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DEVELOPMENT OF BERMUDA: A RADIATION TRANSPORT CODE SYSTEM PART Ⅲ A ONE-DIMENSIONAL ADJOINT NEUTRON TRANSPORT CODE

July 1994

Tomoo SUZUKI*, Akira HASEGAWA**
Shun-ichi TANAKA and Hiroshi NAKASHIMA

日本原子力研究所
Japan Atomic Energy Research Institute

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Development of BERMUDA: A Radiation Transport Code System Part Ⅲ. A One-dimensional Adjoint Neutron Transport Code

Tomoo SUZUKI* , Akira HASEGAWA**, Shun-ichi TANAKA
and Hiroshi NAKASHIMA

Department of Reactor Engineering
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

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A radiation transport code system BERMUDA has been developed for one-, two- and three-dimensional geometry. Purpose of the development is to establish a basis of an accurate shielding calculation method for general use. The time-independent transport equation is numerically solved using a direct spatial integration method in a multigroup model, to obtain spatial, angular and energy distribution of neutron, gamma rays or adjoint neutron flux. In 1992, four neutron transport codes were reported in JAERI 1327 as Part Ⅰ. In 1993, four gamma rays transport codes were reported in JAERI-M 93-143 as Part Ⅱ. In the present report as Part Ⅲ, reported is the development of an adjoint neutron transport code for one-dimensional spherical geometry. Adjoint neutron flux is used in a sensitivity analysis or in a perturbation calculation. As described in Part Ⅰ, use of the spherical harmonics expansion is avoided in representing anisotropy of both angular flux and scattering cross section. A group-angle transfer matrix is obtained by integrating double-differential cross sections numerically, taking energy-angle correlation into account. A first collision source method is utilized for a case of point source. Angular flux distribution is obtained by integrating the transport equation over a line segment along each angular discrete ordinate toward each spatial mesh point. A fine energy grid method is used, with a rebalancing scheme

* Nuclear Energy Data Center
**Nuclear Power Engineering Corporation

concerning the number of gain and loss of particles over each spatial region and also in each energy grid. The 'energy grid' means a 'subgroup' having equal lethargy width to each other in an energy group. As to group constants, the same library, J439B.BERM125X.DATA, is used commonly to the regular (forward) neutron transport codes as in Part I. Validity of the present code BERMUDA-1DNA has been tested for five sample problems by comparing the calculated results with those from the forward neutron transport code BERMUDA-1DN. The tests have shown that accurate results are obtainable with BERMUDA-1DNA. In this report as PartⅢ, described are the derivation of the adjoint equation, the calculational method and the validity tests. Job control languages, input data specifications and output data are also described so that the present report is available as a user's manual.

Keywords: BERMUDA, Radiation Transport, Shielding, Code System, Direct Integration Method, Energy Group, Angular Flux, Anisotropy, Double-differential Cross Section, Angular Discrete Ordinates, Adjoint Neutron Flux, Sensitivity Analysis

JAERI-Data/Code 94-002

放射線輸送コードシステムＢＥＲＭＵＤＡの開発
第Ⅲ部　１次元随伴中性子輸送コード

日本原子力研究所東海研究所原子炉工学部
鈴木　友雄*・長谷川　明**・田中　俊一
中島　　宏

（1994年５月16日受理）

高精度の遮蔽計算を行うコードシステムの完成を目標に，その計算手法の基礎を確立するため，１～３次元の各形状に対する放射線輸送コードシステムＢＥＲＭＵＤＡを開発した。本コードシステムでは，空間に関する直接積分法とエネルギーに関する多群モデルとを組合わせて，定常状態での輸送方程式を数値的に解き，中性子，ガンマ線あるいは随伴中性子の各線束の空間，角度，エネルギー分布を求めている。1992年に第Ⅰ部として中性子輸送コード４本がJAERI 1327に報告された。1993年には第Ⅱ部としてガンマ線輸送コード４本がJAERI-M 93-143に報告された。本報告書は第Ⅲ部として，感度解析あるいは摂動計算に必要な随伴中性子束を求めるための１次元球体系用随伴中性子輸送コードの開発について報告している。第Ⅰ部に述べたように，線束や散乱断面積の非等方性の表現に球面調和関数展開を使用することを避け，数値データを直接積分している。散乱による群・角度遷移マトリックスの算出には，エネルギーと散乱角の相関を考慮して，二重微分散乱断面積の数値積分を行う。さらに，点線源の場合は一回散乱源を求めてから輸送方程式を解く方法を用いている。線束の空間・角度分布は各格子点へ向かって各角度分点の方向へ輸送方程式を積分し、エネルギー群をレサジーで等分割した微細群毎に，領域毎の粒子バランスが成り立つように規格化を行いつつ求める。群定数は第Ⅰ部での通常の中性子輸送コードに用いたものと同一のライブラリー（Ｊ４３９Ｂ・ＢＥＲＭ１２５Ｘ・ＤＡＴＡ）が使用される。本コード（ＢＥＲＭＵＤＡ－１ＤＮＡ）の適用性は５コの例題に対して，通常の１次元中性子輸送コード（ＢＥＲＭＵＤＡ－１ＤＮ）と共に，計算結果の積分を比較することにより行い，十分な精度が得られることが確認された。本報告書では随伴方程式の導出，随伴中性子束の計算法とコードの適用性評価について概説すると共に，コード使用マニュアルとして，ジョブ制御文，入力データの準備，さらに出力データの概要について述べている。

東海研究所：〒319－11　茨城県那珂郡東海村白方字白根２－４
＊　（財）原子力データセンター
＊＊（財）原子力発電技術機構

Contents

目　　次

1. Introduction

The radiation transport code system BERMUDA consists of three subsystems as:

(1) Neutron transport codes,
(2) Gamma rays transport codes and
(3) Adjoint neutron transport code.

