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New efficient numerical methods to describe the heat transfer in a solid medium

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ABSTRACT

The analysis of heat conduction through a solid with heat generation leads to a linear matrix differential equation with separated boundary conditions. We present a symmetric second order exponential integrator for the numerical integration of this problem using the imbedding formulation. An algorithm to implement this explicit method in an efficient way with respect to the computational cost of the scheme is presented. This method can also be used for nonlinear boundary value problems if the quasilinearization technique is considered. Some numerical examples illustrate the performance of this method.

1. Introduction

In this work, we consider the numerical integration of the linear matrix differential equation with separated boundary conditions originated by the spatial heat conduction through a solid with local areas of heat generation. Let us denote by z the direction of the heat flow and by Z the total length of the solid medium. If we consider that the flow in other directions is much smaller, the problem can be approximated in one dimension. Then, we define a control volume of length Δz and cross sectional area A, where we can perform an energy balance in order to derive a conservation equation for thermal energy in terms of temperature. This analysis leads to a boundary value problem (BVP) which describes the temperature along the length of the body in the direction of the flow, see [1]. After rescaling $t = z/Z$, the non-autonomous and non-homogeneous BVP is given by

$$\left.\begin{array}{l} T''(t) + p(t)T'(t) + q(t)T(t) = f(t); \\ K_{11}T(0) + K_{12}T'(0) = \gamma_1, \qquad K_{21}T(1) + K_{22}T'(1) = \gamma_2 \end{array}\right\} \tag{1}$$

where $T(t)$ is the temperature, $f(t)$ is the heat generation, and $p(t)$, $q(t)$ are the advection and convection coefficients, respectively, that can depend on the local position t and its cross section A at this point. The first term in the equation corresponds to the conduction in the direction of flow. With appropriate coefficients and boundary conditions, the system (1) describes also a material process in which a solid body is moving out of a hot region and the heat flow is mainly oriented towards the direction of the motion of the body, like a long slab of steel emerging from a furnace or a metal rod undergoing continuous hardening, for example, see [2] for details.

On the other hand, it is known that many relevant engineering problems can be modelled by a second order nonlinear differential equation, say

$$T'' = f(t, T, T'), \quad 0 \le t \le 1,$$

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subject to similar linear boundary conditions as in (1). Nonlinear BVPs can be numerically solved by quasilinearization. It reduces to solving iteratively the following problems for the unknown function $T_{n+1}(t)$ under the assumption that $T_n(t)$ is known:

$$T''_{n+1} - \left(\frac{\partial f}{\partial T'}\right)_n T'_{n+1} - \left(\frac{\partial f}{\partial T}\right)_n T_{n+1} = F(t, T_n(t), T'_n(t))$$

subject to boundary conditions

$$K_{11}T_{n+1}(0) + K_{12}T'_{n+1}(0) = \gamma_1, \qquad K_{21}T_{n+1}(1) + K_{22}T'_{n+1}(1) = \gamma_2,$$

where $T_0(t)$, $T'_0(t)$ correspond to an initial guess, and $\left(\frac{\partial f}{\partial T'}\right)_n$, $\left(\frac{\partial f}{\partial T}\right)_n$ denote the derivatives where the functions $T(t)$, $T'(t)$ are substituted by $T_n(t)$, $T'_n(t)$, and

$$F = f - \left(\frac{\partial f}{\partial T'}\right)_n T'_n - \left(\frac{\partial f}{\partial T}\right)_n T_n.$$

This linear BVP is solved repeatedly until convergence (e.g. given a tolerance, ϵ, the iteration is repeated until $\max_{0<t<1} |T_{n+1}(t) - T_n(t)| < \epsilon$). The solution obtained is a second order approximation of the nonlinear BVP.

This quasilinearization technique is, in practice, one of the recommended approaches of implementation because it leads to a modular program design. Once we have a program module to solve linear problems with a given method, it can be invoked repeatedly for each iteration of a nonlinear problem by first linearizing it [3].

