Introduction to Simulation - Lecture 20

Finite-Difference Methods for Boundary Value Problems

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Thanks to Jaime Peraire

Outline

- Informal Finite Difference Methods
  - Heat Conducting Bar
- More Formal Analysis of Finite-Difference Methods
  - Heat Equation
  - Consistency + Stability yields Convergence

Heat Flow

1-D Example

Discrete Representation

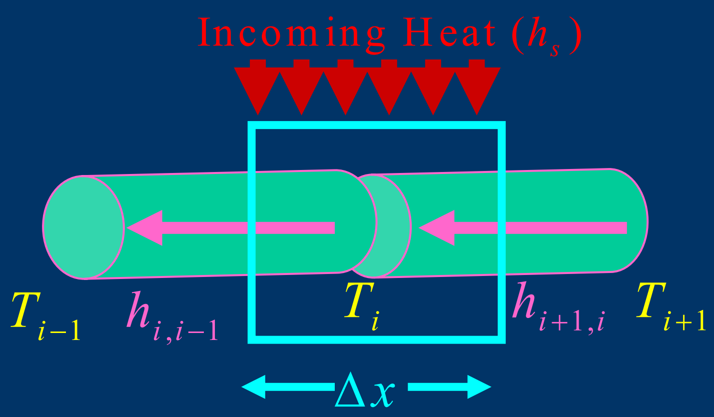
1) Cut the bar into short sections

2) Assign each cut a temperature

Heat Flow

1-D Example

Equation Formulation



$$h_{i+1,i} = \text{heat flow} = \kappa \frac{T_{i+1} - T_i}{\Delta x}$$

$$h_{i+1,i} - h_{i,i-1} = -h_s \Delta x$$

Heat in from left

Heat out from right

Incoming heat per unit length

Limit as the sections become vanishingly small

$$\lim_{\Delta x \to 0} h_s(x) = \frac{\partial h(x)}{\partial x} = \frac{\partial}{\partial x} \kappa \frac{\partial T(x)}{\partial x}$$

Normalized Equation

$$\frac{\partial}{\partial x}\kappa\frac{\partial T(x)}{\partial x} = -h_s \Rightarrow -\frac{\partial^2 u(x)}{\partial x^2} = f(x)$$

$$-u_{xx}(x) = f(x)$$

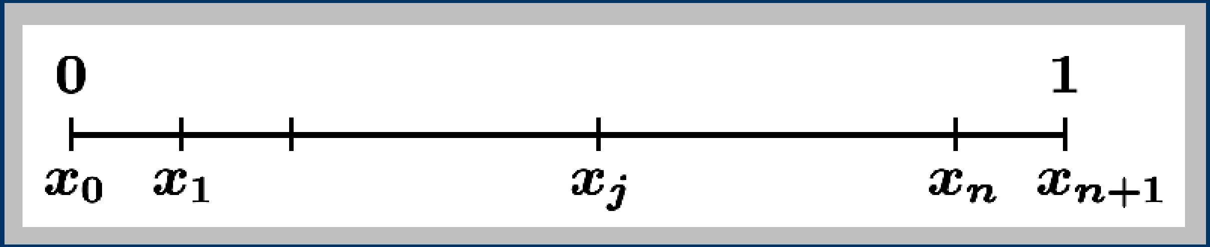
Numerical Solution

Finite Differences

Discretization

Subdivide interval $(0,1)$ into $n+1$ equal subintervals

$$\Delta x = \frac{1}{n+1}$$



$$x_j = j\Delta x, \qquad \hat{u}_j \approx u_j \equiv u(x_j)$$

for $\quad 0 \le j \le n+1$

Numerical Solution

Finite Differences

Approximation

For example . . .

$$
\begin{aligned}
v''(x_j) &\approx \frac{1}{\Delta x}(v'(x_{j+1/2}) - v'(x_{j-1/2})) \\
&\approx \frac{1}{\Delta x}(\frac{v_{j+1} - v_j}{\Delta x} - \frac{v_j - v_{j-1}}{\Delta x}) \\
&= \frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2}
\end{aligned}
$$

for Δx small

Numerical Solution

Finite Differences

Equations...

