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Explicit Stable Methods for the Initial Value Problem for 2^{nd}-Order Parabolic Systems

Nedžad Limić * and Mladen Rogina†

Abstract. A class of numerical methods for ODE which are explicit, absolutely stable, and of any order of convergence, is constructed. Methods can be efficiently applied to those initial value problems for the 2^{nd}-order parabolic system which have solutions with finite L_1-norms. Numerical procedure consists of two basic steps. The space discretizations of elliptic operator must have compartmental structure, and the resulting ODE are solved by constructed numerical methods.

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1. Introduction

A class of numerical methods for the initial value problem for the 2^{nd}-order parabolic system is proposed and analyzed. Methods are explicit, unconditionally stable and of any convergence order. Methods are applicable only to L_1-theory of the initial value problem for the 2^{nd}-order parabolic system. In this article the case of parabolic systems on $\mathbb{R}^d$ is considered although methods are applicable as well to problems on bounded domains. The crucial step of construction is the space discretization of elliptic operator so that its matrix approximations have the compartmental structure. In this way the initial problem is approximated by a sequence of ODE. After the compartmental structure of approximations is gained, methods are defined by approximating the evolution operators of ODE in terms of rational functions with positive terms. The numerator is a polynomial of non-negative matrix valued functions with positive coefficients and the denumerator is the corresponding polynomial of l_1-norms. In turn, such expressions ensure unconditional stability of approximations.

In the second section the mentioned class of methods for ODE is constructed and error bounds are obtained. The basic results regarding the mentioned class of methods for ODE are described in Proposition 1.. In the third section an algorithm for nonhomogeneous ODE is described. In the fourth section conditions on coefficients of elliptic operator are given ensuring solutions in $L_1(\mathbb{R}^d)$. Then it is shown how finite

*Department of Mathematics, University of Zagreb, Bijenička cesta 30, 10000 Zagreb, Croatia, e–mail: nlimic@math.hr

†Department of Mathematics, University of Zagreb, Bijenička cesta 30, 10000 Zagreb, Croatia, e–mail: rogina@math.hr

element techniques can be combined with developed methods for ODE in order to solve numerically 2^{nd}-order parabolic systems.

2. A class of explicit and stable methods for homogeneous ODE

A class of numerical schemes for the initial value problem for a system of ordinary differential equations (ODE) is considered in this section. The system is defined by:

$$\begin{aligned} \frac{d}{dt}v(t) &= A(t)v(t), \\ v(0) &= v_0, \end{aligned} \tag{1}$$

where $v(\cdot)$, $f(\cdot)$ are column valued functions on $[0,\infty)$ of a finite or infinite dimension. Obviously, the column v_0 has the same dimension. The index set of their elements is denoted by J. The matrix valued function $A(\cdot)$ must have a particular structure:

Assumption 2..1 *The matrix-valued function $A(\cdot) = \{a_{ij}(\cdot)\}_{JJ}$, indexed by the set J, has continuous matrix elements on $[0,\infty)$ with the properties:*

(a) $a_{ii}(t) \leq 0$, *for all* $i \in J$, $t \geq 0$,

(b) $a_{ij}(t) \geq 0$, *for all* $i, j \in J$, $i \neq j$, $t \geq 0$,

(c) $a_j(t) = \sum_i a_{ij}(t) \leq 0$ *for all* $j \in J$, $t \geq 0$.

A matrix with prescribed properties is called a *matrix with the compartmental structure*. If the functions a_j are zero for all $j \in J$ the matrix valued function $A(\cdot)$ is called *conservative*. There is a simple result [Ta] concerning solutions of (1). Let q be a positive and measurable function on $[0,\infty)$, bounded on bounded intervals of $[0,\infty)$, such that $|a_{ii}(t)| \leq q(t)$. Then the matrix valued function $A(\cdot)$ generates an evolution family of matrices $Q(t,s), t, s \in [0,\infty)$ such that

$$\| Q(t,s) \|_1 \leq 1, \quad 0 \leq s \leq t < \infty,$$

where $\| \cdot \|_1$ is the l_1-norm. In case of conservative generator $A(\cdot)$ the equality $\| Q(t,s) \|_1 = 1$ is valid.

