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

Sylwester Arabas, Anna Jaruga, Maciej Waruszewski

Atmospheric Physics Seminar
Faculty of Physics, University of Warsaw, Poland

Warsaw, October 23, 2015

Plan of the talk

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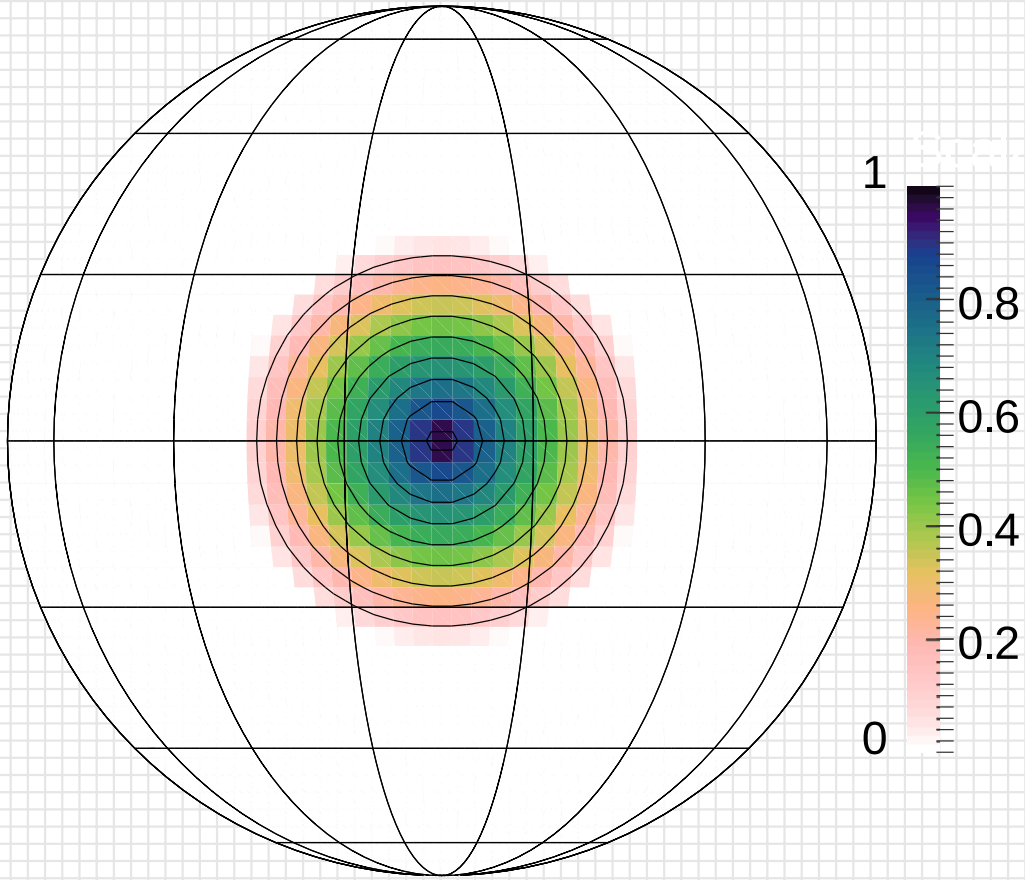

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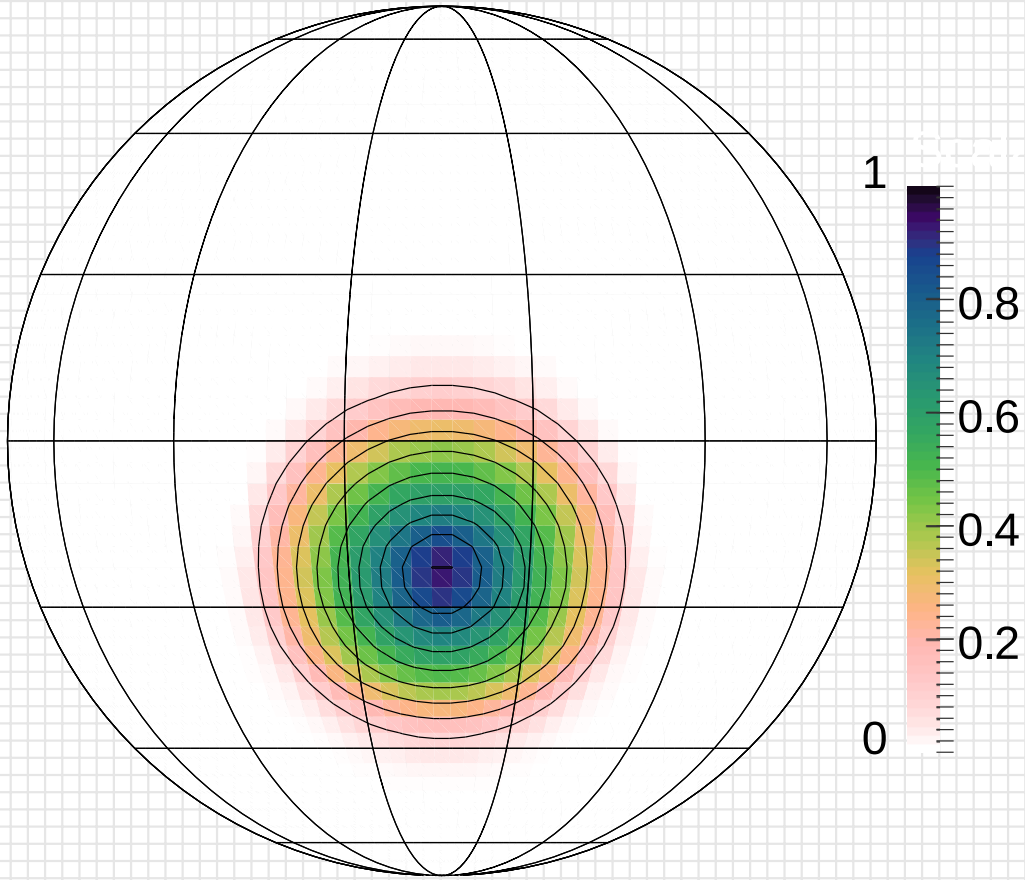

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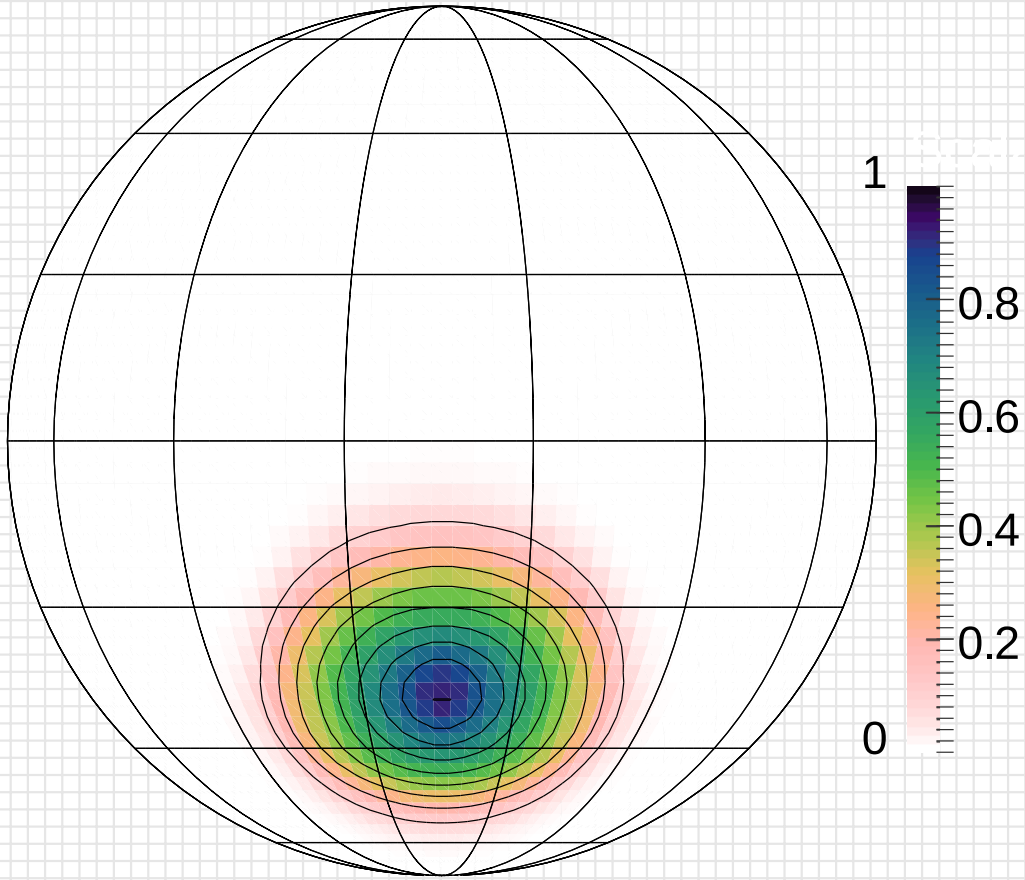

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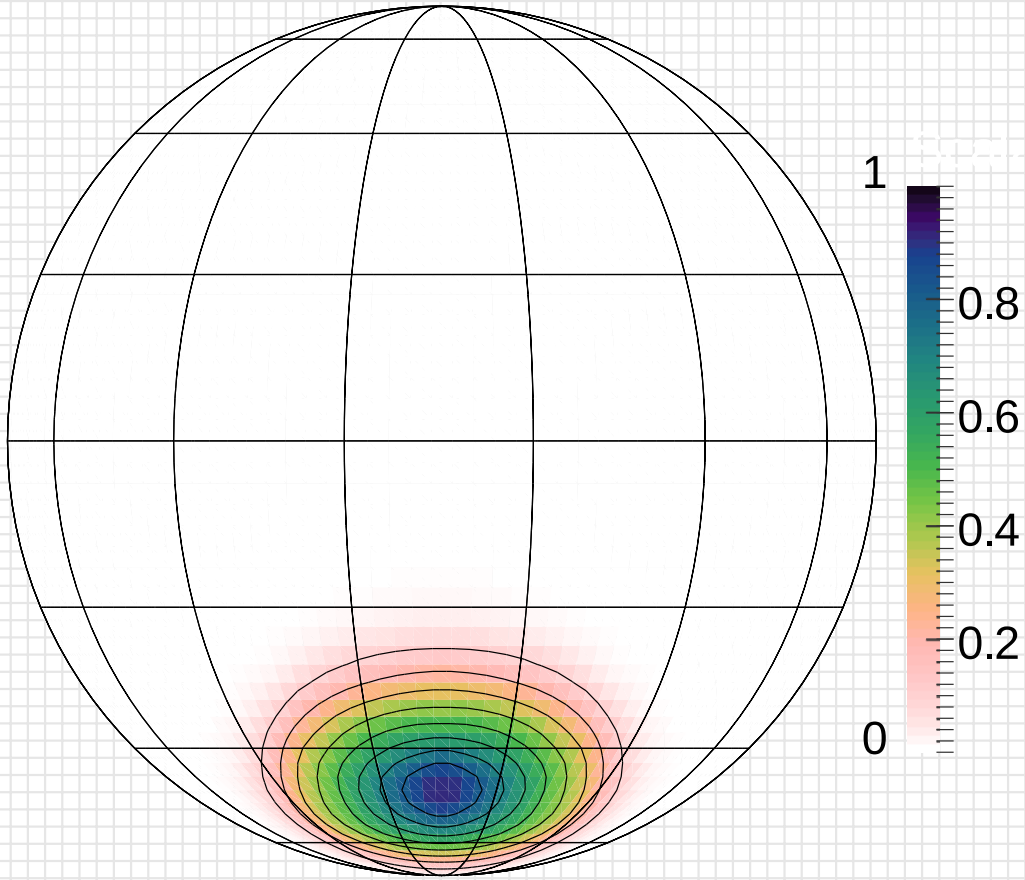

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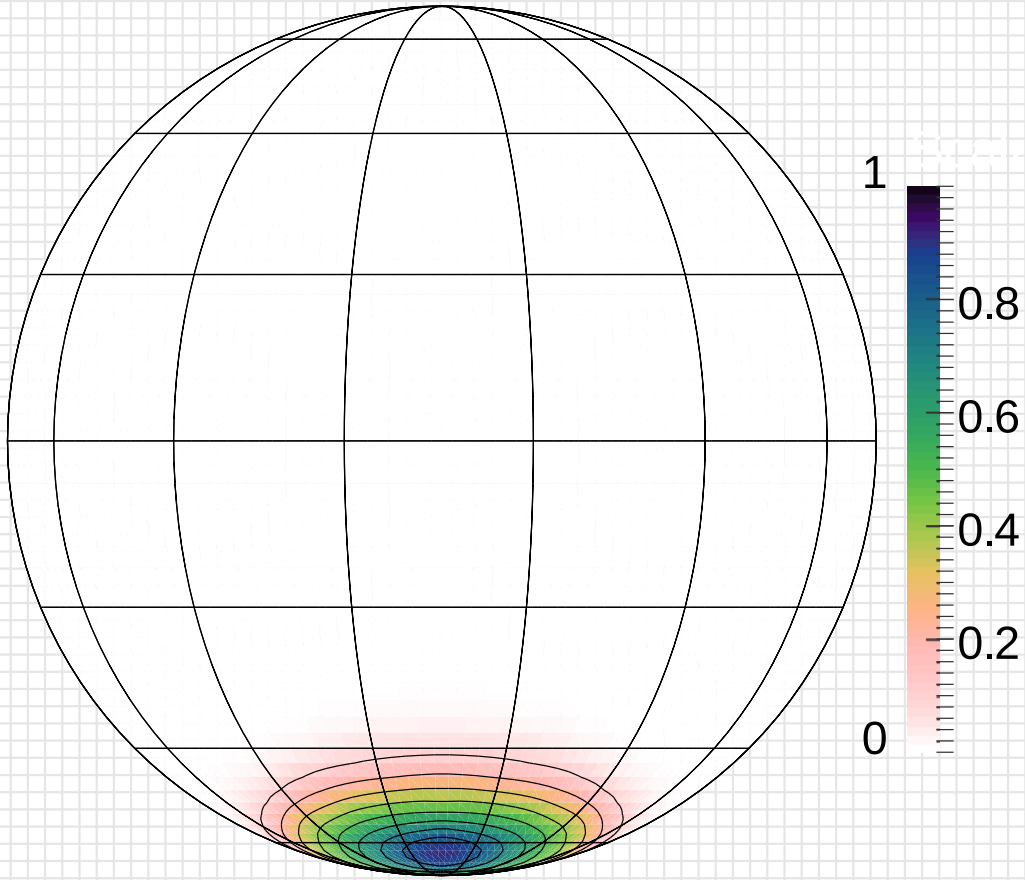

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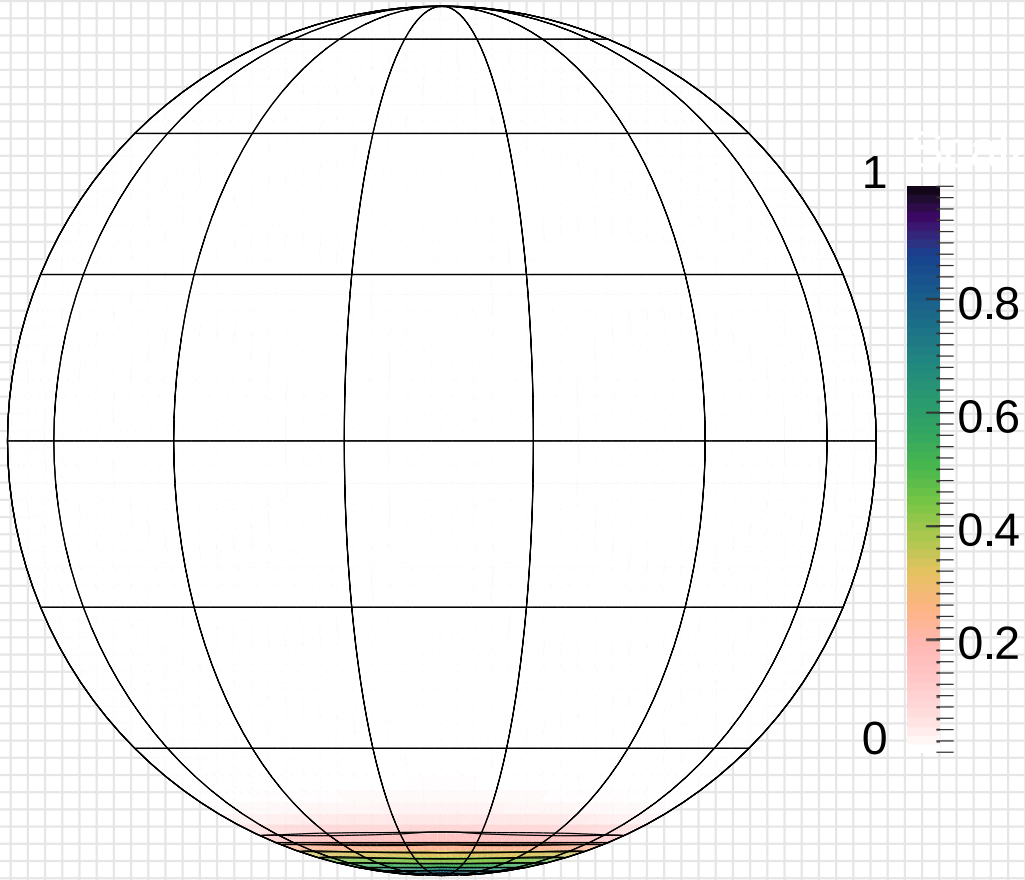

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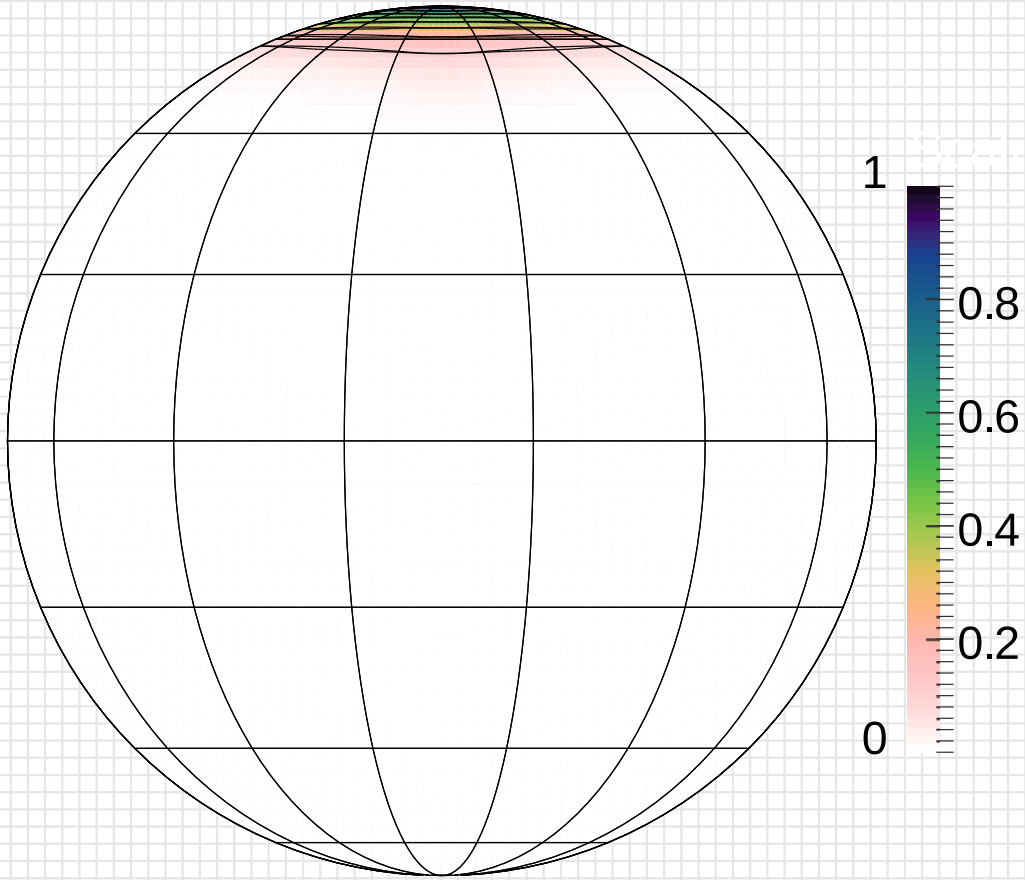

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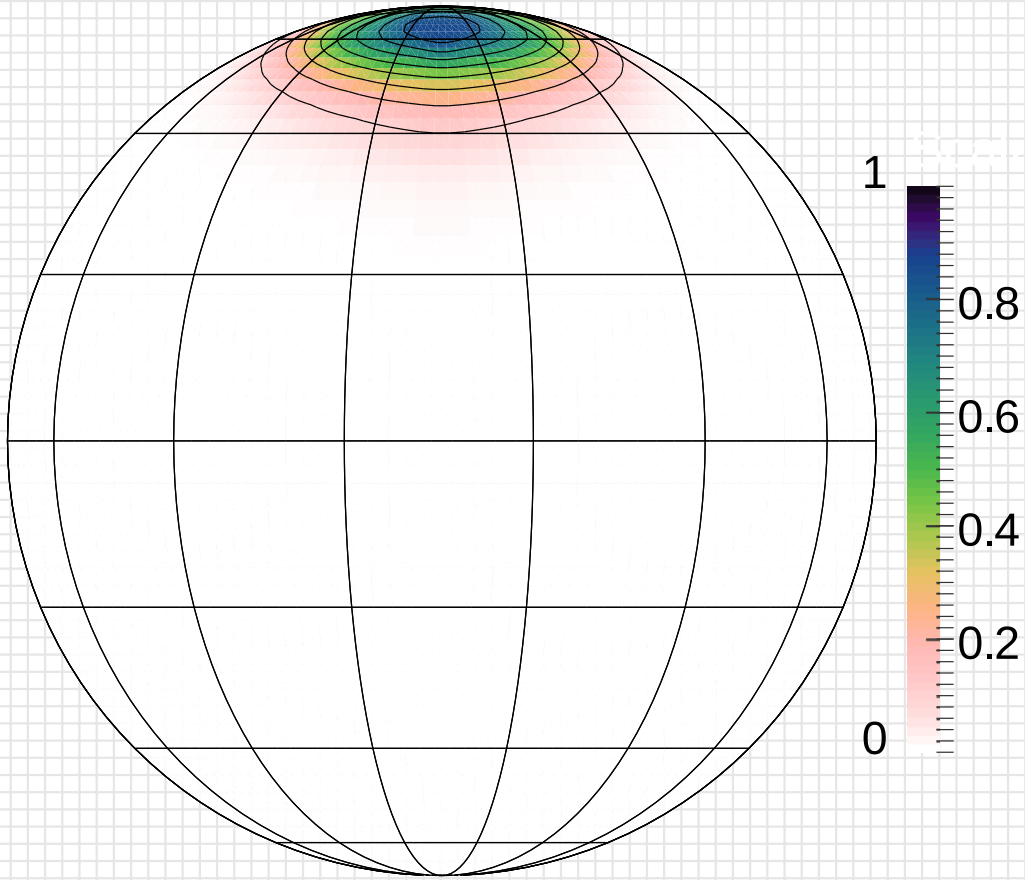

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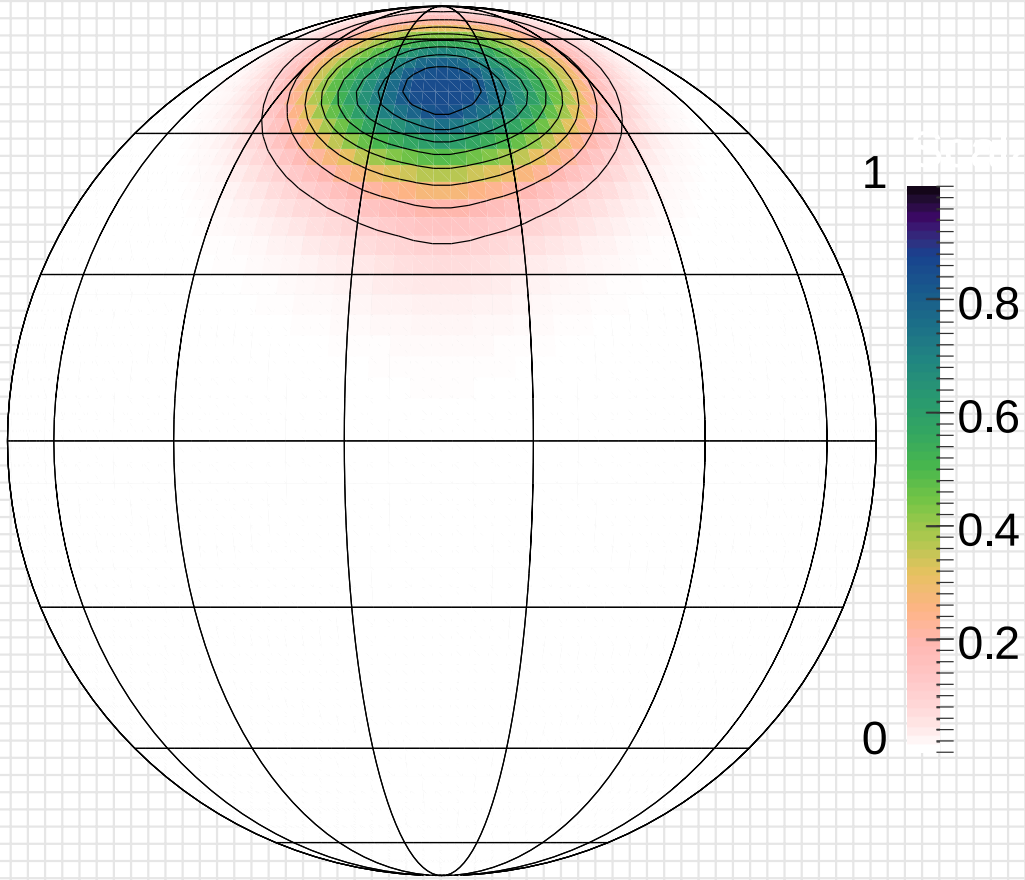

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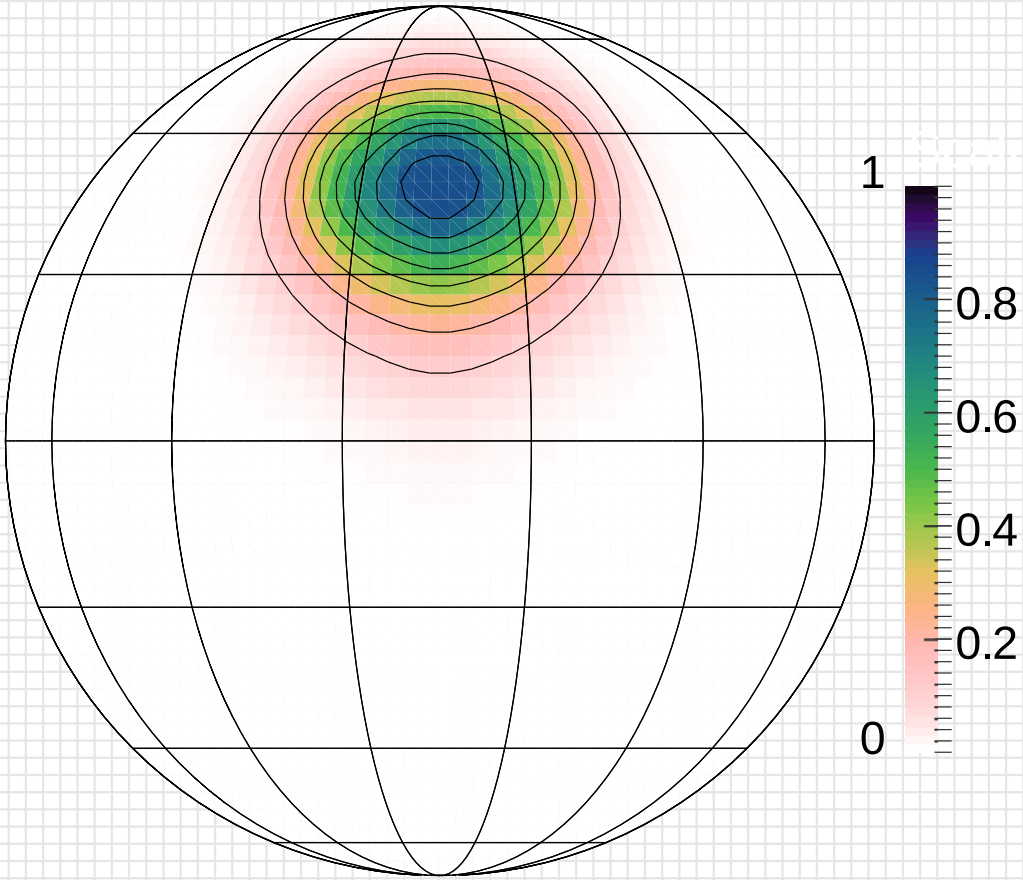

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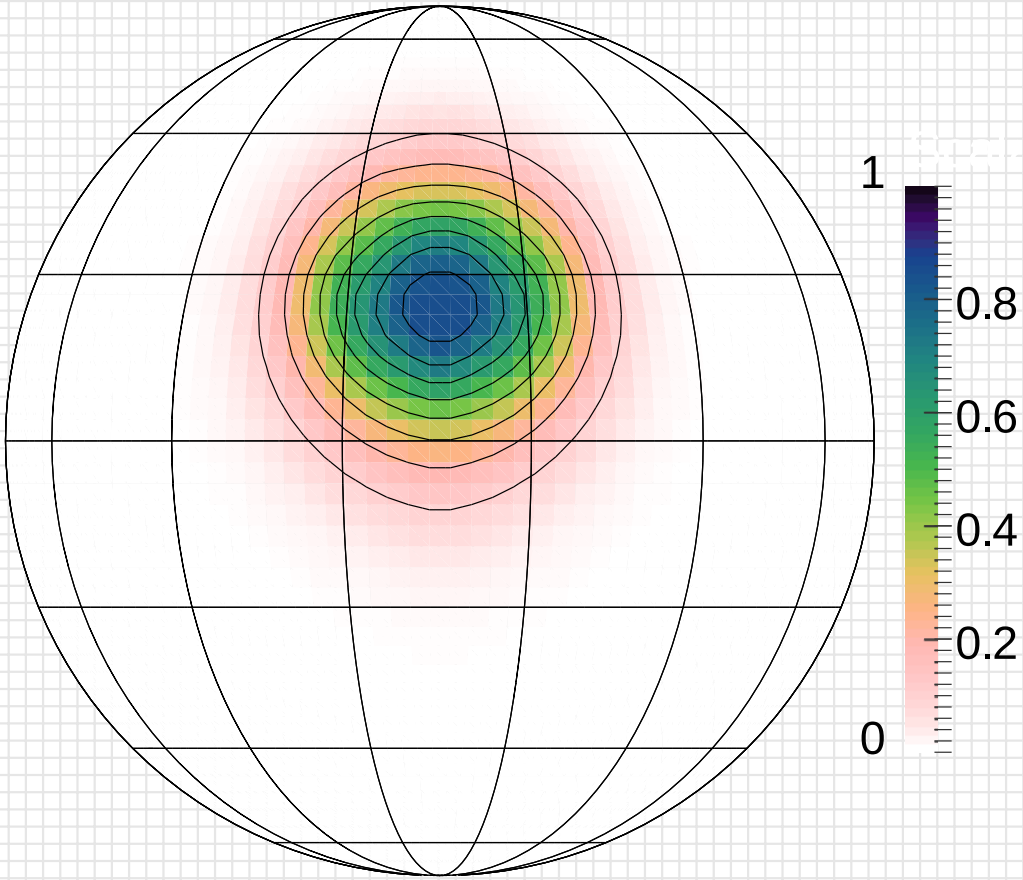

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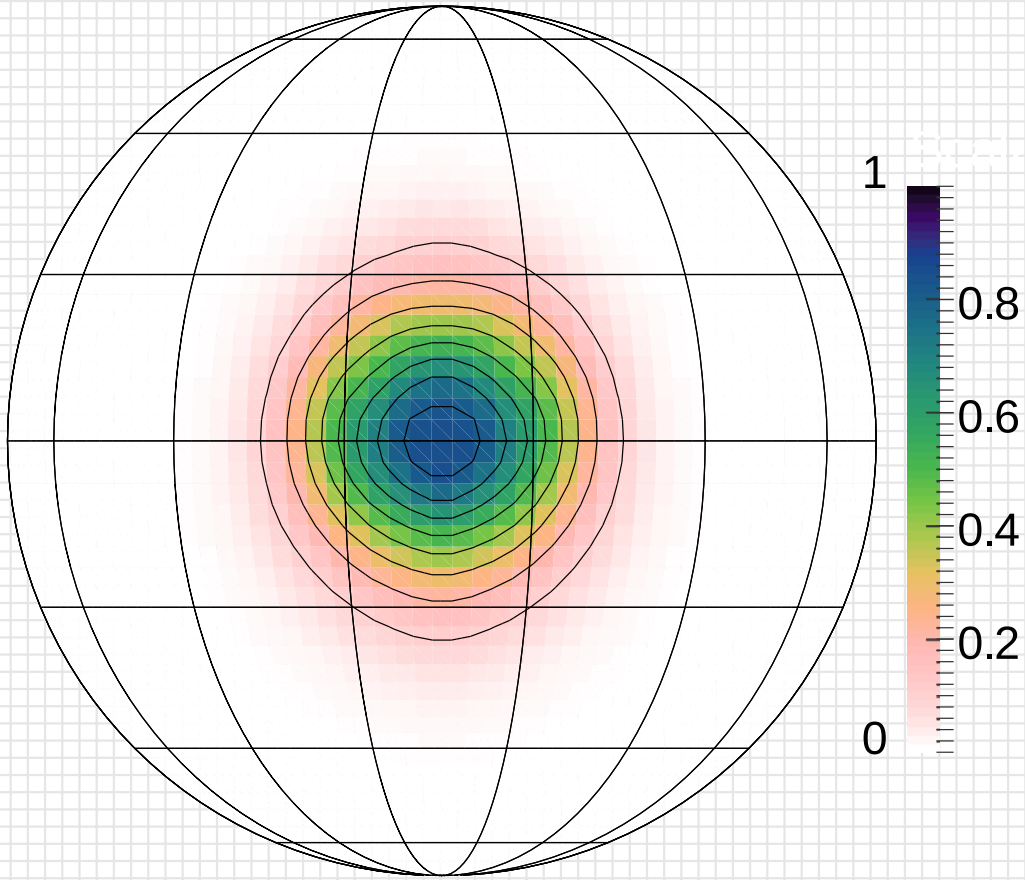

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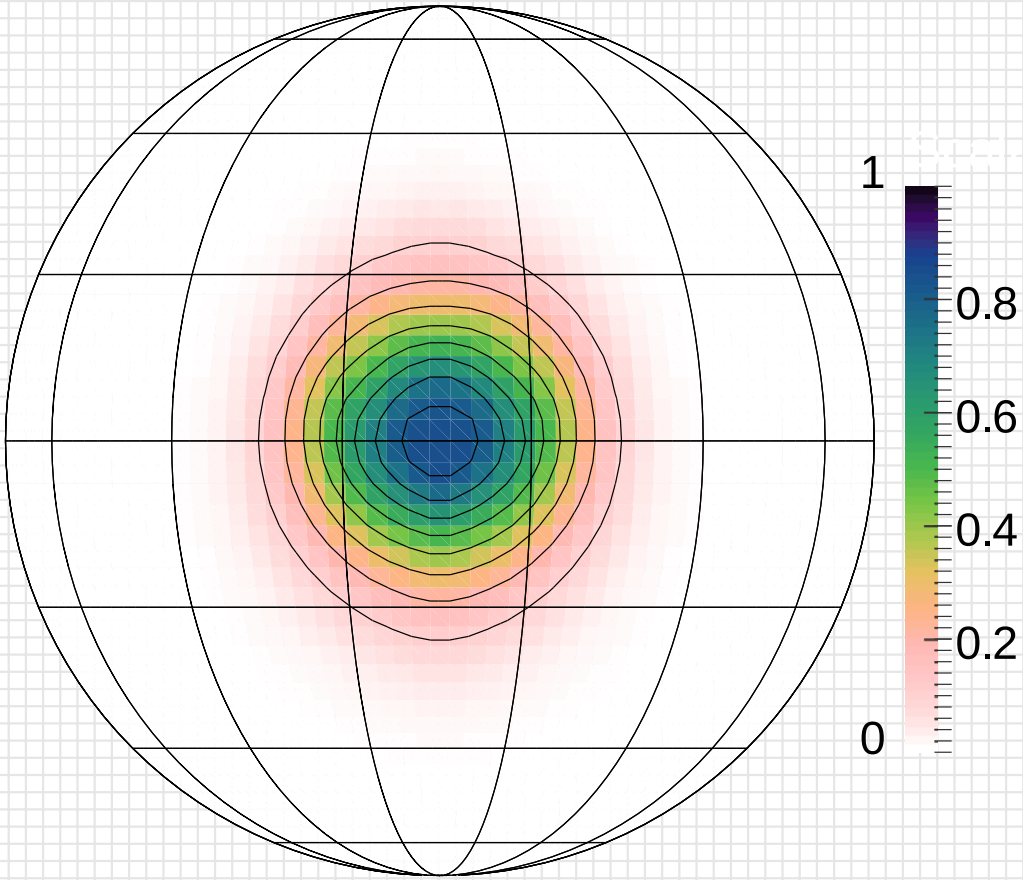

numerical integration using MPDATA

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

features compared with the original F77 implementation:

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

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libmpdata++: aims & design patterns

priority: researchers' productivity

researcher = user

- **ease of obtaining and using**
  ⇝ public repository, documentation, examples
- **result correctness**
  ⇝ multifaceted peer-reviewed automated tests
- **result reproducibility**
  ⇝ atomic versions, no legal nor tech. obstacles

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- **ease of extending**
  ⇝ concise OOP syntax, separation of concerns, automated tests, continuous integration

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Geosci. Model Dev., 8, 1005–1032, 2015
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Geoscientific Model Development
Open Access

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

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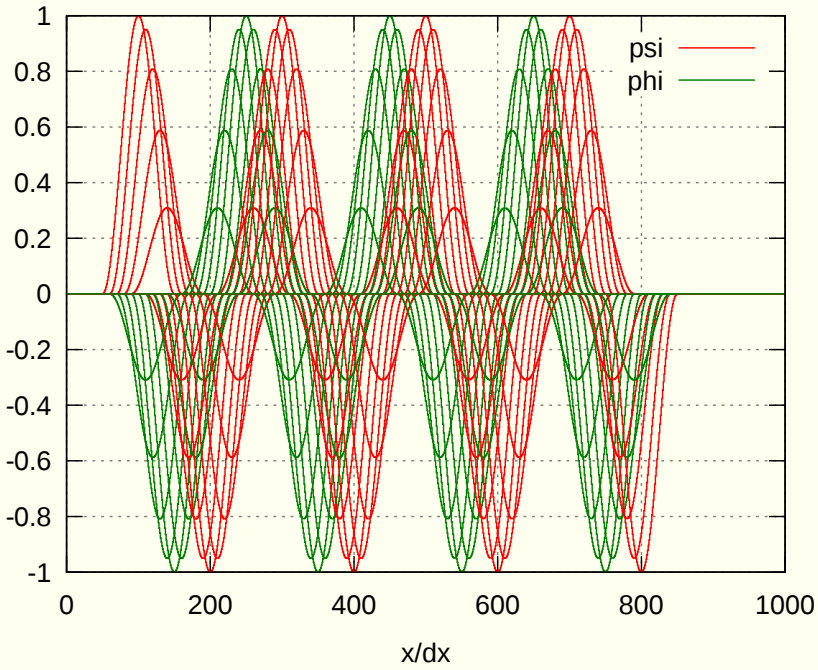

Figure 15. Simulation results of the example presented in Sect. 4.3. Abscissa marks the spatial dimension and ordinate represents the oscillator amplitude. The oscillator state is plotted every 20 time steps.

