

A new separation of variables method for complex geometries

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A procedure has recently been discovered by which the classical separation of variables method can be extended to solve linear boundary value problems for complex geometries. In brief, the procedure consists of embedding the given complex geometry in a larger domain on which complete sets of eigenfunctions exist. The latter are then used to represent the field in the given complex geometry. Since the eigenfunctions are not in general orthogonal on the given boundary, the unknown coefficients are evaluated by a least squares procedure. The details in a specific example, that of two-dimensional heat conduction in a solid of complex shape, are given so that the method can be easily understood and applied. In this case the field satisfies Laplace's equation with given data on the boundary. Since the method is simple and easy to apply, it provides an efficient, extremely accurate and elegant alternative to brute force computation. It is hoped that the method will be taught to college and university students who should have no difficulty in grasping it.

PERHAPS the only fairly general method that all of us learn in college, to solve linear boundary value problems, is the 'method of separation of variables'^{1,2}. This method is also known as the 'Fourier method' or the 'method of eigenfunction expansions'. The method hinges crucially on (i) the variables separating out in the given coordinate system, (ii) the existence of an infinite set of eigenfunctions for the reduced, self-adjoint ordinary differential equation, (iii) the orthogonality of the eigenfunctions permitting the direct evaluation of the coefficients in the series expansion that represents the solution, and (iv) the boundary data being given on constant coordinate lines. The classical method fails if any of these are violated and it is because of these restrictions that the method is considered to be of purely academic interest. Thus, even for linear problems involving complex geometries, it is generally believed that there is no alternative to direct computational methods of solution.

We have recently discovered a way to overcome these limitations, which now permits the method to be used easily and effectively for complex geometries³. The method is so simple that it can be taught to undergraduates and can be used by practising engineers and scientists to solve linear problems involving complex geometries. The purpose of this communication is to give enough details in the solution of a single problem so that anyone wishing to, can learn

the method. It is particularly hoped that college and university teachers will be motivated to teach the method as a superior alternative to brute force computation, at least for linear problems.

Consider steady, two-dimensional heat conduction in the cup-cake-shaped solid shown in Figure 1. The boundary of the complex shape is made up of straight segments AB, DE and EA and the semi-circle BCD; the shape is symmetrical about the line CFG. Let AE be of length $2a$ and DE of length b . The geometry is fully specified by a , b and the angle ϕ_0 . Let us assume that the temperature $\psi(\mathbf{x})$ is known on the boundary of the solid, i.e. $\psi(\mathbf{x}) = \vartheta(\mathbf{x})$ on the boundary, where $\vartheta(\mathbf{x})$ is the given boundary temperature distribution; the field then has to be determined in the interior of the solid, in the domain D . In steady heat conduction, the temperature field $\psi(\mathbf{x})$ has to satisfy Laplace's equation in the interior, i.e.

$$\nabla^2 \psi(\mathbf{x}) = 0 \quad \text{in } D. \quad (1)$$

One observes that there is no obvious coordinate system in which all the boundary segments will be constant coordinate lines. Thus the classical method of separation of variables will not apply to this geometry. Normally, the problem would have to be solved by numerical conformal mapping, a boundary integral type of method or by a direct computational technique.

There are three key steps in the new method suggested by us³: (1) *embed* the domain D with complex geometry in a larger domain D' of simpler geometry, which has on