$-u_{xx} = f$ suggests . . .

$$-\frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} = f(x_j) \quad 1 \le j \le n$$

$$\hat{u}_0 = \hat{u}_{n+1} = 0$$

$$\Longrightarrow \qquad \boxed{A\,\underline{\hat{u}} = \underline{f}}$$

Numerical Solution

Finite Differences

...Equations

$$A = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \vdots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad \underline{\hat{u}} = \begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \vdots \\ \hat{u}_{n-1} \\ \hat{u}_n \end{pmatrix}, \quad \underline{f} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{n-1}) \\ f(x_n) \end{pmatrix}$$

(Symmetric)

$$A \in \mathbb{R}^{n \times n} \qquad \underline{\hat{u}}, \ \underline{f} \in \mathbb{R}^n$$

Numerical Solution

Finite Differences

Solution

Is A non-singular ?

For any $\underline{v} = \{v_1, v_2, \ldots, v_n\}^T$

$$\underline{v}^T A \, \underline{v} = \frac{1}{\Delta x^2}\left(v_1^2 + \sum_{i=2}^{n}(v_i - v_{i-1})^2 + v_n^2\right)$$

Hence $\boxed{\underline{v}^T A \, \underline{v} > 0, \text{ for any } \underline{v} \neq 0}$ (A is **SPD**)

$A \, \underline{\hat{u}} = \underline{f}$: $\underline{\hat{u}}$ **exists** and is **unique**

Numerical Solution

Finite Differences

Example...

$$-u_{xx} = (3x + x^2)e^x, \qquad x \in (0, 1)$$

with

$$u(0) = u(1) = 0.$$

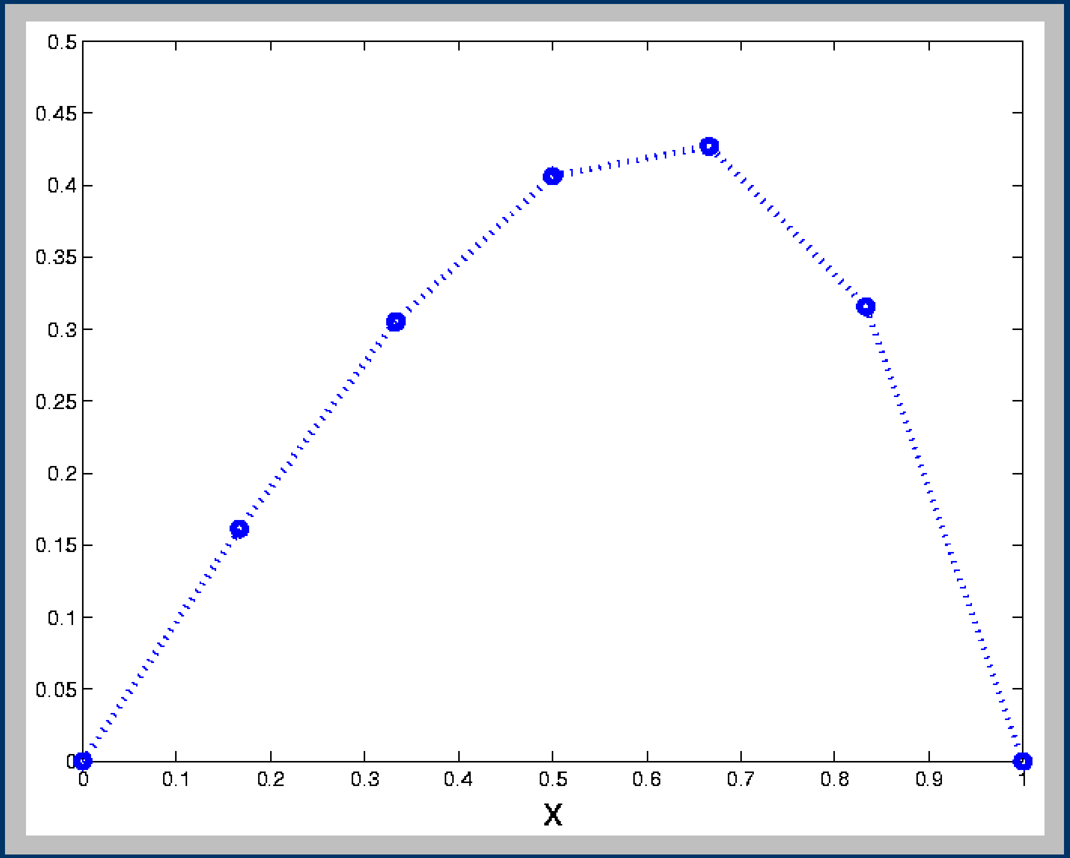
Take $n = 5,\ \Delta x = 1/6\ \ldots$

Numerical Solution

Finite Differences

...Example

$\hat{u}$



Numerical Solution

Finite Differences

Convergence ?

