Reactor physics programming exercise:
Adjoint equation and perturbation calculations

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Let us consider that a small perturbation, such as temperature increase and control rod insertion, is given to a neutron multiplication system. When neutron multiplication factors before and after the perturbation are denoted to as k_1 and k_2, a reactivity inserted by this perturbation ρ can be presented as

$$\rho = \frac{1}{k_1} - \frac{1}{k_2} = \frac{k_2 - k_1}{k_1 k_2}. \tag{1}$$

In reactor physics calculations, it is quite important to accurately evaluate how much reactivity is inserted by perturbation.

Problem 1: Let us consider a one-dimensional slab reactor with width of 50[cm]. This system is homogeneous, and one-group constants are given as $D = 10$[cm], $\Sigma_a = 1$[/cm] and $\nu\Sigma_f = 1$[/cm]. External boundary conditions are zero neutron flux. Calculate reactivity from k_1 and k_2 when Σ_a in a region from 24[cm] to 26[cm] is changed to 1.1, 1.01, 1.001 and 1.0001.

When neutron multiplication factor is numerically calculated, effective digit of calculated k should be finite. When a perturbation is large, inserted reactivity can be easily calculated from two ks before and after the perturbation as shown in Eq. (1), but when a perturbation is small, it is difficult to obtain reactivity with high accuracy. For example, let us consider that we obtain $k_1 = 1.00000$ and $k_2 = 1.00001$ in a perturbation. In this case, we can calculate reactivity only as 0.00001, and this can be 0.000014 and 0.000005. By adopting strict (or rigorous) convergence criteria to iterative calculations, we can obtain numerical results with higher accuracy and then reactivity is numerically calculated with high accuracy, but it requires long computation time in the iterative calculations. To tackle this problem, the perturbation calculations are generally used.

Neutron diffusion equation can be represented by operators as [1]

$$A\phi = \frac{1}{k}F\phi. \tag{2}$$

Adjoint equation to this equation is defined as

$$A^\dagger \phi^\dagger = \frac{1}{k}F^\dagger \phi^\dagger, \tag{3}$$

where $\phi^\dagger$ is *adjoint neutron flux*. $A^\dagger$ and $F^\dagger$ are adjoint operators to A and F, and the following relations hold:

$$\left\langle \phi^\dagger, A\phi \right\rangle = \left\langle \phi, A^\dagger \phi^\dagger \right\rangle, \tag{4}$$

$$\left\langle \phi^\dagger, F\phi \right\rangle = \left\langle \phi, F^\dagger \phi^\dagger \right\rangle, \tag{5}$$

where $\langle\rangle$ is an integration over whole phase spaces. In the present case, this is an integration over whole space and whole energy group, and neutron absorption component in $\left\langle \phi^\dagger, A\phi \right\rangle$ is explicitly represented as

$$\sum_m \sum_g \phi^\dagger_{m,g} \Sigma_{a,m,g} \phi_{m,g} V_m, \tag{6}$$

where $\phi_{m,g}$ is the gth group neutron flux in spatial mesh m and V_m is volume (or width in one-dimension) of mesh m.

Problem 2: Derive the explicit expressions of $\left\langle \phi^\dagger, A\phi \right\rangle$ and $\left\langle \phi^\dagger, F\phi \right\rangle$.

Let us consider that a perturbation is given to a system presented as Eq. (2), operators are changed as $A' = A + \Delta A$ and $F' = F + \Delta F$, and neutron multiplication factor changes to k'. The adjoint equation before the perturbation and the *forward* equation after the perturbation can be written as follows:

$$A^\dagger \phi^\dagger = \frac{1}{k}F^\dagger \phi^\dagger, \tag{7}$$

$$A'\phi' = \frac{1}{k'}F'\phi'. \tag{8}$$

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[1] As shown in this equation, $1/k$ is multiplied to the operator F. Thus the operator F is a neutron generation operator by fissions and can be explicitly presented as $F\phi = \chi_g \sum_{g'} \nu\Sigma_{f,g'}\phi_{g'}$. Scattering is included to the operator A.

