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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

differential equation:

$$u_{xx} = f(u) \tag{6}$$

and mixed boundary conditions

$$u_x(0) = 0 \quad \text{and} \quad u(1) = u_{\text{bulk}}. \tag{7}$$

Here $u_{xx} = \mathrm{d}^2u/\mathrm{d}x^2$. A problem such as this might arise in the study of reaction–diffusion phenomena in a finite slab (Aris, 1975). The data in the model are assumed to be smooth. This means that $f(u)$ is infinitely differentiable. As a consequence of smoothness, there exists a unique function $u = u(x)$ which satisfies the differential equation at every point in the domain as well as the boundary conditions. For $f(u)$ linear in u, is a rather simple task to determine the exact solution. However, in many technical applications, the function is non-linear and a solution can be found in closed form only for some particular cases. Under these circumstances, an approach is to obtain approximate solutions by means of numerical solutions. Here we shall consider approximate solutions under two different schemes; namely, FD and integral-based formulations:

(a) *Finite differences*. Consider a regular grid X_N of size N in the domain $D = [0, 1]$. That is, $X_{N+1} = \{x_0, x_1, \ldots, x_N, x_{N+1}\}$, where $x_j = jh$, $j = 0, \ldots, N+1$, where$h = 1/(N+1)$. For our system, a scheme with central FD for the second-order operator gives

$$\begin{aligned}
&\frac{u_2 - u_1}{h^2} = f(u_1),\\
&\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} = f(u_j), \quad j = 2, \ldots, N-1,\\
&\frac{u_{\text{bulk}} - 2u_N + u_{N-1}}{h^2} = f(u_N),
\end{aligned} \tag{8}$$

where $u_j = u(x_j)$. The result is a set of N non-linear equations that can be solved numerically by means of, e.g., Newton-like methods. The approximation is $\mathrm{O}(h^2)$ and better approximations (i.e., $\mathrm{O}(h^\alpha)$, $\alpha > 2$) are obtained by means of higher-order FD schemes.

(b) *IEF methods*. According to the developments in Appendix A with $x_a = 0$ and $x_b = 1$, one obtains

$$u(x) = u_{\text{bulk}} + \int_0^1 G(z, x) f(u(z))\, \mathrm{d}z. \tag{9}$$

Let $U_{N+2} = (u_0, u_1, \ldots, u_N, u_{N+1})$ be a discrete version for the grid X_{N+1} of the solution $u = u(x)$. If the equality given by Eq. (9) is forced to hold in the grid X_{N+1}, one obtains the following non-linear system:

$$u_j = u_{\text{bulk}} + \int_0^1 G(z, x_j) f(u)\, \mathrm{d}z, \quad j = 1, \ldots, N. \tag{10}$$

Notice that, only the boundary grid points x_0 and x_{N+1} were not considered within the approximation (10) since the Green's function properties force the boundary conditions requirement. Once in this form, similar to FD schemes, system (10) can be solved by existing methods for non-linear systems (Newton-type and direct iteration schemes).

The advantage of FD methods is their strong intuitive flavor that leads to easily implementable algorithms. In fact, FD schemes yield non-linear systems with highly structured Jacobian matrices. For instance, scheme (8) produces a tridiagonal matrix structure that can be exploited for fast matrix inversion. It is known that numerical differentiation can magnify round-off errors. To reduce this adverse effect, numerical schemes based on IEF of the boundary-value problem have been proposed (Mukkavilli et al., 1987bb). Contrary to the FD scheme (8), by virtue of the integration operation, the IEF given by Eq. (10) leads to highly coupled non-linear systems and, hence, to dense Jacobian matrices. On the other hand, FD discretizations of the second-order differential operator are derived from Taylor's series expansions of the underlying function. In this way, it is apparent the absence of a link between the two approximation schemes. In the following section, we will show that, in fact, FD schemes like (8) can be derived from an integral formulation approach. In this way, a Green's function foundation for FD differences schemes is revealed, and potential FD generalizations can be constructed.

4. Subdomain IEF

Consider the following subdomain partition of the domain D with grid $X_{N+1} = \{x_0, x_1, \ldots, x_N, x_{N+1}\}$:

$$D_i = [x_{(i-1)N_s}, x_{iN_s+1}], \quad i = 1, \ldots, M,$$

where M is a divisor of N, and $N_s = N/M$ is the number of internal grid points per subdomain. One has that

(i) $\cup D_i = D$, and
(ii) $D_i \cap D_{i+1} = [x_{iN_s}, x_{iN_s+1}]$.

