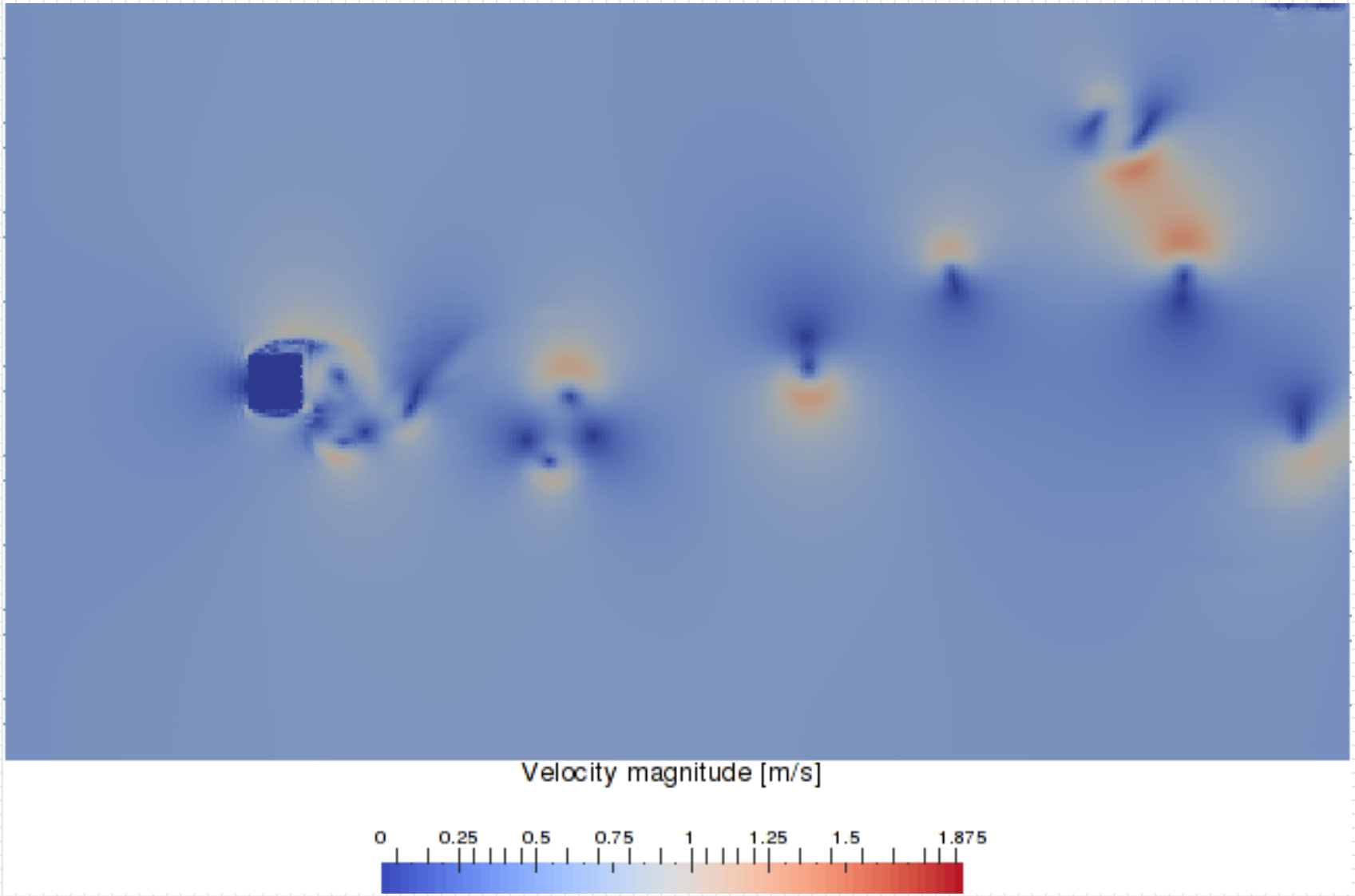