Out of these, four neutron transport codes were reported in JAERI 1327 (Ref.1) as Part I in 1992, and four gamma rays transport codes were reported in JAERI-M 93-143 (Ref.2) as Part II in 1993. The present report is written as Part III for the adjoint neutron transport code.

Almost all of the numerical methods to solve the regular (forward) neutron transport equation are commonly used in the adjoint neutron transport code, except that an adjoint neutron moves in the opposite direction to a forward neutron and also that the adjoint equation in multigroup model is solved from the lowest energy group.

We have developed a computer code, BERMUDA-1DNA, for obtaining space, angle and energy distribution of adjoint neutron flux $\phi^*(\vec{r}, E, \vec{\Omega})$ in one-dimensional spherical geometry. The present report is written as a usage manual for BERMUDA-1DNA.

In Chapter 2, the adjoint neutron transport equation is derived from the forward neutron transport equation. The characteristic features to solve the multigroup adjoint neutron transport equation in the present version of the code system are introduced in Chapter 3. Simple validity tests and their results are given in Chapter 4. Chapter 5 is a guide for users to prepare input data and the job control languages for the FACOM/VP2600 computer. Also, a brief description is given about the output data on printer or disk.

The series of reports on the BERMUDA code system beginning from Part I are completed with this Part III.

2. Derivation of Adjoint Neutron Transport Equation

In BERMUDA-1DNA, fission neutron source is not dealt with. The source term consists only of an independent source and a scattering source. The independent source $S^{*i}(\vec{r}, \vec{\Omega})$ to be input to the present code is a quantity like $\Sigma_a(cm^{-1})$, which can be input as either a point source or a volume source. It is necessary to be conscious of that S^{*i} and ϕ^{*i} for the energy group i are not integrated values over the energy range of group i like S^i and ϕ^i, respectively, but 'average values in the group i.'

From the time-independent neutron transport equation[1], the forward form of it is written using a symbol L as an operator,

$$S(\vec{r}, E, \vec{\Omega}) = L\phi(\vec{r}, E, \vec{\Omega})$$

$$\equiv \vec{\Omega} \cdot \mathrm{grad}\,\phi(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E)\,\phi(\vec{r}, E, \vec{\Omega})$$

$$- \int dE' \int d\vec{\Omega}'\, \phi(\vec{r}, E', \vec{\Omega}')\, \Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega}). \qquad (1)$$

The adjoint operator L^* is derived from the relation[3]:

$$< \phi^*, L\phi > = < \phi, L^*\phi^* > \qquad (2)$$

where $<f, g>$ means an inner product, $\int d\vec{r} \int dE \int d\vec{\Omega}\, f(\vec{r}, E, \vec{\Omega}) g(\vec{r}, E, \vec{\Omega})$, in which each integration is performed over the full range of the variable.

Definite form of the left hand side of Eq. (2) is given as

$$< \phi^*, L\phi > = \int d\vec{r} \int dE \int d\vec{\Omega}\, \phi^*(\vec{r}, E, \vec{\Omega}) \left[\vec{\Omega} \cdot \mathrm{grad}\,\phi(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E)\,\phi(\vec{r}, E, \vec{\Omega}) \right.$$

$$\left. - \int dE' \int d\vec{\Omega}'\, \phi(\vec{r}, E', \vec{\Omega}')\, \Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega}) \right]. \qquad (3)$$

With formulae of vector analysis:

$$\mathrm{div}(\vec{\Omega}\,\phi) = \vec{\Omega} \cdot \mathrm{grad}\,\phi \quad (\vec{\Omega} \text{ is a constant vector in respect of 'grad'}) \text{ and}$$

$$\phi^* \mathrm{div}(\vec{\Omega}\,\phi) = \mathrm{div}(\phi^* \vec{\Omega}\,\phi) - \phi\,\mathrm{div}(\vec{\Omega}\,\phi^*),$$

the first term of Eq. (3) is written,

$$\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi^{*}\vec{\Omega}\cdot\mathrm{grad}\,\phi$$

$$=\int dE\int d\vec{\Omega}\int d\vec{r}\,[\mathrm{div}(\phi^{*}\vec{\Omega}\phi)-\phi\,\mathrm{div}(\vec{\Omega}\phi^{*})]$$

$$=\int dE\int d\vec{\Omega}\int d\vec{s}\,\vec{n}\cdot\vec{\Omega}\,\phi^{*}\phi-\int dE\int d\vec{\Omega}\int d\vec{r}\,\phi\,\vec{\Omega}\cdot\mathrm{grad}\,\phi^{*} \qquad (4)$$

where $\int d\vec{s}$ means the surface integral over the outer boundary, and $\vec{n}$ is the outward normal unit vector at $\vec{s}$. Here we impose the boundary conditions as:

$\phi=0$ for $\vec{n}\cdot\vec{\Omega}<0$ at the outer boundary and

$\phi^{*}=0$ for $\vec{n}\cdot\vec{\Omega}>0$ at the outer boundary,

then from Eq. (4), obtained is

$$\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi^{*}\vec{\Omega}\cdot\mathrm{grad}\,\phi=-\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi\,\vec{\Omega}\cdot\mathrm{grad}\,\phi^{*} \qquad (5)$$

