University of California Berkeley
MATH228B: Numerical Solution of Differential Equations – Spring 2020

Project 1

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1 Problem 1

The objective is to solve the Poisson equation on a non-rectangular domain Ω,

$$\begin{aligned} -\Delta u &= 1 && \text{In } \Omega \\ \nabla u \cdot e_y &= 0 && \text{On P4-P3} \\ -\nabla u \cdot e_x &= 0 && \text{On P1-P4} \\ u &= 0 && \text{On P1-P2 and P2-P3} \end{aligned} \tag{1}$$

Refer to figure 1 for a description of the boundary labels appearing in eq. 1.

1.1 Transformation from reference domain to spatial domain

We consider a linear map T that transforms the domain $\hat{\Omega} = [-1, 1] \times [-1, 1]$ into the domain Ω. The domain Ω is fully specified by providing the coordinates of the four corners $\{P_1, P_2, P_3, P_4\}$. Refer to figure 1 for an illustration.

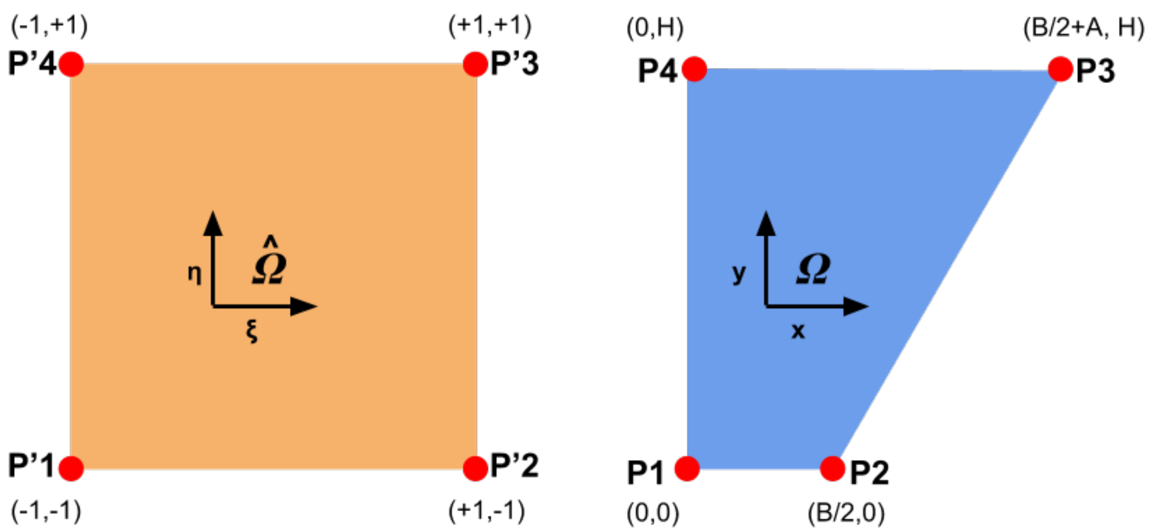


Figure 1: Illustration of the reference domain $\hat{\Omega}$ and the transformed domain Ω.

We will use cartesian coordinates (ξ, η) in the reference domain $\hat{\Omega}$ and cartesian coordinates x, y in the transformed domain Ω. The linear map T is obtained by defining linear shape functions on the reference points $\{P_1', P_2', P_3', P_4'\}$. We refer to these functions as $\{N^1(\xi,\eta), N^2(\xi,\eta), N^3(\xi,\eta), N^4(\xi,\eta)\}$ respectively. They are defined as follows:

$$
\begin{aligned}
N^1(\xi,\eta) &= \frac{(\xi-1)(\eta-1)}{4} \\
N^2(\xi,\eta) &= -\frac{(\xi+1)(\eta-1)}{4} \\
N^3(\xi,\eta) &= \frac{(\xi+1)(\eta+1)}{4} \\
N^4(\xi,\eta) &= -\frac{(\xi-1)(\eta+1)}{4}
\end{aligned} \tag{2}
$$

A point (ξ,η) in the reference domain is interpolated into a point $(x(\xi,\eta), y(\xi,\eta))$ as follows:

$$
\begin{bmatrix} x(\xi,\eta) \\ y(\xi,\eta) \end{bmatrix} = \sum_{I=1}^{4} P_I N^I(\xi,\eta) \tag{3}
$$

Where the $P_I \in \mathbb{R}^2$ are point vectors representing the coordinates of the corresponding corner points in x, y space.

