BEGN 221: Mathematical Methods in Bioengineering

Lecture 16

Finite-Element Methods

References

Haberman APDE, Sec. 6.7.

http://en.wikipedia.org/wiki/Finite_element_method

FINITE ELEMENT METHODS (Haberman Sec. 6.7)

→ Separation of variables (in space) works for simple problems, with geometries that allow for separation of variables in the boundary conditions.

→ Finite element methods offer numerical solutions to diffusion, wave, and other linear PDE problems in bioengineering with complex, arbitrary boundary conditions on real-life geometries (not cubes, cylinders, or spheres).

General linear PDEs (in homogeneous media):

$$\mathcal{L}_t(u(\vec{r},t)) = \Delta u(\vec{r},t) + f(\vec{r},t)$$

e.g.

DIFFUSION EQ.: $\mathcal{L}_t(u) = \dfrac{1}{D}\dfrac{\partial u}{\partial t}$ $\quad \left[D : \dfrac{m^2}{s}\right]$

WAVE EQ: $\mathcal{L}_t(u) = \dfrac{1}{c^2}\dfrac{\partial^2 u}{\partial t^2}$ $\quad \left[c : \dfrac{m}{s}\right]$

CABLE EQ: $\mathcal{L}_t(u) = lC\dfrac{\partial^2 u}{\partial t^2} + rC\dfrac{\partial u}{\partial t}$

$\left[l : \dfrac{H}{m}\right]$ $\quad \left[C : \dfrac{F}{m}\right]$ $\quad \left[r : \dfrac{\Omega}{m}\right]$

General (inhomogeneous) problem:

$$\mathcal{L}_t(u) = \Delta u + \underbrace{f(\vec{r},t)}_{\text{SOURCE}}$$

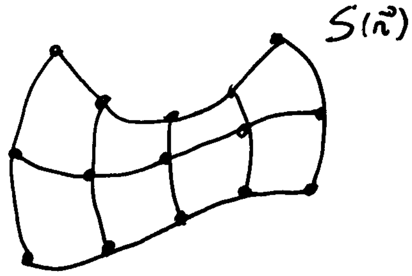
with: I.C. : $u(\vec{r},0) = \underbrace{g(\vec{r})}_{\text{DIFF/WAVE/CABLE}}$, and $\underbrace{\frac{\partial u}{\partial t}(\vec{r},0) = h(\vec{r})}_{\text{WAVE/CABLE}}$

B.C : • VALUE B.C. : $u(S(\vec{r}),t) = u_V(S(\vec{r}))$

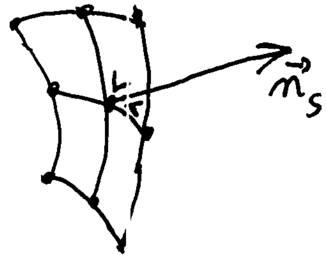
AND/OR

• FLUX B.C. : $\vec{\nabla} u(S,t) \cdot \vec{n}_S = u_F(S(\vec{r}))$

where $S(\vec{r})$ defines a SURFACE in space



and $\vec{n}_S$ is locally perpendicular to the surface S.



Homogeneous problem :

$$\mathcal{L}_t(u_H) = \Delta u_H \quad \text{with} \begin{cases} \text{SOURCE} = 0 & f(\vec{r},t) = 0 \\ \text{VALUE B.C.} = 0 & u_H(S(\vec{r}),t) = 0 \\ \quad\text{AND/OR} & \\ \text{FLUX B.C} = 0 & \vec{\nabla} u_H(S,t) \cdot \vec{n}_S = 0 \end{cases}$$

Separation of space and time (but NOT separation in space):

$$u_H(\vec{r},t) = \phi(\vec{r}) \cdot G(t)$$

TIME : $$\mathcal{L}_t(G(t)) = -\lambda\, G(t)$$

- DIFF. : $\mathcal{L}_t(G) = \frac{1}{D}\frac{d}{dt}G \Rightarrow G(t) = G(0)\cdot e^{-D\lambda t}$
- WAVE : $\mathcal{L}_t(G) = \frac{1}{c^2}\frac{d^2}{dt^2}G \Rightarrow$

$$G(t) = G(0)\cdot\cos(\sqrt{\lambda}\,ct) + \frac{\dot{G}(0)}{\sqrt{\lambda}\,c}\cdot\sin(\sqrt{\lambda}\,ct)$$

