Homework 1: Heat Equation

DN2255
Kevin Mead

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1 Heat Equation

$$q_t = \nabla \cdot (\nabla q) + S$$
$$q(x, y, 0) = 0$$
$$\mathbf{n} \cdot \nabla q = 0$$

$$S(x, y) = exp\left(-\frac{(x - 1/2)^2 + (y - 1/2)^2}{w^2}\right) \tag{1}$$

1.1 Analytical preamble

1. Flux vector from (1), $\vec{F} = -\nabla q$
2. Determine $Q(t) = \int_0^1 \int_0^1 q(x, y, t)dxdy$

2 Discretization and implementation

Let Q_{ij} denote the cell average of q over cell (i,j) so,

$$Q_{ij}(t) = \frac{1}{\Delta x \Delta y} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} q(x_i, y_j, t)dxdy$$

and defining S_{ij} as the cell average of S over cell (i,j),

$$S_{ij}(t) = \frac{1}{\Delta x \Delta y} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} S(x_i, y_j, t)dxdy$$

where $\Delta x = x_{i+1/2} - x_{i-1/2}$ and $\Delta y = y_{j+1/2} - y_{j-1/2}$

1. Derive a finite volume method for the spatial part of (1) by integrating and forming

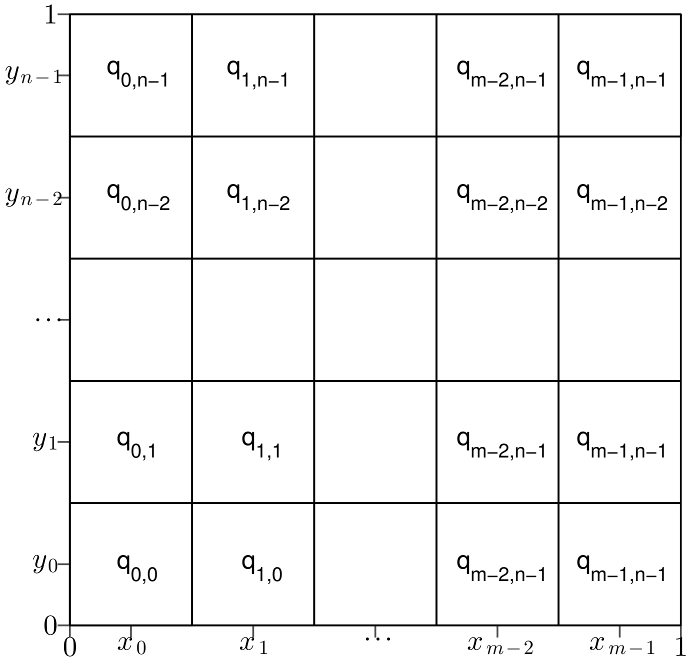


Figure 1: Finite volume grid

cell averages.

$$
\begin{aligned}
q_t &= \nabla \cdot (\nabla q) + S \\
\iint\limits_{\Delta x\, \Delta y} q_t &= \iint\limits_{\Delta x\, \Delta y} \nabla^2 q + \iint\limits_{\Delta x\, \Delta y} S \\
\frac{d}{dt} \iint\limits_{\Delta x\, \Delta y} q &= \iint\limits_{\Delta x\, \Delta y} \left(\frac{d^2 q}{dx^2} + \frac{d^2 q}{dy^2} \right) + \iint\limits_{\Delta x\, \Delta y} S
\end{aligned}
$$

and now dividing everything by the common cell area $\Delta x \Delta y$, we can use (2) and (2) to get

$$
\frac{d}{dt} Q_{ij}(t) = \frac{1}{\Delta x \Delta y} \iint\limits_{\Delta x\, \Delta y} \left(\frac{d^2 q}{dx^2} + \frac{d^2 q}{dy^2} \right) + S_{ij}(t)
$$

I will Taylor expansions to define the Laplacian terms. The Taylor expansions of $q(x_i + \Delta x)$ and $q(x_i - \Delta x)$, taking the derivative with respect to x are

$$
q(x_i + \Delta x) = q(x_i) + \Delta x\, q'(x_i) + \frac{1}{2}(\Delta x)^2 q''(x_i) + \frac{1}{6}(\Delta x)^3 q'''(x_i) + \frac{1}{24}(\Delta x)^4 q^{(4)}(\zeta_+)
$$

$$
q(x_i - \Delta x) = q(x_i) - \Delta x\, q'(x_i) + \frac{1}{2}(\Delta x)^2 q''(x_i) - \frac{1}{6}(\Delta x)^3 q'''(x_i) + \frac{1}{24}(\Delta x)^4 q^{(4)}(\zeta_-)
$$

where the last terms represent a value $\zeta_\pm$ that makes the truncation of the Taylor expansion exactly equal to the infinite series. Since we do not know this value, we must remove it and it will be our truncation error. Adding (1) with (1) and rearranging terms,

$$q''(x_i) = \frac{q(x_i + \Delta x) + q(x_i - \Delta x) - 2q(x_i)}{(\Delta x)^2} - \frac{1}{12}(\Delta x)^2 q^{(4)}(\zeta)$$

and taking off the truncation error,

$$q''(x_i) = \frac{q(x_i + \Delta x) + q(x_i - \Delta x) - 2q(x_i)}{(\Delta x)^2}$$