It is then straightforward to compute the Jacobian and Hessian of this mapping from the derivatives of the shape functions. For example:

$$
\begin{aligned}
\frac{\partial x}{\partial \xi} &= \sum_{I=1}^{4} P_{Ix} \frac{\partial N^I}{\partial \xi} \\
\frac{\partial^2 x}{\partial \xi \partial \eta} &= \sum_{I=1}^{4} P_{Ix} \frac{\partial^2 N^I}{\partial \xi \partial \eta}
\end{aligned}
$$

the other terms of the Jacobian and Hessian may be computed in a similar fashion. Note that because the mapping is linear in ξ and η, the second order derivatives $\partial^2/\partial\xi^2$ and $\partial^2/\partial\eta^2$ are identically zero. The cross terms $\partial^2/(\partial\xi\partial\eta)$ are however non-zero – they are in fact constants equal to 1/4.

1.2 Finite difference scheme for the interior

Our starting point for obtaining a finite difference scheme for the interior of the domain is from Lecture Note 2 which provides a transformation of the Poisson Equation from a non-rectangular domain into a rectangular domain. The equation,

$$
-(u_{xx} + u_{yy}) = f
$$

transforms to,

$$-\frac{1}{J^2}\left(au_{\xi\xi} - 2bu_{\xi\eta} + cu_{\eta\eta} + du_\xi + eu_\eta\right) = f \tag{4}$$

where,

$$\begin{aligned}
&J = x_\xi y_\eta - x_\eta y_\xi \qquad a = x_\eta^2 + y_\eta^2 \\
&b = x_\xi x_\eta + y_\xi y_\eta \qquad c = x_\xi^2 + y_\xi^2 \\
&d = \frac{x_\eta \beta - y_\eta \alpha}{J} \qquad e = \frac{y_\xi \alpha - x_\xi \beta}{J} \\
&\alpha = ax_{\xi\xi} - 2bx_{\xi\eta} + cx_{\eta\eta} \qquad \beta = ay_{\xi\xi} - 2by_{\xi\eta} + cy_{\eta\eta}
\end{aligned} \tag{5}$$

We now use second order accurate finite difference schemes for the derivatives appearing in eq. 4 as follows:

$$\begin{aligned}
u_{\xi\xi} &\approx \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} \\
u_{\xi\eta} &\approx \frac{U_{i+1,j+1} - U_{i+1,j-1} - U_{i-1,j+1} + U_{i-1,j-1}}{4h^2} \\
u_{\eta\eta} &\approx \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} \\
u_\xi &\approx \frac{U_{i,j+1} - U_{i,j-1}}{2h} \\
u_\eta &\approx \frac{U_{i+1,j} - U_{i-1,j}}{2h}
\end{aligned} \tag{6}$$

where $U_{i,j}$ refers to the discrete solution value at a grid point in row i and column j, i.e.:

$$u(\xi_j, \eta_i) \approx U_{i,j}$$

1.3 Finite difference schemes for Neumann boundary conditions

In order to apply the Neumann boundary conditions appearing in eq. 1, we need to transform the normals (e_y for the top boundary and $-e_x$ for the left boundary) into the reference coordinate system. A vector n in the domain Ω can be transformed into a vector N in the reference domain $\hat{\Omega}$ as follows,

$$N = \frac{1}{J}\begin{bmatrix} y_\eta n_x & -x_\eta n_y \\ -y_\xi n_x & x_\xi n_y \end{bmatrix} \tag{7}$$

Where we use $n = e_y$ for the top boundary and $n = -e_x$ for the left boundary.

The boundary condition can now be applied in the reference domain $\hat{\Omega}$ by setting,

$$\frac{1}{J}(u_\xi N_\xi + u_\eta N_\eta) = 0 \tag{8}$$

The derivatives appearing in eq. 8 are approximated by centered differences along the direction of the boundary and by second order one-sided finite differences perpendicular to the boundary.

For the left boundary, we require a one-sided forward finite difference scheme along ξ and centered difference along η:

$$\begin{aligned} u_\xi &\approx \frac{-3U_{i,j} + 2U_{i,j+1} - U_{i,j+2}}{2h} \\ u_\eta &\approx \frac{U_{i+1,j} - U_{i-1,j}}{2h} \end{aligned} \tag{9}$$

For the top boundary, we require a one-sided backward finite difference scheme along η and centered difference along ξ:

$$\begin{aligned} u_\xi &\approx \frac{U_{i,j+1} - U_{i,j-1}}{2h} \\ u_\eta &\approx \frac{3U_{i,j} - 2U_{i-1,j} + U_{i-2,j}}{2h} \end{aligned} \tag{10}$$

The top corner at point P4 requires special treatment: we apply a one sided scheme in both ξ and η.

