A Pedagogical Approach to Introduce Green's Functions to Engineering Students

Leora Maxwell Loftis, Pedro E. Arce, Jennifer Pascal

Department of Chemical Engineering, Tennessee Technological University

Abstract

Nearly all senior undergraduate and graduate engineering students are required to take an advanced engineering mathematics course in which they solve homogeneous partial differential engineering equations (i.e., wave, heat and Laplace equations) using the separation of variables technique. However, real-world applications and cutting edge research may lead to models requiring complementary mathematical approaches such as the use of Green's functions ³. Therefore, it is necessary to introduce senior undergraduate and graduate student researchers (learners) to this approach. Unfortunately, the literature describing this approach varies significantly and does not contain an efficient pedagogical methodology for the students. Furthermore, introducing this approach to students in a methodical, didactic manner remains a challenge that has not been fully addressed in engineering students to learn the Green's function method, building upon knowledge they have gained in mathematics, physics and engineering. The heat equation with a source term will be used as a fundamental, illustrative example of this approach.

Keywords

Green's Functions, Mathematical Modeling

Motivation and Introduction

Due to the fast pace of computational research, many current, complex engineering problems that require mathematical modeling can now be attacked to find a solution. However, solutions to these problems often require very sophisticated, yet inefficient numerical schemes that can take significant amounts of computational power and time. Formal solutions in terms of integral equations whose kernel is based on the Green's function, present an attractive approach to solving some of these more complicated, yet fundamentally important engineering problems. These approaches are often overlooked in favor of overly complex numerical simulations that produce nice pictures, but do not necessarily capture all the trends in the behavior of the system. Furthermore, these approaches are usually not transparent to students (learners). Thus, many engineering undergraduate and graduate researchers are facing these challenging problems without a toolkit that allows them to properly apply and build upon their knowledge to solve these problems. In addition, most engineering graduate programs require students to take a course in partial differential equations in which they (usually) study the three, fundamental engineering partial differential equations (pde's), the heat, wave and Laplace equations. The method of separation of variables is taught in these courses in order to solve special cases of these equations in which there are no source terms, either in the differential equation or in the associated boundary conditions; thus the differential equation and the boundary conditions are homogeneous, so that a Sturm-Liouville problem for the ordinary differential equation (ode) can be solved resulting in the determination of eigenvalues and eigenfunctions³. However, many current engineering problems involve non-homogenous cases of these equations and students are often not exposed to another solution methodology to solve them analytically or semi analytically. Therefore, here we introduce a systematic approach for senior undergraduate and graduate engineering students to apply their knowledge of the separation of variables approach and build on it in order to formulate integral equations that use the Green's function as their kernel. These Green's functions can be readily identified as Fourier sums based on the Sturm-Liouville problem of the differential problem¹.

While Green's functions have been studied and applied extensively in every discipline of engineering, their presentation is different in every venue, making it challenging for students (novices) to educate themselves without the aid of an expert. Green's functions are often presented in abstract mathematical formulations, which are not helpful for most engineering students who are interested in applied mathematics. It is our intention to provide students with a guide, or roadmap to help them apply the Green's function method to solve fundamental engineering research problems. In a future, more in depth contribution, we plan to expand this paper to specific, current biomedical research applications and examine modeling tumor cell response to applied electrical fields.

In this contribution, we use a parabolic type of differential equation, i.e., the heat equation with source terms (in its most general case) as an illustrative example⁷. A visual representation of this system is shown in Figure 1 consisting of a rectangular domain of length, $L_{,}$ in which the temperature, T, at both ends is held at zero, while the initial temperature is some function of the axial position, $x_{,}$ within the rod. First, we illustrate the solution of the

homogeneous problem by using separation of variables in order to identify the Sturm-Liouville problem; its solution leads to the eigenvalues and eigenfunctions^a. Next, we build directly upon



Figure 1: Illustration of system consisting of a long, thin rod held at temperatures of zero at both ends.

this analysis to solve the heat equation with a source term (nonhomogeneous problem) by inverting the differential problem into an integral form via the Green's function approach. The Green's function, i.e., the kernel of the integral equation, is identified as a Fourier sum based on the solution of the homogeneous problem.⁴

Physical Interpretation and Advantages of Green's Function Approach

Green's functions can be viewed, from a physical perspective, as a way to illustrate or elucidate the influence of actions or forces on a particular system. For the example studied here, the heat equation with a source term, the Green's function demonstrates the influence of the initial condition on the temperature profile in the rod (see, for example, ⁶).