1. Does the discrete solution $\hat{u}$ retain the qualitative propeties of the continuous solution $u(x)$?

2. Does the solution become more accurate when $\Delta x \to 0$?

3. Can we make $|u(x_j) - \hat{u}_j|$ for $0 \leq j \leq n+1$ arbitrarily small?

Discretization Error Analysis

Properties of A^{-1}

Let

$$A^{-1} = \{\alpha_{ij}\}_{1 \le i,j \le n}$$

- Non-negativity

$$\alpha_{ij} \ge 0, \qquad \text{for} \qquad 1 \le i, j \le n$$

- Boundedness

$$0 \le \sum_{j=1}^{N} \alpha_{ij} \le \frac{1}{8}, \qquad \text{for} \qquad 1 \le i \le n$$

Discretization Error Analysis

Qualitative Properties of $\hat{u}$

$$f \geq 0 \quad \rightarrow \quad \hat{u} \geq 0$$

$$\underline{\hat{u}} = A^{-1}\, \underline{f}$$

If

$$f_j = f(x_j) \geq 0\,, \qquad \text{for} \quad 1 \leq j \leq n$$

Then

$$\hat{u}_i = \sum_j \alpha_{ij} f_j \geq 0\,, \qquad \text{for} \quad 1 \leq i \leq n$$

Discretization Error Analysis

Qualitative Properties of $\hat{u}$

Discrete Stability

$$\underline{\hat{u}} = A^{-1}\,\underline{f}$$

$$||\underline{\hat{u}}||_\infty = \max_i |\hat{u}_i| = \max_i (|\sum_j \alpha_{ij} f_j|)$$

$$\leq \max_i (\sum_j \alpha_{ij}) \max_i |f_i|$$

$$\leq \frac{1}{8} ||\underline{f}||_\infty$$

Discretization Error Analysis

Truncation Error

For any $v \in C^4$ we can show that

$$\frac{v(x_{j+1}) - 2v(x_j) + v(x_{j-1})}{\Delta x^2} = v''(x_j) + \frac{\Delta x^2}{12} v^{(4)}(x_j + \theta \Delta x)$$

$$-1 \le \theta \le 1$$

Take $u \equiv v \qquad (-u'' = f)$

$$-\frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{\Delta x^2} = f(x_j) \underbrace{- \frac{\Delta x^2}{12} u^{(4)}(x_j + \theta_j \Delta x)}_{\tau_j}$$

Discretization Error Analysis

Error Equation

Let $e_j = u(x_j) - \hat{u}_j$ be the **discretization error**.

$$-\frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{\Delta x^2} = f(x_j) + \tau_j$$

$$-\frac{\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}}{\Delta x^2} = f(x_j)$$

Subtracting

$$-\frac{e_{j+1} - 2e_j + e_{j-1}}{\Delta x^2} = \tau_j, \qquad 1 \le j \le n$$

and

$$e_0 = e_{n+1} = 0$$

Discretization Error Analysis

Error Equation

$$\boxed{A\,\underline{e} = \underline{\tau}}$$

$$\underline{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ \vdots \\ e_N \end{pmatrix}, \qquad \underline{\tau} = \frac{\Delta x^2}{12} \begin{pmatrix} u^{(4)}(x_1 + \theta_1 \Delta x) \\ u^{(4)}(x_2 + \theta_2 \Delta x) \\ \vdots \\ \vdots \\ u^{(4)}(x_N + \theta_N \Delta x) \end{pmatrix}$$

Discretization Error Analysis

Convergence

Using the discrete stability estimate on $\underline{A}\,\underline{e} = \underline{\tau}$