1.4 Dirichlet boundary conditions

Dirichlet boundary conditions are applied directly for all nodes that lie on the boundaries P1-P2 and P3-P4 by setting,

$$U_{i,j} = 0$$

1.5 Integrating the numerical flow rate $\hat{Q}$ in the reference domain

The discretization scheme described so far is second order accurate. In order for us to observe this second order accuracy in the integral of the flow rate, we need to use (at least) a second order accurate numerical integration scheme. The simplest approach is to use Simpson's Rule (i.e. the Trapezoidal Rule) in 2D on a uniform grid:

$$\int_{\hat{\Omega}} \hat{Q} \approx \sum_{i,j=1}^{n} w_{i,j} U_{i,j} \tag{11}$$

where,

$$w_{i,j} = \begin{cases} \frac{1}{4} & \text{i,j is a corner vertex} \\ \frac{1}{2} & \text{i,j is on the boundary but not a corner} \\ 1 & \text{i,j in the interior} \end{cases} \tag{12}$$

1.6 Numerical results

1.6.1 Test Problem: Contours and integral flow value

We first produce a contour plot of the numerical results for the benchmark case. The model parameters are:

$$L = 3.0 \qquad B = 0.5 \qquad H = 1.0 \qquad n = 20$$

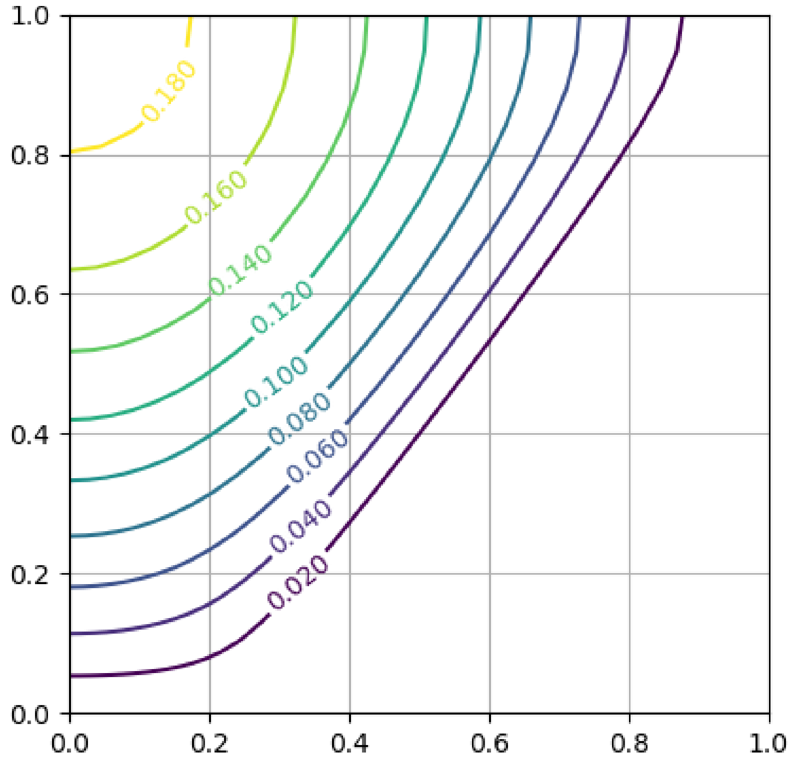


Figure 2: Reference solution with model parameters $L = 3.0$, $B = 0.5$, $H = 1.0$, $n = 20$

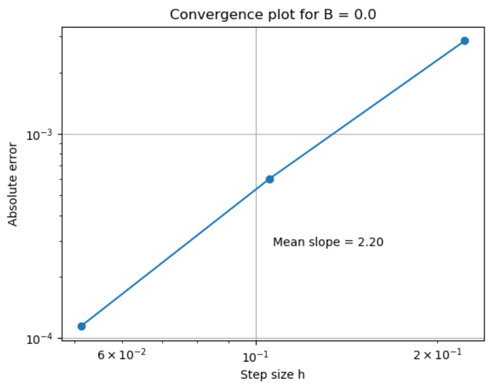
We observe that the Dirichlet condition is met on the bottom and right boundaries, and the normal derivative of the solution respects the Neumann condition at least in the "eye-ball norm".

The corresponding integral of the flow rate in the reference domain is $\hat{Q} = 0.3211$.

