Role of 3D Thermal Diffusivity in the Numerical Resolution of the Heat Equation

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Abstract:- The ad hoc one-dimensional definition of the scalar thermal diffusion coefficient D defined as K / Roh C is short and inadequate to deal with the resolution of the 2D and 3D thermal diffusion equation. We have alternatively applied the chains of matrix B to the solution of the 2D and 3D heat diffusion equation for stationary solutions and time-dependent transient solutions.

The role of 3D thermal diffusivity in the numerical resolution of the heat equation is carefully studied throgh the repeated variation of the main diagonal entry of matrix B,RO in the interval [0,1]. It is obvious that thermal diffusivity is related to RO, one of them produces the other.

The chains of the matrix B using the 3D diffusion coefficient combine D, dt and the Laplace operator in an inseparable block and define a new technique to solve the diffusion of heat in different situations.In this article, we have applied the B chains to solve five different examples of heat diffusion in 2D and 3D geometries for both time-dependent and stationary conditions and the presented digital solutions are surprisingly precise, fast and stable.

I. INTRODUCTION

Below is the equation we are investigating, except we use D for the thermal diffusion coefficient instead of Alpha,
d / dt(partial) U (r, t) = D Nabla^2 (U (r, t) + S (r, t) .. . . (1)

with the boundary conditions B C on the limits of the domain of U and the initial conditions IC of U namely U (0, r).

Where,
S(r,t) is the numerical values of heat energy density source term at the corresponding free nodes in the considered 2D or 3D domain.

In classical numerical methods with finite difference FDM [1,2], when the source term is neglected, Nabla^2 in 3D configuration is expressed numerically as follows,
Nabla^2 U (i, j, k) = {U (i + 1, j, k) + U (i-1, j, k) + U (i, j + 1, k) + U (i, j- 1, k) + U (i, j, k + 1) + U (i, j, k-1) -6 * (U (i, j, k)} / 6 . . . .(2)

and the incremental temporal variation dU is expressed in the form,
dU = D Nabla ^{2} .dt. . . . .(3)

In matrix representation.

The steady state equilibrium solution of Equation (1), which is time independent reduces to,[1]
A (i,j,k) U=b . . . . (4)

And the spatio-teporal evolution or time dependent solution of equation 1) reduces to,[2]
U(r,t+dt) = A . U(r,t) dt. .. . .. .(5)

where r in Cartesian coordinates is given by,
x=i dx, y=j dy and z=k dz.

A is the well-known square Laplace matrix (nxn) known to be tridiagonal for one-dimensional heat diffusion problems and 4-5 diagonal matrix for 2D and 3D problems respectively.

Solving linear systems of algebraic equations (4) is not easy and requires the application of numerical techniques such as Gaussian elimination or more advanced methods.

In addition, the spatio-temporal resolution of Eq 5 by successive iterations is more complicated and suffers from being slow and requires long computation times, especially for large n. Moreover, the solution itself has inherent problems of stability and convergence.

We assume that the complexity of solving equations 4,5, in classical numerical FDM, results from combining alha, nabla squared and dt into a single term by multiplication, i.e. D Nabla ^ 2. dt which would add nothing.

Therefore, we propose the use of matrix chains B [3,4,5,6].

The inherent characteristics of the B chain transition matrix with different values of diagonal elements RO to replace the classic FDM.

Here there is no D, neither Nabla ^ 2 nor dt since all this information is inherent in the inputs of the transition matrix B itself.

In addition, the classical ad hoc one-dimensional definition of thermal diffusivity like D = K / Roh.C is omitted.

In fact, the coefficient D can be expressed as a function of the characteristic time TR of the exponential rise / fall of the digital values of the limit temperature field as explained later in sections 2 and 3..

In the previous articles, we presented the chain transition matrix B and explained its resolution techniques [2,3] which completely neglects the existence of the heat diffusion equation PDE (1) as well as the techniques of FDM finite differences used to solve it.

In other words, the new matrix B-chain techniques [1,2,3] completely neglect Eq.1 as if it never existed and ignore its classic digital FDM solution presented by equations 2-5.