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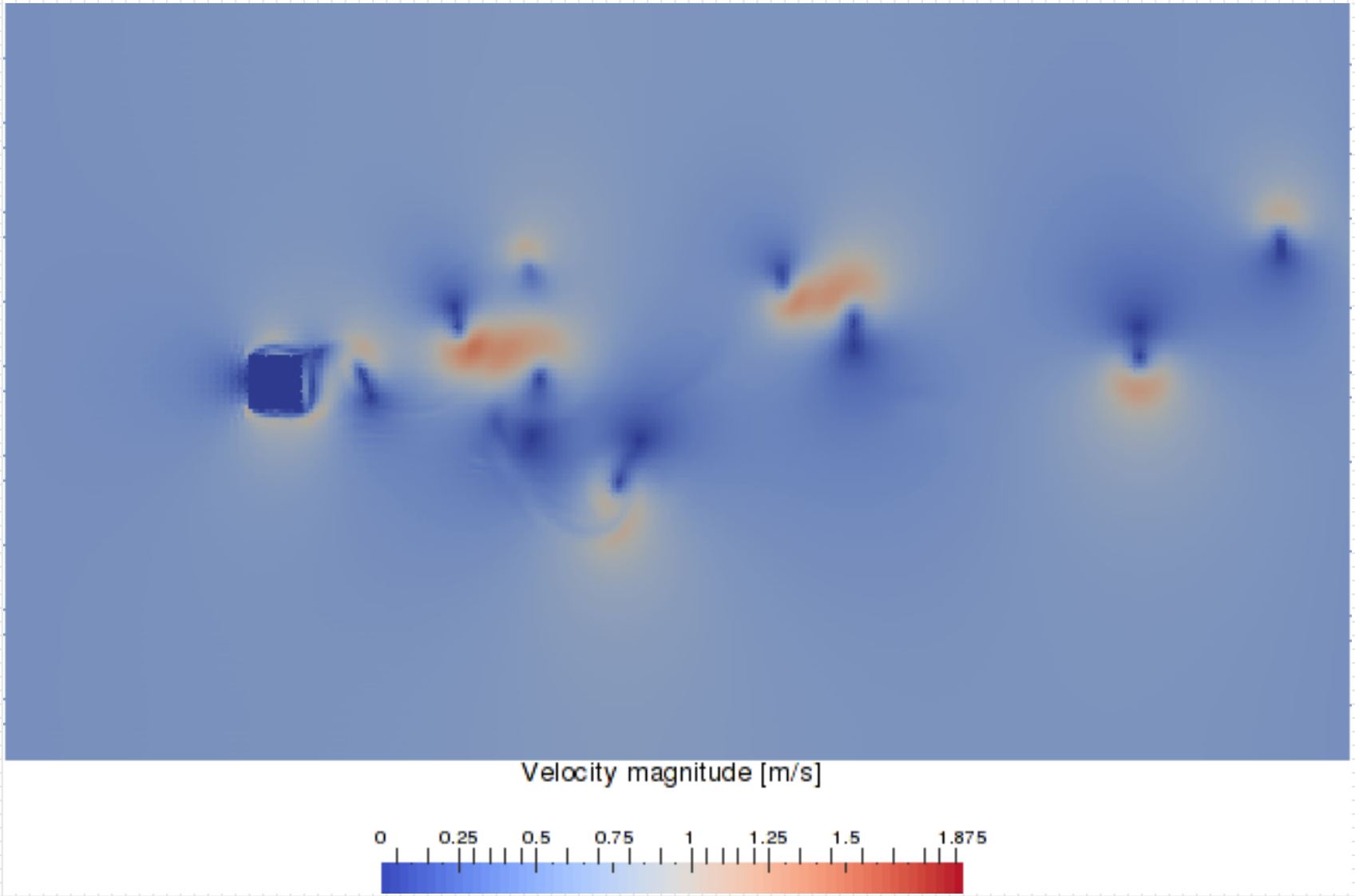

