Derivation of Finite Element Equations

To solve a boundary value problem using the finite element method, we need to perform the following steps:

- 1) Discretise Ω ;
- 2) Choose element shape function ϕ^e ;
- 3) Calculate element matrix K^e and vector F^e ;
- 4) Construct global matrix **K** and vector **F** by assembling contributions from each element;
- 5) Impose boundary conditions;
- 6) Solve the system of equations.

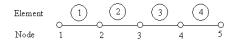
Finite Element Approximation

Consider solving

$$\left\{ \begin{array}{l} -u_{xx} = 2 \quad x \in (a,b) \\ \\ u(a) = \hat{u}_1, \ \frac{du}{dx}(b) = -p_b[u(b) - u_\infty] = \sigma(b). \end{array} \right.$$

Discretization and Topology of finite element mesh

Suppose that we divide [a, b] into 4 equally spaced elements. Within each element, we choose 2 nodes (left and right ends). Then, we design a global numbering scheme for the elements and nodes.



Finite Element Approximation

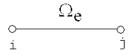
For example, the topology of element 2 can be recorded in the 2nd row of a matrix Node(100,2): Node(2,1)=2 and Node(2,2)=3. For convenience, denote N_i^e as the ith node of element e, i.e., $N_i^e = Node(e,i)$.

Table: System Topology

element	Numbering scheme	
	Local	Global
1	i j	1 2
2	i j	2 3
3	i j	3 4
4	i j	4 5

Galerkin FE formulation

For an arbitrarily chosen element Ω_e , to approximate u(x) over Ω_e by polynomial of degree k, we need to choose (k+1) points within Ω_e . Here we approximate u(x) by a polynomial of degree 1. So we choose two nodes i, j (left and right ends) for Ω_e as shown.



To standardize the calculation of element matrices, we firstly transform the element Ω_e into a standard element defined in [-1,1]. This process is as follows:

Step 1. Introduce local coordinate

$$\xi$$
 with $\left\{ egin{array}{ll} {
m origin} \ \xi = 0 & {
m at \ the \ centre \ of \ element} \\ \xi = -1 & {
m at \ the \ left \ hand \ node} \\ \xi = 1 & {
m at \ the \ right \ hand \ node} \end{array}
ight.$

This can be achieved by a linear transformation

$$\xi = \frac{2x - (x_i + x_{i+1})}{x_{i+1} - x_i}. (1)$$

- * So that points $x \in [x_i, x_{i+1}]$ are transformed to points $\xi \in [-1, 1]$.
- * As every element can be transformed into such element, we call this element as master element denoted by $\bar{\Omega}$
- * then we perform our element calculation on this reference element.

Step 2. For shape functions of degree k, we need to identify (k+1) nodes

(including the end points).

Let ξ_i denote the ξ -coordinate of the ith node,

 u_i^e denote the value of u_h^e at node i.

Then within Ω_e , u(x) can be approximated by the Lagrange polynomial,

$$u_h^e(x) = \sum_{i=1}^{k+1} N_i u_i^e \text{ with } N_i = \prod_{\substack{j=1\\ j \neq j}}^{k+1} \frac{(\xi - \xi_j)}{(\xi_i - \xi_j)}.$$
 (2)

- $u_h^e(x)$ is the local approximation of $u_h(x)$ in Ω_e .
- $N_i(x)$ denote the local interpolating functions of the master element.

$$\begin{array}{ccc} & \overline{\Omega} & & \\ & \overline{\zeta}_1 = -1 & & \zeta_2 = 1 \end{array}$$

eg. For linear interpolation (two nodes in each element)

$$N_1(\xi) = \frac{(\xi - \xi_2)}{(\xi_1 - \xi_2)} = \frac{\xi - 1}{-1 - 1} = \frac{1}{2}(1 - \xi)$$

$$N_2(\xi) = \frac{(\xi - \xi_1)}{(\xi_2 - \xi_1)} = \frac{\xi + 1}{1 + 1} = \frac{1}{2}(1 + \xi)$$