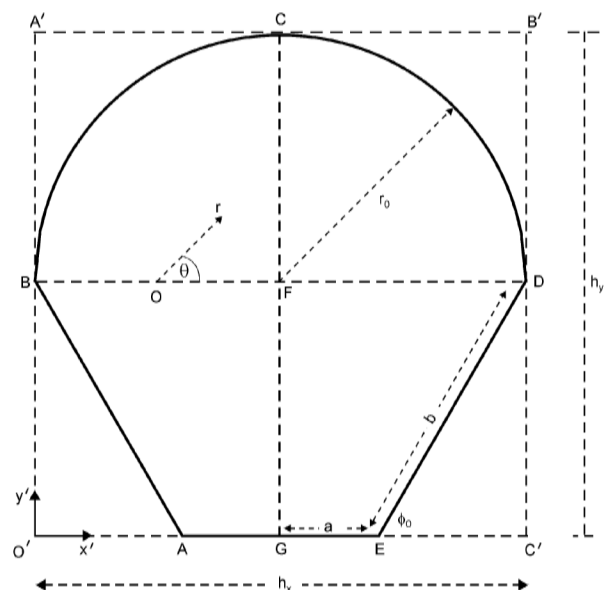


Figure 1. Steady two-dimensional heat conduction in a solid of complex shape. Given the temperature distribution on the boundary ABCDE of the cup-cake-shaped domain D , it is required to determine the temperature $\psi(\mathbf{x})$ in D . The rectangle $O'A'B'C'$ is the embedding domain D' with cartesian coordinate system (x', y') . The origin is at O' .

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it a *complete set* of eigenfunctions, (2) write down the field in the smaller domain D as an infinite series of the members of the complete set of eigenfunctions of D' , and (3) determine the unknown coefficients in the series expansion by truncating it and using the method of least squares to minimize the error on the given boundary data of D . These simple steps will be illustrated here for the problem considered in Figure 1.

It is well known that the rectangular geometry has nice separable solutions for Laplace's equation (eq. (1)). It is therefore natural to embed the given domain D , in this case ABCDE of Figure 1, in the larger dotted rectangle $O'A'B'C'$, which will serve as the embedding domain D' . As shown, the origin of the cartesian coordinate system (x', y') is at O' . For completeness, let us derive the separable solutions $\{\phi_n\}$ to eq. (1) in D' . First assuming that $\phi(x', y')$ vanishes on the vertical boundaries $A'O'$ and $B'C'$, we try $\phi(x', y') \sim X(x')Y(y')$; substitution into eq. (1) and separating the variables leads to $X^{-1}d^2X/dx'^2 = -Y^{-1}d^2Y/dy'^2 = -\lambda^2$, with candidate solutions $\phi(x', y') \sim \exp \pm i\lambda x' \exp \pm \lambda y'$. Since $\phi(x', y')$ has to vanish on $x' = 0, h_x$, it is easy to check that the *eigenvalues* λ_n are given by $\lambda_n = n\pi/h_x$, $n = 1, 2, \dots$ and that the *eigenfunctions* $\phi_n(x', y'; \lambda_n)$ are given by $\phi_n^{\pm}(x', y'; \lambda_n) = \sin \lambda_n x' \exp \pm \lambda_n y'$. It is possible to show that the set $\{\phi_n^{\pm}(x', y'; \lambda_n), n = 1, 2, \dots\}$ is a complete set on D' in the sense that this set can be used to represent the field satisfying eq. (1) in D' , while taking on essentially arbitrary boundary data on $A'B'$ and $O'C'$ and zero boundary data on the vertical sides. In exactly the same way, the set $\{\hat{\phi}_n^{\pm}(x', y'; \mu_n), n = 1, 2, \dots\}$, with $\hat{\phi}_n^{\pm}(x', y'; \mu_n) = \sin \mu_n y' \exp \pm \mu_n x'$ and $\mu_n = n\pi/h_y$, $n = 1, 2, \dots$, is a complete set for arbitrary data on the vertical sides and zero data on the horizontal ones. Together, the two sets $\{\phi_n^{\pm}\}$ and $\{\hat{\phi}_n^{\pm}\}$ can represent essentially arbitrary data on the *whole* boundary of D' .

Following the prescription, we now write the field in D in terms of the complete set of eigenfunctions of D' , i.e. we write

$$\psi(x', y') = \sum_{n=1}^{\infty} [\sin \lambda_n x' \{a_{1n} e^{-\lambda_n y'} + a_{2n} e^{-\lambda_n (h_y - y')}\} + \sin \mu_n y' \{a_{3n} e^{-\mu_n x'} + a_{4n} e^{-\mu_n (h_x - x')}\}], \quad (2)$$

where a_{1n}, a_{2n}, a_{3n} and a_{4n} are real scalars that have to be determined from the given boundary data. The function multiplying a_{2n} in eq. (2) could as well have been written as $\exp \lambda_n y'$, but the form chosen leads to smaller matrix elements; however, this not important or essential. Note that the eigenfunctions on the first line of eq. (2) belong to the set $\{\phi_n^{\pm}\}$, while those on the second line belong to the set $\{\hat{\phi}_n^{\pm}\}$.

