PERGAMON

International Journal of Heat and Mass Transfer 45 (2002) 3585–3596

International Journal of HEAT and MASS TRANSFER

www.elsevier.com/locate/ijhmt

Fast-converging steady-state heat conduction in a rectangular parallelepiped

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Received 14 May 2001; received in revised form 1 February 2002

Abstract

A Green's function approach for precisely computing the temperature and the three components of the heat flux in a rectangular parallelepiped is presented. Each face of the parallelepiped may have a different, but spatially uniform, boundary condition. Uniform volume energy generation is also treated. Three types of boundary conditions are included: type 1, a specified temperature; type 2, a specified flux; or type 3, a specified convection boundary condition. A general form of the Green's function covering all three types of boundary conditions is given. An algorithm is presented to obtain the temperature and flux at high accuracy with a minimal number of calculations for points in the interior as well as on any of the faces. Heat flux on type 1 boundaries, impossible to evaluate with traditional Fourier series, is found by factoring out lower-dimensional solutions. A numerical example is given. This research and resulting computer program was part of a code verification project for Sandia National Laboratories.

Keywords: Green's functions; Laplace equation; Temperature; Series convergence; Parallelepiped

1. Introduction

Although numerical methods and powerful computers are increasingly important in heat conduction, exact solutions still have a role to play. They provide insight into various heat conduction processes. They can be used to assess numerical accuracy and to provide verification of complex numerical programs. For verification, highly accurate solutions for transient three-dimensional problems are particularly important. Although some exact solutions are available in standard references, there are few three-dimensional cases available. Further, accurately evaluating these solutions can require many terms from double or triple series.

This paper addresses *steady* heat conduction in the rectangular parallelepiped by the method of Green's functions. The steady work is important because in many transient solutions, a poorly converging steady-state series term appears [1, p. 185], and an improvement in the convergence speed of this steady term can improve the accuracy of the transient solution. The steady solution can also serve as an independent check on the transient solutions evaluated at large values of time.

In the method of Green's functions, the boundary value problem for the temperature is restated into an integral expression that involves the known boundary conditions and the Green's function (GF). The method of GF is especially advantageous for three-dimensional problems such as the parallelepiped.

The pertinent GF literature is summarized next. Several books give a good overview of the GF method [1–4]. Two books by Butkovskii [5,6] contain many GF organized according to the type of differential equation. The differential equations are categorized according to a

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0017-9310/02/$ - see front matter
PII: S0017-9310(02)00066-2

Nomenclature

B	Biot Number
C	controlling factor, Eq. (34)
f_i	non-homogeneous boundary value, side i
g	energy generation, W/m^2
G	Green's function, m^{-1}, Eq. (10)
h	heat transfer coefficient, $W/(m^2\ K)$
k	thermal conductivity, W/(m K)
L_i	ith parallelepiped dimension, m
n_i	outward normal on side i
N	norm, Eq. (12)
P_{np}	kernel function, Eq. (15)
q	heat flux, W/m^2
S_m	coefficient, Eqs. (17) and (18)
t	time, s
T	temperature, K
V	defined in Eq. (25)
x_i	Cartesian coordinate
X	eigenfunction, Eq. (11)

Subscripts

i,j,k	indices
n,p	summation indices, Eq. (10)
ℓ,m	indices for eigenvalues, Eq. (11)
r	index for direction
1D	one-dimensional

Greek symbols

α	thermal diffusivity, m^2/s
β	eigenvalue, Eq. (14)
δ_{ij}	Kronecker delta
$\delta(x_i - x_i')$	Dirac delta function
Θ	temperature scale, Eq. (33)
λ	eigenvalue, Eq. (11)
χ	generalized eigenfunction, Eq. (32)

number system for the number of spatial dimensions, the order of the highest time derivative, and the order of the highest spatial derivative. Although Butkovskii's number system clearly distinguishes different equations, there are no subdivisions for the various coordinate systems and boundary conditions. Beck et al. [7] give extensive tables of GF for heat conduction and diffusion. The GF are organized with a number system for the number of spatial dimensions, the type of coordinate system, and the type of boundary conditions. Most of the book is devoted to transient heat conduction. Few steady GF, and only one parallelepiped example are given.

Melnikov [8,9] discusses GF for a variety of two-dimensional geometries, including steady heat conduction in Cartesian and cylindrical coordinates. No three-dimensional geometries are treated. Fourier series expansions along one coordinate direction are used to produce single-sum series for the GF. Most importantly, the slowly converging portions of the series for the GF are identified and replaced with closed-form expressions.

Marshall [10] derives Laplace-equation GF for the parallelepiped applied to electrostatic potential problems. Expressions for the GF associated with type 2 (zero-flux) boundaries are given. Although the convergence behavior of the GF is explored with numerical examples, only the point-charge solution is discussed. There is no discussion of distributed sources on the interior or on the boundaries.

Recent work by the second author in a two-dimensional rectangle [11] involved the method of GF to obtain fast-converging expressions for the temperature and heat flux. The present paper is an extension of these methods to the parallelepiped.

The contribution of this paper is fourfold. First, GF for the rectangular parallelepiped are given for any combination of boundaries of types 1, 2, and 3. Second, the important concept of alternative GF is discussed as a means to improve the numerical behavior of the GF method; many alternative GF are given. Third, series convergence is improved by factoring out lower-dimensional solutions. Fourth, an algorithm is presented for efficient, high-accuracy computation of temperature and heat flux in the parallelepiped. This algorithm is part of a code verification project carried out for Sandia National Laboratories.

The remainder of this paper is divided into sections. First the boundary value problem for the temperature is stated, and then the solution with the method of GF is formally stated. The GF itself is next defined and its convergence behavior is explored. The algorithm for efficient computation of the temperature and heat flux is given, along with numerical examples. The GF for the parallelepiped are also available on an internet site devoted to the GF method.

2. Boundary value problem for temperature

The temperature in the parallelepiped with constant and isotropic material properties is governed by the boundary value problem

$$\nabla^2 T = -\frac{g}{k}, \quad 0 < x_r < L_r, \quad r = 1,2,3, \tag{1}$$

$$k_i \frac{\partial T}{\partial n_i} + h_i T = f_i, \quad i = 1,2,\ldots,6. \tag{2}$$

Table 1
Side numbering

i	Side
1	$x_1 = 0$
2	$x_1 = L_1$
3	$x_2 = 0$
4	$x_2 = L_2$
5	$x_3 = 0$
6	$x_3 = L_3$

The subscripts on k, n, h, and f in Eq. (2) denote correspondence to sides of the parallelepiped as given in Table 1. Throughout this paper the sides of the parallelepiped will be referenced using the same convention.

The boundary conditions, given by Eq. (2), can be of three different types: for type 1, $k_i = 0, h_i = 1$, and f_i is a specified temperature; for type 2, $k_i = k$, $h_i = 0$, and f_i is a specified heat flux; and for type 3, $k_i = k$, $h_i = h$, and f_i is a specified product of the convection coefficient and the ambient temperature.