Item (ii) says that the neighbor subdomain D_i and D_{i+1} are overlapping and share the nodes $x_{(i-1)N_s-1}$ and $x_{(i-1)N_s}$. In fact, $x_{(i-1)N_s}$ is the right boundary of D_i and $x_{(i-1)N_s-1}$ is the left boundary of D_{i+1}. Fig. 1 shows a subdomain partition for $M = 3$ and $N_s = 4$. Notice that the subdomains $D_1 = [x_0, x_{N_s+1}]$ and $D_M = [x_{(M-1)N_s}, x_{N+1}]$ contain left and right boundaries, respectively, the boundaries of the physical domain D. The idea is to pose an integral formulation corresponding to the boundary-value problem (6), (7) in each subdomain. In this way, the boundary condition $u_x(0) = 0$ is inherited by an integral formulation in D_1, and the boundary condition $u(1) = u_{\text{bulk}}$ is assigned to an integral formulation in D_M. This observation leads to the following set of boundary-value problems:

$$\begin{aligned}
&u_{xx} = f(u),\\
&x \in D_1, \quad u_x(0) = 0 \quad \text{and} \quad u(x_{N_s+1}) = u_{N_s+1},\\
&u_{xx} = f(u), \quad x \in D_i, \quad i = 2, \ldots, M-1,\\
&u(x_{(i-1)N_s}) = u_{(i-1)N_s} \quad \text{and} \quad u(x_{iN_s+1}) = u_{iN_s+1},\\
&u_{xx} = f(u), \quad x \in D_M,\\
&u(x_{(M-1)N_s}) = u_{(M-1)N_s} \quad \text{and} \quad u(1) = u_{\text{bulk}}.
\end{aligned} \tag{11}$$

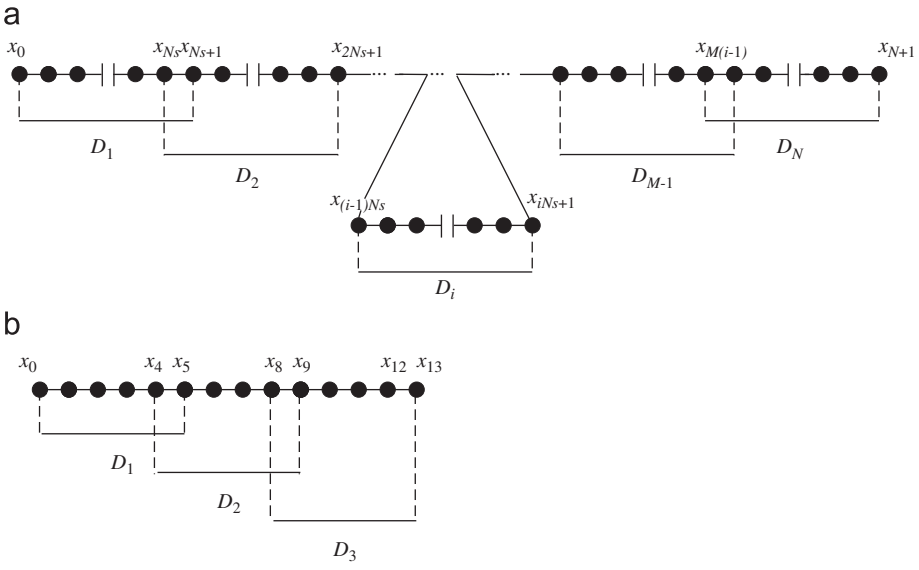

Fig. 1. Example of a subdomain partition with $M = 3$ and $N_s = 4$.

According to the results in Appendix A, the corresponding integral formulations for the above boundary-value problems are the following:

$$
\begin{aligned}
u(x) &= u_{N_s+1} + \int_0^{x_{N_s+1}} G_1(z,x) f(u(z))\,\mathrm{d}z \quad \text{for } x \in D_1,\\
u(x) &= [1 + C_{1,i}(x)]u_{iN_s+1} - C_{1,i}(x)u_{(i-1)N_s}\\
&\quad + \int_{x_{(i-1)N_s}}^{x_{iN_s+1}} G_i(z,x) f(u(z))\,\mathrm{d}z \quad \text{for } x \in D_i \quad \text{and}\\
&\quad i = 2,\ldots,M-1,\\
u(x) &= [1 + C_{1,M}(x)]u_{\text{bulk}} - C_{1,M}(x)u_{(M-1)N_s}\\
&\quad + \int_{x_{(M-1)N_s}}^{1} G_M(z,x) f(u(z))\,\mathrm{d}z \quad \text{for } x \in D_M, \qquad (12)
\end{aligned}
$$

where

$$
\begin{aligned}
G_1(z,x) &= (z-x)H(z-x) - (x_{N_s+1} - x),\\
G_i(z,x) &= (z-x)H(z-x) + C_{1,i}(x)z + C_{2,i}(x)\\
&\quad \text{for } i = 2,\ldots,M, \qquad (13)
\end{aligned}
$$

and the functions $C_{1,i}(x)$ and $C_{2,i}(x)$ are given by

$$
\begin{aligned}
C_{1,i}(x) &= -\frac{x_{iN_s+1} - x}{x_{iN_s+1} - x_{(i-1)N_s}} = -\frac{x_{iN_s+1} - x}{(N_s+1)h},\\
C_{2,i}(x) &= -x_{(i-1)N_s}C_{1,i}(x) \quad \text{for } i = 2,\ldots,M. \qquad (14)
\end{aligned}
$$

