

Adding point-like sinks and sources

$$\frac{\partial u}{\partial t} = D \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + K_{out} \sum_{p=1}^N \delta(r_p - r) - K_{in} \sum_{c=1}^N \delta(r_c - r)$$

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We can discretize the first half-step (x implicit, y explicit) using the following scheme:

$$\frac{u_{i,j}^{k+\frac{1}{2}} - u_{i,j}^k}{\Delta t/2} = D \left(\frac{u_{i+1,j}^{k+\frac{1}{2}} - 2u_{i,j}^{k+\frac{1}{2}} + u_{i-1,j}^{k+\frac{1}{2}}}{\Delta x^2} + \frac{u_{i,j+1}^k - 2u_{i,j}^k + u_{i,j-1}^k}{\Delta y^2} \right) + (S_{out} - S_{in})$$

Where S_{out} and S_{in} are the source and sink terms, respectively:

$$S_{out} = K_{out} \sum_{p=1}^N \delta_\epsilon(r_p - r_{i,j}) \quad \text{and} \quad S_{in} = \frac{K_{in} u_{i,j}^k}{m + u_{i,j}^k} \sum_{c=1}^N \delta_\epsilon(r_c - r_{i,j})$$

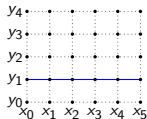
We can define $\alpha = \frac{D\Delta t}{2\Delta x^2} = \frac{D\Delta t}{2\Delta y^2}$ to get

$$-\alpha u_{i-1,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{i,j}^{k+\frac{1}{2}} - \alpha u_{i+1,j}^{k+\frac{1}{2}} = \alpha u_{i,j-1}^k + (1-2\alpha)u_{i,j}^k + \alpha u_{i,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in})$$

We know all the terms in right-hand side of the equation (blue), but we need to compute the left-hand side (red).

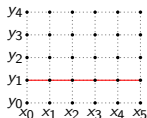
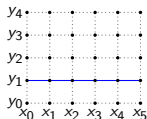
Writing the tridiagonal matrix

Let's fix $j = 1$ and write the equations for $i = 1, 2, 3, 4$:



Writing the tridiagonal matrix

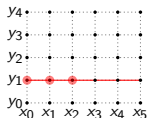
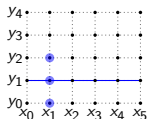
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$$-\alpha u_{0,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} = \alpha u_{1,j-1}^k + (1-2\alpha)u_{1,j}^k + \alpha u_{1,j+1}^k + \frac{\Delta t}{2} (S_{out} - S_{in})$$

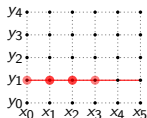
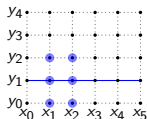


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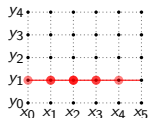
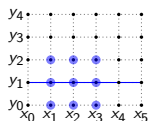
$$-\alpha u_{1,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{2,j}^{k+\frac{1}{2}} - \alpha u_{3,j}^{k+\frac{1}{2}} = \alpha u_{2,j-1}^k + (1-2\alpha)u_{2,j}^k + \alpha u_{2,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in})$$



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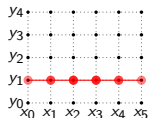
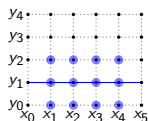
$$\begin{aligned}
 -\alpha u_{0,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} &= \alpha u_{1,j-1}^k + (1-2\alpha)u_{1,j}^k + \alpha u_{1,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\
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 -\alpha u_{2,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{3,j}^{k+\frac{1}{2}} - \alpha u_{4,j}^{k+\frac{1}{2}} &= \alpha u_{3,j-1}^k + (1-2\alpha)u_{3,j}^k + \alpha u_{3,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in})
 \end{aligned}$$



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 -\alpha u_{0,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} &= \alpha u_{1,j-1}^k + (1-2\alpha)u_{1,j}^k + \alpha u_{1,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\
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 \end{aligned}$$

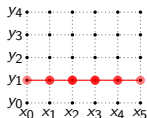
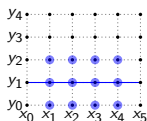


