PSE for SPEED

Lecture 6b: Solution Strategies for Distributed Parameter Models

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Contents

- Partial differential equation types
- Initial and boundary conditions
- Finite difference methods
- Method of lines
- Method of weighted residuals
  - collocation
  - orthogonal collocation

Equation Types

Parabolic

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2}\right)$$

Elliptic

$$0 = D\left(\frac{\partial^2 c}{\partial x^2}\right)$$

Hyperbolic

$$\frac{\partial^2 c}{\partial t^2} = D\left(\frac{\partial^2 c}{\partial x^2}\right)$$

Initial and boundary conditions

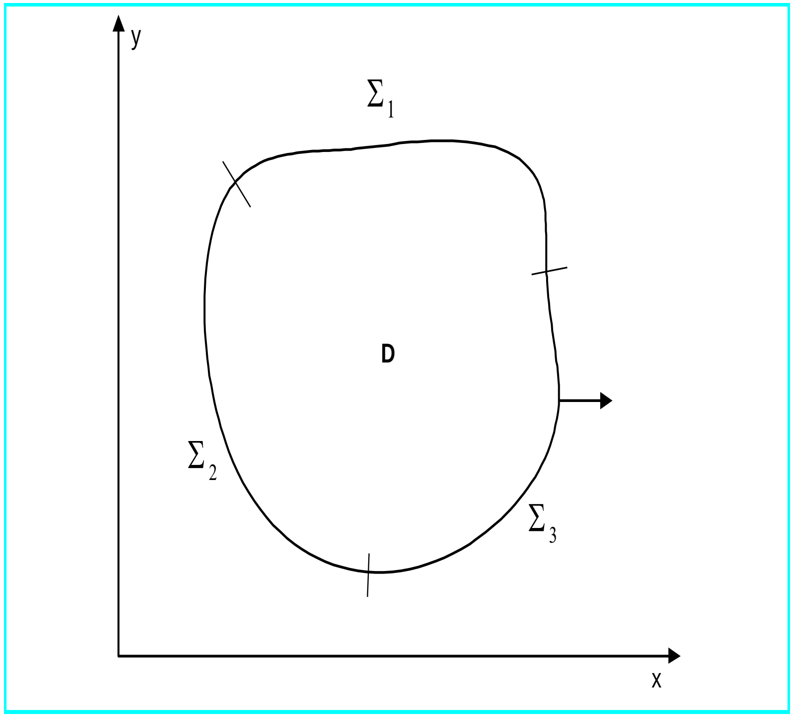
❖ Initial conditions needed for time varying problems

$u(x,y,z,t) = f(u)$ at $t = 0$

❖ Boundary conditions needed to set conditions on the balance volume surfaces. 3 main types exist:

- Dirichlet
- Neumann
- Robbins

Boundary Conditions



Dirichlet condition

$$\Phi = f(x,y) \text{ on } \sum_1$$

Neumann condition

$$\frac{\partial \Phi}{\partial n} = g(x,y) \text{ on } \sum_2$$

Robbins (third) condition

$$a(x,y)\Phi + \beta(x,y)\frac{\partial \Phi}{\partial n} = \gamma(x,y) \text{ on } \sum_3$$

Solution methods for DPS models

Original model

Algebraic equations

Differential equations

Finite difference (FD)

Finite element (FE)

Weighted residuals (WR)

Method of lines (MOL)

Shooting methods (SM)

Own reading: orthogonal collocation methods

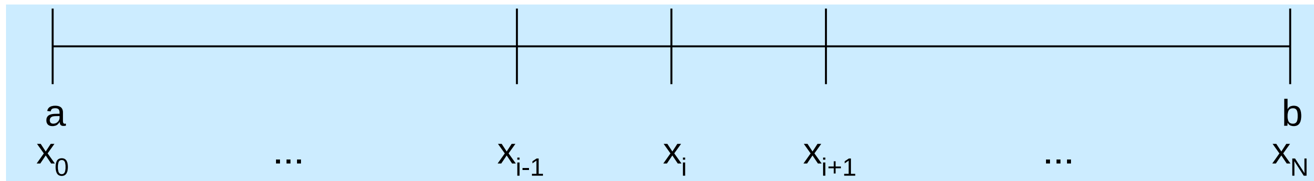
Finite Difference Methods (FDM)

