

Chapter 1

Example problem: Adaptive solution of the 3D Poisson equation in a spherical domain

Following the numerous 2D problems discussed in earlier examples we now demonstrate that the solution of 3D problems is just as easy. For this purpose we discuss the adaptive solution of the 3D Poisson problem

Three-dimensional model Poisson problem

Solve

$$\sum_{i=1}^3 \frac{\partial^2 u}{\partial x_i^2} = f(x_1, x_2, x_3), \quad (1)$$

in the "eighth-of-a-sphere" domain D , with Dirichlet boundary conditions

$$u|_{\partial D} = u_0 \quad (2)$$

where the function u_0 is given.

We choose a source function and boundary conditions for which

$$u_0(x_1, x_2, x_3) = \tanh(1 - \alpha((\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{N})), \quad (3)$$

is the exact solution. Here where $\mathbf{x} = (x_1, x_2, x_3)$

is the vector of the spatial coordinates, and the vectors $\mathbf{x}_0 = (x_1^{(0)}, x_2^{(0)}, x_3^{(0)})$ and $\mathbf{N}_0 = (N_1, N_2, N_3)$ are constants. For large values of the constant α the solution varies rapidly across the plane through \mathbf{x}_0 whose normal is given by \mathbf{N} .

Here are some plots of the exact and computed solutions for $\mathbf{x}_0 = (0, 0, 0)$, $\mathbf{N}_0 = 1/\sqrt{3}(-1, -1, 1)$, and $\alpha = 50$ at various levels of mesh refinement. Note that the plot of the exact solution was produced by setting the nodal values to the exact solution, obtained by evaluating (3) at the nodal positions. The elements' basis functions were then used to interpolate between the nodal values. On the coarse meshes, the interpolation between the "exact" nodal values is clearly inadequate to resolve the rapid variation of the solution.



Figure 1.1 Plot of the solution

1.1 Global parameters and functions

Following our usual practice, we use a namespace, `TanhSolnForPoisson`, to define the source function, the exact solution and various problem parameters.

```

=====start_of_namespace=====
/// Namespace for exact solution for Poisson equation with sharp step
=====
namespace TanhSolnForPoisson
{
    /// Parameter for steepness of step
    double Alpha=1;

    /// Orientation (non-normalised x-component of unit vector in direction
    /// of step plane)
    double N_x=-1.0;

    /// Orientation (non-normalised y-component of unit vector in direction
    /// of step plane)
    double N_y=-1.0;

```

```

/// Orientation (non-normalised z-component of unit vector in direction
/// of step plane)
double N_z=1.0;

/// Orientation (x-coordinate of step plane)
double X_0=0.0;

/// Orientation (y-coordinate of step plane)
double Y_0=0.0;

/// Orientation (z-coordinate of step plane)
double Z_0=0.0;

// Exact solution as a Vector
void get_exact_u(const Vector<double>& x, Vector<double>& u)
{
    u[0] = tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-Y_0)*
        N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*
        N_z/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)));
}

/// Exact solution as a scalar
void get_exact_u(const Vector<double>& x, double& u)
{
    u = tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-Y_0)*
        N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*
        N_z/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)));
}

/// Source function to make it an exact solution
void get_source(const Vector<double>& x, double& source)
{
    double s1,s2,s3,s4;

    s1 = -2.0*tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z)))*(1.0-pow(tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z))),(2.0))*Alpha*Alpha*N_x*N_x/(N_x*N_x+N_y*N_y+N_z*N_z);
    s3 = -2.0*tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z)))*(1.0-pow(tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z))),(2.0))*Alpha*Alpha*N_y*N_y/(N_x*N_x+N_y*N_y+N_z*N_z);
    s4 = -2.0*tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z)))*(1.0-pow(tanh(Alpha*((x[0]-X_0)*N_x/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[1]-
Y_0)*N_y/sqrt(N_x*N_x+N_y*N_y+N_z*N_z)+(x[2]-Z_0)*N_z/sqrt(N_x*N_x+N_y*N_y+N_z*
N_z))),(2.0))*Alpha*Alpha*N_z*N_z/(N_x*N_x+N_y*N_y+N_z*N_z);
    s2 = s3+s4;
    source = s1+s2;
}

} // end of namespace

```

1.2 The driver code

The driver code solves the 3D Poisson problem with full spatial adaptivity – a fairly time-consuming process. To minimise the run-times when the code is executed during `oomph-lib`'s self-tests, we use command line arguments to optionally limit the number of adaptive refinements. If the code is run with a(ny) command line arguments, only a single adaptive refinement is performed; otherwise up to four levels of refinement are permitted. `oomph-lib` provides storage for the command line arguments in the namespace `CommandLineArgs` to make them accessible to other parts of the code.