(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);
```

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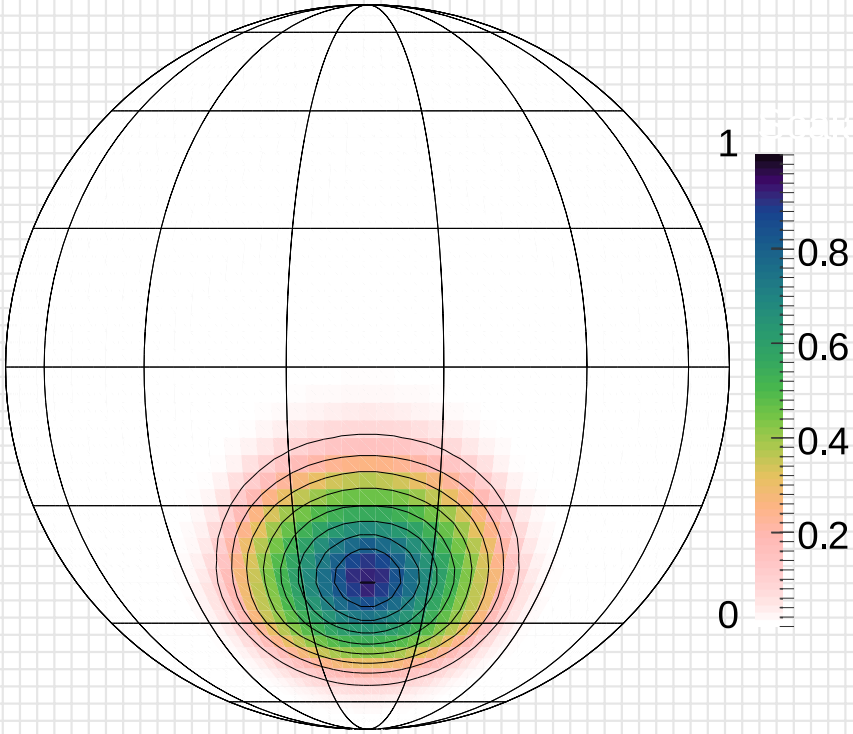
user/test code



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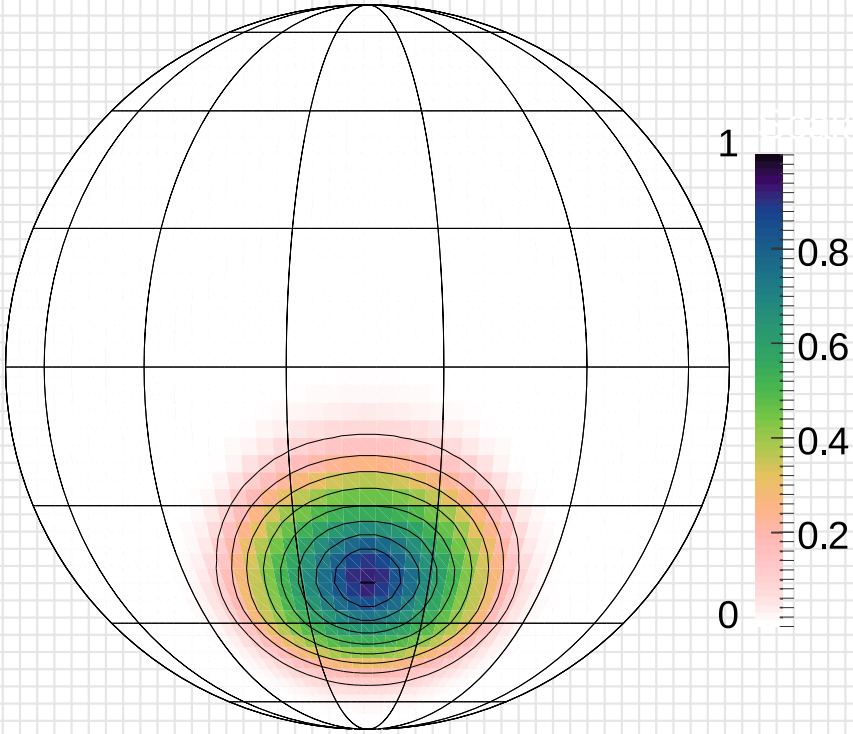

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source terms

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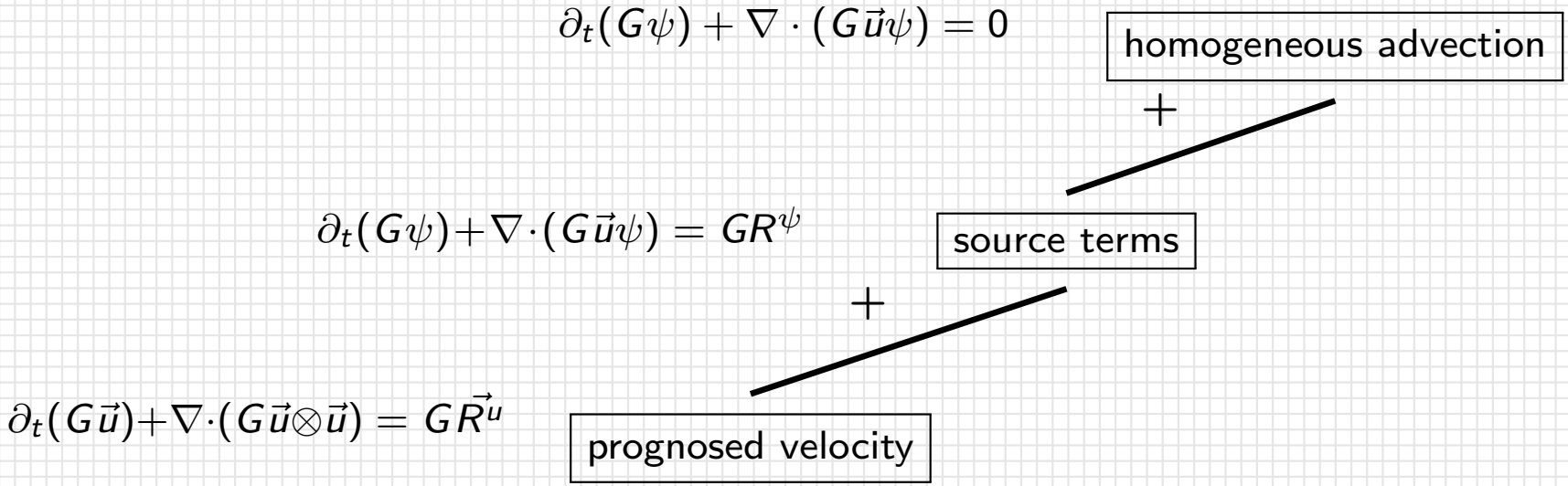

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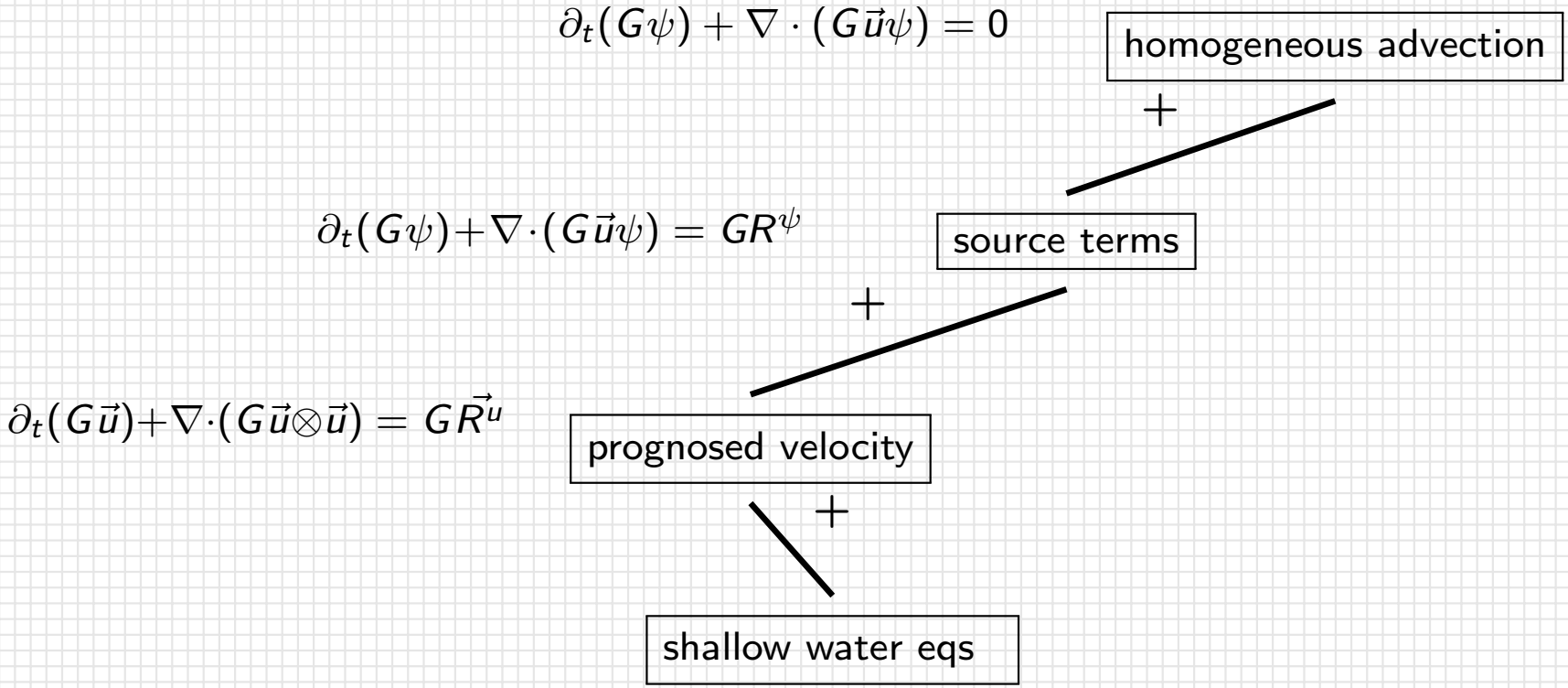

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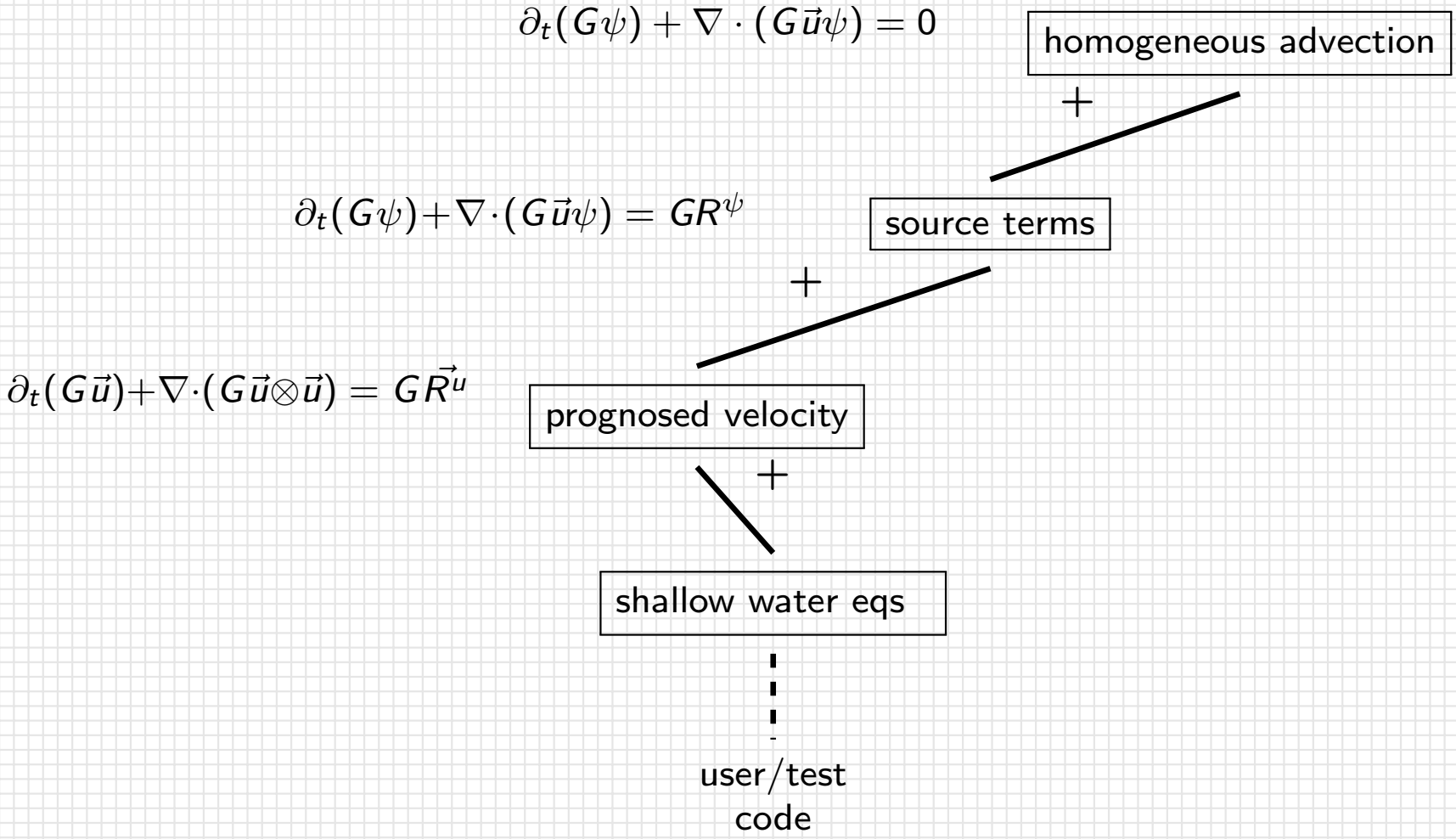
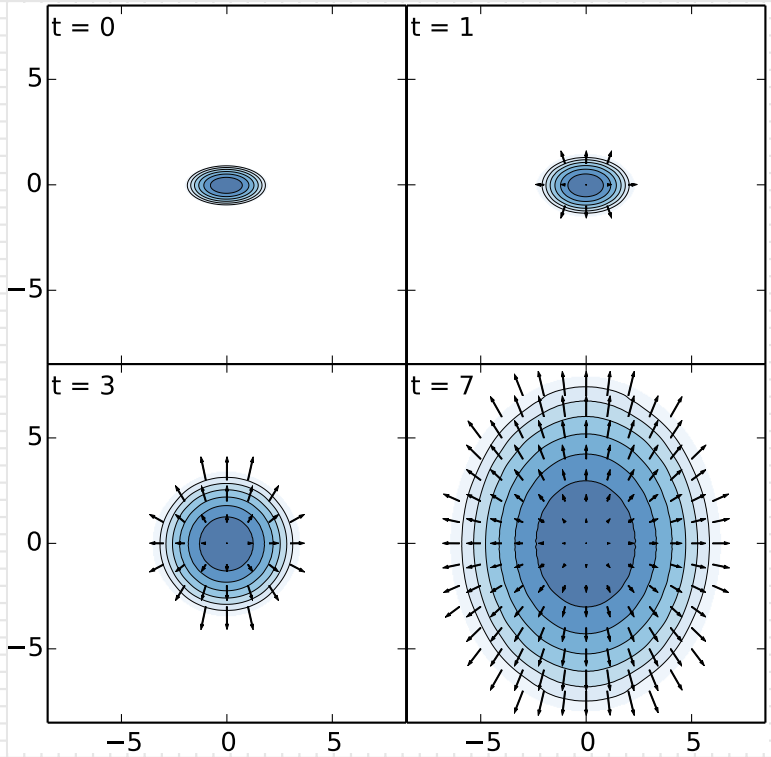


libmpdata++: 3D shallow-water system example



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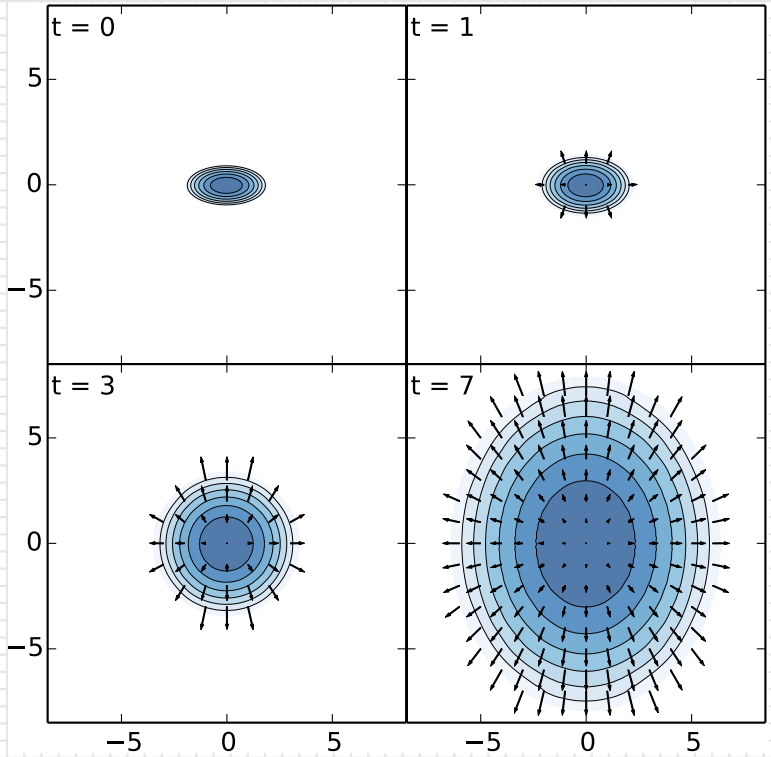

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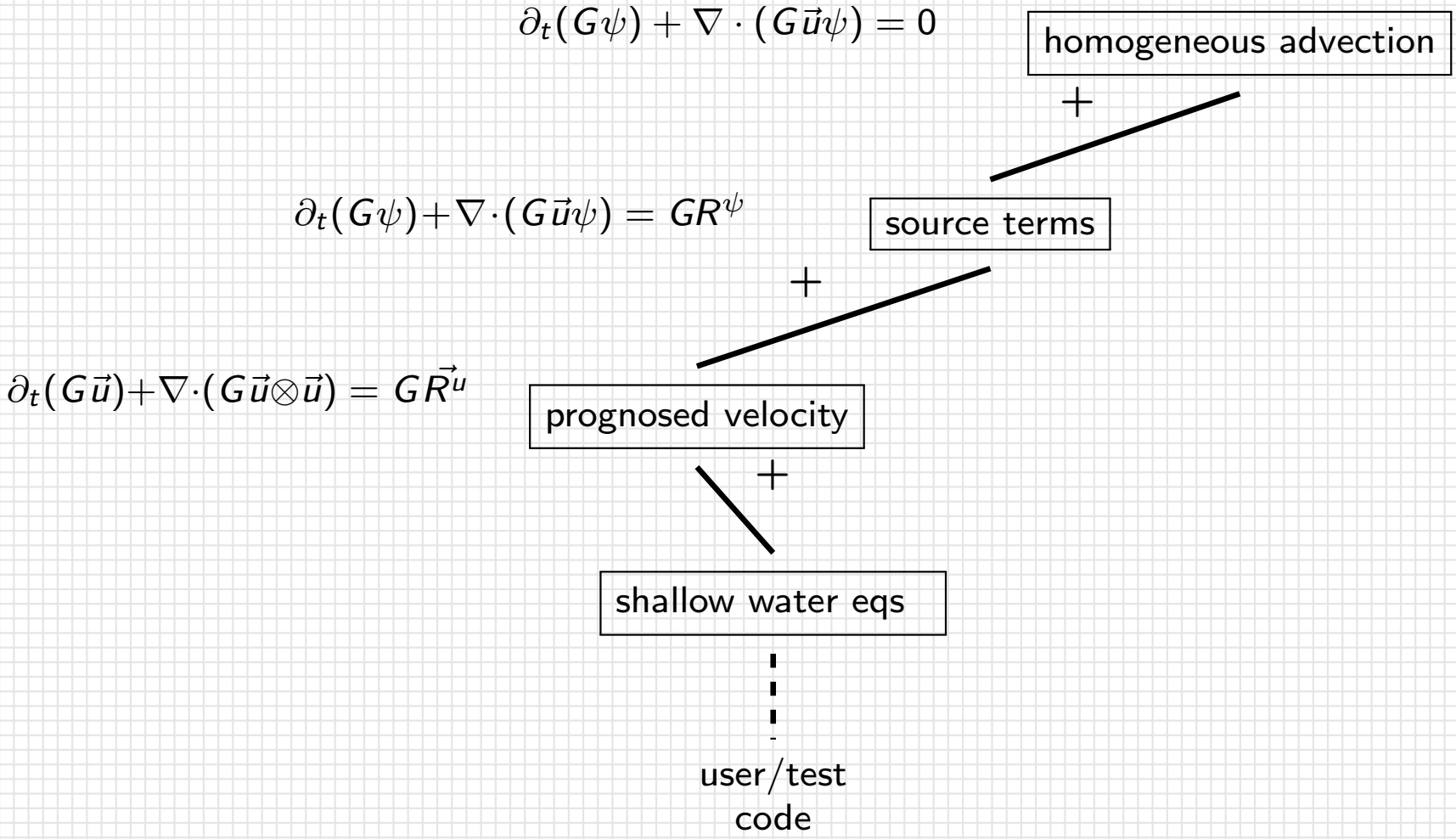

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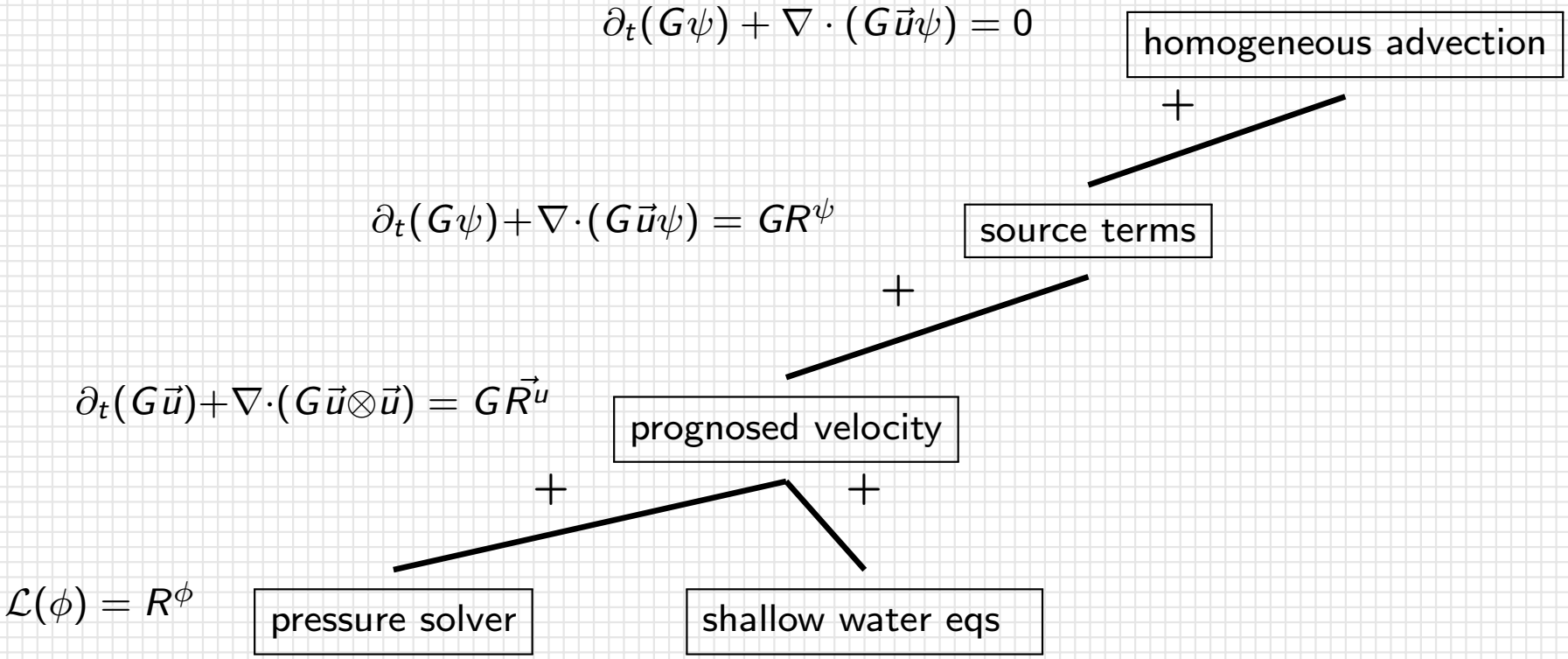

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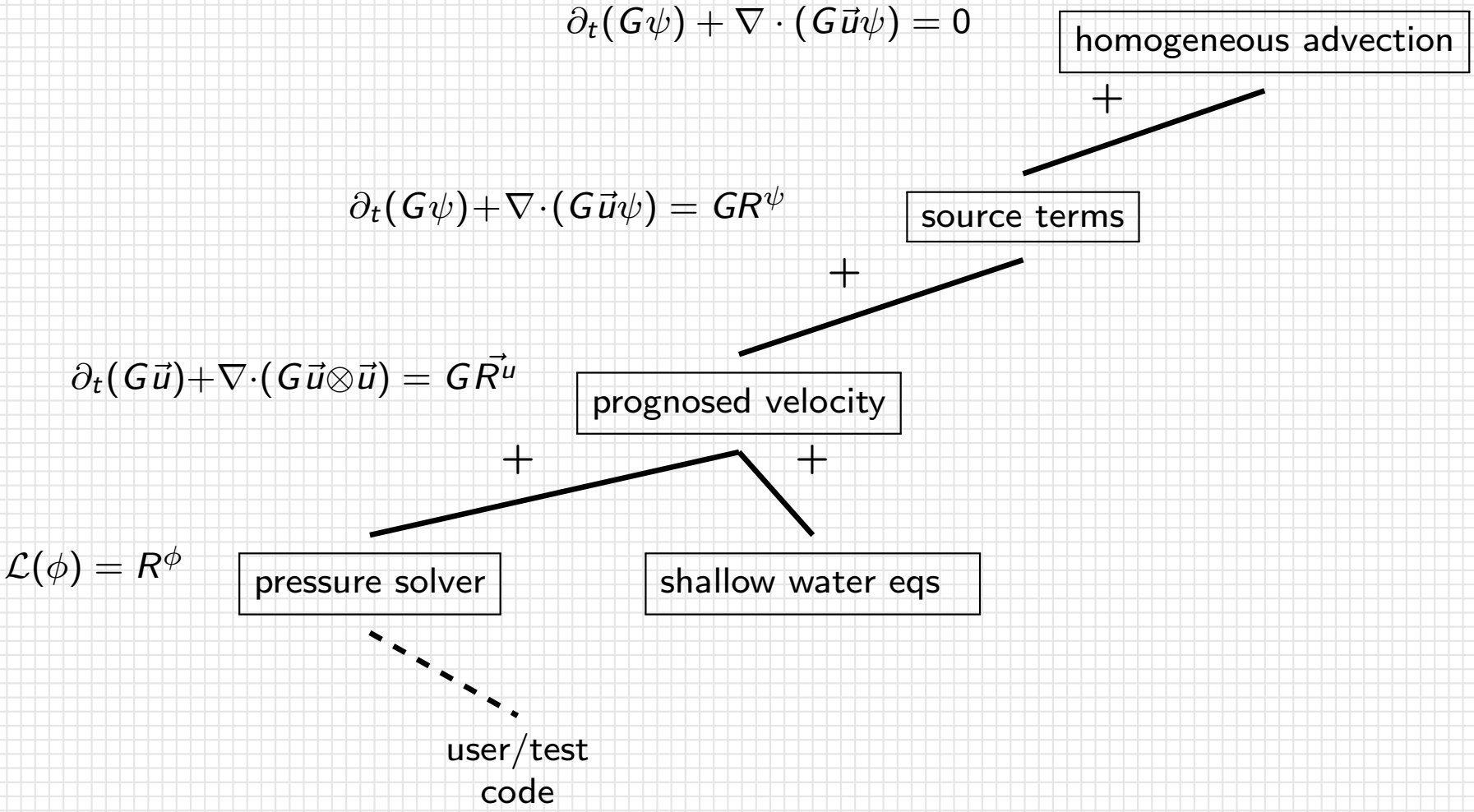

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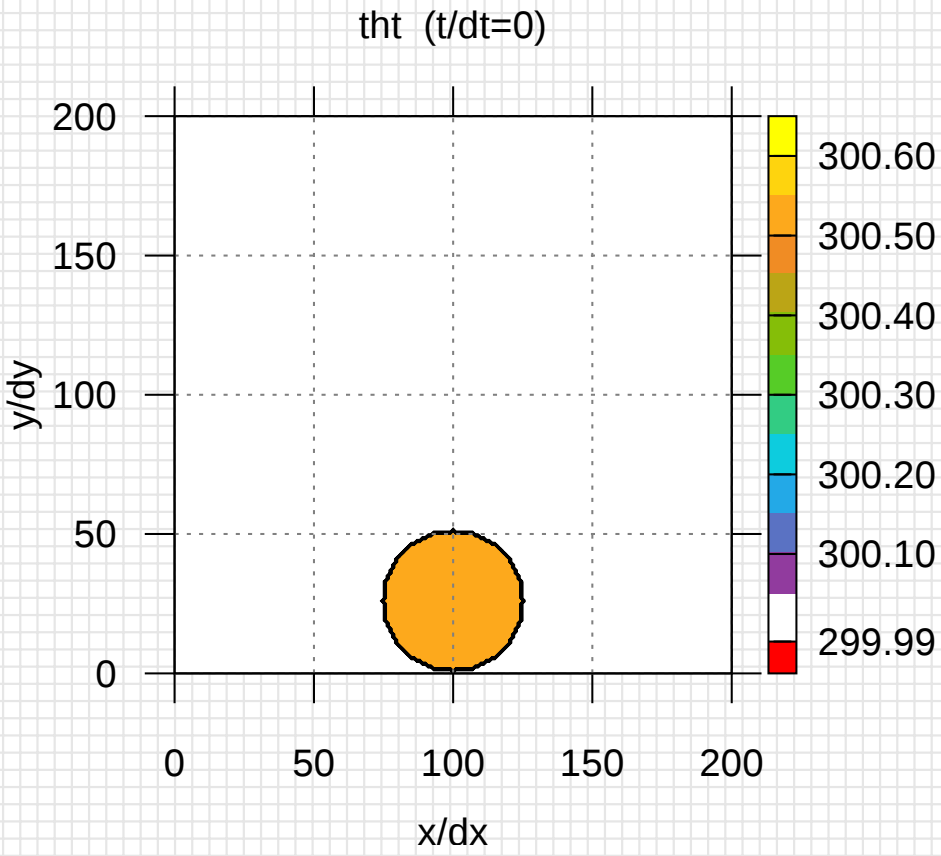

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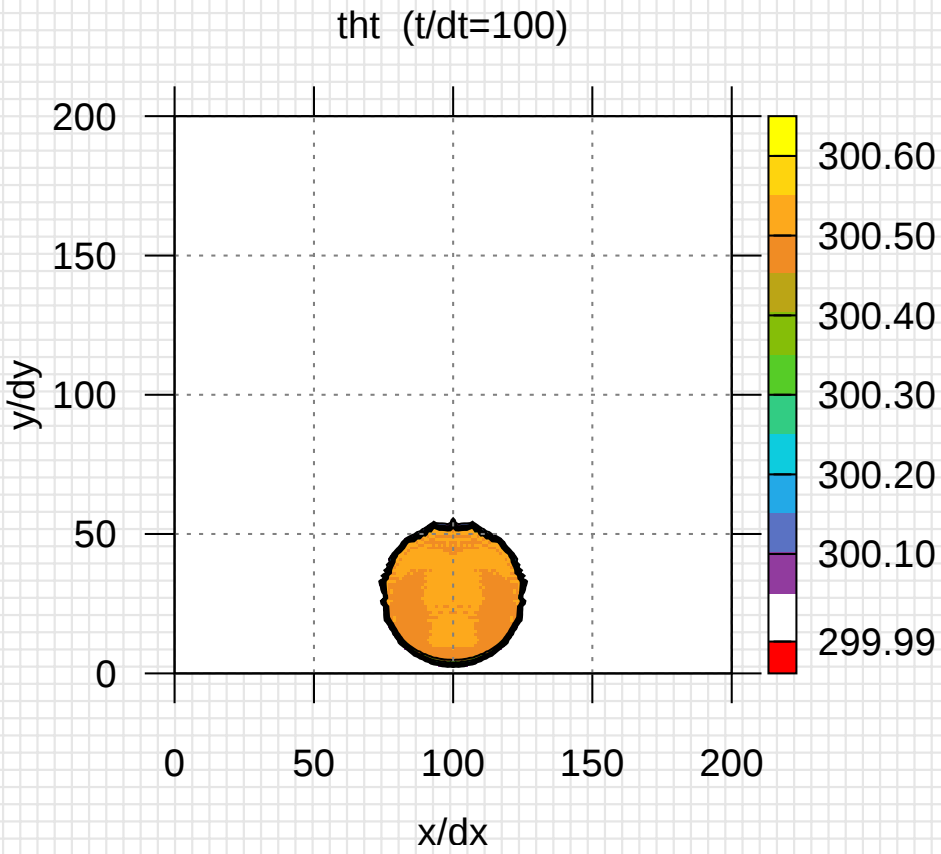

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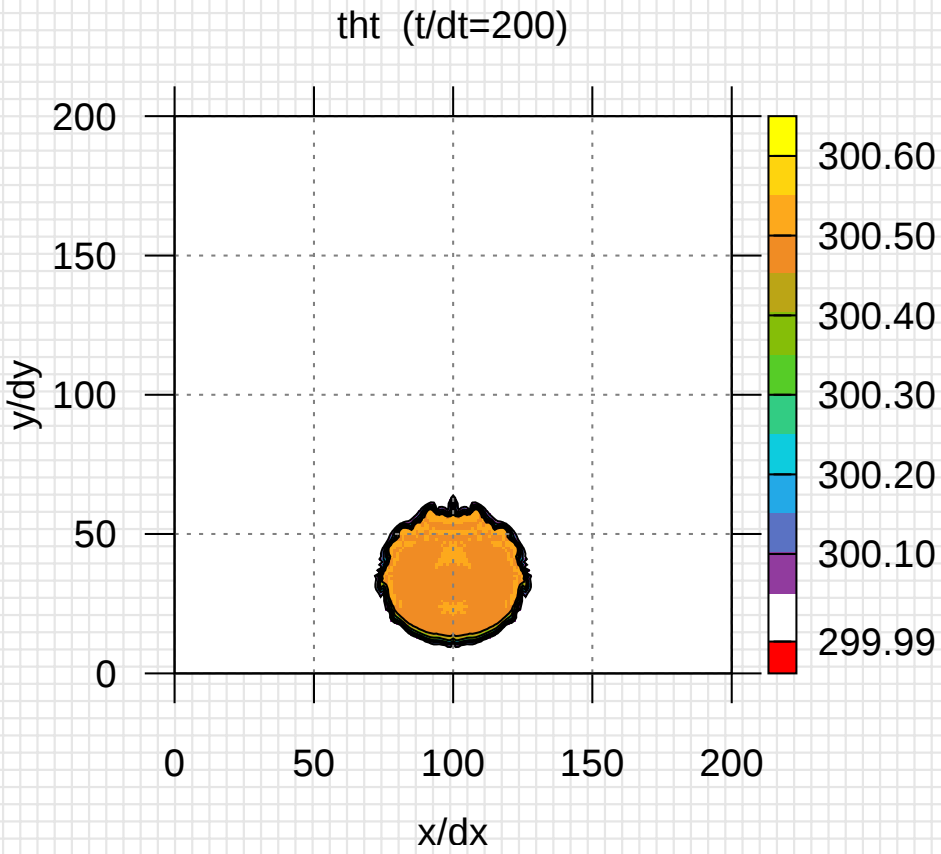

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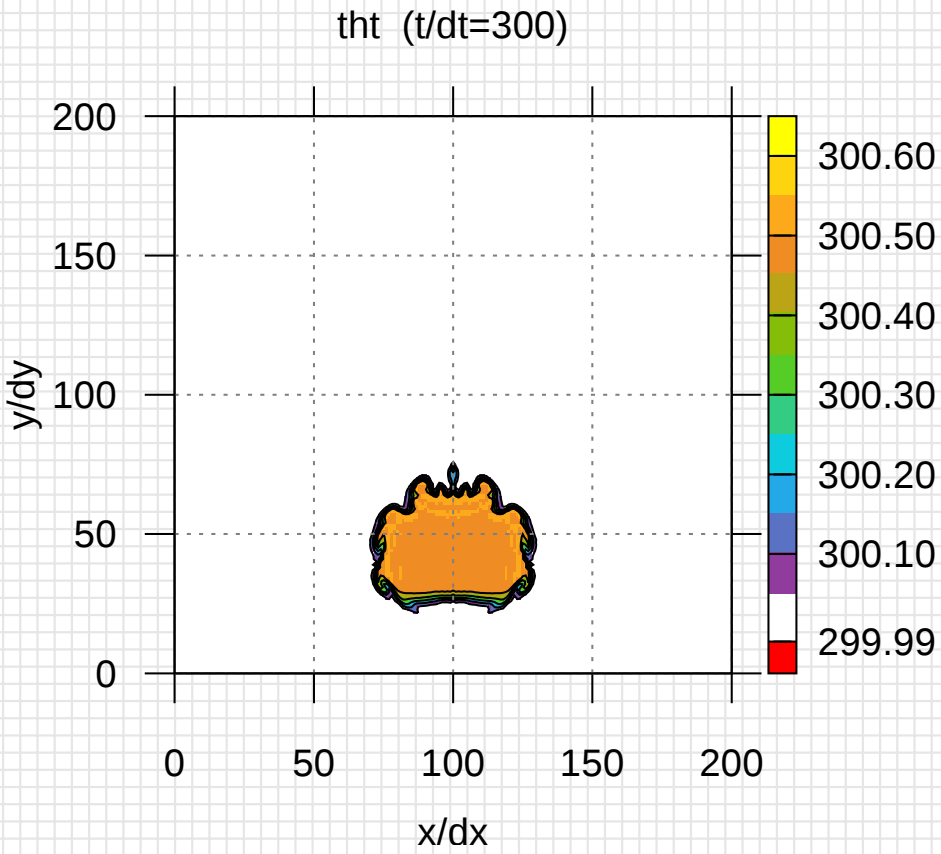

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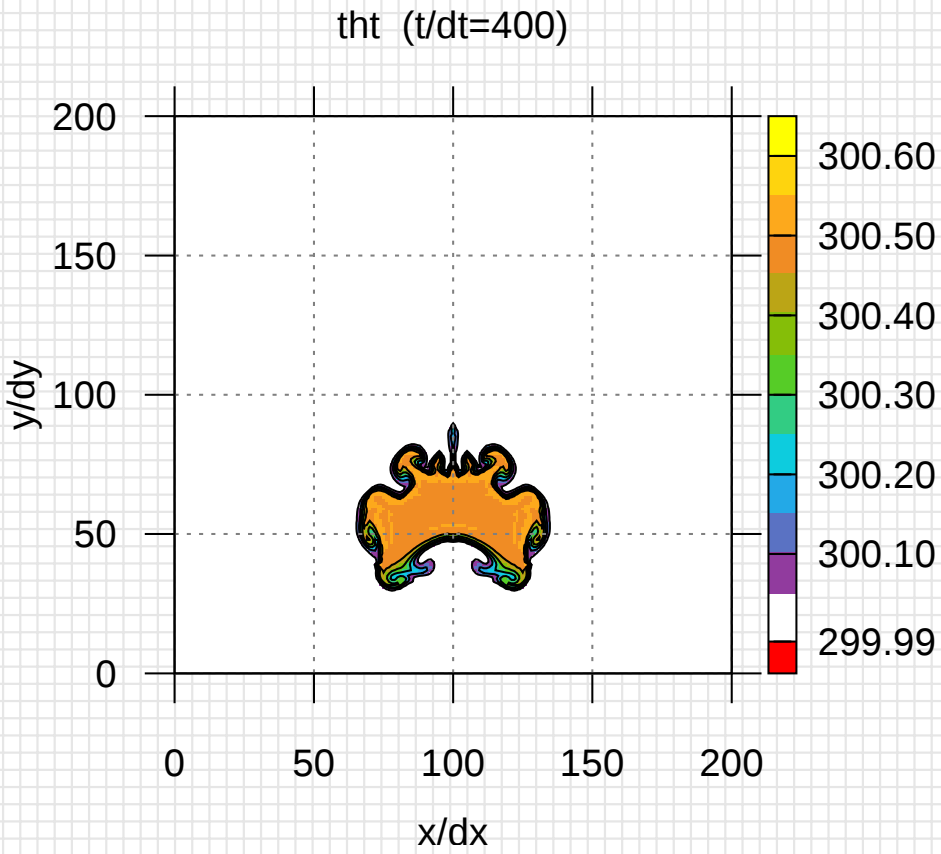

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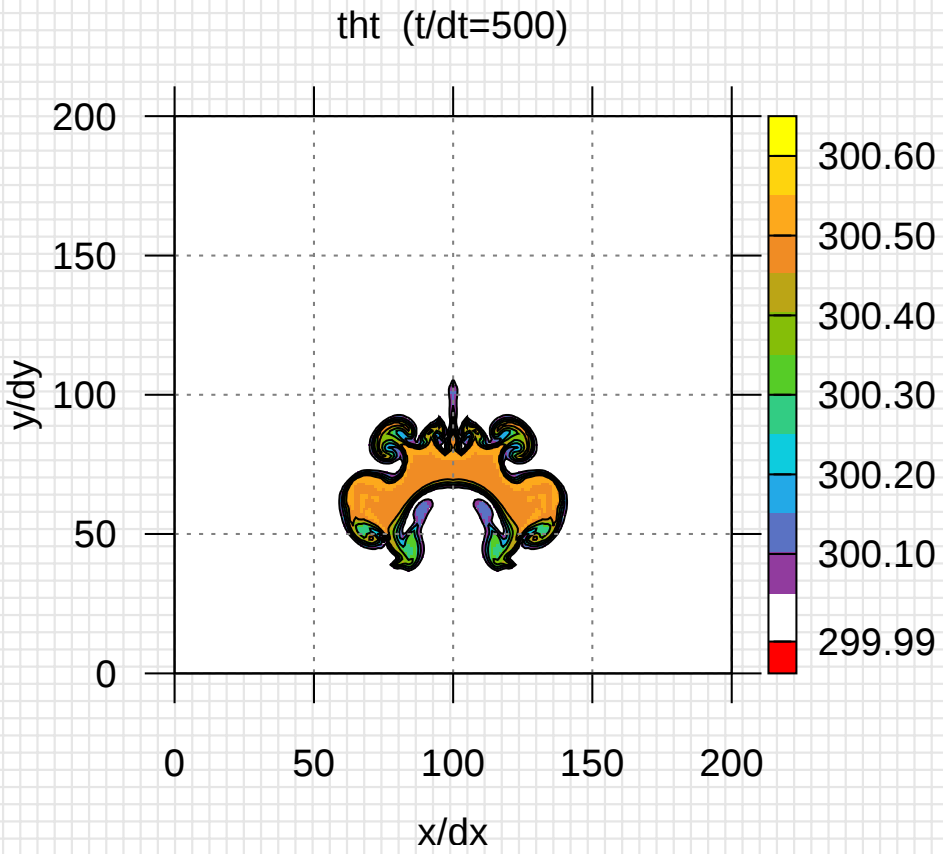

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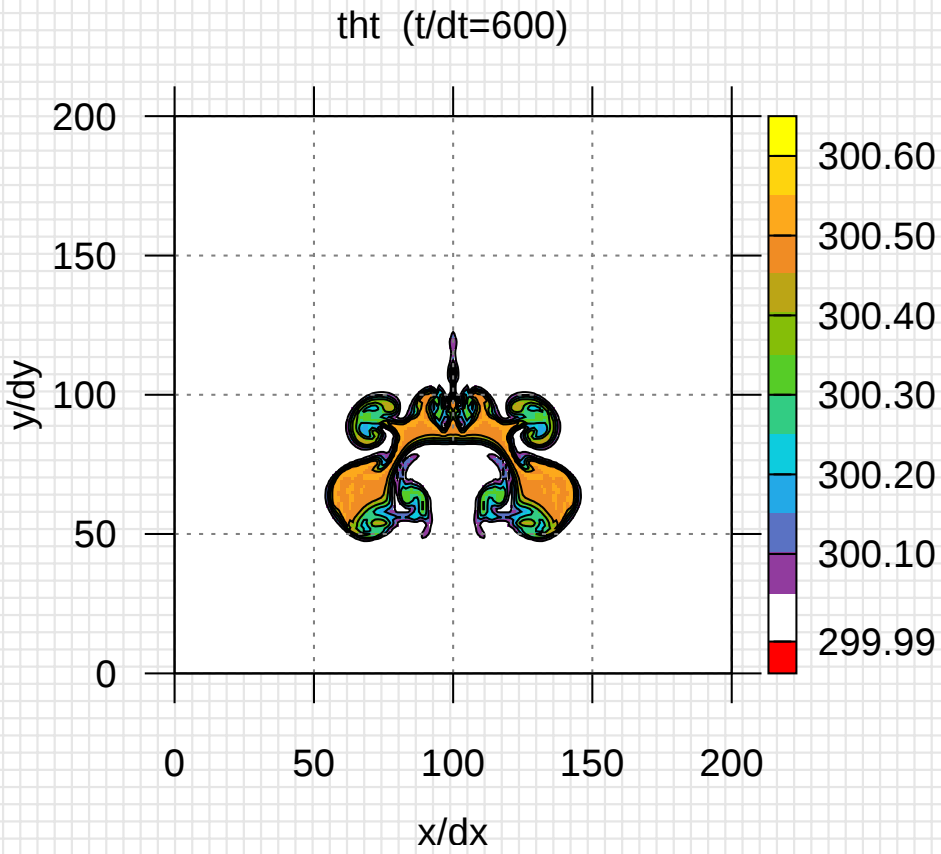