- Popular and simple approach
- Seeks to replace derivative terms with finite difference approximations (FDA)
- Leads to large sets of algebraic equations (difference equations)
- Handles most problems with accuracy adjustable via grid spacing or order of FDA

Finite Difference Approximations (1)

❖ Based on a grid or mesh over the 1D or 2D domain

Grid definition



Grid points

$$\left.\begin{aligned} x_i &= a + i.\Delta x \quad 0 \le \mathrm{i} \le \mathrm{N} \\ \Delta \mathrm{x} &= (\mathrm{b} - \mathrm{a})/\mathrm{N} \end{aligned}\right\} \text{Uniform mesh}$$

❖ Mesh can have equal or non-equal spacing

❖ Uses various manipulations of the Taylor Series to generate FDAs

Finite Difference Approximations (2)

- Taylor series

$$u(x_i+\Delta x)=u(x_i)+\Delta x u'(x_i)+\frac{1}{2}\Delta x^2 u''(x_i)+\frac{1}{6}\Delta x^3 u'''(x_i)+\mathrm{K}$$

$$u(x_i-\Delta x)=u(x_i)-\Delta x u'(x_i)+\frac{1}{2}\Delta x^2 u''(x_i)-\frac{1}{6}\Delta x^3 u'''(x_i)+\mathrm{K}$$

- First order approximations

$$u_i'=\frac{du(x_i)}{dx}\simeq\frac{u_{i+1}-u_i}{\Delta x}+0(\Delta x)$$

$$u_i'=\frac{du(x_i)}{dx}\simeq\frac{u_i-u_{i-1}}{\Delta x}+0(\Delta x)$$

- Second order approximations

$$u_i'=\frac{du(x_i)}{dx}\simeq\frac{u_{i+1}-u_{i-1}}{2\Delta x}+0(\Delta x^2)$$

$$u_i''=\frac{d^2u(x_i)}{dx^2}\simeq\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta x^2}+0(\Delta x^2)$$

FDM - Application (1)

Unsteady diffusion

$$\frac{\partial c}{\partial t} = k\left(\frac{\partial^2 c}{\partial x^2}\right)$$

