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NONLINEAR HEAT TRANSFER

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March 1980

Lawrence Livermore Laboratory

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NONLINEAR HEAT TRANSFER

William E. Mason, Jr.
Methods Development Group

This report consists of a reproduction of the visuals used during the videotaping of the LLL Continuing Education Course CE-3151-6. The course was taped during January and February 1980 and consisted of six sessions which discussed the TACO and TACO3D nonlinear, finite element heat transfer codes and POSTACO, a companion graphics post-processor.

The following table lists the subjects of each session and lists the corresponding page numbers to aid those viewing the videotapes.

Session	Topic(s)	Pages
1.	Finite Element Heat Transfer	1-8
2.	Finite Element Heat Transfer (Cont.)	9-19
3.	TACO Features	20-30
4.	Additional TACO Features and Steady-State Examples	31-36
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NONLINEAR HEAT TRANSFER

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JANUARY 1980

OBJECTIVE:

TO DESCRIBE THE NUMERICAL SOLUTION OF NONLINEAR HEAT TRANSFER PROBLEMS USING THE TACO AND TACO3D FINITE ELEMENT COMPUTER CODES.

FINITE ELEMENT METHOD

VARIATIONAL FORMULATION

1-D STEADY STATE

D.E. $\frac{d}{dx}\left(k\frac{dT}{dx}\right)+Q=0 \qquad 0<x<L$

B.C. $\begin{cases} T=T_0 \quad \text{or} \quad -k\frac{dT}{dx}+q_0=0 \quad \text{at } x=0 \\ T=T_L \quad \text{or} \quad k\frac{dT}{dx}+q_L=0 \quad \text{at } x=L \end{cases}$

EQUIVALENT VARIATIONAL STATEMENT:

$$\delta I = I(T+\delta T)-I(T)=0$$

WHERE

$$I(T)=\int_0^L\left[\frac{k}{2}\left(\frac{dT}{dx}\right)^2-QT\right]dx + \left[q_0 T\Big|_{x=0}+q_L T\Big|_{x=L}\right]$$

$$\delta I = \int_0^L \left[k \frac{dT}{dx} \frac{d(\delta T)}{dx} - Q\delta T \right] dx$$

INTEGRATE BY PARTS

$$+ \left[q_0 \delta T \Big|_{x=0} + q_L \delta T \Big|_{x=L} \right]$$

$$= \left[k \frac{dT}{dx} \delta T \right] \Big|_0^L - \int_0^L \left[\frac{d}{dx}\left(k \frac{dT}{dx} \right) + Q \right] \delta T \, dx$$

$$+ \left[q_0 \delta T \Big|_{x=0} + q_L \delta T \Big|_{x=L} \right]$$

$$\delta I = -\int_0^L \left[\frac{d}{dx}\left(k \frac{dT}{dx} \right) + Q \right] \delta T \, dx$$

$$+ \left[-k \frac{dT}{dx} + q_0 \right] \Big|_{x=0} \left[\delta T \right] \Big|_{x=0}$$

$$+ \left[k \frac{dT}{dx} + q_L \right] \Big|_{x=L} \left[\delta T \right] \Big|_{x=L}$$

$\underline{\delta I = 0} \Rightarrow \frac{d}{dx}\left(k \frac{dT}{dx} \right) + Q = 0 \qquad 0 < x < L$

$\delta T = \delta T_0 = 0$ or $-k \frac{dT}{dx} + q_0 = 0$ at $x = 0$

$\delta T = \delta T_L = 0$ or $k \frac{dT}{dx} + q_L = 0$ at $x = L$

THE CLASSICAL APPROACH TO OBTAINING APPROXIMATE SOLUTIONS FROM THE VARIATIONAL FORMULATION IS VIA THE RITZ PROCEDURE.

RITZ PROCEDURE

$$T(x) \cong \sum_{n=1}^{N} A_n \phi_n(x)$$

A_n = ARBITRARY CONSTANTS
ϕ_n = TRIAL FUNCTIONS

ADMISSIBILITY CONDITIONS:

1. $T(x)$ MUST BE CONTINUOUS.
2. $\frac{dT}{dx}$ MUST BE PIECEWISE CONT.
3. T MUST SATISFY ITS BOUNDARY CONDITIONS.

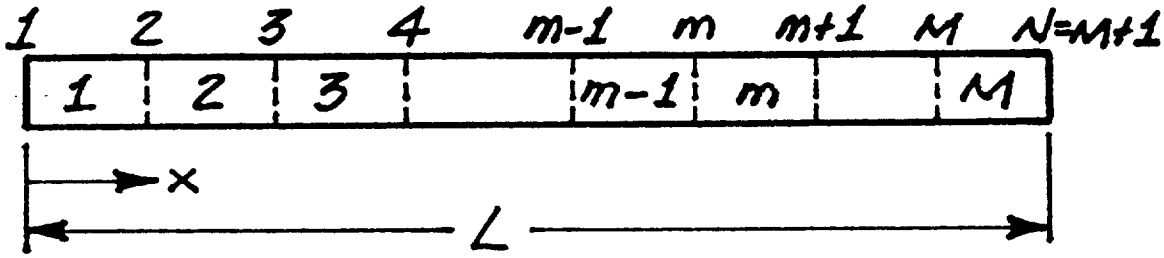
ON SUBSTITUTION

$$I(T) = I(A_1, A_2, \cdots, A_N)$$

$$\delta I = \frac{\partial I}{\partial A_1}\delta A_1 + \frac{\partial I}{\partial A_2}\delta A_2 + \cdots + \frac{\partial I}{\partial A_N}\delta A_N$$

$$\delta I = 0 \Rightarrow \frac{\partial I}{\partial A_1} = 0, \ \frac{\partial I}{\partial A_2} = 0, \cdots, \frac{\partial I}{\partial A_N} = 0$$

FINITE ELEMENT PROCEDURE



$$I(T) = \sum_{m=1}^{M} I^m + \left[q_0 T_1 + q_L T_N \right]$$

$$I^m = \int_{x_m}^{x_{m+1}} \left[\frac{k^m}{2} \left(\frac{dT^m}{dx} \right)^2 - Q^m T^m \right] dx$$

$$T^m(x) = C_1^m + C_2^m x$$

$$= \left(1 - \frac{x - x_m}{\ell^m}\right) T_m + \left(\frac{x - x_m}{\ell^m}\right) T_{m+1}$$

LETTING $\quad T_1^m = T_m \;\&\; T_2^m = T_{m+1}$

: element unknowns

$$N_1^m = \left(1 - \frac{x - x_m}{\ell^m}\right) \;\&\; N_2^m = \left(\frac{x - x_m}{\ell^m}\right)$$

: basis functions

THEN $\quad T^m(x) = \sum_{i=1}^{2} N_i^m T_i^m \equiv N_i^m T_i^m$

$$I^m = \int_{x_m}^{x_{m+1}} \left[\frac{k^m}{2} \left(\frac{dN_i^m}{dx} T_i^m \right) \left(\frac{dN_j^m}{dx} T_j^m \right) - Q^m N_i^m T_i^m \right] dx$$

$$= \frac{1}{2} K_{ij}^m T_i^m T_j^m - F_i^m T_i^m$$

$$K_{ij}^m = \int_{x_m}^{x_{m+1}} k^m \frac{dN_i^m}{dx} \frac{dN_j}{dx} dx = \begin{pmatrix} \text{element} \\ \text{conductivity} \\ \text{array} \end{pmatrix}$$

$$F_i^m = \int_{x_m}^{x_{m+1}} Q^m N_i^m dx = \begin{pmatrix} \text{element thermal} \\ \text{load array} \end{pmatrix}$$

NOTE: ELEMENT CONDUCTIVITY ARRAY (MATRIX) IS SYMMETRIC, I.E.

$$K_{ij}^m = K_{ji}^m \quad (i \neq j)$$

$$K_{ij}^m = \begin{pmatrix} K_{11}^m & K_{12}^m \\ K_{21}^m & K_{22}^m \end{pmatrix} \qquad K_{12}^m = K_{21}^m$$

IF $k^m \neq k^m(x)$

$$Q^m \neq Q^m(x)$$

THEN

$$K_{ij}^m = \frac{k^m}{\ell^m}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$F_i^m = \frac{Q^m \ell^m}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

RELATIONSHIP TO RITZ PROCEDURE:

$$I^m = I^m(T_m, T_{m+1})$$

$$\therefore \; I = I(T_1, T_2, \cdots, T_N)$$

$$\delta I = \frac{\partial I}{\partial T_1}\delta T_1 + \frac{\partial I}{\partial T_2}\delta T_2 + \cdots + \frac{\partial I}{\partial T_N}\delta T_N$$

$$\delta I = 0 \Rightarrow \frac{\partial I}{\partial T_1} = 0, \; \frac{\partial I}{\partial T_2} = 0, \cdots, \frac{\partial I}{\partial T_N} = 0$$

ELEMENT EQUATIONS MUST BE COMBINED INTO SYSTEM EQUATIONS.

$$\frac{\partial I}{\partial T_m} = \frac{\partial I^{m-1}}{\partial T_m} + \frac{\partial I^m}{\partial T_m} = 0$$

$$\frac{\partial I^m}{\partial T_i^m} = K_{ij}^m T_j^m - F_i^m$$

$$\frac{\partial I}{\partial T_m} = \left(K_{21}^{m-1} T_{m-1} + K_{22}^{m-1} T_m - F_2^{m-1}\right)$$

$$+\left(K_{11}^m T_m + K_{12}^m T_{m+1} - F_1^m\right) = 0$$

$\therefore$ FOR EACH INTERIOR NODE $(m = 2, 3, \cdots, N-1)$ THE RESULTING EQUATION IS

$$K_{21}^{m-1} T_{m-1} + \left(K_{22}^{m-1} + K_{11}^m\right) T_m + K_{12}^m T_{m+1} = F_2^{m-1} + F_1^m$$

FORMING ALL OF THESE EQUATIONS (INCLUDING MODIFICATIONS FOR $m = 1$ & N) GIVES

$$[K]\{T\} = \{F\}$$

DIRECT "STIFFNESS" METHOD:

MOST COMMON METHOD FOR FORMING SYSTEM EQUATIONS FROM ELEMENT EQUATIONS.

TERMS IN ELEMENT MATRICES ARE ADDED INTO APPROPRIATE ROWS AND COLUMNS OF SYSTEM MATRICES.

$$
\begin{bmatrix}
K_{11}^{1} & K_{12}^{1} & & & & \\
K_{21}^{1} & K_{22}^{1}+K_{11}^{2} & K_{12}^{2} & & & \\
 & K_{21}^{2} & K_{22}^{2}+K_{11}^{3} & K_{12}^{3} & & \\
 & & & & & \\
 & & & K_{11}^{M-1} & K_{22}^{M-1}+K_{11}^{M} & K_{12}^{M} \\
 & & & & K_{21}^{M} & K_{22}^{M}
\end{bmatrix}
\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ \\ T_{N-1} \\ T_N \end{Bmatrix}
=
\begin{Bmatrix} F_1^{1} \\ F_2^{1}+F_1^{2} \\ F_2^{2}+F_1^{3} \\ \\ F_2^{M-1}+F_1^{M} \\ F_2^{M} \end{Bmatrix}
$$

BOUNDARY CONDITIONS:

SO FAR BOUNDARY CONDITIONS HAVE NOT BEEN APPLIED.

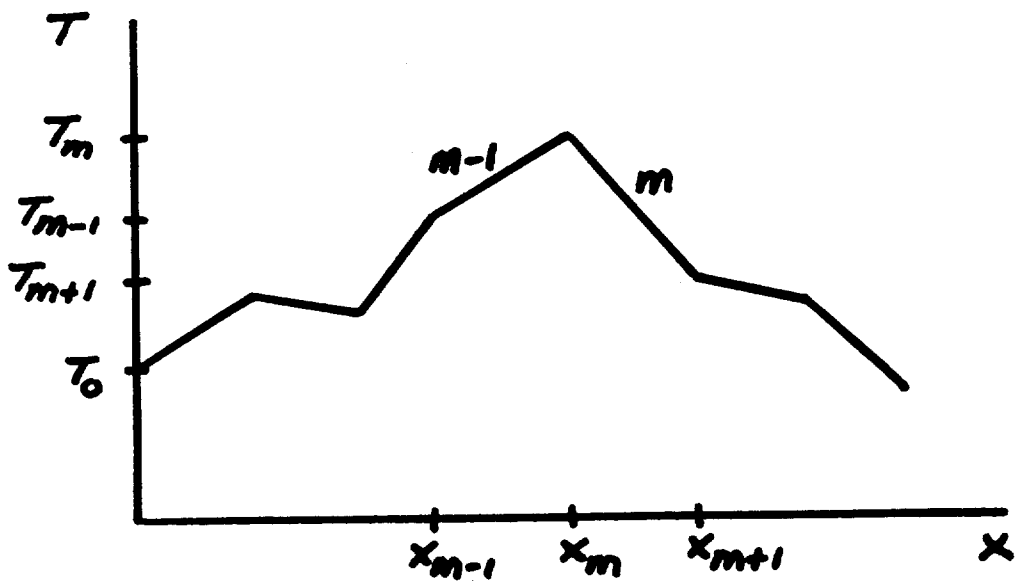
ASSUME, FOR EXAMPLE, THAT $T = T_0$ AT $x = 0$ AND $k\frac{dT}{dx} + q_L = 0$ AT $x = L$

TWO METHODS FOR APPLYING THESE CONDITIONS ARE ILLUSTRATED BELOW.

$$
\begin{bmatrix}
\overset{1}{\cancel{K_{11}^{1}}} & \overset{0}{\cancel{K_{12}^{1}}} & & & & \\
\overset{0}{\cancel{K_{21}^{1}}} & K_{22}^{1}+K_{11}^{2} & K_{12}^{2} & & & \\
 & K_{21}^{2} & K_{22}^{2}+K_{11}^{3} & K_{12}^{3} & & \\
 & & & & & \\
 & & & K_{11}^{M-1} & K_{22}^{M-1}+K_{11}^{M} & K_{12}^{M} \\
 & & & & K_{21}^{M} & K_{22}^{M}
\end{bmatrix}
\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ \\ T_{N-1} \\ T_N \end{Bmatrix}
=
\begin{Bmatrix} \overset{T_0}{\cancel{F_1^{1}}} \\ F_2^{1}+F_1^{2} - K_{21}^{1}T_0 \\ F_2^{2}+F_1^{3} \\ \\ F_2^{M-1}+F_1^{M} \\ F_2^{M}-q_L \end{Bmatrix}
$$

$$
\begin{bmatrix}
\cancel{K_{11}^{1}}^{\,10^{30}} & K_{12}^{1} & & & & \\
K_{21}^{1} & K_{22}^{1}+K_{11}^{2} & K_{12}^{2} & & & \\
 & K_{21}^{2} & K_{22}^{2}+K_{11}^{3} & K_{12}^{3} & & \\
 & & & & & \\
 & & & K_{11}^{M-1} & K_{22}^{M-1}+K_{11}^{M} & K_{12}^{M} \\
 & & & & K_{21}^{M} & K_{22}^{M}
\end{bmatrix}
\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ \\ T_{N-1} \\ T_N \end{Bmatrix}
=
\begin{Bmatrix} \cancel{F_1^{1}}^{\,T_0 \times 10^{30}} \\ F_2^{1}+F_1^{2} \\ F_2^{2}+F_1^{3} \\ \\ F_2^{M-1}+F_1^{M} \\ F_2^{M}-q_L \end{Bmatrix}
$$

NOTE THAT ADMISSIBILITY CONDITIONS HAVE BEEN SATISFIED:



WEIGHTED RESIDUAL METHOD

"WEAK" FORMULATION

$$\int_0^L \phi\left[\frac{d}{dx}\left(k\frac{dT}{dx}\right)+Q\right]dx$$

$$-\left[\phi\left(-k\frac{dT}{dx}+q_0\right)\right]\Big|_{x=0}-\left[\phi\left(k\frac{dT}{dx}+q_L\right)\right]\Big|_{x=L}=0$$

$$=\left[\phi\left(k\frac{dT}{dx}\right)\right]\Big|_0^L-\int_0^L\left[\frac{d\phi}{dx}\left(k\frac{dT}{dx}\right)-\phi Q\right]dx$$

$$-\left[\phi\left(-k\frac{dT}{dx}+q_0\right)\right]\Big|_{x=0}-\left[\phi\left(k\frac{dT}{dx}+q_L\right)\right]\Big|_{x=L}$$

$$=-\int_0^L\left[\frac{d\phi}{dx}\left(k\frac{dT}{dx}\right)-\phi Q\right]dx-q_0\phi\Big|_{x=0}-q_L\phi\Big|_{x=L}$$

WEIGHTED RESIDUAL FORMULATIONS

$$\phi = w_j \quad (j=1,2,3,\cdots,n)$$

(1) POINT COLLOCATION: $w_j=\delta_j=\begin{cases}1 & x=x_j\\ 0 & x\neq x_j\end{cases}$

(2) SUBDOMAIN COLLOCATION:

$$w_j=1 \qquad a_j\le x\le b_j$$

(3) GALERKIN METHOD:

$$w_j=N_j=\text{basis functions}$$

GALERKIN METHOD

$$-\int_0^L \left[\frac{dN_i^m}{dx}\left(k^m \frac{dN_j^m}{dx} T_j^m\right) - N_i^m Q^m\right] dx - q_0 N_i^m\Big|_{x=0} - q_L N_i^m\Big|_{x=L} \qquad (A)$$

$$= -\left[\int_{x_m}^{x_{m+1}} k^m \frac{dN_i^m}{dx}\frac{dN_j^m}{dx} dx\right] T_j^m + \int_{x_m}^{x_{m+1}} N_i^m Q^m dx - q_0 N_i^m\Big|_{x=0} - q_L N_i^m\Big|_{x=L}$$

$$= -K_{ij}^m T_j^m + F_i^m - q_0 N_i^m\Big|_{x=0} - q_L N_i^m\Big|_{x=L}$$

: same as variational formulation

TRANSIENT CASE

GALERKIN FORMULATION

$$\text{D.E.}\left\{ \rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + Q \right.$$

$$\text{B.C.}\begin{cases} T = T_0(t) \text{ or } -k\dfrac{\partial T}{\partial x} + q_0 = 0 & \text{at } x=0 \\ T = T_L(t) \text{ or } k\dfrac{\partial T}{\partial x} + q_L = 0 & \text{at } x=L \end{cases}$$

$$\text{I.C.}\left\{ T = T_i(x) \quad \text{at } t=0 \right.$$

NOW

$$T^m(x,t) \cong N_i^m(x)\,T_i^m(t)$$

NOTE: $$\frac{\partial T^m}{\partial x} = \frac{dN_i^m}{dx}T_i^m$$

$$\frac{\partial T^m}{\partial t} = N_i^m \frac{dT_i^m}{dt}$$

IN (A) $Q^m \rightarrow Q^m - \rho^m c_p^m \frac{\partial T^m}{\partial t}$:

$$-\int_0^L \left[\frac{dN_i^m}{dx}\left(k^m \frac{dN_j^m}{dx} T_j^m\right) - N_i^m\left(Q^m - \rho^m c_p^m N_j^m \frac{dT_j^m}{dt}\right)\right]dx$$

$$-q_0 N_i^m\Big|_{x=0} - q_L N_i^m\Big|_{x=L}$$

$$= -C_{ij}^m \frac{dT_j^m}{dt} - K_{ij}^m T_j^m + F_i^m$$

$$-q_0 N_i^m\Big|_{x=0} - q_L N_i^m\Big|_{x=L}$$

WHERE

$$C_{ij}^m = \int_{x_m}^{x_{m+1}} \rho^m c_p^m N_i^m N_j^m \, dx$$

$$K_{ij}^m = \int_{x_m}^{x_{m+1}} k^m \frac{dN_i^m}{dx}\frac{dN_j^m}{dx}\, dx$$

$$F_i^m = \int_{x_m}^{x_{m+1}} N_i^m Q^m \, dx$$

COMBINING ELEMENT EQUATIONS TO FORM SYSTEM EQUATIONS GIVES

$$[C]\left\{\frac{dT}{dt}\right\}+[K]\{T\}=\{F\}$$

DENOTING $\dot{T}=\frac{dT}{dt}$ AND DROPPING BRACKETS

$$C\dot{T}+KT=F$$

TIME INTEGRATION

$$C_{t+\alpha\Delta t}\dot{T}_{t+\alpha\Delta t}+K_{t+\alpha\Delta t}T_{t+\alpha\Delta t}$$

$$=F_{t+\alpha\Delta t} \quad (0\leq\alpha\leq 1)$$

$C_{t+\alpha\Delta t}=C(T_{t+\alpha\Delta t})$	$\dot{T}_{t+\alpha\Delta t}=\frac{1}{\Delta t}(T_{t+\Delta t}-T_t)$
$K_{t+\alpha\Delta t}=K(T_{t+\alpha\Delta t})$	$T_{t+\alpha\Delta t}=(1-\alpha)T_t+\alpha T_{t+\Delta t}$
$F_{t+\alpha\Delta t}=(1-\alpha)F_t+\alpha F_{t+\Delta t}$	$T_{t+\Delta t}=T_t+\Delta T_t$

COMBINING EQUATIONS GIVES

$$K^*_{t+\alpha\Delta t}\Delta T_t = F^*_{t+\alpha\Delta t}$$

WHERE

$$K^*_{t+\alpha\Delta t} = \frac{1}{\Delta t}C_{t+\alpha\Delta t} + \alpha K_{t+\alpha\Delta t}$$

$$F^*_{t+\alpha\Delta t} = F_{t+\alpha\Delta t} - K_{t+\alpha\Delta t}T_t$$

STABILITY CONSIDERATIONS

FORWARD EXPLICIT:
$\alpha = 0$

CRANK-NICHOLSON:
$\alpha = \frac{1}{2}$

BACKWARD IMPLICIT:
$\alpha = 1$

UNCONDITIONALLY STABLE: $\frac{1}{2} \leq \alpha \leq 1$

TWO-DIMENSIONAL CASE

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + Q \quad \text{in } R$$

$$\text{B.C.} \begin{cases} T = T_s & \text{on } S_1 \\ k_x \frac{\partial T}{\partial x} n_x + k_y \frac{\partial T}{\partial y} n_y + q = 0 & \text{on } S_2 \end{cases}$$

$$\text{I.C.} \left\{ T = T_i \right. \qquad \text{at } t = t_i$$

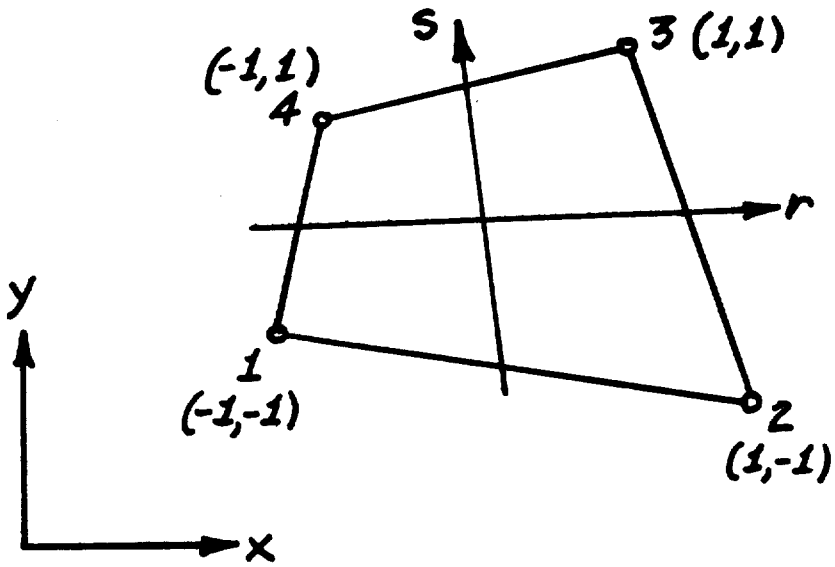
IN GENERAL

$$q = f(T,t)\left(T^a - T_\infty^a\right)^b$$

"LINEARIZED"

$$q = f_0(T,t) + h(T,t)\left(T - T_\infty\right)$$

BILINEAR QUADRILATERAL ELEMENT



$$T(r,s) = \frac{1}{4}(1-r)(1-s)T_1 + \frac{1}{4}(1+r)(1-s)T_2 + \frac{1}{4}(1+r)(1+s)T_3 + \frac{1}{4}(1-r)(1+s)T_4$$

$$\therefore \quad T(r,s,t) = N_i(r,s)\,T_i(t)$$

CAN RELATE LOCAL (r,s) COORDINATES TO GLOBAL (x,y) COORDINATES BY

$$x(r,s) = N_i x_i$$

$$y(r,s) = N_i y_i$$

TO DERIVE ELEMENT EQUATIONS FOLLOW THE GALERKIN METHOD

$$\iint_A N_i\left[\frac{\partial}{\partial x}\left(k_x\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y\frac{\partial T}{\partial y}\right)+Q-\rho c_p\frac{\partial T}{\partial t}\right]dA$$

$$-\int_S N_i\left[k_x\frac{\partial T}{\partial x}n_x+k_y\frac{\partial T}{\partial y}n_y+f_0+h(T-T_\infty)\right]dS=0$$

$\Rightarrow$

$$C_{ij}=\iint_A \rho c_p N_i N_j\,dA$$

$$K_{ij}=\iint_A\left[k_x\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+k_y\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\right]dA+\int_{S_2} hN_iN_j\,dS$$

$$F_i=\iint_A N_iQ\,dA+\int_{S_2} N_i(hT_\infty-f_0)\,dS$$

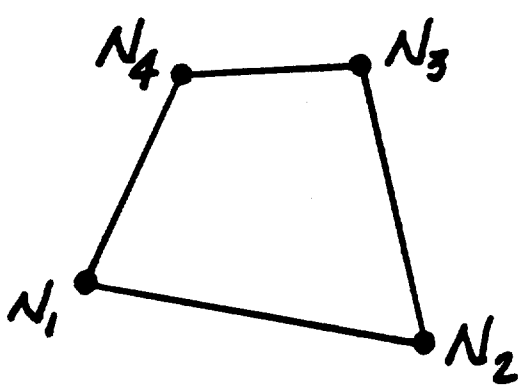
TACO FEATURES

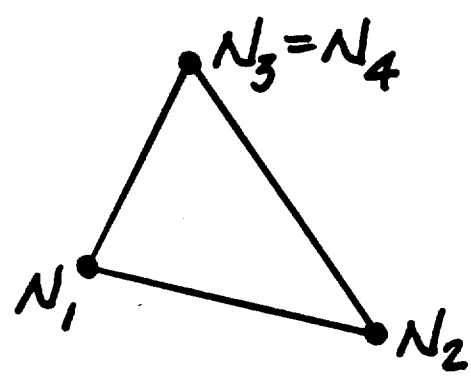
TACO IS AN IMPLICIT, NONLINEAR, TRANSIENT, FINITE ELEMENT CODE

REF.: W.E. MASON
TACO-A FINITE ELEMENT HEAT TRANSFER CODE
UCID-17980

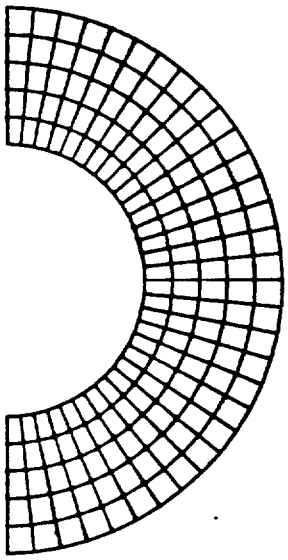
SPATIAL DISCRETIZATION

BASIC ELEMENT:
4-NODE ISOPARAMETRIC QUADRILATERAL





MESH GENERATION



TACO HAS ONLY LIMITED MESH GENERATION CAPABILITY. FOR COMPLICATED MESHES SEPARATE MESH GENERATION CODES MUST BE USED.

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   UCID-17139 (1976)

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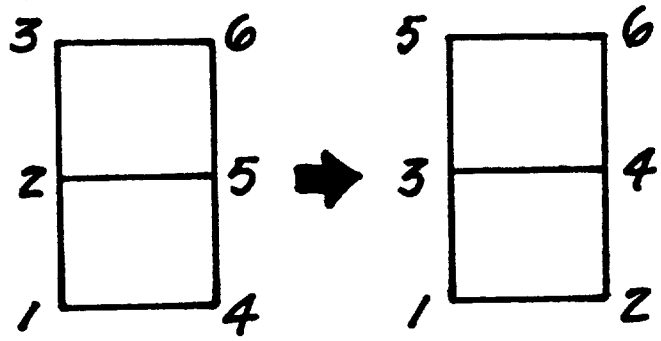
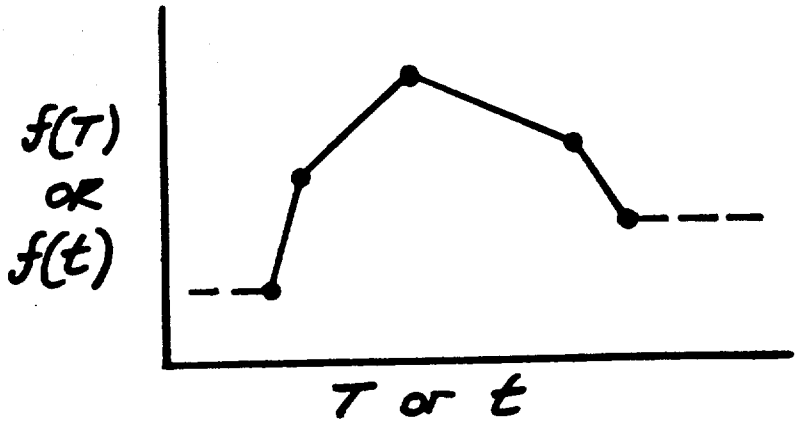
BANDWIDTH AND PROFILE MINIMIZATION

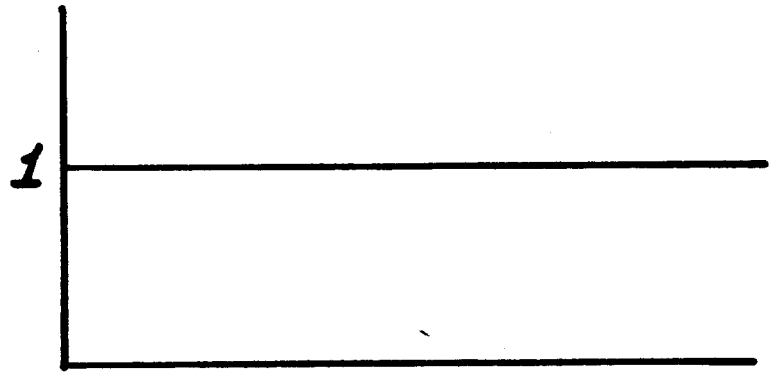


FUNCTIONAL REPRESENTATION

PIECEWISE LINEAR



CONSTANT



USER SUBPROGRAM

4 ENTRY POINTS:

USUB : INITIALIZE

USUB2 : CALCULATE

USUB3 : PRINT

USUB4 : PLOT

CURVE NUMBER (NC)

NC = 0 ⇨ CONSTANT

NC > 0 ⇨ TIME DEP.

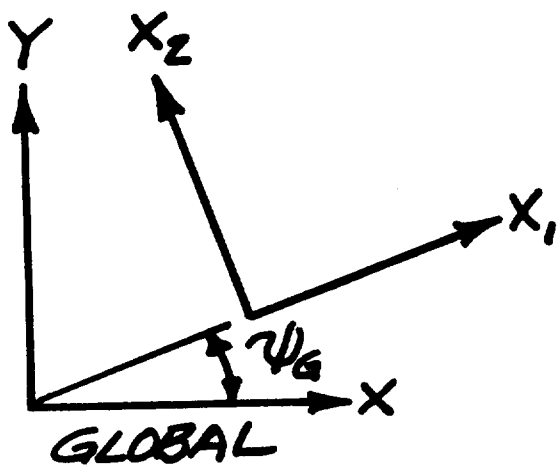
NC < 0 ⇨ TEMP. DEP.

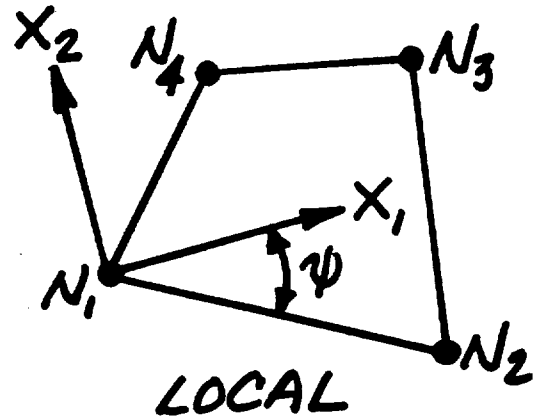
|NC| > 999 ⇨ USER SUB.

MATERIAL PROPERTIES

ISOTROPIC: ρ, c_p, k

ORTHOTROPIC: ρ, c_p, k_1, k_2, ψ





HEAT GENERATION RATES

CAN BE DEFINED BY:

- MATERIAL
- ELEMENT

INITIAL TEMPERATURES

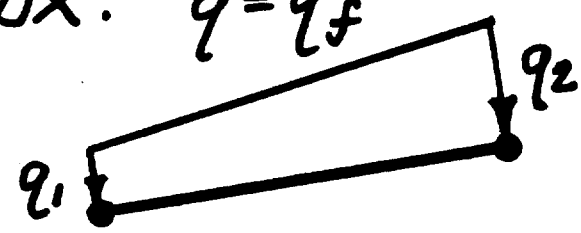
CAN BE DEFINED:

- FOR ENTIRE BODY
- BY NODES

BOUNDARY CONDITIONS

- TEMPERATURE:
  SPECIFIED BY NODES

- FLUX: $q = q_f$



- FORCED CONVECTION: $q = h(t)[T - T_\infty(t)]$

- GENERAL NONLINEAR

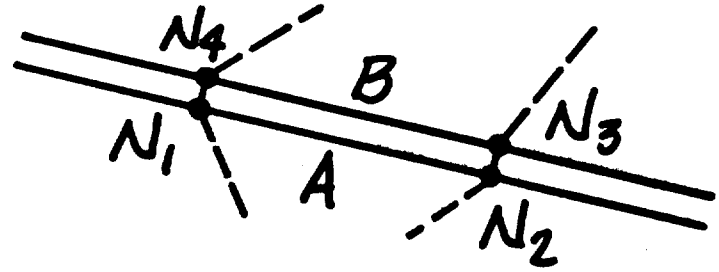
$$q = f(T,t)\left[T^a - T_\infty^a(t)\right]^b$$

EXAMPLE:

RADIATION

$$q = \sigma\epsilon\left[T^4 - T_\infty^4\right]$$

INTERNAL SURFACE CONDITIONS

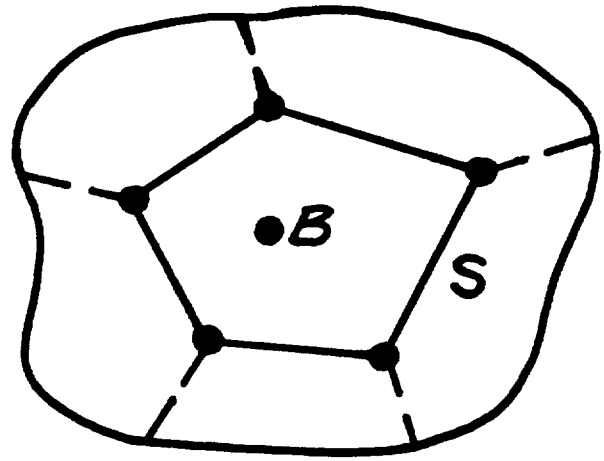


$$q = f(t)\left[T_A^a - T_B^a\right]^b$$

EXAMPLE: CONTACT RESISTANCE

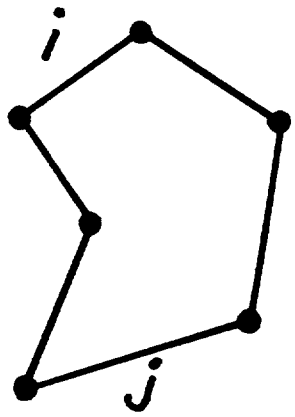
$$q = h\left[T_A - T_B\right]$$

BULK NODES



$$q = f(t)\left[T_S^a - T_B^a\right]^b$$

ENCLOSURE RADIATION



INCOMING FLUX: $\mathcal{H}$

$$\mathcal{H}_i = \sum_{j=1}^{N} F_{i-j} B_j$$

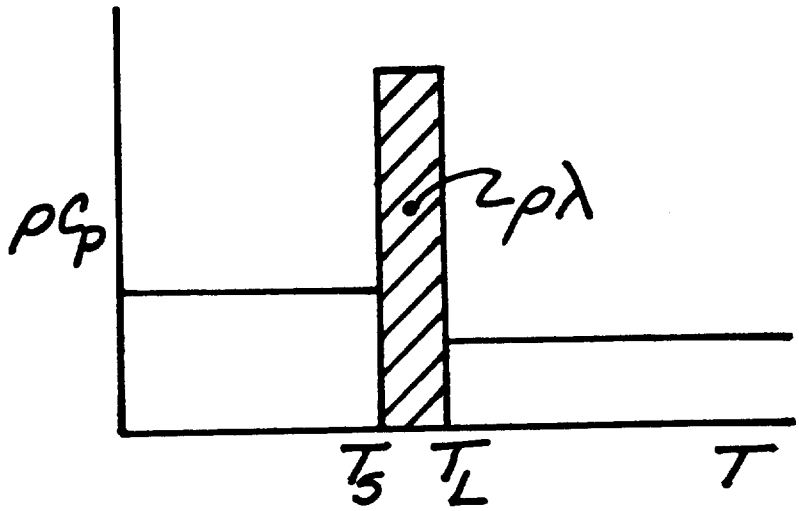
OUTGOING FLUX: B

$$B_i - (1-\epsilon_i)\mathcal{H}_i = \epsilon_i \sigma T_i^4$$

NET FLUX: q

$$q_i = B_i - \mathcal{H}_i$$

PHASE CHANGE



λ = LATENT HEAT

CHEMICAL KINETICS

EXAMPLE:

$$Q = -\sum_{n=1}^{N} \rho_n q_n \frac{\partial c_n}{\partial t}$$

$$\frac{\partial c_n}{\partial t} = -c_n^{p_n} z e^{-E_n/RT}$$

HANDLED IN TACO BY USER SUBPROGRAM

TIME STEP CONTROL

- CONSTANT
- PIECEWISE CONSTANT
- VARIABLE

NONLINEAR PROBLEMS

PROBLEM IS NONLINEAR IF:

$$k = k(T)$$

OR $\rho c_p = \rho c_p(T)$

OR $Q = Q(T)$

OR q NOT LINEAR FUNCTION OF T

NONLINEAR ANALYSIS

$$K^*(T_{t+\alpha\Delta t})\Delta T_t = F^*(T_{t+\alpha\Delta t})$$

TACO SOLUTION SCHEME INVOLVES A MODIFIED DIRECT ITERATION METHOD. STEPS INCLUDE:

1. K^* UPDATE (REFORMATION)
2. F^* UPDATE (ITERATION)

THERMAL STRESS ANALYSIS

MECHANICAL CODES SUCH AS NIKE2D (UCRL-52678) CAN READ TEMPERATURES FROM BINARY PLOT FILES PRODUCED BY TACO TO CALCULATE THERMAL STRESS STATES.

UNITS

MUST BE CONSISTENT!

EXAMPLE:

QUANTITY	UNITS	QUANTITY	UNITS
T	°C	C_p	J/kg·°C
x, y	m	k	W/m·°C
t	s	Q	W/m³
ρ	kg/m³	q	W/m²

AVAILABILITY

ON LLL OCTOPUS SYSTEM
OBTAIN WITH

ON CDC 7600

EXE GLGLIB TACO DR. / t v

ON CRAY

LIB MDGLIB!X TACO!END / t v

EXECUTION

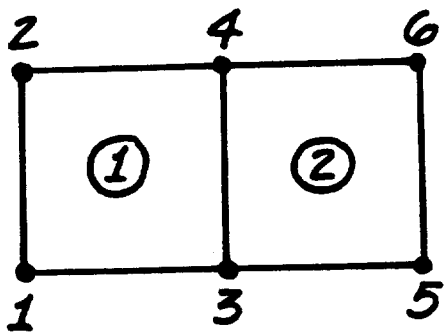
TACO I=<u>infile</u>, O=<u>printfile</u>, P=<u>plotfile</u> / t r

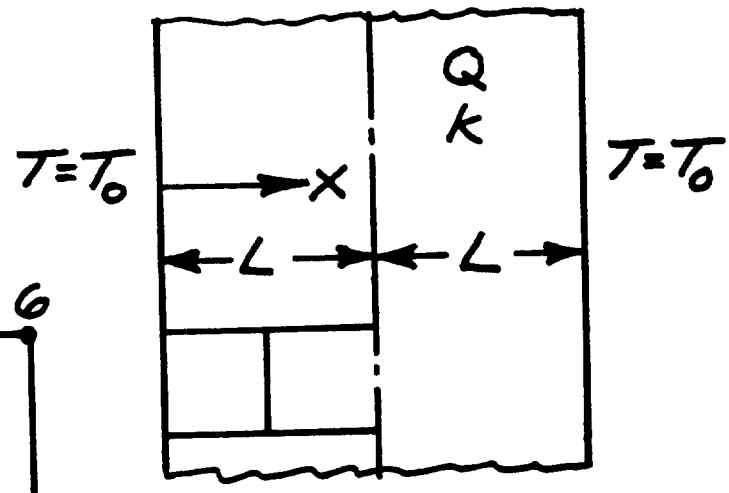
FILE NAMES ARE ORDER INDEPENDENT.
DROPOUTS ARE PERMITTED, E.G.,

TACO P=<u>plotfile</u> / t r

DEFAULT NAMES: I = TACOIN
O = TPRINT
P = TPLOT

EXAMPLE A.





$L=1$ $Q=2$
$k=1$ $T_0=3$

INPUT DATA FOR EXAMPLE A.

```
 1 $ TITLE CARD
 2 TACO EXAMPLE A.
 3 $ CONTROL CARD 1
 4      6     2     1     2     0     2     0     0     0     0     0     0     0     0     0     0
 5 $CONTROL CARD 2
 6      1     2          1.0
 7 $ CONTROL CARD 3
 8      0
 9 $ CONTROL CARD 4 (NOT REQUIRED)
10 $ CONTROL CARD 5
11      0
12 $ CONTROL CARD 6
13      0
14 $ NODAL POINT DATA
15      1                0.0       0.0       0.0
16      5                1.0       0.0       0.0     2
17      2                0.0       0.5       0.0
18      6                1.0       0.5       0.0     2
19 $ ELEMENT DATA
20      1     1     3     4     2     1     1     2
21 $ MATERIAL DATA
22 PSEUDO          1     1       1.0     0             1.0     0             0.0
23      0                1.0
24 $ HEAT GENERATION DATA
25      1     0          2.0     1     1
26 $ TEMPERATURE BOUNDARY CONDITION DATA
27      1     0          3.0     1     1
28 $ END DATA
29 STOP
```

SOLUTION-EXAMPLE A.

$$T_1 = T_2 = 3.00$$

$$T_3 = T_4 = 3.75$$

$$T_5 = T_6 = 4.00$$

EXACT SOLUTION:

$$T(x) = T_0 + \frac{Q}{k}\left(Lx - \frac{1}{2}x^2\right)$$

GIVES SAME VALUES AS ABOVE.

EXAMPLE NO. 1

$$\frac{d}{dx}\left(k\frac{dT}{dx}\right)+Q=0 \qquad 0\le x\le L$$

$$k=A+BT$$

SAME MESH AS EXAMPLE A.

$$-k\frac{dT}{dx}=C(T^4-T_\infty^4) \quad \text{at } x=0$$

$$T=T_L \quad \text{at } x=L$$

$L=1 \qquad A=1 \qquad B=-0.2 \qquad C=0.0025$

$Q=0.2 \qquad T_\infty=4 \qquad T_L=1$

INPUT DATA FOR EXAMPLE NO. 1

```
TACO EXAMPLE NO. 1
& CONTROL CARDS
& CARD 1
    6    2    1    0    0    2    0    0    1    0    0    0    0    1    0    0
& CARD 2
    1    2         1.0
& CARD 3
    0
& CARD 4 (NOT REQUIRED)
& CARD 5
    1
& CARD 6
    0
& NODAL POINT DATA
    1              0.0        0.0        0.0
    5              1.0        0.0        0.0    2
    2              0.0        0.5        0.0
    6              1.0        0.5        0.0    2
& ELEMENT DATA
    1    1    3    4    2    1    1    2
& MATERIAL DATA
PSEUDO         1    1        1.0    0            1.0    0            0.2
   -1
& TEMPERATURE BOUNDARY CONDITIONS
    5    0         1.0    1    1
& NONLINEAR BOUNDARY CONDITIONS
    2    1         0    0.0025         0        4.0       4.0       4.0       1.0
    0
& PIECEWISE LINEAR CURVE DATA
K-CURVE        1    2
        0.0        1.0
        5.0        0.0
STOP
```

SOLUTION-EXAMPLE NO. 1

ITERATION NUMBER	TEMPERATURE x = 0.0	x = 0.5
0	0.0	0.0
1	1.500	1.275
2	1.853	1.446
3	1.955	1.484
4	1.986	1.495
5	1.996	1.499
6	1.999	1.500
7	2.000	1.500

EXACT SOLUTION: $T = 2 - x$

EXAMPLE NO. 2

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \qquad 0 \le x \le L$$

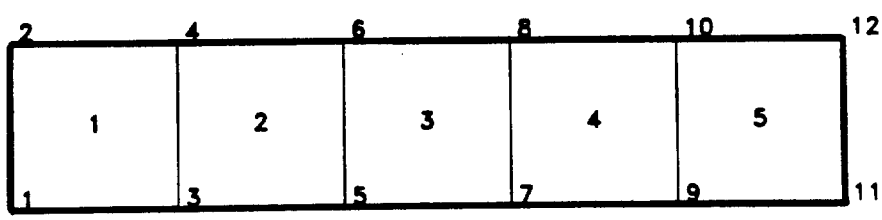
$$T(0,t) = T_0$$

$$-k \frac{\partial T}{\partial x}(L,t) = h\left[T(L,t) - T_\infty\right]$$

$$T(x,0) = T_0$$

$$\rho = C_p = k = L = T_0 = 1 \qquad T_\infty = 0 \qquad h = 0.6$$

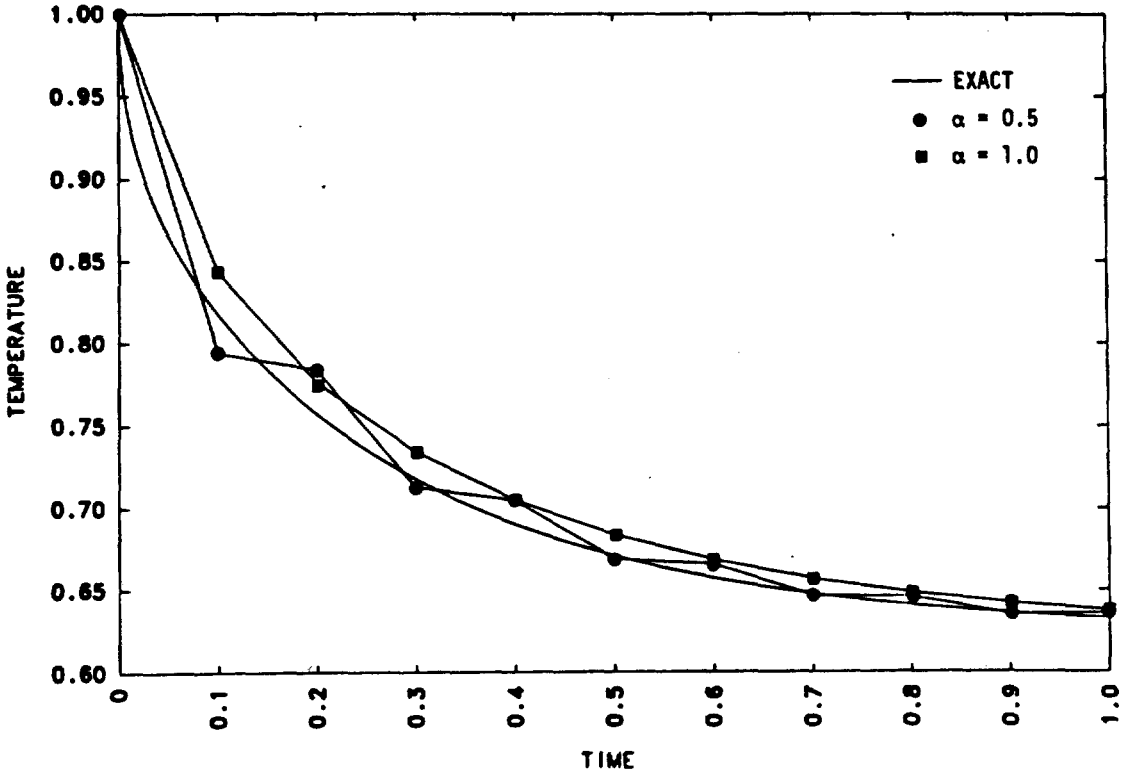
MESH FOR EXAMPLE 2



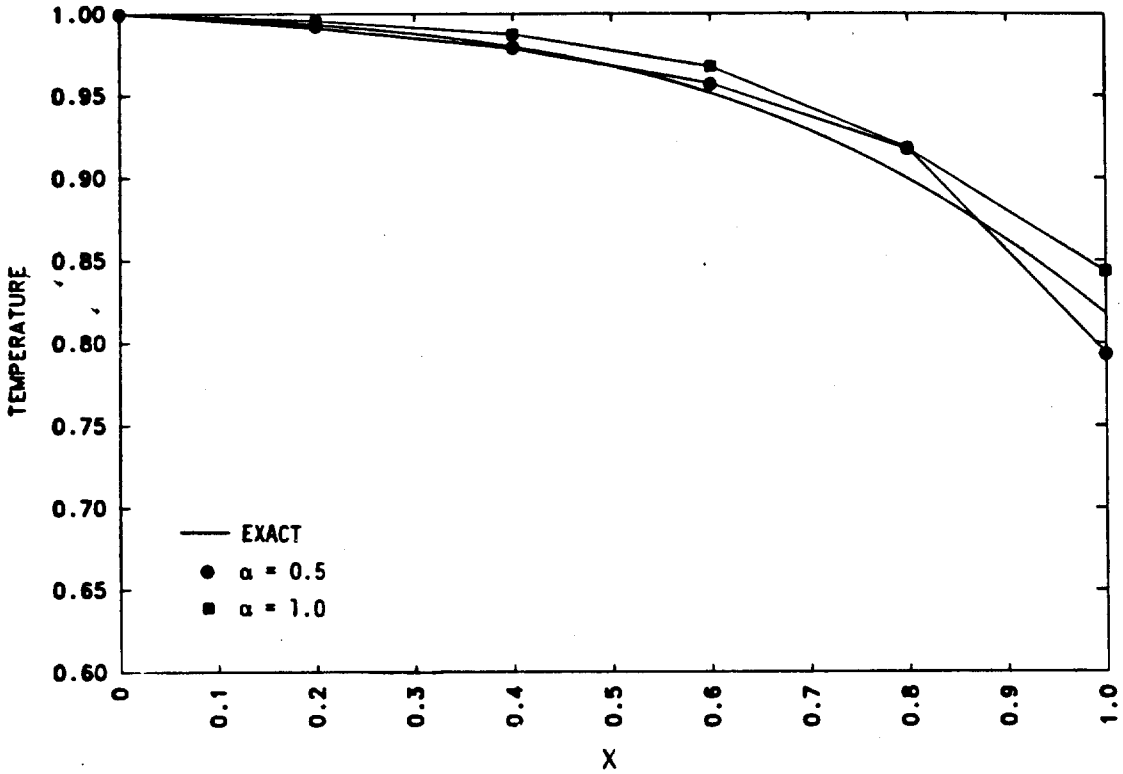
INPUT DATA FOR EXAMPLE NO. 2

```
TACO EXAMPLE NO. 2
& CONTROL CARD NO. 1
   12    5    1    0    0    2    0    1    0    0    0    0    0    0    0    0
& CONTROL CARD NO. 2
    1    2         1.0
& CONTROL CARD NO. 3
    1    0    1    1         0.0       1.0       0.5
& CONTROL CARD NO. 4
        0.1         1.0
& CONTROL CARD NO. 5
    0
& CONTROL CARD NO. 6
    0
& NODAL DATA
    1              0.0       0.0       0.0
   11              1.0       0.0       0.0    2
    2              0.0       0.2       0.0
   12              1.0       0.2       0.0    2
& ELEMENT DATA
    1    1    3    4    2    1    4    2
& MATERIAL DATA
PSEUDO         1    1         1.0    0            1.0    0            0.0
    0              1.0
& TEMPERATURE BOUNDARY CONDITIONS
    1    0         1.0    1    1
& CONVECTION BOUNDARY CONDITIONS
   11   12         0         0.6         0         0.0       0.0
STOP
```

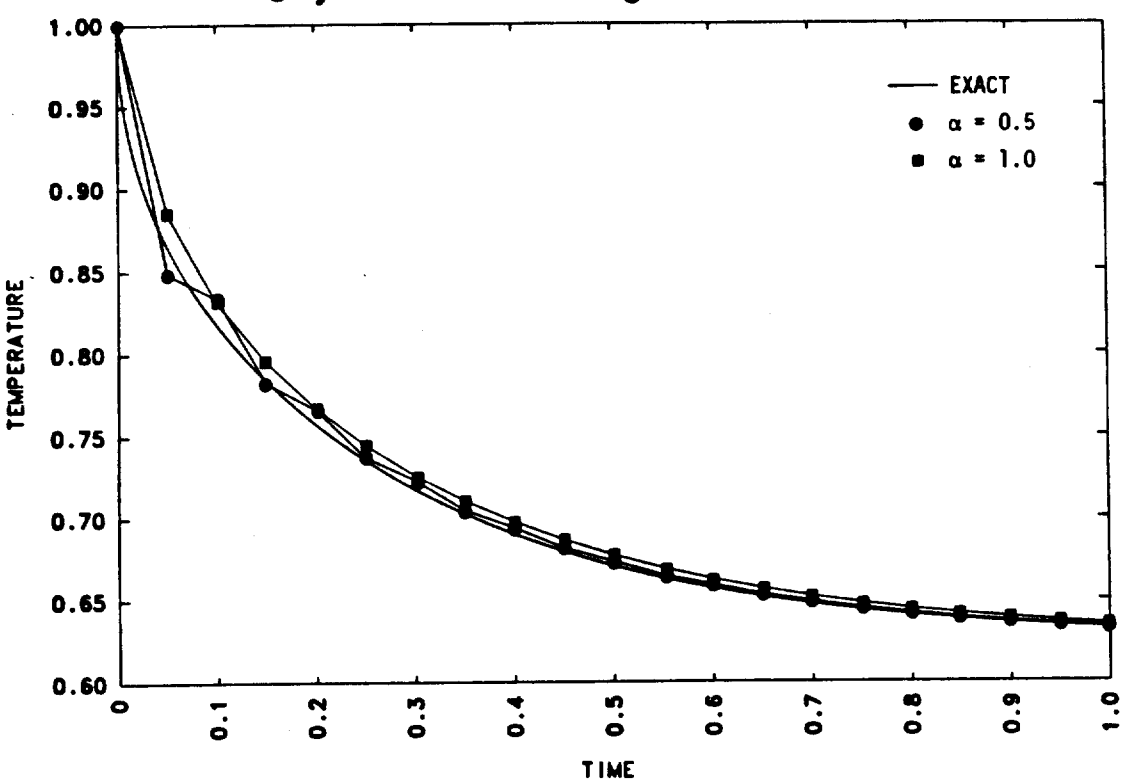
T(t) AT X=1 (Δt=0.1)



$T(x)$ AT $t=0.1$ $(\Delta t=0.1)$



$T(t)$ AT $x=1$ $(\Delta t=0.05)$



POSTACO

A COMPANION GRAPHICS POST-PROCESSOR FOR TACO.

REF: W. E. MASON
POSTACO - A POST-PROCESSOR FOR SCALAR TWO-DIMENSIONAL FINITE ELEMENT CODES
UCID-17979

POSTACO FEATURES

1. MATERIAL OUTLINES
2. MESHES
3. ISOTHERMS
4. PROFILE PLOTS
5. NODAL TIME HISTORY PLOTS & PRINTOUTS

AVAILABILITY

ON LLL OCTOPUS SYSTEM CDC7600 COMPUTERS.

OBTAIN WITH

EXE GLGLIB POSTACO DR./t v

EXECUTION

POSTACO I=infile, P=plotfile, U=uxfile,
BOX=(ann id) / t v

ENTRIES ARE ORDER INDEPENDENT.
DROPOUTS ARE PERMITTED.

DEFAULT NAMES: I=POSTIN
P=TPLOT
U=U

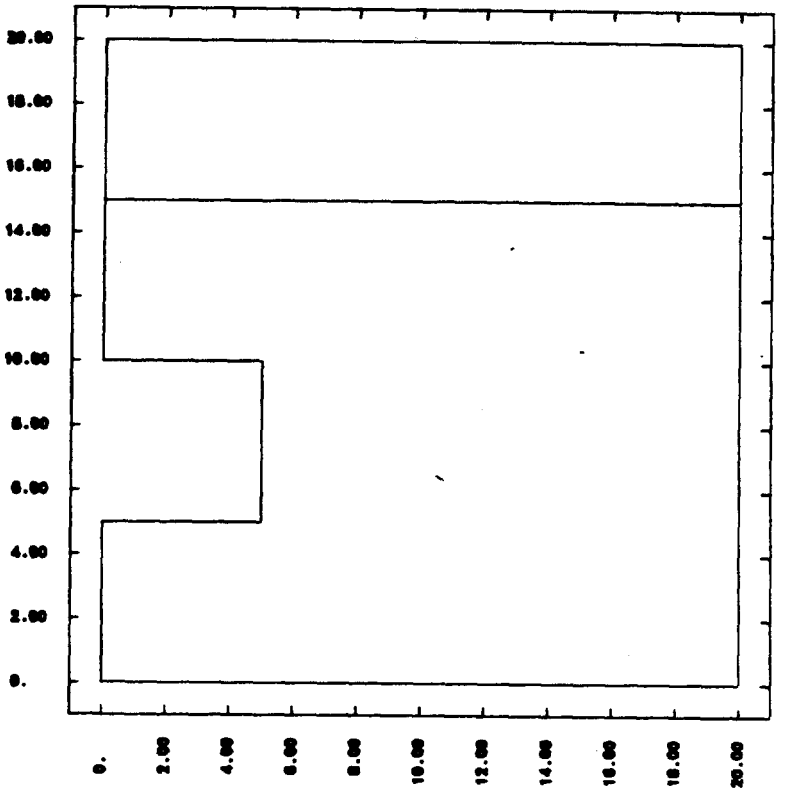
GRAPHICAL OUTPUT

1. TMDS VIEWING (UXTV & UXEDIT)
2. VERSATEC (UXRJ & UXTV)
3. WIDE VERSATEC (UXRJ)
4. HARDCOPY (UXFR)
5. FILM - 35MM & 16MM (UXFR)
6. MICROFICHE (UXFR)
7. NIPS (UXFR + FRTV)

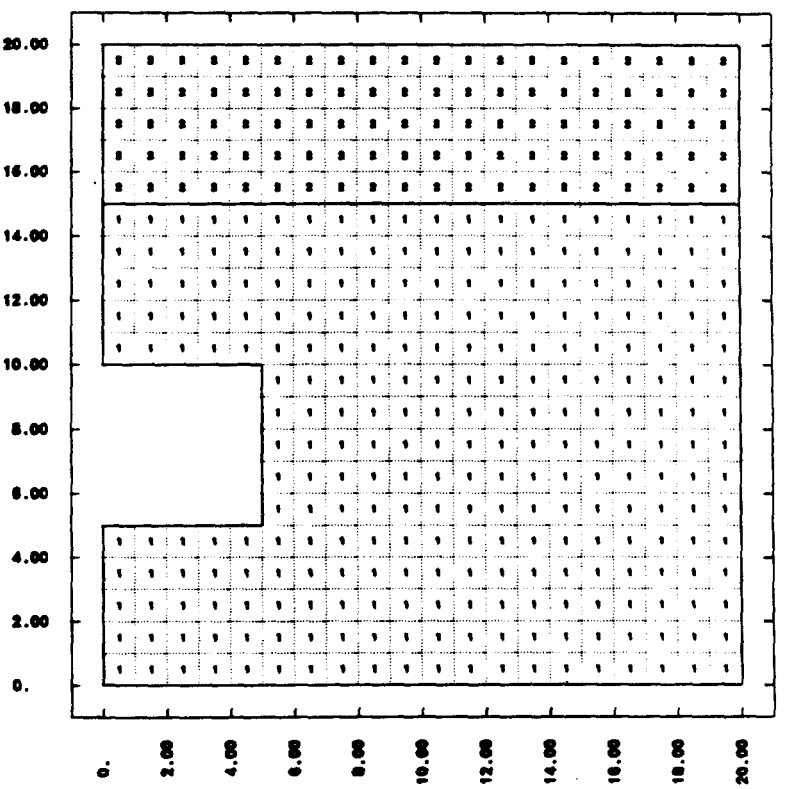
REFERENCES

1. M. BLAIR, "THE UXDD80 GRAPHICS SYSTEM," UCID-30146
2. M. BLAIR, "UTILITY ROUTINE UXFR/ PRELIMINARY USER'S GUIDE"
3. M. BLAIR, "UXEDIT - A UTILITY ROUTINE FOR EDITING UXDD80 PICTURES"

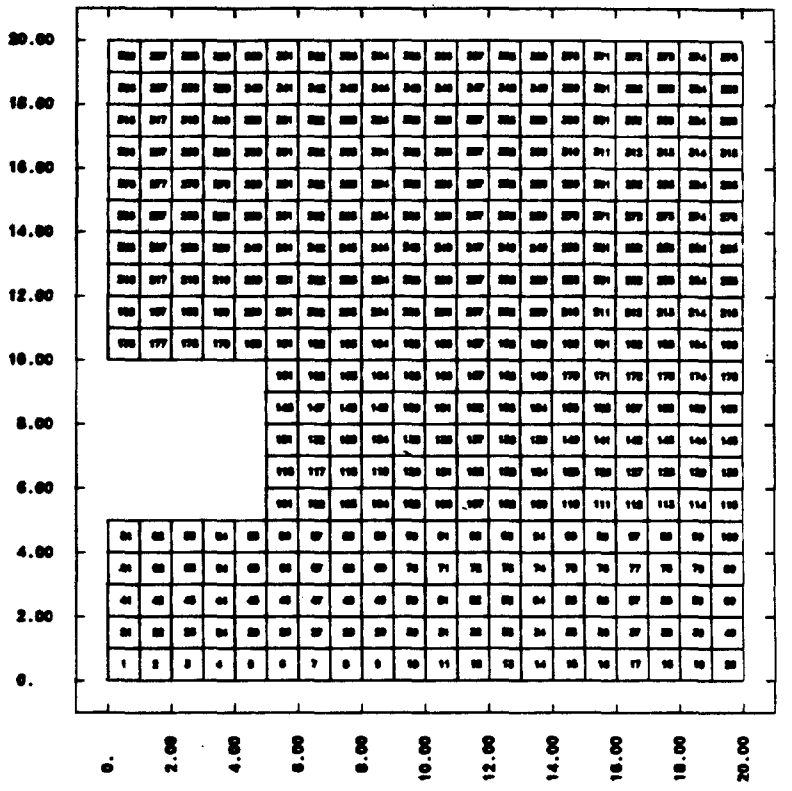
EXAMPLE FOR POSTACO
MATERIAL OUTLINE



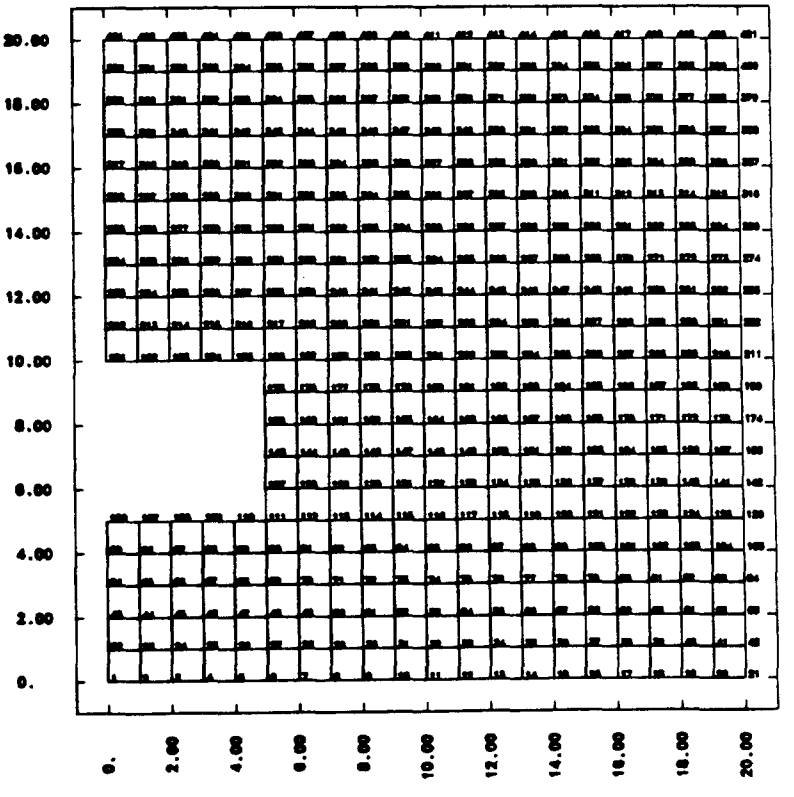
EXAMPLE FOR POSTACO
MATERIAL NUMBERS



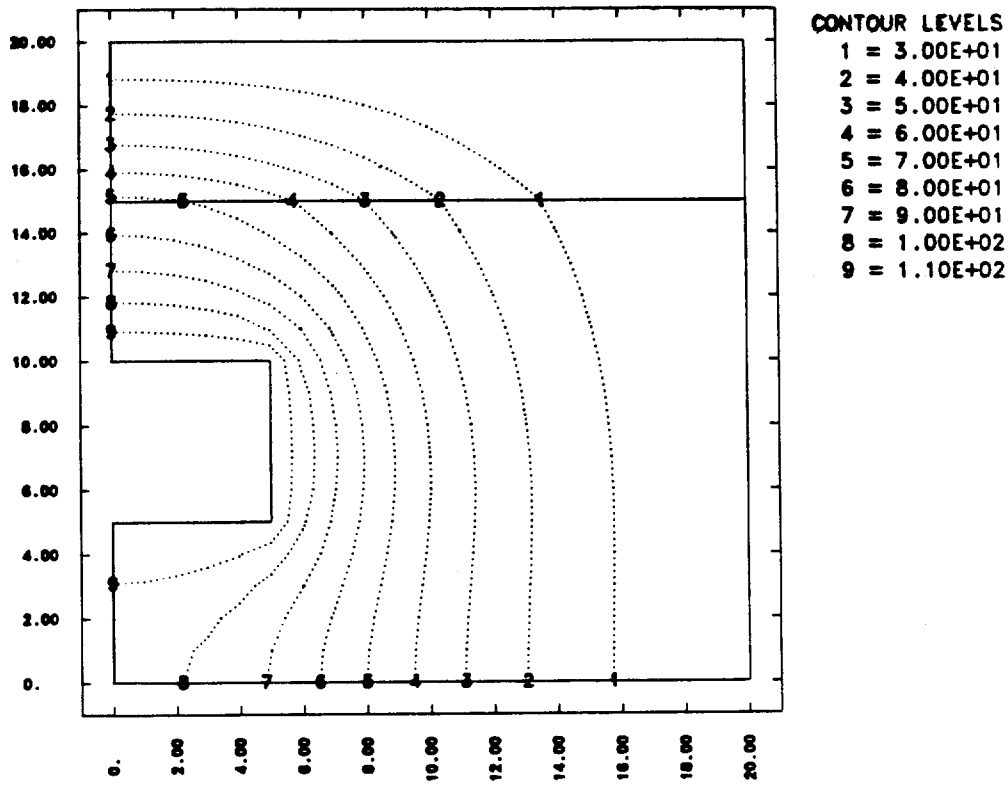
EXAMPLE FOR POSTACO
ELEMENT NUMBERS



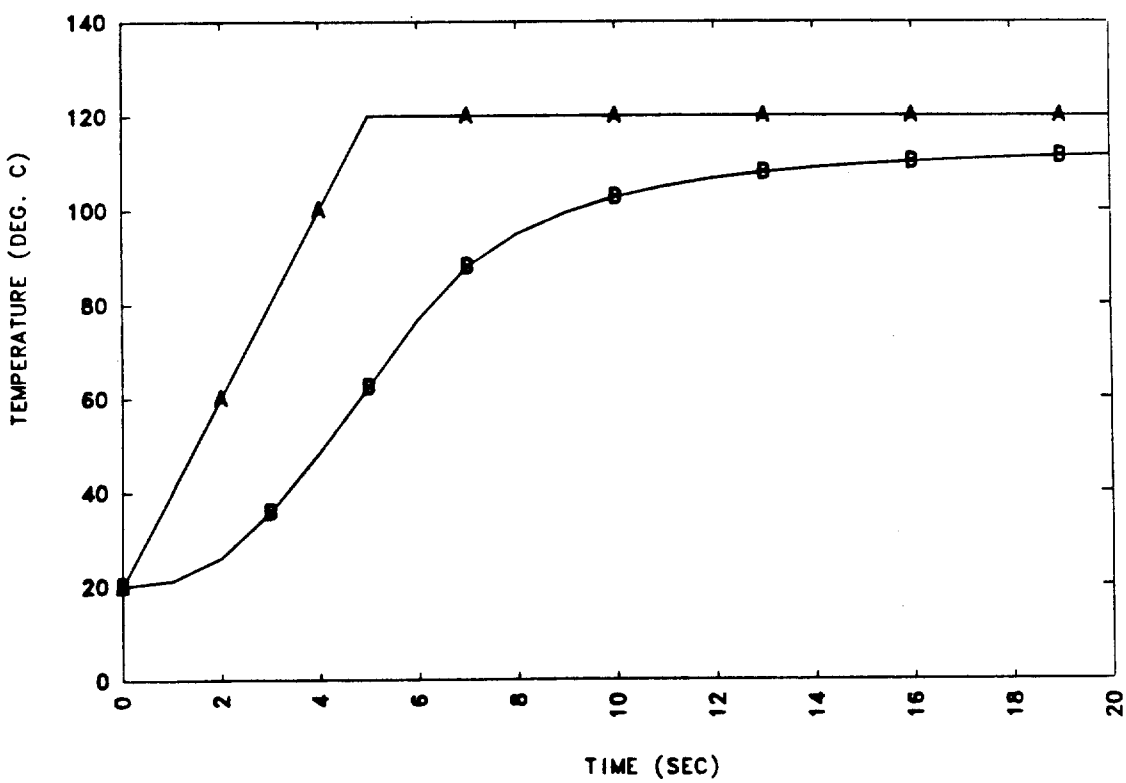
EXAMPLE FOR POSTACO
NODE NUMBERS



EXAMPLE FOR POSTACO
ISOPLOT AT TIME 1.0000E+01

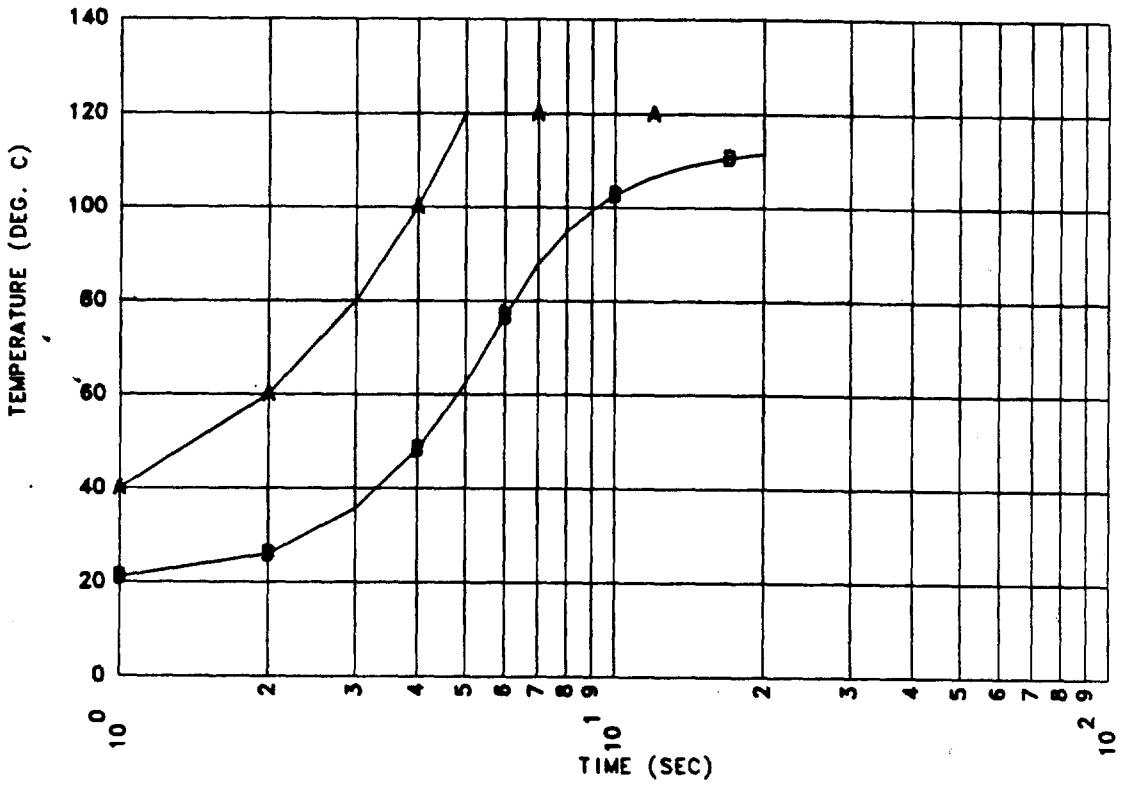


EXAMPLE FOR POSTACO



NODES: 106:A 1:B

EXAMPLE FOR POSTACO



NODES: 106:A 1:B

EXAMPLE FOR POSTACO 18:52:37U 10/21/78 TACO:V1. C:09/19/78

NODE 106. TIME HISTORY FOR TEMPERATURE (DEG. C)

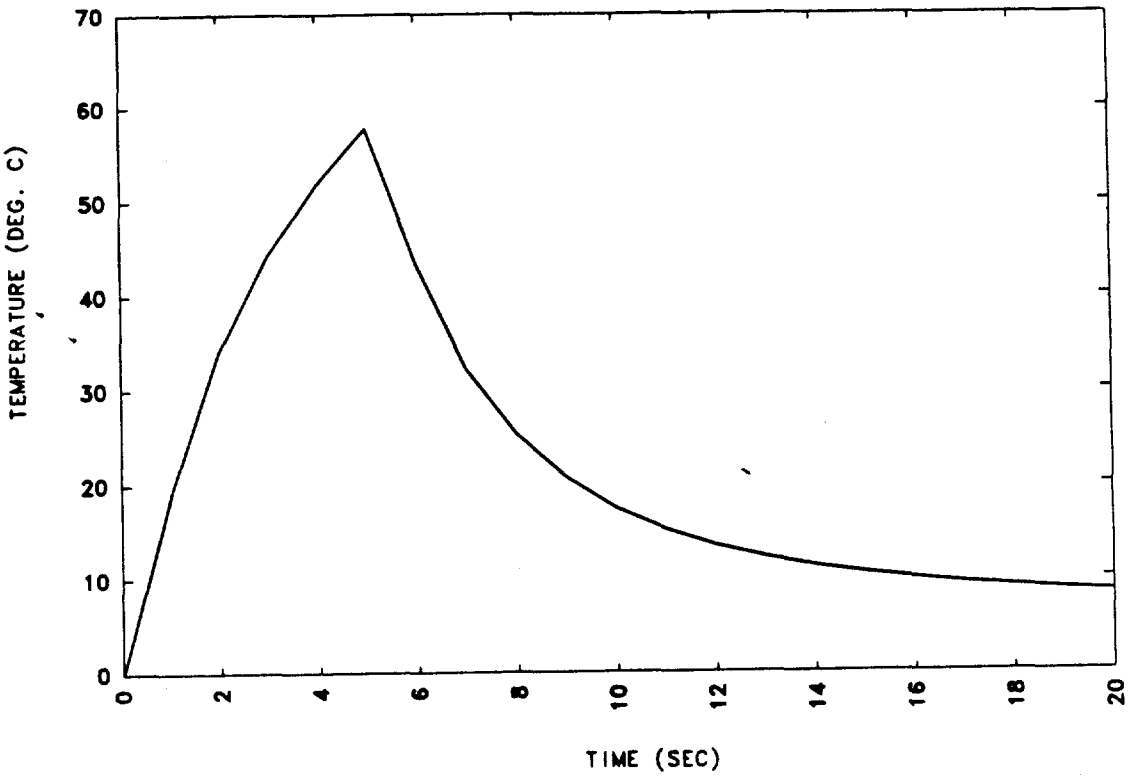
TIME	VALUE	TIME	VALUE	TIME	VALUE	TIME	VALUE
0.	2.0000E+01	6.0000E+00	1.2000E+02	1.2000E+01	1.2000E+02	1.8000E+01	1.2000E+02
1.0000E+00	4.0000E+01	7.0000E+00	1.2000E+02	1.3000E+01	1.2000E+02	1.9000E+01	1.2000E+02
2.0000E+00	6.0000E+01	8.0000E+00	1.2000E+02	1.4000E+01	1.2000E+02	2.0000E+01	1.2000E+02
3.0000E+00	8.0000E+01	9.0000E+00	1.2000E+02	1.5000E+01	1.2000E+02		
4.0000E+00	1.0000E+02	1.0000E+01	1.2000E+02	1.6000E+01	1.2000E+02		
5.0000E+00	1.2000E+02	1.1000E+01	1.2000E+02	1.7000E+01	1.2000E+02		

EXAMPLE FOR POSTACO 18:52:37U 10/21/78 TACO:V1. C:09/19/78

NODE 1. TIME HISTORY FOR TEMPERATURE (DEG. C)

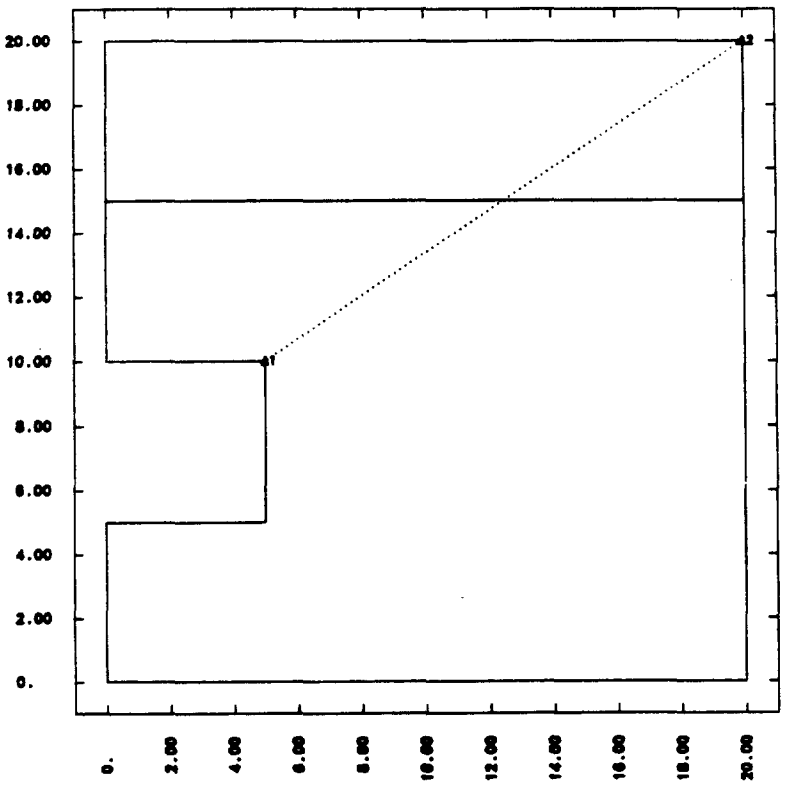
TIME	VALUE	TIME	VALUE	TIME	VALUE	TIME	VALUE
0.	2.0000E+01	6.0000E+00	7.6635E+01	1.2000E+01	1.0657E+02	1.8000E+01	1.1097E+02
1.0000E+00	2.1040E+01	7.0000E+00	8.7817E+01	1.3000E+01	1.0782E+02	1.9000E+01	1.1130E+02
2.0000E+00	2.5041E+01	8.0000E+00	9.4731E+01	1.4000E+01	1.0877E+02	2.0000E+01	1.1156E+02
3.0000E+00	3.5724E+01	9.0000E+00	9.9313E+01	1.5000E+01	1.0952E+02		
4.0000E+00	4.8225E+01	1.0000E+01	1.0263E+02	1.6000E+01	1.1010E+02		
5.0000E+00	6.2296E+01	1.1000E+01	1.0487E+02	1.7000E+01	1.1059E+02		

EXAMPLE FOR POSTACO

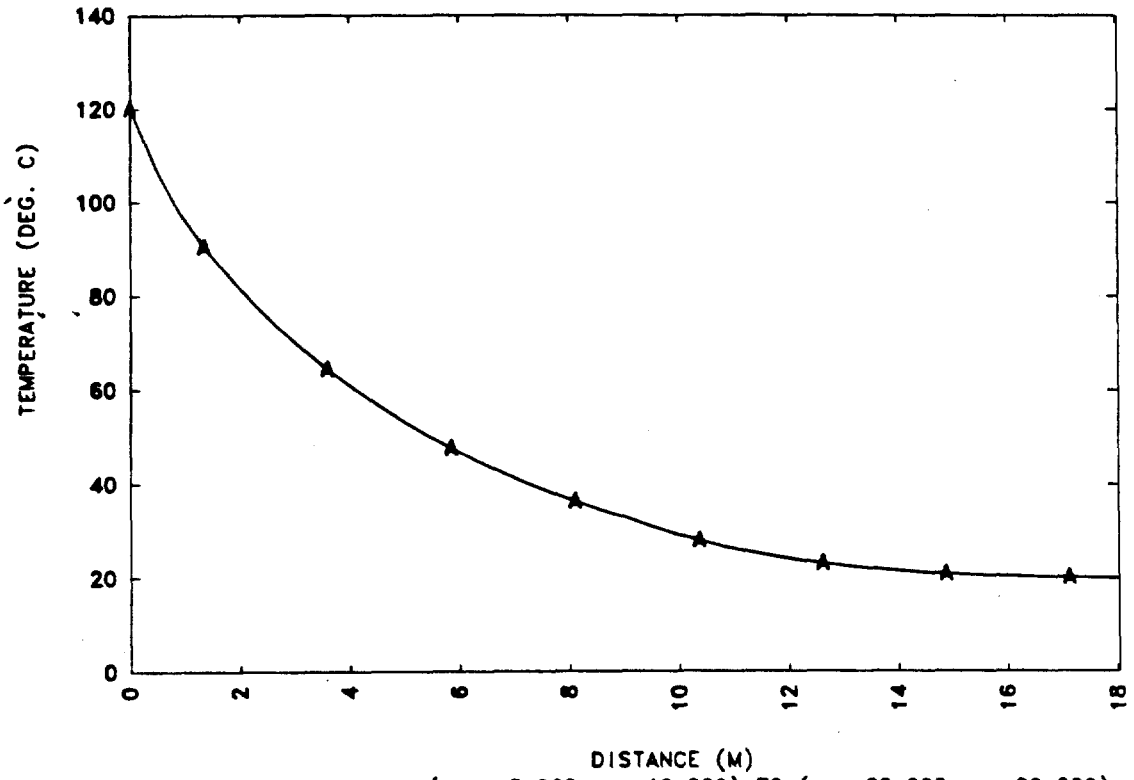


DIFFERENCE BETWEEN NODE 106 AND NODE 1

EXAMPLE FOR POSTACO
PROFILE PLOT GEOMETRY



EXAMPLE FOR POSTACO



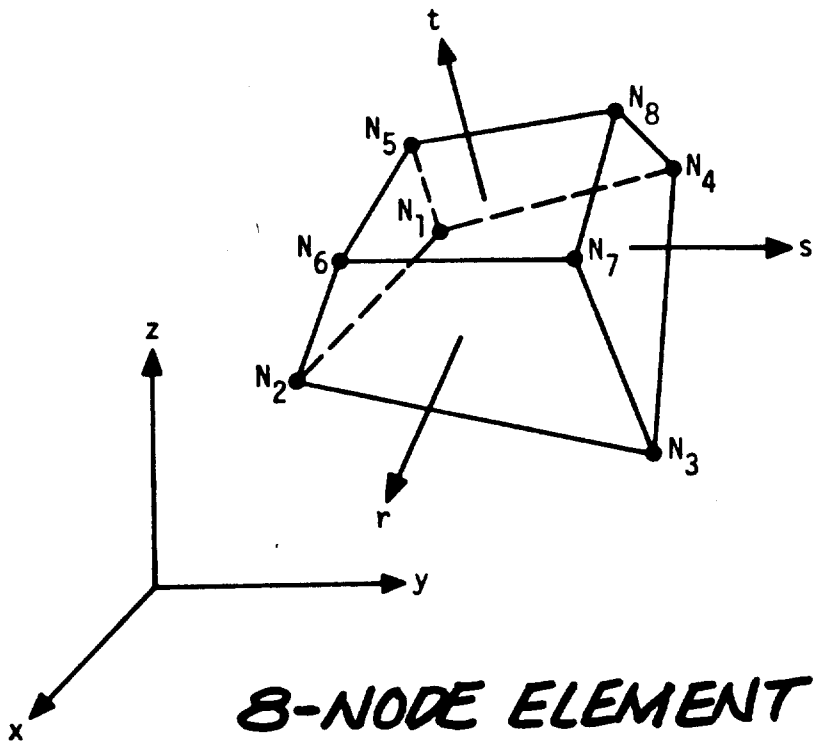
TIME = 1.000E+01 (5.000, 10.000) TO (20.000, 20.000)

TACO3D FEATURES

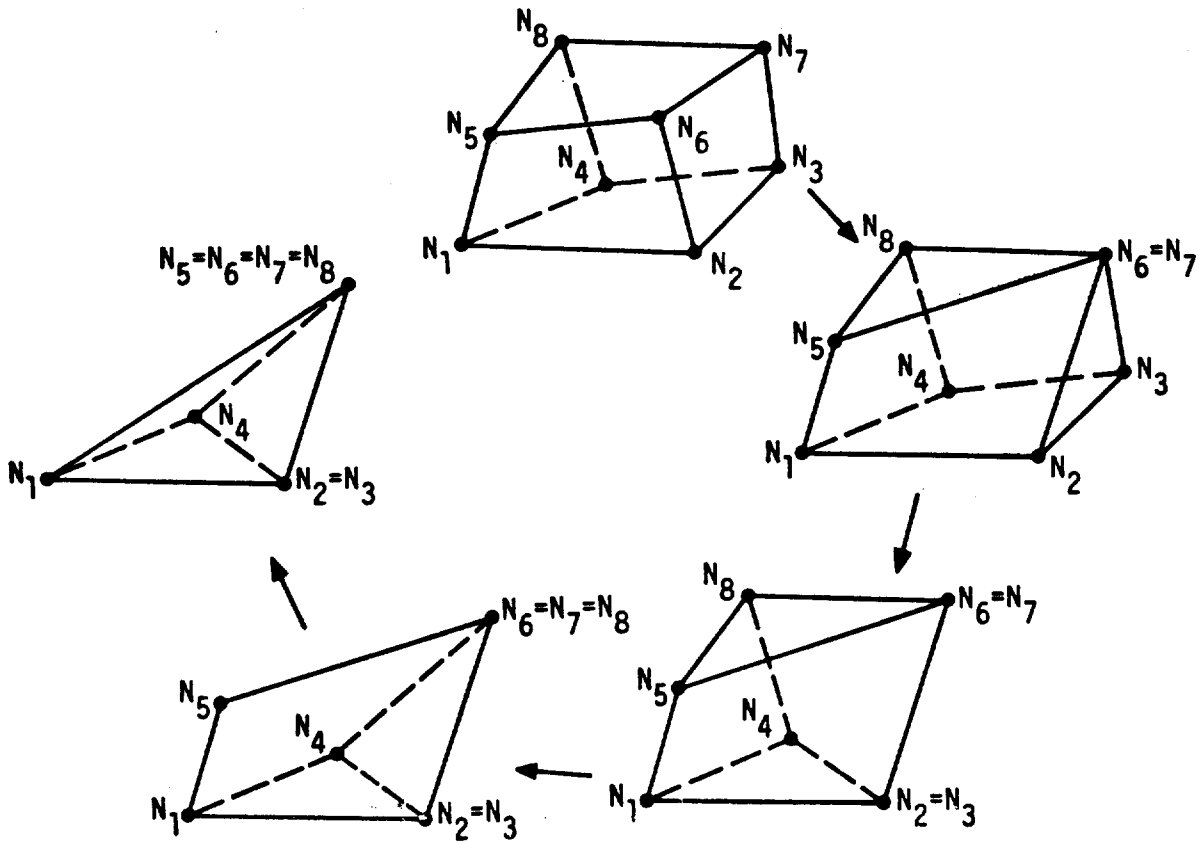
TACO3D IS A THREE-DIMENSIONAL, NONLINEAR, TRANSIENT, FINITE ELEMENT CODE.