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Let's fix $j = 1$ and write the equations for $i = 1, 2, 3, 4$:

$$\begin{aligned} -\alpha u_{0,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} &= \alpha u_{1,j-1}^k + (1-2\alpha)u_{1,j}^k + \alpha u_{1,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{1,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{2,j}^{k+\frac{1}{2}} - \alpha u_{3,j}^{k+\frac{1}{2}} &= \alpha u_{2,j-1}^k + (1-2\alpha)u_{2,j}^k + \alpha u_{2,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{2,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{3,j}^{k+\frac{1}{2}} - \alpha u_{4,j}^{k+\frac{1}{2}} &= \alpha u_{3,j-1}^k + (1-2\alpha)u_{3,j}^k + \alpha u_{3,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{3,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{4,j}^{k+\frac{1}{2}} - \alpha u_{5,j}^{k+\frac{1}{2}} &= \alpha u_{4,j-1}^k + (1-2\alpha)u_{4,j}^k + \alpha u_{4,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \end{aligned}$$

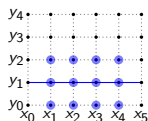
Which can be written as a matrix:



Writing the tridiagonal matrix

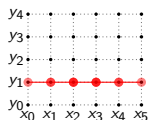
Let's fix $j = 1$ and write the equations for $i = 1, 2, 3, 4$:

$$\begin{aligned} -\alpha u_{0,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} &= \alpha u_{1,j-1}^k + (1-2\alpha)u_{1,j}^k + \alpha u_{1,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{1,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{2,j}^{k+\frac{1}{2}} - \alpha u_{3,j}^{k+\frac{1}{2}} &= \alpha u_{2,j-1}^k + (1-2\alpha)u_{2,j}^k + \alpha u_{2,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{2,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{3,j}^{k+\frac{1}{2}} - \alpha u_{4,j}^{k+\frac{1}{2}} &= \alpha u_{3,j-1}^k + (1-2\alpha)u_{3,j}^k + \alpha u_{3,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \\ -\alpha u_{3,j}^{k+\frac{1}{2}} + (1+2\alpha)u_{4,j}^{k+\frac{1}{2}} - \alpha u_{5,j}^{k+\frac{1}{2}} &= \alpha u_{4,j-1}^k + (1-2\alpha)u_{4,j}^k + \alpha u_{4,j+1}^k + \frac{\Delta t}{2}(S_{out} - S_{in}) \end{aligned}$$



Which can be written as a matrix:

$$\begin{bmatrix} -\alpha & 1+2\alpha & -\alpha & 0 & 0 & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha & 0 & 0 \\ 0 & 0 & -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & 0 & 0 & -\alpha & 1+2\alpha & -\alpha \end{bmatrix} \begin{bmatrix} u_{0,j}^{k+\frac{1}{2}} \\ u_{1,j}^{k+\frac{1}{2}} \\ u_{2,j}^{k+\frac{1}{2}} \\ u_{3,j}^{k+\frac{1}{2}} \\ u_{4,j}^{k+\frac{1}{2}} \\ u_{5,j}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,j} \\ b_{2,j} \\ b_{3,j} \\ b_{4,j} \end{bmatrix}$$

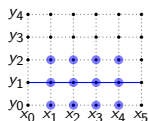


Where $b_{i,j}$ is the right hand side of the equation, which is already known.

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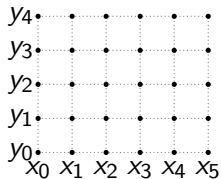
$$\begin{bmatrix} -\alpha & 1+2\alpha & -\alpha & 0 & 0 & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha & 0 & 0 \\ 0 & 0 & -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & 0 & 0 & -\alpha & 1+2\alpha & -\alpha \end{bmatrix} \begin{bmatrix} u_{0,j}^{k+\frac{1}{2}} \\ u_{1,j}^{k+\frac{1}{2}} \\ u_{2,j}^{k+\frac{1}{2}} \\ u_{3,j}^{k+\frac{1}{2}} \\ u_{4,j}^{k+\frac{1}{2}} \\ u_{5,j}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,j} \\ b_{2,j} \\ b_{3,j} \\ b_{4,j} \end{bmatrix}$$

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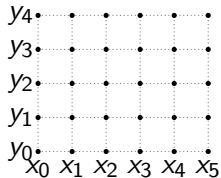
Because of the boundary conditions, we can simplify the matrix to a tridiagonal matrix.

Writing the tridiagonal matrix

We get one system of equations for each j value.

