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RADIATION TRANSPORT
July 1, 1987 – September 30, 1987

by

R. D. O'Dell and Ann Nagy

ABSTRACT

Research and development progress in radiation transport for the Los Alamos National Laboratory's Group X-6 for the fourth quarter of FY 87 is reported. Included are unclassified tasks in the areas of Deterministic Radiation Transport, Monte Carlo Radiation Transport, and Cross Sections and Physics.

I. INTRODUCTION

Research, development, and design analyses performed by Group X-6, Radiation Transport, of the Applied Theoretical Physics Division during the fourth quarter of FY 87 are described in this progress report. Included is the unclassified portion of programs in the Group funded by the U.S. Department of Energy. Our classified work is reported elsewhere. Some of the reported work was performed in direct support of other Laboratory groups and contractors.

This report is divided into three sections: Deterministic Radiation Transport, Monte Carlo Radiation Transport, and Cross Sections and Physics. Authors of individual task reports are listed in parentheses after each task title. Authors not in Group X-6 also have their affiliation noted. Readers are encouraged to contact these cognizant personnel directly for additional information or further published results.

Technical program management for Group X-6 during this reporting period was provided by R. Arthur Forster, Group Leader, and by Associate Group Leaders John S. Hendricks, R. Douglas O'Dell, and Billy D. Meixner.

II. DETERMINISTIC RADIATION TRANSPORT

The deterministic radiation transport effort in Group X-6 is involved in the development and assessment of both numerical and analytical methods and models for deterministic radiation transport; in the development and testing of new and improved deterministic transport codes; in the maintenance, improvement, and support of existing computer codes; and in the application of our codes to nuclear analyses.

A. ONEDANT/TWODANT Code Support (F. W. Brinkley, Jr., and R. D. O'Dell)

During this quarter, much of the work on our multigroup, time independent discrete ordinates codes ONEDANT¹ and TWODANT² was devoted to bug fixes, code export-related work, and user assistance.

A most distressing systems bug was discovered when we found that the arctangent (ATAN) function as supplied by Cray Research, Inc. (CRI), was producing bad results on our Cray-1 class computers when operating in the vector mode. Upon further investigation, we found that this problem had existed at least since February 1987. With assistance and support from R. Boland and R. Frank of Group C-10, we traced the bug to the ATAN function and apprised CRI of the problem. The bug is eliminated. The ATAN function is used in ONEDANT and TWODANT only in calculations involving higher order scatter, and we contacted several users who we knew were running such problems. Fortunately, their previously computed results were not significantly affected by the bug. Nevertheless, it is disconcerting to find that such bad systems routines can be in the Laboratory's computing system and exist undetected for months.

Several other, more minor, bugs were uncovered by users. We found that the TWODANT restart using the scalar fluxes from a previous run as input with the RTFLUX scalar flux interface file was not working properly. This option is rarely used and had not been checked for some time. With assistance from R. Alcouffe (X-6), we readily corrected the problem. W. Walters (X-6) found that rather poor neutron balance was indicated by TWODANT even though the problem was fully converged. Again, with assistance from R. Alcouffe, we located and eliminated the bug. Another minor bug was found by W. Walters in TWODANT. In search calculations, the user normally enters an input value for the parameter EV. In some cases this value may be a negative quantity. Walters found that if a negative value of EV was provided in the input for a nonsearch calculation, namely a k_{eff} calculation, TWODANT would abort with a fatal error of negative fission source. We modified the code to check input value of EV on nonsearch problems and to set the value to zero if it is input as a negative value. Another minor bug in TWODANT was uncovered by Capt. B. Hall and Lt. J. Warsa of the Air Force Weapons Laboratory (AFWL). In attempting to run an inhomogeneous source problem with the source distribution supplied by the SOURCE and SOURCF input arrays, TWODANT was failing. Upon investigation we found and eliminated an indexing problem in the code for the SOURCE/SOURCF combination of input.

In code export-related matters, we prepared and sent a requested IBM-compatible version of ONEDANT/TWODANT to the French center for nuclear studies in Cadarache in response to their request. Assistance was also provided to EG&G, Idaho, in making ONEDANT/TWODANT operational on its Cray X MP/24 computer, which operates under the UNICOS operating system. EG&G had acquired our code package from the Radiation Shielding Information Center (RSIC) in Cray Operating System (COS) form and was encountering problems getting the COS version to run on UNICOS. We discovered that one of the problems was that the COS subroutine MEMORY was not available on their system. MEMORY is used to dynamically adjust memory under COS. By simply fixing the size of the main container array and bypassing memory bounds checking, the EG&G users were able to circumvent this problem. As for a longer-term solution, we should be able to use the same approach that we took in getting our code package to operate on the National Magnetic Fusion Energy Computing Center (NFMECC) at Livermore, which uses the FORTLIB library. UNICOS has a systems routine HPALLOC, which returns a pointer, that could be used much the same as we use it at the NMFECC. We also discovered that SEGLDR, the UNICOS/COS linker at EG&G, Idaho, will not accept our COS input. We gave them instructions that should enable them to correct the problem.

Assistance is also being provided to AFWL personnel in Albuquerque in making our codes operational on their Cray-2 computer. Since we do not have a Cray-2 at Los Alamos, we are having to feel our way through this procedure. We found that AFWL does not intend to allow dynamic memory adjustment, so a fixed container array size will be necessary. We also found that the Cray-2 at AFWL does not have a routine to turn off the divide fault indicator. This lack will cause problems in the TWODANT routine MASWEP. We have provided AFWL with coding changes using IF, THEN, ELSE statements to get around this problem. We will continue to work with them as needed.

As reported in the next section of this report, ONEDANT and TWODANT have been made operational on the Sun Scientific Workstation.

User assistance was provided to numerous users, including B. Wienke (X-4), R. Perkins (San Diego Supercomputer Center), Capt. B. Hall (AFWL), J. Morel (X-6), J. Sapir (N-12).

B. ONEDANT/TWODANT for the Sun SWS (F. W. Brinkley, Jr., and R. D. O'Dell)

With the acquisition of Sun Scientific workstations at Los Alamos and, especially in Group X-6, the desirability of making ONEDANT and TWODANT operational on the Suns has been increasing. During this quarter, we implemented both codes on the Sun.

We began with the VAX version of the code package and began placing sections of the code on the Sun. With the standard Sun F77 compiler that we were using, the machine got hung on a ONEDANT routine named INPUTY. Since F77 compiler is a UNIX product, it must be given the maximum number of EQUIVALENCES, STATEMENT labels, STATEMENTS, and the like—a very cumbersome

requirement. When the EQUIVALENCES were removed from INPUTY, the routine compiled but, of course, was useless. Although the Sun manual suggested several lengthy and uncertain things for the user to try to correct this failure of the compiler, we chose not to try them, and we set the project aside. We subsequently obtained a version of the VMS Sun F77 compiler, which was installed into our system by B. A. Clark (X-6). This compiler worked and soon both ONEDANT and TWODANT were executing problems by remotely logging into a Sun 3.

C. New Cross-Section Library Features for ONEDANT/TWODANT (F. W. Brinkley, Jr., and R. D. O'Dell)

In the preceding section of this report, we described our implementation of the ONEDANT/TWODANT codes on the Sun Scientific Workstation at Los Alamos. It should be noted that the problems that we executed on the Sun were simple ones, which contained their multigroup cross sections within the input file. Most realistic problems obtain their cross sections from separate, usually large, cross-section files. Since the great majority of cross-section files are binary, they are not amenable to transfer to the Suns. Therefore, we considered ways in which we could easily and efficiently get cross-section files onto the Sun system. We quickly decided that to try to ship the raw, isotopic multigroup libraries over would require a prohibitive amount of work for the user and would require, potentially, an enormous amount of storage. Since our ONEDANT/TWODANT packages accept cross-section libraries in a variety of forms but always process these forms into a mixed material multigroup binary file, called MACRXS, of specified format,¹ we focused our attention on that file. The file normally contains mixed material macroscopic cross sections, so it is usually much smaller than the basic isotopic cross-section library and thus imposes less burden on SWS storage. The MACRXS file produced by ONEDANT/TWODANT, however, is a binary file and is thus not amenable to transferring from, say, a Cray to the Sun. We thus chose to provide the codes with a capability to write a BCD (ASCII) version of MACRXS upon user request. This BCD form of MACRXS is named MACBCD. To have the code write and save this MACBCD file, we added an input parameter WRITMXS into Block III of the ONEDANT/TWODANT input, which when the user enters

WRITMXS=MACBCD

causes the code to prepare and save a BCD version of MACRXS. The resultant MACBCD is readily exported to any type of computing environment since it is an ASCII file. We, of course, then had to enable ONEDANT/TWODANT to read and use such a file. This was done and is invoked by specifying

LIB=MACBCD

in the Block III input.

It is important to note that the above procedure presupposes that the user who wishes to create a MACBCD file has both ONEDANT/TWODANT and a master

cross-section library on a production-type computing system (for example, our ICN) in addition to the standalone Sun. The run with WRITMXS=MACBCD is made on the main computing system, and the resultant MACBCD file is placed onto the Sun so that all subsequent runs can be made on the Sun through the LIB=MACBCD option. This capability is now operational.