REF: W.E. MASON
TACO3D - A THREE-DIMENSIONAL FINITE ELEMENT HEAT TRANSFER CODE
UCID-

SPATIAL DISCRETIZATION



8-NODE ELEMENT



MESH GENERATION

TACO3D HAS LIMITED MESH GENERATION CAPABILITY.

REF.: M.A. GERHARD
SLIC: AN INTERACTIVE, GRAPHIC MESH GENERATOR FOR FINITE-ELEMENT AND FINITE-DIFFERENCE APPLICATION PROGRAMS
UCRL-52823 (1979)

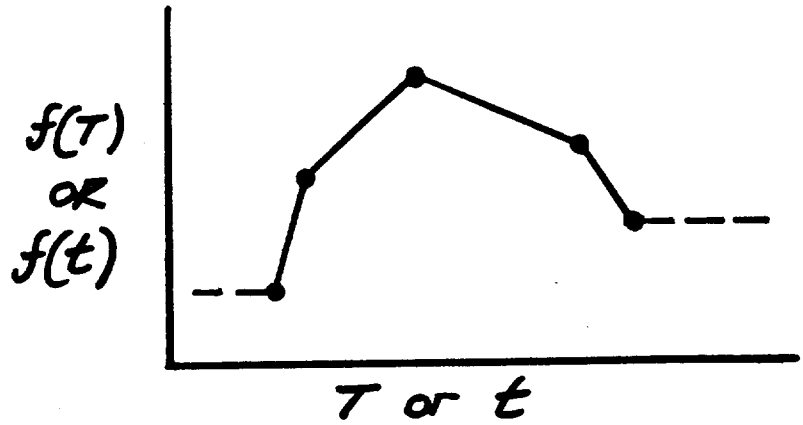
BANDWIDTH AND PROFILE MINIMIZATION

TACO3D USES GPS ALGORITHM.

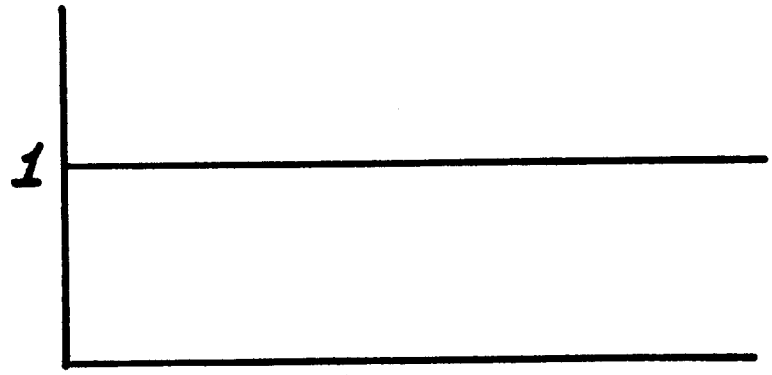
REF: N. GIBBS, W. POOLE, & P. STOCKMEYER
AN ALGORITHM FOR REDUCING THE BANDWIDTH AND PROFILE OF A SPARSE MATRIX
SIAM J. NUM. ANAL., VOL 13, NO. 2

FUNCTIONAL REPRESENTATION

PIECEWISE LINEAR



CONSTANT



USER SUBPROGRAM

4 ENTRY POINTS:

USUB : INITIALIZE

USUB2 : CALCULATE

USUB3 : PRINT

USUB4 : PLOT

CURVE NUMBER (NC)

$NC = 0 \Rightarrow$ CONSTANT

$NC > 0 \Rightarrow$ TIME DEP.

$NC < 0 \Rightarrow$ TEMP. DEP.

$|NC| > 999 \Rightarrow$ USER SUB.

MATERIAL PROPERTIES

ISOTROPIC: ρ, C_p, k

ORTHOTROPIC:
ρ, C_p, k_x, k_y, k_z

HEAT GENERATION RATES

CAN BE DEFINED BY:

- MATERIAL
- ELEMENT

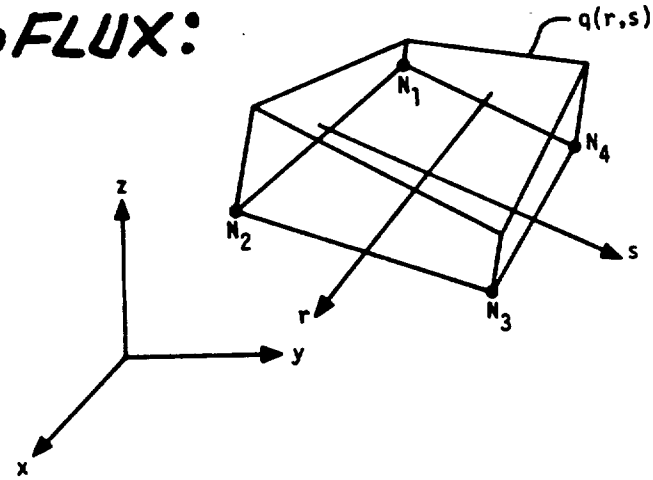
INITIAL TEMPERATURES

CAN BE DEFINED:

- FOR ENTIRE BODY
- BY NODES

BOUNDARY CONDITIONS

- TEMPERATURE: SPECIFIED BY NODE
- FLUX:



- FORCED CONVECTION:

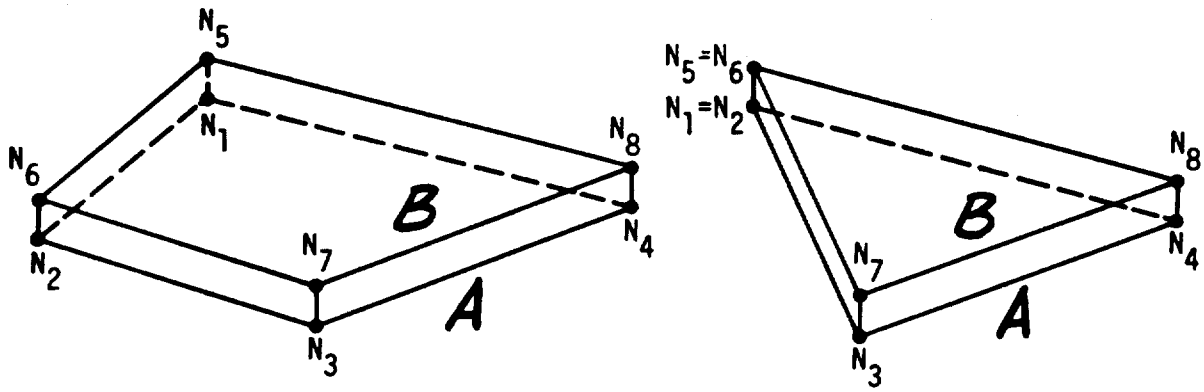
$$q = h(t)\left[T - T_\infty(t)\right]$$

- GENERAL NONLINEAR:

$$q = f(T,t)\left[T^a - T_\infty^a(t)\right]^b$$

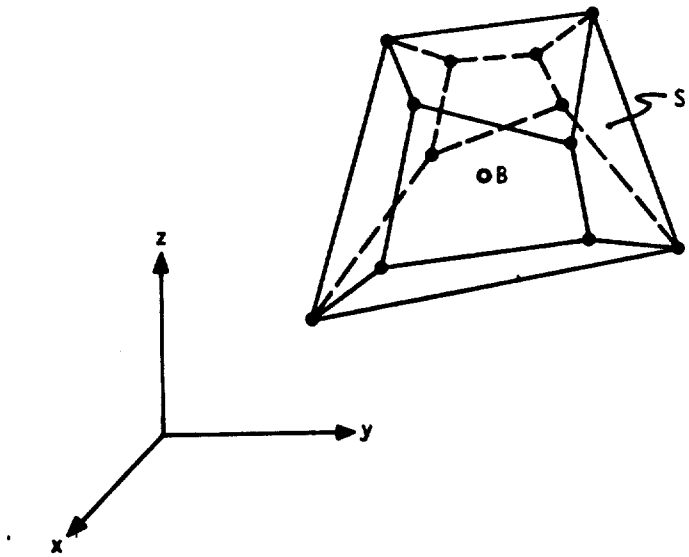
INTERNAL SURFACE CONDITIONS

$$q = f(t)\left[T_A^a - T_B^a\right]^b$$



BULK NODES

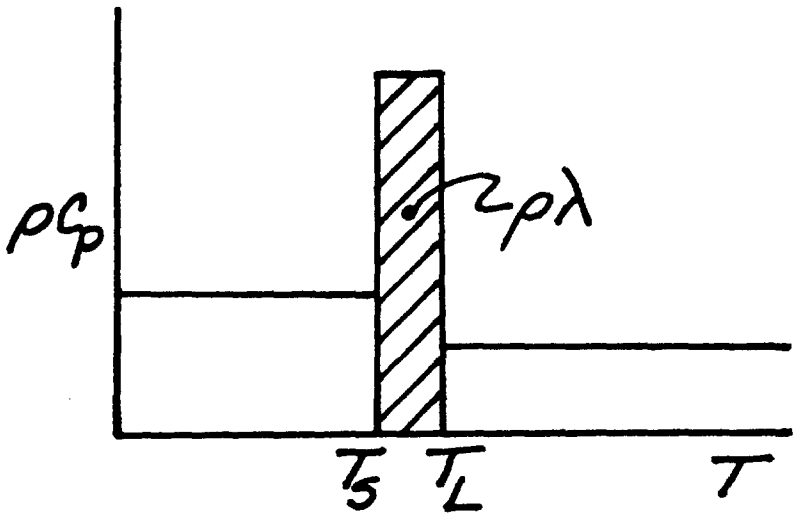
$$q = f(t)\left[T_S^a - T_B^a\right]^b$$



ENCLOSURE RADIATION

NOT AVAILABLE IN TACO3D AT PRESENT.

PHASE CHANGE



λ = LATENT HEAT

CHEMICAL KINETICS

EXAMPLE:

$$Q = -\sum_{n=1}^{N} \rho_n q_n \frac{\partial c_n}{\partial t}$$

$$\frac{\partial c_n}{\partial t} = -c_n^{p_n} z e^{-E_n/RT}$$

HANDLED IN TACO3D BY USER SUBPROGRAM.

TIME STEP CONTROL

- CONSTANT
- PIECEWISE CONSTANT
- VARIABLE

NONLINEAR PROBLEMS

PROBLEM IS NONLINEAR IF:

$$k = k(T)$$

OR $\rho c_p = \rho c_p(T)$

OR $Q = Q(T)$

OR q NOT LINEAR FUNCTION OF T

NONLINEAR ANALYSIS

$$K^*(T_{t+\alpha\Delta t})\Delta T_t = F^*(T_{t+\alpha\Delta t})$$

TACO SOLUTION SCHEME INVOLVES A MODIFIED DIRECT ITERATION METHOD. STEPS INCLUDE:

1. K^* UPDATE (REFORMATION)
2. F^* UPDATE (ITERATION)

THERMAL STRESS ANALYSIS

MECHANICAL CODES (E.G., NIKE3D) CAN READ TEMPERATURES FROM BINARY PLOT FILES PRODUCED BY TACO3D TO CALCULATE THERMAL STRESSES.

AVAILABILITY

ON LLL OCTOPUS SYSTEM

TO OBTAIN

ON CDC 7600

```
EXE GLGLIB TACO3D DR./t r
```

ON CRAY

```
LIB MDGLIB!x TACO3D!END/t r
```

EXECUTION

TACO3D I=infile, O=printfile, P=plotfile /t v

FILE NAMES ARE ORDER INDEPENDENT.
DROPOUTS ARE PERMITTED.

DEFAULT NAMES: I = TACOIN
O = TPRINT
P = TPLOT

POST-PROCESSING

- POSTACO (TIME HISTORY)
- GRAPE (SPATIAL)

REF:

1. W.E. MASON, "POSTACO – A POST-PROCESSOR FOR SCALAR, TWO-DIMENSIONAL FINITE ELEMENT CODES," UCID-17979.

2. B.E. BROWN, "DISPLAYING THE RESULTS OF THREE-DIMENSIONAL ANALYSIS USING GRAPE, PART ONE-VECTOR GRAPHICS," UCID-18507.