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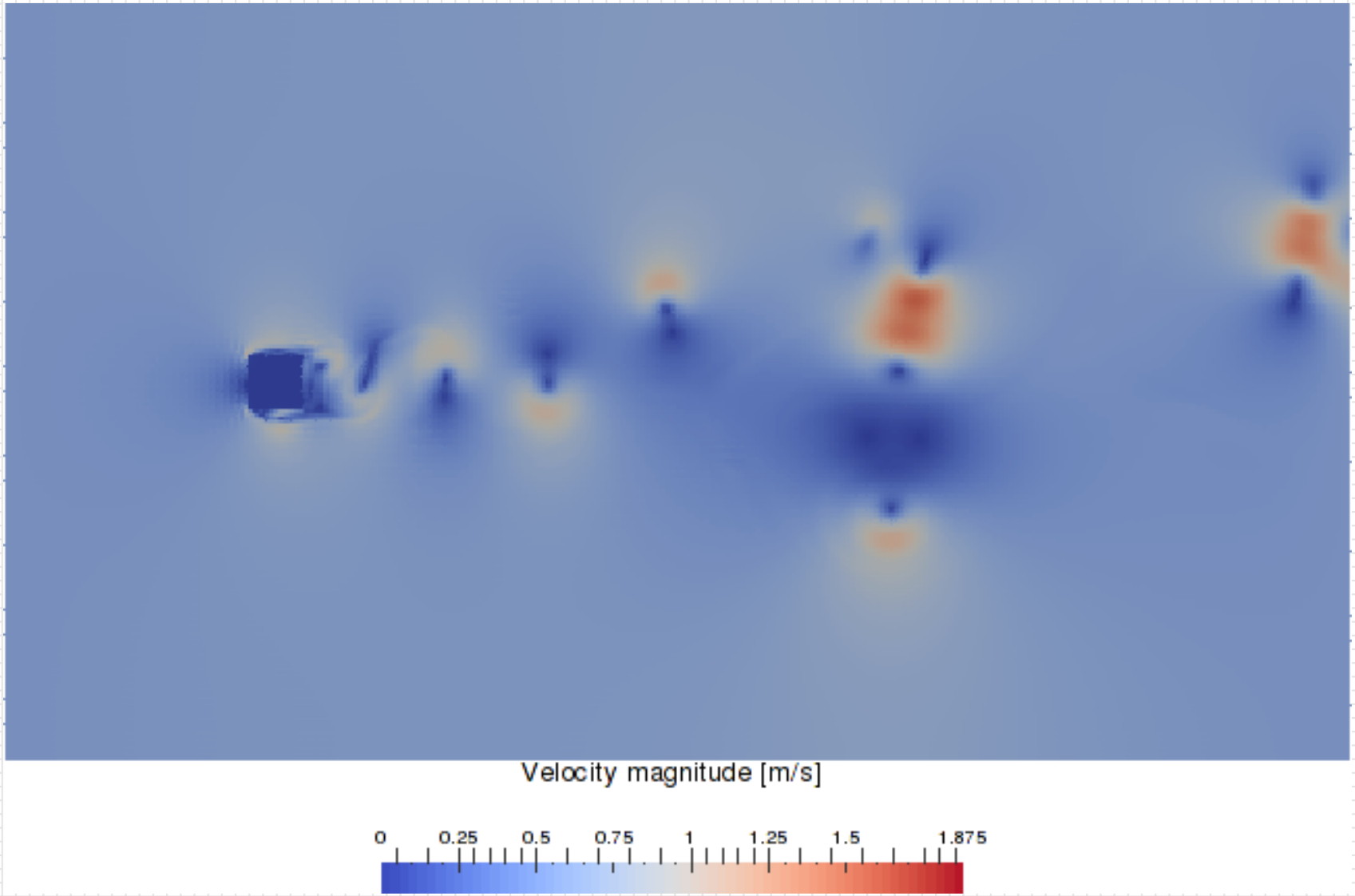

