Numerical Solution of 2D Diffusion-Advection Equation and Nonlinear Problem with Difference Methods

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Abstract

In this project we do an error analysis on and solve the diffusion-advection equation using the finite difference method. We also solve a nonlinear equation modelling a microelectromechanical device. The numerical results were consistent with the theoretical analysis and physical interpretation.

1 Introduction

The main topic of this project is the diffusion-advection equation solved on a two-dimensional domain. The equation describes diffusion, a movement process due to the concentration gradient [2], and advection, which is transport due to bulk motion of some quantity in a given system [3]. We use both Dirichlet and Neumann conditions on rectangular and circular boundaries. An error analysis will be performed and verified numerically. In addition, the report will consider a nonlinear problem, modelling a microelectromechanical device. This problem describes the deflection of an elastic membrane located above a rigid metal plate.

2 Theory

The diffusion-advection equation is given by

$$-\mu \Delta u + \boldsymbol{v} \cdot \nabla u = f \quad \text{in } \Omega. \tag{1}$$

Here Δ is the Laplace operator, ∇ is the gradient and $\mu > 0$ is the diffusion constant. The velocity field $\boldsymbol{v} : \Omega \to \mathbb{R}^2$ and the source function $f : \Omega \to \mathbb{R}$ may depend on the position.

Let $\Omega = (0,1) \times (0,1)$, i.e., the unit square, and use Dirichlet conditions to solve the problem. Discretization of the problem, using central differences, yields

$$\frac{-\mu\big(U_S + U_W + U_N + U_E - 4U_P\big)}{h^2} + v_1 \cdot \frac{U_E - U_W}{2h} + v_2 \cdot \frac{U_N - U_S}{2h} = f_P, \quad (2)$$

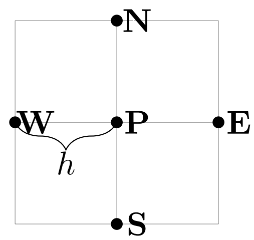


Figure 1: Five-point stensil with definition of the points P, N, S, E and W.

where $\mathbf{v} = [v_1, v_2]$ and the points P, N, S, E, W are defined in Figure 1. Using stepsize $h = \frac{1}{M}$ yields a linear system with $(\mathrm{M}{+}1)^2$ equations and unknowns, which can be represented in vector form as

$$\boldsymbol{AU} = \boldsymbol{F}. \quad (3)$$

Error analysis

Theorem 1 *Given equation* (1) *with* $f \in C^2(0,1)$ *and Dirichlet conditions on the unit square solved by the finite difference scheme* (2). *Assuming* $h \le \frac{2\mu}{\max\{|v_1|,|v_2|\}}$ *and* v_1, v_2 *does not change sign on* Ω, *the global error* $e_p = u_p - U_p, p \in \Omega$, *satisfies the error bound*

$$|e_p| \le \frac{Kh^2}{12} \quad (4)$$

with

$$K = \max_{p\in\Omega}\{|\partial_x^4 u_p|, |\partial_y^4 u_p|\} + \frac{1}{\mu}\max\{|v_1 \partial_x^3 u_p|\} + \frac{1}{\mu}\max\{|v_2 \partial_y^3 u_p|\}.$$

This implies that the scheme is of second order.

Proof Taylor expansion and the mean value theorem gives that

$$\frac{u(x_0+h,y) - u(x_0-h,y)}{2h} = \partial_x u(x_0,y) + \frac{h^2}{6}\partial_x^3 u(\xi,y) \quad \xi \in (x_0-h, x_0+h)$$

$$\frac{u(x_0+h,y) - 2u(x_0,y) + u(x_0-h,y)}{h^2} = \partial_x^2 u(x_0,y) + \frac{h^2}{12}\partial_x^4 u(\xi,y) \quad \xi \in (x_0-h, x_0+h),$$

and equivalent for y. The local truncation error, given by $L_h U_p - L_h u_p$, is thus