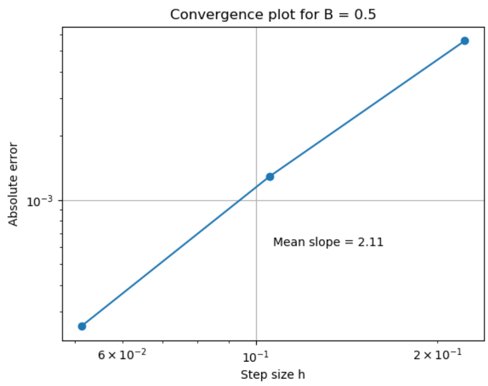
1.6.2 Convergence plots

We now study convergence of the numerical solution under uniform grid refinement in the reference domain. We use the integral of $\hat{Q}$ at a refinement level of $n = 80$ as the "true" solution, and measure convergence against this value for $n = 10, 20, 40$.

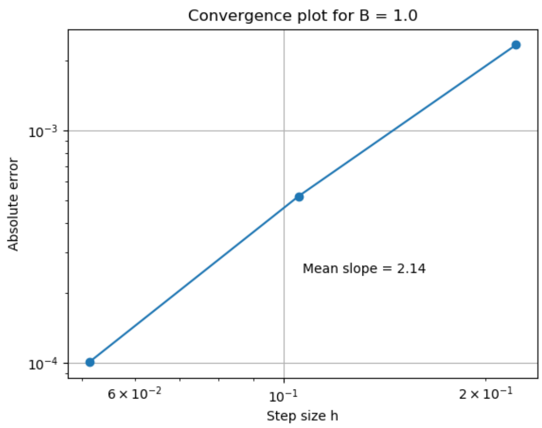
Fig. 3 shows the convergence plots for different values of the parameter B. We observe that the mean slope, which represents the order of convergence, is ≈ 2 which is expected for a globally second order accurate method.



(a) Convergence plot for $B = 0.0$



(b) Convergence plot for $B = 0.5$



(c) Convergence plot for $B = 0.0$

Figure 3: Convergence plots for various values of the geometric parameter B. Observe that the mean rate of convergence is ≈ 2 which is expected for a second order accurate method.

The contour plot for $n = 40$ is produced below:

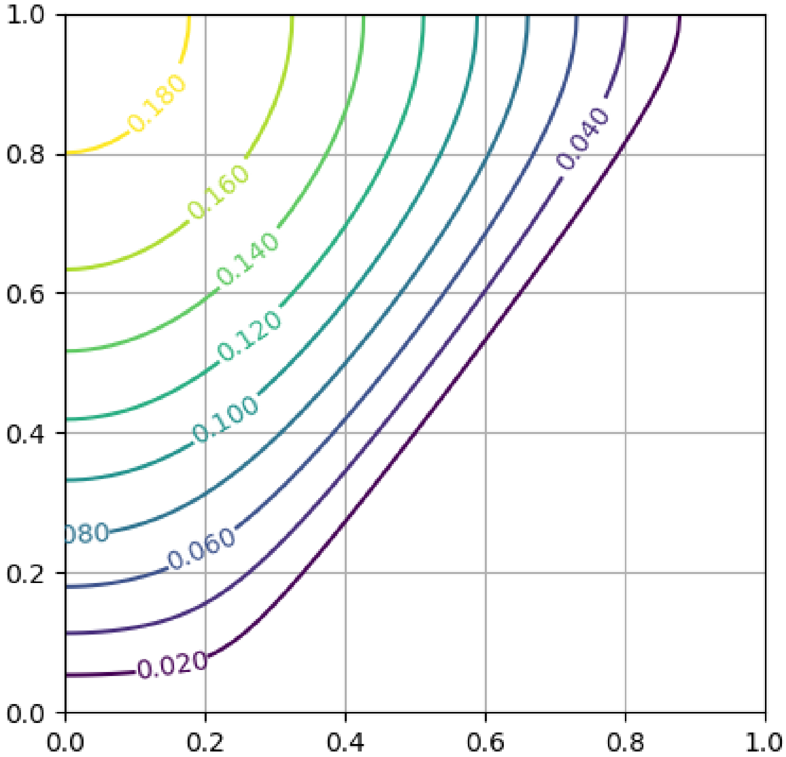


Figure 4: Reference solution with model parameters $L = 3.0$, $B = 0.5$, $H = 1.0$, $n = 40$

2 Problem 2

The given differential equation is:

$$u_t = \kappa u_{xx} - \gamma u \tag{13}$$

We are analyzing the numerical scheme:

$$U_j^{n+1} = U_j^n + \frac{k}{2h^2}\kappa\left[U_{j-1}^n - 2U_j^n + U_{j+1}^n + U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}\right] - k\gamma\left[(1-\theta)U_j^n + \theta U_j^{n+1}\right] \tag{14}$$

