Parabolic Boundary Value Problems

We consider the solution of linear parabolic problems (diffusion problems) governed by the parabolic partial differential equation $(1)_1$ with boundary condition $(1)_2$ and initial condition $(1)_3$ as follows:

$$
\begin{aligned}
& & & u_t - \nabla.(k\nabla u) + bu = f \quad \text{in } \Omega \times \mathrm{I} \\
& \text{subj.} & \text{B.C.} \quad & \frac{\partial u}{\partial n} + \alpha u = \gamma \quad \text{on } \partial\Omega \times \mathrm{I} \\
& & \text{I.C.} \quad & u(\mathbf{x}, 0) = \hat{u}(\mathbf{x}) \quad \text{in } \Omega \\
& & \text{where I} \quad & : [0,\ T]
\end{aligned}
\tag{1}
$$

Semi-discretization in space

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

$$\int_\Omega u_t v \; d\Omega + \int_\Omega (k\nabla u \cdot \nabla v + buv) \; d\Omega + \int_{\partial\Omega} k\alpha uv \; ds = \int_\Omega fv \; d\Omega + \int_{\partial\Omega} k\gamma v \; ds. \tag{2}$$

Thus, we are led to the following variational problem:
Find $u = u(\mathbf{x}, t) \in H^1(\Omega)$ such that for every $t \in I$, $u(\mathbf{x}, 0) = \hat{u}(\mathbf{x})$

$$(u_t, v) + a(u, v) = L(v), \;\; \forall \; v \in H^1(\Omega) \tag{3}$$

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

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

$$\left(\frac{\partial u_h}{\partial t}, v_h\right) + a(u_h, v_h) = L(v_h) \qquad \forall\ v_h \in H_h^1. \tag{4}$$

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.

$$u_h(\mathbf{x}, t) = \sum_{j=1}^{n} u_j\ (t)\varphi_j\ (\mathbf{x}) \tag{5}$$

From (4) and (5), by using the usual finite element formulation, we obtain

$$\mathbf{M}\dot{\mathbf{u}} + \mathbf{A}\mathbf{u} = \mathbf{F} \tag{6}$$

$$\begin{aligned}
\text{where} \quad \mathbf{M} = (m_{ij}) \quad & \text{with} \quad m_{ij} = (\phi_i, \phi_j) = \textstyle\sum_{e=1}^{E} \int_{\Omega_e} \phi_i \phi_j d\Omega \\
\mathbf{A} = (a_{ij}) \quad & \text{with} \quad a_{ij} = a(\phi_i, \phi_j) = \\
& \textstyle\sum_{e=1}^{E} \int_{\Omega_e} \left(k \nabla \phi_i \cdot \nabla \phi_j + b \phi_i \phi_j\right) d\Omega \\
& + \textstyle\sum_{e=1}^{\partial E} \int_{\partial \Omega_e} k \alpha \phi_i \phi_j \, ds \\
\mathbf{F} = (f_i) \quad & \text{with} \quad f_i = L(\phi_i)
\end{aligned}$$

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.*

Definition: 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 (1) with $k = 1,\ b = f = 0,\ u = 0$ on $\partial\Omega$ and let u_n be the corresponding finite element solution using (6). Then $\exists$ constant c such that

$$\max_{t \in I} \parallel u(t) - u_n(t) \parallel \leq c\left(1 + \left|\log \frac{T}{h^2}\right|\right) \max_{t \in I} h^2 \|u(t)\|_{H^2(\Omega)}. \qquad (7)$$

<u>Basic stability inequality</u> (for $f = 0,\ u = 0$ on $\partial\Omega$).
Let $u_h(t)$ satisfy (6), then

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

<u>Proof</u> For $u = 0$ on $\partial\Omega$, (4) becomes (on taking $v_h = u_h$)

$$\begin{aligned}
&(\dot{u}_h, u_h) + a(u_h, u_h) = 0 \\
&\tfrac{1}{2}\ \tfrac{d}{dt}\|u_h\|^2 + a(u_h, u_h) = 0 \\
&\|u_h\|^2 + 2\int_0^t a(u_h(s), u_h(s))ds = \|u_h(0)\|^2
\end{aligned}$$