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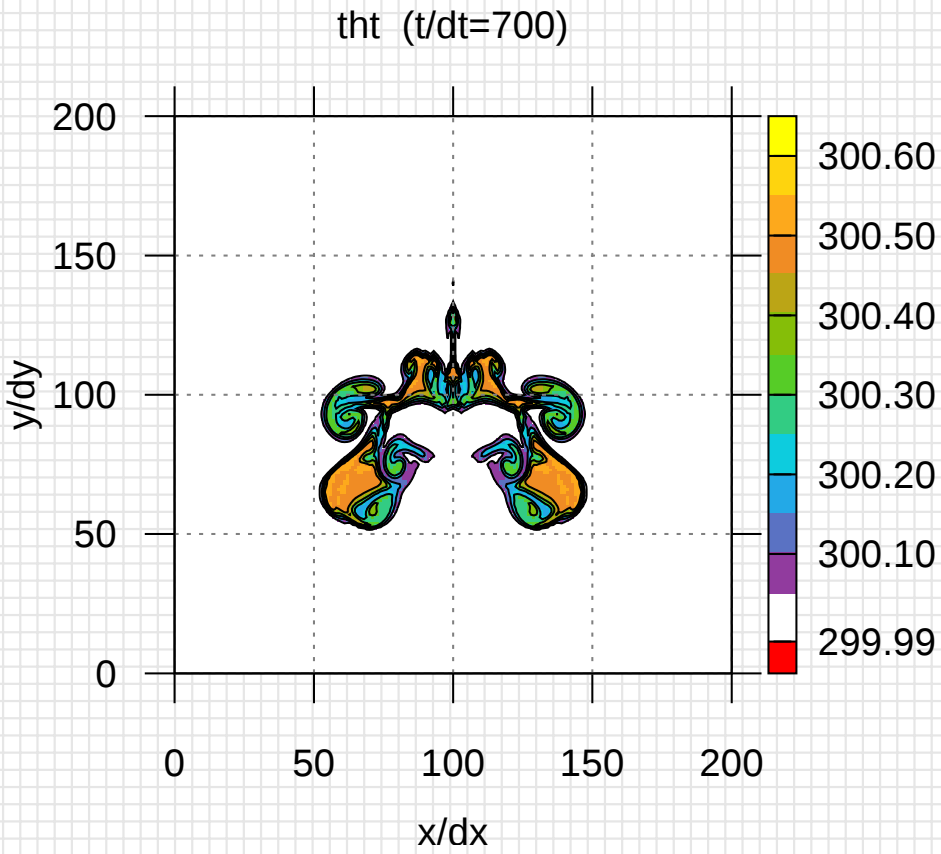

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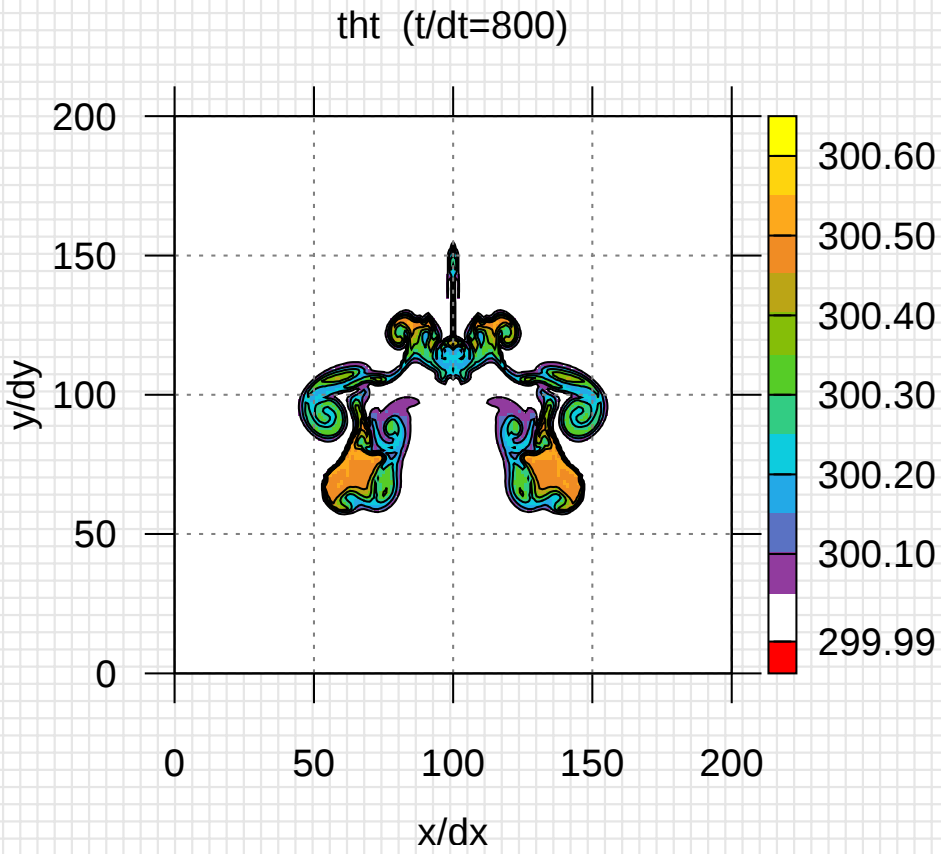

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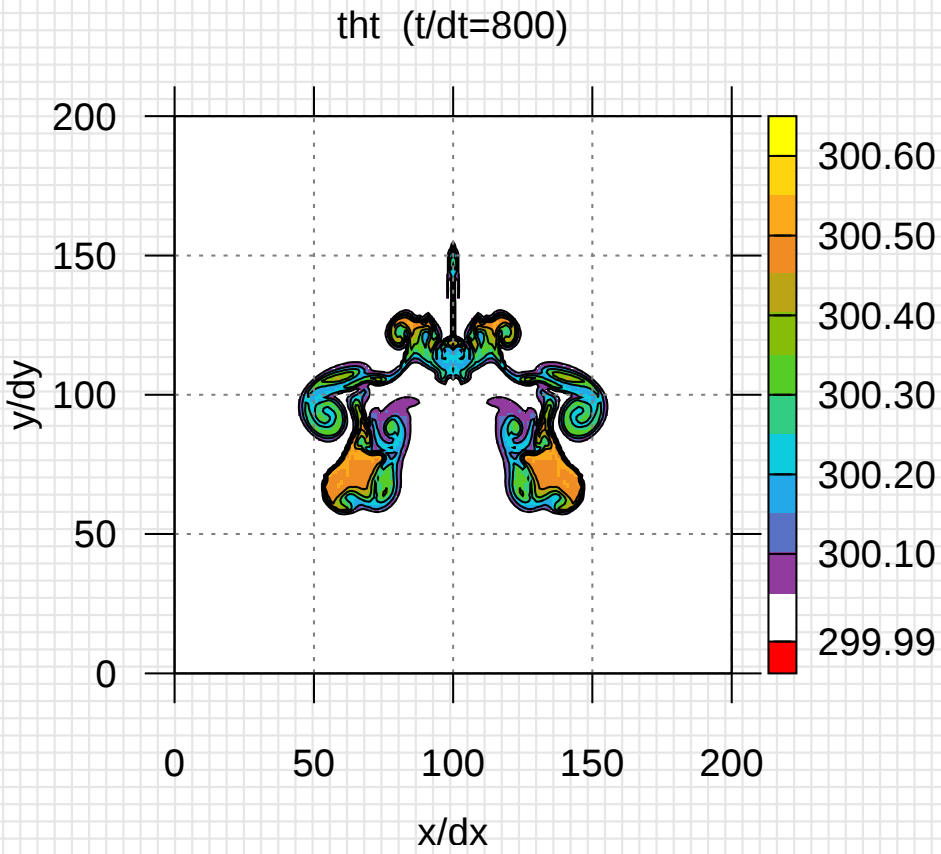

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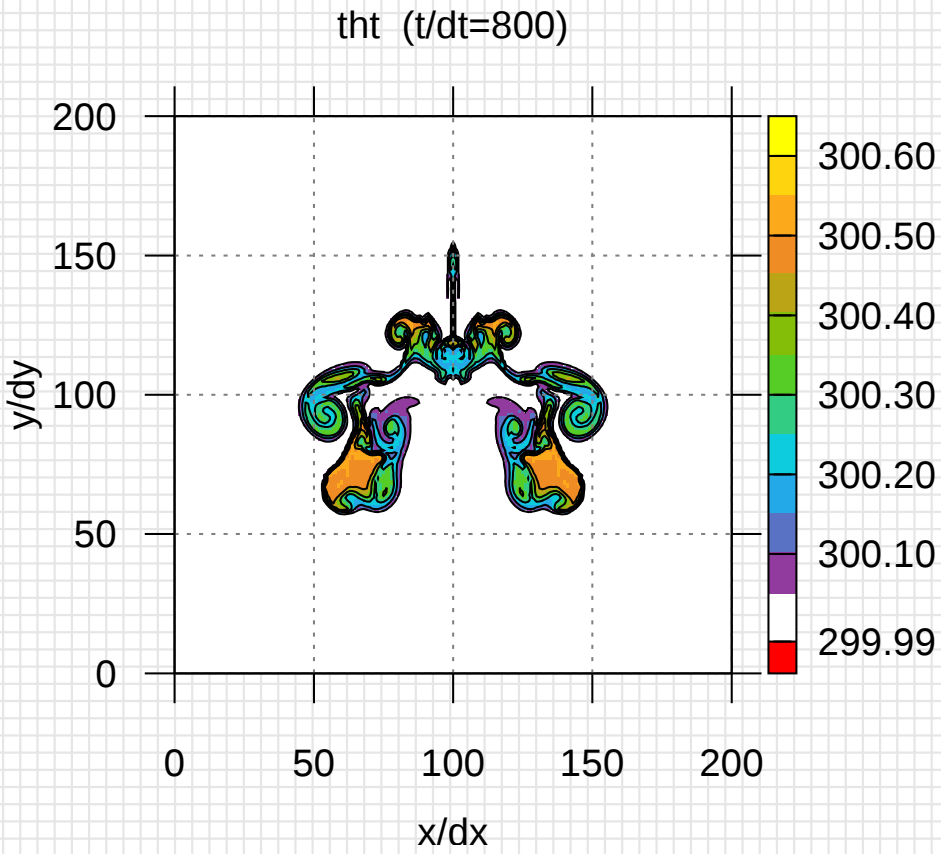

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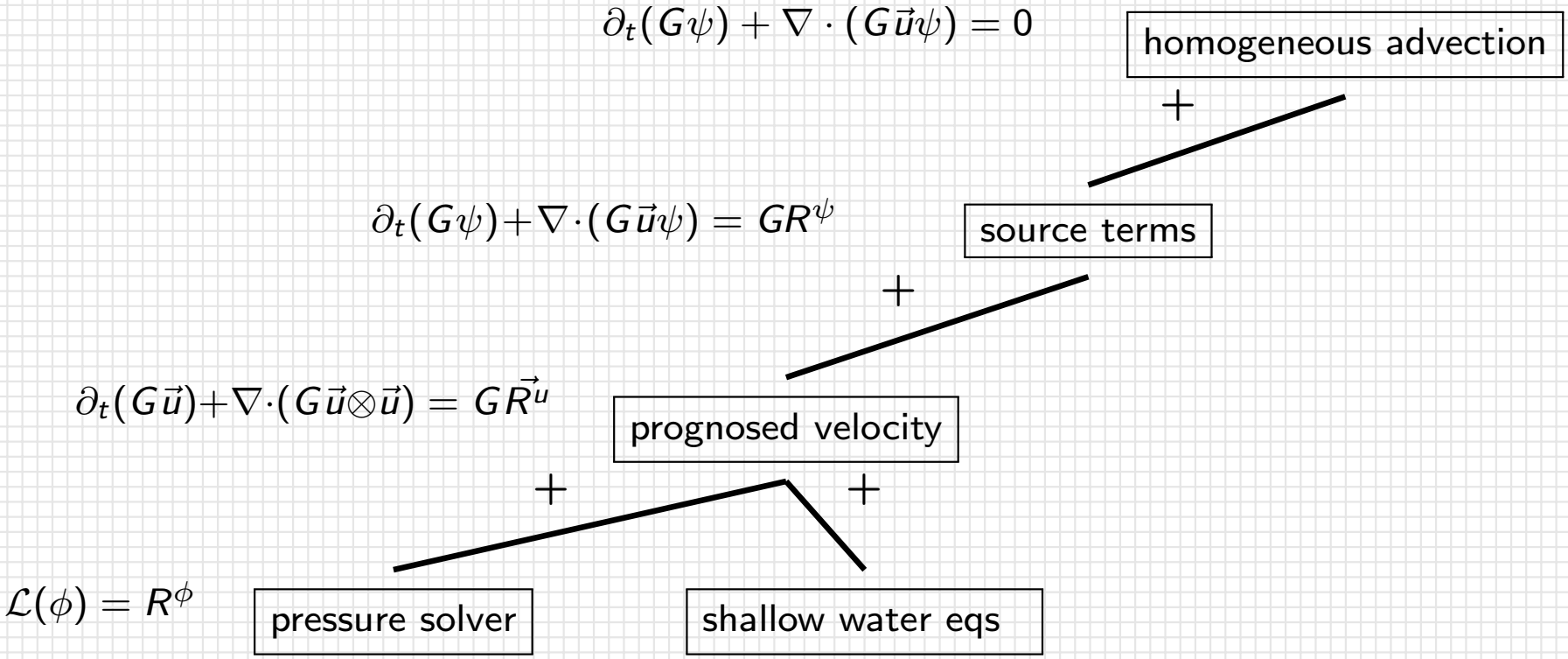

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- support for integration in 1D, 2D & 3D
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Plan of the talk

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

Plan of the talk

libmpdata++ 2.0: summary of features under development

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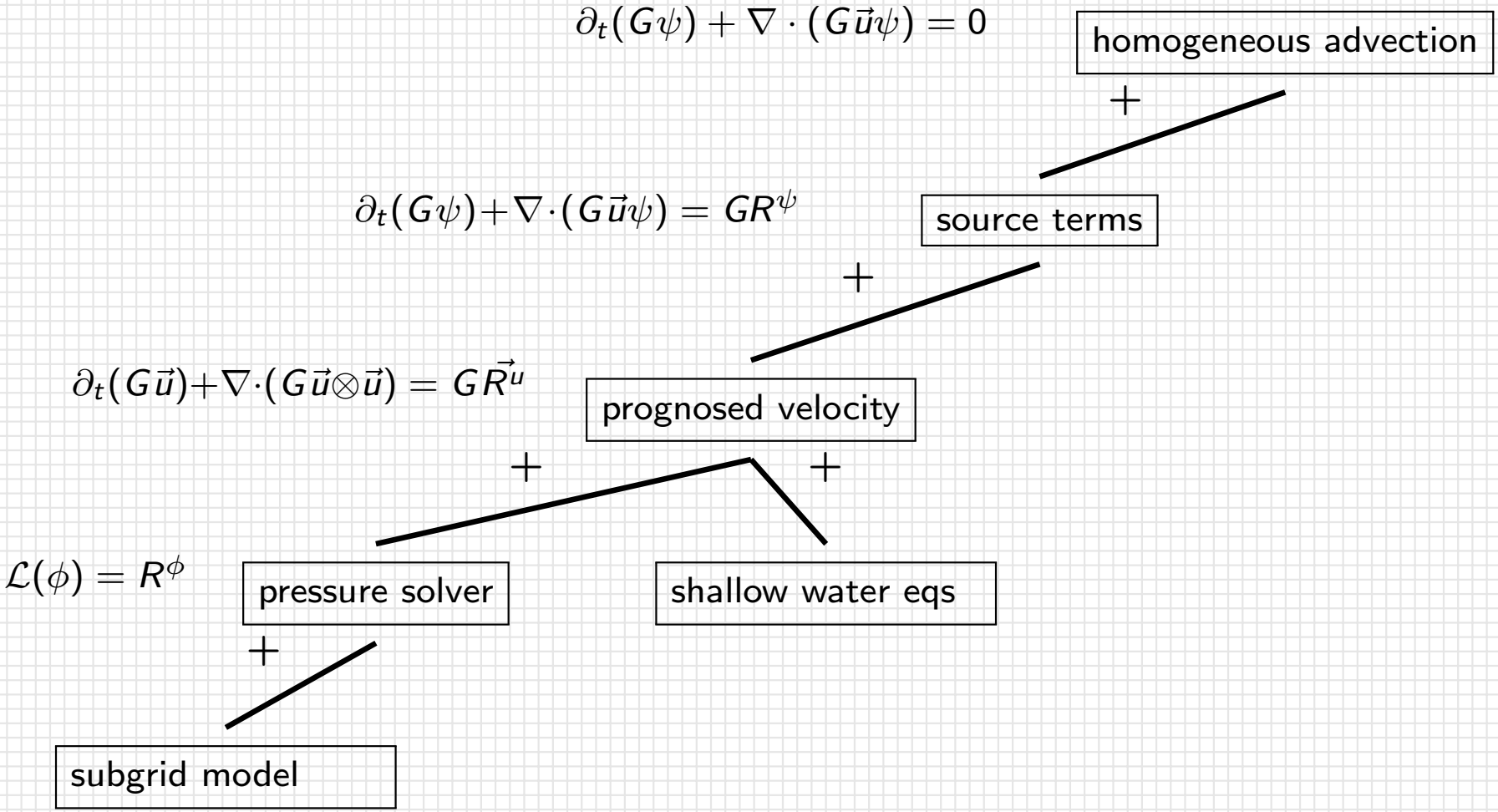
- higher-order operators
  (for DNS/iLES simulations)
- implicit treatment of absorbers
  (for immersed-boundary method)
- adaptive timestepping
- distributed-memory parallelisation
  (using Boost.MPI & HDF5/MPI-IO)

libmpdata++ 2.0: solver/algorithm hierarchy



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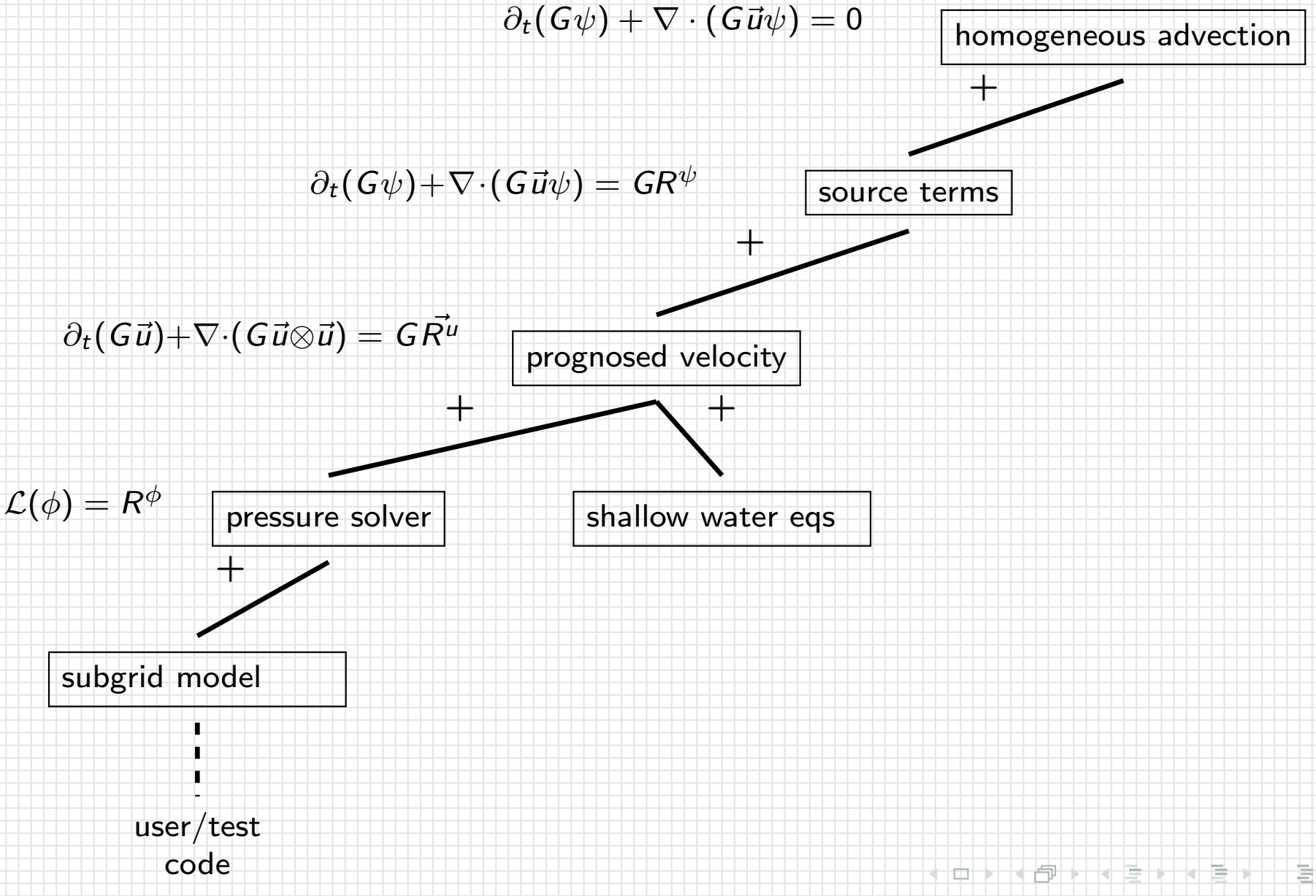

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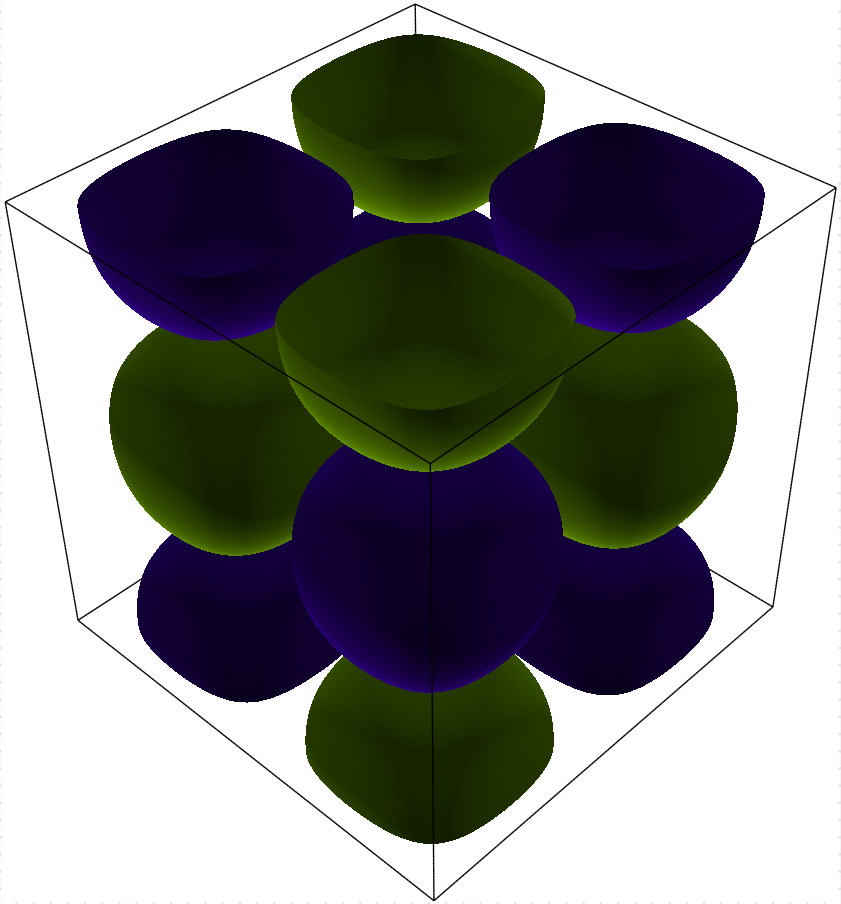

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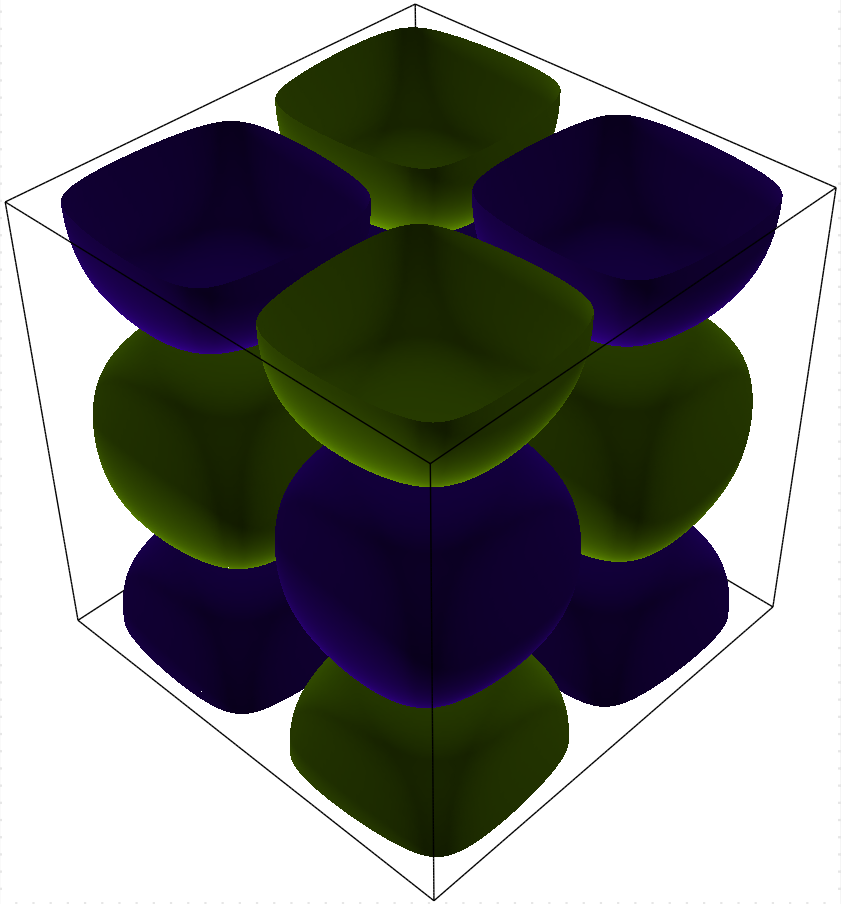

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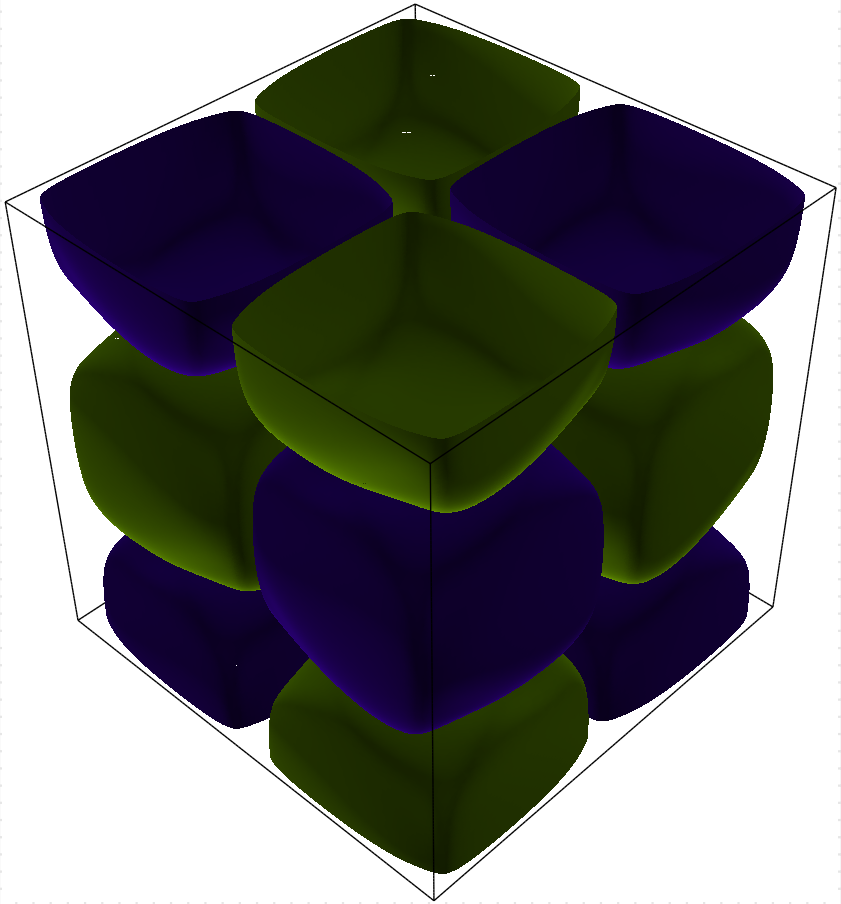

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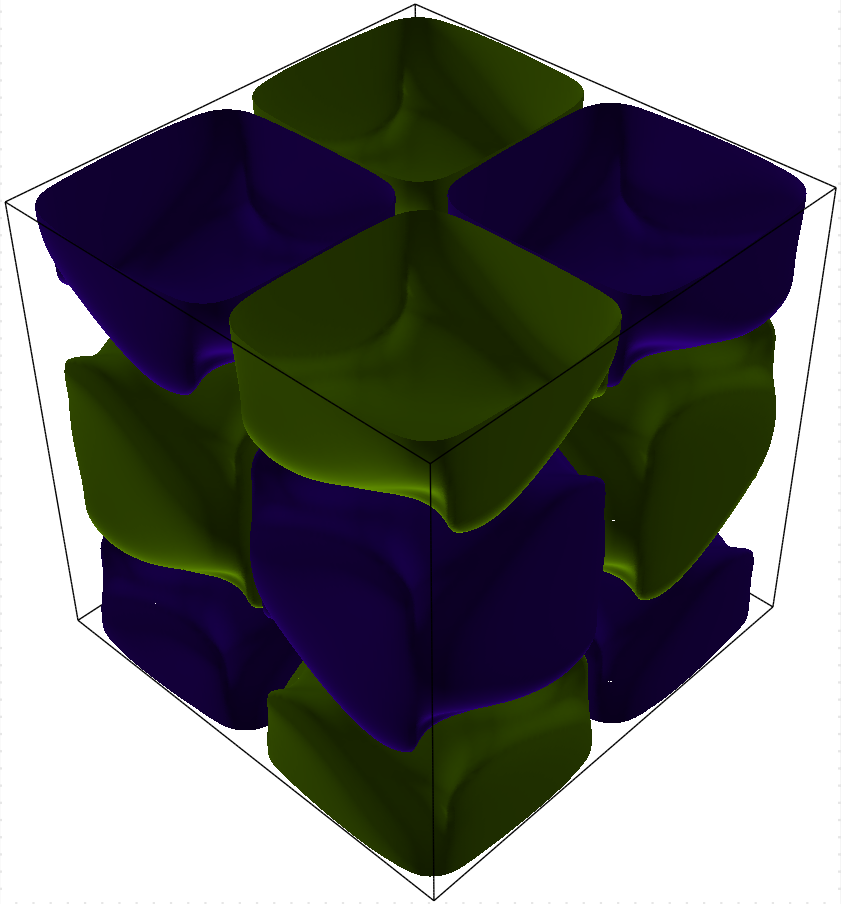

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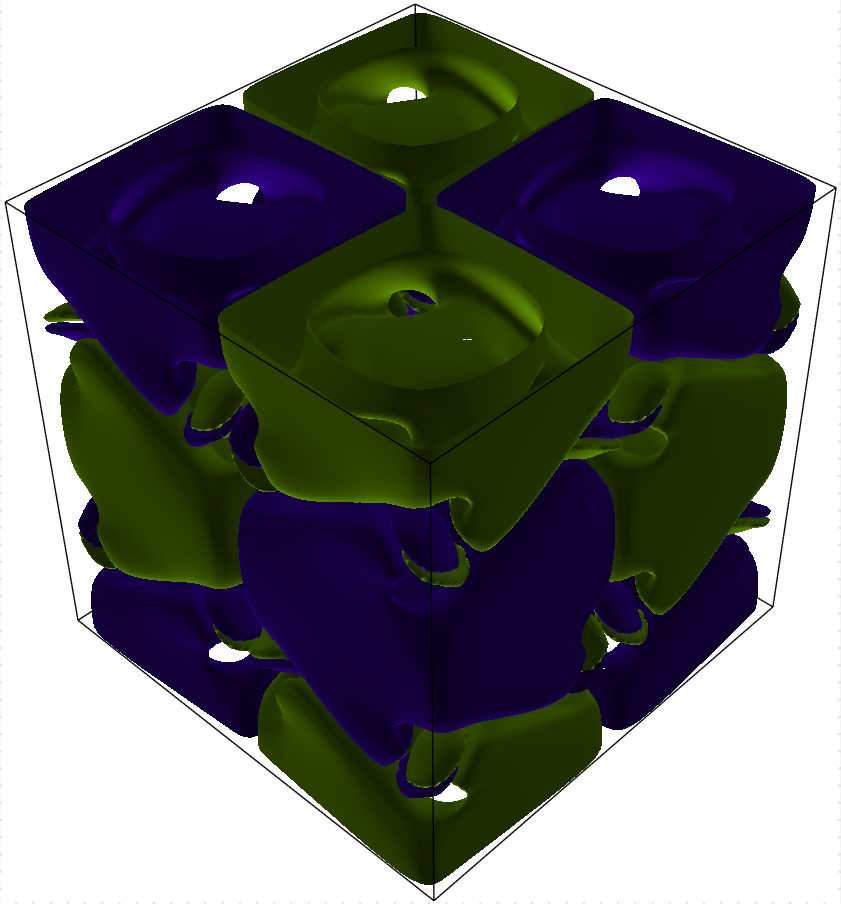

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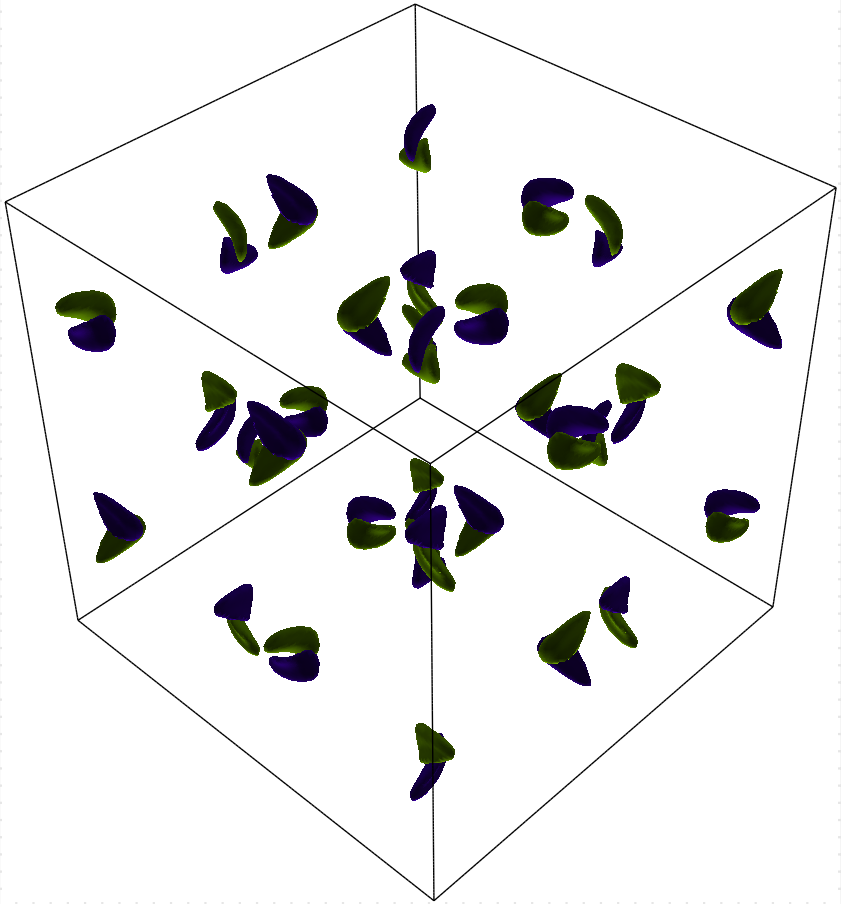

