Computational Science:
Computational Methods in Engineering

Multivariable Finite-Difference Method

Outline

- Staggered Grid
- Derivative Matrices for Staggered Grids
- Example

Staggered Grid

3

Multi-Variable Problems

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \Rightarrow \qquad \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} = ag(x)$$

$$\frac{\partial g(x)}{\partial x} = bf(x) \qquad \qquad \frac{g(x+\Delta x) - g(x-\Delta x)}{2\Delta x} = bf(x)$$

This formulation will work, but it is less accurate than is possible. These finite-difference span $2\Delta x$ across the grid, whereas it is possible to use finite-differences that span only Δx.

EMPossible

4

Tighter Finite-Difference Approximations

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \frac{\partial g(x)}{\partial x} = bf(x)$$

$$\Rightarrow$$

$$\frac{f\left(x+\frac{\Delta x}{2}\right) - f\left(x-\frac{\Delta x}{2}\right)}{\Delta x} = ag(x)$$

$$\frac{g\left(x+\frac{\Delta x}{2}\right) - g\left(x-\frac{\Delta x}{2}\right)}{\Delta x} = bf(x)$$

This formulation would be difficult and tedious to make work because it requires us to know the value of $f(x)$ and $g(x)$ at midpoints. These do not exist and would need to be interpolated.

EMPossible

5

Use Terms Only Where They are Defined

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \frac{\partial g(x)}{\partial x} = bf(x)$$

$$\Rightarrow$$

$$\frac{f(x+\Delta x) - f(x)}{\Delta x} = ag(x)$$

$$\frac{g(x+\Delta x) - g(x)}{\Delta x} = bf(x)$$

Important rule:

All terms in a finite-difference equation must exist at the same point.

The above system of equations is violating this rule because the finite-differences on the left exist at the midpoints while the terms on the right do not.

EMPossible

6

Adopt a Staggered Grid

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \frac{\partial g(x)}{\partial x} = bf(x)$$

$$\Rightarrow$$

$$\frac{f(x+\Delta x) - f(x)}{\Delta x} = ag\left(x + \frac{\Delta x}{2}\right)$$

$$\frac{g\left(x + \frac{\Delta x}{2}\right) - g\left(x - \frac{\Delta x}{2}\right)}{\Delta x} = bf(x)$$

This works! The finite differences are “tighter” approximations and each term in the equations exists at the same point.

The only drawback is that it must be remembered that $f(x)$ and $g(x)$ will be stored at physically different points.

EMPossible 7

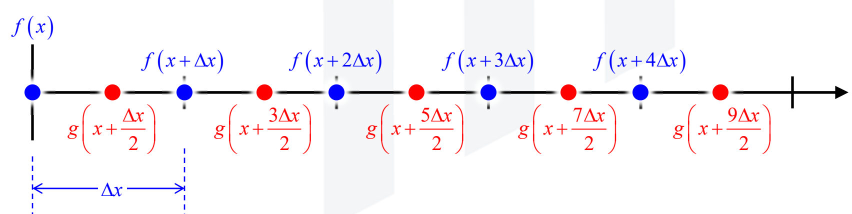
1D Staggered Grid

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \frac{\partial g(x)}{\partial x} = bf(x)$$

$$\Rightarrow$$

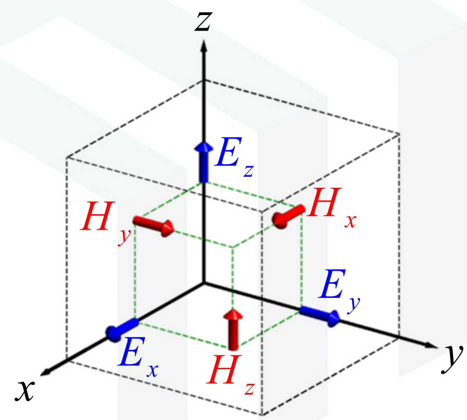
$$\frac{f(x+\Delta x) - f(x)}{\Delta x} = ag\left(x + \frac{\Delta x}{2}\right)$$

$$\frac{g\left(x + \frac{\Delta x}{2}\right) - g\left(x - \frac{\Delta x}{2}\right)}{\Delta x} = bf(x)$$



