Chapter 1

Example problem: Adaptive solution of the 2D advection diffusion equation

In this example we discuss the adaptive solution of the 2D advection-diffusion problem

Two-dimensional advection-diffusion problem in a rectangular domain

Solve

Pe
$$\sum_{i=1}^{2} w_i(x_1, x_2) \frac{\partial u}{\partial x_i} = \sum_{i=1}^{2} \frac{\partial^2 u}{\partial x_i^2} + f(x_1, x_2),$$
 (1)

in the rectangular domain $D=\{(x_1,x_2)\in[0,1]\times[0,2]\}$, with Dirichlet boundary conditions

$$u|_{\partial D} = u_0, \tag{2}$$

where the *Peclet number*, Pe the boundary values, u_0 , the source function $f(x_1, x_2)$, and the components of the "wind" $w_i(x_1, x_2)$ (i = 1, 2) are given.

We choose the forcing function and the boundary conditions such that

$$u_0(x_1, x_2) = \tanh(1 - \alpha(x_1 \tan \Phi - x_2)),$$
 (3)

is the exact solution of the problem. For large values of α , the exact solution approaches a step, oriented at an angle Φ against the x_1 -axis.

In the computations we will impose the "wind"

$$\mathbf{w}(x_1, x_2) = \begin{pmatrix} \sin(6x_2) \\ \cos(6x_1) \end{pmatrix}, \qquad (4)$$

illustrated in this vector plot:

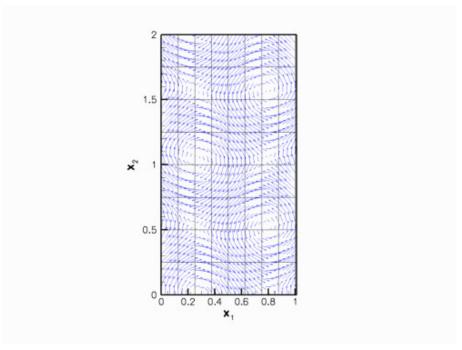


Figure 1.1 Plot of the wind.

The graph below shows a plot of the solution, computed at various levels of mesh adaptation, for $\Phi=45^{\circ},\ \alpha=50$ and a Peclet number of Pe=200.

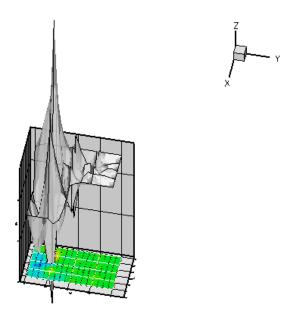


Figure 1.2 Plot of the forced solution at different levels of mesh refinement.

More interesting is the following plot which shows the solution for the same parameter values and boundary conditions, but for a zero forcing function, $f\equiv 0$.

1.1 The driver code 3

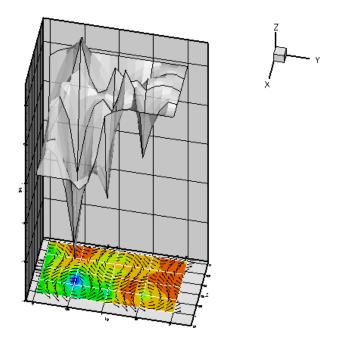


Figure 1.3 Plot of the unforced solution at different levels of mesh refinement.

The plot nicely illustrates the physical effects represented by the (unforced) advection diffusion equation. If $u(x_1,x_2)$ represents the concentration of a chemical that is advected by the velocity field $\mathbf w$, while being dispersed by molecular diffusion, the advection-diffusion equation describes the steady-state concentration of this chemical. In this context the Peclet number is a measure of the relative importance of advective and diffusive effects. For very small Peclet number, the concentration is determined predominantly by diffusive effects – as $\text{Pe} \to 0$, the advection diffusion equation approaches the Poisson equation. Conversely, at large values of the Peclet number, the concentration is determined predominantly by advective effects. The chemical is "swept along" by the flow and diffusive effects are only important in thin "boundary" or "shear" layers in which the concentration varies over short lengthscales. These can be seen clearly in the most finely resolved solution above.