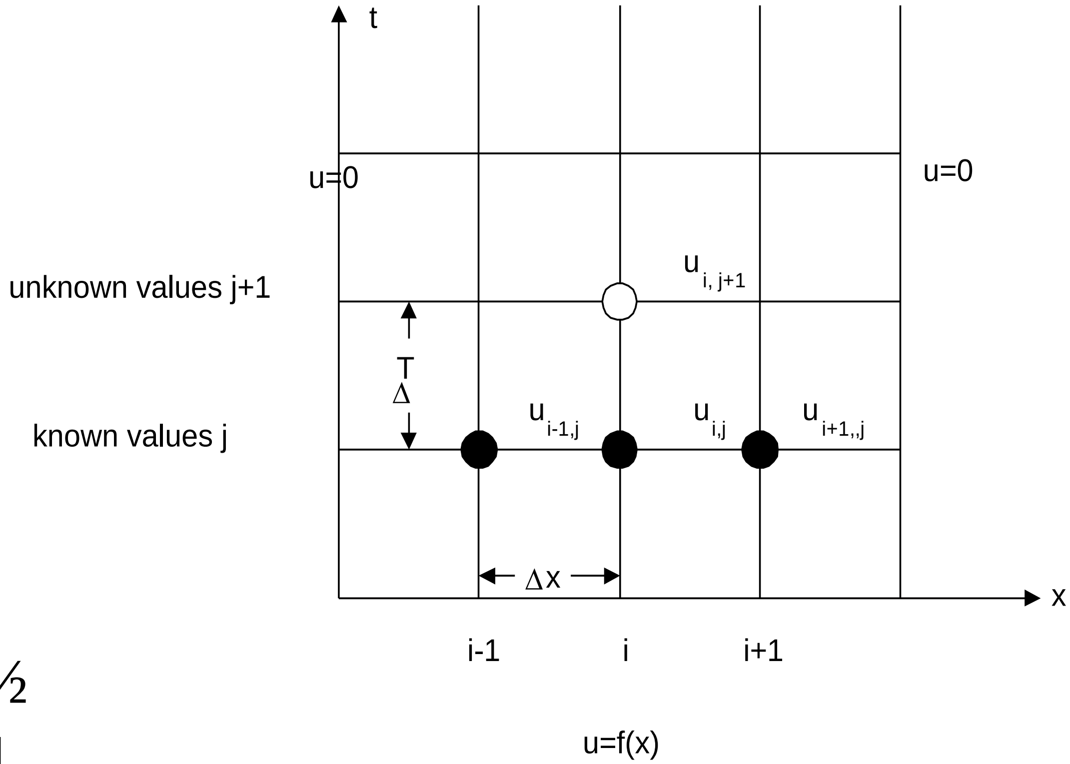
BCs:

u(0,t) = 1; u(1,t) = 0

ICs:

u(x,0) = 2x ;   0 < x ≤ ½

u(x,0) = 2 (1-x) ; ½ < x < 1



FDM - Application (2)

❖ Governing equation

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$$

Finite difference form

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

❖ Rearrange to:

$$u_{i,j+1} = u_{i.,j} + r(u_{i-1,j} - 2u_{i,j} + u_{i+1,j})$$

$$r = \frac{\Delta t}{\Delta x^2}$$

gives a set of algebraic equations to be solved explicitly

❖ Apply boundary conditions to difference equations

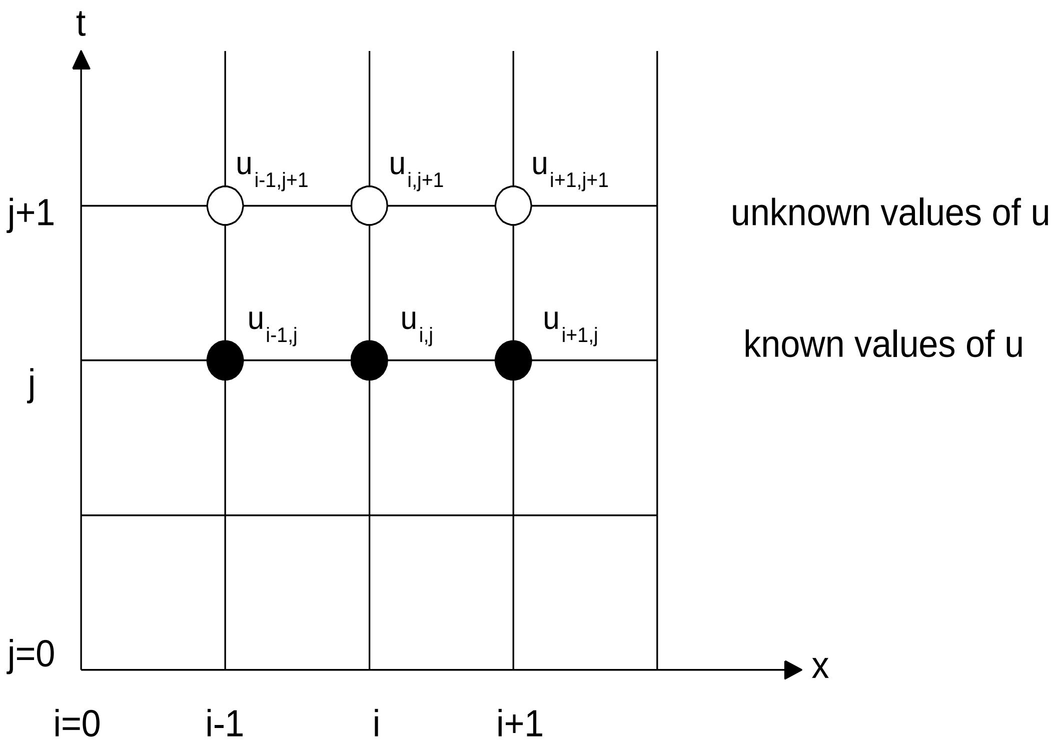
❖ Severe restrictions on *r* due to numerical stability of

