Lecture 24
The Adjoint Transport Equation

1 Introduction

The adjoint transport operator constitutes a powerful tool for efficiently calculating transport responses for arbitrary source functions and for weakly perturbed systems. It is also useful for formulating certain functionals arising in variational transport formulations.

2 Derivation of the Adjoint Transport Operator

2.1 Inner Products

We begin our discussion by considering the definition of an inner product, which is required to define an adjoint operator. Given any two elements of a linear function space, f and g, the inner product of f and g, denoted by $< f, g >$, maps f and g to a scalar. Furthermore, the inner product must have the following properties:

1. linearity:

$$\langle af_1 + bf_2, g\rangle = a\langle f_1, g\rangle + b\langle f_2, g\rangle \,, \tag{1a}$$

where a and b are arbitrary constants.

2. symmetry:

$$\langle f, g\rangle = \langle g, f\rangle\,, \tag{1b}$$

3. strict positivity:

$$\begin{aligned} \langle f, f\rangle &\geq 0\,, \quad \text{for all } f, \\ &= 0\,, \quad \text{if and only if } f = 0. \end{aligned} \tag{1c}$$

A typical inner product for square-integrable phase-space functions is

$$\langle f, g\rangle = \int f(\overrightarrow{P})g(\overrightarrow{P})\,dP\,, \tag{2}$$

where dP denote a differential phase space volume. However, it is important to recognize that there are an infinite number of valid inner products.

2.2 Adjoint Operators

Let $\mathbf{A}$ denote a linear operator defined on an inner product function space. Then $\mathbf{A}$ has an adjoint, denoted $\mathbf{A}^\dagger$, if

$$\langle \mathbf{A}f, g\rangle = \langle f, \mathbf{A}^\dagger g\rangle\,, \quad \text{for all } f \text{ and } g. \tag{3}$$

Note that the adjoint operator will generally be a function of the inner product being used. Thus the adjoint of an operator is only unique for a given inner product.

Let us now consider the 3-D transport operator defined over all space:

$$\mathbf{B}\psi = \overrightarrow{\Omega} \cdot \overrightarrow{\nabla}\psi + \sigma_t\psi = \int_0^\infty \int_{4\pi} \sigma_s \left(E' \rightarrow E, \overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) \psi(\overrightarrow{\Omega}', E')\, d\Omega'\, dE' \,. \tag{4}$$

Assuming the standard inner product for square-integrable functions on this infinite phase-space domain, the adjoint transport operator exists and is easily shown to be given by

$$\mathbf{B}^\dagger\psi = -\overrightarrow{\Omega} \cdot \overrightarrow{\nabla}\psi + \sigma_t\psi = \int_0^\infty \int_{4\pi} \sigma_s \left(E \rightarrow E', \overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) \psi(\overrightarrow{\Omega}', E')\, d\Omega'\, dE' \,. \tag{5}$$

On a finite spatial domain, the adjoint operator does not formally exist, but one can nonetheless show that

$$\langle \mathbf{B}f, g \rangle = \int_0^\infty \int_{4\pi} \oint f g\, \overrightarrow{\Omega} \cdot \overrightarrow{n}\, dA\, d\Omega\, dE + \langle f, \mathbf{B}^\dagger g \rangle \,. \tag{6}$$

3 Response Calculations

Suppose that we wish to compute an integral response from a solution to the transport equation, i.e., we want to compute,

$$\mathcal{R} = \int q^\dagger(\overrightarrow{P})\psi(\overrightarrow{P})\, dP \,, \tag{7}$$

where $q^\dagger(\overrightarrow{P})$ is an arbitrary response function. We can solve for $\mathcal{R}$ in two ways. The first is the standard way, namely, to solve the transport equation and then directly evaluate the response using Eq. (7). The other is to first solve the following adjoint equation:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla}\psi^\dagger + \sigma_t\psi^\dagger = \int_0^\infty \int_{4\pi} \sigma_s \left(E \rightarrow E', \overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) \psi^\dagger(\overrightarrow{\Omega}', E')\ \ d\Omega'\, dE' + q^\dagger \,. \tag{8}$$

Then the response is evaluated with the following expression:

$$\langle q^\dagger, \psi \rangle = \langle q \psi^\dagger \rangle - \int_0^\infty \int_{4\pi} \oint \psi \psi^\dagger \overrightarrow{\Omega} \cdot \overrightarrow{n} \, dA \, d\Omega \, dE \, . \tag{9}$$

The adjoint boundary conditions for Eq. (8) are chosen to ensure that the only forward fluxes contributing to the response via Eq. (9) are those that are known from boundary conditions. Consequently, a single adjoint transport calculation can be used to compute the response for any incident boundary flux or distributed source. In contrast, the standard approach via Eq. (7) requires a separate transport calculation for each incident boundary flux and distributed source. Thus if a particular response is desired for a variety of sources, the adjoint approach is far more efficient than the standard or forward approach.