The integral formulations in Eq. (12) are satisfied for each x in the corresponding subdomain. The following step is to force Eqs. (12) to be pointwise satisfied at each grid point of the corresponding subdomain. This yields to the following set of non-linear equations:

$$
\begin{aligned}
u_j &= u_{N_s+1} + \int_0^{x_{N_s+1}} G_1(z,x_j) f(u(z))\,\mathrm{d}z \quad \forall j = 1,\ldots,N_s,\\
u_{(i-1)N_s+j} &= \gamma_{1,j}(N_s)u_{iN_s+1} + \gamma_{2,j}(N_s)u_{(i-1)N_s}\\
&\quad + \int_{x_{(i-1)N_s}}^{x_{iN_s+1}} G_i(z,x_{(i-1)N_s+j}) f(u(z))\,\mathrm{d}z\\
&\quad \forall i = 2,\ldots,M-1,\ \ \forall j = 1,\ldots,N_s,\\
u_{(M-1)N_s+j} &= \gamma_{1,j}(N_s)u_{\text{bulk}} + \gamma_{2,j}(N_s)u_{(M-1)N_s}\\
&\quad + \int_{x_{(M-1)N_s}}^{1} G_M(z,x_{(M-1)N_s+j}) f(u(z))\,\mathrm{d}z\\
&\quad \forall j = 1,\ldots,N_s, \qquad (15)
\end{aligned}
$$

where

$$
\begin{aligned}
\gamma_{1,j}(N_s) &= \frac{j}{N_s+1}, \quad j = 1,\ldots,N_s,\\
\gamma_{2,j}(N_s) &= \frac{N_s+1-j}{N_s+1}, \quad j = 1,\ldots,N_s. \qquad (16)
\end{aligned}
$$

Eq. (15) is a system of $N = MN_s$ non-linear equations that should be solved for the N-dimensional vector of unknowns $U_N = (u_1,\ldots,u_N)$. As in the case of FD and global integral formulations described in the above section, the approximate solution U_N can be obtained numerically by means of, e.g., Newton-type or direct iteration procedures. The following comments are in order:

- The overlap of neighbor subdomains is necessary in order to establish an equation for the grid points x_{iN_s+1}, $i = 1,\ldots,M-1$. In fact, an equation cannot be assigned to such grid points under no overlapping because they would not belong to any subdomain interior.

- In the limit as $x_{N_s+1} \to 1$, one has that $M = 1$, $N_s = N$ and the approximate global integral formulation given by Eq. (10) is obtained.
- The global integral formulation in Eq. (10) leads to dense Jacobian matrices. In the case of subdomain integral formulation as in Eq. (15), the Jacobian matrix has an overlapping block-diagonal structure with each block being dense, $(N_s + 2) \times (N_s + 2)$-dimensional and with one-dimensional overlaps. In the limit $N_s = 1$ ($M = N$), the resulting Jacobian matrix has a tridiagonal structure.
- The aim of the subdomain integral formulation is to reduce the influence domain of the propagators $G_i(z, x)$. While in global integral formulation, D is the influence domain of the sole Green's function $G(z, x)$, here the influence domain is almost decoupled into the subdomains D_i's. In principle, this should reduce the propagation of round-off and approximation errors through the whole domain D.

4.1. FD as a limit case of subdomain IEF

Here we will show that the approximation scheme given by Eq. (15) is reduced to a classical FD scheme in the case where $N_s = 1$ or $M = N$. That is, we will analyze the situation where each subdomain has only one interior grid point. In such case, $\gamma_{1,1}(1) = \gamma_{2,1}(1) = 1/2$, resulting in the following set of non-linear equations:

$$u_2 - u_1 = -\int_0^{x_2} G_1(z, x_1) f(u(z))\,\mathrm{d}z, \tag{17}$$

$$u_{j+1} - 2u_j + u_{j-1} = -2\int_{x_{j-1}}^{x_{j+1}} G_j(z, x_j) f(u(z))\,\mathrm{d}z \quad \text{for } j = 2, \ldots, N-1,$$

$$u_{\text{bulk}} - 2u_N + u_{N-1} = -2\int_{x_{N-1}}^{1} G_M(z, x_N) f(u(z))\,\mathrm{d}z.$$

In this stage of the analysis, evaluation of the integrals is required:

(a) Since $G_1(z, x_1) = (z - x_1)H(z - x_1) - (x_2 - x_1) = (z - x_1)H(z - x_1) - h$, one has that

$$G_1(z, x_1) = \begin{cases} -h & \text{for } z \in [0, x_1], \\ (z - x_1) - h & \text{for } z \in [x_1, x_2]. \end{cases}$$

By noticing that $G_1(x_2, x_1) = 0$, the usage of a trapezoidal rule based on the three equidistant points $\{x_0, x_1, x_2\}$ gives

$$-2\int_0^{x_2} G_1(z, x_1) f(u(z))\,\mathrm{d}z \approx \frac{3}{2}h^2 f(u_1). \tag{18}$$

