

Unstructured Finite Volume approach for 3-D unsteady Thermo-Structural Analysis using Bi-Conjugate Gradient Stabilized method

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Abstract: The structural members subjected to severe thermal environments are generally encountered in high speed flows. The optimization of these structural members needs a coupled Fluid -Thermo-Structural analysis. As a first step towards a coupled Fluid -Thermo-Structural analysis, an unsteady 3-D Thermo-Structural analysis is attempted in the present work. As finite volume method is the most popular method for fluid flow analysis. The same methodology is adopted for thermo-structural analysis in the present work. An implicit time stepping is adapted to achieve uniform time stepping while solving heat conduction and structural dynamics equation. The implementation of implicit scheme results in a system algebraic equations and are solved using Bi-Conjugate Gradient Stabilized (Bi-CGStab) method. The space discretization is carried out using arbitrarily oriented tetrahedral elements and a new least square based methodology is used for the evaluation of derivatives avoiding the reconstruction of variables at the nodes. As a first step, an unstructured finite volume code for the solution of 3-D unsteady heat conduction equation is developed. The code has been validated for various Neumann and Dirichlet boundary conditions. The results are compared with the analytical solution available for semi-infinite body heat conduction and are found to be in good agreement. Then the code is further extended for the unsteady structural dynamics equations and an integrated linear elastic Thermo-Structural analysis was carried out for the case of internally heated hollow sphere. The unstructured finite volume method in conjunction with Bi-CGStab solver results in an efficient unsteady Thermo-Structural solver and can be easily extended for an integrated Fluid-Thermo-Structural analysis.

Keywords: Unstructured, Finite Volume Method, Unsteady, Thermo-Structural, Bi-CGStab method.

I. INTRODUCTION

The structural members subjected to severe thermal environments are generally encountered in high speed flows. Design of such hypersonic vehicle structures depend on accurate prediction of the aero-thermal loads, structural temperatures and their gradients, as well as structural deformation and stresses. So an integrated multi disciplinary analysis procedure is required for accurate, timely prediction of coupled response of these structural members. To meet the above analysis requirement for hypersonic vehicles the NASA Langley Research Center was developed an integrated Fluid-Thermal-Structural (LIFTS) analyser using Finite element methods [3].

In this project work, the aim is to simulate coupled Thermo-Structural problem, by using the three-dimensional unstructured finite volume method applying Bi-CGStab method [9] as the numerical solution tool. The work deals with the unstructured finite volume method for the analysis because the method takes full advantages of an arbitrary mesh, where large number of options are open for the definition of the control volumes around which the conservation laws are expressed. In addition, by the direct discretization of the integral form of the conservation laws we can ensure that the basic quantities mass, momentum and energy will remain conserved at discrete level. The finite volume method is well established as well as an efficient method for solving fluid flow problems and can be extended to other problems like heat transfer and structural analysis because the fact that the governing equations achieve similarity with fluid flow problems. In this work, tetrahedron elements are used for the space discretization because of its flexibility in meshing and will give very good results for all complex geometries. The unstructured finite volume method is well accepted as the method for CFD, a computer code for the Thermo-Structural analysis using the same method is expected to pave the way for an integrated Fluid-Thermo-Structural analysis methodology using this method.

II. MODELLING AND FORMULATION OF THERMO-STRUCTURAL ANALYSIS

A. Mathematical modelling

The governing equations for the unsteady heat conduction equation and structural dynamics are described in this section A. The resulting equations are cast into a divergence form so that the finite volume method can be applied.

1) Governing equations for thermal analysis.

The general 3D heat conduction equation in Cartesian coordinates without heat generation is given by,

$$\rho C_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial x} \left(-K_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(-K_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(-K_z \frac{\partial T}{\partial z} \right) = 0 \dots\dots\dots (1)$$

Where, ρ is the density, C_p is the specific heat, K_x, K_y, K_z are the orthotropic conductivity along x, y and z directions.

Defining $q_x = -K_x \frac{\partial T}{\partial x}, q_y = -K_y \frac{\partial T}{\partial y}, q_z = -K_z \frac{\partial T}{\partial z}$ the above equation can be written as,

$$\rho C_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial x} (q_x) + \frac{\partial}{\partial y} (q_y) + \frac{\partial}{\partial z} (q_z) = 0 \dots\dots\dots (2)$$

The above equation can be written in divergence form as follows,

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot q = 0 \dots\dots\dots (3)$$

2) Governing equations for Thermo-Structural analysis

The governing equation of structural dynamics is the equilibrium equations. Neglecting the body forces the equilibrium equations are given by,

$$\rho \frac{\partial^2 u}{\partial t^2} - \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) = 0 \dots\dots\dots (4)$$

$$\rho \frac{\partial^2 v}{\partial t^2} - \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right) = 0 \dots\dots\dots (5)$$

$$\rho \frac{\partial^2 w}{\partial t^2} - \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) = 0 \dots\dots\dots (6)$$

Where u, v, w are the displacements in x, y and z directions, $\tau_{xx}, \tau_{yy}, \tau_{zz}$, are the normal stress components, $\tau_{xy}, \tau_{xz}, \tau_{yz}$ are the shear stress components.

The normal stress components can be written in terms of normal strain components as follows,

$$\tau_{xx} = \frac{E}{(1+\sigma)(1-2\sigma)} [(1-\sigma)\epsilon_{xx} + \sigma(\epsilon_{yy} + \epsilon_{zz})] - \beta(T - T_{init}) \dots\dots\dots (7)$$

$$\tau_{yy} = \frac{E}{(1+\sigma)(1-2\sigma)} [(1-\sigma)\epsilon_{yy} + \sigma(\epsilon_{xx} + \epsilon_{zz})] - \beta(T - T_{init}) \dots\dots\dots (8)$$

$$\tau_{zz} = \frac{E}{(1+\sigma)(1-2\sigma)} [(1-\sigma)\epsilon_{zz} + \sigma(\epsilon_{xx} + \epsilon_{yy})] - \beta(T - T_{init}) \dots\dots\dots (9)$$

Where $\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}$ are the strain components along x, y, z directions respectively, $E =$ Young's modulus, $\sigma =$ Poisson's ratio, $\beta = \frac{E\alpha_e}{1-2\sigma}$, Where α_e is the coefficient of thermal expansion.