- CABLE : $\mathcal{L}_t(G) = lC\,\frac{d^2G}{dt^2} + rC\,\frac{dG}{dt}$

(left as an exercise)

SPACE : $\Delta \phi(\vec{r}) + \lambda \phi(\vec{r}) = 0$ (Haberman p.270)

with complex B.C. (value / flux)

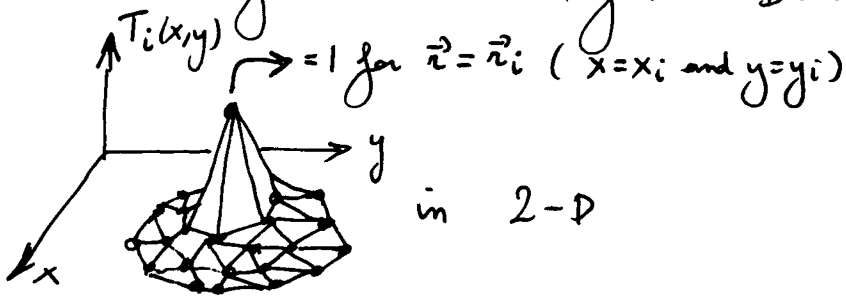
$\longrightarrow$ Solve using FINITE ELEMENTS

- specific to the B.C. geometry and type (value / flux)
- independent of PDE type (diffusion ; wave ; cable ; ...)

Let $\phi(\vec{r}) = \sum_{i=1}^{n} u_i \cdot T_i(\vec{r})$ on a grid with discrete points $\vec{r}_i$ such that :

- $T_i(\vec{r}_i) = 1$
- $T_i(\vec{r}_j) = 0$ for $j \neq i$
- T_i is PIECEWISE LINEAR on segments connecting vertices on the grid
- T_i satisfies all value / flux B.C.

e.g:

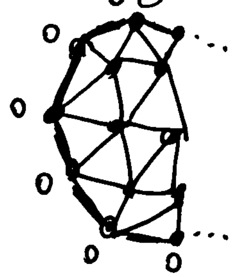


in 2-D

How does T_i satisfy the boundary conditions?

- VALUE B.C. : $T_i(S(\vec{r})) = 0$

$\Rightarrow$ T_i is zero, for each of the i, on each of the vertex points that are on the boundary (as well as the segments that connect them).



- FLUX B.C. : $\vec{\nabla} T_i(s) \cdot \vec{n}_s = 0$

$\Rightarrow$ The gradient (slope) of T_i, for each of the i, is PARALLEL to the surface segments suspended by the vertex points on the boundary.

$\Rightarrow$ The average of T_i values on the vertex points of any polyhedron segment on the boundary should equal the T_i value of the vertex interior point, part of the same polyhedron.

We seek a solution $\phi(\vec{r}) = \sum_{j=1}^{n} u_j T_j(\vec{r})$ that approximates

$$\Delta \phi(\vec{r}) + \lambda \phi(\vec{r}) = 0$$

in integral form:

$$\iiint_V T_i(\vec{r}) \cdot \left(\Delta\phi(\vec{r}) + \lambda \phi(\vec{r}) \right) d^3\vec{r} = 0 \,, \quad i = 1, 2, \dots n$$

over the domain (volume) V enclosed by the B.C. surface S.

Note: $\vec{\nabla}(T_i \vec{\nabla}\phi) = T_i \cdot \underbrace{\vec{\nabla}\cdot\vec{\nabla}\phi}_{\Delta\phi} + \vec{\nabla} T_i \cdot \vec{\nabla}\phi$

$$\Rightarrow \iiint_V T_i \, \Delta\phi \, d^3\vec{r} = \underbrace{\iiint_V \vec{\nabla}(T_i \vec{\nabla}\phi)\, d^3\vec{r}}_{} - \iiint_V \vec{\nabla} T_i \cdot \vec{\nabla}\phi \, d^3\vec{r}$$