This work is addressed to building an algorithm for linear problems which are difficult to solve from the numerical point of view. In particular, we are interested in stiff problems. In those cases, standard explicit methods usually suffer from stability problems and are useless. Implicit methods are, however, computationally expensive and the use of variable time steps is a more challenging task. We consider explicit methods using the imbedding formulation. This requires us to numerically solve a set of non-homogeneous and non-autonomous linear IVPs forward and backward in time. We are interested in symmetric second order methods since they are appropriate for solving the nonlinear BVPs and, if a very high accuracy is desired, the extrapolation technique can also be used. We present symmetric second order exponential integrators which show a high performance for these problems. The scheme proposed can also be trivially used with a variable time step as well as in those cases where the functions $p(t)$, $q(t)$ and $f(t)$ are only known on a given mesh.

2. The matrix boundary value problem

In order to address the problem (1), we consider the numerical integration of a general linear two point boundary value problem of the form

$$\mathbf{y}'(t) = S(t)\mathbf{y}(t) + \mathbf{h}(t); \qquad B_0\mathbf{y}(0) = \gamma_1, \qquad B_1\mathbf{y}(1) = \gamma_2; \quad 0 \le t \le 1. \tag{2}$$

Here $\mathbf{y}(t)$, $\mathbf{h}(t) \in \mathbb{C}^n$, $S(t) \in \mathbb{C}^{n\times n}$, $B_0 \in \mathbb{C}^{p\times n}$, $B_1 \in \mathbb{C}^{q\times n}$, $\gamma_1 \in \mathbb{C}^p$, $\gamma_2 \in \mathbb{C}^q$, with $p + q = n$, and we assume that $\operatorname{rank}(B_0) = p$ and $\operatorname{rank}(B_1) = q$. We consider the case $q \le p$ because the case $p < q$ can be treated in a similar way. Notice that the limit cases $p = 0$ or $q = 0$ correspond to initial and final value problems respectively. Let us denote

$$\mathbf{y}(t) = \begin{bmatrix} \mathbf{y}_1(t) \\ \mathbf{y}_2(t) \end{bmatrix}, \qquad S(t) = \begin{bmatrix} A(t) & B(t) \\ C(t) & D(t) \end{bmatrix}, \qquad \mathbf{h}(t) = \begin{bmatrix} \mathbf{f}_1(t) \\ \mathbf{f}_2(t) \end{bmatrix}.$$

Note that problem (1) corresponds to the particular scalar case when $y_1(t) = T(t)$, $y_2(t) = T'(t)$, $A(t) = 0$, $B(t) = 1$, $C(t) = -q(t)$, $D(t) = -p(t)$, $f_1(t) = 0$ and $f_2(t) = f(t)$, $B_0 = [K_{11} \;\; K_{12}]$, $B_1 = [K_{21} \;\; K_{22}]$. For stiff problems it is convenient to consider the imbedding formulation which we briefly introduce. Let us consider the change of variables

$$\mathbf{y}(t) = Z(t)\mathbf{w}(t) = \begin{bmatrix} I_p & X \\ 0 & I_q \end{bmatrix} \begin{bmatrix} \mathbf{w}_1(t) \\ \mathbf{w}_2(t) \end{bmatrix}. \tag{3}$$

By the imbedding formulation [4,5], the two-point boundary value problem can be replaced by a set of initial value problems (IVPs). This procedure leads to a matrix Riccati differential equation (RDE) that is coupled with other equations. Thus, in the same way as in [5], the original BVP can be solved as follows:

(I) Solve, from $t = 0$ to $t = 1$, the IVPs

$$X'(t) = B(t) + A(t)X(t) - X(t)D(t) - X(t)C(t)X(t), \qquad X(0) = -K_{11}^{-1}K_{12}.$$

(II) Taking into account (3) and the initial condition of the step **I**, solve, from $t = 0$ to $t = 1$, the $\mathbf{w}_1$-equation

$$\mathbf{w}'_1(t) = [A(t) - X(t)C(t)]\mathbf{w}_1(t) - X(t)\mathbf{f}_2(t) + \mathbf{f}_1(t); \qquad \mathbf{w}_1(0) = K_{11}^{-1}\gamma_1.$$

(III) Next, solve from $t = 1$ to $t = 0$, the $\mathbf{w}_2$-equation

$$\mathbf{w}'_2(t) = [D(t) + C(t)X(t)]\mathbf{w}_2(t) + C(t)\mathbf{w}_1(t) + \mathbf{f}_2(t),$$

with the starter final condition $[K_{21}X(1) + K_{22}]\mathbf{w}_2(1) + K_{21}\mathbf{w}_1(1) = \gamma_2$.

