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Hermes2d

C++ library for rapid development of adaptive
hp-FEM / hp-DG solvers

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Hermes2d Overview

What it is?

- C++ multi-platform (Win, Linux, MacOS) library for rapid prototyping of FEM & DG solvers

- "When you want to solve a non-trivial PDE in 2d with the least possible effort. And you know some C/C++."

- "When you want to test drive something small (a preconditioner, error estimate, FE space), and you don't want to write all the rest for it. And you know some OOP in C++."

How can I try it out?

- https://github.com/hpfem/hermes

- On Linux
    - Download, get dependencies via package managers, configure, build

- On Windows
    - Download, get dependencies from https://github.com/l-korous/hermes-windows, configure, build

What technologies are used in Hermes2d?

- (Modern) C++, well documented, and exception-safe

- OpenMP for parallelization of the most CPU-intensive tasks

- Real-time OpenGL visualization

- External linear solvers (UMFPACK, PARALUTION, MUMPS, PETSc)

- Usual exchange formats (XML, BSON, VTK, ExodusII, MatrixMarket, Matlab)

Hermes2d Overview > Features

What can it do?

- Stationary / Time-dependent / Harmonic equations

- Number of manual, and automatic mesh refinement (AMR) options
    - Granular AMR setup based on customizable error estimate calculations

- Nonlinear equation handling using Newton's and Picard's method
    - Fully automatic & configurable Newton's method with damping coefficient control, jacobian reuse control, arbitrary stopping criteria control

- Time-adaptivity, Space-time adaptivity using embedded Runge-Kutta methods
    - Time-error space distribution, arbitrary calculations of any error estimate pluggable into AMR, and time-step controllers

- Weak & Strong coupled problems
    - No matter what the coupling is, when you can write the weak formulation of your problem on paper, you can do that in Hermes2d as well.

What it cannot do (does not do)

- Problem specific optimizations, caching, shortcuts, etc.
    - But #1: In some cases, the Hermes2D API provides methods that can be used for some optimizations.
    - But #2: Due to the use of OOP, users of the library are welcome to sub-class Hermes2d core classes and implement the missing functionality.

Examples > Magnetostatics

In this example, we solve the equation

$$\nabla \times \left[\frac{1}{\mu} (\nabla \times u) \right] = J, \quad u|_{\delta\Omega} = 0$$

Where

- J is the current density,

- μ is (nonlinear) permeability,

- u is the (sought) magnetic vector potential (its z-component),

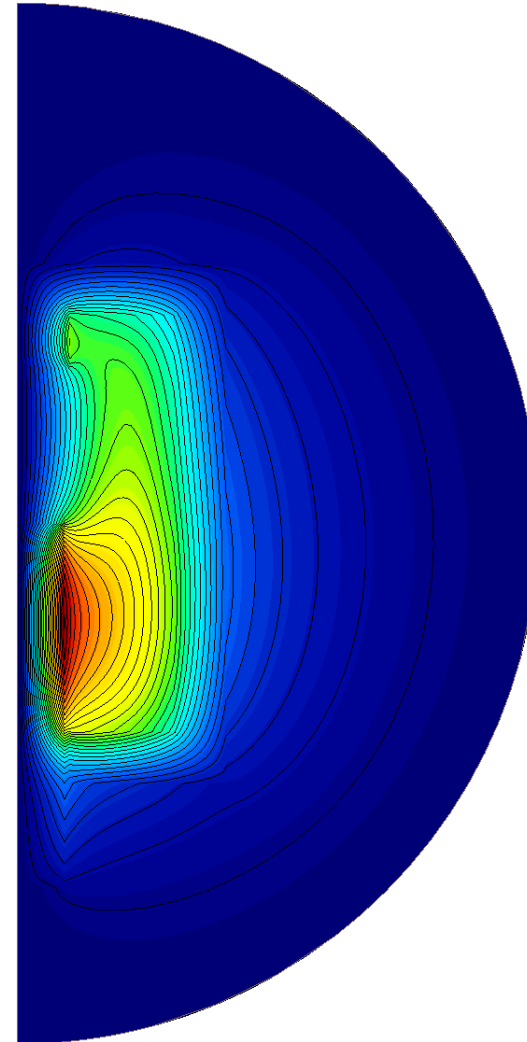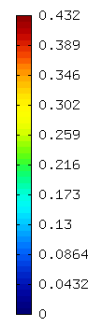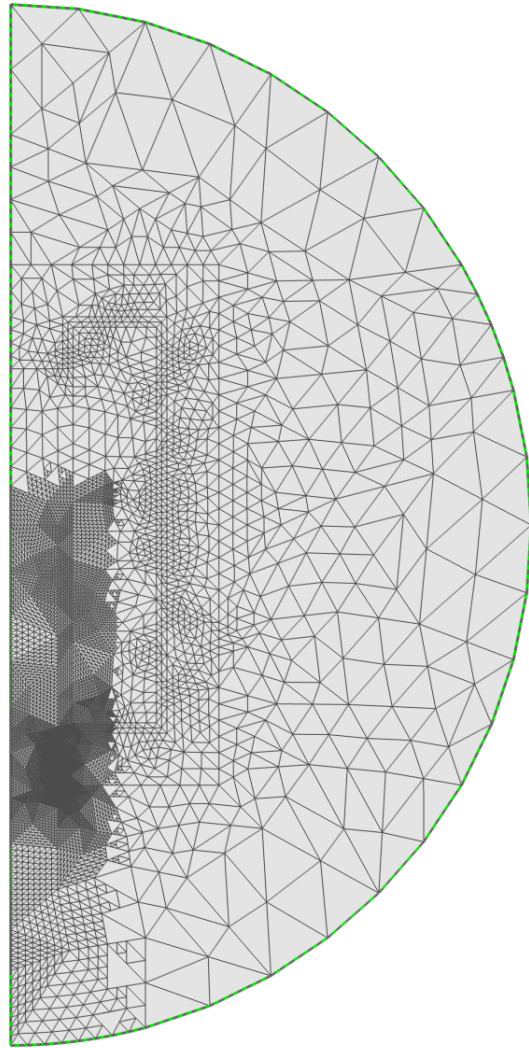- Ω is the space domain (picture on next slide).

The features illustrated on this example are

- Newton's method for nonlinear problems,

- nonlinear term specification using a table of values, and cubic spline interpolation.

Examples > Magnetostatics

Domain Ω with

triangular mesh

Solution –

vector potential u

0.432
0.389
0.346
0.302
0.259
0.216
0.173
0.13
0.0864
0.0432
0

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Examples > Magnetostatics

Refining the mesh according to a criterion

```
mesh->refine_by_criterion(&refinement_criterion);
- header: int refinement_criterion(Element* e), returning whether or not to refine a particular Element.
Used to refine the mesh around the copper <> iron interface.
```

CubicSpline class used for nonlinearity description

```
// Define nonlinear magnetic permeability via a cubic spline.
std::vector<double> mu_inv_pts({ 0.0, 0.5, 0.9, ... });
std::vector<double> mu_inv_val({ 1. / 1500.0, 1. / 1480.0, 1. / 1440.0, ... });
CubicSpline mu_inv_iron(mu_inv_pts, mu_inv_val, ...);
```

Newton's method for a strong nonlinearity

```
// Automatic damping ratio – if a step is unsuccessful, damping factor will be multiplied by this, if successful, it will be divided by this.
newton.set_auto_damping_ratio(1.5);
// Initial damping factor – we can start with a small one, automation will increase it if possible.
newton.set_initial_auto_damping_coeff(.1);
// The redidual norm after a step must be at most this factor times the norm from the previous step to pronounce the step 'successful'.
// Now for very strong nonlinearities, we may even need this > 1.
newton.set_sufficient_improvement_factor(1.25);
// This is a strong nonlinearity, where we can't afford to reuse Jacobian matrix from a step in subsequent steps.
newton.set_max_steps_with_reused_jacobian(0);
// Maximum number of iterations. Hermes will throw an exception if this number is exceeded and the tolerance is not met.
newton.set_max_allowed_iterations(100);
// The tolerance – simple in this case, but can be a combination of relative / absolute thresholds of residual norm, solution norm, solution difference norm, ...
newton.set_tolerance(1e-8, Hermes::Solvers::ResidualNormAbsolute);
```

Examples > Advection

In this example, we solve the equation

$$\nabla \cdot [\,(-x_2, x_1)u\,] = 0, \quad u|_{\delta\Omega} = g$$

Where

- u is the sought solution,

- Ω is the space domain - square (0, 1) x (0, 1),

- g is defined as follows:
  - $g = 1,\ \text{where } (-x_2, x_1) \cdot \vec{n}\,(\vec{x}) > 0,$
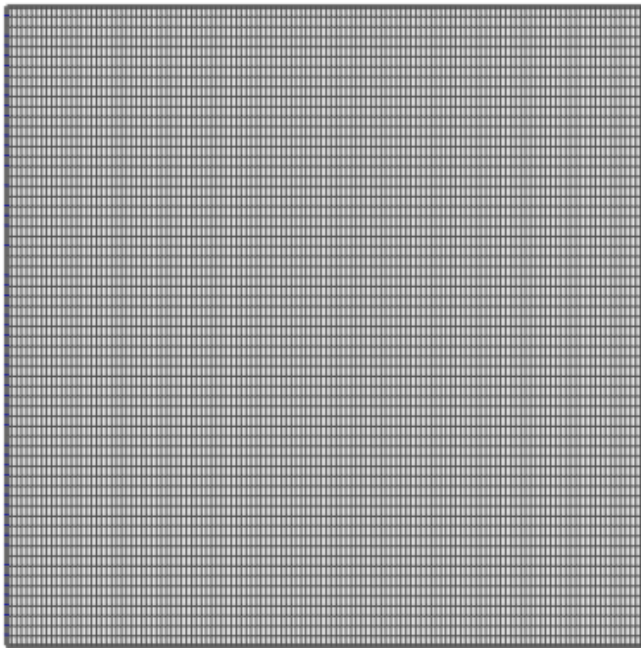 - $g = 0,\ \text{where } (-x_2, x_1) \cdot \vec{n}\,(\vec{x}) \leq 0.$

The features illustrated on this example are

- Discontinuous Galerkin (DG) implementation of integrating over internal edges,

- postprocessing of results – in this case using a limiter preventing spurious oscillations that occur in DG method.

Examples > Advection

Domain Ω with
quadrilateral mesh

Solution

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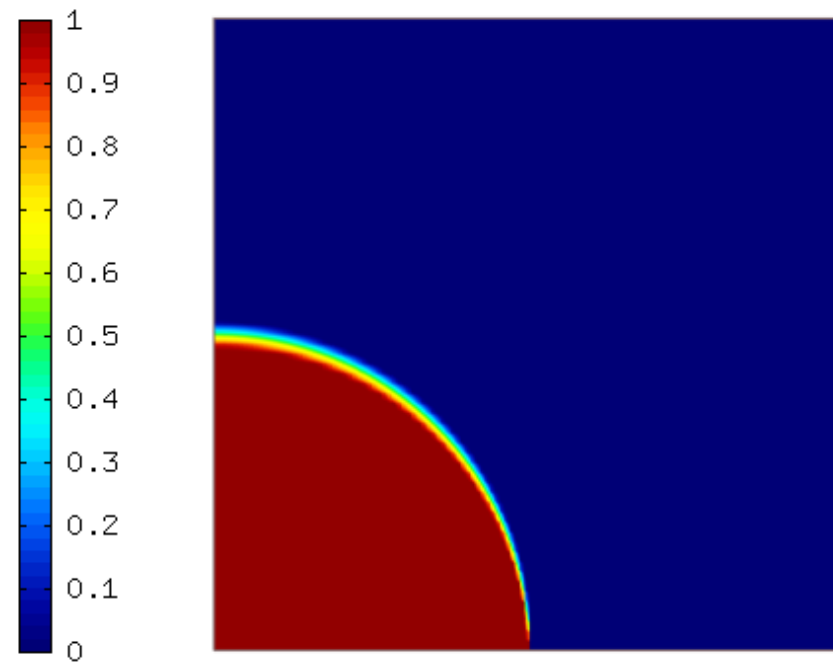
Examples > Advection

Integration over internal edges

- Regular forms (simplified)

  ```
  matrix_form(int n, double *wt, Func<double> *u, Func<double> *v)
  ```
  - n ... Number of integration points
  - wt ... Integration weights
  - u ... Basis function values(, derivatives) in the integration points
  - v ... Test function values(, derivatives) in the integration points

- DG forms (simplified)

  ```
  matrix_form(int n, double *wt, DiscontinuousFunc<double> *u, DiscontinuousFunc<double> *v)
  ```
  - n, wt ... As above
  - u, v ... DiscontinuousFunc<double> = { Func<double> u->central, Func<double>* u->neighbor } ... Only one is filled for each matrix_form call.

Postprocessing

- e.g. Vertex-based limiter (Kuzmin, D.: A vertex-based hierarchical slope limiter for -adaptive discontinuous Galerkin methods, JCAM, 233(12):3077-3085)

  ```
  // sln_vector ... Algebraic system solution
  // space ... FE space of the solution
  // Instantiate the limiter
  PostProcessing::VertexBasedLimiter limiter(space, sln_vector);
  // Get a limited solution, already as a Hermes2D Solution object
  Hermes::Hermes2D::Solution<double> limited_sln = limiter.get_solution();
  ```

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Examples > Advection > Automatic adaptivity (AMR)

We solve the same problem – equation & boundary conditions:

$$\nabla \cdot [\, (-x_2, x_1)u\,] = 0, \quad u|_{\delta\Omega} = g$$

But this time, we start from a very coarse mesh:
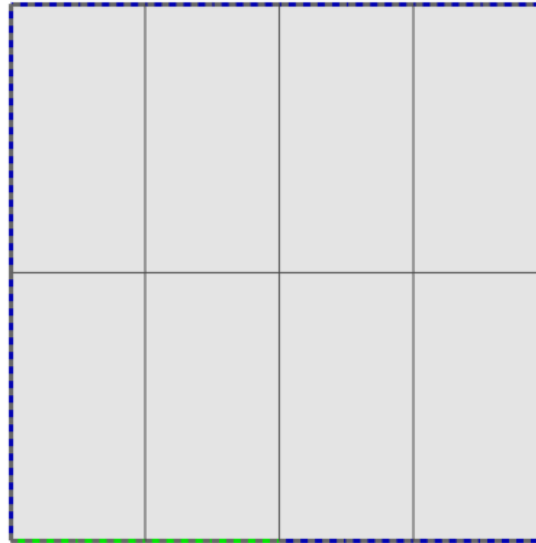
And we employ AMR (h-adaptivity) to get results on the next slide.

Examples > Advection > Automatic adaptivity (AMR)
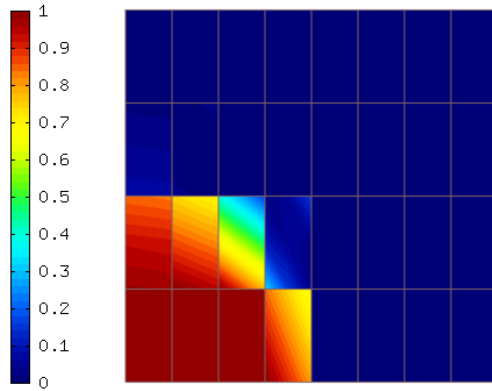
AMR step 1, Element count: 32
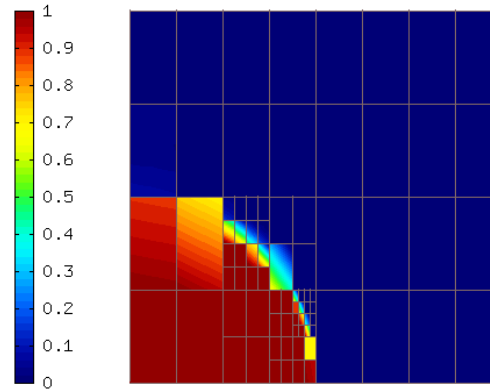
AMR step 2, Element count: 116
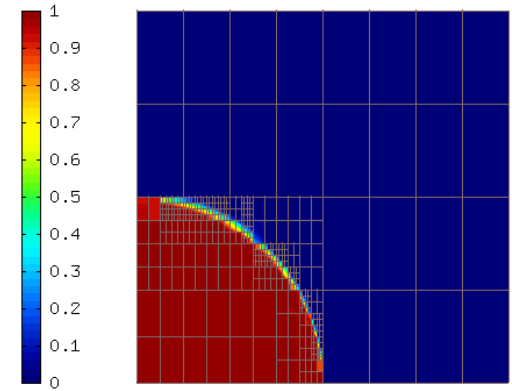
AMR step 3, Element count: 272
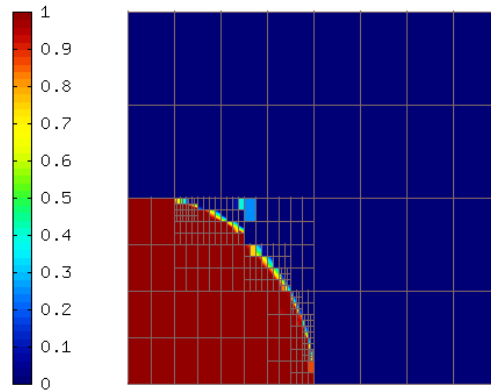
AMR step 4, Element count: 504
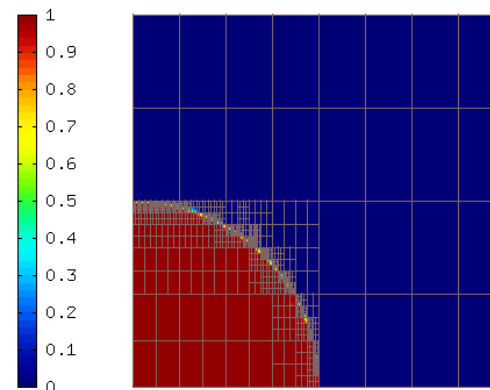
AMR step 5, Element count: 848

Examples > Advection > Automatic adaptivity (AMR)

```cpp
int adaptivity_step = 1; bool done = false;
do
{
    // Construct globally refined reference mesh and setup reference space.
    Mesh::ReferenceMeshCreator ref_mesh_creator(mesh);
    MeshSharedPtr ref_mesh = ref_mesh_creator.create_ref_mesh();
    Space<double>::ReferenceSpaceCreator refspace_creator(space, ref_mesh, USE_TAYLOR_SHAPESET ? 0 : 1);
    SpaceSharedPtr<double> refspace = refspace_creator.create_ref_space();

    // Solve the problem on the reference space.
    linear_solver.set_space(refspace);
    linear_solver.solve();

    // Get the Hermes2D Solution object from the solution vector.
    Solution<double>::vector_to_solution(linear_solver.get_sln_vector(), refspace, refsln);

    // Project the reference solution to the coarse space in L2 norm for error calculation.
    OGProjection<double>::project_global(space, refsln, sln, HERMES_L2_NORM);

    // Calculate element errors and total error estimate.
    errorCalculator.calculate_errors(sln, refsln);
    double total_error_estimate = errorCalculator.get_total_error_squared() * 100;

    // If error is too large, adapt the (coarse) space.
    if (error_estimate > ERR_STOP)
        adaptivity.adapt(&selector);
    else
        done = true;

    // Increase the step counter.
    adaptivity_step++;
} while (done == false);
```

Examples > Navier-Stokes

In this example, we solve the equations

$$\frac{\delta u}{\delta t} - \frac{\Delta u}{Re} + (u \cdot \nabla)u + \nabla p = 0, \quad u|_{\delta\Omega \backslash \Gamma_o} = g$$

$$\nabla \cdot u = 0$$

Where

- Γ_o is the output boundary,
- u, p is the sought solution,
- Ω is the space domain – see next slide,
- g is defined as follows:
    - $g_1 = 0$ everywhere except inlet,
    - $g_2 = 0$ everywhere,
    - g_1 is a parabolic profile on the inlet.