3. Solution in terms of the Green's function

In this section the temperature is found in terms of the GF by splitting the problem into seven subproblems, one for each non-homogeneous boundary and one for internal generation. By superposition the solution can be written as

$$T = T_0 + T_1 + T_2 + T_3 + T_4 + T_5 + T_6, \tag{3}$$

where T_0 satisfies the original partial differential equation, Eq. (1), and homogeneous boundary conditions. For $j \neq 0, T_j$ satisfies the homogeneous partial differential equation corresponding to Eq. (1), the non-homogeneous boundary condition T satisfies on side j, and the associated homogeneous boundary conditions T satisfies on the remaining sides. Explicitly,

$$\nabla^2 T_j = -\frac{g}{k}\delta_{0j}, \quad 0 < x_r < L_r, \quad r = 1,2,3, \tag{4}$$

$$k_i \frac{\partial T_j}{\partial n_i} + h_i T_j = f_i \delta_{ij}, \quad i = 1,2,\ldots,6, \tag{5}$$

where δ_{ij} is the Kronecker delta function and $j = 0,1,\ldots,6$.

Rather than solve for T_j directly for every value of j, we have chosen to use the symmetry of the parallelepiped to streamline the algorithm as follows. For $j = 0,1$ we solve for T_j as defined above. For $j = 2,3,\ldots,6$ the coordinate system may always be rotated so that the non-homogeneous side is at $x_1 = 0$. If (x_1, x_2, x_3) is the original point at which the temperature is desired, the corresponding coordinates for the rotations used are given in Table 2.

Table 2
Rotation of coordinates to place heated face at $x_1 = 0$

Heated side	Replace x_1 by	Replace x_2 by	Replace x_3 by
0[a] or 1	–	–	–
2	$L_1 - x_1$	$L_2 - x_2$	–
3	x_2	$L_1 - x_1$	–
4	$L_2 - x_2$	x_1	–
5	x_3	–	$L_1 - x_1$
6	$L_3 - x_3$	–	x_1

[a] Heating at "side 0" is internal generation.

Therefore, through superposition and rotation only internal generation problems and problems with non-homogeneities at $x_1 = 0$ need to be considered. Dropping the subscript j, the solution to Eqs. (4) and (5) in terms of the Green's Function, G, defined later, is given by

$$T(\mathbf{x}) = \begin{cases} \frac{g}{k}\int_v G(\mathbf{x}\,|\,\mathbf{x}')\,\mathrm{d}v' & \text{if internal generation,} \\ f_1 \int_{s_1} \left.\frac{\partial G(\mathbf{x}\,|\,\mathbf{x}')}{\partial x_1'}\right|_{x_1'=0} \mathrm{d}s_1' & \\ \quad \text{if } s_1 \text{ is non-homogeneous of type 1,} & \\ \frac{f_1}{k}\int_{s_1} G(\mathbf{x}\,|\,\mathbf{x}')\big|_{x_1'=0}\,\mathrm{d}s_1' & \\ \quad \text{if } s_1 \text{is non-homogeneous of type 2 or 3,} & \end{cases} \tag{6}$$

where $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{x}' = (x_1', x_2', x_3')$. The integral for volume generation is over the volume of the parallelepiped, while the integrations for non-homogeneous type 1, type 2 or type 3 boundary conditions on side 1 are surface integrals over side 1, that is $\mathrm{d}v' = \mathrm{d}x_1'\,\mathrm{d}x_2'\,\mathrm{d}x_3'$ and $\mathrm{d}s_1' = \mathrm{d}x_2'\,\mathrm{d}x_3'$.

Using Fourier's law, the three components of heat flux are

$$q_{x_m} = -k\frac{\partial T}{\partial x_m}, \quad m = 1,2,3. \tag{7}$$

Because of the use of superposition and coordinate system rotations, care must be taken when calculating the heat flux in the original coordinates. Table 3 gives the correspondence between the components of heat flux in the rotated coordinates to the components of heat flux in the original coordinates depending on which original side is non-homogeneous.

Table 3
Rotated and original heat flux components

Heated side	Rotated q_{x_1} is	Rotated q_{x_2} is	Rotated q_{x_3} is
0 or 1	q_{x_1}	q_{x_2}	q_{x_3}
2	$-q_{x_1}$	$-q_{x_2}$	q_{x_3}
3	q_{x_2}	$-q_{x_1}$	q_{x_3}
4	$-q_{x_2}$	q_{x_1}	q_{x_3}
5	q_{x_3}	q_{x_2}	$-q_{x_1}$
6	$-q_{x_3}$	q_{x_2}	q_{x_1}

4. Definition of the Green's function

In this section the Green's function needed for the temperature solution is defined. The GF for the parallelepiped is the response at location (x_1, x_2, x_3) caused by a point source of heat at (x'_1, x'_2, x'_3). The GF satisfies the boundary value problem:

$$\frac{\partial^2 G}{\partial x_1^2} + \frac{\partial^2 G}{\partial x_2^2} + \frac{\partial^2 G}{\partial x_3^2} = -\delta(x_1 - x'_1)\delta(x_2 - x'_2)\delta(x_3 - x'_3), \quad 0 < x_r < L_r, \ \ r = 1, 2, 3, \tag{8}$$

$$k_i \frac{\partial G}{\partial n_i} + h_i G = 0 \quad \text{for faces } i = 1, 2, \ldots, 6, \tag{9}$$

where δ is the Dirac delta function and the homogeneous boundary conditions are the same type on each face as in the temperature problem, Eq. (2).

The GF may be written in the form

$$G(\mathbf{x}|\mathbf{x}') = \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \frac{X_n(x_k) X_n(x'_k)}{N(\lambda_{kn})} \times \frac{X_p(x_j) X_p(x'_j)}{N(\lambda_{jp})} P_{np}(x_i, x'_i), \tag{10}$$

where (i, j, k) is some permutation of $(1, 2, 3)$, each $X_\ell(x_m)$ is an eigenfunction, λ is an eigenvalue, and each $P_{np}(x_i, x'_i)$ is a kernel function. Note that the permutation (i, j, k) relates to the directions chosen for the kernel function and eigenfunctions in the rotated coordinate system which was introduced earlier for the temperature.

The double-sum form of the GF is important because it suggests six alternative series for each GF depending on the permutation of $(1, 2, 3)$ used for (i, j, k). There is also a triple-sum form of the steady GF whose poor convergence behavior [7, p. 195] is well known. We will see later that the alternate forms are very important for finding a fast-converging series for the temperature. In the remainder of this section the eigenfunctions and kernel functions will be discussed for any combination of boundary condition types. To organize all of these combinations, a numbering system is needed.