Otherwise the driver code is very similar to that used in the [corresponding 2D Poisson problems](#): We construct the problem, passing the pointer to the source function. Next, we create a `DocInfo` object to specify the output directory, and execute the global self-test to assert that the problem has been set up correctly. Next we solve the problem on the coarse initial mesh (comprising four 27-node brick elements) and then adapt the problem based on the elemental error estimates, until the maximum number of adaptations has been reached or until the adaptation ceases to changes the mesh.

```

//=====start_of_main=====
/// Driver for 3D Poisson problem in eighth of a sphere. Solution
/// has a sharp step. If there are
/// any command line arguments, we regard this as a validation run
/// and perform only a single adaptation.

```

```
//=====
int main(int argc, char *argv[])
{
    // Store command line arguments
    CommandLineArgs::setup(argc,argv);

    // Set up the problem with 27-node brick elements, pass pointer to
    // source function
    EighthSpherePoissonProblem<RefineableQPoissonElement<3,3> >
    problem(&TanhSolnForPoisson::get_source);

    // Setup labels for output
    DocInfo doc_info;

    // Output directory
    doc_info.set_directory("RESULT");

    // Step number
    doc_info.number()=0;

    // Check if we're ready to go
    cout << "Self test: " << problem.self_test() << std::endl;
    // Solve the problem
    problem.newton_solve();
    //Output solution
    problem.doc_solution(doc_info);

    //Increment counter for solutions
    doc_info.number()++;

    // Now do (up to) three rounds of fully automatic adaption in response to
    // error estimate
    unsigned max_solve;
    if (CommandLineArgs::Argc>1)
    {
        // Validation run: Just one adaptation
        max_solve=1;
        cout << "Only doing one adaptation for validation" << std::endl;
    }
    else
    {
        // Up to four adaptations
        max_solve=4;
    }

    for (unsigned isolve=0;isolve<max_solve;isolve++)
    {
        // Adapt problem/mesh
        problem.adapt();

        // Re-solve the problem if the adaptation has changed anything
        if ((problem.mesh_pt()->nrefined() !=0) ||
            (problem.mesh_pt()->nunrefined() !=0))
        {
            problem.newton_solve();
        }
        else
        {
            cout << "Mesh wasn't adapted --> we'll stop here" << std::endl;
            break;
        }

        //Output solution
        problem.doc_solution(doc_info);

        //Increment counter for solutions
        doc_info.number()++;
    }

    // pause("done");
} // end of main
```

1.3 The problem class

The problem class has the usual structure – the only difference to the corresponding 2D codes is that the assignment of the boundary conditions in `actions_before_newton_solve()` now involves three nodal coordinates rather than two.

```
//=====start_of_class_definition=====
/// Poisson problem in refineable eighth of a sphere mesh.
//=====
template<class ELEMENT>
class EighthSpherePoissonProblem : public Problem
```

```

{
public:
    /// Constructor: Pass pointer to source function
    EighthSpherePoissonProblem(
        PoissonEquations<3>::PoissonSourceFctPt source_fct_pt);

    /// Destructor: Empty
    ~EighthSpherePoissonProblem() {}

    /// Overload generic access function by one that returns
    /// a pointer to the specific mesh
    RefineableEighthSphereMesh<ELEMENT>* mesh_pt()
    {
        return dynamic_cast<RefineableEighthSphereMesh<ELEMENT>*>(Problem::mesh_pt());
    }

    /// Update the problem specs after solve (empty)
    void actions_after_newton_solve() {}

    /// Update the problem specs before solve:
    /// Set Dirichlet boundary conditions from exact solution.
    void actions_before_newton_solve()
    {
        // Loop over the boundaries
        unsigned num_bound = mesh_pt()->nboundary();
        for(unsigned ibound=0; ibound<num_bound; ibound++)
        {
            // Loop over the nodes on boundary
            unsigned num_nod=mesh_pt()->nboundary_node(ibound);
            for (unsigned inod=0; inod<num_nod; inod++)
            {
                Node* nod_pt=mesh_pt()->boundary_node_pt(ibound,inod);
                double u;
                Vector<double> x(3);
                x[0]=nod_pt->x(0);
                x[1]=nod_pt->x(1);
                x[2]=nod_pt->x(2);
                TanhSolnForPoisson::get_exact_u(x,u);
                nod_pt->set_value(0,u);
            }
        }

        /// Doc the solution
        void doc_solution(DocInfo& doc_info);

private:
    /// Pointer to source function
    PoissonEquations<3>::PoissonSourceFctPt Source_fct_pt;
}; // end of class definition

```

[See the discussion of the [1D Poisson problem](#) for a more detailed discussion of the function type `PoissonEquations<3>::PoissonSourceFctPt`.]