(b) One has that $G_j(z, x_j) = (z - x_j)H(z - x_j) + C_{1,j}(x_j)z + C_{2,j}(x_j)$, for $j = 2, \ldots, N$ and $z \in [x_{j-1}, x_{j+1}]$. It can be shown that in this case $C_{1,j}(x_j) = -1/2$ and $C_{2,j}(x_j) = x_{j-1}/2$. Therefore, $G_j(z, x_j) = (z - x_j)H(z - x_j) + 1/2(x_{j-1} - z)$ for $j = 2, \ldots, N$, or

$$G_j(z, x_j) = \begin{cases} \frac{1}{2}(x_{j-1} - z) & \text{for } z \in [x_{j-1}, x_j], \\ (z - x_j) + \frac{1}{2}(x_{j-1} - z) & \text{for } z \in [x_j, x_{j+1}]. \end{cases}$$

If one notes that $G_j(x_{j-1}, x_j) = G_j(x_{j+1}, x_j) = 0$, the application of the trapezoidal rule on the three equidistant points $\{x_{j-1}, x_j, x_{j+1}\}$ yields

$$-2\int_{x_{j-1}}^{x_{j+1}} G_j(z, x_j) f(u(z))\,\mathrm{d}z \approx h^2 f(u_j) \quad \text{for } j = 2, \ldots, N-1. \tag{19}$$

In this way, the subdomain IEF scheme given by Eq. (17) becomes

$$\frac{u_2 - u_1}{h^2} = \frac{3}{2}f(u_1),$$

$$\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} = f(u_j), \quad j = 2, \ldots, N-1,$$

$$\frac{u_{\text{bulk}} - 2u_N + u_{N-1}}{h^2} = f(u_N), \tag{20}$$

which corresponds to a classical FD scheme (see Eq. (8)) except for the equation corresponding to the next-to-boundary node x_1 where the non-linear function $f(u)$ evaluated at x_1 is weighted by the factor 3/2. Such a weighting factor results from the effects of the Neumann boundary condition $u_x(0) = 0$ reflected in the shape of the Green's function that does not vanish at $x = 0$ (see Fig. 2). In this way, from a Green's function viewpoint, the classical FD scheme given by Eq. (8) underweights the effects of the Neumann boundary conditions by implicitly assuming that the propagator $G_1(z, x)$ vanishes at the boundary. Under such restriction, one recovers the unity weighting factor, and hence the classical FD scheme.

Based on the results of this subsection, the IEF scheme given by Eq. (15) can be considered as a generalized FD scheme where $\gamma_{1,j}(N_s)u_{iN_s+1} - u_{(i-1)N_s+j} + \gamma_{2,j}(N_s)u_{(i-1)N_s}$ is a type of asymmetric approximation for the second-order differential operator, and the integral $-\int_{x_{(i-1)N_s}}^{x_{iN_s+1}} G_i(z, x_{(i-1)N_s+j}) f(u(z))\,\mathrm{d}z$ "collects" the pointwise effects of the non-linear function on the subdomain D_i. Finally, it is apparent from Eq. (20) that three-point FD is the natural approximation for the second-order differential operation u_{xx}. That is, higher-order approximations for such differential operator can be justified only from a Taylor's series expansion standpoint, but not from the intrinsic propagation properties of the underlying Green's functions.

4.2. Numerical results

Some features of subdomain IEF and its convergence to FD scheme will be illustrated in this subsection by using a customized Fortran program. Consider a linear function $f(u) = \phi^2 u$, which can be describing a first-order chemical reaction in a slab with u and ϕ being the concentration and the Thiele

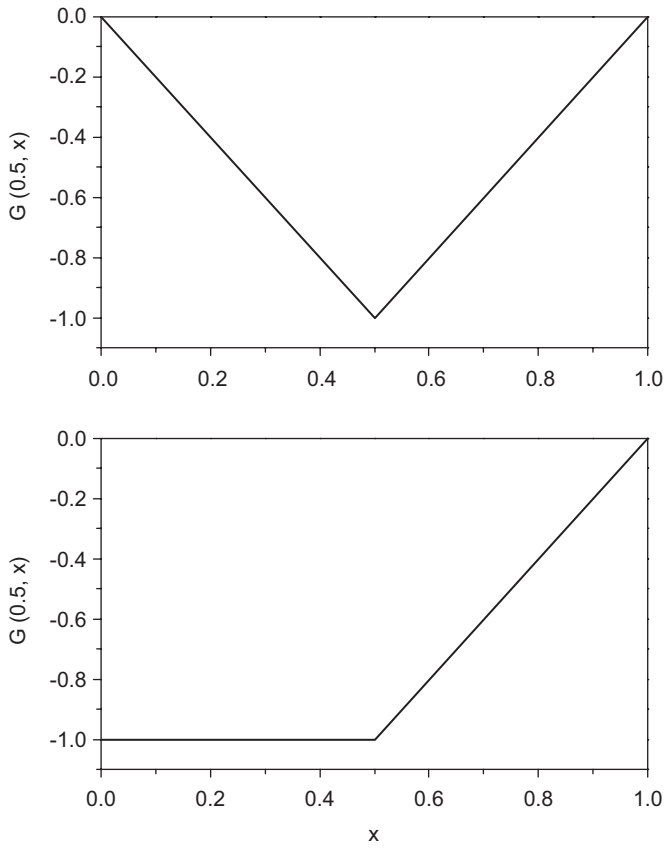

Fig. 2. Green's function for Dirichlet and mixed boundary conditions, for $x_a = 0$, $x_b = 1$ and $z = 0.5$.