Calculation of Element Contributions

Having selected an approximate set of shape functions, we now come to a crucial step in the analysis, i.e., the calculation of element matrices and vectors.

$$\begin{array}{ccc} \Omega_e & & \\ \hline k & & I \end{array}$$

Consider $\Omega_e(x_k, x_l)$

$$k_{ij}^{\mathsf{e}} = \int_{\mathsf{x}_{\mathsf{k}}}^{\mathsf{x}_{\mathsf{l}}} \phi_{i}' \phi_{j}' \; d\mathsf{x}, \qquad f_{i}^{\mathsf{e}} = \int_{\mathsf{x}_{\mathsf{k}}}^{\mathsf{x}_{\mathsf{l}}} 2\phi_{i} \; d\mathsf{x}.$$

Using the following coordinate transformation

$$\xi = \frac{2x - (x_k + x_l)}{x_l - x_k}, \quad d\xi = \frac{2}{x_l - x_k} dx = \frac{2}{h} dx$$

we have

$$k_{ij}^e = rac{h}{2} \int_{-1}^1 N_i' N_j' \ d\xi, \quad f_i^e = rac{h}{2} \int_{-1}^1 2 N_i \ d\xi.$$

Note:

$$\begin{aligned} N_k &= \frac{1}{2} (1 - \xi), & N_l &= \frac{1}{2} (1 + \xi) \\ N_k' &= \frac{dN_k}{dx} = \frac{dN_k}{d\xi} \frac{d\xi}{dx} = -\frac{1}{2} \left(\frac{2}{h}\right) = -\frac{1}{h} \\ N_l' &= \frac{dN_l}{dx} = \frac{dN_l}{d\xi} \frac{d\xi}{dx} = +\frac{1}{2} \left(\frac{2}{h}\right) = \frac{1}{h} \end{aligned}$$

Therefore,
$$k^e = \begin{bmatrix} k_{kk}^e & k_{kl}^e \\ k_{lk}^e & k_{ll}^e \end{bmatrix}$$
, $f^e = \begin{bmatrix} f_k^e \\ f_l^e \end{bmatrix}$ with
$$k_{kk}^e = \frac{h}{2} \int_{-1}^1 N_k' N_k' \ d\xi = \frac{h}{2} \int_{-1}^1 \frac{1}{h^2} \ d\xi = \frac{1}{h}$$

$$k_{lk}^e = k_{kl}^e = \frac{h}{2} \int_{-1}^1 N_k' N_l' d\xi = \frac{h}{2} \int_{-1}^1 (\frac{1}{-h}) (\frac{1}{h}) \ d\xi = -\frac{1}{h}$$

$$k_{ll}^e = \frac{h}{2} \int_{-1}^1 N_l' N_l' \ d\xi = \frac{1}{h}$$

$$f_k^e = h \int_{-1}^1 \frac{1}{2} (1 - \xi) \ d\xi = h$$

i.e. for
$$e = 1, 2, 3, 4$$

$$K^{e} = \frac{1}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$F^e = \left[egin{array}{c} F_k^e \ F_l^e \end{array}
ight] = h \left[egin{array}{c} 1 \ 1 \end{array}
ight].$$

Thus, we can obtain all the element matrices.

For $\Omega_1(x_1, x_2)$,

$$K^1 = \left[\begin{array}{cc} k_{11}^1 & k_{12}^1 \\ & & \\ k_{21}^1 & k_{22}^1 \end{array} \right] = K^e, \quad F^1 = \left[\begin{array}{c} F_1^1 \\ & \\ F_2^1 \end{array} \right] = F^e.$$

For $\Omega_2(x_2, x_3)$,

$$K^2 = \begin{bmatrix} k_{22}^2 & k_{23}^2 \\ k_{32}^2 & k_{33}^2 \end{bmatrix} = K^e, \quad F^2 = \begin{bmatrix} F_2^2 \\ F_3^2 \end{bmatrix} = F^e.$$