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

Time Differencing

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

$$\mathbf{M}\dot{\mathbf{u}} + \mathbf{A}\mathbf{u} \ = \ \mathbf{F} \tag{8}$$

Let $$\frac{d\mathbf{u}}{dt}(t) = \frac{\mathbf{u}(t+\Delta t_r) - \mathbf{u}(t)}{\Delta t}\left(or \frac{d\mathbf{u}_r}{dt} = \frac{\mathbf{u}_{r+1} - \mathbf{u}_r}{\Delta t_r}\right) \tag{9}$$

and use forward difference with $O(\Delta t)$ accuracy, then (8) becomes

$$\mathbf{M}\ \mathbf{u}_{r+1} = (\mathbf{M} - \Delta t_r \mathbf{A})\mathbf{u}_r + \Delta t_r \mathbf{F}_r \tag{10}$$

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

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 $(\mathbf{u}_t = 0)$ in Chapter 4 can be modified to solve this FE system at each time step.

Program Structure

Loop over time steps $r = 0, 1, 2, ...Max_t$

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

For each Ω_e, calculate $a^e, m^e, f^e, \&\ b_r^e = (m^e - \Delta t_r k^e) u_r^e$

Assemble m^e to M & b_r^e to b_r

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

Solve $Mu_{r+1} = b_r$

Stability

To analyze the stability of the forward difference scheme, we consider the system (8) with the initial solution $\mathbf{u}(0) = \hat{\mathbf{u}}$.

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

$$\mathbf{M}(\dot{\mathbf{u}} + \dot{\mathbf{e}}) + \mathbf{A(u{+}e){=}F}. \tag{11}$$

From (8) and (11) $\Rightarrow \quad \mathbf{M\dot{e}} + \mathbf{Ae} = \mathbf{0}$

$$\Rightarrow \quad \frac{d\mathbf{e}}{dt} = -\mathbf{M}^{-1}\mathbf{Ae}.$$

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

$$\mathbf{e}_{r+1} = R^{r+1}\mathbf{e}_0 \ , \ (r = 0, 1, ... \frac{T}{\Delta t}). \tag{12}$$

Let $\lambda_i, \ \{\mathbf{w}_i\}_{i=1}^{N}$ be eigenvalues and eigenvectors of $\mathbf{M}^{-1}\mathbf{A}$.

Then $\mathbf{M}^{-1}\mathbf{A}\mathbf{w}_i \ = \ \lambda_i \mathbf{w}_i$

$\rightarrow$ $\Delta t \mathbf{M}^{-1}\mathbf{A}\mathbf{w}_i \ = \ -\Delta t \lambda_i \mathbf{w}_i$

$$\mathbf{I}\mathbf{w}_i - \Delta t \mathbf{M}^{-1}\mathbf{A}\mathbf{w}_i \ = \ (1 - \Delta t \lambda_i)\mathbf{w}_i$$

$$(\mathbf{I} - \Delta t \mathbf{M}^{-1}\mathbf{A})\mathbf{w}_i \ = \ (1 - \Delta t \lambda_i)\mathbf{w}_i$$

We can approximate the error at r=0 as $\mathbf{e}_0 = \sum_{i=1}^{N} \alpha_i \mathbf{w}_i$.