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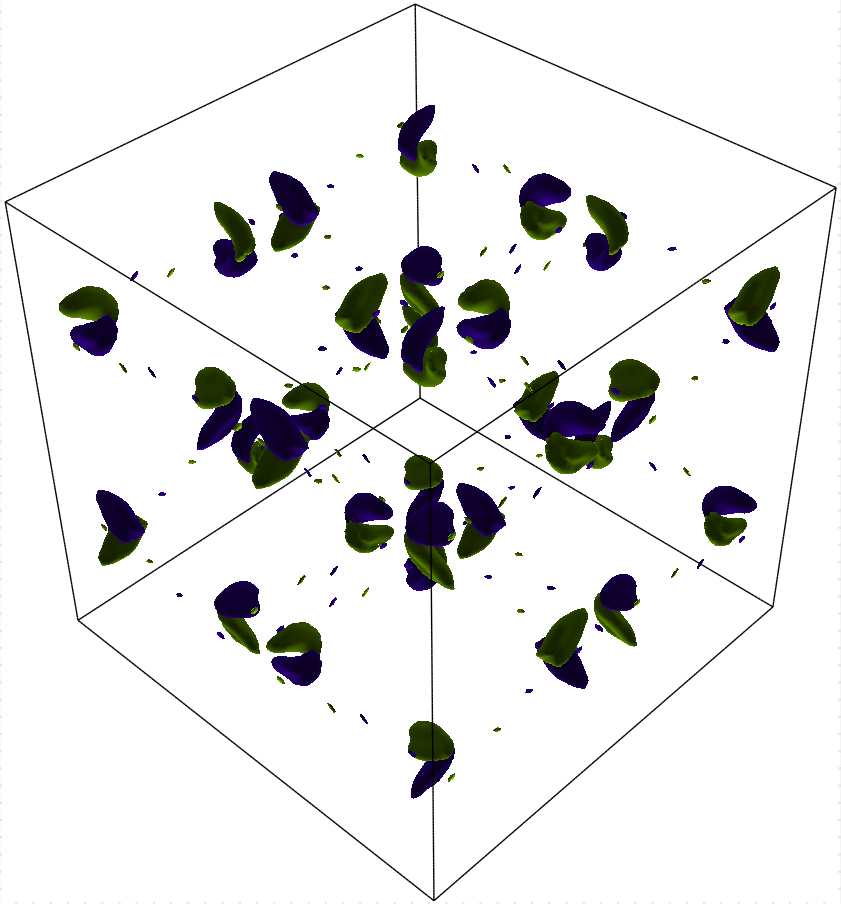

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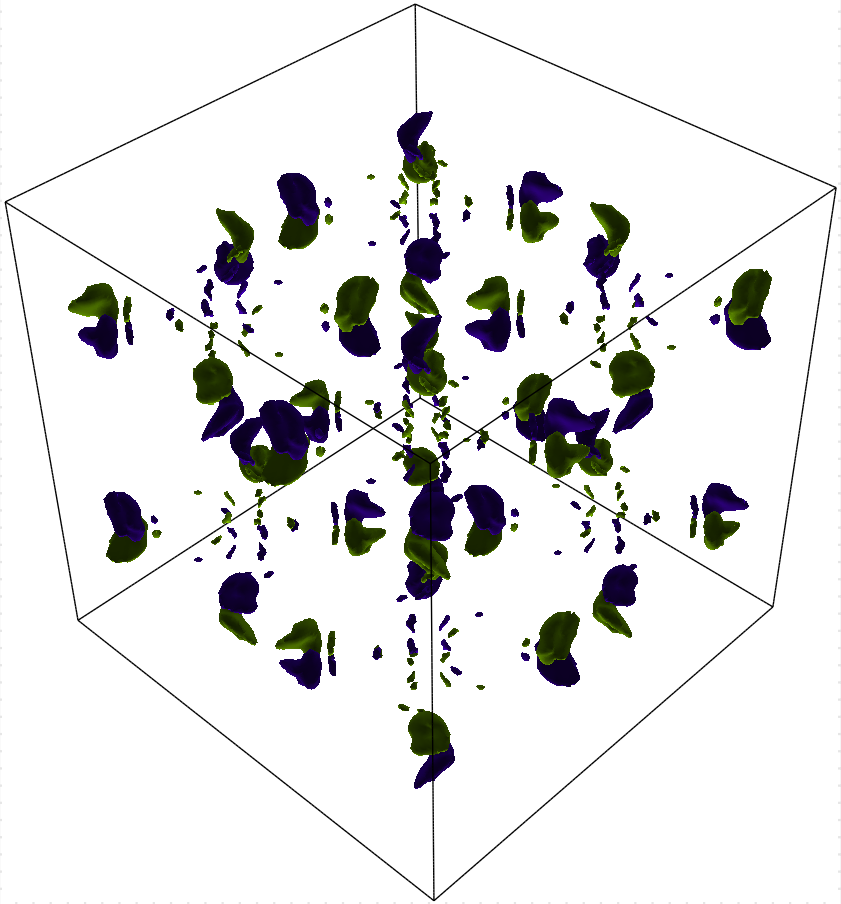

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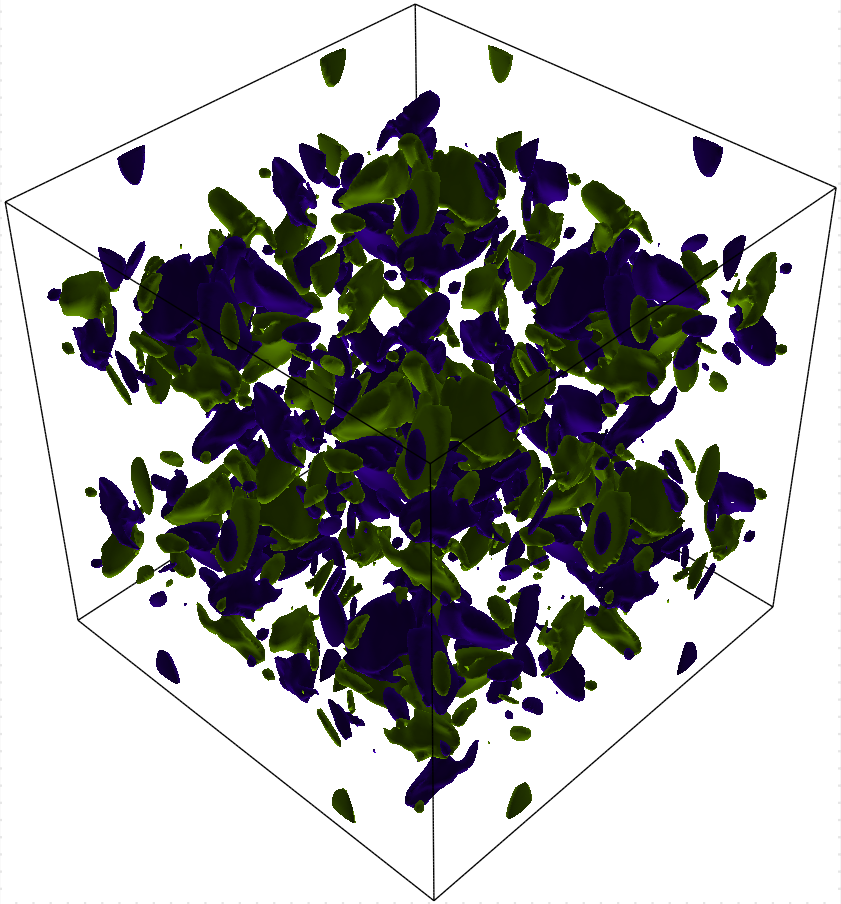

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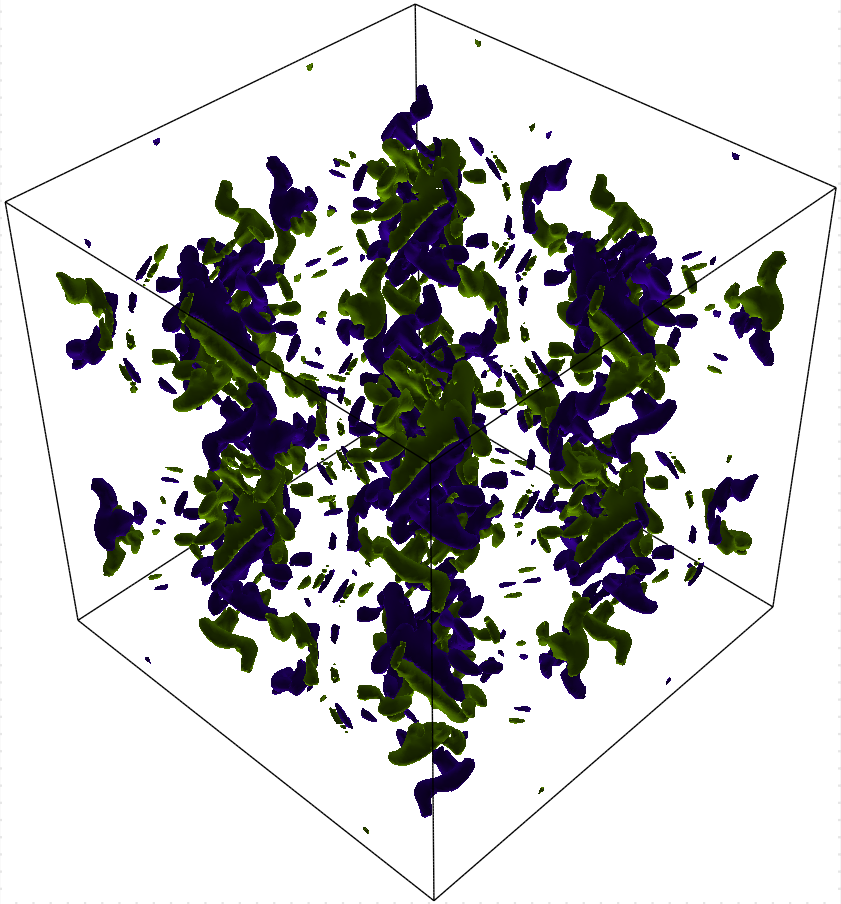

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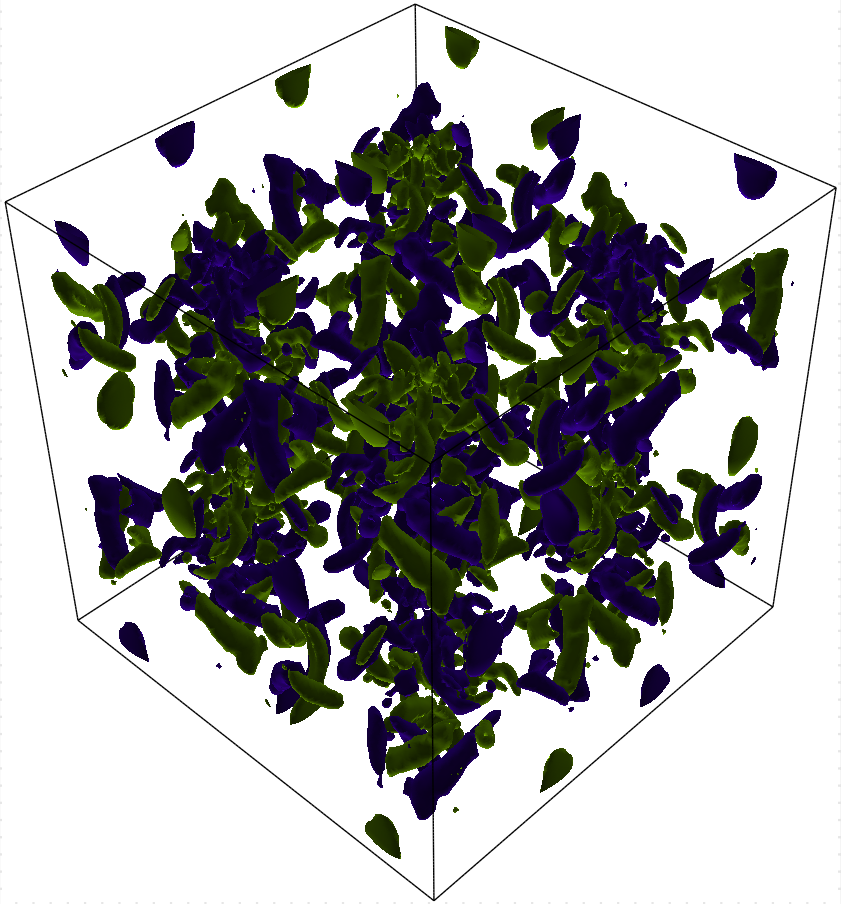

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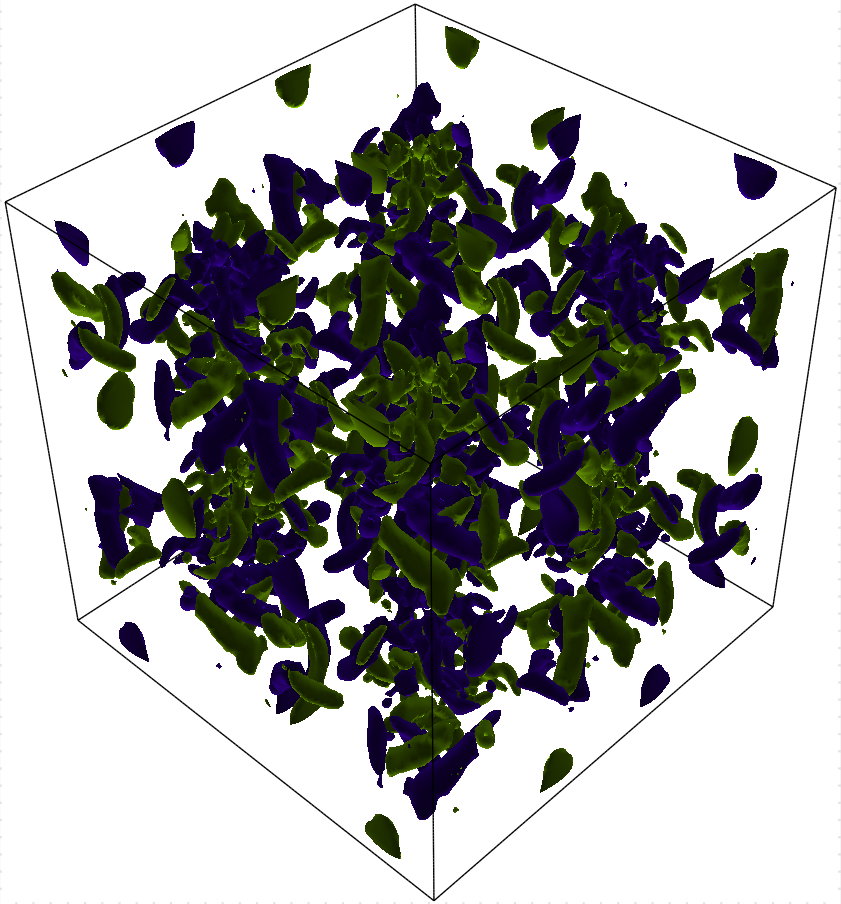

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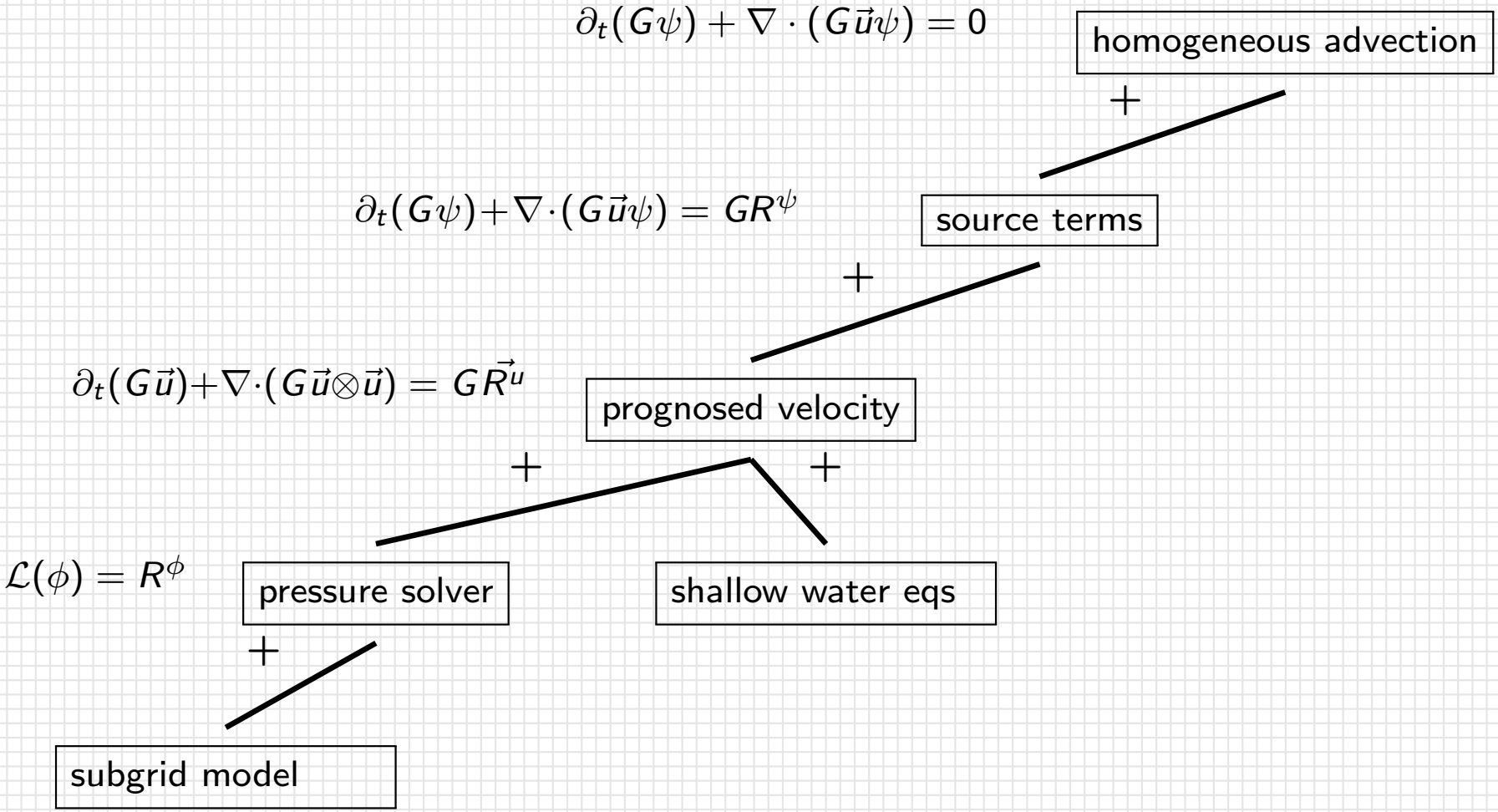

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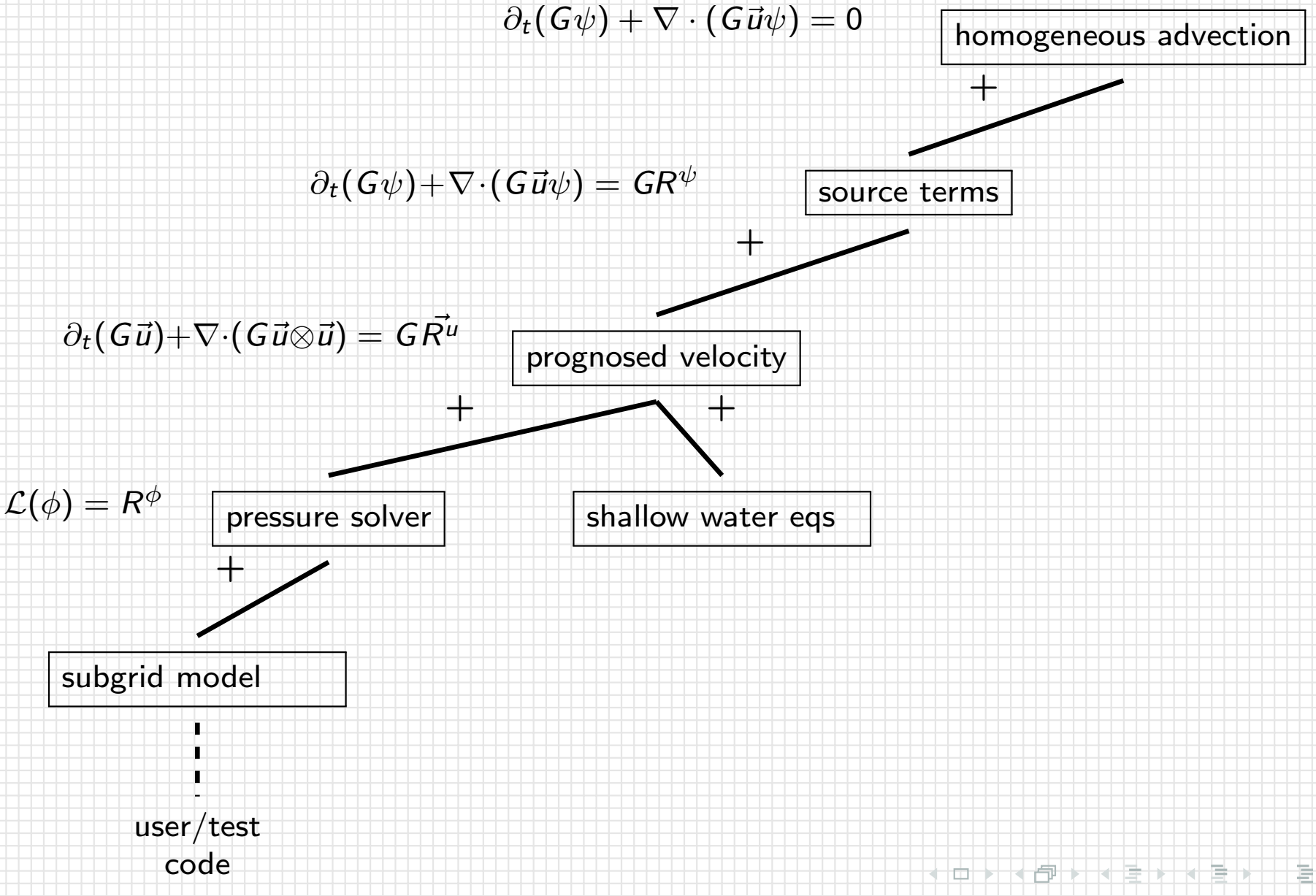

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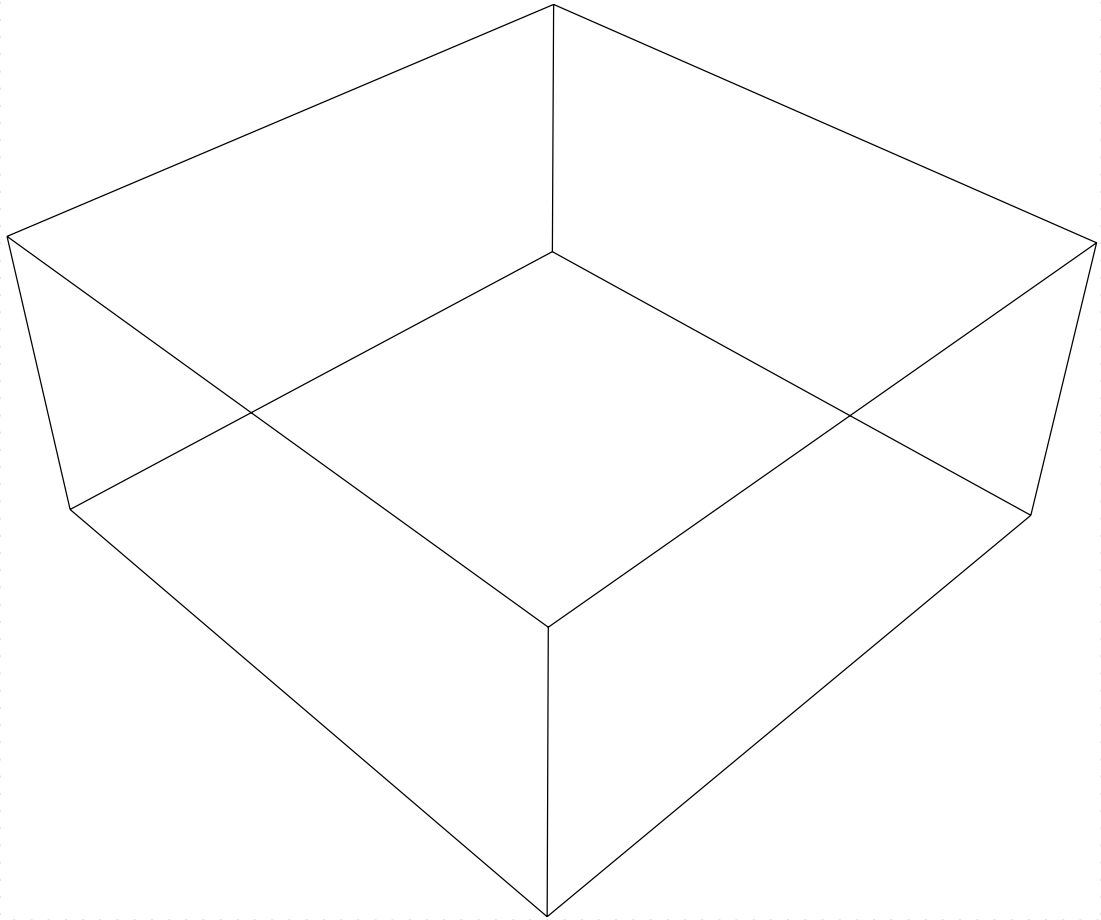

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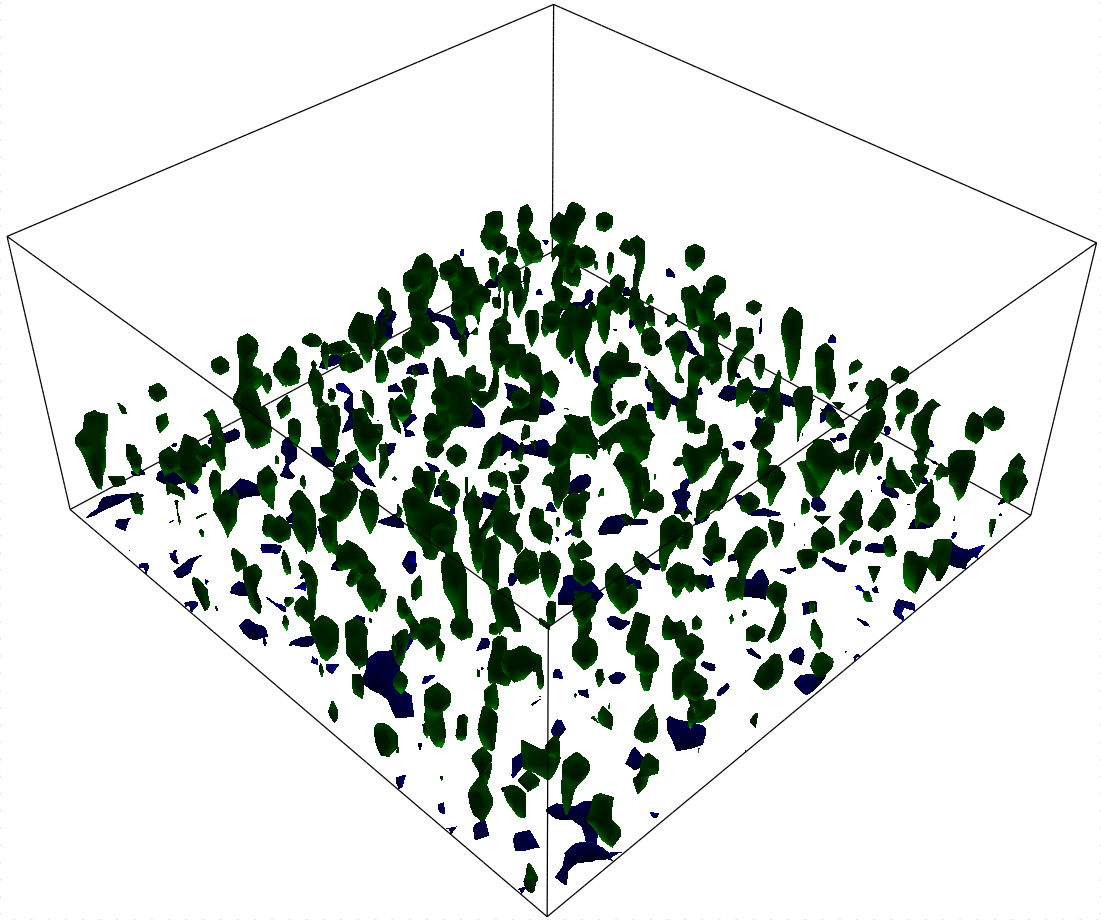

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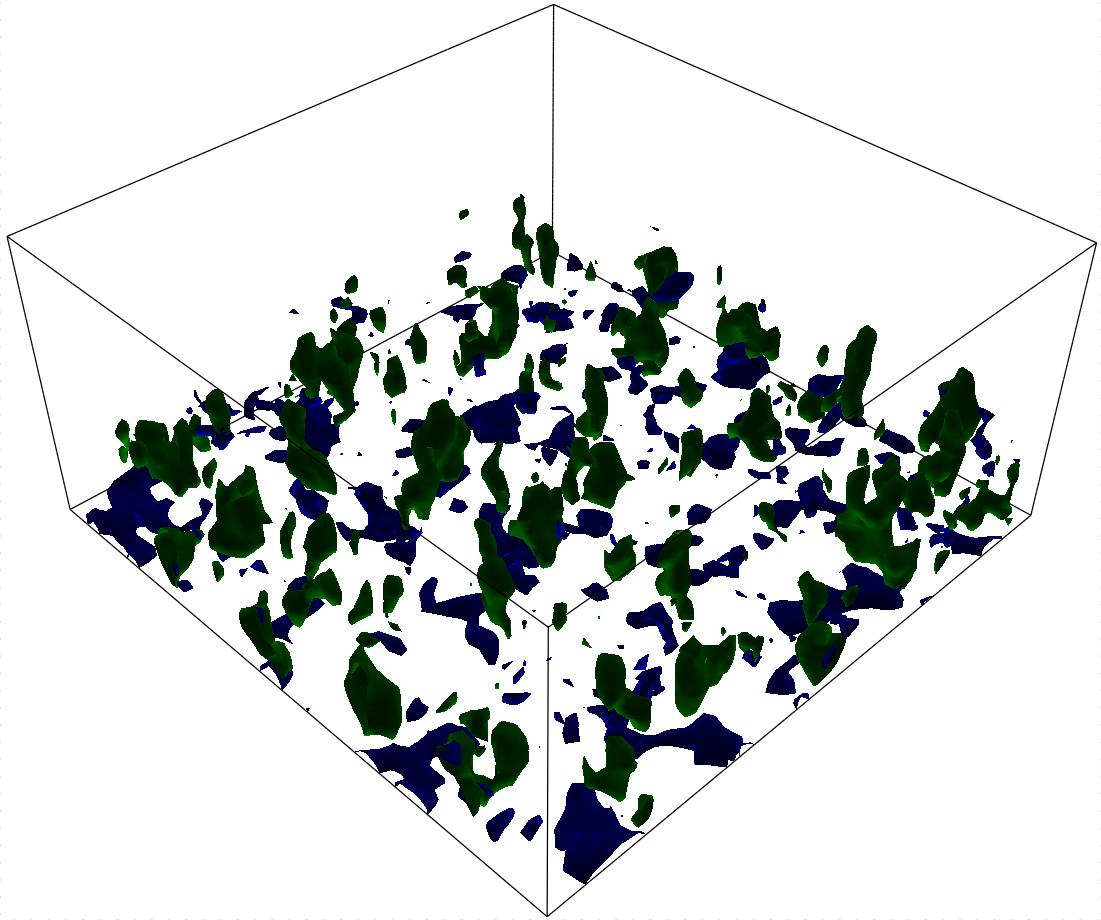

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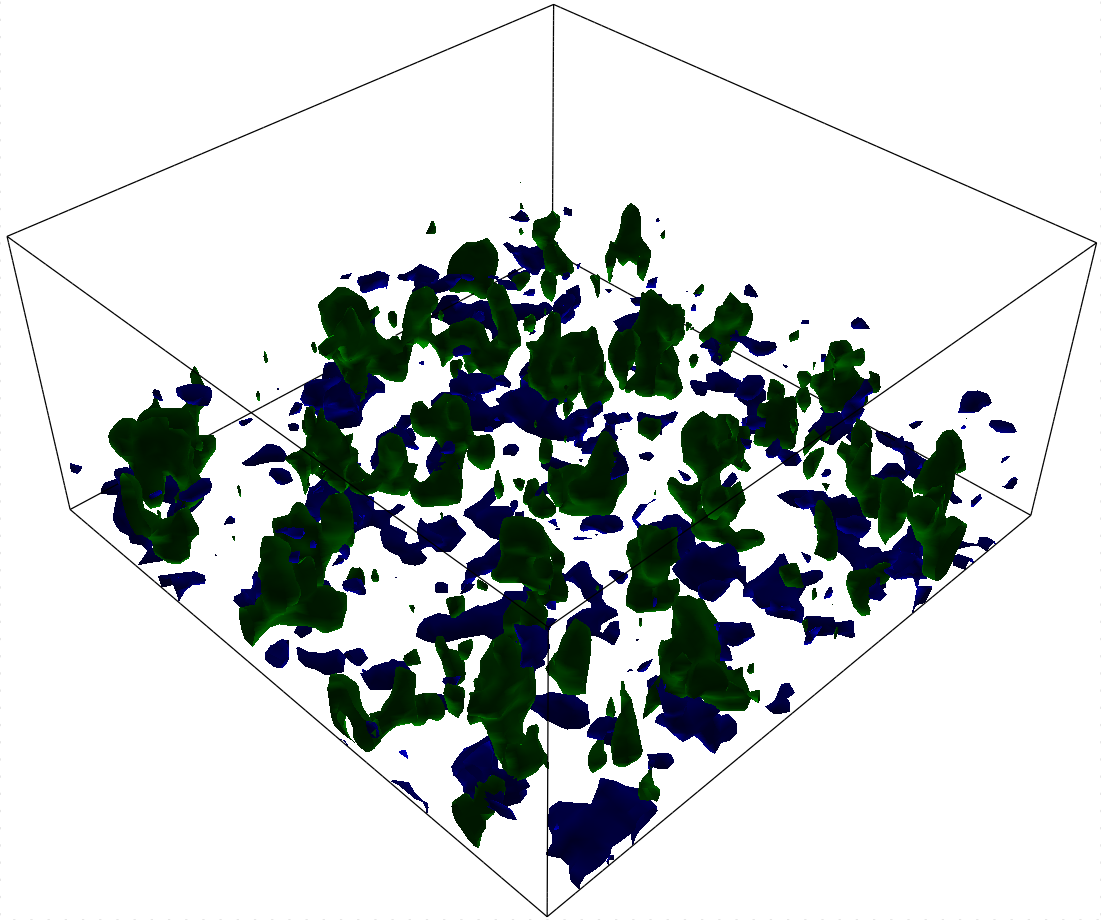

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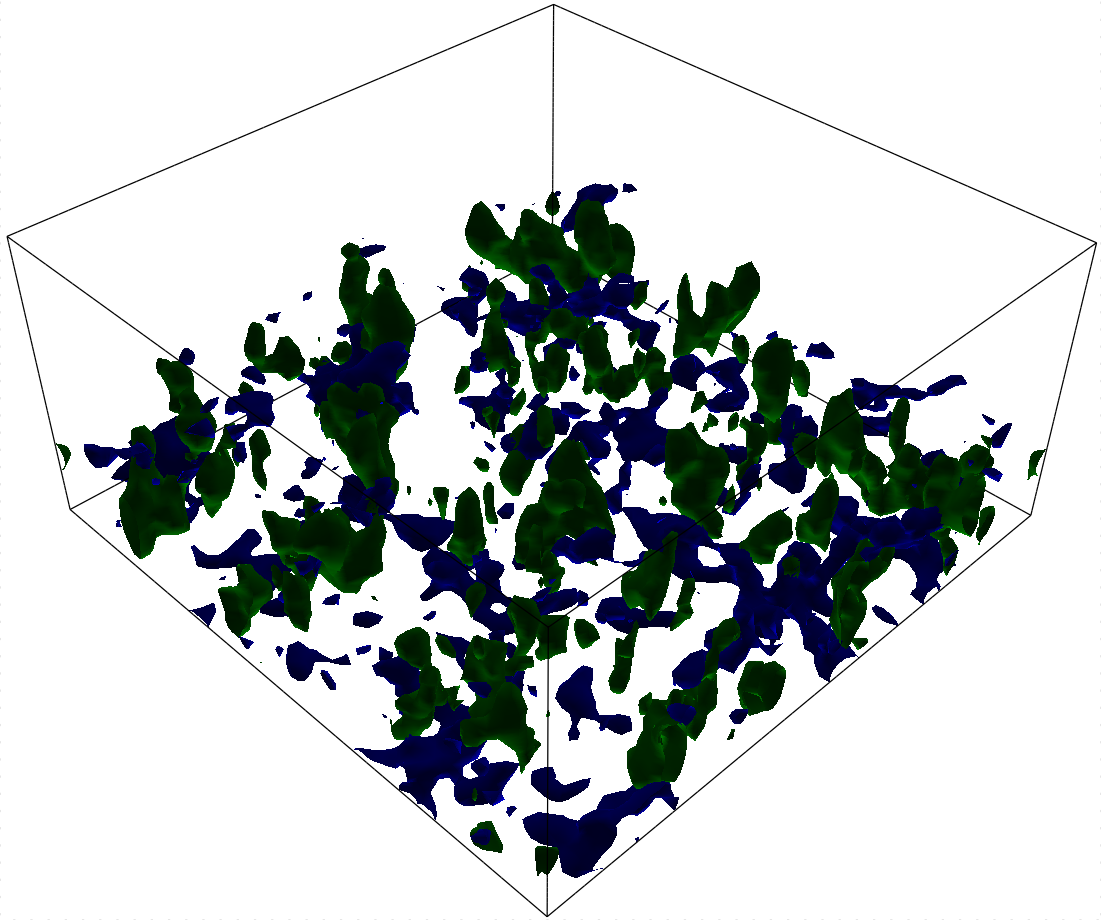

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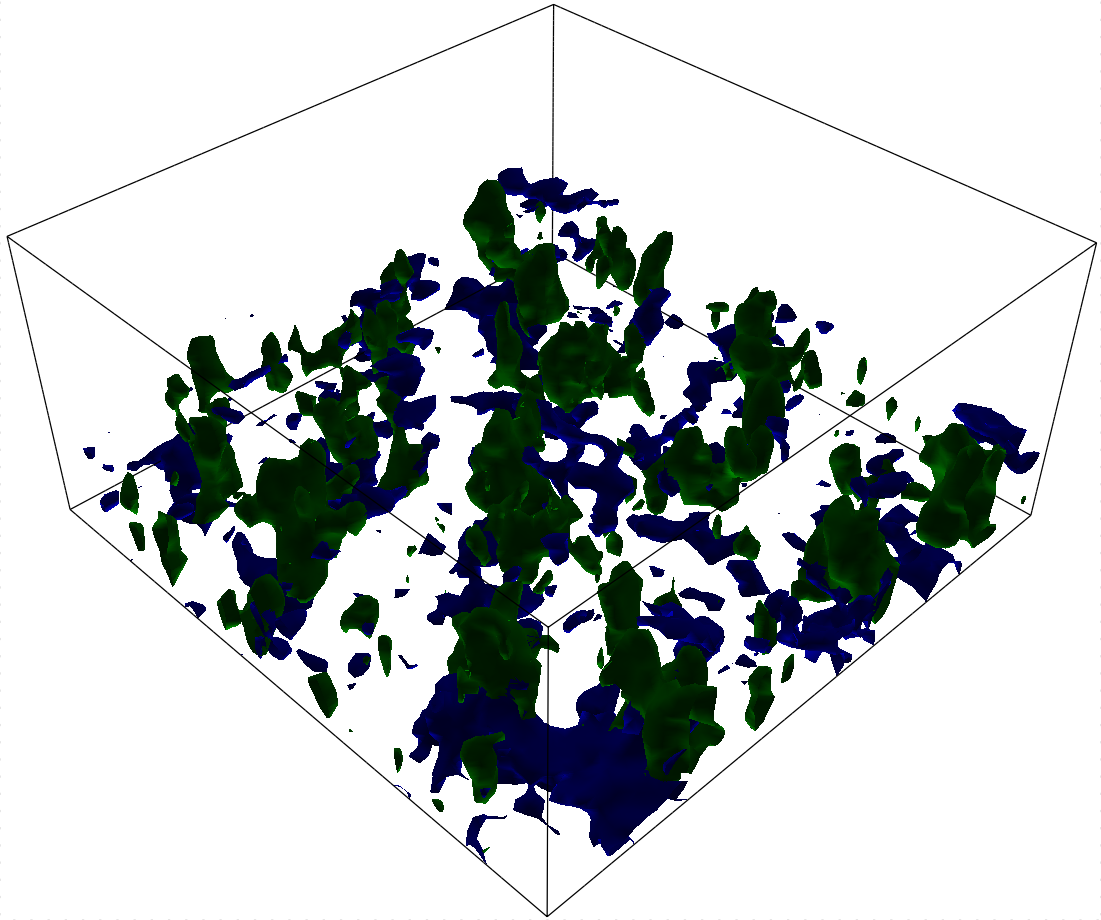

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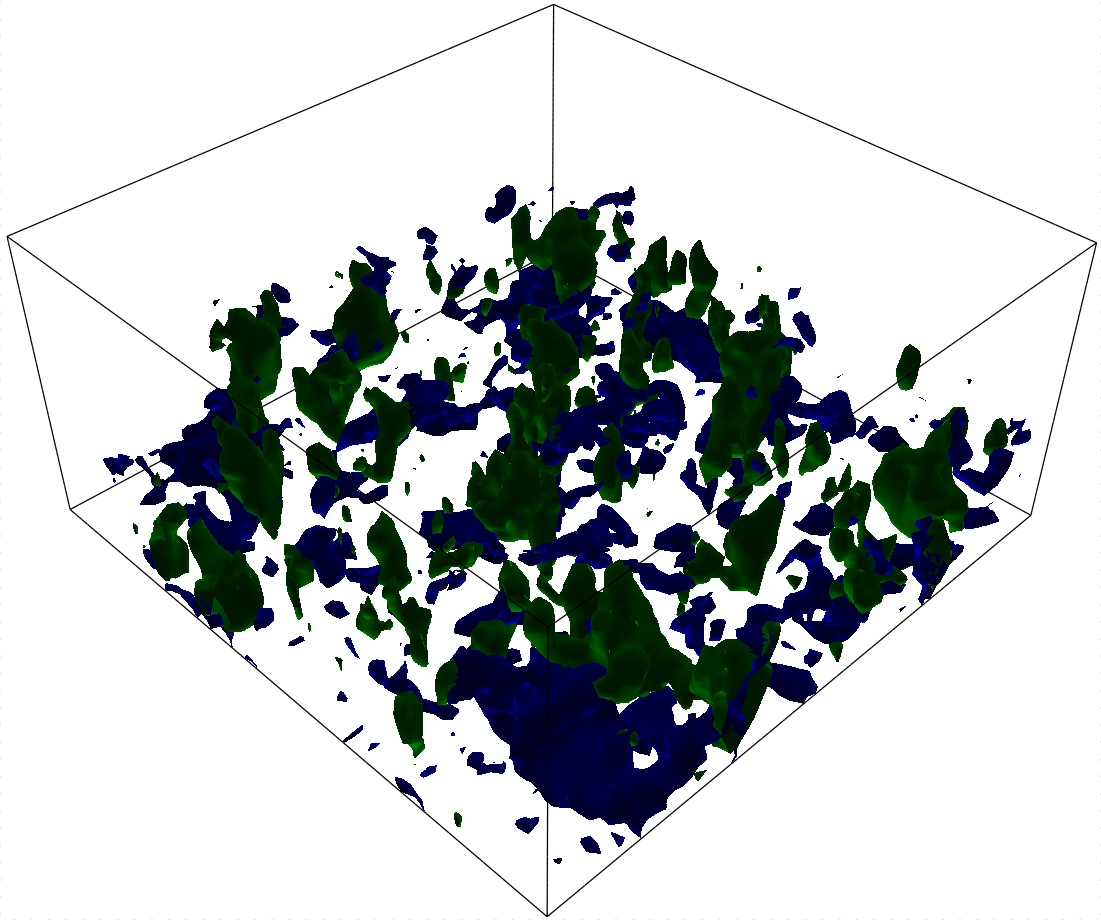

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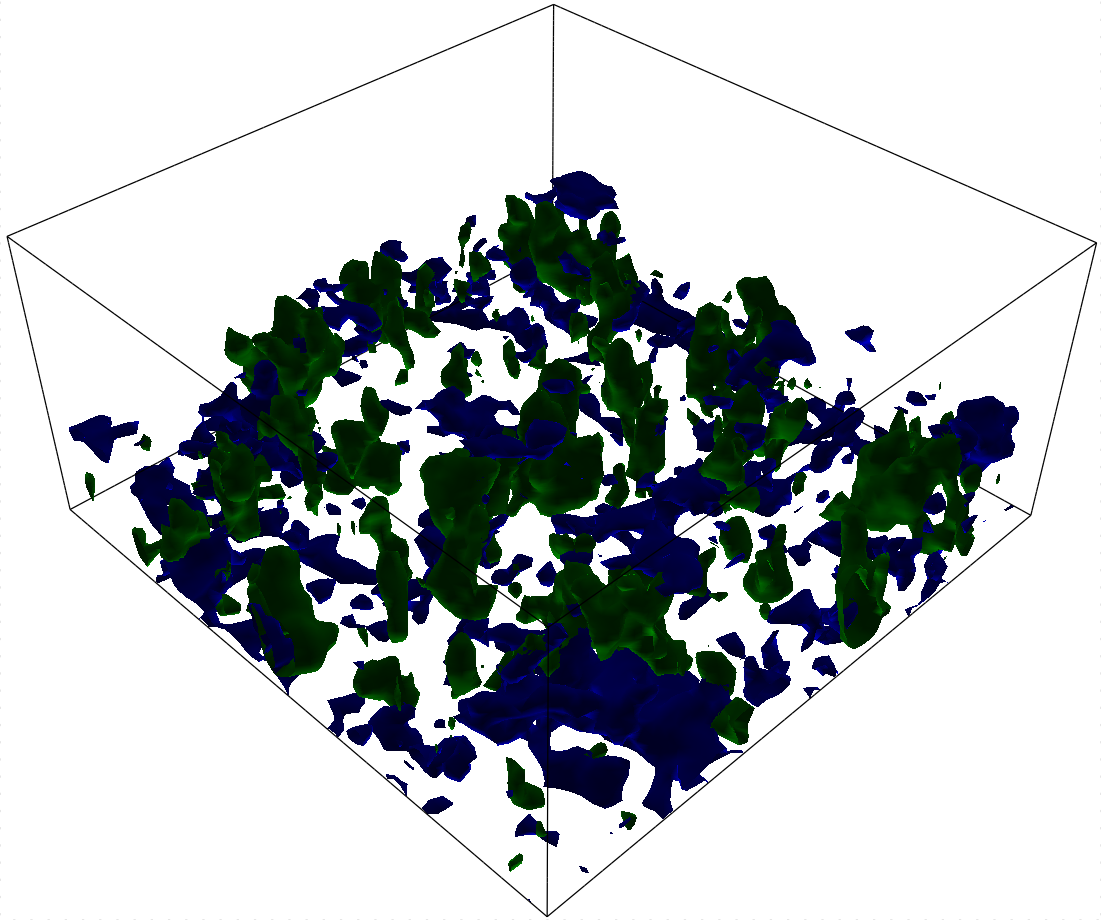

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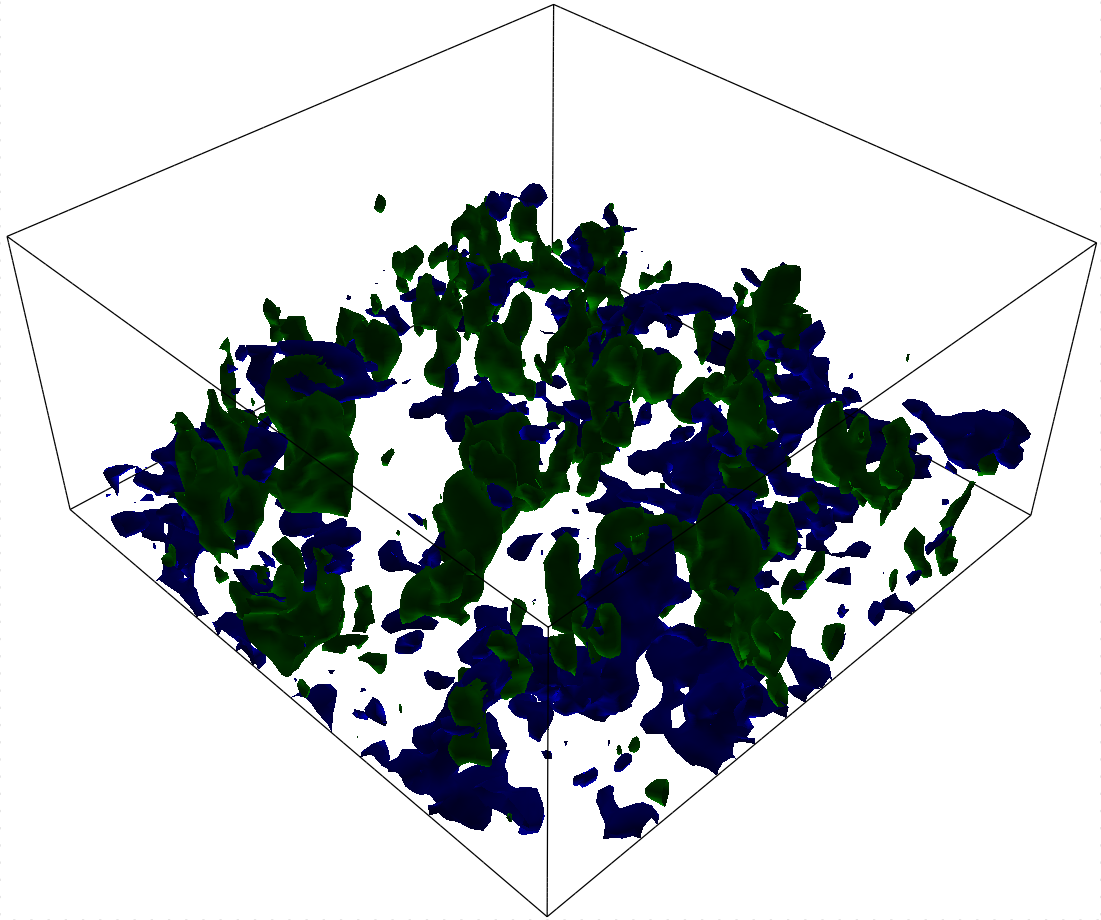

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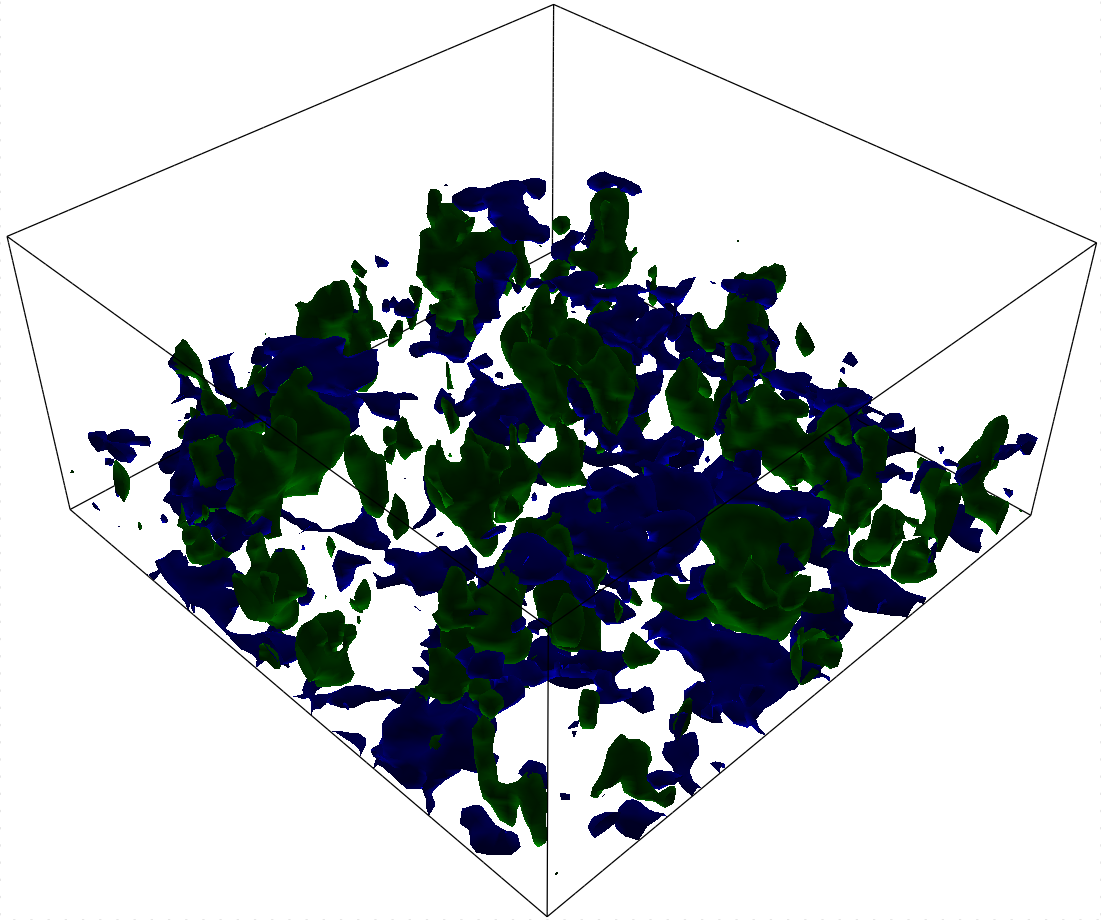