While settling on the above procedure, we also decided that two other forms of a BCD (ASCII) cross-section file that are familiar to many users could also be produced in a manner similar to that for MACBCD. These two forms were the standard Los Alamos-format files, which we refer to as the XSLIB formats. One form of the XSLIB file is the old fixed-field (6E12) format, and the other form uses the FIDO fixed-field format, which permits a compact way of entering repeated data entries. We have added to ONEDANT/TWODANT the capabilities to write and save these two forms through the user input parameter WRITMXS in Block III. They are

WRITMXS=XSLIBE

for the 6E12 fixed-field format form (E denotes the "E" in 6E12) and

WRITMXS=XSLIBF

for the FIDO fixed-field format form (F denotes "FIDO"). Both forms of the XSLIB files contain header, or title, cards before each block of cross-section data.

Writing and saving any of the BCD forms MACBCD, XSLIBE, and XSLIBF can be done independently of the format of the runs input cross-section library (as specified by the LIB= entry).

D. Acceleration of Outer Iterations in Multigroup Diffusion Problems [E. W. Larsen (University of Michigan)]

In obtaining solutions of multigroup diffusion problems, one cycles through the groups, solving the equation for each group one at a time; upon completion of such a cycle an "outer" iteration is said to be performed. One continues this iterative process by performing as many outer iterations as needed to obtain convergence. Occasionally this iteration can be very slowly convergent. The purpose of this report is to describe a method for accelerating convergence. The idea is to perform a group collapse and use a "grey," or one-group, equation to accelerate the convergence of the multigroup equation. This strategy has worked successfully for radiative transfer problems,³ and we speculate that it will also work for multigroup diffusion problems, even with full upscattering.

To begin, let us consider the multigroup diffusion problem

$$\begin{aligned}
-\frac{d}{dx}D_g\frac{d}{dx}\phi_g + \sigma_{Tg}\phi_g &= \sum_{g'=1}^G \sigma_{sg'g}\phi_{g'} \\
&+ \chi_g \sum_{g'=1}^G (\nu\sigma_f)_{g'}\phi_{g'}
\end{aligned} \tag{1}$$

$$\vdash Q_g \quad , \quad 0 < x < X \quad ,$$

$$\phi_g(0) - 2D_g(0)\phi_g(0) = 0 \quad , \tag{2}$$

$$\phi_g(X) + 2D_g(X)\phi_g(X) = 0 \quad . \tag{3}$$

These equations hold for $g = 1, \dots, G$. We have the identities:

$$\sigma_{Tg} = \sigma_{ag} + \sigma_{fg} + \sigma_{sg} = \text{total cross section} \quad , \tag{4}$$

$$\sigma_{sg} = \sum_{g'=1}^G \sigma_{sgg'} = \text{macroscopic scattering cross section} \quad , \tag{5}$$

and we define the macroscopic cross sections:

$$\sigma_{sg}^d = \sum_{g'=g}^G \sigma_{sgg'} = \text{macroscopic downscattering cross section} \quad , \tag{6}$$

$$\sigma_{sg}^u = \sum_{g'=1}^{g-1} \sigma_{sgg'} = \text{macroscopic upscattering cross section} \quad , \tag{7}$$

which will be used later.

Our purpose here is to study the convergence of the outer iteration process for solving Eqs. (1)-(3), and to devise improved iteration strategies based on the grey acceleration method, which has proved successful for radiative transfer problems.

To introduce a simpler notation for the problem (1)-(3), let us define the following vectors and matrices:

$$\underline{\phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_G \end{pmatrix}$$

$$\underline{\underline{D}} = \begin{pmatrix} D_1 & & & 0 \\ & D_2 & & \\ & & \ddots & \\ 0 & & & D_g \end{pmatrix}$$

$$\underline{\underline{\sigma}}_T = \begin{pmatrix} \sigma_{T1} & & & 0 \\ & \sigma_{T2} & & \\ & & \ddots & \\ 0 & & & \sigma_{TG} \end{pmatrix}$$

$$\underline{\underline{\sigma}}_s^d = \begin{pmatrix} \sigma_{S11} & & & 0 \\ \sigma_{S12} & \sigma_{S22} & & \\ \vdots & & \ddots & \\ \sigma_{S1G} & \dots & & \sigma_{SGG} \end{pmatrix} \text{ (downscattering)}$$

$$\underline{\underline{\sigma}}_s^u = \begin{pmatrix} 0 & \sigma_{s21} & \sigma_{s31} & \dots & \sigma_{sG1} \\ & 0 & \sigma_{s32} & \ddots & \vdots \\ & & 0 & \ddots & \\ & 0 & & 0 & \sigma_{sG,G-1} \\ & & & & 0 \end{pmatrix} \text{ (upscattering)}$$

$$\underline{\underline{\chi}} = \begin{pmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_G \end{pmatrix}$$

$$\underline{\underline{\nu\sigma}}_f = ((\nu\sigma_f)_1, (\nu\sigma_f)_2, \dots, (\nu\sigma_f)_G)$$

$$\underline{\underline{Q}} = \begin{pmatrix} Q_1 \\ Q_2 \\ \vdots \\ Q_G \end{pmatrix}.$$

Then, Eqs. (1)-(3) become

$$\begin{aligned}
-\frac{d}{dx}\underline{D} \cdot \frac{d}{dx}\underline{\phi} + \underline{\sigma}_T \cdot \underline{\phi} &= \left(\underline{\sigma}_s^d + \underline{\sigma}_s^u \right) \cdot \underline{\phi} \\
&+ \underline{\chi} \left(\underline{\nu} \underline{\sigma}_f \cdot \underline{\phi} \right) + \underline{Q} \quad ,
\end{aligned} \tag{8}$$

$$\underline{\phi}(0) - 2\underline{D}(0) \cdot \frac{d}{dx}\underline{\phi}(0) = 0 \quad , \tag{9}$$

$$\underline{\phi}(X) + 2\underline{D}(X) \cdot \frac{d}{dx}\underline{\phi}(X) = 0 \quad . \tag{10}$$

The standard outer iteration process is defined by

$$\begin{aligned}
-\frac{d}{dx}\underline{D} \cdot \frac{d}{dx}\underline{\phi}^{(\ell+1)} + \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \underline{\phi}^{(\ell+1)} \\
= \left(\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right) \cdot \underline{\phi}^{(\ell)} + \underline{Q} \quad ,
\end{aligned} \tag{11}$$

$$\underline{\phi}^{(\ell+1)}(0) - 2\underline{D}(0) \cdot \frac{d}{dx}\underline{\phi}^{(\ell+1)}(0) = 0 \quad , \tag{12}$$

$$\underline{\phi}^{(\ell+1)}(X) + 2\underline{D}(X) \cdot \frac{d}{dx}\underline{\phi}^{(\ell+1)}(X) = 0 \quad , \tag{13}$$

and if we define

$$\underline{\Phi}^{(\ell+1)} = \underline{\phi}^{(\ell+1)} - \underline{\phi}^{(\ell)} \quad ,$$

then recursive equations for $\underline{\Phi}^{(\ell)}$, obtained by subtracting Eqs. (11)-(13) for successive values of ℓ , are

$$\begin{aligned}
-\frac{d}{dx}\underline{D} \cdot \frac{d}{dx}\underline{\Phi}^{(\ell+1)} + \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \underline{\Phi}^{(\ell+1)} \\
= \left(\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right) \cdot \underline{\Phi}^{(\ell)} \quad ,
\end{aligned} \tag{14}$$

$$\underline{\Phi}^{(\ell+1)}(0) - 2\underline{D}(0) \cdot \frac{d}{dx}\underline{\Phi}^{(\ell+1)}(0) = 0 \quad , \tag{15}$$

$$\underline{\Phi}^{(\ell+1)}(X) + 2\underline{D}(X) \cdot \frac{d}{dx}\underline{\Phi}^{(\ell+1)}(X) = 0 \quad . \tag{16}$$

To study the convergence of the iteration scheme defined by Eqs. (11)-(13), it is sufficient that we determine how rapidly $\underline{\Phi}^{(\ell)} \rightarrow 0$.

To do this, let us seek eigenvalue error modes:

$$\underline{\Phi}^{(\ell)}(x) = \omega^{(\ell)} \underline{\Phi}(x) \quad ; \tag{17}$$

then, Eqs. (14)-(16) reduce to

$$\begin{aligned}
& -\frac{d}{dx}\underline{D} \cdot \frac{d}{dx}\underline{\Phi} + \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \underline{\Phi} \\
& = \frac{1}{\omega} \left(\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right) \cdot \underline{\Phi} \quad , \quad 0 < x < X \quad ,
\end{aligned} \tag{18}$$

$$\underline{\Phi}(0) - 2\underline{D}(0) \cdot \frac{d}{dx}\underline{\Phi}(0) = 0 \quad , \tag{19}$$

$$\underline{\Phi}(X) - 2\underline{D}(X) \cdot \frac{d}{dx}\underline{\Phi}(X) = 0 \quad , \tag{20}$$

and we seek the largest value of $|\omega|$. Eq. (18) can be written

$$\omega \underline{\Phi} = \left[-\frac{d}{dx}\underline{D} \frac{d}{dx} + \underline{\sigma}_T - \underline{\sigma}_s^d \right]^{-1} \cdot \left[\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\Phi} \quad , \tag{21}$$

and it is clear that the operator on the right side of this equation is positive with "nice" properties. Therefore, the largest (in magnitude) eigenvalue (call it ω_1) will be real and positive, and the corresponding eigenfunction (call it $\underline{\Phi}_1$) will have real and positive components. It is clear from Eq. (18) that if there is no upscattering, $\omega_1 = k_1$, where k_1 is the largest "k-eigenvalue." It is also clear that the original problem is subcritical iff $\omega_1 < 1$, and that this problem is critical iff $\omega_1 = 1$. We will henceforth assume that the problem is subcritical, and we will also assume that it is nearly critical. Then, $0 < \omega_1 < 1$, but $\omega \approx 1$. Hence, since ω_1 is the largest (in magnitude) eigenvalue, the outer iteration scheme (11)-(13) will converge very slowly.

