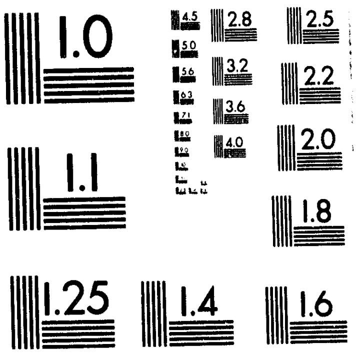
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THE TORSED AND TORSET CODES FOR COUPLING THREE-DIMENSIONAL TORT CALCULATIONS*

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ABSTRACT

Two new codes perform "bootstrapping" of either two- or three-dimensional boundary fluxes to a TORT three-dimensional calculation. TORSED couples a DORT RZ calculation to an XYZ TORT. Two methods of directional remapping are available, each less expensive than methods previously available for this work. TORSED is compatible with the discontinuous mesh features of TORT.

The second code, TORSET, couples two XYZ TORT problems. The second problem may lie entirely inside the first, or it may touch over only a portion of its surface. TORSET can obtain most of its input data from the primary TORT problem or from an automatic mesh generator.

Both codes are available for general use on Cray mainframes and UNIX workstations.

INTRODUCTION

Users of the two-dimensional DOT and DORT codes[1,2,3] have found it important to solve problems in segments, coupling the segments by passing flux or fluence values at an internal boundary of one problem to an external boundary of another. This "bootstrapping" procedure allows the solution of problems too large to be treated as one unit. It also allows the details of a small section to be changed repeatedly without recalculating the flux environment surrounding the section. Bootstrapping is even more important in using the three-dimensional TORT code.[4,5,6] This paper will discuss software for coupling both two- and three-dimensional primary calculations to TORT secondary calculations.

A 1986 code called DOTTOR[7,8] was developed to couple fluence from a DORT air/ground weapons radiation calculation to the surfaces of large concrete buildings to be studied by TORT. DOTTOR assumed that each direction in the quadrature set could be associated with a sector of direction space surrounding it. The code then summed the overlapping sectors in order to perform the directional remapping of flux. Linear interpolation was used to perform the spatial remapping. DOTTOR was successful in its intended application, but it was considered too expensive for application to multi-million-mesh-cell problems. Also, it was not practical to modernize the code to accept new TORT features such as the discontinuous mesh option.

A new code called TORSED[9] now performs the DORT-TORT coupling at a fraction of the CPU and memory cost of DOTTOR, using either of two simplified methods of directional remapping. The "look backward" method is satisfactory except for cases having extreme anisotropy or non-aligned quadrature sets. The "look forward" method is somewhat more expensive, but it has been accurate in the most severe test cases.

The TORSET code couples one TORT problem to another. Indications of the accuracy and cost of both codes are given in the discussion.

THE TORSED CODE FOR DORT-TORT COUPLING

TORSED[9] maps DORT fluxes in RZ geometry into TORT boundary sources in XYZ geometry. There are two elements of this task: performing the spatial interpolation and coping with directional misalignment.

The spatial interpolation is handled in a straightforward way. For a given direction, the mean flux in each DORT cell is associated with a point at the center of the cell, and then the flux at the center of the TORT surface cell is calculated by either linear or logarithmic interpolation. The TORT mesh can be moved about inside the DORT mesh or rotated about the Z axis.

With this done, it is typically found that the DORT quadrature directions are not aligned with the desired TORT directions. This can occur due to rotation of the TORT geometry, to mismatch between the DORT and TORT quadrature, or to the rotation inherent in the transformation from RZ to XYZ geometry. A means of directional remapping is required.

The first method of performing the directional remapping is the "look-backward" method, in which the flux in each TORT direction is set equal to the flux in the nearest DORT direction. This approach has the virtues of simplicity and economy. It was one of the methods used in DOT remapping, and it has been used in various other codes as well. It works best when the flux is a smooth function of direction. It may be inaccurate when the flux has sharp variation between neighboring directions, when the DORT quadrature has unequal weights, and when the direction sets are non-aligned.

