C1 - Assignment 2 Report

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1 Introduction

In this report we study numerical solutions to boundary value problems, in particular for the advection-reaction-diffusion equation under given boundary conditions. In general, we define a boundary value problem as follows

> Let $\Omega \subseteq \mathbb{R}^d$, $d = 1, 2$, be a bounded simply connected open domain. Find, for f, v given, a function u such that
>
> $$\mathcal{L}[u] = f, \quad \text{in } \Omega, \qquad u = v, \quad \text{on } \partial\Omega,$$
>
> where $\mathcal{L} = -\Delta u + \mathbf{p} \cdot \nabla u + qu$, with $\mathbf{p}, q$ given smooth, bounded functions.

In this report, we deal with a *Dirichlet problem*, in which we ask to find the solution of the equation in the interior of Ω while prescribing its value on the boundary $\partial\Omega$.

We obtain numerical solutions of the advection-reaction-diffusion equation through the *finite-difference* (FD) method. The approach of the FD method is to evaluate the given operator $\mathcal{L}$ at a set of discretisation points $(x_j)_{j=1}^{J}$ with the derivatives within replaced by difference quotients of the approximated solution, U. These difference quotients (e.g. $\partial^-, \partial^+, \partial^+\partial^-$) are obtained by truncating the Taylor expansion of the exact solution about the discretisation points x_j. Then after this discretisation, one should obtain a system of equations, which can be rewritten as a linear matrix problem, i.e. $A\mathbf{U} = \mathbf{f}$ for the approximate solution $\mathbf{U}$ and given data $\mathbf{f}$. There are a number of ways in which linear problems can be solved, on that we shall use is the *Gauss-Seidel* method discussed in Assigment 1 of this course.

In section 2 we go through the discretisation of the advection-reaction-diffusion equation throgh the finite difference method and present its numerical implementation. In section 3, we test the numerical scheme obtained in section 2 on the advection-diffusion-reaction equation with known analytical solutions as to deduce the error of the scheme and some analyical results. In section 4, we provide a conclusion to the analysis performed in the previous sections.

2 Problem

The aim of this report is to numerically deduce (throught the method of finite differences) the solutions of the advection-diffusion-reaction equation

$$-\alpha u'' + \beta u' + \gamma u = 0,$$

for given parameter values α, β and γ. In particular, we seek to find the the solutions of the linear advection diffusion equation

$$-\alpha u'' + \beta u' = 0, \quad u(0) = 0, \; u(L) = 1, \tag{1}$$

and the linear diffusion reaction equation

$$-\alpha u'' + \gamma u = 0, \quad u(0) = 0, \; u(L) = 1, \tag{2}$$

in the domain $\Omega = [0, 1]$. For equation (1), define the so-called *Péclet* number, Pe, through

$$Pe = \frac{|\beta| L}{2\alpha},$$

and for the equation (2), the so-called Damköhler number

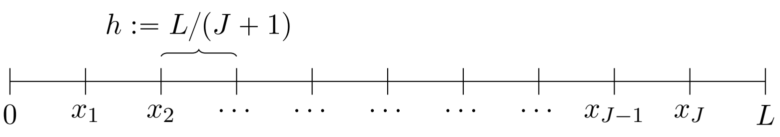
$$Da = \frac{\gamma}{\alpha}.$$

2.1 Discretisation Through Finite-Differences

We begin by discretising the general boundary value problem

$$-\alpha u'' + \beta u' + \gamma u = 0, \quad u(0) = 0, \; u(L) = 1. \tag{3}$$

When we require equation (1) or (2), we choose $\gamma = 0$ or $\beta = 0$ respectively. We discretise equation (3) by finite differences with simple centred schemes for second and first order derivatives. We begin by letting $(x_j)_{j=0}^{J+1}$ be a partition of the interval $\Omega = [0, L]$ such that $0 = x_0 < x_1 < x_2 < \cdots < x_J < x_{J+1} = L$. We denote the jth interval by $I_j = [x_{j-1}, x_j]$ with the mesh size $h_j = |I_j|$. Within this report, we consider a uniform mesh size, and therefore set $h := h_j$ for all j, hence $x_j = jh$. Now let $U_j := u(x_j)$ for each $j \in \{1, \dots, J\}$ and define