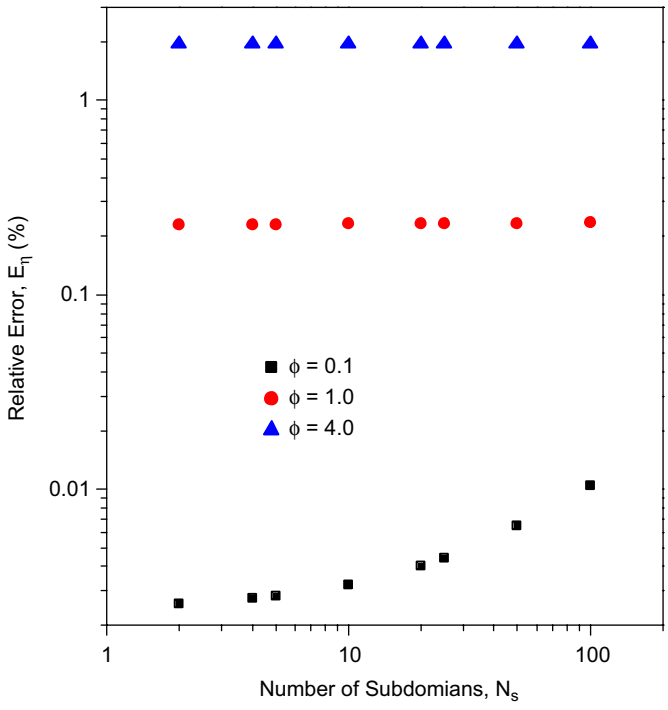

Fig. 3. Relative error as a function of the number of subdomains, for $N = 100$ and three different values of the Thiele modulus.

modulus, respectively. As a single index for measuring approximation errors, we have considered the effectiveness factor η which, in this case, corresponds to the average concentration $\eta = \int_0^1 u(w)\,dw$. It can be shown that, for boundary conditions $u|_{x=1} = 1$ and $u_x|_{x=0} = 0$, $\eta = \tan h(\phi)/\phi$. If η_{ap} is an approximation for η, the relative error is given by $E_\eta = |\eta - \eta_{ap}|/\eta$. Fig. 3 shows the relative error as a function of the number of subdomains, for $N = 100$ and three different values of the Thiele modulus. It is observed that the relative error is almost constant for all values of the number of subdomains, which implies that the domain partition into subdomains preserves the approximation capability of the global IEF. However, as discussed before, the subdomain IEF offers the advantage that the corresponding Jacobian matrix has a block-diagonal structure, and this property can be exploited for more efficient matrix inversion procedures. It is also observed that the approximation error is augmented with the Thiele modulus. This is expected since the corresponding concentration profile is sharper for large values of ϕ, making harder its approximation.

It should be stressed that the subdomain IEF converges to the FD scheme (20) as $N_s \to N$. The only difference with the classical FD scheme is the weighting factor $3/2$ appearing in the equation for the left-hand side boundary. In order to evaluate the effect of such weighting factor, Fig. 4 shows the approximation error E_η as a function of the number of nodes for two different

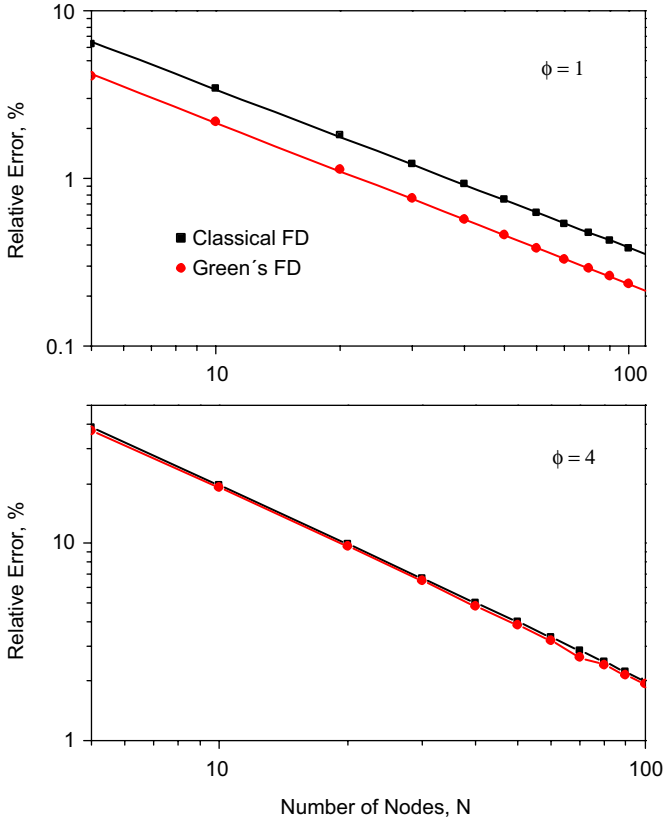

Fig. 4. Approximation error E_η as a function of the number of grid nodes, for two different values of the Thiele modulus.