Doing the same thing for y_j and Δy

$$q''(y_j) = \frac{q(y_j + \Delta y) + q(y_j - \Delta y) - 2q(y_j)}{(\Delta y)^2}$$

Now substituting these equations back into (1), rewriting $q(x_i \pm \Delta x)$ as $q_{i\pm1,j}$, $q(y_j \pm \Delta y)$ as $q_{i,j\pm1}$, and for this problem,$\Delta x = \Delta y$,

$$\frac{d}{dt}Q_{ij}(t) = \frac{1}{\Delta x \Delta y} \iint\limits_{\Delta x\ \Delta y} \left(\frac{q_{i+1,j} + q_{i-1,j} + q_{i,j+1} + q_{i,j-1} - 4q_{i,j}}{\Delta x \Delta y} \right) + S_{ij}(t)$$

Lastly, it can be seen that (1) is the 5-point Laplacian combined with the average of q over a cell which is Q_{ij}, so the equation becomes

$$\begin{aligned}
\frac{d}{dt}Q_{ij}(t) &= \left(\frac{Q_{i+1,j} + Q_{i-1,j} + Q_{i,j+1} + Q_{i,j-1} - 4Q_{i,j}}{\Delta x \Delta y} \right) + S_{ij}(t) \\
\frac{d}{dt}Q_{ij}(t) &= \Delta_5 Q_{ij} + S_{ij}(t)
\end{aligned}$$

At the boundaries, there is no flux, F=0, so $Q_{0,j} = Q_{-1,j}$, $Q_{i,0} = Q_{i,-1}$, $Q_{i,N-1} = Q_{i,N}$, $Q_{M-1,j} = Q_{M,j}$. The stencils for corner boundaries like $i = 0, j = 0$ or $i = m-1, j = n-1$

$$\begin{aligned}
\frac{d}{dt}Q^n_{0,0} &= \left(\frac{Q_{1,0} + Q_{-1,0} + Q_{0,1} + Q_{0,-1} - 4Q_{0,0}}{\Delta x \Delta y} \right) + S_{0,0}(t) \\
&= \left(\frac{Q_{1,0} + Q_{0,1} - 2Q_{0,0}}{\Delta x \Delta y} \right) + S_{0,0}(t) \\
\frac{d}{dt}Q^n_{m-1,j-1} &= \left(\frac{Q_{m-2,j-1} + Q_{m-1,j-2} - 2Q_{m-1,j-1}}{\Delta x \Delta y} \right) + S_{m-1,j-1}(t)
\end{aligned}$$

Equations for boundaries not at a corner look like this:

$$
\begin{cases}
\frac{d}{dt}Q^n_{i,0} = \left(\frac{Q_{i+1,0}+Q_{i-1,0}+Q_{i,1}+-3Q_{i,0}}{\Delta x \Delta y}\right) + S_{i,0}, & \text{if } i \neq 0, m-1 \text{ and } j = 0 \\
\frac{d}{dt}Q^n_{i,0} = \left(\frac{Q_{i+1,0}+Q_{i-1,0}+Q_{i,1}+-3Q_{i,0}}{\Delta x \Delta y}\right) + S_{i,0}, & \text{if } i \neq 0, m-1 \text{ and } j = N-1 \\
\\
\frac{d}{dt}Q^n_{0,j} = \left(\frac{Q_{1,j}+Q_{0,j+1}+Q_{0,j-1}-3Q_{0,j}}{\Delta x \Delta y}\right) + S_{0,j}, & \text{if } i = 0 \text{ and } j \neq 0, N-1 \\
\\
\frac{d}{dt}Q^n_{m-1,j} = \left(\frac{Q_{m-2,j}+Q_{m-1,j+1}+Q_{m-1,j-1}-3Q_{m-1,j}}{\Delta x \Delta y}\right) + S_{m-1,j}, & \text{if } i = m-1 \text{ and } j \neq 0, N-1
\end{cases}
$$

