LA-UR 93-807

CONF-930907--2

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SUBMITTED TO Paper review for the 1993 "Physics and Methods in Criticality Safety" Topical Meeting of the ANS Nuclear Criticality Safety Division. (September 1993 in Nashville, TN)

MASTER

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RECENT DEVELOPMENTS IN THE TWODANT SYSTEM OF CODES FOR CRITICALITY SAFETY

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I. INTRODUCTION

The application of deterministic, discrete ordinates codes to criticality safety problems can be a very useful complement to analyses performed using Monte Carlo methods. This is especially so if there is a need for dose or flux maps of the system or if configuration perturbations are to be studied. In these latter two situations, it is difficult to obtain reliable Monte Carlo results due to statistical effects. Deterministic calculations are also useful as an independent check and verification of Monte Carlo results.

The TWODANT system of discrete ordinates codes[1] has recently been enhanced for criticality safety analysis. In addition to ONEDANT, TWODANT, and TWOHEX, the TWODANT system now includes TWODANT/GQ and THREEDANT. These two new code modules expand the applicability of the TWODANT system. These new capabilities will be demonstrated on a representative sample of nuclear criticality safety problems.

First, TWODANT/GQ and THREEDANT will be described. Salient features of each code module will be discussed. Calculational results obtained by each will be presented and compared with each other and with Monte Carlo results. Finally, some guidelines for the effective use of the TWODANT system on criticality applications will be given.

II. TWODANT/GQ

TWODANT/GQ is a generalized quadrilateral mesh version of TWODANT. TWODANT/GQ may be used in either X Y or R Z geometry, though R Z will be employed exclusively here. This flexible mesh capability allows, for example, TWODANT/GQ to model a sphere nearly exactly in R-Z geometry. This capability will be demonstrated in the calculational results.

Even though a non-orthogonal spatial mesh is used in TWODANT/GQ, the well known and very effective Diffusion Synthetic Acceleration (DSA)[2] is used on both the inner and outer iterations. The coding in TWODANT/GQ is also vectorized except for the one-time ordering of cells for the transport sweeps. The spatial differencing used by TWODANT/GQ can best be described as "diamond-difference-like"[3] and is well behaved in the absence of too many distorted mesh cells. Hence, TWODANT/GQ performs nearly as well as TWODANT on most problems.

About the only difficulty encountered with TWODANT/GQ is the generation of the spatial mesh. Because of the large amounts of information, the geometry input can become tedious. To ease this difficulty, a graphical user interface, ORION, is being developed

III. THREEDANT

THREEDANT is a natural extension of TWODANT to X-Y-Z and R-θ-Z geometries. Only X-Y-Z THREEDANT will be used here. Like TWODANT, THREEDANT uses diamond-differencing, DSA, and diagonal sweep (in each plane) vectorization. THREEDANT's input file and interface file formats are all highly compatible with the rest of the TWODANT system. This means, for example, that a TWODANT input deck may be very easily converted into a THREEDANT input deck.

THREEDANT is currently the only 3D deterministic code which is practical for criticality safety calculations. TORT,[4] a 3D deterministic shielding code, is not efficient for criticality because it lacks outer iteration DSA and diagonal sweep vectorization. TORT is further limited by a restrictive geometrical input. Currently, only rectangular parallelpiped shapes may be input into TORT.

On the other hand, THREEDANT can now be linked to a mesh generation code, FRAC IN THE BOX.[5] FRAC accepts nested region geometry input (including rectangular parallel pipeds, spheres, spherical slices, cylinders, cones, wedges, arbitrary hexahedrons, and general tabular bodies) and generates an X-Y-Z mesh and produces a binary interface file for THREEDANT. FRAC also automatically generates the homogenized material densities inside of each fine mesh cell. Material masses are preserved.

The only practical limitation to FRAC is that all geometric bodies must either be separate from each other or completely enclose each other. At the moment, partial overlap of bodies is not permitted.

Since the problem geometry is not exactly preserved by this "slice and dice" homogenization method, results will be given to show the accuracy of the procedure. At issue is the effect of the discretized surface representation on the solution accuracy. If the spatial mesh is less than a neutron mean free path, then the surface is considered well defined.

IV. CALCULATIONAL PROCEDURES

In order to understand the calculational results in the following sections, some general considerations of discrete ordinates calculations should be reviewed. Unlike Monte Carlo, discrete ordinates calculations require a spatial mesh which mush be fine enough for accuracy but coarse enough for computational efficiency. Similarly, angular quadrature (i.e., the S_N order) must be fine enough for accuracy but coarse enough for computational efficiency. Therefore, for each problem, results from a representative range of spatial mesh configurations and angular quadratures will be presented.