For
$$\Omega_3(x_3, x_4)$$
,

$$K^{3} = \begin{bmatrix} k_{33}^{3} & k_{34}^{3} \\ k_{43}^{3} & k_{44}^{3} \end{bmatrix} = K^{e}, \quad F^{3} = \begin{bmatrix} F_{3}^{3} \\ F_{4}^{3} \end{bmatrix} = F^{e}.$$

For $\Omega_4(x_4, x_5)$,

$$K^4 = \left[\begin{array}{cc} k_{44}^4 & k_{45}^4 \\ & & \\ k_{54}^4 & k_{55}^4 \end{array} \right] = K^e, \quad F^4 = \left[\begin{array}{c} F_4^4 \\ & \\ F_5^4 \end{array} \right] = F^e.$$

To construct the global K and F

i) Expand each element quantity to N dimension, i.e.

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(ii) Add the expanded element quantities to form the global matrices.

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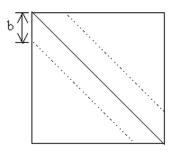
•
$$\mathbf{K} = \sum_{e=1}^{E} K^e$$

$$\bullet = \begin{bmatrix} K_{11}^1 & K_{12}^1 & 0 & 0 & 0 \\ K_{21}^1 & K_{22}^1 + K_{22}^2 & K_{23}^2 & 0 & 0 \\ 0 & K_{32}^2 & K_{33}^2 + K_{33}^3 & K_{34}^3 & 0 \\ 0 & 0 & K_{43}^3 & K_{44}^3 + K_{44}^4 & K_{45}^4 \\ 0 & 0 & 0 & K_{54}^4 & K_{55}^4 \end{bmatrix},$$

$$\bullet \mathbf{F} = \begin{bmatrix} F_1^1 \\ F_2^1 + F_2^2 \\ F_3^2 + F_3^3 \\ F_4^3 + F_4^4 \\ F_5^4 \end{bmatrix}.$$

Remarks

- 1) Consider a typical entry K_{ij} , Contributions to this entry are only from those elements containing both nodes i and j.
- 2) The system matrix **K** has its nonzero terms clustered about its main diagonal while locations distant from the diagonal contain zero terms. The coefficient matrix is said to be banded as well as sparse.



Now the system of equations obtained so far is

$$\begin{bmatrix} K_{11} & K_{12} & & & & \\ K_{21} & K_{22} & K_{23} & & & \\ & K_{32} & K_{33} & K_{34} & & \\ & & K_{43} & K_{44} & K_{45} \\ & & & K_{54} & K_{55} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 + \sigma(b)\phi(b) \end{bmatrix}.$$
(3)

Next, we need to impose the boundary conditions on the above system.

(i) Dirichlet boundary condition (also named essential boundary condition in the finite element method)

$$u(a) = u_1 = \hat{u}_1$$

• As u_1 is known, we move all known quantities $K_{i1}u_1$ in (3) to the right hand side.

Thus

$$\begin{bmatrix} 0 & K_{12} & 0 & 0 & 0 \\ 0 & K_{22} & K_{23} & 0 & 0 \\ 0 & K_{32} & K_{33} & K_{34} & 0 \\ 0 & 0 & K_{43} & K_{44} & K_{45} \\ 0 & 0 & 0 & K_{54} & K_{55} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} F_1 - K_{11}\hat{u}_1 \\ F_2 - K_{21}\hat{u}_1 \\ F_3 - K_{31}\hat{u}_1 \\ F_4 - K_{41}\hat{u}_1 \\ F_5 - K_{51}\hat{u}_1 + \sigma(b) \end{bmatrix}.$$

- * In the variational statement, the test function v(x) is required to satisfy v(a) = 0.
- st However, the 1st equation of the system (3) is obtained by

$$(u_N, \phi_1) = (f, \phi_1) - \sigma \phi_1 \mid_a^b = 0$$

As $\phi_1(a) = 1 \neq 0$, $\phi_1(x)$ is not from the class of admissible test functions, $\phi_1(x) \notin H^1_{oh}$.