2. Integrate with implicit Euler scheme

$$
\begin{aligned}
\frac{Q^{n+1}_{ij} - Q^n_{ij}}{\tau} &= \Delta_5 Q^{n+1}_{ij} + S^n_{ij}(t) \\
Q^{n+1}_{ij} &= (\mathbf{I} - \tau \mathbf{\Delta_5})^{-1}(Q^n + S^n)
\end{aligned}
$$

The implicit Euler scheme is unconditionally stable where the explicit scheme has restrictions on the time step. To find the stability of $\mathbf{Q}^{n+1} = \mathbf{A}\mathbf{Q}^n$, we find the eigenvalues of $\mathbf{A}v_k = \lambda_k v_k$. The temperature at a later time can be written in terms of the initial temperature by multiplying the matrix $\mathbf{A}$ by itself n times, $\mathbf{Q}^{n+1} = \mathbf{A}^n\mathbf{Q}^1$. If any eigenvalue of $\mathbf{A}$ satisfies $|\lambda_k| > 1$, then as $n \to \infty$, $Q \to \infty$.[1] The explicit scheme has a value where the eigenvalue could become greater than one. But the implicit scheme takes the inverse of a matrix before the eigenvalues are calculated, thus making the maximum absolute value of an eigenvalue never greater than zero.

3. The laplacian written as the second derivative in 1D for each dimension is convenient because this allows us to easily define the boundary conditions similar to like we would for a purely 1D system.

   i. The fully discrete problem in matrix form

$$
Q^{n+1}_{ij}(t) = (\mathbf{I} - \tau(\mathbf{T_x} + \mathbf{T_y}))^{-1}(Q^n + S^n)
$$

   where $\mathbf{T_x} = \frac{1}{\Delta x^2}(\delta_{i-1} + \delta_{i+1} - 2\delta_i)$ and $\mathbf{T_y} = \frac{1}{\Delta y^2}(\delta_{j-1} + \delta_{j+1} - 2\delta_j)$.
   Near an x or y boundary, one term from that respective derivative will cancel with the $2\delta_i, j$ term. For example, when $i = 0$, $\mathbf{T_x}$ will become $\frac{1}{\Delta x^2}(\delta_{i+1} - \delta_i)$ because the δ_{i-1} term will cancel with a δ_i term because of boundary conditions.

4. The method was implemented using the operator matrix $\mathbf{A}$[2] and is generated at line 1 in the code. The sparse function was also used on the matrix to save

computational power and time

$$A = \left[\begin{array}{ccc|ccc|ccc} 2 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 & 0 & -1 & 0 & 0 & 0 \\ \hline -1 & 0 & 0 & 3 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 3 & 0 & 0 & -1 \\ \hline 0 & 0 & 0 & -1 & 0 & 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 2 \end{array}\right]$$

3 Numerical results

1. **Solution plots: Show plots of the solution for some time levels before and after t = 1/4, for both source functions S.** Figures 2 and 3 are plots of the solution with a delta function and Gaussian function, Equation (1), as source terms. For both of these plots, space discretization was $m = n = 50$ and time discretization was $dt = 2e - 3$ seconds.

2. **Convergence**

3. **Numerical Conservation**: Demonstrate that the method is numerically conservative by looking at

$$\int q \, \mathrm{d}x\mathrm{d}y = \Delta x \Delta y \sum Q_{ij} \tag{2}$$

   i. **Time-discretization and how your code handles the discontinuity in g(t)**
   My code handles the discontinuity in g(t) by using two loops with the first loop including the source term and going from $t = 0$ to $t = ts \cdot \tau$ where $ts = \mathrm{round}(0.25/\tau)$.

   ii. **Space-discretization; where in the cell does (x,y)=(1/2,1/2) appear? different for odd and even m,n**
   The cell (1/2, 1/2) appears only for odd values of m,n and is at $(m + 1)/2$. For example, if $m = n = 11$, then $(x_6, y_6) = (1/2, 1/2)$.

4 Refinements

Consider

$$q_t = a(y)q_{xx} + b(x)q_{yy} + S$$

instead of the original PDE and choose any coefficients a(y) and b(x) as smooth positive functions.