EMPossible 8

Staggering Functions in Three Dimensions



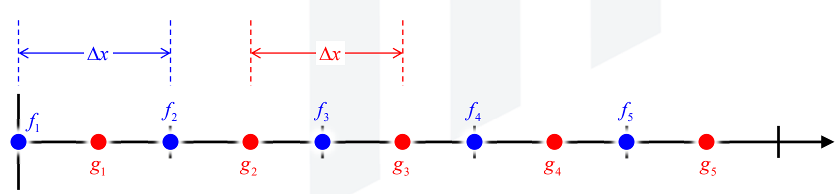
K. S. Yee, "Numerical solution of the initial boundary value problems involving Maxwell's equations in isotropic media," IEEE Trans. Microwave Theory and Techniques, vol. 44, pp. 61–69, 1966.

EMPossible 9

1D Staggered Grid in Terms of Array Indices

$$\frac{\partial f(x)}{\partial x} = ag(x) \qquad \Rightarrow \qquad \frac{f_{i+1} - f_i}{\Delta x} = ag_i$$

$$\frac{\partial g(x)}{\partial x} = bf(x) \qquad \qquad \frac{g_i - g_{i-1}}{\Delta x} = bf_i$$



EMPossible 10

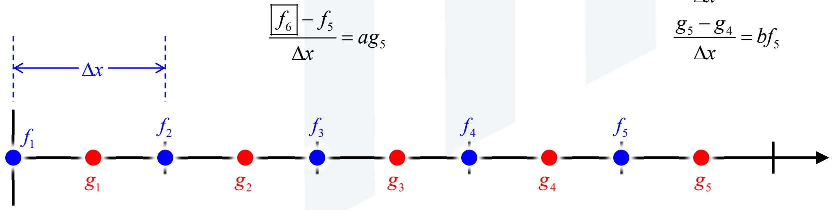
Derivative Matrices for Staggered Grids

Derivative Matrices for Staggered Grids (1 of 2)

Write both of the finite-difference equations at each cell on the grid.

$$\frac{f_{i+1}-f_i}{\Delta x}=ag_i \quad \Rightarrow \quad \begin{aligned} \frac{f_2-f_1}{\Delta x}&=ag_1\\ \frac{f_3-f_2}{\Delta x}&=ag_2\\ \frac{f_4-f_3}{\Delta x}&=ag_3\\ \frac{f_5-f_4}{\Delta x}&=ag_4\\ \frac{\boxed{f_6}-f_5}{\Delta x}&=ag_5 \end{aligned}$$

$$\frac{g_i-g_{i-1}}{\Delta x}=bf_i \quad \Rightarrow \quad \begin{aligned} \frac{g_1-\boxed{g_0}}{\Delta x}&=bf_1\\ \frac{g_2-g_1}{\Delta x}&=bf_2\\ \frac{g_3-g_2}{\Delta x}&=bf_3\\ \frac{g_4-g_3}{\Delta x}&=bf_4\\ \frac{g_5-g_4}{\Delta x}&=bf_5 \end{aligned}$$



EMPossible

Derivative Matrices for Staggered Grids (2 of 2)

Notice the boundary condition fixes for $f(x)$ and $g(x)$ are incorporated at opposite sides of the grid due to the staggering.

$$\frac{f_2-f_1}{\Delta x}=ag_1 \quad \frac{f_3-f_2}{\Delta x}=ag_2 \quad \frac{f_4-f_3}{\Delta x}=ag_3 \quad \frac{f_5-f_4}{\Delta x}=ag_4 \quad \frac{\boxed{f_6}-f_5}{\Delta x}=ag_5$$

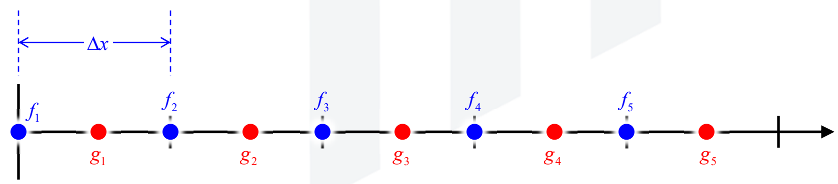
$$\Rightarrow \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}=a\begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \end{bmatrix}$$

