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DØS Perturbation Modules DGRAD/VIP/TPERT

E. T. Tomlinson
R. L. Childs
R. A. Lillie

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TABLE OF CONTENTS

ACKNOWLEDGMENTS	v
ABSTRACT	1
INTRODUCTION	1
DGRAD	3
VIP	8
TPERT	14
REFERENCES	21
APPENDIX	23

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**DØS PERTURBATION MODULES
DGRAD/VIP/TPERT**

E. T. Tomlinson, R. L. Childs and R. A. Lillie

ABSTRACT

The perturbation modules DGRAD, VIP, and TPERT have been upgraded to run under the DØS DRIVER. A brief discussion of each module, its function, and its input requirements is presented in this report. One transport theory and one diffusion theory sample problem are also presented.

INTRODUCTION

The capability of the Discrete Ordinates System¹ (DØS) has been enhanced with the addition of a series of three code modules, DGRAD², VIP³, and TPERT², that enable the user to perform perturbation calculations. All these modules are operational under the DØS DRIVER and have internally consistent input/output formats. Dynamic storage allocation, variable dimensioning and the high efficiency FSAM¹ data transmission routines are used throughout these modules. FIDO input is used by these modules.

The DGRAD module converts a DOT IV¹ diffusion theory scalar flux file in VARFLM¹ format to a transport flux file in VARFLM format. The output file contains the scalar flux and the partial flux gradients at each mesh interval in each energy group.

The VIP module calculates the spatial integral of the forward and adjoint fluxes and moments. This module is applicable to both transport and diffusion calculations.

The TPERT module evaluates the reactivity change due to a given change in material cross sections. TPERT will perform either transport or diffusion theory perturbation calculations using either first-order or exact perturbation theory.

A brief description of each module, its function, and its input requirements are discussed in this report. One transport theory and one diffusion theory sample problem are also presented.

DGRAD

The module, DGRAD, calculates the directional flux gradients or currents from DOTIV diffusion theory scalar flux tapes. The input file is expected to be in VARFLM format. The output file is in the same format.

In order to calculate the reactivity associated with changes in reactor compositions using diffusion theory, it is necessary to fold not only the scalar fluxes with the appropriate cross sections, but also the average flux gradients with the diffusion coefficients. Since DOT diffusion theory does not directly calculate these gradients, it was necessary to calculate the needed quantities external to the DOT code.

Consider the typical mesh cell with cell-centered fluxes

The flux on the left boundary of cell i, j , ϕ_{BL} can be calculated if the current across this boundary is assumed to be continuous.

$$2 D_{i-1,j} \frac{\phi_{BL} - \phi_{i-1,j}}{\Delta_{i-1}} = 2 D_{i,j} \frac{\phi_{i,j} - \phi_{BL}}{\Delta_i}$$

where $D_{i,j}$ is the diffusion coefficient for cell i,j . Solving for ϕ_{BL}

$$\phi_{BR} = \frac{D_{i,j} \phi_{i,j} \Delta_{i-1} + D_{i-1,j} \phi_{i-1,j} \Delta_i}{D_{i-1,j} \Delta_i + D_{i,j} \Delta_{i-1}} .$$

Similarly for the right boundary

$$\phi_{BR} = \frac{D_{i+1,j} \phi_{i+1,j} \Delta_i + D_{i,j} \phi_{i,j} \Delta_{i+1}}{D_{i,j} \Delta_{i+1} + D_{i+1,j} \Delta_i} .$$

The R direction gradient can then be obtained as follows

$$\nabla \phi_{i,j}^R = \frac{\phi_{BR} - \phi_{BL}}{\Delta_i} .$$

Similar arguments are used for the calculation of the Z direction gradients.