$$\overset{\text{GAUSS}}{=} \oiint_{S(V)} T_i \, \vec{\nabla}\phi \cdot \vec{n} \, dS = 0 \quad \text{because:}$$

$$\begin{cases} \bullet\ T_i = 0 \text{ ON VALUE BOUNDARY} \\ \bullet\ \vec{\nabla}\phi \cdot \vec{n} = 0 \text{ ON FLUX BOUNDARY} \\ \quad (\vec{\nabla} T_j \cdot \vec{n} = 0) \end{cases}$$

$$\Rightarrow \iiint_V \vec{\nabla} T_i \cdot \vec{\nabla}\phi \, d^3\vec{r} = \lambda \iiint_V T_i \cdot \phi \, d^3\vec{r}$$

GALERKIN APPROXIMATION

(WEAK FORM)

(Haberman pp. 267–270)

$$\Rightarrow \sum_{j=1}^{n} \underbrace{\iiint_V \vec{\nabla} T_i \cdot \vec{\nabla} T_j \, d^3\vec{r}}_{K_{ij}} \cdot u_j = \lambda \sum_{j=1}^{n} \underbrace{\iiint T_i T_j \, d^3\vec{r}}_{M_{ij}} \cdot u_j$$

STIFFNESS MATRIX $\bar{\bar{K}}$ MASS MATRIX $\bar{\bar{M}}$

$$\Rightarrow \quad \bar{\bar{K}} \, \vec{u} = \lambda \, \bar{\bar{M}} \, \vec{u}$$

$\Rightarrow$ generalized eigenvector-eigenvalue problem for non-zero solutions $\vec{u}$:

$\det(\bar{\bar{K}} - \lambda \bar{\bar{M}}) = 0$ with $\vec{u}$ in the null-space of $\bar{\bar{K}} - \lambda \bar{\bar{M}}$

Solutions to λ and $\vec{u}$ are eigenvalues and eigenvectors of $\bar{\bar{M}}^{-1} \cdot \bar{\bar{K}}$

For any eigenvalue λ, the solution $\phi(\vec{r}) = \sum_{j=1}^{n} u_j T_j(\vec{r})$ is the corresponding EIGENMODE.

Since $\bar{\bar{M}}^{-1} \cdot \bar{\bar{K}}$ is $(n \times n)$, there are n eigenvalues λ_k and n corresponding eigenmodes $\phi_k(\vec{r}) = \sum_{j=1}^{n} (u_k)_j T_j(\vec{r})$

$$\Rightarrow u_H(\vec{r}, t) = \sum_k A_k \, \phi_k(\vec{r}) \cdot G_k(t)$$

HOMOGENEOUS SOLUTION

with $G_k(t) = e^{-D\lambda_k t}$ for DIFFUSION.

How to find the coefficients A_k ?

As with all diffusion / wave problems (satisfying Sturm-Liouville), the eigenmodes $\phi_k(\vec{r})$ are ORTHOGONAL :

PROOF: $\bar{\bar{M}}$ and $\bar{\bar{K}}$ are symmetric (and positive definite)

$\Rightarrow$ eigenvalues λ_k are real (and positive),

and eigenvectors $\vec{u}_k$ are orthogonal w.r.t. $\bar{\bar{M}}$:

$$\vec{u}_k^T \cdot \bar{\bar{M}} \cdot \vec{u}_\ell = c_k \delta_{k\ell}$$

$$\Rightarrow \iiint_V \phi_k(\vec{r})\,\phi_\ell(\vec{r})\,d^3\vec{r} = \sum_i \sum_j (u_k)_i (u_\ell)_j \underbrace{\iiint_V T_i(\vec{r})\,T_j(\vec{r})\,d^3\vec{r}}_{M_{ij}}$$

$$= \vec{u}_k^T \cdot \bar{\bar{M}} \cdot \vec{u}_\ell = c_k \delta_{k\ell} \qquad \text{Q.E.D.}$$

I.C. $$u_H(\vec{r},0) = \sum_k A_k\,\phi_k(\vec{r}) \cdot \underbrace{G_k(0)}_{\substack{\shortparallel \\ 1 \text{ for DIFFUSION}}}$$

$$= g(\vec{r})$$

$$\Rightarrow A_k = \frac{\iiint_V g(\vec{r})\,\phi_k(\vec{r})\,d^3\vec{r}}{\iiint_V \left[\phi_k(\vec{r})\right]^2 d^3\vec{r}} \qquad \text{(as before)}$$

General solution to INHOMOGENEOUS PDE with INHOMOGENEOUS B.C.:

use Green's functions as before.