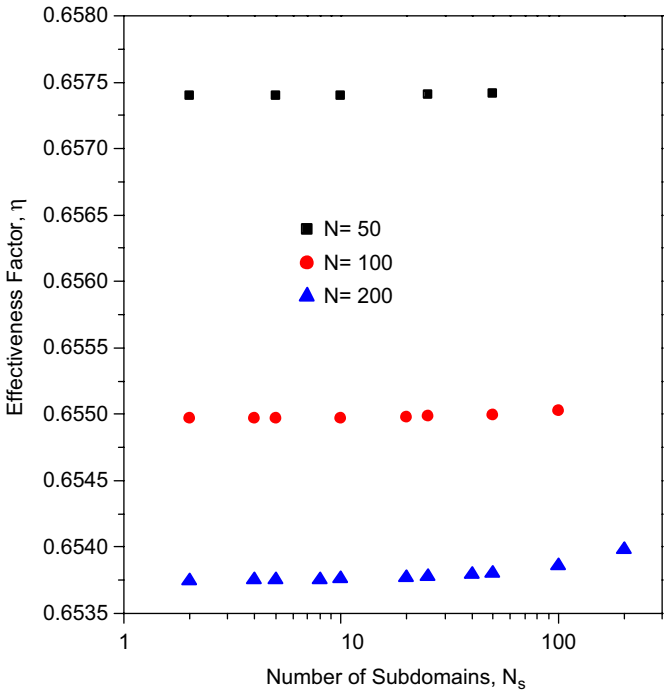

Fig. 5. Effectiveness factor as a function of the number of subdomains, for a second-order reaction rate with $N = 100$ and $\phi = 1$.

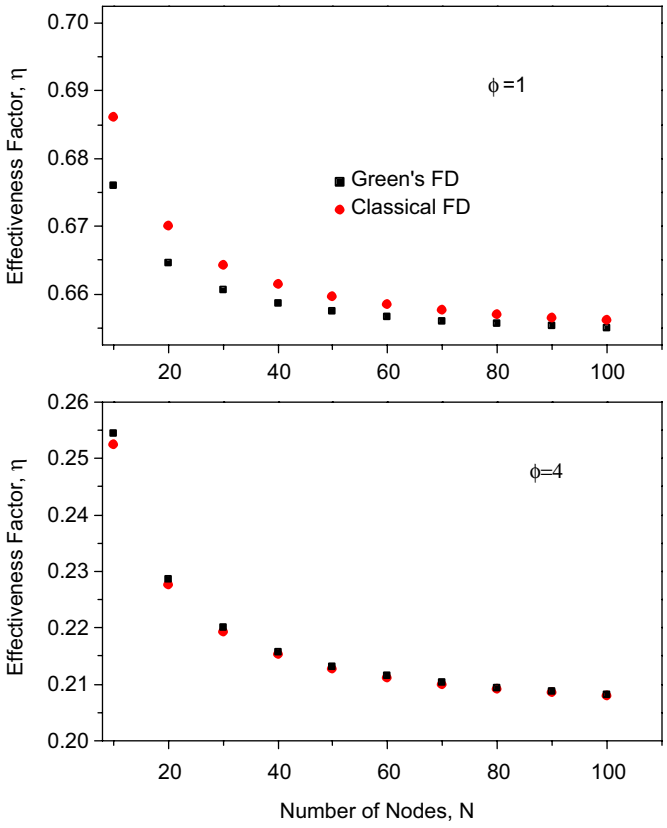

Fig. 6. Effectiveness factor as a function of the number of grid nodes, for a second-order reaction rate and two different values of the Thiele modulus.

values of the Thiele modulus. As expected, the approximation error decreases with the number of computational nodes used, and such decreasing behavior follows a power law with scaling exponent of the order of 0.9 for both the classical and the IEF-based FD schemes. However, the approximation error for the FD scheme with weighting factor is always smaller than that for the classical FD scheme. This shows that the weighting factor $3/2$ has a positive effect on the approximation of the solution $u(x)$ by means of discretization schemes. Such effect is more important for small Thiele modulus values (of the order of 1 and smaller). In fact, for large values of ϕ the concentration profile is sharper in a way that $u(x) \approx 0$ for x's close to the zero-flux boundary. Consequently, the contribution of the nodes close to the boundary where $u_x(0) = 0$ to the average concentration is very small, and both the classical and the IEF-based FD schemes give practically the same approximation.