The features illustrated on this example are

- OpenGL visualization of vector fields,
- Simple time-stepping using implicit Euler scheme.

Examples > Navier-Stokes > OpenGL visualization of vector fields

Solution

- Velocity (vector field) top

- Pressure bottom

- t = 30s
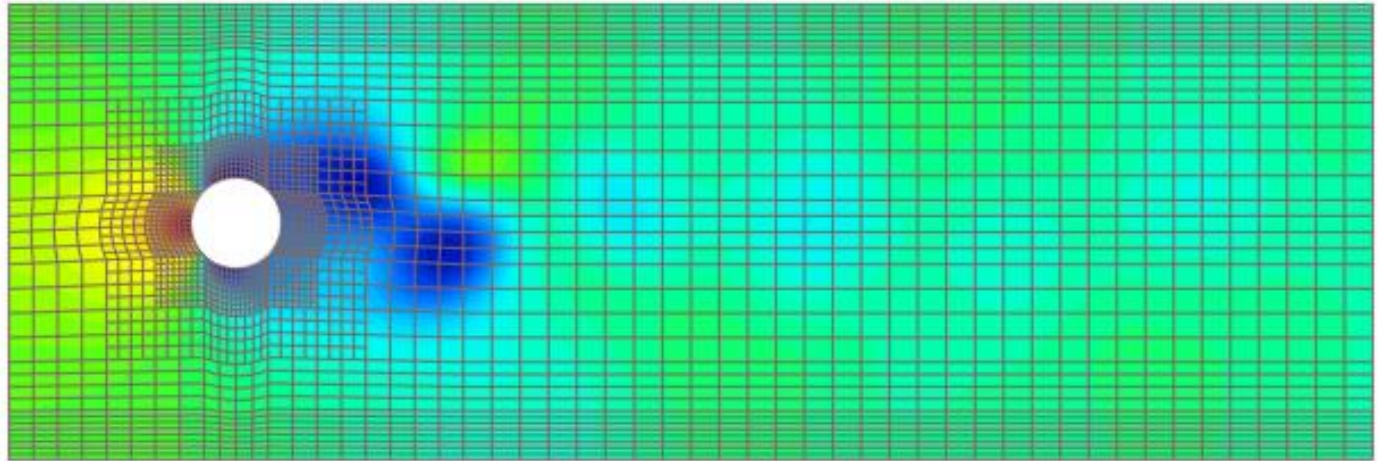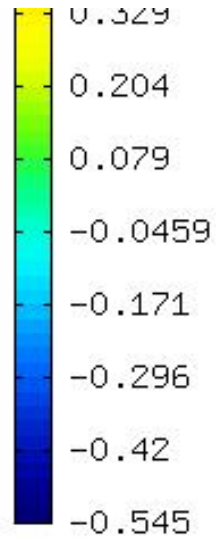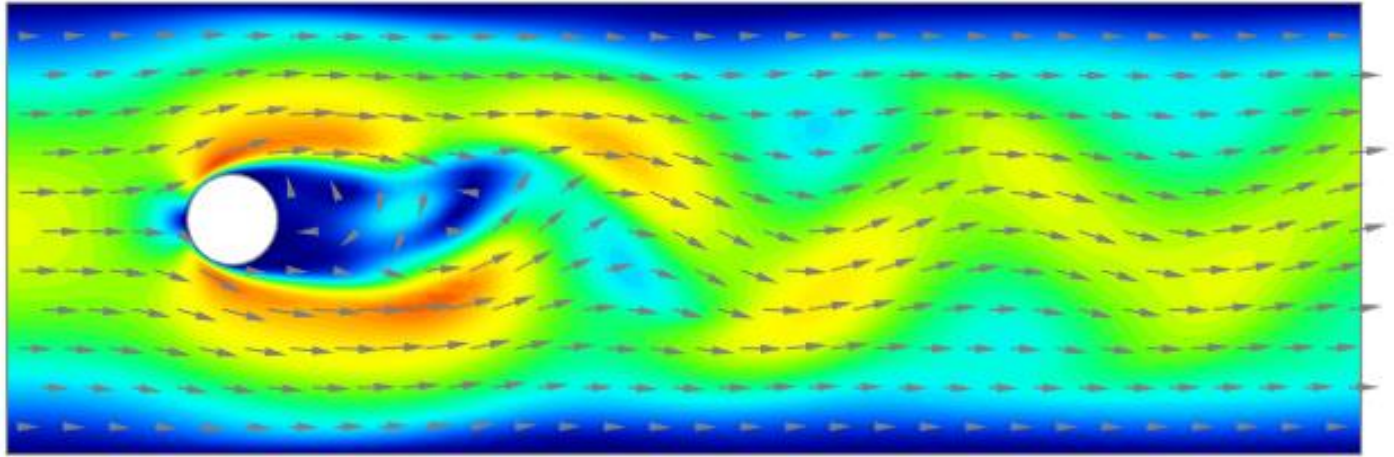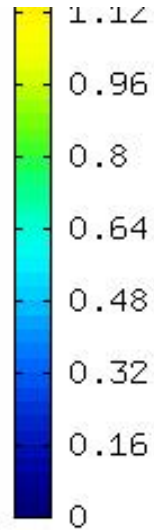
Examples > Navier-Stokes > OpenGL visualization of vector fields

Solution

- Velocity (vector field) top

- Pressure bottom

- t = 40s
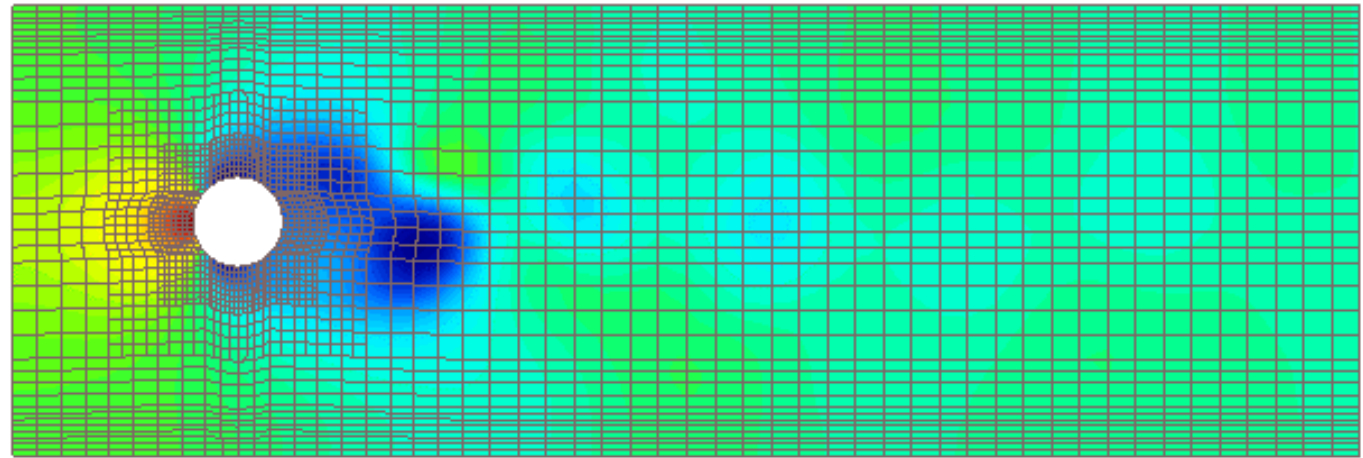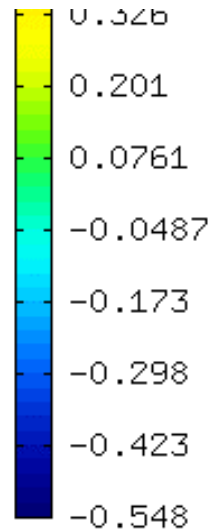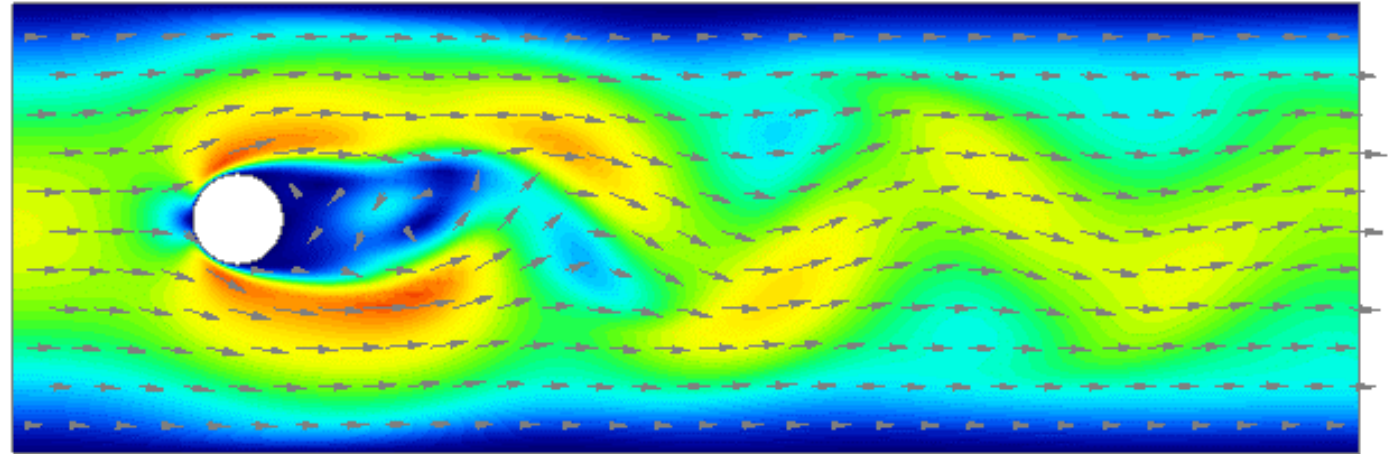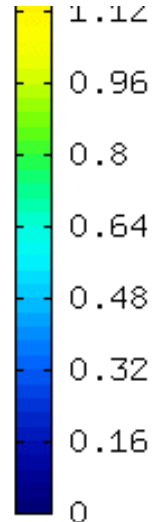
Examples > Navier-Stokes > OpenGL visualization of vector fields

Solution

- Velocity (vector field) top

- Pressure bottom

- t = 55s
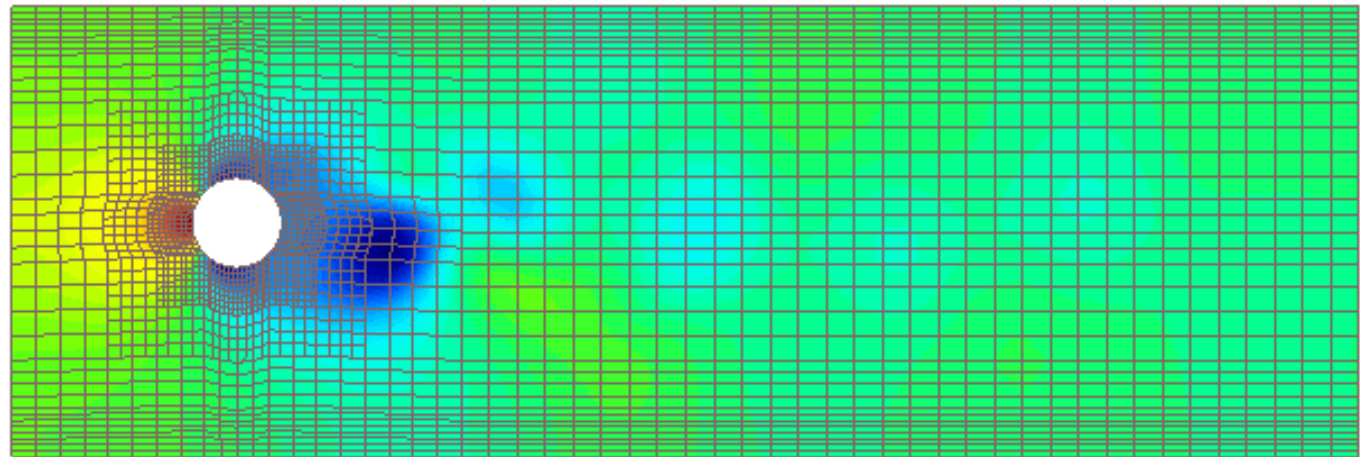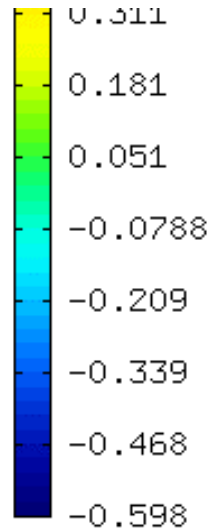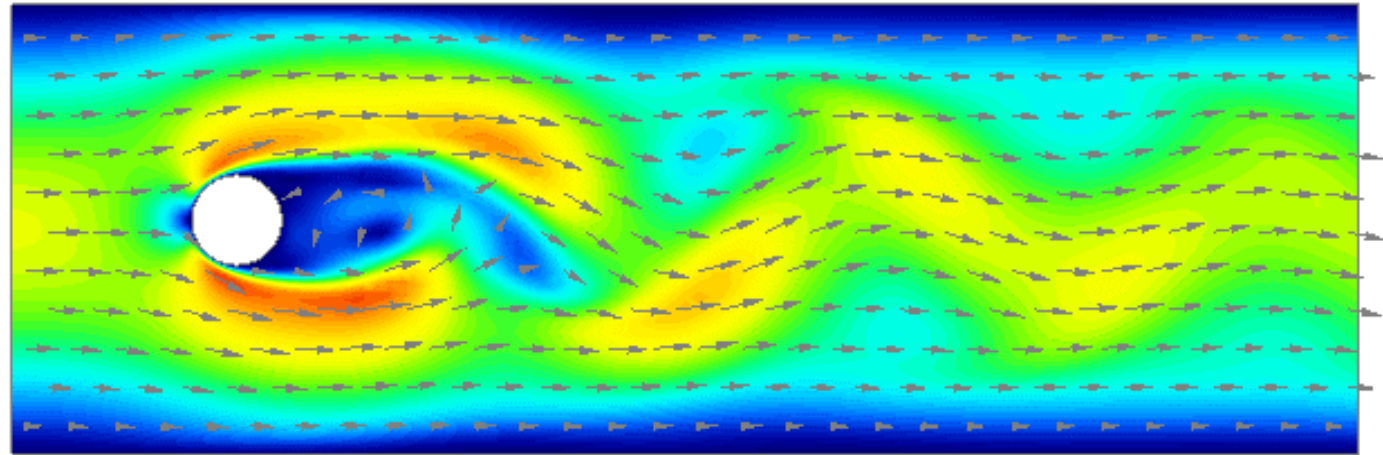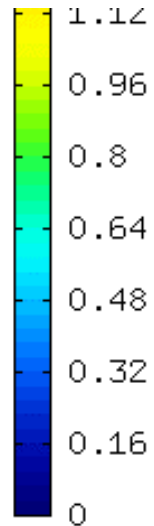
Examples > Navier-Stokes

Simple time-stepping using implicit Euler scheme

```cpp
for (int time_step = 1; time_step <= T_FINAL / TAU; time_step++, current_time += TAU)
{
    // Update time-dependent essential BCs.
    newton.set_time(current_time);

    // Solve Newton.
    // Weak formulation implements the implicit Euler scheme, and uses previous time step solutions.
    newton.solve(coeff_vec);

    // Get the solutions, insert as Hermes2D Solution object into the previous time step solutions.
    Hermes::Hermes2D::Solution<double>::vector_to_solutions(newton.get_sln_vector(), spaces, sln_prev_time);

    // Visualization.
    vview.set_title("Velocity, time %g", current_time);
    vview.show(xvel_prev_time, yvel_prev_time);

    pview.set_title("Pressure, time %g", current_time);
    pview.show(p_prev_time);
}
```

Example > Complex

This problem describes the distribution of the vector potential in a domain comprising a wire carrying electrical current, air, and an iron which is not under voltage. We solve the equation

$$-\frac{1}{\mu}\Delta A + i\omega\sigma A \ - \ = 0, \quad u|_{\Gamma_1} = 0, \left.\frac{\delta u}{\delta n}\right|_{\Gamma_2} = 0$$

Where

- Ω is the space domain - rectangle (0, 0.004) x (0, 0.003),
- Γ_1 is the top and right and left edge of Ω,
- Γ_2 is the bottom edge of Ω,
- A is the sought solution, ω is the given angular velocity, σ given conductivity

The features illustrated on this example are

- hp-adaptive FEM,
- Handling of complex equations in Hermes2D,
- Spatial error inspection.
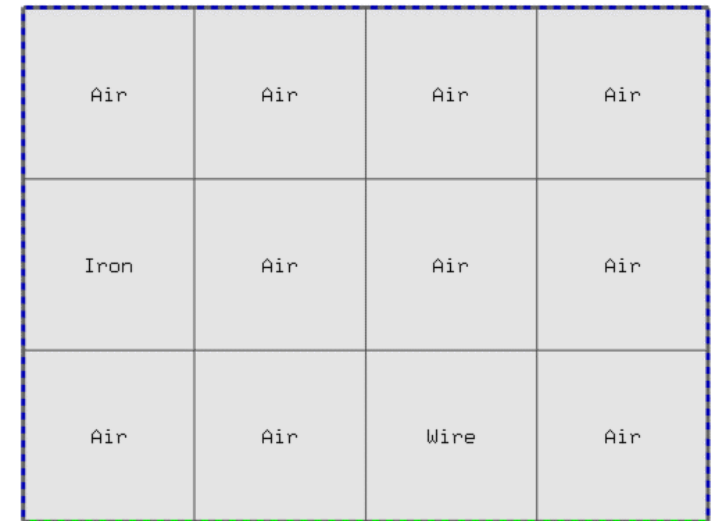
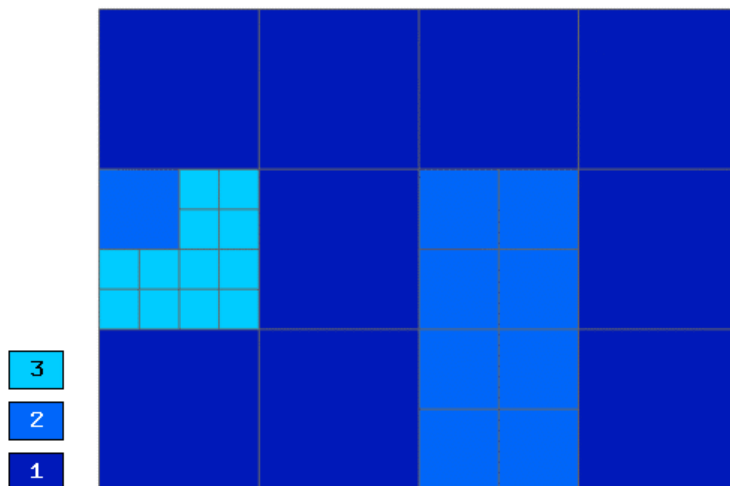# Example > Complex > hp-FEM step #1

Solution
- Reference space
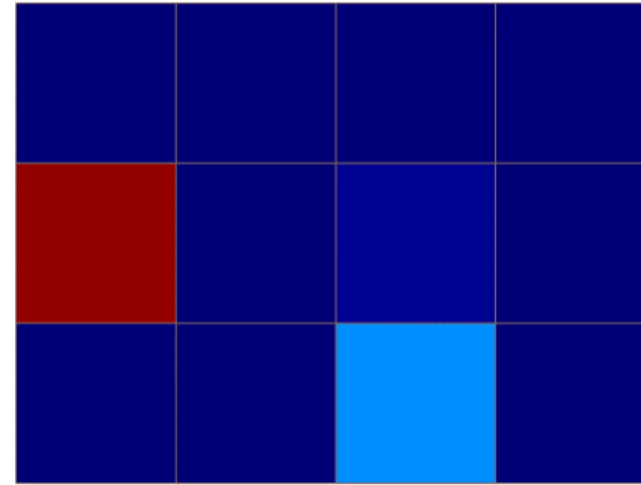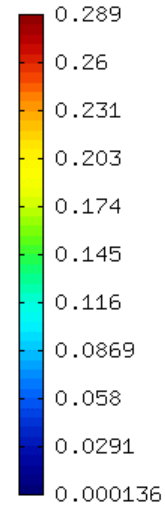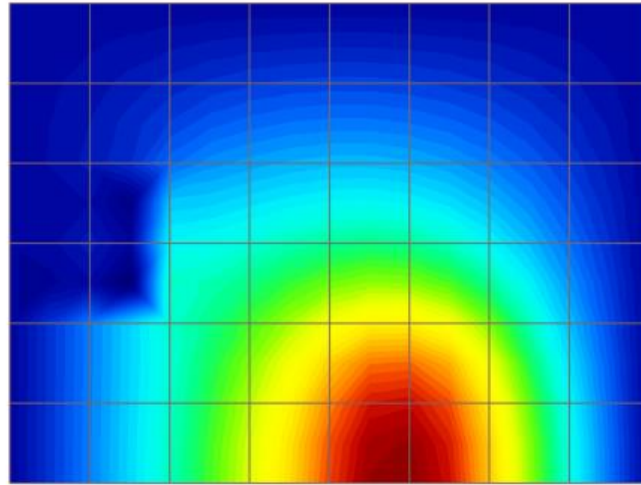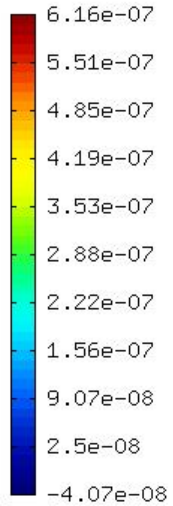
Spatial error inspection
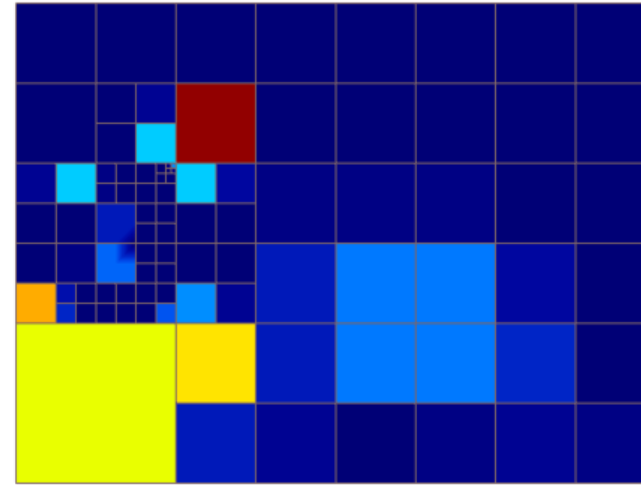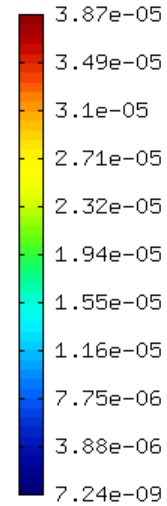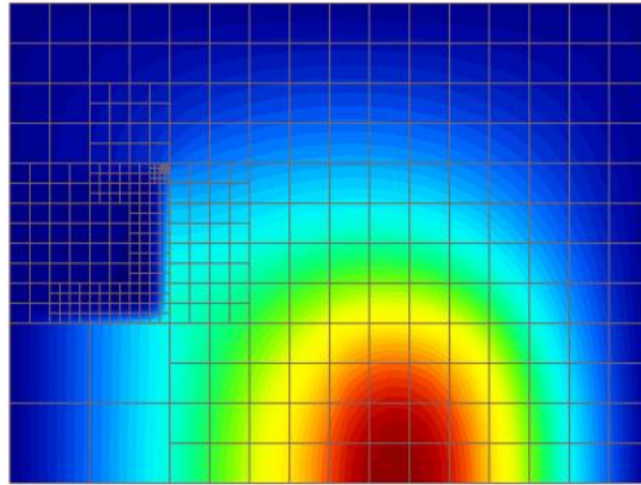
Element-wise error for the coarse mesh
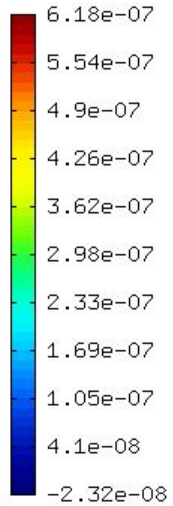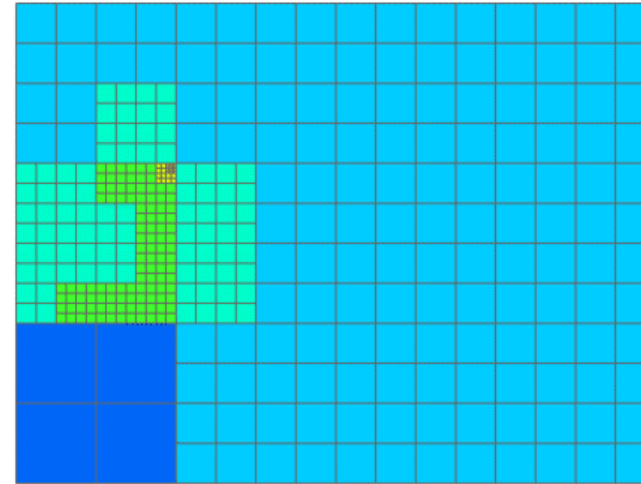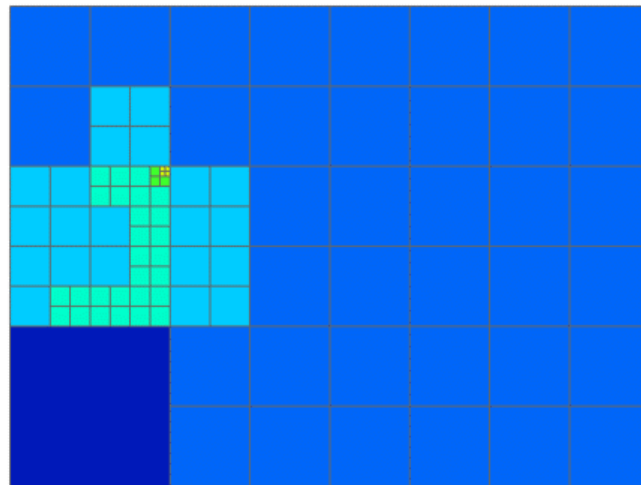

Coarse mesh
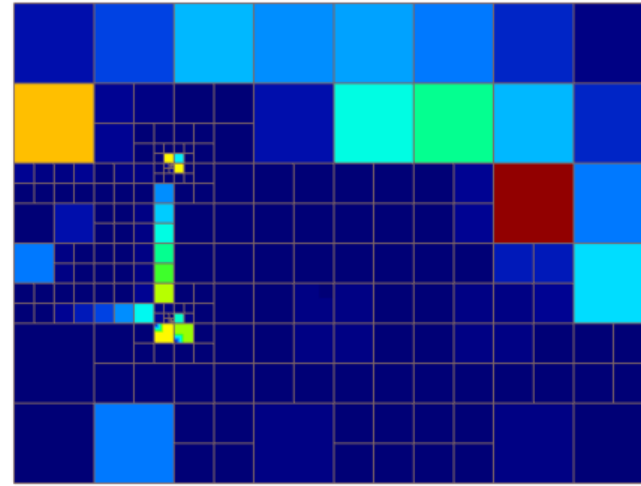

Fine mesh

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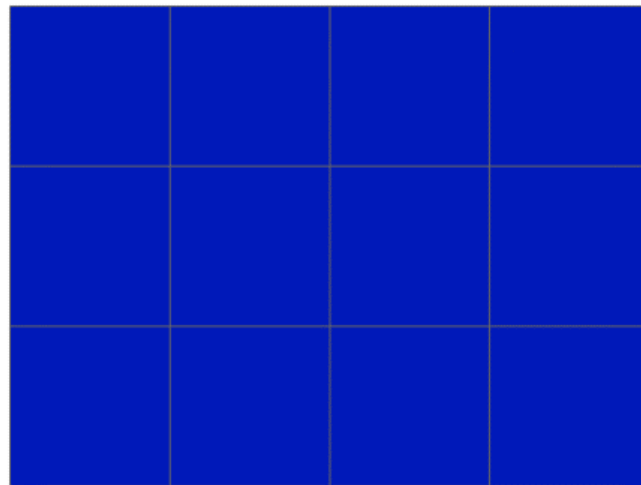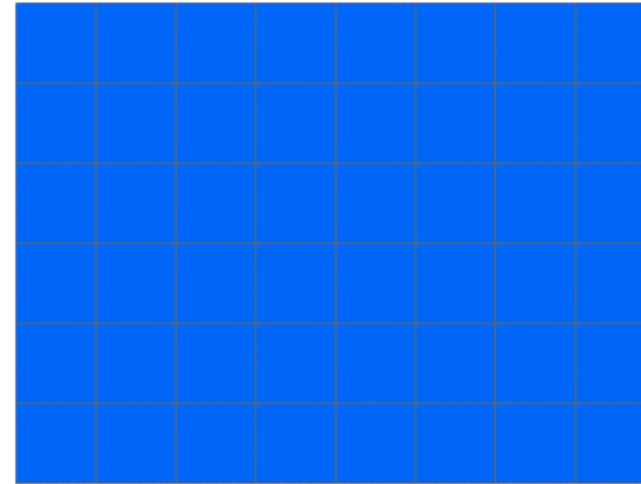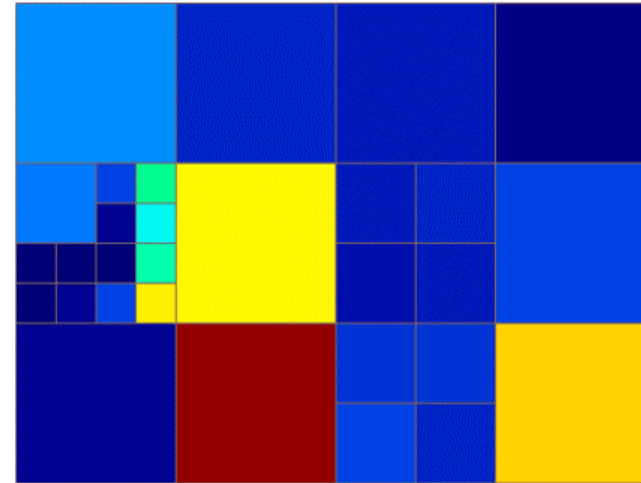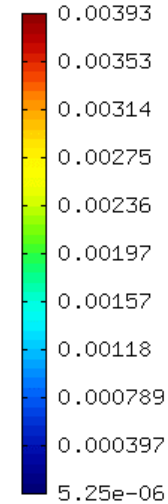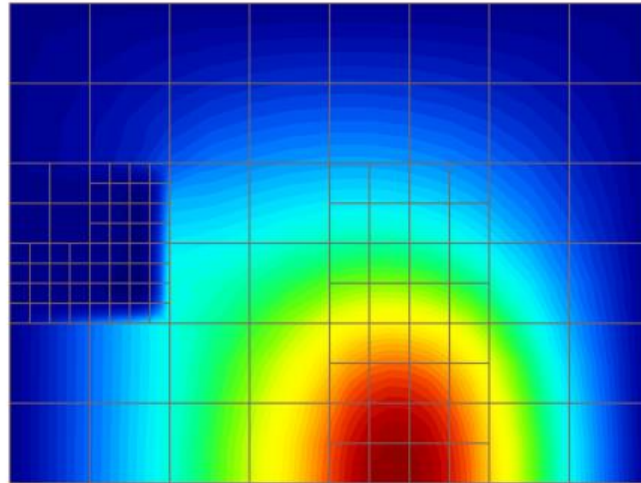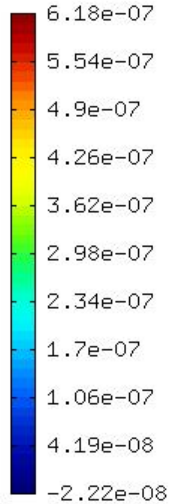
Solution
- Reference space

Spatial error inspection

Element-wise error for the coarse mesh
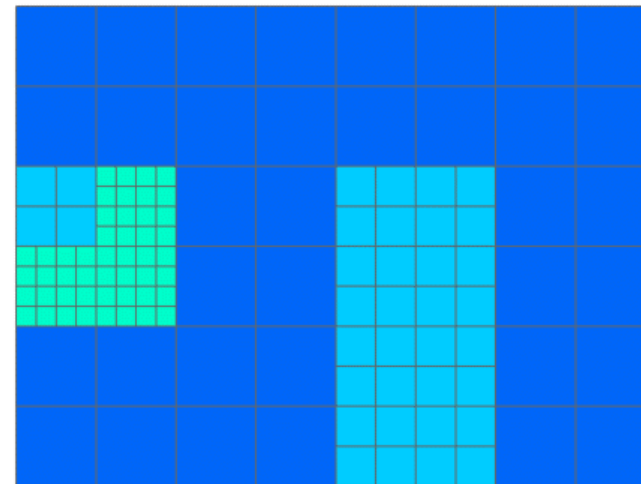
Coarse mesh

Fine mesh

Solution
- Reference space
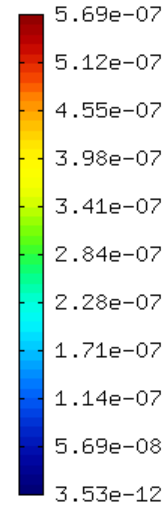
Spatial error inspection
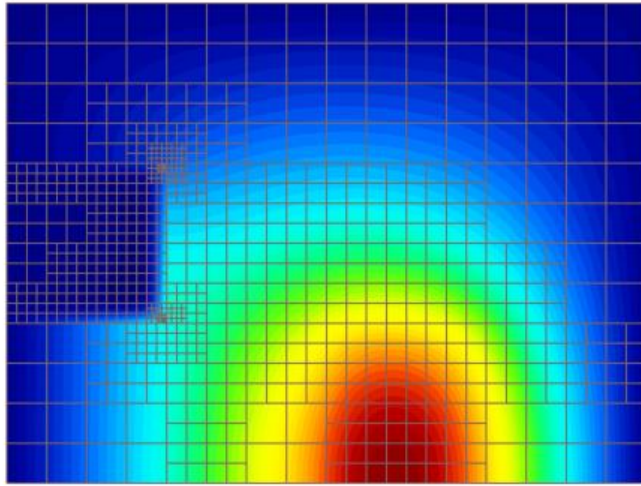
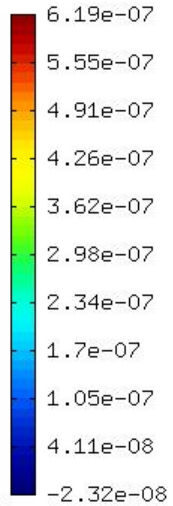Element-wise error for the coarse mesh

Coarse mesh

Fine mesh

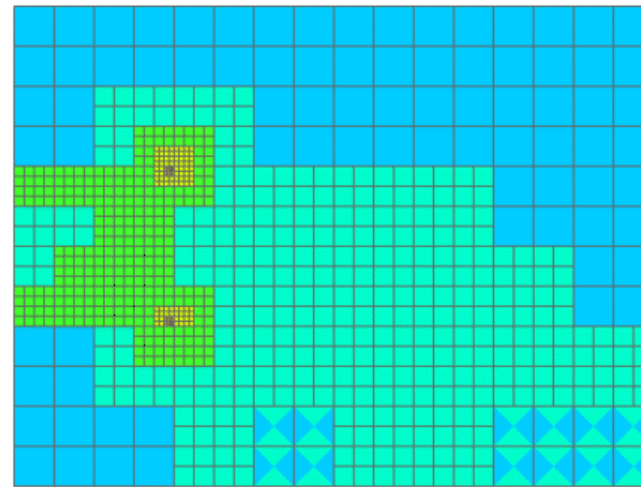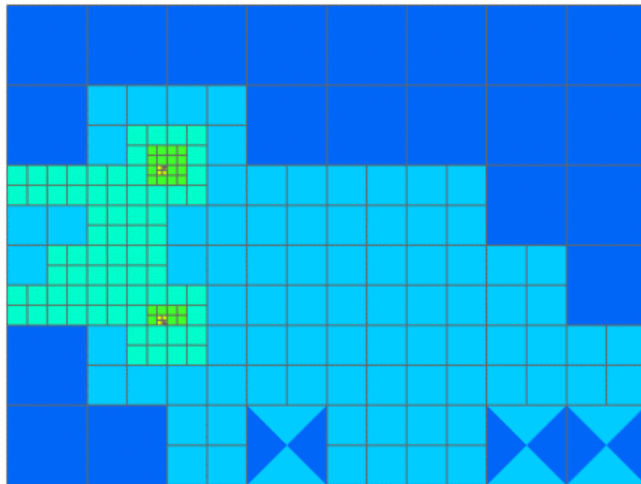# Example > Complex > hp-FEM step #29

Solution
- Reference space

Spatial error inspection

Element-wise error for the coarse mesh

Coarse mesh

Fine mesh

Example > Complex

Handling of complex equations in Hermes2D

- Very easy, all relevant Hermes2d classes have the number (real | complex) as their template argument:
  - For real numbers we use double: `H1Space<std::complex<double> >(mesh, boundary_conditions)`
  - For complex numbers we use std::complex<double>: `H1Space<std::complex<double> >(mesh, boundary_conditions)`

hp-adaptive FEM

- Basic settings to control the AMR process

```cpp
// Error calculation & adaptivity. We specify the norm here, and the type of error
DefaultErrorCalculator<::complex, HERMES_H1_NORM> errorCalculator(RelativeErrorToGlobalNorm);

// Stopping criterion for an adaptivity step. Influences the number of elements refined at each step.
AdaptStoppingCriterionSingleElement<::complex> stoppingCriterion(0.9);

// Adaptivity processor class. Gets the error calculator and stopping criterion
Adapt<::complex> adaptivity(&errorCalculator, &stoppingCriterion);

// Stopping criterion for adaptivity.
const double TOTAL_ERROR_ESTIMATE_STOP = 1e-3;
```

Examples > Wave Equation

In this example, we solve the equations

$$\frac{1}{c^2}\frac{\delta^2 u}{\delta t^2} - \Delta u = 0, \quad u|_{\delta\Omega} = 0, \quad \frac{\delta u}{\delta t}\bigg|_{\delta\Omega} = 0 \quad (1)$$

Where
- u is the sought solution,
- Ω is the space domain – see next slide,
- c is the wave speed.