<u>Coaching Point:</u> Students might immediately ask something like, "Why is that so helpful? Why would a numerical solution not give you the same result?" Here, the instructor can use this as a learning opportunity to delineate the advantages of using Green's functions to solve pde's in comparison to numerical solutions. For example, in numerical approaches, such as the finite difference/element method, a grid must be constructed and the pde's decomposed into algebraic equations at every single node on the grid which can be an extremely time consuming process and require substantial amounts of computational power. Using Green's functions, this entire process can be avoided and the solution can be obtained for every point in time and space directly. Additionally, the Green's function approach described here is very systematic and leads to analytical (formal) solutions in terms of integral equations, which are more beneficial and reliable than numerical solutions based on approaches such as finite difference and finite elements.

The Homogeneous Problem: One Dimensional Heat Equation

The one dimensional (1-D) heat equation (1a) with homogeneous boundary conditions and initial condition (1b) is often the first equation introduced to senior undergraduates/graduate students in engineering during their first partial differential equations course,

^a In the case of the heat equation, the solution of the Sturm-Liouville problem is analytically obtained. For other cases, where the problem at hand is more complex, the final solution results in roots of the characteristic polynomial. Therefore, a root finder is useful for this purpose.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2},\tag{1a}$$

$$T(0,t) = 0 \ T(L,t) = 0$$

$$T(x,0) = f(x) ,$$
(1b)

where T is temperature, t, time, α , thermal diffusivity, x, axial position and f(x) a function describing the initial temperature distribution within the rod. Equation (1a) can be solved using separation of variables approach (see Figure 3) to obtain the following Sturm-Liouville problem^b

$$X'' - \lambda^2 X = 0,$$
 (2a)
X(0) = 0 (2b)

$$X(L) = 0 \quad (2b)$$

where X is the solution of the spatial problem arising from separation of variables and λ is the eigenvalues. The eigenvalues can be determined by studying their three cases ($\lambda = 0$; $\lambda < 0$; $\lambda > 0$) to find the one that does not lead to a nontrivial solution of equation (2a) when the boundary conditions (2b) are applied. As shown in Figure 3 these eigenvalues are numbers at which the function, $\sin\left(\frac{n\pi x}{L}\right)$ is equal to zero. Thus, the associated eigenfunctions for this problem are,

$$X_n(x) = \sin\left(\frac{n\pi x}{L}\right), n=1,2,3...,$$
 (3)

The temporal equation resulting from separation of variables is a linear, first order ordinary differential equation with constant coefficients and a function for $\theta_n(t)$ can be obtained,

$$\theta_n(t) = c e^{-\lambda_n^2 t}$$
(4)

where c is a constant. Combining equations (3) and (4) one can arrive at the solution of the homogeneous 1-D heat equation with homogeneous boundary conditions.

$$\sum_{n=1}^{\infty} T_n(x,t) = \sum_{n=1}^{\infty} A_n \exp(-\lambda_n^2 t) \sin\left(\frac{n\pi x}{L}\right),$$
(5)

where A_n is the coefficient of the Fourier sine series given by,

$$A_n = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx .$$
 (6)

^b Please note that this is for the case of Dirichlet boundary conditions.

Building Upon the Homogeneous Problem: Introducing a Source Term

Now, adding a source term, Q(x,t) equation (1a) becomes nonhomogeneous, but with the same boundary conditions and initial condition⁵. If these conditions are changed, it will lead to a more complicated problem that requires additional terms in the integral-equation solution methodology that is not the focus of the current contribution. This equation can be solved analytically using Laplace transforms or, alternatively, an inversion-type of approach based on Green's functions.^{c²} We choose to focus on the latter here because of its wider applicability to a larger variety of engineering problems. This approach builds directly upon the process outlined in the homogeneous heat equation approach in the previous section. The eigenvalues and eigenfunctions found in that problem are used here.



Figure 2: Overview of solution process applied to nonhomogeneous heat equation.

The overall process for using Green's functions to solve this problem is outlined in Figure 2. First, eigenfunctions expansion is used to express the general solution of the nonhomogeneous problem, where the Fourier series coefficients are a function of the source term. Next, the time derivative of this solution is taken and substituted into the nonhomogeneous heat equation. This is a generalized Fourier sine series, so the term on the right hand side of the equation can be expressed in terms of Fourier sine series.

The spatial term can be integrated by parts to obtain a linear, ordinary differential equation for $b_n(t)$ that can be solved using an integrating factor approach. Once these the coefficient, $b_n(t)$ is determined it can be substituted back into the equation and the Green's function can be identified.

^c A more robust approach that is based on linear operator methods can also be used. However, we focus in this contribution on an introductory course where elements of functional analysis may not be part of the students' knowledge.

