10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
**Lecture #19: Boundary Value Problems (BVPs) Lecture 2.**

## *Finite Differences*

$$\left.\frac{df}{dx}\right|_{x_0} \equiv \frac{f(x_o+\Delta x)-f(x_o-\Delta x)}{2\Delta x}+O\left((\Delta x)^2\right)$$ Relatively good accuracy, better convergence

$$\left.\frac{df}{dx}\right|_{x_0} \equiv \frac{f(x_o+\Delta x)-f(x_o)}{\Delta x}+O(\Delta x)$$ ONE SIDED upwind differencing: The error leads to numerical stability but is a mathematical trick. Adds in error $D_{eff} = D_{true} + {}^{V}{}_{x}\Delta x/2$ and $Pe_{local,\, eff} < 2$. Still wrong, because artificially increased.

$\nabla^2\phi + \underline{v}\cdot\nabla\phi + S(\phi) = 0$

$$\frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{(\Delta x)^2}+\frac{v\phi_{i+1}-\phi_i}{\Delta x}+f\left(\phi(x)\right)=0$$

linear   linear   linear or nonlinear

$$\underline{\underline{M}}\times\underline{\phi}+\begin{pmatrix} f\left(\phi(x_1)\right) & & 0 \\ & f\left(\phi(x_2)\right) & \\ 0 & & \ddots \end{pmatrix}=0$$

$$\underline{\underline{M}}\times\underline{\phi}+\begin{pmatrix} f\left(\phi_1\right) & & 0 \\ & f\left(\phi_2\right) & \\ 0 & & \ddots \end{pmatrix}=0$$

approx. to differential operators

## Newton's Method

$\underline{F}(\underline{\phi}) = 0$

$\underline{\underline{J}}\underline{\Delta}\phi = -\underline{F}$ ← Newton update $\underline{\underline{J}} = \underline{\underline{M}} +$

$$\begin{pmatrix} \left.\frac{\partial f}{\partial\phi}\right|_{\phi_1} & & 0 \\ & \left.\frac{\partial f}{\partial\phi}\right|_{\phi_2} & \\ 0 & & \ddots \end{pmatrix}$$

## Example: Rectangular Duct With Incompressible Flow

Rectangular duct with incompressible fluid being pulled by gravity:

$\nabla^2 v_z(x,y) = \rho g/\mu$ No slip at walls: $v_z(\text{boundaries}) = 0$

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \leftarrow \begin{array}{l} \phi(x_i, y_i) \rightarrow \varphi(n) \\ n = (i-1) * N_y + j \end{array} \qquad \underline{\varphi} = \begin{pmatrix} v_z(x_1, y_1) \\ v_z(x_1, y_2) \\ \vdots \\ v_z(x_1, y_{N_y}) \\ v_z(x_2, y_1) \end{pmatrix}$$

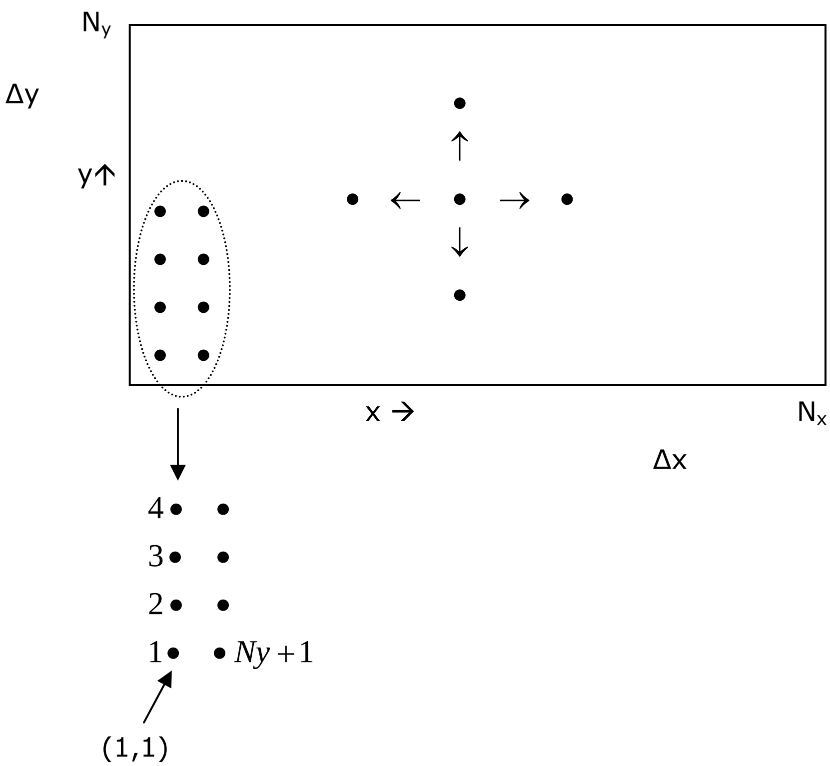



**Figure 1.** Rectangular duct with incompressible flow.

$N_x N_y$ = # points

Interior: $$\frac{v_z(x_{i+1}, y_j) - 2v_z(x_i, y_j) + v_z(x_{i-1}, y_j)}{(\Delta x)^2} + \frac{v_z(x_i, y_{j+1}) - 2v_z(x_i, y_j) + v_z(x_i, y_{j-1})}{(\Delta y)^2}$$

