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A Green's function formulation for finite-differences schemes

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Abstract

The finite-differences (FD) method has been used with remarkable success in solving a wide range of problems in virtually all areas of engineering. Our aim in this paper is to show how FD schemes can be derived from an integral formulation of boundary-value problems from Green's functions. For this purpose, we confine our attention to a simple second-order model representing diffusion and non-linear reaction in a catalytic slab. The classical FD discretization is obtained by forcing the integral equation formulation of the boundary-value problem to hold at the discretization points. Under the Green's function formulation, Dirichlet boundary conditions are incorporated as in classical FD. Interestingly, Neumann boundary conditions modify the discretization at the boundary node, and numerical results show that such modification improves the performance of the FD method.

Keywords: Finite differences; Reaction–diffusion; Green's function

1. Introduction

The finite-differences (FD) method is a general technique for constructing approximate solutions to boundary-value problems. Because of the generality and richness of the ideas underlying the method, it has been used with remarkable success in solving a wide range of problems in virtually all areas of engineering. For instance, recent work has shown that an accurate numerical scheme for parabolic PDEs plays a central role to obtain reduced-order (i.e., finite-dimensional) models for state estimation and feedback control purposes (Christofides and Daoutidis, 1997; Baker and Christofides, 2000; Christofides, 2001). General and customized FD methods are now standard for solving many applications in chemical engineering. A plethora of results and studies on FD methods can be found in the literature, including stability analysis, improved performance and robustness. In general, derivation of FD schemes are made from Taylor's series expansions or Newton's FD calculus. It seems, at least from an engineering perspective, that research work should focus on refined applications and detailed grid or mesh constructions. However, in this paper we will reveal a novel link with another formulation from boundary-value problems; namely, integral equation formulations (IEF) obtained from Green's function approaches (Barton, 1989; Beck et al., 1992; Melnikov, 1995; Duffy, 2001). In fact, in the chemical engineering literature, IEF based on Green's functions have been proposed as an alternative to most traditional FD schemes. Amundson and Schilson (1961) obtained the Green's function for isothermal linear reaction in a sphere, and solved the resulting linear Fredholm integral equation via a successive approximation technique. Kesten (1969) applied Green's function analysis to obtain concentration profiles for ammonia decomposition in a spherical catalytic pellet. Dixit and Tavlarides (1982) were the first to use Newton iteration schemes to solve non-linear Fredholm equations arising from reaction in a sphere, and applied their results to the Fischer–Tropsch synthesis. Subsequently, Mukkavilli et al. (1987a) presented and solved numerically an IEF for reaction in a finite cylinder with Dirichlet boundary conditions.

Numerical schemes based on IEF offer interesting implementation advantages, including exact incorporation of boundary conditions and enhanced stability in the face of round-off

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error smoothing (Beck et al., 1992). On the other hand, FD schemes are well studied and optimized computer codes are available both publicly and commercially. On the one hand, Green's functions provide an important theoretical and physical backup for IEF schemes. On the other hand, FD methods have an intuitive flavor with theoretical backup from well-studied function approximation theory. It is apparent that FD and IEF are two different techniques to obtain approximate solutions for boundary-value problems. The aim of this paper is to show a link between the two techniques. Specifically, it is shown that FD schemes can be obtained as a particular case from IEF methods. The departing point for establishing such connection is the description of the boundary-value problem as a *subdomain* IEF. The classical FD scheme is obtained by forcing the subdomain IEF to have zero residues at the discretization points. Under the Green's function formulation, Dirichlet boundary conditions are incorporated as in classical FD. Interestingly, mixed (i.e., Neumann plus Dirichlet) boundary conditions modify the discretization at the boundary node, and numerical results show that such modification improves the performance of the FD method. Numerical results with both linear and non-linear examples are used to illustrate our findings.

It should be stressed that, since our aim in this paper is to motivate the usage of Green's functions to derive FD schemes, we confine our attention to the simplest, most transparent example: a one-dimensional, two-point boundary-value problem characterized by a simple non-linear ordinary differential equation (ODE) of second-order, together with a pair of boundary conditions. We shall refer to this example as our "model problem". Although the simplicity of the model problem, both its mathematical structure and our approach in formulating its IEF approximation are essentially the same in more complex problems.