Because of the minus sign in front of the gradient term in Eq. (5), adjoint particles in direction $\overrightarrow{\Omega}$ actually travel in the direction $-\overrightarrow{\Omega}$. Thus while adjoint boundary fluxes are specified for incoming directions, such directions actually correspond to $\overrightarrow{\Omega} \cdot \overrightarrow{n} > 0$ rather than $\overrightarrow{\Omega} \cdot \overrightarrow{n} < 0$. If the forward solution satisfies incident flux or vacuum boundary conditions, the adjoint solution must satisfy vacuum conditions, and if the forward solution satisfies reflective conditions, the adjoint solution must satisfy reflective conditions.

Equation (9) is derived as follows. First we take the inner product of $\psi^\dagger$ with Eq. (4):

$$\langle \mathbf{L}\psi, \psi^\dagger \rangle = \langle q, \psi^\dagger \rangle \, . \tag{10}$$

Next we take the inner product of ψ with Eq. (5):

$$\langle \mathbf{L}^\dagger \psi^\dagger, \psi \rangle = \langle q^\dagger, \psi \rangle \,. \tag{11}$$

Equation (10) is then subtracted from Eq. (11):

$$\langle q^\dagger, \psi \rangle = \langle \mathbf{L}^\dagger \psi^\dagger, \psi \rangle - \langle \mathbf{L}\psi, \psi^\dagger \rangle + \langle q, \psi^\dagger \rangle \,. \tag{12}$$

Substituting from Eq. (7) into Eq. (12), we get

$$\langle q^\dagger, \psi \rangle = \langle \mathbf{L}^\dagger \psi^\dagger, \psi \rangle - \langle \mathbf{L}\psi, \psi^\dagger \rangle + \langle q, \psi^\dagger \rangle \,. \tag{13}$$

Finally, substituting from (6) into (13), we obtain Eq. (9).

4 First-Order Perturbation Theory

Suppose that we wish to determine the perturbation in a particular transport response due to a perturbation in the source and/or the transport operator, e.g., a small change in geometry, cross sections, etc. The straightforward way to compute a perturbation in a response would be to first compute the transport solution for the both the unperturbed and perturbed systems, and subtract the unperturbed response from the perturbed response. This approach can suffer from calcellation errors, and requires a calculation for each perturbed system. An alternative approach is to use first-order perturbation theory, which

allows the direct calculation of *any* perturbed response using forward and adjoint solutions for the *unperturbed* system.

We begin the derivation of this result by considering the unperturbed forward and adjoint solutions, respectively:

$$\mathbf{L}\psi = q\,, \tag{14}$$

and

$$\mathbf{L}^\dagger\psi^\dagger = q^\dagger\,. \tag{15}$$

The perturbed forward solution satisfies:

$$(\mathbf{L} + \delta\mathbf{L})\,(\psi + \delta\psi) = q + \delta q\,. \tag{16}$$

Algebraically manipulating Eq. (16), we get:

$$\mathbf{L}\psi + \mathbf{L}\delta\psi + \delta\mathbf{L}\psi + \delta\mathbf{L}\delta\psi = q + \delta q\,. \tag{17}$$

Dropping the second-order term in Eq. (17), we obtain a simplified perturbed forward equation that is accurate through first order:

$$\mathbf{L}\psi + \mathbf{L}\delta\psi + \delta\mathbf{L}\psi = q + \delta q\,. \tag{18}$$

Taking the inner product of $\psi^\dagger$ with Eq. (18) gives:

$$\langle\mathbf{L}\psi, \psi^\dagger\rangle + \langle\mathbf{L}\delta\psi, \psi^\dagger\rangle + \langle\delta\mathbf{L}\psi, \psi^\dagger\rangle = \langle q, \psi^\dagger\rangle + \langle\delta q, \psi^\dagger\rangle\,. \tag{19}$$

Taking the inner product of $\psi + \delta\psi$ with Eq. (15) gives:

$$\langle \mathbf{L}^\dagger \psi^\dagger, \psi \rangle + \langle \mathbf{L}^\dagger \psi^\dagger, \delta\psi \rangle = \langle q^\dagger, \psi \rangle + \langle q^\dagger, \delta\psi \rangle \,. \tag{20}$$

