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THE ADJOINT SPACE IN HEAT TRANSPORT THEORY

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Abstract – The mathematical concept of adjoint operators is applied to the heat transport equation and an adjoint equation is defined with a detector function as source term. The physical meaning of the solutions for the latter equation is outlined together with an application in the field of perturbation analysis.

NOMENCLATURE

c, specific heat capacity [J/(kg · K)];
$\mathbf{n}$, unit normal vector;
O, operator;
O^+, adjoint operator;
q, heat source density [W/m^3];
$\mathbf{r}$, position vector;
R, detector reading;
S, surface [m^2];
t, time [s];
T, temperature [K];
T^+, adjoint function;
$\mathbf{v}$, velocity vector [m/s];
V, volume [m^3].

Greek symbols

α, heat-transfer coefficient [W/(m^2 · K)];
ε, detector efficiency;
λ, heat conductivity [W/(m · K)];
ρ, density [kg/m^3];
ϕ, heat flux density [W/m^2];
ψ, arbitrary function.

Subscripts

b, boundary;
f, final;
i, initial;
o, unperturbed;
s, source;
th, thermometer.

INTRODUCTION

IN CALCULATIONS on neutron transport in nuclear reactors the use of the mathematical concept of so-called adjoint operators has proven to be very useful for certain types of problems. Neutron transport problems are often characterized by their complexity, mainly because of the number of variables defining the neutron field (position, velocity, direction of movement and time) and the geometrical complexities which occur in practice. Even with modern computers it is only possible to calculate approximate solutions and any technique to increase the calculational efficiency is welcome. Against this background the adjoint calculational techniques have found widespread use in reactor physics, for instance in such areas as variational techniques for constructing approximate solutions [1], perturbation techniques for calculation of effects of small parameter changes [1, 2] and efficient techniques for Monte Carlo calculations [3]. As a result, the technique itself has developed considerably and may find fruitful applications in other areas of physics. In connection with research on reactor dynamics, the present authors have applied the adjoint technique to the heat-transport equations in order to calculate temperature and neutron density fluctuations in a reactor, which is an application in the field of perturbation theory. Recently an application in the area of sensitivity theory for thermal-hydraulics problems was published, also emanating from the nuclear reactor field [4].

In the next paragraphs the principle of the adjoint technique is outlined and an example of an application is presented; this sample problem has been chosen as simple as possible in order to focus on principles.

THE ADJOINT HEAT TRANSPORT EQUATION

We start from the heat transport equation, which reads in usual notation:

$$\rho c \frac{\partial T}{\partial t} = -\rho c \mathbf{v} \cdot \nabla T + \nabla \cdot \lambda \nabla T + q, \tag{1}$$

where the space and time variables have been omitted for the sake of convenience. Equation (1) can be written as

$$OT = q, \tag{2}$$

where O denotes the transport operator. The solution T should satisfy boundary conditions and initial conditions, imposed by the physics of the system under consideration.

We now introduce a detector function $\varepsilon(\mathbf{r}, t)$ which gives the sensitivity of a 'thermometer', positioned in the system, such that the reading of the detector is given by:

$$R = (\varepsilon, T) = \int_{t_i}^{t_f} \mathrm{d}t \int_V \mathrm{d}\mathbf{r} \varepsilon T, \tag{3}$$

where t_i and t_f are the initial and final time of the time interval under consideration and V the total volume of the system, and where a parentheses notation for integration over phase space is introduced.

Suppose we can find an operator O^+ that satisfies the following relation:

$$(\psi, OT) = (O^+\psi, T), \tag{4}$$

where ψ should satisfy boundary conditions to be specified, but remains arbitrary for the rest. We shall call O^+ *adjoint* to O. Then we can define an adjoint function T^+ that satisfies the equation:

$$O^+T^+ = \varepsilon. \tag{5}$$

From equations (2), (4) and (5) we obtain:

$$R = (\varepsilon, T) = (q, T^+). \tag{6}$$

From this it follows that the function T^+ is a measure for the influence exerted on the temperature in the detection region by an amount of heat injected into the system. This becomes even more apparent by choosing a simple detector function:

$$\varepsilon = \varepsilon_{th}\delta(\mathbf{r} - \mathbf{r}_{th}) \cdot \delta(t - t_{th}) \tag{7a}$$

and as source term a heat injection pulse at time t_s and position $\mathbf{r}_s$:

$$q = q_s\delta(\mathbf{r} - \mathbf{r}_s) \cdot \delta(t - t_s). \tag{7b}$$

In equations (7a) and (7b) δ denotes the Dirac delta distribution. The particular choice of detector function implies that at time t_{th} the temperature in position $\mathbf{r}_{th}$ is read. Substitution in (6) gives:

$$q_sT^+(\mathbf{r}_s, t_s) = \varepsilon_{th}T(\mathbf{r}_{th}, t_{th}). \tag{8}$$

In other words: the function T^+ gives the temperature response in Kelvin per Joule. One is tempted to call T^+ an "adjoint temperature" but it should be stressed that such a nomenclature is not in accordance with its physical dimension.

For the sake of simplicity we restrict ourselves further to stationary cases, for which the regular equation reads:

$$-\rho c\mathbf{v} \cdot \nabla T + \nabla \cdot \lambda \nabla T + q = 0 \tag{9}$$

and try out as adjoint equation:

$$\nabla \cdot \rho c\mathbf{v}T^+ + \nabla \cdot \lambda\nabla T^+ + \varepsilon = 0. \tag{10}$$

The dimension of T^+ is Kelvin per Watt, in case that ε is a thermometer.

We multiply equation (9) by T^+ and equation (10) by T, subtract and integrate over the total system volume. In order to satisfy equation (4), both the convection terms and the conduction terms should cancel. For the conduction terms we get:

$$\begin{aligned}\int_V \mathrm{d}\mathbf{r}\{T^+\nabla \cdot \lambda\nabla T - T\nabla \cdot \lambda \nabla T^+\} &= \int_V \mathrm{d}\mathbf{r}\{\nabla \cdot (T^+\lambda\nabla T - T\lambda\nabla T^+)\} \\ &= \int_S \mathrm{d}S\{T^+\lambda\nabla T \cdot \mathbf{n} - T\lambda\nabla T^+ \cdot \mathbf{n}\},\end{aligned} \tag{11}$$

where the surface integration is over the bounding surface of the system, on which the boundary conditions are imposed; $\mathbf{n}$ is a unit vector in the direction of the outward normal on the surface. The last step in the derivation above is based on Gauss' divergence theorem.

By appropriate choice of boundary conditions, the two terms in (11) will cancel. If, for instance, the direct boundary condition is:

$$(-\lambda\nabla T \cdot \mathbf{n})_b = \alpha T_b, \tag{12a}$$

we should choose:

$$(-\lambda\nabla T^+ \cdot \mathbf{n})_b = \alpha T_b^+. \tag{12b}$$

The subscript b refers to the boundary of the system.

The heat transport equation (1) determines the temperature distribution, except for a constant which can be chosen arbitrarily. If we take as reference value a constant temperature of the surroundings of the system, such that T is the difference with this surrounding temperature, α in equation (12a) denotes the coefficient of heat transfer to these surroundings. In case the system is imbedded in an infinitely good heat conductor, the boundary conditions (12a) and (12b) can be written as $T_b = 0$ and $T_b^+ = 0$. The conduction operator is said to be *self-adjoint*, because both operators and boundary conditions are identical in regular space and adjoint space.

For the convection terms the forementioned procedure gives:

$$\begin{aligned}\int_V \mathrm{d}\mathbf{r}\{T\nabla \cdot \rho c\mathbf{v}T^+ + T^+\rho c\mathbf{v} \cdot \nabla T\} &= \int_V \mathrm{d}\mathbf{r}\nabla \cdot \rho c\mathbf{v}TT^+ \\ &= \int_S \mathrm{d}S\rho c\mathbf{v}TT^+ \cdot \mathbf{n},\end{aligned} \tag{13}$$

where again the last step is based on Gauss' theorem. This term applies only to stream tubes; $T\rho c\mathbf{v} \cdot \mathbf{n}$ is the enthalpy flow density.