$$|\tau_p| = \mu\frac{h^2}{12}(\partial_x^4 u(\xi_p,y) + \partial_y^4 u(x,\eta_p) + v_1\frac{h^2}{6}\partial_x^3 u(\mu_p,y) + v_2\frac{h^2}{6}\partial_y^3 u(x,\rho_p),$$

and a bound for this truncation error is

$$|\tau_p| \le \frac{\mu \cdot Kh^2}{6}.$$

Define a function ϕ by

$$\phi(x,y) =: \frac{Kh^2}{4}\begin{cases}(x^2-2x)+(y^2-2y) & \text{if } v_1, v_2 \geq 0\\ (x^2-1)+(y^2-2y) & \text{if } v_1 < 0, v_2 \geq 0\\ (x^2-2x)+(y^2-1) & \text{if } v_1 \geq 0, v_2 < 0\\ (x^2-1)+(y^2-1) & \text{if } v_1, v_2 < 0.\end{cases} \tag{5}$$

Note that $L_h e_p = \tau_p$. Then

$$L_h(\phi \pm e) = -\mu K h^2 + v_1 \partial_x \phi + v_2 \partial_y \phi \pm \mu K h^2,$$

and since $v_1 \partial_x \phi \leq 0$ and $v_2 \partial_y \phi \leq 0$ it follows that

$$L_h(\phi \pm e) \leq 0.$$

To be able to the use the discrete maxium principle [1](p. 76), the following equations must be satisfied

$$\begin{array}{ll}\frac{\mu}{h^2} - \frac{v_1}{2h} > 0, & \frac{\mu}{h^2} + \frac{v_1}{2h} > 0\\ \frac{\mu}{h^2} - \frac{v_2}{2h} > 0, & \frac{\mu}{h^2} + \frac{v_2}{2h} > 0\end{array}. \tag{6}$$

Making the assumption $h \leq \frac{2\mu}{\max\{|v_1|,|v_2|\}}$, the discrete maximum principle then gives that

$$|e_p| \leq \frac{Kh^2}{12}. \tag{7}$$

Curved Boundary

Solving the problem with irregular boundaries requires extra attention. With the unit circle in the first quadrant as the domain, using the same regular grid as above yields the discretization shown in Figure 2.

Then, most inner points can be calculated using the scheme in (2). However, points near the boundary require a modified scheme. If **E** is outside the boundary, the following approximations for the first and second derivatives with respect to x are used:

$$\begin{aligned}\frac{\partial u_P}{\partial x} &= \frac{U_{E'} - U_W}{h(1+\Theta^x)},\\ \frac{\partial^2 u_P}{\partial x^2} &= \frac{2}{h^2\Theta^x(1+\Theta^x)}(\Theta^x U_W - (1+\Theta^x)U_P + U_{E'}),\end{aligned} \tag{8}$$

where **E'** and Θ^x are as defined in Figure 3 and the second derivative is found by differentiating twice the interpolation polynomial through $\mathbf{W}, \mathbf{P}$ and **E'**. The value of Θ^x is easily found using that the boundary is the unit circle:

$$\Theta^x = \frac{x_{E'} - x_P}{h}, \quad x_{E'} = \sqrt{1 - y_P^2}. \tag{9}$$

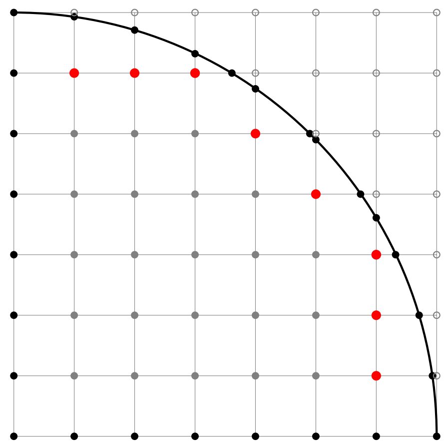


Figure 2: Discretization of a partly circular domain with $M = 7$. Black points are boundary points with known solutions, points outside the boundary are set to zeros, gray points are inner points where the usual scheme can be used, whereas red points demand a modified scheme.