$$0 < r \leq ½$$

FDM – Crank-Nicholson methods

- Introduce some implicit character to FDA of governing equation
- Improve numerical stability
- Three main methods
  - fully explicit method (cf. Euler)
  - Crank-Nicholson (original) method
  - fully implicit method (cf. Backward Euler)

Crank-Nicholson mesh



Explicit method:

$u_{i,j}$ only

C-N method:

mix $u_{i,j+1}$; $u_{i,j}$

Implicit method:

$u_{i-1,j+i}$, $u_{i,j+1}$, $u_{i+1,j+1}$

Crank-Nicolson application

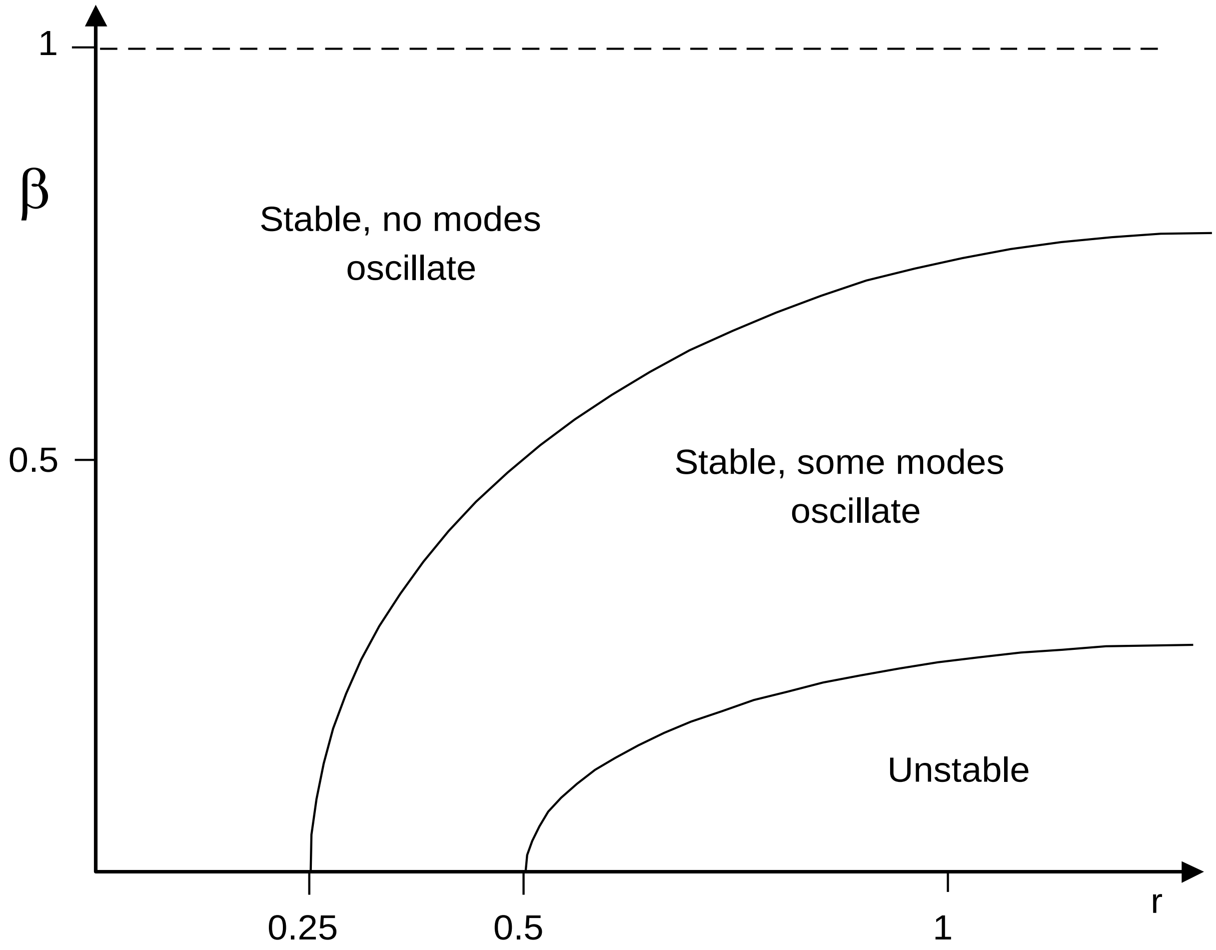
Governing equation: $$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