The matrix $A(t)$ can be represented as $A(t) = D(t) + B(t)$, where $D(t)$ is a diagonal matrix with diagonal elements $a_{ii}(t)$, and $B(t)$ is a matrix with nonnegative elements and zero diagonal elements. It is easy to describe the schemes for matrices A satisfying Assumption 2..1 and having all diagonal elements equal. First we consider the case of t-independent matrices so that $a_{ii} = -p$. Let τ be increment in time, and $t_m = m\tau$, $m = 0, 1, ...$ Let v_m be the approximations of $v(t_m)$. For t-independent A, the approximations of order L are defined by:

$$v_m = V_L(\tau)v_{m-1}, \quad m \in \mathbb{N}, \quad V_L(\tau) = P_L(\tau,p)^{-1} P_L(\tau,B),$$

where the polynomial $P_L(\tau,x)$ of order L is equal to the first $L+1$ terms of expansion of $x \to \exp(\tau x)$, i.e. $P_L(\tau,x) = \sum_{r=0}^{L} \tau^r x^r / r!$. The l_1-matrix norm of the numerator

$P_L(\tau, B)$ is not larger than the norm of denominator, so that $\|V_L(\tau)\|_1 \leq \exp(-\kappa\tau)$, where $\kappa = inf_i\ |a_i|$. The order of convergence is L, as follows from the corresponding local error bounds:

$$\|v_m - v(t_m)\|_1 \leq \|V_L(\tau)\|_1 \|v_{m-1} - v(t_{m-1})\|_1 + \frac{2(p\tau)^{L+1}}{(L+1)!}\|v(t_{m-1})\|_1.$$

If all $a_i = 0$, then $\|v_m\|_1 = \|v_0\|_1, \quad m \in \mathbb{N}$. The matrix $V_L(\tau)$ is obviously an approximation of $Q(\tau, 0)$ of the order $L+1$.

An extension to t-dependent matrices $A(\cdot)$ is simple. Let

$$A(t) = -p(t)I + B(t),$$

where both, p and matrix elements of B, are smooth enough, so that integration formulæ, to be used in proceeding construction, have desired error bounds. Let $W(t,s)$ be the evolution family generated by $B(\cdot)$. In the proposed generalization the matrix $Q(m\tau, (m-1)\tau)$ is approximated by the ratio in which the numerator approximates $W((m-1)\tau, m\tau)$ and the denominator approximates the corresponding function of p. In the first step of construction the numerator contains the first $L+1$ terms of expansion of $W((m-1)\tau, m\tau)$ and the denominator must contain the corresponding $L+1$ terms of expansion of exponential function having the integral of p in the exponent. In the second step of construction each term of expansion must be approximated by an integration formula, with an error bound of the order $L+1$. So obtained numerator and denominator are denoted by $X_L(\tau, m, B)$ and $X_L(\tau, m, p)$, respectively. The sequence

$$v_m = V_L(\tau, m) v_{m-1}, \quad V_L(\tau, m) = X_L(\tau, m, p)^{-1}\, X_L(\tau, m, B), \tag{2}$$

obtained in this way, converges to the solution of (1) with the order L. For lower order convergence integration formulæ are simple. The third order scheme is defined by the third degree polynomial:

$$\begin{aligned} X_3(\tau, m, g) \ = \ 1 + \frac{\tau}{6}\Big[g(t_b) + 4g(t_m) + g(t_e)\Big] + \\ \frac{\tau^2}{12}\Big[g(t_e)g(t_b) + g(t_e)^2 + 2g(t_m)^2 + 2g(t_m)g(t_b)\Big] + \frac{\tau^3}{6} g(t_e)g(t_m)g(t_b), \end{aligned} \tag{3}$$

where t_b, t_m and t_e are the beginning, midpoint and endpoint of the interval $[(m-1)\tau, m\tau]$, respectively. In order to apply the scheme to non-commuting matrices $B(t), t \in [0, \infty)$, the order of factors $B(t)$ must be respected.

