May 30, 2021

1 Quick derivation of finite difference scheme

The finite difference approximation of the two dimensional biharmonic operator $\nabla^4\psi = \psi_{xxxx} + 2\psi_{xxyy} + \psi_{yyyy}$ can be found by using the following standard approximations

$$\psi_{xxxx(i,j)} \approx \frac{\psi_{i,j-2} - 4\psi_{i,j-1} + 6\psi_{i,j} - 4\psi_{i,j+1} + \psi_{i,j+2}}{\Delta x^4} \tag{1.1}$$

$$\psi_{yyyy(i,j)} \approx \frac{\psi_{i-2,j} - 4\psi_{i-1,j} + 6\psi_{i,j} - 4\psi_{i+1,j} + \psi_{i+2,j}}{\Delta y^4} \tag{1.2}$$

$$\psi_{xxyy(i,j)} \approx \frac{\psi_{i-1,j-1} - 2\psi_{i-1,j} + \psi_{i-1,j+1} - 2(\psi_{i,j-1} - 2\psi_{i,j} + \psi_{i,j+1}) + \psi_{i+1,j-1} - 2\psi_{i+1,j} + \psi_{i+1,j+1}}{\Delta x^2 \Delta y^2} \tag{1.3}$$

If we take our $M \times N$ solution grid for ψ which has $(M-2)\times(N-2)$ unknowns and stack each row of the grid of unknowns on top of each other in a column vector $\boldsymbol{\psi}$ we can obtain a finite difference matrix operator on this vector approximating the biharmonic operator as the following $(M-2)\times(M-2)$ block pentadiagonal matrix

$$\nabla^4_{FD} = \begin{pmatrix} \mathsf{R} & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & 0 & \dots & 0 \\ \mathsf{T} & \mathsf{R} & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & \dots & 0 \\ \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R} & \mathsf{T} & \dots & 0 \\ 0 & \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \mathsf{R} \end{pmatrix} \tag{1.4}$$

where I is the $(N-2)\times(N-2)$ identity matrix and

$$\mathsf{R} = \begin{pmatrix} R_d & R_{d1} & R_{d2} & 0 & \dots & 0 \\ R_{d1} & R_d & R_{d1} & R_{d2} & \dots & 0 \\ R_{d2} & R_{d1} & R_d & R_{d1} & \dots & 0 \\ 0 & R_{d2} & R_{d1} & R_d & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & R_d \end{pmatrix} \tag{1.5}$$

is a $(N-2)\times(N-2)$ matrix where

$$R_d = \frac{6}{\Delta x^4} + \frac{8}{\Delta x^2 \Delta y^2} + \frac{6}{\Delta y^4} \tag{1.6}$$

$$R_{d1} = -(\frac{4}{\Delta x^4} + \frac{4}{\Delta y \Delta x^2}) \tag{1.7}$$

$$R_{d2} = \frac{1}{\Delta x^4} \tag{1.8}$$

and

$$\mathsf{T} = \begin{pmatrix} T_d & T_{d1} & 0 & 0 & \dots & 0 \\ T_{d1} & T_d & T_{d1} & 0 & \dots & 0 \\ 0 & T_{d1} & T_d & T_{d1} & \dots & 0 \\ 0 & 0 & T_{d1} & T_d & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & T_d \end{pmatrix} \tag{1.9}$$

is a $(N-2)\times(N-2)$ matrix where

$$T_d = -\left(\frac{4}{\Delta x^2 \Delta y^2} + \frac{4}{\Delta y^4}\right) \tag{1.10}$$

$$T_{d1} = \frac{2}{\Delta x^2 \Delta y^2}. \tag{1.11}$$

The second order no flux boundary condition at the bottom of the domain is implemented by adding the block $\mathsf{I}/\Delta y^4$ to the bottom right block in the finite difference operator. The no flux conditions on the side walls are implemented to second order accuracy by adding to every R block in the finite difference operator the following

$$\mathsf{Q}_1 = \begin{pmatrix} \frac{1}{\Delta x^4} & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{\Delta x^4} \end{pmatrix} \tag{1.12}$$

If we call the top line of points in the solution grid 'end', then the stress boundary condition is approximated by

$$\alpha\frac{\psi_{end+1,j}+\psi_{end-1,j}}{\Delta y^2} = \frac{4(\psi_{end-1,j+1}-2\psi_{end-1,j}+\psi_{end-1,j-1})-(\psi_{end-2,j+1}-2\psi_{end-2,j}+\psi_{end-2,j-1})}{2\Delta y \Delta x^2} \tag{1.13}$$

using a standard one sided difference for ψ_{xxy}, and taking advantage of the fact that $\psi = 0$ on these 'end' gridpoints ($y = 0$). We can use this to solve for a general point on the 'end+1' ghost row of points above the domain. Therefore the vector of points on this ghost row must be given in terms of the 'end-1' and 'end-2' rows respectively as

$$\boldsymbol{\psi}_{end+1} = \left(\frac{2\Delta y}{\alpha \Delta x^2}\mathsf{Q}_2 - \mathsf{I}\right)\boldsymbol{\psi}_{end-1} - \frac{\Delta y}{2\alpha\Delta x^2}\mathsf{Q}_2\boldsymbol{\psi}_{end-2} \tag{1.14}$$

where

$$\mathsf{Q}_2 = \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} \tag{1.15}$$