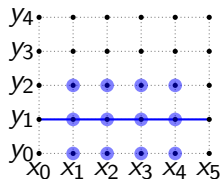


$\Delta t/2$

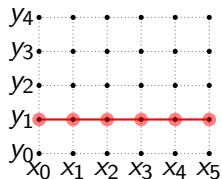


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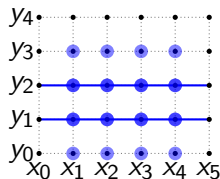
\downarrow
 $\Delta t/2$



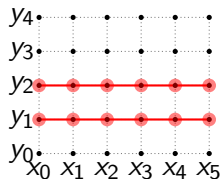
$$\begin{bmatrix}
 1 + \alpha & -\alpha & 0 & 0 \\
 -\alpha & 1 + 2\alpha & -\alpha & 0 \\
 0 & -\alpha & 1 + 2\alpha & -\alpha \\
 0 & 0 & -\alpha & 1 + \alpha
 \end{bmatrix}
 \begin{bmatrix}
 u_{1,1}^{k+\frac{1}{2}} \\
 u_{2,1}^{k+\frac{1}{2}} \\
 u_{3,1}^{k+\frac{1}{2}} \\
 u_{4,1}^{k+\frac{1}{2}}
 \end{bmatrix}
 =
 \begin{bmatrix}
 b_{1,1} \\
 b_{2,1} \\
 b_{3,1} \\
 b_{4,1}
 \end{bmatrix}$$

Writing the tridiagonal matrix

We get one system of equations for each j value.



\downarrow
 $\Delta t/2$

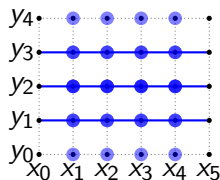


$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,1}^{k+\frac{1}{2}} \\ u_{2,1}^{k+\frac{1}{2}} \\ u_{3,1}^{k+\frac{1}{2}} \\ u_{4,1}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,1} \\ b_{2,1} \\ b_{3,1} \\ b_{4,1} \end{bmatrix}$$

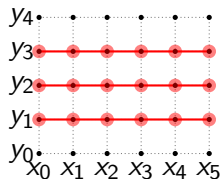
$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,2}^{k+\frac{1}{2}} \\ u_{2,2}^{k+\frac{1}{2}} \\ u_{3,2}^{k+\frac{1}{2}} \\ u_{4,2}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,2} \\ b_{2,2} \\ b_{3,2} \\ b_{4,2} \end{bmatrix}$$

Writing the tridiagonal matrix

We get one system of equations for each j value.



\downarrow
 $\Delta t/2$



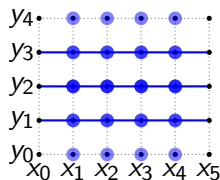
$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,1}^{k+\frac{1}{2}} \\ u_{2,1}^{k+\frac{1}{2}} \\ u_{3,1}^{k+\frac{1}{2}} \\ u_{4,1}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,1} \\ b_{2,1} \\ b_{3,1} \\ b_{4,1} \end{bmatrix}$$

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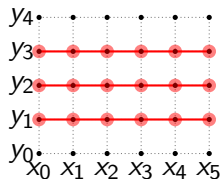
$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,3}^{k+\frac{1}{2}} \\ u_{2,3}^{k+\frac{1}{2}} \\ u_{3,3}^{k+\frac{1}{2}} \\ u_{4,3}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,3} \\ b_{2,3} \\ b_{3,3} \\ b_{4,3} \end{bmatrix}$$

Writing the tridiagonal matrix

We get one system of equations for each j value.



\downarrow
 $\Delta t/2$



$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,1}^{k+\frac{1}{2}} \\ u_{2,1}^{k+\frac{1}{2}} \\ u_{3,1}^{k+\frac{1}{2}} \\ u_{4,1}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,1} \\ b_{2,1} \\ b_{3,1} \\ b_{4,1} \end{bmatrix}$$

$$\begin{bmatrix} 1+\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \begin{bmatrix} u_{1,2}^{k+\frac{1}{2}} \\ u_{2,2}^{k+\frac{1}{2}} \\ u_{3,2}^{k+\frac{1}{2}} \\ u_{4,2}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} b_{1,2} \\ b_{2,2} \\ b_{3,2} \\ b_{4,2} \end{bmatrix}$$

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Now we can use the Thomas algorithm for solving each tridiagonal system.

Implementing Neumann Boundary Conditions

Neumann boundary conditions specify that the derivative of the concentration at the boundary is zero:

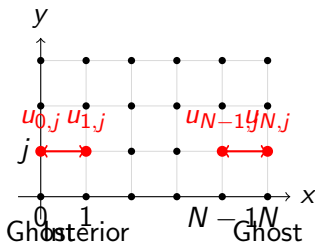
$$\left. \frac{\partial u}{\partial x} \right|_{x=0} = 0 \quad \text{and} \quad \left. \frac{\partial u}{\partial x} \right|_{x=L} = 0$$

In the discretized form, this means:

$$\frac{u_{1,j} - u_{0,j}}{\Delta x} = 0 \quad \Rightarrow \quad u_{0,j} = u_{1,j}$$

$$\frac{u_{N,j} - u_{N-1,j}}{\Delta x} = 0 \quad \Rightarrow \quad u_{N,j} = u_{N-1,j}$$

These conditions state that the ghost points ($u_{0,j}$ and $u_{N,j}$) have the same value as their adjacent interior points.