If the diagonal elements (functions) a_{ii} of A are not mutually equal, the proposed schemes can be used after a slight adjustment. Let $[0, T]$ be the interval of interest. It is assumed that there exists a continuous function p on the considered interval such that $p(t) \geq -a_{ii}(t)$ for all i, and $t \in [0, T]$. After splitting $A(t) = -p(t)I + B(t)$ the proposed schemes can be used. Obviously, the matrix valued function $B(\cdot)$ has nontrivial diagonal elements. It is clear that the optimal error is achieved by choosing the function p as small as possible. Apparently, the best estimate is obtained when all the diagonal elements are mutually equal.

In order to apply integration formulae to the scheme (2) optimally, it is useful to assume that the following error estimates are valid:

$$\begin{aligned} \sup_{0\le m\le K} \, |Z_L(\tau,m,p) \, - \, X_L(\tau,m,p)| \;&\le\; \tau^{L+1}\,\alpha(L,p), \\ \sup_{0\le m\le K} \, \|Z_L(\tau,m,B) \, - \, X_L(\tau,m,B)\|_1 \;&\le\; \tau^{L+1}\,\beta(L,B), \end{aligned}$$

where the error bounds α and β are τ-independent. It has to be pointed out that the error bounds α and β are equal to zero for t-independent matrices A.

To write expressions as briefly as possible we use the following notation:

$$|p|_T = \sup\{|p(t)| \, : \, t\in[0,T]\}, \qquad \mu_T = \inf\{|p(t)| \, : \, t\in[0,T]\}.$$

Apart from this we need a magnitude of oscillation over intervals $I(r) = [(r-1)\tau, r\tau]$,

$$|\Delta p|_T \;=\; \max_{r\le K}\Big\{\max\{p(t) \;:\; t\in I(r)\} \;-\; \min\{p(t) \;:\; t\in I(r)\}\Big\}.$$

The convergence of numerical schemes (2) to solutions of (1) is described by the next result.

Proposition 1. *Let the interval* $[0,T]$ *be discretized by* $t_k = k\tau$, $k = 0,1,\ldots,K$, *where* $\tau = T/K$.

(i) Then $\|V_L(\tau,m)\|_1 \le 1$, *and* $\|V_L(\tau,m)\|_1 = 1$ *for conservative* $A(\cdot)$.

(ii) Let $Q(t,s)$ *be the evolution family associated with (1). Then*

$$\begin{gathered} \big\|\, Q(T,0) \;-\; V_L(\tau,K)V_L(\tau,K-1)\,\cdots\,V_L(\tau,1)\,\big\|_1 \;\le \\ \tau^L\,\frac{2T|p|_T^{L+1}}{(L+1)!}\,\exp\left(\tau\,|\Delta p|_T\right) \;+\; \tau^L\,\frac{T(\alpha(L,p)+\beta(L,B))}{\exp(\tau\,\mu_T)}. \end{gathered} \tag{4}$$

An implementation of the method (2) essentially reduces to an efficient implementation of the multiplication of matrix with column. This fact must be manifested as an advantage for problems with sparse stiffness matrices having a larger band as demonstrated in the second example.

Example 1. To demonstrate the method the initial value problem (1) is solved with the t-independent matrix $A = -2I + I_- + I_-$, of the order $n = 10000$, where $I_\pm$ are the first off-diagonals. The problem is solved numerically on the interval $[0,1]$ with the time increment $\tau = 10^{-3}$. The system is solved by the method (2) with $L = 3$ (expression (3)) and Euler implicit method. The method (2) is slightly faster and the ratio of computing times is 0.73.