We shall now describe an acceleration strategy modeled directly on the algorithm that has worked for radiative transfer calculations. We begin with an outer iteration of the form described by Eqs. (11)-(13):

$$\begin{aligned}
& -\frac{d}{dx}\underline{D} \cdot \frac{d}{dx}\underline{\phi}^{(\ell+\frac{1}{2})} + \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \underline{\phi}^{(\ell+\frac{1}{2})} \\
& = \left(\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right) \cdot \underline{\phi}^{(\ell)} + \underline{Q} \quad ,
\end{aligned} \tag{22}$$

$$\underline{\phi}^{(\ell+\frac{1}{2})}(0) - 2\underline{D}(0) \cdot \frac{d}{dx}\underline{\phi}^{(\ell+\frac{1}{2})}(0) = 0 \quad , \tag{23}$$

$$\underline{\phi}^{(\ell+\frac{1}{2})}(X) + 2\underline{D}(X) \cdot \frac{d}{dx}\underline{\phi}^{(\ell+\frac{1}{2})}(X) = 0 \quad . \tag{24}$$

Notice that the solution of these equations is $\underline{\phi}^{(\ell+\frac{1}{2})}$, not $\underline{\phi}^{(\ell+1)}$. We will now describe the extra steps needed to generate $\underline{\phi}^{(\ell+1)}$.

We define the "unit" vector, where components are all equal to one:

$$\underline{u} = (1, 1, \dots, 1) \quad , \tag{25}$$

$$\phi = \underline{u} \cdot \underline{\phi} = \sum_{g=1}^G \phi_g \quad . \quad (26)$$

We also introduce a “spectral” function:

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_G \end{pmatrix} \quad , \quad (27a)$$

satisfying

$$1 = \underline{u} \cdot \theta = \sum_{g=1}^G \theta_g \quad . \quad (27b)$$

Now, we operate on Eqs. (22)-(24) by $\underline{u} \cdot (\quad)$ and get

$$\begin{aligned} -\frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\phi}^{(\ell+\frac{1}{2})} + \underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \underline{\phi}^{(\ell+\frac{1}{2})} \\ = \left(\underline{u} \cdot \underline{\sigma}_s^u + \nu \underline{\sigma}_f \right) \cdot \underline{\phi}^{(\ell)} + \underline{u} \cdot \underline{Q} \quad , \end{aligned} \quad (28)$$

$$\phi^{(\ell+\frac{1}{2})} (0) - 2 \underline{u} \cdot \underline{D} (0) \cdot \frac{d}{dx} \underline{\phi}^{(\ell+\frac{1}{2})} (0) = 0 \quad , \quad (29)$$

$$\phi^{(\ell+\frac{1}{2})} (X) + 2 \underline{u} \cdot \underline{D} (X) \cdot \frac{d}{dx} \underline{\phi}^{(\ell+\frac{1}{2})} (X) = 0 \quad , \quad (30)$$

and then we write

$$\underline{\phi}^{(\ell+\frac{1}{2})} = \underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \quad ,$$

and Eqs. (28)-(30) become

$$\begin{aligned} -\frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \left[\underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \right] \\ + \underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \cdot \left[\underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \right] \\ = \left(\underline{u} \cdot \underline{\sigma}_s^u + \nu \underline{\sigma}_f \right) \cdot \left[\underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left(\underline{\phi}^{(\ell)} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \right] \\ + \underline{u} \cdot \underline{Q} \quad , \end{aligned}$$

$$\phi^{(\ell+\frac{1}{2})} (0) - 2 \underline{u} \cdot \underline{D} (0) \cdot \frac{d}{dx}$$

$$\left[\underline{\theta} (0) \phi^{(\ell+\frac{1}{2})} (0) + \left(\underline{\phi}^{(\ell+\frac{1}{2})} (0) - \underline{\theta} (0) \phi^{(\ell+\frac{1}{2})} (0) \right) \right] = 0 \quad ,$$

$$\phi^{(\ell+\frac{1}{2})}(X) + 2\underline{u} \cdot \underline{D}(X) \cdot \frac{d}{dx}$$

$$\left[\underline{\theta}(X) \phi^{(\ell+\frac{1}{2})}(X) + \left(\underline{\phi}^{(\ell+\frac{1}{2})}(X) - \underline{\theta}(X) \phi^{(\ell+\frac{1}{2})}(X) \right) \right] = 0 \quad ,$$

or

$$\begin{aligned} & - \frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\theta} \phi^{(\ell+\frac{1}{2})} \\ & = \left[\frac{d}{dx} \underline{u} \cdot \underline{D} \frac{d}{dx} - \underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \right] \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \\ & + \left(\underline{u} \cdot \underline{\sigma}_s^u + \underline{\nu} \underline{\sigma}_f \right) \cdot \left(\underline{\phi}^{(\ell)} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) + \underline{u} \cdot \underline{Q} \quad , \end{aligned} \quad (31)$$

$$\begin{aligned} & \phi^{(\ell+\frac{1}{2})}(0) - 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \underline{\theta}(0) \phi^{(\ell+\frac{1}{2})}(0) \\ & = 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \left[\underline{\phi}^{(\ell+\frac{1}{2})}(0) - \underline{\theta}(0) \phi^{(\ell+\frac{1}{2})}(0) \right] \quad , \end{aligned} \quad (32)$$

$$\begin{aligned} & \phi^{(\ell+\frac{1}{2})}(X) + 2\underline{u} \cdot \underline{D}(X) \cdot \frac{d}{dx} \underline{\theta}(0) \phi^{(\ell+\frac{1}{2})}(X) \\ & = - 2\underline{u} \cdot \underline{D}(X) \cdot \frac{d}{dx} \left[\underline{\phi}^{(\ell+\frac{1}{2})}(X) - \underline{\theta}(X) \phi^{(\ell+\frac{1}{2})}(X) \right] \quad . \end{aligned} \quad (33)$$

To obtain equations for $\phi^{(\ell+1)}$, we simply replace $\phi^{(\ell)}$ by $\underline{\phi}^{(\ell+\frac{1}{2})}$ [in the last line of Eq. (31)], and $\underline{\phi}^{(\ell+\frac{1}{2})}$ by $\underline{\phi}^{(\ell+1)}$ on the left sides of Eqs. (31)-(33). We get

$$\begin{aligned} & - \frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta} \phi^{(\ell+1)} + \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\theta} \phi^{(\ell+1)} \\ & = \left[\frac{d}{dx} \underline{u} \cdot \underline{D} \frac{d}{dx} - \underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right) \right] \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) \\ & + \left(\underline{u} \cdot \underline{\sigma}_s^u + \underline{\nu} \underline{\sigma}_f \right) \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) + \underline{u} \cdot \underline{Q} \quad , \end{aligned} \quad (34)$$

$$\begin{aligned} & \phi^{(\ell+1)}(0) - 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \underline{\theta}(0) \phi^{(\ell+1)}(0) \\ & = 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \left[\underline{\phi}^{(\ell+\frac{1}{2})}(0) - \underline{\theta}(0) \phi^{(\ell+\frac{1}{2})}(0) \right] \quad , \end{aligned} \quad (35)$$

$$\begin{aligned}
& \phi^{(\ell+1)}(X) + 2\underline{u} \cdot \underline{D}(X) \cdot \frac{d}{dx} \underline{\theta}(X) \phi^{(\ell+1)}(X) \\
& = -2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \left[\underline{\phi}^{(\ell+\frac{1}{2})}(X) - \underline{\theta}(X) \phi^{(\ell+\frac{1}{2})}(X) \right] .
\end{aligned} \tag{36}$$

Similarly, if we use

$$\underline{\phi}^{(\ell+\frac{1}{2})} = \underline{\theta} \phi^{(\ell+\frac{1}{2})} + \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) , \tag{37}$$

we can define

$$\underline{\phi}^{(\ell+1)} = \underline{\theta} \phi^{(\ell+1)} + \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) . \tag{38}$$

Eqs. (34)-(36) are the acceleration equations. Their “driving” terms are all of the form

$$\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} , \tag{39}$$

for which

$$\underline{u} \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\theta} \phi^{(\ell+\frac{1}{2})} \right) = 0 . \tag{40}$$

The spectral function $\underline{\theta}$, which at this point is required only to satisfy Eq. (27b), must still be selected.