We transform (1) into

$$\frac{\delta u}{\delta t} = v$$

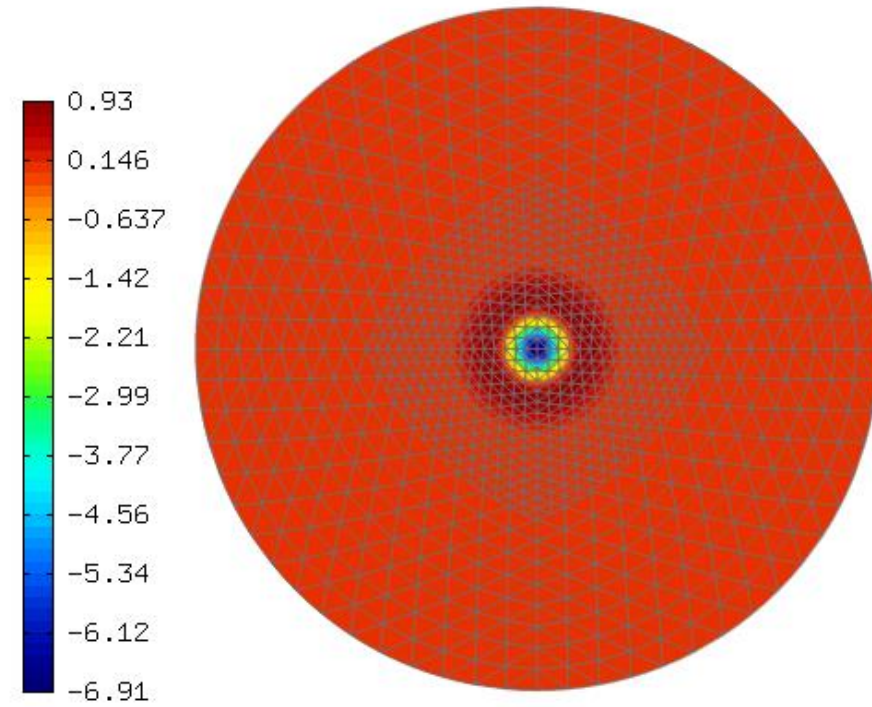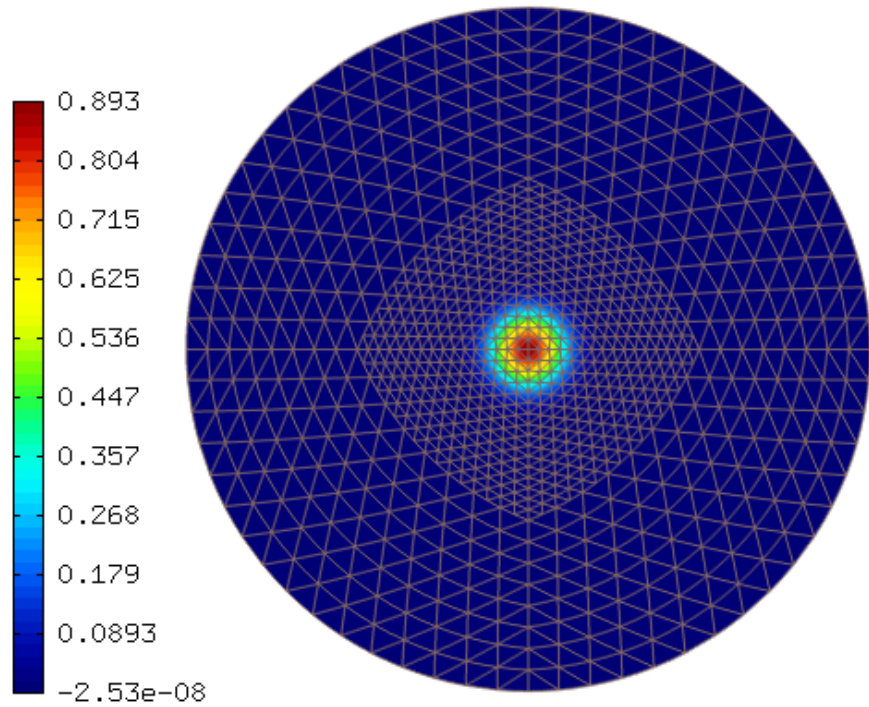$$\frac{\delta v}{\delta t} = c^2 \Delta u$$

The features illustrated on this example are

- Using an arbitrary Runge-Kutta method for time discretization,

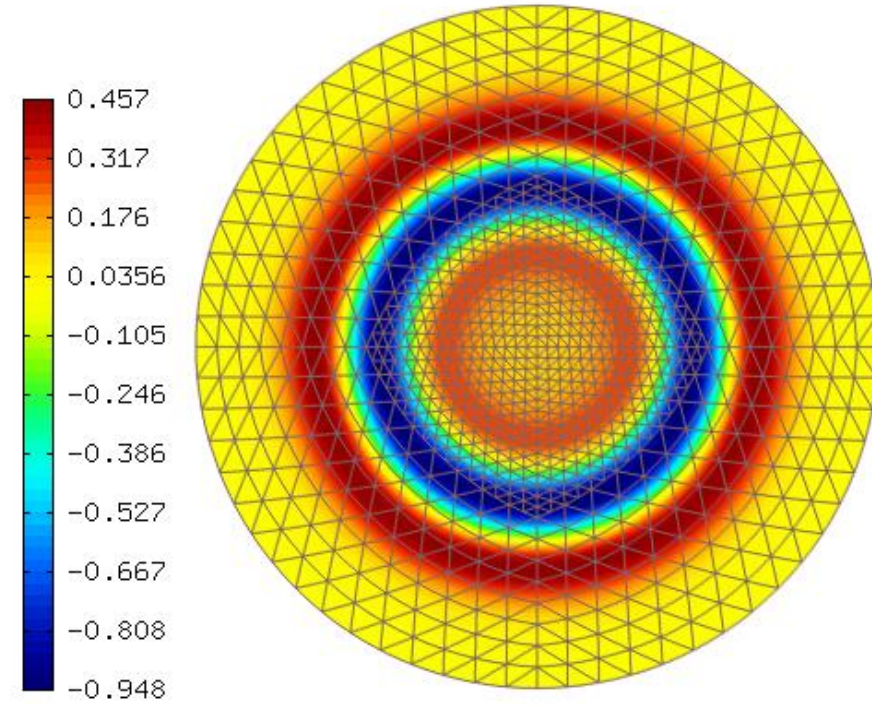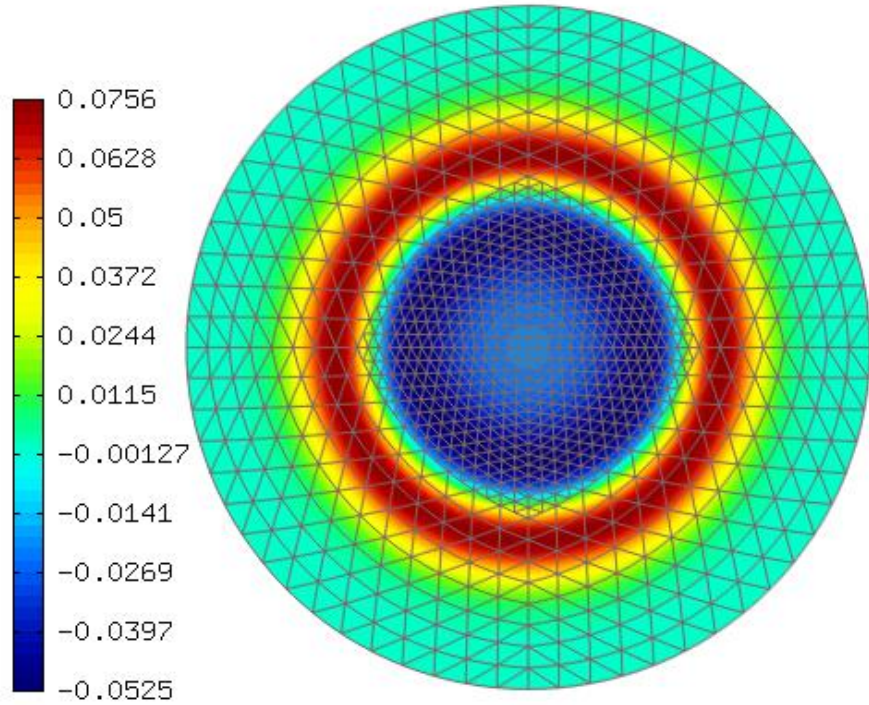- Time-adaptivity using embedded Runge-Kutta methods.

Example > Wave Equation
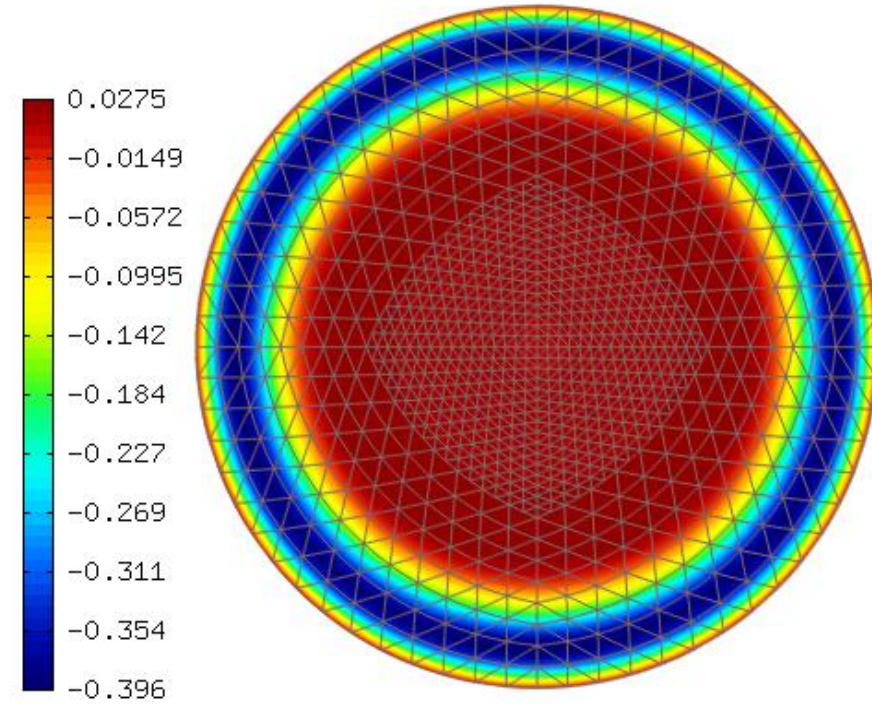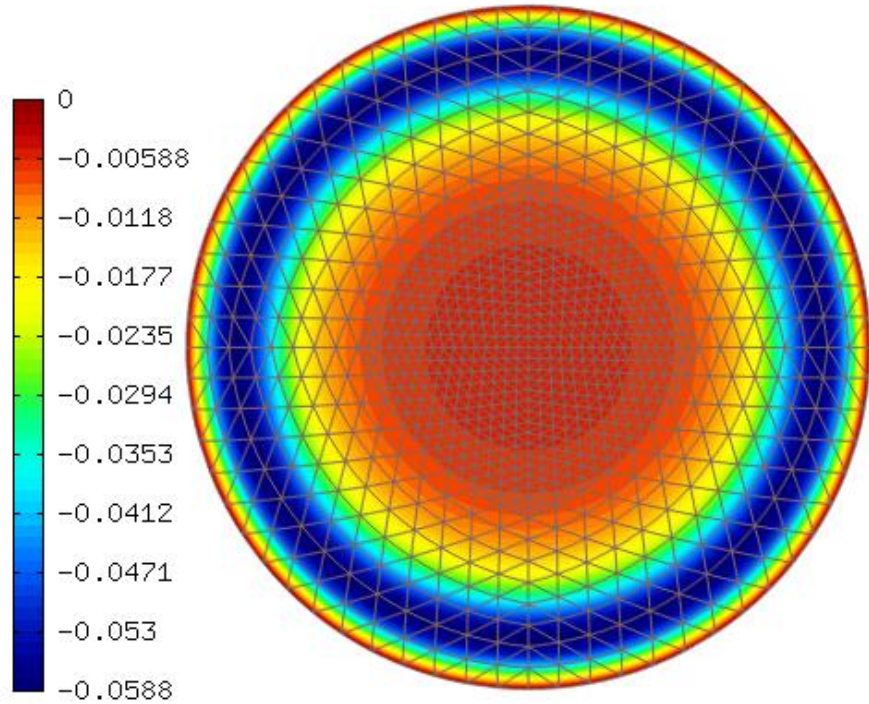
u (left), v(right), t = 1e-2s

Example > Wave Equation
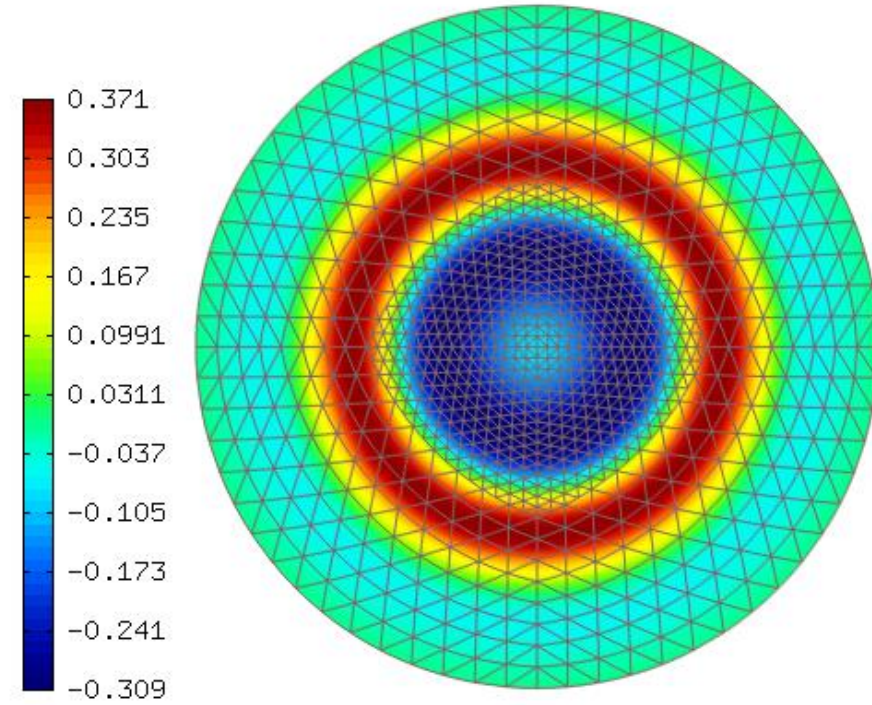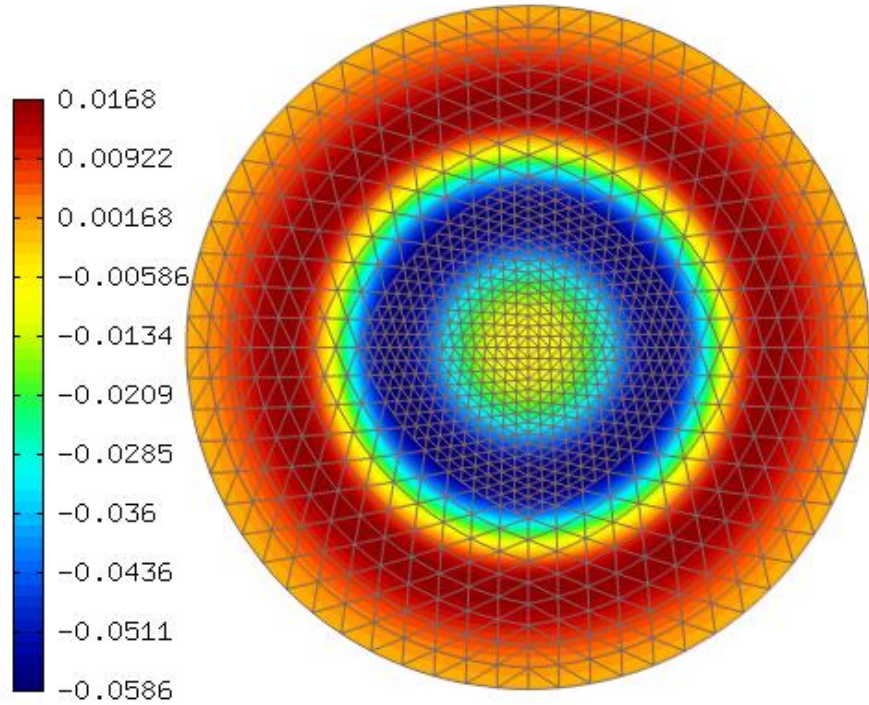
u (left), v(right), t = 5.1e-1s

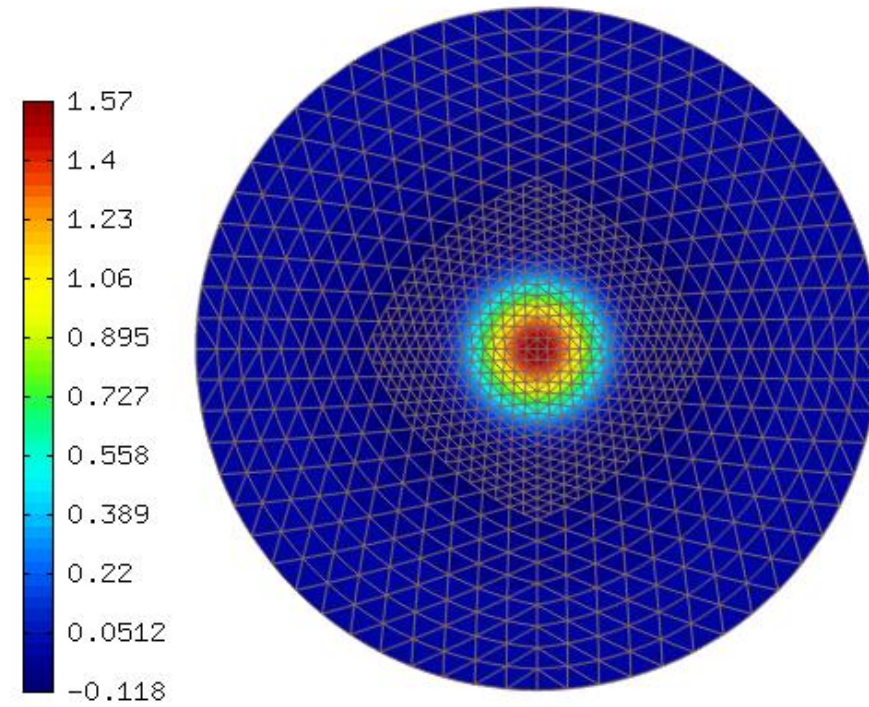# Example > Wave Equation
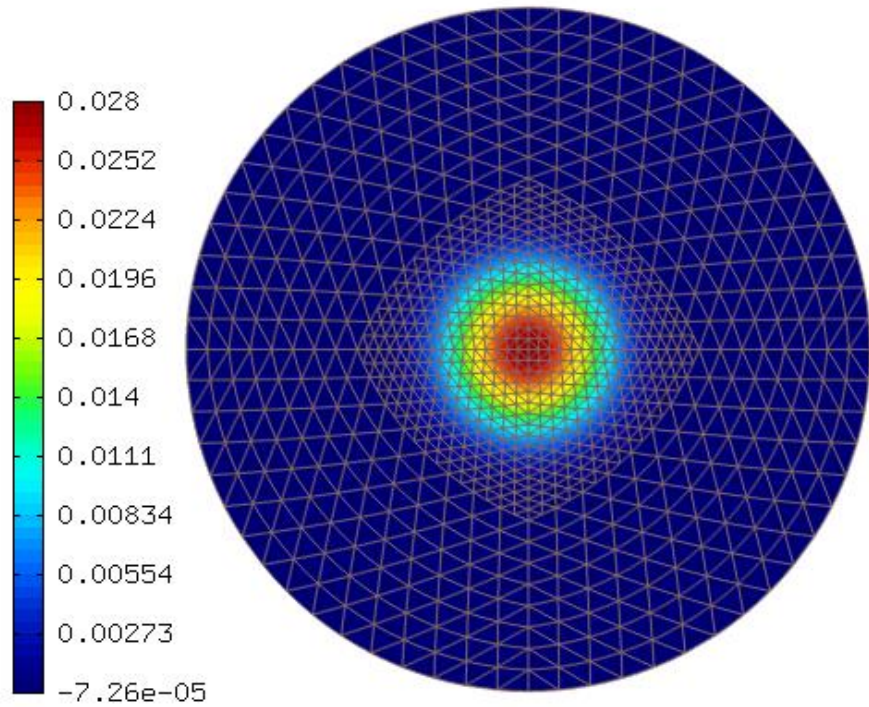
u (left), v(right), t = 1.01s

Example > Wave Equation

u (left), v(right), t = 1.51s

Example > Wave Equation

u (left), v(right), t = 2.01s

Example > Wave Equation

Time-adaptivity using embedded Runge-Kutta methods

```
runge_kutta.rk_time_step_newton(previous_solution, new_solution, time_error_function);
...
Hermes::Hermes2D::Views::ScalarView time_error_view;
time_error_view.show(time_error_function);
...
DefaultNormCalculator<double, HERMES_H1_NORM> normCalculator;
normCalculator.calculate_norms(time_error_function);
double relative_time_error_estimate = normCalculator.get_total_norm_squared() * 100.;
```


Image – temporal error in u (top), v (bottom), t = 0.3s
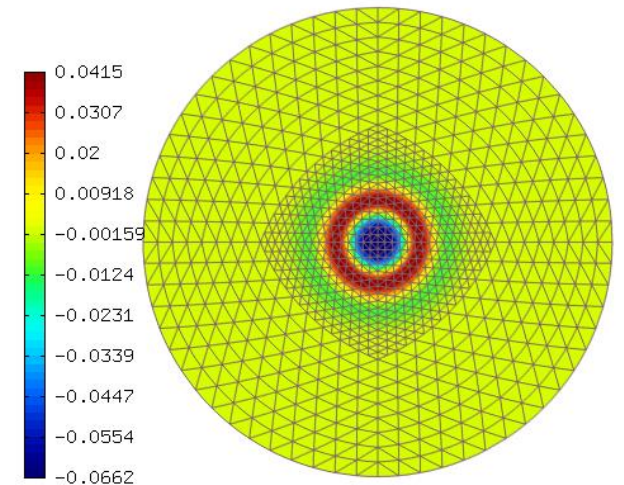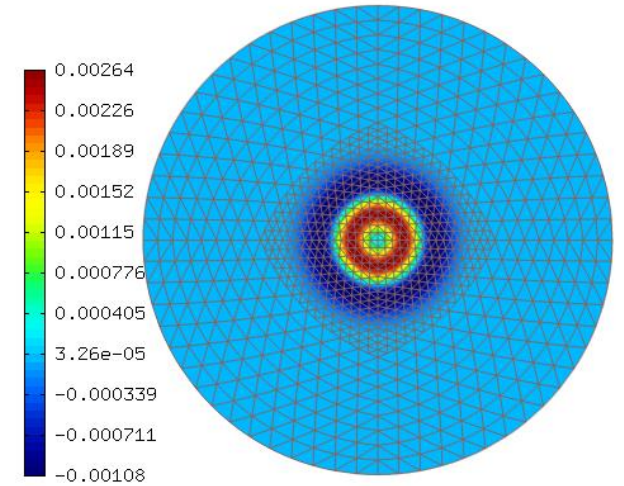
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Example > Wave Equation

Time-adaptivity using embedded Runge-Kutta methods

```
runge_kutta.rk_time_step_newton(previous_solution, new_solution, time_error_function);
...
Hermes::Hermes2D::Views::ScalarView time_error_view;

time_error_view.show(time_error_function);
...
DefaultNormCalculator<double, HERMES_H1_NORM> normCalculator;

normCalculator.calculate_norms(time_error_function);

double relative_time_error_estimate = normCalculator.get_total_norm_squared() * 100.;
```
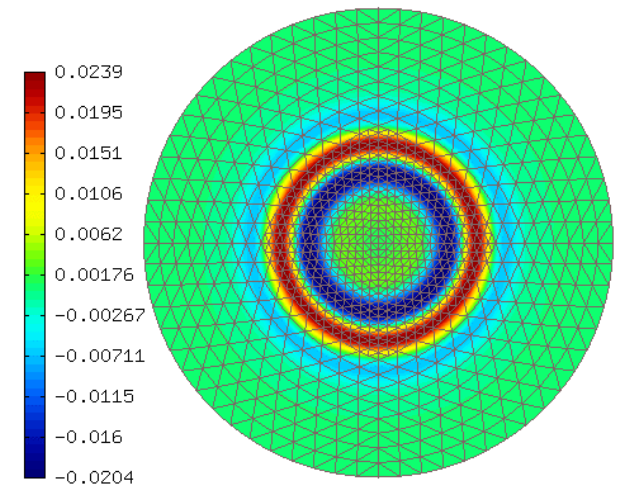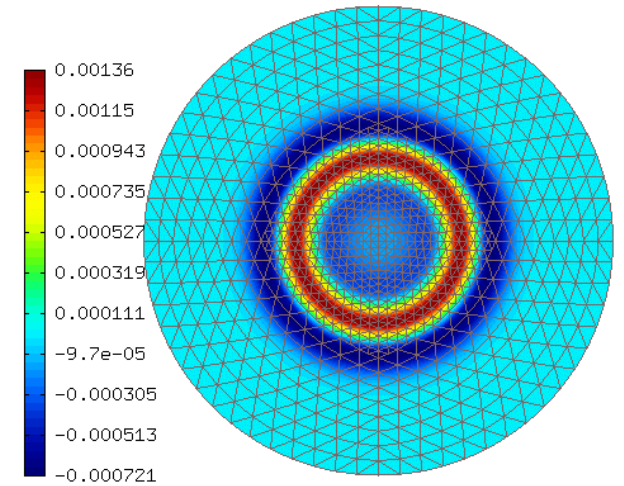

Image – temporal error in u (top), v (bottom), t = 0.8s

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Example > Benchmark Interior Layer

We solve the equation

$$-\Delta u = f, \quad u|_{\delta\Omega} = \tilde{f}$$

Where

- Ω is the space domain - square (0, 1) x (0, 1),
- $\tilde{f}$ is the (known) exact solution,
- f is the Laplacian of the exact solution,
- u is the sought solution
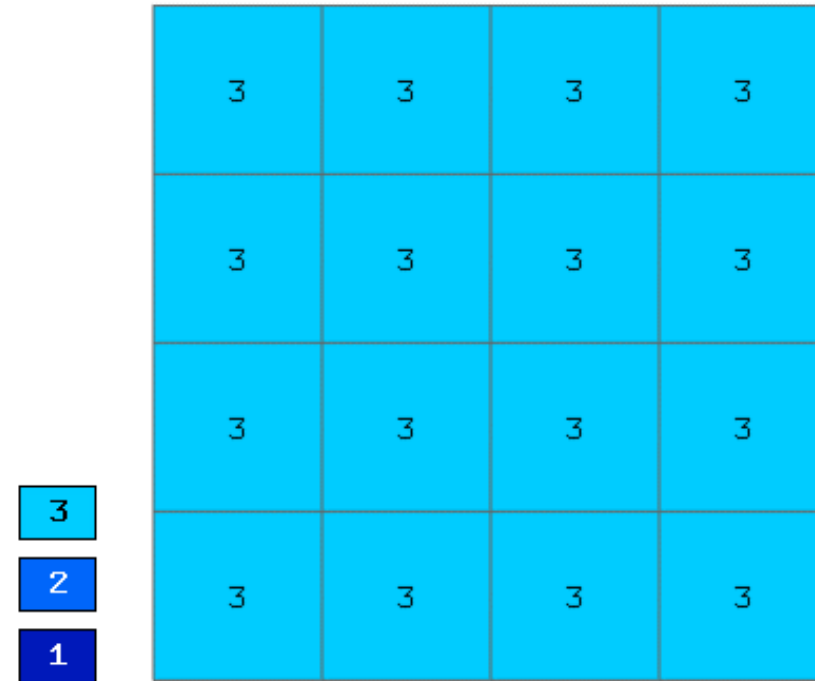
The features illustrated on this example are

- Calculating exact error,
- Anisotropic refinements usage in AMR.

Example > Benchmark Interior Layer

solution (left), FE space (right), adaptivity step #1
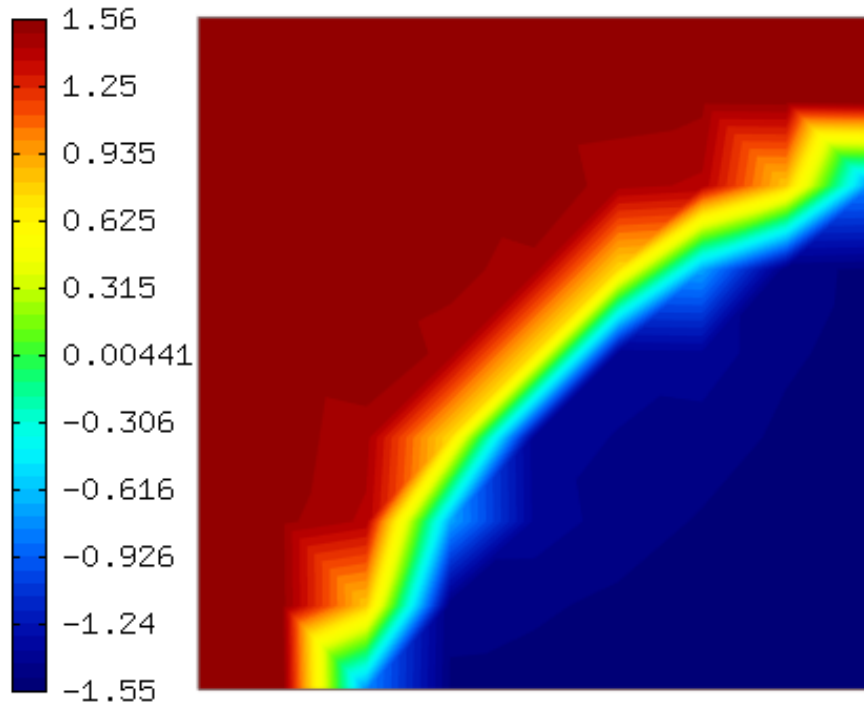
Example > Benchmark Interior Layer

solution (left), FE space (right), adaptivity step #2

Example > Benchmark Interior Layer

solution (left), FE space (right), adaptivity step #3

Example > Benchmark Interior Layer

solution (left), FE space (right), adaptivity step #6

Example > Benchmark Interior Layer

solution (left), FE space (right), adaptivity step #11
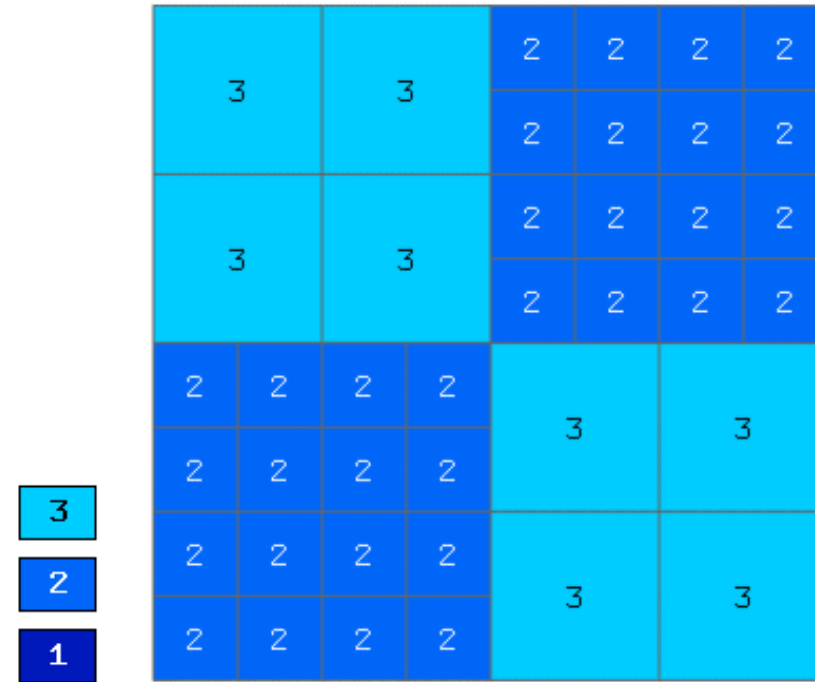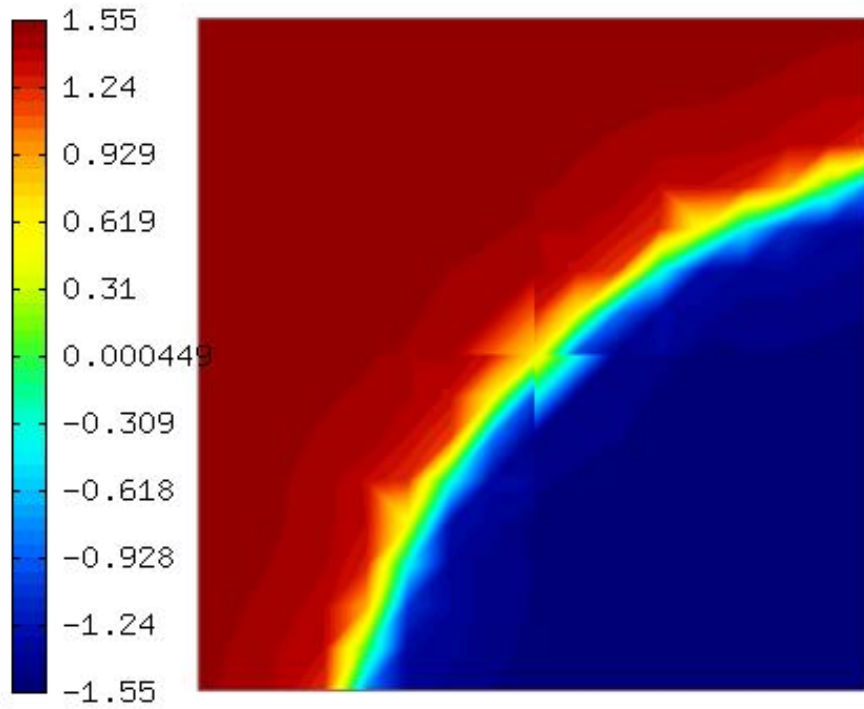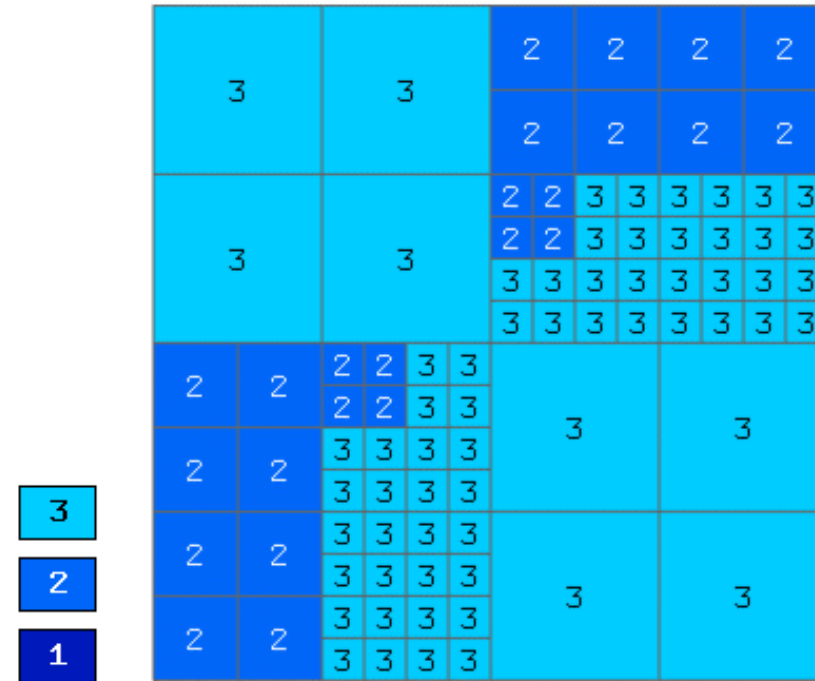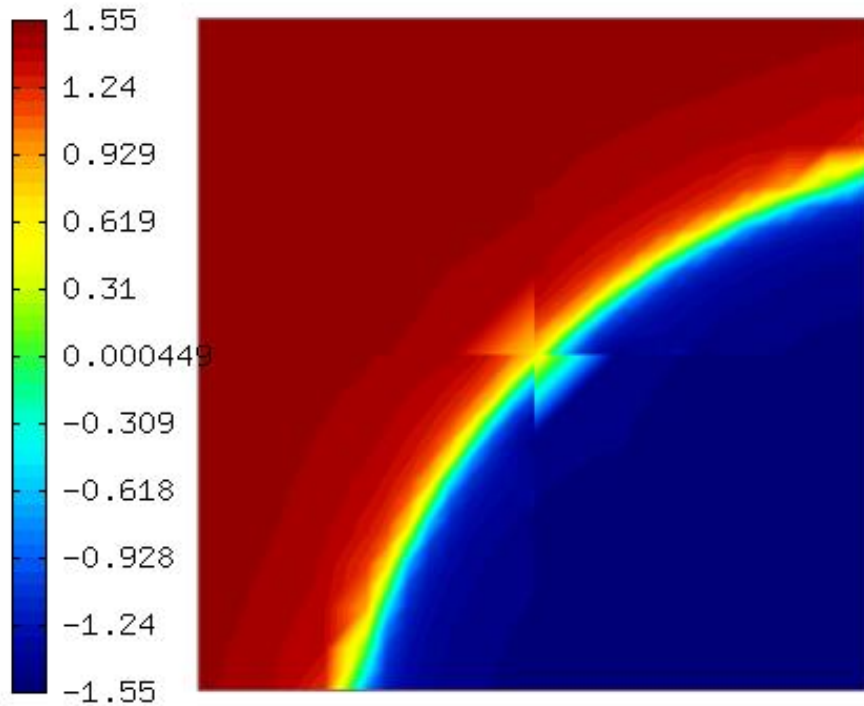
Example > Benchmark Interior Layer