The second term of Eq. (3) is easily transformed. The third term is transformed with interchanging $(E,\vec{\Omega})$ and $(E',\vec{\Omega}')$ with each other,

$$\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi^{*}(\vec{r},E,\vec{\Omega})\,[-\int dE'\int d\vec{\Omega}'\,\phi(\vec{r},E',\vec{\Omega}')\,\Sigma_{s}(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})]$$

$$=\int d\vec{r}\int dE\int d\vec{\Omega}\int dE'\int d\vec{\Omega}'\,[-\phi^{*}(\vec{r},E',\vec{\Omega}')\,\phi(\vec{r},E,\vec{\Omega})\,\Sigma_{s}(\vec{r},E\to E',\vec{\Omega}\to\vec{\Omega}')]$$

$$=\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi(\vec{r},E,\vec{\Omega})\,[-\int dE'\int d\vec{\Omega}'\,\phi^{*}(\vec{r},E',\vec{\Omega}')\,\Sigma_{s}(\vec{r},E\to E',\vec{\Omega}\to\vec{\Omega}')]\,. \qquad (6)$$

By the relations of Eqs. (5) and (6), Eq. (3) becomes

$$<\phi^{*},L\phi>=\int d\vec{r}\int dE\int d\vec{\Omega}\,\phi(\vec{r},E,\vec{\Omega})\,[-\vec{\Omega}\cdot\mathrm{grad}\,\phi^{*}(\vec{r},E,\vec{\Omega})+\Sigma_{t}(\vec{r},E)\,\phi^{*}(\vec{r},E,\vec{\Omega})$$

$$-\int dE'\int d\vec{\Omega}'\,\phi^{*}(\vec{r},E',\vec{\Omega}')\,\Sigma_{s}(\vec{r},E\to E',\vec{\Omega}\to\vec{\Omega}')]\,.$$

Finally we obtain the adjoint operator as

$$S^*(\vec{r}, E, \vec{\Omega}) = L^* \phi^*(\vec{r}, E, \vec{\Omega})$$

$$\equiv -\vec{\Omega} \cdot \mathrm{grad}\, \phi^*(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E)\, \phi^*(\vec{r}, E, \vec{\Omega})$$

$$-\int dE' \int d\vec{\Omega}'\, \phi^*(\vec{r}, E', \vec{\Omega}')\, \Sigma_s(\vec{r}, E \rightarrow E', \vec{\Omega} \rightarrow \vec{\Omega}'). \qquad (7)$$

In order to derive the multigroup equation, the adjoint neutron flux for group i is defined as:

$$\phi^{*i}(\vec{r}, \vec{\Omega}) = \int_{\Delta E_i} \phi^*(\vec{r}, E, \vec{\Omega})\, dE / \Delta E_i$$

where ΔE_i is the group energy width.

Discretizing the angular variable $\vec{\Omega}$ as $\vec{\Omega}_n$, and using the same kernel as in Ref. 1, the multigroup adjoint neutron transport equation can be written as:

$$-\vec{\Omega}_n \cdot \mathrm{grad}\, \phi^{*i}(\vec{r}, \vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})\, \phi^{*i}(\vec{r}, \vec{\Omega}_n)$$

$$= \sum_{j=i}^{IMAX} \sum_{n'} \phi^{*j}(\vec{r}, \vec{\Omega}_{n'})\, (\Delta \vec{\Omega}_{n'} / \Delta \vec{\Omega}_n) K^{i \rightarrow j,\, n \rightarrow n'}(\vec{r}) + S^{*i}(\vec{r}, \vec{\Omega}_n). \qquad (8)$$

where IMAX is the number of energy groups.

From Eqs. (1), (2) and (7), the relation

$$\langle \phi^*, S \rangle = \langle \phi, S^* \rangle \qquad (9)$$

is derived, which is used for validity tests of the present code, BERMUDA-1DNA, in Chapter 4.

3. Numerical Method to Solve Adjoint Equation

The reciprocity relation between scattering kernels

$$\Delta\vec{\Omega}_n K^{i\to j,n'\to n}(\vec{r}) = \Delta\vec{\Omega}_{n'} K^{i\to j,n\to n'}(\vec{r}) \tag{10}$$

is obtained from the equation written at 3 lines below Eq. (3.22) in Ref. 1. It is rewritten as

$$(\Delta\vec{\Omega}_{n'} / \Delta\vec{\Omega}_n) K^{i\to j,n\to n'}(\vec{r}) = K^{i\to j,n'\to n}(\vec{r}),$$

and substituting the latter into Eq. (8), we obtain

$$-\vec{\Omega}_n \cdot \mathrm{grad}\,\phi^{*i}(\vec{r},\vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})\,\phi^{*i}(\vec{r},\vec{\Omega}_n)$$
$$= \sum_{j=1}^{IMAX}\sum_{n'}\phi^{*j}(\vec{r},\vec{\Omega}_{n'})K^{i\to j,n'\to n}(\vec{r}) + S^{*i}(\vec{r},\vec{\Omega}_n). \tag{11}$$

So as to make Eq. (10) more accurate in numerical sense than the calculational method for $W^*_{n',nm'}$ in Ref. 1, twenty points of n in the domain $\Delta\vec{\Omega}_n$ on the unit sphere (twenty points of $\omega_n = \cos\theta_n$ on the longitude contained in $\Delta\vec{\Omega}_n$) is adopted, instead of five points as in Ref. 1, to calculate $W^*_{n',nm'}$ values. And the average of the twenty values is used as the objective $W^*_{n',nm'}$ value. After that, $\Delta\phi_{n',nm'}$ is obtained in the same formula as Eq. (3.22) in Ref. 1, that is,

$$\Delta\phi_{n',nm'} = [2\pi\,\Delta\vec{\Omega}_{n'} / \sum_L \Delta\vec{\Omega}_L W^*_{n',Lm'}]\, W^*_{n',nm'}.$$

The forward code, BERMUDA-1DN, has also been improved to obtain the same accurate $W^*_{n',nm'}$ and $\Delta\phi_{n',nm'}$ values.

