Problem 1

Question 1

Using the Taylor series expansion, show that the central difference method for the second derivative is second-order accurate

Solution:

Using Taylor series (for some small h) we can write next two relations:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(x)}{2!} + h^3 \frac{f'''(x)}{3!} + O(h^4)$$

And

$$f(x-h) = f(x) - hf'(x) + \frac{h^2 f''(x)}{2!} - h^3 \frac{f'''(x)}{3!} + O(h^4)$$

Adding these two relations we get:

$$f(x+h) + f(x-h) = 2f(x) + 2h^2 \frac{f''(x)}{2!} + 2O(h^4)$$

Thus:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

So, we can state for this that this method is second-order accurate

Question 2

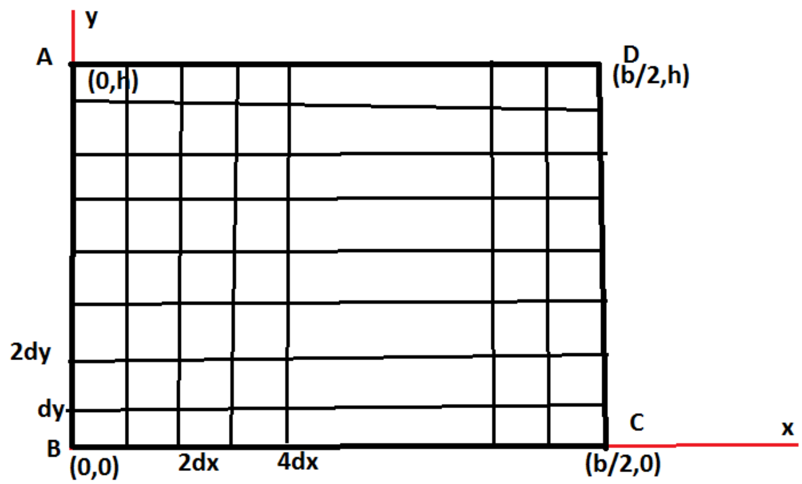
Use a second-order central difference method to derive the finite difference schemes for the discretisation of all derivative terms for equation (6) in the interior of the domain. Use a simpler first-order scheme for the Neumann boundary points. You do not have to derive special schemes for the corner points, use the left boundary scheme at corner A, and u=0 at the other three corners.

Solution:

Equation 6 is:

$$\frac{\partial u^2}{\partial^2 x} + \frac{\partial u^2}{\partial^2 y} = -1$$

Lets show the grid:



So, we have N-1 steps in each (x,y) direction with stepvalues:

$$\Delta x = \frac{b}{2(N-1)}, \quad \Delta y = \frac{h}{N-1},$$

And let I will be number of node in x direction and j – number of node in y direction.

Then, we can write the second-order central difference method for equation (6) as:

$$\frac{u(i+1,j) - 2u(i,j) + u(i-1,j)}{\Delta x^2} + \frac{u(i,j+1) - 2u(i,j) + u(i,j-1)}{\Delta y^2} = -1, \quad i,j = 2 \dots N-1$$

This we give us next 5-point stencil:

$$\begin{pmatrix} 0 & 1/\Delta y^2 & 0 \\ 1/\Delta x^2 & -\dfrac{2}{\Delta x^2} - \dfrac{2}{\Delta y^2} & 1/\Delta x^2 \\ 0 & 1/\Delta y^2 & 0 \end{pmatrix}$$

For AB and Ad we have Neumann boundary, using first order scheme for first derivative (for AB for $\partial u/\partial y$, and for AD for $\partial u/\partial x$) we can write:

$$\frac{u(i,N) - u(i-1,N)}{\Delta x} = 0, \qquad \frac{u(1,j) - u(1,j-1)}{\Delta y} = 0, \quad i,j = 1 \dots N$$

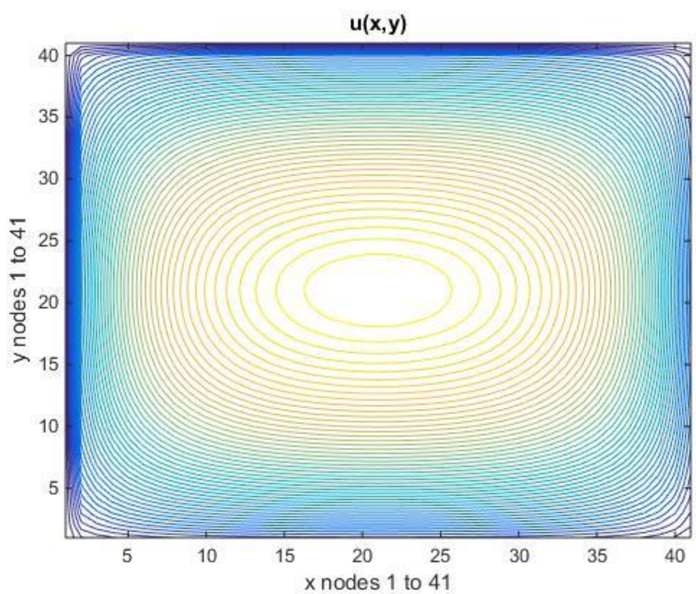
Also, due to conditions to BC and CD:

$$u(i,1) = 0, \qquad u(N,j) = 0, \quad i,j = 1 \dots N$$

And these equations above are our seeking scheme for solving the equation.

Question 3

For this question we write the function (see prob1.m and additional function velocity.m) using our described scheme above with mixed conditions also presented above. As a result we got the next contour plot for resulting u(x,y)



Question 4.

Write a Matlab programme to calculate the flow rate from the final $(x,)$ values resulting from question 3.

Solution:

We done this using provided equations for numerical integration scheme using trapezoidal rule and using next relations:

$$I(y_j) \cong \frac{\Delta x}{2}\left[u(x_1, y_j) + 2\sum_{i=2}^{N-1} u(x_i, y_j) + u(x_N, y_j)\right]$$

$$Q \cong \frac{\Delta y}{2}\left[I(y_1) + 2\sum_{i=2}^{N-1} I(y_i) + I(y_N)\right]$$

The corresponding code is in program prob1.m.

And the output for the FlowRate is:

total flowrate is 0.0178

Question 5

Write a Matlab programme to calculate the convergence rate for the L_2 norm of the solution. Use the grid sizes N=11,21,41,81. Since we don't know the exact solution, use the solution for N=81 as a reference. To calculate the L_2 norm, only use the reference grid points that correspond to the coarsest grid. This will avoid interpolation problems, keeping the complexity of your code at a minimum. Comment on your results.

Solution:

We calculated norm rate using provided algorithm in points which are the same for different size of grid (for N=81 and for others cases N=11,21,41).

To find this we wrote two additional functions (mymesh.m and myerr.m) and used these functions in main program named prob1.m

Here are the results:

L2 norm of error at N=11

er11 = 2.9591e-04

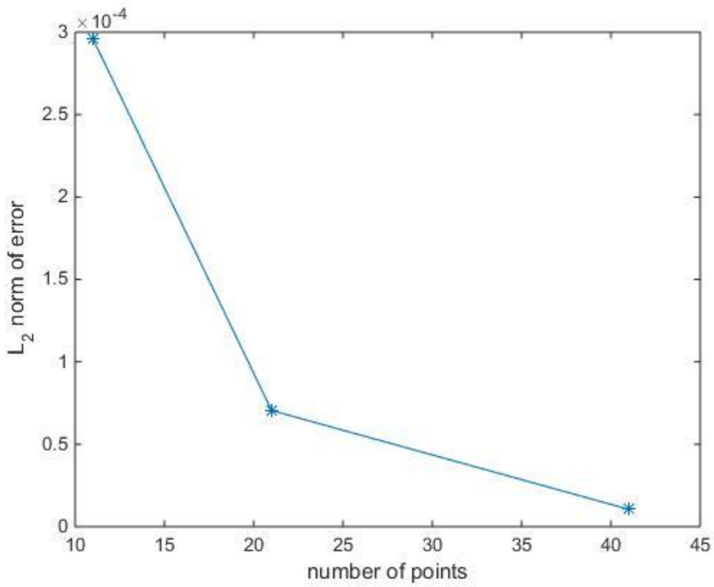
L2 norm of error at N=21

er21 =   7.0513e-05

L2 norm of error at N=41

er41 =   1.0543e-05

And for these values we built the next plot:



Analyzing this graph we can see the dependence – with increasing number of nodes in our grid for finite difference scheme we will get the lower value for L_2 norm of error. This mean – the higher number of nodes - the closer to optimal result we will get, and this least statement are correlate with that we know from the theory.

Problem 2

Question 1

Consider the simpler 1D diffusion equation (not the more complex reaction-diffusion equations set up above):

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$$

where ν - is the viscosity. Determine whether equation is elliptic, parabolic or hyperbolic. Show your reasoning and calculations.