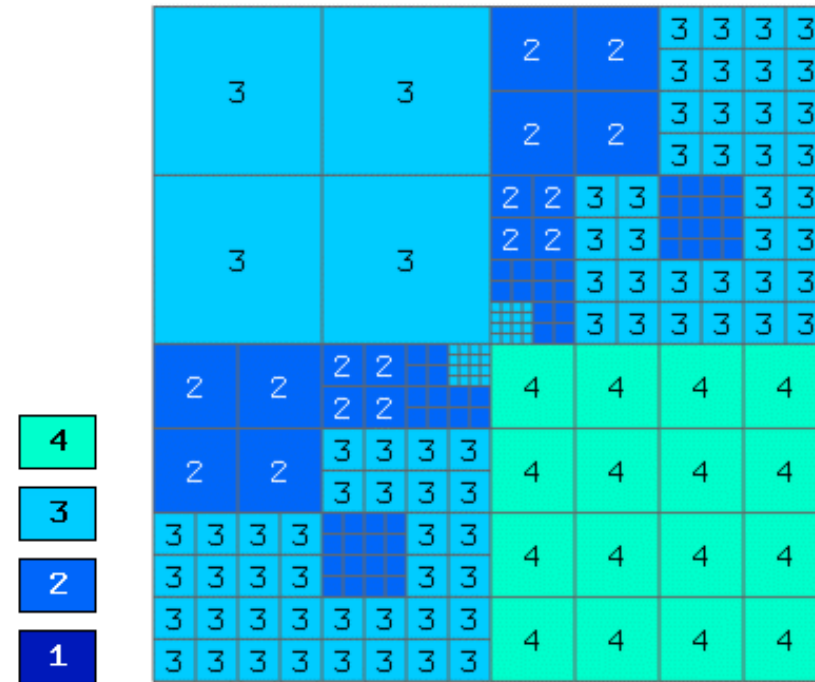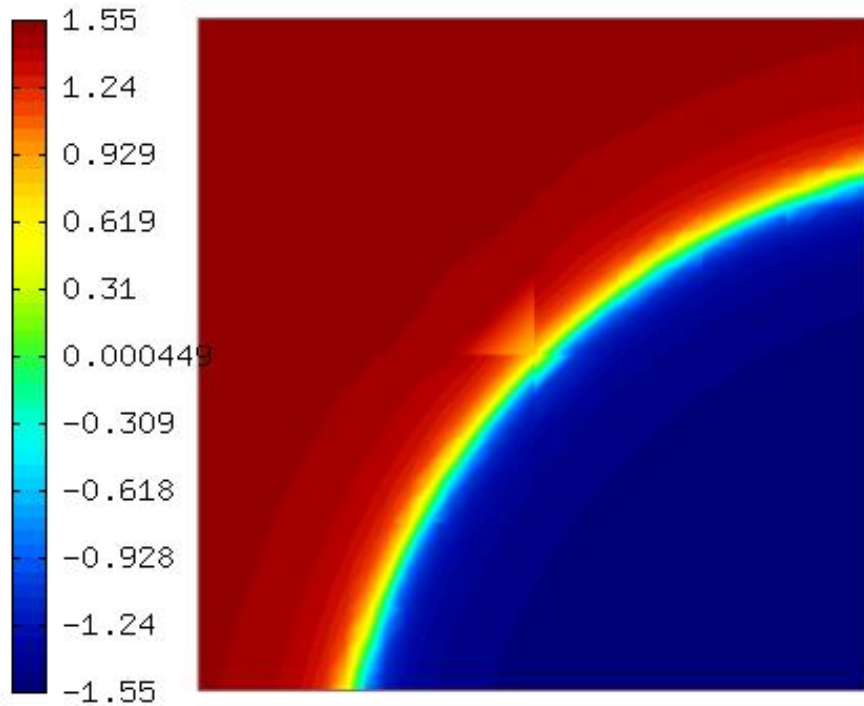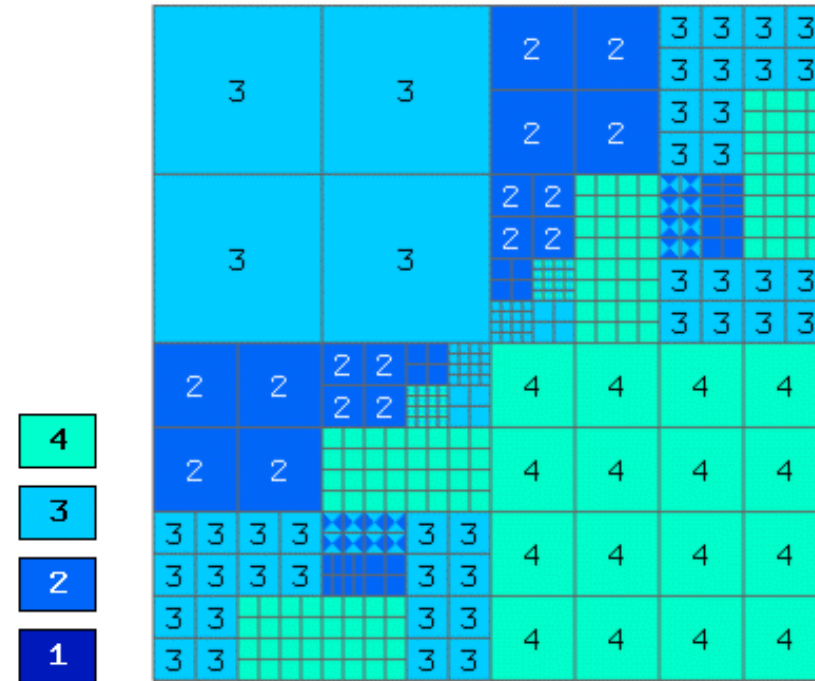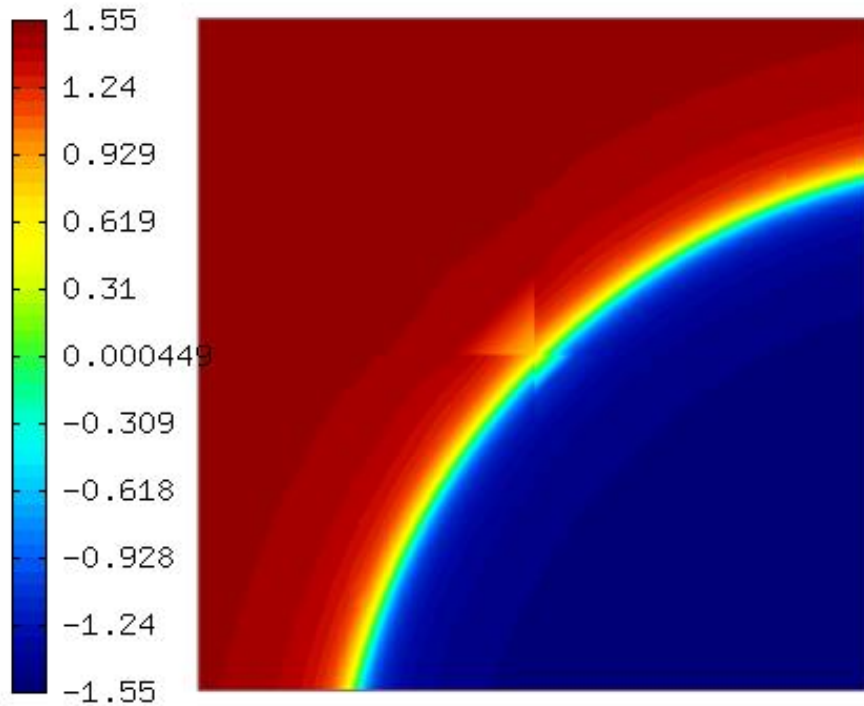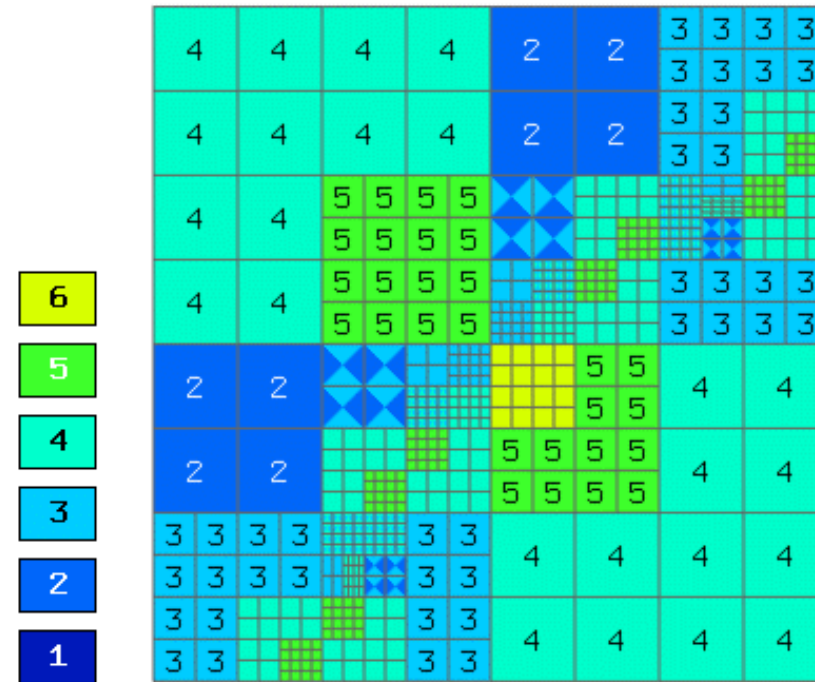solution (left), FE space (right), adaptivity step #19
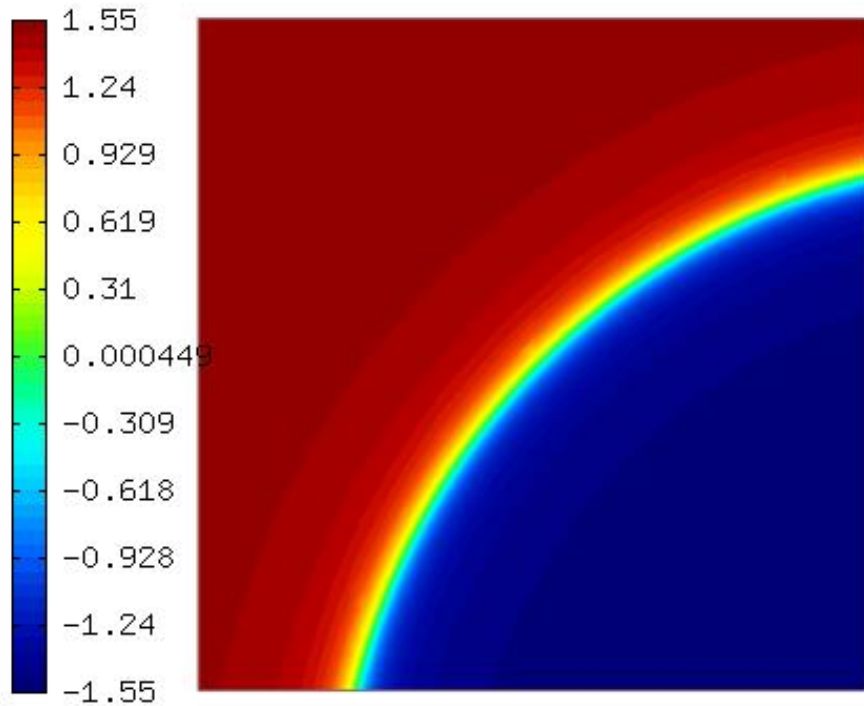
Example > Benchmark Interior Layer

Calculating exact error – through sub-classing existing Hermes2D class **ExactSolutionScalar<double>**:

```cpp
class CustomExactSolution : public ExactSolutionScalar<double>{
public:
  // Implement the actual function expression.
  virtual double value(double x, double y) const;

  // Implement the derivatives expression.
  virtual void derivatives (double x, double y, double& dx, double& dy) const;

  // Overwrite the expression calculating polynomial order (for integration order deduction).
  virtual Ord value(Ord x, Ord y) const;
};
```

- and then employing standard ErrorCalculator<double> class for error calculation

Anisotropic refinements usage in AMR

```cpp
// Predefined list of element refinement candidates.
// H2D_HP_ANISO stands for h-, and p-candidates, anisotropic in shape, and polynomial orders.
const CandList CAND_LIST = H2D_HP_ANISO;
// Class which for each element selected for refinement, selects the best refinement candidate.
H1ProjBasedSelector<double> selector(CAND_LIST);
...
// As before, adapt the FE space – using the selector provided
adaptivity.adapt(&selector);
```

Example > Heat and Moisture

We solve the system of equations

$$c^{TT}\frac{\delta T}{\delta t} + c^{Tw}\frac{\delta w}{\delta t} - d^{TT}\Delta T - d^{Tw}\Delta w = 0,$$

$$c^{wT}\frac{\delta T}{\delta t} + c^{ww}\frac{\delta w}{\delta t} - d^{wT}\Delta T - d^{ww}\Delta w = 0.$$

Where

- T, w is the sought solution,

- c^{ab}, d^{ab} are thermal capacity and thermal conductivity properties,

- (complicated) boundary conditions (Axisymmetric, Dirichlet, Newton) are prescribed.

The features illustrated on this example are

- Multimesh,

- Dynamical meshes.

Example > Heat and Moisture
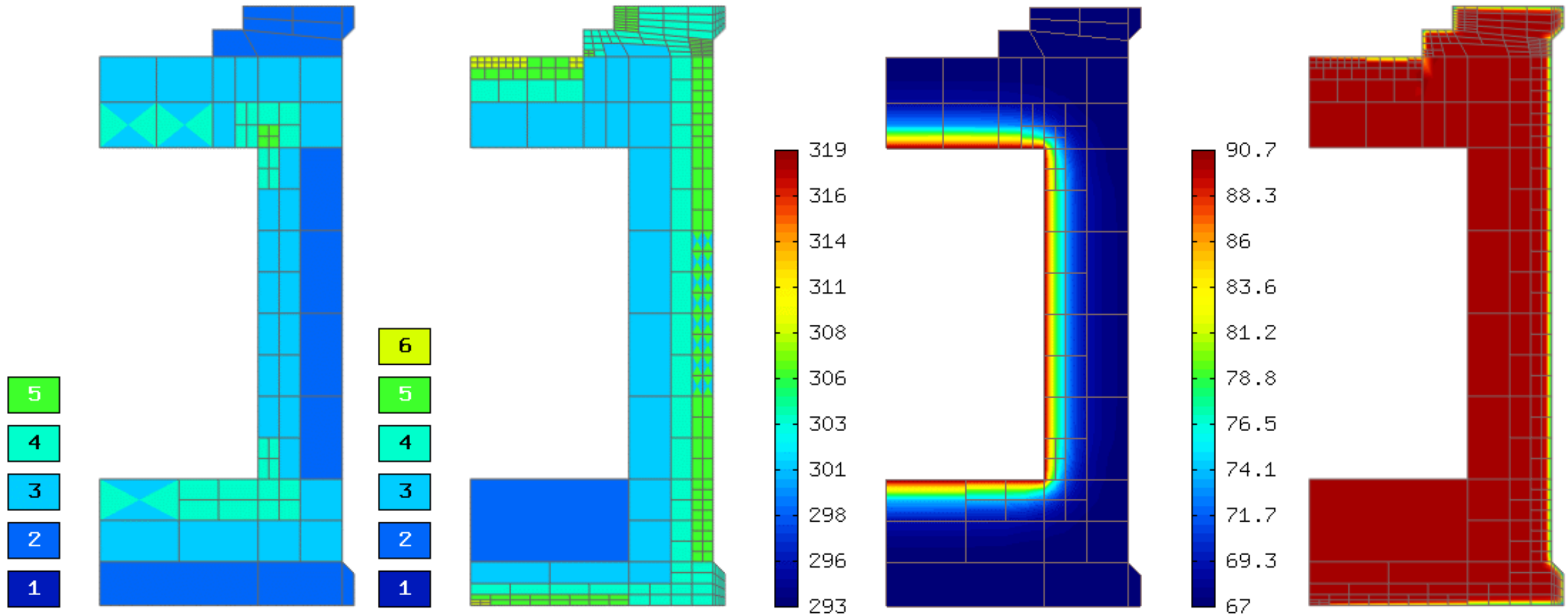
Meshes for T, w (left); Solutions for T, w (right), t = 10 days.