2016 ASEE Southeast Section Conference



Figure 3: Outline of mathematical process applied to nonhomogeneous heat equation.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + Q(x,t) \,. \tag{7}$$

Now, the method of eigenfunctions expansion can be employed,

$$T(x,t) = \sum_{n=1}^{\infty} b_n(t)\phi_n(x), \qquad (8)$$

where $b_n(t)$ are coefficients of the Fourier series and $\phi_n(x)$ are the eigenfunctions of the homogeneous problem. Taking the time derivative of the right hand side of equation (8) a generalized Fourier series is obtained. Thus, by definition, this Fourier series can be expressed as follows,

$$\frac{2}{L}\int_{0}^{L} \left(\alpha \frac{\partial^2 T}{\partial x^2} \phi_n(x) \right) dx + \frac{2}{L} \int_{0}^{L} Q(x,t) \phi_n(x) dx , \qquad (9)$$

where all terms have been previously defined. Integrating the left hand side using integration by parts (learned by students in calculus 2) and applying the homogeneous boundary conditions when appropriate, this can be simplified to $-\alpha\lambda_n^2$. Thus, one can arrive at a linear, ordinary differential equation with constant coefficients for $b_n(t)$.

$$\frac{db_n}{dt} + \alpha \lambda_n^2 b_n(t) = q_n(t) , \qquad (10)$$

where $q_n(t) = \frac{2}{L} \int_0^L Q(x,t)\phi_n(x) dx$. This equation can be solved using the integrating factor

method learned by students in undergraduate differential equations and substituted back into the eigenfunctions expansion (equation 8) to obtain an equation for T(x,t). Using Fubini's Theorem ⁷ to switch the order of summation and integration, the students can arrive at the equation for T(x,t) shown on the right hand side of Figure 3. The Green's function can be identified to simplify this equation to the following formal solution to the nonhomogeneous heat equation:

$$T(x,t) = \int_{0}^{L} g(x_0) G(x,t;x_0,t_0) dx_0 + \int_{0}^{L} \int_{0}^{t} G(x,t;x_0,t_0) Q(x_0,t_0) dt_0 dx_0,$$
(11)

where $G(x,t;x_0,t_0)$ is defined in Figure 3.

Summary and Concluding Remarks

Here we have briefly outlined a systematic approach to apply the Green's function method to solve the nonhomogeneous heat equation. We believe this contribution can help engineering students who are working in mathematical modeling gain a more fundamental understanding of their system through the process of obtaining an analytical solution, described here. Just by using the method illustrated in Figures 2 and 3 students (learners) can implement this to their particular problem, since this builds directly upon the skills (separation of variables) they gain in an introductory partial differential equations course. In a future contribution, we will expand upon this to include a more in depth analysis of this method applied to a biomedical application.

Leora Maxwell

Leora Maxwell Loftis is a graduate student in chemical engineering at Tennessee Technological University (TTU). She is involved in research of mathematical modeling for cancer treatments utilizing electric fields. She obtained her Bachelor's degree from TTU in 2015. She has presented her research at multiple conferences, one at which she earned a national award for a poster presentation. Also, Leora has won multiple awards in the chemical engineering department and College of Engineering at TTU.

Pedro E. Arce

Pedro E. Arce is a University Distinguished Faculty Fellow, Professor and Chair of the Department of Chemical Engineering at Tennessee Technological University. He has contributed to numerous approaches for increasing student learning and enhancing collaborative approaches and innovation-driven learning. Dr. Arce is the only faculty that has received four Thomas C. Evans Award recognitions for these contributions and has conducted numerous workshops at the ASEE-SE annual meetings to expose colleagues to these developments. Dr. Arce received a Diploma from the Universidad Nacional del Litoral, Santa Fe, Argentina, a Master of Science and a PhD from Purdue University. All degrees are in Chemical Engineering.

Jennifer Pascal

Jennifer Pascal is an assistant professor of chemical engineering at Tennessee Technological University (TTU) whose research focuses on mathematical modeling of electrical field-based cancer treatments. She earned her Bachelor's and Doctoral degrees from TTU in 2006 and 2011, respectively. She was recognized for her work in fluid-particle separations in 2010 with a national award. She received a National Institutes of Health (NIH) Postdoctoral Fellowship at the University of New Mexico where she worked on modeling drug delivery to tumors prior to her appointment at TTU. She has taught fluid mechanics, mass transport, introduction to chemical engineering and a graduate course on modeling biological systems.

References

1. Amundson, N. R. The mathematical understanding of chemical engineering systems. : Elsevier, 2014.

2. Arce, P., B. Locke, and I. Trigatti. An integral-spectral approach for reacting Poiseuille flows. AIChE J. 42:23-41, 1996.

3. Haberman, R. Applied partial differential equations with Fourier series and boundary value problems. AMC 10:12, 2004.

4. Jerri, A. Introduction to integral equations with applications. : John Wiley & Sons, 1999.

5. Loney, N. W. Applied Mathematical Methods for Chemical Engineers. : CRC Press, 2006.

6. Ozisik, M. N. Heat conduction. : John Wiley & Sons, 1993.

7. Zill, D., W. S. Wright, and M. R. Cullen. Advanced engineering mathematics. : Jones & Bartlett Learning, 2011.