1.1 The driver code

Overall, the structure of the driver code is very similar to that in the <u>corresponding Poisson example</u>. The only difference is that we have to specify function pointers to the source and the "wind" functions, which are passed to the problem constructor. We create the problem, perform a self-test, set the global parameters that affect the solution and solve the problem using <code>oomph-lib's "black-box"</code> adaptive Newton solver.

```
start_of_main=
/// Driver code for 2D AdvectionDiffusion problem
int main()
 //Set up the problem
 // Create the problem with 2D nine-node refineable elements from the
 // RefineableQuadAdvectionDiffusionElement family. Pass pointer to
 // source and wind function.
Refineable {\tt AdvectionDiffusionProblem} < Refineable {\tt QAdvectionDiffusionElement} < 2, \\
 3> > problem(&TanhSolnForAdvectionDiffusion::source_function,
               &TanhSolnForAdvectionDiffusion::wind_function);
 // Check if we're ready to go:
 cout « "\n\n\nProblem self-test ";
   (problem.self_test() == 0)
   cout « "passed: Problem can be solved." « std::endl;
else
   throw OomphLibError("Self test failed",
                       OOMPH_CURRENT_FUNCTION,
```

```
OOMPH_EXCEPTION_LOCATION);

}

// Set the orientation of the "step" to 45 degrees

TanhSolnForAdvectionDiffusion::TanPhi=1.0;

// Choose a large value for the steepness of the "step"

TanhSolnForAdvectionDiffusion::Alpha=50.0;

// Solve the problem, performing up to 4 adptive refinements

problem.newton_solve(4);

//output the solution

problem.doc_solution();

} // end of main
```

1.2 Global parameters and functions

The specification of the source function and the exact solution in the namespace TanhSolnForAdvectionDiffusion is similar to that for the Poisson examples. The only difference is the inclusion of the Peclet number and the "wind" function.

```
/// with "sharp" step
namespace TanhSolnForAdvectionDiffusion
   /// Peclet number
  double Peclet=200.0;
   /// Parameter for steepness of step
  double Alpha;
   /// Parameter for angle of step
  double TanPhi;
   /// Exact solution as a Vector
  void get_exact_u(const Vector<double>& x, Vector<double>& u)
     u[0] = tanh(1.0-Alpha*(TanPhi*x[0]-x[1]));
   /// Exact solution as a scalar
  void get_exact_u(const Vector<double>& x, double& u)
     u=tanh(1.0-Alpha*(TanPhi*x[0]-x[1]));
   /// Source function required to make the solution above an exact solution
  void source_function(const Vector<double>& x_vect, double& source)
     double x=x vect[0];
     double v=x vect[1];
     source
2.0* \\ tanh (-0.1E1 + \\ Alpha* (TanPhi*x-y))* (1.0-pow(tanh (-0.1E1 + \\ Alpha* (TanPhi*x-y)))* (1.0-pow(tanh (-0.1E1 + \\ Alpha*x-y)))* (1.0-pow(tanh (-0.1E1 +
 TanPhi*x-y)),2.0))*Alpha*Alpha*TanPhi*TanPhi+2.0*tanh(-0.1E1+Alpha*(TanPhi*x-y)
)*(1.0-pow(tanh(-0.1E1+Alpha*(TanPhi*x-y)),2.0))*Alpha*Alpha-Peclet*(-sin(6.0*y
) * (1.0-pow(tanh(-0.1E1+Alpha*(TanPhi*x-y)),2.0)) *Alpha*TanPhi+cos(6.0*x) * (1.0-
pow(tanh(-0.1E1+Alpha*(TanPhi*x-y)),2.0))*Alpha);
   /// Wind
  void wind_function(const Vector<double>& x, Vector<double>& wind)
     wind[0]=sin(6.0*x[1]):
     wind[1]=\cos(6.0*x[0]);
} // end of namespace
```