4.1. Numbering system

In all there are 729 different combinations of boundary condition types for the parallelepiped, each with its own GF. Each GF has six possible forms (given explicitly later) for a total of 4374 different summations that could be used to calculate the temperature (or heat flux). There are, however, only nine eigenfunctions and nine kernel functions. Each summation for temperature (or heat flux) consists of a different combination of these 18 basic functions, their integrals, or their derivatives. The particular eigenfunctions or kernel function needed is determined by the boundary conditions on the faces perpendicular to their directions. Therefore, a numbering system is used to identify each function.

For eigenfunctions, the designation *XIJ* is used to identify the eigenfunction in the x_m direction with a boundary condition of type $I = 1, 2,$ or 3 at $x_m = 0$ and a boundary condition of type $J = 1, 2,$ or 3 at $x_m = L_m$. For example $X12$ represents eigenfunctions placed in the x_m direction with a boundary condition of type 1 at $x_m = 0$ and a boundary condition of type 2 at $x_m = L_m$. For kernel functions, a similar system is used. The designation *PIJ* ($I, J = 1, 2,$ or 3) is used to denote the kernel function in the x_i direction with a boundary condition of type I at $x_i = 0$ and a boundary condition of type J at $x_i = L_i$. Note in this numbering system, although it is related to the numbering system for GF [7, Chapter 2], the coordinate direction is not given explicitly since any of the eigenfunctions or kernel functions could be placed in any direction and which function is used depends on the type of boundary conditions, not the particular direction.

4.2. Eigenfunctions

The eigenfunctions in Eq. (10), $X_\ell(x_m)$, satisfy the ordinary differential equations

$$X''_\ell(x_m) + \lambda_{m\ell}^2 X_\ell(x_m) = 0, \tag{11}$$

where λ_{ml} are the eigenvalues. The boundary conditions are the same as those satisfied by the GF at $x_m = 0$ and $x_m = L_m$. Additionally, each norm, $N(\lambda_{m\ell})$, is chosen such that

$$\sum_{\ell=0}^{\infty} \frac{X_\ell(x_m) X_\ell(x'_m)}{N(\lambda_{m\ell})} = \delta(x_m - x'_m). \tag{12}$$

There are nine possible different eigenfunctions depending on the type of boundary conditions on the faces perpendicular to the direction x_m. All of the eigenfunctions are linear combinations of sines and cosines and are given along with their norms and their eigenvalues or eigenconditions in Table 4. The sum in Eq. (12) only begins at zero if both boundaries are of type 2. In this case, $\lambda_{m0} = 0$, otherwise all of the eigenvalues are real and positive.

4.3. General kernel function

With the above choices for $X_\ell(x_m)$ and $N(\lambda_{m\ell})$, the kernel function $P_{np}(x_i, x'_i)$ must satisfy

$$\frac{\mathrm{d}^2 P_{np}}{\mathrm{d}x_i^2} - \beta_{np}^2 P_{np} = -\delta(x_i - x'_i), \tag{13}$$

where β_{np} is given by

$$\beta_{np} = \sqrt{\lambda_{kn}^2 + \lambda_{jp}^2}. \tag{14}$$

Table 4
Eigenfunction, norm, and eigenvalues for nine required cases

(a) Eigenfunctions

Cases	$X_\ell(x_m)$
$X11$, $X12$, and $X13$	$\sin(\lambda_{m\ell}x_m)$
$X21$, $X22$, and $X23$	$\cos(\lambda_{m\ell}x_m)$
$X31$, $X32$, and $X33$	$\lambda_{m\ell}L_m\cos(\lambda_{m\ell}x_m)+B_I\sin(\lambda_{m\ell}x_m)$

(b) Inverse norm and eigenvalues or conditions

Case	$N(\lambda_{m\ell})^{-1}$	$\lambda_{m\ell}$ or eigencondition
$X11$	$2/L_m$	$\ell\pi/L_m$
$X12$	$2/L_m$	$(2\ell-1)\pi/2L_m$
$X13$[a]	$2\phi_m/L_m$	$\lambda_{m\ell}L_m\cot(\lambda_{m\ell}L_m)=-B_J$
$X21$	$2/L_m$	$(2\ell-1)\pi/2L_m$
$X22$	$2/L_m$, $\lambda_{m\ell}\neq 0$	$\ell\pi/L_m$
	$1/L_m$, $\lambda_{m\ell}=0$	
$X23$[a]	$2\phi_m/L_m$	$\lambda_{m\ell}L_m\tan(\lambda_{m\ell}L_m)=B_J$
$X31$	$2/[(\lambda_{m\ell}L_m)^2+B_I^2+B_I]$	$\lambda_{m\ell}L_m\cot(\lambda_{m\ell}L_m)=-B_I$
$X32$	$2/[(\lambda_{m\ell}L_m)^2+B_I^2+B_I]$	$\lambda_{m\ell}L_m\tan(\lambda_{m\ell}L_m)=B_I$
$X33$[b]	$2\Phi_m/L_m$	$\tan(\lambda_{m\ell}L_m)=[\lambda_{m\ell}L_m(B_I+B_J)]/[(\lambda_{m\ell}L_m)^2-B_IB_J]$

Here $B_I=h_{2m-1}L_m/k$ is the Biot number at $x_m=0$ and $B_J=h_{2m}L_m/k$ is the Biot number at $x_m=L_m$. Index $\ell=1,2,\ldots$ for all cases except $X22$ with $\ell=0,1,2,\ldots$

[a] $\phi_m=[(\lambda_{m\ell}L_m)^2+B_J^2]/[(\lambda_{m\ell}L_m)^2+B_J^2+B_J]$.

[b] $\Phi_m=\phi_m\div[(\lambda_{m\ell}L_m)^2+B_I^2+B_I\phi_m]$.

The kernel function, suppressing the *np* subscript, may be written as

$$P(x_i,x_i')=\frac{S_J^-(S_I^-\mathrm{e}^{-\beta(2L_i-|x_i-x_i'|)}+S_I^+\mathrm{e}^{-\beta(2L_i-x_i-x_i')})}{2\beta(S_I^+S_J^+-S_I^-S_J^-\mathrm{e}^{-2\beta L_i})}+\frac{S_J^+(S_I^+\mathrm{e}^{-\beta(|x_i-x_i'|)}+S_I^-\mathrm{e}^{-\beta(x_i+x_i')})}{2\beta(S_I^+S_J^+-S_I^-S_J^-\mathrm{e}^{-2\beta L_i})},\tag{15}$$

where the indices I and J are just the numbers of the sides perpendicular to the x_i direction and are given by

$$I=2i-1,\quad J=2i\tag{16}$$

while the parameters S_{M}^+ and S_{M}^- depend on the boundary conditions on side M and are given by

$$S_{\mathrm{M}}^+=\begin{cases}1 & \text{if side M is type 1 or type 2,}\\ \beta L_i+B_{\mathrm{M}} & \text{if side M is type 3,}\end{cases}\tag{17}$$

$$S_{\mathrm{M}}^-=\begin{cases}-1 & \text{if side M is type 1,}\\ 1 & \text{if side M is type 2,}\\ \beta L_i-B_{\mathrm{M}} & \text{if side M is type 3.}\end{cases}\tag{18}$$

Here $B_{\mathrm{M}}=L_ih_{\mathrm{M}}/k$ is the Biot Number for side M, where k is the conductivity of the parallelepiped.