C-N-FDA:

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

Stable for: $$r = \frac{\Delta t}{\Delta x^2} \le \frac{0.5}{(1-2\beta)}$$

C-N - Stability Regions



Solving the finite difference equations

- Obtain matrix form: $Au_{j+1} = f(u_j)$
  (This is equivalent to the system: Ax=b)

- Solve using linear matrix methods
  - Matlab solution: x=A\b
  - Matlab factorization: [L,U]=lu(A) ;
    y=L\b ; x=U\y ;
- Iterate if nonlinear (F(x)=0)
  - Matlab solution: e.g. 'fsolve' routine

C-N solution example

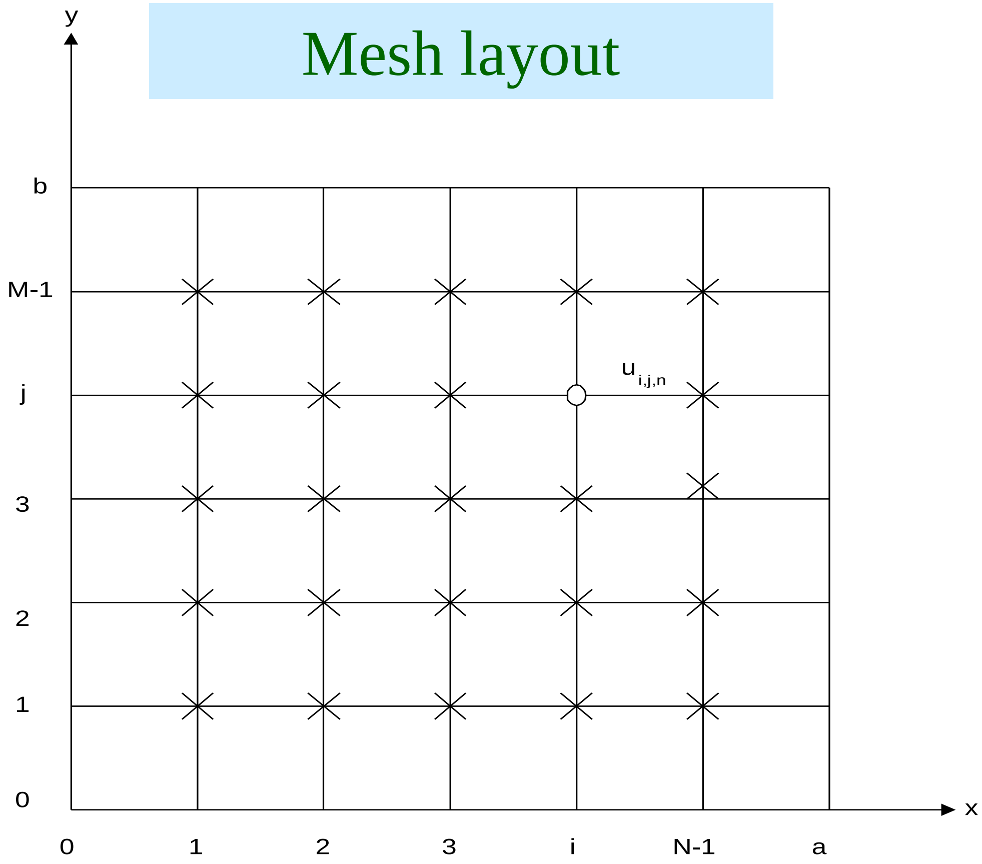
for $\beta = \dfrac{1}{2}$

get: $-u_{i-1,j+1} + 4u_{i,j+1} - u_{i+1,j+1} = u_{i-1,j} + u_{i+1,j}$

$$
\begin{pmatrix}
4 & -1 & & & & & & & & \\
-1 & 4 & -1 & & & & & & & \\
 & \ddots & \ddots & \ddots & & & & & & \\
 & & \ddots & \ddots & \ddots & & & & & \\
 & & & \ddots & \ddots & \ddots & & & & \\
 & & & & \ddots & \ddots & \ddots & & & \\
 & & & & & \ddots & \ddots & \ddots & & \\
 & & & & & & \ddots & \ddots & \ddots & \\
 & & & & & & & -4 & 4 & -1 \\
 & & & & & & & & -1 & 4
\end{pmatrix}