We will now use the method of least squares to determine the unknown coefficients to, in principle, any required degree of accuracy. Truncate the series in eq. (2) to N terms and write

$$\psi(x', y') = \sum_{n=1}^N \{f_1(x', y')a_{1n} + f_2(x', y')a_{2n} + f_3(x', y')a_{3n} + f_4(x', y')a_{4n}\}, \quad (3)$$

where

$$f_1(x', y') = \sin \lambda_n x' e^{-\lambda_n y'}, \quad f_2(x', y') = \sin \lambda_n x' e^{-\lambda_n (h_y - y')} \\ f_3(x', y') = \sin \mu_n y' e^{-\mu_n x'}, \quad f_4(x', y') = \sin \mu_n y' e^{-\mu_n (h_x - x')}. \quad (4)$$

One notes that now there are $4N$ real scalars to be determined from the given boundary data $\vartheta(\mathbf{x})$. Distribute M ($M > 4N$) points, not necessarily equi-spaced, on the boundary of D and let ϑ_k , $k = 1, 2, \dots, M$ be the given temperatures at these points. Similarly, let $f_{ik} = f_i(x'_k, y'_k)$, $k = 1, 2, \dots, M$ be the values of $f_i(x')$ at these points and similarly for the other functions in eq. (4). We can then define the error, e_k , at the k th point by

$$e_k = -\vartheta_k + \sum_{n=1}^N \{f_{1k}a_{1n} + f_{2k}a_{2n} + f_{3k}a_{3n} + f_{4k}a_{4n}\}, \quad (5)$$

and the total error squared at all the M chosen points on the boundary by

$$E^2 = \sum_{k=1}^M e_k^2 = \sum_{n=1}^M \left[-\vartheta_k + \sum_{n=1}^N \{f_{1k}a_{1n} + f_{2k}a_{2n} + f_{3k}a_{3n} + f_{4k}a_{4n}\} \right]^2. \quad (6)$$

One could also define the total error squared as an integral of eq. (5) over the boundary, but the simple definition in eq. (6) is adequate for our purposes. One can now regard E^2 as a function of the $4N$ scalars, $a_{11}, a_{21}, a_{31}, a_{41}, \dots, a_{4N}$ and ask what these should be in order that E^2 be a minimum. A necessary condition is that $\partial E^2 / \partial a_{ni} = 0$ for $n = 1, 2, 3, 4$ and $i = 1, 2, \dots, N$. For example, with $n = 1$

$$\frac{\partial E^2}{\partial a_{1i}} = \sum_{k=1}^M \left[-\vartheta_k + \sum_{n=1}^N \{f_{1k}a_{1n} + f_{2k}a_{2n} + f_{3k}a_{3n} + f_{4k}a_{4n}\} \right] f_{1ki} \\ f_{1i} = 0, \quad i = 1, 2, \dots, N. \quad (7)$$

Thus we have $4N$ linear algebraic equations for the $4N$ real scalars and these can be solved by standard routines. One would expect that as N becomes larger and larger, the error will decrease and this is what is found. As long as $M > 4N$, the exact value of M is unimportant, especially as N and M become large. However, it appears that for better accuracy for small N , it is a good idea to keep M to be two to three times the number of unknowns, in this case $4N$.

Figure 2 shows the results of calculations done by the above procedure for a particular choice of boundary data and geometry. In this case the geometrical parameters are $a = 0.25$, $b = 0.75$ and $\phi_0 = 60^\circ$. Moreover, since we wish to demonstrate the accuracy of the method, we choose a field that is known exactly and use the resulting data on the boundary to test the efficacy and accuracy of the proposed method. The temperature field is given exactly by