Subtracting Eq. (19) from Eq. (20), and using Eqs. (6) and (9) to simplify, we get

$$\langle q^\dagger, \delta\psi \rangle = \langle \delta q, \psi^\dagger \rangle - \langle \delta\mathbf{L}\psi, \psi^\dagger \rangle - \int_0^\infty \int_{4\pi} \oint \delta\psi \, \psi^\dagger \overrightarrow{\Omega} \cdot \overrightarrow{n} \, dA \, d\Omega \, dE \,. \tag{21}$$

As long as geometric perturbations are limited to the interior of the transport domain, it will be possible to evaluate the surface integral in Eq. (21).

First-order perturbation theory can be used to calculate derivatives of a response with respect to a perturbation parameter. For instance, suppose that we express an operator perturbation as a function of a parameter, α as follows:

$$\delta\mathbf{L}(\alpha) = \alpha \delta\mathbf{L}_0 \,, \tag{22}$$

where $\delta\mathbf{L}_0$ denotes a fixed perturbation. Substituting from Eq. (22) into Eq. (21), and assuming that only this operator perturbation is non-zero, we obtain

$$\begin{aligned} \delta\mathcal{R}(\alpha) &= -\langle \delta\mathbf{L}\psi, \psi^\dagger \rangle \,, \\ &= -\alpha \langle \delta\mathbf{L}_0 \psi, \psi^\dagger \rangle \,. \end{aligned} \tag{23}$$

Note that

$$\frac{\delta\mathcal{R}(\alpha)}{\alpha} = \frac{\mathcal{R}(\alpha) - \mathcal{R}(0)}{\alpha} = -\langle \delta\mathbf{L}_0 \psi, \psi^\dagger \rangle \,. \tag{24}$$

Trivially taking the limit of the above expression as $\alpha \to 0$, we get

$$\frac{d\mathcal{R}}{d\alpha} = -\langle \delta \mathbf{L}_0 \psi, \psi^\dagger \rangle \,. \tag{25}$$

Such derivaties are very useful for sensitivity analysis.

5 Adjoint Calculations with Standard S_n Codes

Very few changes have to be made to a standard multigroup S_n code to do an adjoint calculation. In fact one need only perform certain operations on the cross section data rather than make changes to the discretization or solution algorithm. For instance, consider the following multigroup forward transport equation:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi_g + \sigma_{t,g} \psi_g = \sum_{g'=1}^{G} \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \frac{2\ell+1}{4\pi} \sigma_{\ell,g' \to g} \phi_{\ell,g'}^m Y_\ell^m(\overrightarrow{\Omega}) + q_g(\overrightarrow{\Omega}) \,. \tag{26}$$

If we assume the following inner product that is a combination of the standard inner product and the multigroup dot product:

$$\langle \overrightarrow{\psi}, \overrightarrow{\psi}^\dagger \rangle = \int \int_{4\pi} \sum_{g=1}^{G} \psi_g \psi_g^\dagger \, d\Omega \, dV \,, \tag{27}$$

the corresponding equation adjoint to Eq. (26) is

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi_g^\dagger + \sigma_{t,g} \psi_g^\dagger = \sum_{g'=1}^{G} \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \frac{2\ell+1}{4\pi} \sigma_{\ell,g \to g'} \phi_{\ell,g'}^{m,\dagger} Y_\ell^m(\overrightarrow{\Omega}) + q_g^\dagger(\overrightarrow{\Omega}) \,. \tag{28}$$

Note that the only real change other than the change of sign of the streaming term is the transposition of the group-to-group transfer cross sections. Note that although we have not explicitly included fission or other more general interactions, all interactions can be represented in terms of a removal cross section and group-to-group transfer cross section coefficients. For instance, the transfer coefficients for fission are isotropic and given by:

$$\sigma_{0,g'\to g} = \chi_g \nu \sigma_{f,g'} \,. \tag{29}$$

Thus there is no loss of generality in our presentation. Also note that using the multigroup dot product makes it easy to form the adjoint multigroup equation, but this dot product does not go over to the standard analytic energy inner product in the limit as the number of groups increases. This is not a problem *per se*, but it is an important point to remember when defining responses. The response function must be defined to obtain the desired response using the chosen inner product. If the inner product changes, the response function must also change.