On the outer boundaries of the problem the following conditions are imposed

For reflected boundaries at

$i=1$	$\phi_{0,j} = \phi_{1,j}$	$j=1$	$\phi_{1,0} = \phi_{1,1}$
	$\Delta_{0,j} = \Delta_{1,j}$		$\Delta_{1,0} = \Delta_{1,1}$
	$D_{0,j} = D_{1,j}$		$D_{1,0} = D_{1,1}$

$$\begin{array}{ll}
 i=IM & \phi_{IM+1,j} = \phi_{IM,j} \\
 & \Delta_{IM+1,j} = \phi_{IM,j} \\
 & D_{IM+1,j} = D_{IM,j} \\
 j=JM & \phi_{i,JM+1} = \phi_{i,JM} \\
 & \Delta_{i,JM+1} = \Delta_{i,JM} \\
 & D_{i,JM+1} = D_{i,JM}
 \end{array}$$

For non-return boundaries the flux is assumed to equal zero at the extrapolated boundary

$$\begin{array}{ll}
 i=1 & \phi_{0,j} = 0.0 \\
 & \Delta_{0,j} = 1.42089/\epsilon_{TR} \\
 & D_{0,j} = D_{1,j} \\
 j=1 & \phi_{i,0} = 0.0 \\
 & \Delta_{i,0} = 1.42089/\epsilon_{TR} \\
 & D_{i,0} = D_{i,1} \\
 i=IM & \phi_{IM+1,j} = 0.0 \\
 & \Delta_{IM+1,j} = 1.42089/\epsilon_{TR} \\
 & D_{IM+1,j} = D_{IM,j} \\
 j=JM & \phi_{i,JM+1} = 0.0 \\
 & \Delta_{i,JM+1} = 1.42089/\epsilon_{TR} \\
 & D_{i,JM+1} = D_{i,JM}
 \end{array}$$

The DGRAD module is limited to X-Y, R-Z, and R- θ geometries and regularly meshed problems.

DGRAD INPUT**Title Card (20A4)**

1\$\$ IFLX - 0/1 Forward/Adjoint
 IM - No. of Radial Intervals
 JM - No. of Axial Intervals
 MZ - No. of Material Zones
 ITL - Cross-Section Table Length
 IHT - Position of the Transport Cross Section
 MT - Total Number of Materials
 IGM - No. of Energy Groups
 IBL - Left Boundary Condition 0=VAC 1=REF
 IBR - Right Boundary Condition
 IBT - Top Boundary Condition
 IBB - Bottom Boundary Condition
 IPI - 0/1 Diffusion/Hybrid Output⁴ (see Note 2)
 NIN - Flux Input Unit
 NOUT - Flux Output Unit
 NSEC - Cross-Section Input Unit (see Note 3)
 ISCRT - Scratch Unit (RV=2)
 IPRT - 0/1 Print/No Print Flux and Gradients

Data Block must be terminated with a T.

4** (IM+1) Radial Boundaries
 5** (JM+1) Axial Boundaries
 6\$\$ (IM*JM) Zone Number By Interval
 7\$\$ (MZ) Material By Zone

Data Block must be terminated with a T.

Note 1. To run multiple cases, simply supply a new title card and input all the arrays and T's.

Note 2. If IPI is set equal to zero, the scalar flux and the flux gradients are output for the TPRT diffusion perturbation calculation. If IPI is set equal to 1, the scalar flux and the partial currents are output for the VIP transport integral calculation. VIP is then run as if it were doing a normal P_1 transport problem. The latter option allows for including the P_1 scattering effects and implicit calculation of neutron leakage worths.

Note 3. The cross sections are expected in the group independent format. A forward GIP¹ file is required for the forward flux and an adjoint GIP file is required for the adjoint flux.

DGRAD UNIT DESCRIPTION

<u>UNIT</u>	<u>DESCRIPTION</u>
N5	CARD INPUT (5)
N6	PRINTER OUTPUT (6)
NIN	FLUX INPUT
NOUT	FLUX OUTPUT
NSEC	CROSS SECTION INPUT (GIP FORMAT)
ISCRT	SCRATCH (RV=2)

VIP

The VIP module calculates the spatial integral of the forward and adjoint fluxes and moments. The code allows for grouping of mesh intervals into larger regions.

