10.34, Numerical Methods Applied to Chemical Engineering Professor William H. Green

Lecture #21: TA Tutorial on BVPs, FEMLAB®.

BVPs

What methods to use for each situation:

- 1D
- Finite Differences
- ODE's
 - 2nd order: → Two 1st order
 - 1st order: → Shooting



- 2D
- o Finite Differences
- o Method of Lines
 - Stiff
- o Non-uniform grid
- 3D
- o Finite Element

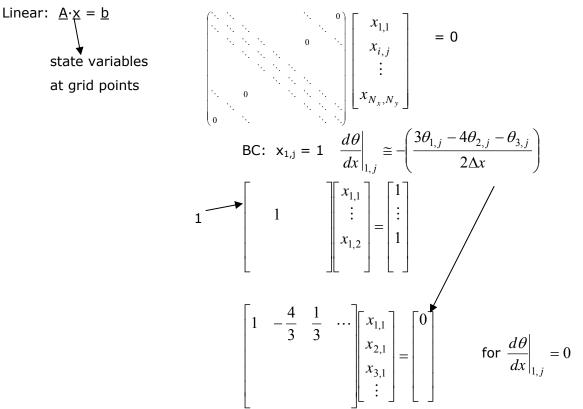
Figure 1. Boundary layer.

Capture the fast

portion of reaction with adaptive time stepping

Finite Element
 Figure 2. Adaptive time stepping.
 Finite Volume

Coding Boundary Conditions



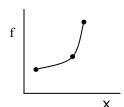
Cite as: William Green, Jr., course materials for 10.34 Numerical Methods Applied to Chemical Engineering, Fall 2006. MIT OpenCourseWare (http://ocw.mit.edu), Massachusetts Institute of Technology. Downloaded on [DD Month YYYY].

Nonlinear use fsolve

BC:
$$x_{1,j} = 1 \longrightarrow x_{1,j} - 1 = 0$$
 {set to zero}

Non-Uniform Grid

Throw out all original equations



$$p(x) = \Sigma f_i L_i(x)$$

polynomial between three points
$$p(x) = \sum_{i=0}^{N} f_i L_i(x) \qquad L_i(x) = \prod_{k=0}^{N} \left[\frac{x - x_k}{x_i - x_k} \right]$$

Figure 3. A graph of a polynomial fit of three points.

$$f(x) = f_1 \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} + f_2 \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} + f_3 \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}$$

 $\frac{df}{dx}$: differentiate the above expression f(x) and evaluate at x₂.

$$\frac{df}{dx}\bigg|_{x_2} = f_1 \frac{(x_2 - x_3)}{(x_1 - x_2)(x_1 - x_3)} + f_2 \frac{2x_2 - x_3 - x_1}{(x_2 - x_1)(x_2 - x_3)} + f_3 \frac{(x_2 - x_1)}{(x_3 - x_1)(x_3 - x_2)}$$

$$\left. \frac{d^2 f}{dx^2} \right|_{x_2} = \frac{2f_1}{(x_1 - x_2)(x_1 - x_3)} + \frac{2f_2}{(x_2 - x_1)(x_2 - x_3)} + \frac{2f_3}{(x_3 - x_1)(x_3 - x_2)}$$

MatLAB Equation: *nonuniform_example*

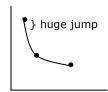


Figure 4. Graph of a function that is steep in the beginning.

Scaling

$$v_{z} \frac{\partial C_{A}}{\partial z} = D \left[\frac{\partial^{2} C_{A}}{\partial z^{2}} + \frac{\partial^{2} C_{A}}{\partial y^{2}} \right] + k(C_{A}C_{B} - C_{AB} / K)$$

$$Z = \frac{z}{L}$$

$$Y = \frac{y}{b}$$

$$\frac{\partial C_{A}}{\partial Z} = \left(\frac{DL}{v_{z}b^{2}} \right) \frac{\partial^{2} C_{A}}{\partial Y^{2}} + \left(\frac{D}{v_{z}L} \right) \frac{\partial^{2} C_{A}}{\partial Z^{2}} + \left(\frac{L}{v_{z}} \right) R$$

$$\frac{\partial C_A}{\partial Z} = 10^{-3} \frac{\partial^2 C_A}{\partial Y^2} \Rightarrow (dy)^2 = 10^{-3} \delta_Z$$

so if $\delta z = 10^{-1}$, choose $\delta y = 10^{-2}$

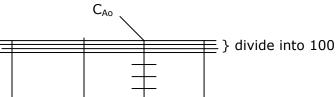


Figure 6. Non-uniform grid.

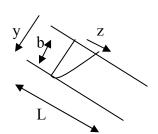


Figure 5. Diagram of pipe flow with reaction and diffusion.

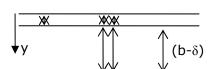
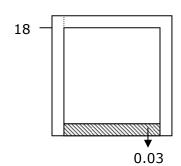


Figure 7. Division of problem into δ and (b- δ) regions.

$$\frac{\partial C_A}{\partial z} = 10^{-9} \frac{\partial^2 C_A}{\partial z^2}$$

Using FEMLAB®

* space dimension: axial symmetry 2D



axis/grid setting: $r_{min} = -0.01$

 $r_{\text{max}} = 0.06$

 $z_{min} = -1$

 $z_{max} = 20$

Figure 8. Diagram of FEMLAB Example.

Subdomain settings:

 $r = 0.001(r-(r/0.05)^2)$

Boundary settings:

mesh mode puts in finite elements.

Solve the problem.

DONE IN UNDER 3 MINUTES!!!