A nonlinear choice is to take

$$\underline{\theta} = \underline{\theta}^{(\ell+\frac{1}{2})} = \underline{\phi}^{(\ell+\frac{1}{2})} / \phi^{(\ell+\frac{1}{2})} .$$

Then the terms (39) vanish, and we are left with

$$\underline{\theta}^{(\ell+\frac{1}{2})} = \underline{\phi}^{(\ell+\frac{1}{2})} / \phi^{(\ell+\frac{1}{2})} , \tag{41}$$

$$\begin{aligned}
& -\frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta}^{(\ell+\frac{1}{2})} \phi^{(\ell+1)} + \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \sigma_f \right] \\
& \cdot \underline{\theta}^{(\ell+\frac{1}{2})} \phi^{(\ell+1)} = \underline{u} \cdot \underline{Q} .
\end{aligned} \tag{42}$$

$$\phi^{(\ell+1)}(0) - 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \underline{\theta}^{(\ell+\frac{1}{2})}(0) \phi^{(\ell+1)}(0) = 0 , \tag{43}$$

$$\phi^{(\ell+1)}(X) + 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \underline{\theta}^{(\ell+\frac{1}{2})}(X) \phi^{(\ell+1)}(X) = 0 , \tag{44}$$

$$\underline{\phi}^{(\ell+1)} = \underline{\theta}^{(\ell+\frac{1}{2})} \phi^{(\ell+1)} . \tag{45}$$

The full acceleration method is then defined by Eqs. (22)-(24) and (41)-(45). The main idea is that if Eqs. (22)-(24) determine the spectral function $\underline{\theta} = \underline{\phi}\phi$ fairly rapidly, but the amplitude ϕ fairly slowly, then Eqs. (41)-(45) will give a much-improved value of ϕ .

A linear method would involve a choice for $\underline{\theta}$ that is independent of ϕ and is based on a Fourier analysis. To do this, we assume an infinite medium and take, in Eq. (21),

$$\underline{\Phi}(x) = \hat{\underline{\Phi}}e^{i\lambda x}$$

to get

$$\omega \underline{\Phi} = \underline{M}_\lambda \cdot \hat{\underline{\Phi}} \quad ,$$

$$\underline{M}_\lambda = \left[\lambda^2 \underline{D} + \underline{\sigma}_T - \underline{\sigma}_s^d \right]^{-1} \cdot \left[\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right] \quad , \quad (46a)$$

and it is obvious that $\underline{M}_\lambda$ is a positive matrix but is a decreasing function of λ . Therefore, the "largest" eigenvalue will be positive and simple and have a positive eigenfunction, and the eigenvalue will be a decreasing function of λ . Thus, the largest value of $|\omega|$ will occur at $\lambda = 0$:

$$\omega_1 \hat{\underline{\Phi}}_1 = \left(\underline{\sigma}_T - \underline{\sigma}_s^d \right)^{-1} \cdot \left(\underline{\sigma}_s^u + \underline{\chi} \underline{\nu} \underline{\sigma}_f \right) \cdot \hat{\underline{\Phi}}_1 \quad . \quad (46b)$$

The choice of $\underline{\theta}$ then should be

$$\underline{\theta} = \hat{\underline{\Phi}}_1 / \underline{u} \cdot \hat{\underline{\Phi}}_1 \quad .$$

Then, one can subtract Eqs. (31)-(33) from (34)-(36), and (37) from (38), and the result is

$$\underline{\theta} = \hat{\underline{\Phi}}_1 / \underline{u} \cdot \hat{\underline{\Phi}}_1 \quad , \quad (47)$$

$$- \frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta} f^{(\ell+1)} + \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\theta} f^{(\ell+1)} \quad (48)$$

$$= \left(\underline{u} \cdot \underline{\sigma}_s^u + \underline{\nu} \underline{\sigma}_f \right) \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\phi}^{(\ell)} \right) \quad ,$$

$$f^{(\ell+1)}(0) - 2\underline{u} \cdot \underline{D}(0) \cdot \frac{d}{dx} \underline{\theta}(0) f^{(\ell+1)}(0) = 0 \quad , \quad (49)$$

$$f^{(\ell+1)}(X) + 2\underline{u} \cdot \underline{D}(X) \cdot \frac{d}{dx} \underline{\theta}(x) f^{(\ell+1)}(X) = 0 \quad , \quad (50)$$

$$\underline{\phi}^{(\ell+1)} = \underline{\phi}^{(\ell+\frac{1}{2})} + \underline{\theta} f^{(\ell+1)} \quad . \quad (51)$$

This method “kills” the eigenvalue corresponding to $\lambda = 0$. Thus, the spectral radius will likely be determined by $|\omega_2|$, where ω_2 is the second largest (in magnitude) eigenvalue of the matrix $\underline{\underline{M}}_0$. [See Eqs. (46)]. If $|\omega_2|$ is not close to one, then the method should converge very quickly, but if $|\omega_2|$ is close to one, which can occur if there is weak coupling between the energy groups, then this method will not converge as quickly. However, in any case, it ought to converge more quickly than the unaccelerated method.

Note that the following quantities in Eq. (48) can be written

$$\begin{aligned}
& \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\theta} \\
&= \underline{u} \cdot \left[\underline{\sigma}_T - \underline{\sigma}_s - \chi \underline{\nu} \underline{\sigma}_f \right] \cdot \underline{\theta} \\
&= \sum_g \sum_{g'} \left[\sigma_{Tg'} \delta_{g'g} - \sigma_{sg'g} - \chi_g (\nu \sigma_f)_{g'} \right] \theta_{g'} \\
&= \sum_{g'} \left[\sigma_{Tg} - \sigma_{sg'} - (\nu \sigma_f)_{g'} \right] \theta_{g'} \\
&= \sum_{g'} \left[\sigma_{ag} - (\nu \sigma_f)_g \right] \theta_g
\end{aligned} \tag{52}$$

$$\begin{aligned}
& \left(\underline{u} \cdot \underline{\sigma}_s^u + \underline{\nu} \underline{\sigma}_f \right) \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} \dots \underline{\phi}^{(\ell)} \right) \\
&= \sum_{g=1}^G \left(\sum_{g'=g+1}^G \sigma_{sg'g} + (\nu \sigma_f)_g \right) \left(\phi_g^{(\ell+\frac{1}{2})} - \phi_g^{(\ell)} \right) \\
&= \sum_{g'=1}^G \left(\sum_{g=1}^{g'-1} \sigma_{sg'g} + (\nu \sigma_f)_{g'} \right) \left(\phi_{g'}^{(\ell+\frac{1}{2})} - \phi_{g'}^{(\ell)} \right) \\
&= \sum_{g=1}^G \left(\sigma_{sg}^u + (\nu \sigma_f)_g \right) \left(\phi_g^{(\ell+\frac{1}{2})} - \phi_g^{(\ell)} \right) ,
\end{aligned} \tag{53}$$

where σ_{sg}^u is defined in Eq. (7).

It is also worth noting that in Eqs. (47)-(52) one can conceptually ignore the terms

$$\frac{d}{dx} \underline{\theta}$$

and get:

$$\underline{\theta} = \hat{\Phi}_1 / \underline{u} \cdot \hat{\Phi}_1 \quad , \quad (54)$$

$$\begin{aligned} & - \frac{d}{dx} \left(\underline{u} \cdot \underline{D} \cdot \underline{\theta} \right) \frac{d}{dx} f^{(\ell+1)} + \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \sigma_f \right] \cdot \underline{\theta} f^{(\ell+1)} \\ & = \left(\underline{u} \cdot \underline{\sigma}_s^u + \underline{\nu} \sigma_f \right) \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\phi}^{(\ell)} \right) \quad , \end{aligned} \quad (55)$$

$$f^{(\ell+1)}(0) - 2 \left[\underline{u}(0) \cdot \underline{D}(0) \cdot \underline{\theta}(0) \right] \frac{d}{dx} f^{(\ell+1)}(0) = 0 \quad , \quad (56)$$

$$f^{(\ell+1)}(X) + 2 \left[\underline{u}(X) \cdot \underline{D}(X) \cdot \underline{\theta}(X) \right] \frac{d}{dx} f^{(\ell+1)}(X) = 0 \quad . \quad (57)$$

These equations have a symmetric diffusion operator, and they may be easier to deal with in 2-D. In particular, these equations are now precisely of the form of each of the within-group equations in the original multigroup formalism [see Eqs. (1)-(3)].

An issue which needs to be considered is whether or not the one-group equations, (42) and (48), are actually solvable. In other words, do the operators on the left sides of these equations represent fictitious one-group media which are subcritical? For example, the fictitious one-group absorption cross section in Eqs. (48) is

$$\begin{aligned} \tilde{\sigma}_a &= \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \sigma_f \right] \cdot \underline{\theta} \\ &= \sum_{g=1}^G \left[\sigma_{Tg} \theta_g - \sum_{g'=1}^G \sigma_{sg'g} \theta_{g'} - (\nu \sigma_f)_g \theta_g \right] \\ &= \sum_{g=1}^G \left[\sigma_{Tg} - \sigma_{sg} - (\nu \sigma_f)_g \right] \theta_g \\ &= \sum_{g=1}^g \left[\sigma_{ag} - (\nu \sigma_f)_g \right] \theta_g \\ &= \sum_{g=1}^g \left\{ \sigma_{rg} + [(1 - \nu) \sigma_f]_g \right\} \theta_g \quad , \quad [\sigma_r = \text{capture}] \quad , \end{aligned}$$

and this quantity can be negative.

In other words, because we are treating fission explicitly, it appears to be possible that a multigroup problem, which is subcritical for a finite medium, can “collapse” to a one-group problem which is supercritical. At least, I do not see how to exclude this possibility, if fission is present. (If fission is not present, then everything should work properly.)

