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TITLE: **3-D RESEARCH TRANSPORT CODES AT LOS ALAMOS**

AUTHOR(S): J.E. Morel
J.M. McGhee
W.F. Walters

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Los Alamos New Mexico 87545

3-D RESEARCH TRANSPORT CODES AT LOS ALAMOS

J.E. Morel, J.M. McGhee, and W.F. Walters
Computer Research and Applications Group
Group CIC-3, Mail Stop B265
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
jim@lanl.gov, mcghee@lanl.gov, and wfw@lanl.gov

ABSTRACT

We describe 3-D research transport codes which have been developed at Los Alamos National Laboratory over the last three years. Some simple example calculations are presented.

I. INTRODUCTION

The purpose of this paper is to describe the 3-D research codes developed at Los Alamos National Laboratory over the last three years. These are research codes in the sense that they serve as testbeds for new 3-D numerical transport methods. Although they are capable of fully realistic calculations, these codes are not suitable for general distribution and are therefore limited to in-house use. There are three basic classes of codes: unstructured tetrahedral-mesh even-parity codes, rectangular-mesh even-parity codes, and rectangular-mesh first-order (as opposed to even-parity) codes. All of the codes were developed with funding for massively-parallel computing research and applications, and all of them run on the Connection Machine CM-200 and CM-5 massively-parallel computers in the Advanced Computing Laboratory at LANL. Many of the codes have both a multigroup neutron/gamma version as well as a thermal radiation (infrared and x-ray) version. In the remainder of this paper, the angular discretization methods, spatial discretization methods, and solution techniques associated with each code are discussed. Finally, some simple example calculations are presented.

II. THE NIKE EVEN-PARITY S_N and SP_N CODES

The NIKE multigroup neutron/gamma code solves either the even-parity S_n equations or the even-parity SPn equations with anisotropic scattering on unstructured tetrahedral meshes using a source iteration technique in conjunction with diffusion-synthetic acceleration of the within-group scattering source and one-group diffusion-acceleration of the fission-source. We stress that this solution technique applies to *both* the S_n and SP_n equations. This is possible because we express the SP_n equations in a non-standard "canonical" form which reduces to the even-parity S_n equations with Gauss quadrature in the 1-D case. A parallel preconditioned conjugate-gradient method is used to solve the source-iteration equations. Thus there are three iteration levels: the conjugate-gradient iterations are on the first (innermost) level,

followed by the within-group source iterations on the second level, followed by the fission source iterations on the third (outermost) level. Since the acceleration equations themselves are diffusion equations, they are also solved with the conjugate-gradient technique. A linear-continuous finite-element discretization is used for the spatial variables. Options exist for time-dependent, alpha-eigenvalue, k-eigenvalue, and steady-state source calculations. The algorithm is optimized for time-dependent calculations. The S_n solution and acceleration techniques used in these codes are described in References 1 and 2. The SP_n solution and acceleration techniques used in these codes are described in Reference 3. Both a rectangular-mesh neutron/gamma version and an unstructured tetrahedral-mesh thermal radiative transfer version of the NIKE code exist.