T is temperature at the specified location in the material and is obtained by solving the heat conduction equation.

T_{init} is the initial temperature of the body.

The shear stress components can be written in terms of shear strain components as follows,

$$\tau_{xy} = 2\mu\epsilon_{xy} \dots\dots\dots (10)$$

$$\tau_{yz} = 2\mu\epsilon_{yz} \dots\dots\dots (11)$$

$$\tau_{xz} = 2\mu\epsilon_{xz} \dots\dots\dots (12)$$

$2\mu = \frac{E}{(1+\sigma)}$, where μ is the lames constant and also known as shear modulus.

The strain components are given in a matrix form,

$$\epsilon_{ij} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & \frac{\partial w}{\partial z} \end{bmatrix} \dots\dots\dots (13)$$

Substituting the above strain-displacement relationships in stress-strain relationships and then substituting these stress-strain relationships in the equilibrium equations, we get the equations in the divergence form as,

$$\rho \frac{\partial^2 U}{\partial t^2} - \nabla \cdot \tau = 0 \dots\dots\dots (14)$$

The above equations are similar to that of heat conduction equation and the finite volume method can be applied. The unsteady Thermo-Structural analysis is performed in two steps at every time level. First the temperature distribution is computed for the time step from the initial condition by solving the heat conduction equation with appropriate

boundary conditions. The temperature distribution obtained is used along with structural boundary conditions to obtain the displacements u , v , and w by solving the structural dynamics equation for the same time step. The above methodology is repeated for time marching. The solution methodology and details are given in the next section B.

B. Finite volume formulation

1) Finite volume formulation for thermal analysis

As explained in the previous section, for Thermo-Structural analysis first we need to solve the heat conduction equation to get the temperature distribution in the body.

By integrating equation (3) we get,

$$\int_V \left(\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot q \right) dV = 0 \dots\dots\dots (15)$$

$$\rho C_p V_i \frac{dT_i}{dt} + \int_S q \cdot n \cdot dS = 0 \Rightarrow \rho C_p V_i \frac{dT_i}{dt} + \sum_{All\ faces\ of\ CV} q \cdot n \cdot S = 0$$

For discretization we have used unstructured tetrahedron elements so the above equation can be written as,

$$\Rightarrow \rho C_p V_i \frac{dT_i}{dt} + \sum_1^4 q \cdot n \cdot S = 0 \dots\dots\dots (16)$$

$$\Rightarrow \rho C_p V_i \frac{dT_i}{dt} + (q_{1x} \cdot S_{1x} + q_{1y} \cdot S_{1y} + q_{1z} \cdot S_{1z} + q_{2x} \cdot S_{2x} + q_{2y} \cdot S_{2y} + q_{2z} \cdot S_{2z} + q_{3x} \cdot S_{3x} + q_{3y} \cdot S_{3y} + q_{3z} \cdot S_{3z} + q_{4x} \cdot S_{4x} + q_{4y} \cdot S_{4y} + q_{4z} \cdot S_{4z}) = 0 \dots\dots\dots (17)$$

Where, V_i is the volume of element, S_{1x} , S_{1y} , S_{1z} are the projected face area of the face-1 along x, y and z respectively, S_{2x} , S_{2y} , S_{2z} are the projected face area of the face-2 along x, y and z respectively, S_{3x} , S_{3y} , S_{3z} are the projected face area of the face-3 along x, y and z respectively and S_{4x} , S_{4y} , S_{4z} are the projected face area of the face-4 along x, y and z respectively. The different faces of the tetrahedron are shown in the Fig.1. The convention used is the face opposite to node 1 is named as Face 1 and so on.

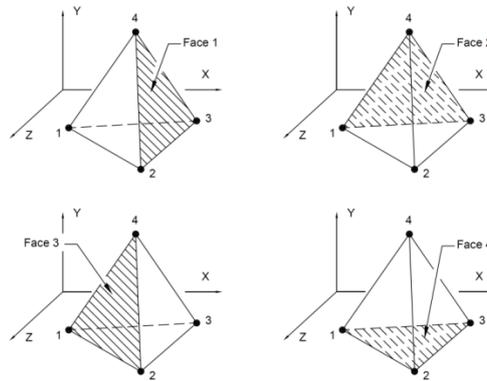


Fig.1. Different faces of a tetrahedron element

$$\Rightarrow \rho C_p V_i \frac{dT_i}{dt} + \sum_{j=1}^4 \left[\left(-K_x \cdot \frac{\partial T}{\partial x} \right)_j S_{j-x} + \left(-K_y \cdot \frac{\partial T}{\partial y} \right)_j S_{j-y} + \left(-K_z \cdot \frac{\partial T}{\partial z} \right)_j S_{j-z} \right] \dots\dots\dots (18)$$

The above can written as follows,

$$\Rightarrow \rho C_p V_i \frac{dT_i}{dt} + F_i = 0 \dots\dots\dots (19)$$

Explicit and implicit time stepping schemes can be used for the integration of these system of ordinary differential equations. Explicit schemes are conditionally stable and many times the time steps become extremely small for many practical problems. The advantage is that the residue can be explicitly evaluated from the values of the primitive variables known at the previous time step. Though the implicit schemes are unconditionally stable, the residues are to be computed on the current time level which involves the solution of the matrix system which is symmetric/non-symmetric. The iterative solution technique, Bi-CGStab method can be used effectively here as it can be modified as an element-by-element solver.

