Numerical Techniques for PDE

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A good many times I have been present at gatherings of people who, by the standards of traditional culture, are thought highly educated and who have with considerable gusto been expressing their incredulity at the illiteracy of scientists. Once or twice I have been provoked and have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative. Yet I was asking something which is about the scientific equivalent of: Have you read a work of Shakespeare’s?”  
C. P. Snow, The Two Cultures and the Scientific Revolution
Canonical Forms and Important PDE

Hyperbolic:

First-Order:
\[ u_t + cu_x = 0 \]
\[ u(0, x) = f(x) \]

Solution: \( u(t, x) = f(x - ct) \)

Second-Order:
\[ u_{tt} - c^2 u_{xx} = 0 \]
\[ u(0, x) = f(x), \quad u_t(0, x) = g(x) \]

Solution: \[ u(t, x) = \frac{1}{2} [f(x - ct) + f(x + ct)] + \frac{1}{2c} \int_{x-ct}^{x+ct} g(y) \, dy \]
Canonical Forms and Important PDE

**Parabolic** e.g., Heat equation

\[ u_t = \alpha u_{xx} \]

\[ u(0, x) = f(x) \]

\[ u(t, 0) = u(t, L) = 0 \]

Solution:

\[ u(t, x) = \sum_{n=1}^{\infty} a_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x) \]

where \( \lambda_n = \frac{n\pi}{L} \) and

\[ a_n = \frac{2}{L} \int_0^L f(x) \sin(\lambda_n x) \, dx \]
Canonical Forms and Important PDE

**Elliptic** e.g., Laplace’s equation

\[ u_{xx} + u_{yy} = 0, \quad (x, y) \in \Omega \]
\[ u(x, y) = f(x, y), \quad (x, y) \in \partial \Omega \]

Solution:

\[ u(x, y) = \sum_{n=1}^{\infty} B_n \sin(\lambda_n x) \sinh(\lambda_n y) \]

where \( \lambda_n = \frac{n\pi}{a} \) and

\[ B_n = \frac{2}{a \sinh(\lambda_n b)} \int_{0}^{a} f_2(x) \sin(\lambda_n x) dx \]

**Physical Examples:** Steady state heat behavior; steady state structural deformations
Canonical Forms and Important PDE

Rod Model:

\[ \rho A \frac{\partial^2 u}{\partial t^2} - Y A \frac{\partial^2 u}{\partial x^2} - c A \frac{\partial^3 u}{\partial x^2 \partial t} = f \]

Boundary Conditions:

\[ u(t, 0) = 0 \]

\[ N(t, \ell) = -k]\ell u(t, \ell) - c\ell \frac{\partial u}{\partial t}(t, \ell) - m\ell \frac{\partial^2 u}{\partial t^2}(t, \ell) \]

Weak Formulation:

\[
\int_0^\ell \rho A \frac{\partial^2 u}{\partial t^2} \phi dx + \int_0^\ell \left[ Y A \frac{\partial u}{\partial x} + c A \frac{\partial^2 u}{\partial x \partial t} \right] \frac{d\phi}{dx} dx \\
= \int_0^\ell f \phi dx - \left[ k\ell u(t, \ell) + c\ell \frac{\partial u}{\partial t}(t, \ell) + m\ell \frac{\partial^2 u}{\partial t^2}(t, \ell) \right] \phi(\ell)
\]

for all \((\phi, \varphi) = (\phi, \phi(\ell)) \in V\)
Canonical Forms and Important PDE

Beam Model:

\[ \rho \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = f(t, x) \]

\[ w(t, 0) = \frac{\partial w}{\partial x}(t, 0) = 0 \]

\[ M(t, \ell) = \frac{\partial M}{\partial x}(t, \ell) = 0 \]

where \( M(t, x) = -Y I(x) \frac{\partial^2 w}{\partial x^2} - cI \frac{\partial^3 w}{\partial x^2 \partial t} + k_p(x)V(t) \)