2. IEF of boundary-value problems

A brief description of Green's functions and related concepts will be described below. Consider the following class of linear differential equations:

$$Lu(x) = ku(x), \quad x \in D \subset \mathbb{R}^n \tag{1}$$

with suitable boundary conditions. Here, L represents a *linear* differential operator of a given order. Let $G(z, x)$ be an integral kernel, called *Green's function*, which will be defined later. Then, repeated integration by parts over $\int_D G(z, x)Lu(z)\,\mathrm{d}z$ yields (Barton, 1989; Melnikov, 1995)

$$\int_D G(z, x)Lu(z)\,\mathrm{d}z = [\ldots]|_{\partial D} + \int_D u(z)L^*G(z, x)\,\mathrm{d}z, \tag{2}$$

where z is a dummy integration variable, $[\ldots]|_{\partial D}$ are terms evaluated at the boundary of D, and L^* is the formal adjoint differential operator associated with L. Computation of the IEF requires the computation of the adjoint operator L^*. One says that L is self-adjoint if $L^* = L$. Notice from Eq. (1) that $Lu(x)=ku(x)$, which can be used in the left-hand side of Eq. (2) to obtain

$$\int_D G(z, x)ku(z)\,\mathrm{d}z = [\ldots]|_{\partial D} + \int_D u(z)L^*G(z, x)\,\mathrm{d}z.$$

On the other hand, if one poses the differential problem on $G(z, x)$ as

$$L^*G(z, x) = \delta(z - x), \tag{3}$$

where $\delta(z - x)$ is the delta function, one obtains that $\int_D u(z)\delta(z - x)\,\mathrm{d}z = u(x)$ (Greenberg, 1971). In this way, Eq. (2) is reduced to the expression $\int_D G(z, x)f(u(z))\,\mathrm{d}z = [\ldots]|_{\partial D} + u(x)$, or

$$u(x) = -[\ldots]|_{\partial D} + \int_D G(z, x)ku(z)\,\mathrm{d}z. \tag{4}$$

This equation corresponds to a Fredholm IEF for the differential problem (1). Notice that Eq. (4) becomes a linear integral equation. The Green's function $G(z, x)$ is computed from the *linear* differential equation (3) with suitable boundary conditions. Notice that if L is self-adjoint, the Green's function problem is simply

$$LG(z, x) = \delta(z - x) \tag{5}$$

and the boundary conditions depend directly from the original system boundary conditions. It should be noticed that, in some sense, the IEF via Green's function can be seen as the inverse of the linear differential operator L.

As commented in the introduction, numerical and analytical procedures have been reported in the literature to deal with the linear integral equation (4). However, the most interesting practical problems are non-linear due to a source term; namely,

$$Lu(x) = f(x, u(x)), \quad x \in D \subset \mathbb{R}^n.$$

In this way, if $f(z, u(z))$ is a linear function, an explicit solution for the boundary-value problem (1) can be obtained. However, if $f(z, u(z))$ is a non-linear function, Eq. (4) is a semi-analytical solution where inversion of operators is carried out only on the linear differential operators. This leads to a non-linear integral equation of the form

$$u(x) = -[\ldots]|_{\partial D} + \int_D G(z, x)f(z, u(z))\,\mathrm{d}z.$$

It is noticed that, in order to obtain an IEF for the boundary-value problem (1), full linearity of the differential equation is not required. Of course, if $f(z, u(z))$ is non-linear, the semi-analytical formulation given by Eq. (4) should be complemented by a suitable numerical scheme to obtain a finite-dimensional (i.e., approximate) solution. As we will show in the following sections, a formulation of Eq. (4) in subdomains leads to standard FD schemes.

3. Statement of the problem

We begin by considering the problem of finding a function $u = u(x)$, $x \in [0, 1]$, which satisfies the following linear