Leaving re-entrant flows out of discussion, injection of heat at the exit of a stream tube can have no influence on a thermometer reading inside the system and the boundary condition is:

$$T^+ = 0 \quad \text{for } \mathbf{v} \cdot \mathbf{n} > 0. \tag{14}$$

The integral over surfaces with entrant flows remains and depends on the boundary condition of T. In case that the entrant flows have the temperature of the surroundings, viz. $T = 0$, the surface integral cancels.

We conclude that the convection operator has no adjoint in the complete sense of equation (4). Equations (9), (10) and (13) can be combined to give:

$$\int_V \mathrm{d}\mathbf{r}\varepsilon T = \int_V \mathrm{d}\mathbf{r}qT^+ - \int_S \mathrm{d}S\rho c\mathbf{v}TT^+ \cdot \mathbf{n}. \tag{15}$$

The last term accounts for convective transport from the surroundings and can be incorporated in the second term by defining a surface heat source density:

$$q_{\text{surface}} = \rho c\mathbf{v}T \cdot \mathbf{n}. \tag{16}$$

Finally it should be remarked that adjoint operators can only be defined for linear operators, which in the present context implies that ρ, c and $\mathbf{v}$ may not depend on T. For an extension of the adjoint technique to time-dependent phenomena, we refer to the reactor physics literature listed in the references.

PERTURBATION ANALYSIS

The adjoint function T^+ is a measure for the influence of heat injection on a fixed temperature detector. The heat injection and the detector may have arbitrary spatial distributions. This means that the quantity T^+ is very useful for the calculation of the effect of system perturbations. In order to illustrate this, we assume that the heat conductivity in the system undergoes a small change $\delta\lambda(\mathbf{r})$ and we ask for the change in detector reading δR.

We define $\lambda = \lambda_o + \delta\lambda$ and $T = T_o + \delta T$, where λ_o and T_o refer to the unperturbed state or reference system. The equations pertinent to this problem read:

$$-\rho c\mathbf{v}\cdot\nabla T + \nabla\cdot\lambda\nabla T + q = 0, \tag{17}$$

boundary: $$\lambda\nabla T\cdot\mathbf{n} = -\alpha T, \tag{17a}$$

$$\nabla\cdot\rho c\mathbf{v}T^+ + \nabla\cdot\lambda_o\nabla T^+ + \varepsilon = 0, \tag{18}$$

boundary: $$\lambda_o\nabla T^+\cdot\mathbf{n} = -\alpha T. \tag{18a}$$

In line with the procedure described in the preceding paragraph it follows:

$$R = \int_V \mathrm{d}\mathbf{r}\varepsilon T = \int_V \mathrm{d}\mathbf{r} q T^+ - \int_V \mathrm{d}\mathbf{r}\delta\lambda\nabla T\cdot\nabla T^+ - \int_S \mathrm{d}S T T^+\rho c\mathbf{v}\cdot\mathbf{n}. \tag{19}$$

For the unperturbed state we have:

$$R_o = \int_V \mathrm{d}\mathbf{r}\varepsilon T_o = \int_V \mathrm{d}\mathbf{r} q T^+ - \int_S \mathrm{d}S T_o T^+\rho c\mathbf{v}\cdot\mathbf{n}. \tag{20}$$

Subtraction gives:

$$\delta R = \int_V \mathrm{d}\mathbf{r}\varepsilon\delta T = -\int_V \mathrm{d}\mathbf{r}\delta\lambda\nabla T\cdot\nabla T^+ - \int_S \mathrm{d}S\delta T\cdot T^+\rho c\mathbf{v}\cdot\mathbf{n}. \tag{21}$$

Neglecting the second-order term $\delta\lambda\nabla\delta T$ in this equation and putting $\delta T = 0$ on entrant flow surfaces, gives the first-order perturbation expression:

$$\delta R = -\int_V \mathrm{d}\mathbf{r}\delta\lambda\nabla T_o\cdot\nabla T^+. \tag{22}$$

This technique can be applied to perform sensitivity analysis on system parameters, i.e. to answer the question how the temperature in a certain point or region of a system varies in case the system parameters are varied. With the help of equation (22) one can for instance find the optimum positioning of isolating material in a system in order to attain a maximum temperature increase in the detection region, as is shown in the following example.