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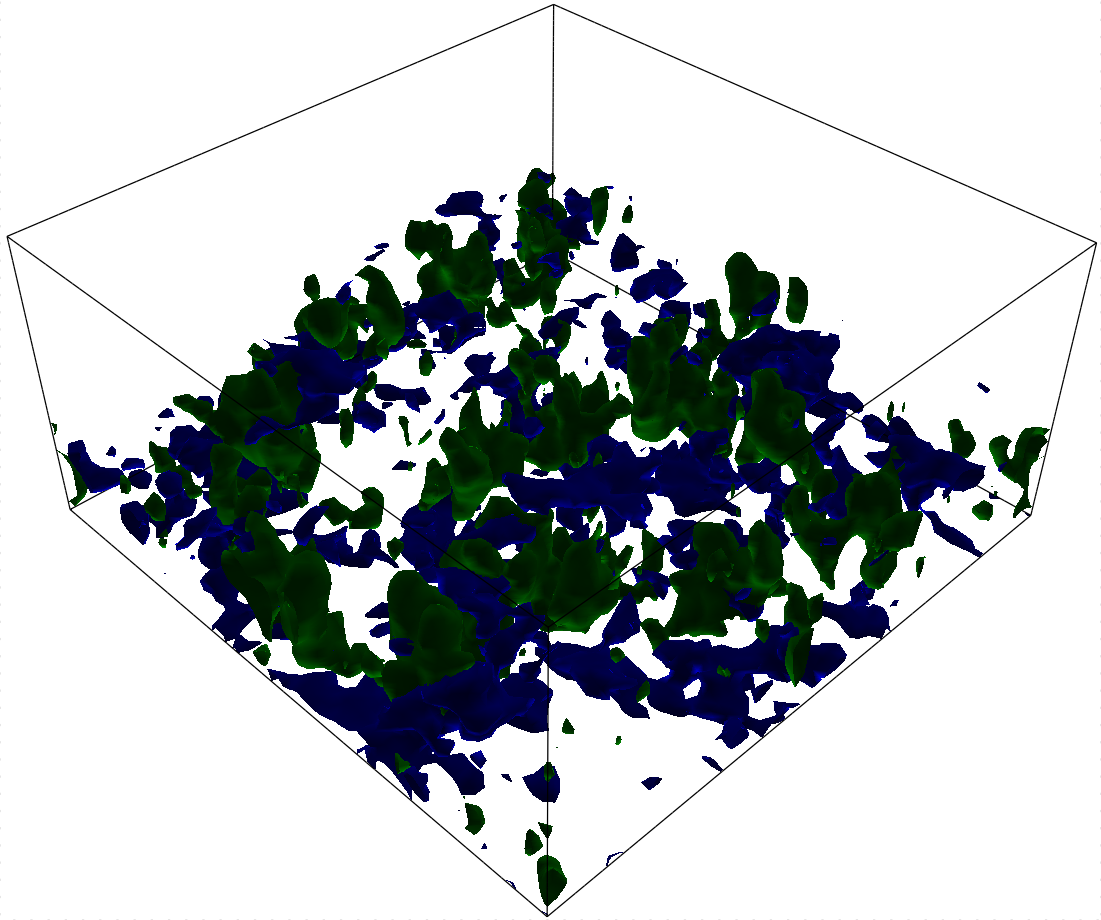

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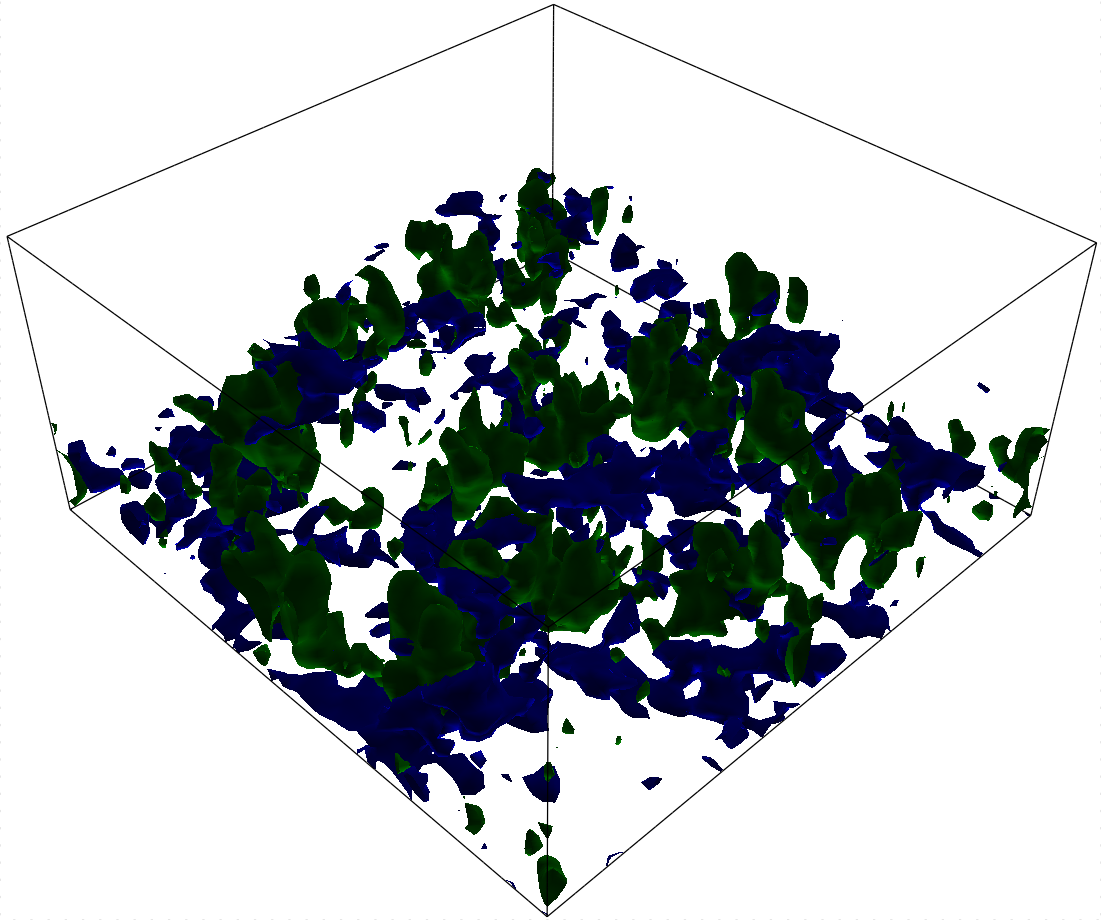

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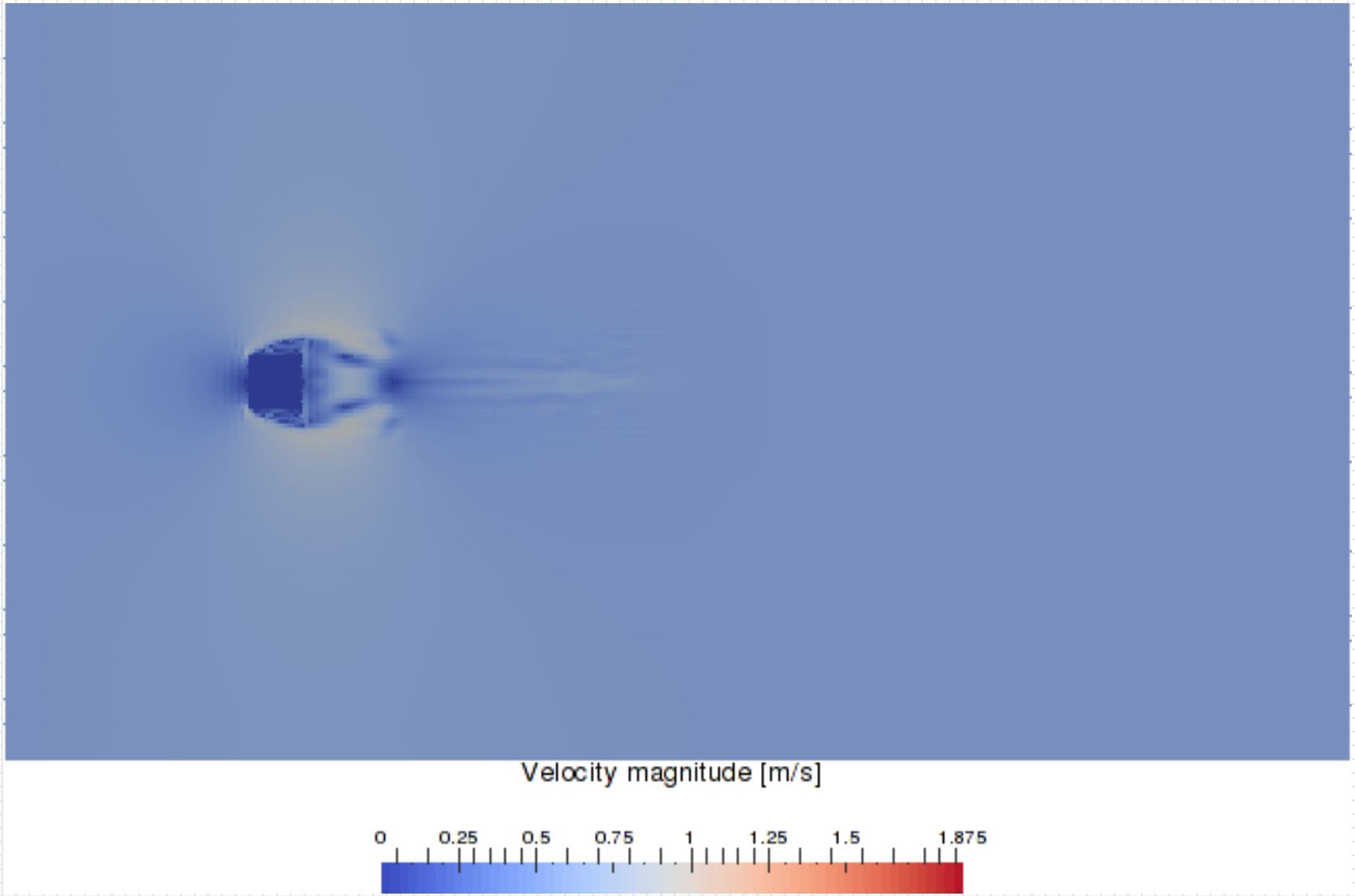

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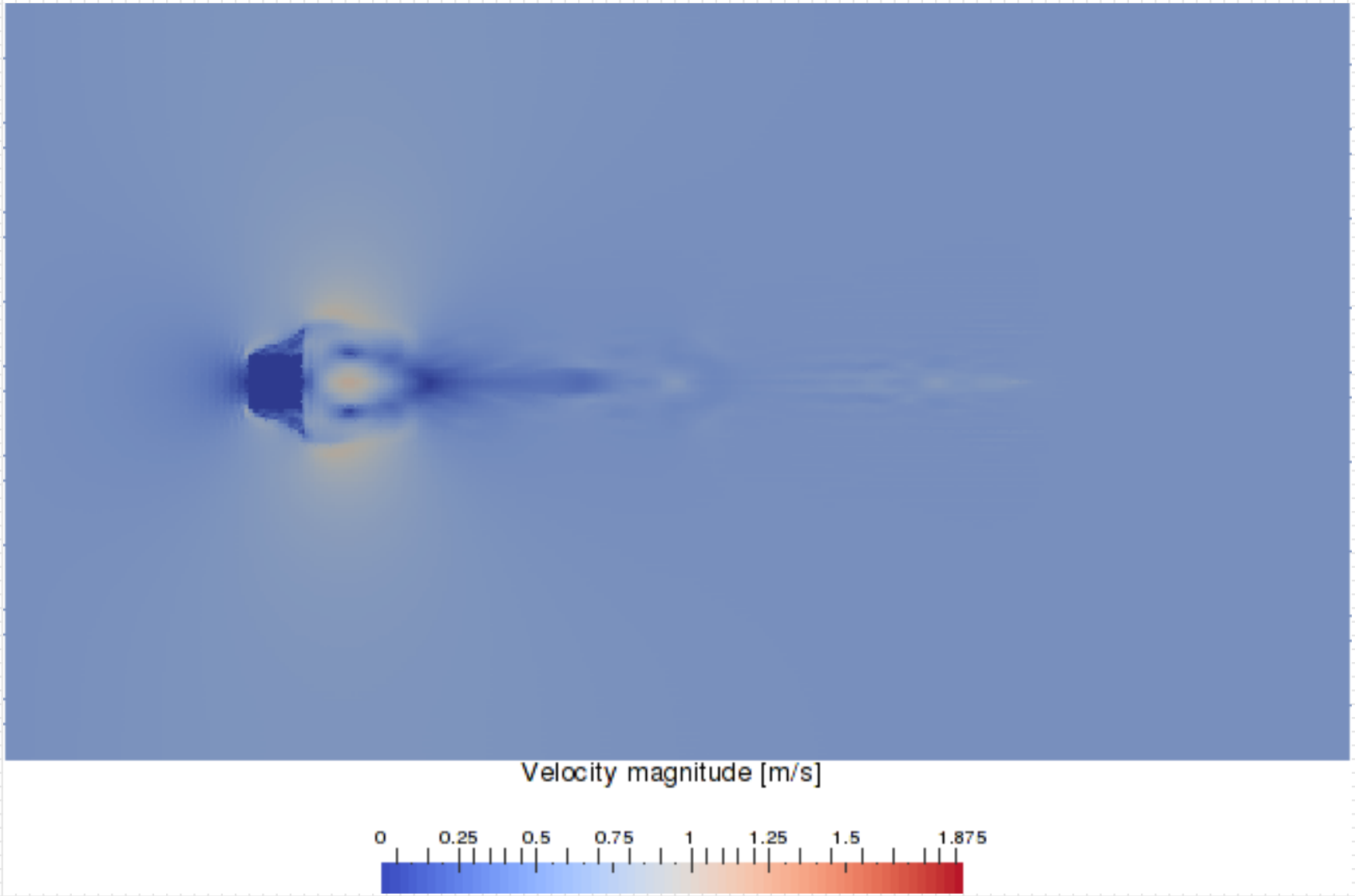

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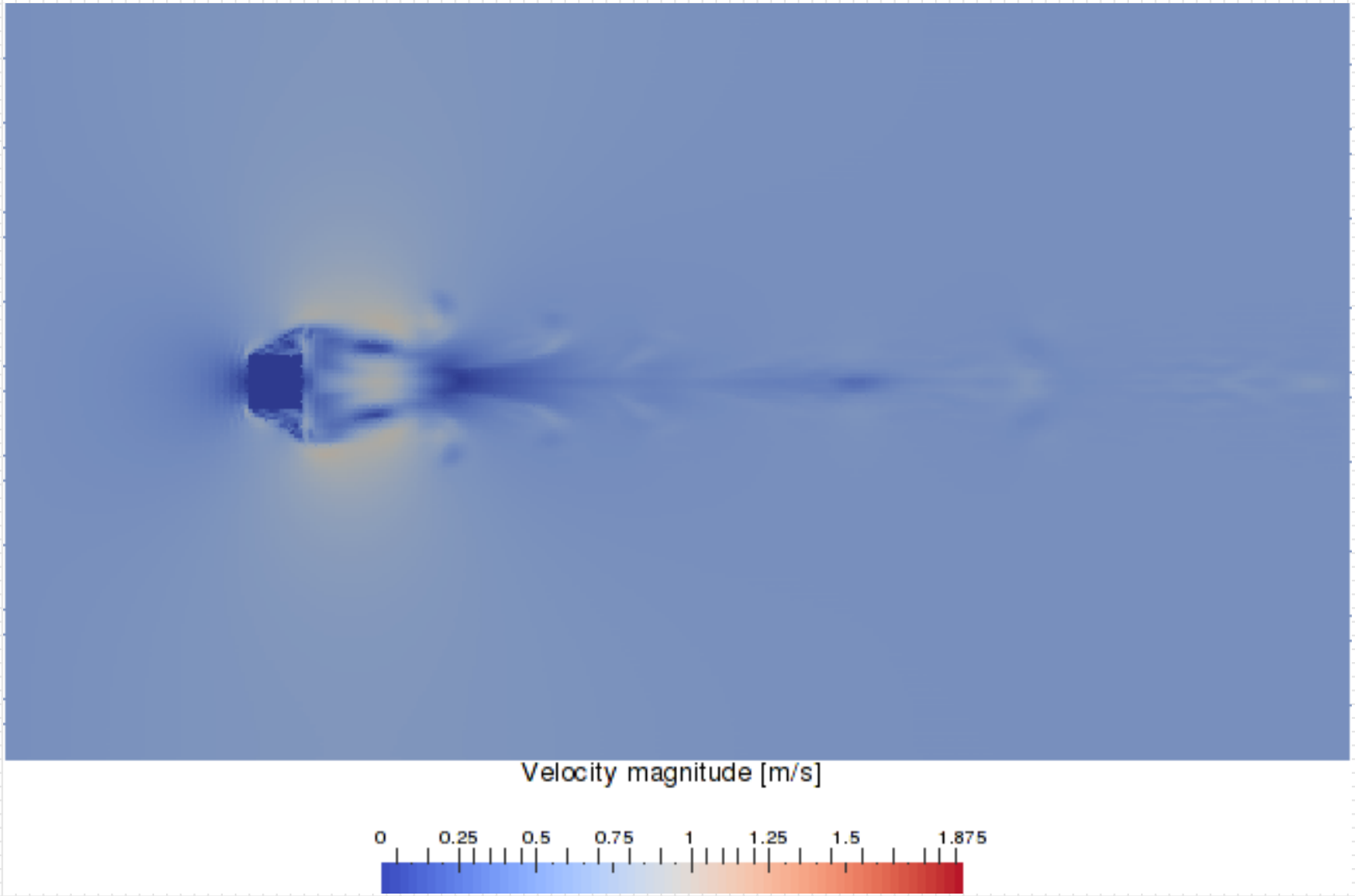

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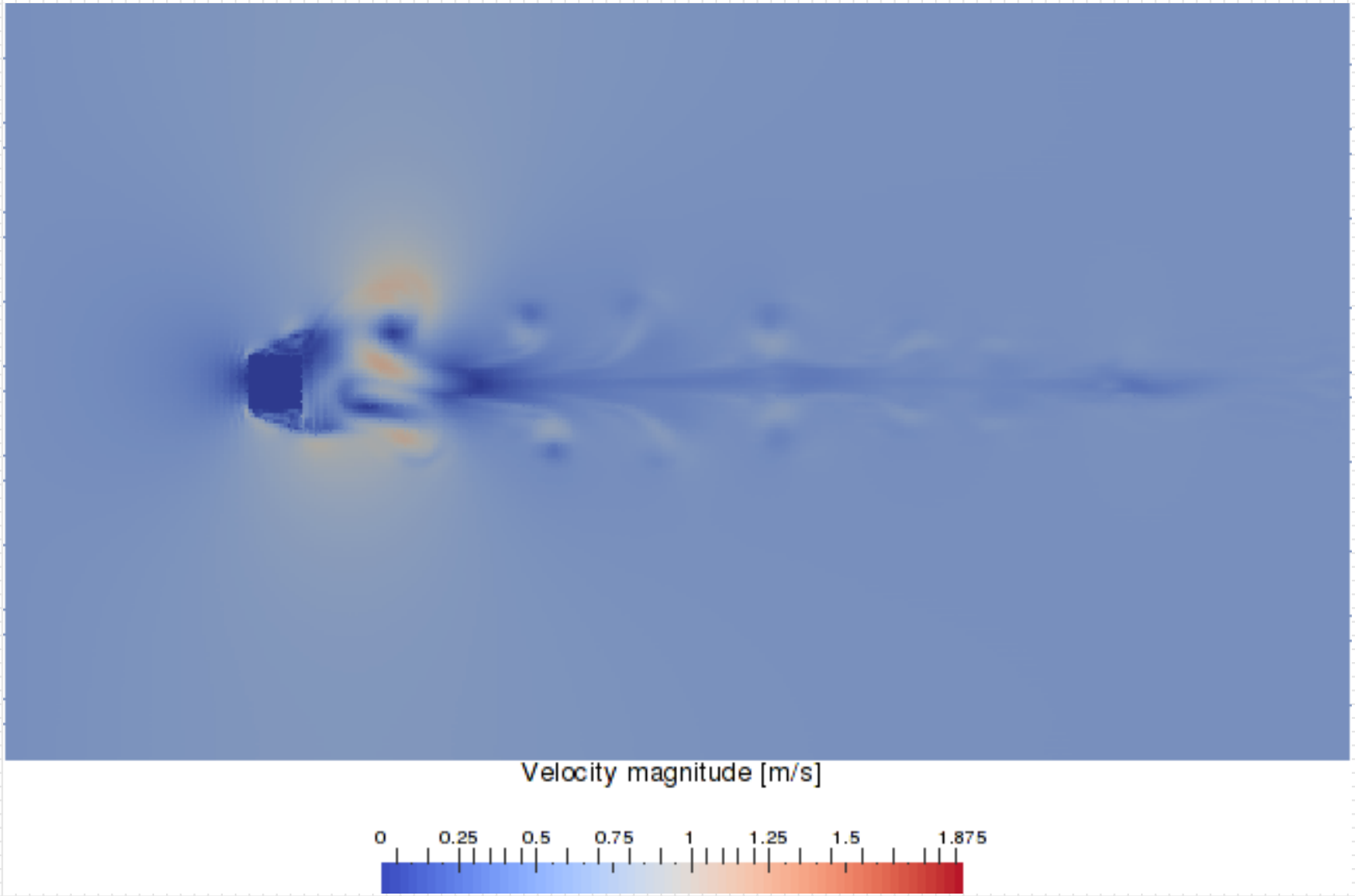

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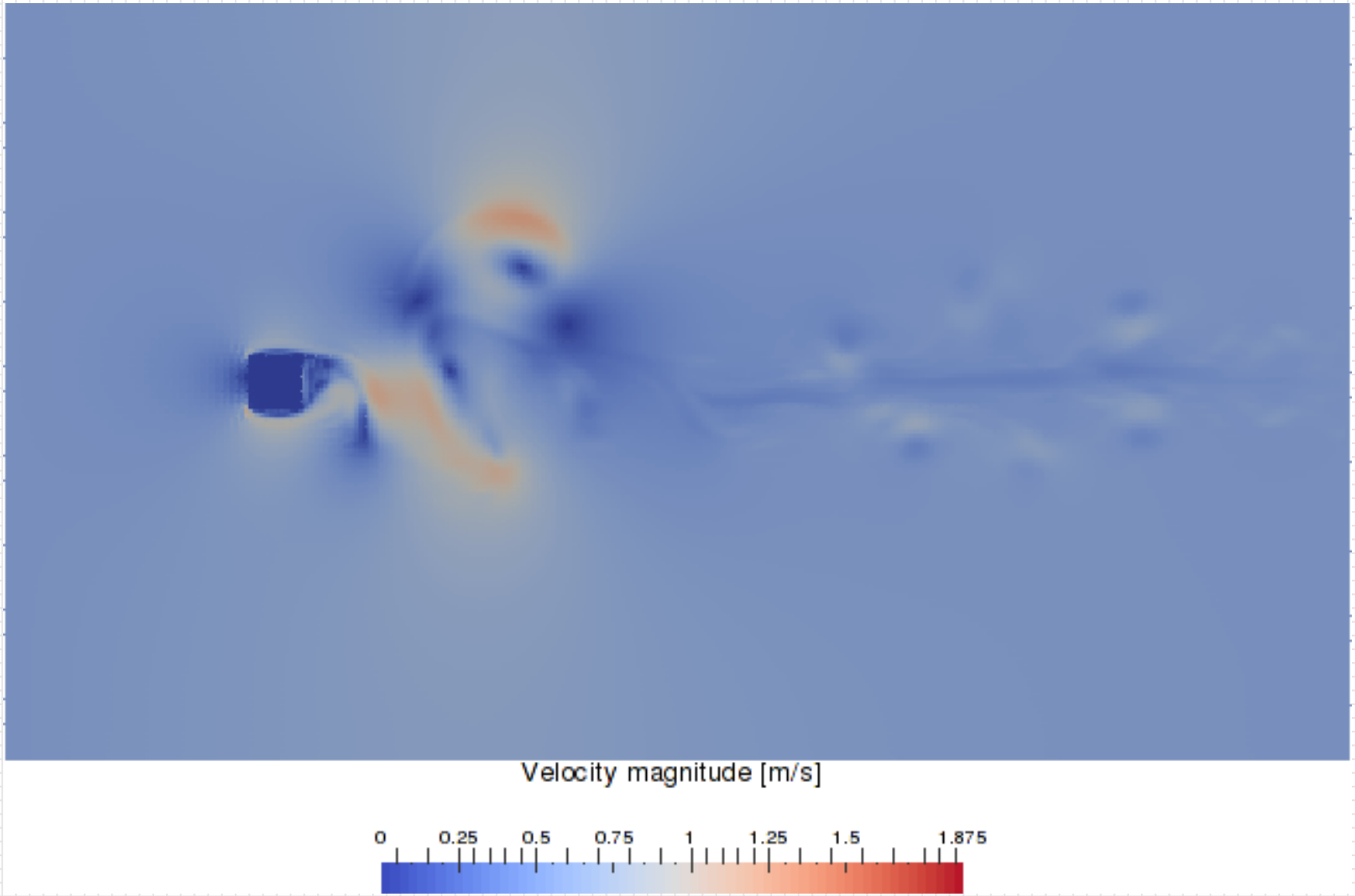

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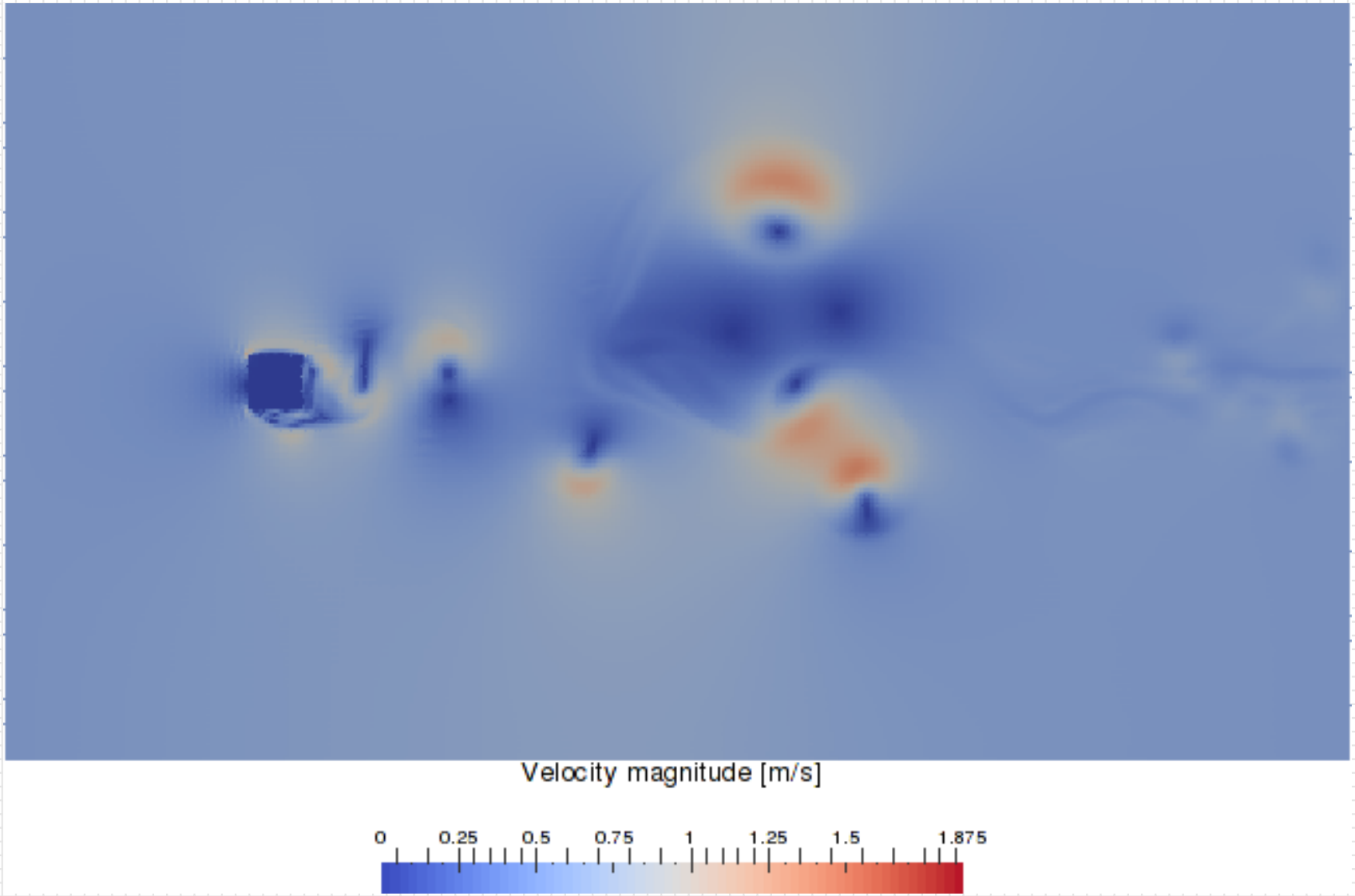

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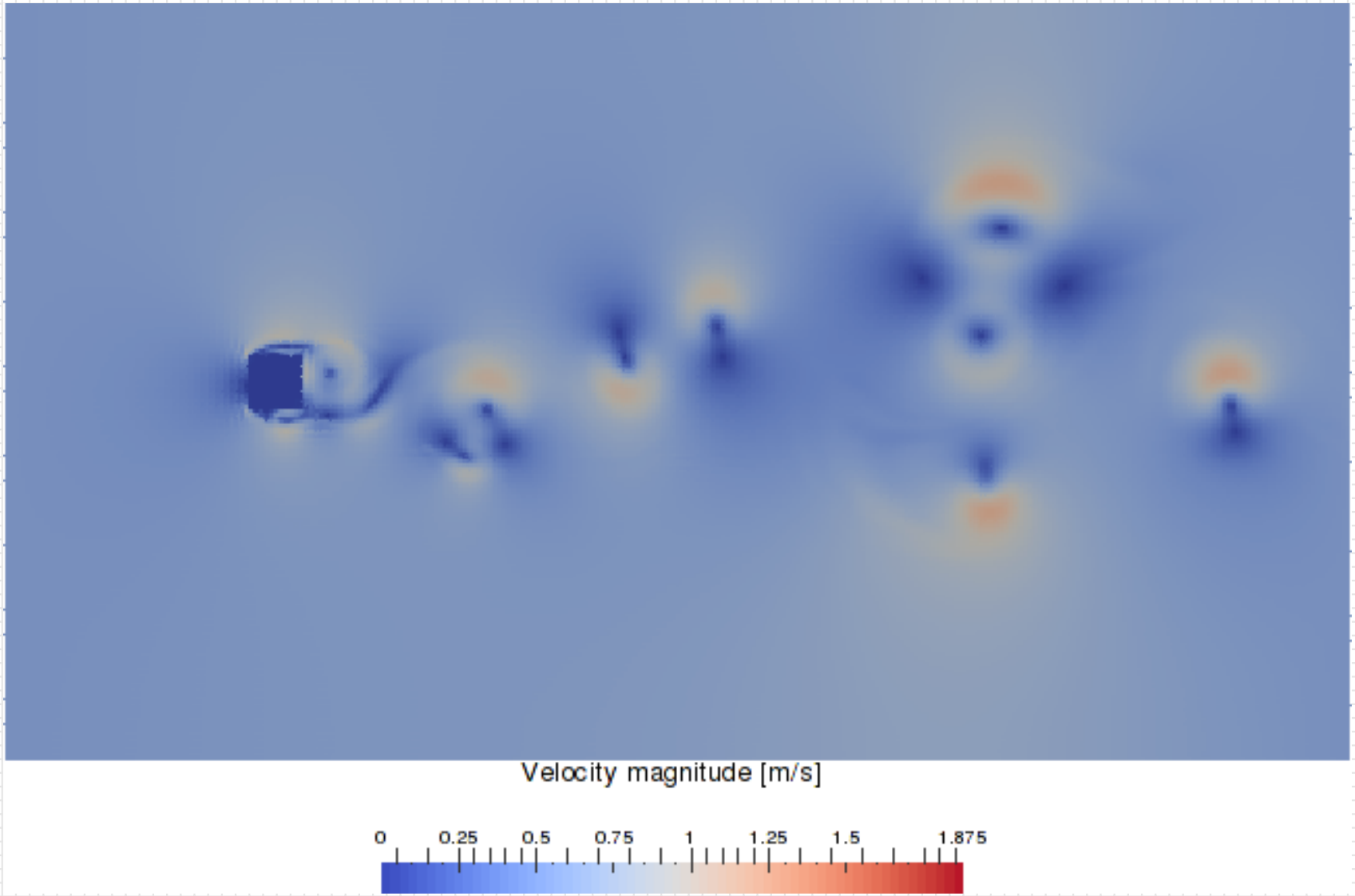

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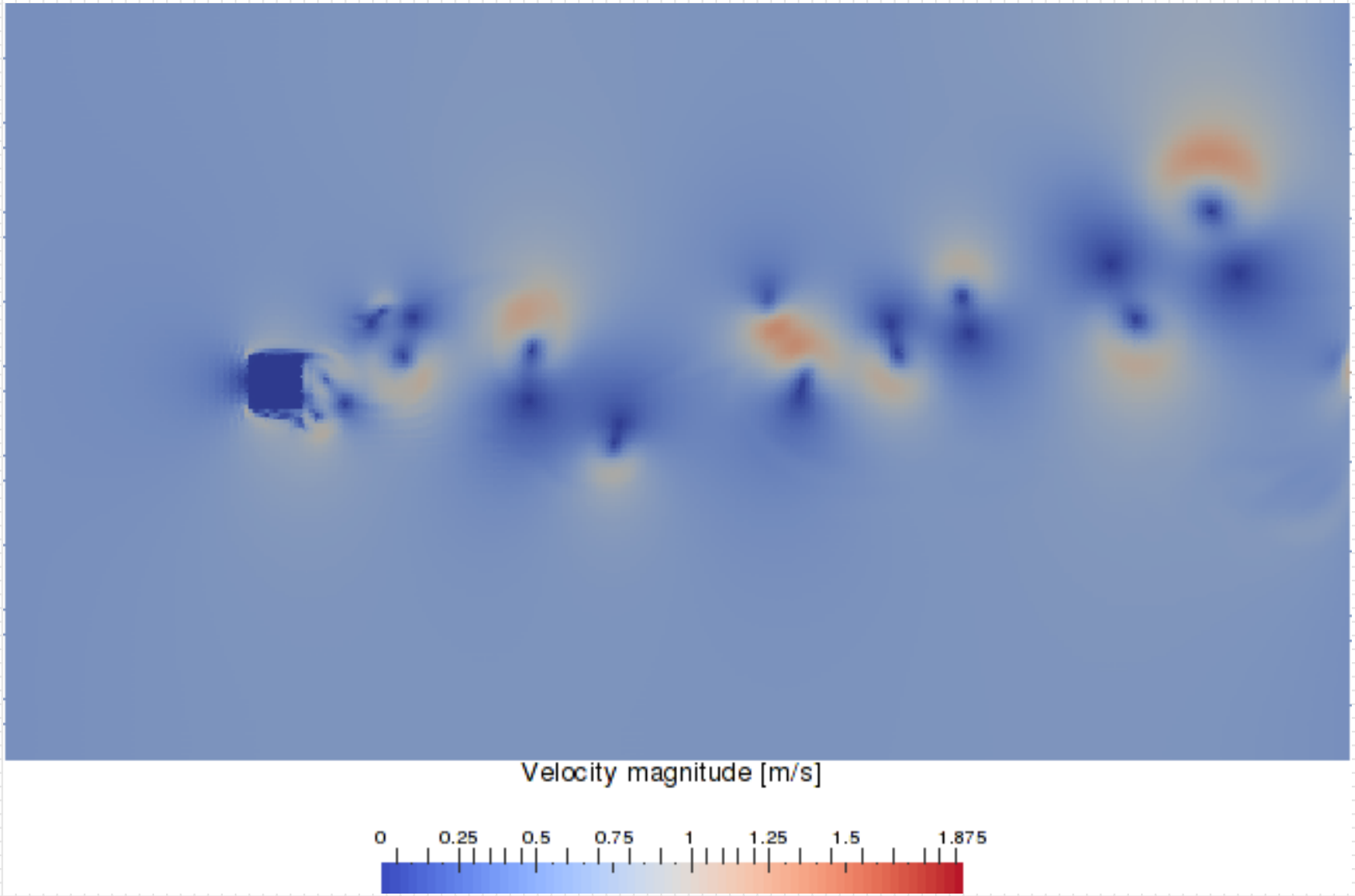

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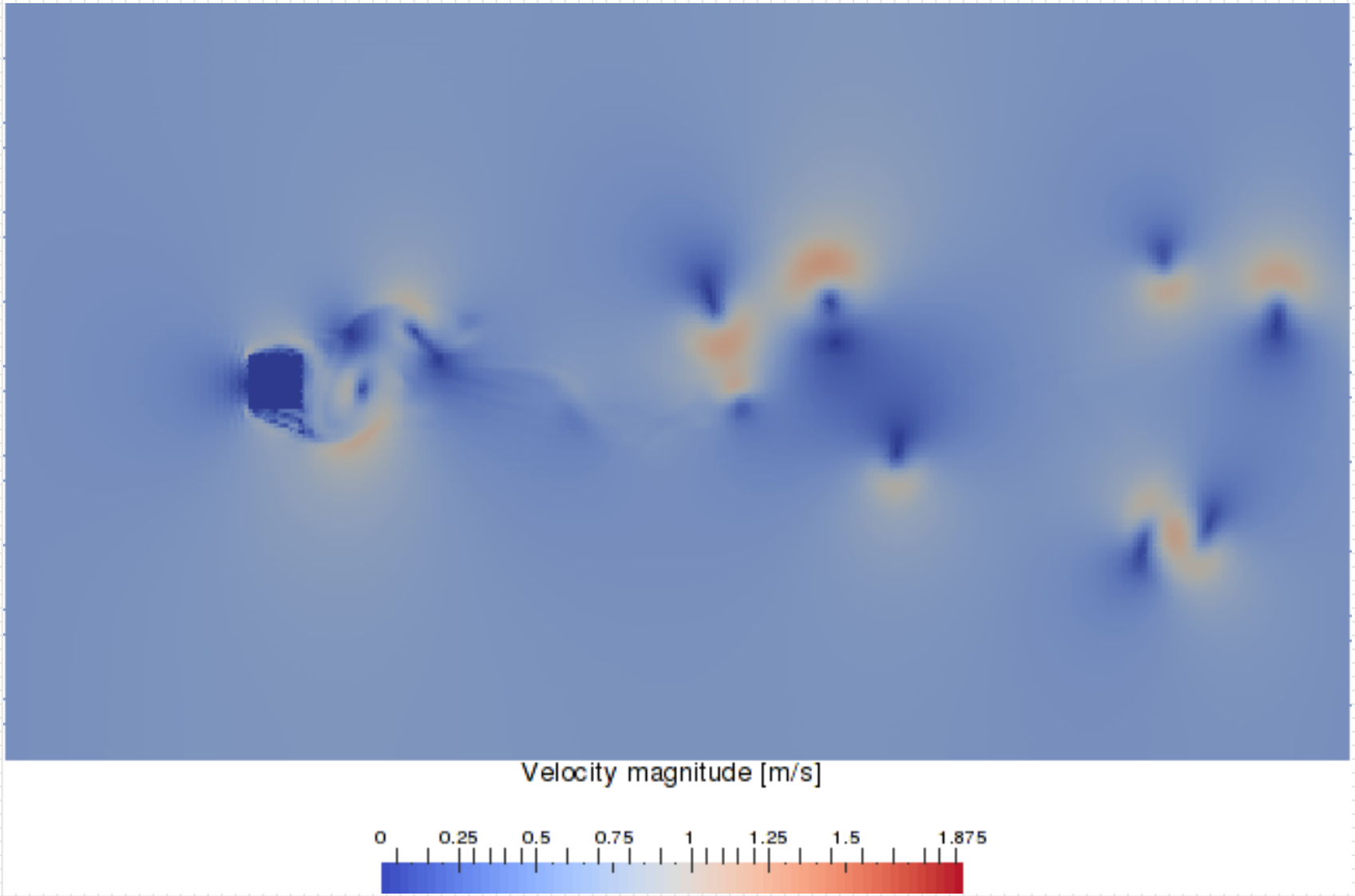

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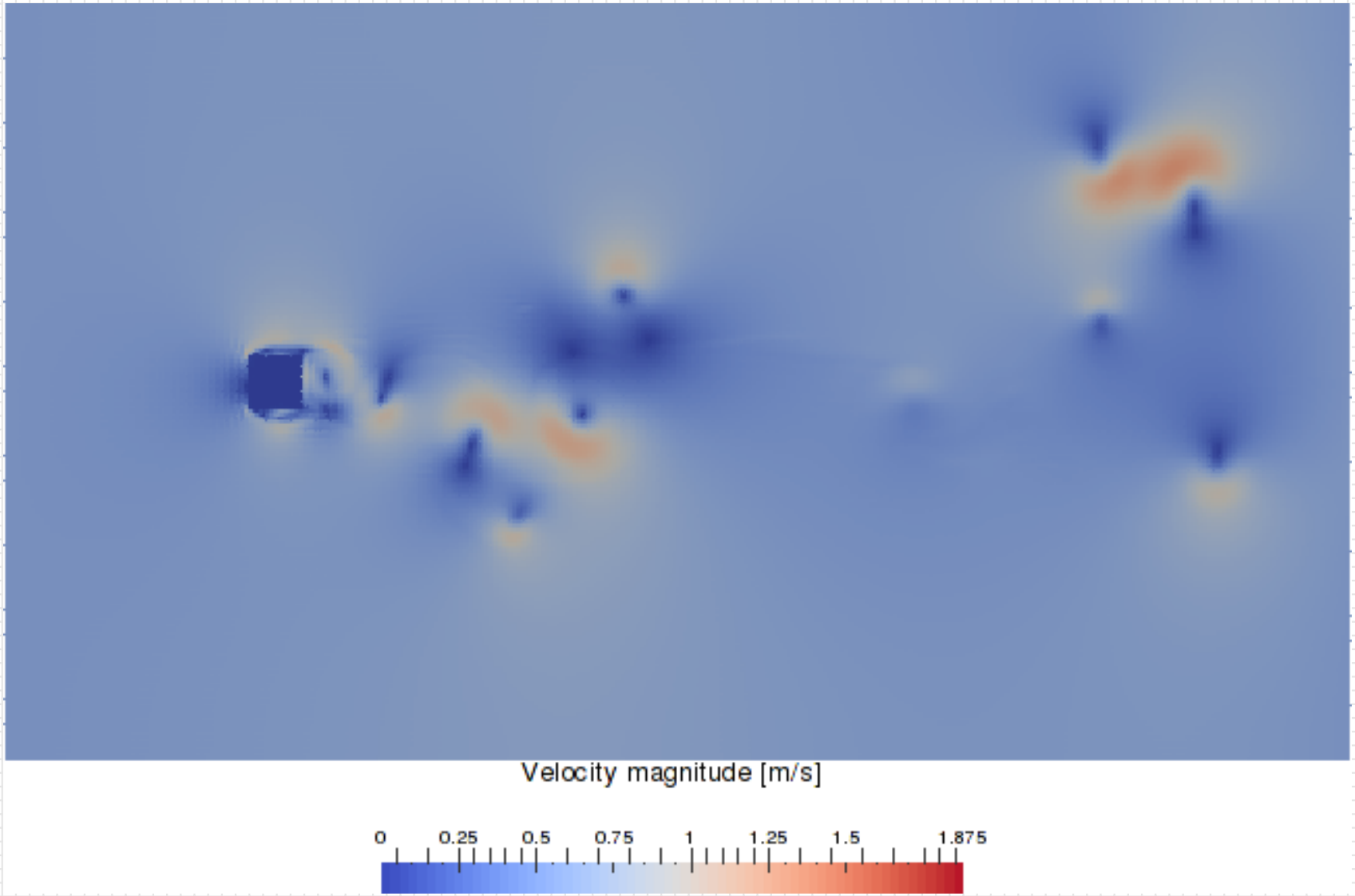

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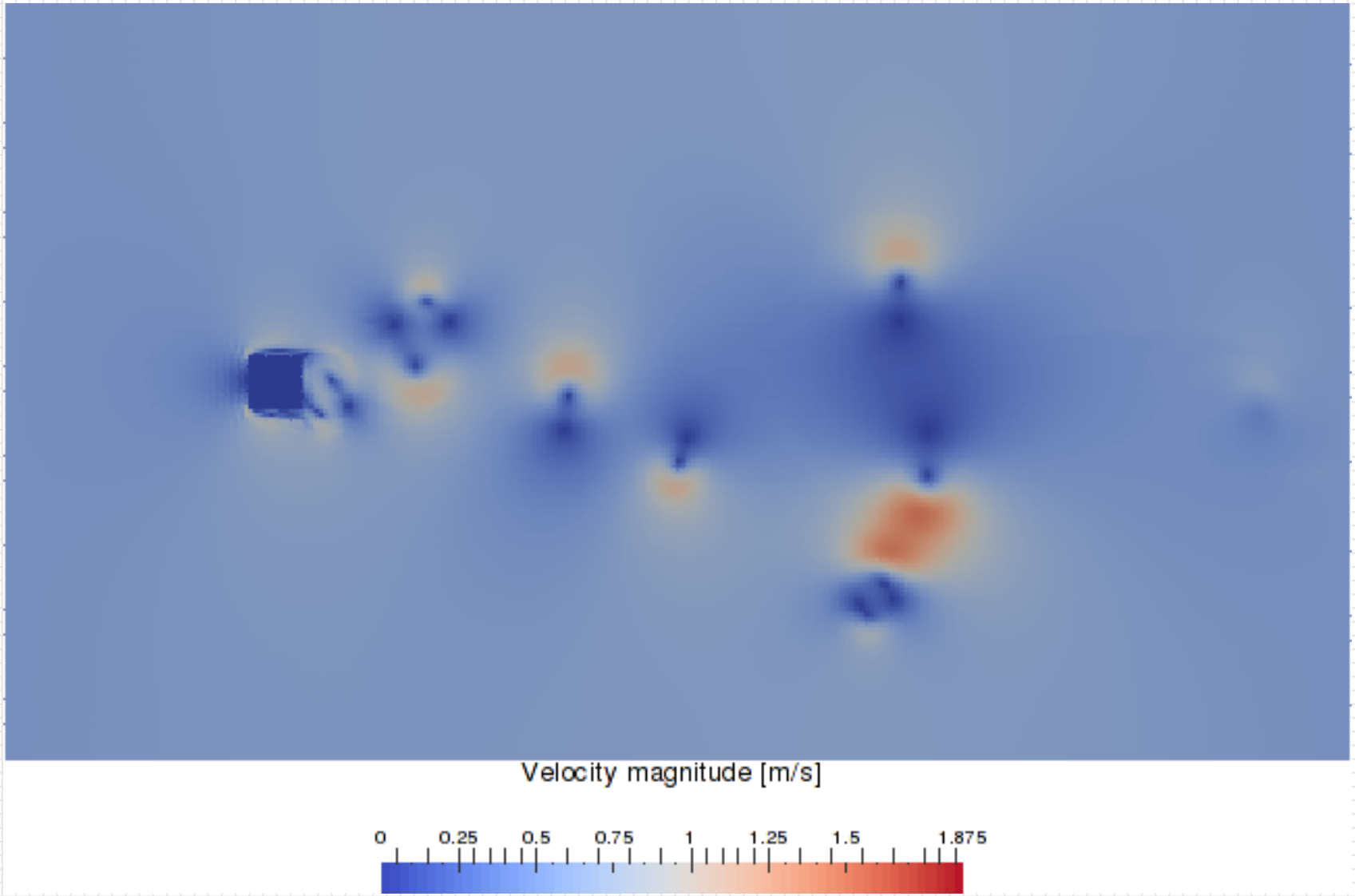

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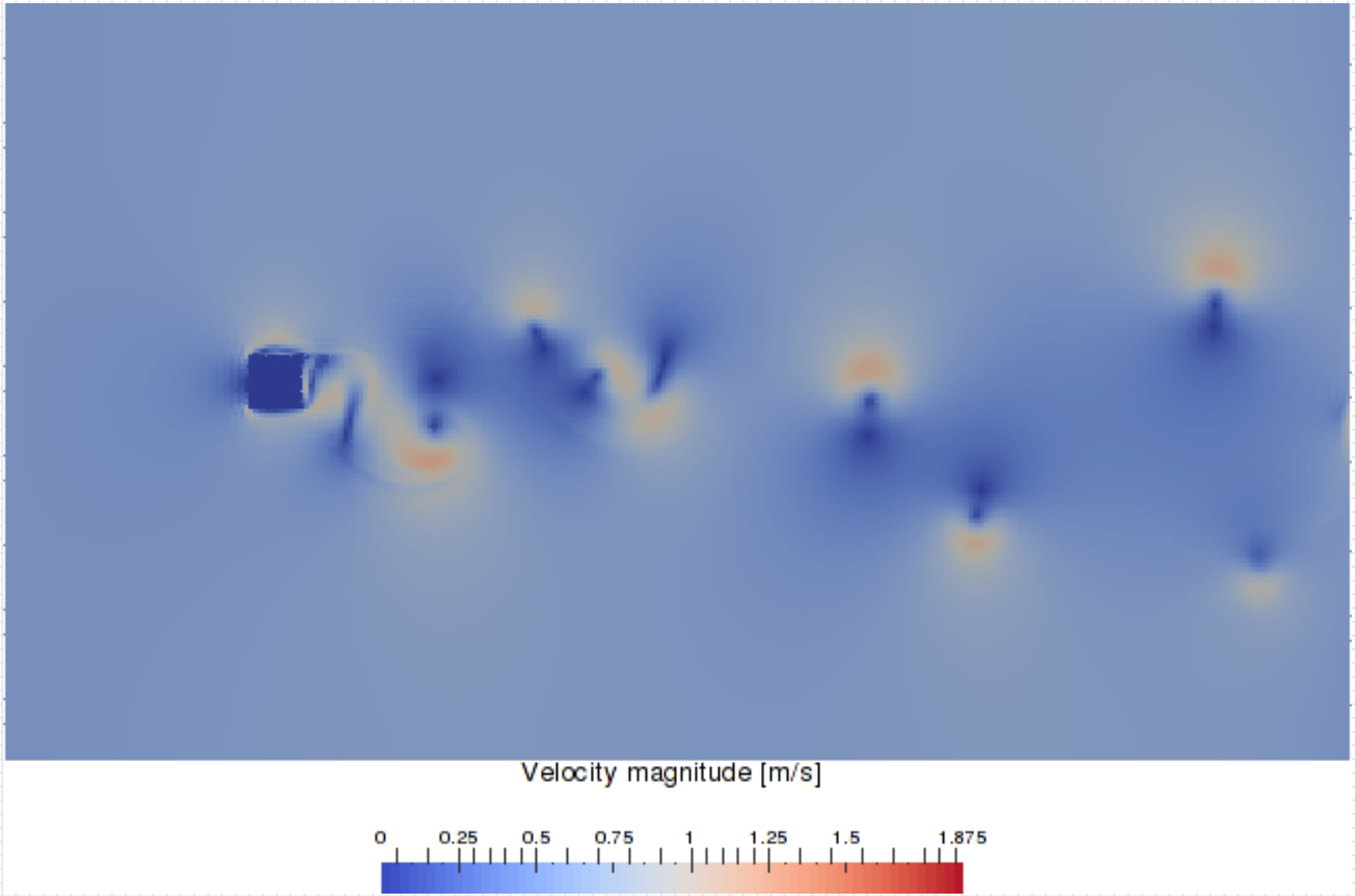

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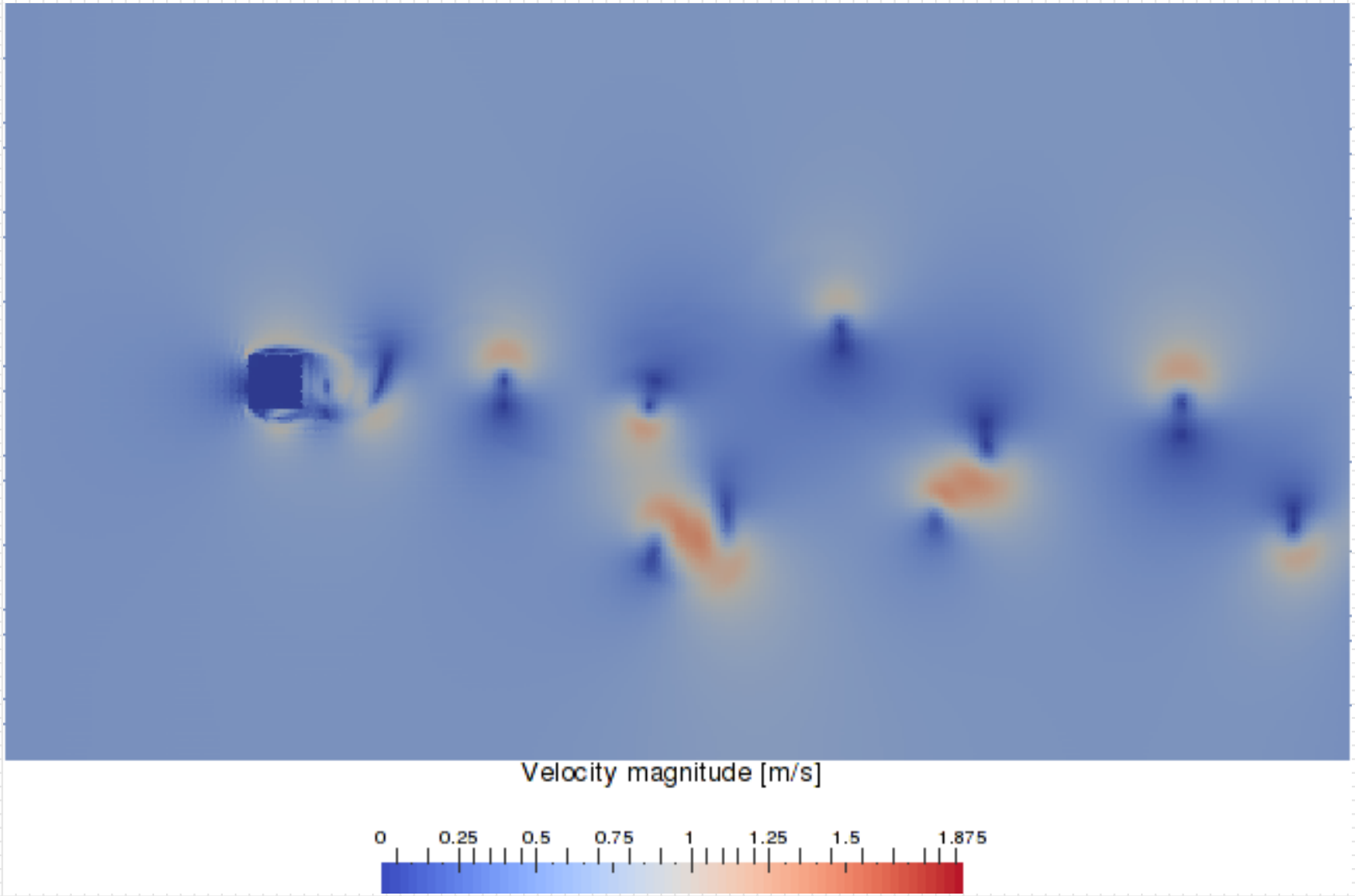

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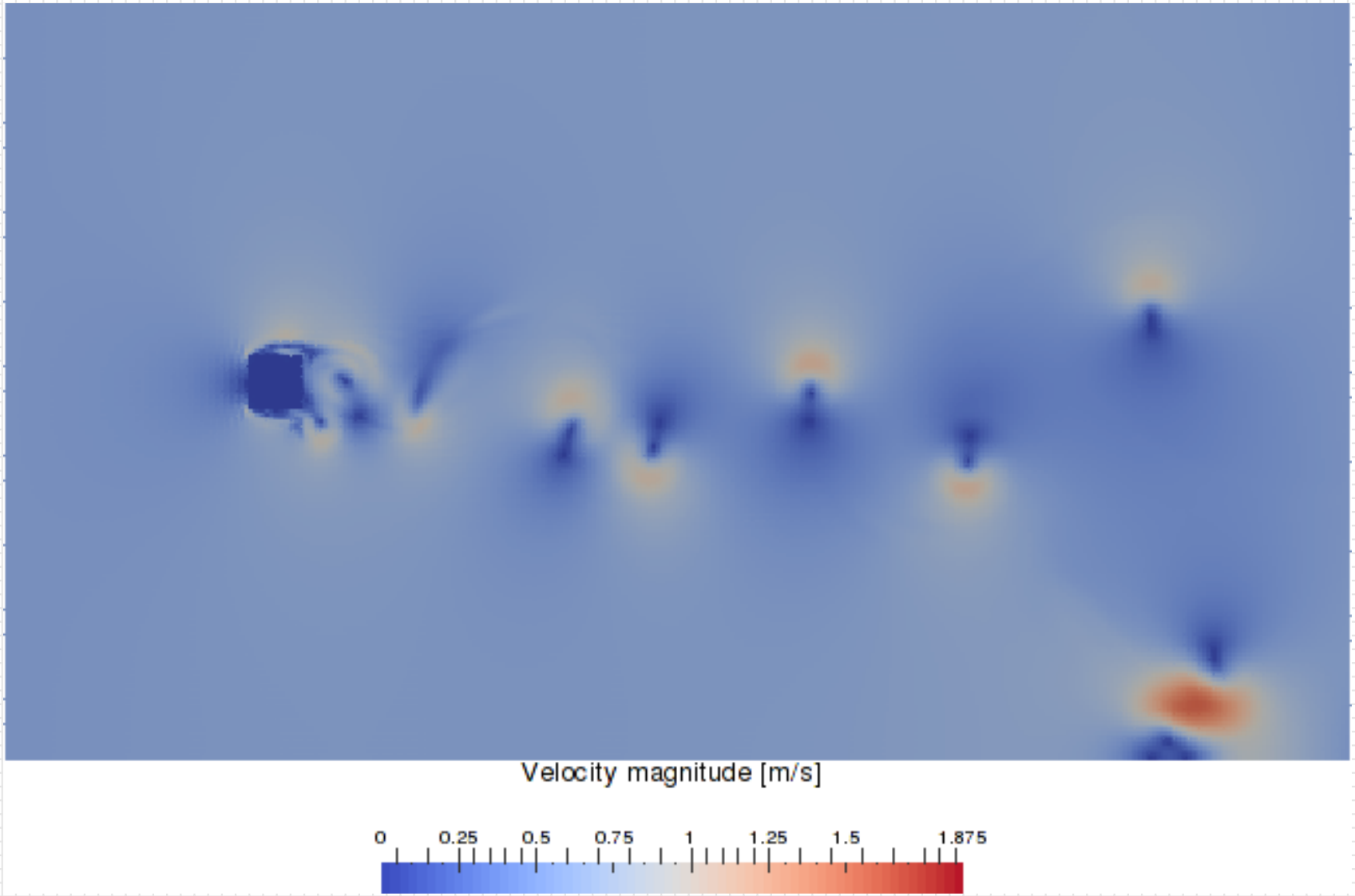

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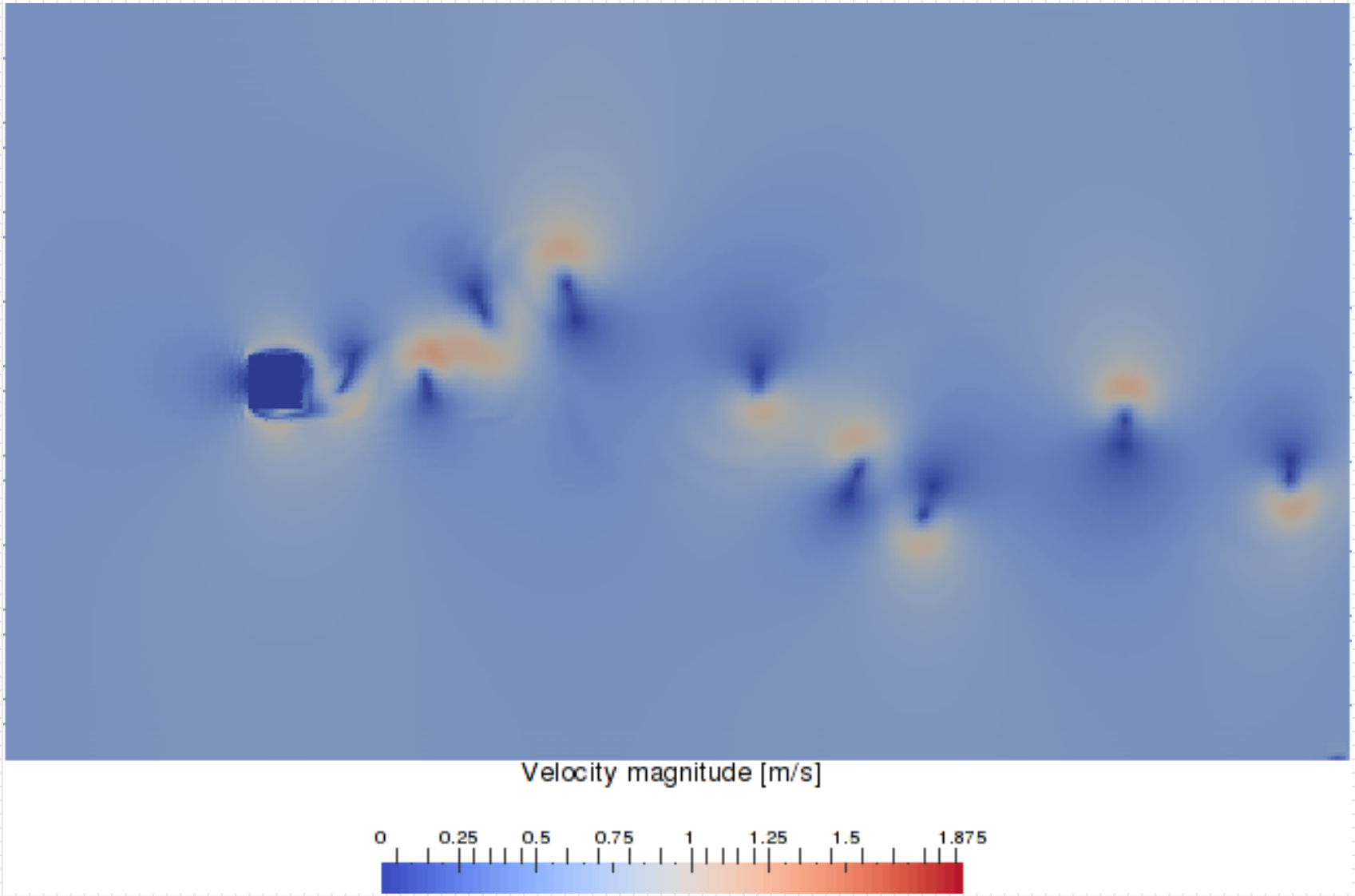

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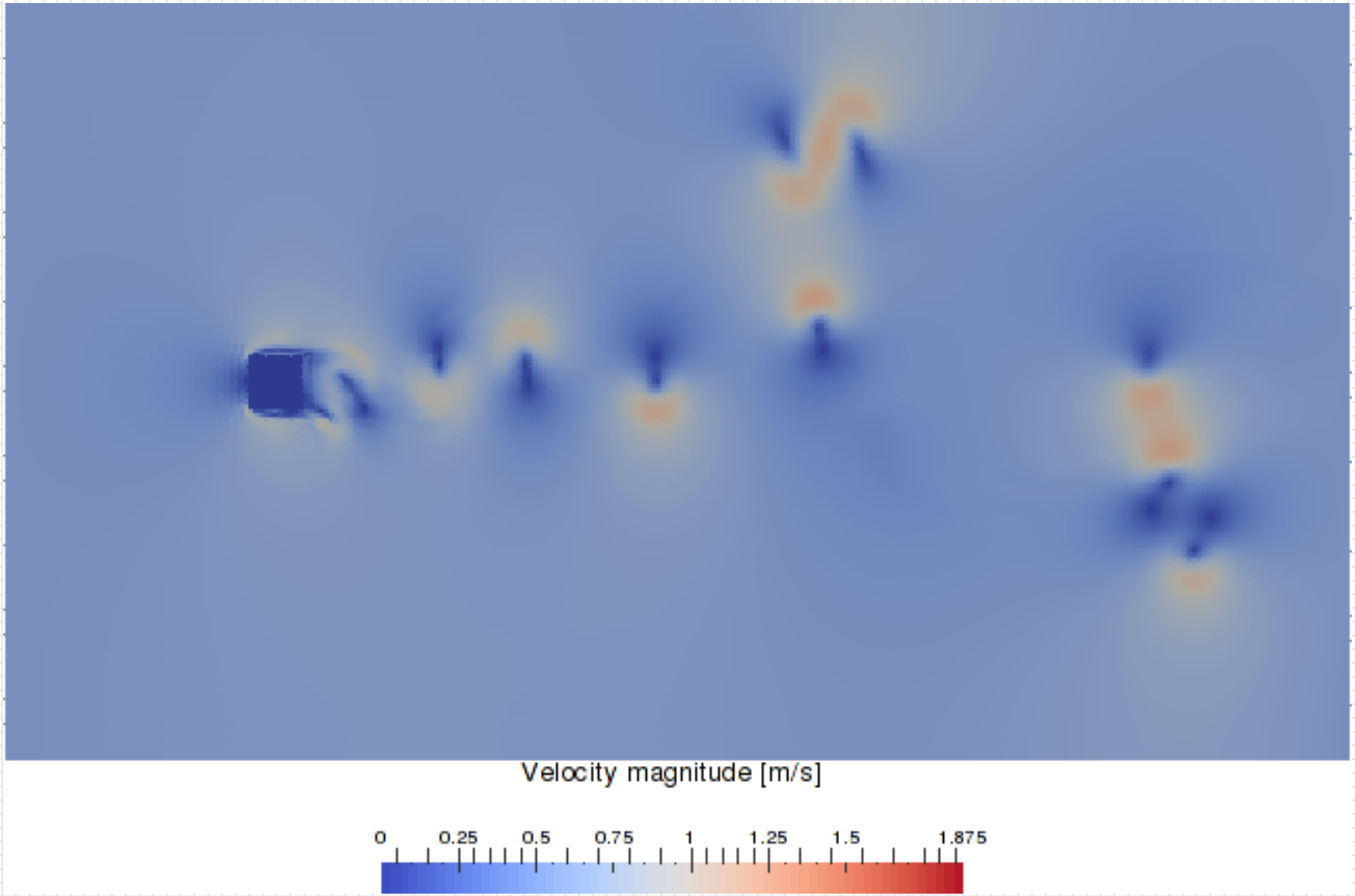

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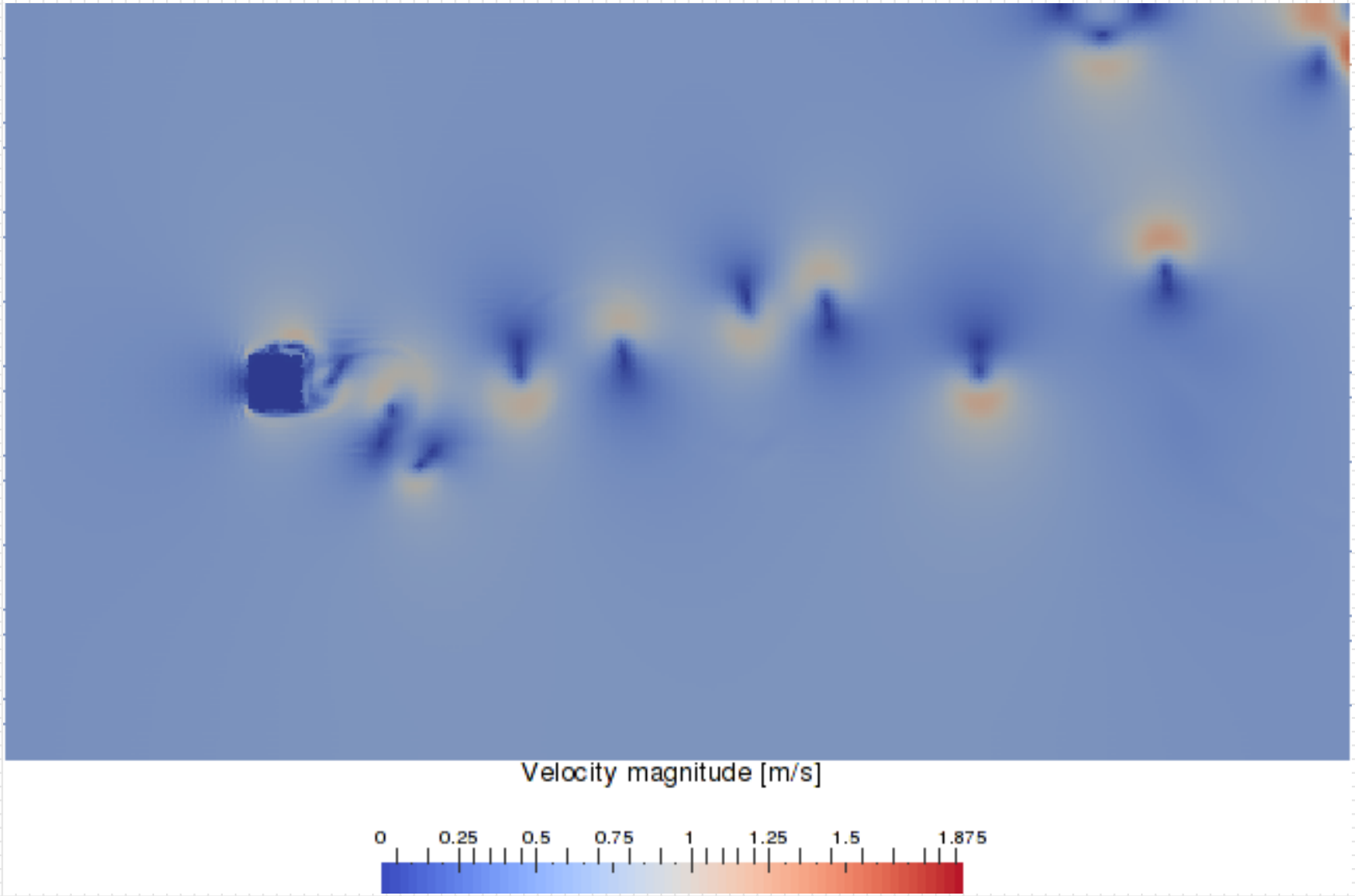