The above equation (19) is solved by pure implicit time integration (for implicit scheme “F” is evaluated for T_i^{n+1} i.e. for the value at the next time step ($t+\Delta t$) as follows,

$$\Rightarrow \rho C_p V_i \frac{T_i^{n+1} - T_i^n}{\Delta t} + F_i^{n+1} = 0 \dots\dots\dots (20)$$

$$\Rightarrow \rho C_p V_i \frac{T_i^{n+1}}{\Delta t} + F_i^{n+1} - \rho C_p V_i \frac{T_i^n}{\Delta t} = 0 \dots\dots\dots (21)$$

As first step for finding the fluxes (F) over the four faces of the tetrahedron, we need the derivatives to be evaluated at these faces and it requires the evaluation of T and its derivatives in x, y and z directions. The primitive variables are averaged between the elemental values on either side of the face and the derivative evaluation is explained in section 3. The present method of derivative evaluation totally avoids the reconstruction of variables from elemental value to nodal values. With the evaluation primitive variables and their derivatives, the fluxes on each of the four faces of the tetrahedron can be evaluated. Multiplied by the projected surface areas and summing up gives the residue for each element and the above equation reduces to a form AX-B=0 and is solved using Bi-CGStab method. The algorithm for Bi-CGStab this method is given below,

Compute $r_0 = B - Ax_0$ for some initial guess x_0

$$\rho_0 = a_0 = \omega_0 = 1; \quad v_0 = p_0 = 0$$

Iteration starts $n=1,2,3 \dots\dots\dots$ do

$$\rho_n = r_0^T r_{n-1} ; \quad \beta_n = \frac{\rho_n}{\rho_{n-1}} \cdot \frac{a_{n-1}}{\omega_{n-1}}$$

$$p_n = r_{n-1} + \beta_n (p_{n-1} - \omega_{n-1} \cdot v_{n-1})$$

$$v_n = Ap_n ; \quad a_n = \frac{\rho_n}{r_0^T v_n}$$

$$S_n = r_{n-1} - a_n \cdot v_n$$

$$t_n = AS_n ; \quad \omega_n = \frac{t_n^T S_n}{t_n^T t_n}$$

$$x_n = x_{n-1} + a_n p_n + \omega_n S_n$$

$$r_n = S_n - \omega_n t_n$$

Check convergence; continue if necessary

End do

The main advantage of the Bi-CGStab solver is that it requires always the residue B-AX or the column vector [A]{x} which totally avoids the assembly of matrix [A]. For iterative improvement of the solution, the L.H.S of the above equation is computed with different values of unknown T and the solution proceeds to make L.H.S-R.H.S to zero. It is reported that the convergence of Bi-CGStab method is fast. Hence this solver is used in the present effort to solve the system of equations resulting from the application of unstructured finite volume method to the 3D unsteady heat conduction equation. Once the temperature distributions are known, the next step is to solve the structural dynamics equation for a coupled Thermo-Structural analysis and is discussed in the following section 2.

2) Finite volume formulation for thermo-structural analysis

To solve for “u” displacement integrate equation (14)

$$\int \left(\rho \frac{\partial^2 u}{\partial t^2} - \nabla \cdot \tau \right) dV = 0 \dots\dots\dots (22)$$

$$\Rightarrow \rho V_i \frac{d^2 u_i}{dt^2} - \int_S \tau \cdot n \cdot dS = 0 \dots\dots\dots (23)$$

$$\Rightarrow \rho V_i \frac{d^2 u_i}{dt^2} - \sum_{All\ faces\ of\ CV} \tau \cdot n \cdot S = 0 \dots\dots\dots (24)$$

For a tetrahedron it can be written as,

$$\Rightarrow \rho V_i \frac{d^2 u_i}{dt^2} - \sum_1^4 \tau \cdot n \cdot S = 0 \dots\dots\dots (25)$$

$$\Rightarrow \rho V_i \frac{d^2 u_i}{dt^2} - \sum_{j=1}^4 (\tau_{xx-j} \cdot S_{j-x} + \tau_{xy-j} \cdot S_{j-y} + \tau_{xz-j} \cdot S_{j-z}) = 0 \dots\dots\dots (26)$$

Where, τ_{xx-j} is the normal stress component along x-direction on face-j, τ_{xy-j} is the shear stress component along y-direction on face-j, τ_{xz-j} is the shear stress component along z-direction on face-j and S_{x-j} , S_{y-j} , S_{z-j} are the projected face area of the face-j along x, y, z-directions respectively.

The above equation can be written as,

$$\rho V_i \frac{d^2 u_i}{dt^2} - \sum_{j=1}^4 \left\{ \left[2\mu \left(\frac{\partial u}{\partial x} \right)_j - \beta(T_j - T_{ref}) \right] S_{j-x} + \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)_j \right] S_{j-y} + \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)_j \right] S_{j-z} \right\} = 0 \dots\dots\dots (27)$$

Similarly we can write for “v” as,

$$\rho V_i \frac{d^2 v_i}{dt^2} - \sum_{j=1}^4 \left\{ \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)_j \right] S_{j-x} + \left[2\mu \left(\frac{\partial v}{\partial y} \right)_j - \beta(T_j - T_{ref}) \right] S_{j-y} + \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)_j \right] S_{j-z} \right\} = 0 \dots\dots\dots (28)$$

Similarly we can write for “w” as,

$$\rho V_i \frac{d^2 w_i}{dt^2} - \sum_{j=1}^4 \left\{ \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)_j \right] S_{j-x} + \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)_j \right] S_{j-y} + \left[2\mu \left(\frac{\partial w}{\partial z} \right)_j - \beta(T_j - T_{ref}) \right] S_{j-z} \right\} = 0 \dots\dots\dots (29)$$