We should discard this equation and hence the system of equations becomes

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & K_{22} & K_{23} & 0 & 0 \\ 0 & K_{32} & K_{33} & K_{34} & 0 \\ 0 & 0 & K_{43} & K_{44} & K_{45} \\ 0 & 0 & 0 & K_{54} & K_{55} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} 0 \\ F_2 - K_{21}\hat{u}_1 \\ F_3 - K_{31}\hat{u}_1 \\ F_4 - K_{41}\hat{u}_1 \\ F_5 - K_{51}\hat{u}_1 + \sigma(b) \end{bmatrix}.$$

Finally, we can either delete the 1st equation to yield an 4×4 system or add equation $u_1 = \hat{u}_1$ into the system to obtain

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & K_{22} & K_{23} & 0 & 0 \\ 0 & K_{32} & K_{33} & K_{34} & 0 \\ 0 & 0 & K_{43} & K_{44} & K_{45} \\ 0 & 0 & 0 & K_{54} & K_{55} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \hat{u}_1 \\ F_2 - K_{21}\hat{u}_1 \\ F_3 - K_{31}\hat{u}_1 \\ F_4 - K_{41}\hat{u}_1 \\ F_5 - K_{51}\hat{u}_1 + \sigma(b) \end{bmatrix}.$$
(4)

(ii) General natural boundary condition

$$k\frac{du(b)}{dx}=-p_b(u(b)-u_\infty)=\sigma(b).$$

The above natural boundary condition has been brought into the variational statement and consequently the 5th equation of (4) is

$$K_{54}u_4 + K_{55}u_5 = F_5 - K_{51}\hat{u}_1 - p_bu_5 + p_bu_\infty$$

$$\Rightarrow K_{54}u_4 + (K_{55} + p_b)u_5 = F_5 - K_{51}\hat{u}_1 + p_bu_\infty$$

Therefore system (4) becomes

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & K_{22} & K_{23} & 0 & 0 \\ 0 & K_{32} & K_{33} & K_{34} & 0 \\ 0 & 0 & K_{43} & K_{44} & K_{45} \\ 0 & 0 & 0 & K_{54} & (K_{55} + p_b) \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \hat{u}_1 \\ F_2 - K_{21} \hat{u}_1 \\ F_3 - K_{31} \hat{u}_1 \\ F_4 - K_{41} \hat{u}_1 \\ F_5 - K_{51} \hat{u}_1 + p_b u_{\infty} \end{bmatrix}.$$

which can then be solved to find u_2 , u_3 , u_4 and u_5 .

Error Estimates

- * Suppose that the actual solution u of our boundary value problem has the property that its derivatives of order s are square-integrable on Ω , but those of order s+1 and higher are not, s being an integer greater than unity.
- * Further, suppose that we use shape functions that contain complete polynomial of degree $\leq k$ and a uniform mesh of elements of equal length h.
- * Then the approximate error, measured in H_1 -norm, can be shown to satisfy the asymptotic error estimate

$$\| u - u_n \|_{1} \le ch^{\mu} \quad \text{(note } \| v \|_{1} = \left[\int_{a}^{b} (v'^2 + v^2) dx \right]^{1/2}$$

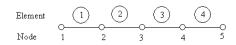
where c is a constant independent of h and $\mu = min(k, s)$.



Exercise

Using a standardised (master) linear element to construct a global system $\mathbf{K}\mathbf{u} = \mathbf{F} + \mathbf{F}_b$ of the BVP:

$$\begin{cases} -u_{xx} = \delta(x-2) & x \in (0,4) \\ u(0) = 2, \ u_x(4) = -2(u(4) - 1). \end{cases}$$



Semi-discretization in space

Consider the solution of linear parabolic problems (diffusion problems) as follows:

$$u_{t} - \nabla \cdot (k\nabla u) + bu = f \quad \text{in } \Omega \times I$$
subj. B.C.
$$\frac{\partial u}{\partial n} + \alpha u = \gamma \quad \text{on } \partial\Omega \times I$$
I.C.
$$u(\mathbf{x}, 0) = \hat{u}(\mathbf{x}) \quad \text{in } \Omega$$
where I : $[0, T]$ (5)