The Green's function is the homogeneous solution $u_H(\vec{r},t)$ with I.C. $u_H(\vec{r},t') = \delta(\vec{r}-\vec{r}')$

$$\underbrace{u_H(\vec{r},t')}_{\text{INITIAL ACTIVATION AT TIME } t'} = \underbrace{\delta(\vec{r}-\vec{r}')}_{\text{IMPULSE AT LOCATION } \vec{r}'}$$

for DIFFUSION

$$\Rightarrow \sum_k A_k \, \phi_k(\vec{r}) \, . \, e^{-D\lambda_k t'} = \delta(\vec{r}-\vec{r}')$$

$$\Rightarrow \sum_k A_k \underbrace{\iiint_V \phi_k(\vec{r})\,\phi_\ell(\vec{r})\,d^3\vec{r}}_{c_k \delta_{k\ell}} \; e^{-D\lambda_k t'} = \underbrace{\iiint_V \delta(\vec{r}-\vec{r}')\,\phi_\ell(\vec{r})\,d^3\vec{r}}_{\phi_\ell(\vec{r}')}$$

$$\Rightarrow A_\ell = \frac{1}{c_\ell}\,\phi_\ell(\vec{r}')\,.\, e^{+D\lambda_k t'}$$

$$G(\vec{r},t;\vec{r}',t') = u_H(\vec{r},t) = \sum_k A_k\,\phi_k(\vec{r})\,.\, e^{-D\lambda_k t}$$

$$= \sum_k \frac{1}{c_k}\,\phi_k(\vec{r}')\,\phi_k(\vec{r})\; e^{-D\lambda_k (t-t')}$$

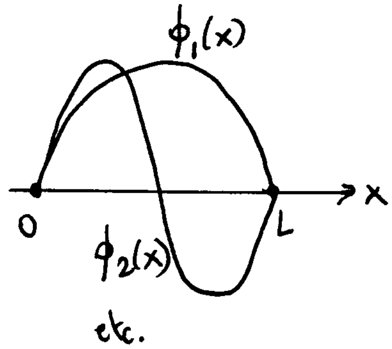
(as before!)

with $c_k = \iiint_V (\phi_k(\vec{r}'))^2 \, d^3\vec{r}'$

EXAMPLE : Diffusion in 1-D

on $[0, L]$ with VALUE-VALUE B.C.

$$\Rightarrow \quad u_H(x,t) = \sum_k A_k \underbrace{\sin\left(\frac{k\pi x}{L}\right)}_{\phi_k(x)} \cdot \underbrace{e^{-D\left(\frac{k\pi}{L}\right)^2 t}}_{G_k(t)}$$

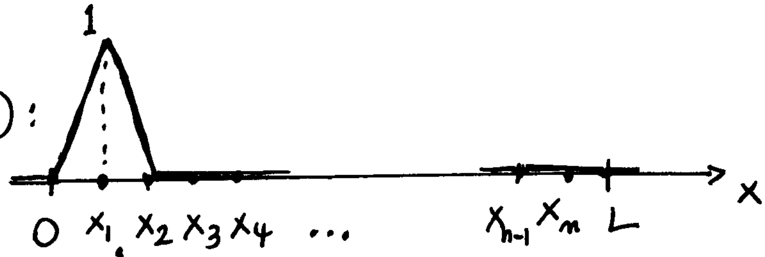


$$\lambda_k = \left(\frac{k\pi}{L}\right)^2$$

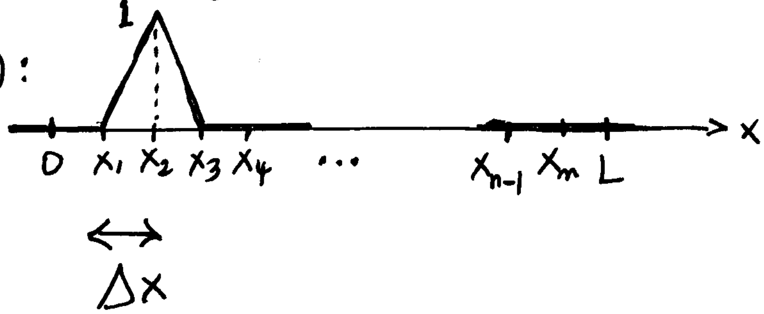
ANALYTICAL SOLUTION

FINITE ELEMENTS

$T_1(x)$:

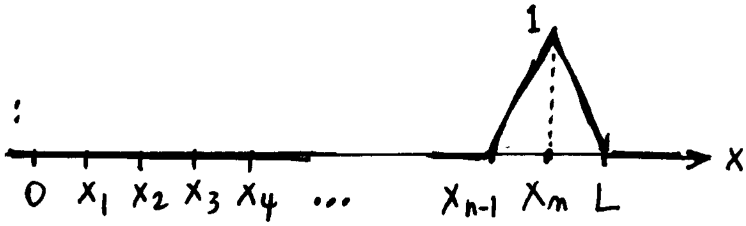


$T_2(x)$:



⋮

$T_n(x)$:



$$\Rightarrow \quad K_{ij} = \int_0^L \frac{dT_i}{dx}(x)\,\frac{dT_j}{dx}(x)\,dx = \begin{cases} \frac{2}{\Delta x} & \text{for } i = j \\ -\frac{1}{\Delta x} & \text{for } i = j \pm 1 \end{cases}$$

$$M_{ij} = \int_0^L T_i(x)\,T_j(x)\,dx = \begin{cases} \frac{2}{3}\Delta x & \text{for } i = j \\ \frac{1}{6}\Delta x & \text{for } i = j \pm 1 \end{cases}$$

```matlab
%%% Finite Elements: Linear (1-D) Diffusion with value-value B.C.
%%% BENG 221 example, 11/17/2011

L = 1;    % length
n = 100;  % number of finite elements
ne = 10;  % number of displayed eigenmodes
don = diag(ones(n,1),0); % on-diagonal, all ones
doff = diag(ones(n-1,1),1); % off-diagonal, all ones

dx = 1 / (n+1); % grid spacing, uniform
x = (0:n+1)' * L / (n+1);  % vertex points, including 0 and L boundary points
K = 1/dx * (2*don - doff - doff'); % stiffness matrix