The new matrix chain B techniques are defined and based on the statistical recurrence formula [1],

$\mathbf{U_{i,j,k}^{(N+1)} = B\,(U^{N} + b + S)}$**. . . (6)**

Where b is the vector of Dirichlet boundary conditions arranged in the prop order and S is the energy density source / sink term at the specified free node points.
It follows that the numerical statistical solution of the heat diffusion equation is simply given by,U(r,t)=(B^0+B+B^2+B^3+. . . . .B^N). (b+S) + B^N .U(r,0) . . . . (7)

For large values of the number of iterations N, B ^ N and the initial condition term B ^ N. U (r, 0) tends to zero for any initial arbitrary distribution U (r, 0) and will be neglected in the following to analysis .

It is obvious that the matrix summation B^0+B+B^2+B^3+. . . . .B^N for any number of iterations N is the required transient time-dependent solution of the heat diffusion equation.Moreover

The propsed new techniques presents the solution for Dirichlet boundary value problem of PDE 1 ,U(r,t)=(B^0+B+B^2+B^3+. . . . .B^N). (b+S) =E . (b+S). . . (7)

Where the transfer matrix E at given N , is given by,
E(N)=
B^0+B+B^2+B^3+. . . . .B^N . . . . (8)

b is the BC conditions vector arranged in proper adequate order and S is the energy density source/sink term at the concerned free nodes. Both b and S vectors are expressed in the same units as U.

What is striking about equation (7) is that it exactly follows the rise / fall of the exponential curve of time when multiplied by the boundary condition vector b, i.e. say that it follows namely Exp -t / TR or 1- Exp -t / TR.

the dimensionless time is given by,
t ^ = t / TR. . . . . (9)

Where TR is the characteristic time = 1 / Alpha.

Here, the elapsed time appears in the form N t ^ or more simply N.

It has been shown that the transition matrix B combines D, Nabla ^ 2 and dt in an inseparable block. And has been successfully applied [1,2,3,4] to systematically solve many Laplace PDE and Poisson PDE situations as well as the heat diffusion equation.

The proposed B-techniques apply for any arbitrary distribution of the source / sink term S and for all types and geometries of boundary conditions BC which is the decisive factor in the statistical solution of PDE boundary value problems. We first deal with the simplest case, namely Dirichlet BC.

During this work we extend the B techniques to the role of thermal diffusivity in the numerical resolution of the heat equation which is the subject of this article.

II. THEORY

The theory of this work is explained in 4 consecutive steps namely,
I-Define the geometrical configuration 2D or 3D and discretize the space in n equidistant free nodes.
ii-Construct the transition matrix B for the prescribed domain with an arbitrary diagonal entry RO.
The B-matrix is well defined [1,2] by the conditions i-iv.
iii-Use the B-matrix chains ,Equation 7, to find both the steady state solution or the time dependent spatio-temporal evolution of the solution of heat diffusion equation in either 2D or 3D.
Note that the classic equations 1 - 5 have been replaced by a single equation 6.
iv-Repeat step iii for different values of the diagonal input RO in the closed interval of [0,1] to obtain the equivalence relations of alpha or TR = 1 / alpha vs RO.

This produces the connection between 3D alpha and RO as shown in Tables I and II.

In other words, the construction of the B-matrix nxn would suffice to define the spatio-temporal evolution of the solution U (r, t) for any BC and any value of the diffusion coefficient D which is a function of RO of the matrix B itself.

As a general rule, starting from zero initial conditions, The numerical results of solution (7) show that it exactly follows an exponential rise in time for all the free nodes in a given 2D or 3D configuration, namely U (t) = Umax (1- Exp -ALPHA .t)The above rule is used to find the variation of Alpha with RO by finding the exponential fit of the time curve for any thermal diffusivity value D included in the variable RO

In other words, the time solution for U (r, t) exactly follows an exponential curve of time in the form U (t) = U (t) max. (1- Exp (-D .t)) for all values of RO.

The insertion of the dimensionless time t ^ and the length h ^ is simple.
t ^ = t / TR and dimensionless coordinates x ^ = x ^ / h, y ^ = y / h and z ^ = z / h where h is the spacing between two successive free nodes.

It follows that the dimensionless spacing between two successive free nodes h ^ is given by,
h^ = 1 / (n + 1) . . . .(10)
It is obvious that the time t in equation 7 is given by N dt, N being the number of iterations.

Unlike conventional FDM, in the proposed B-chain techniques, there are no stability issues besides rapid convergence.

Note that Equation 7 predicts two important physical facts,
i-The value of U at the free node of position r1 is interchangeable with the source term at position r2, i.e. if S (r1) gives a numerical value of the energy at r2, then a source similar to r2 gives the same numerical value of energy at r1.
ii-The temporal evolution of the energy density of a 2D rectangle is the same as that of a cube or a 3D rectangloid provided that the rectangle has the same distribution of free nodes as that of the base of the rectagloid, See Figs, 1, 2,3, 4,5.