Next, substitutions $\vec{\Omega}_n \to -\vec{\Omega}_n$ and $\vec{\Omega}_{n'} \to -\vec{\Omega}_{n'}$ are performed in Eq. (11). As described in Ref. 1, $\vec{\Omega}_n$'s are defined with the Gaussian quadrature set of order 20, so that $-\vec{\Omega}_n = \vec{\Omega}_{21-n}$ holds. Then

$$\vec{\Omega}_n \cdot \mathrm{grad}\,\phi^{*i}(\vec{r},-\vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})\,\phi^{*i}(\vec{r},-\vec{\Omega}_n)$$
$$= \sum_{j=1}^{IMAX}\sum_{n'}\phi^{*j}(\vec{r},-\vec{\Omega}_{n'})K^{i\to j,(21-n')\to(21-n)}(\vec{r}) + S^{*i}(\vec{r},-\vec{\Omega}_n).$$

Denoting $-\vec{\Omega}_n$ and $-\vec{\Omega}_{n'}$ as $\vec{\Omega}_{\bar{n}}$ and $\vec{\Omega}_{\bar{n}'}$, respectively, relations of $\bar{n}=21-n$ and $\bar{n}'=21-n'$ are apparent from the symmetrical property of the Gaussian set. Then

$$\vec{\Omega}_n \cdot \mathrm{grad}\,\phi^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}}) + \Sigma_t{}^i(\vec{r})\,\phi^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}})$$

$$= \sum_{j=i}^{IMAX} \sum_{n'} \phi^{*j}(\vec{r}, \vec{\Omega}_{\bar{n}'}) K^{i\to j, \bar{n}'\to\bar{n}}(\vec{r}) + S^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}}).$$

In this equation, we write $F^i(\vec{r}, \vec{\Omega}_n)$ in place of $\phi^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}})$, so that $F^i(\vec{r}, \vec{\Omega}_n)$ obeys the same outer boundary condition as that for the forward flux $\phi^i(\vec{r}, \vec{\Omega}_n)$.

$$\vec{\Omega}_n \cdot \mathrm{grad}F^i(\vec{r}, \vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})F^i(\vec{r}, \vec{\Omega}_n)$$

$$= \sum_{j=i}^{IMAX} \sum_{n'} F^j(\vec{r}, \vec{\Omega}_{n'}) K^{i\to j, \bar{n}'\to\bar{n}}(\vec{r}) + S^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}}).$$

From the symmetrical property of the twenty belt zones on the unit sphere in the longitudinal direction (see the zone surrounded with dotted lines in Fig. 3.2 in Ref. 1)

$$K^{i\to j, \bar{n}'\to\bar{n}}(\vec{r}) = K^{i\to j, n'\to n}(\vec{r})$$

is easily proved, so that the both sides of the above equation have numerically equal values. Thus we finally obtain the adjoint equation to be solved numerically:

$$\vec{\Omega}_n \cdot \mathrm{grad}F^i(\vec{r}, \vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})F^i(\vec{r}, \vec{\Omega}_n)$$

$$= \sum_{j=i}^{IMAX} \sum_{n'} F^j(\vec{r}, \vec{\Omega}_{n'}) K^{i\to j, n'\to n}(\vec{r}) + S^{*i}(\vec{r}, \vec{\Omega}_{\bar{n}}). \qquad (12)$$

Comparing Eq. (12) with the forward equation given as Eq. (3.25) in Ref. 1:

$$\vec{\Omega}_n \cdot \mathrm{grad}\,\phi^i(\vec{r}, \vec{\Omega}_n) + \Sigma_t{}^i(\vec{r})\,\phi^i(\vec{r}, \vec{\Omega}_n)$$

$$= \sum_{j=1}^{i} \sum_{n'} K^{j\to i, n'\to n}(\vec{r})\,\phi^j(\vec{r}, \vec{\Omega}_{n'}) + S^i(\vec{r}, \vec{\Omega}_n), \qquad (13)$$

the differences between Eqs. (12) and (13) are that $\sum_{j=1}^{i}$ in Eq. (13) becomes $\sum_{j=1}^{IMAX}$ in

Eq. (12), and that $\vec{\Omega}_n$ in S^i becomes $\vec{\Omega}_{\bar{n}}$ in S^{*i}. The boundary conditions for ϕ^i and P^i are common.

$S^{*i}(\vec{r}, \vec{\Omega}_n)$ is inverted in the order of n of $\vec{\Omega}_n$, after the values for S^{*i} are given as input data. Then Eqs. (12) and (13) can be almost analogously solved except that Eq. (12) must be conversely solved from the energy group IMAX consecutively up to the energy group 1.