The expression for P in Eq. (15) is symmetric if x_i and x_i' are interchanged and covers all nine possible boundary condition combinations provided $\beta\neq 0$. A derivation of Eq. (15) is given in Appendix A.

4.4. Kernel functions for $\beta=0$

If all of the faces parallel to the kernel direction are of type 2, then the zero eigenvalue exists. Provided the boundary conditions on the faces perpendicular to the direction of the kernel function are not also both of type 2, the kernel function must satisfy

$$\frac{\partial^2P_{00}}{\mathrm{d}x_i^2}=-\delta(x_i-x_i')\tag{19}$$

as well as the boundary conditions at $x_i=0$ and $x_i=L_i$. The nine kernel functions for this case are given in Table 5. In the table, I and J are as in Eq. (16) and the i subscript has been dropped. The special case when all six boundaries of the parallelepiped are of type 2 is covered in the next section.

4.5. Special case: all type 2 boundary conditions

For the special case when all six boundaries are of type 2, the usual GF does not exist and the usual GF solution cannot be used to find the temperature. In this section a pseudo GF is discussed that can be used instead [4, Chapter 6].

In this case, the input data to the temperature problem must satisfy a constraint – the sum of the heat passing through the boundaries of the body must be equal to the (negative of the) integral of the heat

Table 5
Kernel function for $\beta = 0$

Case	$P_{00}(x,x')$ for $x > x'$ (use $P_{00}(x',x)$ for $x < x'$)
$P11$	$x'(1 - x/L)$
$P12$	x'
$P13$	$x'[1 - B_J(x/L)/(1 + B_J)]$
$P21$	$L - x$
$P22$[a]	$((x')^2 + x^2)/(2L) - x + L/3$
$P23$	$L(1 + 1/B_J - x/L)$
$P31$	$(B_I x' - B_I x'x/L + L - x)/(1 + B_I)$
$P32$	$L(1/B_I + x'/L)$
$P33$	$(B_I B_J x' + B_I x' - B_I B_J x'x/L - B_J x + B_J L + L) \div (B_I B_J + B_I + B_J)$

[a] Special temperature solution needed with this pseudo GF.

introduced by volume energy generation. This is equivalent to satisfying an energy balance over the volume of the parallelepiped. In addition, the solution is only unique within an additive constant.

The pseudo GF, G_{PS}, satisfies the following differential equation:

$$\frac{\partial^2 G_{PS}}{\partial x_1^2} + \frac{\partial^2 G_{PS}}{\partial x_2^2} + \frac{\partial^2 G_{PS}}{\partial x_3^2} = -\delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3') + \frac{1}{L_1 L_2 L_3}. \quad (20)$$

If the pseudo GF is assumed to be in the same form as the GF in Eq. (10) and the eigenfunctions are assumed to satisfy Eqs. (11) and (12) then the kernel functions $P_{np}(x_i, x_i')$ for n and p not both zero satisfy Eq. (13) and are given by Eq. (15). However, $P_{00}(x_i, x_i')$, the kernel function for $\beta = 0$, must satisfy

$$\frac{d^2 P_{00}}{dx_i^2} = -\delta(x_i - x_i') + \frac{1}{L_i}. \quad (21)$$

A solution for P_{00} is given by

$$P_{00}(x_i, x_i') = \begin{cases} \left[x_i^2 + (x_i')^2\right]/(2L_i) - x_i' + L_i/3, & x_i < x_i', \\ \left[x_i^2 + (x_i')^2\right]/(2L_i) - x_i + L_i/3, & x_i' < x_i. \end{cases} \quad (22)$$

This solution is only unique up to an additive constant. The constant chosen, $L_i/3$, causes the integral of P_{00} with respect to x_i' over $(0, L_i)$ to be zero.

To find the temperature from the pseudo GF the following integral equation must be used:

$$T(\mathbf{x}) = \begin{cases} \frac{f_1}{k} \int_{s_1} G_{PS}(\mathbf{x}\,|\,\mathbf{x}')\, ds_1' \\ \quad \text{if side 1 is non-homogeneous,} \\ \frac{g}{k} \int_v G_{PS}(\mathbf{x}\,|\,\mathbf{x}')\, dv' \\ \quad \text{if internal generation.} \end{cases} \quad (23)$$

This solution gives a spatial average temperature in the parallelepiped of zero. If a different average temperature is desired, simply add this average temperature to the computed temperature at every point.

4.6. Internet site for Green's functions

More information on the GF method is given in an internet site called the Green's Function Library (http://www.engr.unl.edu/~glibrary). A variety of GF for other geometries are available there for both steady and transient heat conduction. The GF available in the GF Library are organized by differential equation, coordinate system, body shape, and type of boundary conditions. The purpose of the GF Library is to provide wide availability of Green's Functions and to promote the GF method.

5. Convergence

In this section the convergence behavior of the series for the temperature is discussed. Of the six possible forms of the GF, one resulting form of the temperature expression will generally converge faster than the others depending on the point of evaluation, the shape of the parallelepiped, the type of boundary conditions, and the thermal properties of the parallelepiped. To evaluate the temperature and heat flux several additional functions are needed. Depending on the type of problem being solved and the direction chosen for the kernel function, the additional functions include: either the integral from 0 to L_i of the kernel function with respect to x_i'; the kernel function evaluated at $x_i' = 0$; or, the derivative of the kernel function with respect to x_i' evaluated at $x_i' = 0$. Next these additional functions are discussed with respect to their impact on series convergence.