Example 2. The function

$$u(t,x_1,x_2) \;=\; \exp(\,-\,\pi^2\sigma^2 t\,)\; sin(\pi x_1) sin(\pi x_2)$$

is a solution of the parabolic initial value problem with the elliptic operator $A = (\sigma^2/2)\Delta$ on $D = (0,1) \times (0,1)$, and the homogeneous Dirichlet boundary conditions. In this example the following values of parameters are taken, $\sigma^2 = 0.1/\pi^2, t = 1$. This boundary value problem is numerically approximated in the usual way choosing the grid-step $h = 2^{-6}$. The resulting ODE (1) is solved by the method (2) with $L = 3$ and Euler implicit method with various time increments, $\tau = 1/K$, $K = 100, 300, 500$. Algebraic systems appearing in Euler method, defined by band matrices, are solved by Gaussian eliminations without pivoting. The ratios of computing times of the two methods are given in Table 1. All calculations were carried out in double precision, with the same level of optimization, on SUN-SPARC (Ultra-Enterprise). The error bounds (4) are given in the last row of Table.

Table 1. Ratio of computing times

K	*100*	*300*	*500*
$\dfrac{tim((3))}{tim(Eul.meth.)}$	*1.29E-03*	*1.33E-03*	*.34E-03*
$\varepsilon(3,\tau)$	*0.2208E+00*	*0.4670E-02*	*0.9019E-03*

Apparently, the efficiency of method (3) is emphasized when applied to parabolic systems with space dimension higher than 1.

3. Nonhomogeneous ODE

Now we consider the system

$$\begin{aligned} \frac{d}{dt}v(t) &= A(t)v(t) + f(t), \\ v(0) &= v_0, \end{aligned} \tag{5}$$

and describe a second order method, based on the constructed methods of Section 2., which can be efficiently used to solve nonhomogeneous ODE. The solution of (5) has the form

$$u(T) = Q(T,0)v_0 + \int_0^T Q(T,s)\, f(s)\, ds.$$

The objective of present discussion is a numerical approximation of the second term on the right hand side:

$$u(T) = \int_0^T Q(T,s)\, f(s)\, ds = \sum_{k=1}^{K} \int_{(k-1)\tau}^{k\tau} Q(T,s)\, f(s)\, ds, \tag{6}$$

Only the second order convergence is discussed here. In the first step of approximation the interval $[0,T]$ is divided into K subintervals of the length τ. The points of subdivision are denoted by $t_k = k\tau, k = 0, 1, \ldots, K$. Then the trapezoidal rule is used at each subinterval of division in order to approximate integrals by sums. In the second step of approximation the matrices $U(T, k\tau)$ are approximated by $V_L(\tau, k)$ of (2), where $L \geq 2$. The obtained expression approximating (6) has the form:

$$\begin{array}{rcl} u_{app}(T) & = & \frac{\tau}{2}\, f(T) + \\ & = & \tau V_L(\tau, K)\, f(T - tau) + \\ & = & \tau V_L(\tau, K) V_L(\tau, K-1)\, f(T - 2\tau) + \\ & & \cdots\cdots\cdots\cdots\cdots\cdots \\ & = & \tau V_L(\tau, K) V_L(\tau, K-1)\, \cdots\, V_L(\tau, 2)\, f(\tau) + \\ & = & \frac{\tau}{2} V_L(\tau, K) V_L(\tau, K-1)\, \cdots\, V_L(\tau, 1)\, f(0). \end{array} \tag{7}$$

When an approximation of the first term of (5) is summed with the obtained approximation of $u(T)$, we get a rule analogous to rules of linear one-step methods. There are K steps of computations as follows:

$$\begin{array}{lcl} w(0) = v_0 \, + \, \frac{\tau}{2}\, f(0) & \to & w(1) \, = \, V_L(\tau, 1)\, w(0) \\ w(1) \, + \, \tau\, f(\tau) & \to & w(2) \, = \, V_L(\tau, 2)\, \big(w(1) \, + \, \tau\, f(\tau)\big) \\ w(2) \, + \, \tau\, f(2\tau) & \to & w(3) \, = \, V_L(\tau, 3)\, \big(w(2) \, + \, \tau\, f(2\tau)\big) \\ \ldots\ldots & & \ldots\ldots\ldots \\ w(K-1) \, + \, \tau\, f(T-\tau) & \to & w(K) \, = \, V_L(\tau, K)\, \big(w(K-1) \, + \, \tau\, f(T-\tau)\big) \\ w(k) \, + \, \frac{\tau}{2}\, f(T) & \to & v_{app} \, = \, w(k) \, + \, \frac{\tau}{2}\, f(T) \end{array}$$

Higher order approximations, with the same time increment τ, can be obtained by using higher order integration formulae such as Simpson rule.