By multiplying ϕ' to the both sides of Eq. (7) and $\phi^\dagger$ to the both sides of Eq. (8), and integrating them over whole phase spaces, the following equation can be derived:

$$\langle \phi', A^\dagger \phi^\dagger \rangle \;=\; \frac{1}{k} \langle \phi', F^\dagger \phi^\dagger \rangle, \tag{9}$$

$$\langle \phi^\dagger, A' \phi' \rangle \;=\; \frac{1}{k'} \langle \phi^\dagger, F' \phi' \rangle. \tag{10}$$

When we consider the nature of the adjoint operators as shown in Eqs. (4) and (5), Eq. (9) can be rewritten as

$$\langle \phi^\dagger, A\phi' \rangle = \frac{1}{k} \langle \phi^\dagger, F\phi' \rangle. \tag{11}$$

By substituting Eq. (11) from Eq. (10), the following equation is derived:

$$\langle \phi^\dagger, \Delta A \phi' \rangle = \left(\frac{1}{k'} - \frac{1}{k} \right) \langle \phi^\dagger, F'\phi' \rangle + \frac{1}{k} \langle \phi^\dagger, \Delta F \phi' \rangle. \tag{12}$$

From this equation, it can be found that reactivity inserted by this perturbation can be calculated by the following equation:

$$\rho = \frac{1}{k} - \frac{1}{k'} = \frac{\frac{1}{k} \langle \phi^\dagger, \Delta F \phi' \rangle - \langle \phi^\dagger, \Delta A \phi' \rangle}{\langle \phi^\dagger, F'\phi' \rangle}. \tag{13}$$

This equation suggests that small reactivity can be accurately calculated because reactivity is obtained from simple integral calculations.

Furthermore, when we introduce an approximation $\phi' \approx \phi$ to Eq. (13), the following equation is derived:

$$\rho = \frac{\frac{1}{k} \langle \phi^\dagger, \Delta F \phi \rangle - \langle \phi^\dagger, \Delta A \phi \rangle}{\langle \phi^\dagger, F'\phi \rangle}. \tag{14}$$

] The perturbation calculation presented in Eq. (13) is referred to as *the rigorous perturbation* and that in Eq. (14) is as *the first-order perturbation.* In the rigorous perturbation calculations, adjoint neutron flux before the perturbation $\phi^\dagger$ and forward neutron flux after the perturbation ϕ' are required, so calculations of ϕ' should be done for each perturbation. On the other hand, in the first-order perturbation calculations, forward neutron flux ϕ and adjoint neutron flux ϕ^* before the perturbation are required, so reactivity given by arbitrary perturbation can be calculated from these quantities. This theory is generally used in sensitivity calculations.

One-group neutron diffusion eigenvalue adjoint equation can be written as

$$-\frac{d}{dx}\left(D(x)\frac{d}{dx}\phi^\dagger(x) \right) + \Sigma_a(x)\phi^\dagger(x) = \frac{1}{k}\nu\Sigma_f(x)\phi^\dagger(x). \tag{15}$$

This is the exactly same as the one-group forward equation; $\phi(x) = \phi^\dagger(x)$.

> Problem 3: Calculate reactivity given by a perturbation in the problem 1 by using the first-order perturbation theory; $\phi(x)$ and $\phi^\dagger(x)(= \phi(x))$. Compare results with those in problem 1.

Perturbation is given only to Σ_a in the problem 1, so $\Delta F = 0$.

> Problem 3: Calculate reactivity in the problem 1 by the rigorous perturbation theory; $\phi'(x)$ and $\phi^\dagger(x)(= \phi(x))$.

On the other hand, multi-group adjoint equation is different from multi-group forward equation. Multi-group adjoint equation is presented as

$$-\frac{d}{dx}\left(D_g(x)\frac{d}{dx}\phi_g^\dagger(x) \right) + \Sigma_{a,g}(x)\phi_g^\dagger(x) + \sum_{g'}\Sigma_{g\to g'}\phi_g^\dagger(x) = \frac{1}{k}\nu\Sigma_{f,g}\sum_{g'}\chi_{g'}(x)\phi_{g'}^\dagger(x) + \sum_{g'}\Sigma_{g\to g'}\phi_{g'}^\dagger(x). \tag{16}$$