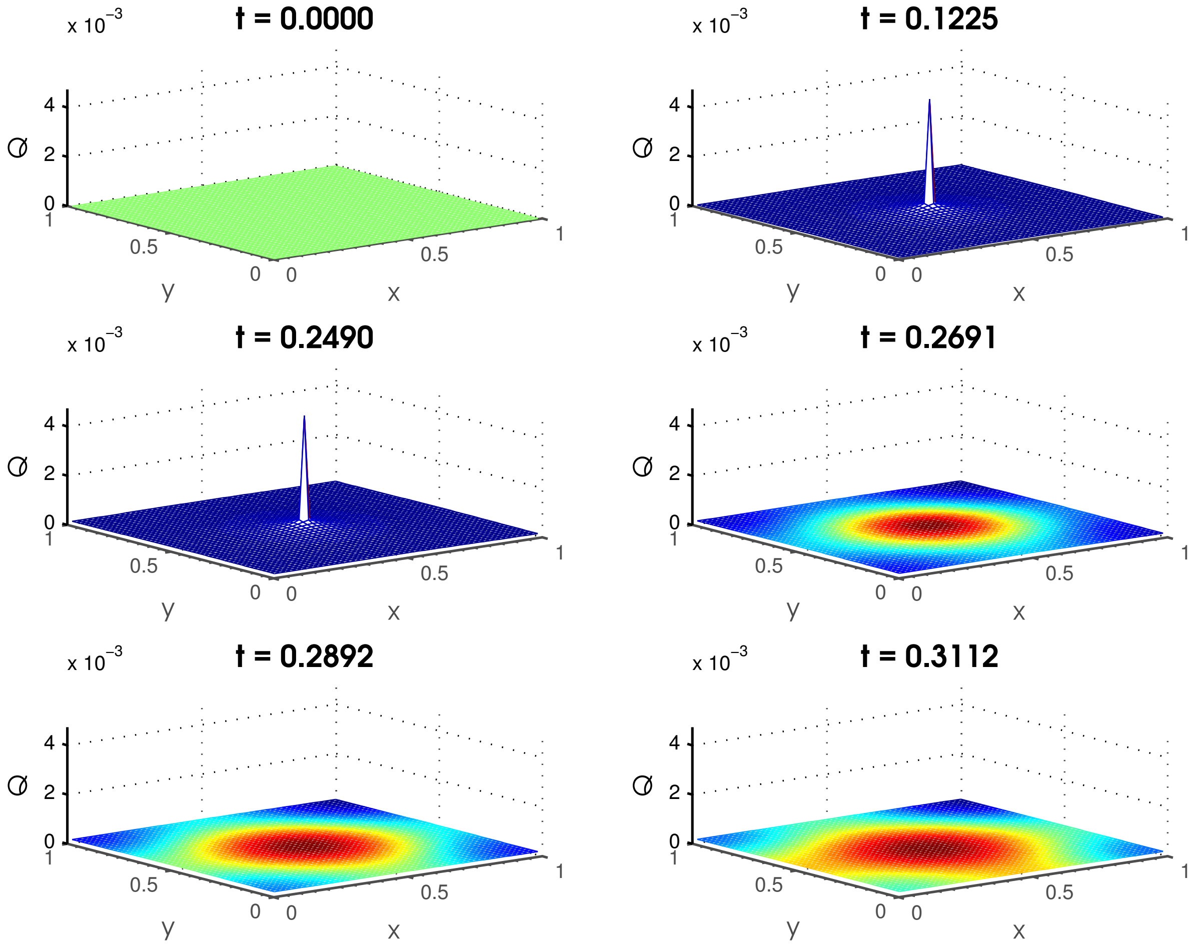


Figure 2: Results with a delta function at the center as a source.

