Fundamental Solutions and Functionally Graded Materials

P. A. Martin

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1. Introduction

A fundamental solution (or Green's function) is a singular solution of a governing partial differential equation (PDE). They can be constructed easily when the PDE has constant coefficients. They are useful for reducing boundary-value problems to boundary integral equations (BIEs). We begin by describing simple properties of fundamental solutions, and then comment on the use and construction of half-space Green's functions.

We then move on to consider functionally graded materials (FGMs). These are inhomogeneous materials: their properties vary with position. Modelling FGMs leads to PDEs with variable coefficients, and this makes the construction of fundamental solutions more difficult.

In this paper, we consider FGMs where the properties vary exponentially in one prescribed direction; such 'exponentially graded' materials provide a reasonable model of certain real situations. We discuss the construction of fundamental solutions for steady-state heat conduction and for three-dimensional elasticity. These solutions should be useful in the development of boundary integral methods for FGMs.

2. What is a Fundamental Solution?

As a prototypical example, consider Laplace's equation in three dimensions, $\nabla^2 u = 0$. A fundamental solution for this PDE is

$$G(P, P') = G(\mathbf{x}, \mathbf{x}') = R^{-1},$$

where the points P and P' have position vectors $\mathbf{x}$ and $\mathbf{x}'$, respectively, with respect to an origin O, and $R = |\mathbf{x} - \mathbf{x}'|$ is the distance between P and P'. Notice that $\nabla^2_P G(P, P') = 0$ and $\nabla^2_{P'} G(P, P') = 0$ for $P \neq P'$.

We can use G in order to reduce boundary-value problems to boundary integral equations. For example, suppose that one wants to solve $\nabla^2 u = 0$ inside a bounded region V with a Dirichlet condition, $u = f$, on the boundary of V, S. A careful application of Green's theorem in V to $u(P)$

and $G(P,P')$, with $P' \in V$, gives the integral representation

$$u(P') = \frac{1}{4\pi}\int_S \left\{ G(p,P')\,\frac{\partial u}{\partial n} - f(p)\,\frac{\partial G}{\partial n_p} \right\} ds_p, \quad P' \in V, \tag{1}$$

where the unit normal to S points *out* of V. To obtain this well-known formula, one has to excise a small sphere from V (of radius ε and centred at P') prior to using Green's theorem, and then lets the radius $\varepsilon \to 0$.

The unknown boundary values of $\partial u/\partial n$ in (1) can then be found by solving a BIE; such equations can be obtained by, for example, considering the limit $P' \to p' \in S$ in (1), or by calculating the normal derivative of (1) at p'.

So far, we have used the simplest choice for G, namely $G = R^{-1}$. In fact, G could be modified in various ways. Thus, we could use

$$AR^{-1} + H(P,P'),$$

where A is any constant or any function of P', and H is any non-singular solution of $\nabla_P^2 H = 0$ (at least in the neighbourhood of P'). These modifications may sometimes be exploited to good effect.

As a second example, suppose that one wants to consider the radiation of acoustic waves in the unbounded region outside S, with a Neumann condition, $\partial u/\partial n = g$, on S. The governing PDE is the three-dimensional Helmholtz equation, $(\nabla^2 + k^2)u = 0$. In order to have a unique solution, we impose the Sommerfeld radiation condition at infinity; this implies that

$$u \sim r^{-1}\, e^{ikr}\, f(\theta,\phi) \quad \text{as} \quad r \to \infty,$$

where r, θ and ϕ are spherical polar coordinates and f is the (unknown) far-field pattern.