Variational statement

Multiplying (5), for a given t, by $v \in H^1$, then integrating over Ω and using Green's theorem, we get

$$\int_{\Omega} u_t v \ d\Omega + \int_{\Omega} (k \nabla u \cdot \nabla v + buv) \ d\Omega + \int_{\partial \Omega} k \alpha uv \ ds = \int_{\Omega} fv \ d\Omega + \int_{\partial \Omega} k \gamma v \ ds.$$
(6)

Thus, we are led to the following variational problem:

Find
$$u = u(\mathbf{x}, t) \in H^1(\Omega)$$
 such that for every $t \in I$
$$(u_t, v) + a(u, v) = L(v) \quad \text{for all } v \in H^1(\Omega) \tag{7}$$

$$u(\mathbf{x},0) = \hat{u}(\mathbf{x}) \tag{8}$$

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where
$$(\cdot, \cdot)$$
 = inner product $a(u, v) = \int_{\Omega} (k \nabla u \cdot \nabla v + buv) d\Omega + \int_{\partial\Omega} k \alpha uv \ ds.$ $L(v) = \int_{\Omega} fv \ d\Omega + \int_{\partial\Omega} k \gamma v \ ds.$

Finite Element Approximation

Let H_h^1 be a finite dimensional subspace of H^1 with basis functions $\{\phi_1,\phi_2,...\phi_n\}$. Then, the variational problem is approximated by : Find $u_h(\mathbf{x},t)\in H_h^1$ such that $u_h(\mathbf{x},0)=\hat{u}(\mathbf{x})$ and

$$\left(\frac{\partial u_h}{\partial t}, v_h\right) + a(u_h, v_h) = L(v_h) \quad \forall \ v_h \in H_h^1.$$
 (9)

In the usual way, we introduce a discretization of Ω as a union of elements Ω_e , i.e. $\Omega \to \bigcup_{e=1}^E \Omega_e$ and approximate $u(\mathbf{x},t)$ at t by.

$$u_h(\mathbf{x},t) = \sum_{j=1}^n u_j(t)\varphi_j(\mathbf{x})$$
 (10)

Finite Element Approximation

From (9) and (10), by using the usual finite element formulation, we obtain

where
$$\mathbf{M}\dot{\mathbf{u}} + \mathbf{A}\mathbf{u} = \mathbf{F}$$

 $\mathbf{u}(0) = \hat{\mathbf{u}}$ (11)
where $\mathbf{M} = (m_{ij})$ with $m_{ij} = (\varphi_i, \varphi_j) = \sum_{e=1}^{E} \int_{\Omega_e} \varphi_i \varphi_j d\Omega$
 $\mathbf{A} = (a_{ij})$ with $a_{ij} = a(\varphi_i, \varphi_j)$
 $= \sum_{e=1}^{E} \int_{\Omega_e} (k \nabla \varphi_i \cdot \nabla \varphi_j + b \varphi_i \varphi_j) d\Omega$
 $+ \sum_{e=1}^{\partial E} \int_{\partial \Omega_e} k \alpha \varphi_i \varphi_j ds$
 $\mathbf{F} = (f_i)$ with $f_i = L(\varphi_i)$

Consistency and Stability

Definition: consistency

By **consistency** we mean that the numerical scheme converges to the correct governing equation as the mesh size and the time stepping independently go to zero.

<u>Definition:</u> stability By **stability** we generally mean that a scheme is stable if the error measured in an appropriate norm does not become unbounded as time increases.

Error estimate theorem

Let u be the solution of (5) with k=1, b=f=0, u=0 on $\partial\Omega$ and let u_n be the corresponding finite element solution using (11). Then \exists a constant c such that

$$\max_{t \in I} \| u(t) - u_n(t) \| \le c \left(1 + \left| \log \frac{T}{h^2} \right| \right) \max_{t \in I} h^2 \| u(t) \|_{H^2(\Omega)}.$$
 (12)

Consistency and Stability

Basic stability inequality (for f = 0, u = 0 on $\partial\Omega$).