Hence,

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

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

Therefore,

$$\mathbf{e}_{r+1} = R^{r+1}\mathbf{e}_0 = \sum_{1}^{N} (1 - \lambda_i \Delta t)^{r+1} \alpha_i \mathbf{w}_i \tag{13}$$

Remarks

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

$$|1 - \lambda_i \Delta t| < 1, \ \texttt{i.e.} \ \Delta t < \frac{2}{\lambda_i} \ \ (i = 1, 2, ..., N), \tag{14}$$

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 (14) implies

$$\Delta t \leq \frac{2}{\beta} h^2 = ch^2 \tag{15}$$

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 $$\frac{d\mathbf{u}}{dt}(t + \frac{\Delta t}{2}) = \frac{\mathbf{u}(t+\Delta t) - \mathbf{u}(t)}{\Delta t}$$

$$\mathbf{u}(t + \frac{\Delta t}{2}) = \frac{1}{2}(\mathbf{u}(t) + \mathbf{u}(t + \Delta t))$$

Then (8) becomes

$$(\mathbf{M} + \frac{\Delta t}{2}\mathbf{A})\mathbf{u}_{r+1} = (\mathbf{M} - \frac{\Delta t}{2}\mathbf{A})\mathbf{u}_r + \Delta t \mathbf{F}_{r+\frac{1}{2}} \tag{16}$$

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

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

<u>Stability</u>

We consider an initial error $\mathbf{e}_0$ and analyze the error growth in the recursion (16). Pre-multiplying (16) by $\mathbf{M}^{-1}$, we obtain

$$(I + \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{A})\mathbf{e}_{r+1} = (I - \frac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{A})\mathbf{e}_r, \tag{17}$$

$$\mathbf{e}_{r+1} = R_+^{-1} R_- \mathbf{e}_r = (R_+^{-1} R_-)^{r+1}\mathbf{e}_0, \tag{18}$$

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

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

$$\mathbf{e}_0 = \textstyle\sum_1^N \alpha_i \, \mathbf{w}_i,$$

$$R_\pm \mathbf{w}_i = (I \pm \tfrac{\Delta t}{2}\mathbf{M}^{-1}\mathbf{A})\mathbf{w}_i = (1 \pm \tfrac{\Delta t}{2}\lambda_i)\mathbf{w}_i,$$

$$R_+^{-1} \, \mathbf{w}_i = (1 + \tfrac{\Delta t}{2}\lambda_i)^{-1}\mathbf{w}_i.$$

Therefore,

$$\mathbf{e}_{r+1} = (R_+^{-1}R_-)^r \; R_+^{-1}(R_- \, \mathbf{e}_0) = (R_+^{-1}R_-)^r \; \sum R_+^{-1}(1 - \frac{\Delta t}{2}\lambda_i)\alpha_i \mathbf{w}_i$$

$$= (R_+^{-1}R_-)^r \; \sum_{i=1}^{N} \frac{1 - \frac{\Delta t}{2}\lambda_i}{1 + \frac{\Delta t}{2}\lambda_i}\alpha_i \mathbf{w}_i \; = \; \sum_{i=1}^{N} \rho_i^{r+1}\alpha_i \mathbf{w}_i.$$

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.

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

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

Using the similar procedure, it can be shown that the above scheme is

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

Time Integration

Two different kinds of integration schemes, implicit and explicit, can be utilized to solve the system of parabolic finite element equations.

`eg. Backward Euler:` $\dot{M}\frac{U_{n+1}-U_n}{\triangle t} + A(U_{n+1})U_{n+1} = F_{n+1}$

`-- implicit`

`Forward Euler:` $M\frac{U_{n+1}-U_n}{\triangle t} + A(U_n)U_n = F_n$

`-- explicit.`

Note: In constructing a time integration scheme, questions of numerical stability and accuracy must be considered.

EXERCISE

Consider the convection-diffusion-problem

$$\frac{\partial u}{\partial t} - \mu \Delta u + \beta_1 \frac{\partial u}{\partial x_1} + \beta_2 \frac{\partial u}{\partial x_2} = f \quad \text{in } \Omega \times I$$

$$u \ = \ 0 \ \text{ on } \ \partial\Omega \times I$$

$$u(\mathbf{x}, 0) = u_0 \quad \text{on} \ \ \Omega$$

a) Find the variational statement of the problem.

b) Determine the finite element equation.