\begin{pmatrix}
u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{i,j+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{9,j+1}
\end{pmatrix}
=
\begin{pmatrix}
u_{0,j} + u_{2,j} \\ u_{1,j} + u_{3,j} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ u_{8,j} + u_{10,j}
\end{pmatrix}
$$

FD methods for Parabolic Equations

Mesh layout



Mesh definition

$$u(i\Delta x,\, j\Delta y,\, u\Delta t) = u_{i,j,n}$$

where

$$x = i\Delta x$$
$$y = j\Delta y$$
$$t = n\Delta t$$

FDM example - Parabolic Equation

❖ Governing equation:

$$\frac{\partial u}{\partial t} = k\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

❖ Explicit FDA:

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

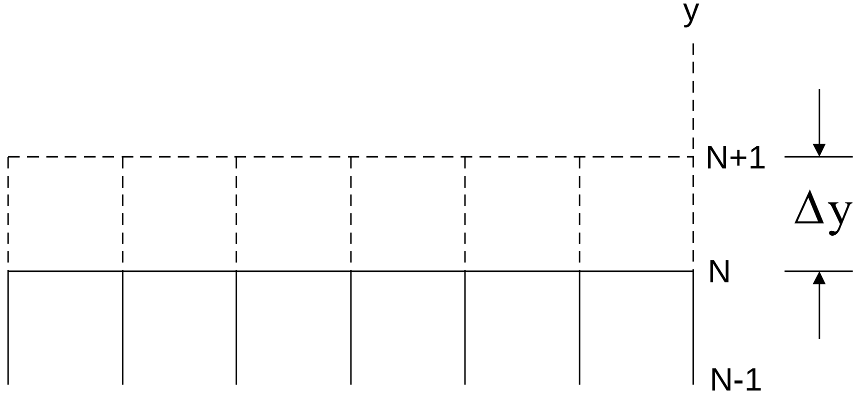
❖ Stability limit is:

$$k\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)\Delta t \le \frac{1}{2}$$

Handling Derivative Boundary Conditions

- ❖Neumann condition $$\frac{\partial T}{\partial y} = -T \quad \text{on} \quad y = 1$$

- ❖Create "false" boundary



- ❖Write central difference approximation for BC at j=N.