For the three-dimensional Helmholtz equation, a fundamental solution is

$$\frac{\cos kR}{R} \sim \frac{1}{R} \quad \text{as} \quad R \to 0.$$

Another is

$$A\,\frac{\cos kR}{R} + B\,\frac{\sin kR}{R}.$$

Usually, we want a fundamental solution that also satisfies the radiation condition, so we can take $A = 1$ and $B = i$, giving

$$G(P,P') = \frac{e^{ikR}}{R}.$$

We can use G to obtain a BIE for u on S; the standard equation is

$$2\pi u(p) - \int_S u(q)\,\frac{\partial G}{\partial n_q}\,ds_q = -\int_S g(q)\,G(q,p)\,ds_q, \quad p \in S.$$

For more information on BIEs for the Helmholtz equation, see [1].

3. Half-Space Green's Functions

It is common to construct (and use) fundamental solutions that also satisfy an additional boundary condition (just as we selected a fundamental solution that satisfied a radiation condition). To give a flavour of these, we discuss briefly a few examples of *half-space Green's functions*. These are singular solutions of a PDE in a half-space $y > 0$, say, that also satisfy a boundary condition on $y = 0$ (together with a condition at infinity). They are used to derive BIEs when the half-space contains an obstacle with boundary S; the result is a BIE over S.

The simplest examples of half-space Green's functions are for Laplace's equation or the Helmholtz equation with the boundary condition $u = 0$ or $\partial u/\partial y = 0$ on $y = 0$: such fundamental solutions are easily constructed by the method of images.

If the half-space is filled with water, the governing PDE is Laplace's equation and the appropriate boundary condition on the free surface is the Robin condition $Ku + \partial u/\partial y = 0$, where K is a given positive constant. Appropriate fundamental solutions are known [2]. Fundamental solutions are also known when the PDE is the Helmholtz equation [3].

If the half-space is filled with a homogeneous isotropic elastic solid, with a traction-free boundary, corresponding fundamental solutions are known: the static solutions were obtained by Melan (two dimensions) and Mindlin (three dimensions) in the 1930's. Time-dependent solutions were obtained by Lamb in 1904, and are discussed in books on elastic waves [4].

Finally, we mention a recent construction for a bi-material half-plane, where two solid quarter-planes (made from different materials) are welded together, and a point force acts inside one of them. This problem can be solved using Mellin-transform techniques [5]. The solution can be used to analyse cracks near the intersection of the interface and the traction-free surface.

All these half-space Green's functions are more complicated than the corresponding 'full-space' Green's functions. Thus, an issue arises: should one use a simple full-space Green's function, leading to a BIE over both S and the half-space boundary; or should one use a half-space Green's function, leading to a BIE over S only? There is a trade-off here, which can have computational repercussions. Little has been done by way of comparison, but see reference [6] for some comparisons in time-harmonic elastodynamics.

4. Steady-State Heat Conduction

Let us now consider inhomogeneous media. We begin with the problem of steady-state heat conduction in an anisotropic inhomogeneous material. This is a scalar problem. The governing PDE can be written as

$$\frac{\partial}{\partial x_i}\left(k_{ij}(\mathbf{x})\,\frac{\partial u}{\partial x_j}\right) = 0, \tag{2}$$

where the usual summation convention is employed and the conductivity matrix $k(\mathbf{x})$ with entries $k_{ij}(\mathbf{x})$ is symmetric. Little can be done for 'arbitrary' $k(\mathbf{x})$. To make progress, we assume that $k(\mathbf{x})$ has a specific functional form,

$$k_{ij}(\mathbf{x}) = K_{ij} \exp(2\mathbf{b} \cdot \mathbf{x}), \tag{3}$$

where $K_{ij} = K_{ji}$ are constants and $\mathbf{b}$ is a given constant vector. We say that the material is *exponentially graded*, with $\mathbf{b}$ giving the *grading direction*. This choice for $k(\mathbf{x})$ is convenient mathematically, of course, but it also gives a reasonable model for certain thermal barrier coatings; it is also a good prototype for analogous elasticity problems.