$$||\underline{e}||_\infty \leq \frac{1}{8}||\underline{\tau}||_\infty$$

or

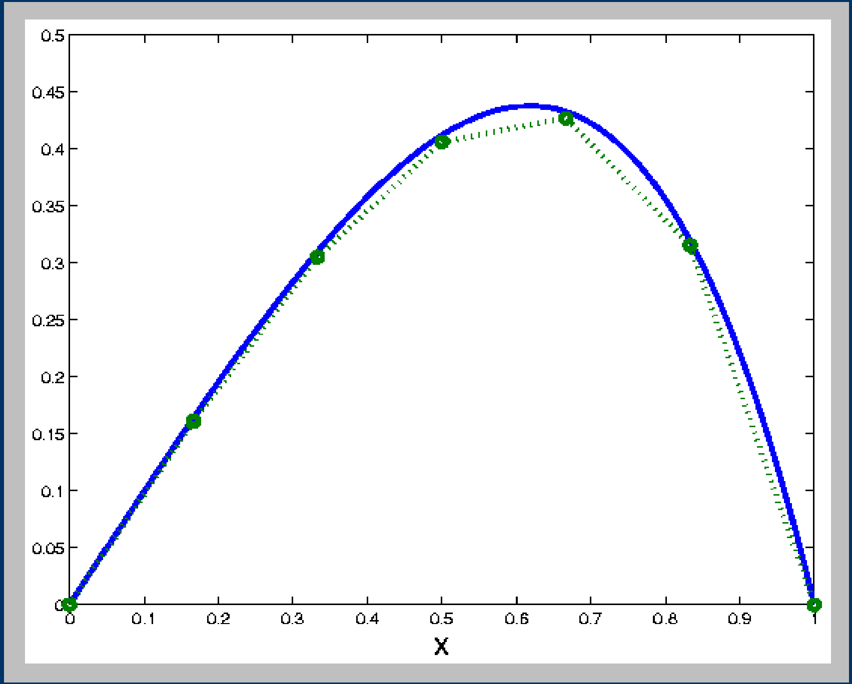
$$\max_{1 \leq i \leq n} |u(x_i) - \hat{u}_i| \leq \frac{\Delta x^2}{96} \max_{0 \leq x \leq 1} |u^{(4)}(x)|$$

A-priori Error Estimate

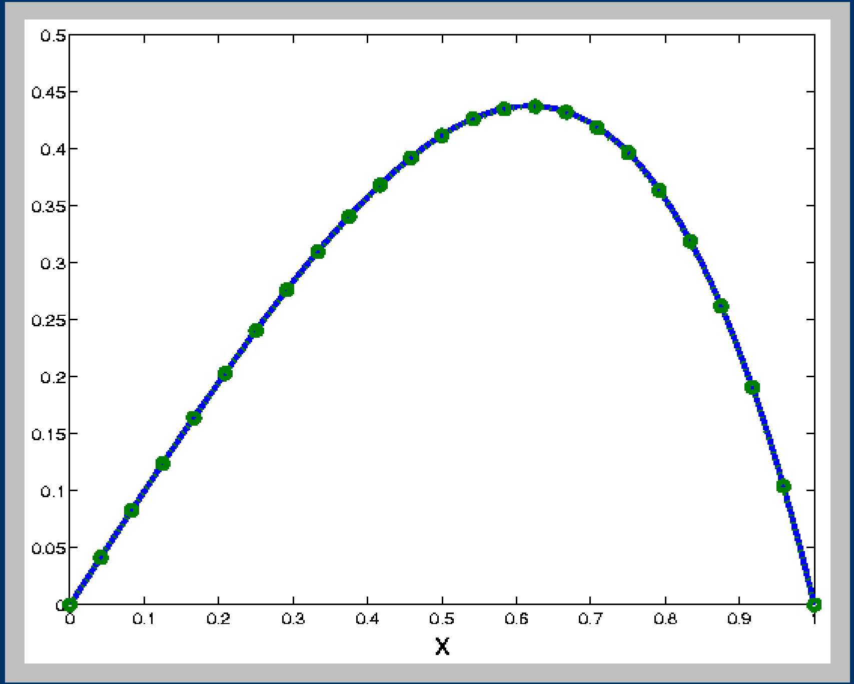
Discretization Error Analysis

Numerical Example

$$-u_{xx} = (3x + x^2)e^x, \quad x \in (0,1), \quad u(0) = u(1) = 0$$



$\Delta x = 1/6$



$\Delta x = 1/24$

Discretization Error Analysis

Numerical Example

EXAMPLE : $-u_{xx} = (3x + x^2)e^x, \; x \in (0,1)$

$n+1$	$\|\|\underline{u} - \underline{\hat{u}}\|\|_\infty$
3	0.0227
6	0.0059
12	0.0015
24	$3.756e-04$
48	$9.404e-05$
96	$2.350e-05$
192	$5.876e-06$

Asymptotically,

$$\|\underline{u} - \underline{\hat{u}}\|_\infty \approx C \Delta x^\alpha$$

$$C = 0.216623$$

$$\alpha = 2.000$$

Summary

- For a simple model problem we can produce numerical approximations of **arbitrary accuracy**.