EXAMPLE

For illustration purposes computer calculations were performed on a two-dimensional purely conductive system as shown in Fig. 1; the system is

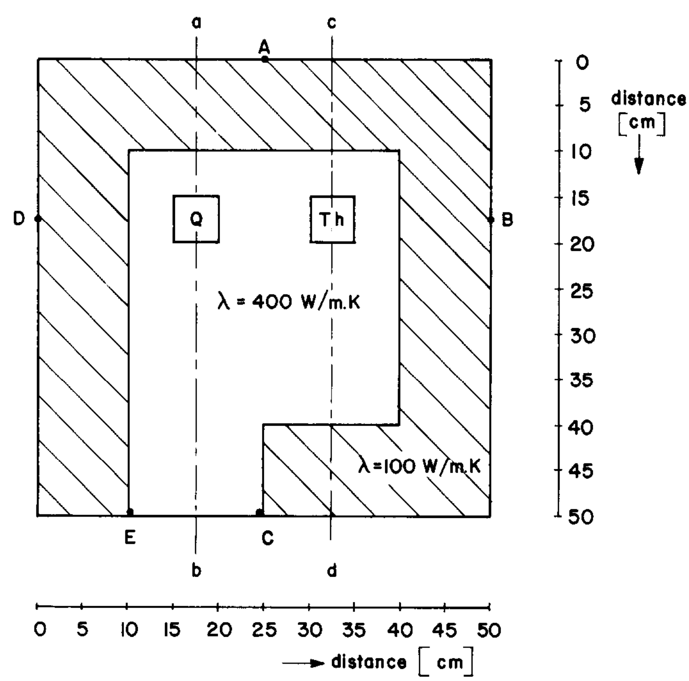

FIG. 1. Configuration of sample problem.

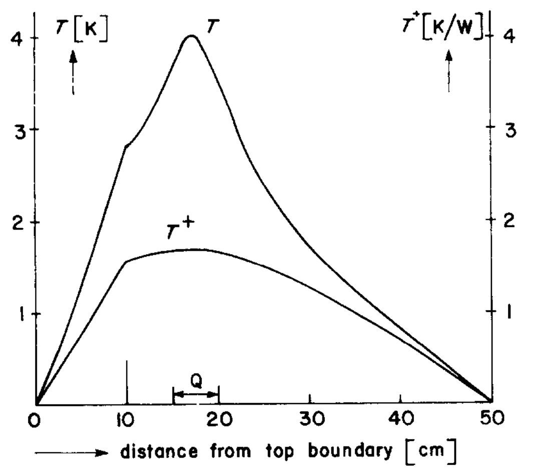

FIG. 2. Distribution of temperature T and adjoint function T^+ along the line a–b of Fig. 1.

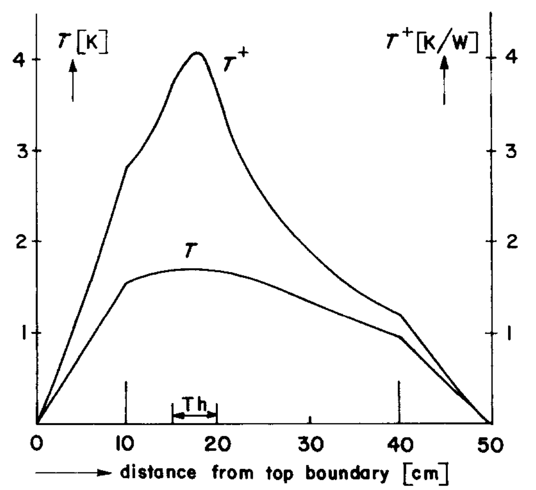

FIG. 3. Distribution of temperature T and adjoint function T^+ along the line c–d of Fig. 1.

infinitely long in the direction perpendicular to the plane of drawing. The materials differ by a factor of 4 in heat conductivity; Q is the heat source region and Th the thermometer region. As boundary condition a fixed temperature was chosen. In Figs. 2 and 3 some results are shown of the solution of the regular and adjoint heat transport equation; the temperature values are related to a heat source density of 1 W/cm^3 in region Q. If we replace a piece of material at the system boundary by perfect isolation material ($\lambda = 0$), the temperature increase in the detection region can be calculated in first-order approximation with equation (22). In this case $\delta\lambda = -100$ W/m·K or -400 W/m·K, depending on the position of the isolation material. The behaviour of the integrand of equation (22) along the system boundary is shown in Fig. 4, together with the heat flux density ϕ at the boundary. The optimal position for placement of isolation is seen to be position A (Fig. 1), followed by positions B, C and D which are about equivalent, and finally position E.