In order not to worry too much about the theory and the details of its predictions, we go directly to 2D and 3D geometric spatial applications as follows:

III. APPLICATIONS AND NUMERICAL RESULTS

We present the applications and the numerical results of this article in two parts, namely the transient and stationary solutions.

III-A.Transient Solutions

Consider the simplest case of 3D geometric configuration. A 3D cube of 8 equidistant free nodes and 8 boundary conditions as shown in figure-1.

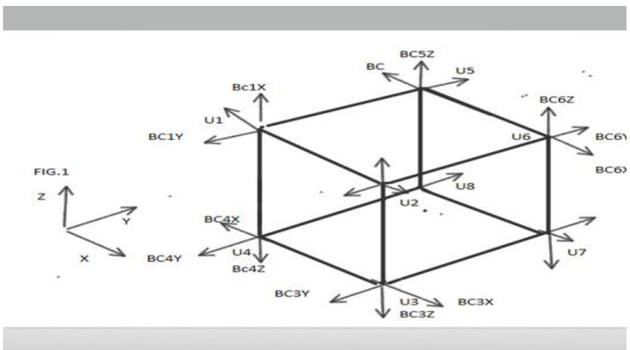

Fig. 1. Transient heat diffusion equation in a 3D cube of 8 free nodes with 8 Dirichlet BC.

For simplicity, the cube in Figure -1 has an initial zero temperature condition and is placed inside a larger cube of which all fixed Dirichlets BC are assumed to be unity.

The chains of matrix B, Eq. 7, are used to find the temporal rate of exponential rise over time for different RO elements of the interval [0,1] and the numerical results are shown in Table I.

Table I. Numerical results for RO vs alpha up to equation 7 for the 3D cube 8 free nodes

RO	0.	0.2	0.4	0.6	0.8	1.0
ALPHA	0.693	0.511	0.357	0.223	0.105	0.000
ALPHA-LOG	Log 2	Log 1.667	Log 1.429	Log 1.25	Log1.111	Log1.0

Note that Table I precisely prescribes the prediction relation between 3D Alpha and RO as a logarithmic relation,
ALPHA = Log {1 / (1/2 + RO / 2)},. . . Relationship. . . . (1)

Now consider another simple case of rectangular or square 2D geometric configuration. A 2D square of 9 equidistant free nodes and 9 boundary conditions as shown in Figure 2.

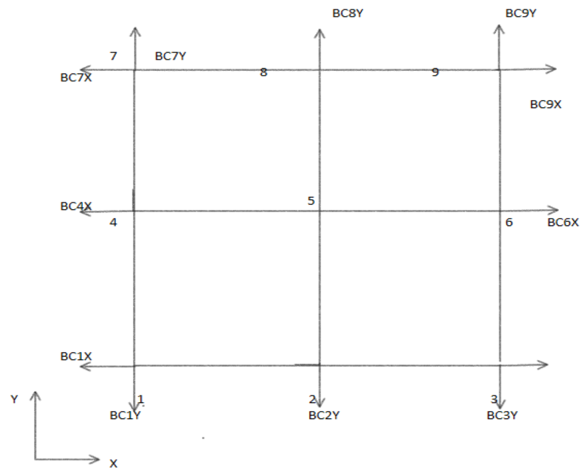

Fig. 2 - 2D square of 9 equidistant free nodes and 9 Dirichlet boundary conditions.

The numerical results of Eq. 6 are shown in Table II, as follows,

Table II. Numerical results for RO vs alpha up to equation 7 for the 2D square 9 free nodes

.2RO	0.	0.2	0.4	0.6	0.8	1.0
ALPHA-LOG	0.376	0.282	0.206	0.129	0.0636	0.0

A slightly more complicated 3D application is shown in Fig. 3

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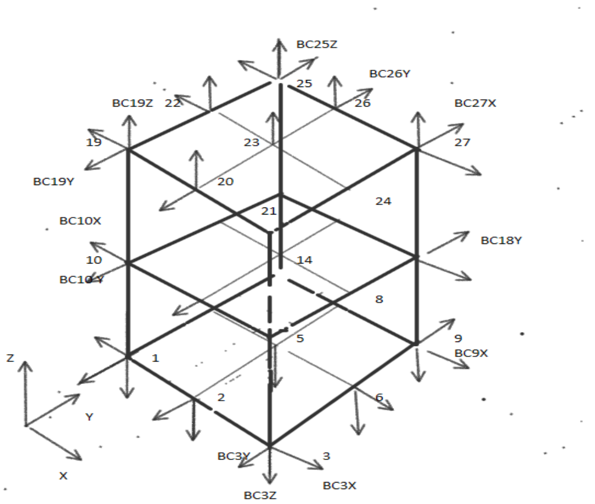

Fig. 3 - Heat diffusion in 3D paralleloid of 27 equidistant free nodes and 26 Dirichlet boundary conditions.