Substitution of (3) in (2) gives

$$K_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + 2b_i K_{ij} \frac{\partial u}{\partial x_j} = 0. \tag{4}$$

We are going to transform this equation into a Helmholtz equation. First, we remove the first-derivative terms by changing the dependent variable: putting

$$u = v \exp(-\mathbf{b} \cdot \mathbf{x})$$

gives

$$K_{ij} \frac{\partial^2 v}{\partial x_i \partial x_j} - b_i b_j K_{ij} v = 0.$$

This is beginning to resemble a Helmholtz equation. To go further, we change the independent variables to

$$y_i = \Omega_{ij} x_j \quad \text{with} \quad \Omega K \Omega^T = I;$$

here, $K = (K_{ij})$ and $\Omega = (\Omega_{ij})$. This gives

$$(\nabla_y^2 - \kappa^2) v = 0 \quad \text{with} \quad \kappa^2 = \mathbf{b}^T K \mathbf{b}.$$

The PDE for v is known as the *modified Helmholtz equation*. A typical fundamental solution is

$$A \frac{e^{-\kappa R}}{R},$$

where

$$R^2 = (\mathbf{y} - \mathbf{y}')^T (\mathbf{y} - \mathbf{y}') = (\mathbf{x} - \mathbf{x}')^T K^{-1} (\mathbf{x} - \mathbf{x}').$$

Reverting to the original variables, we find that a fundamental solution for (4) is

$$A \exp(-\mathbf{b} \cdot \mathbf{x}) \frac{e^{-\kappa R}}{R},$$

or, with symmetry,

$$B \exp\{-\mathbf{b} \cdot (\mathbf{x} + \mathbf{x}')\} \frac{e^{-\kappa R}}{R}.$$

More details and information on thermal applications of FGMs can be found in [7]. This paper also contains an alternative method, based on the use of Fourier transforms. We will use this method for exponentially graded elastic solids, because the 'transformation method' described above for the scalar equation (4) does not extend to vector problems.

5. Exponentially Graded Elastic Solids

Consider an anisotropic inhomogeneous elastic solid: the stiffnesses $c_{ijk\ell}$ satisfy $c_{ijk\ell} = c_{jik\ell} = c_{k\ell ij}$. The Green's function $\mathbf{G}(\mathbf{x};\mathbf{x}')$ is a 3×3 matrix with entries G_{ij} that satisfy

$$\frac{\partial}{\partial x_j}\left\{c_{ijk\ell}(\mathbf{x})\,\frac{\partial G_{\ell m}}{\partial x_k}\right\} = -\delta_{im}\,\delta(\mathbf{x}-\mathbf{x}'), \quad i=1,2,3, \tag{5}$$

where δ_{ij} is the Kronecker delta and $\delta(\mathbf{x})$ is the three-dimensional Dirac delta. As usual, $G_{ij}(\mathbf{x};\mathbf{x}')$ gives the i-th component of the displacement at $\mathbf{x}$ due to a point force acting in the j-th direction at $\mathbf{x}'$. A standard argument shows that $\mathbf{G}$ is symmetric,

$$G_{ij}(\mathbf{x};\mathbf{x}') = G_{ji}(\mathbf{x}';\mathbf{x}). \tag{6}$$

Evaluating the left-hand side of (5) gives

$$c_{ijk\ell}(\mathbf{x})\,\frac{\partial^2 G_{\ell m}}{\partial x_j \partial x_k} + \left(\frac{\partial}{\partial x_j} c_{ijk\ell}(\mathbf{x})\right)\frac{\partial G_{\ell m}}{\partial x_k} = -\delta_{im}\,\delta(\mathbf{x}-\mathbf{x}'). \tag{7}$$