Let $u_h(t)$ satisfy the system (11), then

$$||u_h(t)|| \le ||u_h(0)|| \le ||\hat{u}||, \ t \in I$$

Proof

For u = 0 on $\partial\Omega$, (9) becomes (on taking $v_h = u_h$)

$$(\dot{u}_h,u_h)+a(u_h,u_h)=0$$

$$\frac{1}{2} \frac{d}{dt} ||u_h||^2 + a(u_h, u_h) = 0$$

$$||u_h||^2 + 2 \int_0^t a(u_h(s), u_h(s)) ds = ||u_h(0)||^2$$

Therefore, $||u_h|| \leq ||\hat{u}||$

Note: we have used the notation $||w|| = (w, w)^{1/2} = (\int w^2 d\Omega)^2$.



Time Differencing

We now consider the numerical technique to solve the following system of ordinary differential equations.

$$\mathbf{M}\dot{\mathbf{u}} + \mathbf{A}\mathbf{u} = \mathbf{F} \tag{13}$$

Forward Difference Scheme

Let
$$\frac{d\mathbf{u}}{dt}(t) = \frac{\mathbf{u}(t + \Delta t_r) - \mathbf{u}(t)}{\Delta t} \left(or \frac{d\mathbf{u}_r}{dt} = \frac{\mathbf{u}_{r+1} - \mathbf{u}_r}{\Delta t_r}\right)$$
(14)

and use forward difference with $O(\Delta t)$ accuracy, then (9) becomes

$$\mathbf{M} \ \mathbf{u}_{r+1} = (\mathbf{M} - \Delta t_r \mathbf{A}) \mathbf{u}_r + \Delta t_r \mathbf{F}_r \tag{15}$$

where $\sum_{r=1}^{n} \Delta t_r = T$

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Forward Difference Scheme

Hence, starting with \mathbf{u}_0 at r=0, we can generate a sequence of solutions $\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_n$ corresponding to $t_1, t_2, ..., T$.

Remarks:

- 1) If k, b and α depend on time, then A is a function of time, so that in the forward difference scheme, \mathbf{A} is replaced by $\mathbf{A}(t)$.
- 2) Finite element code for the equilibrium problem ($\mathbf{u}_t = 0$) can be modified to solve this FE system at each time step.