- An **a-priori error estimate** gives the asymptotic dependence of the solution error on the discretization size Δx.

Generalizations

Definitions

Consider a linear elliptic **differential equation**

$$\boxed{\mathcal{L}\, u = f}$$

and a **difference scheme**

$$\boxed{\hat{\mathcal{L}}\, \underline{\hat{u}} = \underline{\hat{f}}}$$

Generalizations

Consistency

The difference scheme is **consistent** with the differential equation if:

For **all** smooth functions v

$$(\hat{\mathcal{L}}\underline{v} - \underline{\hat{f}})_j - (\mathcal{L}v - f)_j \to 0, \quad \text{for } j = 1, \ldots, n$$

when $\Delta x \to 0$.

$$(\hat{\mathcal{L}}\underline{v} - \underline{\hat{f}})_j - (\mathcal{L}v - f)_j = \mathcal{O}(\Delta x^p) \text{ for all } j$$

$\Rightarrow$ p is **order of accuracy**

Generalizations

Truncation Error

$$(\hat{\mathcal{L}}\underline{u} - \underline{\hat{f}})_j - \underbrace{(\mathcal{L}u - f)_j}_{=0} = \tau_j, \quad \text{for} \ \ j = 1, \ldots, n$$

or,

$$\hat{\mathcal{L}}\underline{u} - \underline{\hat{f}} = \underline{\tau} \ .$$

The truncation error results from inserting the exact solution into the difference scheme.

Consistency $\Rightarrow \ ||\underline{\tau}||_\infty = \mathcal{O}(\Delta x^p)$

Generalizations

Error Equation

Original scheme

$$\hat{\mathcal{L}}\,\underline{\hat{u}} = \underline{\hat{f}}$$

Consistency

$$\hat{\mathcal{L}}\,\underline{u} = \underline{\hat{f}} + \underline{\tau}$$

The error $\underline{e} = \underline{u} - \underline{\hat{u}}$ satisfies

$$\boxed{\hat{\mathcal{L}}\underline{e} = \underline{\tau}\ .}$$

Generalizations

Stability

Matrix norm

$$||M||_\infty = \sup_{\underline{v} \in \mathbb{R}^n} \frac{||M\underline{v}||_\infty}{||\underline{v}||_\infty}$$

The difference scheme is **stable** if

$$||\hat{\mathcal{L}}^{-1}||_\infty \leq C \quad \text{(independent of } \Delta x\text{)}$$

Generalizations

Stability

$$\|M\|_\infty = \sup_{\|\underline{v}\|_\infty = 1} \|M\underline{v}\|_\infty$$

$$= \sup_{\|\underline{v}\|_\infty = 1} \left(\max_i \left| \sum_{j=1}^{n} m_{ij} v_j \right| \right)$$

$$= \max_i \left(\sup_{\|\underline{v}\|_\infty = 1} \left| \sum_{j=1}^{n} m_{ij} v_j \right| \right) \qquad v_j = \text{sign}(m_{ij})$$

$$= \max_i \sum_{j=1}^{n} |m_{ij}|$$ **(max row sum)**

Generalizations

Convergence

Error equation

$$\underline{e} = \hat{\mathcal{L}}^{-1} \, \underline{\tau}$$

Taking norms

$$||\underline{e}||_\infty = ||\hat{\mathcal{L}}^{-1} \, \underline{\tau}||_\infty$$

$$\leq ||\hat{\mathcal{L}}^{-1}||_\infty \, ||\underline{\tau}||_\infty$$

$$\leq \underbrace{||\hat{\mathcal{L}}^{-1}||_\infty \, C}_{C_1} \, \Delta x^p = C_1 \, \Delta x^p$$

Generalizations

Summary

Consistency + Stability $\Rightarrow$ Convergence

Convergence		Stability		Consistency
$\|\|\underline{e}\|\|_\infty$	$\leq$	$\|\|\hat{\mathcal{L}}^{-1}\|\|_\infty$	$\cdot$	$\|\|\underline{\tau}\|\|_\infty$

Summary

- Informal Finite Difference Methods
  - Heat Conducting Bar
- More Formal Analysis of Finite-Difference Methods
  - Heat Equation
  - Consistency + Stability yields Convergence