$$\left[D_x^f\right][f]=a[g]$$

$$\frac{g_1-\boxed{g_0}}{\Delta x}=bf_1 \quad \frac{g_2-g_1}{\Delta x}=bf_2 \quad \frac{g_3-g_2}{\Delta x}=bf_3 \quad \frac{g_4-g_3}{\Delta x}=bf_4 \quad \frac{g_5-g_4}{\Delta x}=bf_5$$

$$\Rightarrow \frac{1}{\Delta x}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \end{bmatrix}=b\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

$$\left[D_x^g\right][g]=b[f]$$



Final Matrix Equations

Here is what has been done so far

$$\frac{\partial f(x)}{\partial x}=ag(x) \qquad \frac{\partial g(x)}{\partial x}=bf(x) \quad \Rightarrow \quad \left[D_x^f\right][f]=a[g] \qquad \left[D_x^g\right][g]=b[f]$$

With practice, this step will be obvious and not require any intermediate work.

There are two options for solving this system of matrix equations.

Solve Simultaneously

$$\begin{bmatrix} \left[D_x^f\right] & -a[I] \\ -b[I] & \left[D_x^g\right] \end{bmatrix}\begin{bmatrix} [f] \\ [g] \end{bmatrix}=\begin{bmatrix} [0] \\ [0] \end{bmatrix}$$

Solve Individually

$$\left(\left[D_x^g\right]\left[D_x^f\right]-ab[I]\right)[f]=[0]$$

$$[g]=\frac{1}{a}\left[D_x^f\right][f]$$

Second-Order Derivative Matrix?

An interesting thing happened on the last slide.

$$\left(\left[D_x^g \right] \left[D_x^f \right] - ab \left[I \right] \right) \left[f \right] = \left[0 \right]$$

Recall last time a second-order derivate matrix was calculated from two first-order derivative matrices? It did not work well.

$$\mathbf{D}_x^{(1)} \mathbf{D}_x^{(1)} = \frac{1}{(2\Delta x)^2} \begin{bmatrix} -1 & 0 & 1 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ 0 & 1 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix} \qquad \mathbf{D}_x^{(2)} = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

So what is happening with $\left[D_x^g \right] \left[D_x^f \right]$?

$$\left[D_x^g \right] \left[D_x^f \right] = \frac{1}{\Delta x} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \cdot \frac{1}{\Delta x} \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix} = \frac{1}{(\Delta x)^2} \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

Perfect!

EMPossible

15

$\left[D_x^f \right]$ and $\left[D_x^g \right]$ are Related

After inspecting the two derivative matrices,

$$\left[D_x^f \right] = \frac{1}{\Delta x} \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix} \qquad \left[D_x^g \right] = \frac{1}{\Delta x} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

…it can be seen that the derivative matrices are related through

$$\left[D_x^g \right] = -\left[D_x^f \right]^H$$

This holds for many of the common boundary conditions.

Confirmed BC's
- Dirichlet
- Periodic
- Floquet

Exceptions
- Neumann
- ??

EMPossible

16

Final Notes

- It is usually best to form matrix equations early in the formulation process.
- Usually, only first-order derivative matrices are ever needed on staggered grids. First-order derivative matrices can be multiplied to get second-order derivative matrices.
- For most boundary conditions, the derivative matrices are related through

$$\left[D_x^g\right] = -\left[D_x^f\right]^H$$

When this is the case, only one derivative matrix has to be built.

- Even more magic happens when there are expressions like

$$\frac{\partial}{\partial x}\left[a(x)\frac{\partial}{\partial y}\right] \rightarrow \left[D_x^g\right][A]\left[D_x^f\right]$$

Very simple for us! ☺

EMPossible

17

Example

18

Example (1 of 5)

Solve the following coupled differential equation in the interval $1 < x < 10$.

$$\frac{df(x)}{dx} = 2g(x)$$
$$\frac{dg(x)}{dx} = -f(x)$$
$$f(0) = 1 \qquad f(10) = 0$$

EMPossible

Example (2 of 5)

Formulation (done on paper)

Step 1 – Write equations in matrix form

$$\begin{aligned}\frac{df(x)}{dx} &= 2g(x) \\ \frac{dg(x)}{dx} &= -f(x)\end{aligned} \quad \rightarrow \quad \begin{aligned}\left[D_x^f\right][f] &= 2[g] \\ \left[D_x^g\right][g] &= -[f]\end{aligned}$$