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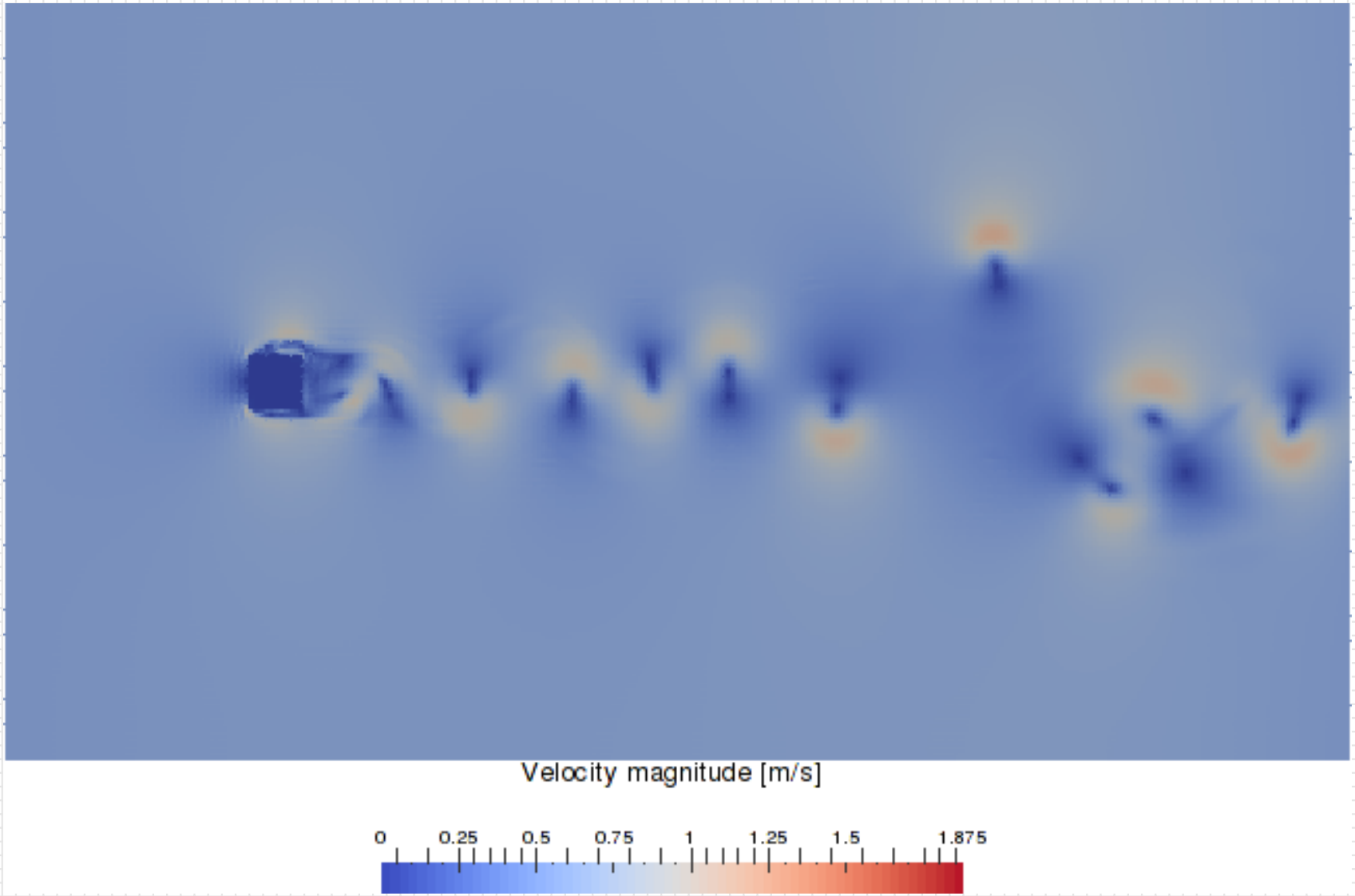

