

AN A-STABLE THREE-LEVEL METHOD FOR THE GALERKIN SOLUTION OF QUASILINEAR PARABOLIC PROBLEMS

I. FARAGÓ – A. GALÁNTAI

Abstract. Parabolic partial differential equations are often solved by semidiscrete Galerkin methods. These methods first make a finite element discretization in the space variables reducing the problem to solution of the Cauchy-problem of a system of ordinary differential equations. This problem is then solved by a highly stable difference or Runge-Kutta method.

In this paper we investigate the numerical solution of the semidiscretized Cauchy-problem for a class of nonlinear partial differential equations used in the modelling of chemical reactors and other areas.

1. Introduction

Consider the following initial-boundary value problem

$$(1) \quad \frac{\partial u}{\partial t} = Pu, \quad ((x, t) \in \Omega \times (0, T])$$

$$(2) \quad Bu = 0 \quad ((x, t) \in \Gamma \times (0, T])$$

$$(3) \quad u(x, 0) = u_0(x) \quad (x \in \bar{\Omega}).$$

where $x = (x_1, x_2, \dots, x_N) \in \Omega \subset R^N, t \in (0, T], T > 0, \Omega$ is a bounded domain with a sufficiently smooth boundary. The operator P is defined by

$$(4) \quad Pu = \sum_{i,j=1}^N \frac{\partial}{\partial x_i} (F_{i,j}(x) \frac{\partial u}{\partial x_j}) - F_0(u, x, t).$$

The operator B is representing some classical boundary condition and $u_0(x)$ is given function. Assume that the following conditions are satisfied.

- (i) There is only one generalized solution of the problem (1)-(3) in $H^1(\Omega)$ for arbitrary fixed $t \in (0, T]$ (see Ladizhenskaya [13] and Lions [7]).
- (ii) For arbitrary fixed $x \in \bar{\Omega}$ the matrix $[F_{i,j}(x)]_{i,j=1}^N$ is symmetric and uniformly positive definite, that is there exist such positive numbers k_0, k_1 that for any vector $\xi = (\xi_1, \xi_2, \dots, \xi_N) \in R^N$ the inequality

$$(5) \quad k_0 \sum_{i=1}^N \xi_i^2 \leq \sum_{i,j=1}^N F_{i,j}(x) \xi_i \xi_j \leq k_1 \sum_{i=1}^N \xi_i^2$$

holds.

- (iii) The function F_0 is continuous and uniformly Lipschitzian in its first variable, that is there exists a constant $L_0 > 0$ such that

$$(6) \quad |F_0(s_1, x, t) - F_0(s_2, x, t)| < L_0 |s_1 - s_2|$$

is satisfied for all $s_1, s_2 \in R$ and for all $(x, t) \in \bar{\Omega} \times [0, T]$.

We also assume that there exists a space V_h^l of finite elements which is a finite dimensional subspace of $H^1(\Omega)$ and it satisfies the approximation property that for given $l \in \mathbf{N}^+$ and an arbitrary $u \in H^1(\Omega) \cap H^{l+1}(\bar{\Omega})$ there is an element $\tilde{u} \in V_h^l$ such that

$$(7) \quad \|u - \tilde{u}\|_0 + h \|u - \tilde{u}\|_1 \leq ch^{l+1} \|u\|_{l+1},$$

where c is a positive constant and h is the maximal diameter of the discretization. (For the existence of such spaces of finite elements see Strang [8], Molchanov [14], Faragó [3].)