The calculations presented below are meant to be benchmark solutions. Hence, the pointwise flux iteration convergence criteria was used. This particular criteria can be relaxed considerably if only the deterministic eigenvalue is desired.

All of the calculations carried out with the TWODANT system used the LANL 118 isotope 16-group Hansen-Roach cross-section library. Appropriate selection of fissile and fissionable isotopes was based on the potential scattering of light isotopes per absorber atom. Standard default quadrature sets were used for all of the deterministic calculations. Any problem symmetries which were present were utilized to reduce the size of the calculations.

All of the calculations reported here were carried out on a 8 processor 128 Megaword CRAY YMP. None of the calculations were multitasked, however. Currently, the CRAY YMP has a maximum field length of ~800 Mbytes and disk space of ~45 Gbytes. The fact that the CRAY is a vector machine is very important to the TWODANT system of codes. Deterministic codes are generally more vectorizable than Monte Carlo codes. Thus, much of the execution speed of the TWODANT system is due to vectorization.

V. CALCULATIONAL RESULTS

A. Part I Bare Assemblies

As a first example of the new capabilities of the TWODANT system, we have chosen to analyze 2 bare critical assemblies. The first is the well known GODIVA core and the other is a cylindrical assembly with intermediate U 235 enrichments. We will demonstrate that TWODANT/GQ can indeed model a sphere and that the "slice and dice" discretization and homogenization used in THREEDANT can be used to analyze criticality problems. The particular problem descriptions used here were taken from a MCNP neutron benchmark report.[6]

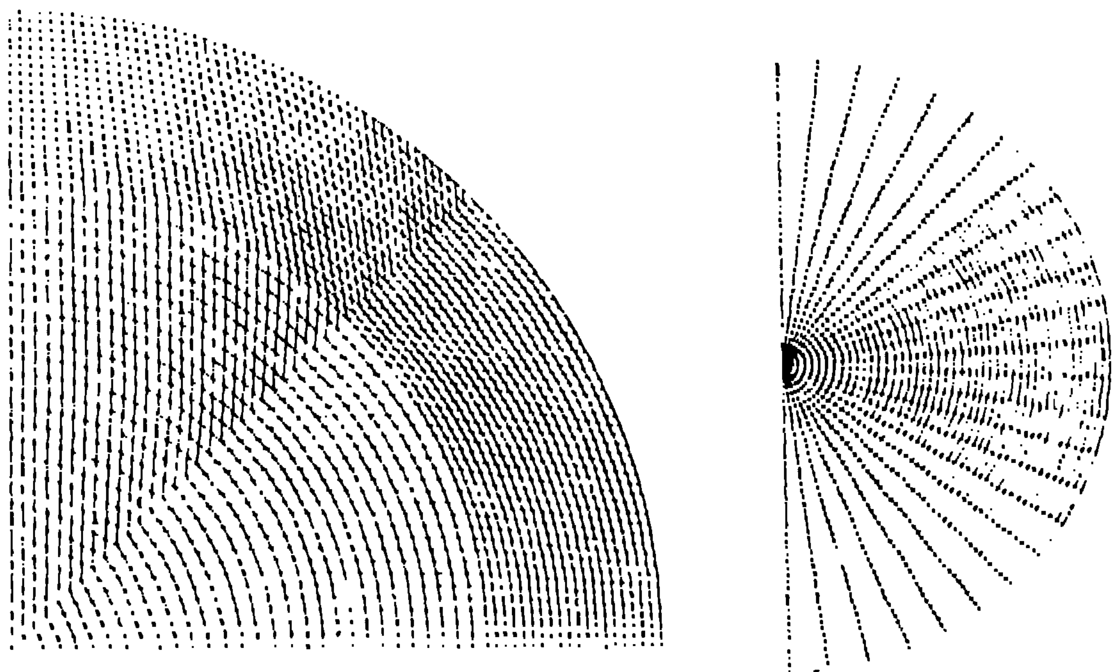
For GODIVA, two different TWODANT/GQ meshings were used. They are illustrated in Fig. 1. Results from the GODIVA analyses are given in Table I. All deterministic calculations reported here were run with a convergence criteria of 10^{-3} or 10^{-4} on the pointwise fluxes. Quite a few results for different quadratures are given to show that X-Y-Z THREEDANT is somewhat less quadrature sensitive than ONE or TWODANT in curvilinear geometries. This is believed to be related to the fact that the basic discrete ordinates formulation is simpler in cartesian than it is in curvilinear geometries. There is no angular redistribution in cartesian geometries. The practical result of this is that low order quadratures may generally be used in THREEDANT.