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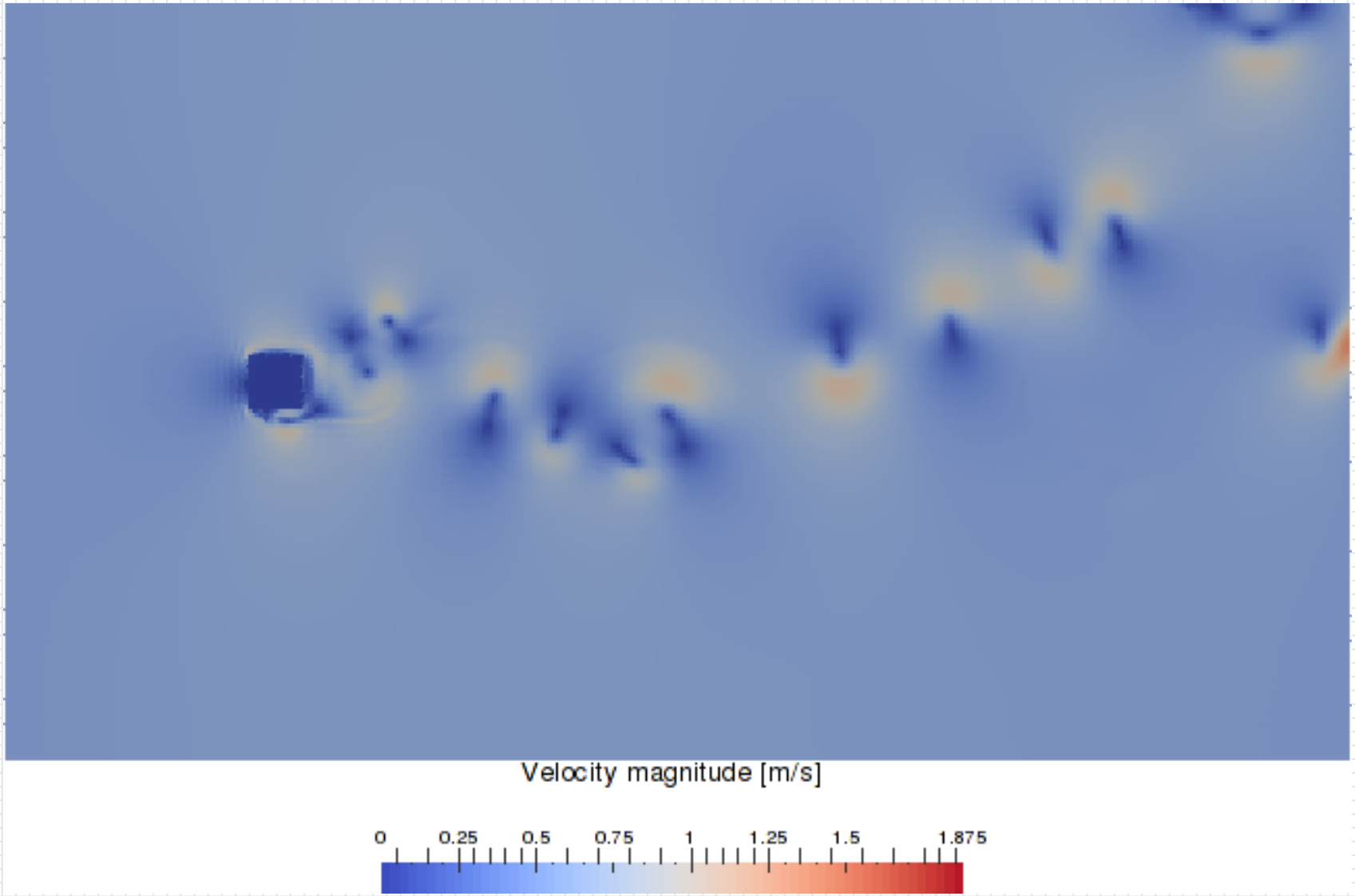

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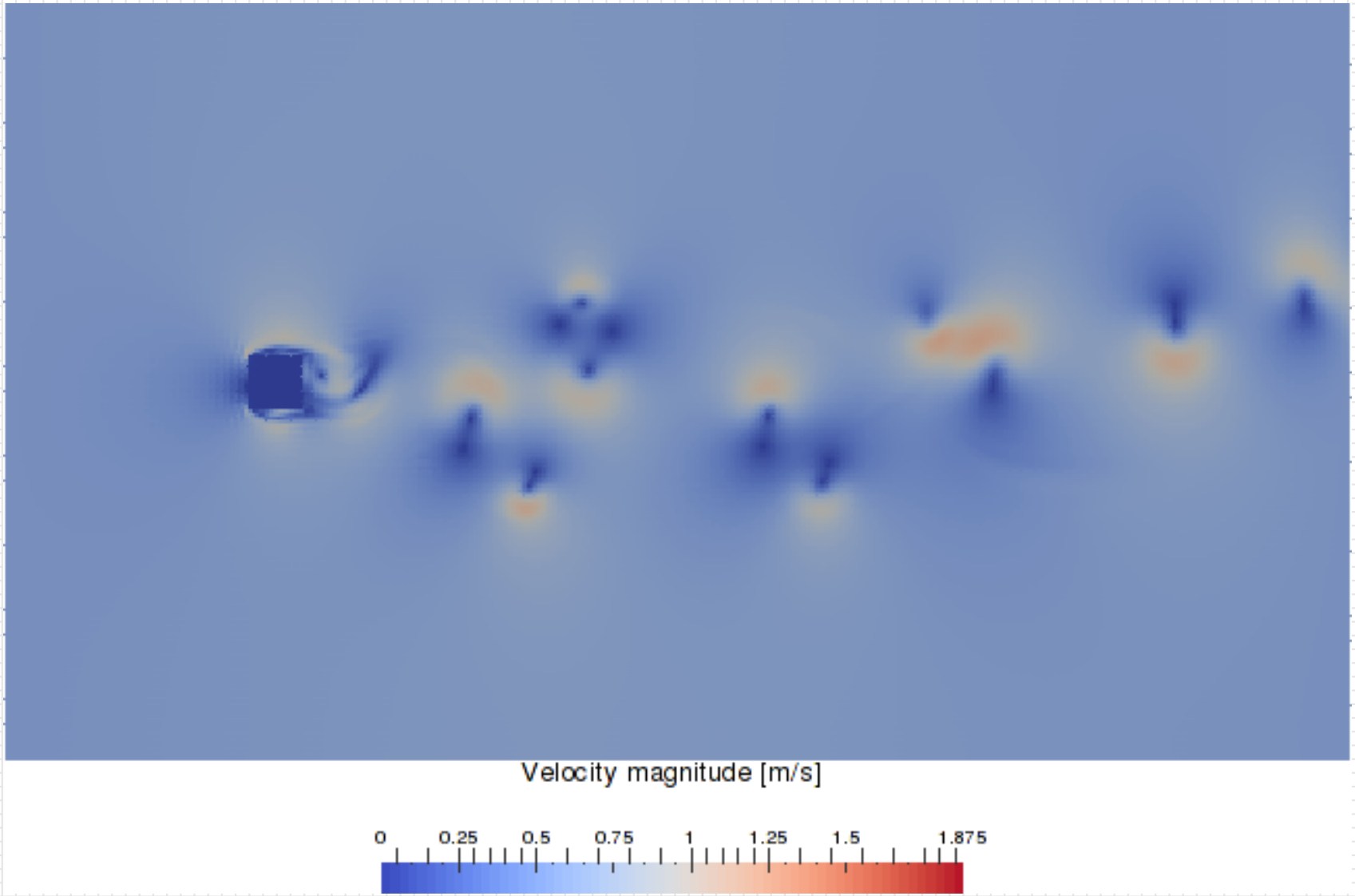

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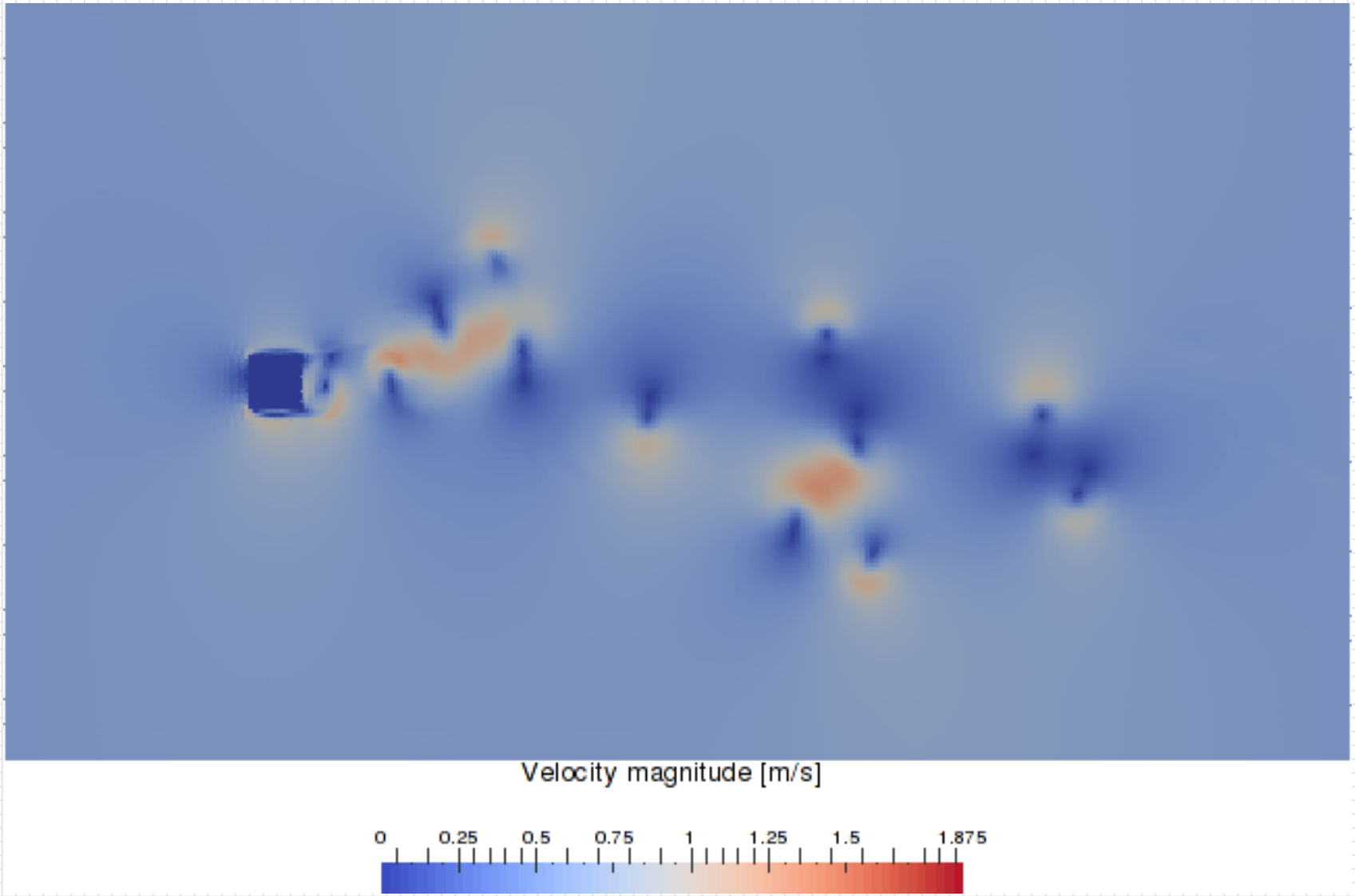

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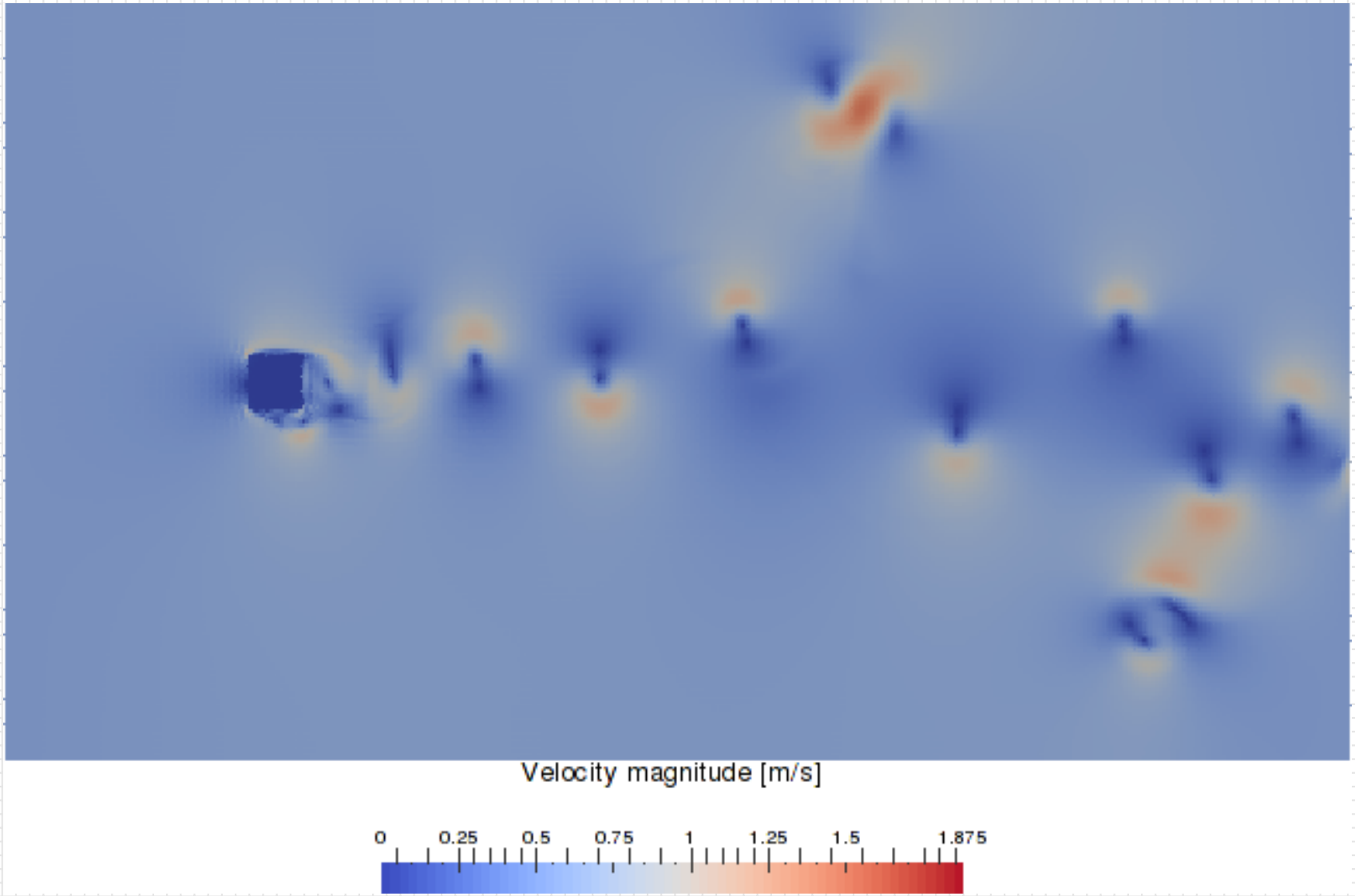

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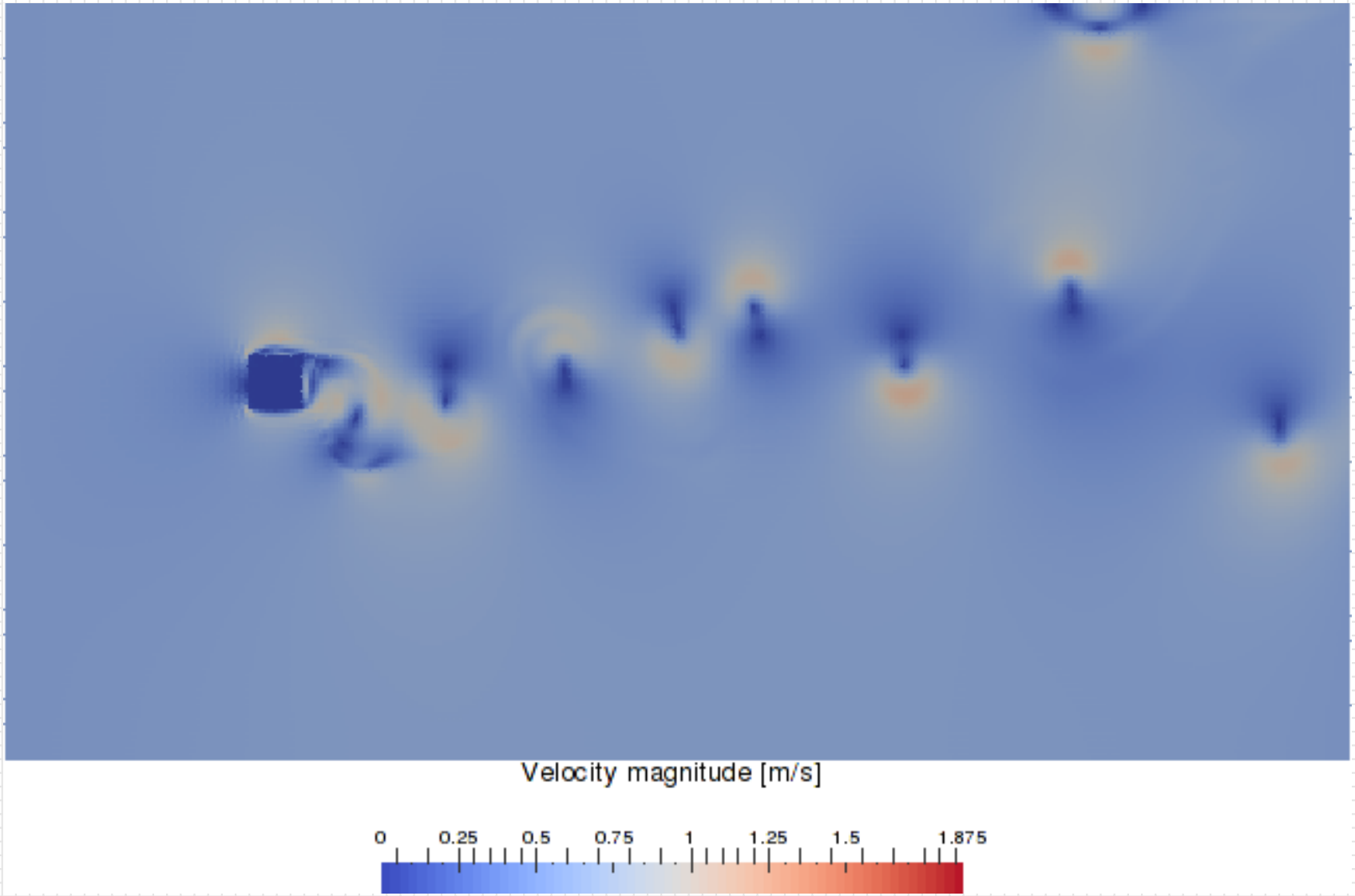

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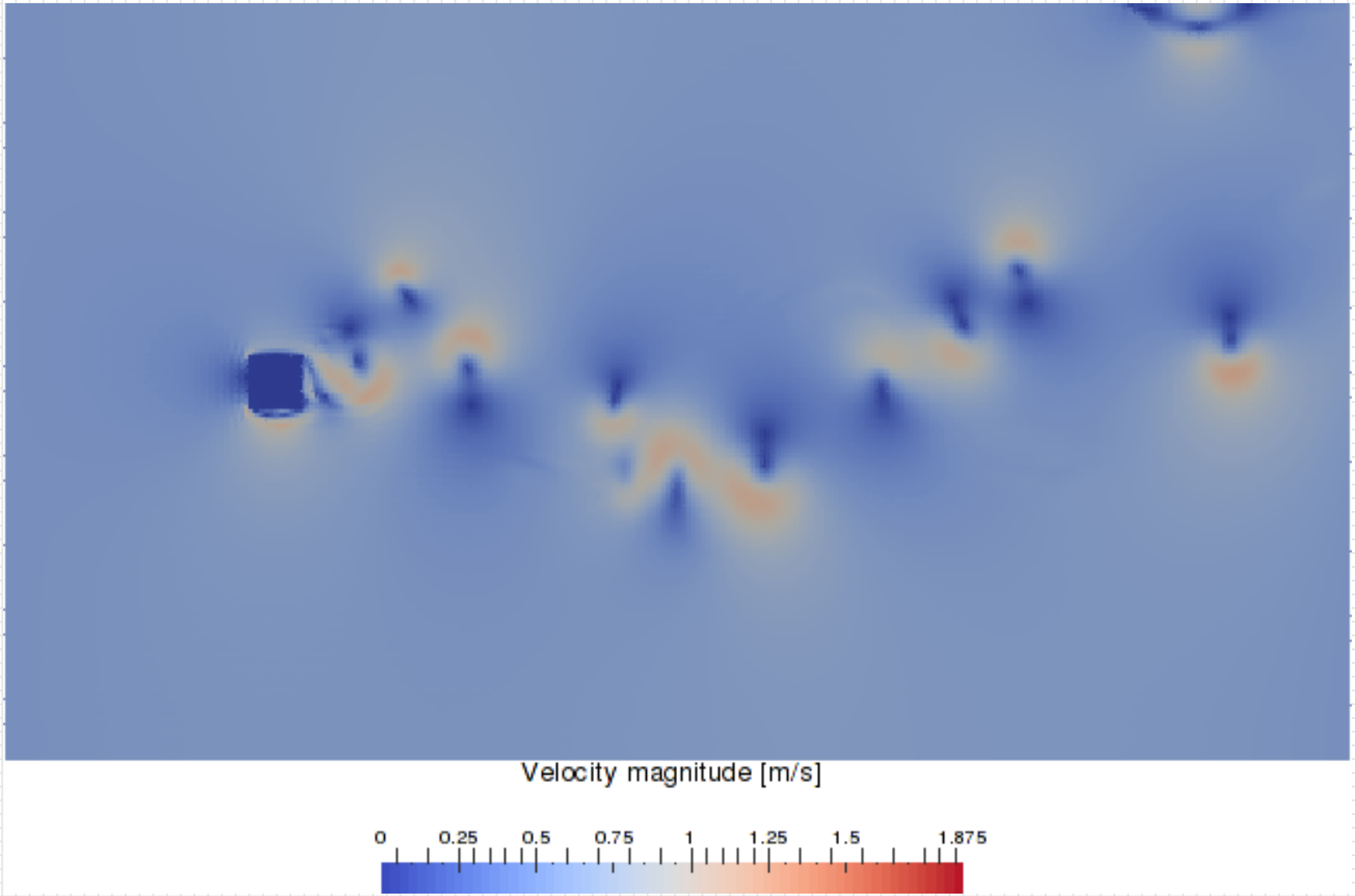

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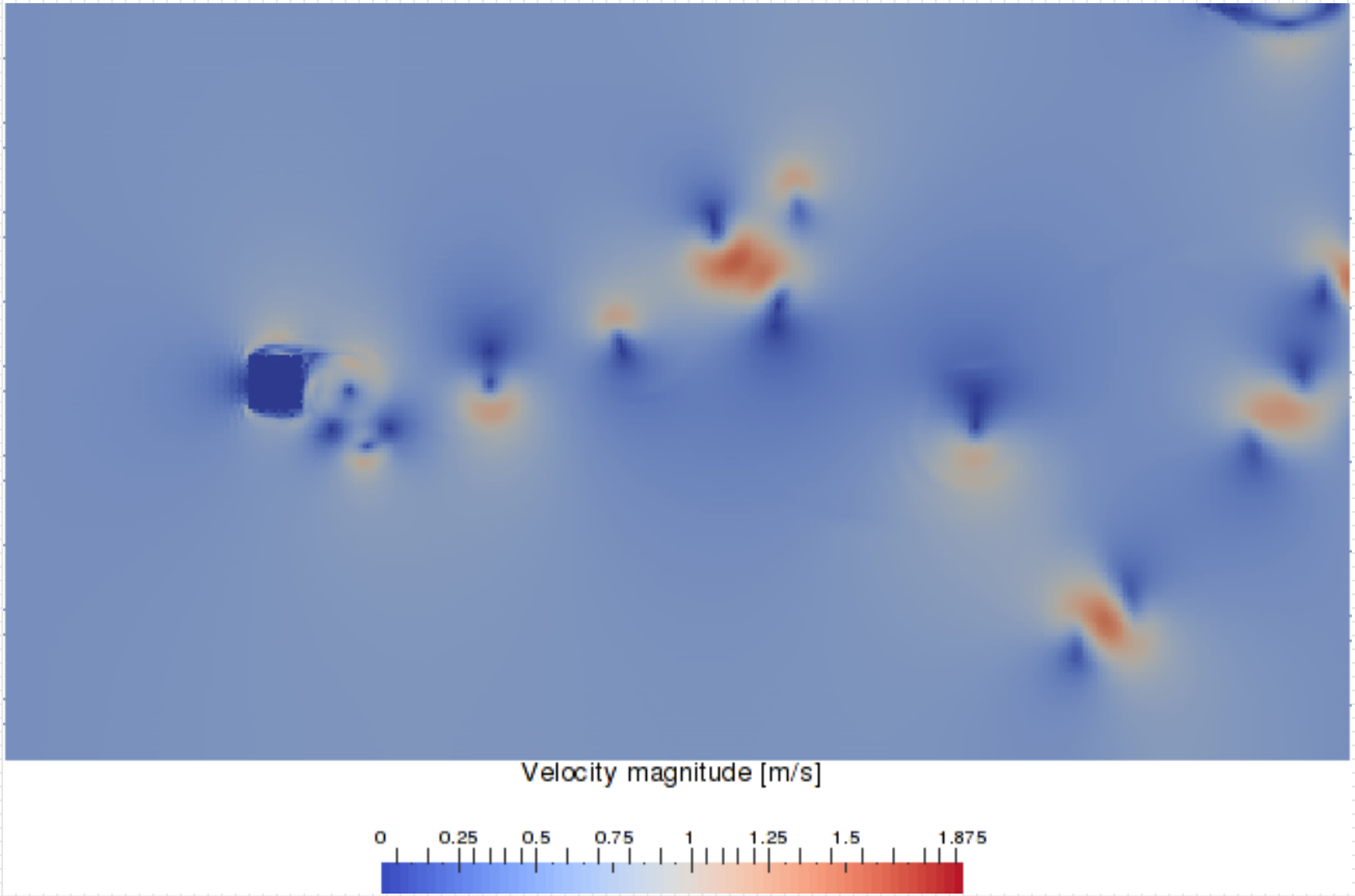

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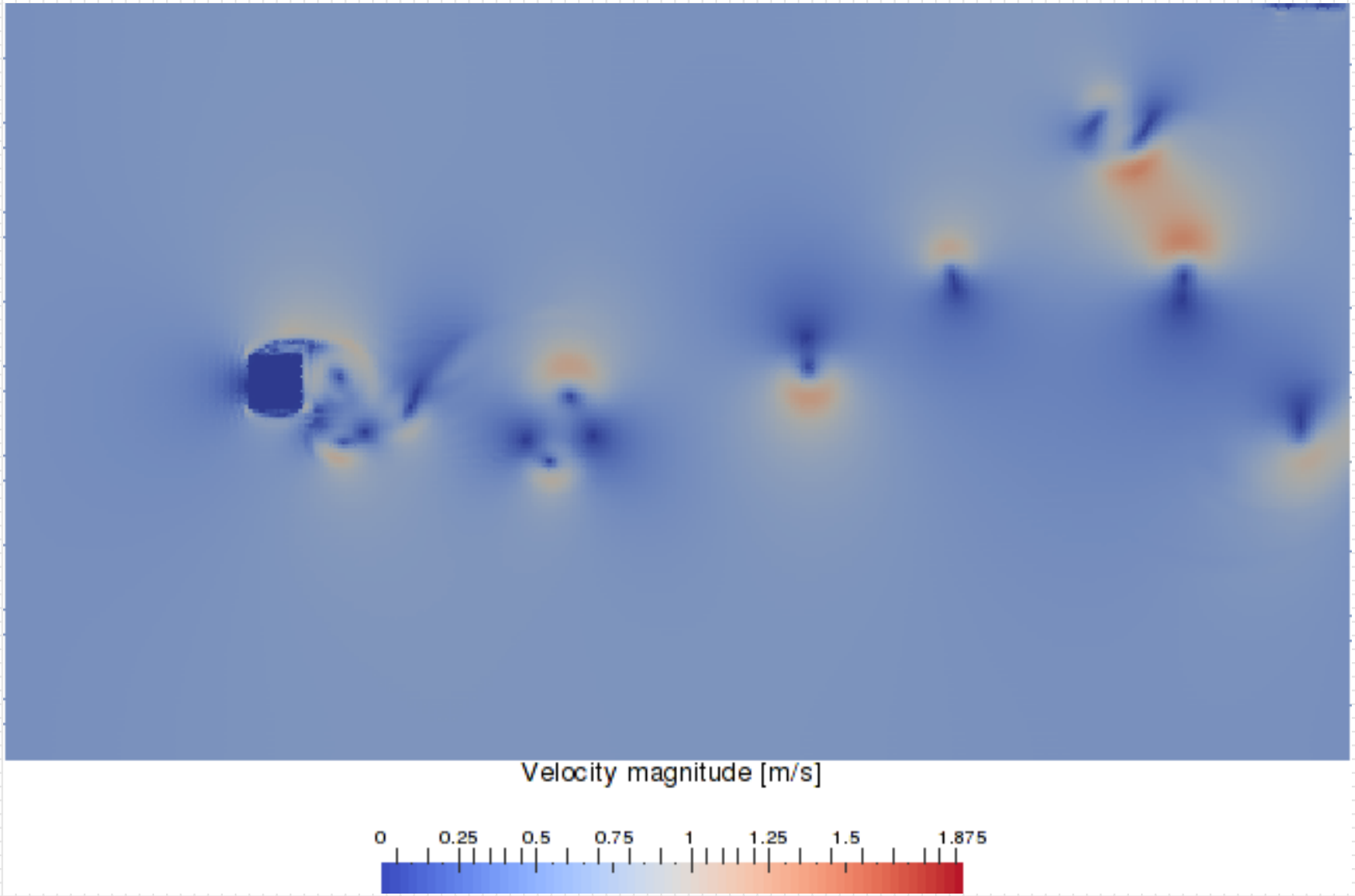

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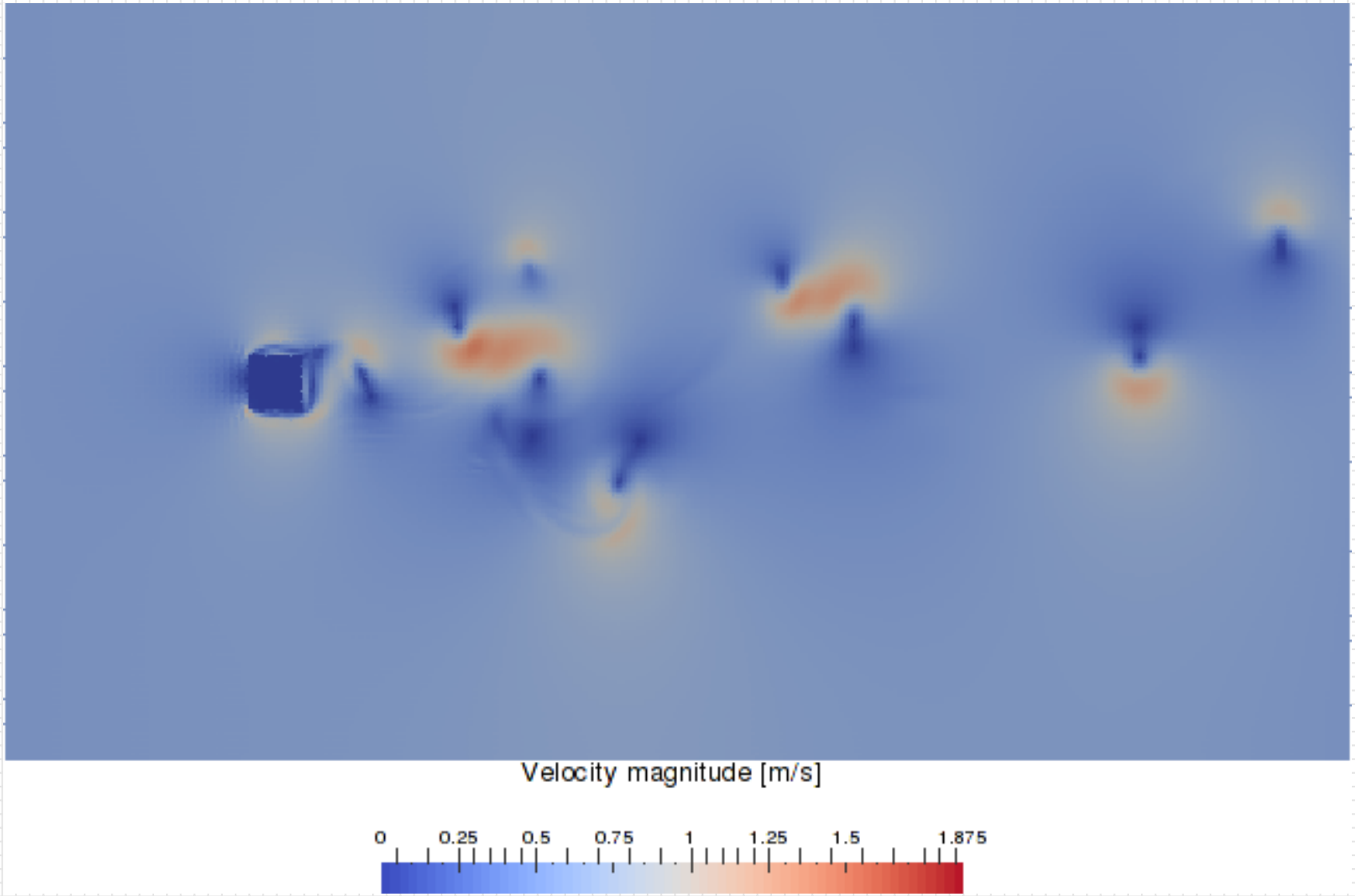

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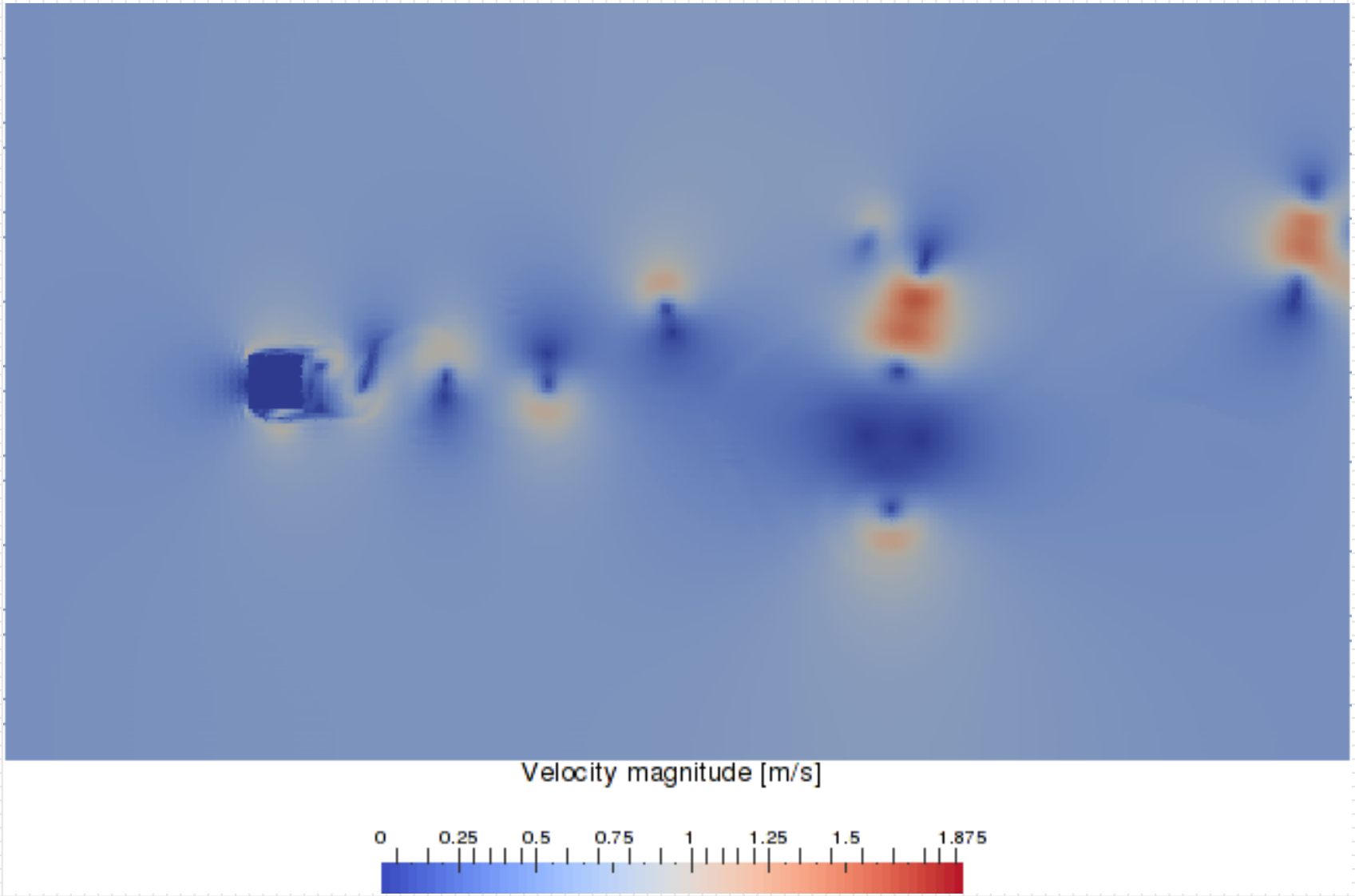

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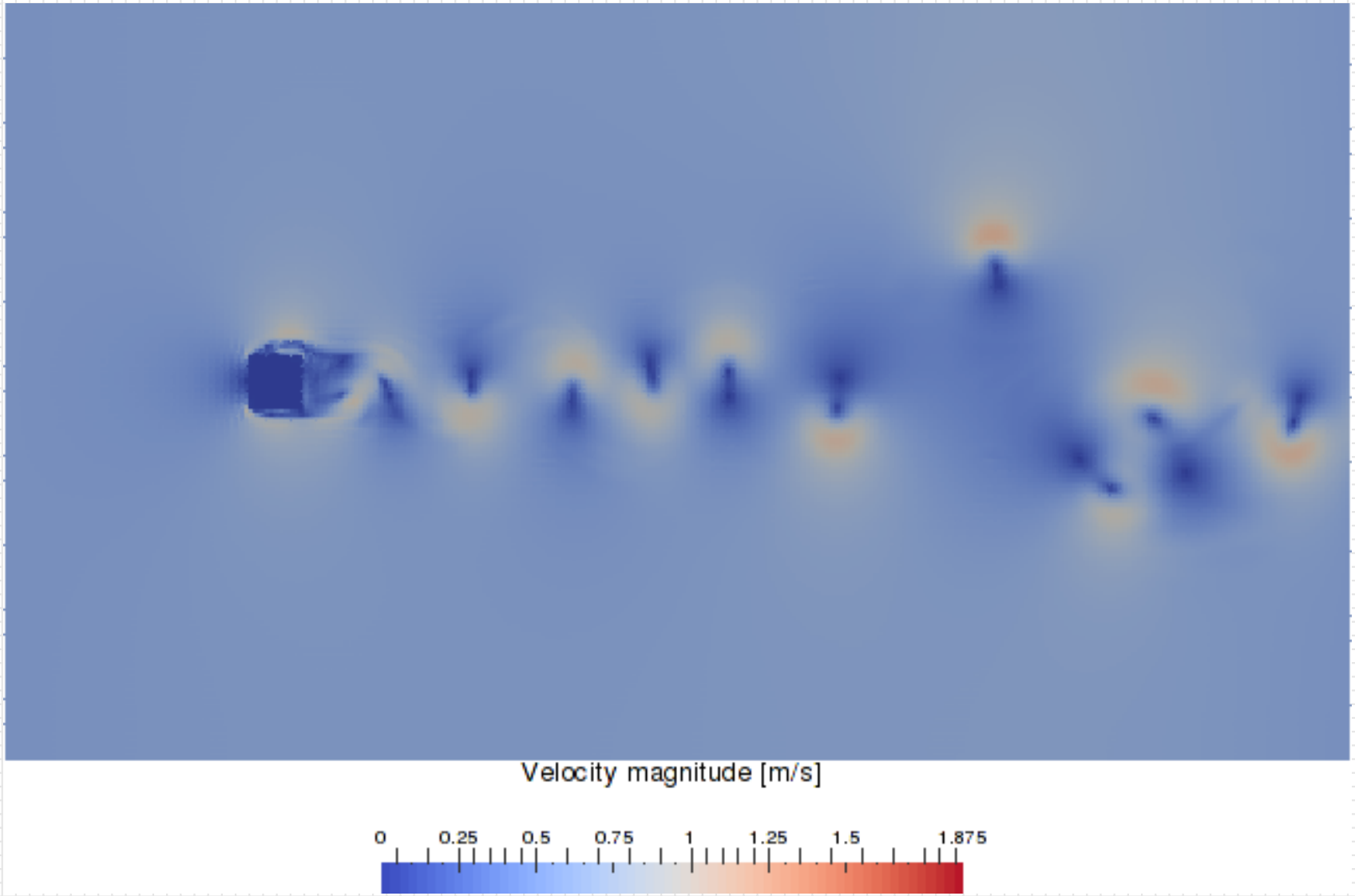

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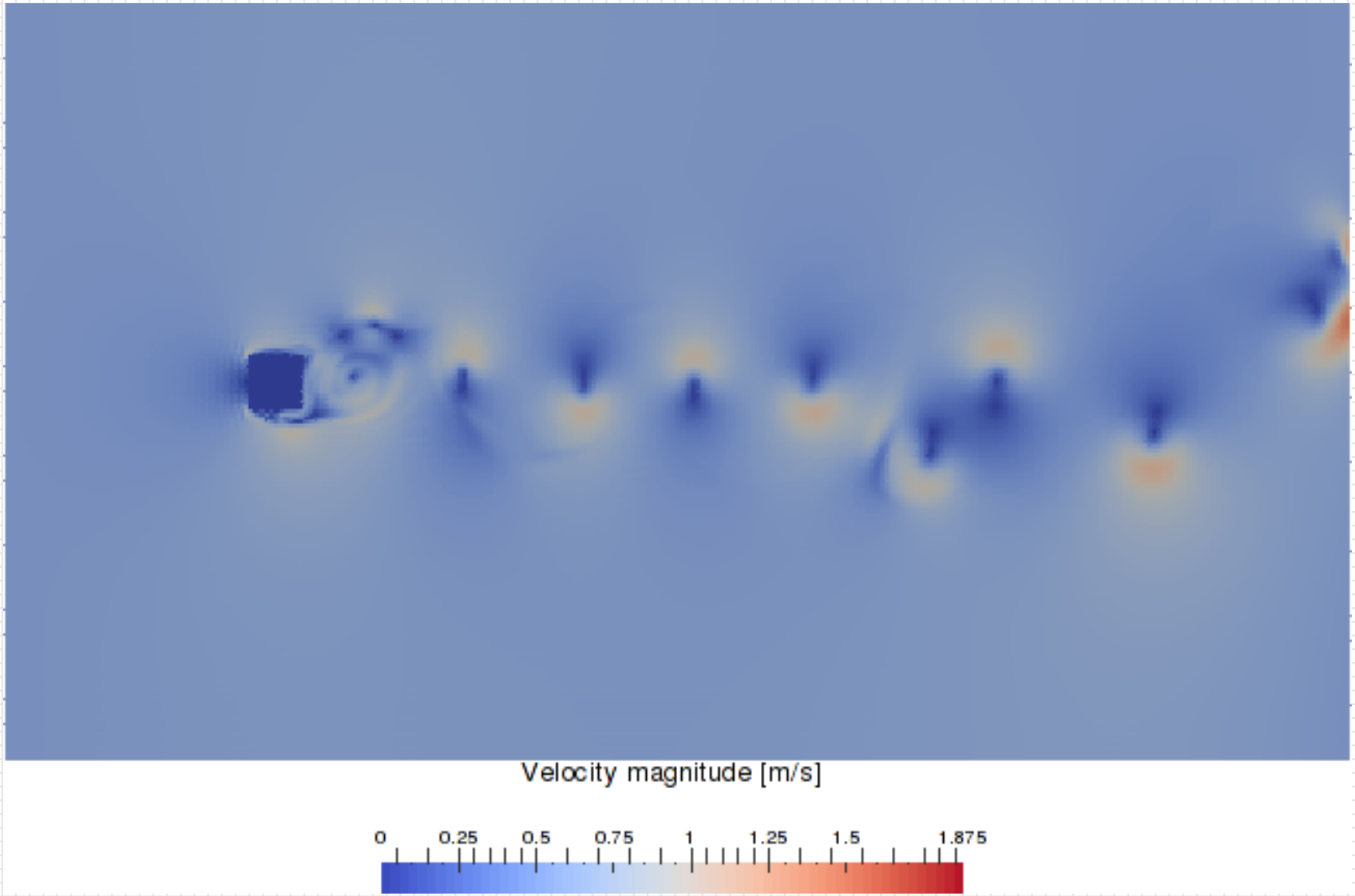

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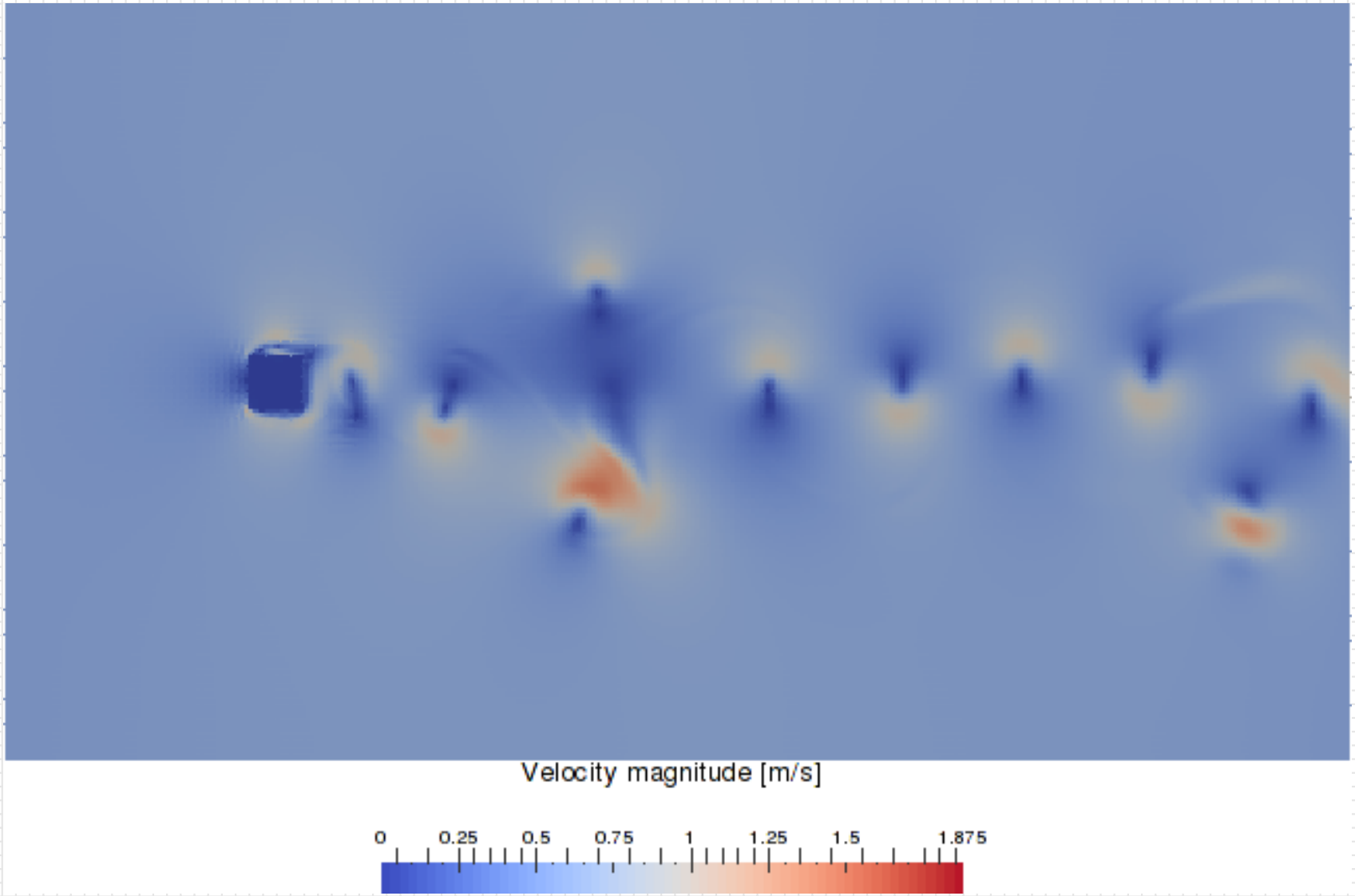

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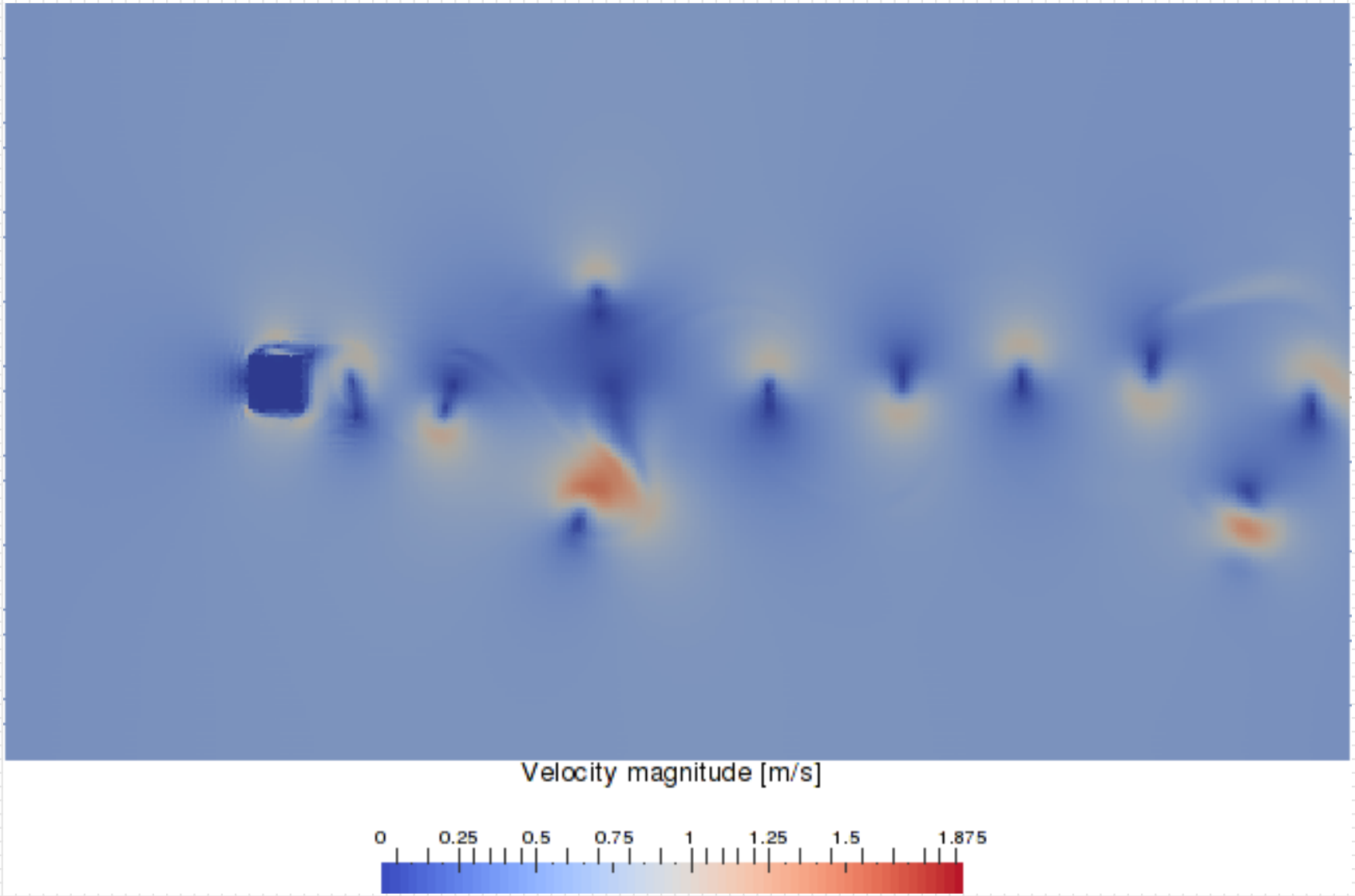

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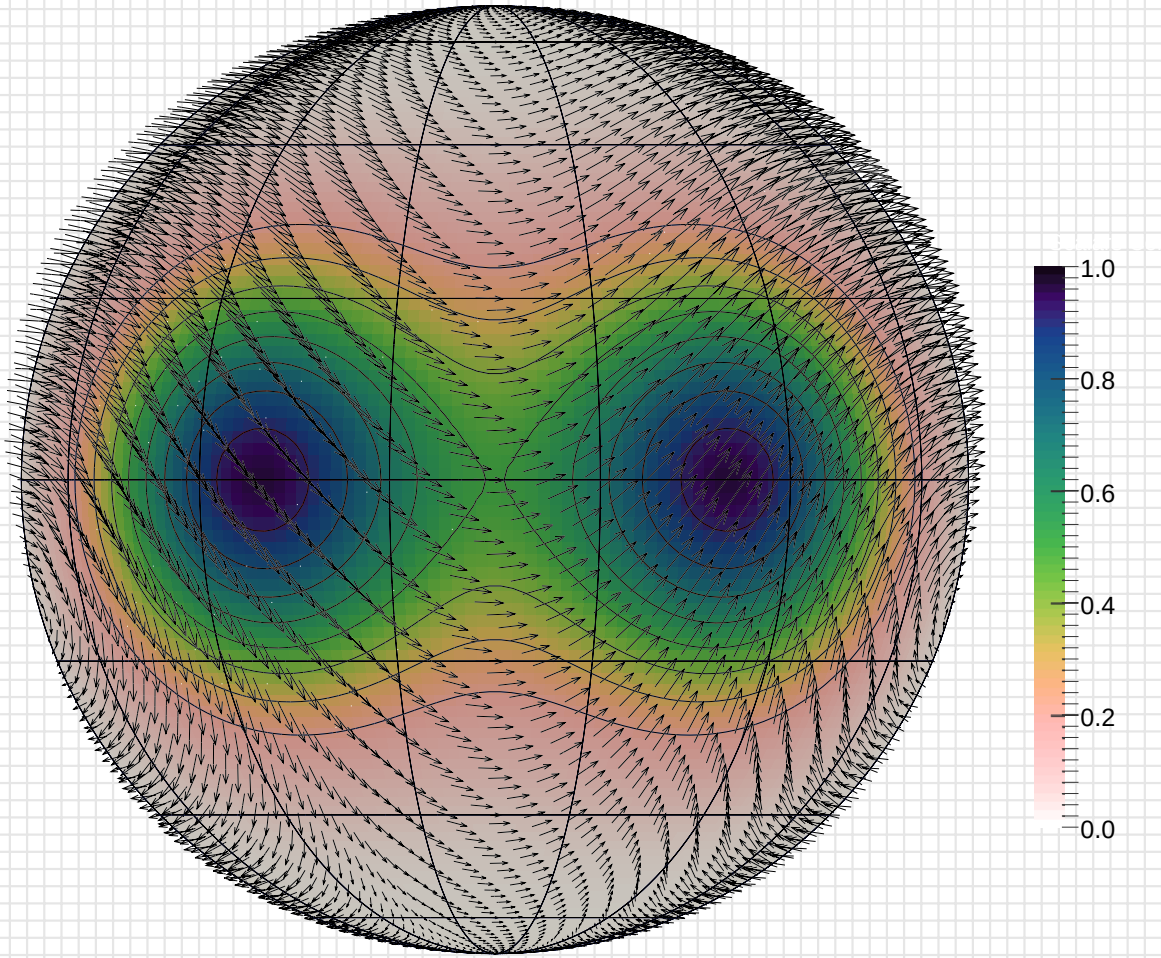

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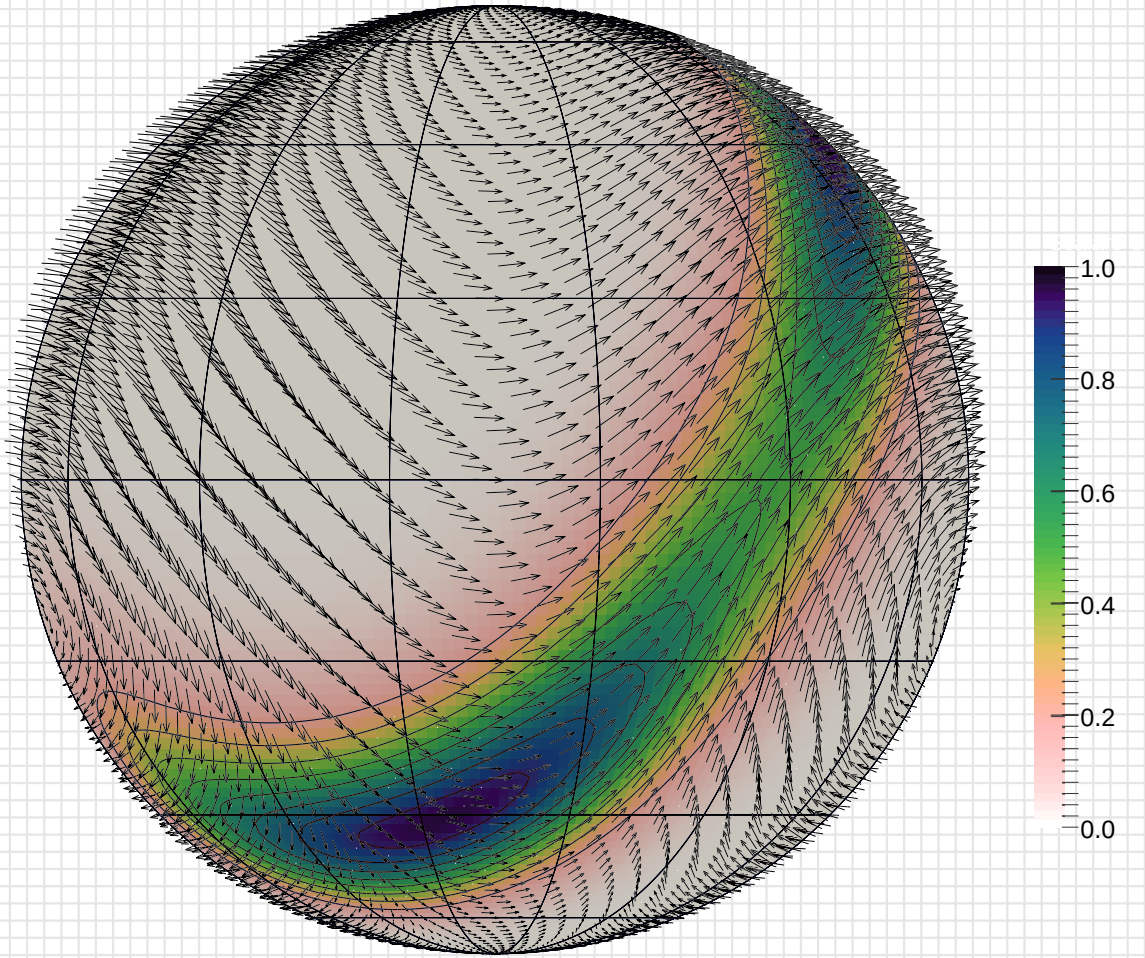

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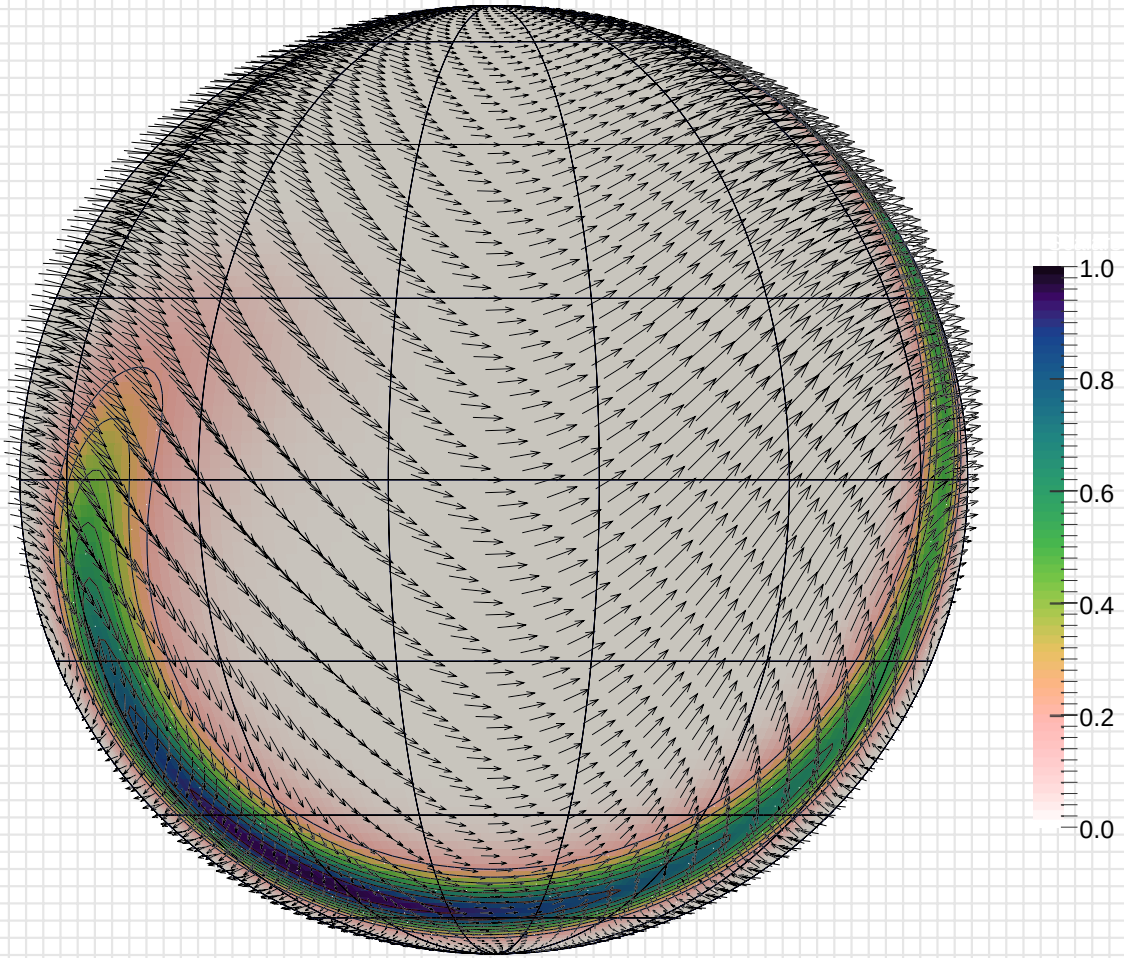

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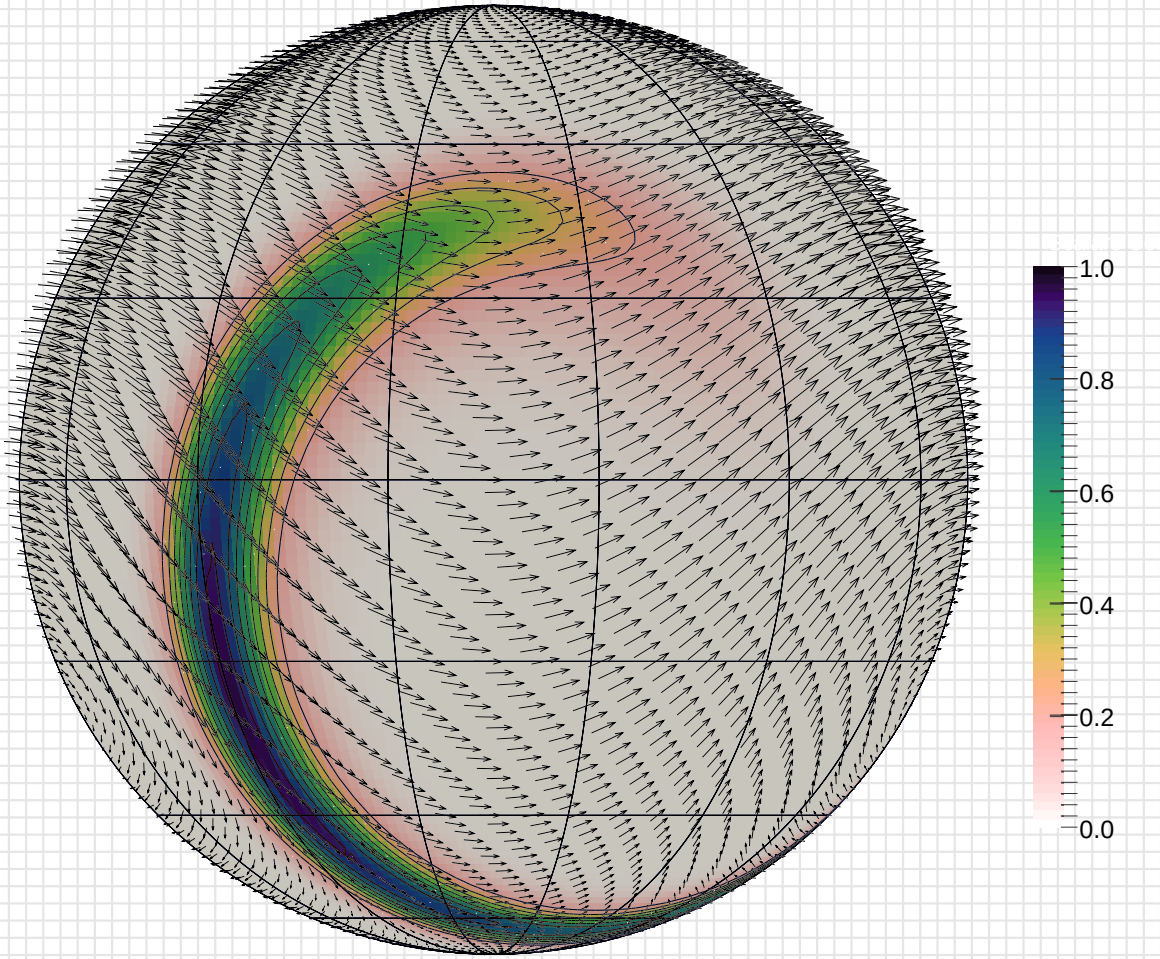

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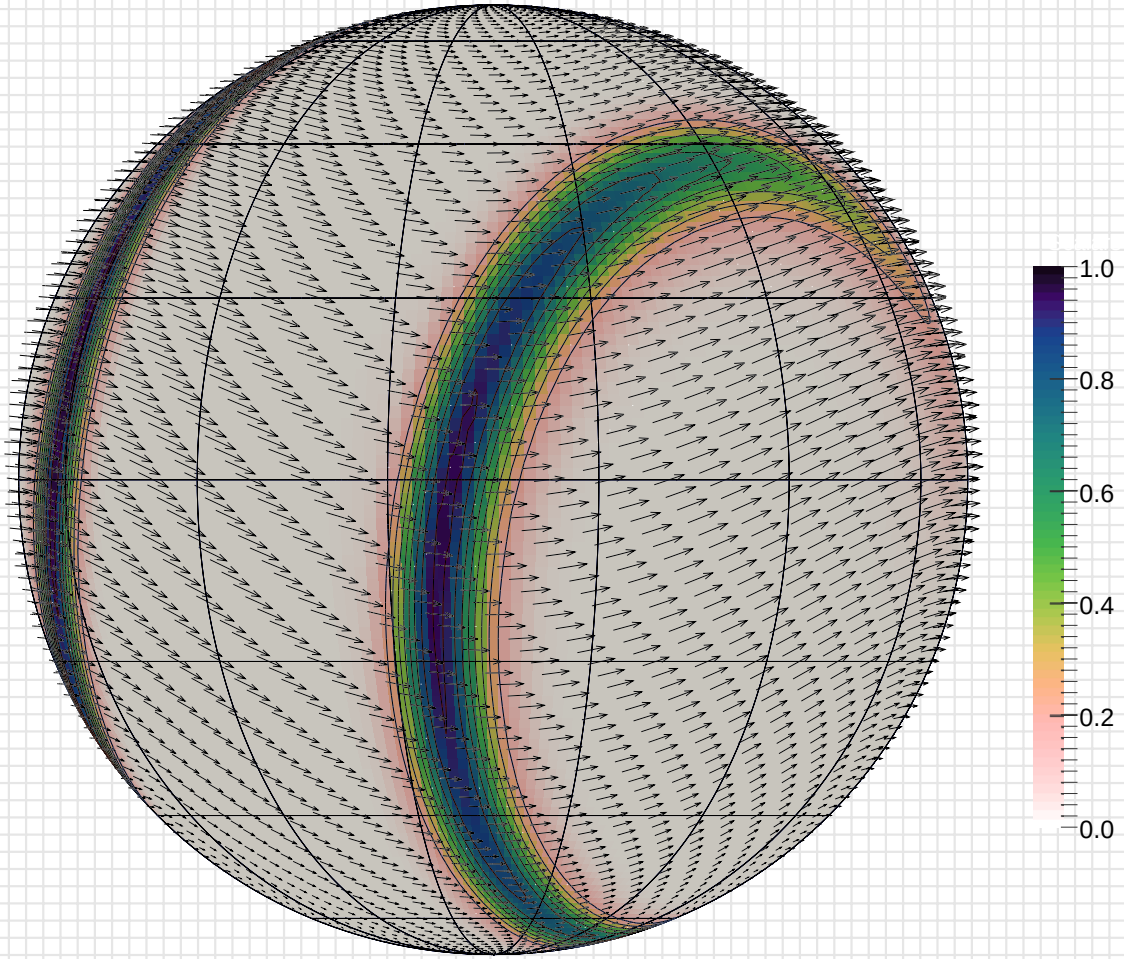