Changes in a response, R , can be calculated using the perturbation theory relationship

$$\Delta R \approx \iiint \phi^*(r, E, \Omega) \left[\iint \delta \Sigma_g(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \times \phi(r, E', \Omega') dE' d\Omega' - \delta \Sigma_t(r, E) \phi(r, E, \Omega) \right] dE d\Omega dr, \quad (1)$$

where the perturbation is represented by the changes in the total and scattering cross sections and ϕ and ϕ^* are the forward and adjoint fluxes. The spatial and energy integrations are easily evaluated by replacing the integrals with summations over energy groups and a space mesh. The angular integrations are more complicated and are considered in more detail.

The scattering term in Eq. (1) requires the evaluation of an integral of the form

$$\int_{4\pi} \phi^*(\Omega) \int_{4\pi} \phi(\Omega') \sigma(\Omega \cdot \Omega') d\Omega' d\Omega.$$

The cross section is expanded in a Legendre series as

$$\sigma(\Omega \cdot \Omega') = \frac{1}{4\pi} \sum_{l=0}^{\infty} \sigma_l P_l(\Omega \cdot \Omega'), \quad (2)$$

where $\sigma_l = (2l + 1) \int_{4\pi} \sigma(\Omega \cdot \Omega') P_l(\Omega \cdot \Omega') d\Omega$. Similarly, the angular fluxes may be expanded in a spherical harmonic series as

$$\phi(\Omega) = \sum_{l=0}^{\infty} \sum_{m=0}^l \frac{2l+1}{4\pi} j_{l,m} A_l^m(\Omega), \quad (3)$$

and

$$\phi^*(\Omega) = \sum_{l=0}^{\infty} \sum_{m=0}^l (-1)^l (2l+1) j_{l,m}^* A_l^m(\Omega), \quad (4)$$

where

$$j_{l,m} = \int_{4\pi} \phi(\Omega) A_l^m(\Omega) d\Omega,$$

$$j_{l,m}^* = \frac{1}{4\pi} \int_{4\pi} \phi^*(-\Omega) A_l^m(\Omega) d\Omega,$$

$$A_l^m(\Omega) = \left[\frac{2}{1+\delta_{0,m}} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\eta) \cos m\psi,$$

$$\int_{4\pi} d\Omega = \int_0^{2\pi} \int_{-1}^1 d\eta d\psi,$$

and

$$A_l^m(-\Omega) = (-1)^l A_l^m(\Omega).$$

The form of the above equations was chosen to conform with the equations programmed in DOT. The $(-1)^l$ and $-\Omega$ factors arise because the adjoint problem is solved for $\phi^*(-\Omega)$.

The addition theorem for Legendre polynomials is (ignoring terms that vanish under integration)

$$P_l(\Omega \cdot \Omega') = \sum_{m=0}^l A_l^m(\Omega) A_l^m(\Omega'). \quad (5)$$

Substitution of Eqs. (2), (3), (4), and (5) into the desired integral and use of the orthogonality relationship,

$$\int_{4\pi} A_l^m(\Omega) A_l^{m'}(\Omega) d\Omega = \frac{4\pi}{2l+1} \delta_{l,l'} \delta_{m,m'} \quad (6)$$

yields the final result

$$\begin{aligned} & \int_{4\pi} \phi^*(\Omega) \int_{4\pi} \phi(\Omega') \sigma(\Omega \cdot \Omega') d\Omega' d\Omega \\ &= \sum_{l=0}^{\infty} \sum_{m=0}^l (-1)^l \sigma_l j_{l,m} j_{l,m}^* \end{aligned} \quad (7)$$