Program Structure

Program Structure

```
Loop over time steps r=0,1,2,...N_t

Loop over elements e=1,2,...N_e

For each \Omega_e, calculate a^e,m^e,f^e,\&~b^e_r=(m^e-\Delta t_r k^e)u^e_r

Assemble m^e to M~\&~b^e_r to b_r

Modify M~\&~b_r to satisfy essential B.C.'s

Solve Mu_{r+1}=b_r
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Stability

To analyze the stability of the forward difference scheme, we consider the system (13) with the initial solution $\mathbf{u}(0) = \hat{\mathbf{u}}$.

Error Analysis

Suppose $\mathbf{e}(t) := \text{error in } \mathbf{u}(t)$ due to a small change in $\hat{\mathbf{u}}$, then

$$M(\dot{u} + \dot{e}) + A(u+e) = F. \tag{16}$$

(16)-(13)
$$\Rightarrow$$
 $\mathbf{M}\dot{\mathbf{e}} + \mathbf{A}\mathbf{e} = \mathbf{0}$
 $\Rightarrow \frac{d\mathbf{e}}{dt} = -\mathbf{M}^{-1}\mathbf{A}\mathbf{e}.$

Thus, using forward difference scheme,

$$\mathbf{e}_{r+1} = (\mathbf{I} - \Delta t_r \mathbf{M}^{-1} \mathbf{A}) \mathbf{e}_r = R_r \mathbf{e}_r = \left(\Pi_{i=0}^r R_i \right) \mathbf{e}_0.$$

If $\Delta t_r = \Delta t$ (constant), then

$$\mathbf{e}_{r+1} = R^{r+1} \mathbf{e}_0 \ , \ (r = 0, 1, \dots \frac{T}{\Lambda t}).$$
 (17)

Error Analysis

 λ_i , $\{\mathbf{w}_i\}_{i=1}^N$ be eigenvalues and eigenvectors of $\mathbf{M}^{-1}\mathbf{A}$. Let $\mathsf{M}^{-1}\mathsf{A}\mathsf{w}_i = \lambda_i\mathsf{w}_i$ Then $\Delta t \mathbf{M}^{-1} \mathbf{A} \mathbf{w}_i = -\Delta t \lambda_i \mathbf{w}_i$ $\mathbf{I}\mathbf{w}_{i} - \Delta t \mathbf{M}^{-1} \mathbf{A} \mathbf{w}_{i} = (1 - \Delta t \lambda_{i}) \mathbf{w}_{i}$ $(\mathbf{I} - \Delta t \mathbf{M}^{-1} \mathbf{A}) \mathbf{w}_i = (1 - \Delta t \lambda_i) \mathbf{w}_i$ We can approximate the error at r=0 as

$$\mathbf{e}_0 = \sum_{i=1}^N \alpha_i \mathbf{w}_i.$$

Hence,
$$R\mathbf{e}_0 = \sum_1^N \alpha_i (I - \Delta t \mathbf{M}^{-1} \mathbf{A}) \mathbf{w}_i = \sum_i \alpha_i (1 - \lambda_i \Delta t) \mathbf{w}_i$$

 $R^2 \mathbf{e}_0 = \sum_1^N (1 - \lambda_i \Delta t) \alpha_i (I - \Delta t \mathbf{M}^{-1} \mathbf{A}) \mathbf{w}_i = \sum_1^N (1 - \lambda_i \Delta t)^2 \alpha \mathbf{w}_i$.
Therefore,

$$\mathbf{e}_{r+1} = R^{r+1} \mathbf{e}_0 = \sum_{1}^{N} (1 - \lambda_i \Delta t)^{r+1} \alpha_i \mathbf{w}_i$$
 (18)

Remarks:

1) The error will not grow and the scheme is stable if

$$|1 - \lambda_i \Delta t| < 1$$
, i.e. $\Delta t < \frac{2}{\lambda_i}$ $(i = 1, 2, ..., N)$, (19)

- 2) The larger the value of λ_i , the greater the restriction on the time step.
- 3) The value of λ_i is related to the finite element mesh. For example, for linear element, from a study of the eigenvalue problem, the highest frequency for an operator of order 2m is $\lambda_m = \beta h^{-2m}$ for a constant β . In the diffusion problem considered, m=1 and inequality (19) implies

$$\Delta t \le \frac{2}{\beta} h^2 = ch^2 \tag{20}$$

Central and Backward Difference (Crank-Nicolson Method)

The forward difference extrapolation leads to the restriction on the time step size to ensure stability. Here, we derive a scheme with unconditional stability.

Crank-Nicolson Scheme

Let $\frac{\frac{d\mathbf{u}}{dt}(t+\frac{\Delta t}{2})}{\mathbf{u}(t+\frac{\Delta t}{2})} = \frac{\mathbf{u}(t+\Delta t)-\mathbf{u}(t)}{\Delta t}$ $\mathbf{u}(t+\frac{\Delta t}{2}) = \frac{1}{2}(\mathbf{u}(t)+\mathbf{u}(t+\Delta t)) \text{ Then (13) becomes}$