We simply multiply by a factor of $1/\Delta y^4$ and add this to the top block row of the linear system to implement this boundary condition. We therefore obtain the linear system

$$\alpha \begin{pmatrix} \mathsf{R}+\mathsf{Q}_1-\frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & 0 & \dots & 0 \\ \mathsf{T} & \mathsf{R}+\mathsf{Q}_1 & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & \dots & 0 \\ \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R}+\mathsf{Q}_1 & \mathsf{T} & \dots & 0 \\ 0 & \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R}+\mathsf{Q}_1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \mathsf{R}+\mathsf{Q}_1+\frac{1}{\Delta y^4}\mathsf{I} \end{pmatrix}\boldsymbol{\psi}$$

$$= \begin{pmatrix} -\frac{2}{\Delta x^2\Delta y^3}\mathsf{Q}_2 & \frac{1}{2\Delta x^2 \Delta y^3}\mathsf{Q}_2 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}\boldsymbol{\psi} \tag{1.16}$$

which is the full version of the linear system given in the text as (**??**).

$$\mathsf{B}\boldsymbol{\psi} = \alpha\mathsf{C}\boldsymbol{\psi} \tag{1.17}$$

1.1 Surface diffusion

We can also add surface diffusion into the problem. The only change in the boundary conditions is given by altering the stress condition such that it becomes

$$\alpha\psi_{yy} = -\psi_{xxy} - \bar{D}\psi_{xxyy} \tag{1.18}$$

where $\hat{D}$ is the normal non dimensional diffusion coefficitn divided by $\bar{\Gamma}$. We first need to find the finite difference approximation for ψ_{xxyy} which is a one sided difference for y. We have a central difference approximation

$$\psi_{xx(i,j)} = \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{\Delta x^2} \tag{1.19}$$

and a one sided approximation

$$\psi_{yy(end,j)} = \frac{2\psi_{end,j} - 5\psi_{end-1,j} + 4\psi_{end-2,j} - \psi_{end-3,j}}{\Delta y^2} \tag{1.20}$$

we know that $\psi_{end,j} = 0$, so combining these using this we have

$$\begin{aligned}
\psi_{xxyy} &= \frac{\frac{-5\psi_{end-1,j+1}+4\psi_{end-2,j+1}-\psi_{end-3,j+1}}{\Delta y^2} - 2\frac{-5\psi_{end-1,j}+4\psi_{end-2,j}-\psi_{end-3,j}}{\Delta y^2} + \frac{-5\psi_{end-1,j-1}+4\psi_{end-2,j-1}-\psi_{end-3,j-1}}{\Delta y^2}}{\Delta x^2} \\
&= \frac{(-5\psi_{end-1,j+1} + 4\psi_{end-2,j+1} - \psi_{end-3,j+1}) - 2(-5\psi_{end-1,j} + 4\psi_{end-2,j} - \psi_{end-3,j}) + (-5\psi_{end-1,j-1} + 4\psi_{end-2,j-1} - \psi_{end-3,j-1})}{\Delta x^2 \Delta y^2} \\
&= \frac{-5\psi_{end-1,j+1} + 4\psi_{end-2,j+1} - \psi_{end-3,j+1} + 10\psi_{end-1,j} - 8\psi_{end-2,j} + 2\psi_{end-3,j} - 5\psi_{end-1,j-1} + 4\psi_{end-2,j-1} - \psi_{end-3,j-1}}{\Delta x^2 \Delta y^2}
\end{aligned} \tag{1.21}$$