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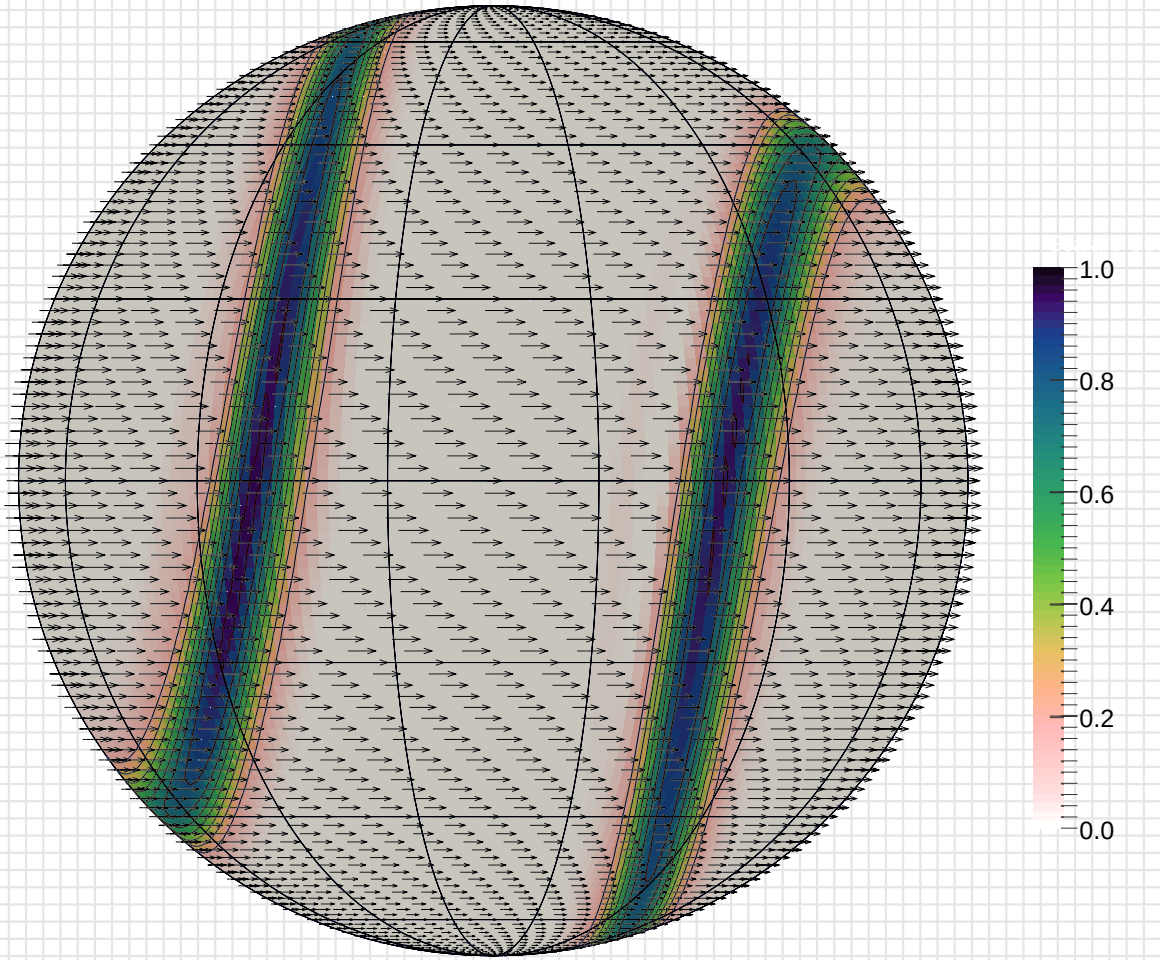

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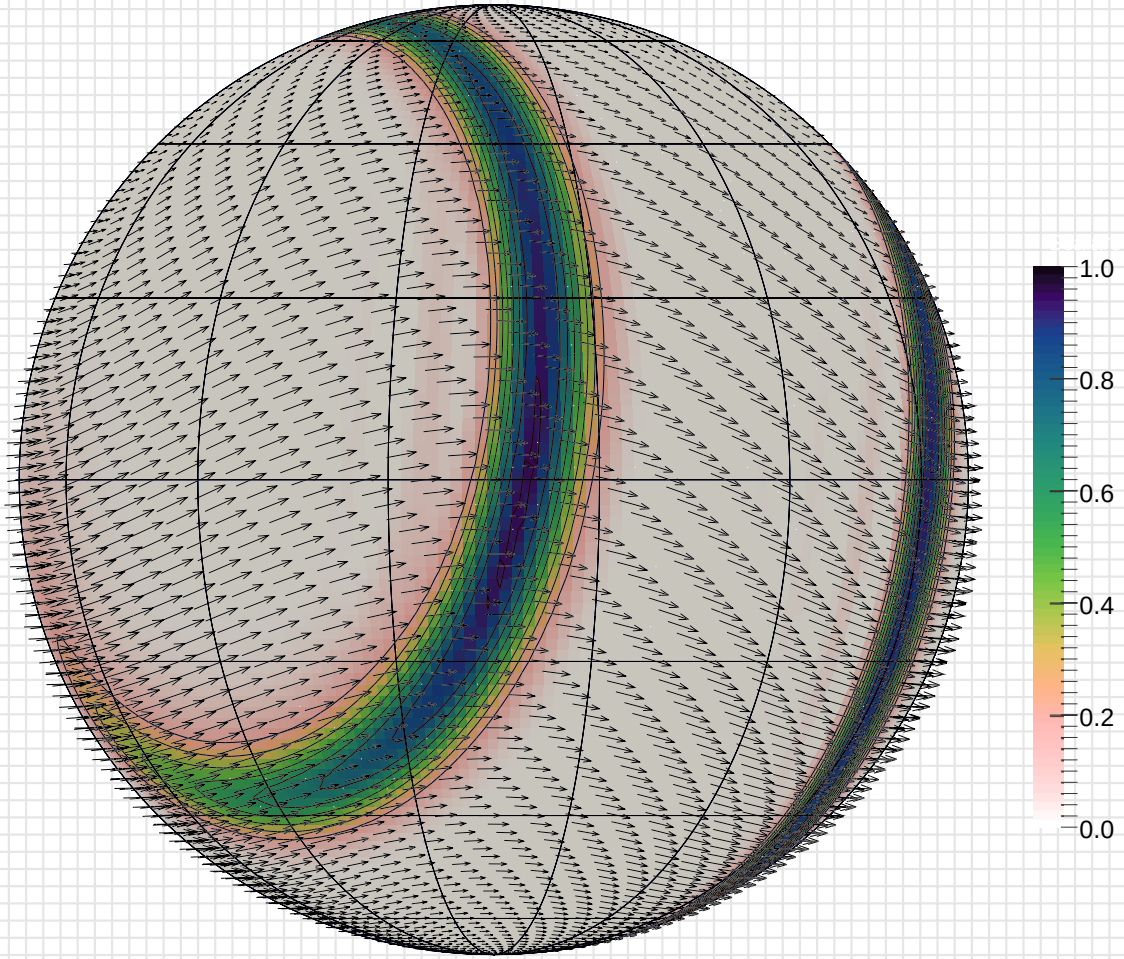

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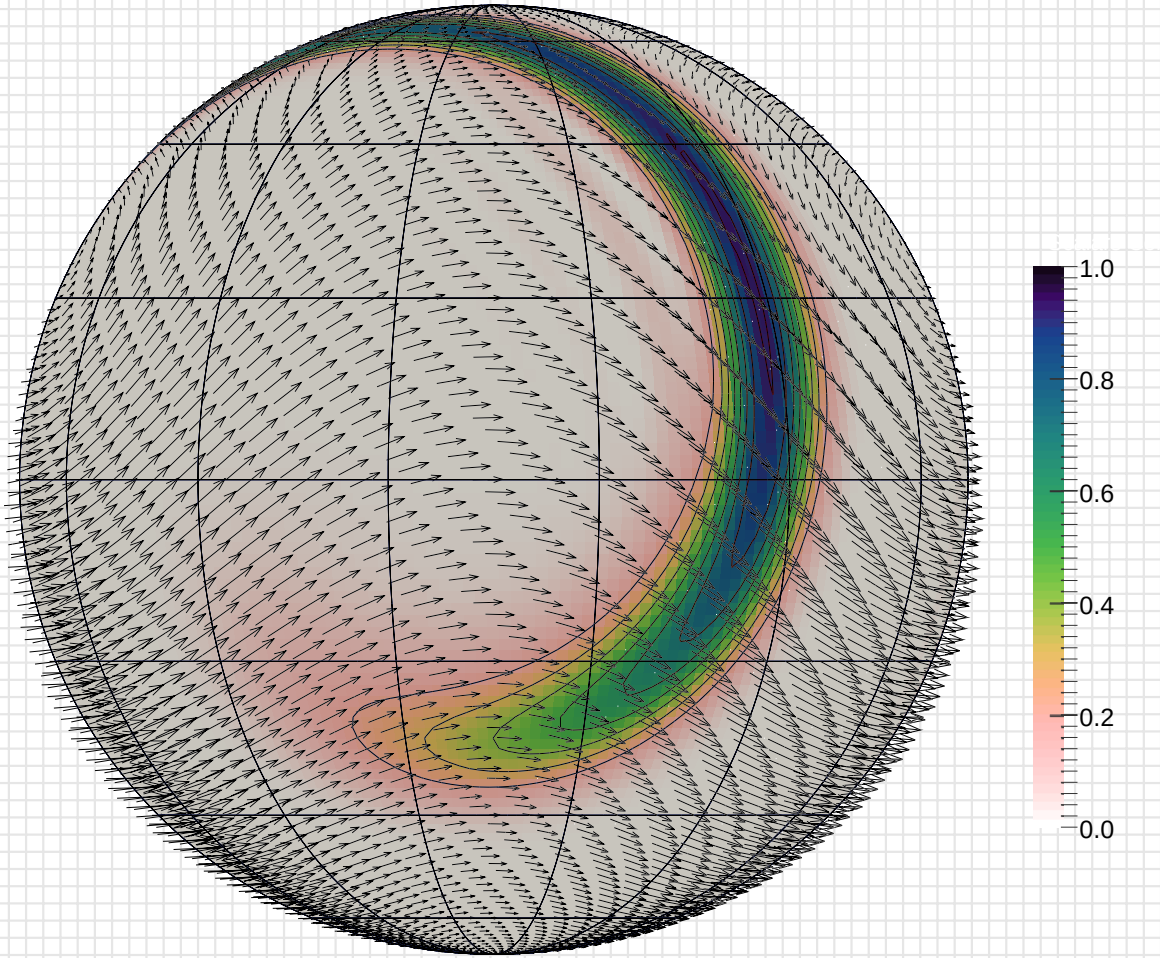

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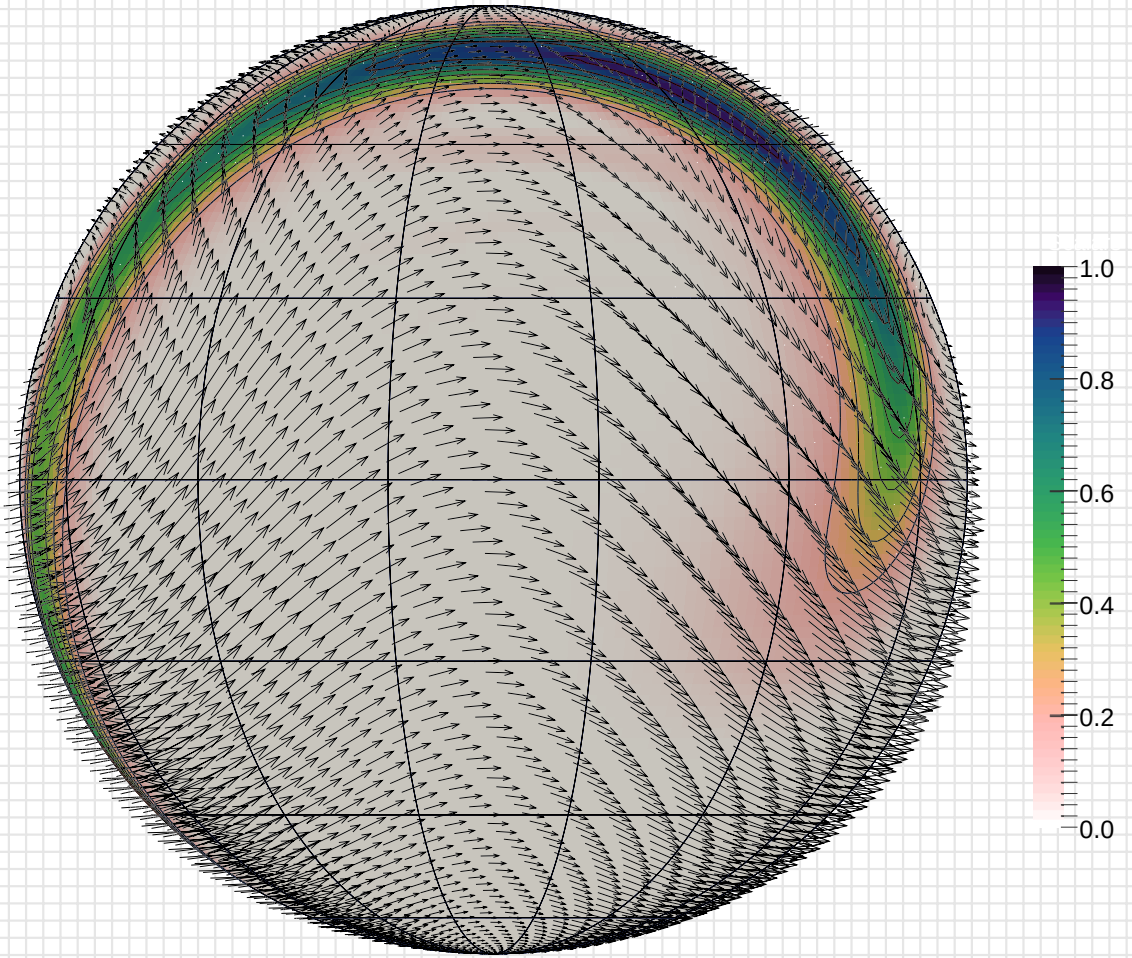

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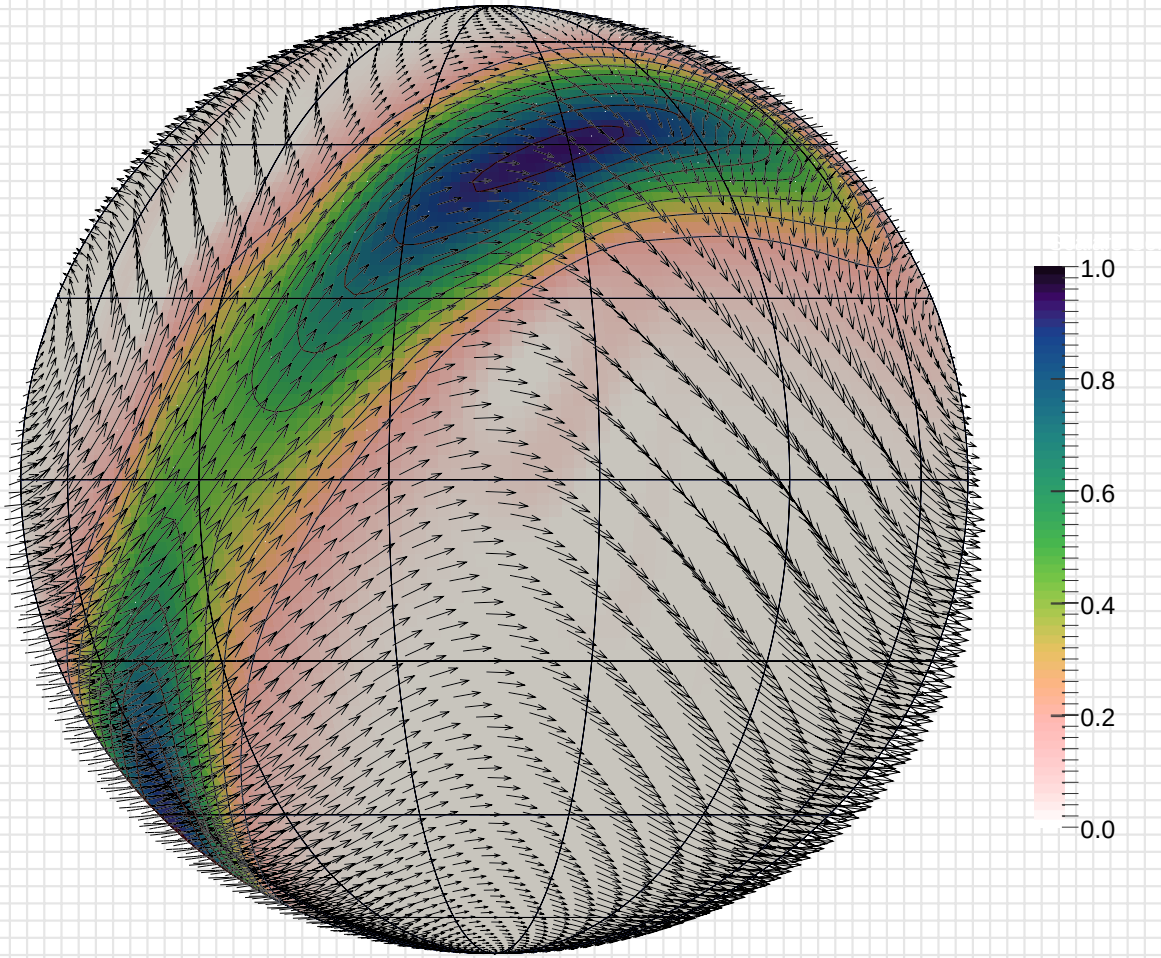

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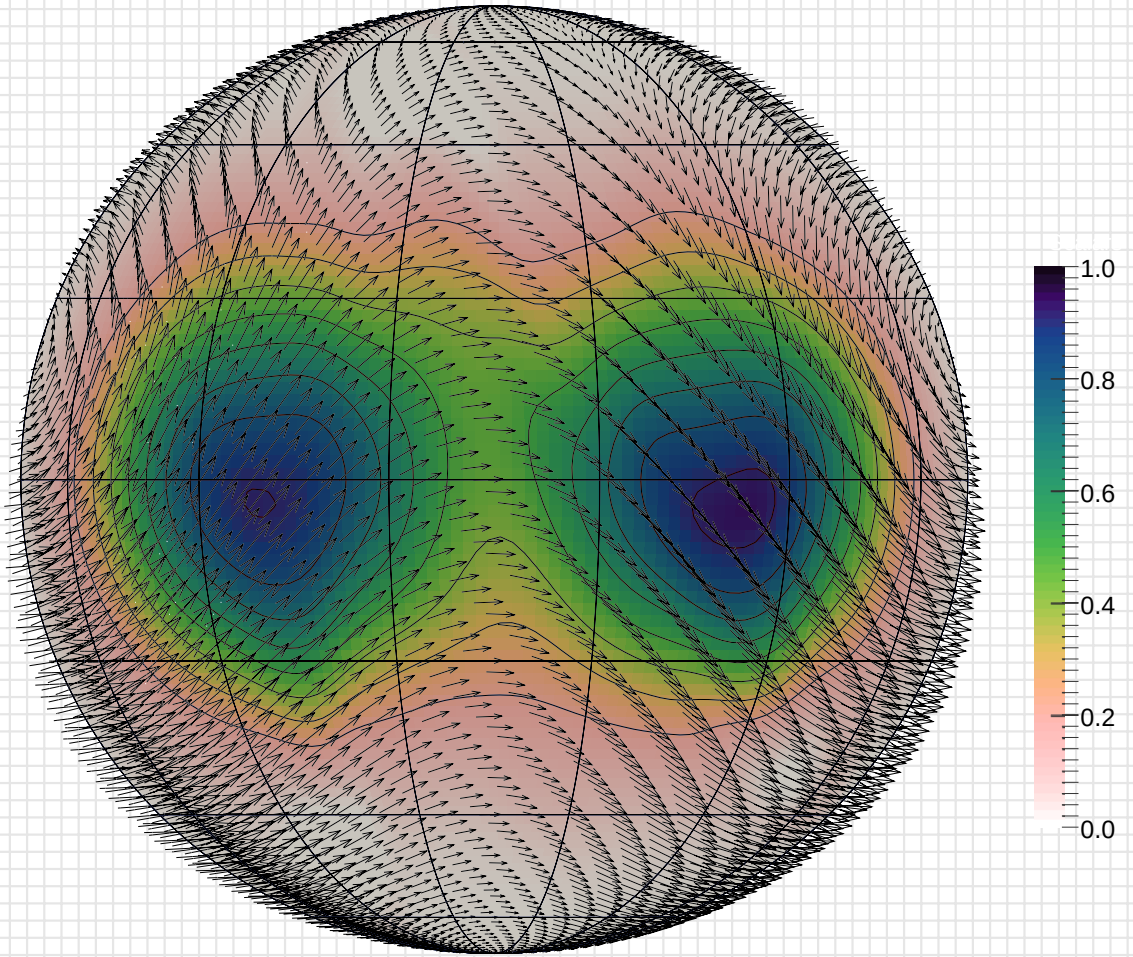

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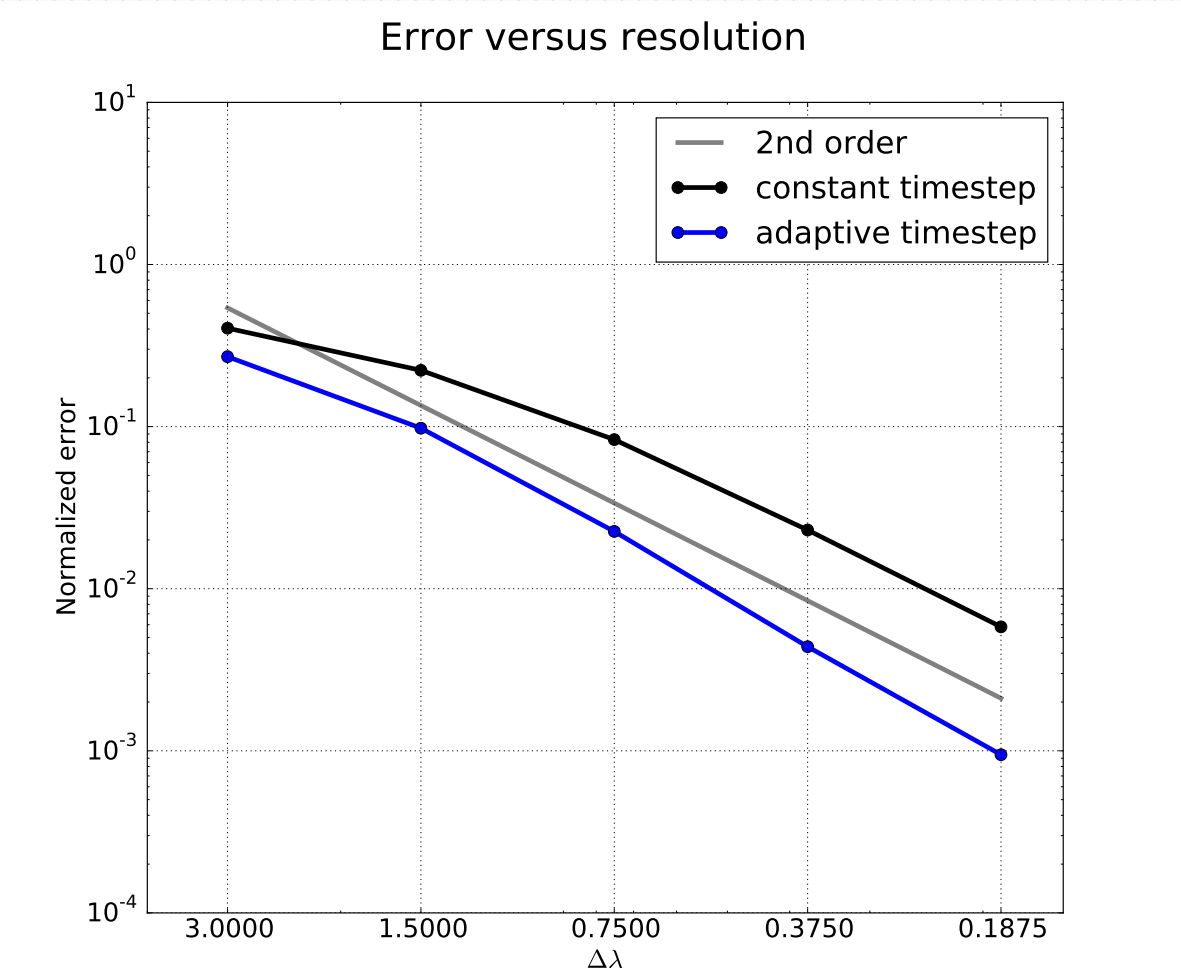

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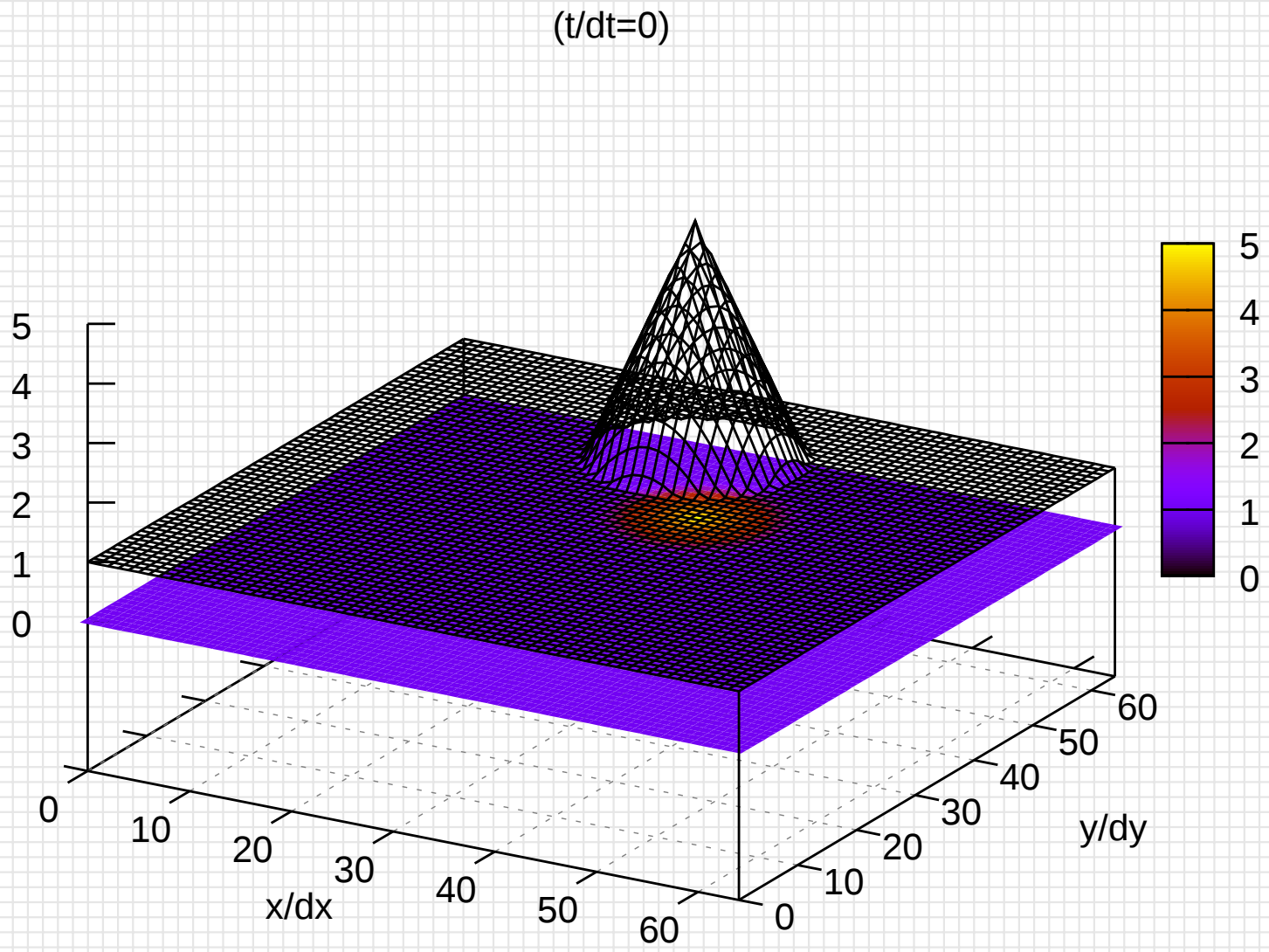
coded by
Maciej Waruszewski

Plan of the talk

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

Plan of the talk

libmpdata++: rotating cone test



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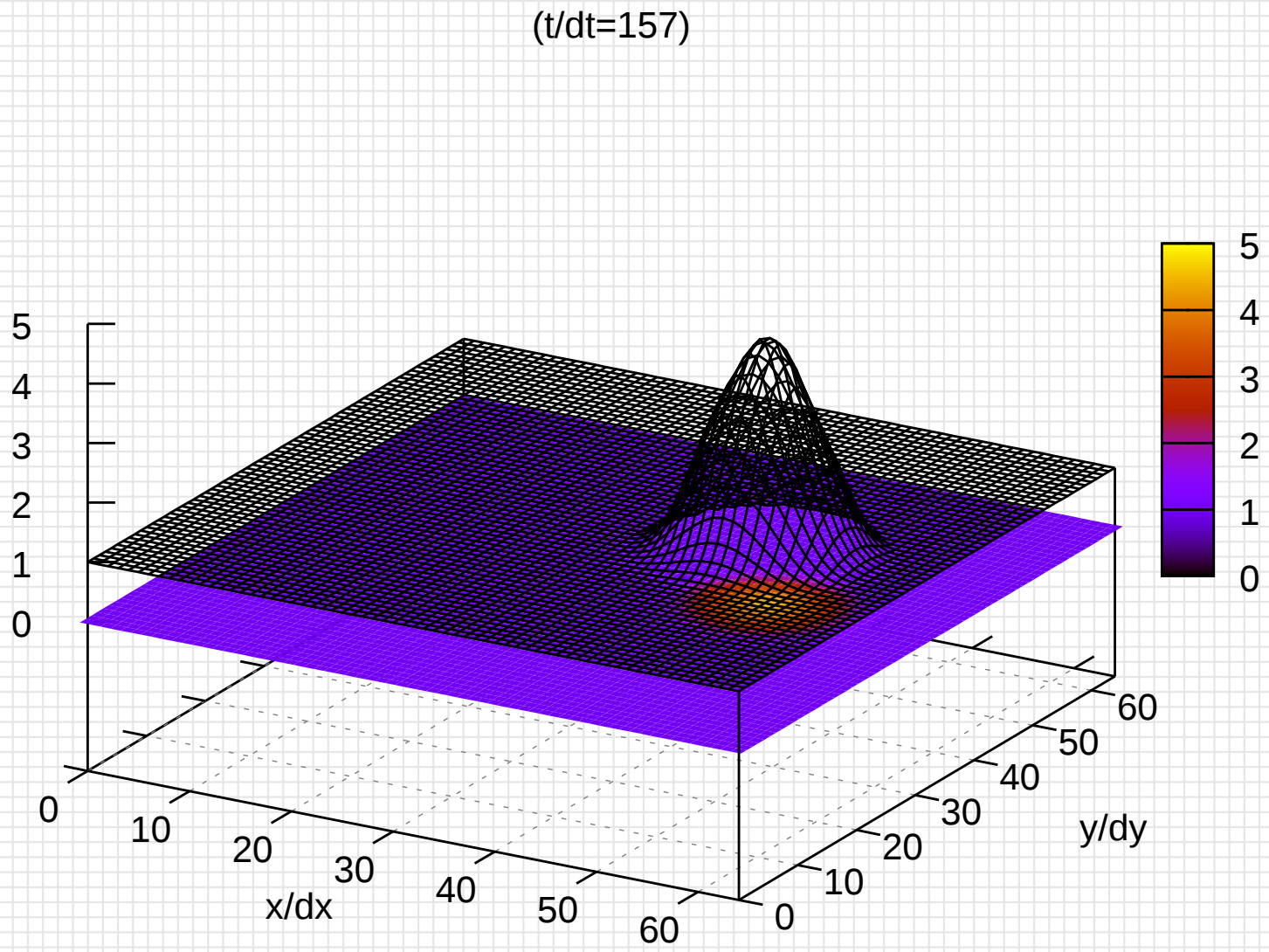

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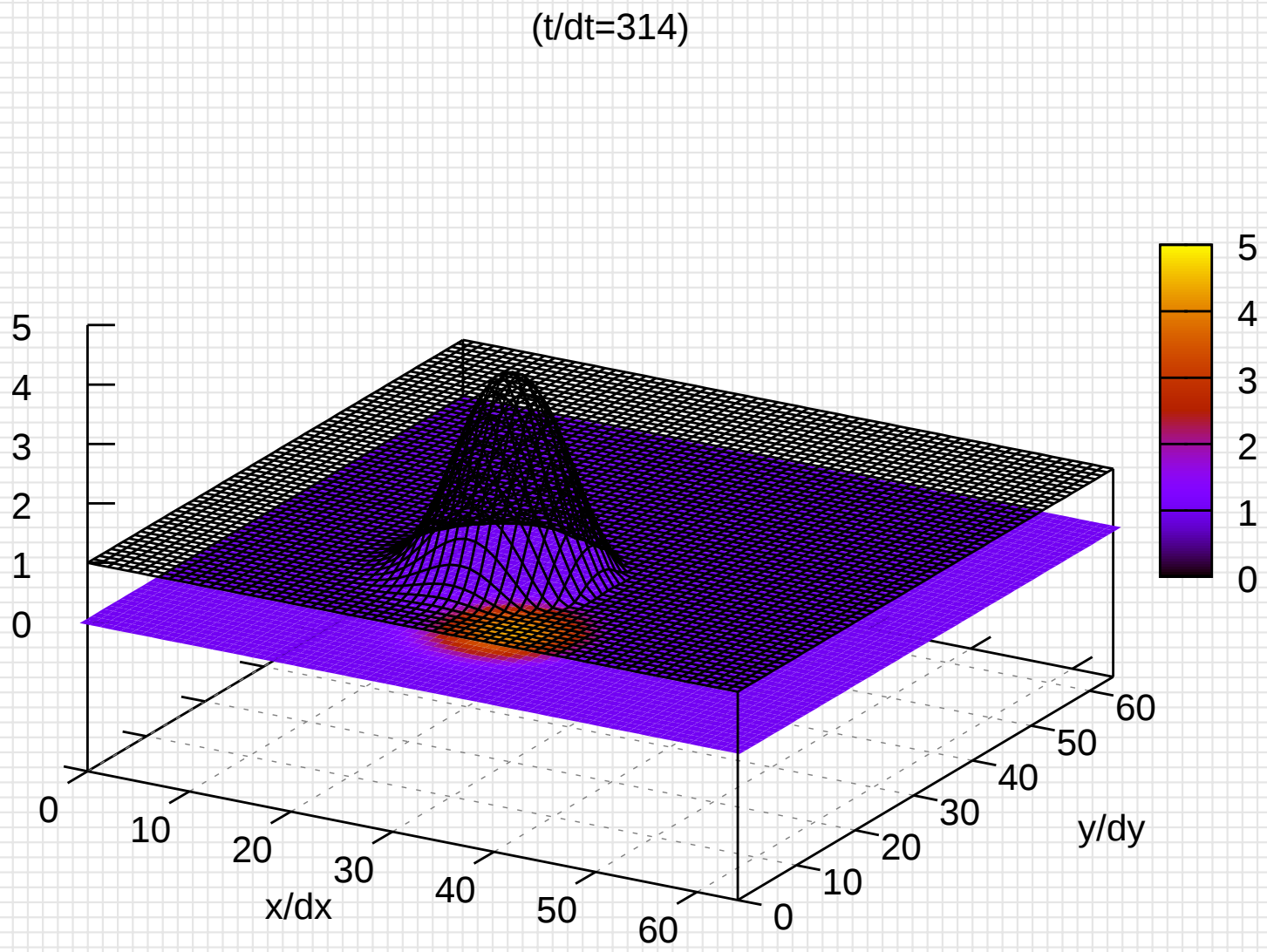

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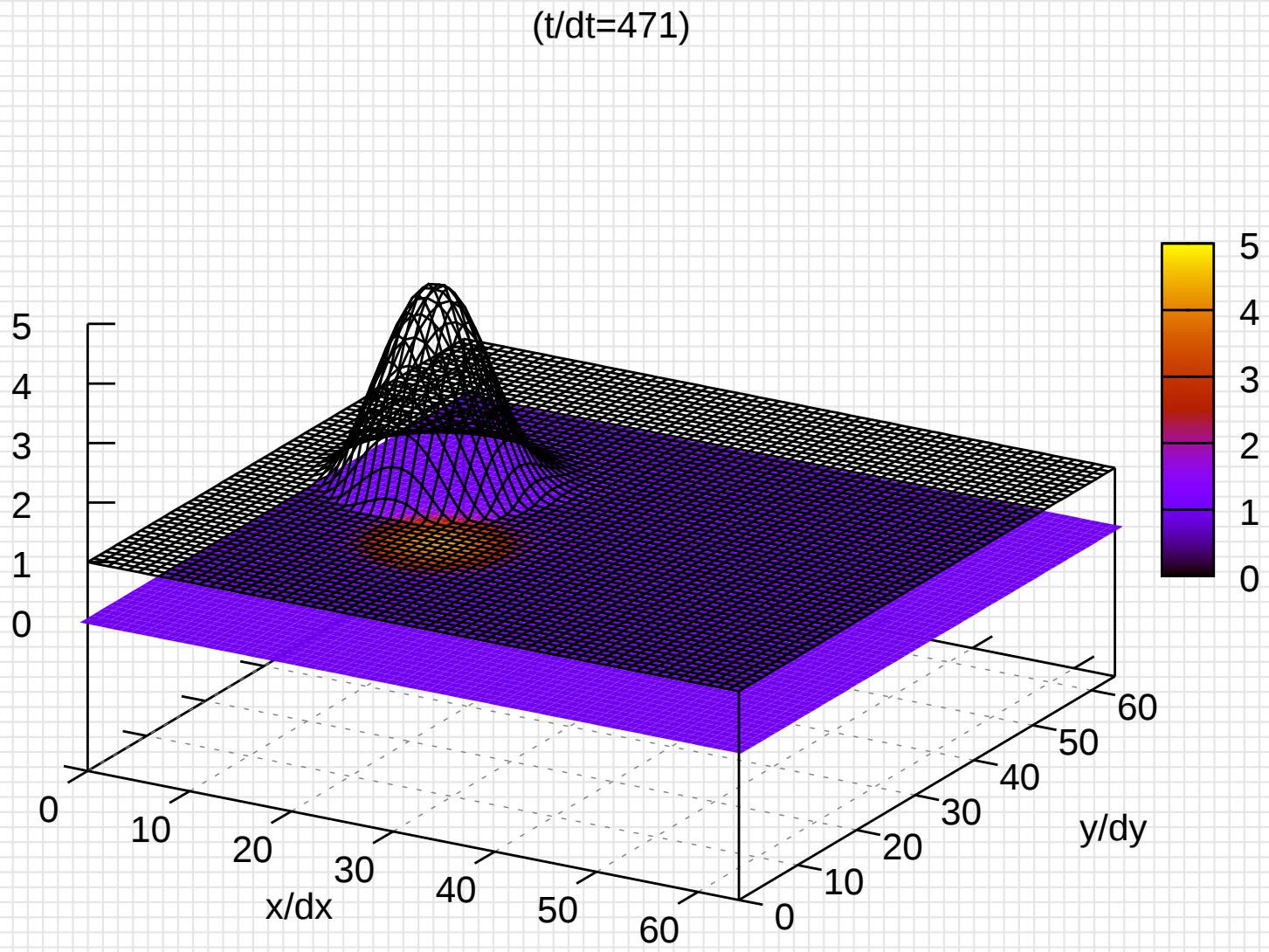

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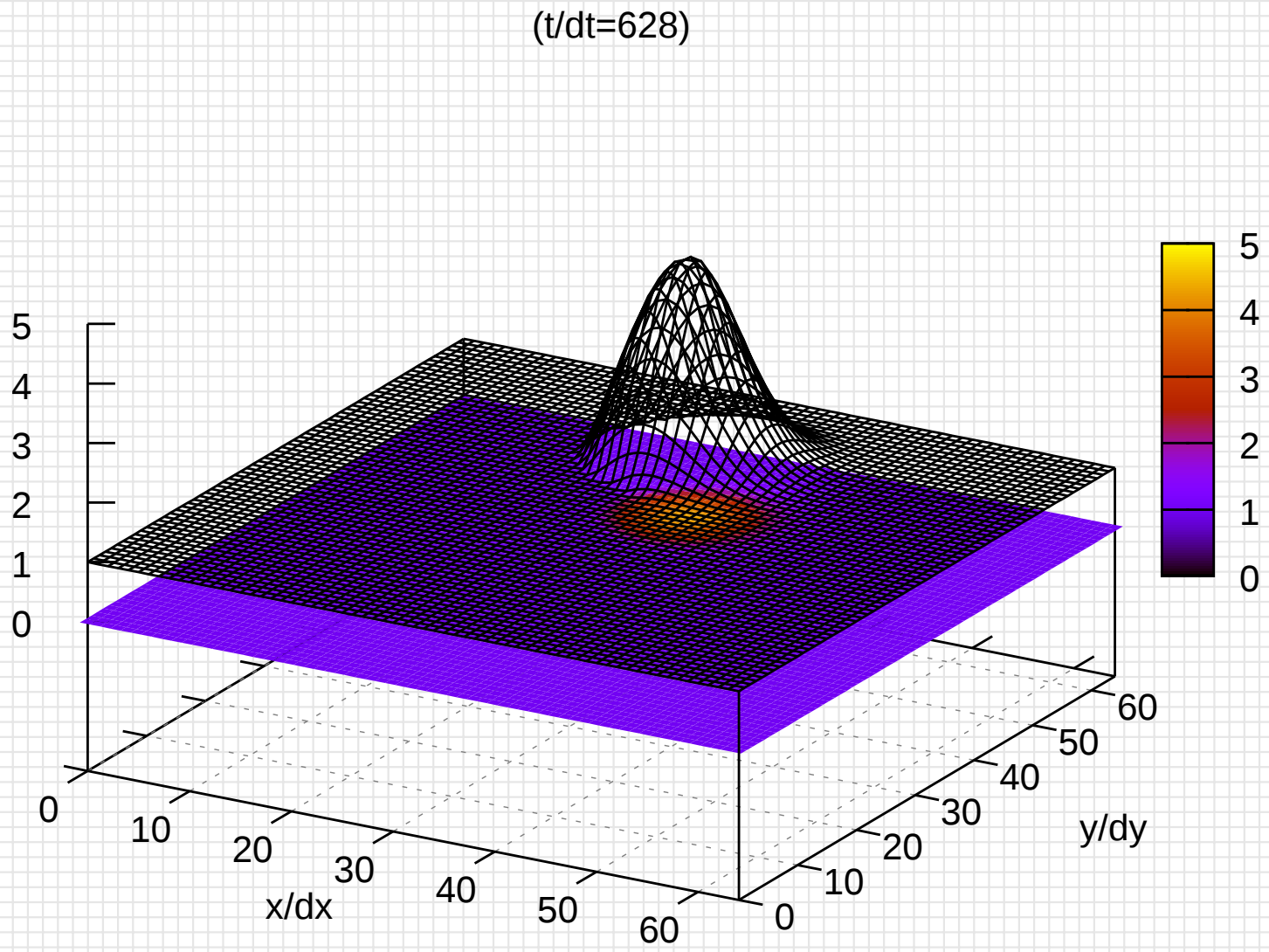

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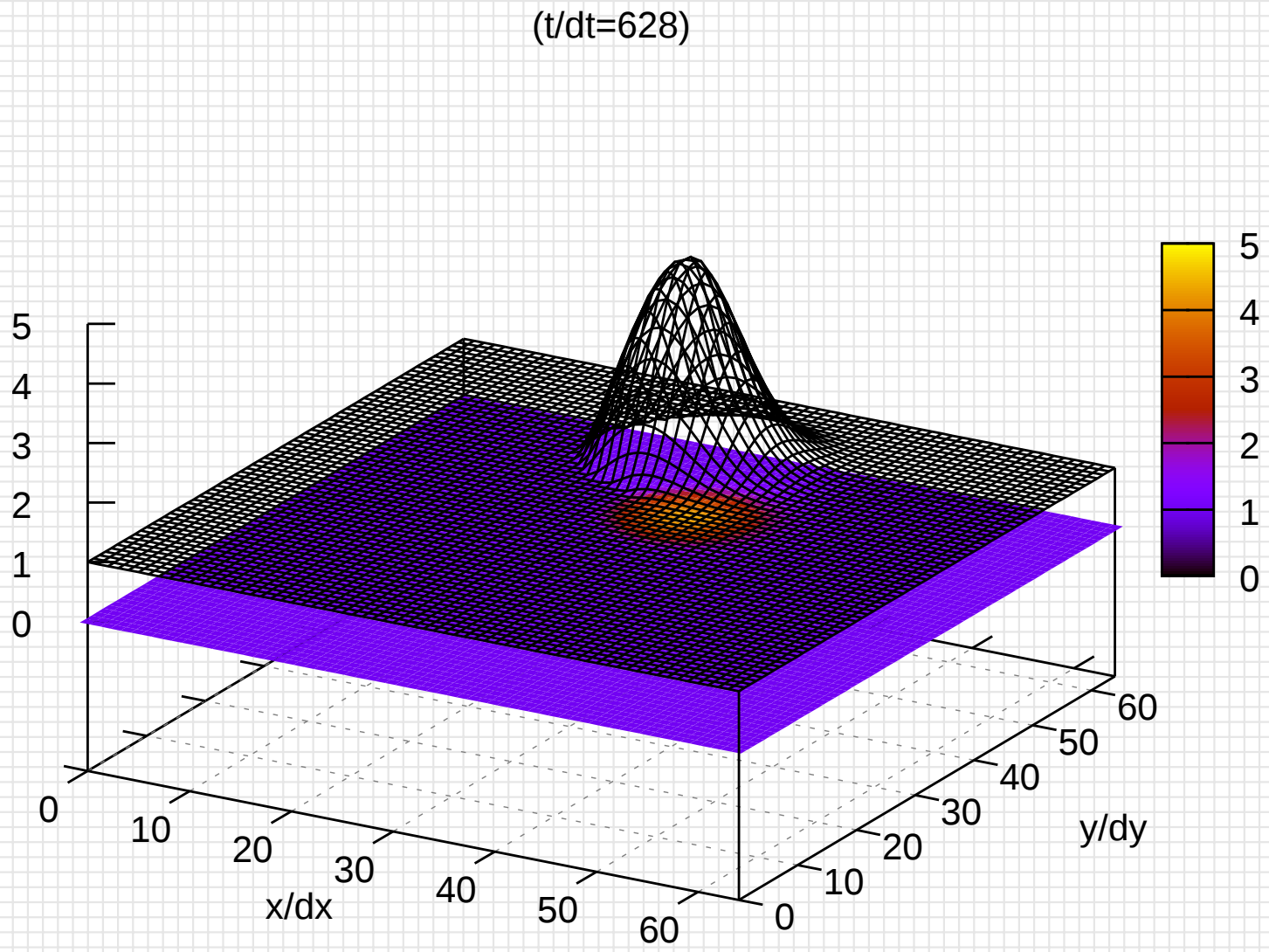

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```cpp
#include <libmpdata++/solvers/mpdata.hpp>
#include <libmpdata++/concurr/serial.hpp>
#include <libmpdata++/output/gnuplot.hpp>

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 }
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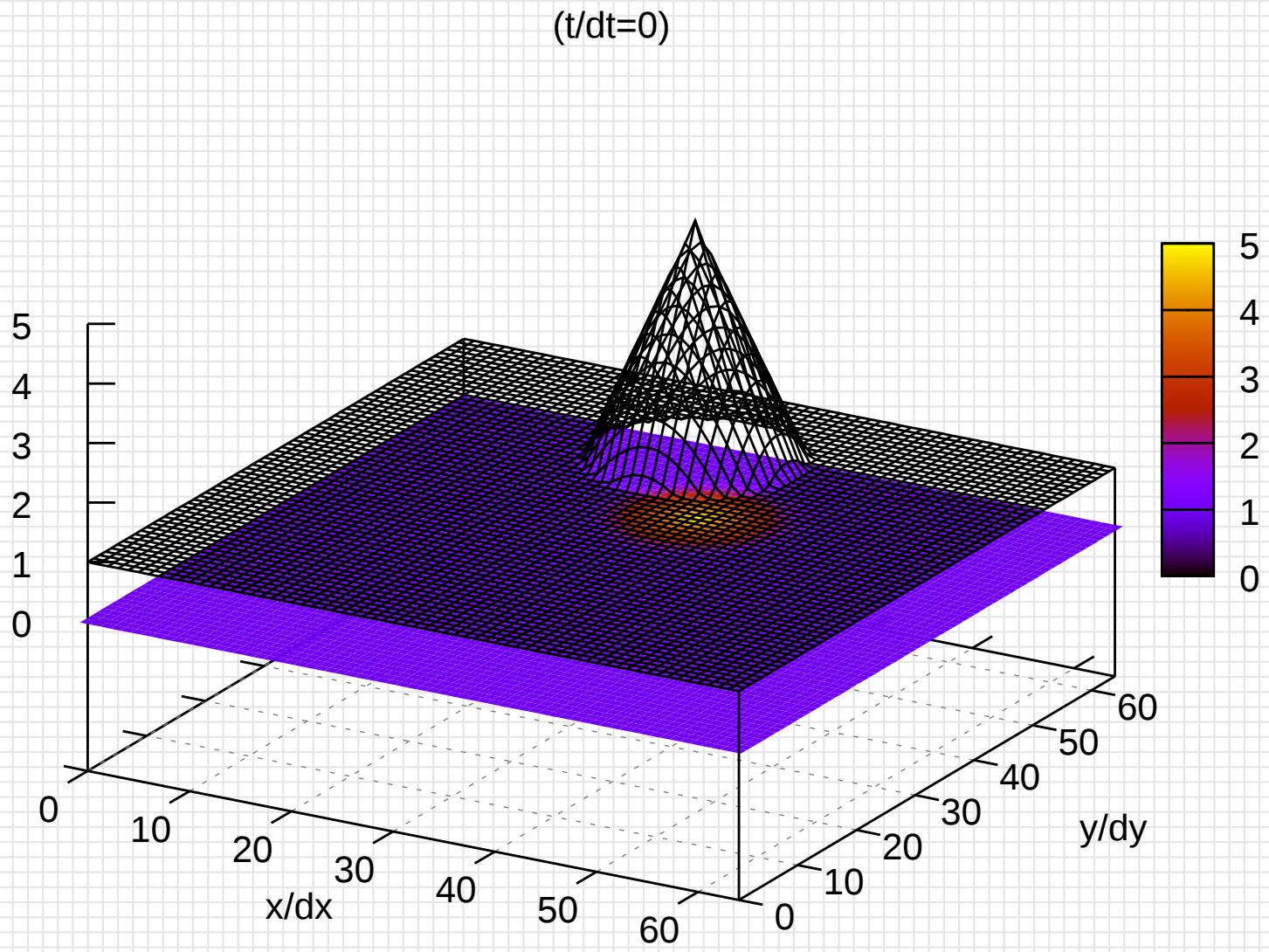
CMakeLists.txt