TORSED also allows use of a "look-forward" method of directional remapping that is similar to the DOTTOR method in result, although not in detail or cost. In this new method, the flux in each DORT direction is apportioned among TORT nearest-neighbor directions according to a "closeness" criterion. If the DORT and TORT directions lie in common "eta levels", i.e. bands having a common angle with the Z axis, then linear interpolation in the azimuthal angle between two nearest neighbors is used, and the inverse of the sine of the angle between directions is used as the closeness criterion. If the directions do not lie in common eta levels, the interpolation is performed in both azimuthal and polar angles between three nearest neighbors, and the square of the inverse of the sine is used as the closeness criterion.

This method is generally valid for all combinations of directional flux variation, axis rotation, and quadrature mismatch. One potential shortcoming is the possibility of uneven TORT fluxes. An extreme example might be the mapping of an S-2 DORT flux into an S-16 TORT quadrature. In each octant of the TORT flux, no more than three directions would have non-zero flux -- true to the fundamental assumptions of discrete ordinates, but not desirable to the user.

A more practical test is one in which an isotropic S-6 DORT flux is mapped into an S-6 TORT quadrature rotated about the Z axis through 1-degree increments. The maximum and root-mean-square (RMS) deviation from unity in TORT flux are taken as a measure of accuracy. In Table 1, two variations of the look-forward strategy are shown. In the first, nearest neighbors are selected only from the octant in which the DORT direction lies. In the second, close directions in adjacent octants are allowed to be neighbors.

The second method is significantly more expensive to execute than the first, but still much cheaper than the DOTTOR method and within acceptable limits. Accordingly, it was adopted for use in TORSED.

As with any bootstrapping, the user must choose the remapping boundary such that perturbations inside the boundary do not alter the incoming boundary flux significantly. In general, this is true if the boundary is far from the location of the perturbation, or if the enclosed volume is so small that the probability of entry, reflection or transmission, and re-entry is small.

Construction and use of the code are described in ORNL/TM-12359,[9] although certain details of the input, such as how to select the look-forward method, have changed. The user can specify rotation of the TORT geometry about the Z axis, and the TORT mesh may be of the discontinuous type. That type of mesh is described in an appendix of the ORNL document.[9] The VISA code, required as an interface between DORT and TORSED, is also described.

An extensive set of test problems is described in the report. In one, a cylindrical source is surrounded by water and air. Two groups of a 20-group library are solved. A region adjacent to the corner of the source region is chosen for modeling by TORT, as shown in Fig. 1. The outer surface of the DORT cylinder must be represented in stairstep fashion for TORT solution, of course. Even so, TORT boundary fluxes match the corresponding DORT fluxes within 7%.

Another problem maps all 20 groups of DORT flux onto the surface of a 104,247-cell concrete building for which DOTTOR was developed. Significant running statistics for both look-backward and look-forward methods as well as for DOTTOR solution are given in Table 2.

THE TORSET CODE FOR TORT-TORT COUPLING

Another code, TORSET, allows preparation of a TORT boundary source based on files written by another TORT problem. TORSET is particularly easy to set up and use, in that most of the input data can be obtained from the primary TORT problem or from a geometry input file such as that produced by COGEDIF.[10] Because of the potentially-large volume of directional fluxes from the primary problem, the user is allowed to select a sector of the problem over which the fluxes are to be output.

The secondary geometry may be entirely contained within the sector specified in the interface file, or it may overlap only partially, as indicated in Fig. 2. Zero flux is supplied on non-overlapping surfaces. Either linear or logarithmic spatial interpolation is allowed. The secondary mesh may be of the discontinuous type. Rotation of the secondary mesh and interpolation between non-matching direction sets are to be added soon.

One of the available demonstration problems is a simulation of a concrete box sitting on a pad in front of a reactor source as depicted in Fig. 3. Two groups of a 20-group cross section library are solved. The primary TORT calculation was solved both with and without the concrete box. The fluxes from the calculation without the concrete box were transformed into a boundary source for calculation of the box region alone in a secondary TORT calculation. Key flux values at the points indicated in the figure matched the full simulation within 4%.