$$\psi(r, \theta) = r^n \sin n\theta, \quad (8)$$

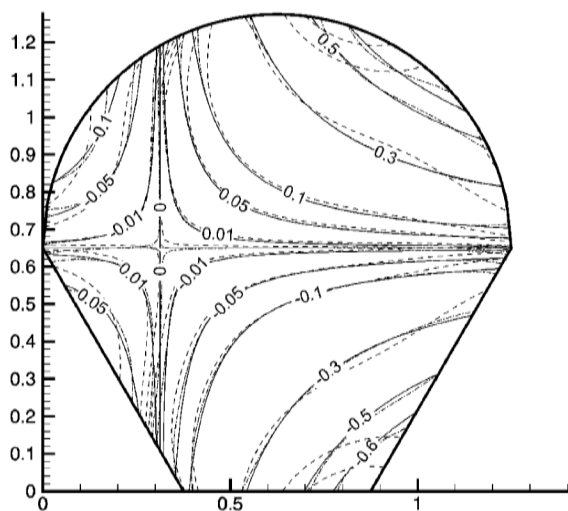


Figure 2. Temperature distribution $\psi(\mathbf{x})$ in D when the exact solution is $r^2 \sin 2\theta$ with the origin of the polar coordinate system located at O in Figure 1. $a = 0.25$, $b = 0.75$, $\phi_0 = 60^\circ$. —, the exact solution $\psi(r, \theta = r^2 \sin 2\theta)$; - - -, $N = 2$; - · - · -, $N = 5$; ·····, $N = 10$.

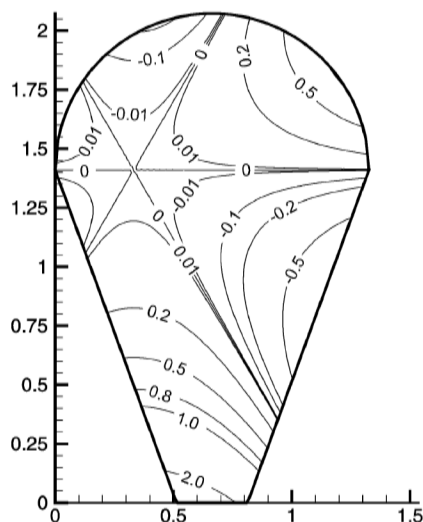


Figure 3. Temperature distribution in the solid when the exact field is $r^3 \sin 3\theta$ and $a = 0.15$, $b = 1.5$, $\phi_0 = 70^\circ$. The exact field and the eigenfunction expansion with $N = 10$ are indistinguishable.

where the origin of the polar coordinate system (r, θ) is located at O , the mid-point of BF , as shown in Figure 1. Needless to say, ψ as defined in eq. (8) satisfies Laplace's equation (eq. (1)). Now, if (x_b, y_b) is a point on the boundary of D , the boundary data $\vartheta(x_b, y_b)$ are given by just evaluating the right-hand side of eq. (8) at the point (x_b, y_b) . We can then proceed with the eigenfunction expansion procedure as described above.

In Figure 2 the given field corresponds to the case where $n = 2$ in eq. (8), and the computed fields with $N = 2$, 5 and 10 are shown with $M = 10N$ in each case. On this scale the computed fields, especially for the larger N , will be insensitive to the exact choice of M . Figure 2 shows that even with N as small as 5, the overall field is reasonably described by the eigenfunction expansion, while with $N = 10$ the results are indistinguishable on this scale. One can obtain a more quantitative appreciation of the increase in accuracy with increasing N from the data in Table 1, which shows the magnitude of the maximum error on the boundary, ϵ_m , as a function of N . While the maximum error is already as low as about 0.27×10^{-4} when $N = 10$ it reduces drastically to 0.19×10^{-7} when $N = 50$; such accuracies are not achievable by any other method, certainly not with as little effort. The calculation with $N = 50$, including the computation of the field at 100×100 field points takes 3 s on a Pentium III running at 866 MHz. Figure 3 shows the results for an ice-cream cone-shaped geometry; here the field is given by eq. (8) with $n = 3$. The results for $N = 10$ are once again indistinguishable from the exact solution.

The example considered here was chosen for its simplicity so that the details of the method would be transparent. However, the same method applies, with exactly the same steps, to three-dimensional problems and to other linear operators³. Thus the eigenfunction method is a powerful one for solving linear boundary value problems. It is conceptually simple, the field equations are satisfied exactly, it is fast and can be extremely accurate, it has the potential to yield the asymptotic nature of the field, it does not require any gridding or panelling and it permits one to store the details of the field in a relatively small number of coefficients. The only weakness of the method till now was that its use was restricted to rather simple geometries, not to those of practical importance. With the present ex-

Table 1. Magnitude of maximum error on the boundary ϵ_m as a function of N , the number of terms in the series for $\psi(x', y')$

| N | Number of scalars | ϵ_m |
|-----|-------------------|------------------------|
| 1 | 4 | 0.518 |
| 2 | 8 | 0.164 |
| 5 | 20 | 0.497×10^{-1} |
| 10 | 40 | 0.268×10^{-4} |
| 25 | 100 | 0.105×10^{-5} |
| 50 | 200 | 0.190×10^{-7} |

tension to complex geometries, the scope of the method has been extended greatly, making it the method of choice to solve linear boundary value problems on complex geometries.