Implementing Neumann Boundary Conditions in the Tridiagonal System

For the first half-step (x-direction), we need to modify the tridiagonal system to incorporate the boundary conditions.

For the left boundary ($i = 1$), the original equation is:

$$-\alpha u_{0,j}^{k+\frac{1}{2}} + (1 + 2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} = \text{RHS}_{1,j}$$

With the Neumann condition $u_{0,j} = u_{1,j}$, we substitute:

$$-\alpha u_{1,j}^{k+\frac{1}{2}} + (1 + 2\alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} = \text{RHS}_{1,j}$$

Simplifying:

$$(1 + \alpha)u_{1,j}^{k+\frac{1}{2}} - \alpha u_{2,j}^{k+\frac{1}{2}} = \text{RHS}_{1,j}$$

For the right boundary ($i = N - 1$), the original equation is:

$$-\alpha u_{N-2,j}^{k+\frac{1}{2}} + (1 + 2\alpha)u_{N-1,j}^{k+\frac{1}{2}} - \alpha u_{N,j}^{k+\frac{1}{2}} = \text{RHS}_{N-1,j}$$

With the Neumann condition $u_{N,j} = u_{N-1,j}$, we substitute:

$$-\alpha u_{N-2,j}^{k+\frac{1}{2}} + (1 + 2\alpha)u_{N-1,j}^{k+\frac{1}{2}} - \alpha u_{N-1,j}^{k+\frac{1}{2}} = \text{RHS}_{N-1,j}$$

Simplifying:

$$-\alpha u_{N-2,j}^{k+\frac{1}{2}} + (1 + \alpha)u_{N-1,j}^{k+\frac{1}{2}} = \text{RHS}_{N-1,j}$$

Implementation in the Code

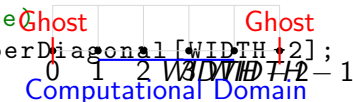
In the JavaScript implementation, the boundary conditions are applied as follows:

```
1 // Apply boundary conditions for the x-direction
2 // Left boundary (reflective)
3 mainDiagonal[1] += lowerDiagonal[1];
4 lowerDiagonal[1] = 0;
5
6 // Right boundary (reflective)
7 mainDiagonal[WIDTH-2] += upperDiagonal[WIDTH-2];
8 upperDiagonal[WIDTH-2] = 0;
```

This code modifies the tridiagonal system to incorporate the Neumann boundary conditions.

Why mainDiagonal[1] and not mainDiagonal[0]?

The key insight is that the computational domain is indexed from 1 to WIDTH-2, with indices 0 and WIDTH-1 being ghost points.



The tridiagonal system is set up for the interior points (1 to WIDTH-2), so the first equation corresponds to index 1, not 0.

Detailed Explanation of Boundary Condition Implementation

For the left boundary, the original tridiagonal system has:

$$\text{lowerDiagonal}[1] = -\alpha$$

$$\text{mainDiagonal}[1] = 1 + 2\alpha$$

$$\text{upperDiagonal}[1] = -\alpha$$

The code modifies this to:

$$\begin{aligned}\text{mainDiagonal}[1] + &= \text{lowerDiagonal}[1] \\ &= (1 + 2\alpha) + (-\alpha) \\ &= 1 + \alpha\end{aligned}$$

And sets $\text{lowerDiagonal}[1] = 0$, effectively removing the dependency on the ghost point.

This implementation correctly enforces the Neumann boundary conditions by modifying the tridiagonal system coefficients to account for the equality between ghost points and their adjacent interior points.

Similarly, for the right boundary:

$$\text{lowerDiagonal}[\text{WIDTH}-2] = -\alpha$$

$$\text{mainDiagonal}[\text{WIDTH}-2] = 1 + 2\alpha$$

$$\text{upperDiagonal}[\text{WIDTH}-2] = -\alpha$$

The code modifies this to:

$$\begin{aligned}\text{mainDiagonal}[\text{WIDTH}-2] + &= \text{upperDiagonal}[\text{WIDTH}-2] \\ &= (1 + 2\alpha) + (-\alpha) \\ &= 1 + \alpha\end{aligned}$$

And sets $\text{upperDiagonal}[\text{WIDTH}-2] = 0$, removing the dependency on the ghost point.