In a problem designed to test the running speed in a large problem, all 20 groups of flux near the outer boundary of the 104,274-cell problem described earlier were mapped onto another mesh with the same number of cells, but with slightly smaller geometry. This was a "worst case", since the file of directional flux was huge, and each secondary TORT surface cell corresponded to a different cell in the primary TORT mesh, requiring an I/O of a new record. Even so, performance was acceptable, as shown in Table 3. A normal problem would probably be less I/O bound.

AVAILABILITY

TORSED, TORSET, and VISA have been included in the Version 2.8 release of the DORT/TORT package. This can be obtained through the Radiation Shielding Information Center (RSIC) at Oak Ridge. A charge is made for handling.

Operation has been demonstrated on Cray mainframes and on IBM RS/6000 workstations. Installation procedures are also provided for SUN, DEC, and HP workstations.

TABLES

Table 1. Accuracy of two variations of the lock-forward method in remapping isotropic flux

	RMS error	**Maximum error, any rotation**
Octant restricted	16%	54%
Unrestricted	5%	16%

Table 2. Operating costs of TORSED and DOTTOR on the large concrete building problem

	Memory words	**Cray CPU minutes**
TORSED LB option	37,000	0.18
TORSED LF option	121,000	0.76
DOTTOR	486,000	1.81

Table 3. Machine requirement for a "worst case" TORSET problem

	Memory words	**Execution seconds**
Cray X-MP	253,168	72 CPU + 431 system
IBM RS6000/320h	253,168	505

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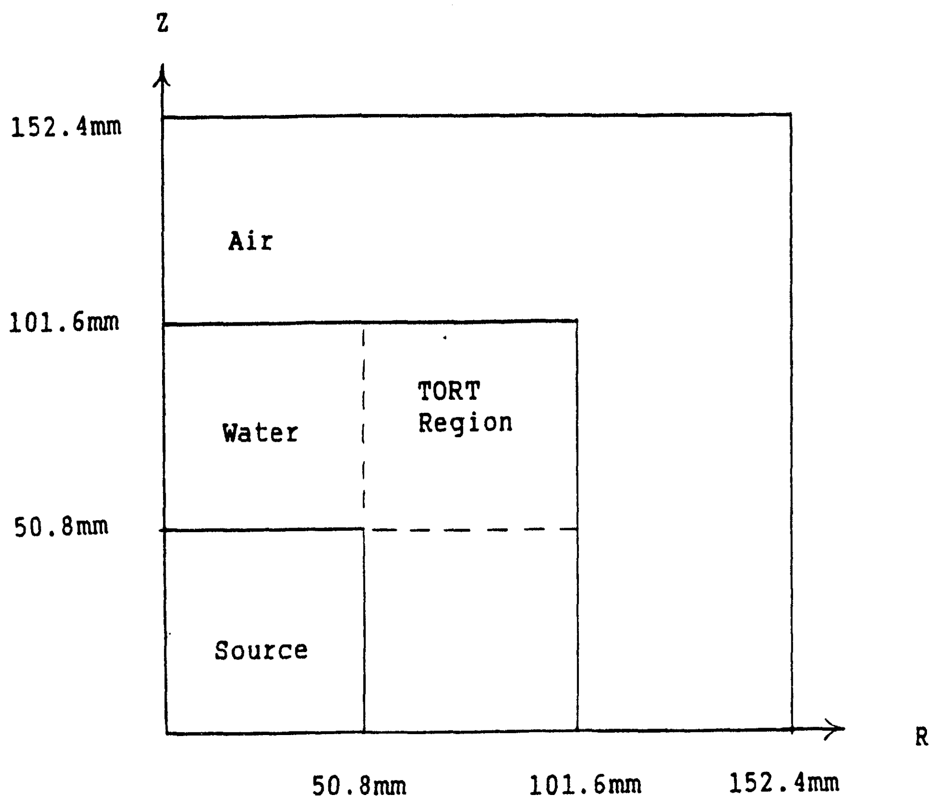

Fig. 1. Coupling of RZ DORT Reactor Calculation to XYZ TORT Geometry.