Without the analysis with the adjoint equation one is inclined to select positions with higher heat leakage. Wrongly positioned C would have been chosen and on the upper boundary a position too far to the left. Position D would have been considered much more important than B, whereas in fact B is slightly more important than D. It is also remarkable that the positions C and E differ by about a factor of two in importance, which is not expected on the basis of the small difference in heat flux densities.

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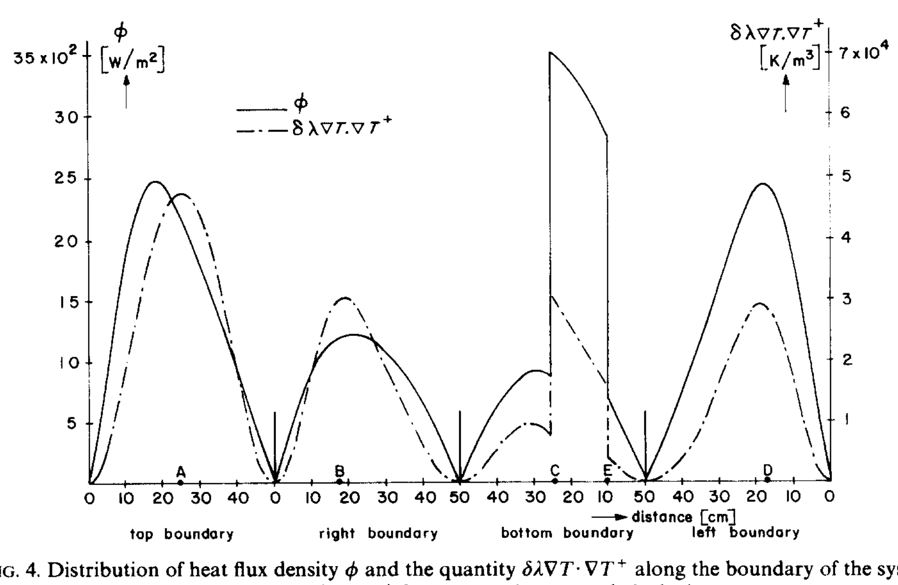

FIG. 4. Distribution of heat flux density ϕ and the quantity $\delta\lambda\nabla T\cdot\nabla T^+$ along the boundary of the system, starting at the top left corner, going around clockwise.

L'ESPACE ADJOINT DANS LA THEORIE DU TRANSPORT DE CHALEUR

Résumé — Le concept mathématique des opérateurs adjoints est appliqué à l'équation du transport de chaleur et une équation adjointe est définie avec une fonction de détection comme terme source. La signification physique des solutions de la dernière équation est dégagée avec une application dans le domaine de l'analyse de perturbation.

DER ADJUNGIERTE RAUM IN DER THEORIE DES WÄRMETRANSPORTS

Zusammenfassung — Das mathematische Konzept adjungierter Operatoren wird auf die Wärmetransportgleichung angewendet und eine adjungierte Gleichung mit einer Detektor-Funktion als Quellenterm definiert. Die physikalische Bedeutung der Lösung dieser Gleichung und ihre Anwendung auf dem Gebiet der Störungsanalysis werden erläutert.

СОПРЯЖЕННОЕ ПРОСТРАНСТВО В ТЕОРИИ ТЕПЛОПЕРЕНОСА

Аннотация — Математическая концепция сопряженных операторов применена к уравнениям переноса тепла, а сопряженное уравнение определяется с помощью детекторной функции в качестве источника. Излагается физический смысл решений последнего уравнения и приводится пример использования этих решений в теории возмущений.