Element Transformation

Calculation of element matrices in x, y coordinates is awkward as integration region is complex and limit of integration changes from element to element. If we can find a transformation

$$T_e \; : \quad \begin{cases} x = x(\xi, \eta) \\ y = y(\xi, \eta) \end{cases}$$

which maps an arbitrarily chosen element e into a standard (master) element $\bar{\Omega}$, then the calculation of element matrices can be standardized using numerical quadrature.

(1) Master Element & Its Connection with Finite Element Mesh

The geometry of the master element is chosen as simple as possible, eg. the square as shown.

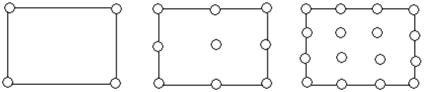


Figure: Square elements with 4 nodes (linear element), 9 nodes (quadratic element) and 16 nodes (cubic element)

Element Calculation

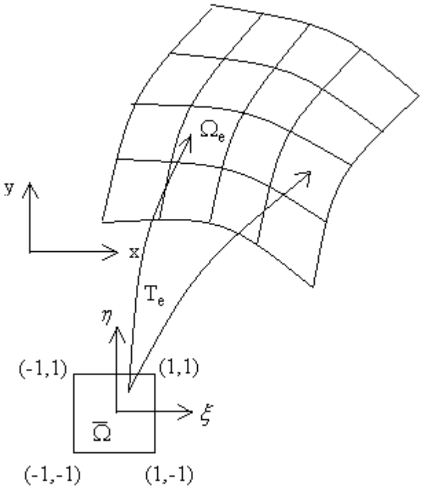


Figure: Element transformation T_e

Element Calculation

• A point $P(\xi = \alpha, \eta = \beta)$ in the standard element $\bar{\Omega}$ is mapped into a point

$$P[x(\alpha, \beta), y(\alpha, \beta)]$$

in local element Ω_e.
• A line $(\xi = \alpha)$ in $\bar{\Omega}$ is mapped into a curve

$$[x = x(\alpha, \eta), y = y(\alpha, \eta)]$$

in the plane, which is called the curvilinear coordinate line $(\xi = \alpha)$.

Element Calculation

• A finite element mesh can be viewed as a sequence of transformation $\{T_1,\ T_2, ... T_E\}$ of the fixed master element. Each element Ω_e is the image of the master element $\bar{\Omega}$ under a coordinate map T_e.

• All properties of a given type of elements (number and location of nodes, shape functions, stiffness and etc) can be prescribed for the fixed element $\bar{\Omega}$, and then carried to any Ω_e in the mesh by using the map T_e.

Relations between dx, dy with $d\xi$ and $d\eta$

Suppose $x(\xi,\eta)$ and $y(\xi,\eta)$ are continuously differentiable, then

$$dx = \frac{\partial x}{\partial \xi} d\xi + \frac{\partial x}{\partial \eta} d\eta \text{ and}$$

$$dy = \frac{\partial y}{\partial \xi} d\xi + \frac{\partial y}{\partial \eta} d\eta$$

$$\text{or} \quad \begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{bmatrix} \begin{bmatrix} d\xi \\ d\eta \end{bmatrix} = J \begin{bmatrix} d\xi \\ d\eta \end{bmatrix}, \qquad (19)$$

where $J =$ Jacobian matrix of the transformation.

(2) Properties of Coordinate Transformation

If at point (ξ, η) we have $|J| = det(J) \neq 0$
then an inverse map $T_e^{-1}(x, y \to \xi, \eta)$ exists at this point and thus

$$\begin{bmatrix} d\xi \\ \\ d\eta \end{bmatrix} = J^{-1} \begin{bmatrix} dx \\ \\ dy \end{bmatrix} \tag{20}$$

and

$$T_e^{-1} \ : \quad \begin{array}{c} \xi = \xi(x, y) \\ \eta = \eta(x, y) \end{array} \tag{21}$$

defines a map $(x, y) \to (\xi, \eta)$.