1.4 The Problem constructor

In the Problem constructor, we set the "steepness parameter" α to a large value and create the mesh for a sphere of radius 5. Next, we create the error estimator and pass it to the adaptive mesh.

```

//=====start_of_constructor=====
/// Constructor for Poisson problem on eighth of a sphere mesh
//=====
template<class ELEMENT>
EighthSpherePoissonProblem<ELEMENT>::EighthSpherePoissonProblem(
    PoissonEquations<3>::PoissonSourceFctPt source_fct_pt) :
    Source_fct_pt(source_fct_pt)
{
    // Setup parameters for exact tanh solution
    // Steepness of step
    TanhSolnForPoisson::Alpha=50.0;

    /// Create mesh for sphere of radius 5
    double radius=5.0;
    Problem::mesh_pt() = new RefineableEighthSphereMesh<ELEMENT>(radius);

    // Set error estimator
    Z2ErrorEstimator* error_estimator_pt=new Z2ErrorEstimator;
    mesh_pt()->spatial_error_estimator_pt()=error_estimator_pt;
}

```

We adjust the targets for the mesh adaptation so that the single mesh adaptation performed during a validation run

produces a non-uniform refinement pattern. (The error targets for this case were determined by trial and error.) The tighter error tolerances specified otherwise are appropriate to properly resolve the solution, as shown in the animated gif files at the beginning of this document.

```
// Adjust error targets for adaptive refinement
if (CommandLineArgs::Argc>1)
{
    // Validation: Relax tolerance to get nonuniform refinement during
    // first step
    mesh_pt()->max_permitted_error()=0.7;
    mesh_pt()->min_permitted_error()=0.5;
}
else
{
    mesh_pt()->max_permitted_error()=0.01;
    mesh_pt()->min_permitted_error()=0.001;
} // end adjustment
```

Next, we assign the boundary conditions. In the present problem all boundaries are Dirichlet boundaries, therefore we loop over all nodes on all boundaries and pin their values. If only a subset of the mesh boundaries were of Dirichlet type, only the nodes on those boundaries would have to be pinned. "Usually" the numbering of the mesh boundaries is (or at least should be!) documented in the mesh constructor but it can also be obtained from the function `Mesh::output_boundaries(...)` whose use is illustrated here.

```
//Doc the mesh boundaries
ofstream some_file;
some_file.open("boundaries.dat");
mesh_pt()->output_boundaries(some_file);
some_file.close();

// Set the boundary conditions for this problem: All nodes are
// free by default -- just pin the ones that have Dirichlet conditions
// here (all the nodes on the boundary)
unsigned num_bound = mesh_pt()->nboundary();
for(unsigned ibound=0; ibound<num_bound; ibound++)
{
    unsigned num_nod= mesh_pt()->nboundary_node(ibound);
    for (unsigned inod=0; inod<num_nod; inod++)
    {
        mesh_pt()->boundary_node_pt(ibound, inod)->pin(0);
    }
} // end of pinning
```

Finally we loop over all elements to assign the source function pointer, and then call the generic `Problem::assign_eqn_numbers()` routine to set up the equation numbers.

```
//Find number of elements in mesh
unsigned n_element = mesh_pt()->nelement();

// Loop over the elements to set up element-specific
// things that cannot be handled by constructor
for(unsigned i=0; i<n_element; i++)
{
    // Upcast from FiniteElement to the present element
    ELEMENT *el_pt = dynamic_cast<ELEMENT*>(mesh_pt()->element_pt(i));

    //Set the source function pointer
    el_pt->source_fct_pt() = Source_fct_pt;
}

// Setup equation numbering
cout <<"Number of equations: " << assign_eqn_numbers() << std::endl;
} // end of constructor
```

1.5 Post-processing

The function `doc_solution(...)` writes the FE solution and the corresponding exact solution, defined in `TanhSolnForPoisson::get_exact_u(...)` to disk. The `DocInfo` object specifies the output directory and the label for the file names. [See the discussion of the

1D Poisson problem for a more detailed discussion of the generic `Mesh` member functions `Mesh::output(...)`, `Mesh::output_fct(...)` and `Mesh::compute_error(...)`].

```
//=====start_of_doc=====
// Doc the solution
//=====
template<class ELEMENT>
void EighthSpherePoissonProblem<ELEMENT>::doc_solution(DocInfo& doc_info)
{
    ofstream some_file;
    char filename[100];

    // Number of plot points
    unsigned npts;
```

```

npts=5;

// Output solution
//-----
sprintf(filename,"%s/soln%i.dat",doc_info.directory().c_str(),
        doc_info.number());
some_file.open(filename);
mesh_pt()->output(some_file,npts);
some_file.close();

// Output exact solution
//-----
sprintf(filename,"%s/exact_soln%i.dat",doc_info.directory().c_str(),
        doc_info.number());
some_file.open(filename);
mesh_pt()->output_fct(some_file,npts,TanhSolnForPoisson::get_exact_u);
some_file.close();

// Doc error
//-----
double error,norm;
sprintf(filename,"%s/error%i.dat",doc_info.directory().c_str(),
        doc_info.number());
some_file.open(filename);
mesh_pt()->compute_error(some_file,TanhSolnForPoisson::get_exact_u,
                        error,norm);
some_file.close();
cout << "error: " << sqrt(error) << std::endl;
cout << "norm : " << sqrt(norm) << std::endl << std::endl;
} // end of doc

```

1.6 Source files for this tutorial

- The source files for this tutorial are located in the directory:

`demo_drivers/poisson/eighth_sphere_poisson/`

- The driver code is:

`demo_drivers/poisson/eighth_sphere_poisson/eighth_sphere_poisson.cc`

1.7 PDF file

A [pdf version](#) of this document is available.