1.3 The problem class

The problem class is very similar to those used in the corresponding Poisson examples. The only change is that we use the function Problem::actions_before_adapt() to document the progress of the automatic spatial adaptation. For this purpose, we store a DocInfo as private member data in the Problem. This allows us to increment the counter that labels the output files, accessible from DocInfo::number(), whenever a new solution has been documented.

```
/// with refineable 2D QAdvectionDiffusion elements. The specific type
/// of element is specified via the template parameter.
template < class ELEMENT>
class RefineableAdvectionDiffusionProblem : public Problem
public:
 /// Constructor: Pass pointer to source and wind functions
RefineableAdvectionDiffusionProblem(
  AdvectionDiffusionEquations<2>::AdvectionDiffusionSourceFctPt source_fct_pt,
  AdvectionDiffusionEquations<2>::AdvectionDiffusionWindFctPt wind fct pt);
 /// Destructor. Empty
 ~RefineableAdvectionDiffusionProblem(){}
 /// \short Update the problem specs before solve: Reset boundary conditions /// to the values from the tanh solution.
 void actions_before_newton_solve();
 /// Update the problem after solve (empty)
 void actions_after_newton_solve(){}
 /// Actions before adapt: Document the solution
 void actions_before_adapt()
   // Doc the solution
   doc_solution();
   // Increment label for output files
   Doc info.number()++;
 /// \short Doc the solution.
void doc_solution();
 /// \short Overloaded version of the problem's access function to /// the mesh. Recasts the pointer to the base Mesh object to
 /// the actual mesh type.
 RefineableRectangularQuadMesh<ELEMENT>* mesh_pt()
   return dynamic_cast<RefineableRectangularQuadMesh<ELEMENT>*>(
   Problem::mesh_pt());
private:
 /// DocInfo object
DocInfo Doc_info;
 /// Pointer to source function
AdvectionDiffusionEquations<2>::AdvectionDiffusionSourceFctPt Source_fct_pt;
 /// Pointer to wind function
AdvectionDiffusionEquations<2>::AdvectionDiffusionWindFctPt Wind_fct_pt;
}; // end of problem
```

1.4 The Problem constructor

The constructor is practically identical to the constructors used in the various Poisson examples. We specify the output directory in the Problem's DocInfo object, create the mesh and an error estimator, and apply the boundary conditions by pinning the nodal values on the Dirichlet boundaries.

```
==start_of_constructor
/// \short Constructor for AdvectionDiffusion problem: Pass pointer to
/// source function.
template<class ELEMENT>
RefineableAdvectionDiffusionProblem<ELEMENT>::RefineableAdvectionDiffusionProblem(
{\tt AdvectionDiffusionEquations<2>::AdvectionDiffusionSourceFctPt\ source\_fct\_pt,}
AdvectionDiffusionEquations<2>::AdvectionDiffusionWindFctPt wind_fct_pt)
      : Source_fct_pt(source_fct_pt), Wind_fct_pt(wind_fct_pt)
// Set output directory
Doc_info.set_directory("RESLT");
// Setup mesh
// # of elements in x-direction
unsigned n_x=4;
// # of elements in y-direction
unsigned n_y=4;
// Domain length in x-direction
double l_x=1.0;
// Domain length in y-direction
double 1_y=2.0;
// Build and assign mesh
Problem::mesh_pt() =
```

```
new RefineableRectangularQuadMesh<ELEMENT>(n_x,n_y,l_x,l_y);
// Create/set error estimator
mesh_pt()->spatial_error_estimator_pt()=new Z2ErrorEstimator;

// Set the boundary conditions for this problem: All nodes are
// free by default -- only need to pin the ones that have Dirichlet
// conditions here
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 loop over boundaries
```