The total cross-section term in Eq. (1) requires the evaluation of an integral of the form

$$\int_{4\pi} \phi(\Omega) \phi^*(\Omega) d\Omega.$$

This integral can be evaluated using the angular fluxes from the discrete ordinates calculation as had been done in 1-D calculations. However, because of the tremendous quantity of numbers to be stored in 2-D problems (70 million for the example in the appendix), it is highly desirable to avoid storing the angular flux if possible. A way to avoid treating the angular flux may be found by substituting Eqs. (3) and (4) into the desired integral and using Eq. (6) to obtain

$$\int_{4\pi} \phi(\Omega) \phi^*(\Omega) d\Omega = \sum_{l=0}^{\infty} \sum_{m=0}^l (-1)^l (2l+1) j_{l,m} j_{l,m}^* \quad (8)$$

Thus, Eq. (1) can be evaluated using only the flux moments, $j_{l,m}$ and $j_{l,m}^*$, provided the series in Eqs. (7) and (8) can be truncated after a

few terms without serious error. Present experience indicates that a third-order expansion (through $l=3$) is sufficient for many problems.

Like DGRAD, VIP is limited to X-Y, R-Z, and R- θ problems that have a regular mesh.

VIP INPUT

TITLE CARD (20A4)

1\$\$ ID - Problem identification number (>0)
 IM - Number of radial intervals
 JM - Number of axial intervals
 IZM - Number of zones
 ISCT - Maximum order of scattering
 IGM - Number of energy groups
 IGE - 0/1/2 X-Y, R-Z/R- θ geometry
 IHT - Table position of total cross section in SWANLAKE
 ITL - Cross section table length
 IFISS - 1/2 No fission SWANLAKE/fission SWANLAKE
 IPRT - 0/N No effect/Print the $\langle\phi, \phi^*\rangle$ matrix for region
 1 through N

2\$\$ NUF - 0/N No effect/Read uncollided forward flux
 moments from unit N
 NAU - 0/N No effect/Read uncollided adjoint flux
 moments from unit N
 NFF - Logical unit for forward flux file (see Note 1)
 NUF - Logical unit for adjoint flux file
 NTP - Output unit number for $\langle\phi, \phi^*\rangle$ tape (see Note 2)
 NIN - Input unit (5)
 NOU - Output unit (6)
 NBUF - K-bytes for buffer space

Terminate Data Block 1 with a T.

2** Axial interval boundaries (JM+1)
 4** Radial interval boundaries (IM+1)
 8\$\$ Zone number by interval (IM*JM)
 9\$\$ Region by zone (IZM)

Terminate Data Block 2 with a T.

Note 1. Forward and adjoint flux files are expected to be in VARFLM format.

Note 2. VIP $\langle\phi, \phi^*\rangle$ output files are not in a CCCC format since none exists. A file that is internally consistent with IPERT and SWANLAKE has been retained.

VIP UNIT DESCRIPTION

<u>UNITS</u>	<u>DESCRIPTION</u>
NIN	Card Input (5)
NOU	Printer Output (6)
NUF	Uncollided forward flux file
NUA	Uncollided adjoint flux file
NFF	Forward flux file
NAF	Adjoint flux file
NTP	$\langle \phi, \phi^* \rangle$ file

TPERT

A perturbation code, TPERT, has been written to obtain exact and first-order reactivity changes. The purpose of this section is to provide a brief review of the expressions evaluated by TPERT and to provide a detailed description of the required input. TPERT couples with VIP¹ which generates adjoint-forward flux tables, i.e., ϕ^* tables, using DOT-IV¹ scalar flux tape information. The general scheme consists of passing the spatially integrated ϕ^* tables from VIP into TPERT which in turn folds the ϕ^* tables with the pertinent cross section changes.

The reactivity associated with a change in reactor composition, i.e., a perturbation, may be obtained from:

$$\Delta\rho = \langle \phi^*, (\Delta F/k - \Delta\Sigma + \Delta S) \phi' \rangle / \langle \phi^*, F' \phi' \rangle \quad (9)$$

where

$\Delta\rho$ = reactivity change

ΔF = change in fission operator

$\Delta\Sigma$ = change in total cross section operator

ΔS = change in scattering operator

k = unperturbed state eigenvalue

ϕ^* = unperturbed adjoint flux

ϕ' = perturbed forward flux

$F' = F + \Delta F$ = perturbed fission operator.