After Eq. (12) is solved up to the group 1, the order of n of $\vec{\Omega}_n$ in $P^i(\vec{r}, \vec{\Omega}_n)$ is inverted, and $\phi^{*i}(\vec{r}, \vec{\Omega}_n)$ is obtained.

The definite formula of the scattering kernel is[1)]

$$K^{i\to j, n'\to n}(\vec{r}) = (1/4\pi)\,\Sigma_{iso}{}^{i\to j}(\vec{r}) + \sum_m N^m(\vec{r}) \int_{\Delta E_i} (dE/\Delta E_i) \int_{\Delta E_j} dE' \int_{\Delta \vec{\Omega}_{n'}} d\vec{\Omega}' \sum_L F_L{}^{mi}\,\sigma\,(E\to E', \vec{\Omega}'\to\vec{\Omega}_n)$$

where $F_L{}^{mi}$ is the resonance self-shielding factor and has meaning only in the case of elastic scattering ($L=0$). If $L\neq 0$, then $F_L{}^{mi}\equiv 1$. The N^m is the atomic number density for nuclide m.

In order to solve the Eq. (12), at first, for the thermal (IMAX-th) group, it has become clear that a 'Coarse Mesh Rebalance' technique[1)] is necessary like in BERMUDA-2DN etc. notwithstanding a one-dimensional code, because Σ_t is large in the thermal group. So, the technique has been applied not only to BERMUDA-1DNA, but also to the one-dimensional forward neutron transport code, BERMUDA-1DN.

4. Validity Tests

The sample problem used for testing BERMUDA-1DN in 117 energy groups (Fig. 5.1 in Ref. 1) is again chosen to test BERMUDA-1DNA as well as BERMUDA-1DN newly improved in $W^*_{n',nm'}$ and 'Coarse Mesh Rebalance (CMR)' calculations as mentioned in the previous chapter.

The tests are performed using Eq. (9),

$$<\phi^*, S> = <\phi, S^*>. \tag{9}$$

In the case of energy group model, ϕ and S in Eq. (9) are the integrated values over the range of energy group width, whereas ϕ^* and S^* are averaged values over the same range.

BERMUDA-1DNA is tested for the following five problems comparing the calculated results with those from BERMUDA-1DN:

(1) 4 regions problem with the same configuration and composition as in Fig. 5.1 in Ref. 1,

(2) 6 regions problem made by dividing the second region of the problem (1), containing Li_2O, into three regions having equal thickness in $\vec{r}$ direction,

(3) 2 regions problem made by removing the outer 2 regions of problem (1) (the regions of carbon and framework),

(4) 4 regions problem made by dividing the second region of the problem (3), containing Li_2O, into three regions having equal thickness in $\vec{r}$ direction and

(5) 1 region problem made by removing the outer 3 regions of problem (1).

For simplicity in comparing, all of five problems are calculated using an isotropic point source of magnitude 1 at the origin. The forward calculations with BERMUDA-1DN use the isotropic point source in the first energy group, and the adjoint calculations with BERMUDA-1DNA use the isotropic point source in the last thermal energy group (IMAX-th or 117th group).

Then from Eq. (9), it is sufficient to show that

$$\Phi^{117}(0) = \Phi^{*1}(0)$$

holds, where Φ's are the scalar flux defined as

$$\Phi^{i}(0) = \sum_{n=1}^{20} \Delta \vec{\Omega}_n \phi^{i}(0, \vec{\Omega}_n) \quad \text{and}$$

$$\Phi^{*i}(0) = \sum_{n=1}^{20} \Delta \vec{\Omega}_n \phi^{*i}(0, \vec{\Omega}_n),$$

respectively.

The results of the present tests are summarized in Table 1. The relative errors are all less than factor 3 or 4 after total 234 groups (2×117 groups) calculations. It can be considered that the availability of BERMUDA-1DNA is confirmed.

Table 1 Results of test calculations

Case No.	$\Phi^{117}(0)$	$\Phi^{*1}(0)$	$\Phi^{*1}(0) / \Phi^{117}(0)$
(1)	4.783×10^{-10}	1.463×10^{-9}	3.058
(2)	4.873×10^{-10}	1.411×10^{-9}	2.895
(3)	4.804×10^{-10}	1.455×10^{-9}	3.030
(4)	4.837×10^{-10}	1.399×10^{-9}	2.892
(5)	3.954×10^{-10}	$1.527\times10^{+26}$ [a]	3.863

[a] For Case No. (5), $S^{*117}(0)$ is multiplied by 10^{+35} so as to avoid troublesome underflows.

5. User's Manual

As the present code is programmed for one-dimensional spherical geometry, the spatial point $\vec{r}$ in the previous chapters is written as r in this chapter.

5.1 JCL

The JCL (a set of job control languages) for the BERMUDA-1DNA execution on the FACOM/VP2600 computer in JAERI is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.05 W.03 C.00 I.07 E.01 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=2,NOTIFY=Jxxxx
      OPTP PASSWORD=xxxxxxxx
//    EXEC LMGOEX,LM=J9091.BERMUDA,PNM=BERM1DNA (*1)
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FLUX1DNA.DATA (*2)
//FT02F001 DD UNIT=WK10,SPACE=(TRK,(100,50)),DISP=(NEW,DELETE,DELETE),
//    DSN=&&WORK,DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT04F001 DD DISP=SHR,DSN=J439B.BERM125X.DATA,LABEL=(,,,IN)
//SYSIN     DD DISP=SHR,DSN=Jxxxx.DATA1DNA.DATA (*3)
++
//
```

(*1) There has already been a load module J9091.BERMUDA.LOAD(BERM1DNA) prepared for a public use in JAERI.

If necessary, a new load module is able to be created on a disk from the source module J9091.BERMUDA.FORT77(BERM1DNA). The JCL for creating a new load module is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
```

```
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.03 W.01 C.08 I.02 E.02 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),NOTIFY=Jxxxx,PASSWORD=xxxxxxxx
//    EXEC FORTEXVP,SO=J9091.BERMUDA,A='ELM(BERM1DNA),NOVMSG',LCT=62
//    EXEC LKEDCTEX,LM=Jxxxx.BERM1DNA,UNIT=xxxxx,MODS='07,07,1',A=MAP
++
//
```