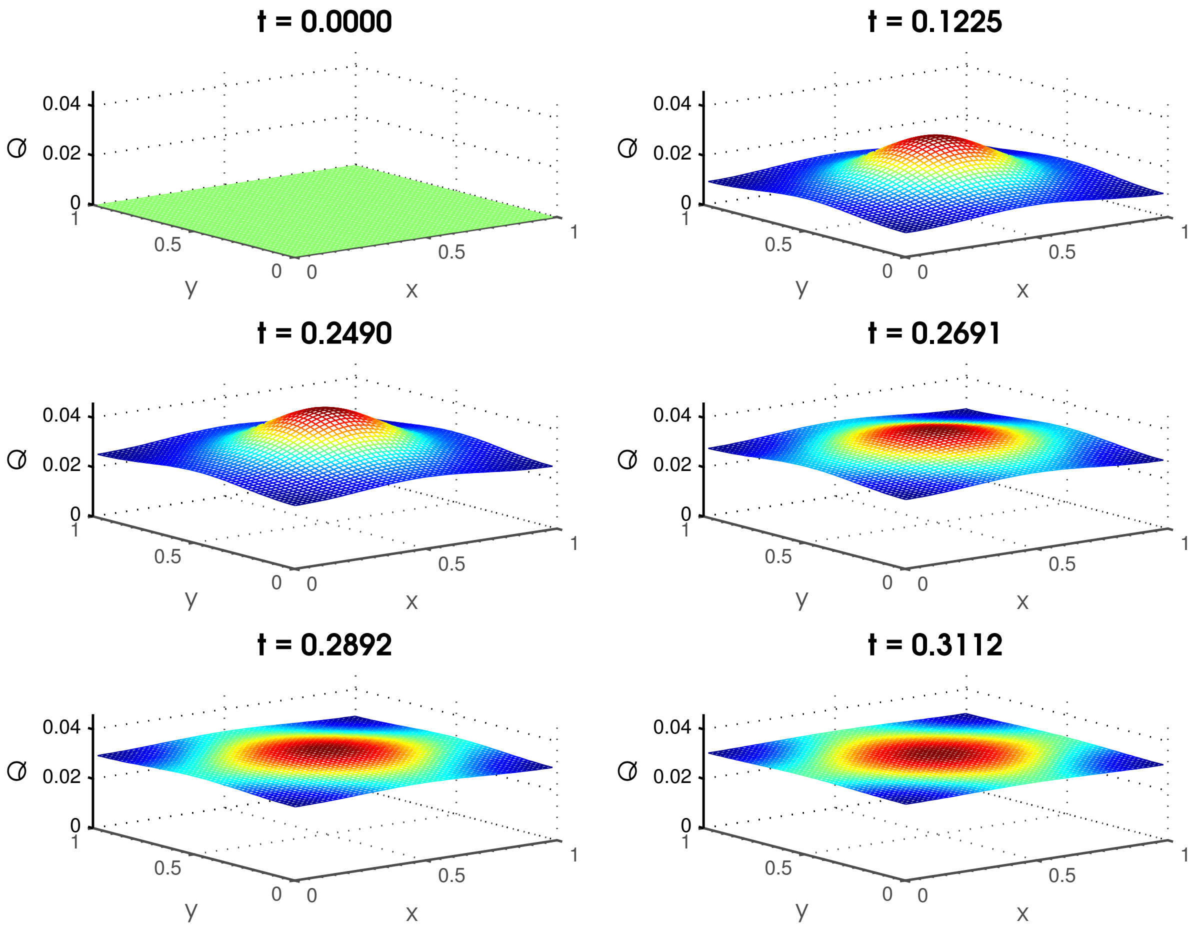
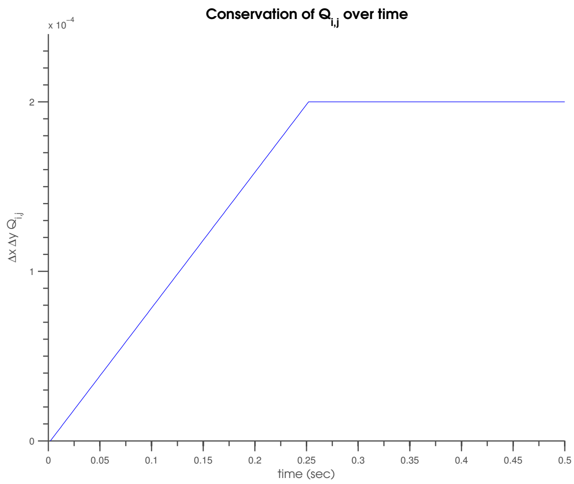
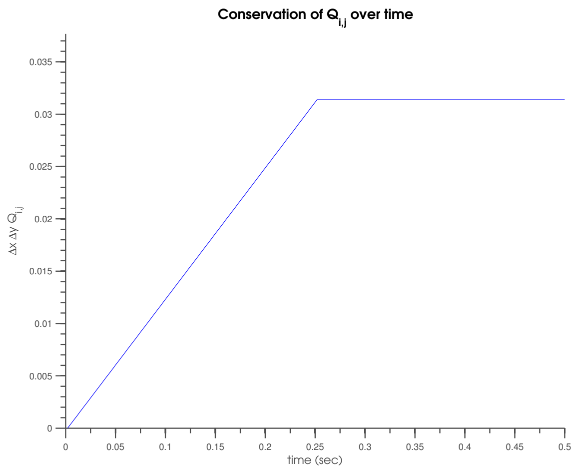


Figure 3: Results with Equation (1) as the source function.



(a) Source - Delta Function at center



(b) Source - Gaussian Distribution at center

Figure 4: Plot of Equation (2) to show conservation of the quantity $Q_{i,j}$ over time. The plot has a source term adding heat to the system, but after $t = 0.25$ s, the source is shut off and the amount of Q does not change over time.

4.1 Variable Coefficients

1. Formulate the fully discrete problem for the variable coefficient case, preferably in the Kronecker notation. Hint: Multiplication from the left with a diagonal matrix scales each row of a matrix. How do you scale the columns?