Let $V_h^t = \text{span}[\varphi, \dots, \varphi_n]$ and seek the approximate solution in the following form

$$(8) \quad u_n(x, t) = \sum_{i=1}^n \alpha_i(t) \varphi_i(x)$$

Then for the unknown vector $\alpha(t) = [\alpha_1(t), \dots, \alpha_n(t)]$ we have the Cauchy-problem of the form

$$(9) \quad M\alpha' + Q\alpha = F(\alpha, t) \quad (0 < t \leq T)$$

$$(10) \quad M\alpha(0) = \tilde{\alpha}_0,$$

where M and Q are positive definite matrices, $F : R^{n+1} \rightarrow R^n$ and the initial value $\tilde{\alpha}_0$ are also given (see [3], [8]). Hence the matrix M^{-1} exists and the problem (9)-(10) equivalent with the problem

$$(11) \quad \alpha' = A\alpha + f(\alpha, t)$$

$$(12) \quad \alpha(0) = \alpha_0.$$

It can be shown ([8], [5]) that the problem (11)-(12) satisfies the following two properties

- (iv) The matrix A has only negative eigenvalues and it is diagonalizable.
- (v) The map $f : R^{n+1} \rightarrow R^n$ is continuous and there exists a constant $L \geq 0$ such that

$$(13) \quad \|f(y_1, t) - f(y_2, t)\| \leq L\|y_1 - y_2\| \quad (y_1, y_2 \in R^n)$$

holds for all $t \in [0, T]$.

It is known ([1], [2], [11]) that the problem (11)-(12) can be considered as a stiff system. Therefore we need to choose a highly stable method to solve it.

In this paper we are going to investigate linear two-step methods. Two-step methods of the form (ζ, σ) can be defined by their characteristic polynomials

$$(14) \quad \zeta(\xi) = \sum_{s=0}^2 \zeta_s \xi^s; \quad \sigma(\xi) = \sum_{s=0}^2 \sigma_s \xi^s,$$

where $\sigma(1) = 1$ is assumed. The method (ζ, σ) is of order two if the coefficients satisfy the following conditions:

$$(15) \quad \begin{aligned} \zeta_1 &= 1 - 2\zeta_2, & \zeta_0 &= -1 + \zeta_2, \\ \sigma_1 &= \frac{1}{2} + \zeta_2 - 2\sigma_2, & \sigma_0 &= \frac{1}{2} - \zeta_2 + \sigma_2 \end{aligned}$$

DEFINITION 1. Consider the test problem

$$(16) \quad y' = \lambda y, \quad y(0) = y_0 \quad (\lambda \in \mathbb{C})$$

Let $z = \lambda\tau$ ($\tau > 0, \lambda \in \mathbb{C}$) and denote by y_m the numerical solution of (16) at the point $t_m = m\tau$ ($m \geq 0$). The set S of those values of z for which $\{y_m\}_{m=0}^{\infty}$ converges to 0 for all y_0 is said to be the region of absolute stability of the method.

DEFINITION 2. A method is said to be A_0 -stable if $(-\infty, 0) \subset S$. The method is said to be A -stable if $\mathbb{C}^- \subset S$, where $\mathbb{C}^- = \{z | \operatorname{Re}(z) < 0\}$.

Applying the method (14) to the problem (11)-(12) we obtain the recursion

$$(17) \quad \sum_{s=0}^2 \zeta_s \alpha^{m+s} = \tau A \left(\sum_{s=0}^2 \sigma_s \alpha^{m+s} \right) + \tau \sum_{s=0}^2 \sigma_s f(\alpha^{m+s}, t_{m+s})$$

which is nonlinear systems of algebraic equations for the unknown vector α^{m+2} (α^m is the approximation of $\alpha(t)$ on the time level $t_m = m\tau$). In order to avoid the solution of this nonlinear system we linearize it using axtrapolation ([10]). Keeping the accuracy of the scheme we change t_{m+2} and α^{m+2} to $t_{\overline{m+2}}$ and $\alpha^{\overline{m+2}}$, where

$$(18) \quad \begin{aligned} t_{\overline{m+2}} &= t_m + (2\sigma_2 + \sigma_1)\tau, \\ \alpha^{\overline{m+2}} &= (2\sigma_2 + \sigma_1)\alpha^{m+1} + (\sigma_0 - \sigma_2)\alpha^m \end{aligned}$$

are extrapolated values. Substituting (18) into the righthand side of (17) one obtains a linear algebraic system.

