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A FORTRAN PROGRAM FOR CALCULATING
THE TEMPERATURE DISTRIBUTION RESULTING
FROM VOIDS IN LAMINATED STRUCTURES

*Gordon D. Lassahn
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U. S. ATOMIC ENERGY COMMISSION
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CONTENTS

Abstract	1
Introduction	1
Boundary Conditions Used in the Calculation	1
Description of the Program	2
Use of the Program	4
Sample Run	5
References	6
Appendix	7

A FORTRAN PROGRAM FOR CALCULATING THE TEMPERATURE DISTRIBUTION RESULTING FROM VOIDS IN LAMINATED STRUCTURES

Gordon D. Lassahn and Raymond D. Dixon

Abstract: Described is a FORTRAN time-sharing program that calculates the steady-state temperature distribution resulting from heat flowing around a void at the interface of a two-layer metal structure. One exterior surface of the structure is heated, and the heat is conducted through the metal plates and across the metal-metal interface to the opposite exterior surface, where the heat is dissipated to the air.

The void at the interface is a rectangular cross-section slot in one of the metal plates. The conductivities of the two metals and of the interface, the dimensions of the plates and of the slot, and the boundary temperatures are variable. A sample calculation is presented.

INTRODUCTION

The computer program described in this report was written in support of a study to determine the feasibility of using infrared thermography to detect bond defects in laminated metal structures.¹ The program calculates the steady-state temperature distribution for the model shown in Figure 1. The model consists of a block with a slot across the top (the defect) and a plate on top of the block. The model is heated from the bottom with a hot plate, and it dissipates heat into the air from all the other surfaces. The purpose of the calculation was to predict the temperature variation on the top surface of the plate caused by the presence of the slot in the block. Adjustable parameters are the sizes of the slot, block, and plate, the hot plate and air temperatures, the plate and block thermal conductivities, and the coefficients for heat transfer across the various surfaces.

BOUNDARY CONDITIONS USED IN THE CALCULATION

At each interface, i.e., the plate-block interface, the hot plate-block interface, and the block-air and plate-air interfaces, the heat flow is approximated as being proportional to the temperature difference across the interface:

Figure 1. The Model Used for Calculations. Dimensions are labeled with the names of the corresponding computer program input variables.

$$J = C (T_1 - T_2), \text{ where}$$

J is the heat flux from surface 1 to surface 2 (energy · area⁻¹ · time⁻¹),

C is the thermal conductance per unit area (energy · area⁻¹ · time⁻¹ · degree⁻¹), and

T_1 and T_2 are the temperatures of surfaces 1 and 2 at the interface (degree).

Both the hot plate and the outside air are held at constant temperatures. Heat is conducted directly between the air in the slot and the outside air.

DESCRIPTION OF THE PROGRAM

For the calculations, a rectangular coordinate system is used. The origin is chosen to be at the center of the top surface of the plate (see Figure 1). The positive Z-axis is normal to the plate and in the direction of the hot plate. The Y-axis is parallel to the slot. The X-axis is normal to the slot. The X-Z plane and the Y-Z plane are symmetry planes, and therefore it is sufficient to calculate the temperature in one-fourth of the assembly, say for $X > 0$ and $Y > 0$.

A three-dimensional rectangular lattice of points is constructed throughout the $X > 0, Y > 0$ region. The program adjusts the positions of the interior boundaries (the slot surfaces and the plate-block interface) to coincide with the nearest parallel planar array of points. The single points on these interior boundaries are replaced by pairs of points, one on each side of the boundary. These points are labeled with indexes I, J, and K for the Z, X, and Y directions, respectively. The K labeling is straightforward, with $K = 1$ at $Y = 0$. Figure 2 shows two sketches of points in a plane parallel to the X-Z plane, for the $X > 0$ region. The I and J labelings are indicated in the top and bottom sketches, respectively. The points denoted by triangles are not part of the regular array, but are used as dummy points to simplify the program.

The calculations consist mainly of solving a system of linear equations in which the unknowns are the temperatures of all the points. Of course, there must be as many equations as there are points, and there is a simple correspondence between the equations and the points. The equation for each point states that the net heat flow into the region around that point is zero. This condition follows from the requirement that the temperature of the point be constant in time (that is, the steady state solution is sought), so there can be no change in the heat content of the region around the point.

The (approximate) finite difference equations expressing this condition can be obtained by integrating the (exact) equation of continuity over the region around the point in question, with the time derivative of the temperature not equal to zero:

$$0 = \iiint_V (-\rho c \frac{\partial T}{\partial t}) dV = \iiint_V \nabla \cdot \mathbf{J} dV = \iint_A \mathbf{J} \cdot d\mathbf{A},$$

where ρ is the density of the material, c is the specific heat, and $\mathbf{J}$ is the heat current. The region of integration is a rectangular solid surrounding the point, as indicated by the dashed lines in Figure 3 for an example point on the surface of the plate.

Figure 2. Labeling of Points in the X-Z Plane.

The surface integral can be written as the sum of six integrals, one for each face of the region of integration. Each of the six integrals can be approximated:

$$\iint \mathbf{J} \cdot d\mathbf{A} = C(T_{\text{inside}} - T_{\text{outside}})A$$

for a surface at a boundary of the model (the top surface in the example of Figure 3), or

$$\iint \mathbf{J} \cdot d\mathbf{A} = -\sigma \frac{\partial T}{\partial n} A$$

for a surface in the interior of one of the parts of the model. Here n is the coordinate pointing out of the region, perpendicular to the area A . The $\partial T/\partial n$ is approximated by a finite difference of the form $[T(n + \delta n) - T(n)]/\delta n$, and A is just the area of the surface ($\delta X \delta Y$ and $\frac{1}{2} \delta X \delta Z$ for the top and front surfaces in Figure 3).

Figure 3. The 1, J, K Point and the Neighboring Points Used in Writing the Temperature Equation for the 1, J, K Point.

The finite difference equation obtained by this scheme for the example point (1, J, K) of Figure 3 is:

$$0 = [T(2, J, K) - T(1, J, K)] \sigma \delta X \delta Y / \delta Z \\ + [T(1, J+1, K) - T(1, J, K)] \sigma \delta Y \frac{1}{2} \delta Z / \delta X \\ + [T(1, J-1, K) - T(1, J, K)] \sigma \delta Y \frac{1}{2} \delta Z / \delta X \\ + [T(1, J, K+1) - T(1, J, K)] \sigma \delta X \frac{1}{2} \delta Z / \delta Y \\ + [T(1, J, K-1) - T(1, J, K)] \sigma \delta X \frac{1}{2} \delta Z / \delta Y \\ + [T_{\text{air}} - T(1, J, K)] C \delta X \delta Y,$$

where σ is the conductivity of the plate material, C is the previously mentioned conductance per area of the plate-air interface, δX , δY , δZ are the dimensions of one cell in the model, and T_{air} is the temperature of the surrounding air (a known constant). An equation of this form (simplified by dividing by a factor like $\sigma \delta X \delta Y \delta Z / 2$) is used for each point in the model.

This system of linear equations is solved by the Gauss-Seidel iterative method with over-relaxation.² In this method, the temperature of each point in turn is recalculated in each iteration. The most recent previously calculated (or estimated, on the first iteration) values of the temperatures of that point and its neighboring points are used to calculate the correction to the temperature of the point in question. The temperature of the (1, J, K) point is corrected by the amount

$$R [B(1, J, K) + \sum_{I', J', K'} A(1, J, K, I', J', K') \\ T(I', J', K') - T(1, J, K)]$$

where R is the relaxation factor, the A 's are the coefficients of the temperatures of the neighboring points, and B is the constant term in the linear equation. For the previously mentioned example, in which $I = 1$, we would have

$$B(1, J, K) = DT_{\text{air}} 2C/(\sigma \delta Z), \\ A(1, J, K, 2, J, K) = 2D/(\delta Z)^2, \\ A(1, J, K, 1, J+1, K) = A(1, J, K, 1, J-1, K) = \\ D/(\delta X)^2, \text{ and} \\ A(1, J, K, 1, J, K+1) = A(1, J, K, 1, J, K-1) = \\ D/(\delta Y)^2, \text{ where} \\ D = 1/[2C/(\sigma \delta Z) + 2/(\delta X)^2 + 2/(\delta Y)^2 + 2/(\delta Z)^2].$$

All other A 's in this example are zero.

The iteration process will converge for any value of R between 1 and 2, but there is an optimum value in this range which will give fastest convergence. This optimum value of R depends on the particular problem being worked, and can not be determined before all the model parameters (size and shape of model, thermal conductivities, etc.) are known. In this program, the value of R is large at the beginning of the iteration procedure and is decreased whenever the sum of all the temperature corrections in one iteration is of the opposite algebraic sign from that of the previous iteration. Intuitively, the large R at the beginning causes rapid convergence of the iteration procedure and overshooting the solution to the equations. When the maximum overshoot is reached, the temperature corrections change sign. At this point, R is reduced to decrease the speed of convergence and the overshoot for the next approach to the solution. In this manner, R is decreased in steps as the iteration procedure continues, but R is never allowed to be less than 1. The procedure continues in this manner until either the number of iterations reaches the maximum allowed or the sum of the squares of all the temperature corrections in one step of the iteration is below some preselected value. In either case, the temperatures of selected points on the top surface are then printed out, and the iteration procedure is resumed with the value of R fixed at one. Normally, only one more step in the iteration will be done before the sum-of-the-squares criterion causes final termination of the calculation and a final printout of the temperature distribution. However, for some cases the first termination may be due to the limit placed on the number of iterations rather than being caused by the sum of the squares criterion. In any case, as many as five more iterations ($R = 1.0$) can be performed before the calculation terminates. These last

few iteration steps often complete the convergence of a calculation that had been converging slowly with a larger relaxation factor.

USE OF THE PROGRAM

Table I defines the input variables needed for the program. The input data are in two parts, read in lines 104 and 116. The program is listed in the Appendix. After the tempera-

Table I. Input Variables

Variable Name	Definition
DSLOT	Thickness of slot.*
ERMAX	Value of the sum of the squares of all the temperature corrections in one iteration, for which the calculation is considered converged.
IM, JM, KM	Number of cells in the Z, X, and Y directions, respectively, into which the X>0, Y>0 region is divided.
LENGTH	Length of slot.*
NMAX	Maximum allowable number of iterations.
RO	Initial value of the over-relaxation factor.
S1	Thermal conductivity of top plate material.
S2	Thermal conductivity of the block material.
S3	Thermal conductivity of the air in the slot.
S12	Thermal conductance per unit area across the block-plate interface.
S13	Thermal conductance per unit area across the interface between the block and the air in the slot.
S23	Thermal conductance per unit area across the interface between the top plate and the air in the slot.
SAIR	Thermal conductance per unit area across the exterior surfaces that dissipate heat to the air.
SMO	Thermal conductance per unit area across the hot plate-block interface.
TA	Air temperature.
TBOO	Thickness of the bottom block.*
TH	Hot plate temperature.
TTOP	Thickness of top plate.*
WIDTH	Width of block in direction perpendicular to slot.*

*See Figure 1.

ture calculations are finished for one set of data, the program returns to line 116 to read new values of only those parameters for the next calculation. The values of the parameters read in line 104 are retained from the previous calculation, and the temperature distribution from the previous calculation is used as the beginning of the next calculation. This feature saves computer time when the variables read in line 116 are frequently changed by small amounts. However, if the value of TTOP, the first variable read in line 116, is zero or negative, the program returns to line 104 and reads new values for all the input

variables in both lines 104 and 116, and sets all the temperatures equal to the hot plate temperature for the beginning of the calculation. If IM, the first variable read in line 104, is zero or negative, the program stops. Therefore, a single blank input record causes the program to start over at the beginning, and two blank records in a row cause the program to stop.

For the program to function correctly, the input data must satisfy the following compatibility requirements:

$KM \geq 1$
 $JM > 2.5 \times \text{WIDTH} / \text{WSLOT}$
 $JM > 1.5 \times \text{WIDTH} / (\text{WIDTH} / \text{SLOT})$
 $IM > 1.5 \times (TTOP + TBOO) / TTOP$
 $IM > 1.5 \times (TTOP + TBOO) / (TBOO - \text{DSLOT})$
 $IM > 2 \times (TTOP + TBOO) / \text{DSLOT}$
 $NMAX > 5$
 $\text{LENGTH} > 0$

$S1 > 0$

$S2 > 0$

$S3 > 0$

$2 > RO \geq 1$

The dimensions of the array T, specified in Lines 102 and 342, must be greater than or equal to (IM + 3, JM + 2, KM + 1).

The input data must be specified in a consistent set of units.

Obviously, one would expect larger values of IM, JM, and KM to give more accurate results, and also to take more computer time and storage space. These factors are best weighed by the user for a particular problem. One aspect to be considered is that if the interior boundaries of the model do not coincide with a plane of points of the array, these model boundaries will be moved by the program, to coincide with the nearest plane of points. Often, IM and JM can be chosen to make the cell size exactly or nearly commensurate with the specimen dimensions, thus eliminating or minimizing the error caused by moving the interfaces.

For the input parameters used in this work, it was found that convergence was fastest when the value of RO was about 1.93. It was also found that a highly conductive block-hot plate interface (large SMO) greatly speeded the convergence of the calculation of the temperature distribution without affecting the result of interest (the size of the surface temperature decreased caused by the slot). Using IM, JM, KM = 24, 18, 8, with the other parameters approximately equal to those used in the sample run, it was found that NMAX = 400 was sufficient to allow convergence of most calculations.

For each iteration, the sum of the squares of all the temperature corrections (SCOR2) is calculated. This is used as an indication of whether the calculation has converged. It is assumed that SCOR2 becomes small when convergence is attained. The examples that were studied verified that the value of SCOR2 does fall off very rapidly at some point in the calculation, and this is assumed to represent convergence. In this program, the iteration procedure stops when SCOR2 is less than the input variable ERMAX.

The best value of ERMAX depends mainly on the number of points, and is limited by the accuracy of the computer. Experience indicates that the maximum value for ERMAX should be about $10^{-7} \times IM \times JM \times KM$. The minimum value should be the product of $IM \times JM \times KM$ multiplied by the square of the smallest non-zero change the computer can make in a temperature value. For example, a seven-digit machine working with temperatures between 20° and 60° cannot make a non-zero temperature correction smaller than 10^{-5} . Then ERMAX should not be smaller than $10^{-10} \times IM \times JM \times KM$.

The output includes a list of the input variable values after the boundary position adjustments have been made, and the temperatures at 50 points on the top surface of the $X > 0, Y > 0$ portion of the plate. These points are as evenly spaced as possible with five rows in the Y direction and ten rows in the X direction. The X coordinates and the Y coordinates of these points are listed. Also listed are the number of iterations performed, the last value of the relaxation factor used, and the sum of the squares of all the temperature corrections made in the last iteration. These three numbers and the temperature distribution are printed twice for each calculation, as previously described.

If the number of iterations is greater than NMAX-5 for the first listing of the temperatures or greater than 5 for the second listing, the user should assume that convergence has not been attained and that the temperatures indicated might be far from the correct values.

SAMPLE RUN

This sample run was done on a time-sharing digital computer using a FORTRAN compiler. It is listed in Table II. The parameters were selected to give an example representative of problems with which the authors are experienced, and also to give quick convergence. The parameters are:

plate material: stainless steel, thermal conductivity =
 $0.14 \text{ watt} \cdot \text{cm}^{-1} \cdot ^\circ\text{K}^{-1}$
 plate thickness: 0.159 cm

block material: copper, thermal conductivity:
 $4.00 \text{ watts} \cdot \text{cm}^{-1} \cdot ^\circ\text{K}^{-1}$

block thickness: 1.27 cm

block width: 6.00 cm

slot depth: 0.635 cm

slot width: 1.27 cm

slot length: 2.54 cm

hot plate temperature: 60°C

air temperature: 20°C

Solder between the plate and the block.

Exterior surfaces are painted black; emissivity is approximately 1 for these surfaces.

Surfaces facing the slot are bare unpolished metal; emissivity is estimated to be about 0.75.

Carslaw and Jaeger³ give formulas for the conductance per unit area for the various surfaces. These give:

$$SAIR = 0.0008 \text{ watt} \cdot \text{cm}^{-2} \cdot ^\circ\text{K}^{-1}$$

$$S13 = 0.0006 \text{ watt} \cdot \text{cm}^{-2} \cdot ^\circ\text{K}^{-1}$$

$$S23 = 0.0006 \text{ watt} \cdot \text{cm}^{-2} \cdot ^\circ\text{K}^{-1}$$

$$S12 = 8.36 \text{ watt} \cdot \text{cm}^{-2} \cdot ^\circ\text{K}^{-1}$$

The value of SMO should be approximately 0.02, but the unreasonably high value of $300 \text{ watt} \cdot \text{cm}^{-2} \cdot ^\circ\text{K}^{-1}$ is used to save computer time, as has been mentioned.

The thermal conductivity of air is $0.00023 \text{ watt} \cdot \text{cm}^{-1} \cdot ^\circ\text{K}^{-1}$.

The values $IM = 18$, $JM = 15$, and $KM = 4$ satisfy the previously mentioned compatibility requirements.

RO is chosen to be 1.93, NMAX is 400, and ERMAX is 10^{-5} , which is about $10^{-8} \times IM \times JM \times KM$.

These input values are fed into the computer in the proper order in response to the two requests for input at the beginning of the sample run (lines 104 and 116).

In the computer output, WSLLOT is listed as 1.200 rather than the input value of 1.27. This is a result of the shifting of a specimen boundary in the X direction to make it coincide with the nearest cell boundary. The other boundaries already matched and there was no shifting in the Z direction.

The output variable SMH is the same as the input variable SMO. Because it was chosen so large, it could not be printed in the specified format.

Since the output indicates that the number of iterations required, 37, was below NMAX-5, 395, and that the sum of the squares of the temperature corrections in the last

TABLE II. Sample Run

RUN

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INPUT: 00104

? 18, 15, 4, 20., 60., 1.27, 2.54, .00023, 300., .0008, .0006, .0006,
 ? 1.93, 4.00, 4.36, 400, .00001

INPUT: 00116

? .159, .635, 1.27, 6.0, .14

TTOP, TBOT, D SLOT, IM, I2, I1 = 0.159 1.270 0.635 18 12 3
 WIDTH, W SLOT, JM, J1, LENGTH, KM = 6.000 1.200 15 4 2.540 4
 TA, TH, ERMAX, RO, NMAX = 20. 60. .0000100 1.93 400

S1	S2	S3	S12	S13	S23	SAIR	SMH
0.140000	4.000000	0.000230	8.360000	0.000600	0.000600	0.000800	*.000000
X-COORDINATES							
0.000	0.400	0.600	1.000	1.400	1.600	2.000	2.400 2.600 3.000
Y-COORDINATES							
0.000	0.317	0.635	0.952	1.270			
37 1.5839	0.0000085						
59.62	59.75	59.88	59.94	59.94	59.94	59.94	59.94 59.91
59.62	59.74	59.88	59.94	59.94	59.94	59.94	59.94 59.91
59.60	59.73	59.88	59.93	59.94	59.94	59.94	59.93 59.91
59.56	59.71	59.87	59.93	59.93	59.93	59.93	59.93 59.91
59.50	59.66	59.84	59.91	59.92	59.92	59.91	59.91 59.89
1 1.0000	0.0000009						
59.62	59.75	59.88	59.94	59.94	59.94	59.94	59.94 59.91
59.62	59.74	59.88	59.94	59.94	59.94	59.94	59.94 59.91
59.60	59.73	59.88	59.93	59.94	59.94	59.94	59.93 59.91
59.56	59.71	59.87	59.93	59.93	59.93	59.93	59.93 59.91
59.50	59.66	59.84	59.91	59.92	59.92	59.91	59.91 59.89

INPUT: 00116

? 8

COMPUTER UNITS: 290.4

READY

iteration, 0.0000085, is below the reasonable value of ERMAX, it can be assumed that the calculation has converged. Further indications of convergence are that only one more iteration was done after the first set and that the temperatures in the two listings agree.

In the array of 50 temperatures listed, the left column of numbers are temperatures of points on the Y-axis, and the top row of numbers are temperatures of points on the X-axis. Since the width of the slot (WSLOT) is 1.2 cm, the edge of the slot must be at X = 0.6 cm. The list of the X-coordinates indicates that the third column of numbers are temperatures of the surface at X = 0.6 cm, so these points are directly above the edge of the slot.

The temperature above the center of the slot is 59.62, and the temperature along the X-axis away from the slot is 59.94. Therefore, the presence of the slot caused a 0.32 degree temperature decrease along the X-axis. Along the edge of the top surface, all the temperatures are lower

than along the X-axis, and the slot has a greater effect, causing a temperature drop of 0.42 degrees.

After completing the temperature calculation for one set of data, the computer requested a second set of data and the operator terminated execution of the program.

This run required about 12 minutes of terminal time and 39,344 bytes of computer storage space.

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3. H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids*, (Oxford University Press, London) 2nd Edition 1959, p 20.

APPENDIX

GDL6 TUE.06/15/71 #01

```

101 REAL LENGTH
102 DIMENSION T(21,17,5), TOUT(10)
103 COMMON T,KMAX,R,TA,SCOR,SCOR2
104 56 READ, IM,JM,KM,TA,TH,TB00,LENGTH,S3,SMO,SAIR,S13,S23,R0
105 & ,S2,S12,NMAX,ERMAX
107 IF (IM) 58,58,59
108 58 STOP
109 59 IH=IM+3
110 JC=JM+2
111 KMAX=KM+1
112 DO 13 I=1,IH
113 DO 13 J=1,JC
114 DO 13 K=1,KMAX
115 13 T(I,J,K)=TH
116 50 READ , TTOP,DSL0T,WSLOT,WIDTh,S1
118 IF (TTOP) 56,56,57
119 57 R=R0
120 SOLD=-1.
121 DELZ=(TTOP+TB00)/FLOAT(IM)
122 I1=IFIX(TTOP/DELZ+.5)+1
123 TTOP=DELZ*FLOAT(I1-1)
124 I2=I1+IFIX(DSL0T/DELZ+.5)+1
125 DSL0T=DELZ*FLOAT(I2-I1-1)
126 TB0T=DELZ*FLOAT(IM+1-I1)
127 DELX=WIDTh/FLOAT(JM)/2.
128 J1=IFIX(WSLOT/2./DELX+.5)+1
129 WSLOT=2.*DELX*FLOAT(J1-1)
130 DELY=LENGTH/2./FLOAT(KM)
131 PRINT 3, TTOP,TB0T,DSL0T,IM,I2,I1
132 3 FORMAT (" TTOP,TB0T,DSL0T,IM,I2,I1= ",3(F5.3,1X),3(I3,1X))
133 PRINT 4, WIDTh,WSLOT,JM,J1,LENGTH,KM
134 4 FORMAT (" WIDTh,WSLOT,JM,J1,LENGTH,KM= ",
135 & 2(F5.3,1X),2(I3,1X),F5.3,1X,I3)
136 PRINT 5, TA,TH,ERMAX,R0,NMAX
137 5 FORMAT (" TA,TH,ERMAX,R0,NMAX = ",2(F4.0,1X),F8.7,1X,F4.2,15)
138 PRINT 6, S1,S2,S3,S12,S13,S23,SAIR,SMO
139 6 FORMAT ("      S1      S2      S3      S12      S13      S23
140 &      SAIR      SMH"/8(1X,F8.6))
141 DO 11 I=1,10
142 11 TOUT(I)=DELX*FLOAT(IFIX(.5+FLOAT(I-1)*FLOAT(JM)/9.))
143 PRINT 7, (TOUT(I),I=1,10)
144 7 FORMAT (" X-COORDINATES"/10(1X,F6.3))
145 DO 12 I=1,5
146 12 TOUT(I)=DELY*FLOAT(IFIX(.5+FLOAT(I-1)*FLOAT(KM)/4.))
147 PRINT 8, (TOUT(I),I=1,5)
148 8 FORMAT (" Y-COORDINATES"/10(1X,F6.3))
149 JA=JM-1
150 JB=JM+1
151 JD=J1-1
152 JE=J1+1
153 JF=J1+2
154 JG=J1-2
155 IA=I1-1
156 IB=I1+1
157 IC=I1+2
158 ID=I2-1
159 IE=I2+1
160 IF=I2+2

```

APPENDIX

GDL6 TUE.06/15/71 #02

```

161 IG=IM+2
162 X=1./DELX**2
163 Y=1./DELY**2
164 Z=1./DELZ**2
165 X2=2.*X
166 Y2=2.*Y
167 Z2=2.*Z
168 S12Z=2.*S12/S1/DELZ
169 S13Z=2.*S13/S1/DELZ
170 S21Z=2.*S12/S2/DELZ
171 S23Z=2.*S23/S2/DELZ
172 S23X=2.*S23/S2/DELX
173 S31Z=2.*S13/S3/DELZ
174 S32Z=2.*S23/S3/DELZ
175 S32X=2.*S23/S3/DELX
176 SMH=2.*SM0/S2/DELZ
177 SX1=2.*SAIR/S1/DELX
178 SX2=2.*SAIR/S2/DELX
179 SY1=2.*SAIR/S1/DELY
180 SY2=2.*SAIR/S2/DELY
181 SZ1=2.*SAIR/S1/DELZ
182 D1=S13Z/2.
183 D2=S12Z/2.
184 B1=(S23X+S23Z)/2.
185 IKON=1
186 MLIM=NMAX-5
187 91 DO 51 M=1,MLIM
188 SCOR=0.
189 SCOR2=0.
190 CALL RUNK (1,1,2,Z2,2,1,X2,1,2,0.,0,0,0.,0,0,0.,0,0,
191&1,SZ1,TA,0.,0.,Y,Y2,SY1)
192 DO 21 J=2,JM
193 JU=J+1
194 JV=J-1
195 21 CALL RUNK (1,J,3,Z2,2,J,X,1,JU,X,1,JV,0.,0,0,0.,0,0,
196& 1,SZ1,TA,0.,0.,Y,Y2,SY1)
197 CALL RUNK (1,JB,2,Z2,2,JB,X2,1,JM,0.,0,0,0.,0,0,0.,0,0,
198& 2,SZ1,TA,SX1,TA,Y,Y2,SY1)
199 DO 31 I=2,IA
200 IH=I+1
201 IV=I-1
202 CALL RUNK (I,1,3,Z,IU,1,Z,IV,1,X2,I,2,0.,0,0,0.,0,0,
203& 0,0.,0.,0.,0.,Y,Y2,SY1)
204 DO 22 J=2,JM
205 JU=J+1
206 JV=J-1
207 22 CALL RUNK (I,J,4,Z,IU,J,Z,IV,J,X,I,JU,X,I,JV,0.,0,0,
208& 0,0.,0.,0.,0.,Y,Y2,SY1)
209 31 CALL RUNK (I,JB,3,X2,I,JM,Z,IU,JB,Z,IV,JB,0.,0,0,0.,0,0,
210& 1,SX1,TA,0.,0.,Y,Y2,SY1)
211 CALL RUNK (I1,1,3,S13Z,IB,1,Z2,IA,1,X2,I1,2,0.,0,0,0.,0,0,
212& 0,0.,0.,0.,0.,Y,Y2,SY1)
213 DO 23 J=2,JD
214 JU=J+1
215 JV=J-1
216 23 CALL RUNK (I1,J,4,Z2,IA,J,S13Z,IB,J,X,I1,JU,X,I1,JV,0.,0,0,
217& 0,0.,0.,0.,0.,Y,Y2,SY1)
218 CALL RUNK (I1,J1,5,Z2,IA,J1,X,I1,JD,X,I1,JE,D1,IB,J1,D2,IB,JE,

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APPENDIX

GDL6

TUE.06/15/71 #03

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219& 0,0.,0.,0.,0.,Y,Y2,SY1)
220 DO 24 J=JE,JM
221 JU=J+1
222 JV=J-1
223 24 CALL RUNK (I1,J,4,Z2,IA,J,S12Z,IB,JU,X,I1,JU,X,I1,JV,0.,0,0,
224& 0,0.,0.,0.,0.,Y,Y2,SY1)
225 CALL RUNK (I1,JB,3,Z2,IA,JB,X2,I1,JM,S12Z,IB,JC,0.,0,0,0.,0,0,
226& 1, SX1,TA,0.,0.,Y,Y2,SY1)
227 CALL RUNK (IB,1,3,Z2,IC,1,X2,IB,2,S31Z,I1,1,0.,0,0,0.,0,0,
228& 0,0.,0.,0.,0.,Y,Y,Y)
229 DO 25 J=2,JD
230 JU=J+1
231 JV=J-1
232 25 CALL RUNK (IB,J,4,Z2,IC,J,S31Z,I1,J,X,IB,JU,X,IB,JV,0.,0,0,
233& 0,0.,0.,0.,0.,Y,Y,Y)
234 CALL RUNK (IB,J1,4,Z2,IC,J1,X2,IB,JD,S31Z,I1,J1,S32X,IB,JE,
235& 0.,0,0,0,0.,0.,0.,0.,Y,Y,Y)
236 CALL RUNK (IB,JE,4,Z2,IC,JE,X2,IB,JF,S21Z,I1,J1,S23X,IB,J1,
237& 0.,0,0,0,0.,0.,0.,0.,Y,Y2,SY2)
238 DO 26 J=JF,JB
239 JU=J+1
240 JV=J-1
241 26 CALL RUNK (IB,J,4,Z2,IC,J,X,IB,JU,X,IB,JV,S21Z,I1,JV,0.,0,0,
242& 0,0.,0.,0.,0.,Y,Y2,SY2)
243 CALL RUNK (IB,JC,3,Z2,IC,JC,X2,IB,JB,S21Z,I1,JB,0.,0,0,0.,0,0,
244& 1, SX2,TA,0.,0.,Y,Y2,SY2)
245 DO 32 I=IC,ID
246 IU=I+1
247 IV=I-1
248 CALL RUNK (I,1,3,Z,IU,1,Z,IV,1,X2,I,2,0.,0,0,0.,0,0,
249& 0,0.,0.,0.,0.,Y,Y,Y)
250 DO 27 J=2,JD
251 JU=J+1
252 JV=J-1
253 27 CALL RUNK (I,J,4,Z,IU,J,Z,IV,J,X,I,JU,X,I,JV,0.,0,0,
254& 0,0.,0.,0.,0.,Y,Y,Y)
255 CALL RUNK (I,J1,4,Z,IU,J1,Z,IV,J1,X2,I,JD,S32X,I,JE,0.,0,0,
256& 0,0.,0.,0.,0.,Y,Y,Y)
257 CALL RUNK (I,JE,4,Z,IU,JE,Z,IV,JE,X2,I,JF,S23X,I,J1,0.,0,0,
258& 0,0.,0.,0.,0.,Y,Y2,SY2)
259 DO 28 J=JF,JB
260 JU=J+1
261 JV=J-1
262 28 CALL RUNK (I,J,4,Z,IU,J,Z,IV,J,X,I,JU,X,I,JV,0.,0,0,
263& 0,0.,0.,0.,0.,Y,Y2,SY2)
264 32 CALL RUNK (I,JC,3,X2,I,JB,Z,IU,JC,Z,IV,JC,0.,0,0,0.,0,0,
265& 1, SX2,TA,0.,0.,Y,Y2,SY2)
266 CALL RUNK (I2,1,3,Z2,ID,1,S32Z,IE,1,X2,I2,2,0.,0,0,0.,0,0,
267& 0,0.,0.,0.,0.,Y,Y,Y)
268 DO 29 J=2,JD
269 JU=J+1
270 JV=J-1
271 29 CALL RUNK (I2,J,4,Z2,ID,J,S32Z,IE,J,X,I2,JU,X,I2,JV,0.,0,0,
272& 0,0.,0.,0.,0.,Y,Y,Y)
273 CALL RUNK (I2,J1,4,Z2,ID,J1,X2,I2,JD,S32X,I2,JE,S32Z,I2,JE,
274& 0.,0,0,0,0.,0.,0.,0.,Y,Y,Y)
275 CALL RUNK (I2,JE,5,Z2,IF,J1,Z,ID,JE,X2,I2,JF,X,IE,JD,B1,I2,J1,
276& 0,0.,0.,0.,0.,Y,Y2,SY2)

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APPENDIX

GDL6

TUE.06/15/71 #04

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277 DO 41 J=JF,JB
278 JU=J+1
279 JV=J-1
280 41 CALL RUNK (I2,J,4,Z,IF,JV,Z,ID,J,X,I2,JU,X,I2,JV,0.,0,0,
281& 0,0.,0.,0.,0.,Y,Y2,SY2)
282 CALL RUNK (I2,JC,3,Z,IF,JB,Z,ID,JC,X2,I2,JB,0.,0,0,0.,0,0,
283& 1,SX2,TA,0.,0.,Y,Y2,SY2)
284 CALL RUNK (IE,1,3,Z2,IF,1,X2,IE,2,S23Z,I2,1,0.,0,0,0.,0,0,
285& 0,0.,0.,0.,0.,Y,Y2,SY2)
286 DO 42 J=2,JG
287 JU=J+1
288 JV=J-1
289 42 CALL RUNK (IE,J,4,Z2,IF,J,X,IE,JU,X,IE,JV,S23Z,I2,J,0.,0,0,
290& 0,0.,0.,0.,0.,Y,Y2,SY2)
291 CALL RUNK (IE,JD,4,Z2,IF,JD,X,IE,JG,X,I2,JE,S23Z,I2,JD,0.,0,0,
292& 0,0.,0.,0.,0.,Y,Y2,SY2)
293 DO 43 J=J1,JB
294 JU=J+1
295 43 CALL RUNK (IE,J,1,1.,I2,JU,0.,0,0,0.,0,0,0.,0,0,0.,0,0,
296& 0,0.,0.,0.,0.,0.,0.,0.)
297 DO 33 I=IF,IG
298 IU=I+1
299 IV=I-1
300 CALL RUNK (I,1,3,Z,IU,1,Z,IV,1,X2,I,2,0.,0,0,0.,0,0,0,
301& 0,0.,0.,0.,0.,Y,Y2,SY2)
302 DO 44 J=2,JM
303 JU=J+1
304 JV=J-1
305 44 CALL RUNK (I,J,4,Z,IU,J,Z,IV,J,X,I,JU,X,I,JV,0.,0,0,
306& 0,0.,0.,0.,0.,Y,Y2,SY2)
307 33 CALL RUNK (I,JB,3,Z,IU,JB,Z,IV,JB,X2,I,JM,0.,0,0,0.,0,0,
308& 1,SX2,TA,0.,0.,Y,Y2,SY2)
309 CALL RUNK (IH,1,2,Z2,IG,1,X2,IH,2,0.,0,0,0.,0,0,0.,0,0,
310& 1,SMH,TH,0.,0.,Y,Y2,SY2)
311 DO 45 J=3,JM
312 JU=J+1
313 JV=J-1
314 45 CALL RUNK (IH,J,3,Z2,IG,J,X,IH,JU,X,IH,JV,0.,0,0,0.,0,0,
315& 1,SMH,TH,0.,0.,Y,Y2,SY2)
316 CALL RUNK (IH,JB,2,Z2,IG,JB,X2,IH,JM,0.,0,0,0.,0,0,0.,0,0,
317& 2,SMH,TH,SX2,TA,Y,Y2,SY2)
318 IF (SCOR2-ERMAX) 73,73,72
319 72 IF(SOLD*SCOR) 74,74,75
320 74 R=R+.19-.468/R
321 75 SOLD=SCOR
322 IF (R-1.) 81,51,51
323 81 R=1.
324 51 CONTINUE
325 73 PRINT 9, M,R,SCOR2
326 9 FORMAT (IX,I5,IX,F6.4,IX,F10.7)
327 DO 14 K=1,5
328 KK=IFIX(.5+FLOAT(K-1)*FLOAT(KM)/4.)+1
329 DO 15 J=1,10
330 JJ=IFIX(.5+FLOAT(J-1)*FLOAT(JM)/9.)+1
331 15 TOUT(J)=T(1,JJ,KK)
332 14 PRINT 2,(TOUT(J),J=1,10)
333 2 FORMAT (10(IX,F6.2))
334 GO TO (92,50),IKON

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APPENDIX

GDL6

TUE.06/15/71 #05

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335 92 IKON=2
336 MLIM=5
337 R=1.
338 GO TO 91
339 END
340 SUBROUTINE RUNK (I,J,N,A,I1,J1,B,I2,J2,C,I3,J3,D,I4,J4,E,I5,J5,
341& M,F,T1,G,T2,Y,YE,CE)
342 DIMENSION T(21,17,5)
343 COMMON T,KMAX,R,TA,SCOR,SCOR2
344 MM=M+1
345 DO 1 K=1,KMAX
346 V=0.
347 U=0.
348 GO TO (10,11,12),MM
349 12 V=V+G
350 U=U+G*T2
351 11 V=V+F
352 U=U+F*T1
353 10 GO TO (13,14,15,16,17),N
354 17 V=V+E
355 U=U+E*T(I5,J5,K)
356 16 V=V+D
357 U=U+D*T(I4,J4,K)
358 15 V=V+C
359 U=U+C*T(I3,J3,K)
360 14 V=V+B
361 U=U+B*T(I2,J2,K)
362 13 V=V+A
363 U=U+A*T(I1,J1,K)
364 IF (K-1) 18,18,19
365 18 U=U+2.*Y*T(I,J,2)
366 GO TO 22
367 19 IF (K-KMAX) 20,21,21
368 20 U=U+Y*(T(I,J,K-1)+T(I,J,K+1))
369 22 V=V+2.*Y
370 GO TO 2
371 21 U=U+YE*T(I,J,K-1)+CE*TA
372 V=V+YE+CE
373 2 COR=U/V-T(I,J,K)
374 SCOR=SCOR+COR
375 SCOR2=SCOR2+(R*COR)**2
376 1 T(I,J,K)=T(I,J,K)+R*COR
377 RETURN
378 END
```