For the bare cylinder problems, THREEDANT results are compared to TWODANT in Table II. At 10.9% enrichment, the critical height was estimated to be 119.4 cm. At 14.11% enrichment, the critical height was measured to be 44.24 cm. The THREEDANT results are seen to be very consistent with the geometrically exact results from TWODANT.

It is also apparent from Table II that the LANL 118 isotope Hansen-Roach cross sections are not appropriate for this problem. That the problem is set up correctly was verified by rerunning this analysis with another cross section library the LANL MENDF5 library. All of the calculated eigenvalues were then found to be ~.99. This is considered "critical" since MENDF5 does not account for delayed neutrons.

B. Part 2 - Reflected Cores

To add geometric complexity to our analysis, we now turn to reflected cores. The problems which we have selected are a graphite reflected uranium sphere, a water reflected uranium sphere, and a uranium sphere supported by plexiglass and submerged under water. The first two problems were taken from the MCNP neutron benchmark report.[6] The third problem is from the MCNP criticality benchmark report.[7] It is also sample problem 15 of the standard 25 test problem set for KENO.[8]



Mesh 1 Mesh 2

Fig. 1 TWODANT/GQ meshes for GODIVA.

TABLE I

GODIVA ANALYSIS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
ONEDANT	50	.17cm	S_8	.9979	< 0.1 mins
			S_{12}	.9965	< 0.1
			S_{16}	.9960	< 0.1
			S_{24}	.9957	< 0.1
TWODANT/GQ	#1 49x49	.18cm	S_8	.9970	0.5 mins
			S_{12}	.9961	0.7
			S_{16}	.9958	1.0
	#2 14x25	.20cm	S_8	.9967	0.3 mins
			S_{12}	.9958	0.5
			S_{16}	.9955	0.4
THREEDANT	25x25x25	.34cm	S_4	.9942	1.7 mins
			S_6	.9942	1.9
			S_8	.9942	2.5
THREEDANT	50x50x50	.17cm	S_4	.9950	6.2 mins
			S_6	.9950	8.3
			S_8	.9950	11.5

TABLE II

BARE CYLINDRICAL REACTOR ANALYSIS

Code	U-235 Enrichment	mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
TWODANT	10.9%	55x125	.48cm	S_8	.9754	0.4 mins
				S_{12}	.9750	0.7
				S_{16}	.9749	1.1
THREEDANT*	10.9%	55x55x125	.48cm	S_6	.9749	39.3 mins
				S_8	.9747	50.8
TWODANT	14.11%	55x55	.48cm	S_8	.9764	0.2 mins
				S_{12}	.9761	0.4
				S_{16}	.9760	0.6
THREEDANT*	14.11%	55x55x55	.48cm	S_6	.9755	13.7 mins
				S_8	.9756	20.8

*10^{-3} pointwise convergence

For the graphite reflected uranium sphere, our results are given in Table III. Our results from the water reflected sphere are in Table IV and sample problem 15 results are found in Table V. A picture of the TWODANT/GQ interior region mesh for sample problem 15 is shown on Fig. 2.

The somewhat greater sensitivity to spatial mesh seen in Tables IV and V is not surprising. Both of these problems contain water which has a mean free path of ~.33 cm in group 16 of the Hansen-Roach energy structure. It is also known that diamond differencing generally requires a spatial mesh less than or equal to 1 2 mean free paths for accuracy. In fact, the same general mean free path considerations apply to the "slice and dice" discretization and homogenization procedure used in FRAC for THREEDANT. Therefore, a spatial mesh which is refined enough for the diamond differencing will generally be refined enough for the "slice and dice" homogenization.