5.1. Solutions with an integral of the kernel function

In this section solutions containing an integral of the kernel function are discussed. These arise from Eq. (6) when the temperature (or heat flux) is caused by internal generation or by a non-homogeneous boundary if the kernel function is not placed in the x_1-direction ($i \neq 1$). Suppressing the np subscripts this integral is given by

$$\int_0^{L_i} P(x_i, x_i')\, dx_i' = \frac{1}{\beta^2} + V(\beta, x_i), \quad (24)$$

where

$$V(\beta, x_i) = \frac{(S_I^- - S_I^+)(S_J^- e^{-\beta(2L_i - x_i)} + S_J^+ e^{-\beta x_i})}{2\beta^2(S_I^+ S_J^+ - S_I^- S_J^- e^{-2\beta L_i})} + \frac{(S_J^- - S_J^+)(S_I^- e^{-\beta(L_i + x_i)} + S_I^+ e^{-\beta(L_i - x_i)})}{2\beta^2(S_I^+ S_J^+ - S_I^- S_J^- e^{-2\beta L_i})}. \quad (25)$$

Note that all the exponents are negative unless x_i is located on a boundary of type 1 or 3. Ignoring the $1/\beta^2$

term, convergence in the series resulting from the substitution of Eq. (10) into Eq. (6) is controlled by the smallest (negative) exponent in the numerator of Eq. (24). For this reason, points on type 1 or 3 boundaries are referred to as troublesome points because they result in slowly convergent or divergent series due to one of the exponentials becoming unity. Generally at the troublesome points the heat flux convergence is slower than that for temperature (due to differentiation of the Fourier series) and in many cases the series for heat flux diverges. A technique that improves the temperature convergence and allows for the evaluation of the heat flux, factoring out lower-dimensional solutions, is presented in the next section. For evaluation on type 2 boundaries the factor pre-multiplying the "troublesome" exponential is zero and such points are not considered troublesome.

5.1.1. Factoring out lower-dimensional solutions

At a non-troublesome point, the convergence of the series is improved by noting that the integral of the kernel function is of the form

$$\begin{aligned}\int_0^{L_i} P(x_i,x_i')\,\mathrm{d}x_i' &= \frac{1}{\beta^2}+V(\beta,x_i)\\ &= \int P\,\mathrm{d}x_i' \text{ (if type 2 on both } x_i \text{ faces)}\\ &\quad + V(\beta,x_i),\end{aligned} \tag{26}$$

where first term corresponds to the result if the sides at $x_i = 0$ and $x_i = L_i$ had type 2 boundary conditions. For any problem in this case, the boundary conditions on those sides in the corresponding temperature problem are homogeneous. Thus the first term corresponds to insulation in the x_i-direction. The resulting sum from this term multiplied by the eigenfunctions in the x_k and x_j directions is therefore the solution to the two-dimensional problem in the $x_k x_j$-plane. Convergence is improved if this two-dimensional problem is not calculated as a double summation, but rather as an equivalent single summation with an eigenfunction in one direction and a kernel function in the other [11]. At non-troublesome points the convergence of the sum resulting from multiplication of the eigenfunctions by the second term in Eq. (26), $V(\beta,x_i)$, is controlled by the exponents in the numerator. All of the exponents are negative and the eigenvalues are increasing. Therefore the sum converges fairly rapidly.

In an analogous fashion, if the kernel function in the single-summation two-dimensional problem is not placed in the x_1-direction or if it is an internal generation problem, the integral of the kernel function in the two-dimensional problem will also have two terms, one of which is a *one-dimensional* problem in the x_k-direction. This one-dimensional single-summation problem can be evaluated as a closed-form polynomial to provide a large reduction in computation time. Refer to [11] for a full discussion of this procedure.

5.1.2. Example

Consider the temperature evaluated at a non-troublesome point with a kernel function in the x_3-direction for the three-dimensional problem, a kernel function in the x_2-direction for the two-dimensional problem, and a type 1 non-homogeneous boundary condition at $x_1 = 0$. The temperature is given by

$$\begin{aligned}T(\mathbf{x}) = f_1 \sum_{n=0}^{\infty}\sum_{p=0}^{\infty} &\frac{X_n(x_1)}{N(\lambda_{1n})}\left.\frac{\mathrm{d}X_n(x_1')}{\mathrm{d}x_1'}\right|_{x_1'=0}\\ &\times \frac{X_p(x_2)\int_0^{L_2} X_p(x_2')\,\mathrm{d}x_2'}{N(\lambda_{2p})}\int_0^{L_3} P_{np}(x_3)\,\mathrm{d}x_3'\end{aligned} \tag{27}$$

or after factoring out the lower-dimensional solution in the x_1x_2 plane and then factoring out the one-dimensional solution in the x_1 direction:

$$\begin{aligned}T(\mathbf{x}) = f_1 \sum_{n=0}^{\infty}\sum_{p=0}^{\infty} &\frac{X_n(x_1)}{N(\lambda_{1n})}\left.\frac{\mathrm{d}X_n(x_1')}{\mathrm{d}x_1'}\right|_{x_1'=0}\\ &\times \frac{X_p(x_2)\int_0^{L_2} X_p(x_2')\,\mathrm{d}x_2'}{N(\lambda_{2p})}V(\beta_{np},x_3)\\ &+ f_1 \sum_{n=0}^{\infty}\frac{X_n(x_1)}{N_x(\lambda_{1n})}\left.\frac{\mathrm{d}X_n(x_1')}{\mathrm{d}x_1'}\right|_{x_1'=0}V(\lambda_{2n},x_2)+T_{1\mathrm{D}}(x_1),\end{aligned} \tag{28}$$

where $T_{1\mathrm{D}}(x_1)$ is the temperature for the one-dimensional problem in the x_1-direction. The nine possible one-dimensional temperature solutions are given in Table 6.

5.2. Solutions without integrals of the kernel function

If the boundary condition on side 1 is non-homogeneous of type 1 and a kernel function is placed in the x_1-direction then $\partial P/\partial x_1'(x_1,0)$ is needed as part of the temperature solution

$$\frac{\partial P}{\partial x_1'}(x_1,0) = \frac{(S_1^+ - S_1^-)(S_2^-\mathrm{e}^{-\beta(2L_1-x_1)} + S_2^+\mathrm{e}^{-\beta x_1})}{2(S_1^+S_2^+ - S_1^-S_2^-\mathrm{e}^{-2\beta})}. \tag{29}$$

If the boundary condition on side 1 is non-homogeneous of type 2 or type 3 and a kernel function is placed in the

Table 6
One-dimensional temperature solutions

Case	$T_{1\mathrm{D}}(x_1)$
$X11$	$f_1(1-x_1/L_1)$
$X12$	f_1
$X13$	$f_1(1-[B_2/(1+B_2)]x_1/L_1)$
$X21$	$\frac{f_1}{k}(L_1-x_1)$
$X22$[a]	$\frac{f_1}{k}(x_1^2/(2L_1)-x_1+L_1/3)$
$X23$	$\frac{f_1}{k}(L_1+L_1/B_2-x_1)$
$X31$	$\frac{f_1}{k}(L_1-x_1)/(1+B_1)$
$X32$	$\frac{f_1}{k}L_1/B_1$
$X33$	$\frac{f_1}{k}(L_1-B_2x_1+L_1B_2)/(B_1+B_2+B_1B_2)$

[a] Constructed from the pseudo GF.

x_1-direction then $P(x_1,0)$ is needed as part of the temperature solution

$$P(x_1,0)=\frac{(S_1^+ + S_1^-)(S_2^- \mathrm{e}^{-\beta(2L_1-x_1)} + S_2^+ \mathrm{e}^{-\beta x_1})}{2\beta(S_1^+ S_2^+ - S_1^- S_2^- \mathrm{e}^{-2\beta})}. \tag{30}$$

In either case, troublesome points are at $x_1 = 0$, regardless of the type of boundary condition and the lower-dimensional solution cannot be factored out. Despite not being able to factor out the lower-dimensional problem placing the kernel function in the x_1 direction may still be preferable to other directions if it produces faster decaying exponential terms in the two-dimensional sum.