These steps of compilation and linkage are executed rather rapidly on the FACOM/M780 scalar computer. The new load module is applied by replacing the above "LM=J9091.BERMUDA,PNM=BERM1DNA" (\$1) with "LM=Jxxxx.BERM1DNA".

(\$2) The adjoint neutron flux file Jxxxx.FLUX1DNA.DATA has to be allocated beforehand as:

```
//FT01F001 DD UNIT=xxxxx,SPACE=(TRK,(60,10)),
//    DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLUX1DNA.DATA,
//    DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the spatial distributions of angular and scalar fluxes of adjoint neutron for all of the calculated energy groups. It can be used for editing the output results with the forward neutron flux file, Jxxxx.FLUX1DN.DATA, and the group constants library, J439B.BERM125X.DATA.

(\$3) The input data file Jxxxx.DATA1DNA.DATA has to be allocated beforehand as:

```
//FT05F001 DD UNIT=xxxxx,SPACE=(TRK,(01,01)),
//    DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.DATA1DNA.DATA,
//    DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120,DSORG=PS)
```

The contents of this file are described in Sec.5.2. If the one line of the JCL (\$3) is substituted with

```
//SYSIN    DD *
      [input data described in Sec.5.2]
/*
```

without allocating the Jxxxx.DATA1DNA.DATA, some trouble may occur in the DTLIST routine (the subroutine for printing out initially the data in the input queue (SYSIN) in 80-bit image) in the new environment of the Operating System concerning FORTEXVP, LKEDEX and LMGOEX.

5.2 Input Data

#01 (2I3) 1 line

- ITMAX : maximum number of iteration times for each energy grid of the groups except the thermal group
  (ITMAX = 1, 2 or 3)
- IH : selection of scattering cross section of Hydrogen in the thermal group

$$IH = \begin{cases} 1 \cdots \sigma_s^H = 29.028\text{barn for a simple H (free gas model)} \\ 2 \cdots \sigma_s^H = 46.367\text{barn for H in } H_2O \text{ (Nelkin model)} \\ 3 \cdots \sigma_s^H = 30.798\text{barn for H in polyethylene)} \end{cases}$$

#02 (18A4) 1 line

- Problem title : any characters, numbers or blanks describing the problem on columns 1～72

#03 (7I6, 2E12.5) 1 line

- IMAX : total number of energy groups for this problem (≦125)
- IP(≡2) : geometry (sphere only)
- MMAX : number of kinds of mixture (≦20)
- KMAX : number of spatial regions (MMAX≦KMAX≦20)
  (In a region, mixture is assigned to be homogeneous and mesh sizes (Δr) are assigned to be equal to each other. A region is namely a 'Coarse Mesh.')
- IMAXL : total number of groups of the group constants library used
  (IMAXL = 125 for J439B.BERM125X.DATA)
- I1LIB : group no. "on the group constants library" where the group 1 is to be defined
  (IMAX+I1LIB≦IMAXL+1)

In BERMUDA, the I1LIB-th group on the library is called as "group 1".

- IPS : type of the fixed source

$$IPS = \begin{cases} 0 \cdots \text{volume source} \\ 1 \cdots \text{point source (only at the center of the sphere)} \end{cases}$$

・ER : upper energy (eV) for the group 1 of the problem
EUP(I1LIB+1)＜ER≦EUP(I1LIB)

・EPS : convergence criterion (for angular flux) to be used to terminate the thermal group iteration, or the grid iteration if convergence is attained before ITMAX times
(usually EPS＝10^{-3})

#04 (20I3) 1 line

・(MM(MK), MK＝1, MMAX) : number of nuclides to be included in each mixture
For a vacuum, assign one dummy nuclide which is contained in another mixture. Input its code number in #08 and atomic number density (0.) in #09. (1≦MM(MK)≦10)

#05 (10I6) [(KMAX+9)/10] lines

The brackets [⋯] means the integer discarding the fractions.

・(MR(K), K＝1, KMAX) : mixture no. (≡MK defined in #04) to be assigned to each region

#06 (10I6) [(KMAX+9)/10] lines

・(INTER(K), K＝1, KMAX) : number of mesh intervals between the 'origin' and the outer boundary of each region (even numbers only)