TABLE III

GRAPHITE REFLECTED URANIUM SPHERE ANALYSIS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
ONEDANT	180	.07cm	S_8	1.0000	< 0.1 mins
			S_{12}	.9983	< 0.1
			S_{16}	.9977	< 0.1
THREEDANT	50x50x50	.25cm	S_4	.9988	10.7 mins
			S_6	.9986	15.8
MCNP				.9981±.0010	19.4 mins

TABLE IV

WATER-REFLECTED URANIUM SPHERE RESULTS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
ONEDANT	180	.17cm	S_8	.9951	< 0.1 mins
			S_{12}	.9932	< 0.1
			S_{16}	.9924	< 0.1
ONEDANT	60	0.50cm	S_8	1.0024	< 0.1 mins
			S_{12}	1.0003	< 0.1
			S_{16}	0.9997	< 0.1
THREEDANT*	50x50x60	0.60cm	S_4	1.0023	20.5 mins
	60x60x70	0.50cm	S_4	1.0003	30
			S_6	1.0003	58
	70x70x70	0.44cm	S_4	.9989	43
	80x80x80	0.38cm	S_4	.9977	58
MCNP				.9956±.0022	123 mins

* 10^{-4} pointwise convergence

TABLE V

SAMPLE PROBLEM 15 RESULTS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
TWODANT/GQ	73x102	$\sim$.5cm	S_8	1.0028	1.4 mins
			S_{12}	1.0019	2.0
			S_{16}	1.0015	3.8
THREEDANT*	70x70x100	.44cm	S_6	1.0051	76 mins
	100x100x125	.35cm	S_6	1.0025	152 mins
MCNP				1.0016±.0011	330 mins

* 10^{-4} pointwise convergence

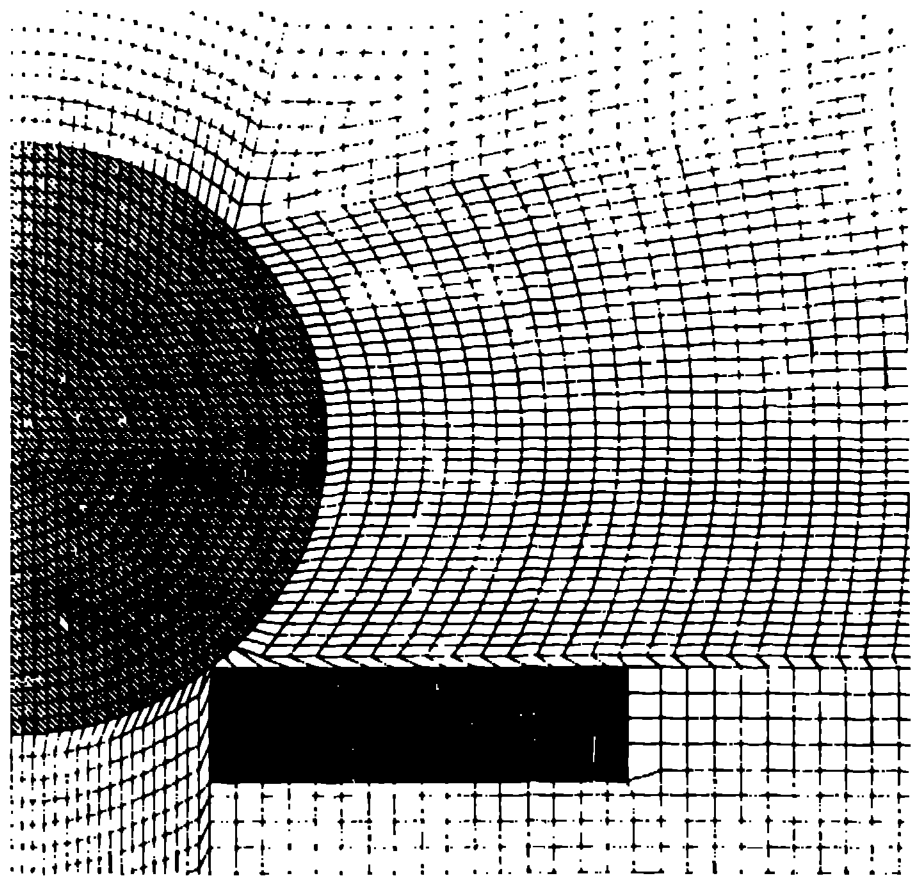


Fig. 2. Interior mesh for TWODANT/GQ on Sample Problem 15

As the THREEDANT calculations begin to be "large" (and the definition of large would be machine dependent), cpu time can be reduced by relaxing the THREEDANT pointwise flux convergence criteria from 10^{-4} to 10^{-1}. In all of the problems run to date, this has been found to speed up the calculation significantly and to change k_{eff} by less than 0.0003.

C. Part 3 - Solutions and Arrays

Results from several additional calculations will now be provided to further demonstrate the capabilities of TWODANT/GQ and THREEDANT. The first problem in this section is sample problem 21 from the KENO test problem set.[7,8] It is a spherical aluminum tank mostly filled with a solution of highly enriched uranyl fluoride. Results are given on Table VI.