There are possible ways to get around this problem. In Eq. (42), let us define

$$\tilde{\sigma}_a = \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \sigma_f \right] \cdot \underline{\theta}^{(\ell+\frac{1}{2})} \quad . \quad (58)$$

Then, we rewrite Eq. (42) as:

$$\begin{aligned} & - \frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta}^{(\ell+\frac{1}{2})} \phi^{(\ell+1)} + \frac{1}{2} [|\tilde{\sigma}_a| + \tilde{\sigma}_a] \phi^{(\ell+1)} \\ & = \underline{u} \cdot \underline{Q} + \frac{1}{2} [|\tilde{\sigma}_a| - \tilde{\sigma}_a] \phi^{(\ell+\frac{1}{2})} \quad . \end{aligned} \quad (59)$$

Then, if $\tilde{\sigma}_a > 0$, absorption is treated implicitly, but if $\tilde{\sigma} < 0$, it is treated as an explicit source.

In Eq. (48), we define

$$\hat{\sigma}_a = \left[\underline{u} \cdot \left(\underline{\sigma}_T - \underline{\sigma}_s \right) - \underline{\nu} \sigma_f \right] \cdot \underline{\theta} \quad (60)$$

and then we can rewrite Eq. (48) as

$$\begin{aligned} & - \frac{d}{dx} \underline{u} \cdot \underline{D} \cdot \frac{d}{dx} \underline{\theta} \phi^{(\ell+1)} + \frac{1}{2} [|\hat{\sigma}_a| + \hat{\sigma}_a] \phi^{(\ell+1)} \\ & = \left(\underline{u} \cdot \underline{\sigma}_s + \nu \sigma_f \right) \cdot \left(\underline{\phi}^{(\ell+\frac{1}{2})} - \underline{\phi}^{(\ell)} \right) \quad . \end{aligned} \quad (61)$$

Here, if $\hat{\sigma}_a < 0$, we simply remove $\hat{\sigma}_a$ from the problem.

Both these methods amount to not accelerating certain components of the problem. These prescriptions are also overly conservative in that one can always live with a small amount of negative absorption, but exactly how much is difficult to determine.

It is not clear how these methods will perform, and only implementation and experimentation seem likely to provide a firm and thorough understanding of their strengths and weaknesses.

E. Distorted Mesh Solver for Radiation Transport (R. E. Alcouffe)

We have begun a project to develop and implement a distorted mesh solver for the TWODANT² and SHORTIE^{4,5} codes. To develop a tractable solver, we have made the following restrictions on the composition and connectivity of the mesh. First, the mesh must be logically rectangular in its connectivity; that is, at each point of intersection of mesh lines, four—and only four—quadrilaterals are joined. The only exception to this is on the axis of symmetry in (r,z) geometry, where triangular meshes are permitted. This condition permits centers of convergence to be modeled. Second, the mesh is restricted to a rectangular domain in the logical space, but the boundaries of the solution domain need not lie on the exterior boundaries if they are on the axis of symmetry. With these restrictions, it is possible to construct an ordering of the problem mesh that allows the mesh sweeping to be vectorized to

the fullest extent. The vectorization depends upon the ordering routine to pick out groups of cells that can be solved simultaneously. On the logical mesh, this means picking out cells which lie on diagonals, so this is quite similar to the diagonal sweeper now used in the orthogonal codes TWODANT and SHORTIE.

The ordering is done for each angle so that the transport operator is inverted non-iteratively by sweeping the spatial mesh. Thus, just as in the orthogonal methods, the iterations involved in solving radiation transport problems on a nonorthogonal mesh are source iterations. The solution method is the same as previously developed for the orthogonal codes in that diffusion acceleration is used to accelerate the transport iterations, and the multifrequency-grey method is used to accelerate the multifrequency diffusion iterations. This approach has been successful in solving radiative flow problems in two-dimensional orthogonal meshes, and the task in this project is to determine whether it can be as successful for nonorthogonal (distorted) meshes.

At present, the main goals of this project are to develop an efficient, reliable transport solver for a general quadrilateral but logically rectangular mesh and to develop a source iteration acceleration method that is efficient, effective, and as robust as practical. We want to establish numerical values for these goals to be better able to ascertain the practicality of our methods for solving radiation flow problems using the present-generation machines (Cray X-MP/48). To this end we assume the mesh ordering and sweeping to take $1-2 \mu\text{s}$ per phase space cell on the X-MP. We also assume that the diffusion accelerator and the grey accelerator will be as effective on the distorted mesh as on a corresponding orthogonal mesh, that is, 2-4 transport iterations per time step and 1-5 diffusion iterations per transport iteration. Thus, the mean time to solve a medium sized radiation flow problem of 5000 spatial meshes, S_8 angular quadrature, and 10 frequency groups should be from 4.5 to 1.5 s per time step. Thus, a 1000 time step problem of this size should be solved in under 4 h if these goals are met.

As mentioned above, the first task in developing a distorted mesh solver is to develop an ordering routine. The job of the ordering routine is to pick out the sequence of spatial meshes in an order that will allow the solver to invert the transport operator noniteratively. This can always be done since the transport operator is first order in both the spatial and angular derivatives. However, there is an additional task that the ordering routine must perform to take advantage of the architecture of the Cray X-MP computers. Since those computers are vector machines, an ordering must be chosen so the mesh sweeping can be vectorized for maximum solution speed. Thus, groups of cells that can be solved simultaneously must be found by the ordering routine; on the logical mesh these cells will lie on diagonals.

We do the ordering on the logical mesh by typing cells as to how many sides are visible. Only two side-visible cells can be solved simultaneously. Operationally, the ordering routine collects the following information: 1) the starting cell number, 2) the starting cell type, and 3) the number of cells in the diagonal. The mesh sweeper can then take this information and process it in order and efficiently invert the transport operator on the vector machine. Thus, the main difference between sweeping on a distorted mesh and on an orthogonal mesh is making provisions in

the mesh sweeper to solve one-side-visible and three-side-visible quadrilaterals (and the special case of triangles).

The spatial and angular discretization and solution method is based upon the diamond differencing algorithm as derived by Hill and Paternoster⁶ for arbitrary quadrilaterals. This method is supplemented by a set-to-zero fixup in case the angular intensity extrapolates to a negative value. As with the orthogonal mesh, the diamond differencing is the simplest method having the diffusion limit. The simplicity allows for efficient coding with minimum storage requirements, and the diffusion limit allows the accelerator to perform efficiently and yet obtain an accurate solution when the transport solution is diffusion-like. This certainly is an appropriate first attempt with the S_N method itself.

The diffusion acceleration method, a source iteration accelerator for radiation transport problems, involves the following ingredients: 1) formation of an appropriate diffusion equation whose solution is the same as the scalar intensity solution of the transport equation, 2) a solution method for inverting the resulting diffusion operator for each frequency group, and 3) an iteration method for solving the multi-group diffusion equation. For the general distorted mesh, it is not yet clear what the best method is for addressing each of the above aspects. To assess where the chief difficulties might be, we have begun with a straightforward approach based upon the method for orthogonal mesh.

To form the diffusion operator, we take the transport balance equation for each cell and add those equations for four adjoining cells. It is this four-cell-balance equation that is used to form the basic diffusion acceleration equation. That is, we form a diffusion equation with correction terms derived from this transport balance such that upon convergence the scalar intensity solutions to the diffusion equation and the transport equation are the same. We have used, as a first try, the source correction method with a conventional five-point diffusion operator where the unknowns are on the mesh corners. The main point of uncertainty is the use of a five-point diffusion operator because for conventional diffusion theory it is known that generally a nine-point operator is required for accuracy. However, in the transport accelerator, the five-point operator correction terms should be accurate enough, but the efficiency of the accelerator depends to some extent upon how "close" the diffusion operator is to the corresponding transport operator. This is something that cannot be predicted and must be determined by empirical tests.

We invert the diffusion operator with the standard multigrid method as currently incorporated in the TWODANT code. Since the diffusion equation is five point, this has required no change in the multigrid solver itself.

Last, the solution to the multifrequency diffusion equation requires source iteration acceleration. To this end we use the same multifrequency-grey method as in the SHORTIE code. Again, we can do this because the diffusion operator is five point. We know from experience with SHORTIE that this grey accelerator will perform well in converging the diffusion iterations.

It should be obvious by now that the success of the above-outlined transport solution method depends heavily upon the representation of the diffusion acceleration equation as a five-point operator. This five-point representation is not an essential

restriction, but it certainly does simplify the implementation of the method for distorted meshes.

To date, we have coded corrections into SHORTIE that should implement the above-described method for solving radiation flow problems on a distorted mesh. Some restructuring of the core storage was required, as was a linking mechanism to a code that would prepare the geometric input. The ordering routine is by far the most complicated aspect of the method. The routine is now mostly complete although some known deficiencies remain. The mesh sweeping routine is quite straightforward to implement and is now being documented. The accelerator is also mostly completed in its five-point form. Thus, at present, we have available a prototype code that can solve the time-dependent radiation transport equation on a general distorted mesh. Below we present some selected results that show current capabilities of the code and how close we are to meeting the goals stated above.

We estimate that the ordering routine is about 90% finished. It is not yet as robust as it ultimately must be, but it is becoming quite reliable. With the present routine, we can order a general mesh of quadrilaterals and the selected triangles on a logical domain, shown in Fig. 1. In performing preliminary timing studies, we estimate that we can order a mesh at a cost of 5-10 μ s per mesh cell per angle. This high cost exists because almost none of the coding can be vectorized. However, it should be kept in mind that ordering is not group dependent and need be done only for those angles and time steps where the mesh has changed enough that the cell types have changed. It is expected, therefore, that ordering costs for the typical problem will be minimal.

Fig. 1. An example logical mesh for the ordering routine.