For the evaluation of “u “equation (27) can written as follows,

$$\Rightarrow \rho V_i \frac{d^2 u_i}{dt^2} + F_i \dots\dots\dots (30)$$

The above equation can be solved implicitly. For Implicit scheme “F” is evaluated for u_i^{n+1} i.e. for the value at the next time step (t+Δt),

$$\Rightarrow \rho V_i \left(\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} \right) + F_i^{n+1} = 0 \dots\dots\dots (31)$$

$$\Rightarrow \rho V_i \frac{u_i^{n+1}}{\Delta t^2} + F_i^{n+1} + \rho V_i \left(\frac{-2u_i^n + u_i^{n-1}}{\Delta t^2} \right) = 0 \dots\dots\dots (32)$$

In the similar way we can evaluate v and w as follows,

$$\Rightarrow \rho V_i \frac{v_i^{n+1}}{\Delta t^2} + F_i^{n+1} + \rho V_i \left(\frac{-2v_i^n + v_i^{n-1}}{\Delta t^2} \right) = 0 \dots\dots\dots (33)$$

$$\Rightarrow \rho V_i \frac{w_i^{n+1}}{\Delta t^2} + F_i^{n+1} + \rho V_i \left(\frac{-2w_i^n + w_i^{n-1}}{\Delta t^2} \right) = 0 \dots\dots\dots (34)$$

The computation of fluxes over the four faces requires the evaluation of u, v and w its derivatives in x, y and z directions. The primitive variables are averaged between the elemental values on either side of the face and the derivative evaluation is explained in section 3. Once the computation of the fluxes over all the faces are completed, the above equation reduces to a form AX-B=0 and is solved using Bi-CGStab method to get u, v and w.

3) Evaluation of derivatives

To calculate the flux terms, the first order derivatives like $\frac{\partial \Phi}{\partial x}$, $\frac{\partial \Phi}{\partial y}$, $\frac{\partial \Phi}{\partial z}$ that appear in the implicit formulation are to be evaluated at faces of the tetra element. The derivatives are calculated at face using Taylor series based least square method. Let “Φ “be the variable (u, v, w or T) and from the Taylor series we can write Φ as,

$$\Phi(x, y, z) \cong \Phi_f + (x - x_f) \frac{\partial \Phi}{\partial x} + (y - y_f) \frac{\partial \Phi}{\partial y} + (z - z_f) \frac{\partial \Phi}{\partial z} + (\text{Higher order terms}) \dots\dots\dots(35)$$

Higher order terms are neglected since the value is small. If the values of the function are known at a points or neighbours (i = 1 to n, n = total number of neighbours and the subscript “ f “ represents the face center value), we can approximate the derivatives of the function at the reference node (face centered value) by solving a system of linear equations. For such an approximation we select the points i = 1 to n, we are in the immediate neighbourhood of the reference point. The above equation can be written in the form,

$$\Phi(x, y, z) \cong \Phi_f + (x - x_f).a + (y - y_f).b + (z - z_f).c$$

Where, $a = \frac{\partial \Phi}{\partial x}$, $b = \frac{\partial \Phi}{\partial y}$, $c = \frac{\partial \Phi}{\partial z}$

$$(\Phi - \Phi_f) - (x - x_f).a - (y - y_f).b - (z - z_f).c = 0 \dots\dots\dots (36)$$

The above equation is of the form,

$$\Phi(x, y, z) = ax + by + cz$$

The derivative evaluation for each face is to be unique as the face is shared by two elements on either side having two cell-centre values of the variable which is insufficient to compute the derivatives. One option is to reconstruct the three

nodal values of the variables from the neighbouring cell centre values and then use them along with the two cell centre values to get the derivatives. This is quite time and memory consuming process. Hence an efficient and unique derivative evaluation directly from the cell centre values is developed. As the face is shared by two elements, we have the cell centre values of all the four neighbours of each element (see Fig.2). As we have now three unknowns (a, b and c) and eight equations, a least square based methodology is used to determine the derivatives.

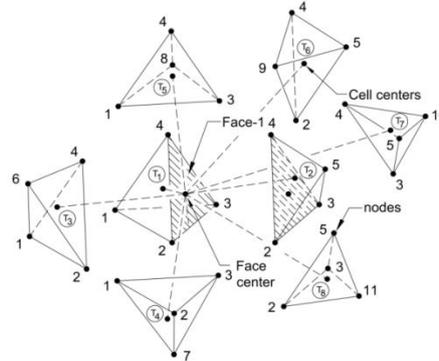


Fig.2. Cell center values used for the evaluation of the gradient through faces

The Least square method of evaluating gradients is as follows,

$$R = \sum_{i=1}^8 [(\Phi_i - \Phi_f) - (x_i - x_f).a - (y_i - y_f).b - (z_i - z_f).c] \dots \dots \dots (37)$$

To evaluate a, b and c, we need to differentiate R^2 w.r.t a, b, c and equate to zero i.e. $\frac{\partial R^2}{\partial a} = 0, \frac{\partial R^2}{\partial b} = 0, \frac{\partial R^2}{\partial c} = 0$

Differentiating w.r.t “ a “ we get, $\frac{\partial R^2}{\partial a} = 2R \frac{\partial R}{\partial a} = 0 \Rightarrow R \frac{\partial R}{\partial a} = 0$

$$\begin{aligned} & \left[\sum_{i=1}^8 [(\Phi_i - \Phi_f) - (x_i - x_f).a - (y_i - y_f).b - (z_i - z_f).c] \right] \times \sum_{i=1}^8 (x_i - x_f) = 0 \\ \Rightarrow & \sum_{i=1}^8 (x_i - x_f).(x_i - x_f).a + \sum_{i=1}^8 (y_i - y_f).(x_i - x_f).b + \sum_{i=1}^8 (z_i - z_f).(x_i - x_f).c = \sum_{i=1}^8 (\Phi_i - \Phi_f).(x_i - x_f) \end{aligned}$$