We first define the following operators:

$$\mathcal{D}_x^2 u(x,t) := \frac{1}{h^2}\left[u(x-h,t) - 2u(x,t) + u(x+h,t)\right] \tag{15}$$

$$\mathcal{D}_t^+ := \frac{1}{k}\left[u(x,t+k) - u(x,t)\right] \tag{16}$$

Then, inserting the true solution $u(x,t)$ into the finite difference scheme eq. 14, we can write the local truncation error as:

$$\tau(x,t) = \mathcal{D}_t^+ u(x,t) - \frac{\kappa}{2}\left[\mathcal{D}_x^2 u(x,t) + \mathcal{D}_x^2 u(x,t+k)\right] + \gamma\left[(1-\theta)u(x,t) + \theta u(x,t+k)\right] \tag{17}$$

We now perform Taylor expansions of the expressions in eq. 15 and 16. First we expand the space derivative $\mathcal{D}_x^2 u(x,t)$:

$$\begin{aligned}\mathcal{D}_x^2 u(x,t) = \frac{1}{h^2}\Bigg(& u(x,t) - hu_x(x,t) + \frac{h^2}{2!}u_{xx}(x,t) - \frac{h^3}{3!}u_{xxx}(x,t) \\ & -2u(x,t) + u(x,t) + hu_x(x,t) + \frac{h^2}{2!}u_{xx}(x,t) + \frac{h^3}{3!}u_{xxx}(x,t) + \mathcal{O}(h^4)\Bigg) \\ \mathcal{D}_x^2 u(x,t) = {}& u_{xx}(x,t) + \mathcal{O}(h^2)\end{aligned} \tag{18}$$

Similarly, we expand $\mathcal{D}_x^2 u(x,t+k)$ to get:

$$\begin{aligned}\mathcal{D}_x^2 u(x,t+k) &= u_{xx}(x,t+k) + \mathcal{O}(h^2) \\ &= u_{xx}(x,t) + ku_{xxt}(x,t) + \frac{k^2}{2!}u_{xxtt}(x,t) + \mathcal{O}(h^2+k^3)\end{aligned} \tag{19}$$

Finally, we Taylor expand the reaction term as:

$$\begin{aligned}(1-\theta)u(x,t) + \theta u(x,t+k) &= (1-\theta)u(x,t) + \theta\left(u(x,t) + ku_t(x,t) + \frac{k^2}{2!}u_{tt}(x,t) + \mathcal{O}(k^3)\right) \\ &= u(x,t) + \theta k u_t(x,t) + \frac{\theta k^2}{2!}u_{tt}(x,t) + \mathcal{O}(k^3)\end{aligned} \tag{20}$$

We now combine equations 18, 19, and 20 and insert it into the equation for the local truncation error eq. 17 to get:

$$\begin{aligned}\tau(x,t) = & u_t(x,t) + \frac{k}{2}u_{tt}(x,t) + \mathcal{O}(k^2) \\ & -\frac{\kappa}{2}\left(2u_{xx}(x,t) + ku_{xxt}(x,t) + \frac{k^2}{2!}u_{xxtt}(x,t) + \mathcal{O}(h^2+k^3)\right) \\ & +\gamma\left(u(x,t) + \theta k u_t(x,t) + \frac{\theta k^2}{2!}u_{tt}(x,t) + \mathcal{O}(k^3)\right)\end{aligned}$$

We now use the differential equation eq. 13, and also observe:

$$\begin{aligned} & u_t = \kappa u_{xx} - \gamma u \\ \implies & u_{tt} = \kappa u_{xxt} - \gamma u_t\end{aligned} \tag{21}$$

Using the above two expressions, we have the local truncation error as:

$$\tau(x,t) = \frac{k}{2}\left(u_{tt}(x,t) - \kappa u_{xxt}(x,t) + 2\gamma\theta u_t(x,t)\right) + \mathcal{O}(h^2 + k^2) \tag{22}$$

Now note that if $\theta = 1/2$, then the term in parentheses in eq. 22 vanishes due to eq. 21. For any other value of θ, the leading order in time is $\mathcal{O}(k)$. Thus we have,

$$\tau(x,t) = \begin{cases} \mathcal{O}(k + h^2) & \theta \neq \frac{1}{2} \\ \mathcal{O}(k^2 + h^2) & \theta = \frac{1}{2} \end{cases} \tag{23}$$