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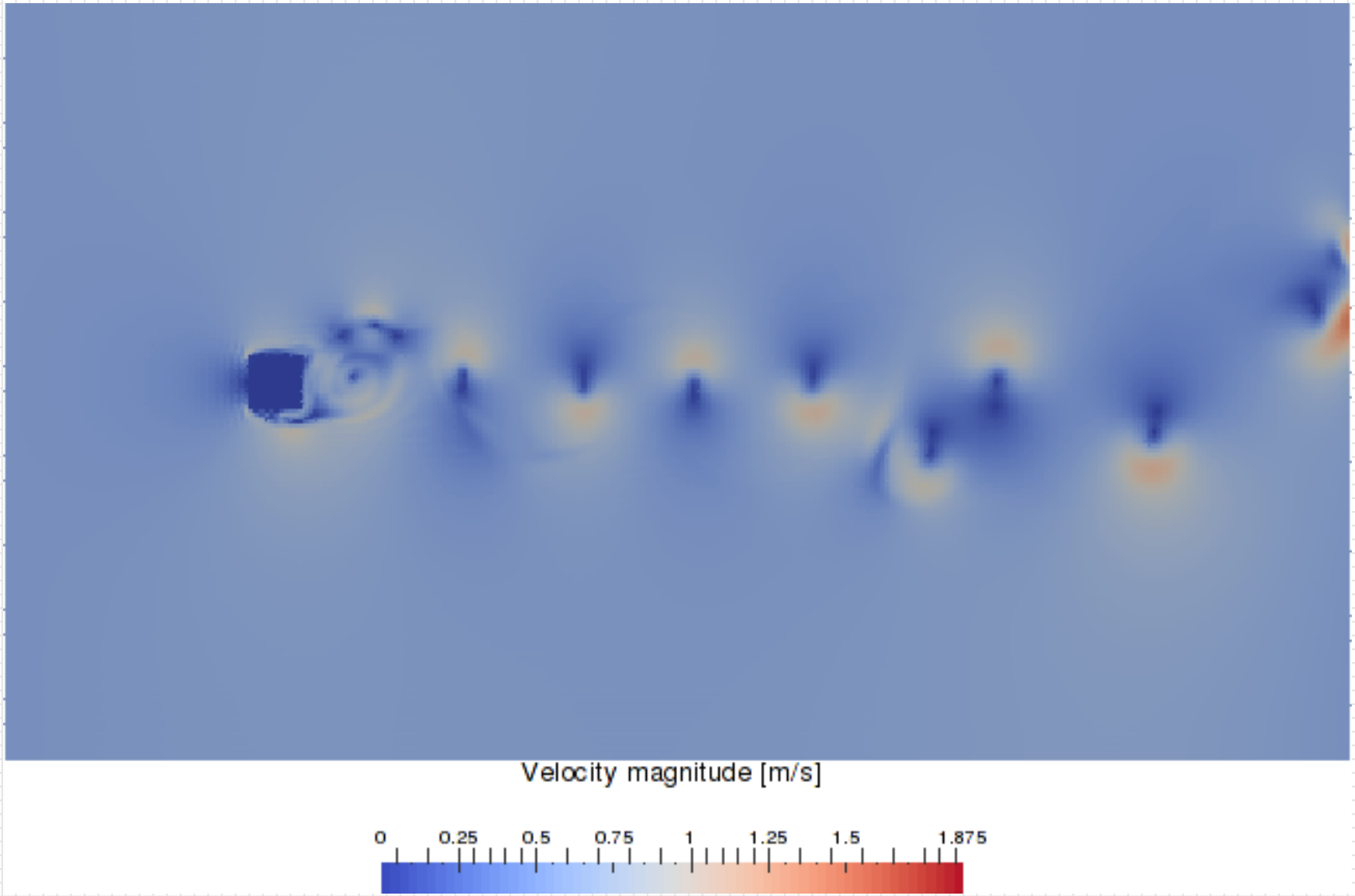