5.3. Solutions with derivatives: heat flux

Each component of the heat flux is found from a derivative of the temperature, given by Eq. (6), through Fourier's law, Eq. (7). The required derivatives fall onto the components of the GF given by Eq. (10). Thus, calculating the components of the heat flux requires finding a derivative of either a kernel function or an eigenfunction with respect to the coordinate in the direction of the heat flux component. This derivative degrades the convergence of each of the forms of the summations by introducing another factor of the eigenvalue into the numerator of each of the summations. However, it does not alter the relative convergence of the different forms of the GF and the definition of troublesome points remains the same.

6. Algorithm for temperature and heat flux

To calculate the temperature and heat flux at a point in the parallelepiped there are six different forms of the expression for temperature (and for each component of the heat flux) depending on the directions chosen for the kernel functions. After substituting Eq. (10) into Eq. (6), and factoring out lower-dimensional solutions when possible, the equation for temperature may be written compactly as

$$\begin{aligned}\frac{T(\mathbf{x})}{\Theta} = &\sum_{p=0}^{\infty}\sum_{n=0}^{\infty}\chi_p(x_k)\chi_n(x_j)C(\beta_{np},x_i)\\ &+\sum_{n=0}^{\infty}\chi_n(x_k)C(\lambda_{ni},x_j)(1-\delta_{1i})\\ &+T_{1\mathrm{D}}(x_k)(1-\delta_{1i})(1-\delta_{1j}),\end{aligned} \tag{31}$$

where δ_{1i} is the Kronecker delta function and where

$$\chi_\ell(x_m)=\frac{X_\ell(x_m)}{N(\lambda_{m\ell})} \times \begin{cases} X_\ell(0) & \text{if } m=1 \text{ and } s_1 \text{ is type 1,}\\ X'_\ell(0) & \text{if } m=1 \text{ and } s_1 \text{ is type 2 or 3,}\\ \int_0^{L_m} X_\ell(x'_m)\,\mathrm{d}x'_m & \text{otherwise.}\end{cases} \tag{32}$$

The temperature scale Θ is given by

$$\Theta = \begin{cases} \frac{g}{k} & \text{if internal generation,}\\ f_1 & \text{if } s_1 \text{ is type 1,}\\ \frac{f_1}{k} & \text{if } s_1 \text{ is type 2 or 3}\end{cases} \tag{33}$$

and

$$C(\eta,x_\ell) = \begin{cases} P(x_\ell,0) & \text{if } \ell=1 \text{ and } s_1 \text{ is type 1,}\\ \frac{\partial P(x_\ell,0)}{\partial x'_\ell} & \text{if } \ell=1 \text{ and } s_1 \text{ is type 2 or 3,}\\ V(\eta,x_\ell) & \text{otherwise.}\end{cases} \tag{34}$$

The factor $C(\eta,x_\ell)$ is called the controlling factor and is given explicitly in Eqs. (25), (29), and (30). The quantity $V(\eta,x_\ell)$ is defined by Eq. (25). There are six different forms for the GF that can be used in Eq. (31) depending on the permutation of $(1,2,3)$ used for (i,j,k).

An algorithm was sought to choose the form of the GF to give the most rapid convergence of the sums and requiring the fewest possible terms for the computation of the temperature and heat flux to a specified precision. Convergence of the sums is primarily determined by the exponents in the controlling factors. All of the exponents consist of a non-positive constant multiplied by an eigenvalue. The constants depend upon the location of the point of evaluation relative to the sides of the parallelepiped perpendicular to the direction of the kernel function. The constants are only zero at troublesome points.

The eigenvalues increase with the indices of the summations. Therefore, the controlling factors decay quickly and the resulting sum converges quickly if the eigenvalues increase rapidly. The eigenvalues in the controlling factors within double summations depend upon the eigenvalues in the other directions through Eq. (14). The eigenvalues in the other directions depend on the boundary conditions, thermal properties, and the dimensions of the parallelepiped as per Table 4. This dependence is either given by a simple algebraic expression or a transcendental equation.

Because of the complicated dependencies of the exponents of the controlling factors on other aspects of the problem, the following procedure was used to choose the form of the GF. It was noticed that by about the fifth eigenvalue the eigenvalues became well-ordered. That is, if the fifth eigenvalue in one direction was larger than the fifth eigenvalue in another direction, then the same was true of all succeeding eigenvalues. Based on this observation a choice between the six different forms of the GF could be made.

The form of the GF was chosen to require the fewest terms in the double-sum portion of Eq. (31). For each of the three possible directions of the kernel function in the double sum, the smallest exponent of the controlling factor was found using the fifth eigenvalue in the other directions. The kernel function direction was chosen

corresponding to the controlling factor with the largest (negative) of these three exponents (with the intent to choose the fastest-converging double sum).

If the single sum was needed ($i \neq 1$), the direction of the second kernel function was chosen in an analogous manner. That is, it was placed in the direction that resulted in a controlling factor whose smallest (negative) exponent using the fifth eigenvalue was larger than the smallest (negative) exponent of the controlling factor if it was placed in the other direction.

Since the controlling factor for a particular direction of kernel function in the expressions for the heat flux components is found from the derivative of the temperature expression, it has the same exponents. Thus the directions chosen for the kernel functions used to find the temperature are also used when computing the components of the heat flux.

Troublesome points are only located on sides of the parallelepiped and are caused by an exponent in the controlling factor becoming zero. Therefore provided the point of evaluation is not on an edge or corner of the parallelepiped, the algorithm also automatically avoids evaluation using a controlling factor with a troublesome point. Temperatures and fluxes on edges and corners are often not well defined and are not treated here. However, on edges and corners where the temperature and flux are well defined the algorithm will give the correct value. At any point inside or on a face of the parallelepiped, the algorithm picks a fast converging form of the GF. The algorithm is summarized below:

0. Initialize temperature and heat flux components
1. Let side = 0, 6 (0 for internal generation)
   1.1 Rotate coordinates to place the non-homogeneous side at $x_1 = 0$
      1.11 Pick the first kernel direction such that the smallest exponent using the fifth eigenvalues is as large as possible.
      1.12 If a two-dimensional problem is to be factored out, pick the second kernel direction such that the smallest exponent using the fifth eigenvalues is as large as possible.
   1.3 Find the temperatures and flux components
   1.4 Add the results to the temperatures and fluxes in original coordinates
2. Process the next side
3. Print results

7. Numerical example

Various problems and geometries were used to test the algorithm's ability to find a fast converging form of the GF. One of the test cases is given here in detail. Additional information on the algorithm and the computer program is given elsewhere [12]. The parallelepiped was $3.0 \times 5.0 \times 1.0$ with an internal volume generation of 210 and a conductivity of 0.7. The units could be taken to be any consistent set. The type of boundary conditions, the boundary values, and convection coefficients are summarized in Table 7.