Weak Formulation:

\[ \int_0^\ell \rho \frac{\partial^2 w}{\partial t^2} \phi \, dx + \int_0^\ell \gamma \frac{\partial w}{\partial t} \phi \, dx + \int_0^\ell Y I \frac{\partial^2 w}{\partial x^2} \frac{d^2 \phi}{dx^2} \, dx + \int_0^\ell c I \frac{\partial^3 w}{\partial x^2 \partial t} \frac{d^2 \phi}{dx^2} \, dx = \int_0^\ell f \phi \, dx + \int_0^\ell k_p V(t) \frac{d^2 \phi}{dx^2} \, dx \]

for all \( \phi \in V = H_0^2(0, \ell) \)
Approximation Techniques for the Rod Model: Galerkin

Linear Basis:

\[ \phi_j(x) = \frac{1}{h} \begin{cases} 
  x - x_{j-1}, & x_{j-1} \leq x < x_j \\
  x_{j+1} - x, & x_j \leq x \leq x_{j+1} \\
  0, & \text{otherwise}
\end{cases} \]

Approximate Solution:

\[ u^N(t, x) = \sum_{j=1}^{N} u_j(t) \phi_j(x) \]

System:

\[ \sum_{j=1}^{N} \int_{0}^{\ell} \rho A \phi_i \phi_j \, dx + \sum_{j=1}^{N} \int_{0}^{\ell} c A \phi'_i \phi'_j \, dx + \sum_{j=1}^{N} u_j(t) \int_{0}^{\ell} Y A \phi'_i \phi'_j \, dx \]

\[ = \int_{0}^{\ell} f \phi_i \, dx - \left( k_\ell u_N(t) \phi_N(\ell) + c_\ell \ddot{u}_N(t) \phi_N(\ell) + m_\ell \dddot{u}_N(t) \phi_N(\ell) \right) \phi_N(\ell) \]

for \( i = 1, \cdots, N \)
Approximation Techniques for the Rod Model: Galerkin

2nd-Order Vector System:

\[ \mathbf{M} \ddot{\mathbf{u}}(t) + \mathbf{Q} \dot{\mathbf{u}} + \mathbf{K} \mathbf{u}(t) = \mathbf{f}(t) \]

where \( \mathbf{u}(t) = [u_1(t), \ldots, u_N(t)]^T \) and

\[
[M]_{ij} = \begin{cases} 
\int_0^\ell \rho A \phi_i \phi_j \, dx , & i \neq N \text{ or } j \neq N \\
\int_0^\ell \rho A \phi_i \phi_j \, dx + m_\ell , & i = N \text{ and } j = N
\end{cases}
\]

\[
[K]_{ij} = \begin{cases} 
\int_0^\ell Y A \phi_i' \phi_j' \, dx , & i \neq N \text{ or } j \neq N \\
\int_0^\ell Y A \phi_i' \phi_j' \, dx + k_\ell , & i = N \text{ and } j = N
\end{cases}
\]

\[
[Q]_{ij} = \begin{cases} 
\int_0^\ell c A \phi_i' \phi_j' \, dx , & i \neq N \text{ or } j \neq N \\
\int_0^\ell c A \phi_i' \phi_j' \, dx + c_\ell , & i = N \text{ and } j = N
\end{cases}
\]

\[
[f]_i = \int_0^\ell f \phi_i \, dx
\]
Approximation Techniques for the Rod Model: Galerkin

Matrices: Constant coefficients

\[
\mathbf{M} = \rho A h \begin{bmatrix}
\frac{2}{3} & \frac{1}{6} & 0 & \cdots & 0 \\
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
0 & \cdots & 0 & \frac{1}{6} & \frac{1}{3} + \frac{m_\ell}{h}
\end{bmatrix}, \quad \mathbf{K} = \frac{YA}{h} \begin{bmatrix}
2 & -1 & 0 & \cdots & 0 \\
-1 & 2 & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & -1 & 1 + h k_\ell
\end{bmatrix}
\]