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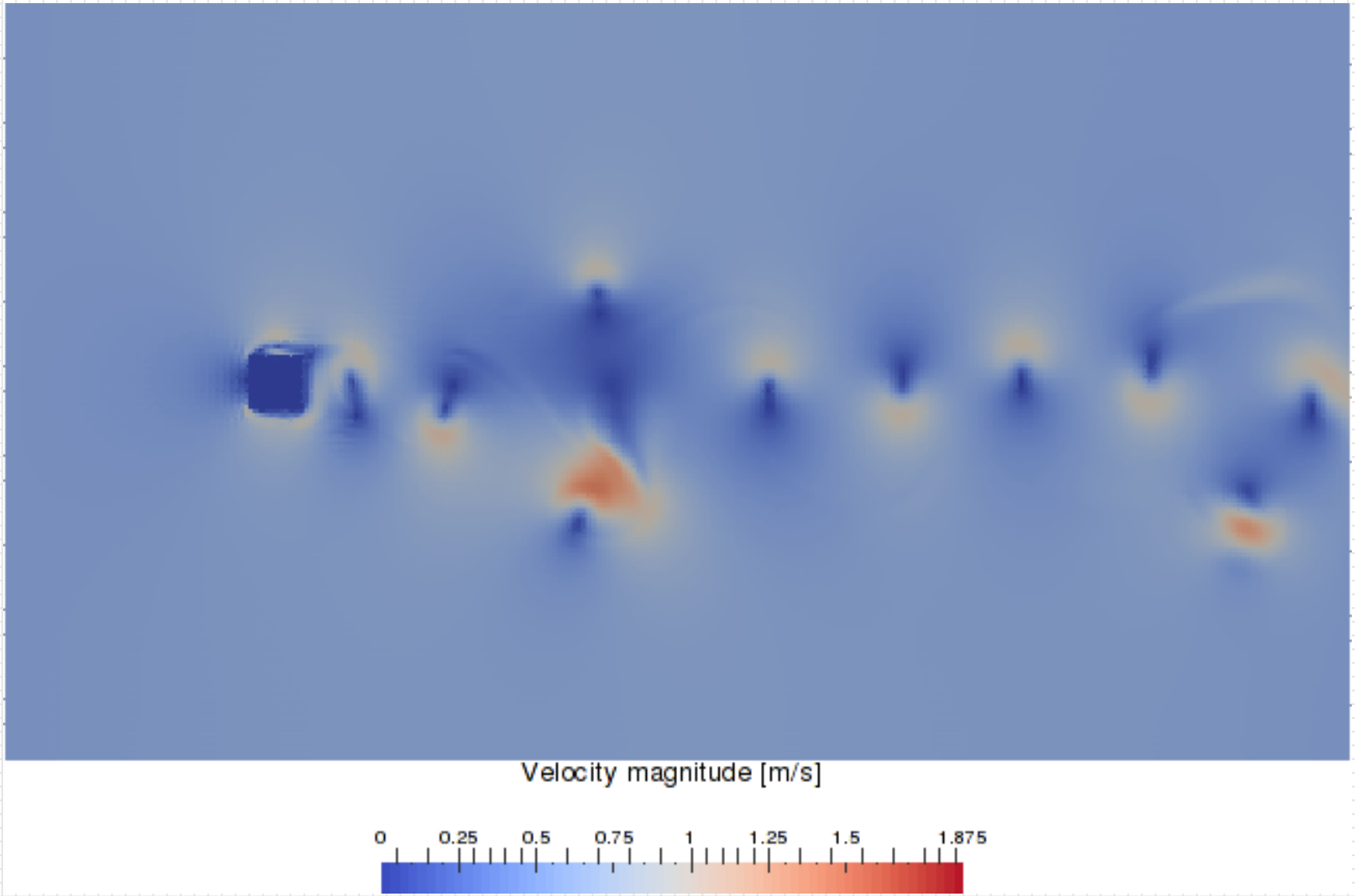