   The variable coefficients used were

   $$a(y) = y$$
   $$b(x) = x$$

   The matlab code was adjusted at the line defining $T_{N \times N}$,

   ```
   TNxN = kron(TN,diag(h/2:h:L)) + kron(diag(h/2:h:L),TN)
   ```

   whereas before it was

   ```
   TNxN = kron(TN,eye(N)) + kron(eye(N),TN)
   ```

   This adjustment scales linearly according to the position.

2. Implement a solver for the variable coefficient problem. With the Kronecker product construction, this should be fairly simple. Present convergence and conservation results as in Section 3. Figures 5 and 6 shows that with a smooth variable coefficient, energy is still conserved. The variable coefficients that I've chosen lead to changes that are easily seen at x=0 and y=0 because the amount of heat doesn't increase at that point.

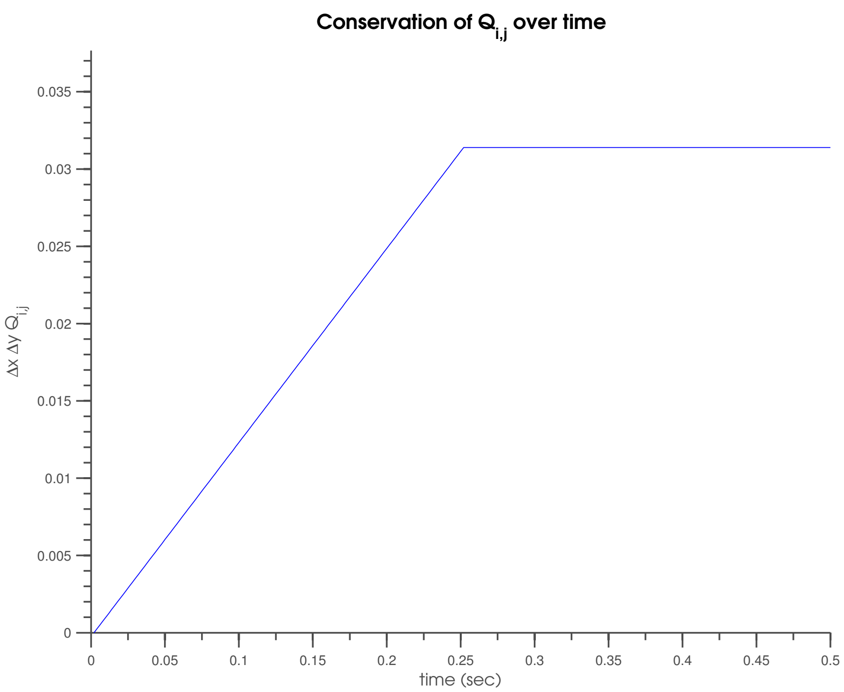


Figure 5: Conservation Results for a smooth source function.