Element Calculation

As in (19), we have

$$\begin{bmatrix} d\xi \\ \\ d\eta \end{bmatrix} = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} \begin{bmatrix} dx \\ \\ dy \end{bmatrix}. \tag{22}$$

Hence, by equating terms in (22) and (20), we have the following relations

$$\frac{\partial \xi}{\partial x} = \frac{1}{|J|}\frac{\partial y}{\partial \eta}, \quad \frac{\partial \xi}{\partial y} = -\frac{1}{|J|}\frac{\partial x}{\partial \eta}, \quad \frac{\partial \eta}{\partial x} = -\frac{1}{|J|}\frac{\partial y}{\partial \xi}, \quad \frac{\partial \eta}{\partial y} = \frac{1}{|J|}\frac{\partial x}{\partial \xi} \tag{23}$$

(3) Construction of the Transformations T_e

Criteria for selection of T_e

(i) Within $\Omega_e, \xi(x, y)$ and $\eta(x, y)$ must be invertible and continuously differentiable.

(ii) $\{T_e\}_{e=1}^{E}$ must generate a mesh with no spurious gaps between elements and with no element overlapping another.

(iii) T_e should be easy to construct from the geometric data of the element.

(3) Construction of the Transformations T_e

Construction of T_e

The transformation T_e is constructed based on the element shape functions.

Let ψ_j be the shape function defined on $\bar{\Omega}$ for $j = 1, 2...N$, where N is the total number of nodes in $\bar{\Omega}$.

Then, any function $g = g(\xi, \eta)$ in $\bar{\Omega}$ can be approximated by

$$\bar{g}(\xi, \eta) = \sum g_j \psi_j(\xi, \eta). \tag{24}$$

(3) Construction of the Transformations T_e

Let $g = x$ and $g = y$ respectively, from (24) we have

$$T_e \;:\; \begin{array}{c} x = \sum_{j=1}^{N} x_j \psi_j(\xi, \eta), \\ \\ y = \sum_{j=1}^{N} y_j \psi_j(\xi, \eta), \end{array} \tag{25}$$

which maps $\bar{\Omega}$ to Ω_e. To see this, consider a node i in $\bar{\Omega}$, the coordinates is (ξ_i, η_i). From (25), this point is mapped into point $x = x_i$, $y = y_i$ in the $x - y$ plane i.e, node i.

Remark

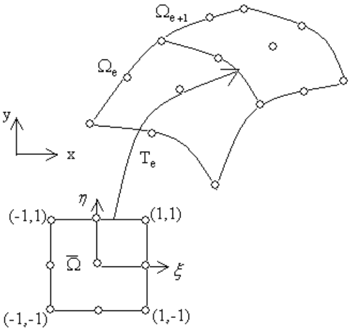
1) Criterion (iii) is easily verified. T_e is readily constructed from element data $(x_i,\ y_i,\ \ldots)$.
2) Criterion (ii) is usually not difficult to satisfy.
3) For T_e to be invertible, we require $det(J) \neq 0$. In addition, from the integration theory,

$$dxdy = |J|\ d\xi d\eta.$$

Clearly, for the mapping defined by (21) to be acceptable, we must have positive values of $|J|$ at all points in $\bar{\Omega}$. The satisfaction of this condition is not assured in general for all maps of the form (25). Each set of shape functions must be examined to ensure that $|J| > 0$ throughout $\bar{\Omega}$.

Straight sides of $\bar{\Omega}$ map to curved sides of Ω_e

The quadratic shape function on the master square maps the element to the corresponding elements Ω_e in the $x - y$ plane in such a way that straight sides of the $\bar{\Omega}$ are mapped to quadratic curved sides of Ω_e.
On a given curved side between Ω_e and Ω_{e+1}, the maps T_e and T_{e+1} reduce to the same quadratic functions.



Example

The following figure shows a 4-node master element $\bar{\Omega}$ and 2 elements Ω_1 and Ω_2 generated from it using the map (25). The shape function defined on $\bar{\Omega}$ are

$$\varphi = \frac{1}{4}(1 + \xi\xi_i)(1 + \eta\eta_i), \quad (i = 1, ..., 4)$$

where (ξ_i, η_i) are coordinates of node i.