Computer Code Abstract

SNCONV

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1. Program Identification: SNCONV is a flexible neutron transport computer code useful for studying the convergence properties of discrete ordinates methods for different space and angle discretizations, and selecting an optimum discretization procedure.

2. Function: The SNCONV computer code permits the study of the convergence properties for combined spatial and angular discretizations[1] of the discrete ordinates method used to solve the linear transport equation for anisotropically scattering, subcritical slab media. Unified estimates analysis can be obtained for general classes of finite difference methods, such as characteristic methods and balance equation methods. The code provides the information on the role played by various spatial moments of the approximate fluxes in determining global discretization errors and superconvergence at certain points in the mesh cells. However, an extremely tight convergence criterion must be used to obtain the asymptotic convergence rates. More importantly, the code can be used to select an optimum discretization procedure with little computational time. This is achieved by running the code for a given transport problem on a few very coarse meshes for a small number of iterations with various spatial discretizations. The output will provide error norms and ratio of overall error norms for these discretizations. The user will simply compute the arithmetic operation counts and time estimates (which are machine dependent) for each method per calculational step and then select the most economic discretization procedure, based on a comparative study with the output from the code.

3. Method of Solution: The standard method of source iteration is employed, which involves iterations through the space-angle mesh in directions of neutron motion. The appropriate recursion formulas affecting one iteration for a typical scheme[2] in the usual notations are the following:

$$\begin{aligned}\psi_i[x_{j+(\nu/2)}] &= f_{i,j}\psi_i[x_{j-(\nu/2)}] + (1-f_{i,j})[M_0S]_{i,j} \\ &\quad + 2\nu(M_1S)_{i,j}[1-(\tfrac{1}{2}+d_{i,j})(1-f_{i,j})] + (M_2S)_{i,j} \\ &\quad \times\{(1-f_{i,j}) - 12d_{i,j}[1-(\tfrac{1}{2}+d_{i,j})(1-f_{i,j})]\} ,\end{aligned} \tag{1}$$

$$(M_0\psi)_{i,j} = (M_0S)_{i,j} - \nu d_{i,j}[\psi_i(x_{j+1/2}) - \psi_i(x_{j-1/2})] , \tag{2}$$

$$(M_1\psi)_{i,j} = (M_1S)_{i,j} - 3\nu d_{i,j}[\psi_i(x_{j+1/2}) + \psi_i(x_{j-1/2}) - 2(M_0\psi)_{i,j}] , \tag{3}$$

and

$$M_2(\psi)_{i,j} = (M_2S)_{i,j} - 5\nu d_{i,j}[\psi_i(x_{j+1/2}) - \psi_i(x_{j-1/2}) - 2(M_1\psi)_{i,j}] , \tag{4}$$

where

$$f_{i,j} = \exp(-|\epsilon_{ji}|) ,$$
$$d_{i,j} = |\epsilon_{ji}|^{-1} ,$$

and

$$\epsilon_{ji} = \sigma_j h_j/\mu_i .$$

Here, h_j is the width of a spatial cell $c_j = [x_{j-1/2}, x_{j+1/2}]$; the terms $\psi_i(x_{j+1/2})$ and $\psi_i(x_{j-1/2})$ are right-edge and left-edge fluxes, respectively, for the direction μ_i, and S is the total source. The moments M_ℓ are defined as $(M_\ell f)_i(x) = \langle p_{\ell,j}, f_i\rangle p_{\ell,j}(x)$, where

$$\langle p_{\ell,j}, f_i\rangle = \left(\frac{2l+1}{h_j}\right)\int_{c_j} p_{\ell,j}(x) f_i(x)\,dx .$$

Here,

$$p_{\ell,j}(x) = p_\ell\left[\frac{2(x-x_j)}{h_j}\right] ,$$

where p_ℓ is the ℓ'th Legendre polynomial. The parameter $\nu = \pm 1$ in Eqs. (1) through (4) is used for a sweep to right or left, respectively, depending on neutron direction.

The code provides information on both angular and

scalar fluxes for various approximate methods and calculates the error norms for the following: the angular flux defined at the cell edges for each discrete angle, the scalar flux at the cell edges and average scalar flux defined in a spatial cell. The typical error norm for the cell-edge scalar flux is given by

$$\|\Phi\| = \max_j |\Phi_{j+1/2} - \Phi^{exact}_{j+1/2}| \ .$$

When exact solution of the problem is not available, the "exact" answer for the comparison purpose is obtained in the code by solving the test problem on a relatively fine mesh with a high-order method.

4. Related Material: No additional programs are required. A suitable acceleration method may be used with each spatial difference scheme for faster convergence of the iterations. However, this acceleration is not necessary for studies of convergence of the approximations as the space-angle mesh is refined. A small addition to the code may also allow it to compare the performance of higher moments of angular flux.

5. Restrictions: The errors in a numerical calculation consist of a sum of the discretization error and the error due to roundoff. Therefore, to accurately estimate the convergence rates for a particular method, one needs to utilize high-precision arithmetic. Also, the convergence criteria for the iterations should be set tight.

6. Computers: The code was developed on the SIEMENS 7-551 and VAX-11/780 and modified for Cray X-MP.

7. Running Time: The information on computer time is usually difficult to obtain in an interactive computing environment. For our purposes, we compare the performance of high-order methods with low-order methods from an arithmetic operational count of computing the edge fluxes, the flux moments, and the appropriate source moments over a spatial cell for each direction and each iteration. For example, the time estimate of the quadratic characteristic method is ~1.5 times that of the linear characteristic method.[3]

8. Machine Requirement: None.

9. Programming Language: Fortran IV.

10. Operating System: VMS(VAX), CTSS/COS(CRAY).

11. Additional Programming Information: The program has ~1100 lines of coding.

12. Materials Available: The code and documentation may be obtained from the authors.

13. References:

[1]E. J. ALLEN, H. D. VICTORY, Jr., and K. GANGULY, "On the Convergence of Finite-Differenced Multigroup Discrete-Ordinates Methods for Anisotropically Scattering Slab Media," *SIAM J. Numer. Anal.*, **26**, 88 (1989).

[2]R. VAIDYANATHAN, "A Finite Moments Algorithm for Particle Transport Problems," *Nucl. Sci. Eng.*, **71**, 46 (1979).

[3]H. D. VICTORY, Jr., and K. GANGULY, "On Finite-Difference Methods for Solving Discrete-Ordinates Transport Equations," *SIAM J. Numer. Anal.*, **23**, 78 (1986).