First-Order System:

\[
\dot{\mathbf{z}}(t) = \mathbf{A} \mathbf{z}(t) + \mathbf{F}(t)
\]
\[
\mathbf{z}(0) = \mathbf{z}_0
\]

where

\[
\mathbf{A} = \begin{bmatrix}
0 & \mathbb{I} \\
-\mathbf{M}^{-1} \mathbf{K} & -\mathbf{M}^{-1} \mathbf{Q}
\end{bmatrix}, \quad \mathbf{F}(t) = \begin{bmatrix}
0 \\
\mathbf{M}^{-1} \mathbf{f}(t)
\end{bmatrix}
\]

Note: Codes available at http://www4.ncsu.edu/~rsmith/Smart_Material_Systems/Chapter8/
Approximation Techniques for the Rod Model: Finite Element

Motivating Problem: \[ \rho A \frac{\partial^2 u}{\partial t^2} + YA \frac{\partial^2 u}{\partial x^2} = 0 \]

Local Basis Elements: Take

\[ u(t, x) = a_0(t) + a_1(t)x \]
\[ = \varphi^T(x)a(t) \]

where \( a(t) = [a_0(t), a_1(t)]^T \) and \( \varphi(x) = [1, x]^T \). Then

\[
\begin{bmatrix}
u_L(t) \\
u_R(t)
\end{bmatrix} =
\begin{bmatrix}
1 & 0 \\
1 & h
\end{bmatrix}
\begin{bmatrix}
a_0(t) \\
a_1(t)
\end{bmatrix}
\]

\[ \Rightarrow u(t) = Ta(t) \]

By observing that \( a(t) = Su(t) \), where

\[ S = T^{-1} =
\begin{bmatrix}
1 & 0 \\
-\frac{1}{h} & \frac{1}{h}
\end{bmatrix}, \]

it follows that displacements can be represented as

\[ u(t, x) = \phi^T(x)u(t) \]

where \( \phi^T(x) = [1 - \frac{x}{h}, \frac{x}{h}] \).
Approximation Techniques for the Rod Model: Finite Element

`Action' Integral:

\[ A = \int_{t_0}^{t_1} [K - U] dt \]
\[ = \int_{t_0}^{t_1} \frac{1}{2} \int_{0}^{h} \left[ \rho \dot{u}_x^2(t, x) - Y A u_x^2(t, x) \right] dx dt \]

Here

\[ u_x^2(t, x) = u^T(t) S^T D(x) S u(t), \quad \dot{u}_x^2(t, x) = \dot{u}^T(t) S^T F(x) S \dot{u}(t) \]

where

\[ D(x) = \varphi_x(x) \varphi_x^T(x) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad F(x) = \varphi(x) \varphi^T(x) = \begin{bmatrix} 1 & x \\ x & x^2 \end{bmatrix} \]

Thus

\[ A[U] = \int_{t_0}^{t_1} \frac{1}{2} \left[ \dot{u}^T(t) M_e \ddot{u}(t) - u^T(t) K_e u(t) \right] dt \]

where \( U = (u, \dot{u}) \) and

\[ M_e = \rho A S^T \cdot \int_{0}^{h} F(x) dx \cdot S, \quad K_e = Y A S^T \cdot \int_{0}^{h} D(x) dx \cdot S \]

\[ M_e = \rho A h \begin{bmatrix} \frac{1}{3} & \frac{1}{6} & \frac{1}{3} \\ \frac{1}{6} & \frac{1}{3} & \frac{1}{6} \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, \quad K_e = \frac{Y A}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \]

\( M_e: \text{Local Mass Matrix} \)
\( K_e: \text{Local Stiffness Matrix} \)
Approximation Techniques for the Rod Model: Finite Element