We consider a particular inhomogeneous material in which the stiffnesses vary exponentially, so that

$$c_{ijk\ell}(\mathbf{x}) = C_{ijk\ell}\,\exp(2\mathbf{b}\cdot\mathbf{x}),$$

where $\mathbf{b} = (b_1, b_2, b_3)$ and $C_{ijk\ell}$ and b_i are given constants. Hence

$$(\partial/\partial x_j)c_{ijk\ell}(\mathbf{x}) = 2C_{ijk\ell}\,b_j\,\exp(2\mathbf{b}\cdot\mathbf{x}) = 2b_j\,c_{ijk\ell}(\mathbf{x}). \tag{8}$$

Using (8), (7) becomes

$$\begin{aligned} C_{ijk\ell}\,\frac{\partial^2 G_{\ell m}}{\partial x_j \partial x_k} + 2b_j\,C_{ijk\ell}\,\frac{\partial G_{\ell m}}{\partial x_k} &= -\delta_{im}\,\exp(-2\mathbf{b}\cdot\mathbf{x})\,\delta(\mathbf{x}-\mathbf{x}') \\ &= -\delta_{im}\,\exp(-2\mathbf{b}\cdot\mathbf{x}')\,\delta(\mathbf{x}-\mathbf{x}') \end{aligned} \tag{9}$$

for $i = 1,2,3$. Note that we can replace the right-hand side of (9) by

$$-\delta_{im}\,\exp(-\mathbf{b}\cdot[p\mathbf{x}+p'\mathbf{x}'])\,\delta(\mathbf{x}-\mathbf{x}'), \tag{10}$$

where p and p' are any constants that satisfy the constraint $p+p'=2$; this flexibility will be exploited soon.

Let us introduce $\mathbf{G}^0$, the Green's function for a *homogeneous* solid with constant stiffnesses $C_{ijk\ell}$. It is defined by

$$C_{ijk\ell}\,\frac{\partial^2 G^0_{\ell m}}{\partial x_j \partial x_k} = -\delta_{im}\,\delta(\mathbf{x}-\mathbf{x}'), \quad i=1,2,3. \tag{11}$$

Comparing these equations with (9) suggests writing

$$\mathbf{G}(\mathbf{x};\mathbf{x}') = \exp(-2\mathbf{b}\cdot\mathbf{x}')\,\left\{\mathbf{G}^0(\mathbf{x};\mathbf{x}') + \mathbf{G}^1(\mathbf{x};\mathbf{x}')\right\}, \tag{12}$$

whence $\mathbf{G}^1$ is found to satisfy

$$C_{ijk\ell}\,\frac{\partial^2 G^1_{\ell m}}{\partial x_j \partial x_k} + 2b_j\,C_{ijk\ell}\,\frac{\partial G^1_{\ell m}}{\partial x_k} = -2b_j\,C_{ijk\ell}\,\frac{\partial G^0_{\ell m}}{\partial x_k} \tag{13}$$

for $i=1,2,3$. Equation (13) is a system of three coupled second-order PDEs, with constant coefficients. However, the decomposition (12) has a disadvantage: the symmetry property (6) is not inherited by $\mathbf{G}^1$. Thus, we change the right-hand side of (9), using (10) with $p=p'=1$, giving

$$C_{ijk\ell}\,\frac{\partial^2 G_{\ell m}}{\partial x_j \partial x_k} + 2b_j\,C_{ijk\ell}\,\frac{\partial G_{\ell m}}{\partial x_k} = -\delta_{im}\,\exp\{-\mathbf{b}\cdot(\mathbf{x}+\mathbf{x}')\}\,\delta(\mathbf{x}-\mathbf{x}'), \tag{14}$$

and we replace (12) by

$$\mathbf{G}(\mathbf{x};\mathbf{x}') = \exp\{-\mathbf{b}\cdot(\mathbf{x}+\mathbf{x}')\}\,\left\{\mathbf{G}^0(\mathbf{x};\mathbf{x}') + \mathbf{G}^g(\mathbf{x};\mathbf{x}')\right\}, \tag{15}$$