We complete the problem setup by passing the function pointers to the source and wind functions, and the pointer to the Peclet number to the elements. Finally, we set up the equation numbering scheme.

```
// Complete the build of all elements so they are fully functional
// Loop over the elements to set up element-specific
// things that cannot be handled by the (argument-free!) ELEMENT
// constructor: Pass pointer to source function
unsigned n_element = mesh_pt()->nelement();
for(unsigned i=0;i<n_element;i++)
{
    // Upcast from GeneralsedElement 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;
    //Set the wind function pointer
    el_pt->wind_fct_pt() = Wind_fct_pt;
    // Set the Peclet number
    el_pt->pe_pt() = &TanhSolnForAdvectionDiffusion::Peclet;
}
// Setup equation numbering scheme
cout «"Number of equations: " « assign_eqn_numbers() « std::endl;
// end of constructor
```

1.5 Actions before solve

As before, we use the Problem::actions_before_newton_solve() function to set/update the boundary conditions.

```
========start_of_actions_before_newton_solve===
/// Update the problem specs before solve: (Re-)set boundary conditions
/// to the values from the tanh solution.
template<class ELEMENT>
void RefineableAdvectionDiffusionProblem<ELEMENT>::actions before newton solve()
 // How many boundaries are there?
unsigned num_bound = mesh_pt()->nboundary();
 //Loop over the boundaries
 for(unsigned ibound=0;ibound<num_bound;ibound++)</pre>
  {
  // How many nodes are there on this boundary?
  unsigned num_nod=mesh_pt()->nboundary_node(ibound);
   // Loop over the nodes on boundary
   for (unsigned inod=0;inod<num_nod;inod++)</pre>
     // Get pointer to node
     Node* nod_pt=mesh_pt()->boundary_node_pt(ibound,inod);
     // Extract nodal coordinates from node:
     Vector<double> x(2);
     x[0] = nod_pt -> x(0);
     x[1] = nod_pt -> x(1);
     // Compute the value of the exact solution at the nodal point
     Vector<double> u(1);
     TanhSolnForAdvectionDiffusion::get_exact_u(x,u);
     // Assign the value to the one (and only) nodal value at this node
     nod_pt->set_value(0,u[0]);
   // end of actions before solve
```

1.6 Post-processing

The function $doc_solution(...)$ is identical to that in the Poisson example. We output the solution, the exact solution and the error.

```
template<class ELEMENT>
void RefineableAdvectionDiffusionProblem<ELEMENT>::doc_solution()
ofstream some file:
char filename[100];
 // Number of plot points: npts x npts
unsigned 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,TanhSolnForAdvectionDiffusion::get_exact_u);
 some_file.close();
 // Doc error and return of the square of the L2 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,TanhSolnForAdvectionDiffusion::get_exact_u,
                           error, norm);
some_file.close();
 // Doc L2 error and norm of solution
cout « "\nNorm of error : " « sqrt(error) « std::endl; cout « "Norm of solution: " « sqrt(norm) « std::endl « std::endl;
```

1.7 Comments and Exercises

- 1. Explore the change in the character of the solution of the unforced problem when the Peclet number is slowly increased from 0 to 200, say. Note how at small Peclet number, strong diffusive effects smooth out the rapid spatial variations imposed by the boundary conditions. Conversely, at large values of the Peclet number, the behaviour is dominated by advective effects. As a result, in regions where the "wind" is directed into the domain, the value of u set by the Dirichlet boundary conditions is "swept" into the domain. In regions where the "wind" is directed out of the domain, the value of u "swept along" by the flow in the interior "clashes" with the value prescribed by the boundary conditions and the solution adjusts itself over a very short length scale, leading to the development of thin "boundary layers".
- 2. Explore the character of the solution on coarse meshes at large and small Peclet numbers. Note how at large Peclet numbers the solution on the coarse meshes displays strong "wiggles" throughout the domain. These only disappear once the mesh adaptation fully resolves the regions of rapid variation. We will explore this issue further in another example.

1.8 Source files for this tutorial

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

```
demo_drivers/advection_diffusion/two_d_adv_diff_adapt/
```

· The driver code is:

```
\label{lem:demo_drivers} $$ demo_drivers/advection_diffusion/two_d_adv_diff_adapt/two_d_adv_diff_{$\leftarrow$} $$ adapt.cc
```

1.9 PDF file

A pdf version of this document is available.