(IV) Finally, recover $\mathbf{y}(t) = Z(t)\mathbf{w}(t)$, with $Z(t)$ given by (3).

3. Exponential integrators for the matrix RDE

From [6], in a simple way, the study of our matrix RDEs reduces to the study of the IVP

$$Y'(t) = \begin{bmatrix} V'(t) \\ W'(t) \end{bmatrix} = S(t)Y(t), \qquad Y(0) = \begin{bmatrix} X_0 \\ I_q \end{bmatrix}, \qquad S(t) = \begin{bmatrix} A(t) & B(t) \\ C(t) & D(t) \end{bmatrix} \tag{4}$$

with $Y \in \mathbb{C}^{n\times q}$ and $S \in \mathbb{C}^{n\times n}$. Then, the solution of the RDE is given by $X(t) = V(t)W^{-1}(t)$, with $V \in \mathbb{C}^{p\times q}$, $W \in \mathbb{C}^{q\times q}$, in the region where $W(t)$ is invertible. If $W(t)$ has no inverse in some point of the interval $[0, 1]$, the error for $X(t)$ will cause large errors in $\mathbf{w}_1$ and $\mathbf{w}_2$ which are then propagated, leading to large errors for the solutions $\mathbf{y}_1$ and $\mathbf{y}_2$, because the equations are coupled. However, this problem can be solved easily by covering the interval $[0, 1]$ by a finite set of intervals where the problem can be reformulated with appropriate permutation matrices, see Lemma 3.1 of [5] for more details. This multiple imbedding implies that for each subinterval one has to solve a different linear differential equation where the inverse of the matrix appearing in (4) is far from being singular.

Now, let us present an explicit symmetric second order Lie group integrator to solve (4) numerically. If we denote by $\Phi(t, t_0)$ the fundamental solution of (4), then

$$\exp\left(\int_t^{t+h} S(t)\mathrm{d}t\right) = \Phi(t+h, t) + \mathcal{O}(h^3)$$

corresponds to the first order approximation (second order in the time step, h) for most exponential methods like e.g. the Magnus, Fer or Wilcox expansions, see [7] and the references therein for details. Here, it suffices to approximate the integral by a second order symmetric rule, like the trapezoidal rule so

$$\Psi(t+h, t) \equiv \exp\left(\frac{h}{2}(S(t+h) + S(t))\right) = \Phi(t+h, t) + \mathcal{O}(h^3).$$

The non-homogeneous problem can be treated in a similar way.

4. Solving the thermal energy equation

Applying the exponential integrator method presented in the above section to our system of coupled IVPs presented at the end of Section 2, we obtain

$$\begin{bmatrix} W_{n+1} \\ V_{n+1} \end{bmatrix} = \exp\left(\frac{h}{2}(S(t_{n+1}) + S(t_n))\right) \begin{bmatrix} W_n \\ V_n \end{bmatrix} \Rightarrow X_{n+1} = V_{n+1}W_{n+1}^{-1}$$

where $X_n = X(t_n) + \mathcal{O}(h^3)$, $t_n = nh$. In this way, the matrix functions $A(t_n)$, $B(t_n)$, $C(t_n)$, $D(t_n)$ are computed at the same mesh points as the approximations X_n to $X(t_n)$. The second step is the integration of the $\mathbf{w}_1$-equation by a symmetric second order exponential integrator for non-homogeneous linear equations

$$\mathbf{w}_{1,n+1} = \exp\left(\frac{h}{2}(A_{n+1} + A_n - X_nC_n - X_{n+1}C_{n+1})\right)\left(\mathbf{w}_{1,n} + \frac{h}{2}\mathbf{g}_n\right) + \frac{h}{2}\mathbf{g}_{n+1},$$

where $\mathbf{g}_n = -X_n\mathbf{f}_{2,n} + \mathbf{f}_{1,n}$. Next, we approximate the non-homogeneous $\mathbf{w}_2$-equation backward in time by