Example > Heat and Moisture

Meshes for T, w (left); Solutions for T, w (right), t = 10 days.
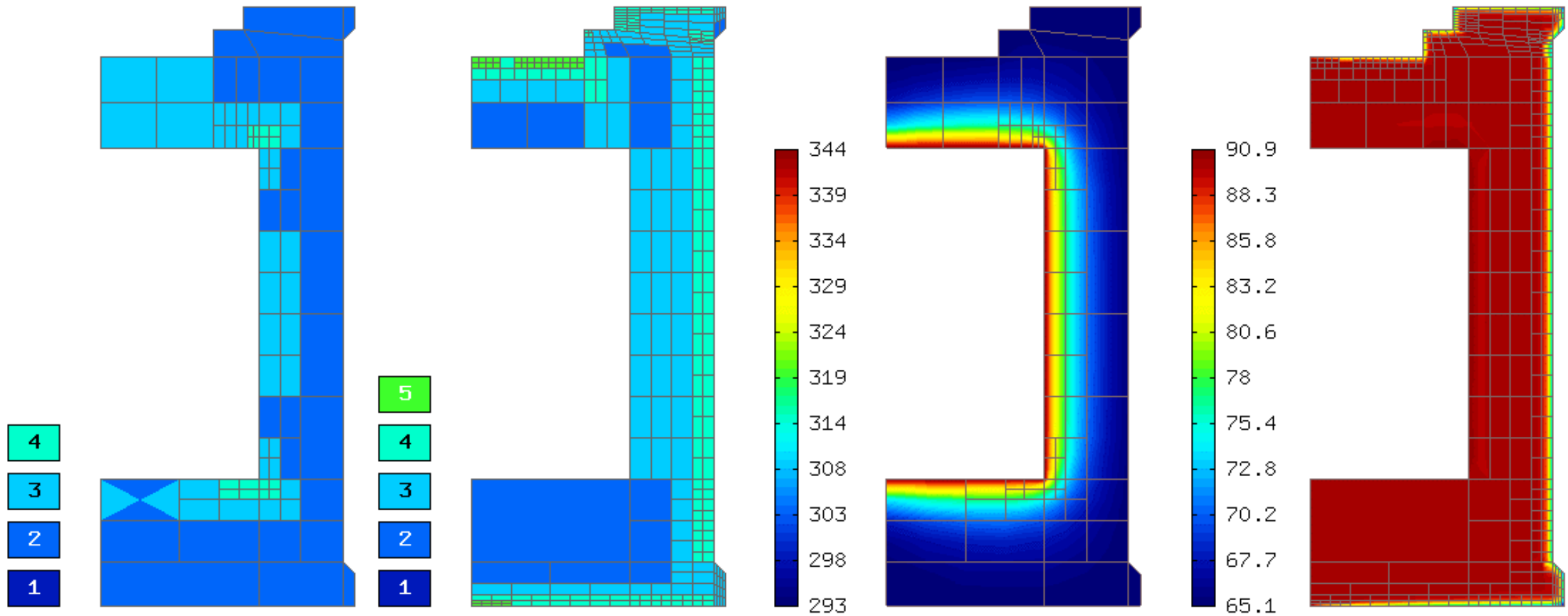
Example > Heat and Moisture

Meshes for T, w (left); Solutions for T, w (right), t = 10 days.
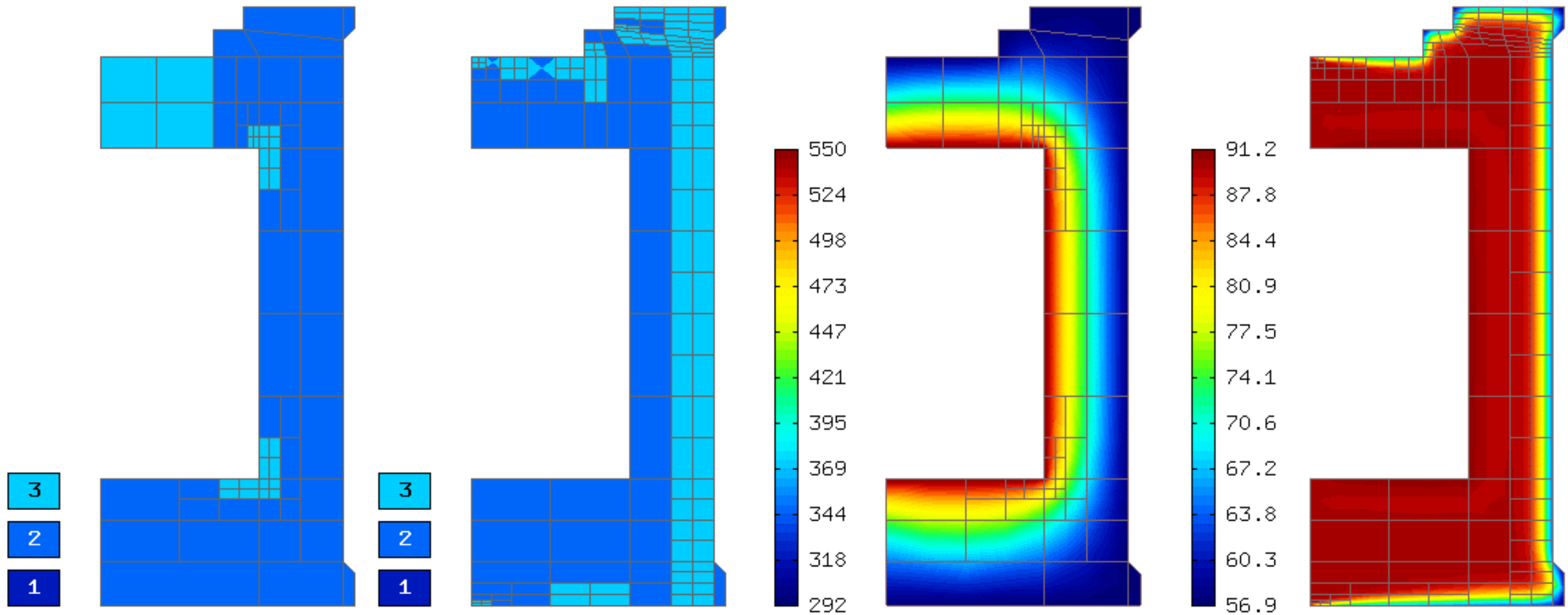
Example > Heat and Moisture

Meshes for T, w (left); Solutions for T, w (right), t = 10 days.
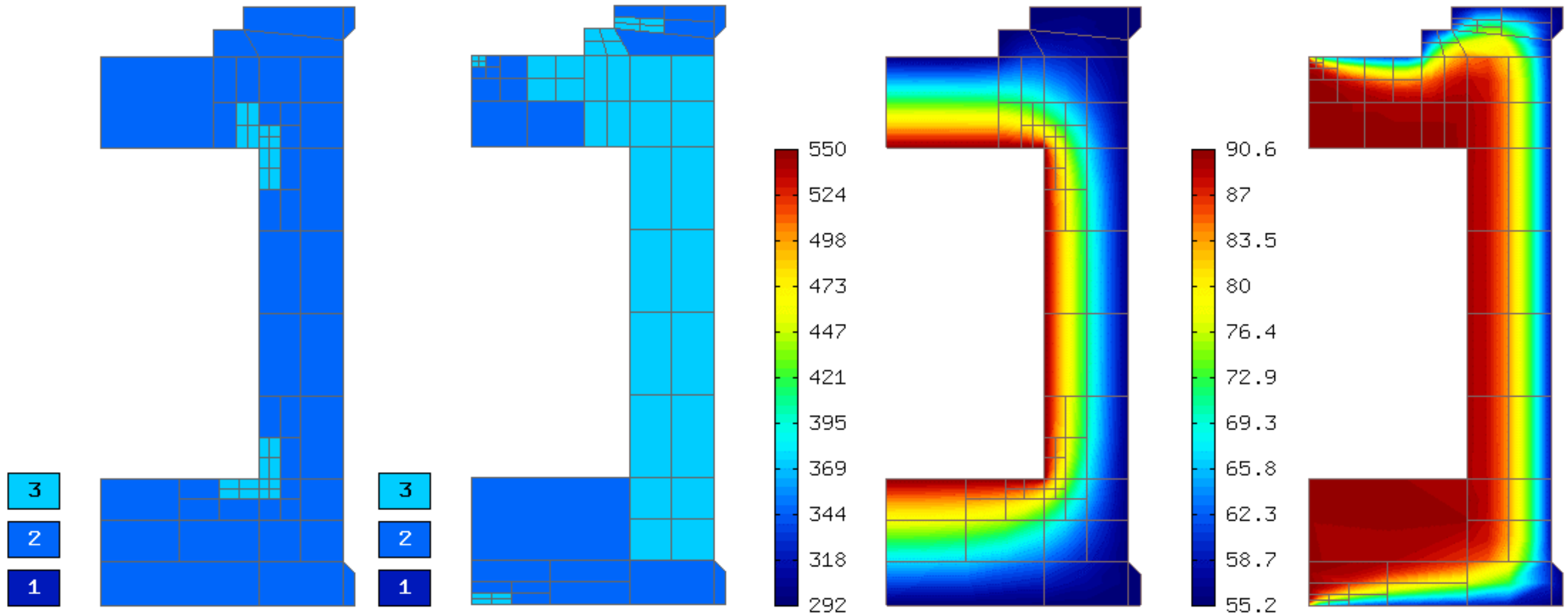
Example > Heat and Moisture

- Multimesh & Dynamical meshes
    - The key functionality here is de-refining the FE space, either periodically or when some indicator indicates us to.

```cpp
if (should_unrefine_in_this_step)
{
    // Unrefine one layer of refinements on the mesh for T.
    T_mesh->unrefine_all_elements();
    // Also coarsen the polynomial order.
    T_space->adjust_element_order(-1);

    // Do the above also for the mesh for w.
    w_mesh->unrefine_all_elements();
    w_space->adjust_element_order(-1);

    // Assign DOFs after the change.
    T_space->assign_dofs();
    w_space->assign_dofs();
}
```

- Note:
    - In the above, it is clearly seen that there are two Space, and two Mesh structures – different for each component.
    - This is enough input from the user to achieve multi-mesh behavior. Hermes2D takes care of the rest.

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Example > GAMM channel

We solve the Euler equations of compressible flow

$$\frac{\mathbf{w}^{n+1} - \mathbf{w}^n}{\tau} + \frac{\partial \mathbf{f}_x(\mathbf{w}^{n+1})}{\partial x} + \frac{\partial \mathbf{f}_y(\mathbf{w}^{n+1})}{\partial y} + \frac{\partial \mathbf{f}_z(\mathbf{w}^{n+1})}{\partial z} = 0$$

Where

$$\mathbf{w} = \begin{pmatrix} \varrho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ E \end{pmatrix} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} \quad \mathbf{f}_x = \begin{pmatrix} \rho u_1 \\ \rho u_1^2 + p \\ \rho u_1 u_2 \\ \rho u_1 u_3 \\ u_1(E+p) \end{pmatrix} = \begin{pmatrix} w_1 \\ \frac{w_1^2}{w_0} + p \\ \frac{w_1 w_2}{w_0} \\ \frac{w_1 w_3}{w_0} \\ \frac{w_1}{w_0}(w_4 + p) \end{pmatrix} \quad \mathbf{f}_y = \begin{pmatrix} \rho u_2 \\ \rho u_2 u_1 \\ \rho u_2^2 + p \\ \rho u_2 u_3 \\ u_2(E+p) \end{pmatrix} = \begin{pmatrix} w_2 \\ \frac{w_2 w_1}{w_0} \\ \frac{w_2^2}{w_0} + p \\ \frac{w_2 w_3}{w_0} \\ \frac{w_2}{w_0}(w_4 + p) \end{pmatrix} \quad \mathbf{f}_z = \begin{pmatrix} \rho u_3 \\ \rho u_3 u_1 \\ \rho u_3 u_2 \\ \rho u_3^2 + p \\ u_3(E+p) \end{pmatrix} = \begin{pmatrix} w_3 \\ \frac{w_3 w_1}{w_0} \\ \frac{w_3 w_2}{w_0} \\ \frac{w_3^2}{w_0} + p \\ \frac{w_3}{w_0}(w_4 + p) \end{pmatrix}$$

$$p = \frac{R}{c_v}\left(E - \tfrac{1}{2}\rho\left(u_1^2 + u_2^2 + u_3^3\right)\right) = \frac{R}{c_v}\left(w_4 - \frac{w_1^2 + w_2^2 + w_3^2}{2w_0}\right)$$

- **w** is the sought solution,

- R, c_v are constants

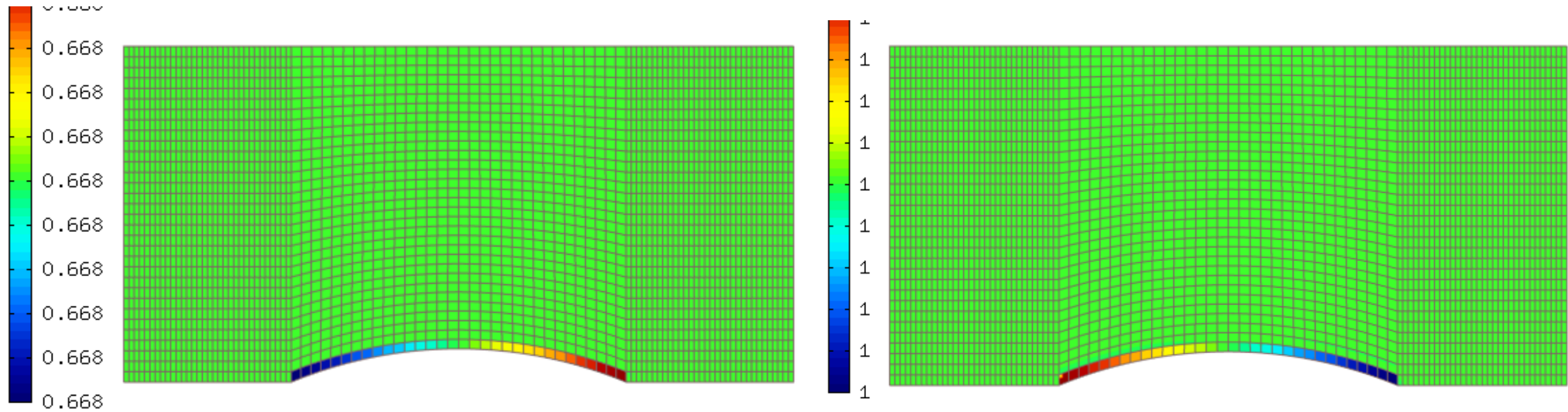- (complicated) Boundary conditions (reflective, 'do nothing', and inlet) are prescribed.

The feature illustrated on this example are:

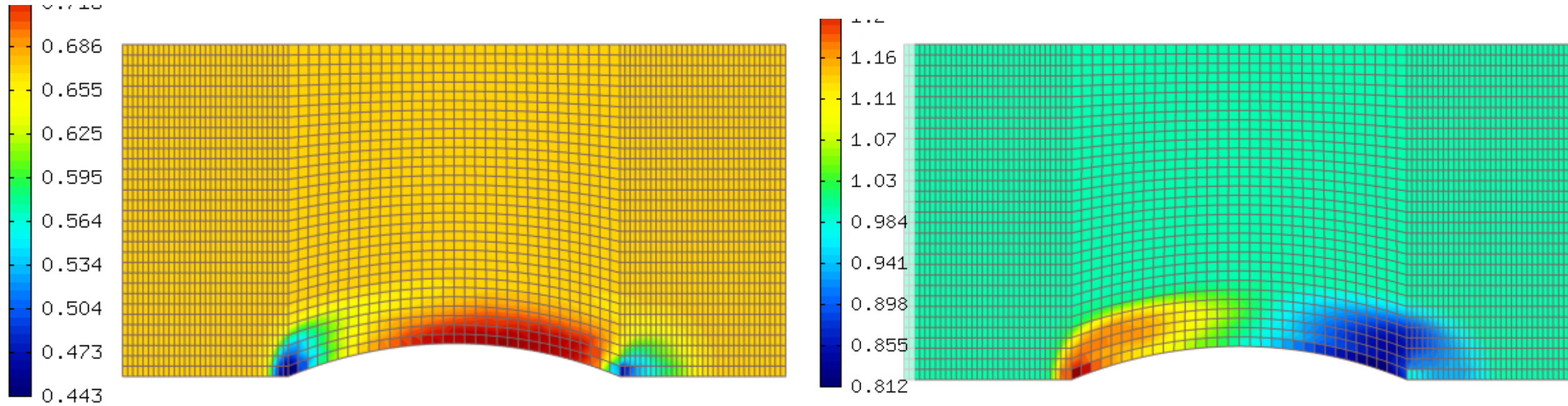- Post-processing filters (calculating Mach number, pressure)

Example > GAMM channel

Mach number (left), Pressure (right), t = 3e-4 s.

Example > GAMM channel

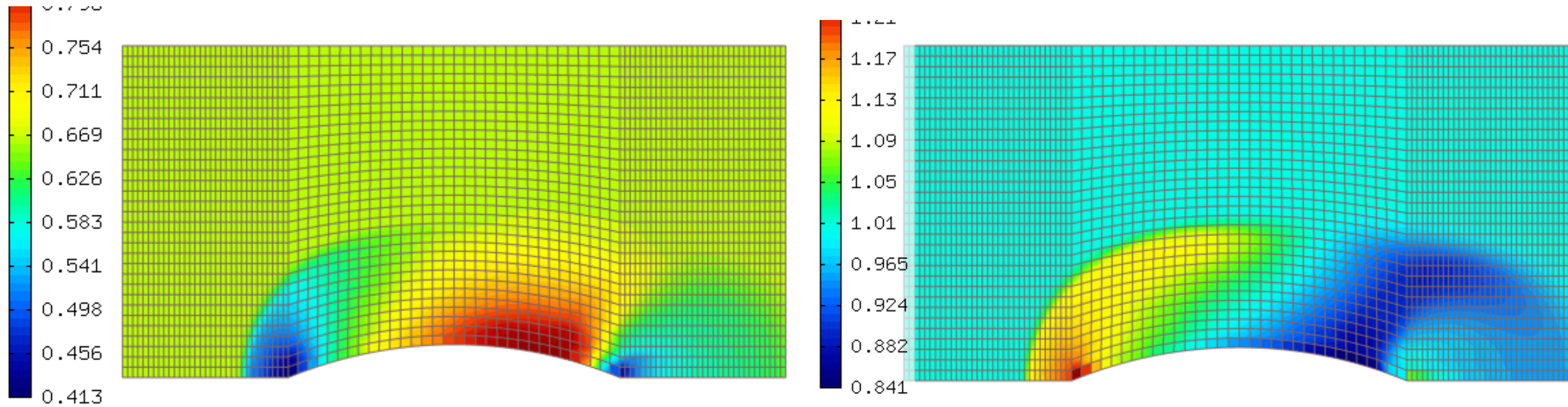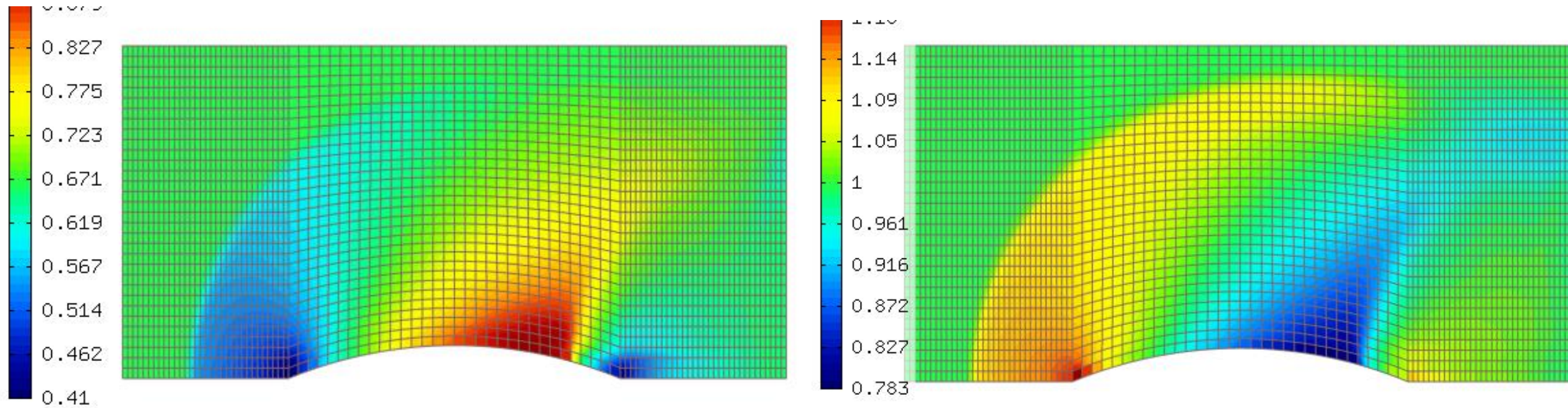Mach number (left), Pressure (right), t = 0.09 s.