Step 2 – Solve first equation for $[g]$

$$[g] = 0.5\left[D_x^f\right][f]$$

Step 3 – Substitute this expression for $[g]$ into the second equation and simplify.

$$\left[D_x^g\right][g] = -[f]$$
$$\left[D_x^g\right]\left(0.5\left[D_x^f\right][f]\right) = -[f]$$
$$\left[D_x^g\right]\left[D_x^f\right][f] + 2[f] = [0]$$
$$\left(\left[D_x^g\right]\left[D_x^f\right] + 2[I]\right)[f] = [0]$$

Step 4 – Write final matrix equation in standard form.

$$[A][f] = [0]$$
$$[A] = \left[D_x^g\right]\left[D_x^f\right] + 2[I]$$

EMPossible

Example (3 of 5)

Implementation (done in MATLAB)

Step 1 – Initialize MATLAB

```
% staggered_grid.m

% INITIALIZE MATLAB
close all;
clc;
clear all;

% OPEN FIGURE WINDOW
fig = figure('Color','w');

% DEFINE PROBLEM PARAMETERS
xa = 0;
xb = 10;
fa = 1;
fb = 0;
Nx = 1000;
```

Step 2 – Calculate Grid

```
% COMPUTE GRID
dx = (xb - xa)/(Nx - 1);
x  = linspace(xa,xb,Nx);
```

Step 3 – Build Derivative Matrices

```
% BUILD DERIVATIVE MATRICES
DFX = sparse(Nx,Nx);
DFX = spdiags(-ones(Nx,1),0,DFX);
DFX = spdiags(+ones(Nx,1),1,DFX);
DFX = DFX / dx;

DGX = - DFX';
```

EMPossible 21

Example (4 of 5)

Implementation (done in MATLAB)

Step 4 – Build Standard Matrix Equation

```
% BUILD A (DIRICHLET)
I = speye(Nx,Nx);
A = DGX*DFX + 2*I;
```

Step 5 – Incorporate Boundary Values

```
% INCORPORATE BOUNDARY VALUES
b = zeros(Nx,1);

A(1,:) = 0;
A(1,1) = 1;
b(1)   = fa;

A(Nx,:)  = 0;
A(Nx,Nx) = 1;
b(Nx)    = fb;
```

Step 6 – Solve Matrix Equation

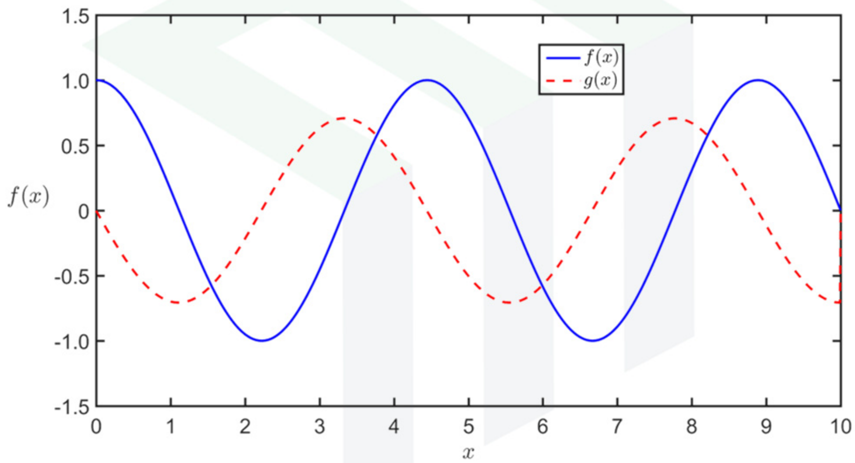
```
% SOLVE MATRIX EQUATION
f = A\b;
g = 0.5*DFX*f;
```

Step 7 – Visualize Results

```
% VISUALIZE RESULTS
h = plot(x,f,'-b','LineWidth',2); hold
on;
plot(x,g,'-r','LineWidth',2); hold off;
h2 = get(h,'Parent');
set(h2,'LineWidth',2,'FontSize',18);
xlabel('x');
ylabel('f(x)');
```

EMPossible 22

Example (5 of 5)



EMPossible