M = dx/6 * (4*don + doff + doff'); % mass matrix


% finite differences: eigenvalue-eigenmode problem K*U = Lambda*dx*U with Lambda diagonal
help eig
% [U, Lambda] = eig(K/dx);
[U, Lambda] = eig(K, dx*don);
lambda_fd = diag(Lambda); % eigenvalues
phi_fd = [zeros(1,n); U; zeros(1,n)]; % eigenmodes; including 0 and L boundary points
phi_fd = phi_fd * diag(sign(phi_fd(2,:))); % flip eigenmodes with negative slope at zero

% finite elements: generalized eigenvalue-eigenmode problem K*U = Lambda*M*U with Lambda diagonal
[U, Lambda] = eig(K, M);
lambda_fe = diag(Lambda); % eigenvalues
phi_fe = [zeros(1,n); U; zeros(1,n)]; % eigenmodes; including 0 and L boundary points
phi_fe = phi_fe * diag(sign(phi_fe(2,:))); % flip eigenmodes with negative slope at zero

% analytical solution; ground truth
lambda_anal = (pi * (1:n) / L).^2; % analytical eigenvalues (separation of variables)
phi_anal = sqrt(2) * sin(pi * x * (1:n) / L); % analytical eigenmodes (separation of variables)


% plot eigenvalues
figure(1)
semilogy(lambda_fd, 'k:')
hold on
semilogy(lambda_fe, 'k-')
semilogy(lambda_anal, 'k--')
hold off
xlabel('Mode{\it k}')
ylabel('Eigenvalue {\it \lambda_k}')
legend('Finite Differences', 'Finite Elements', 'Analytical', 'Location', 'NorthWest')
print -dpdf 'linfinelem_eigenvalues.pdf'

% plot eigenmodes
figure(2)
plot(x, phi_fd(:,1:ne), ':')
hold on
plot(x, phi_fe(:,1:ne), '-')
plot(x, phi_anal(:,1:ne), '--')
hold off
xlabel('{\it x/L}')
ylabel('Eigenmodes {\it \phi_k}')
print -dpdf 'linfinelem_eigenmodes.pdf'
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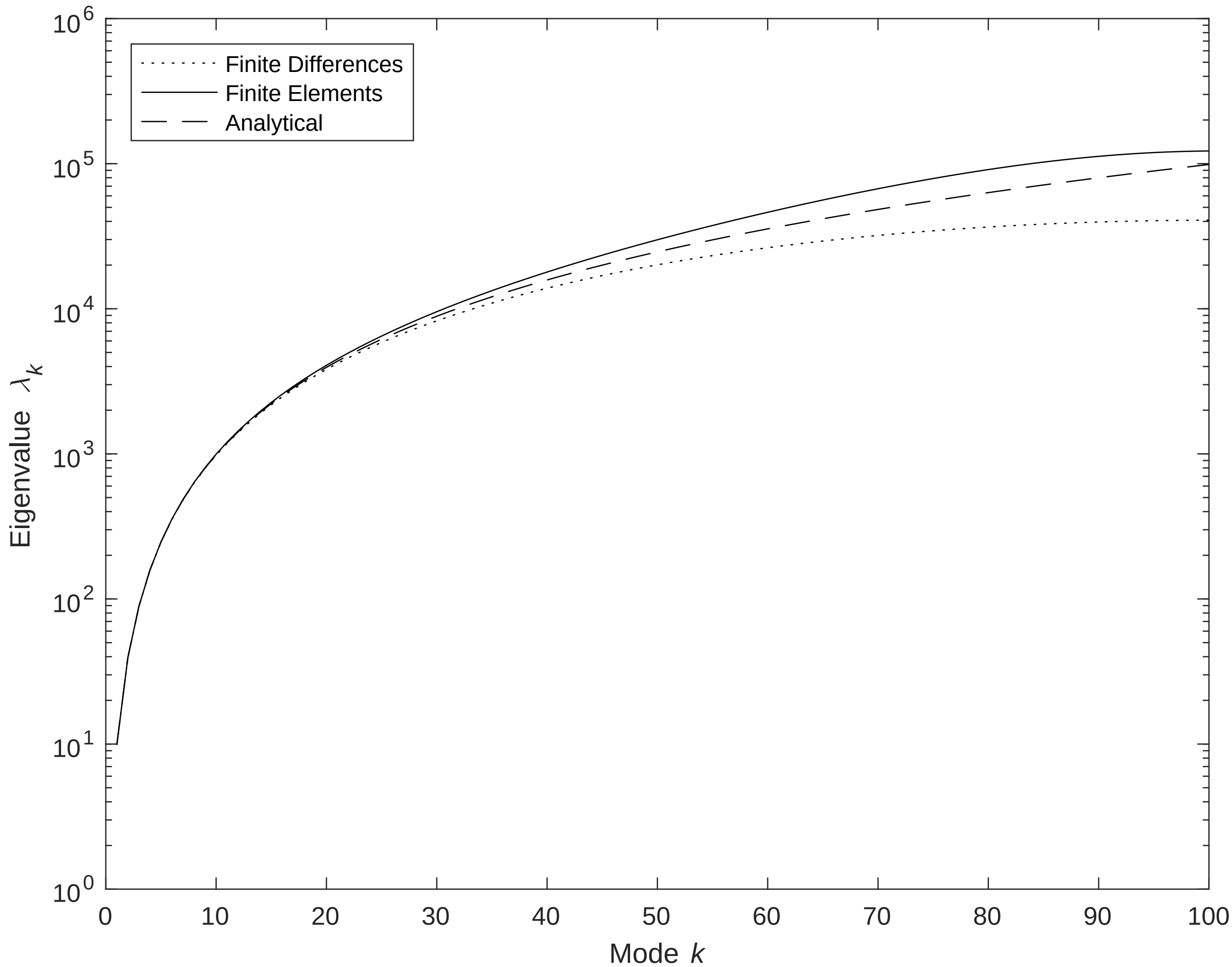
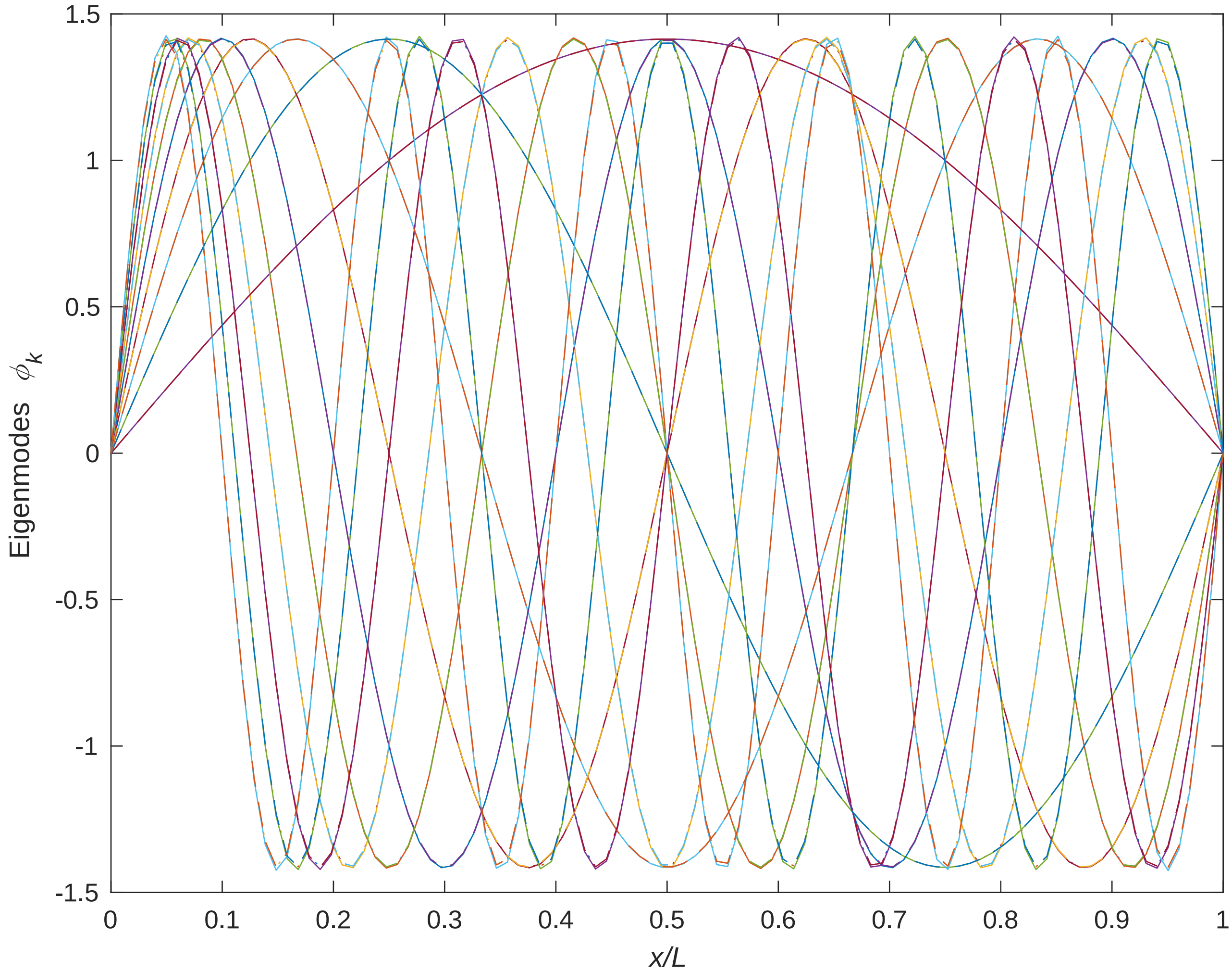


Finite Differences
Finite Elements
Analytical
10^6
10^5
10^4
10^3
10^2
10^1
10^0
Eigenvalue λ_k
0
10
20
30
40
50
60
70
80
90
100
Mode k



1.5
1
0.5
0
-0.5
-1
-1.5
Eigenmodes ϕ_k
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x/L