Numerical procedure to solve multi-group adjoint equation is basically the same as that for the forward equation, but an order of energy group in the procedure is different. In two-group problems, fission neutron source is initially assumed, and then adjoint neutron flux is calculated for group 2, and then calculation is performed for group 1. Note that fission neutron source in group g is $\nu\Sigma_{f,g}\sum_{g'}\chi_{g'}\phi_{g'}$ in the adjoint equation. Since computer program for the forward equation

might be extended to adjoint equation treatment, it is better that scalar fission source is defined as $F = \sum_{g'} \chi_{g'} \phi_{g'}$ and fission source in each group is defined as $\nu\Sigma_{f,g} F$. Neutron multiplication factor at the nth outer iteration k^n can be guessed by $k^n = F^n/(F^{n-1}/k^{n-1})$, but is the initial fission source of the outer iteration is set as $F^0 = 1$ and $k^0 = 1$ is also assumed, $k^n = F^n$ since $F^{n-1}/k^{n-1} = 1$.

Problem 5: Let us consider a one-dimensional slab with width of $100[\text{cm}]$ and constants are given in the table below. External boundary conditions are zero neutron flux. Obtain k and $\phi_g^\dagger$ by solving the adjoint equation, and confirm that the calculated k coincides with k obtained by solving the forward equation of the same system.

Energy group	D	Σ_a	$\Sigma_{g,g+1}$	$\nu\Sigma_f$	χ
1	1.5	0.01	0.02	0.005	1.0
2	0.4	0.1	-	0.141	0.0

Problem 6: Obtain reactivity by the rigorous perturbation calculations when $\sigma_{a,1}$ is increased by 5% in a range from $48[\text{cm}]$ to $52[\text{cm}]$ in the slab reactor given in the problem 5. Also calculate reactivity induced by different perturbation which are given to $\nu\Sigma_{f,2}$ and $\Sigma_{1\rightarrow2}$ in the same spatial range.

Problem 7: On the slab reactor given the problem 6, calculate reactivity when D_1 and D_2 are increased by 1% in a whole region.

Reactivity calculations for diffusion coefficients perturbation are a bit complicated, so descriptions are provided below.

When a perturbation is given to diffusion coefficients, numerator of perturbation equation ρ^{nume} is calculated as follows:

$$\rho^{nume} = \int dx \left\{ \phi^\dagger \frac{d}{dx}\left(\Delta D \frac{d\phi'}{dx} \right) \right\} \tag{17}$$

$$= \left[\phi^\dagger \Delta D \frac{d\phi'}{dx} \right] - \int dx \left\{ \left(\frac{d\phi^\dagger}{dx} \right) \Delta D \left(\frac{d\phi'}{dx} \right) \right\}. \tag{18}$$

Since an integration in Eq. (17) is done over whole spatial region, so quantities of the first term of the right hand side of Eq. (18) should be on external boundaries, and those are zero. [2] Finally ρ^{nume} can be presented as

$$\rho^{nume} = -\int dx \left\{ \left(\frac{d\phi^\dagger}{dx} \right) \Delta D \left(\frac{d\phi'}{dx} \right) \right\} \tag{19}$$

Neutron current J is represented as follows in the diffusion approximation:

$$J = -D \frac{d\phi}{dx}. \tag{20}$$

Thus Eq. (19) can be rewritten by using neutron current as

$$\rho^{nume} = -\int dx \left\{ \left(\frac{J^\dagger}{D} \right) \Delta D \left(\frac{J'}{D'} \right) \right\}. \tag{21}$$

In general numerical procedure to diffusion equation, neutron current j on the mesh surface is defined from neutron flux at mesh surface and mesh center, so J should be constant in left-half and right-half in each mesh. When these are denoted to as J_{left} and J_{right}, ρ^{nume} can be written as

$$\rho^{nume} = -\frac{\Delta D}{DD'} \frac{\Delta x_i}{2} \left(J_{left}^\dagger J_{left}' + J_{right}^\dagger J_{right}' \right) \tag{22}$$

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[2]In the zero neutron flux condition, $\phi^\dagger = 0$ on the boundary. In the reflective boundary condition, $d\phi'/dx = 0$ on the boundary.