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The Three-Dimensional, Discrete Ordinates Neutral Particle Transport Code TORT: An Overview*

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THE THREE-DIMENSIONAL, DISCRETE ORDINATES NEUTRAL PARTICLE TRANSPORT CODE TORT: AN OVERVIEW*

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Abstract

The centerpiece of the Discrete Ordinates Oak Ridge System (DOORS), the three-dimensional neutral particle transport code TORT is reviewed. Its most prominent features pertaining to large applications, such as adjustable problem parameters, memory management, and coarse mesh methods, are described. Advanced, state-of-the-art capabilities including acceleration and multiprocessing are summarized here and detailed in other papers in these Proceedings. Future enhancement of existing graphics and visualization tools is briefly presented.

Introduction

The Discrete Ordinates Oak Ridge System (DOORS) is comprised of several computer codes developed over the years at Oak Ridge National Laboratory to solve a wide variety of neutral particle transport problems arising in applications. The first release of DOORS 3.1 in 1995 was characterized by a modernized installation procedure and an expanded list of peripheral codes included in the distribution, as well as other new features.[1,2] Bringing the member codes together in DOORS is the first step in establishing smoother connections between them which will eventually be manipulated via a user friendly Graphical User Interface (GUI).

As the power and capacity of electronic computers expanded over the past three decades the work horse of the transport calculations evolved in dimensionality from one-, to two-, to three-dimensional. Time consuming cross section generation is often still performed using one-dimensional models, and two-dimensional models still suffice for many applications. Hence DOORS includes codes for these purposes; the focus of this paper, however, is the three-dimensional code TORT.[3]

TORT was conceived in the mid eighties to compute radiation dose profiles in large multistory concrete buildings. While largely based on its two-dimensional predecessor, DORT, it quickly evolved in an individual fashion suited to the difficulties associated with the problems it is applied to, primarily size. Thus high order, coarse mesh methods, vectorization of the mesh sweep, discontinuous mesh, among others, are features developed and implemented exclusively for TORT.[3] These

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and other unique features of the code made it an invaluable computational tool for large problems in a wide variety of applications. A high level of confidence in TORT's reliability and computational efficiency has been established over the years through the experiences of many researchers and engineers working in different areas.

While TORT is a general purpose transport code it has gained particular notoriety for accurately solving large problems with complex configurations. At present the largest TORT application employs 3.6 million computational cells, S_{16} angular quadrature, P_3 anisotropic scattering expansion, and 11 energy groups, a monumental challenge to the computational resources typically available at research institutions. The code's *production* attributes, such as robustness, efficiency, accuracy, and reliability, resulted in its proliferation into many areas of application new to deterministic transport methodologies. These include medical applications,[4,5] charged particle transport,[6] and time dependent calculations,[7] in addition to the traditional reactor physics and shielding applications; see for example Refs. 8,9.

In the remainder of this paper we present an overview of TORT emphasizing its most salient features that make it particularly suitable for large production level applications. We start with a brief description of DOORS and its member code, then we discuss adjustable problem parameters including discontinuous mesh, and the memory management capability. The three spatial approximations available in TORT are reviewed next, then acceleration schemes for the iterative process are described, followed by a brief section on multiprocessing with TORT. The last section is dedicated to graphical routines currently available and visualization tools planned for the future.

Discrete Ordinates Oak Ridge System (DOORS)

DOORS is a collection of codes built around the discrete-ordinates codes ANISN, DORT, and TORT gives the user a wide range of capabilities to pre- and post-process data in transition from one computation to the next. These codes represent a total investment of many man-years of effort contributed by many researchers over the past three decades. While most codes included in the present version of DOORS are in their original condition, they have been packaged and will be maintained in unisome in the future. DOORS also introduced modern maintenance and installation procedures, e.g. makefiles, that facilitate updating activities and extend the package's compatibility into the future. ORNL supports DOORS on UNIX-based platforms, Cray supercomputers, and a variety of workstations; PC versions of some of the member codes have been reported and are available from RSICC.