Similarly differentiating w.r.t “ b “ we get

$$R \frac{\partial R}{\partial b} \Rightarrow \sum_{i=1}^8 (x_i - x_f).(y_i - y_f).a + \sum_{i=1}^8 (y_i - y_f).(y_i - y_f).b + \sum_{i=1}^8 (z_i - z_f).(y_i - y_f).c = \sum_{i=1}^8 (\Phi_i - \Phi_f).(y_i - y_f)$$

Similarly differentiating w.r.t “ c “ we get

$$R \frac{\partial R}{\partial c} \Rightarrow \sum_{i=1}^8 (x_i - x_f).(z_i - z_f).a + \sum_{i=1}^8 (y_i - y_f).(z_i - z_f).b + \sum_{i=1}^8 (z_i - z_f).(z_i - z_f).c = \sum_{i=1}^8 (\Phi_i - \Phi_f).(z_i - z_f)$$

The above set of equations can be written in matrix form as follows

$$\begin{bmatrix} \sum_{i=1}^8 (x_i - x_f).(x_i - x_f) & \sum_{i=1}^8 (y_i - y_f).(x_i - x_f) & \sum_{i=1}^8 (z_i - z_f).(x_i - x_f) \\ \sum_{i=1}^8 (y_i - y_f).(x_i - x_f) & \sum_{i=1}^8 (y_i - y_f).(y_i - y_f) & \sum_{i=1}^8 (z_i - z_f).(y_i - y_f) \\ \sum_{i=1}^8 (z_i - z_f).(x_i - x_f) & \sum_{i=1}^8 (z_i - z_f).(y_i - y_f) & \sum_{i=1}^8 (z_i - z_f).(z_i - z_f) \end{bmatrix} \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^8 (\Phi_i - \Phi_f).(x_i - x_f) \\ \sum_{i=1}^8 (\Phi_i - \Phi_f).(y_i - y_f) \\ \sum_{i=1}^8 (\Phi_i - \Phi_f).(z_i - z_f) \end{bmatrix} \dots \dots \dots (38)$$

To improve the accuracy, the weights have been incorporated for the evaluation of derivatives. i.e. from considering the distance from eight cell center values. The above matrix can be solved for a, b, c using crammers rule. After evaluating the derivatives of T, u, v, and w on each face, the average fluxes $q_x, q_y, q_z, \tau_{xx}, \tau_{yy}, \tau_{zz}, \tau_{xy}, \tau_{xz}, \tau_{yz}$ are evaluated and summed over all the four faces for each tetrahedron to compute A and B of the system of equations which is solved using Bi-CGStab method.

III. SOLUTION OF HEAT CONDUCTION AND INTEGRATED THERMO-STRUCTURAL ANALYSIS

A. Solution of unsteady heat conduction equation

As a first step the unstructured finite volume methodology described in the previous chapters, first applied to the solution of 3-D unsteady heat conduction equation. To test the efficiency and accuracy of the code, a standard test case of a one dimensional semi-infinite solid slab is considered for the validation of the heat conduction solver for various boundary conditions. A rectangular slab (50mm×5mm×5mm) as shown in Fig.3 was considered as the computational domain.

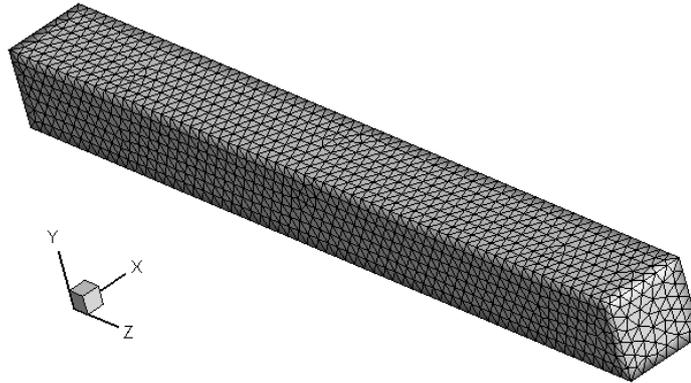


Fig.3. Semi-infinite body

The length and time were selected to ensure the semi-infinite condition. The computational domain is discretized into tetrahedron elements having 17143 elements and 3861 nodes. The aspect ratio of the tetrahedral elements was kept close to one. The Gambit software was used to generate the mesh and a FORTRAN code was written to get the unsteady temperature distribution. The grid independency test was also carried out to check the grid dependency of the solution.

1) Validation of heat flux boundary condition

For the validation of heat flux boundary condition, one end of the slab is suddenly exposed to a heat flux of quantity “q” and all the other faces are insulated. Initially the slab was at a temperature T₀. The analytical solution for a semi-infinite body with a heat flux boundary condition is given in J.P. Holman [10]. The unsteady temperature at any point in a semi-infinite solid for a heat flux boundary condition is given by,

$$T(z,t) = T_0 + \left(\frac{2q}{k}\right) \left(\sqrt{\frac{\alpha_t t}{\pi}}\right) \exp\left(\frac{-z^2}{4\alpha_t t}\right) - \left(\frac{qz}{k}\right) \left(1 - \operatorname{erf}\left(\frac{z}{2\sqrt{\alpha_t t}}\right)\right) \dots\dots(39)$$

Where,

T is the temperature at any point, T₀ is the initial temperature, q is the applied heat flux and z is the distance from the hot XY plane to a point where the temperature is measured at time “t” and α_t is the thermal diffusivity.

Following are the properties used for the validation of the heat flux boundary condition,

Density, ρ = 1000 kg/m³, Specific heat, C_p= 2000 J/kgK, Conductivity, K_x, K_y, K_z = 20 W/mK

i) Boundary condition (B.C):- q=10000 W/m² at Z=0.0 All other faces are insulated.

ii) Initial condition (I.C):- T(x, y, z, 0) =T₀= 300.0 K

With the above boundary and initial conditions, the code results are exactly matching with the analytical solutions as shown in Fig.4 (a). From this figure we can see that the temperature increases with time at any point in the slab. Since the considered computational domain is just to validate the heat conduction code, the time integration is selected in such a way that the semi-infinite condition is not violated. The contour plots for the slab after 10sec is shown in Fig.4 (b).