The numerical results of Eq. 7 as applied for FIG. 3 are shown in Table III, as follows,

Table III. Numerical results for RO vs alpha up to equation 7 for the 3D paralleloid 27 free nodes

RO	0.	0.2	0.4	0.6	0.8	1.0
ALPHA	0.376	0.282	0.206	0.129	0.0636	0.0

Note that the numerical values for RO and Alpha in Table III are exactly the same as those in Table II according to equation 10 and prediction ii.

Figure 4 shows the heat diffusion equation in a 2D rectangle of 25 equidistant free nodes with 16 Dirichet BC.

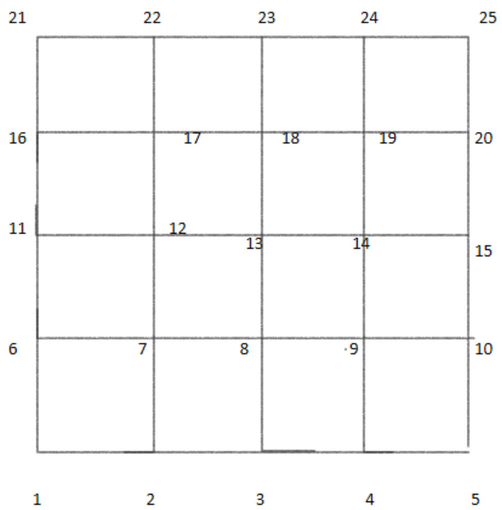

Fig.4 diffusion equation in 2D rectangle of 25 equally spaced free nodes with 16 Dirichet BC.

The numerical results of Eq. 7 as applied for FIG. 4 are shown in Table IV, as follows,

Table IV. Numerical results for RO vs alpha up to equation 7 for the 2D square 25 free nodes

RO	0.	0.2	0.4	0.6	0.8	1.0
ALPHA	0.167	0.127	0.0923	0.0558	0.0323	0.0

III-B. Steady state solutions

The steady-state equilibrium solution is defined mathematically in Equation 1 as,

dU / dt) patiel = 0

It follows that D Nabla ^ 2 = 0 is the same as Nabla ^ (r) = 0.

Therefore, it is evident that the distribution of the equilibrium temperature field does not depend on the value of thermal diffusivity D. It only affects the time elapsed to reach the final destination of the steady-state temperature distribution.

However, in the steady-state digital solution of matrix B, it is obtained by one of two methods, namely,

1-summation of E = B ^ 0 + B + B ^ 2 ...... + B ^ N .... (8) for N sufficiently large.
2-Using the equivalence relation,
E = (I-B) ^ - 1. . . . . (11)

And finally the solution in steady state of equilibrium is given by the matrix D = E-I, [1,3,6] and,
U = D. (B + S) .... (12)

We consider here two cases,

Case 1

Figure 2 was considered by Mathews [1] to find the steady-state temperature distribution by reducing the PDE .1 into nine linear algebraic equations, then solving the algebraic system by Gaussian elimination.

He assumed an arbitrary boundary conditions vector b of 9 elements in degrees C as,
b = (100,20,20,80,0,0,260,180,180) T

And he got the steady-state temperature distribution vector in the form,
U = (55.7143, 43.2143, 27.1429, 79.6429, 70.0000, 45.3571, 112.858, 111.786, 84.2857) T
If we use Eq. 7 with the same BC, then the corresponding results of Eq. 7 after N = 30 iterations are,
U = (55.7126, 43211, 27.142, 79.6396, 69.9968, 45.3555, 112.8560, 111.7841, 84.2846) T

The agreement between the Mathews results and the results of matrix B chain is excellent.