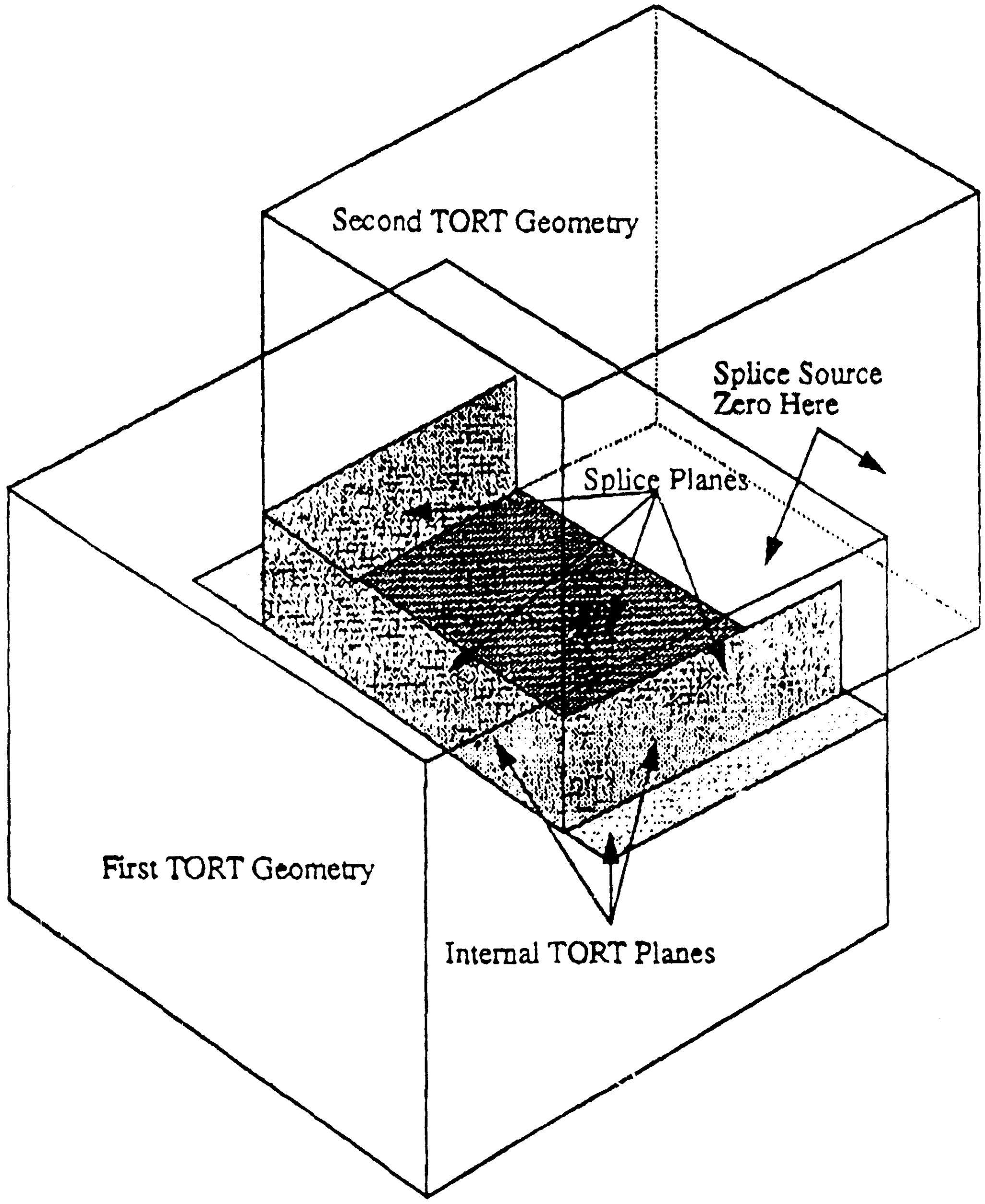

Fig. 2. Treatment of Non-overlapping TORT Meshes.