4. Initial value problem for parabolic systems

In order to apply developed methods of Sections 3. and 3.. to an initial value problem for the 2^{nd}-order parabolic system it is necessary to approximate the parabolic system with ODE having the compartmental structure. In accordance with definitions in the previous section the initial value problem is considered on $[0, \infty) \times \mathbb{R}^d$.

Let the measurable functions $a_{ij} = a_{ji}$, b_i $(i, j = 1, 2, \ldots, d)$ and c be defined on $[0, \infty) \times \mathbb{R}^d$ and satisfy the following conditions:

$$\begin{array}{c} |b_i|, |c| \quad \leq M, \quad c \leq 0, \\ M\, |z|_2^2 \geq \displaystyle\sum_{i,j=1}^{d} a_{ij}(t, \mathbf{x}) z_i \bar{z}_j \geq \mu |z|_2^2, \quad \mu > 0, \quad \mathbf{x} \in \mathbb{R}^d, \ t \geq 0, \end{array} \tag{8}$$

where, M and μ are positive constants, z_i are complex numbers, and $|z|_2$ is the corresponding l_2-norm. The associated family of elliptic differential operator in divergence form

$$A(t, \mathbf{x}) \, = \, \sum_{i,j=1}^{d} \partial_i a_{ij}(t, \mathbf{x}) \partial_j \, + \, \sum_{j=1}^{d} \partial_j b_j(t, \mathbf{x}) \, + \, c(t, \mathbf{x}), \quad t \geq 0, \tag{9}$$

is considered on $\mathbb{R}^d$.

The 2^{nd}-order parabolic system is formally defined by

$$\begin{aligned} \left(\frac{\partial}{\partial t} - A(t)\right) u(t) &= f(t), \\ u(0) &= u_0. \end{aligned} \tag{10}$$

Let $\|\cdot\|_p$ denote the $L_p(\mathbb{R}^d)$-norm and let $(\cdot|\cdot)$ be the scalar product in $L_2(\mathbb{R}^d)$. The Sobolev space of functions on $\mathbb{E}_T = (0,T)\times\mathbb{R}^d$ having one space derivative is denoted by $W_2^{0,1}(\mathbb{E}_T)$. The quadratic form on $W_2^1(\mathbb{R}^d))$ defined by elliptic operator (9) is denoted by $a(t,\cdot,\cdot)$. We assume that the functions b_i, c are such that the form is coercitive:

$$a(t,u,u) \;\geq\; \alpha \sum_{i=1}^{d} \|\partial_i u\|_2^2, \quad t \geq 0,$$

for some $\alpha > 0$. The variational formulation of (10) is defined by:

$$\begin{aligned} \big(v(t)|u(t)\big) \;-\; \textstyle\int_0^t \big(\dot v(s)|u(s)\big)\,ds \;+\; \int_0^t a(s,v(s),u(s))\,ds \;=& \\ \big(v(0)|u_0\big) \;+\; \textstyle\int_0^t \big(v(s)|f(t)\big)\,ds,& \end{aligned} \tag{11}$$

for any $t \in (0,T)$ and any $v \in C_0^1([0,T], W_2^1(\mathbb{R}^d))$. There exists a unique solution of (11) in $W_2^{0,1}(\mathbb{E}_T)$, such that $t \to \|u(t)\|_2$ is a continuous function on $[0,T]$ (sse [Li]).