2. A special two step method and its stability

We derive a one-parameter class of two-step methods which are based on the extrapolation principle mentioned in the previous section. The method must be of order 2. We start with the standard two-step methods and choose the parameters as follows

$$(19) \quad \varsigma_2 = \frac{1}{2}, \quad \sigma_2 = \Theta \quad (\Theta \in R).$$

Then we have the following coefficients

$$(20) \quad \begin{aligned} \varsigma_0 &= -\frac{1}{2}, \quad \varsigma_1 = 0, \quad \varsigma_2 = \frac{1}{2} \\ \sigma_0 &= \Theta, \quad \sigma_1 = 1 - 2\Theta, \quad \sigma_2 = \Theta. \end{aligned}$$

If we apply this scheme to the problem (11)-(12) and use the notations

$$(21) \quad \alpha^{m+1,\Theta} = \Theta\alpha^{m+2} + (1 - 2\Theta)\alpha^{m+1} + \Theta\alpha^m,$$

$$(22) \quad \begin{aligned} f^{m+1,\Theta} &= \Theta f(\alpha^{m+2}, t_{m+2}) + (1 - 2\Theta)f(\alpha^{m+1}, t_{m+1}) + \\ &+ \Theta f(\alpha^m, t_m) \end{aligned}$$

then we obtain the recursion

$$(23) \quad \frac{\alpha^{m+2} - \alpha^m}{2\tau} = A\alpha^{m+1,\Theta} + f^{m+1,\Theta} \quad (m \geq 0).$$

The extrapolation formula(18) has now the form

$$(24) \quad t_{\frac{m+2}{2}} = t_m + \tau = t_{m+1}, \quad \overline{\alpha^{m+2}} = \alpha^{m+1}$$

and $f^{m+1,\Theta} \sim f(t_{m+1}, \alpha^{m+1})$ for small τ 's. Thus we have the following linearized form of scheme (23)

$$(25) \quad \frac{\alpha^{m+2} - \alpha^m}{2\tau} = A\alpha^{m+1,\Theta} + f(t_{m+1}, \alpha^{m+1})$$

($m = 0, 1, \dots$).

Next we investigate the stability properties of the method (25). If we apply (25) to the test problem (16) then we get the difference equation

$$(26) \quad \frac{y^{m+2} - y^m}{2\tau} = \lambda y^{m+1,\Theta} \quad (m \geq 0)$$

which is equivalent to the recursion

$$(27) \quad (1 - 2\Theta z)y^{m+2} - 2(1 - 2\Theta)zy^{m+1} - (1 + 2\Theta z)y^m = 0$$

The characteristic equation of (27) has the form

$$(28) \quad \Pi(\xi, z) = (1 - 2\Theta z)\xi^2 - 2(1 - 2\Theta)z\xi - (1 + 2\Theta z) = 0.$$

Theorem 1. *The method (25) is A_0 -stable iff $\Theta > \frac{1}{4}$.*

Proof. The solution of (27) is tending to 0 for all y_0 if the zeros of the characteristic equation (28) lie in the disk $\{w \in \mathbb{C} : |w| < 1\}$. Hence it is enough to show that for all $z < 0$ this

condition is satisfied if and only if $\Theta > \frac{1}{4}$. If $z < 0$ the coefficients of (28) are real and we can use a special case of the Schur-Cohn criterion (Kobza [6]): A real polynomial of the form

$$(29) \quad a_2 x^2 + a_1 x + a_0 \quad (a_2 > 0)$$

has its both zeros in the open unit disk if and only if the coefficients satisfy the system

$$(30) \quad a_2 + a_1 + a_0 > 0, \quad a_2 - a_0 > 0, \quad a_2 - a_1 + a_0 > 0.$$

Using (30) one can show that the zeros of (28) lie in the open unit disk for all $z < 0$ if and only if $\Theta > \frac{1}{4}$.

