Numerical solution of the 3D Poisson equation

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Introduction

The Poisson equation is solved numerically using the finite volume method. Central differencing is applied to the diffusion terms. The resulting linear system is solved using the incomplete Cholesky factorization conjugate gradient method (ICCG).

Model equations

The Poisson equation is given by:

$$\lambda \nabla^2 T + q = 0 \tag{1}$$

With T the dependent variable, λ a constant and q a function depending on the coordinates x, y and z of the domain V. Both Dirichlet and Neumann boundary conditions are applicable. The Dirichlet boundary conditions are:

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

Where f is some function which specifies the value of T at the boundary ∂V. The Neumann boundary conditions are:

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

Where g is some function which specifies the value of the derivative of T with respect to some spatial coordinate at the boundary, $\mathbf{x}$ is the position vector and $\mathbf{n}$ the unit vector normal to the boundary.

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 equation (1), $\mathbf{x}$ is the distribution of T 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 T 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 a case is considered for which an analytical solution can be obtained. The analytical solution is then compared with the solution obtained numerically. The following form of the Poisson equation can be solved analytically:

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

With boundary conditions:

$$T = 0 \qquad \forall x, y, z \in \partial V \tag{11}$$

The corresponding analytical solution to equation (10) above is:

$$T = -\frac{\sin(\pi x)\sin(\pi y)\sin(\pi z)}{3\pi^2} \tag{12}$$

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 %.

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.