$\mathbf{U} = (U_1, \dots, U_J)$, which denotes the approximation of u on the interior of the partitioning of $[0, L]$. Then the discrete problem approximating the continuous problem (3) is given by

$$-\alpha \partial^- \partial^+ U_j + \beta \partial^0 U_j + \gamma U_j = 0, \tag{4}$$

for $j = 1, \dots, J$ with $U_0 = u(0) = 0$ and $U_{J+1} = u(L) = 1$, where

$$\partial^- \partial^+ U_j = \frac{U_{j-1} - 2U_j + U_{j+1}}{h^2}, \quad \partial^0 = \frac{U_{j+1} - U_{j-1}}{2h}.$$

Equation (4) can be rewritten as

$$\left(-\frac{\alpha}{h^2}-\frac{\beta}{2h}\right)U_{j-1}+\left(\frac{2\alpha}{h^2}+\gamma\right)U_j+\left(-\frac{\alpha}{h^2}+\frac{\beta}{2h}\right)=0,$$

for $j=1,\ldots,J$, which gives rise to the following linear equation

$$A\mathbf{U}=\mathbf{f}, \tag{5}$$

where $A=(a_{ij})\in\mathbb{R}^{J\times J}$ is such that

$$a_{ij}=\begin{cases}-\frac{\alpha}{h^2}-\frac{\beta}{2h} & \text{if } j=i-1,\\ \frac{2\alpha}{h^2}+\gamma & \text{if } j=i,\\ -\frac{\alpha}{h^2}+\frac{\beta}{2h} & \text{if } j=i+1,\end{cases}$$

and $\mathbf{f}=(f_i)\in\mathbb{R}^J$ is such that

$$f_i=\begin{cases}0 & i\neq J,\\ \frac{\alpha}{h^2}-\frac{\beta}{2h} & i=J.\end{cases}$$

We make note of the fact that the matrix A is sparse and tridiagonal. This completes the finite difference discretisation, and we may now apply numerical inversion techniques to the matrix A to deduce the numerical solution, $\mathbf{U}$, of the problem (3). If A is made diagonally dominant, then we may use the Gauss-Seidel numerical scheme implemented in Assignment 1 to solve the linear system.

2.2 Numerical Implementation

To implement the above discretisation into a numerical scheme, we begin by creating a class called `FiniteDifference` shown below.

```
class FiniteDifference
{
public:
   FiniteDifference(); // Default Constructor
   FiniteDifference(int J, double L, double alpha, double beta, double gamma, double
       b_0, double b_L);
   FiniteDifference(const FiniteDifference& scheme); // Copy Constructor
   ~FiniteDifference(); // Destructor

   int getJ();
   double getL();
   double getAlpha();
   double getBeta();
   double getGamma();
   double getb_0();
   double getb_L();

   SparseMatrix constructMatrix(); // Constructs the "differential operator" matrix A

private:
   int J_; // The number of points in the discretisation
   double L_; // Length of interval
   double b_0_, b_L_; // Boundary conditions
   double alpha_, beta_, gamma_; // Equation parameters
};
```

To carry out the finite difference method described above, we define the member function `constructMatrix` of the class `FiniteDifference` to constuct the matrix A define in equation (5).

```
SparseMatrix FiniteDifference::constructMatrix()
{
   double h = L_/(double) (J_ + 1); // Setting the mesh size
   SparseMatrix A = SparseMatrix(J_,J_);
   double D = 2*alpha_/(double) (h*h) + gamma_; // Diagonal terms of A
   double UD = -(alpha_ - h*beta_/2.0)/(double) (h*h); // Upper-diagonal terms of A
   double LD = -(alpha_ + h*beta_/2.0)/(double) (h*h); // Lower-diagonal terms of A
   for (int i = 0; i < J_; ++i)
   {
      for (int j = 0; j < J_; ++j)
      {
         if(j == i + 1) // Upper-diagonal entries
         {
            A.addEntry(i, j, UD);
         }
         else if(j == i) // Diagonal entries
         {
            A.addEntry(i, j, D);
         }
         else if (j == i - 1) // Lower-diagonal entries
         {
         A.addEntry(i, j, LD);
         }
      }
   }
   return A;
}
```

We then proceed to solve the linear system in equation (5) by inverting it against $\mathbf{f}$ using the Gauss-Seidel numerical scheme, described in the previous assignment, to obtain the approximate solution to the problem (3) in the form of a STL vector $\mathbf{U}$.