The brackets, i.e., $\langle \rangle$, in Eq. (9) indicate integration over space, energy and angle. Equation (9) is normally called the exact perturbation equation since there are no approximations employed in its

development. The first-order, or linear, approximation to Eq. (9) may be obtained by simply substituting the unperturbed forward flux ϕ and the unperturbed fission operator F for ϕ' and F' , respectively.

$$\Delta\rho = \langle \phi^*, (\Delta F/k - \Delta\Sigma + \Delta s)\phi \rangle / \langle \phi^*, F\phi \rangle . \quad (10)$$

The evaluation of the integrals in Eqs. (9) and (10) is carried out in two steps. The first step is performed by VIP and results in the generation of $(L+1)$, where L is the order of scattering anisotropy, $\phi^*\phi$ tables for each region in which material changes occur or in which fissionable nuclides appear. These tables are ordered in a manner similar to ANISN formatted cross-section tables.

The terms which fold with the total cross section in TPRT are located in position IHT. These terms have the form:⁴

$$T_g = -\sum_L \sum_{l=0}^L \sum_{m=0}^l (-1)^{l+1} (2l+1) j_{l,m,1,g}^* j_{l,m,1,g} V_1 \quad (11)$$

where

$j_{l,m,1,g}^*$ = the DOT l_m^{th} adjoint flux moment in space cell 1 and group g

$j_{l,m,1,g}$ = the DOT forward flux moment.

V_1 = volume of 1^{th} space cell.

The terms which fold with the scattering and fission operators are stored in positions IHS through IHS+G-1 where G represents the total number of groups. These terms have the form:

$$T_{l,g,g'} = \sum_l \sum_m (-1)^{l+1} j_{l,m,1,g}^* j_{l,m,g'} V_1 . \quad (12)$$

For a given group g , the subscript g' may take on two values. In positions IHS through $IHS+g-1$:

$$g' = g-k+1 \text{ for } k=1, \dots, g$$

and in positions $IHS+g$ through $IHS+G-1$:

$$g' = k \text{ for } k=g+1, \dots, G.$$

The second step in the evaluation of the integrals in Eqs. (9) and (10) is carried out by TPRT. This step consists of folding the terms represented by Eqs. (11) and (12) with the appropriate cross-section changes for each region. The folding process is described by the following:

$$\langle \phi^*, \frac{\Delta F}{k} \phi \rangle_r = \sum_g \sum_{g'} \chi_g \frac{\Delta \nu \Sigma_{fg'}}{k} T_{0,g,g'}, \quad (13a)$$

$$- \langle \phi^*, \Delta \Sigma \phi \rangle_r = \sum_g \Delta \Sigma_{Tg} T_g, \quad (13b)$$

and

$$\langle \phi^*, \Delta S \phi \rangle_r = \sum_g \sum_{g'} \sum_l \Delta \Sigma_{sl,g'+g} T_{l,g,g'} \quad (13c)$$

where

χ_g = fraction of fission neutrons born in group g ,

$\Delta \nu \Sigma_{fg'}$ = change in nu times the fission cross section in group g

$\Delta \Sigma_{Tg}$ = change in total cross section in group g ,

$\Delta \Sigma_{sl,g'+g}$ = change in l^{th} order scattering coefficient for scattering from group g' to group g .

In Eqs. (13), the subscript r has been introduced to denote different material regions. The perturbation denominators, i.e., $\langle \phi^*, F' \phi' \rangle$ and $\langle \phi^*, F \phi \rangle$ are evaluated by simply substituting $v \Sigma_{f'g'}$ or $v \Sigma_{fg'}$ into Eq. (13a) for $\Delta v \Sigma_{fg'}$. Summing the region contributions to $\Delta \rho$ completes the reactivity calculation.