Rows of $\underline{M}$ look like this:

$$\underline{\underline{M}} = \left( 0.....\frac{1}{(\Delta x)^2} 000 \frac{1}{(\Delta y)^2} - 2\left( \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right) 00 \frac{1}{(\Delta x)^2} 00 \frac{1}{(\Delta y)^2} 00 \right)$$

$\underline{\underline{M}}\underline{\phi} = \rho g/\mu$ $\{\underline{\underline{M}}\underline{\phi} = \underline{b}\}$

*Shown in MATLAB*

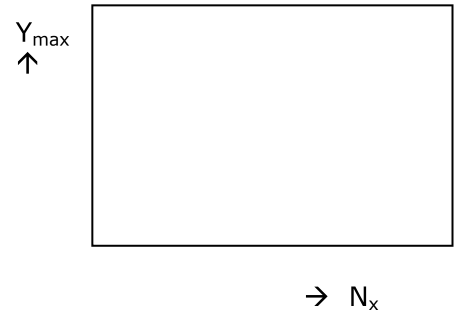
function makeAforLaplacian(Nx,Ny,Xmax,Ymax)

Non-sparse: A(n, n+1) = $1/(\Delta y)^2$

Sparse format: $m_{vec}(k) = n$

$\eta_{vec}(k) = n+1$

$A_{vec}(k) = 1/(\Delta y)^2$




## MATLAB for Sparse Matrix

```
Nx = 20;  Ny = 30;
Xmax = 40;  Ymax = 10;
A_sparse = makeA_sparse(Nx,Ny,Xmax,Ymax);
b = zeros(Nx*Ny,1);  % unknown vector
b = b+1;
phi = A_sparse\b;
check = A_sparse*phi;
      check(400)  ans = 1.0
bbig = 1e7*b
phi = A_sparse\bbig;
check = A_sparse*phi;
      ans = 1e7
```

How do know if correct?

```
V_shaped = reshape(phi, Ny, Nx);
      surf(V_shaped)
```

Makes a beautiful plot of the solution

## Adding Convection

Peclet number $Pe = {}^{vL}/_{D}$

$Pe_{local} = {}^{vx\Delta x}/_{D}$

$\nabla(v\phi) + D\nabla^2\varphi + S(\varphi) = 0$

$$\frac{\partial v_x}{\partial x}\varphi + v_x\frac{\partial \varphi}{\partial x} + D\frac{\partial^2 \varphi}{\partial x^2} + S(\varphi) = 0$$

$$\frac{\partial}{\partial x}\begin{pmatrix}\varphi \\ \varphi'\end{pmatrix} = \begin{pmatrix}\varphi' \\ \frac{-v_x}{D}\varphi' - \frac{1}{D}\frac{\partial v_x}{\partial x}\varphi - \frac{S}{D}\end{pmatrix} \qquad \frac{\partial \varphi}{\partial x}$$

Recall from ODE discussion:

$$\frac{\partial \varphi}{\partial t} = -\lambda\varphi \qquad \Delta t < \frac{2}{\lambda}$$ numerical stability of explicit solvers

$$\frac{\partial(\varphi')}{\partial x} = -\frac{v_x}{D}\varphi' + stuff \qquad \frac{v_x}{D} = \lambda \qquad \Delta x < \frac{2}{\lambda} \Rightarrow \Delta x < \frac{2}{\frac{v_x}{D}}$$

$$\boxed{\mathrm{Pe}_{\mathrm{local}} < 2}$$

Achieve $\mathrm{Pe}_{\mathrm{local}} < 2$ by making Δx smaller. This leads to stiffness. Difficulties when implicit solving. Use adaptive meshing with Gear predictor-corrector.

$$D_{eff} = D_{true} + \frac{v_x \Delta x}{2} \qquad \left.\frac{\partial f}{\partial x}\right|_{xD} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} + O(\Delta x)$$

$$\mathrm{Pe}_{\mathrm{local}} < 2$$

Method of lines for flow only in x-direction

$$v_x\frac{\partial \varphi}{\partial x} + D\nabla^2\varphi + .....$$

$$v_x\frac{\partial \varphi}{\partial x} + D\frac{\partial^2 \varphi}{\partial x^2} + D\left(\frac{\varphi(x, y+\Delta y, z) - 2\varphi(x,y,z) + \varphi(x, y-\Delta y, z)}{(\Delta y)^2}\right) + .....$$

PDE → ODE {works only if: $v_y$, $v_z$ ~ negligible; $\mathrm{Pe}_{\mathrm{local}} < 2$}

Equations like this for all discrete z and y values in mesh.