$$(\mathbf{M} + \frac{\Delta t}{2}\mathbf{A})\mathbf{u}_{r+1} = (\mathbf{M} - \frac{\Delta t}{2}\mathbf{A})\mathbf{u}_r + \Delta t\mathbf{F}_{r+\frac{1}{2}}$$
(21)

Remarks: The only essential difference from the forward scheme lies in the actual form of the element matrix and vector contributions.

$$m^e + \frac{\Delta t}{2}a^e$$
, and $(m^e - \frac{\Delta t}{2}a^e)\mathbf{u}_r^e + \Delta t f_{r+\frac{1}{2}}^e$.

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Stability

We consider an initial error \mathbf{e}_0 and analyze the error growth in the recursion (21). Pre-multiplying (21) by \mathbf{M}^{-1} , we obtain

$$(I + \frac{\Delta t}{2} \mathbf{M}^{-1} \mathbf{A}) \mathbf{e}_{r+1} = (I - \frac{\Delta t}{2} \mathbf{M}^{-1} \mathbf{A}) \mathbf{e}_r, \tag{22}$$

$$\mathbf{e}_{r+1} = R_{+}^{-1} R_{-} \mathbf{e}_{r} = (R_{+}^{-1} R_{-})^{r+1} \mathbf{e}_{0},$$
 (23)

where $R_{\pm} = \mathbf{I} \pm \frac{\Delta t}{2} \mathbf{M}^{-1} \mathbf{A}$.

Stability

Further, assume that $\mathbf{M}^{-1}\mathbf{A}$ has N linearly independent eigenvectors \mathbf{w}_i , then

$$\mathbf{e}_0 = \sum_1^N \alpha_i \ \mathbf{w}_i, R_{\pm} \mathbf{w}_i = (I \pm \frac{\Delta t}{2} \mathbf{M}^{-1} \mathbf{A}) \mathbf{w}_i = (1 \pm \frac{\Delta t}{2} \lambda_i) \mathbf{w}_i, R_{+}^{-1} \ \mathbf{w}_i = (1 + \frac{\Delta t}{2} \lambda_i)^{-1} \mathbf{w}_i.$$

Therefore,

$$\mathbf{e}_{r+1} = (R_{+}^{-1}R_{-})^{r} R_{+}^{-1}(R_{-}\mathbf{e}_{0}) = (R_{+}^{-1}R_{-})^{r} \sum_{i=1}^{R_{-}^{-1}} (1 - \frac{\Delta t}{2}\lambda_{i})\alpha_{i}\mathbf{w}_{i}$$

$$= (R_{+}^{-1}R_{-})^{r} \sum_{i=1}^{N} \frac{1 - \frac{\Delta t}{2}\lambda_{i}}{1 + \frac{\Delta t}{2}\lambda_{i}}\alpha_{i}\mathbf{w}_{i} = \sum_{i=1}^{N} \rho_{i}^{r+1}\alpha_{i}\mathbf{w}_{i}.$$

As the eigenvalues λ_i are all positive, $\rho_i = \frac{1 - \frac{\Delta t}{2} \lambda_i}{1 + \frac{\Delta t}{2} \lambda_i} \leq 1$. Consequently, the error will not grow and the scheme is stable.

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Remarks:

- 1) If $\lambda_i < \frac{2}{\Delta t}$, then $\rho_i > 0$ and the error components decay monotonically; if $\lambda_i > \frac{2}{\Delta t}$, then $\rho_i < 0$ and the error components decay in an oscillatory manner from one step to the next. Therefore, we can define $\lambda^* = \frac{2}{\Delta t}$ as natural frequency.
- 2) The highest frequency depends inversely on the mesh size h with $\lambda_n = \beta h^{-2m}$ for a constant β . Accordingly, if the finite element mesh is repeatedly refined, inevitably when $h^{2m} < \beta \frac{\Delta t}{2}$, some of the higher order components enter and decaying oscillations appear. For m=1 and linear element in our diffusion problem in one dimension, the oscillations in components occur when $\frac{\Delta t}{h^2} > \frac{2}{\beta}$, which is, incidentally, the stability limit of the previous forward scheme.

Backward difference scheme

 $\underline{\mathsf{Scheme}}:\left(\mathbf{M}+\Delta t\mathbf{A}\right)\mathbf{u}_{r+1}=\mathbf{M}\mathbf{u}_r+\Delta t\mathbf{F}_{r+1}.$

Using the procedure similar to that in (ii), it can be shown that the above scheme is

- $O(\Delta t)$ accuracy,
- unconditionally stable,
- $\rho_i = (1 + \lambda_i \Delta t)^{-1}.$