- ❖Eliminate fictitious value $T_{i,N+1}$ by substitution of FDA of BC into FDA of equation.

Method of Lines (MOL)

Key features:

- Converts parabolic PDEs to ODEs
- Discretizes the spatial variable(s) by using finite difference approximations
- Can result in sets of stiff ODEs
- Simple computer implementation

Method of Lines - application

Governing equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

Discretize spatial terms to get:

$$\frac{du_i}{dt} = f_i(u) \qquad i = 0(1)N$$

Apply appropriate boundary conditions (at i=0, i=N)

Method of Lines - example

Problem:

$$\frac{\partial c}{\partial t} = \alpha \nabla^2 c + \beta R(c)$$

$$\frac{\partial c}{\partial r} = 0 \text{ at } r = 0; \quad \frac{\partial c}{\partial r} = Bi_w(c(1,z) - c_w(Z))$$

MOL gives:

$$\frac{dc_i}{dt} = \alpha\left(\frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta r^2} + \left(\frac{\alpha - 1}{r_i}\right)\frac{c_{i+1} - c_{i-1}}{2\Delta r}\right) + \beta R_i$$

BCs give:

$$\frac{c_1 - c_{-1}}{2\Delta r} = 0 \quad ; \quad \frac{c_{N+1} - c_{N-1}}{2\Delta r} = Bi_w(c_N - c_w)$$

$$c_{-1} = c_1 \quad ; \quad c_{N+1} = c_{N-1} + 2\Delta r Bi_w(c_N - c_w)$$

Method of Lines – example (cont.)

Final equation set:

$$\frac{dc_0}{dt} = \frac{2a\alpha}{\Delta r^2}(c_1 - c_0) + \beta R_c$$

$$\frac{dc_i}{dt} = \alpha\left(\frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta r^2} + \left(\frac{\alpha - 1}{r_i}\right)\frac{c_{i+1} - c_{i-1}}{2\Delta r}\right) + \beta R_i \quad i = 1(1)N-1$$

$$\frac{dc_N}{dt} = \alpha\left(\frac{2c_{N-1} + Bi_w 2\Delta r(c_N - c_w) - 2c_N}{\Delta r^2} + (a-1)(2\Delta r Bi_w (c_N - c_w)\right) + \beta R_N$$

Method of Weighted Residuals (MOWR)

Key characteristics:

It is a polynomial approximation method with the following steps:

- choose a polynomial form
- fit the BCs to the polynomial
- substitute approximate solution into PDE
- distribute the error by making residual zero:
    - *collocation, least squares*
    - *Galerkin, subdomain, moments*

It is a powerful technique with accurate results from low order polynomials

MOWR - Application Example (1)

Problem: $$\frac{d}{dx}\left[(1+\alpha u)\frac{du}{dx}\right] = (1+\alpha u)\frac{d^2u}{dx^2} + \alpha\left(\frac{du}{dx}\right)^2 = 0 \;\; ; \;\; u(0)=0, \; u(1)=1$$

Trial function: $$\phi_N = \sum_{i=0}^{N+1} c_i x^i$$ (power series in x)

Fit BCs:

$$\phi_N(0) = 0 \rightarrow c_0 = 0$$ BC at x=0

$$\phi_N(1) = 1 \rightarrow \sum_{i=1}^{N+1} c_i = 1$$ BC at x=1

$$\phi_N = x + \sum_{i=1}^{N} A_i\left(x^{i+1} - x\right)$$ modified trial function

Terms:

$$\phi_1 = x + A_1(x^2 - x)$$
$$\phi_1' = 1 + A_1(2x - 1)$$
$$\phi_1'' = 2A_1$$

trial functions for N=1

MOWR - Application Example (2)