Now, consider a second-order reaction rate $f(u) = \phi^2 u^2$. Since for this case an analytical solution is not available, we have obtained an estimate of the effectiveness factor using classical FD scheme with $N = 1000$. For $\phi = 1$ and 4, one has that $\eta = 0.6537$ and 0.2079, respectively. For $\phi = 1$, Fig. 5 shows the estimated effectiveness factor as a function of the number of subdomains for three different values of the number of grid points. For $N = 200$, the estimated effectiveness factor has deviations not larger than 0.5% for all values of the number of subdomains. This shows that, even for non-linear reaction rates the FD scheme based on subdomain IEF is stable. Such feature is demonstrated for small values of the number of grid nodes. In fact, it is observed that despite the Green's function formulation has been partitioned into many subdomains, the estimated effectiveness factor displays insignificant variations. As in the linear case, the effect of the weighting factor $3/2$ was also evaluated. For two different values of the Thiele modulus, Fig. 6 shows the variations of the effectiveness factor with the number of nodes, both for Green's based and classical FD schemes. For small values of ϕ, the classical FD scheme overestimates the effectiveness factor converging slower to the "true" one. This effect is less pronounced for larger Thiele modulus where the penetration of the concentration front affects no-flux where $u_x(0) = 0$. These results show that, rather than being effects of non-linearities, the differences between the results from Green's function and classical FD schemes are due to the differences in the propagation structure around the domain boundaries.

5. Concluding remarks

For boundary-value problems, we have shown how FD schemes can be obtained from Green's function formulations. An advantage over the classical FD derivations is that the effect of boundary conditions is naturally incorporated via boundary propagators. Regarding our results and their potential extensions for more involved cases, we have the following comments:

- *Main advantage and drawback*. For Neumann boundary conditions, the resulting FD scheme is different from the classical one for those grid nodes close to the boundary.

Numerical simulations have shown that such slight modifications improve the performance of FD schemes, leading to smaller approximation error for the same number of grid points. A possible drawback of the Green's function approach is that, while derivation of classical FD schemes is now a more or less standard procedure, the present one requires previous analytical work to compute Green's functions. Fortunately, Green's functions are available in the open literature for a wide variety of physical systems of practical interest.

- *Higher dimensional cases*. We have shown that a subdomain IEF for reaction–diffusion equations leads to a FD scheme similar to the classical one. Specifically, the discretization scheme into the system domain agrees with the classical FD discretization. The only difference is a correction at boundaries due to Neumann boundary conditions (see Eq. (20)). Heuristically, extension of the present FD scheme to the high-dimensional case is straightforward; namely, carry out a classical discretization for the system domain and add the correction factor $3/2$ at boundary directions affected by Neumann boundary conditions. However, the issue deserves a more detailed analysis that should be considered in subsequent work.
- *Curvilinear coordinates*. As a first approach, aimed to show a link between FD and IEF, we have constrained to the Cartesian case (see Eq. (6)). Reaction–diffusion equations in cylindrical and spherical coordinates like $(1/x^m)(\mathrm{d}/\mathrm{d}x)(x^m(\mathrm{d}u/\mathrm{d}x)) = f(x,u(x))$, $m = 1$ or 2, $x \in [0,1]$, appear commonly in engineering applications. The question is how the FD scheme derived from IEF can be extended for non-Cartesian cases. Here, the differential operator is

$$L_m = \frac{1}{x^m}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^m\frac{\mathrm{d}}{\mathrm{d}x}\right).$$

  In contrast to the Cartesian case, the operator L_m is not self-adjoint. An alternative to overcome this situation is to compute the formal adjoint differential operator, say L_m^*, associated with L_m. A more practical one is to look for an integration factor $\phi_m(x)$ such that $\mathscr{L}_m = \phi_m(x)L_m$ is self-adjoint. It can be shown that the integration factor is $\phi_m(x) = x^m$, such that $\mathscr{L}_m = \mathrm{d}/\mathrm{d}x(x^m(\mathrm{d}/\mathrm{d}x))$ is actually a linear self-adjoint operator. In this way, the resulting boundary-value problem to be addressed is $\mathscr{L}_m(u(x)) = x^m f(x,u(x))$, and the Green's function problem corresponds to the operator $\mathscr{L}_m = \mathrm{d}/\mathrm{d}x(x^m(\mathrm{d}/\mathrm{d}x))$. From this point, although the procedure involves complex algebraical manipulations, it is possible to arrive to a FD scheme for curvilinear coordinates. The issue is beyond the scope of this paper and results will be reported in a future work.
- *Unsteady-state case*. Consider the boundary-value problem (6) under unsteady-state conditions