```
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



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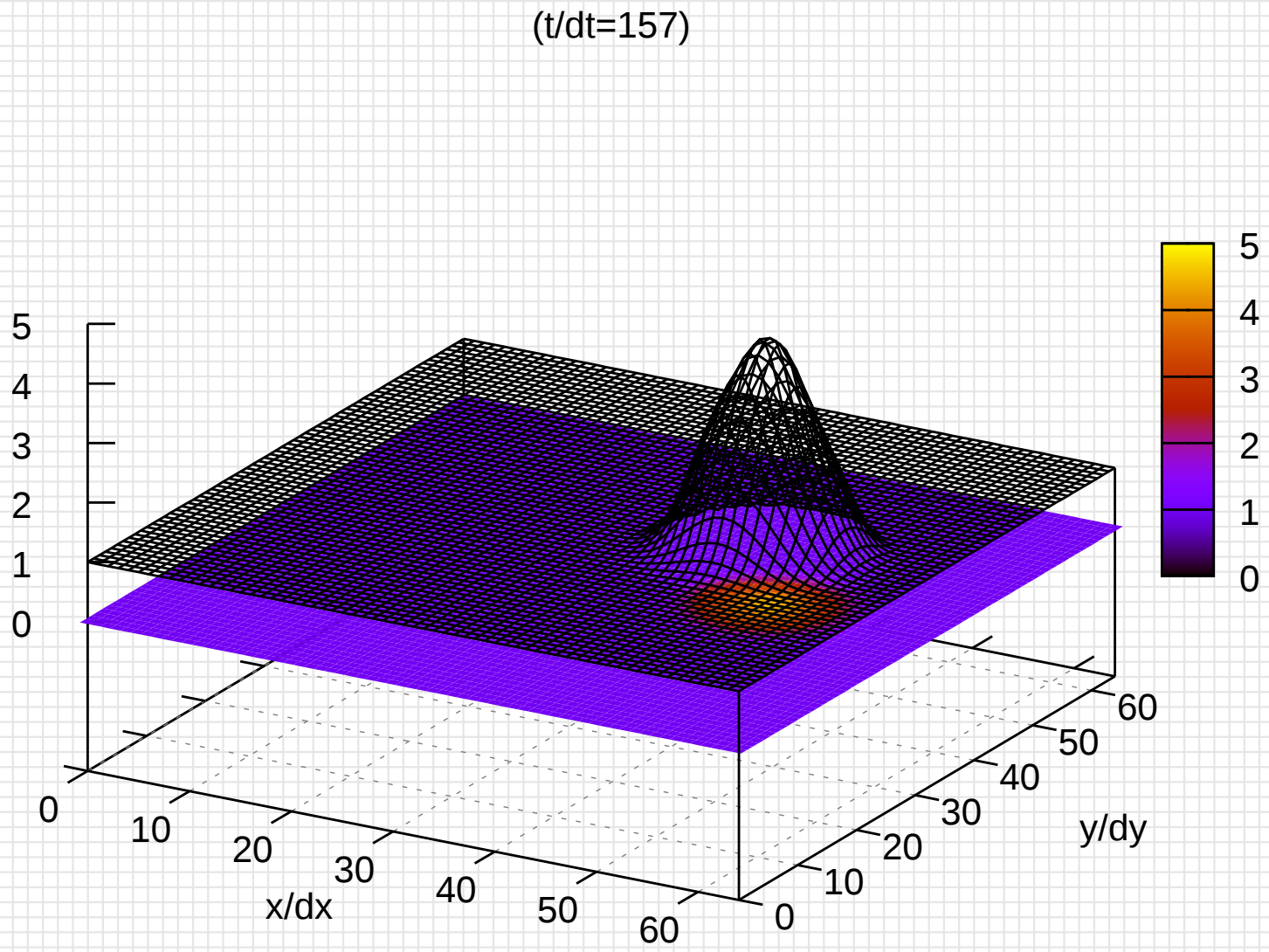

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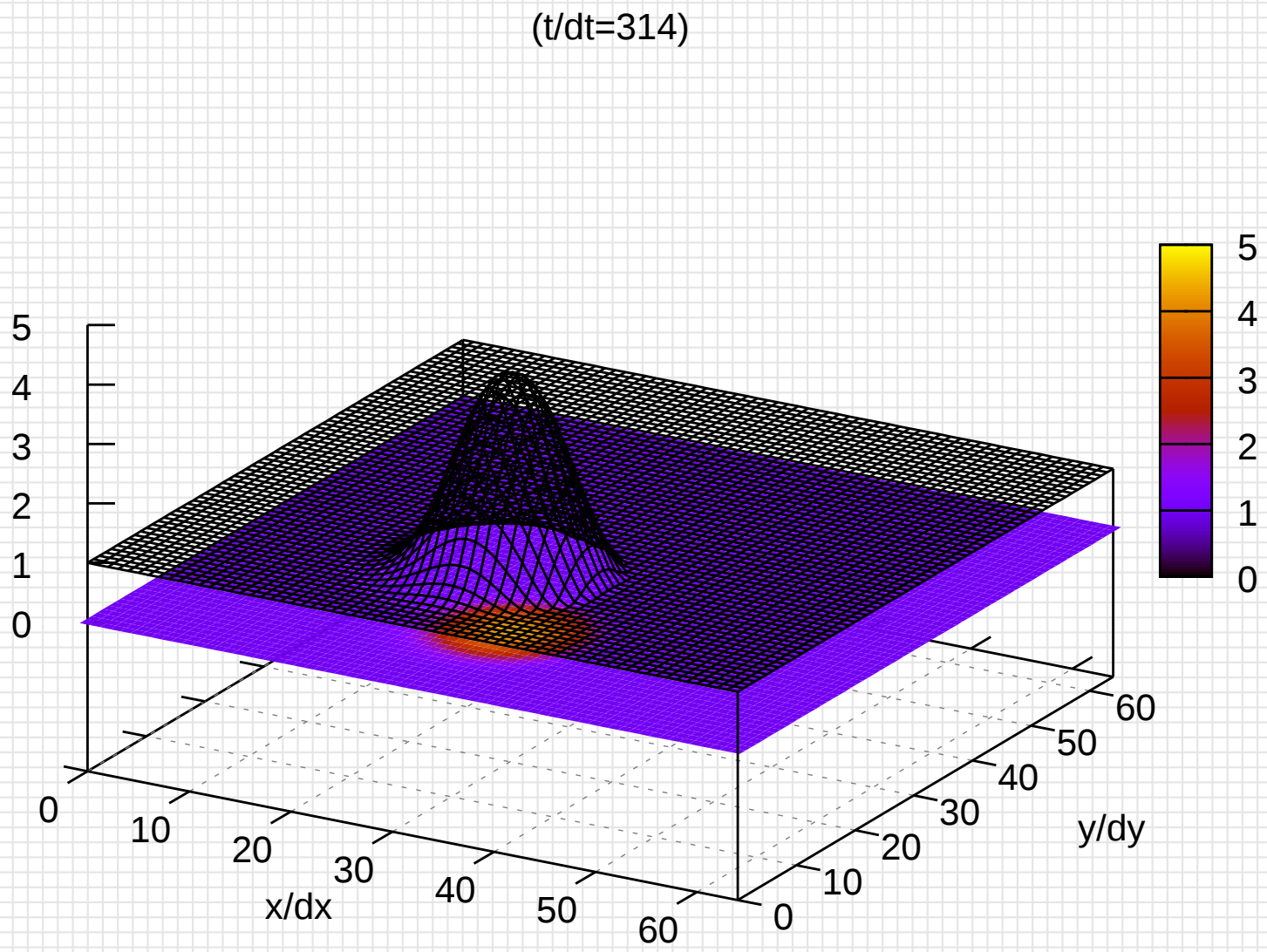

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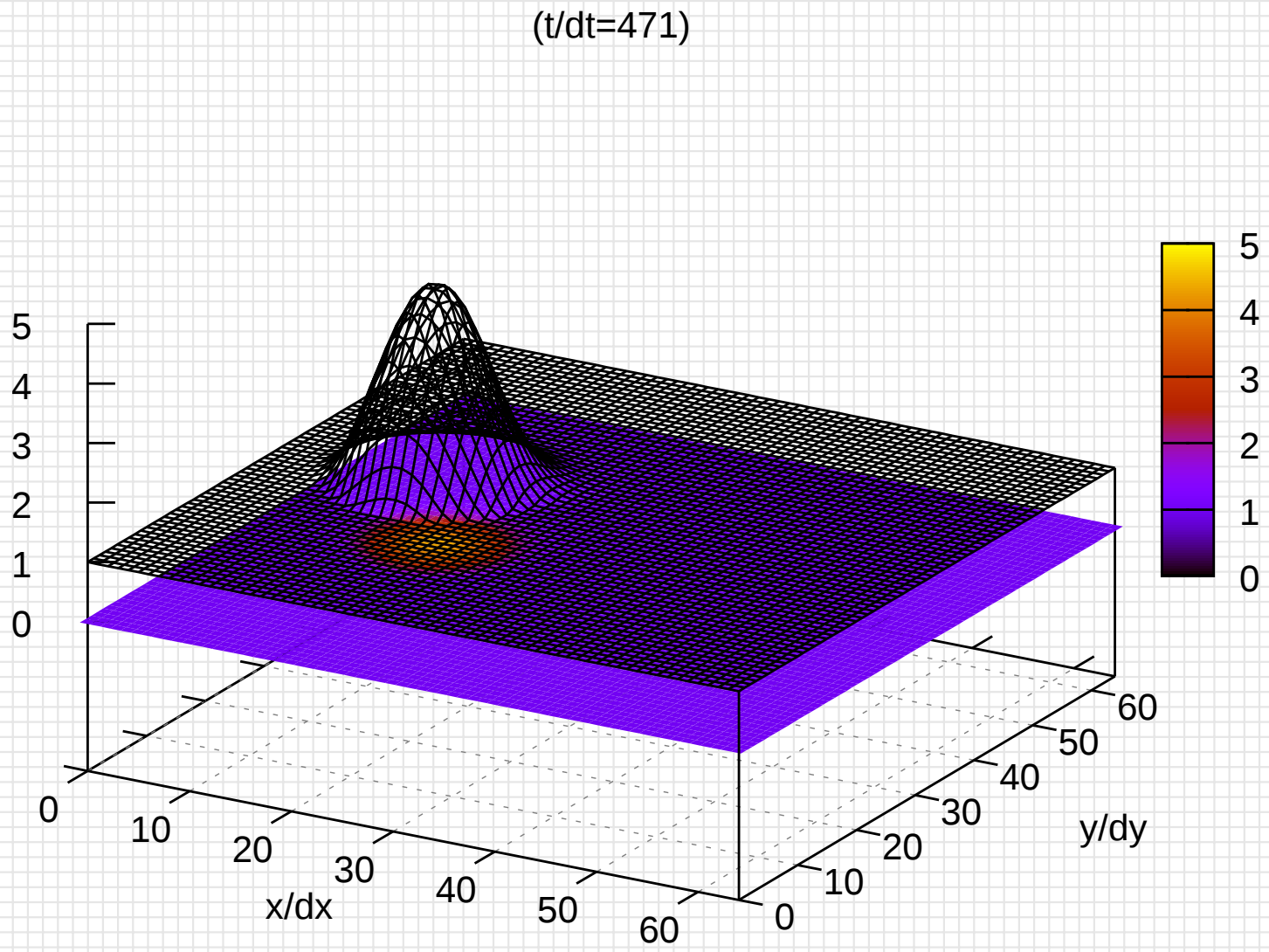

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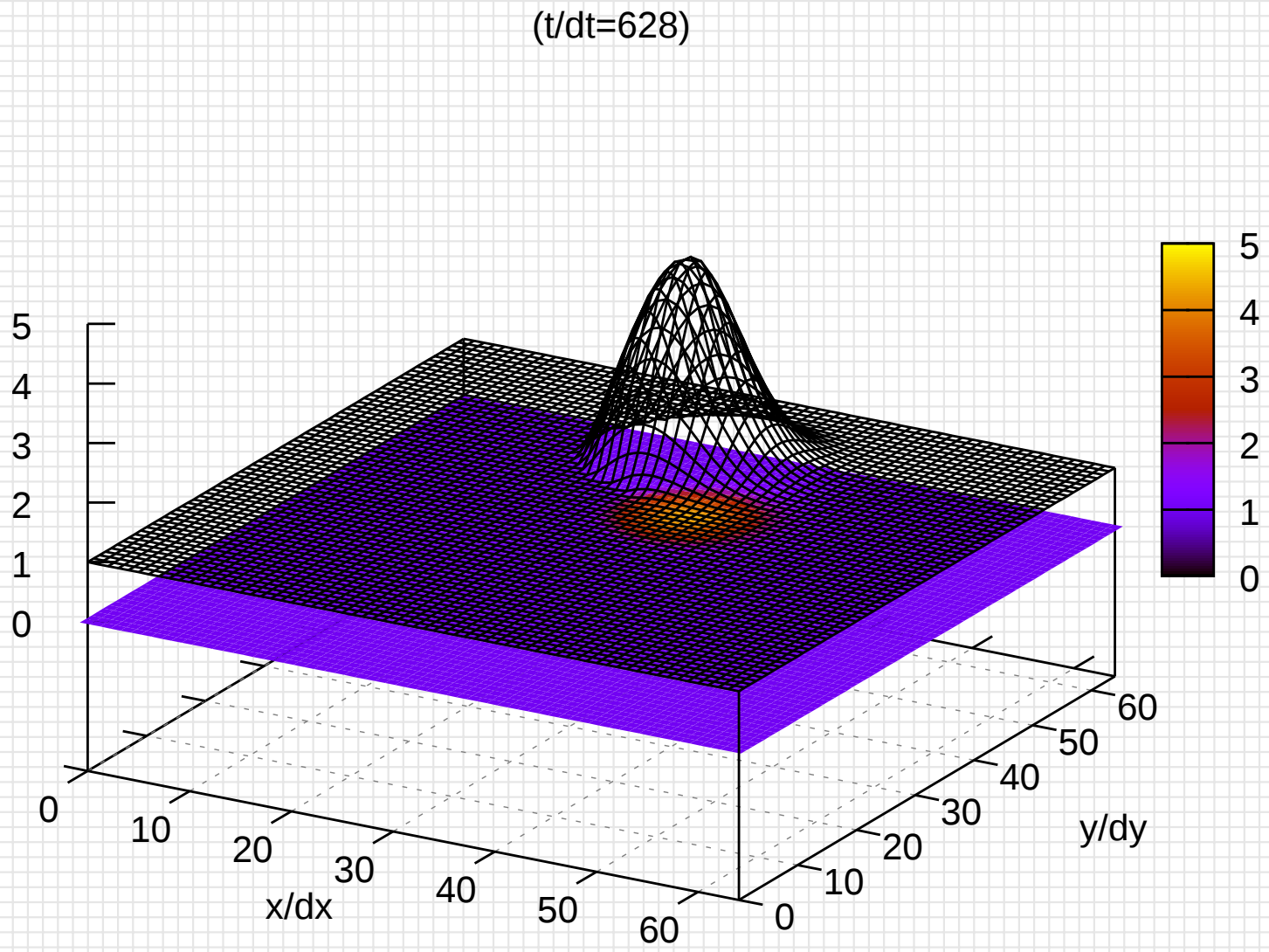

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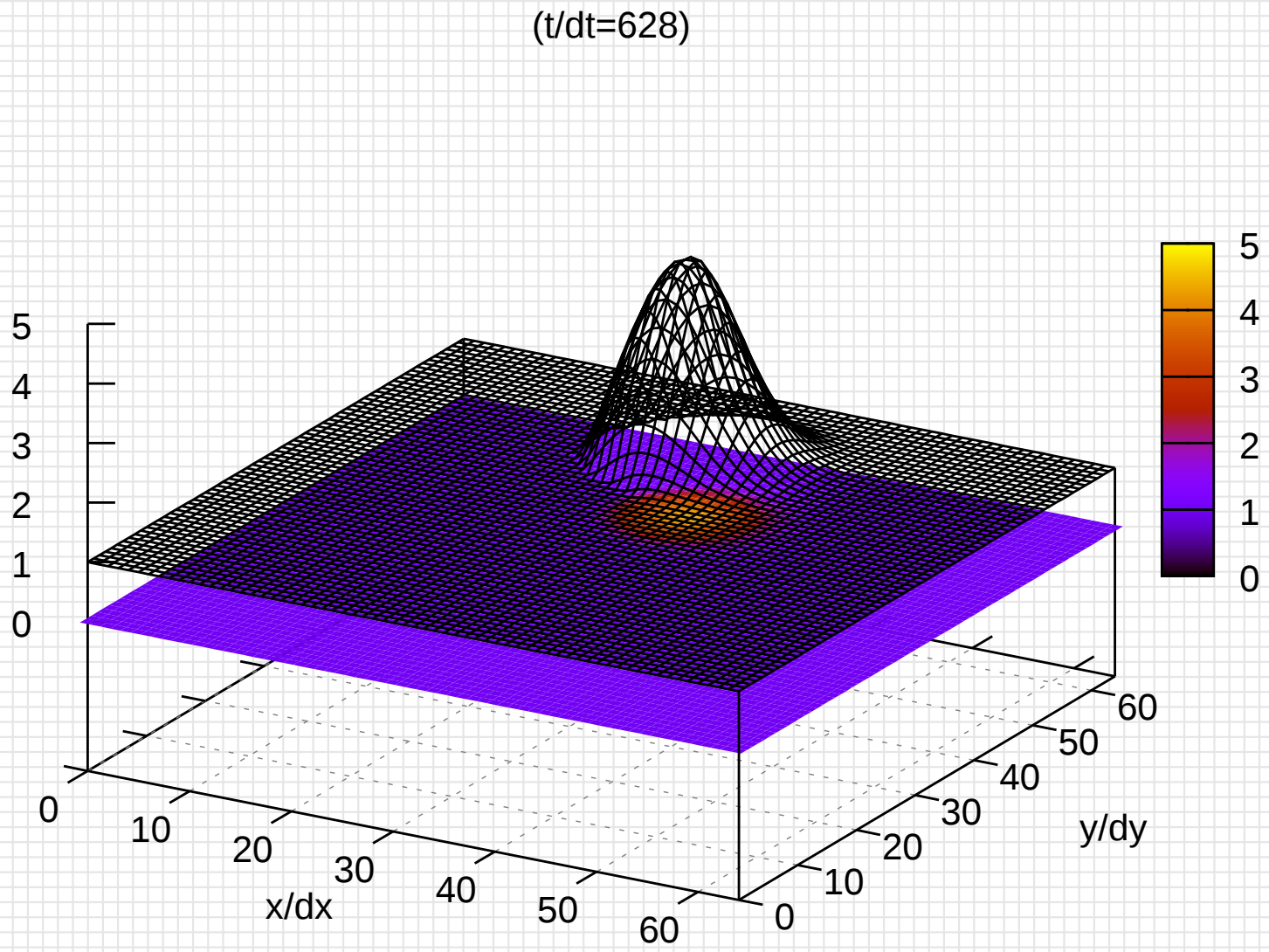

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side note: concurrency nomenclature

problem decomposition method

- domain decomposition (data parallelism)
- ...

process interaction method (hardware related)

- shared-memory (e.g., multi-core CPU)
  $\rightsquigarrow$ synchronisation-based concurrency, e.g., OpenMP
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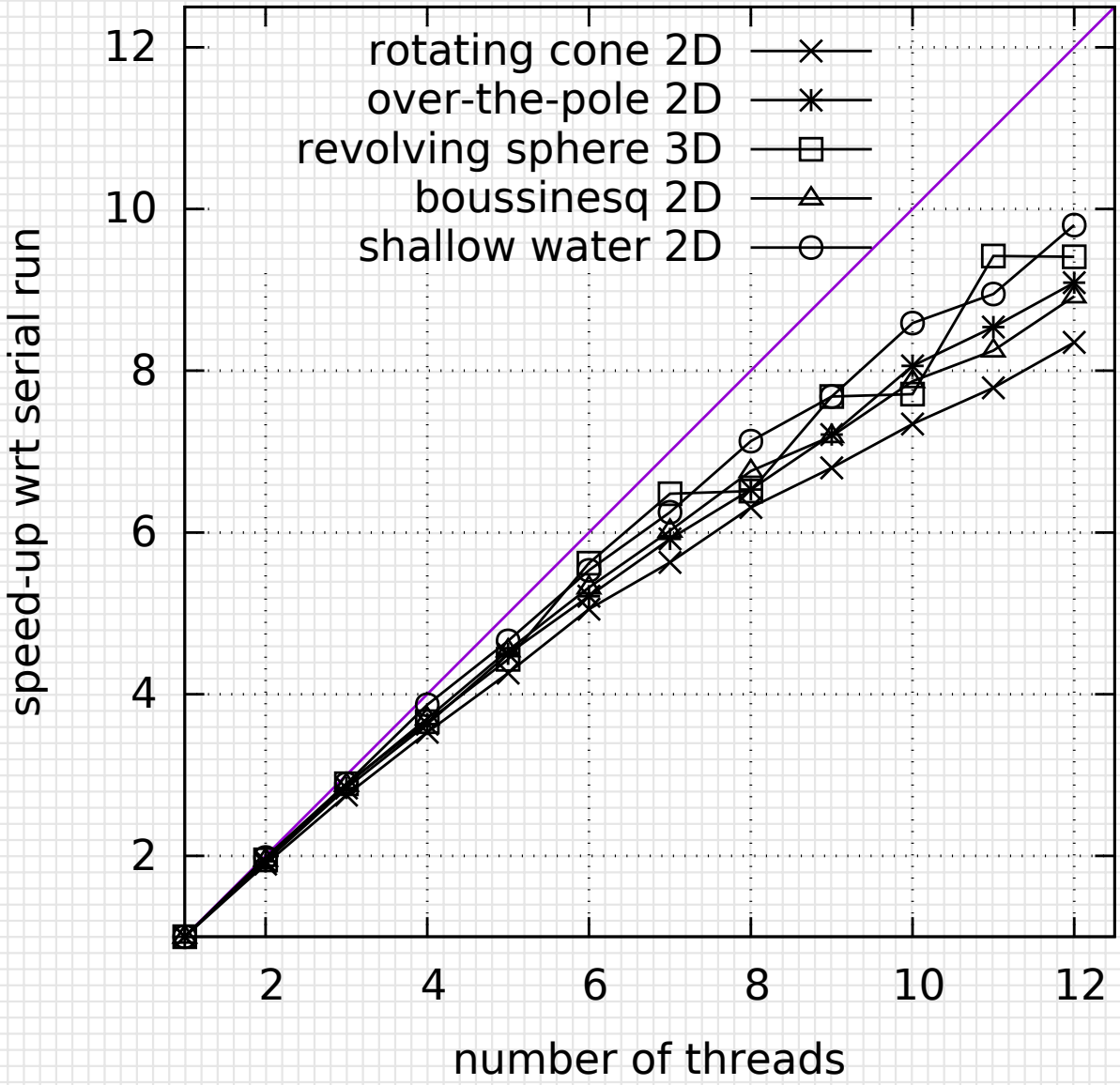
with multi-threading ⇝ also 64 LOC!

```
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%
...
```

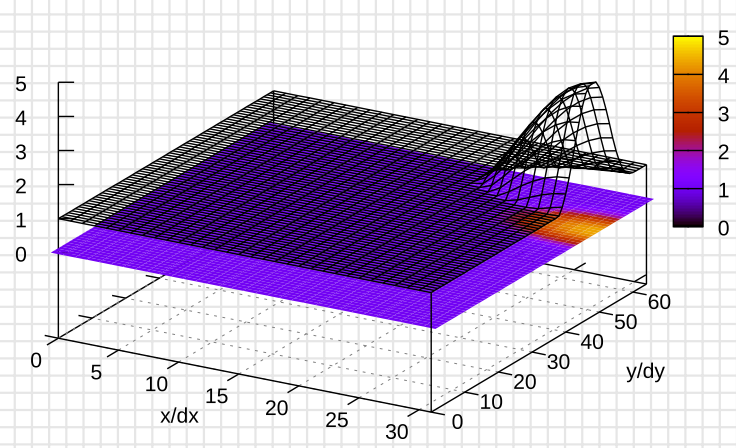
libmpdata++: multi-threading performance scaling

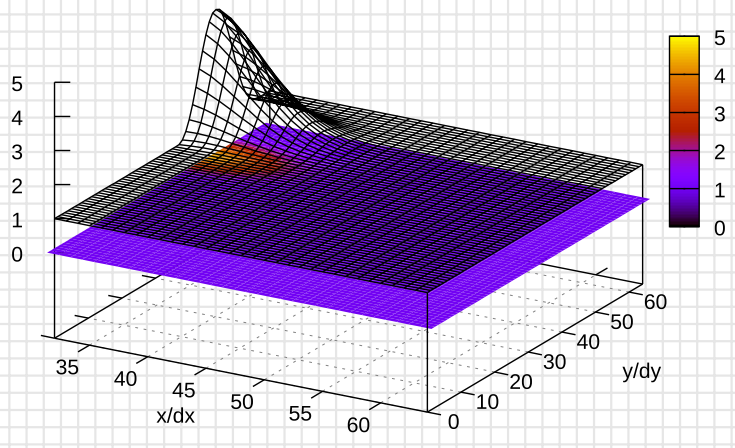


MPI + threads $\rightsquigarrow$ also 64 LOC!!! (recompilation only)

```
$ 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%
...
```





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ECMWF

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

libmpdata++

a prospective dynamical core for LES

Thank you for your attention

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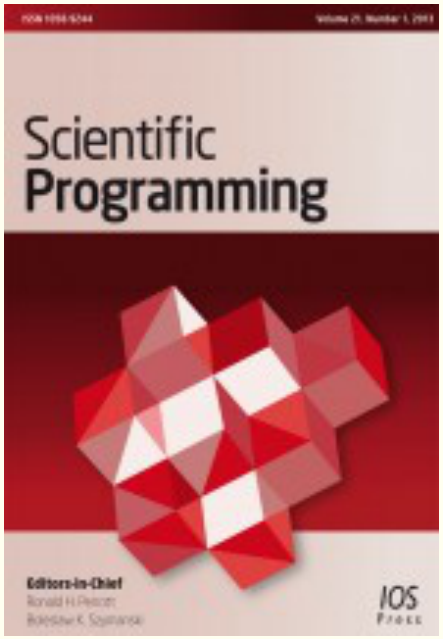
C++ vs. FORTRAN: language-choice tradeoffs



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

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

libmpdata++ vs. F77-MPDATA: CPU-time ratios

(3D, homogeneous advection, serial)

grid	59^3	$(2\times59)^3$	$(4\times59)^3$	$(6\times59)^3$
ratio	4.8	2.0	1.4	0.9

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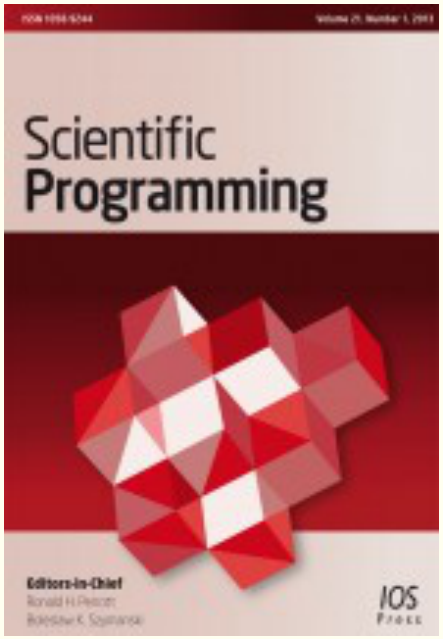

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libmpdata++: some design choices

legal

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

library components

- solvers/algorithms:
  - ...
- boundary conditions:
  - ...
- output handlers:
  - HDF5/XDMF (MPI-IO)
  - gnuplot
- shared-mem concurrency:
  - OpenMP
  - Boost.Thread
  - C++11 threads
- distributed-mem concurr.:
  - MPI

dependencies

- C++ compiler (C++11 & OpenMP)
- Blitz++
- Boost (ptr_container, timer, thread, preprocessor, filesystem, format, property_tree, MPI)
- CMake, CTest
- MPI
- HDF5
- gnuplot-iostream

API

- header-only library
- template-based component selection
- inheritance-based component extensions
- user exposed to Blitz++ API