Equivalent approximations for ∂_y and ∂_{yy} are found when **N** is outside the boundary. Whether $\mathbf{E}, \mathbf{N}$ or both are outside the boundary is found by checking if $\Theta^x, \Theta^y \leq 1$. A new scheme for the points near the boundary is found by replacing the relevant derivaties with these new approximations in equation (2).

In the error analysis, we obtained order 2 as the symmetry of the five point stencil and central difference approximations make certain terms in the Taylor expansions cancel eachother. In the modified scheme, this symmetry, and hence convergence order 2, is lost.

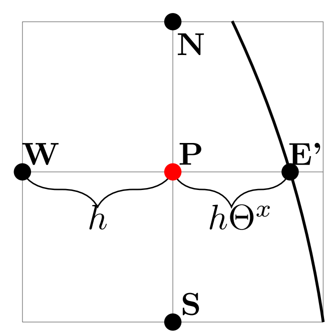


Figure 3: Definition of Θ^x and the point **E'** lying outside of the regular grid.

Neumann Conditions

To incorporate Neumann conditions, $\partial_y u_P = g^N$ on the edge where $y = 0$, we use a fictitious point s laying outside the the domain. Central difference gives that

$$\partial_y u_P = \frac{u_N - u_s}{2h} = g^N.$$

Rearranging and inserting this into the scheme gives

$$\frac{-\mu\big(U_W + 2U_N + U_E - 4U_P - 2h\cdot g^N\big)}{h^2} + v_1 \cdot \frac{U_E - U_W}{2h} + v_2 \cdot g^N = f_P. \quad (10)$$

A similar modification can be made to incorporate Neumann Conditions on the other edges. After this modification the scheme still has order two [1] (p. 19).

Modified scheme

The error analysis showed that the scheme should converge whenever $h \leq \frac{2\mu}{\max\{|v_1|,|v_2|\}}$. To avoid this restriction on h, the scheme can be modified by approximating $\partial_x u$ using the backward difference when $v_1 > 0$ and the forward difference when $v_1 < 0$, and the same for $\partial_y u$. These approximations are of order 1, but give a scheme which converges for every choice of h. For $v_1 > 0$ and $v_2 < 0$ the scheme would be

$$\frac{-\mu\big(U_S + U_W + U_N + U_E - 4U_P\big)}{h^2} + v_1 \cdot \frac{U_P - U_W}{h} + v_2 \cdot \frac{U_N - U_P}{h} = f_P, \quad (11)$$

and the necessary conditions on the coefficients in the discrete maximum principle [1] (p. 76),

$$\frac{\mu}{h^2} + \frac{v_1}{h} > 0, \quad \frac{\mu}{h^2} - \frac{v_2}{h} > 0, \quad \frac{4\mu}{h^2} + \frac{v_1 - v_2}{h} > 0, \quad (12)$$

are statisfied for all h.

Nonlinear problems - Modelling a microelectromechanical device

The nonlinear system consists of two surfaces located at $z = 0$ and $z = 1$, where the upper is an elastic membrane fixed at the boundaries and the lower is a rigid metal plate. Mathematically, the deflection u of the elastic membrane when putting on an electrical potential can be modelled by

$$\begin{aligned} \Delta u &= \frac{\lambda}{u^2} \quad \text{in } \Omega \\ u &= 1 \quad \text{on } \partial\Omega, \end{aligned} \quad (13)$$

where λ is a constant proportional to an electrical potential working on the device [4]. The domain Ω is once again the unit square, i.e., $(0,1)\times(0,1)$, and discretizing this domain gives

$$\frac{(U_S + U_W + U_N + U_E - 4U_P)\cdot U_P^2}{h^2} - \lambda = 0 \quad (14)$$

for all inner points U_P. This is a nonlinear system of equations, which can be denoted in vector form as

$$G_h(U) = 0. \quad (15)$$

As the system is nonlinear, the Newton method will be used to solve it iteratively. The method is given by

$$U^{(k+1)} = U^{(k)} - J_h(U^{(k)})^{-1} G_h(U^{(k)}),$$

where $J_h(U)$ is the Jacobian of $G_h(U)$.