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Received and accepted 15 December 2004

Is there a need for variable density option in making combined mass correction to gravity data acquired over high relief?

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Traditional gravity data processing involves terrain and Bouguer corrections with uniform density. However, inclusion of variable densities honouring surface geology in such corrections is a long-felt need. This matter assumes fundamental importance for gravity data acquired over high relief. So, improved Bouguer and terrain correction scheme is proposed and its utility is demonstrated on a gravity profile along Mahe–Sumdo–Tso Morari of Ladakh Himalaya.

A maximum difference of about 50–70 mGal in the final Bouguer anomaly is observed between data processed through normal procedure with uniform Bouguer density ($= 2.67 \text{ g/cm}^3$) and those proposed with variable density. This underlines the importance of the proposed scheme.

THE purpose of making corrections to gravity data is to arrive at Bouguer anomaly free of non-geologic effects that are unavoidable components of the basic measurement. In-depth analysis of gravity data corrections is clearly missing in basic English language textbooks¹. In recent years, La Fehr² and Talwani³ have dealt with the problem of making Bullard *B* correction. The method proposed by Banerjee⁴ for gravity data acquired over high relief uses a digital terrain model and constant Bouguer density.

Northwestern Himalaya is characterized by high elevations and severely tectonized zones with steep dips, which pose challenging problems for geophysical data processing in general and gravity data, in particular. A new improved gravity data reduction method is proposed, involving variable density information. The effectiveness of the proposed procedure is illustrated on a gravity profile along Mahe–Sumdo–Tso Morari of Ladakh Himalaya.

The conventional land Bouguer gravity, Δg_B based on single constant density for combined mass correction is given by

$$\Delta g_B = g_{\text{obs}} - LC \pm FAC \mp BC + TC, \quad (1)$$

where g_{obs} refers to observed gravity reading, LC is latitude correction, FAC is free-air correction, BC is Bouguer correction and TC is terrain correction.

To incorporate the terrain correction term with variable density option in eq. (1), let us adopt Hammer's template for the terrain around the gravity station covered by N circles of radii R_i ($i = 1, n$ for the inner zone and $i = n + 1, N$ for the outer zone), with $m(i)$ compartments the inner zone ($j = 1, m(i)$) and $M(i)$ compartments in the outer zone ($j = 1, M(i)$). Then TC in eq. (1) can be expressed as

$$TC = \sum_{i=1}^n \sum_{j=1}^{m(i)} f_{ij} \rho_{ij} + \sum_{i=n+1}^N \sum_{j=1}^{M(i)} f_{ij} \sigma, \quad (2)$$

where ρ_{ij} and σ are the variable and constant Bouguer densities of the inner and outer zones (Figure 1) respectively, and following Grushinsky and Sazhina⁵, one can have

$$f_{ij} = \frac{1}{C} (2\pi G ((R_{i+1} - R_i) + \sqrt{R_i^2 + h_{ij}^2} - \sqrt{R_{i+1}^2 + h_{ij}^2})), \quad (3)$$

where

$$C = \begin{cases} m(i), i = 1, n, & \text{for the inner zone} \\ M(i), i = n + 1, N, & \text{for the outer zone.} \end{cases} \quad (4)$$

h_{ij} are elevation differences of the ij th curvilinear prism of topography with respect to station elevation d . G is the universal gravitational constant. It is to be noted that the topographic masses around a gravity station delimited by n zones of Hammer's chart in the first summation are for a variable density inner zone and the remaining $(N - n)$ zones in the second summation constitute the outer zone with a constant density σ respectively.

So far, we have made necessary modifications in terrain correction term for the case of variable density option. However, this situation also demands a modification of Bouguer correction term.

BC in the absence of variable densities is given by

$$BC = 2\pi G \sigma d. \quad (5)$$

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