3 Results

We can test the finite-difference approximation by analysing the error (using the L^∞ norm) between the numerical and analytical solution. For this, we consider the cases of equations (1) and (2) separately.

3.1 Linear Advection-Diffusion Equation

We can in fact solve equation (1) analytically with the given boundary conditions to obtain a unique solution of the following form

$$u(x) = \frac{1 - \exp\left(\frac{\beta x}{\alpha}\right)}{1 - \exp\left(\frac{\beta L}{\alpha}\right)}, \quad x \in [0, L], \tag{6}$$

for $\alpha \neq 0$ and $\beta \in \mathbb{R}$. We note that as $\beta = 0$, $u(x) = x$, which is the limiting behaviour of the solution (6). To be able to use the Gauss-Seidel algorithm, we require that the discretisation matrix A is diagonally dominant. We can guarantee this as along as

$$\left|\frac{2\alpha}{h^2}\right| \geqslant \left|-\frac{\alpha}{h^2} - \frac{\beta}{2h}\right| + \left|-\frac{\alpha}{h^2} + \frac{\beta}{2h}\right| \geqslant \left|\frac{\beta}{h}\right|,$$

that is $2|\alpha| > h|\beta|$. Since $h := \frac{L}{J+1}$, where J denotes the number of discretisation points, it follows that

$$J + 1 \geqslant \frac{|\beta| L}{|\alpha|} \geqslant Pe.$$

Thus if the number of disretisation points J is greater that the Peclét number minus one ($J > Pe - 1$), then we are guaranteed to have convergence of the approximate solution to the correct solution through the use of Gauss-Seidel. Taking this into account, along with knowing the analytical solution, we can deduce the error, $\|u_h - u\|_\infty$, of the numerical solution with respect to the analytical solution for various different values of α, β, γ and number of discritisation points J. The error plots for this can be seen in Figure 1. From Figure 1, we see that the error between

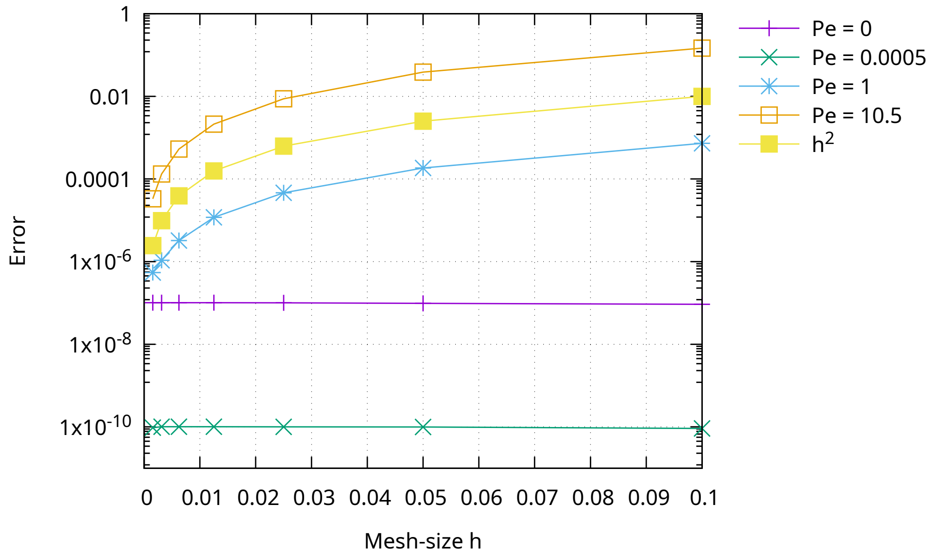


Figure 1: Error between the analyical and numerical solution of equation (1) for variaous Peclét numbers Pe and discretisation points J.

the analytical solution and the numerical solution decreases exponentially for Peclet numbers of order at least 1, but when $Pe = 0.0005$, we observe that the error is very small and decreases extremely slowly as the number of points J increases. We know that by stability

$$\|r_h u - U\|_\infty \leqslant C \|\mathcal{L}_h(r_h u) - \mathcal{L}_h U\|_\infty,$$

for some constant C. By Taylor expansion we know that

$$\|r_h u - u_h\|_\infty \leqslant \frac{h^2}{12} \|u^{(4)}\|_\infty, \quad \|r_h u' - u_h'\|_\infty \leqslant \frac{h^2}{6} \|u^{(3)}\|_\infty.$$