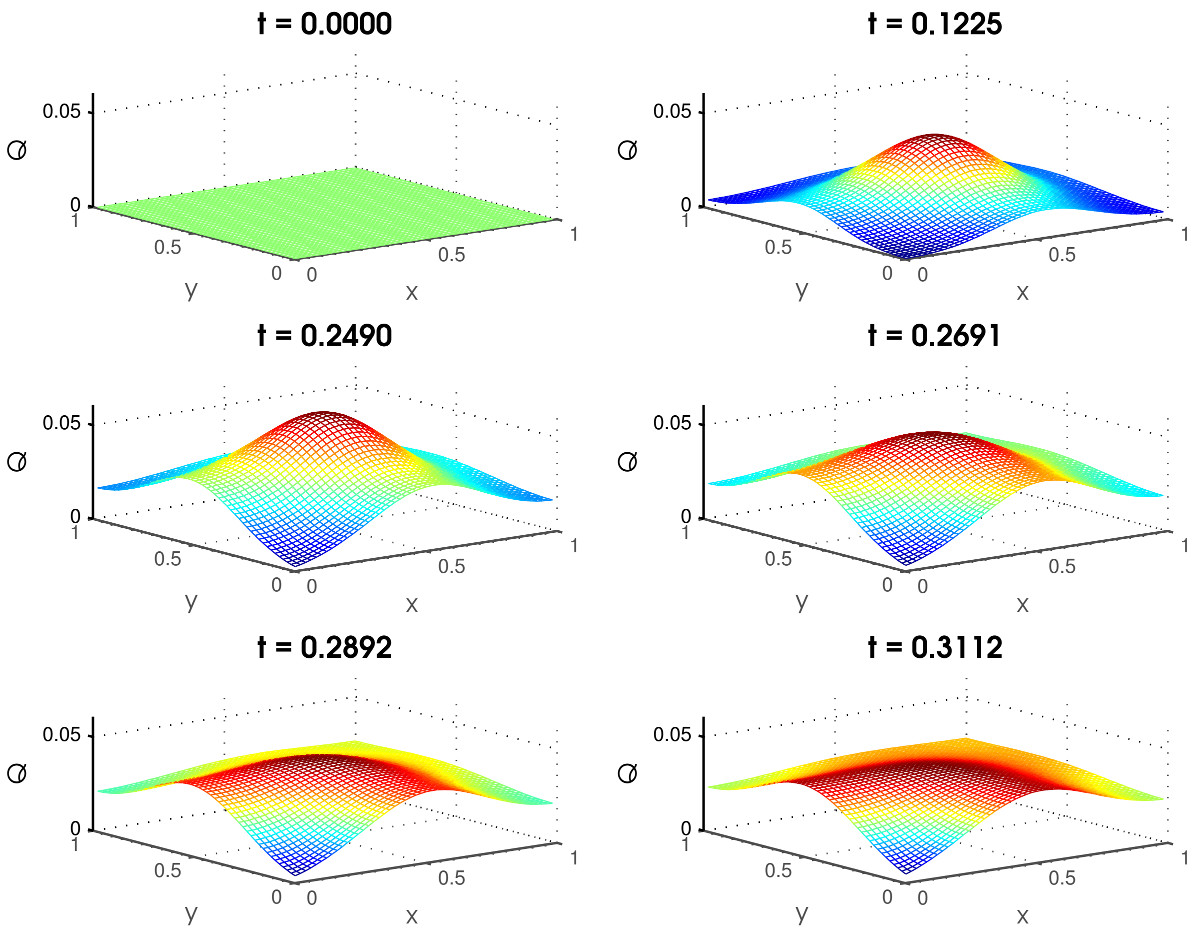


Figure 6: Results of variable coefficients at different times.

4.2 Boundary conditions

Change the boundary conditions to

$$\begin{aligned} q_x(0,y,t) = q_x(1,y,t) &= -1 \\ q(x,0,t) &= \frac{1}{\pi}\sin(\pi x) \\ q(x,1,t) &= \frac{1}{3\pi}\sin(3\pi x) + 1 \end{aligned} \tag{3}$$

You may choose a different set of boundary conditions if you want to, as long as you include at least one non-homogeneous Neuman and Dirichlet condition.

Figures 7 and 8 show the conservation plot and multiple times plot with the new boundary conditions. The code implemented the boundary conditions on $q(x,0,t)$ and $q(x,1,t)$ by setting the values at every time step. The q_x boundary conditions were set by adjusting the matrix in each dimension and setting the boundary conditions. Kronecker delta products were used to create the combination of the x and y matrices.

From the conservation plot, we can see that q was not conserved in this case. The reason is that we did not implement periodic or no flux boundary conditions, and therefore, heat was allowed to escape from the boundaries.

Implement this new boundary condition with the following approach: Construct 1D difference matrices for each dimension and make sure they express the right boundary conditions. Then assemble the 2D difference matrix from the 1D matrices using Kronecker products.

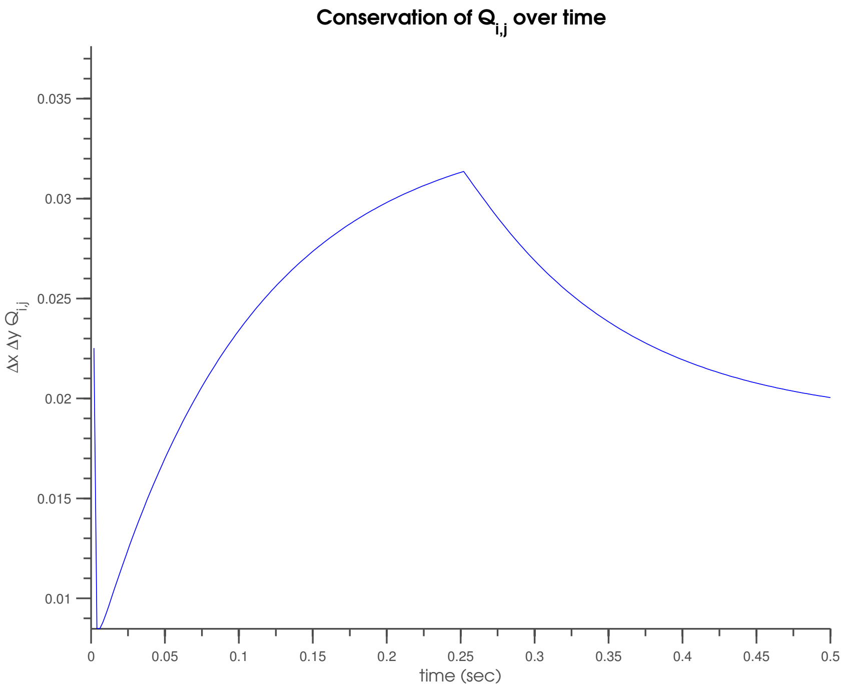


Figure 7: Conservation plot with new boundary conditions (3).