A complete list of the codes comprising the DOORS package at present is shown in Table 1. Among these perhaps the best known are the one-, and two-dimensional sister codes ANISN, and DORT, respectively. While TORT has a one-, and two-dimensional solution capability, these codes are easier to use, and have additional features, e.g. some curvilinear geometry options, which have been more thoroughly tested over the years. Furthermore, because their lower dimensionality is hardwired into them, ANISN and DORT utilize computational resources more efficiently and are more likely to provide faster execution. For this reason they are often used in scoping calculations that require repetitive solution of slightly differing problem configurations. In this regard the adjoint capability of all DOORS transport codes sometimes aides the search for optimal configurations.[5]

The TORSED and TORSET codes implement splicing and bootstrapping techniques that permit the solution of problems that are too large to solve with TORT in their entirety. Essentially these methods amount to a split of the problem domain into two, or more, subdomains that are loosely coupled in only one direction from the source, *primary,* to the observable, *secondary,* configurations, with weak feedback. For details of these techniques and their implementation in important example which has proven extremely valuable in solving very large problems with substantial geometric detail is the discontinuous mesh option in TORT. This feature allows the user to employ more computational cells where fine geometric structure exists, and fewer cells elsewhere. This is achieved by allowing the user, within some constraints, to adjust the number and boundaries of individual cells within a row, not necessarily coinciding with those in adjacent rows. The fact that the solution algorithm in TORT reduces the most general problem to a sequence of sweeps along a row of computational cells in the x–dimension in a given direction allows each row to be processed individually then the boundary angular flux incoming to adjacent rows are inter- or extrapolated to that row's cell structure.

Other adjustments to problem parameters not related to phase space size include, for example, setting iteration number by group, etc. These typically pertain more to reducing execution time by avoiding tight convergence of groups that are inconsequential to the purpose of the computation.

Recent research aimed at providing TORT with the capability to account for heterogeneous material, combinatorial geometry objects by manipulating the spatial weights in the discrete-variable equations is detailed in Ref. 11.

Memory Management

In spite of the flexibility afforded the user in concentrating the computational effort at regions of high sensitivity to the level of detail it is customary in scientific research and engineering design to constantly push the capability limits in order to make progress. Thus the insatiable demand for finer detail kept pace with the phenomenal growth in memory size and external storage options available. Virtual memory is a generic solution to this problem available on many platforms that is designed to conduct the I/O activity at the operating system level thereby relieving the programmer from the burden of foreseeing and accommodating a wide variety of hardware configurations and run time conditions. Nevertheless, the price of this flexibility is paid by the user in the form of long execution times because the generic I/O scheme does not take into account natural *breakpoints* in the solution algorithm of transport problems.

In recognition of this fact, and also to accommodate a variety of platforms with a disparate range of memory sizes TORT attempts to meet a *memory objective* set by the user at run time. First TORT tries to fit the entire problem in the memory objective; if this is not possible it attempts to fit one group at a time within the memory objective and I/O flux and cross section data to scratch files. If this too fails, the code breaks up the geometric configuration into blocks of planes, each of which can fit within the memory objective, and I/O to scratch files is used to maintain and update the data during the calculation. If a single plane does not fit in the memory objective TORT tries to obtain additional memory beyond that specified by the memory objective, assuming it is less than all that is available on the machine, and if this fails it informs the user of its attempts then terminates execution unsuccessfully. Clearly this sequence of attempts is designed to minimize the adverse effect of I/O on performance while enabling the solution of ever larger problems.

Spatial Discretization Methods

TORT is based on the discrete ordinates approximation of the independent angular variable, and the multigroup discretization of the energy variable. Three approximation methods for the spatial dependence are available in the code to accommodate a broad spectrum of applications.

The oldest is the θ–weighted method, which was originally implemented in DORT, represents a whole set of methods parametrized by the single parameter θ set by the user at run time in the

Table 1. Member Codes in the DOORS Package

Code	Function
anisn	Solve one-dimensional transport problems
gbanisn	**anisn** with group band option for thermal upscatter
dort	Solve two-dimensional transport problems
tort	Solve three-dimensional transport problems
torset	Couple primary to secondary **tort** calculations
torsed	Couple *rz*–**dort** to *xyz*–**tort** calculations
visa	Prepare **torsed** input from **dort** output file
alc	Maintenance of cross section library
gip	Prepare cross section library
grtuncl	Estimate uncollided flux and first collided source
falstf	Project last collision source to point detector
bndrys	Convert internal boundary flux to internal boundary source
rtflum	Convert flux moment file across formats
isoplot	Generate contour plot of flux or response
xtorid	Extract planar slice from **tort** output to plot with **isoplot**
jdos	Execute sequence of calculations
drv	Driver module called by **jdos**
cmp	Maintenance of code system*
rscors	Graphics library*

* Public domain software from Sandia National Laboratory

TORT see Ref. 10.