Therefore, we can obtain the following bound on the error

$$\begin{aligned}
\|r_h u - u_h\|_\infty &\leqslant C \| - \alpha r_h u'' + \beta r_h u' + \alpha u_h'' - \beta u_h' \|_\infty \\
&\leqslant C \left(|\alpha| \|r_h u'' - u_h''\|_\infty + |\beta| \|r_h u' - u_h'\|_\infty \right) \\
&\leqslant C \left(\frac{|\alpha| h^2}{12} \|u^{(4)}\|_\infty + \frac{|\beta| h^2}{6} \|u^{(3)}\|_\infty \right).
\end{aligned}$$

Since we know the analytical solution, for $k = 3, 4$

$$u^{(k)}(x) = -\frac{\left(\frac{\beta}{\alpha}\right)^k}{1 - \exp\left(\frac{\beta L}{\alpha}\right)} \exp\left(\frac{\beta x}{\alpha}\right),$$

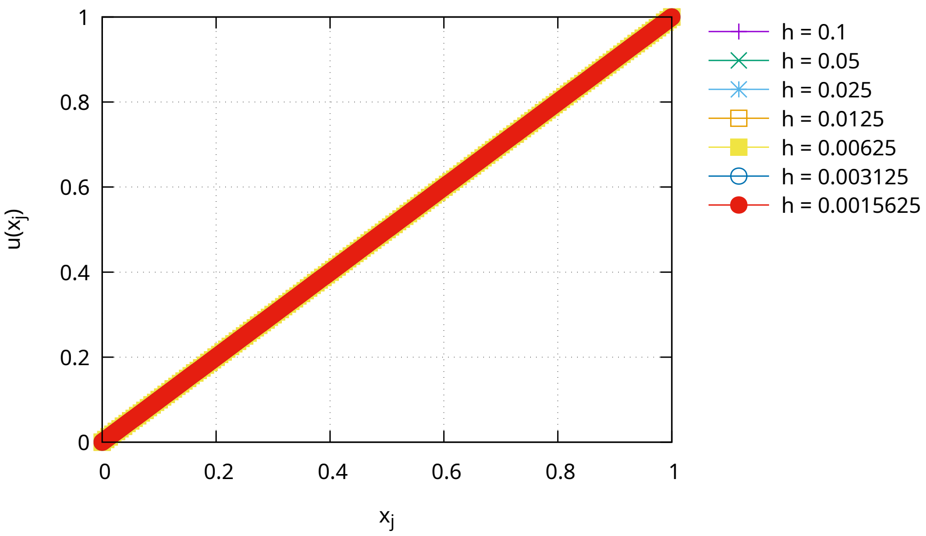
therefore, for $k = 3, 4$

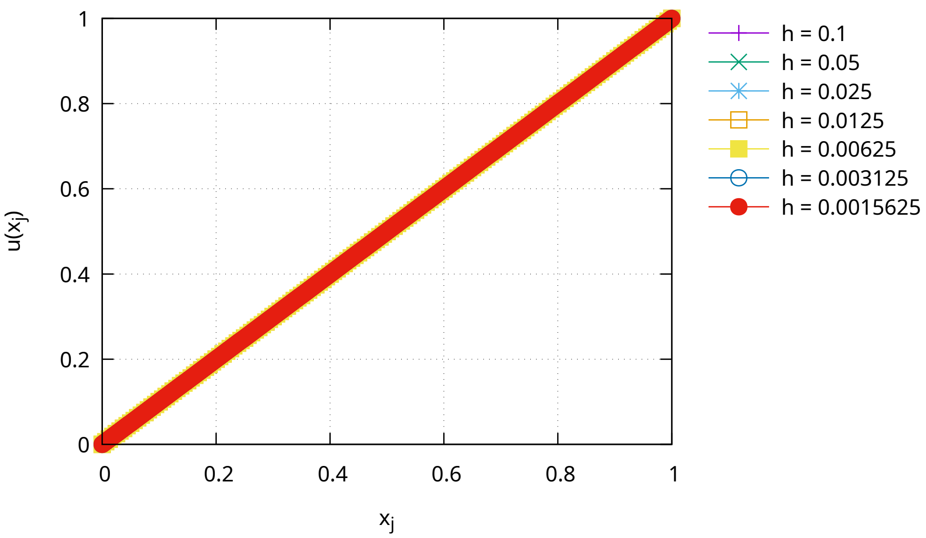
$$\|u^{(k)}\|_\infty = \left|\frac{\beta}{\alpha}\right|^k \left|\frac{\exp\left(\frac{\beta L}{\alpha}\right)}{1-\exp\left(\frac{\beta L}{\alpha}\right)}\right| =: g(\alpha, \beta).$$