Next we define an angular flux, $\hat{\psi}_g$, as follows:

$$\hat{\psi}_g(-\overrightarrow{\Omega}) = \psi_g^\dagger(\overrightarrow{\Omega}) \,. \tag{30}$$

Substituting from Eq. (30) into Eq. (28), we get

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \hat{\psi}_g(-\overrightarrow{\Omega}) + \sigma_{t,g} \hat{\psi}_g(-\overrightarrow{\Omega}) = \sum_{g'=1}^{G} \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \frac{2\ell+1}{4\pi} \sigma_{\ell,g\to g'} \phi_{\ell,g'}^{m,\dagger} Y_\ell^m(\overrightarrow{\Omega}) + q_g^\dagger(\overrightarrow{\Omega}) \,. \tag{31}$$

Evaluating Eq. (31) at $-\overrightarrow{\Omega}$ gives:

$$\overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\hat{\psi}_g(\overrightarrow{\Omega})+\sigma_{t,g}\hat{\psi}_g(\overrightarrow{\Omega})=\sum_{g'=1}^{G}\sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell}\frac{2\ell+1}{4\pi}\sigma_{\ell,g\to g'}\phi_{\ell,g'}^{m,\dagger}Y_\ell^m(\overrightarrow{-\Omega})+q_g^\dagger(-\overrightarrow{\Omega})\,. \quad (32)$$

Now, the spherical-harmonics are even for ℓ even and odd for ℓ odd. So it follows that

$$Y_\ell^m(-\overrightarrow{\Omega})=(-1)^\ell Y_\ell^m(\overrightarrow{\Omega})\,. \quad (33)$$

and further that

$$\begin{aligned}\int_{4\pi}\hat{\psi}(\overrightarrow{\Omega})Y_\ell^m(\overrightarrow{\Omega})\,d\Omega &= \\ &= \int_{4\pi}\psi^\dagger(-\overrightarrow{\Omega})Y_\ell^m(\overrightarrow{\Omega})\,d\Omega\,,\\ &= \int_{4\pi}\psi^\dagger(\overrightarrow{\Omega})Y_\ell^m(-\overrightarrow{\Omega})\,d\Omega\,,\\ &= (-1)^\ell\int_{4\pi}\psi^\dagger(\overrightarrow{\Omega})Y_\ell^m(-\overrightarrow{\Omega})\,d\Omega\,. \quad (34)\end{aligned}$$

From Eqs. (33) and (34) it follows that

$$\phi_{\ell,g'}^{m,\dagger}Y_\ell^m(\overrightarrow{-\Omega})=\hat{\phi}_{\ell,g'}^{m}Y_\ell^m(\overrightarrow{\Omega}) \quad (35)$$

Substituting from Eq. (35) into Eq. (32), we obtain

$$\overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\hat{\psi}_g(\overrightarrow{\Omega})+\sigma_{t,g}\hat{\psi}_g(\overrightarrow{\Omega})=\sum_{g'=1}^{G}\sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell}\frac{2\ell+1}{4\pi}\sigma_{\ell,g\to g'}\hat{\phi}_{\ell,g'}^{m}Y_\ell^m(\overrightarrow{-\Omega})+q_g^\dagger(-\overrightarrow{\Omega})\,. \quad (36)$$

Note that this is just the forward equation for $\hat{\psi}$ with two exceptions:

1. the group-to-group transfer coefficients are transposed in initial and final group index,

2. the distributed source is evaluated at $-\overrightarrow{\Omega}$ rather than $\overrightarrow{\Omega}$.

The boundary conditions for $\hat{\psi}$ follow from those for $\psi^{\dagger}$:

$$\hat{\psi}(\overrightarrow{\Omega}) = \psi^{\dagger}(-\overrightarrow{\Omega}), \quad \text{for } \overrightarrow{\Omega} \cdot \overrightarrow{n} < 0. \tag{37}$$

Thus one can effectively compute $\psi^{\dagger}$ by first solving Eq. (36) for $\hat{\psi}$ and then solving for $\psi^{\dagger}$ via Eq. (30).

It is important to remember that an S_n version of Eq. (28) having the same spatial discretization as Eq. (26) might not be discretely adjoint to Eq. (26). If this is the case, the forward and adjoint values computed for a given response will not be the same for any given spatial mesh and S_n order. However, if the discrete space-direction inner product used converges as the mesh is refined to the standard space-direction inner product used to define Eq. (28), the forward and adjoint values for a given response will become equal as the spatial mesh is refined and the S_n order is increased.

6 Adjoint Functionals

The adjoint operator is also useful for forming functionals used in variational transport formulations. However, since variational transport formulations is a major topic in itself, we defer a discussion of adjoint functionals to a discussion of variational transport formulations.