Adjustable Problem Parameters

Perhaps the factor that most contributes to the difficulty of transport calculations is the large size of the discrete variable system of equations that must be solved numerically. This is a direct consequence of the high dimensionality of phase space, a fact that is easily illustrated by considering a a steady state transport problem in d–dimensional geometry. In such case the phase space is of dimension $2d$: d variables representing physical space, $d-1$ representing the particles direction of motion (discrete ordinates), and one energy variable. It is critical, therefore, to *conserve* discrete variables as much as possible without jeopardizing the accuracy and reliability of the solution. This is accomplished in TORT by permitting the user to adjust the level of detail in a variety of problem parameters according to the anticipated local rate of change in the solution.

For example, sharp flux and cross section anisotropies are more notable at the high energy end of the spectrum. Hence TORT permits the user to select a high order angular quadrature set and high order P_l expansion of the cross sections in the high energy groups, and lower orders in the low energy groups thereby reducing the problem size without sacrificing accuracy. Another range [0,1). This is a weighted diamond difference method spanning the range from the diamond difference scheme (optically thin cells) to the Step method (optically thick cells) where the weights are computed to ensure positivity of the outgoing angular flux given positive incoming flux and volumetric source. Due to the relative simplicity of its equations and its low order approximation, the θ–weighted method is the least computationally intensive option among TORT's spatial approximation methods. Also, it is the least accurate on a given mesh.

The Linear Nodal (LN) method was installed in TORT to enable using optically thick cells while retaining high accuracy of the computed angular flux. This is achieved by computing the first spatial moment of the angular and scalar flux, in addition to the average quantities computed in the θ–weighted method.[12,13] Many modifications to the original method have been implemented over the years in order to improve method accuracy and efficiency, and solution positivity to the extent that, at present, LN is the recommended method for most large applications with optically thick regions in TORT.

The Linear Characteristic (LC) method[15] also computes the first spatial moment of the flux on each cell's surfaces and volume using the exact characteristic paths from incoming to outgoing surfaces, then projecting the resulting expression onto the basis functions (constant and linear). As far as accuracy is concerned LC is competitive with LN with each method gaining an edge over the other for some, but not all, problems. LC executes faster than LN on scalar machines, but due to the high level of vectorization of the LN it is about four times faster on Cray computers.[14]

On a given mesh LN and LC run longer, require more memory, and consume larger disk space but provide more accurate solutions than the θ–weighted method. However, for a fixed accuracy the latter method typically requires eight times as many computational cells than either of the linear schemes. Ultimately for the same solution accuracy requirement, the linear methods end up utilizing less computational resources, i.e. CPU time, memory, and disk space, than the θ–weighted method.[14]

Iteration Acceleration Methods

The recommended method for accelerating the iterative convergence of the inner iterations in TORT is the Partial Current Rebalance (PCR) method.[3] This method is based on reinforcing the balance of neutrons over each computational cell using the cell-surface partial currents resulting from the latest mesh sweep. The discrete variable equation resulting from PCR has the same cell-coupling stencil as a discretized cell-centered diffusion equation but does not necessarily possess some of its important features like diagonal dominance, etc. The PCR matrix equation is solved via a Successive Over-Relaxation (SOR) scheme with the relaxation factor computed numerically from the SOR iterates.

For most TORT applications PCR has proven robust and efficient. However, recent advances in the analysis of the spectral properties of iterative procedures for solving the transport equation have provided the basis for powerful acceleration operators that, at least theoretically, exceed the performance of PCR. The most notable example of such new methods is Diffusion Synthetic Acceleration (DSA) whose spectral radius is bounded from above by 0.25 for model problem configurations, i.e. homogeneous material composition and uniform mesh. The most serious limitation of the class of unconditionally stable DSA operators as far as large three dimensional applications is concerned is that they are edge-centered. Since there are many more surfaces than computational cells the DSA matrix equation can be prohibitively large; this difficulty is compounded further in high order methods, i.e. LN and LC, if the first spatial moments of the flux are to be accelerated also.