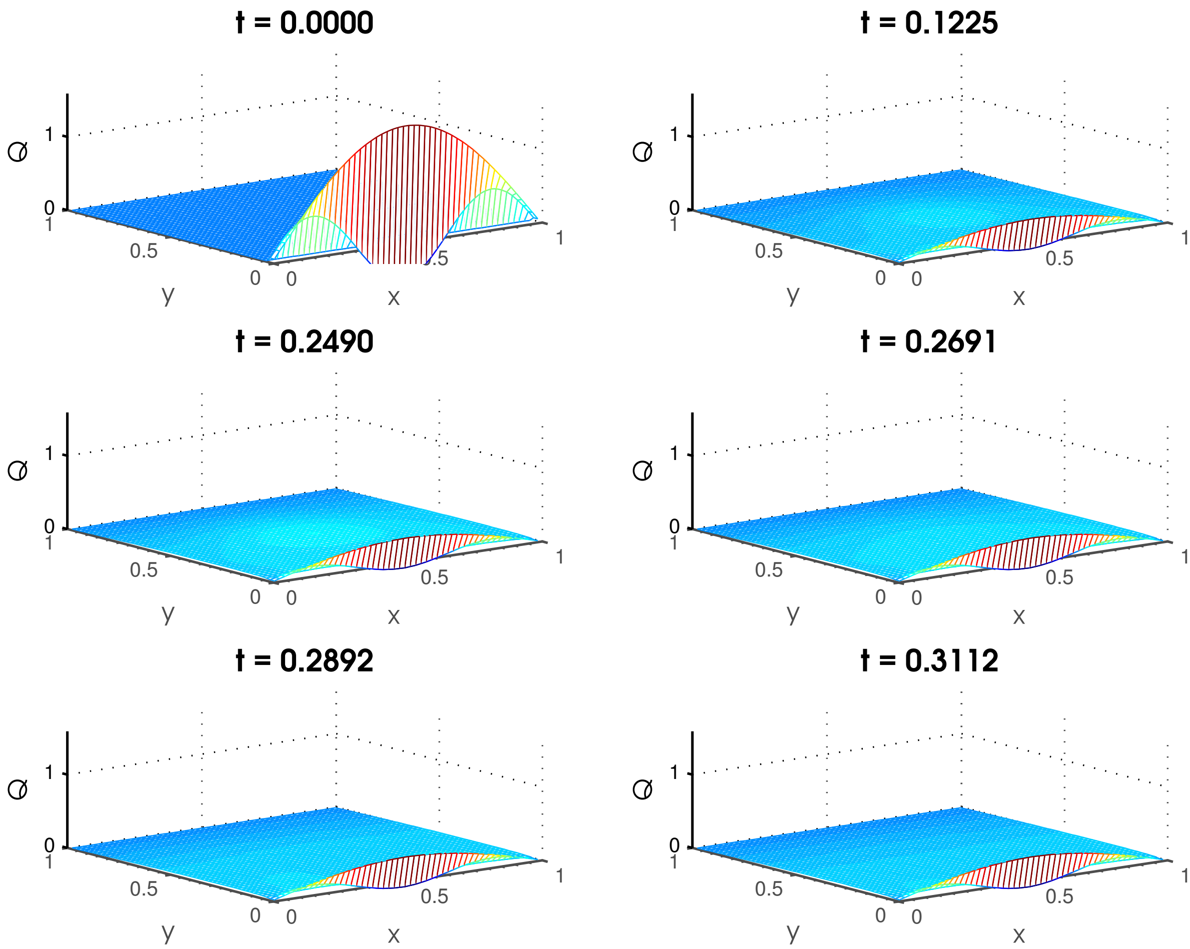


Figure 8: Multiple plots at different times with new boundary conditions (3).

References

[1] A. Garcia, *Numerical methods for physics*. Prentice Hall, 2000. [Online]. Available: http://books.google.ca/books?id=MPVAAQAAIAAJ

[2] J. W. Demmel, *Applied Numerical Linear Algebra*. Philadelphia, PA, USA: Society for Industrial and Applied Mathematics, 1997.