We have tested the sweeper on a limited range of problems. We can compute the solution of a general mesh of quadrilaterals (no triangles as yet) with all of the accelerators turned on. It appears from some rather simple test problems that the

accelerators are working about as well as they do on an orthogonal mesh, which is encouraging. We can best illustrate the current status of the code by showing results on a problem derived from a Kershaw-type mesh that has been used to challenge diffusion solver. The mesh used in this study is shown in Fig. 2. The medium is modeled as polyethylene at a density of 2.45 g/cm^3 . The problem was modeled with SHORTIE using 10 frequency groups and an S_4 angular quadrature. For comparison a uniform orthogonal mesh representation of the same problem was also solved. In Figs. 3a and 3b, we present the spatial temperature distribution at two times from the distorted mesh. In Figs. 4a and 4b, we present the same distributions computed from the orthogonal mesh. An examination of the two solutions will show that essentially the same results are obtained. This leads us to conclude that the coding of the method for distorted meshes is essentially correct and that physically reasonable results are being obtained for radiation flow. The usefulness of the method now depends upon the efficiency with which the computations are being performed.

Fig. 2. Distorted mesh test problem.

Fig. 3a. Temperature profile at time = 2.5 ns on the distorted mesh.

Fig. 3b. Temperature profile at time = 7.5 ns on the distorted mesh.

Fig. 4a. Temperature profile at time = 2.5 ns with an orthogonal mesh.

Fig. 4b. Temperature profile at time = 7.5 ns with an orthogonal mesh.

We have performed a very limited set of timing comparisons with the following results. The mesh sweeper has been timed for a moderate (50 x 50) mesh at 1.5 μ s per cell where the mesh is essentially orthogonal. On more complicated but smaller meshes, the time per cell is around 3 μ s. Thus, it appears we are about a factor of two from the goal stated above. At present, the overall solution time, including the accelerators for the problem described above, is around 7 s per time step extrapolated to an S₈, 10 group 5000 mesh problem. This appears to be within our goal; however, the above problem does not challenge the DSA accelerator very much since the time steps are small (0.01 ns) and iteration acceleration is not very important. We can say that in simpler problems where acceleration is important, the accelerator is performing about as well as for the orthogonal mesh.

We are very encouraged by the results thus far and will continue development along these lines.

III. MONTE CARLO RADIATION TRANSPORT

The Monte Carlo radiation transport effort in Group X-6 is devoted to the development, implementation, assessment, and application of Monte Carlo methods and computer codes for radiation transport.

A. MCNP Code Support and Improvement (T. N. K. Godfrey)

Debugging and minor polishing work continues on Version 3B of MCNP, our continuous energy Monte Carlo code.⁷ A new friendly-user version was made available on August 13. We expect to be using Version 3B sometime this winter.

The scope of the next version of MCNP is not yet defined. The changes might even be so great that we will want to call it Version 4 instead of Version 3C. Two significant improvements appear likely to be included: tree-structured random numbers and graphics improvements.

MCNP has always had some degree of tree structure—adequate for debugging and multitasking—in its random-number system. A small patch has been written that extends it to allow users to add, delete, or modify the following features in a problem without affecting the rest of the problem: tallies, DXTRAN, and neutron-induced protons. This change will also make it cheaper to investigate the effects of small perturbations. Only tracks that pass through a perturbed region will be affected by the perturbation.

We are working on several aspects of the graphics in MCNP. We want to eliminate all remaining unnecessary differences between PLOT and MCPLOT, both in the user interface and internally. We would like to use the graphics standard GKS as much as possible for greater portability. Where GKS is well implemented or is the only graphics system, MCNP will use it directly. Where the implementation is poor, as it is here, MCNP will use its own GKS subroutines, which call CGS, DISSPLA, or PLOT10 library subroutines. We will provide our own high-level subroutines such as for drawing and labeling axes to eliminate dependence on high-level library subroutines. We want to add optional axes and grids to geometry plots and to give

the user more control over the location and appearance of the titles, legends, and captions in plots.

B. Testing of the BFP Package in MCNP for Coupled Electron/Photon Transport (J. F. Briesmeister and J. E. Morel)

During this reporting period, we began testing the hybrid multigroup/continuous-energy Monte Carlo method for coupled electron/photon transport using a Boltzmann-Fokker-Planck approach.⁸ A package embodying this technique has been developed and placed in Version 3B of MCNP. The testing of this patch is intended to shake out any bugs or deficiencies in the code and to provide us greater familiarity with this potentially valuable computational approach.

C. MCNPE Code Support and Improvements (R. G. Schrandt)

Our electron/photon Monte Carlo package MCNPE⁹ incorporates the electron and photon physics from the ITS¹⁰⁻¹² codes into MCNP.⁷ MCNPE will now handle the uncollided contribution to a photon point detector or DXTRAN sphere (see pp. 128-135 of Ref. 7) from bremsstrahlung photons. The bremsstrahlung angular distribution is anisotropic and is a function of the electron energy and direction and the photon sampled energy. The probability density function $p(\mu)$, where μ is the cosine of the angle between the particle direction and the detector, is calculated with an ITS code approximation to the angle of emission. This approximation samples the angle independent of the photon energy.

An electron cell energy cutoff has been added to the code. The cutoff is useful in reducing the time spent tracking electrons in unimportant cells.

More extensive MCNPE use, where more of the options of MCNP are exercised, has revealed a number of bugs, including some in the DXTRAN and point detector diagnostics. These have been eliminated, and additional diagnostics have been added to better understand the bremsstrahlung contributions.

D. SABRINA Tabular Body Capability (J. T. West)

A tabular body capability has been added to SABRINA, our three-dimensional interactive geometry modeler for MCNP.¹³ Now a geometric body can be described as collection of (r,z) points symmetric about the x, y, or z axis. If the last point is the same as the first, a complicated, very bumpy torus may be described. The tabular body can be multiple re-entrant, allowing for describing some very complicated, contorted shapes. The tabular body is treated the same as a simple SABRINA combinatorial body in the tracking logic; therefore, tabular bodies used in zone descriptions can be used with intersections, differences, or union operations as can any other simple body. Tabular bodies referenced in a zone description need not have the same axis of symmetry. An example of a toroidal tabular body is shown in Fig. 5.

Fig. 5. Toroidal tabular body from SABRINA.

E. HETC Code Development (R. E. Prael)

The principal effort in HETC¹⁴ code development has been to implement a model for the effect of the Coulomb barrier for charged particles incident on a nucleus. The results of this effort are discussed in detail in the following section.

The intranuclear tracking algorithms within the ISABEL¹⁵ routines were improved by providing energy-dependent step size limits. The change limits the error induced by approximations in the tracking algorithm, even for very-low-energy particles.

A third major HETC-related effort was the recoding of the INCA and FBRK codes. The effort included the generation of in-code documentation, in preparation for distribution of the codes inside and outside the laboratory. These two codes are expected to be employed in the effort to generate cross-section libraries for both protons and neutrons on light nuclei at energies up to 200 MeV.

F. A Coulomb Barrier for HETC (R. E. Prael)

At incident energies near the Coulomb energy at the nuclear surface, the interaction of a charged particle with a nucleus is inhibited by the Coulomb barrier seen by the incident particle. The effect of the Coulomb barrier on the initial interaction of the incident particle has not been treated in HETC (or in the intranuclear cascade codes VEGAS and ISABEL) although an impenetrable Coulomb barrier limits particle escape in the intranuclear cascade and barrier penetration is modeled in the evaporation process that follows the intranuclear cascade. In most transport problems for which HETC is considered appropriate, the lack of a Coulomb barrier is not a major deficiency since charged particles that have slowed down to low energies probably will not interact in any case; the nuclear interaction length is much greater than the range of the particle in the material. However, for transport problems starting with beam energies below 100 MeV, noticeable effects due to a Coulomb barrier may appear, particularly in heavy materials where the height of the Coulomb barrier may be 10 to 20 MeV. At these lower energies, the probability of a nuclear interaction is small; however, when one does occur, it would be modified significantly by the Coulomb barrier.

To explore the effect of including a Coulomb barrier in HETC, the code was modified with two barrier penetration models. In both models, a probability of barrier penetration is calculated at the kinetic energy of the charged particle attempting a nuclear interaction. The interaction is rejected if a sampled random number exceeds the penetration probability. If the interaction is allowed, the standard intranuclear cascade calculation is permitted.

In the first, and simplest, model the interaction probability is assumed to be

$$P = \max(1.0 - E_c/E, 0.0) \quad , \quad (62)$$

where E_c is the Coulomb energy at an appropriate charge radius and E is the kinetic energy in the center of mass. This model is purely "classical" and allows no interaction below the Coulomb barrier while reducing the interaction probability above the Coulomb barrier. In the following plots, this model is designated as the Coulomb barrier model.

The second model tested takes the barrier penetration probability from an approximate fit to realistic calculated Coulomb barrier penetration factors; the transmission probability is nonzero at and below the Coulomb energy although it diminishes rapidly with energy. In the following plots, this model is designated as the Coulomb penetration model.

In Fig. 6, the effect of employing a Coulomb barrier model is shown for the reaction cross section for protons on ^{27}Al . For comparison, the evaluated data supplied by Group T-2 is also shown. In Fig. 7, the effect of the Coulomb barrier models is shown for a low-energy transport problem in which a 50-MeV proton beam is incident on a stopping length natural lead target. Note that the limitations of the intranuclear cascade/evaporation model itself at these lower energies are probably much greater than the effect of imposing any Coulomb barrier model.