TPERT INPUT

Title Card (18A4)

1\$\$ IHT - Position of total cross section
 IHS - Position of self-scatter cross section
 ITL - Cross-section table length
 IGM - Number of energy groups
 NR - Number of "VIP" regions (see Note 1)
 ISCT - Order of scattering anisotropy
 NMAT - Number of materials from tape (see Note 2)
 ITAB - Logical unit number of VIP ϕ tables
 NCR - No effect
 NDCR - No effect
 NSRT - No effect
 NTAB - No effect
 JFLAG - 0 - use perturbed $v\Sigma_f$ denominator
 1 - use unperturbed $v\Sigma_f$ denominator
 ITOD - 0 - transport calculation (see Note 5)
 1 - diffusion calculation
 NBUF - Buffer space (K-bytes)

Terminate data block 1 with a T.

2** CHI (IGM) - Fission spectrum

3** VEL5 (IGM) - Group inverse velocities - fill with 1.0's if
 inverse velocity folding is not desired (see Note 4)

Arrays 5\$\$ through 10** apply to the following relationships for a
 given VIP region:

$$\Sigma \text{ unperturbed} = U1*\Sigma_1 + U2*\Sigma_2$$

$$\Sigma \text{ perturbed} = P1*\Sigma_1 + P2*\Sigma_2$$

5\$\$ MAT1 (NR) - P_0 material numbers on direct access storage for
 Σ_1 cross sections by VIP region - use negative
 number if region has fissionable material but no
 perturbation.

6** U1 (NR) - Unperturbed multiplier for Σ_1 by VIP region

7** P1 (NR) - Perturbed multiplier for Σ_1 by VIP region

8\$\$ MAT2 (NR) - P_0 material numbers on direct access storage for
 Σ_2 cross sections by VIP region - use a zero if
 only Σ_1 occurs in a region

9** U2 (NR) - Unperturbed multiplier for Σ_2 by VIP region

10** P2 (NR) - Perturbed multiplier for Σ_2 by VIP region

11** EIG - Unperturbed K_{eff}

BETA - Total delayed neutron fraction

DNORM - Perturbation integral denominator - enter 0.0
 if code is to calculate

Terminate data block 2 with a T.

Note 1: Each region which contains a perturbation, i.e., change in cross section, or which contains fissionable material is a VIP region.

Note 2: TPERT, as presently programmed will only accept cross sections in GIP format.

Note 3: To run multiple cases, simply supply a new title card and change the appropriate arrays. Be sure to include a terminator, e.g. T, for both data blocks.

Note 4: TPERT will evaluate the quantity $\langle \phi^*, 1/v \phi \rangle$ which is useful in certain time-dependent reactivity calculations.

Note 5: To run diffusion cases, it is necessary to set ISCT=1 in VIP and input the flux tapes generated by DGRAD.

TPERT UNIT DESCRIPTION

<u>UNIT</u>	<u>DESCRIPTION</u>
8	Cross section input file
N5	Card input (5)
N6	Printer output (6)
ITAB	VIP $\langle \phi, \phi^* \rangle$ integral file
NCR	Cross section scratch file (2)
NDCR	Direct access scratch (91)
NSRT	Scratch (3)
NTAB	Scratch (4)

REFERENCES

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3. R. L. Childs, D. E. Bartine, and W. W. Engle, Jr., "Perturbation Theory and Sensitivity Analysis for Two-Dimensional Shielding Calculations," Trans. Am. Nucl. Soc., 21: 543, June, 1975.
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APPENDIX

SAMPLE PROBLEMS

Two sample problems are included to aid the analyst in using these modules. The first sample problem is a transport theory problem and uses only the VIP and TPERT modules. The second sample problem is the same as the first only run with diffusion theory. All three modules are used in this problem.

The input and output for these problems is presented on the enclosed microfiche.