Counting internal generation there were seven non-homogeneities and therefore seven individual problems to be solved, the results of which were superposed to produce the final result. For the purposes of this example, for each of the seven problems, the temperature and all three components of the heat flux were calculated at three different points using all six possible forms of the GF. All possible combinations of forms of the GF produced the same end results for the temperature and the heat flux within the requested tolerance (1.0×10^{-10}) and are given to nine significant figures in Table 8.

The temperature was computed using Eq. (31) in the reverse order it is presented. In effect, the temperature was first approximated as the one-dimensional temperature in the x_k direction and then adjusted to the two-dimensional temperature in the $x_k x_j$ plane and then finally corrected to the desired temperature of the three-dimensional problem. This order was found to improve the convergence of all forms of the GF. The heat flux components were computed in the same order.

The decision to terminate each individual sum was only made at every fifth iteration. If the sum of the absolute values of the last five terms divided by the temperature computed thus far was less than the tolerance, then the sum was terminated. This same procedure was used on the inner and outer sums of the double summation. Specifically, if the sum of the absolute values of the last five terms of the inner sum divided by the temperature calculated so far was less than the tolerance then the inner sum was terminated and the index of the outer sum was increased by one. The outer sum was terminated when the sum of the absolute value of all the terms added to the temperature from five iterations of the outer index divided by the temperature was less than the tolerance. In Table 9, the total number of series terms needed to calculate the temperature and all three components of the heat flux at each point is given. For each row in the table, one entry is marked to indicate the form of the GF selected by the algorithm presented above.

Table 7
Test case boundary information

Side	Type	f_i	h_i
1	3	100	6
2	2	200	–
3	1	50	–
4	3	150	30
5	1	10	–
6	2	300	–

Table 8
Temperature and heat flux at three points

x_1/L_1	x_2/L_2	x_3/L_3	T	q_x	q_y	q_z
0.02	0.9	0.5	56.9918775	−149.509509	35.5070857	−60.4939038
0.5	0.02	0.9	131.376455	−5.57720000	−519.370005	−153.387409
0.9	0.5	0.02	28.9540610	−8.26653408	.0242271805	−661.107672

The coordinates given in Table 9 are the original coordinates. The actual solution is found by first rotating the coordinate system to place the non-homogeneous side at $x_1 = 0$. The directions of successive kernel functions are given in the rotated coordinates since that is when the algorithm is applied. If the first kernel direction is in the x_1 direction and the result for internal generation (side 0) is not being computed then there is not a second kernel direction.

In Table 9, note that for some rows the worst choice of directions for the kernel functions can require millions of terms, up to 7000 times more terms than the best choice. Although the algorithm does not always pick the best directions for the kernel functions, when it does err it picks the second-best choice which is several orders of magnitude better than the worst choice. There are various reasons the algorithm does not always pick the best possible form of the GF: the way the tolerance criteria was used; the order in which the double sum was computed; whether the location of evaluation was near a null of an eigenfunction; and the way Eq. (31) was used.

Computing the temperature (and fluxes) as first a one-dimensional problem then adjusting it to the two-dimensional problem and the three-dimensional problem improves the convergence of some forms of the GF more than others. The choices of the directions of the kernel functions determines which one-dimensional and two-dimensional solutions are used. If a lower-dimensional solution closely approximates the next higher-dimensional solution then fewer terms of the higher-dimensional solution's sum are needed. How well a lower-dimensional solution approximates the next

Table 9
Total number of series terms required for temperature and heat flux

Heated side	Direction of kernel functions					
	x_1, x_2	x_1, x_3	x_2, x_3	x_2, x_1	x_3, x_1	x_3, x_2
(a) *Evaluated at* $x_1/L_1 = .02$, $x_2/L_2 = 0.9$, $x_3/L_3 = 0.5$						
0	26,687	33,102	1782[a]	1872	5417	4732
1	81,255	93,385	2431[a]	2620	8075	6746
2	330[a]	950	3152	3025	9145	15,462
3	260	645[a]	163,322	162,060	13,740	15,462
4	1975	3225[a]	69,597	69,430	7625	8842
5	7690	8970	2121	1930[a]	72,340	72,171
6	6070	7180	1807	1665[a]	46,000	45,842
(b) *Evaluated at* $x_1/L_1 = 0.5$, $x_2/L_2 = 0.02$, $x_3/L_3 = 0.9$						
0	622	1502[a]	11,457	11,417	2257	2522
1	635	1705[a]	27,821	27,760	3220	3692
2	570	1580[a]	24,122	24,060	3220	3692
3	25,030	30,215	1197[a]	1310	3775	3267
4	260[a]	630	1532	1380	5040	5102
5	3350	4055	23,051	23,105	670[a]	786
6	67,965	58,245	12,992	13,410	1275	652[a]
(c) *Evaluated at* $x_1/L_1 = .9$, $x_2/L_2 = 0.5$, $x_3/L_3 = 0.02$						
0	342[a]	4072	1867	492	432,282	432,272
1	370[a]	1015	3781	565	2,241,815	2,241,806
2	6115	10,880	2947	555[a]	1,064,340	1,064,057
3	325	765	7087	730[a]	2,192,560	2,192,577
4	325	765	6317	730[a]	1,705,080	1,705,097
5	2,092,815	2,454,975	341	3245	6390	356[a]
6	2640	3205	337	390	465	362[a]

[a] Direction selected by algorithm.

Table 10
Number of terms needed depending on accuracy requested

Accuracy	Total terms for 1000 points	Average terms of each double sum	Average terms of each single sum
1.0×10^{-10}	16,113,320	544 (24×24)	30
1.0×10^{-7}	11,701,800	392 (20×20)	25
1.0×10^{-4}	8,453,340	281 (17×17)	21

higher-dimensional solution is not taken into account in the algorithm and this is the chief reason the algorithm at times does not pick the best order of directions for the kernel functions.

Terminating the sums only at every fifth term resulted in five terms being the smallest possible difference in the number of terms required by two different single sums and 25 terms being the smallest possible difference in the number of terms required by two different double sums. Thus small differences in the number of terms required are not that meaningful and could be reduced by using a different stopping criteria. It also would be more efficient to add up the terms of the double sum diagonally. That is, first adding all the terms whose indices sum to 1 then all of the terms whose indices sum to two, etc.

Another factor not taken into account is if the point of evaluation is near the null of an eigenfunction then as much as every other term may be close to zero for some choice of kernel function directions.