Case 2

Case 2 investigates the steady-state temperature in Fig. 3 of 27 equidistant 3D free nodes. The initial conditions are assumed to be zero and the 26 boundary conditions of vector b are assumed to be zero, except that b (1), b (2), b (3) are assumed to be maintained at 100 degrees C.ie.,

b=(100, 100, 100, 0,0,0,0,0,0. . ……0,0……. 0,0,0)T
we have applied Eq. 7 to the rectangle in Fig. 3 and

the resulting steady-state temperature distribution after 22 iterations is shown in three figures, namely Fig. 5, Fig. 6, Fig 7 for the three plane levels, namely nodes 1-9, nodes 10-18 and nodes 19-27

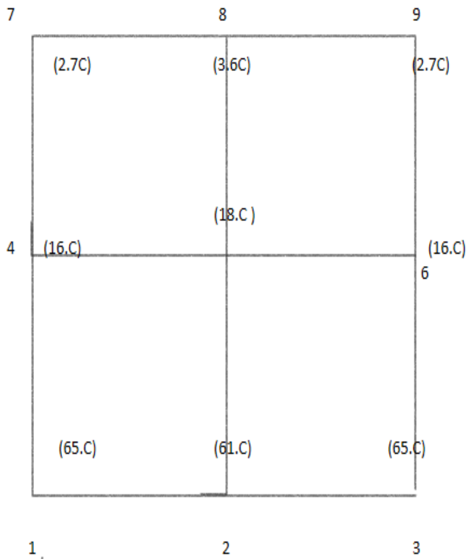

Fig. 5 The temperature distribution for Fig. 3 level one, i.e. free nodes 1-9.

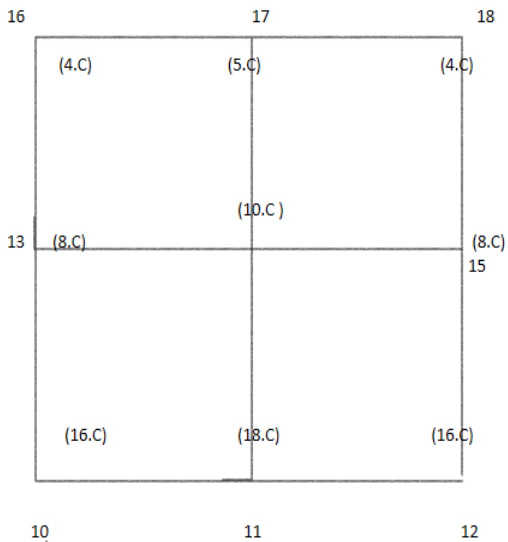

Fig. 6 The temperature distribution for Fig. 3 level two, i.e. free nodes 1-9.

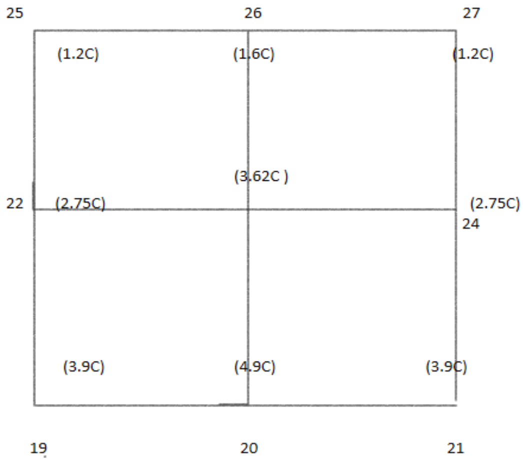

Fig.7 Temperature distribution for Fig. 3 level three, i.e. free nodes 19-27.

IV. CONCLUSIONS

The ad hoc one-dimensional definition of the thermal diffusion coefficient D is short and insufficient to deal with 2D and the 3D heat diffusion equation in both the steady state and the time dependent transient state.

The classical multiplication of the diffusion coefficient D by the operator Nabla ^ 2 dt adds nothing.

We propose the use of matrix chains B where the 3D diffusion coefficient, dt and the Laplace operator are combined in an inseparable block.

We repeatedly applied the B-chains with different ROs in the interval [0,1], to solve five different examples of heat diffusion in 2D and 3D time-dependent and steady-state situations and the numerical solutions were surprisingly precise, fast and stable.

This technique is valuable because there are a large number of newly discovered materials and alloys for which the study of their thermal properties is of great interest. Replacing FDM with new B matrix chain techniques to measure these properties by solving the heat diffusion equation would be promising.

N.B. All calculations in this article have been produced with the author's double precision algorithm to ensure maximum precision, as followed by Ref. 9 for example

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