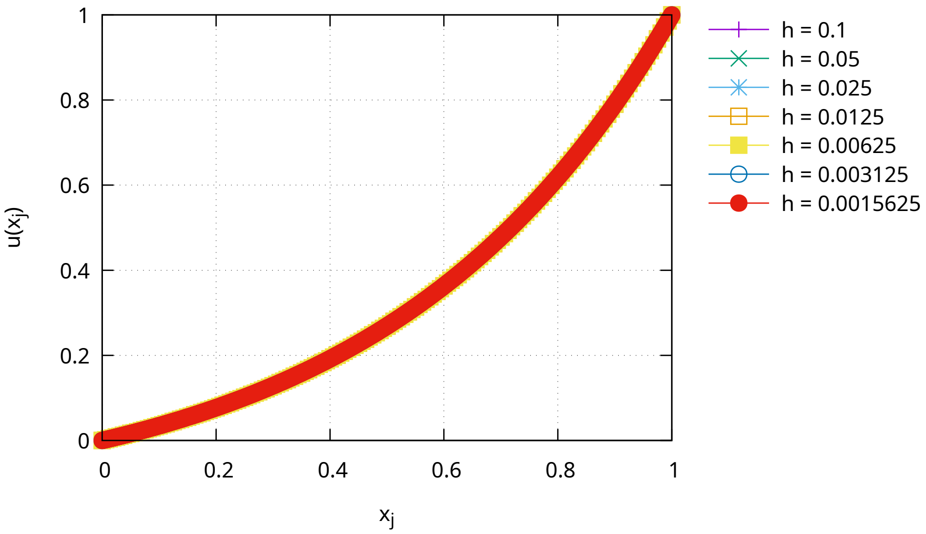
Then

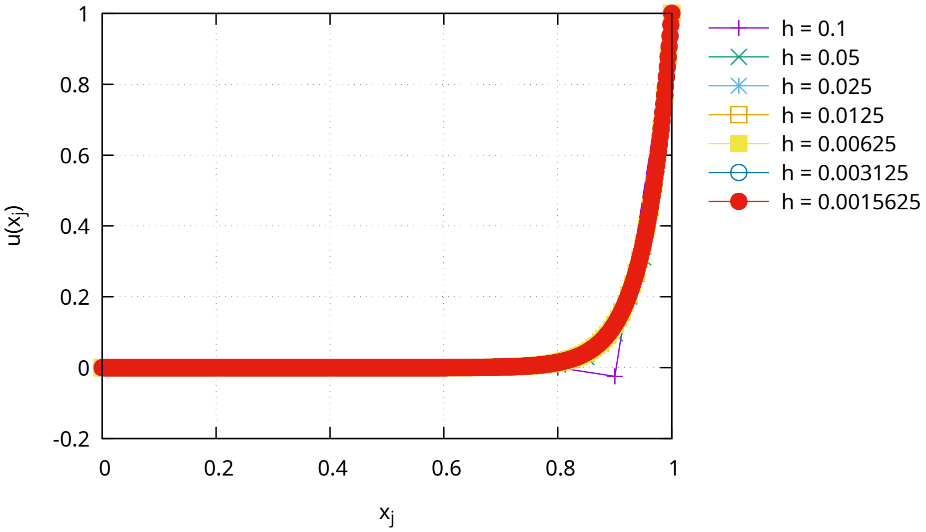
$$\|r_h u - u_h\|_\infty \leqslant C\frac{h^2}{4}\frac{|\beta|^4}{|\alpha|^3} g(\alpha, \beta).$$

Therefore, the order of convergence is at least of order 2, which was expected since that is the order of consistency.









3.2 Linear Diffusion-Reaction Equation

We can also solve equation (2) analytically with the given boundary conditions to obtain a unique solution of the following form

$$u(x) = \frac{\sinh\left(\sqrt{\frac{\gamma}{\alpha}}x\right)}{\sinh\left(\sqrt{\frac{\gamma}{\alpha}}L\right)}, \quad x \in [0, L].$$

4 Conclusion