$$u_t + au_{xx} = f(u)$$

  with suitable boundary and initial conditions. Under classical FD schemes, spatial coordinates are discretized to arrive to a finite set of ODEs. Eventually, these ODEs are integrated via standard integration methods (e.g., Runge–Kutta). The same procedure can be followed for the IEF-based FD scheme; namely, discretize in spatial coordinates to obtain a finite-dimensional set of ODEs. Although the present FD scheme can give better performance, as has been pointed out in above sections, our contribution relies more on showing a link between classical FD schemes and IEF via Green's functions, rather than on providing more efficient numerical schemes for reaction–diffusion equations.
- *Advection systems*. Equations involving convection phenomena are also treated with FD schemes. However, the case offers important stability issues given the tendency of first-order differential terms to produce numerical instabilities. While stable discretization of diffusion operators are well established, FD schemes for convection operators are commonly made on the basis of heuristic methodologies. For instance, for Cartesian coordinates the heuristic rule is to carry out a backward discretization with respect to the convective flow. An interesting question is whether or not such rule can be backed-up by the Green's function methodology presented in above sections. The main obstacle to tackle the problem is that the combined advection–diffusion operator is not self-adjoint. As in the case of curvilinear coordinates, one can look for an integration factor in order to obtain a modified linear differential operator that be self-adjoint. Although computation of such integration factor is an easy issue, it is apparent that the resulting boundary-value problem for the Green's function (see Eq. (5)) has not an easy analytical solution. As a matter of fact, the availability of an analytical expression for the Green's function is at the heart of the procedure described before. An alternative that is being explored consists in carrying out a partial inversion of the linear differential operator. That is, given that the diffusion operator is self-adjoint, the idea is to invert it to obtain an IEF where the convective operator is incorporated into the integral kernel. In this way, round-off instabilities that are commonly introduced by first-order operators are filtered by virtue of the smoothing integral operation.

Appendix A. Green's functions

Consider the differential equation

$$u_{xx} = f(u), \quad x \in [x_a, x_b],$$

where $u_{xx} = \mathrm{d}^2u/\mathrm{d}x^2$. By using integration by parts, the following integral expression can be obtained:

$$u(x) = -[G(z,x)u_z(z) - G_z(z,x)u(z)]|_{x_a}^{x_b} + \int_{x_a}^{x_b} G(z,x)f(u(z))\,\mathrm{d}z, \tag{A.1}$$

and the Green's function equation is

$$G_{zz}(z,x) = \delta(z-x), x \in [x_a, x_b]. \tag{A.2}$$

Some particular features for imposing boundary conditions and solving Eq. (A.2) depend on the boundary conditions for the differential equation (Beck et al., 1992; Duffy, 2001).

- *Dirichlet boundary conditions*. In this case, the boundary conditions are $u(x_a) = u_a$ and $u(x_b) = u_b$. Notice that the boundary values $u_x(x_a)$ and $u_x(x_b)$ are not available. In this way, the unwelcome terms $[G(z,x)u_z(z)]|_{x_a}^{x_b}$ can be removed from Eq. (A.1) by requiring that the Green's function $G(z,x)$ meets the boundary conditions $G(x_a,x) = 0$ and $G(x_b,x) = 0$. It is not hard to show that the Green's function solutions is

$$G(z,x) = (z-x)H(z-x) + C_1(x)z + C_2(x),$$

where $H(z-x)$ is the Heaviside step function,

$$C_1(x) = -\frac{x_b - x}{x_b - x_a}$$

and

$$C_2(x) = -x_a C_1(x).$$

Notice that $G_z(z,x) = H(z-x)+C_1(x)$, so that $G_z(x_a,x) = C_1(x)$ and $G_z(x_b,x) = 1 + C_1(x)$. This leads to the expression

$$u(x)=C_1(x)u_b-[1+C_1(x)]u_a+\int_{x_a}^{x_b} G(z,x)f(u(z))\,\mathrm{d}z.$$

Notice that $C_1(x) < 0$ and $1 + C_1(x) > 0$.

- *Mixed* (*Dirichlet and Neumann*) *boundary conditions*. The boundary conditions are $u_x(x_a) = 0$ and $u(x_b) = u_b$. Here, the data $u(x_a)$ and $u_x(x_b)$ are unknown, so that the conditions $G_z(x_a,x) = 0$ and $G(x_b,x) = 0$ are imposed. Then, the Green's function solution takes the form

$$G(z,x) = (z-x)H(z-x) - (x_b - x).$$

From this expression, it is possible to show that $G_z(x_b,x) = 1$. Then, the IEF becomes

$$u(x) = u_b + \int_{x_a}^{x_b} G(z,x)f(u(z))\,\mathrm{d}z.$$

The Green's function $G(z,x)$ describes the solution of the boundary-value problem under an impulse (i.e., pointwise) source located at $x = z$. In this way, the solution of the original boundary-value problem with distributed source $f(u(x))$ is given by the collected (i.e., integrated) impulse response $G(z,x)$. In this way, $G(z,x)$ can be seen as a propagator of the pointwise effects. Fig. 2 shows the Green's function for Dirichlet and mixed boundary conditions. Here we have taken $x_a = 0$, $x_b = 1$ and $z = 0.5$. Notice the similarity between the Green's function with $z = 0.5$ and the hat-shaped basis element functions used in finite-elements methods (Becker et al., 1981).

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