To evaluate the impact of the accuracy desired on the number of terms required, the temperature and three components of the heat flux for the same test case were also computed at 1000 equally spaced points throughout the parallelepiped for three values of accuracy. The number of terms required for all of the accuracies requested are summarized in Table 10. To compute all of the values, with a requested accuracy of 1.0×10^{-10}, it took a total of 16,113,320 terms including 15,240,040 terms from double sums, 853,280 terms from single sums and 20,000 one-dimensional solutions. Since in all there were 1000 points, four values computed per point, and seven non-homogeneities per value, this means that on average each time a single sum was used it required 30 terms to converge and each time a double sum was used it required 544 terms to converge, which is about 24 iterations of the inner and outer sum. Regardless of the accuracy requested, 20,000 one-dimensional solutions were used for the 1000 points.

8. Summary

In this paper the method of Green's functions has been applied to steady heat conduction in the parallelepiped. A total of $3^6 = 729$ different combinations of boundary conditions are treated for boundaries of types 1, 2, and 3. Alternative forms of each GF are given that may be used to compute numerical values rapidly and accurately anywhere in the parallelepiped. The use of lower-dimensional solutions improves series convergence and provides a convergent series for heat flux on type 1 boundaries. A detailed algorithm is described for computation of the temperature and heat flux efficiently and accurately anywhere in the parallelepiped or on its faces when the heating effects are spatially uniform. Numerical examples are given.

Acknowledgements

The authors gratefully acknowledge support from Sandia National Laboratories under the supervision of contract monitor Dr. Kevin Dowding.

Appendix A. Derivation of Kernel function

Consider a kernel function placed in the x_1-direction. Suppressing the subscripts on P and x, the kernel function satisfies the boundary value problem

$$\frac{\mathrm{d}^2 P}{\mathrm{d}x^2} - \beta^2 P = -\delta(x - x'), \quad 0 < x < L, \tag{A.1}$$

$$k_i \frac{\partial P}{\partial n_i} + h_i P = 0, \quad i = 1, 2. \tag{A.2}$$

The homogeneous solution to Eq. (A.1) is

$$P^{\mathrm{h}} = A\mathrm{e}^{-\beta x} + B\mathrm{e}^{\beta x}. \tag{A.3}$$

Assuming the particular solution is of the form

$$P^{\mathrm{p}} = u_1 \mathrm{e}^{-\beta x} + u_2 \mathrm{e}^{\beta x} \tag{A.4}$$

then

$$\begin{aligned} u_1 &= \int \frac{\mathrm{e}^{\beta x}\delta(x - x')}{W(\mathrm{e}^{-\beta x}, \mathrm{e}^{\beta x})} = \frac{\mathrm{e}^{\beta x'}}{2\beta} U(x - x'), \\ u_2 &= -\int \frac{\mathrm{e}^{-\beta x}\delta(x - x')}{W(\mathrm{e}^{-\beta x}, \mathrm{e}^{\beta x})} = -\frac{\mathrm{e}^{-\beta x'}}{2\beta} U(x - x'), \end{aligned} \tag{A.5}$$

where $U(x - x')$ is the Heaviside function and $W(\mathrm{e}^{-\beta x}, \mathrm{e}^{\beta x}) = 2\beta$ is the Wronskian. Therefore the general solution is

$$P(x,x') = A\mathrm{e}^{-\beta x} + B\mathrm{e}^{\beta x} + \frac{\mathrm{e}^{-\beta(x-x')} - \mathrm{e}^{\beta(x-x')}}{2\beta} U(x-x'). \tag{A.6}$$

Applying the boundary condition at $x = 0$ with a general (type 3) boundary condition gives

$$A = \frac{k_1\beta - h_1}{k_1\beta + h_1} B = \frac{L\beta - B_1}{L\beta + B_1} B \equiv \frac{S_1^-}{S_1^+} B. \tag{A.7}$$

Applying the boundary conditions at $x = L$ (after careful algebraic manipulation) yields

$$B = \frac{S_1^+(S_2^-\mathrm{e}^{-\beta(L-x')} + S_2^+\mathrm{e}^{-\beta(L-x)})}{2\beta(S_1^+S_2^+\mathrm{e}^{\beta L} - S_1^-S_2^-\mathrm{e}^{-\beta L})}, \tag{A.8}$$

$$A = \frac{S_1^-(S_2^-\mathrm{e}^{-\beta(L-x')} + S_2^+\mathrm{e}^{-\beta(L-x)})}{2\beta(S_1^+S_2^+\mathrm{e}^{\beta L} - S_1^-S_2^-\mathrm{e}^{-\beta L})}. \tag{A.9}$$

Substituting Eqs. (A.8) and (A.9) into the general solution, Eq. (A.6) yields

$$\begin{aligned} D(\beta)P(x,x') = {} & S_1^-S_2^-\mathrm{e}^{-\beta L}[(\mathrm{e}^{-\beta(x-x')})(1-U(x-x')) \\ & + \mathrm{e}^{-\beta(x'-x)}U(x-x')] + S_1^+S_2^+\mathrm{e}^{\beta L} \\ & \times [(\mathrm{e}^{\beta(x-x')})(1-U(x-x')) \\ & + \mathrm{e}^{\beta(x'-x)}U(x-x')] + S_1^-S_2^+\mathrm{e}^{\beta(L-x-x')} \\ & + S_1^+S_2^-\mathrm{e}^{-\beta(L-x-x')} \end{aligned} \tag{A.10}$$

or

$$\begin{aligned} D(\beta)P(x,x') = {} & S_1^-S_2^-\mathrm{e}^{-\beta(L-|x-x'|)} + S_1^+S_2^+\mathrm{e}^{\beta(L-|x-x'|)} \\ & + S_1^-S_2^+\mathrm{e}^{\beta(L-x-x')} + S_1^+S_2^-\mathrm{e}^{-\beta(L-x-x')}, \end{aligned} \tag{A.11}$$

where

$$D(\beta) = 2\beta(S_1^+S_2^+\mathrm{e}^{\beta L} - S_1^-S_2^-\mathrm{e}^{-\beta L}). \tag{A.12}$$

Therefore the general solution may be written in a form suitable for computation as

$$\begin{aligned} P(x,x') = {} & \frac{S_2^-(S_1^-\mathrm{e}^{-\beta(2L-|x-x'|)} + S_1^+\mathrm{e}^{-\beta(2L-x-x')})}{2\beta(S_1^+S_2^+ - S_1^-S_2^-\mathrm{e}^{-2\beta L})} \\ & + \frac{S_2^+(S_1^+\mathrm{e}^{-\beta(|x-x'|)} + S_1^-\mathrm{e}^{-\beta(x+x')})}{2\beta(S_1^+S_2^+ - S_1^-S_2^-\mathrm{e}^{-2\beta L})}. \end{aligned} \tag{A.13}$$

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