Form the residual equation (substitute trial function):

$$R(x,\phi_1) = \{1+\alpha[x+A_1(x^2-x)]\}2A_1 + \alpha[1+A_1(2x-1)]^2$$

for collocation at x = ½, α = 1 residual R(½, ϕ_1)=0 is:

$$-\frac{1}{2}A_1^2 + 3A_1 + 1 = 0$$
$$A_1 = -0.3166$$

Approximate first order solution is therefore:

$$\phi_1 = x - 0.3166(x^2 - x)$$

$$\varphi_1 = 0.5795; at, x = 0.5; (true = 0.5811)$$

MOWR - Orthogonal Collocation

❖Similar to standard collocation except polynomials are orthogonal with predefined roots

❖Solve directly for solution *y(x)* and collocation point *x*;

❖Use of symmetric or non-symmetric polynomials depending on whether problem has symmetry, e.g. $\frac{\partial c}{\partial y} = 0 \quad \text{at} \quad x = 0$

❖Handles major geometries easily (built into polynomials)

- planar
- cylindrical
- spherical

Orthogonal Collocation with Symmetry

Problem: Diffusion and reaction in a planar catalyst pellet

$$\frac{d^2y}{dx^2} = \phi^2 R(y) \quad ; \; R(y) = y^2$$

BCs

$$\frac{dy}{dx} = 0 \quad at \; x = 0 \; ; \; y(1) = 1$$

Residual equations obtained by substituting for terms as:

For N=1: $$\sum_{i=1}^{N+1} B_{ji} y_i = \phi^2 R(y_j) \quad j = 1(1)N$$

$$B_{11} y_1 + B_{12} y_2 = \phi^2 y_1^2$$

$$B_{11} = -2.5 \; ; \; B_{12} = 2.5$$

These are pre-calculated coefficients

BC: $y_2 = 1$

Solution: $$y_1 = \frac{-2.5 + \sqrt{6.25 + 10\phi^2}}{2\phi^2}$$

Example: OC without symmetry

Problem:

$$\frac{d}{dx}\left[c(u)\frac{du}{dx}\right]=0$$

$$u(0)=0 \quad u(1)=1$$

$$c(u)=1+u$$

$$(1+u)\frac{d^2u}{dx^2}+\left(\frac{du}{dx}\right)^2=0$$

Residual equations:

$$(1+u_j)\sum_{i=1}^{N+2} B_{ji}u_i+\left[\sum_{i=1}^{N+2} A_{ji}u_i\right]^2=0 \quad j=2(1)(N+1)$$

BCs:

$$u_1=0$$

$$u_{N+2}=1$$

For N=1:

$$(1+u_2)\sum_{i=1}^{3} B_{2i}u_i+\left(\sum_{i=1}^{3} A_{2i}u_i\right)^2=0 \quad j=2$$

$$(1+u_2)(4u_1-8u_2+4u_3)+(-u_1+u_3)^2=0$$

Solution is:

$$u_1=0 \quad , \quad u_3=1 \quad , \quad u_2=0.579$$

Orthogonal collocation on elements

- Useful technique for problems with sharp fronts
- Extension of standard OC method
- Easily implemented technique (convert PDEs and ODEs with polynomial coeffi cients **A** as a function of time; solve ODEs)
- Allows low order polynomials on the elements
- Computationally efficient

Example: OC for parabolic PDE

Problem: $$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x} \right) + R(u)$$

BCs: $u(0,t) = 1 \;\; ; \;\; u(1,t) = 0$ ICs: $u(x,0) = 0$

Residual equations: $$\frac{du_j}{dt} = \sum_{i=1}^{N+2} A_{j,i} D(u_i) \sum_{z=1}^{N+2} A_{i,z} u_z + R(u_j) \qquad j = 1,\dots, N$$

BCs: $u_1(t) = 1 \;\; ; \;\; u_{N+2}(t) = 0$

Solve as a set of N ODEs

Modelling exercise – 5c: Solution of PDEs

Solve the following problems with MoT

* 2nd order PDE
* Unsteady state heat-transfer
* 1st- & 2nd-order PDAE

Model equations will be given in class