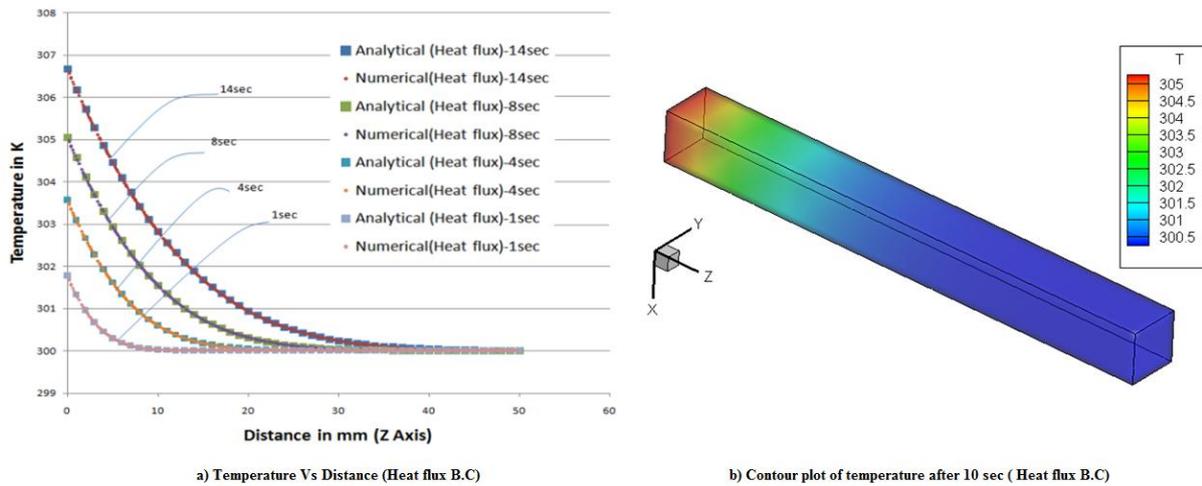


Fig.4. Temperature Vs Distance and contour plot of temperature after 10sec (Heat flux B.C)

2) Validation of convection boundary condition

For the validation of convection boundary condition, one end of the slab is suddenly exposed to convection and all the other faces are insulated. Initially the slab was at a temperature T_0 . The analytical solution for a semi-infinite body for a convection boundary condition is given in J.P. Holman [10]. The unsteady temperature at any point in a semi-infinite solid for a convective boundary condition is given by,

$$T(z,t) = T_0 + (T_\infty - T_0) \left[\left(1 - \operatorname{erf} \left(\frac{z}{2\sqrt{\alpha t}} \right) \right) - \exp \left(\frac{hz}{k} + \frac{h^2 \alpha t}{k^2} \right) \left(1 - \operatorname{erf} \left(\frac{z}{2\sqrt{\alpha t}} + \frac{h\sqrt{\alpha t}}{k} \right) \right) \right] \dots (40)$$

Where,

T_∞ is the ambient temperature and h is the heat transfer coefficient.

Following are the properties values used for the validation of the boundary condition,

Density, $\rho = 7900 \text{ kg/m}^3$, Specific heat, $C_p = 545 \text{ J/kgK}$, Conductivity, $K_x, K_y, K_z = 35 \text{ W/mK}$, Heat transfer coefficient $h_{\text{coeff}} = 1500 \text{ W/m}^2 \text{ K}$

i) Boundary condition (B.C):- $T_\infty = 2200 \text{ K}$ at $Z=0.0$, All other faces are insulated.

ii) Initial condition (I.C):- $T(x, y, z, 0) = T_0 = 300.0 \text{ K}$

With the above boundary and initial conditions, the code results are exactly matching with the analytical solutions as shown in Fig.5 (a). The contour plots for the slab after 10sec is shown in Fig.5 (b).

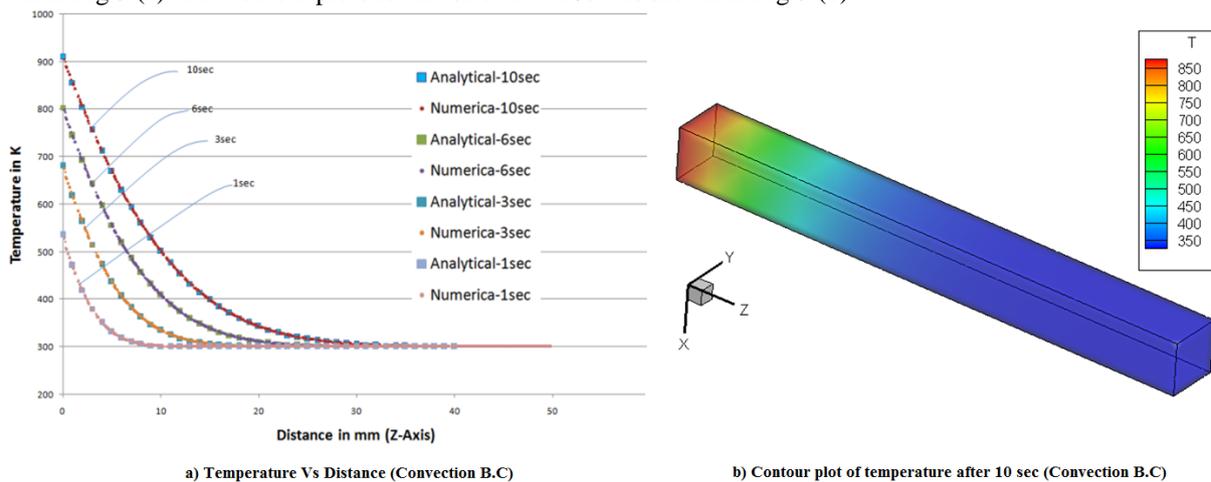


Fig.5. Temperature Vs Distance and contour plot of temperature after 10sec (Convection B.C)

3) Validation of isothermal boundary condition

For the validation of isothermal boundary condition, one end of the slab is suddenly exposed to a constant temperature and all the other faces are insulated. Initially the slab was at a temperature T_0 . The analytical solution for a semi-infinite body for an isothermal boundary condition is given in J.P. Holman [10]. The unsteady temperature at any point in a semi-infinite solid for an isothermal boundary condition is given by,

$$T(z,t) = T_s + (T_0 - T_s) \operatorname{erf} \frac{z}{2\sqrt{at}} \dots\dots(41)$$

Where,

T_s is the temperature applied at one end of the boundary.