$$\mathbf{w}_{2,n} = \exp\left(\frac{-h}{2}(D_{n+1} + D_n + C_nX_n + C_{n+1}X_{n+1})\right)\left(\mathbf{w}_{2,n+1} - \frac{h}{2}\mathbf{h}_{n+1}\right) - \frac{h}{2}\mathbf{h}_n,$$

where $\mathbf{h}_n = C_n\mathbf{w}_{1,n} + \mathbf{f}_{2,n}$. Finally, the solution given by $\mathbf{y}(t) = (\mathbf{w}_1(t) + X(t)\mathbf{w}_2(t), \mathbf{w}_2(t))$, is approximated at the mesh points $t_i = t_0 + ih,\ i = 0, 1, \ldots, N$, by $\mathbf{y}_{1,n} = \mathbf{w}_{1,n} + X_n\mathbf{w}_{2,n}$, $\mathbf{y}_{2,n} = \mathbf{w}_{2,n}$, $n = 0, 1, \ldots, N$. A variable step procedure can also be used.

Let us now consider some numerical examples to compare the performance of this new algorithm with respect to the results obtained by finite differences on some problems where explicit shooting methods are badly conditioned and cannot be used.

Example 4.1 (*Radiation Fin of Trapezoidal Profile*)**.** The temperature distribution associated to a radiation fin in a one-dimensional form of the energy equation is given by [1]

$$\frac{\mathrm{d}^2T}{\mathrm{d}R^2} + \left(\frac{1}{R+\rho} - \frac{\tan\alpha}{(1-R)\tan\alpha + \theta}\right)\frac{\mathrm{d}T}{\mathrm{d}R} - \frac{\beta T^4}{(1-R)\tan\alpha + \theta} = 0 \tag{5}$$

for $0 \le R \le 1$, and boundary conditions $T(0) = 1,\ T'(1) = 0$. Here, α, β, ρ and θ are parameters which depend on the temperature at the boundary, the emissivity of the fin, Planck's constant, the heat conductivity, the radius of the base and the tip, and the angle of inclination of the top surface (see [1, page 86]). We consider the following values: $\alpha = 30°$, $\beta = 0.2$,

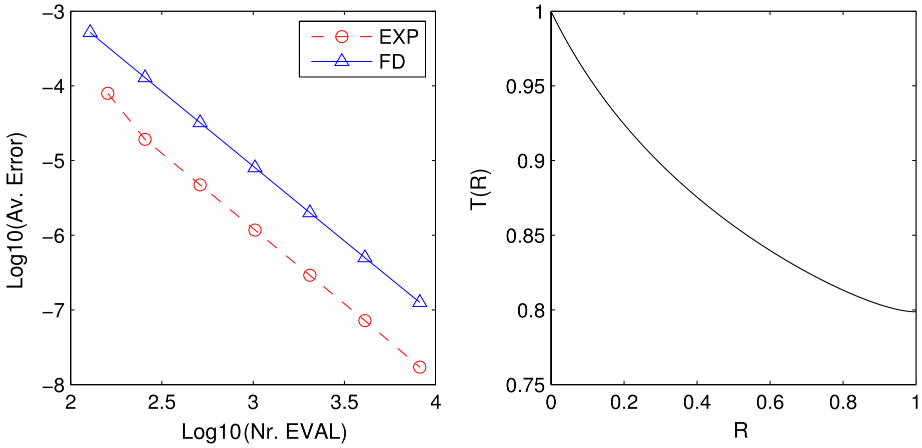

Fig. 1. Left panel: average error versus the number of evaluations for the finite differences (FD) and the exponential integrator when considering the imbedding formulation (EXP). Right panel: Solution, $T(R)$, of the nonlinear BVP (5).