Hamilton’s Principle: See Chapters 7, 8 and Appendix of Smith, 2005

\[ \frac{d}{d\varepsilon} A[U + \varepsilon \gamma] \bigg|_{\varepsilon=0} = 0 \]

where \( \gamma = (\eta, \dot{\eta}) \) and it is assumed that \( \eta(t_0) = \eta(t_1) = 0 \). Here

\[ A[U + \varepsilon \gamma] = \int_{t_0}^{t_1} \frac{1}{2} \left[ (\dot{\mathbf{u}} + \varepsilon \dot{\eta})^T M_e (\dot{\mathbf{u}} + \varepsilon \dot{\eta}) - (\mathbf{u} + \varepsilon \eta)^T K_e (\mathbf{u} + \varepsilon \eta) \right] dt \]

\[ \Rightarrow \frac{d}{d\varepsilon} A[U + \varepsilon \gamma] = \int_{t_0}^{t_1} \frac{1}{2} \left[ \dot{\eta}^T M_e (\dot{\mathbf{u}} + \varepsilon \dot{\eta}) + (\dot{\mathbf{u}} + \varepsilon \dot{\eta})^T M_e \dot{\eta} - \eta^T K_e (\mathbf{u} + \varepsilon \eta) + (\mathbf{u} + \varepsilon \eta)^T K_e \eta \right] dt \]

\[ \Rightarrow \frac{d}{d\varepsilon} A[U + \varepsilon \gamma] \bigg|_{\varepsilon=0} = \int_{t_0}^{t_1} \left[ \dot{\eta}^T M_e \dot{\mathbf{u}} - \eta^T K_e \mathbf{u} \right] dt \quad \text{(since} \quad \dot{\mathbf{u}}^T M_e \dot{\eta} = \dot{\eta}^T M_e \dot{\mathbf{u}}) \]

\[ = -\int_{t_0}^{t_1} \eta \left[ M_e \ddot{\mathbf{u}} + K_e \mathbf{u} \right] dt \quad \text{(integration by parts)} \]

Local System:

\[ M_e \ddot{\mathbf{u}}(t) + K_e \mathbf{u} = 0 \]
Approximation Techniques for the Rod Model: Finite Element

**Global Matrices:** Consider two subregions so $h = \frac{\ell}{2}$. Here

$$\mathbf{u}(t) = [u_{1\ell}(t), u_{2\ell}(t), u_{2r}(t)]^T$$

and

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = 0$$

where

$$\mathbf{M} = \rho A h \begin{bmatrix} \frac{1}{3} & \frac{1}{6} & 0 \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ 0 & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, \quad \mathbf{K} = \frac{Y A}{h} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}.$$  

**Note:** Second row obtained by summing

$$\rho A h \left( \frac{1}{6} \ddot{u}_{1\ell} + \frac{1}{3} \ddot{u}_{2\ell} \right) + \frac{Y A}{h} (-u_{1\ell} + u_{2\ell}) = 0$$

$$\rho A h \left( \frac{1}{3} \ddot{u}_{2\ell} + \frac{1}{6} \ddot{u}_{2r} \right) + \frac{Y A}{h} (u_{2\ell} - u_{2r}) = 0$$

after enforcing $u_{1r} = u_{2\ell}$ and $\ddot{u}_{1r} = \ddot{u}_{2\ell}$. 
Finite Difference Techniques for the Rod Model

Consider first

\[ u_{tt} - K^2 u_{xx} = F \]
\[ u(t, 0) = u(t, \ell) = 0 \]
\[ u(0, x) = f(x), \; u_t(0, x) = g(x) \]

Grid: \( \Delta = \{ (x_i, t_j) \mid x_i = ih, t_j = jk \} \)

System: \( m = K \frac{k}{h} \)

\[ \frac{1}{k^2} [u_{i,j-1} - 2u_{i,j} + u_{i,j+1}] - \frac{K^2}{h^2} [u_{i-1,j} - 2u_{i,j} + u_{i+1,j}] = F(t_j, x_i) \]

\[ \Rightarrow u_{i,j+1} = m^2 [u_{i+1,j} + u_{i-1,j}] + 2(1 - m^2)u_{i,j} - u_{i,j-1} + k^2 F(t_j, x_i) \]