If we put this into the boundary condition (1.18) along with the standard finite difference approximations for the other derivatives calculated in the previous subsection we get

$$\begin{aligned}
&\alpha\frac{\psi_{end+1,j} + \psi_{end-1,j}}{\Delta y^2} = \frac{4(\psi_{end-1,j+1} - 2\psi_{end-1,j} + \psi_{end-1,j-1}) - (\psi_{end-2,j+1} - 2\psi_{end-2,j} + \psi_{end-2,j-1})}{2\Delta y \Delta x^2} \\
&-\hat{D}\frac{-5\psi_{end-1,j+1} + 4\psi_{end-2,j+1} - \psi_{end-3,j+1} + 10\psi_{end-1,j} - 8\psi_{end-2,j} + 2\psi_{end-3,j} - 5\psi_{end-1,j-1} + 4\psi_{end-2,j-1} - \psi_{end-3,j-1}}{\Delta x^2 \Delta y^2}
\end{aligned} \tag{1.22}$$

which becomes

$$\begin{aligned}
&\psi_{end+1,j} = \frac{2\Delta y}{\alpha\Delta x^2}(\psi_{end-1,j+1} - 2\psi_{end-1,j} + \psi_{end-1,j-1}) - \frac{\Delta y}{2\alpha\Delta x^2}(\psi_{end-2,j+1} - 2\psi_{end-2,j} + \psi_{end-2,j-1}) - \psi_{end-1,j} \\
&-\frac{\hat{D}}{\alpha\Delta x^2}(-5\psi_{end-1,j+1} + 4\psi_{end-2,j+1} - \psi_{end-3,j+1} + 10\psi_{end-1,j} - 8\psi_{end-2,j} + 2\psi_{end-3,j} - 5\psi_{end-1,j-1} + 4\psi_{end-2,j-1} - \psi_{end-3,j-1})
\end{aligned} \tag{1.2}$$

We can write this in matrix form as

$$
\begin{aligned}
\boldsymbol{\psi}_{end+1} = {} & \left(\frac{2\Delta y}{\alpha \Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} - \mathsf{I} \right) \boldsymbol{\psi}_{end-1} - \frac{\Delta y}{2\alpha \Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} \boldsymbol{\psi}_{end-2} \\
& + 5\frac{\hat{D}}{\alpha \Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} \boldsymbol{\psi}_{end-1} - 4\frac{\hat{D}}{\alpha \Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} \boldsymbol{\psi}_{end-2} \\
& + \frac{\hat{D}}{\alpha \Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ 0 & 0 & 1 & -2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -2 \end{pmatrix} \boldsymbol{\psi}_{end-3}
\end{aligned} \tag{1.24}
$$

using the matrix Q_2 as defined in the previous subsection, we then have then

$$
\boldsymbol{\psi}_{end+1} = \left(\frac{2\Delta y}{\alpha \Delta x^2} \mathsf{Q}_2 + 5\frac{\hat{D}}{\alpha \Delta x^2} \mathsf{Q}_2 - \mathsf{I} \right) \boldsymbol{\psi}_{end-1} + \left(-\frac{\Delta y}{2\alpha \Delta x^2} \mathsf{Q}_2 - 4\frac{\hat{D}}{\alpha \Delta x^2} \mathsf{Q}_2 \right) \boldsymbol{\psi}_{end-2} + \frac{\hat{D}}{\alpha \Delta x^2} \mathsf{Q}_2 \boldsymbol{\psi}_{end-3} \tag{1.25}
$$

Then we need to add $1/\Delta y^4$ multiplied by this to the top block row of the solution as before in the previous subsection. This will give us the linear system

$$
\begin{aligned}
& \alpha \begin{pmatrix} \mathsf{R} + \mathsf{Q}_1 - \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & 0 & \dots & 0 \\ \mathsf{T} & \mathsf{R} + \mathsf{Q}_1 & \mathsf{T} & \frac{1}{\Delta y^4}\mathsf{I} & \dots & 0 \\ \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R} + \mathsf{Q}_1 & \mathsf{T} & \dots & 0 \\ 0 & \frac{1}{\Delta y^4}\mathsf{I} & \mathsf{T} & \mathsf{R} + \mathsf{Q}_1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \mathsf{R} + \mathsf{Q}_1 + \frac{1}{\Delta y^4}\mathsf{I} \end{pmatrix} \boldsymbol{\psi} \\
& = \begin{pmatrix} -\left(\frac{2}{\Delta x^2 \Delta y^3} + \frac{5\hat{D}}{\Delta x^2 \Delta y^4} \right) \mathsf{Q}_2 & \left(\frac{1}{2\Delta x^2 \Delta y^3} + \frac{4\hat{D}}{\Delta x^2 \Delta y^4} \right) \mathsf{Q}_2 & -\frac{\hat{D}}{\Delta x^2 \Delta y^4}\mathsf{Q}_2 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix} \boldsymbol{\psi}
\end{aligned} \tag{1.26}
$$

which is the full version of the linear system given in the paper as

$$
\mathsf{B}\boldsymbol{\psi} = \alpha \mathsf{C} \boldsymbol{\psi} \tag{1.27}
$$

We also need to implement another boundary condition of no flux of surfactant at the corners of the domain. As we are saying that $v_z = -\Gamma_y$, this amounts to saying that $v_z = \psi_{zz} = 0$ at the top corners of the domain. As $\psi = 0$ on the left hand and right hand edges of the domain this boundary condition is implemented anyway.