Following are the properties values used for the validation of the boundary condition,

Density, $\rho = 1000 \text{ kg/m}^3$, Specific heat $C_p = 2000 \text{ J/kgK}$, Conductivity, $K_x, K_y, K_z = 20 \text{ W/ mK}$

i) Boundary condition (B.C):- $T_s = 500 \text{ K}$ at $Z=0.0$, All other faces are insulated.

ii) Initial condition (I.C):- $T(x, y, z, 0) = T_0 = 300.0 \text{ K}$

With the above boundary and initial conditions, the code results are exactly matching with the analytical solutions as shown in Fig.6 (a). The contour plots for the slab after 10sec is shown in Fig.6 (b).

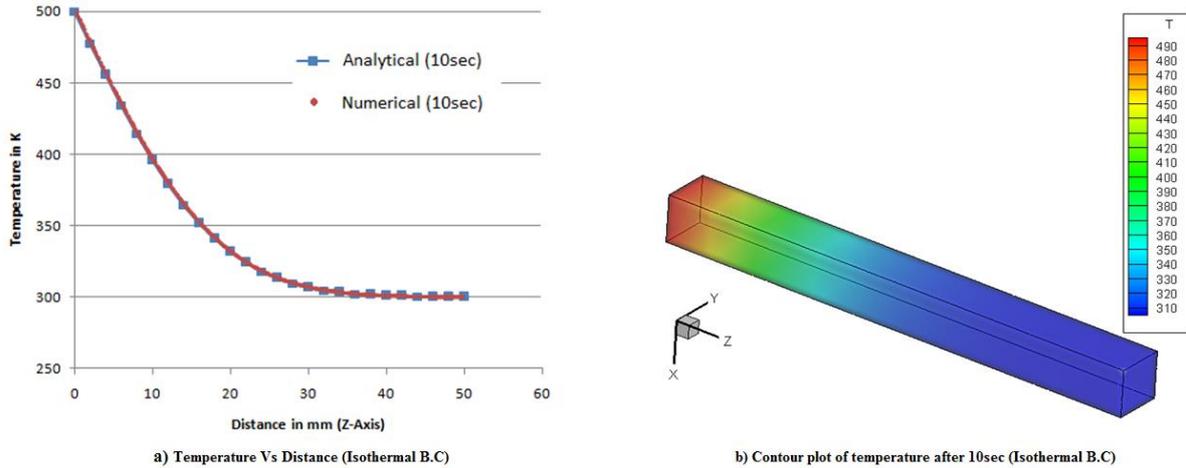


Fig.6. Temperature Vs Distance and contour plot of temperature after 10sec (Isothermal B.C)

4) Summary of heat conduction simulations

The computer code developed for 3-D unsteady heat conduction equation is validated against the analytical solutions as well as published numerical solutions for isothermal, heat flux, convective and radiation boundary conditions available for the semi infinite slab for various boundary conditions. It was found that the solution methodology is accurate, robust using Bi-CGStab solver. The code is now extended for the simultaneous solution of heat conduction equation and structural dynamics equation for an integrated thermo structural analysis.

B. Solution of integrated thermo-structural analysis

As the results of the structural deformation are not affecting the heat conduction solution, the heat conduction and thermo structural solution is solved in an uncoupled manner. From the initial condition the temperature distribution in the body is computed for the first time step by solving the unsteady heat conduction equation. Using this temperature distribution the equations for the displacements $u, v,$ and w are solved. The above process is repeated till steady state is achieved.

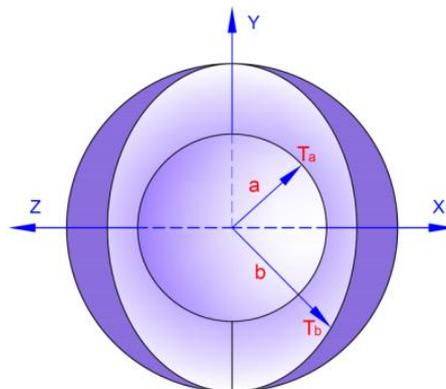


Fig.7. Spherical shell

As analytical solutions are not available for unsteady Thermo-Structural analysis, for the validation of the integrated Thermo-structural solver a hollow sphere [11] shown in Fig.7 with a steady heat flow case was considered. The temperature distributions obtained were used to determine the deformation of the hollow sphere.

Assuming (i) No body force acts on the sphere,

(ii) The temperature distribution in the sphere is,

$$T = \frac{T_b b - T_a a}{b - a} + \frac{(T_b - T_a) ab}{(b - a)R} \dots\dots(42)$$

Where,

a and b are the inner and outer radius of the hollow sphere (see Fig.7.).

T_a and T_b are the temperatures at the inner and outer surfaces.

iii) The surfaces at R = a and R = b are traction free.

The radial displacement in the hollow sphere as follows,

$$u_r = \frac{\alpha_e (T_b - T_a) a}{(1 - \sigma)(b^3 - a^3)} \left[(1 + \sigma)b(a^2 + ab + b^2) + 2(\sigma a^2 - a^2 - \sigma ab - \sigma b^2)R - (1 + \sigma)\frac{a^2 b^3}{R^3} \right] + \alpha_e T_b R \dots\dots(43)$$

Where,

σ is the Poisson's ratio and α_e is the coefficient of thermal expansion.