A more general framework for acceleration schemes, the Adjacent-cell Preconditioning method, has been implemented recently in TORT and is reviewed in Ref. 15. AP is cell-centered and has the same coupling scheme as a discretized cell-centered diffusion equation but its elements are not based on the diffusive properties of a computational cell. Rather, the preconditioner elements are set to provide a vanishing spectral radius of the flat eigenmode of the homogeneous model problem, with reciprocal averaging across material heterogeneity interfaces. Therefore, the preconditioning stage of the iterative process is comprised of a system of discrete-variable equations that is amenable to solution via the same SOR routines in TORT used to solve the PCR equations.

Testing of the AP in TORT demonstrated its effectiveness in reducing the number of iterations required to achieve convergence for all members of the Burre Suite of Test Problems (BSTeP) covering a wide range in parameter space. In fact AP converged in fewer iterations than PCR or TWODANT's DSA for the vast majority of cases comprising BSTeP. However, these tests illustrated the deterioration in spectral properties in cases with sharp material discontinuity contradicting behavior predicted by the homogeneous model problem analysis. Furthermore, this undesirable behavior seems to be commonly shared with other acceleration schemes including PCR and DSA. Analysis of a model problem with material discontinuity, the Periodic Horizontal Interface (PHI), has been analyzed to verify and investigate this phenomenon.[15]

Multiprocessing

A multitasking capability at the macrotasking level is available in TORT for execution on multiprocessor Cray computers running the UNICOS operating system. It is based on a coarse-grained angular domain decomposition which typically produces good parallel efficiency due to the relatively large computation load to parallelization overhead ratio. Since angular domain decomposition in Cartesian geometry is intrinsic there is a one-to-one correspondence (within arithmetic precision) between the sequential and parallel intermediate and final results, so that the number of iterations required to achieve convergence is independent of the number of concurrent processes. The multitasking option, selected by the user at run time, has been tested on Cray Y/MP, C90, and J90 systems and have exhibited significant wall clock speedup factors even for modestly large problems. The problem with quantifying parallel performance on time-shared computers such as the Cray is its sensitivity to machine loading during execution. Nevertheless it was possible to quantify the parallelization overhead for two test problems and conclude the necessity to reduce it sharply.

Recently, a performance model was constructed and validated for the parallelization overhead as a function of the number of participating tasks and other problem parameters. Parametric studies with this model identified the major contributors to parallelization penalty, and efforts were made to reduce their effect on parallel speedup.[16] As a result the present multitasking algorithm incurs only 25-35% of the parallelization penalty previously measured, and improvement in wall clock speedup of up to 50% has been observed in some cases.

Graphics and Visualization

Earlier development of graphics capabilities for DORT utilized a commercial library to provide elementary graphics constructs. More recently ORNL has opted for public-domain-based development of our neutronic codes graphics capabilities in order to facilitate distribution of the package in a self-contained form for the users' convenience. For this purpose we adopted Sandia National Laboratory's RSCORS graphics library which is distributed with future releases of DOORS; see Table 1.

The user of TORT can generate plots of flux or activities from formatted or unformatted files generated by the code using the XTORID and ISPL3D codes.[17] Two dimensional plots are generated for selected planes in the TORT geometry, and can be viewed on-screen for a variety of platforms, or in hardcopy. Several options are available for displaying the plotted quantity: color and greyscale shading, symbol and line contours. In addition, the geometric configuration of the selected plane can be overlaid on the plot.

Another ORNL graphics capability that was originally developed for use with the combinatorial geometry models of the MASH shielding code is the Oak Ridge Geometry Analysis and Modeling Interface (ORIGAMI). ORIGAMI is XWindows based and has been developed and tested on IBM workstations. Its primary function verification and debugging of computational models, and visualization of computed results. ORIGAMI is not distributed in the present release of DOORS, but might be included in the future. Finally, users with specific interfacing needs develop their own pre- and post-processors for TORT.[18]

The seemingly endless increase in computational power, i.e. speed and storage size, has caused applications to grow in size resulting in extremely large data sets that are becoming harder to manage. The need for an interactive Graphical User Interface (GUI) is evident and we hope to begin constructing one for DOORS soon.

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