Now we impose conditions on the coefficients of elliptic operator in order to get solutions in $L_1(\mathbb{R}^d)$ [LR]. Let the coefficients have the following representation:

$$\begin{aligned} a_{ij}(t,\mathbf{x}) &= \hat a_{ij}(t,\mathbf{x}) + \delta_{ij}, \\ b_i(t,\mathbf{x}) &= \hat b_i(t,\mathbf{x}) + \gamma_i. \end{aligned} \qquad i,j \;=\; 1,2,\ldots,d. \tag{12}$$

Lemma 1. *Let $T > 0$, $u_0 \in W_2^1(\mathbb{R}^d) \cap L_1(\mathbb{E}_T)$ and $f \in L_2(\mathbb{E}_T) \cap L_1(\mathbb{E}_T)$. Let $a_{ij}(t), b_i(t)$ have the representation (12), where $\hat a_{ij}(t,\cdot), \hat b_i(t,\cdot)$ are elements of $L_2(\mathbb{R}^d)$ uniformly with respect to $t \in [0,T]$. Then*

$$\|u(t)\|_1 \;\leq\; \|u_0\|_1 + \|f\|_{L_1(\mathbb{E}_T)}, \quad \text{for allt} \in [0,\mathrm{T}].$$

The orthogonal coordinate system in $\mathbb{R}^d$ is determined by unit vectors $\mathbf{e}_i$. For each $n \in \mathbb{N}$, points $\mathbf{x} = h\sum_{l=1}^d k_l \mathbf{e}_l$, $h = 2^{-n}$, $k_l \in \mathbb{Z}$, define a numerical grid G_n on $\mathbb{R}^d$. Elements of G_n are called grid-knots. Let $\mathbf{x} \to \phi(\mathbf{w},\mathbf{x})$ be basis functions centred at grid-knots $\mathbf{w}$, having piecewise continuous first-order partial derivatives. Basis functions span a linear space $\mathcal{L}_n \subset W_2^1(\mathbb{R}^2)$. When the variational formulation (11) is applied to the linear spaces $\mathcal{L}_n$ the result is a sequence of ODE,

$$\begin{aligned} \tfrac{d}{dt} u_n(t) &= A_n(t) u_n(t), \\ u_n(0) &= u_{0n}, \end{aligned} \tag{13}$$

defining numerical approximations of (11). Numerical approximations $u_n(t) \in W_2^{0,1}(\mathbb{E}_T)$ converge to the solution of (11) in $W_2^{0,1}(\mathbb{E}_T)$ for each $T > 0$. If in addition, the conditions of of Lemma 1. are valid the convergence in $L_1(\mathbb{R}^d)$ is also ensured.

Unfortunately, finite element techniques do not usually produce ODE with a compartmental structure. In some cases, such as for Laplace operator, the corresponding approximations $A_n(t)$ have compartmental structure. Only such cases are considered here. The systems (13) can be solved by the method (2) in order to get numerical approximations of $u_n(t_k)$ at a discrete sequence of times $t_k, k = 0, 1, \ldots, K$. An advantage of utilizing the method (2) is already discussed at the end of previous section.

To get compartmental structure for general 2^{nd}-order parabolic system finite element techniques must be avoided. Numerical methods ensuring compartmental structure for general cases are described in [LR].

5. Discussion

Although applicability and efficiency of methods of Section 2. is demonstrated for parabolic systems on $\mathbb{R}^d$ for which solutions have finite L_1-norms, the methods can be applied as well to problems on bounded domains. In case of an initial value problem for the 2^{nd}-order parabolic system on a bounded domain with homogeneous Dirichlet condition, the procedure of Section 4.. can be straightforwardly applied. In case of other boundary conditions the compartmental structure of approximations $A_n(t)$ must be ensured.

Finiteness of L_1-norm of solution of the initial value problem for the 2^{nd} -order parabolic system on $\mathbb{R}^d$ seams to be restrictive, while in case of bounded domains seams to be superfluous. Our intention was to develop methods for problems related to diffusion and derived from diffusion such as behaviour of probability distributions of Markov processes generated by elliptic operators. In this way approximations with compartmental structure are directly related to approximations of Markov process (or/and diffusion) by a sequence of Markov jump processes.

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