The various calculations of the Coulomb barrier transmission probability are illustrated in Fig. 8; the vertical line locates the Coulomb barrier energy with

respect to the particle energy in the laboratory system. The solid line represents the approximate fit to "realistic" barrier penetration factors (the fitting procedure results in some distortion visible near the barrier energy); this is an example of the transmission probability described above as the Coulomb penetration model. The dotted line illustrates the transmission probability from Eq. (62), described above as the Coulomb barrier model. The dashed line illustrates a third approximation

$$P = \max(1.0 - kE_c/E, 0.0) \quad , \quad (63)$$

in which $k < 1$ attempts to reflect the quantum mechanical effect of barrier penetration. In Eq. (63), the factor k is chosen to match the transmission probability at the energy of the Coulomb barrier. The use of a penetration factor k has always been employed in the evaporation model of HETC and is probably quite effective if the Coulomb energy is chosen properly.

Fig. 6. Effect of Coulomb barrier model for proton reactions in ^{27}Al .

Fig. 7. Effect of Coulomb barrier model for a low-energy transport problem.

P+CU63

Fig. 8. Coulomb barrier transmission probabilities.

G. Implicit Splitting (T. E. Booth)

The implicit splitting scheme described in the preceding progress report¹⁶ was modified to approximately emulate the good feature of the forced collision technique. This modification was in response to user requests and is now available for friendly users.

H. Intelligent Random Numbers (T. E. Booth)

The perturbation method alluded to on page 5 of Ref. 17 has been developed and successfully implemented in a small test code. The results are very encouraging; the figure of merit now uniformly increases as the data base of previous experience increases.

The perturbation method divides the phase-space and the random number space by playing several "what-if" games. For example, suppose a particle's history is described by

$$\vec{P}_0, r_{01}, r_{02}, r_{03}, \vec{P}_1, r_{11}, r_{12}, r_{13}, \vec{P}_2, r_{21}, X \quad \text{score} = 1 \quad ,$$

where $\vec{P}_i$ are the physical phase-space coordinates, r_{ij} are the random numbers thrown between the phase-space positions, and X is a termination type (for example, escape). What if $\vec{P}_i$ had been slightly different? Would the same random numbers used from $\vec{P}_i'$ produce the same score? If not, there is some difference between $\vec{P}_i$ and $\vec{P}_i'$. If the same score results, $\vec{P}_i$ and $\vec{P}_i'$ are allowed to be in the same phase-space region. A similar procedure is followed in the random number space. That is, r_{ij} is changed to r'_{ij} and the remaining random numbers are unaltered. If the score changes, the random number space should be divided between r_{ij} and r'_{ij} .

This perturbation technique needs very little data to decide how to divide the phase and random number spaces because the technique is no longer trying to infer differences from uncorrelated data as in Ref. 18. However, the fact that the spaces are known to be different does not mean that the correct (score-weighted) distribution of random numbers is known. There are several ways this problem can be approached; the most successful is described next.

I. Generalization of the Quasi-Deterministic Method (T. E. Booth)

The quasi-deterministic method¹⁹ for estimating the expected score (importance function) for physical phase-space regions has been generalized to work in the random number space as well. The random number biasing is determined from this quasi-deterministic importance estimate in the complete physical-random number space.

To derive the quasi-deterministic method, we use the pictorial representation in Fig. 9. Note that each physical box i is connected to a number of random number boxes ij . The random number boxes ij are connected to physical boxes k . For a particle currently in physical box i , the next physical box k will be determined by

1. the location in box i,
2. the selection of box i,j, and
3. the selection of the random sequence $\bar{r}$ from box i,j.

Fig. 9. Connection of physical boxes to random number boxes.

For each random number box i,j, a physical point is randomly selected in box i, a random sequence is randomly selected in box i,j, and the new physical box k is determined. This process is repeated until an empirical estimate of

$$P_{ijk}, = \text{probability of going from box i,j to box k} \quad (64)$$

$$S_{ijk}, = \text{average score in going from box i,j to box k} \quad (65)$$

Let

$$M_i = \text{average score from box i} \quad (66)$$

$$M_{ij} = \text{average score from random box i,j} \quad (67)$$

$$V_{ij} = \text{volume of random number box i,j} \quad (68)$$

$$P_{ij} = \text{probability of picking random box i,j} \quad (69)$$

The average score, M_i , is determined by the averaging over all possible choices of j and k . There is an immediate score, S_{ijk} , in going from box i through box j to box k plus the average score subsequent to reaching box k , namely M_k . Thus

$$M_i = \sum_j \sum_k P_{ij} P_{ijk} (S_{ijk} + M_k) \quad . \quad (70)$$

Noting that the probability of picking random box j is equal to its volume V_j and rearranging the sums yields

$$M_i = \sum_k \sum_j V_j P_{ijk} (S_{ijk} + M_k) \quad . \quad (71)$$

This is a set of linear equations for the M_i and can be deterministically solved. After the M_i are obtained the average score from box i, j is determined from

$$M_{ij} = \sum_k P_{ijk} (S_{ijk} + M_k) \quad . \quad (72)$$

The intelligent random number technique chooses random number sequences proportional to their expected score M_{ij} . Thus letting

$$q_{ij} = \text{biased probability for selecting random number box } i, j \\ \text{from physical box } i \quad , \quad (73)$$

and recalling $P_{ij} = V_j$ yields

$$q_{ij} = V_j M_{ij} \left\{ \sum_{\ell} M_{i\ell} \right\}^{-1} \quad (74)$$

for the intelligent random number technique.

J. High-Altitude Fluorescent Radiation Transport (D. G. Collins)

The discrepancy between the forward and adjoint calculations of the fluorescent radiation for narrow fields of view has not been resolved. After correction of an error in the computation of the derivative of retarded time as a function of distance, the direct fluorescence computed with the forward and adjoint calculations is in good agreement. However, there is still disagreement in the scattered fluorescence computed with the two methods. To verify the concept, the forward and adjoint calculations were applied to a simple single-scattering model involving isotropic scattering and constant cross sections. Good agreement was obtained for the single-scattered fluorescence calculated with the forward and adjoint methods for the simple model. A continuing search will be conducted to resolve the differences for the more complex model.

IV. CROSS SECTIONS AND PHYSICS

Part of our work in X-6 is devoted to the acquisition, validation, and creating of libraries of cross sections for use in our deterministic and probabilistic codes; to the development of codes for accessing and producing atomic and nuclear data, for example, for use in our codes; and to supporting research and evaluation of physics models for radiation transport problems of interest. We also devote time to computing systems-related matters.

A. Unresolved Resonance Treatment for MCNP (H. M. Fisher)

During this reporting period, much time was spent collaborating with J. Arkusewski of EIR, the Swiss Federal Institute for Reactor Research at Wurenlingen, on the preparation of a patch employing the probability table (PT) method for unresolved resonance cross sections for MCNP calculations. The patch, named MCNPURES, has been written and tested on various problems; however, after discussions with R. C. Little (X-6), it was decided that the unresolved resonance patch should undergo several additional basic tests before we could state with confidence that the patch is working correctly. It was decided that the following tests should suffice to validate the patch.

1. Neutron Transport – run the patch both with PT method turned on and with it turned off; note the results for the case in which the unresolved resonances are of little importance.
2. DXTRAN Spheres
3. Detectors
4. Gamma production/heating
5. FM_n cards
6. An unphysical problem composed only of ^{238}U in which the transmission and average cross sections are determined, that is, $t = \exp(-N\sigma_t t)$ and $\phi\sigma_t/\phi$, where σ_t of the transmission result should mimic the σ_t of the average cross-section result.

Tests 1 and 5 have already been performed quite successfully. Details of these calculations will be given in a forthcoming memorandum. We expect to complete the remaining tests by the end of October 1987, and we expect the unresolved resonance patch to be ready for MCNP friendly users not long thereafter.

B. XDATAP Manual (H. M. Fisher)

The documentation for XDATAP, the data diagnostic and cross-section plotting code,¹⁶ has been completed and is now being edited. Barring unforeseen difficulties, the manual will be available to the MCNP user community before the end of 1987.

C. The Cross-Section Data Handbook (H. M. Fisher)

Work on the cross-section data handbook¹⁷ is continuing although progress is slow because of other tasks. During the reporting period, the utility software to produce the handbook was changed from L^AT_EX to T_EX and the files, text, and plots were moved over to the Apollo Scientific Workstation from the VAX system. We hope to have the handbook ready for publication by the end of January 1988.

D. The TOPS/SPOT Codes (R. E. H. Clark)

A longstanding bug in the TOPS²⁰ and SPOT¹⁷ opacity data codes has been eliminated. Previously, if the user modified the atomic weight, that is, chose a different isotope, or requested a normal density different from what was on the OPLIB files, the opacity calculation used the correct updated atomic weight and normal density. However, the updated values were not written to the SESAME formatted file²¹ of gray opacities. Thus, if a code read in the SESAME file and used the composition listed, it would be inconsistent with the opacity data on the file. This has now been fixed. The composition listed on the SESAME file is now consistent with the opacities. The problem never occurred for the multigroup files, so they are unchanged.

The TOPS/SPOT codes now accept an infile command so that using a controller is no longer necessary. To use the command, first use a text editor to prepare a file of commands exactly as you would type them for the code interactively. Then run the code using the execute line

```
TOPS  INFILE = fname
```

or

```
SPOT  INFILE = fname ,
```

where fname is the name of the file of commands. If fname is not in your local file space, the code will print a message and return control to the tty. If the code finds an end of file in fname, it will NOT return command to the tty; it will end the run. To return control to the tty from an input file, the command

```
INFILE  tty
```

must be included in the file. If you are running the code interactively, you can transfer control to fname with the command

```
INFILE  fname
```

at any time.