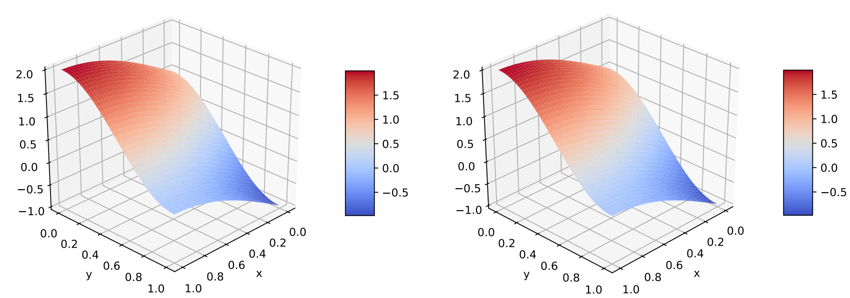
3 Numerical experiments

To solve the linear numerical problem, an index mapping and a class for a general BVP, taking in a boundary condition, source function, intervals, μ, the velocity field and the exact solution, are defined. Furthermore, the finite difference scheme is implemented, as well as a function for creating the right hand side of the equation. The error analysis was performed using multiple stepsizes, and the error for each stepsize was found using the supremum norm.

First, let Ω be the unit square and consider the diffusion-advection (1) where

$$\begin{aligned} Lu(x,y) &= f(x,y) \\ &= \frac{1}{4}\pi^2 \sin(\frac{1}{2}\pi x) + \pi^2 \cos(\pi y) + \frac{1}{2}\pi x \cos(\frac{1}{2}\pi x) - \pi y \sin(\pi y) \text{ in } \Omega \\ u(x,y) &= \sin(\frac{1}{2}\pi x) + \cos(\pi y) \quad \text{on } \partial\Omega \\ v(x,y) &= [x,y], \quad \mu = 1, \quad \Omega = (0,1)\times(0,1) \end{aligned} \tag{16}$$

with exact solution $u(x,y)$ on Ω and using Dirichlet conditions. With values $M = [10, 20, 39, 76, 150]$, the convergence order of the solution of (16) on the unit square was found to be $1.995 \approx 2$. Plots of the numerical and exact solutions can be seen in Figure 4. Figure 5 shows the error together with the theoretical error bound given by (7).



(a) Numerical solution

(b) Exact solution

Figure 4: Numerical and exact solution when the diffusion-advection equation is solved on the unit square in Problem (16).

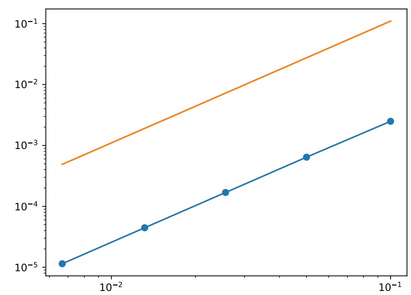
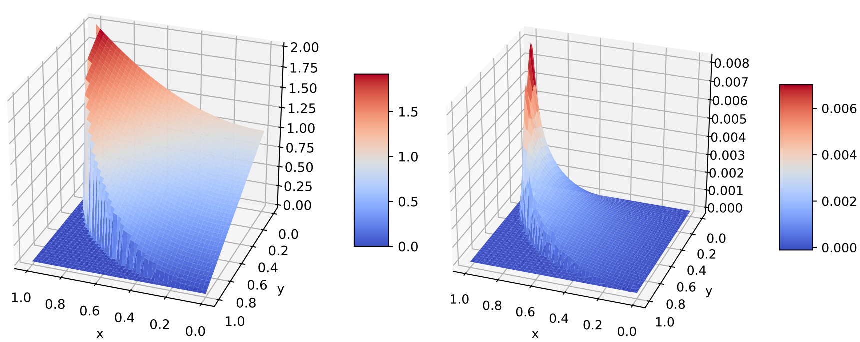


Figure 5: A loglog plot of the error in Problem (16). The orange line is the theoretical error bound, while the blue dots are the numerical errors for different stepsizes.