(2≦INTER(1)＜INTER(2)＜⋯＜INTER(KMAX)≦260-KMAX)

#07 (10F6.3) [(KMAX+9)/10] lines

・(DR(K), K＝1, KMAX) : mesh size Δr (cm) for each region
(not the region thickness)

#08 (10I6) MMAX lines

・(MCODE(M, MK), M＝1, MM(MK)) : code no. of each nuclide in the mixture MK defined in the group constants library used
(In case of using J439B.BERM125X.DATA, see Table 2.2 in Ref.1.)
The order of nuclides in a mixture is able to be arbitrary.

Repeat this in the order of MK＝1, ⋯, MMAX renewing the line for each mixture.

#09 (6E12.5)　　[{MM(MK)+5}/6] lines for each mixture

・(AN(M,MK),M=1,MM(MK)) : effective number density ($10^{24}cm^{-3}$) of each nuclide in the mixture MK

The order of nuclides in a mixture must be the same as in #08.

Repeat this in the order of MK=1,…,MMAX renewing the line for each mixture.

#10 (2I6)　　1 line

・N1 : the first mesh point no. to give spatial distribution of non-zero independent adjoint neutron source in #11

・N2 : the last mesh point no. to give spatial distribution of non-zero independent adjoint neutron source in #11

If IPS=1 in #03, then N1=N2=1. Otherwise, $1 \leqq N1 < N2 \leqq NMAX$.

(NMAX: See (3) below.)

In BERMUDA, the numbering of the mesh points is as follows:

(1) "1" for the origin,

(2) doubly (twice) numbered as "INTER(K)+K" and "INTER(K)+K+1" for the interface between the K-th and the (K+1)-th regions where K=1,…, KMAX-1 (for treating spatial discontinuity of the macroscopic cross sections and the source distribution at the interfaces) and

(3) "NMAX=INTER(KMAX)+KMAX" ($\leqq 260$) for the outermost mesh point.

#11 (6E12.5)　　{[(N2-N1)/6]+1} lines

・(S1(N),N=N1,N2) : spatial distribution of independent adjoint neutron source

Independent adjoint neutron source is given in the form of a function with separation of variables as S1(N)×S2(I)×S3(L). (Each of the S1, S2 and S3 should be normalized to its correct magnitude, respectively. However, it is also valid that the product of the S1, S2 and S3 has the correct normalized value for each energy group(*).)

#12 (2I6)　　1 line

・I1 : the first energy group no. to give energy spectra of non-zero independent adjoint neutron source in #13

・I2 : the last energy group no. to give energy spectra of non-zero independent adjoint neutron source in #13
See Table 2.1 in Ref.1, but note that the group no. is defined so that the I1LIB-th group in Table 2.1 in Ref.1 is 'group 1.'
If the source is of mono-energy (monochromatic), I1＝I2＝IMAX.
Otherwise, 1≦I1＜I2≦IMAX.

#13 (6E12.5) {[(I2-I1)/6]+1} lines
・(S2(I), I＝I1, I2) : energy spectra of independent adjoint neutron source
(As an adjoint neutron source is a quantity like a macroscopic absorption cross section Σ_a, S2(I) is given not as an integrated value, but as an averaged value for the group i having energy width ΔE_i.)
The S2(I) is generally normalized to be 1 integrated over energy, that is,

$$\sum_{I=I1}^{I2} S2(I)\,\Delta E(I) = 1.$$

(However, note the proviso(*) under #11.)

#14 (2I6) 1 line
・L1 : the first ordinate no. to give angular distribution of non-zero independent adjoint neutron source in #15
・L2 : the last ordinate no. to give angular distribution of non-zero independent adjoint neutron source in #15
If the source is isotropic, then L1＝1 and L2＝20. And if it is mono-directional, then L1＝L2. Otherwise, 1≦L1＜L2≦20.

#15 (6E12.5) {[(L2-L1)/6]+1} lines
・(S3(L), L＝L1, L2) : angular distribution of independent adjoint neutron source
The S3(L) is generally normalized to be 1 integrated over the unit sphere, that is,

$$2\pi \sum_{L=L1}^{L2} W_L S3(L) = 1,$$

where W_L is the weight for the Gaussian quadrature set of order 20.

(However, note the proviso(*) under #11.)

An example of input data for the BERMUDA-1DNA code is shown in Fig.1.