E. Work on the HANDI Atomic Data Processing Code (G. W. Pfeufer)

During the fourth quarter of FY 1987, I completed Version 2gc of the HANDI code.^{16,22} This version improves the graphics support for the first curve family and implements full graphics support for the second curve family. In HANDI, the first curve family includes the single independent variable held constant for SESAME plots²¹ and for STYX format²³ gray opacity plots and the first independent variable held constant for STYX multigroup plots; the second curve family includes the second independent variable held constant for STYX multigroup plots. For example, in a plot of Rosseland absorption opacity as a function of photon energy for constant temperature and density, temperature values constitute the first curve family and density values constitute the second curve family. The new graphics package in the code fulfills user requirements for scrutinizing and comparing voluminous quantities of multigroup opacity data and incorporates user suggestions for the form of the command input to manipulate the data and to generate the plots. In this version of HANDI, I unite a sophisticated set of two-dimensional graphics capabilities specifically developed for plotting and comparing Rosseland and Planck multigroup opacity data in STYX format with existing capabilities for plotting and comparing equation of state data in SESAME format and comparing Rosseland and Planck gray opacity data in SESAME and STYX formats.

In the previous quarter,¹⁶ I completed intermediate Versions 2ga and 2gb of the code. In these versions, I reorganized the management and storage of the original data for each SESAME and STYX material, making the two schemes as consistent as possible. In particular, SESAME material data are no longer kept in core; rather, as with STYX material data, they are reread from disk for each plot request.

Building upon these versions, I completed the following major modifications and additions to the graphics capabilities in Version 2gc of HANDI:

1. Generalized the management and storage of the plot data for SESAME and STYX materials to accommodate the second curve family. The plot data for each value in the second curve family are manipulated and stored as a SESAME-like plot. This concept is fundamental to the management of plot data in the code. The original material data in each curve family are fetched from disk to construct a plot of a single material on its default, tabulated, or interpolated curve sets for each curve family. For comparison plots, the original material data in each curve family for subsequent materials in the plot are interpolated onto the x-axis values, and the curve sets are defined for the first material in the plot.
2. Modified the CURVES Command to interpolate tabulated curve values for the two curve families onto specified curve sets. An interpolated curve set is specified independently for each curve family, so a plot can display any combination of default, tabulated, or interpolated curve sets for the two curve families. For example, the plot can display the default curve set for the first curve family and an interpolated curve set for the second curve family.
3. Added the RCURVES Command to recall interpolation curve sets for plot defined with the CURVES Command.

4. Modified the CDISPLAY Command to report coordinate values for the second curve family.
5. Added the TABCURVE Command to select tabulated curve values from the two curve families for plot. A tabulated curve set is specified independently for each curve family. Hence, a plot can display any combination of default, tabulated, or interpolated curve sets for the two curve families. For example, the plot can display a tabulated curve set for the first curve family and an interpolated curve set for the second curve family.
6. Added the RTABCURV Command to recall tabulated curve sets for plot specified with the TABCURVE Command.
7. Added the TABCURVE Option to the STEP Command to move backward and forward through tabulated curves for each curve family for a plot. The steps are specified independently for each curve family and apply to plots displayed with the default curve set or a tabulated curve set specified with the TABCURVE Command.

The news file for Version 2gc summarizes the changes and additions to the graphics capabilities in the code. The on-line documentation for each modified or new command was revised. After I tested the version on my favorite SESAME and STYX materials, Version 2gc was released to friendly users in late September. Users were invited to judge the adequacy of the the news file and the revised on-line documentation for understanding and using the new graphics capabilities and to test the code and report errors and difficulties. After the friendly-user period, Version 2gc will be made available to all users of HANDI.

F. Graphics on the Apollo Scientific Workstation (K. A. Van Riper)

I am continuing to develop an integrated system for preparing PostScript graphics, displaying these plots on the screen, and incorporating them into T_EX documents. New features and removal of some undocumented features in the graphics and display programs continues. An interactive capability for modifying plots is under development. One can now select a position and angle on a graph with the mouse and then enter any string written on the plot at a selectable character size.

The Hershey character set is a collection of about 2000 vector symbols; these were the characters used by REDPP. I have used the Hershey character codings to prepare "stroke" fonts for the APOLLO screen graphics (DOMAIN 2D Graphics Metafile Resource). Unlike pixel fonts, the stroke fonts can be displayed in any size and at any orientation. The REDPP alphabet coding, translated to PostScript encoding, was used to prepare APOLLO fonts corresponding to all the REDPP styles (Roman Sans-Serif, Roman Serif, Script, Greek, English Gothic, German Gothic, Hebrew, etc.).

Transferring PostScript files from the X-6 APOLLO network to the IS Division phototypesetter continues to be painful. Red partition UNIX format files must be changed to unclassified, green partition files in VMS format and moved to an open

VAX running VMS. This takes several steps, some of which must be done on each individual plot file.

REFERENCES

1. R. D. O'Dell, F. W. Brinkley, Jr., and D. R. Marr, "User's Manual for ONEDANT: A Code Package for One-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport," Los Alamos National Laboratory report LA-9184-M (February 1982).
2. R. E. Alcouffe, F. W. Brinkley, Jr., D. R. Marr, and R. D. O'Dell, "User's Guide for TWODANT: A Code Package for Two-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport," Los Alamos National Laboratory report LA-10049-M, Rev. (October 1984).
3. R. E. Alcouffe, B. A. Clark, and E. W. Larsen, in *Multiple Time Scales*, edited by J. V. Brackbill and B. Cohen, Academic Press, Orlando, Fla., p. 73 (1985).
4. R. D. O'Dell, "Radiation Transport, April 1, 1986 - June 30, 1986," Los Alamos National Laboratory report LA-10844-PR (January 1987).
5. R. D. O'Dell, "Radiation Transport, January 1, 1986 - March 31, 1986," Los Alamos National Laboratory report LA-10792-PR (September 1986).
6. T. R. Hill and R. R. Paternoster, "Two Dimensional Spatial Discretization Methods on a Lagrangian Mesh," in Proc. of Meeting on Deterministic Transport Methods, held in Bruyeres-le-Chatel, France, April 19-23, 1982, Vol. I.
7. Judith F. Briesmeister, Ed., "MCNP - A General Monte Carlo Code for Neutron and Photon Transport, Version 3A," Los Alamos National Laboratory report LA-7396-M, Rev. 2 (September 1986).
8. R. D. O'Dell, "Radiation Transport, January 1, 1985 - March 31, 1985," Los Alamos National Laboratory report LA-10591-PR (January 1986).
9. R. D. O'Dell and A. Nagy, "Radiation Transport, July 1, 1986 - September 30, 1986," Los Alamos National Laboratory report LA-11030-PR (August 1987).
10. J. A. Halbleib and T. A. Mehlhorn, "ITS: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAN 84-0573 (November 1984).
11. H. Grady Hughes and Joseph M. Mack, "Integrated TIGER Series at Los Alamos," Los Alamos National Laboratory memorandum X-6:HGH-85-306 (June 17, 1985).

12. H. Grady Hughes, "New Los Alamos Version of the I.T.S." Los Alamos National Laboratory memorandum X-6:HGH-86-121 (March 27, 1986).
13. James T. West, III, "SABRINA: An Interactive Three-Dimensional Geometry-Modeling Program for MCNP," Los Alamos National Laboratory report LA-10688-M (October 1986).
14. R. E. Prael and H. Lichtenstein, "User Guide to the HETC Code System," Los Alamos National Laboratory, Interim Documentation (October 30, 1986).
15. M. R. Clover, R. M. DeVries, N. J. Giacomo, and Y. Yariv, "Low Energy Antiproton-Nucleus Interactions," Phys. Rev. C 26, 2138 (November 1982).
16. R. D. O'Dell and H. Byers, "Radiation Transport, April 1, 1987 - June 30, 1987," Los Alamos National Laboratory report LA-11188-PR (April 1988).
17. R. D. O'Dell and A. Nagy, "Radiation Transport, January 1, 1987 - March 31, 1987," Los Alamos National Laboratory report LA-11180-PR (February 1988).
18. T. E. Booth, "The Intelligent Random Number Technique in MCNP," Proc. Int'l. Topical Meeting in Adv. in Reactor Physics, Math., and Comp., Paris, France, April 27-30, 1987.
19. T. E. Booth, "A Quasi-Deterministic Approximation of the Monte Carlo Importance Function," Trans. Am. Nucl. Soc. 55, 358 (1987).
20. J. Abdallah, Jr. and R. E. H. Clark, "TOPS: A Multigroup Opacity Code," Los Alamos National Laboratory report LA-10454 (October 1985).
21. J. Abdallah, Jr., G. I. Kerley, B. I. Bennett, J. D. Johnson, R. C. Albers, and W. F. Heubner, "HYDSES: A Subroutine Package for Using Sesame in Hydrodynamic Codes," Los Alamos Scientific Laboratory report LA-8209 (June 1980).
22. Gary W. Pfeufer, "Version 2gc of HANDI for Friendly Users," Los Alamos National Laboratory memorandum X-6:GWP-87-493 (September 24, 1987).
23. W. Spangenberg, "Structure of Collapsed STYX Data Files," Los Alamos National Laboratory internal memorandum X-7-84-U200 (July 23, 1984).