Let Ω be the part of the unit circle in the first quadrant. Again solving (1), we use the following test problem with Dirichlet conditions:

$$\begin{aligned} Lu(x,y) &= f(x,y) = -2 + 2x^2 - y \quad \text{in } \Omega \\ u(x,y) &= x^2 - y + 1 \quad \text{on } \partial\Omega \\ v(x,y) &= [x,y], \quad \mu = 1, \quad \Omega = \{x,y : x,y \geq 0, x^2+y^2 \leq 1\}, \end{aligned} \tag{17}$$

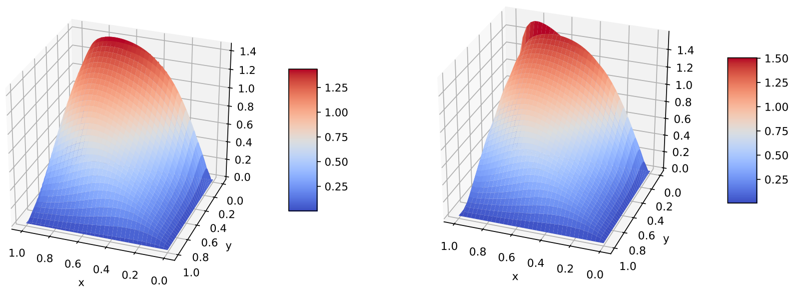
with exact solution $u(x,y)$ on Ω. The numerical solution and error $e = u(x,y) - U(x,y)$ are shown in Figure 6. The error is small, and largest near the curved boundary. Using values $M = [20, 38, 76, 150]$, the numerical convergence order was found to be approximately 0.85. Solving problems with other solutions on the same domain results in different convergence orders, varying between 0.7 and 1.8.



(a) Numerical solution with $h = 1/40$

(b) Error $e = u(x,y) - U(x,y)$

Figure 6: Numerical solution to (17) and its corresponding error plot.



(a) Stepsize $h = 1/100$

(b) Stepsize $h = 1/35$

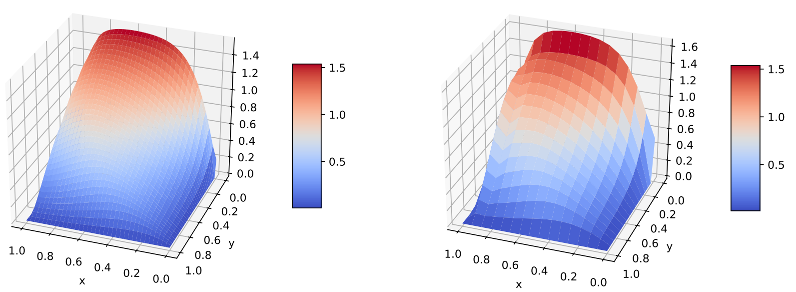
Figure 7: Numerical solution to problem (18), with Diriclet conditions.

Let again Ω be the unit square, and let

$$
\begin{aligned}
Lu(x,y) &= f(x,y) = 1 \quad \text{in } \Omega \\
u(x,y) &= 0 \quad \text{on } \partial\Omega \\
\mu = 10^{-2}, \quad \mathbf{v} &= [y, -x], \quad \Omega = (0,1) \times (0,1)
\end{aligned}
\tag{18}
$$

be an instance of (1). The numerical solution of (18) can be seen in Figure 7, where plot 7a has stepsize $\frac{1}{100}$ and plot 7b has stepsize $\frac{1}{35}$. The plot shows clearly that the solution breaks down when $h = \frac{1}{35}$ and closer inspection show that in fact it breaks down for stepsize $h \gtrsim \frac{1}{50}$.