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Example > GAMM channel

Mach number (left), Pressure (right), t = 0.21 s.

Example > GAMM channel

Mach number (left), Pressure (right), t = 0.36 s.

Example > GAMM channel

Post-processing filters

- Implemented by sub-classing Filter classes

```cpp
class MachNumberFilter : public Hermes::Hermes2D::SimpleFilter<double>
{
  // Constructors, etc.
  ...

  // Overriden method performing the actual calculation
  virtual void filter_fn(int n, const std::vector<const double*>& source_values, double* result)
  {
    // Calculate result for each integration point.
    for (int i = 0; i < n; i++)
    {
      double density = source_values.at(0)[i];
      double momentum_x = source_values.at(1)[i];
      double momentum_y = source_values.at(2)[i];
      double energy = source_values.at(3)[i];

      // Expression to calculate Mach number in the integration point.
      result[i] = std::sqrt((momentum_x / density) * (momentum_x / density) + (momentum_y / density) * (momentum_y / density))
        / std::sqrt(kappa * QuantityCalculator::calc_pressure(density, momentum_x, momentum_y, energy, kappa) / density);
    }
  }
};
```
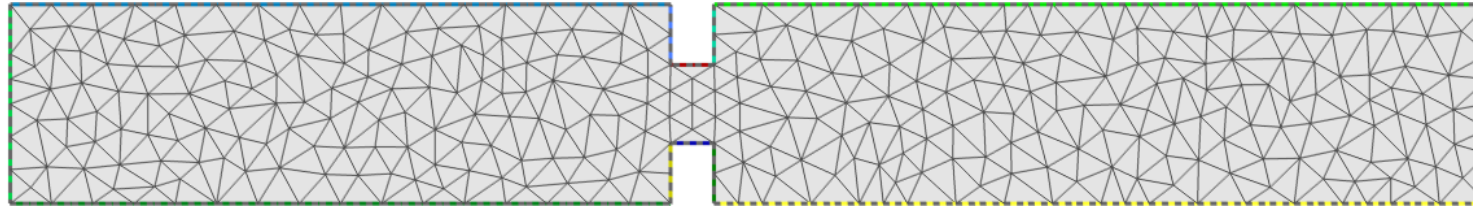
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Example > Helmholtz Waveguide

This example shows how to model harmonic steady state in parallel plate waveguide. We solve the (complex) equation

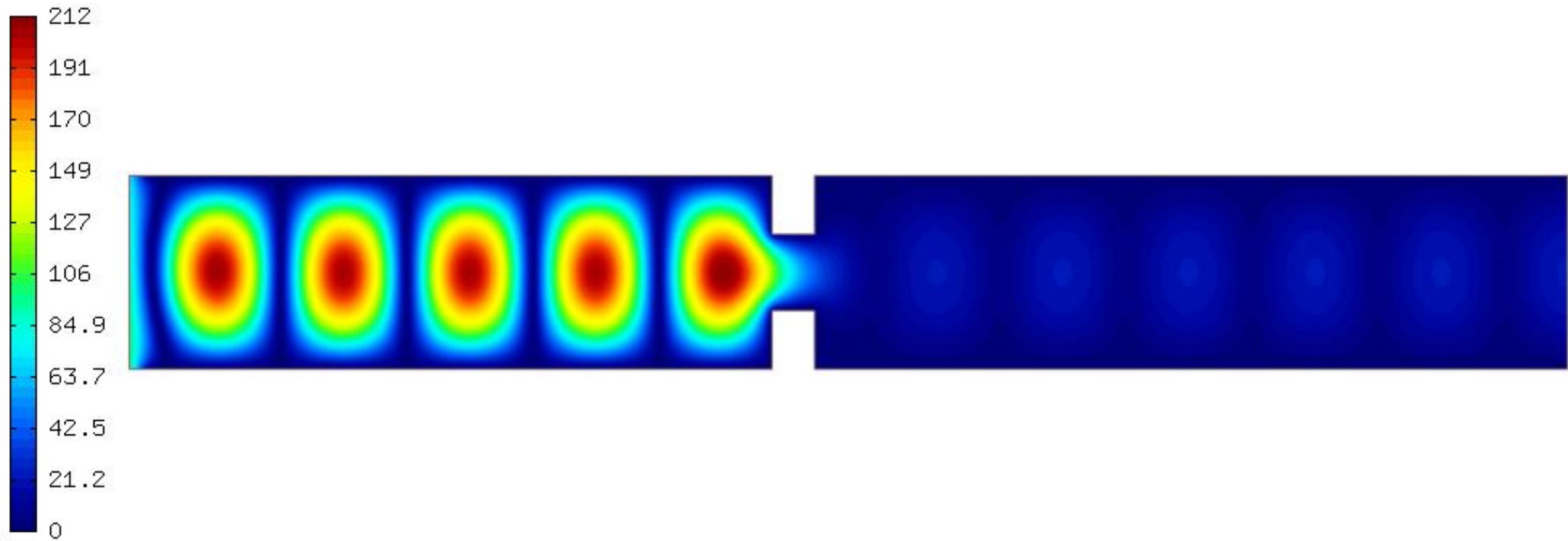$$-\Delta E - \omega^2 \mu\varepsilon E + j\omega\sigma\mu = 0,$$

In this domain:

Where

- E is the sought solution,

- ω is angular velocity,

- σ is conductivity,

- ε is permittivity,

- μ is permeability,

- (complicated) boundary conditions (perfect conductor, impedance, Dirichlet) are prescribed.

The feature illustrated on this example is
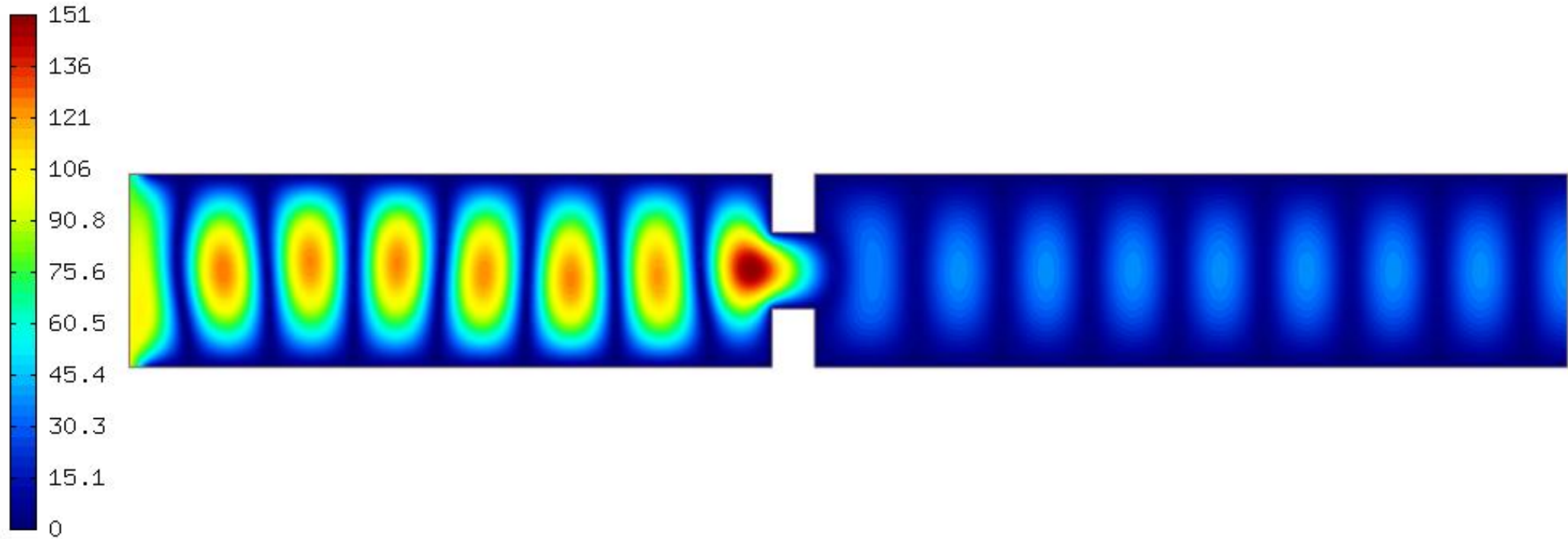
- writing a simple program using Hermes2d.

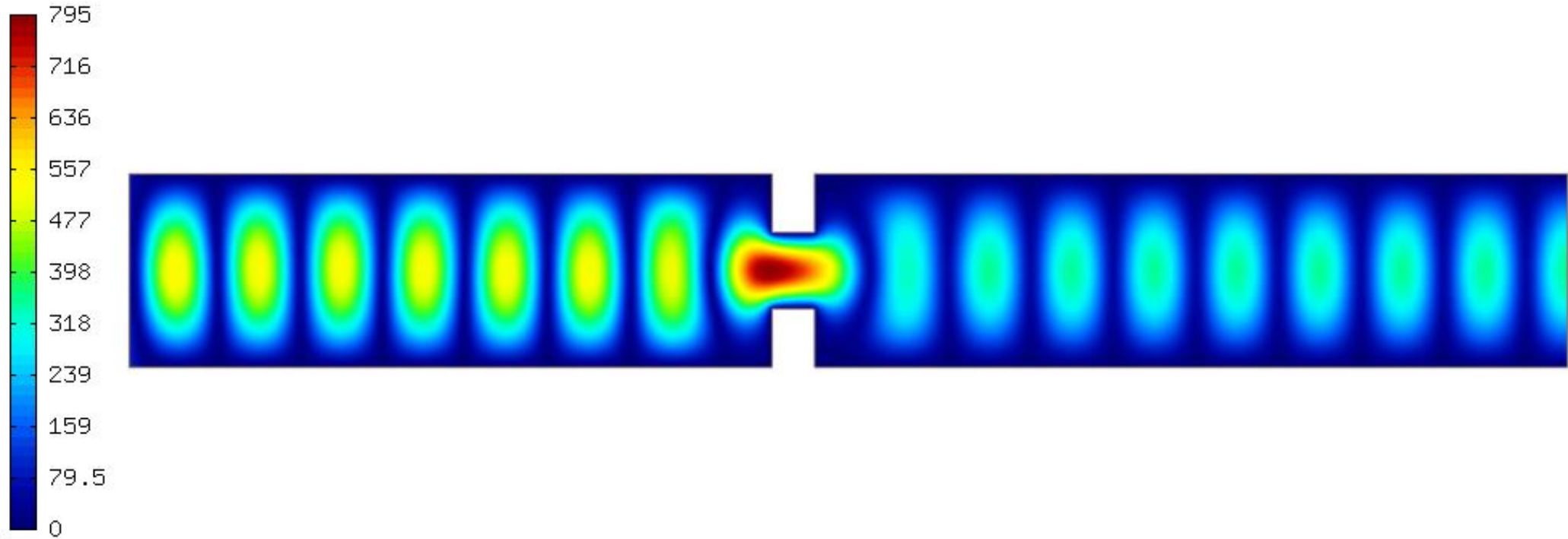# Example > Helmholtz Waveguide


```cpp
std::cout << "Done?";
std::cin >> change_state;
if (!strcmp(change_state, "y"))
    break;
std::cout << "Frequency change [1e9 Hz]: ";
std::cin >> frequency_change;
```

Example > Helmholtz Waveguide


```cpp
std::cout << "Done?";
std::cin >> change_state;
if (!strcmp(change_state, "y"))
    break;
std::cout << "Frequency change [1e9 Hz]: ";
std::cin >> frequency_change;
```

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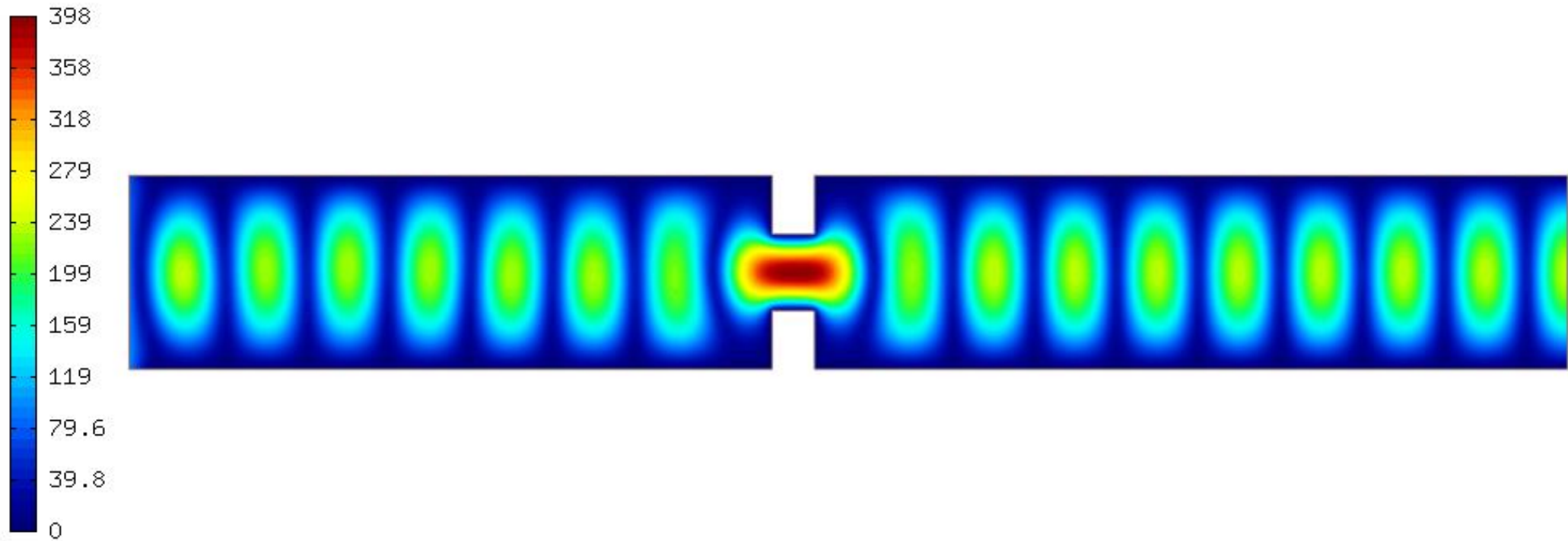# Example > Helmholtz Waveguide


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std::cout << "Done?";
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std::cout << "Frequency change [1e9 Hz]: ";
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```

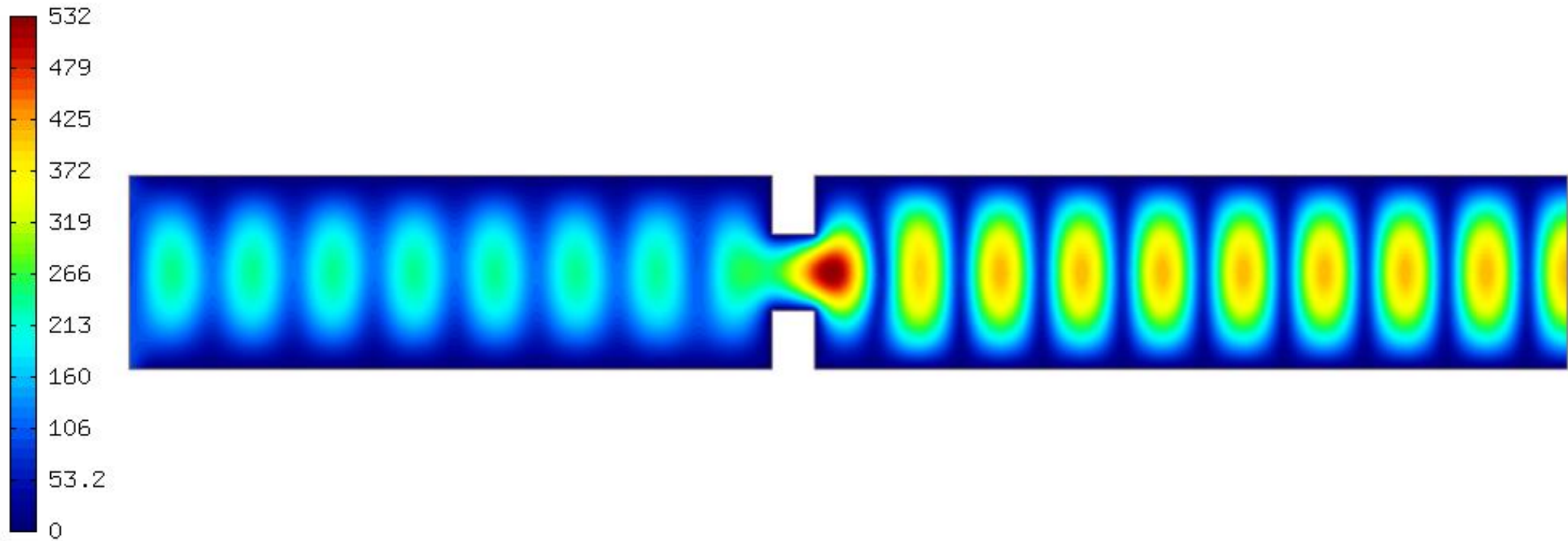# Example > Helmholtz Waveguide


```cpp
std::cout << "Done?";
std::cin >> change_state;
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std::cout << "Frequency change [1e9 Hz]: ";
std::cin >> frequency_change;
```

Example > Helmholtz Waveguide


```cpp
std::cout << "Done?";
std::cin >> change_state;
if (!strcmp(change_state, "y"))
    break;
std::cout << "Frequency change [1e9 Hz]: ";
std::cin >> frequency_change;
```