A hollow sphere of inner radius 50mm and outer radius 60mm is analysed using the computer code developed. The symmetry is not utilized and the problem is analysed as a 3-D Thermo Structural analysis. The inner temperature is kept as 500K and outer temperature as 300K. The properties for the analysis are, Density, ρ = 2700 kg/m³, Specific heat, C_p = 903.0 J/kgK, Conductivity, K_x, K_y, K_z = 237.0 W/ mK

Young's modulus, E = 70.0E9N/m², Poisson's ratio, σ = 0.35, Coefficient of thermal expansion, α_e = 23.1E-6 m/mK

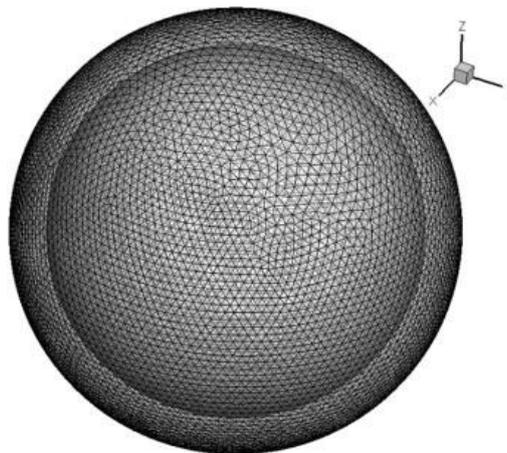


Fig.8. Computational domain of Sphere

The computational domain as shown in Fig.8 was discretized using unstructured tetrahedron elements having 111014 elements and 25333 nodes. For the validation the computer code developed, first the steady state temperature distribution was obtained and this temperature distribution was used to find the displacements. The steady state results for displacements obtained by the solver are discussed in the following sections.

1) Internally heated sphere

For an internally heated sphere, the inner surface temperature is kept as 500K and outer surface temperatures as 300K. As a first step the steady state temperature distribution obtained for the above boundary conditions. This temperature distribution was used to determine the deformation in the hollow sphere. The results obtained from code developed were accurate enough. The radial displacements is shown in Fig.9 (a) and the contour plots for u, v and w are shown in Fig.9 (b), (c), (d) respectively.

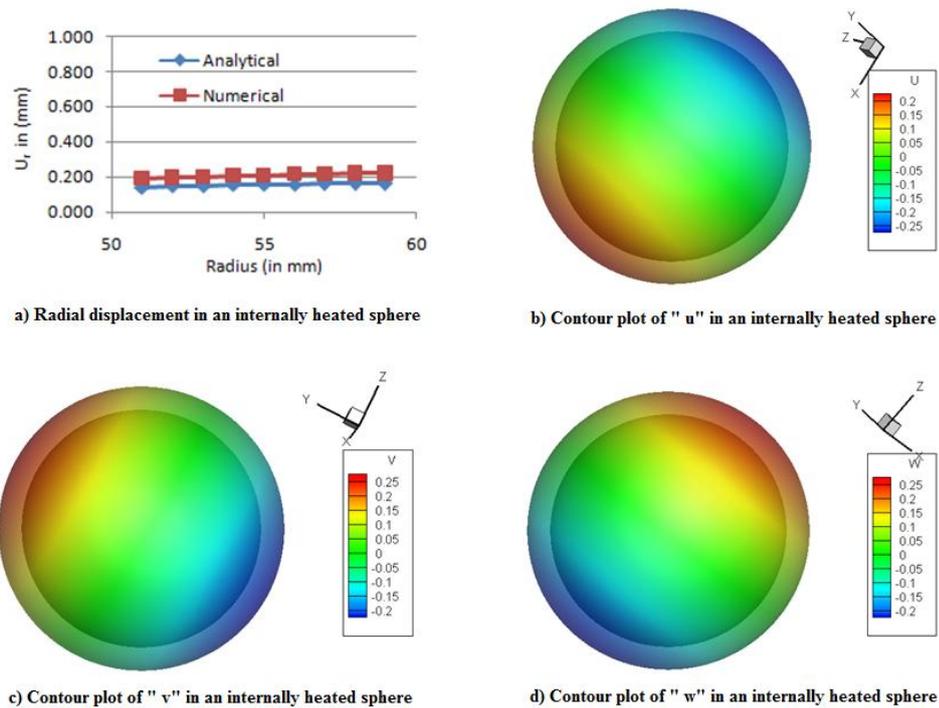


Fig.9. Radial displacement and Contour plots of u, v and w in an internally heated sphere.

2) Summary of Thermo-Structural analysis

The computer code developed for 3-D unsteady integrated thermo structural analysis is validated against analytical solutions for the case of internally heated hollow sphere. It was found that solution methodology is accurate and versatile using Bi-CGStab solver. The code is now can be extended for a coupled Fluid-Thermo-Structural analysis in future.

IV. CONCLUSION

An unstructured finite volume method is developed for 3-D unsteady integrated thermo structural analysis. An implicit time stepping method is adopted and the resulting system of algebraic equations are solved using an efficient Bi-CGStab solver. A unique least square based methodology is used for the derivative evaluation using cell-centre values avoiding time consuming nodal reconstruction. As a first step, an unstructured finite volume code for the solution of 3-D unsteady heat conduction equation is developed. The code has been validated for various Neumann and Dirichlet boundary conditions. The results are compared with the analytical solutions available for semi-infinite body heat conduction and are found to be in good agreement. Then the code is further extended for the unsteady structural dynamics equations and an integrated linear elastic Thermo-Structural analysis is carried out for the case of internally heated hollow sphere. The unstructured finite volume method in conjunction with Bi-CGStab solver results in an efficient unsteady Thermo-Structural solver.

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