so that

$$G^g_{ij}(\mathbf{x};\mathbf{x}') = G^g_{ji}(\mathbf{x}';\mathbf{x}).$$

To find an equation for the *grading term* $\mathbf{G}^g$, we simply substitute (15) in (14), making use of (11); the result is

$$C_{ijk\ell}\,\frac{\partial^2 G^g_{\ell m}}{\partial x_j \partial x_k} + L_{i\ell}\,G^g_{\ell m}(\mathbf{x};\mathbf{x}') = -L_{i\ell}\,G^0_{\ell m}(\mathbf{x};\mathbf{x}') \tag{16}$$

for $i=1,2,3$, where the first-order differential operator $L_{i\ell}$ is defined by

$$L_{i\ell} = (C_{ijk\ell} - C_{ikj\ell})b_j(\partial/\partial x_k) - C_{ijk\ell}b_jb_k.$$

It remains to solve (16); we can do this using three-dimensional Fourier transforms. Before doing that, it is instructive to review the known results for $\mathbf{G}^0$, the so-called *anisotropic Green's function*.

6. The Anisotropic Green's Function

Consider solving (11) by Fourier transforms, which we define by

$$\mathcal{F}\{u\} = \hat{u}(\mathbf{k}) = \int u(\mathbf{x}) \exp(i\mathbf{k} \cdot \mathbf{x})\, d\mathbf{x},$$

where $\mathbf{k}$ is the vector of transform variables. When inverting the Fourier transform to obtain $\mathbf{G}^0$, we have to integrate over $\mathbf{k}$. The relevant integral turns out to involve the vector $\mathbf{r} = \mathbf{x} - \mathbf{x}'$, and it simplifies by choosing spherical polar coordinates with $\mathbf{r}$ along the polar axis. Moreover, the integrand contains $[\mathbf{Q}(\mathbf{k})]^{-1}$, where

$$Q_{im}(\mathbf{k}) = C_{ij\ell m} k_j k_\ell \tag{17}$$

and $C_{ijk\ell}$ are the constant stiffnesses; thus, $\mathbf{Q}$ is homogeneous,

$$\mathbf{Q}(t\mathbf{k}) = t^2 \mathbf{Q}(\mathbf{k}) \quad \text{for any } t \neq 0,$$

and this fact simplifies the calculation. Specifically, we have

$$\begin{aligned} \mathbf{G}^0 &= (2\pi)^{-3} \int [\mathbf{Q}(\mathbf{k})]^{-1} \exp(-i\mathbf{k} \cdot \mathbf{r})\, d\mathbf{k} \\ &= (2\pi)^{-3} \iint k^{-2} [\mathbf{Q}(\hat{\mathbf{k}})]^{-1} \cos(kr \cos\varphi)\, k^2\, dk\, d\hat{\mathbf{k}} \end{aligned}$$

where $r = |\mathbf{r}|$, $k = |\mathbf{k}|$, $\mathbf{k} = k\hat{\mathbf{k}}$ and we have observed that both $\mathbf{G}^0$ and $\mathbf{Q}$ are real. Using spherical polar coordinates (k, φ, χ), where $\varphi = 0$ is the polar axis, we have $d\hat{\mathbf{k}} = \sin\varphi\, d\varphi\, d\chi$ whence

$$\begin{aligned} \mathbf{G}^0 &= (2\pi)^{-3} \lim_{X\to\infty} \int_0^\pi \mathbf{S}(\varphi) \int_0^X \cos(kr\cos\varphi)\, dk\, \sin\varphi\, d\varphi \\ &= \frac{1}{8\pi^3 r} \lim_{X\to\infty} \int_{-1}^1 \mathbf{S}(\cos^{-1}\mu)\, \frac{\sin(Xr\mu)}{\mu}\, d\mu, \end{aligned}$$

where

$$\mathbf{S}(\varphi) = \int_0^{2\pi} [\mathbf{Q}(\hat{\mathbf{k}})]^{-1}\, d\chi.$$