The next problem is sample problem 20 from the KENO benchmark problem set.[7,8] Seven cylinders of uranyl fluoride are arranged in a triangular pitch pattern. Results are given in Table VII.

TABLE VI

SAMPLE PROBLEM 21 RESULTS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
TWODANT/GQ	50x100	.69cm	S_6	1.0041	0.6 mins
			S_8	1.0038	0.8
THREEDANT*	70x70x140	.50cm	S_6	1.0018	50 mins
			S_8	1.0019	94
MCNP			--	.9962±.0008	143 mins

* 10^{-3} pointwise convergence

TABLE VII

SAMPLE PROBLEM 20 RESULTS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
THREEDANT*	57x67x37	.50cm	S_4	.9907	10.1 min
			S_6	.9851	13.2
			S_8	.9845	17.7
THREEDANT*	85x93x54	.34cm	S_4	.9911	26.1mins
			S_6	.9864	37.2
			S_8	.9846	51.0
MCNP				.9960±.0012	35.5 mins

* 10^{-4} pointwise convergence

The final problem is sample problem 18 from the KENO benchmark problem set.[7,8] Twenty seven cylinders of uranyl nitrate solution are arranged in a 3x3x3 array and placed inside of a 6 inch paraffin reflector box. Results for this problem are given in Table VIII.

TABLE VIII

SAMPLE PROBLEM 18 RESULTS

Code	Mesh	Avg. Mesh	Quadrature	k_{eff}	cpu time
THREEDANT	90x90x90	.78cm	S_8	1.0092	181 mins
THREEDANT	100x100x100	.71cm	S_8	1.0096	230 mins
THREEDANT	110x110x110	.64cm	S_8	1.0098	330 mins
THREEDANT	135x135x135	.52cm	S_8	1.0095	801 mins
KENO V.a	—	—	—	1.0084±.0013	40 mins
MCNP*	—	—	--	1.0302±.0012	329 mins

* Lacks a paraffin $S(\alpha,\beta)$ treatment.

The THREEDANT results are non-monotonic since the unevenly spaced mesh pattern used on the first three calculations was not used on the last calculation. The last calculation was evenly spaced in its spatial mesh.

This last problem has a spatial domain dimension of ~70 cm (after symmetry boundary conditions are used). This large domain is difficult for THREEDANT because of the very large number of mesh cells required. The fine mesh requirement of diamond differencing and "slice and dice" homogenization thus limits THREEDANT to criticality applications which, after symmetry, are relatively small in spatial domain. A practical limit for our CRAY-YMP would be about250 mean free paths. (125 mesh x 2 mfp per mesh).

D. CPU Time Comparisons

The cpu times quoted herein should be understood to be approximate in nature. Both TWODANT/GQ and THREEDANT are still evolving and calculational speed-ups are expected. Furthermore, all cpu time comparisons are highly machine and calculation dependent.

Just as Monte Carlo calculations can be shortened or lengthened by statistical error requirements, discrete ordinates calculational times are dependent on spatial meshing and angular quadrature requirements. It is for this reason that we have presented a spread of discrete ordinates results for each problem.

The extremely large 135x135x135 calculation performed on Sample Problem 18 should be considered a demonstration calculation only. It required ~600 Mbytes of the "core" memory on our CRAY-YMP. The calculation's scratch files required disk space much larger than that. Therefore, this calculation is very near the limit of our calculational capability with THREEDANT on our CRAY-YMP. More typical calculations (50-100 mesh cells in each dimension) required from ~50 to ~200 Mbytes of core.

VI. SUMMARY AND CONCLUSIONS

It has been shown that TWODANT/GQ and THREEDANT broaden the capability of discrete ordinates codes in criticality safety calculations. The rather general geometric capabilities of TWODANT/GQ and THREEDANT have been demonstrated on a sampling of benchmark criticality problems. Relatively good agreement with published Monte Carlo results and critical experiments has been seen.

The fine mesh requirements for THREEDANT have been seen to limit discrete ordinates calculations with respect to the size of the spatial domain. Fortunately, however, X-Y-Z THREEDANT calculations have been shown to be somewhat less quadrature dependent than curvilinear ONEDANT or TWODANT calculations. Furthermore, the default point-wise flux convergence criteria of 10^{-4} in TWODANT/GQ and THREEDANT may be relaxed to 10^{-3} on criticality applications.

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