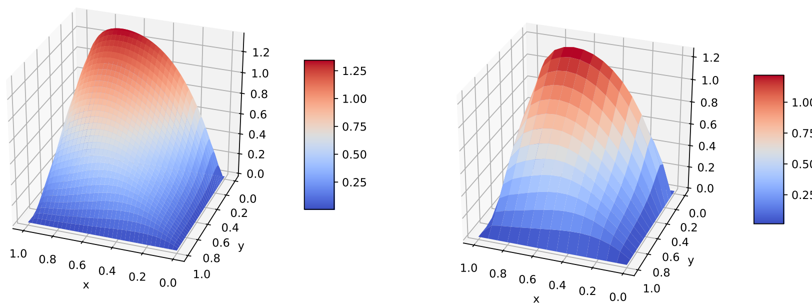
The edge at $y = 0$ has a very sharp front and this edge in particular also seems to have a stability issue. To possibly solve this problem, Neumann conditions, $\partial_n u = 0$ are tested on this edge as in (10). The results can be seen in Figure 8. This gives a smooth solution for $h = \frac{1}{35}$, but the solution breaks down for larger h such as $h = \frac{1}{15}$.



(a) Stepsize $h = 1/35$

(b) Stepsize $h = 1/15$

Figure 8: Numerical solution to problem (18), with Neumann conditions on one side and Diriclet conditions on the rest.



(a) Stepsize $h = 1/35$

(b) Stepsize $h = 1/15$

Figure 9: Numerical solution to problem (18), with a modified scheme.

As discussed in the theory section, a modified scheme can be made as in (11). Implementing this gives the result shown in Figure 9. With this implementation, the result is qualitatively correct for any choice of h.

The result of solving the nonlinear problem (13) is shown in Figure 10. Here, the stepsize is $h = \frac{1}{70}$ and the tolerance is 10^{-6} for the Newton iterations. Increasing λ makes the deflection bigger. Equally, if the sign of λ is changed, it is deflected in the other direction. For $\lambda > 2,5$ the solution breaks down.

4 Discussion

Solving the problem given by equation (16), the numerical order is approximately 2. This verifies the theoretical results found in (7). Furthermore, Figure 5 shows that the theoretical error bound holds for all chosen values of M.

When solving the problem with curved boundary given in (17), the second-order convergence is lost, which is consistent with the predictions in the theory section. Moreover, it makes sense that the error is largest near the curved boundary, where the deviation from the higher-order scheme is largest.

When Ω, μ and the velocity field are as given in (18), it is known from the theoretical error analysis that convergence is not guaranteed for $h \geq \frac{2 \cdot \mu}{1} = 0.02$. The numerical results are consistent with this in that the solution is stable when this restriction is satisfied. When it is not satisfied, we observe that the solution does

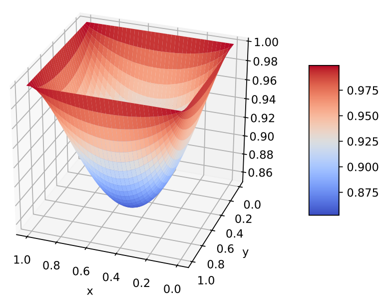


Figure 10: Numerical solution to problem (13) with stepsize $h = 1/70$.

actually break down.

By using Neumann conditions the solution seems to be stable for bigger stepsizes than before, but there are still stability problems if h is too big. This problem is even easier to detect if one chooses a smaller μ which in turn gives a stricter restriction on h.

The modified scheme of lower order should in theory converge for all stepsizes. This is verified by the numerical results.

The solution to the nonlinear system given by equation (13) makes sense from a physical point of view. Increasing λ, equivalent to increasing the electrical potential working on the device, makes the deflection bigger, i.e. the membrane is stretched more downwards. Equally, if the sign of λ is changed, the membrane is deflected the other direction, away from the lower plate. The scheme breaking down with a large λ makes sense since this would give $u \to 0$.

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