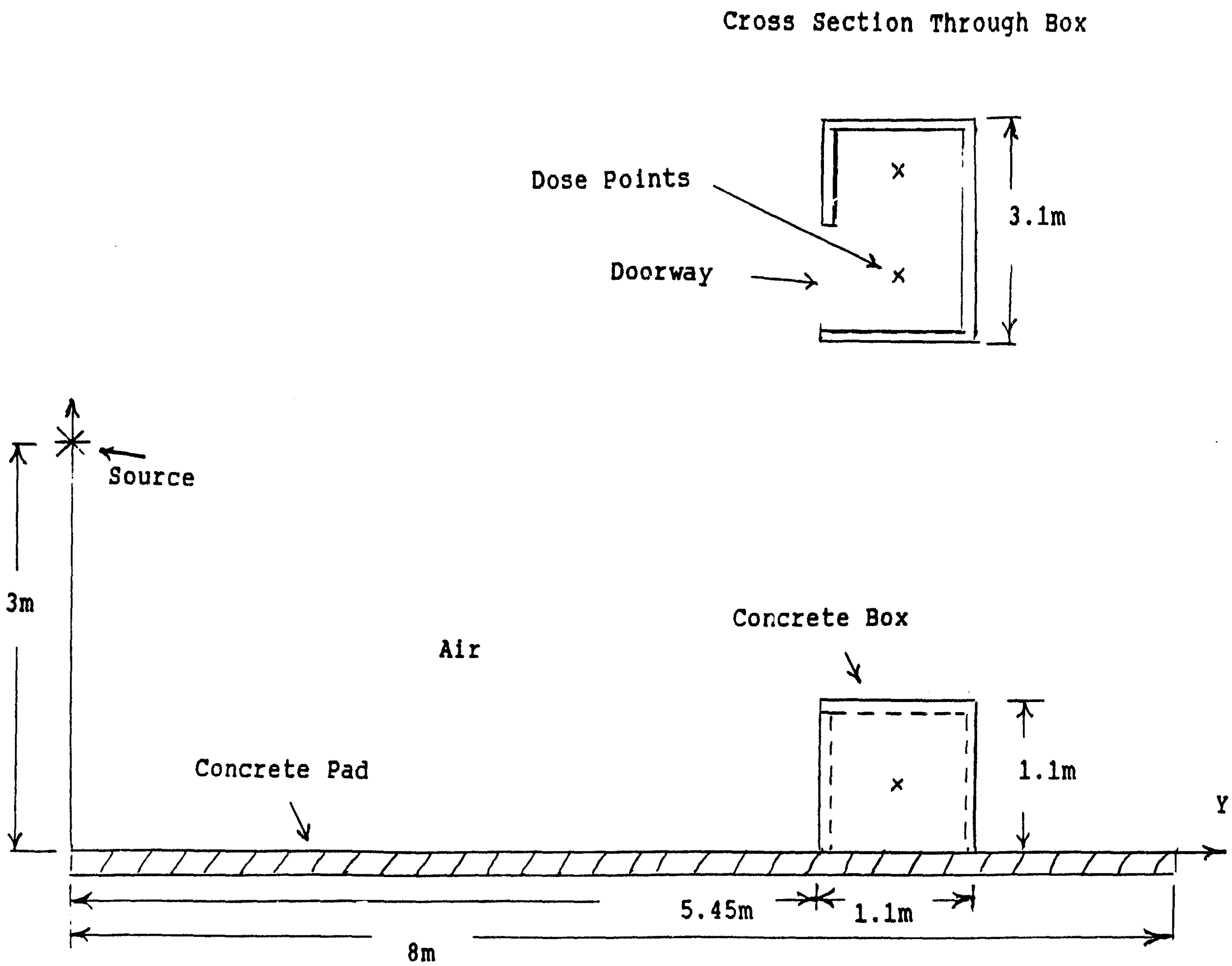

Fig. 3. Coupling of XYZ TORT Environmental Calculation to XYZ TORT Concrete Box Model.

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