Numerical solution of the 3D transient heat conduction equation

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Introduction

The transient heat conduction equation is solved numerically using the finite volume method. Central differencing is applied to the diffusion terms and time discretization is fully implicit. The resulting linear system is solved using the incomplete Cholesky factorization conjugate gradient method (ICCG).

Model equations

From an energy balance at an arbitrary location in the domain V it follows that the equation for transient heat conduction is given by:

$$\rho C_p \frac{\partial T}{\partial t} = \lambda \nabla^2 T + q \tag{1}$$

With ρ the density, C_p the heat capacity, T the temperature, λ the heat conduction coefficient and q the source term. The source term q can be a function of the domain coordinates.

The temperature f or flux g is specified at the boundaries ∂V. Both Dirichlet and Neumann boundary conditions are therefore applicable. The Dirichlet boundary conditions are:

$$T(\mathbf{x}) = f(\mathbf{x}) \qquad \forall x, y, z \in \partial V \tag{2}$$

The Neumann boundary conditions are:

$$\lambda \nabla T(\mathbf{x}) \cdot \mathbf{n} = g(\mathbf{x}) \qquad \forall x, y, z \in \partial V \tag{3}$$

With $\mathbf{x}$ the position vector and $\mathbf{n}$ the unit vector normal to the boundaries and x, y and z the coordinates.

ICCG algorithm

The ICCG algorithm computes the solution to the linear system:

$$M\mathbf{x} = \mathbf{y} \tag{4}$$

Where M is symmetric and positive definite and is the linear system obtained from discretization of the transient heat conduction equation, $\mathbf{x}$ is the temperature distribution to be computed and $\mathbf{y}$ is the set of source terms of the discretized equations.

Before the algorithm is executed, incomplete Cholesky factorization is applied to M resulting in a lower triangular matrix L with the same sparcity as M and an initial estimate $\mathbf{x}_0$ of the temperature distribution is made. Then, the initial residuals $\mathbf{r}_0 = \mathbf{y} - M\mathbf{x}_0$ and the quantity $\mathbf{p}_0 = (LL^T)^{-1}\mathbf{r}_0$ are calculated. Now, the required initial quantities have been calculated and the algorithm can be executed.

The algorithm consists of the following steps [1]:

$$\alpha_i = (\mathbf{r}_i \cdot (LL^T)^{-1}\mathbf{r}_i)/(\mathbf{p}_i \cdot M\mathbf{p}_i) \tag{5}$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{p}_i \tag{6}$$

$$\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha_i M\mathbf{p}_i \tag{7}$$

$$\beta_i = (\mathbf{r}_{i+1} \cdot (LL^T)^{-1}\mathbf{r}_{i+1})/(\mathbf{r}_i \cdot (LL^T)^{-1}\mathbf{r}_i) \tag{8}$$

$$\mathbf{p}_{i+1} = (LL^T)^{-1}\mathbf{r}_{i+1} + \beta_i \mathbf{p}_i \tag{9}$$

Steps (5) to (9) are repeated until the error $|\mathbf{r}|$ is below some threshold ϵ.

Verification

To verify the algorithm is working properly some cases are considered for which analytical solutions can be obtained. These are then compared with the results obtained from simulation.

Steady state solution

For long exposure times the system achieves thermal equilibrium. An example of such a case, for which an analytical solution can be obtained is:

$$\nabla^2 T - \sin(\pi x)\sin(\pi y)\sin(\pi z) = 0 \tag{10}$$

The corresponding analytical solution to the equation above is:

$$T = -\frac{\sin(\pi x)\sin(\pi y)\sin(\pi z)}{3\pi^2} \tag{11}$$

With boundary conditions:

$$T = 0 \qquad \forall x, y, z \in \partial V \tag{12}$$

Comparison of numerical results, obtained with a grid resolution of 20 nodes along each axis and grid coordinates x, y and z ranging from 0 to 1, with the analytical solution shows that the difference between numerical and analytical solutions is 0.21 %.

Short exposure times

For short exposure times, such that the temperature at the center of the material does not change appreciably (i.e.: for small Fourier numbers $Fo = \alpha t/d^2 < 0.1$), penetration theory can be applied to determine the flux g at the boundary:

$$g = \lambda \frac{T_1 - T_0}{\sqrt{\pi \alpha t}} \tag{13}$$

Where T_1 is the temperature at the boundaries, T_0 is the initial temperature, α the thermal diffusivity and t time. Setting the boundary temperature T_1 to

1, the initial temperature T_0 to 0, the heat conduction coefficient to 1 and the thermal diffusivity to 1 gives the following relation for the flux:

$$g = \frac{1}{\sqrt{\pi t}} \tag{14}$$

Equation (14) is compared with the flux computed numerically using a system with a grid resolution of 40 nodes along each axis and grid coordinates x, y and z ranging from 0 to 1. Results are shown in table 1.

Table 1: Numerical and analytical flux data.

t	Flux analytical	Flux numerical	error %
0.0025	11.28	11.52	2.1
0.005	7.98	8.07	1.2
0.0075	6.51	6.57	0.9
0.01	5.64	5.67	0.6
0.0125	5.05	5.04	0.03
0.015	4.61	4.56	1.1
0.02	3.99	3.81	4.5

Moderate exposure times

For moderate exposure times, such that $Fo = \alpha t/d^2 > 0.1$, the temperature distributions $M = (T_1 - T_c)/(T_1 - T_0)$ obtained from simulations are compared with data tabulated in [2], where T_1 is the temperature of the boundary, T_c the temperature at the center and T_0 is the initial temperature distribution. Results are given in table 2.

Table 2: Temperature distribution data.

Fo	M tabulated	M simulation
0.05	0.53	0.46
0.1	0.11	0.11
0.15	0.025	0.026
0.2	0.056	0.060
0.25	0.0012	0.0014

References

[1] David S. Kershaw. The incomplete Cholesky-conjugate gradient method for the iterative solution of systems of linear equations. *J. Comp. Phys.* 26, 43-65, 1978.

[2] L.P.B.M Janssen and M.M.C.G Warmoeskerken. Transport phenomena data companion. 2006.