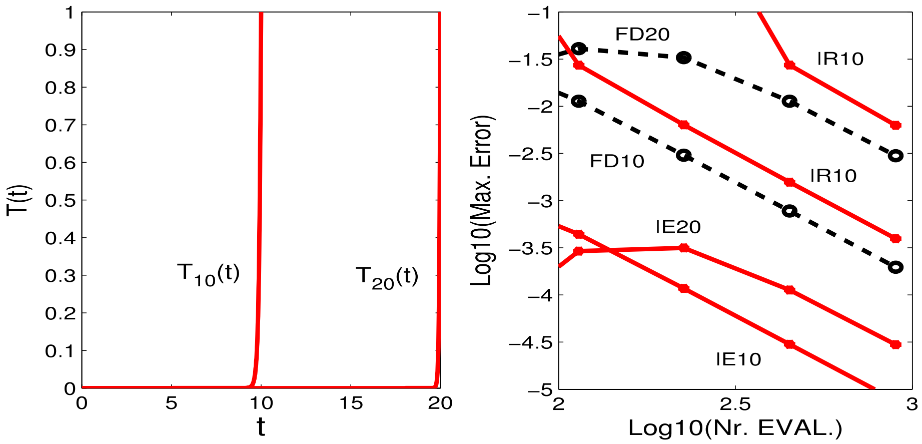

Fig. 2. Left panel: solution, $T_b(t)$, of the problem (7) for $b = 10$ and $b = 20$. Right panel: maximum error, in logarithmic scale, versus the number of evaluations for the following second order time-symmetric methods: finite differences (FDb) and the exponential integrator (IEb) and Runge–Kutta with the trapezoidal rule (IRb) when considering the imbedding formulation.

$\rho = 0.25, \theta = 0.05$, which correspond to a not very stiff problem. The corresponding linearized equation is given by the recursive scheme

$$T''_{n+1} + \left(\frac{1}{R+\rho} - \frac{\tan\alpha}{C(R)}\right)T'_{n+1} - \frac{4\beta T_n(R)^3}{C(R)}T_{n+1} = -\frac{3\beta T_n(R)^4}{C(R)} \tag{6}$$

with $C(R) = (1-R)\tan\alpha + \theta$, and the boundary conditions: $T_{n+1}(0) = 1$, $T'_{n+1}(1) = 0$. At each iteration we solve the non-autonomous and non-homogeneous linear BVP (6). The function $T_n(R)$ is known in a mesh (for simplicity, we take an equispaced mesh, but an adaptive mesh can also be used) and then we use both the second order finite difference method adapted to the matrix linear problem (2) and the second order exponential method. This way provides new solutions for $T_{n+1}(R)$ at the same mesh. The iteration stops when we reach convergence (to compare $T_{n+1}(R)$ with $T_n(R)$ on the mesh) and this solution corresponds to a second order (in the time step) approximation. We consider as the exact solution the numerical solution obtained using a very small time step. Fig. 1 shows the results obtained. For this non-stiff problem the imbedding formulation with the exponential method is still superior to finite differences.

Example 4.2. Let us now consider a homogeneous problem where the convection is proportional to the local temperature and grows with the time. Let us consider also that the solid is a flat plate and then, by [1], the coefficient $p(t) = 0$. In particular, we consider the following thermal energy equation:

$$T''(t) = (1+t^2)T(t); \qquad T(0) = 0, \qquad T(b) = 1; \quad 0 \le t \le b. \tag{7}$$

The solution of this problem is $T(t) = e^{t^2/2}(C_1 + C_2\, erf(t))$ with appropriate values of the constants C_1, C_2, and then, for large values of b, the problem is very stiff (standard explicit shooting methods fail to solve this problem for $b > 9$ [4]). In Fig. 2 we show the solution for $b = 10$ and $b = 20$.

We compute the maximum error of the solution on the mesh for different values of the time step (a constant time step is used for the comparison, but a variable time step could be used for the exponential integrators in the imbedding formulation). We compare the results obtained by the second-order finite difference method (FDb) and the exponential integrator in the imbedding formulation (IEb) for an integration until the final time b. To show the interest of the exponential methods for the integration of the IVPs, we repeated the computation in the imbedding formulation, but the exponential method is replaced by the implicit trapezoidal Runge–Kutta method (IRb). In Fig. 2 we show the results obtained for $b = 10$ and $b = 20$. The superiority of the imbedding formulation is manifest (but only when the IVPs are solved using the exponential integrator) and it increases with the final time b. This relative performance of the exponential method increases when the extrapolation technique is used to increase the order of accuracy of all methods.

We have presented a simple time-symmetric exponential integrator for BVPs in the imbedding formulation. This formulation is of interest for stiff problems and the methods proposed can be easily used for solving nonlinear BVPs when the quasilinearization technique is used. The numerical examples illustrate the interest of this technique and clearly show its superiority when the problem is very stiff.

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