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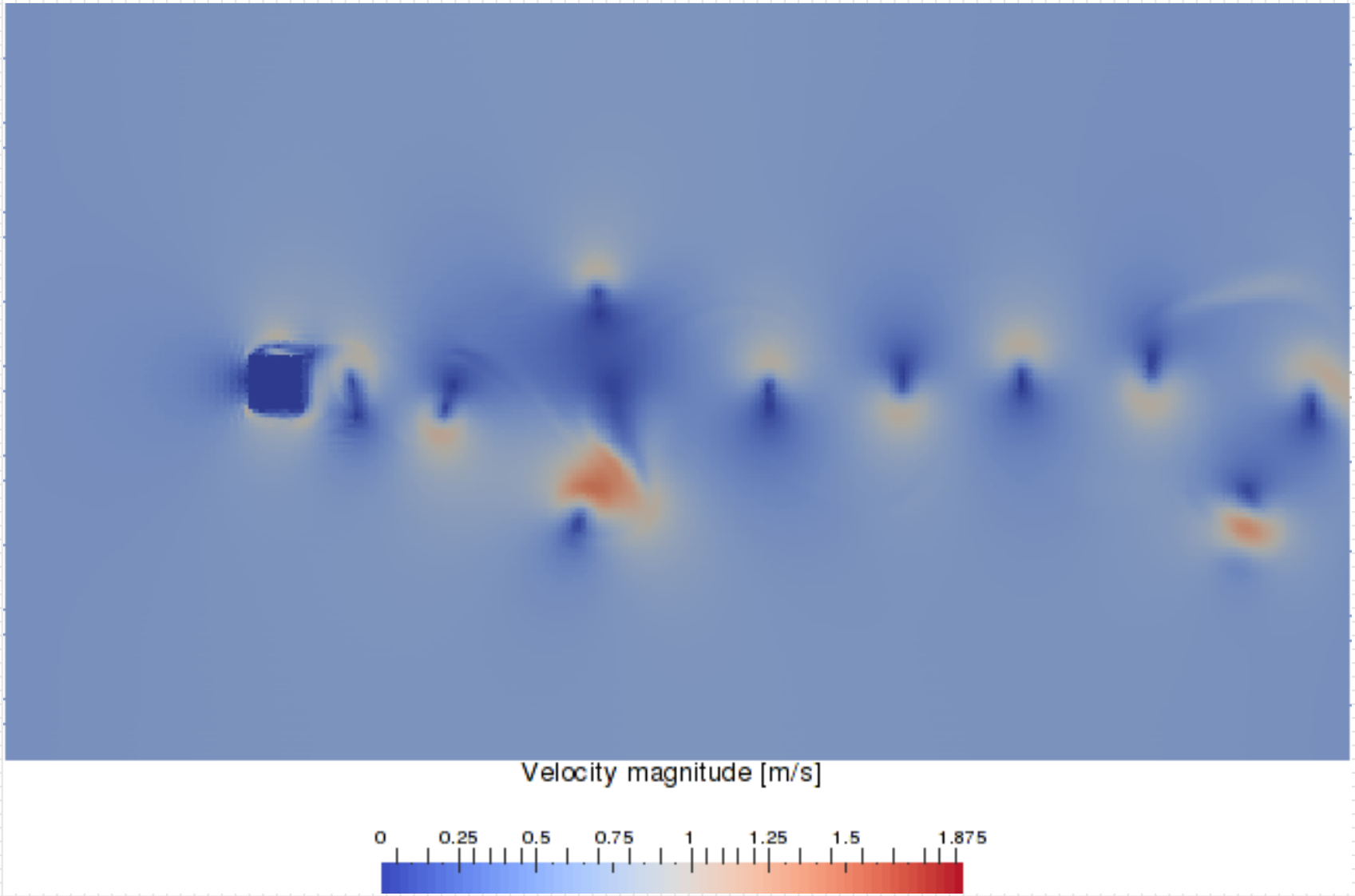

Plan of the talk

1. what's libmpdata++
2. libmpdata++: a hello-world program
3. libmpdata++ 1.0: summary of features
4. libmpdata++ 2.0: new features under development
5. closing remarks

Plan of the talk

libmpdata++: some design choices

legal

- license: GPL
- repo: github.com/igfuw/

library components

- solvers/algorithms
- boundary conditions
- output handlers
- shared-memory concurrency
- distributed-memory concurrency

dependencies

- Blitz++
- Boost
- CMake, CTest
- MPI
- NetCDF

API

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- repo: github.com/igfuw/

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