Note that we have evaluated the integral over k and then put $\mu = \cos\varphi$. The integral over μ is known as a *Dirichlet integral*; its limiting value as $X \to \infty$ is $\pi\mathbf{S}(0)$ (see, for example, p. 365 of reference [8]), whence

$$\mathbf{G} = \frac{1}{8\pi^2 r} \oint [\mathbf{Q}(\hat{\mathbf{k}})]^{-1}\, d\chi,$$

where the integral is taken around the unit circle, centred at the origin and lying in the plane perpendicular to $\mathbf{r}$. The remaining one-dimensional integral must be evaluated numerically, in general.

The derivation given above can be found on p. 412 of the book by Synge [9]; other derivations (involving divergent integrals and generalized functions) are available.

7. Calculating the Graded Term

Recall that we have to solve (11) for $\mathbf{G}^g$, using Fourier transforms. We find that

$$\mathbf{G}^g(\mathbf{x}; \mathbf{x}') = (2\pi)^{-3} \int \mathbf{E}(\mathbf{b}, \mathbf{k}) \exp(-i\,\mathbf{k} \cdot \mathbf{r})\, d\mathbf{k}, \tag{18}$$

where $\mathbf{r} = \mathbf{x} - \mathbf{x}'$,

$$\mathbf{E}(\mathbf{b}, \mathbf{k}) = -\{\mathbf{Q}(\mathbf{k}) + \mathbf{B}(\mathbf{b}, \mathbf{k})\}^{-1} \mathbf{B}(\mathbf{b}, \mathbf{k})\,[\mathbf{Q}(\mathbf{k})]^{-1},$$
$$B_{im}(\mathbf{b}, \mathbf{k}) = i(C_{ij\ell m} - C_{i\ell jm}) b_j k_\ell + C_{ij\ell m} b_j b_\ell$$

and $\mathbf{Q}(\mathbf{k})$ is defined by (17). Note that, unlike $\mathbf{Q}(\mathbf{k})$, $\mathbf{E}(\mathbf{b}, \mathbf{k})$ is not a homogeneous function of $\mathbf{k}$.

How should we evaluate (18)? The integrand involves *three* vectors, namely $\mathbf{r}$, $\mathbf{b}$ and $\mathbf{k}$, where $\mathbf{r}$ and $\mathbf{b}$ may be regarded as fixed. Compare this with the integral for $\mathbf{G}^0$, which involves *two* vectors, $\mathbf{r}$ and $\mathbf{k}$: there, we evaluated the integral by using spherical polar coordinates for $\mathbf{k}$ with $\mathbf{r}$ along the polar axis. For $\mathbf{G}^g$, it turns out to be better to choose spherical polar coordinates for $\mathbf{k}$ *with* $\mathbf{b}$ *along the polar axis.*

We have not done these calculations in general, but only when the underlying material is isotropic [10]. Thus, we suppose that the solid has Lamé moduli given by

$$\lambda(\mathbf{x}) = \lambda_0 \exp(2\mathbf{b} \cdot \mathbf{x}) \quad \text{and} \quad \mu(\mathbf{x}) = \mu_0 \exp(2\mathbf{b} \cdot \mathbf{x}),$$

where λ_0 and μ_0 are constants. (Evidently, Poisson's ratio is constant for such a solid.) Then, $\mathbf{G}^0$ is known explicitly (it is the *Kelvin solution*) and $\mathbf{E}$ can be calculated explicitly. The details are complicated. The result is that the triple Fourier integral defining $\mathbf{G}^g$, (18), can be reduced to the sum of an explicit term, some finite single integrals of modified Bessel functions I_n and some finite double integrals of elementary functions. As $\mathbf{G}^g$ is bounded as $|\mathbf{x} - \mathbf{x}'| \to 0$ (the singularity is contained within the Kelvin solution), having it available only as a computable quantity is not an impediment for a boundary integral implementation.

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