Solution:

The general form for partial derivative equation (PDE) is :

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + F = 0$$

In our case we can write y=t; and then we need to find the relation:

$$B^2 - AC$$

As we see , in our case

$$B = 0, \;\; A = \nu, \;\; C = 0. \quad Then\, B^2 - AC = 0$$

And as

$$B^2 - AC = 0$$

This is **parabolic PDE**

Question 2

Discretise the reaction-diffusion equations (7) in both the interior of the domain and the boundaries. Use a forward-time, central-space (FTCS) scheme for the interior points. Use zero Neumann boundary conditions on all sides of the domain and discretise using a first order special scheme; at the corners, use the zero Neumann boundary condition along x (in other terms: consider the corner as part of either the left or the right boundaries, not the bottom or top ones).

Solution:

We have a system of equations:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1-u)$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F+k)v$$

Let our functions have discretisations as:

$$u(t_l, x_i, y_j) \equiv u(l,i,j) \;\; and \;\; v(t_l, x_i, y_j) \equiv v(l,i,j)$$

For forward time we can write:

$$\frac{\partial u}{\partial t} \cong \frac{u(l+1,i,j) - u(l,i,j)}{\Delta t}, \quad \frac{\partial v}{\partial t} \cong \frac{v(l+1,i,j) - v(l,i,j)}{\Delta t}$$

For central space (using that $\Delta x = \Delta y = \delta$):

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{u(t,i+1,j) - 2u(t,i,j) + u(t,i-1,j)}{\delta^2} + \frac{u(t,i,j+1) - 2u(t,i,j) + u(t,i,j-1)}{\delta^2}$$

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = \frac{v(t,i+1,j) - 2v(t,i,j) + v(t,i-1,j)}{\delta^2} + \frac{v(t,i,j+1) - 2v(t,i,j) + v(t,i,j-1)}{\delta^2}$$

Then, we can write :

$$\frac{u(l+1,i,j) - u(l,i,j)}{\Delta t} = D_u \left(\frac{u(t,i+1,j) - 4u(t,i,j) + u(t,i-1,j) + u(t,i,j+1) + u(t,i,j-1)}{\delta^2} \right) - u(l,i,j)v^2(l,i,j) + F(1 - u(l,i,j)$$

$$\frac{v(l+1,i,j) - v(l,i,j)}{\Delta t} = D_v \left(\frac{v(t,i+1,j) - 4v(t,i,j) + v(t,i-1,j) + v(t,i,j+1) + v(t,i,j-1)}{\delta^2} \right) + u(l,i,j)v^2(l,i,j) - (F+k)v(l,i,j)$$

Question 3

Here we have next values for constants in our problem :

$$N = 192 - grid\ points, \qquad domain\ x_{max} = y_{max} = l = 5\ m, \qquad \Delta x = \Delta y = \delta = l/N$$

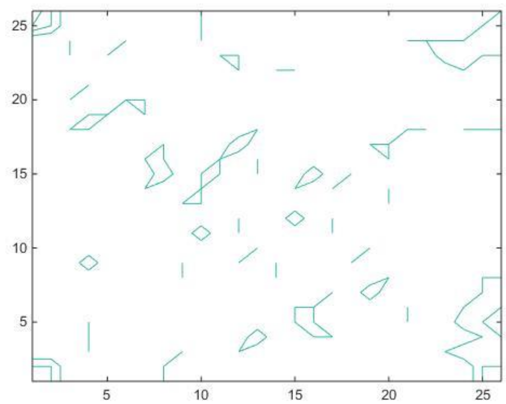
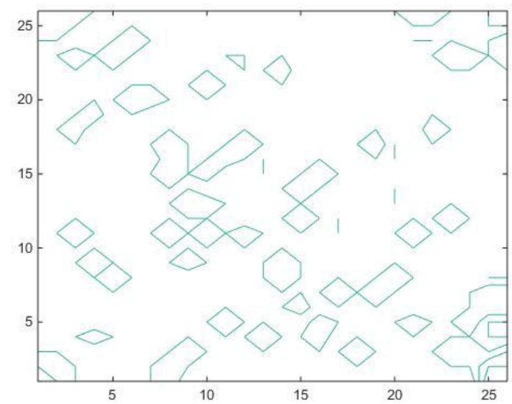
$$D_u = 0.00016, \quad D_v = 0.0008, \qquad F = 0.035, \quad k = 0.065$$

$$t_e = 8000 - (a_{urn} + 1)b_{urn}$$

$$\Delta t = \left(\frac{9}{40}\right)\frac{\delta^2}{\max(D_u, D_v)}$$

Solution:

For this we wrote the program – see prob2.m and got next results:

Final solution for specie u	Final solution for specie v
	

Question 4.

Write a Matlab programme to calculate the evolution in time of the average concentration of the two species over the whole domain:

$$\bar{u}(y) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} u(x_i, y_j, t)$$

$$\bar{v}(y) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} v(x_i, y_j, t)$$

Solution:

We wrote this part (see prob2.m) and got the next graph: