

NE 155, Topic 15, S21
2-D Finite Difference/Volume methods
April 8, 2021

Much of this can be found in Duderstadt and Hamilton, Chp. 5 Section II.B.

PDEs

We'll start by considering PDEs in general, and then move on to the Diffusion Equation specifically.

Recall: a partial differential equation is an equation containing an unknown function of two or more variables and its derivatives with respect to those variables.

If the PDE is linear in u and all derivatives of u , then we say that the PDE is linear.

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + F u = G$$

This equation is a **2nd order** PDE in two variables. It is **linear** if A through G do not depend on u (they may depend on x and y).

Recall that we can classify second order PDEs based on the geometric behavior of their solutions.

- Elliptic if $B^2 - 4AC < 0$.
- Hyperbolic if $B^2 - 4AC > 0$
- Parabolic if $B^2 - 4AC = 0$

Elliptic Equations

Recall that the 2-D Laplacian for the function $u(x, y)$ is

The Laplacian is used in many of the equations that are commonly found in physics:

- Laplace's equation

$$\nabla^2 u(x, y) = 0$$

- Poisson's equation

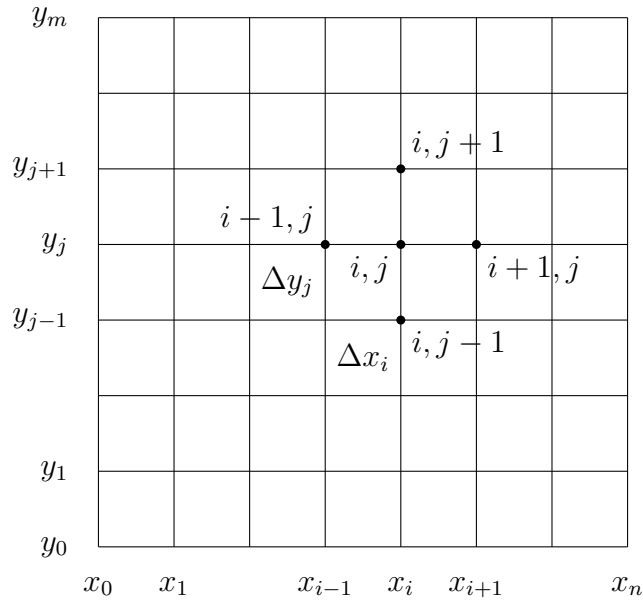
$$\nabla^2 u(x, y) = g(x, y)$$

- Helmholtz's equation (recall that we can make the DE look like this)

$$\nabla^2 u(x, y) + f(x, y)u(x, y) = g(x, y)$$

Meshing

We will use 5 points to define our central-differenced Laplacian:



$$u(x_i, y_j) = u_{i,j} \quad u(x_{i+1}, y_j) = u_{i+1,j}$$

$$\frac{\partial^2 u_{i,j}}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial u_{i,j}}{\partial x} \right) = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x_i^2}$$

$$\frac{\partial^2 u_{i,j}}{\partial y^2} = \frac{\partial}{\partial y} \left(\frac{\partial u_{i,j}}{\partial y} \right) = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y_j^2}$$

All together this gives

If we apply this to Laplace's equation and have fixed boundary conditions:

$$\begin{aligned}u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} &= 0, \quad i = 1, 2, \dots, n-1, \quad j = 1, 2, \dots, m-1 \\u_{0,j} &= BC_L, \quad j = 1, 2, \dots, m-1 \\u_{i,0} &= BC_B, \quad i = 1, 2, \dots, n-1 \\u_{n,j} &= BC_R, \quad j = 1, 2, \dots, m-1 \\u_{i,m} &= BC_T, \quad i = 1, 2, \dots, n-1\end{aligned}$$

Make sure to check how the corners need to be defined.

We could apply this directly the the 2-D diffusion equation.

2-D Finite Volume Method, Diffusion Equation

Remember that in 1-D we were solving this

$$-\frac{d}{dx}D(x)\frac{d\phi(x)}{dx} + \Sigma_a(x)\phi(x) = S(x)$$

with an equilibrium (reflecting) condition at the centerline ($x_0 = 0$) and vacuum on the right ($x_n = a$):

$$\begin{aligned}\frac{d}{dx}\phi(x)|_{x=0} &= 0 && \text{zero net current,} \\ \phi(\tilde{a}) &= 0 && \tilde{a} = a + 2D.\end{aligned}$$

We imposed a spatial mesh and said material discontinuities will coincide with the cell edges, x_i . Thus, we can assume that the cross sections and the diffusion coefficient are constant in each cell. The unknown fluxes and known sources are defined at the mesh or cell edges. We then went on to

define things for the finite volume method.

Now, we're going to extend all of that to two dimensions. We'll start with the multi-D equation:

$$-\nabla \cdot (D(\vec{r})\nabla\phi(\vec{r})) + \Sigma_a(\vec{r})\phi(\vec{r}) = S(\vec{r}) .$$

This equation is elliptic:

- in general, this is the Helmholtz equation.
- if $\Sigma_a(\vec{r}) = 0$ and $D(\vec{r}) = \text{constant}$, then this takes the form of the Poisson equation.
- if $\Sigma_a(\vec{r}) = 0$ and $S(\vec{r}) = 0$, then this becomes Laplace's equation.

In 2-D:

For now we're going to say we have fixed boundary conditions:

$$\phi(-a, y) = \Phi_L , \quad \phi(a, y) = \Phi_R , \quad \phi(x, -b) = \Phi_B , \quad \phi(x, b) = \Phi_T ,$$

with $x \in [-a, a]$ and $y \in [-b, b]$.

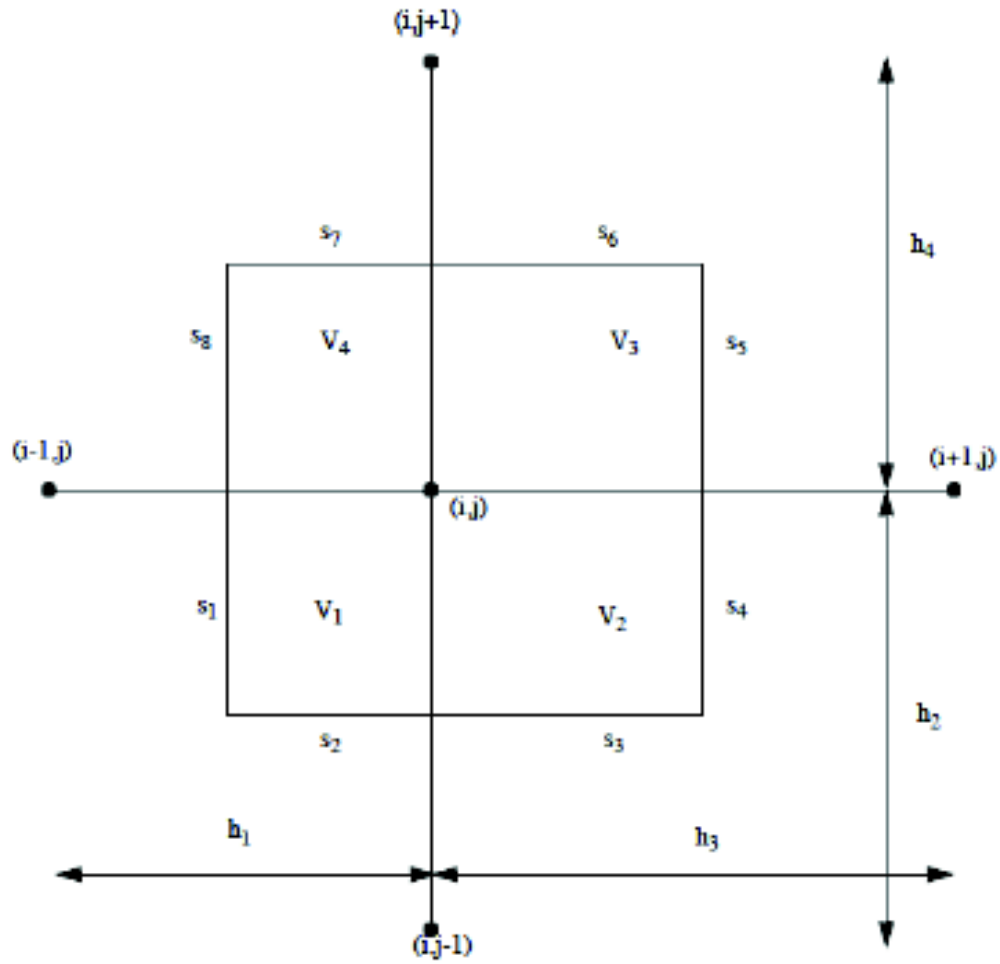
Finite Volume

We assume the diffusion coefficient, absorption cross section, and source are constant in each cell (cell-centered), e.g., for $V_{i,j}$:

$$\begin{aligned} D(x, y) &= D_{i,j} , & x_{i-1} \leq x \leq x_i \text{ and } y_{j-1} \leq y \leq y_j \\ \Sigma_a(x, y) &= \Sigma_{a,i,j} , & x_{i-1} \leq x \leq x_i \text{ and } y_{j-1} \leq y \leq y_j \\ S(x, y) &= S_{i,j} , & x_{i-1} \leq x \leq x_i \text{ and } y_{j-1} \leq y \leq y_j \\ \Delta x_i &\equiv \delta_i = x_i - x_{i-1} \\ \Delta y_j &\equiv \epsilon_j = y_j - y_{j-1} \end{aligned}$$

And analogously for the other 3 cells.

We further assume that the fluxes are constant over the interval centered around (x_i, y_j) (edge-centered):



Now, we integrate the 2-D equation over 4 rectangular partial-volumes (well, areas, technically):

$$V = V_{i,j} + V_{i+1,j} + V_{i,j+1} + V_{i+1,j+1}.$$

$$\int_V d\vec{r} [-\nabla \cdot (D(\vec{r})\nabla\phi(\vec{r})) + \Sigma_a(\vec{r})\phi(\vec{r}) = S(\vec{r})]$$

Streaming Term

Use Gauss Theorem to replace the first volume integral with a surface integral:

Next, we define the partial derivative w.r.t. direction on each surface, using $O(h)$ forward and backward difference schemes since they're simple:

$$\begin{aligned}
 \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{i,j-1} - \phi_{i,j}}{\epsilon_j} && \text{on } S_2, S_3 \\
 &= \frac{\phi_{i,j+1} - \phi_{i,j}}{\epsilon_{j+1}} && \text{on } S_7, S_6 \\
 &= \frac{\phi_{i-1,j} - \phi_{i,j}}{\delta_i} && \text{on } S_1, S_8 \\
 &= \frac{\phi_{i+1,j} - \phi_{i,j}}{\delta_{i+1}} && \text{on } S_4, S_5
 \end{aligned}$$

We then use the midpoint rule for the integration and integrate along each surface. Recall that the physics values are cell-centered while the flux is edge-centered. E.g., surfaces S_2 and S_3 :

$$\begin{aligned}
 - \int_{S_2+S_3} d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \boxed{\frac{\phi_{i,j} - \phi_{i,j-1}}{\epsilon_j} \left(\frac{D_{i,j}\delta_i + D_{i+1,j}\delta_{i+1}}{2} \right)}, \\
 S_6 + S_7 &= \boxed{\frac{\phi_{i,j+1} - \phi_{i,j}}{\epsilon_{j+1}} \left(\frac{D_{i,j+1}\delta_i + D_{i+1,j+1}\delta_{i+1}}{2} \right)}, \\
 S_1 + S_8 &= \boxed{\frac{\phi_{i-1,j} - \phi_{i,j}}{\delta_i} \left(\frac{D_{i,j}\epsilon_j + D_{i,j+1}\epsilon_{j+1}}{2} \right)}, \\
 S_4 + S_5 &= \boxed{\frac{\phi_{i+1,j} - \phi_{i,j}}{\delta_{i+1}} \left(\frac{D_{i+1,j}\epsilon_j + D_{i+1,j+1}\epsilon_{j+1}}{2} \right)},
 \end{aligned}$$

and we do this for each set of surfaces.

Absorption Term

To integrate absorption, we do four integrals - one over each sub-volume:

Again applying the midpoint scheme and using our edge-centered flux definition:

$$\begin{aligned} \int \int dxdy \Sigma_a(x, y) \phi(x, y) &= \boxed{\phi_{i,j} (\Sigma_{a,i,j} V_{i,j} + \Sigma_{a,i+1,j} V_{i+1,j} + \Sigma_{a,i+1,j+1} V_{i+1,j+1} + \Sigma_{a,i,j+1} V_{i,j+1})} \\ &\equiv \Sigma_{a,ij} , \end{aligned}$$

where

$$V_{i,j} = \frac{1}{4} \delta_i \epsilon_j , \quad V_{i+1,j} = \frac{1}{4} \delta_{i+1} \epsilon_j , \quad V_{i+1,j+1} = \frac{1}{4} \delta_{i+1} \epsilon_{j+1} , \quad V_{i,j+1} = \frac{1}{4} \delta_i \epsilon_{j+1} .$$

Source Term

Using the same procedure for the source, we get:

$$\begin{aligned} \int \int dxdy S(x, y) &= \boxed{S_{i,j} V_{i,j} + S_{i+1,j} V_{i+1,j} + S_{i+1,j+1} V_{i+1,j+1} + S_{i,j+1} V_{i,j+1}} \\ &\equiv S_{ij} . \end{aligned}$$

Discretized Equations

The lower index is the cell to which you are coupling, and the upper index is which cell you are in—this becomes important when we’re ordering our matrix.

$$\begin{aligned}
 a_{i-1,j}^{ij} &= -\frac{D_{i,j}\epsilon_j + D_{i,j+1}\epsilon_{j+1}}{2\delta_i} \\
 &\quad (a_L^{ij} \text{ capturing influence of **left** flux on center cell}) \\
 a_{i+1,j}^{ij} &= -\frac{D_{i+1,j}\epsilon_j + D_{i+1,j+1}\epsilon_{j+1}}{2\delta_{i+1}} \\
 &\quad (a_R^{ij} \text{ capturing influence of **right** flux on center cell}) \\
 a_{i,j-1}^{ij} &= -\frac{D_{i,j}\delta_i + D_{i+1,j}\delta_{i+1}}{2\epsilon_j} \\
 &\quad (a_B^{ij} \text{ capturing influence of **lower** flux on center cell}) \\
 a_{i,j+1}^{ij} &= -\frac{D_{i,j+1}\delta_i + D_{i+1,j+1}\delta_{i+1}}{2\epsilon_{j+1}} \\
 &\quad (a_T^{ij} \text{ capturing influence of **upper** flux on center cell}) \\
 \\
 a_{i,j}^{ij} &= \Sigma_{a,ij} - (a_{i-1,j}^{ij} + a_{i+1,j}^{ij} + a_{i,j-1}^{ij} + a_{i,j+1}^{ij}) . \\
 &\quad (a_C^{ij})
 \end{aligned}$$

In this formulation we now have $(n + 1) \times (m + 1)$ unknowns.

Matrix Form

To write the system in a way that looks like $\mathbf{A}\vec{x} = \vec{b}$, we need to choose an ordering strategy for how we want to store the points. Let’s look at a 3×3 example:

(0, 2)	(1, 2)	(2, 2)
(0, 1)	(1, 1)	(2, 1)
(0, 0)	(1, 0)	(2, 0)

6	7	8
3	4	5
0	1	2

Our solution vector length in this example is 9 (3×3). Our matrix size is therefore going to be 9×9 . We can think of this as a 3×3 matrix of 3×3 matrices:

$$\underbrace{\left(\begin{array}{ccc} \begin{pmatrix} a_{0,0}^{00} & a_{1,0}^{00} & 0 \\ a_{0,0}^{10} & a_{1,0}^{10} & a_{2,0}^{10} \\ 0 & a_{1,0}^{20} & a_{2,0}^{20} \end{pmatrix} & \begin{pmatrix} a_{0,1}^{00} & 0 & 0 \\ 0 & a_{1,1}^{10} & 0 \\ 0 & 0 & a_{2,1}^{20} \end{pmatrix} & \begin{pmatrix} 0 \end{pmatrix} \\ \begin{pmatrix} a_{0,0}^{01} & 0 & 0 \\ 0 & a_{1,0}^{11} & 0 \\ 0 & 0 & a_{2,0}^{21} \end{pmatrix} & \begin{pmatrix} a_{0,1}^{01} & a_{1,1}^{01} & 0 \\ a_{0,1}^{11} & a_{1,1}^{11} & a_{2,1}^{11} \\ 0 & a_{1,1}^{21} & a_{2,1}^{21} \end{pmatrix} & \begin{pmatrix} a_{0,2}^{01} & 0 & 0 \\ 0 & a_{1,2}^{11} & 0 \\ 0 & 0 & a_{2,2}^{21} \end{pmatrix} \\ \begin{pmatrix} 0 \end{pmatrix} & \begin{pmatrix} a_{0,1}^{02} & 0 & 0 \\ 0 & a_{1,1}^{12} & 0 \\ 0 & 0 & a_{2,1}^{22} \end{pmatrix} & \begin{pmatrix} a_{0,2}^{02} & a_{1,2}^{02} & 0 \\ a_{0,2}^{12} & a_{1,2}^{12} & a_{2,2}^{12} \\ 0 & a_{1,2}^{22} & a_{2,2}^{22} \end{pmatrix} \end{array} \right)}_{\mathbf{A}} \underbrace{\begin{pmatrix} \phi_{0,0} \\ \phi_{1,0} \\ \phi_{2,0} \\ \phi_{0,1} \\ \phi_{1,1} \\ \phi_{2,1} \\ \phi_{0,2} \\ \phi_{1,2} \\ \phi_{2,2} \end{pmatrix}}_{\vec{\phi}} = \underbrace{\begin{pmatrix} S_{00} \\ S_{10} \\ S_{20} \\ S_{01} \\ S_{11} \\ S_{21} \\ S_{02} \\ S_{12} \\ S_{22} \end{pmatrix}}_{\vec{S}}$$

Another way to think of \mathbf{A} is

$$\left(\begin{array}{ccc} \begin{pmatrix} a_C^{00} & a_R^{00} & 0 \\ a_L^{10} & a_C^{10} & a_R^{10} \\ 0 & a_L^{20} & a_C^{20} \end{pmatrix} & \begin{pmatrix} a_T^{00} & 0 & 0 \\ 0 & a_T^{10} & 0 \\ 0 & 0 & a_T^{20} \end{pmatrix} & \begin{pmatrix} 0 \end{pmatrix} \\ \begin{pmatrix} a_B^{01} & 0 & 0 \\ 0 & a_B^{11} & 0 \\ 0 & 0 & a_B^{21} \end{pmatrix} & \begin{pmatrix} a_C^{01} & a_R^{01} & 0 \\ a_L^{11} & a_C^{11} & a_R^{11} \\ 0 & a_L^{21} & a_C^{21} \end{pmatrix} & \begin{pmatrix} a_T^{01} & 0 & 0 \\ 0 & a_T^{11} & 0 \\ 0 & 0 & a_T^{21} \end{pmatrix} \\ \begin{pmatrix} 0 \end{pmatrix} & \begin{pmatrix} a_B^{02} & 0 & 0 \\ 0 & a_B^{12} & 0 \\ 0 & 0 & a_B^{22} \end{pmatrix} & \begin{pmatrix} a_C^{02} & a_R^{02} & 0 \\ a_L^{12} & a_C^{12} & a_R^{12} \\ 0 & a_L^{22} & a_C^{22} \end{pmatrix} \end{array} \right)$$

This gives us a 5-banded matrix, which is not so difficult to represent with built in functions in Python or MATLAB. We could still solve this directly with Gaussian elimination or LU decomposition, but the size of the system increases pretty rapidly with mesh size.

Therefore using an iterative method like Jacobi, GS, or SOR is probably a better plan.

Boundary Conditions

This all works fine for central points, but what about the boundaries? When we're at the edges, we get four entries rather than five because the edge values are known. For corners we have only three entries.

Let's see how this impacts our equations. Recall:

$$\phi(-a, y) = \Phi_L, \quad \phi(a, y) = \Phi_R, \quad \phi(x, -b) = \Phi_B, \quad \phi(x, b) = \Phi_T.$$

Let's choose what to do at the corners, and then define the rest of the boundaries:

Let's look at how this would impact the left ($i = 0$) boundary. The $i = 0$ equations are simply the boundary condition:

- Change the $a_C^{0,j}$ entries to 1s,
- the $a_x^{0,j}$, where x is R, T , and B to 0, and
- the $S_{0,j}$ entries to Φ_L .

For the $i = 1$ equations:

$$\underbrace{a_{2,j}^{1j}}_R \phi_{2,j} + \underbrace{a_{1,j-1}^{1j}}_B \phi_{1,j-1} + \underbrace{a_{1,j+1}^{1j}}_T \phi_{1,j+1} + \underbrace{a_{1,j}^{1j}}_C \phi_{1,j} = S_{1j} - \underbrace{a_{0,j}^{1j}}_L \phi_L$$

And analogously for the rest of the edges.

Larger Matrix

What about a bigger matrix?

(0, 3)	(1, 3)	(2, 3)	(3, 3)	12	13	14	15
(0, 2)	(1, 2)	(2, 2)	(3, 2)	8	9	10	11
(0, 1)	(1, 1)	(2, 1)	(3, 1)	4	5	6	7
(0, 0)	(1, 0)	(2, 0)	(3, 0)	0	1	2	3

Our solution vector length in this example is 16 (4×4). Our matrix size is therefore going to be 16×16 . We can think of this as a 4×4 matrix of 4×4 matrices:

$$\underbrace{\left(\begin{array}{c} \left(\begin{array}{cccc} a_{0,0}^{00} & a_{1,0}^{00} & 0 & 0 \\ a_{0,0}^{10} & a_{1,0}^{10} & a_{2,0}^{10} & 0 \\ 0 & a_{1,0}^{20} & a_{2,0}^{20} & a_{3,0}^{20} \\ 0 & 0 & a_{2,0}^{30} & a_{3,0}^{30} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,0}^{01} & 0 & 0 & 0 \\ 0 & a_{1,0}^{11} & 0 & 0 \\ 0 & 0 & a_{2,0}^{21} & 0 \\ 0 & 0 & 0 & a_{3,0}^{31} \end{array} \right) \\ 0 \\ 0 \end{array} \right)}_{\mathbf{A}}
 \left(\begin{array}{c} \left(\begin{array}{cccc} a_{0,1}^{00} & 0 & 0 & 0 \\ 0 & a_{1,1}^{10} & 0 & 0 \\ 0 & 0 & a_{2,1}^{20} & 0 \\ 0 & 0 & 0 & a_{3,1}^{30} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,1}^{01} & a_{1,1}^{01} & 0 & 0 \\ a_{0,1}^{11} & a_{1,1}^{11} & a_{2,1}^{11} & 0 \\ 0 & a_{1,1}^{21} & a_{2,1}^{21} & a_{3,1}^{21} \\ 0 &) & a_{2,1}^{31} & a_{3,1}^{31} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,1}^{02} & 0 & 0 & 0 \\ 0 & a_{1,1}^{12} & 0 & 0 \\ 0 & 0 & a_{2,1}^{22} & 0 \\ 0 & 0 & 0 & a_{3,1}^{32} \end{array} \right) \\ 0 \end{array} \right)
 \left(\begin{array}{c} 0 \\ \left(\begin{array}{cccc} a_{0,2}^{01} & 0 & 0 & 0 \\ 0 & a_{1,2}^{11} & 0 & 0 \\ 0 & 0 & a_{2,2}^{21} & 0 \\ 0 & 0 & 0 & a_{3,2}^{31} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,2}^{02} & a_{1,2}^{02} & 0 & 0 \\ a_{0,2}^{12} & a_{1,2}^{12} & a_{2,2}^{12} & 0 \\ 0 & a_{1,2}^{22} & a_{2,2}^{22} & a_{3,2}^{22} \\ 0 & 0 & a_{2,2}^{32} & a_{3,2}^{32} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,2}^{03} & 0 & 0 & 0 \\ 0 & a_{1,2}^{13} & 0 & 0 \\ 0 & 0 & a_{2,2}^{23} & 0 \\ 0 & 0 & 0 & a_{3,2}^{33} \end{array} \right) \end{array} \right)
 \left(\begin{array}{c} 0 \\ 0 \\ \left(\begin{array}{cccc} a_{0,3}^{02} & 0 & 0 & 0 \\ 0 & a_{1,3}^{12} & 0 & 0 \\ 0 & 0 & a_{2,3}^{22} & 0 \\ 0 & 0 & 0 & a_{3,3}^{32} \end{array} \right) \\ \left(\begin{array}{cccc} a_{0,3}^{03} & a_{1,3}^{03} & 0 & 0 \\ a_{0,3}^{13} & a_{1,3}^{13} & a_{2,3}^{13} & 0 \\ 0 & a_{1,3}^{23} & a_{2,3}^{23} & a_{3,3}^{23} \\ 0 & 0 & a_{2,3}^{33} & a_{3,3}^{33} \end{array} \right) \end{array} \right)
 \end{array}$$

$$\underbrace{\begin{pmatrix} \phi_{0,0} \\ \phi_{1,0} \\ \phi_{2,0} \\ \phi_{3,0} \\ \\ \phi_{0,1} \\ \phi_{1,1} \\ \phi_{2,1} \\ \phi_{3,1} \\ \\ \phi_{0,2} \\ \phi_{1,2} \\ \phi_{2,2} \\ \phi_{3,2} \\ \\ \phi_{0,3} \\ \phi_{1,3} \\ \phi_{2,3} \\ \phi_{3,3} \end{pmatrix}}_{\vec{\phi}} = \underbrace{\begin{pmatrix} S_{00} \\ S_{10} \\ S_{20} \\ S_{30} \\ \\ S_{01} \\ S_{11} \\ S_{21} \\ S_{31} \\ \\ S_{02} \\ S_{12} \\ S_{22} \\ S_{32} \\ \\ S_{03} \\ S_{13} \\ S_{23} \\ S_{33} \end{pmatrix}}_{\vec{S}}$$

$(0, m)$	$(1, m)$	$(n - 1, m)$	(n, m)
\vdots			$(n, m - 1)$
$(0, 1)$	$(1, 1)$		$(n, 1)$
$(0, 0)$	$(1, 0)$	\cdots	$(n, 0)$

12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

Our solution vector length in this example is $1 \times nm$. Our matrix size is therefore going to be $nm \times nm$. We can think of this as a $n \times m$ matrix of $n \times m$ matrices: (n rows; m columns)

$$\begin{pmatrix} \phi_{0,0} \\ \phi_{1,0} \\ \phi_{n-1,0} \\ \phi_{n,0} \\ \\ \phi_{0,1} \\ \phi_{1,1} \\ \phi_{n-1,1} \\ \phi_{n,1} \\ \\ \phi_{0,m-1} \\ \phi_{1,m-1} \\ \phi_{n-1,m-1} \\ \phi_{n,m-1} \\ \\ \phi_{0,m} \\ \phi_{1,m} \\ \phi_{n-1,m} \\ \phi_{n,m} \end{pmatrix} = \begin{pmatrix} S_{00} \\ S_{10} \\ S_{(n-1)0} \\ S_{n0} \\ \\ S_{01} \\ S_{11} \\ S_{(n-1)1} \\ S_{n1} \\ \\ S_{0(m-1)} \\ S_{1(m-1)} \\ S_{(n-1)(m-1)} \\ S_{n(m-1)} \\ \\ S_{0m} \\ S_{1m} \\ S_{(n-1)m} \\ S_{nm} \end{pmatrix}$$

$\underbrace{\hspace{15em}}_{\vec{\phi}}$

$\underbrace{\hspace{15em}}_{\vec{S}}$