II. THE NIKE/DANTE EVEN-PARITY P_N CODE

The NIKE/DANTE code solves the multigroup even-parity P_n equations with anisotropic scattering for infrared radiative transfer on unstructured tetrahedral meshes. A linear-continuous finite-element discretization technique is used for the spatial variables. The moment equations for each group are solved simultaneously using a parallel preconditioned conjugate-gradient technique. One of its most important characteristics is that it does not require the huge amount of memory usually required to store the coefficient matrix. The matrix-vector multiply associated with each conjugate-gradient iteration is performed in "blocks" and each matrix block is generated as it is needed and then discarded once it has been used. On a serial or vector machine, this might be a prohibitively expensive strategy in terms of excessive CPU times, but preliminary result indicate that it works quite well on the CM-200 and CM-5 computers. NIKE/DANTE uses rigorous Marshak boundary conditions rather than the extrapolation distances used in some other P_n codes.[4] This causes difficulties at the boundaries because all of the moments become coupled on the boundary whereas the coupling is sparse at interior points. Furthermore, the angular integrals which must be performed to generate the boundary matrix elements cannot be evaluated analytically on the arbitrarily-oriented face of a tetrahedron. This difficulty is dealt with by decomposing the total matrix into the sum of an interior matrix and a boundary matrix, and exactly evaluating the boundary matrix integrals using half-range Gauss-Chebychev quadrature formulae. The boundary integrals are evaluated only once and then stored in memory. The memory requirement associated with these boundary integrals is the dominant requirement in high-order calculations. NIKE/DANTE is our latest research code. It is still undergoing extensive testing and characterization, but appears quite promising.

III. THE THOR NODAL S_N CODE

The THOR code solves the multigroup neutron/gamma S_N equations with anisotropic scattering on rectangular meshes. A nodal method based upon a linear representation within each cell and a constant represention on each face is used for spatial discretization. Diffusion-synthetic acceleration is applied to the inner iterations. The acceleration equations are solved using either a preconditioned bi-conjugate-gradient-squared algorithm or a generalized minimum residual algorithm. The sweep eauations are solved using a parallel block-Jacobi iteration that is par-

ticularly effective for eigenvalue calculations. There are theoretical reasons to believe that this iteration scheme will also be very effective for time-dependent calculations, but only eigenvalue calculations can currently be performed with THOR. The block-Jacobi iteration represents a useful alternative to the parallel sweeping technique of Koch, Baker, and Alcouffe.[5]

IV. COMPUTATIONAL EXAMPLES

In this section we give two computational examples generated with our unstructured-mesh NIKE code. We first consider a computational comparison of the multigroup SP_1, SP_3, and S_4 methods with anisotropic scattering for calculating the k-eigenvalue of a small supercritical sphere of uranium. The uranium has a density of 37.4 g/cm^3 and is composed the isotopes U^{234}, U^{235}, and U^{238} with atomic fractions of 0.001054, 0.93737, and 0.05209, respectively. The sphere has a radius of 6.9355 *cm*. All calculations were performed with the NIKE code. The sphere was modeled with 2587 nodes and 13,120 tetrahedra. All of the calculations were performed on the massively-parallel Connection Machine-200 computer at LANL using a 12-group P_1 set of MENDF-5 cross-sections[6].

The computational results are given in Table 1. It can be seen that the SP_3 eigenvalue differs from the S_4 eigenvalue by about one percent whereas the SP_1 eigenvalue differs from the S_4 eigenvalue by about five percent. Comparing CPU times we find that the SP_3 method is about four times faster than the S_4 method. Although the SP_1 method appears less than twice as fast as the SP_3 method, the particular solution algorithm used in NIKE is not optimal for the SP_1 method and runs about twice as long as an optimal algorithm would. Thus an optimal SP_1 method would be about three times faster than the SP_3 method. Overall, our SP_n method behaves as expected. For the problem considered, the SP_3 method is much more accurate than diffusion (SP_1,) but much less costly than the S_4 method.

Table 1. Eigenvalue Comparison

Method	keff	CPU Time (s)
SP_1	1.328	211
SP_3	1.408	300
S_4	1.390	1351

We next consider a computational comparison of the multigroup SP_1, SP_3, and S_4 methods with anisotropic scattering for calculating the dynamic behavior of the same critical sphere of uranium modeled in the previous set of calculations. The cross-sections,the spatial grid, and the computer used in the dynamic calculations are identical to those used in the first set of calculations. The fluxes in the sphere were initialized to a spatially-constant isotropic value of unity for each group at every point in the sphere. The system was then advanced in time for 27 steps of one nanosecond each. The dynamic alpha-eigenvalue of the sphere was estimated using

the following expression:

$$\alpha_n \approx \frac{1}{\Delta t} ln(\mathcal{N}^n / \mathcal{N}^{n-1}) \quad , \tag{1}$$

where α_n is the dynamic alpha-eigenvalue at time step n, Δt is the time step, and $\mathcal{N}^n$ is the total number of neutrons in the system at step n. The dynamic alpha-eigenvalue is plotted as a function of time for the SP_1, SP_3, and S_4 methods in Fig.1, and the total CPU times for each calculation are given in Table 2. The results show the same trends as those associated with the previous k-eigenvalue calculations. The relative CPU times and the relative accuracy of the three method remain essentially the same. As expected, the basic result is that the SP_3 method is much more accurate than diffusion (SP_1,) but much less costly than the S_4 method.

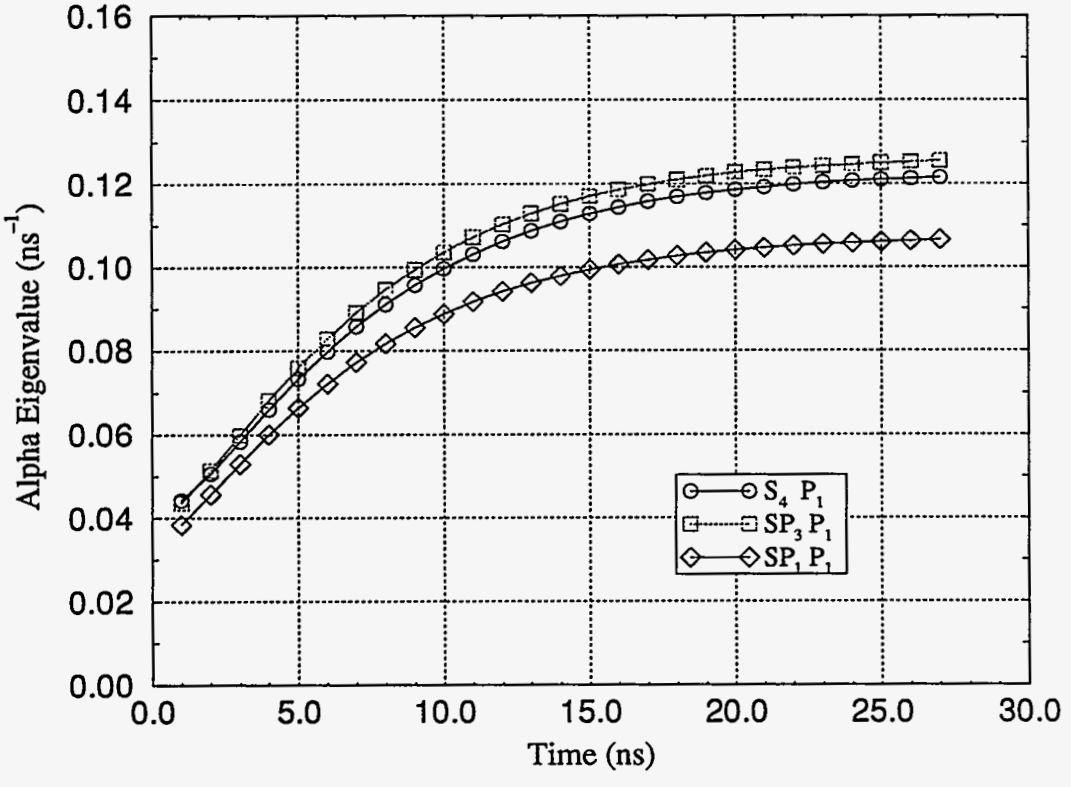

Figure 1: Comparison of Alpha Eigenvalues

Table 2. CPU Times for Alpha Eigenvalue Calculations

Method	CPU Time (s)
SP_1	394
SP_3	502
S_4	2306

Thus it is very convenient to have both an S_n and an SP_n option in the same code. The SP_n technique is very economical and sufficiently accurate for many applications, but the S_n method is available when necessary.

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