```
----+-----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
 3  2                                                                    #01
      J.N.S.T. VOL.14,210  BY SEKI,MAEKAWA      LI-C ASSEMBLY            #02
   117    2     4    4   125     9     1 1.455    +7 1.0     -3          #03
     4  6  5  4                                                         #04
        1     2     3     4                                            #05
       20    44    66    82                                            #06
  0.5  1.0058.96136.91938                                              #07
       240   260   280   250                                           #08
         36    37   240   260   280   250                             #09
         60   240   260   280   250                                     "
        240   260   280   250                                          "
    1.751    -3 6.349   -3 7.303   -4 8.185   -5                      #10
    2.507    -3 3.128   -2 3.086   -3 1.075   -2 1.374   -3 2.023  -4  "
    6.930    -2 1.751   -3 6.349   -3 7.303   -4 8.185   -5            "
    1.161    -3 4.159   -3 4.821   -4 5.632   -5                      #11
       1     1                                                         #12
  1.                                                                   #13
    117   117                                                          #14
  1.                                                                   #15
       1    20                                                         "
  7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2  "
  7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2  "
  7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2  "
  7.957747 -2 7.957747 -2                                              "
```

Fig.1 Sample Input Data for Case (1)

5.3 Output Data

The output data of BERMUDA-1DNA are stored on the magnetic disk FT01 (Jxxxx.FLUX1DNA.DATA; see Sec.5.1 ($2)) and are also given on the printer.

The data on the output disk are the following FORTRAN records repeated IMAX times for each group i (i = 1, ···, IMAX) in the binary form,

((PHIA(L,N),L = 1,20),N = 1,260),(TPHIA(N),N = 1,260),

where PHIA(L,N) : $\phi^{*i}(r_N, \omega_L)$
(without component of uncollided adjoint neutron flux),

TPHIA(N) : $\Phi^{*i}(r_N) = 2\pi \sum_{L=1}^{20} W_L \phi^{*i}(r_N, \omega_L) + \Phi_0^{*i}(r_N)$
(scalar adjoint neutron flux) and

$\Phi_0^{*i}(r_N)$: uncollided adjoint neutron flux.

The data on the output print are as follows:

(a) list of input file Jxxxx.DATA1DNA.DATA (see Sec.5.1 ($3)) like Fig.1,
(b) list of the main input parameters with explanatory captions,

(The items (c)～(g) below are repeated for each energy group i in the reverse order (i = IMAX, ···, 1).)

(c) CPU+VU time (sec) accumulated from the start of computation (EXEC LMGOEX) until the end of each main calculational item,
(d) when the convergence has been attained or ITMAX iterations have been finished for the first (chronologically last) grid,
・adjoint neutron balance parameters; F, GAIN, ABBS, SELF, XLEK (see Sec.3.7 in Ref.1) for $F^{i}(r_N, \omega_L)$ in Eq.(12) integrated over the entire spatial region dealing with it as a single coarse mesh region,

・group no. i, iteration times IT, residual VERGF,

where $VERGF = \max_{N,L} \left| \{F^{i(IT-1)}(r_N, \omega_L) / F^{i(IT)}(r_N, \omega_L)\} - 1 \right| < \varepsilon$,

(N,L : except the cases where $F^{i(IT)}(r_N, \omega_L) = 0$),

IT : iteration times (IT = 1, 2, ···),

(As the energy grid model is used for groups except thermal, these printed adjoint neutron balance parameters and VERGF are meaningless for those groups, because the iteration is terminated by ITMAX (ITMAX≦3) times. In addition, these parameters are obtained only from the data of the first (chronologically last) grid in the group i.)

(e) integrated scalar adjoint neutron flux for each spatial region k (k = 1, ···, KMAX),

$$\int_{V_k} dV \Phi^{*i}(r),$$

where V_k : volume of the spatial region k,

$dV = 4\pi r^2 dr$,

(f) ・the upper energy boundary EUP(i) (eV),

・the lower energy boundary EUP(i+1) (eV),

・the energy width ΔE_i (eV),

(g) scalar adjoint neutron flux $\Phi^{*i}(r_N)$ for N = 1, ···, NMAX and

(h) angular adjoint neutron flux $\phi^{*i}(r_N, \omega_L)$ without the uncollided component for the spatial region 1 only for the groups 1 and IMAX.

The STOP code 2222 indicates that the input fixed adjoint neutron source for the group IMAX is zero.

6. Concluding Remarks

An adjoint neutron transport code named BERMUDA-1DNA in the radiation transport code system BERMUDA has been developed for one-dimensional spherical geometry.

To solve the adjoint neutron transport equation numerically, the deterministic direct integration method is adopted in a multigroup model, same as in the regular (forward) neutron transport codes reported in Part I.[1] Use of the Legendre polynomial expansion is avoided in representing the strong anisotropy of angular flux, and also in calculating numerically the group-angle transfer matrix from the double-differential cross section. For the energy groups except the thermal one, a fine energy grid method dividing an energy group into ten subgroups having equal lethargy widths is also applied as in the forward neutron transport codes.

A Coarse Mesh Rebalance (CMR) method is essential especially when an adjoint point source is given in the thermal group, because the absorption cross section is so large in the low energy region that the spatial distribution of scalar and angular fluxes attenuate to 10^{-30} or less. The one-dimensional forward neutron transport code, BERMUDA-1DN, has also been improved to perform CMR in each spatial region.

Both of the BERMUDA-1DNA and the BERMUDA-1DN codes have been enhanced in accuracy to calculate the azimuthal weight of scattering angle $W^*_{n'nm'}$ by averaging the values at '20' points of n in the angular mesh region $\Delta\vec{\Omega}_n$. The azimuthal angle weight was formerly obtained by averaging the values at only '5' points of n.

Validity tests for BERMUDA-1DNA have been performed giving an isotropic point source in the lowest energy group, by comparing the results with those from BERMUDA-1DN being given an isotropic point source in the highest energy group. Five configurations have been used in these tests. The comparison has shown a satisfactory agreement, so that the validity of BERMUDA-1DNA is confirmed to calculate accurate adjoint neutron flux $\phi^{*i}(\vec{r}, \vec{\Omega}_n)$, which is necessary to sensitivity analyses or perturbation theory calculations.

The compiler for the supercomputer used in JAERI was changed in 1993 from FORT77VP to FORTEXVP and its optimization level has become higher. So the total nine source programs in the BERMUDA code system have been updated to be suitable to the new compiler.

Containing the revised BERMUDA-1DN, the source programs of the following nine transport codes:

(1) BERMUDA-1DN,
(2) BERMUDA-2DN,
(3) BERMUDA-2DN-S16,
(4) BERMUDA-3DN,
(5) BERMUDA-1DG,
(6) BERMUDA-2DG,
(7) BERMUDA-2DG-S16,
(8) BERMUDA-3DG and
(9) BERMUDA-1DNA

will be available to the public within 1994 through the Code Center of JAERI. The Code Center is acted by the Nuclear Energy Data Center (NEDAC) formally from April 1994.

The work in these fifteen years has finished with the publication of the present report.

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