Initial Conditions:

\[ g(x_i) \approx \frac{u_{i,1} - u_{i,-1}}{2k} \Rightarrow u_{i,-1} = u_{i,1} - 2kg(x_k) \]

\[ \Rightarrow u_{i,1} = \frac{m^2}{2} [f(x_{i+1}) + f(x_{i-1})] + (1 - m^2)f(x_i) + kg(x_i) + \frac{k^2}{2} F(t_0, x_i) \]
Finite Difference Techniques for the Rod Model

Now consider

\[ u_{tt} - c^2 u_{xx} - K^2 u_{xx} = F \]

\[ u(t, 0) = u(t, \ell) = 0 \]

\[ u(0, x) = f(x), \quad u_t(0, x) = g(x) \]

**Question:** What is finite difference scheme?
Galerkin Method for Beam Model

Weak Formulation: See Section 8.3 of Smith, 2005

\[
\int_0^\ell \rho \frac{\partial^2 w}{\partial t^2} \phi \, dx + \int_0^\ell \gamma \frac{\partial w}{\partial t} \phi \, dx + \int_0^\ell YI \frac{\partial^2 w}{\partial x^2} \frac{d^2 \phi}{dx^2} \, dx \\
+ \int_0^\ell cI \frac{\partial^3 w}{\partial x^2 \partial t} \frac{d^2 \phi}{dx^2} \, dx = \int_0^\ell f \phi \, dx + \int_0^\ell k_p V(t) \frac{d^2 \phi}{dx^2} \, dx
\]

for all \( \phi \in V = H_{0}^2(0, \ell) \)

Basis:

\[
\phi_j(x) = \begin{cases} 
\hat{\phi}_0(x) - 2\hat{\phi}_{-1}(x) - 2\hat{\phi}_1(x), & j = 1 \\
\hat{\phi}_j(x), & j = 2, \ldots, N + 1 
\end{cases}
\]

where

\[
\hat{\phi}_j(x) = \frac{1}{h^3} \begin{cases} 
(x - x_{j-2})^3, & x \in [x_{j-2}, x_{j-1}) \\
h^3 + 3h^2(x - x_{j-1}) + 3h(x - x_{j-1})^2 - 3(x - x_{j-1})^3, & x \in [x_{j-1}, x_j) \\
h^3 + 3h^2(x_{j+1} - x) + 3h(x_{j+1} - x)^2 - 3(x_{j+1} - x)^3, & x \in [x_j, x_{j+1}) \\
(x_{j+2} - x)^3, & x \in [x_{j+1}, x_{j+2}) \\
0, & \text{otherwise} 
\end{cases}
\]
Galerkin Method for Beam Model

Approximate Solution:

\[ w^N(t, x) = \sum_{j=1}^{N+1} w_j(t) \phi_j(x) \]

System:

\[ \mathbf{M} \ddot{\mathbf{w}} + \mathbf{Q} \dot{\mathbf{w}} + \mathbf{K} \mathbf{w} = \mathbf{f} + V(t) \mathbf{b} \]

where

\[ \mathbf{w}(t) = [w_1(t), \ldots, w_{N+1}(t)]^T \]

and

\[ [\mathbf{M}]_{ij} = \int_0^\ell \rho \phi_i \phi_j dx \]

\[ [\mathbf{Q}]_{ij} = \int_0^\ell \left[ \gamma \phi_i \phi_j + c I \phi_i'' \phi_j'' \right] dx \]

\[ [\mathbf{K}]_{ij} = \int_0^\ell Y I \phi_i'' \phi_j'' dx \]

\[ [\mathbf{f}]_i = \int_0^\ell f \phi_i dx \ , \ [\mathbf{b}]_i = \int_0^\ell \phi_i'' dx \]