Theorem 2. *The method (25) is A-stable if $\Theta > \frac{1}{4}$.*

Proof It is enough to show that for all $z \in \mathbb{C}^-$ the zeros of (28) lie in the open unit disk. Consider the Moebius-transformation

$$(31) \quad \zeta = (p + 1)/(p - 1)$$

which maps the open unit disk onto the half plane $Re(p) < 0$, that is $|\zeta| < 1$ iff $Re(p) < 0$. Furthermore, let be $q = -z$ and consider the equation

$$(32) \quad H(p, q) = (p - 1)^2 \Pi((p + 1)/(p - 1), -q) = 0.$$

The method is A-stable if and only if $Re(q) > 0$ implies $Re(p(q)) < 0$ where $p(q)$ denotes any zero of (32) as a function of q . Similarly, if $q(p)$ denotes the zero of (32) as a function of p then the latter condition is equivalent to the condition, that $Re(p) \geq 0$ implies $Re(q(p)) \leq 0$. By elementary calculations one gets

$$(33) \quad H(p, q) = 4p + 2q(p^2 + 4\Theta - 1) = 0.$$

It is easy to see that for $p^2 = 1 - 4\Theta$ there is no zero of (33). Hence we can solve (33) in the form

$$(34) \quad q = -2p/(p^2 + 4\Theta - 1) = -2[\bar{p}|p|^2 + (4\Theta - 1)p]/|p^2 + 4\Theta - 1|^2.$$

For $\Theta > \frac{1}{4}$ and $Re(p) \geq 0$ we have

$$Re[\bar{p}|p|^2 + (4\Theta - 1)p] \geq 0$$

which implies $Re(q(p)) \leq 0$. Thus the theorem is proved.

It is noted that A-stability implies A_0 -stability. This is the reason for the assumption $\Theta > \frac{1}{4}$ of Theorem 2. It is also worth noting that the method (25) is I -stable for $\Theta > \frac{1}{4}$ which also implies the A-stability (see Wanner-Hairer-Norsett [9]).

3. The convergence of the method

We construct an error estimation for the global error from which the convergence of the algorithm follows.

Rewrite the method (25) in the form

$$(35) \quad \alpha^{m+2} - \alpha^m = 2\tau[A\alpha^{m+1, \Theta} + f(t_{m+1}, \alpha^{m+1})]$$

and let $\hat{\alpha}^m = \alpha(t_m)$, where $\alpha(t)$ is the exact solution of (11)-(12). The local error of the method at $t_m = m\tau$ is defined by

$$(36) \quad \hat{\alpha}^{m+2} - \hat{\alpha}^m = 2\tau[A(\Theta\hat{\alpha}^{m+2} + (1 - 2\Theta)\hat{\alpha}^{m+1} + \Theta\hat{\alpha}^m) + 2\tau f(t_{m+1}, \hat{\alpha}^{m+1}) + T_m].$$

Introduction the notation $e_m = \alpha^m - \hat{\alpha}^m$ for the global error of the method at the point t_m we obtain

$$(37) \quad e_{m+2} - e_m = 2\tau A[\Theta e_{m+2} + (1 - 2\Theta)e_{m+1} + \Theta e_m] + R_m,$$

where

$$(38) \quad R_m = 2\tau[f(t_{m+1}, \alpha^{m+1}) - f(t_{m+1}, \hat{\alpha}^{m+1})] - T_m.$$

By simple calculation one has

$$(39) \quad (I - 2\Theta\tau A)e_{m+2} - 2(1 - 2\Theta)\tau Ae_{m+1} - (I + 2\Theta\tau A)e_m = R_m$$

and

$$(40) \quad \begin{aligned} e_{m+2} = & 2(1 - 2\Theta)(I - 2\Theta\tau A)^{-1}\tau A e_{m+1} + \\ & + (I - 2\Theta\tau A)^{-1}(I + 2\Theta\tau A)e_m + (I - 2\Theta\tau A)^{-1}R_m. \end{aligned}$$

Introduce the notations

$$(41) \quad E_m = \begin{bmatrix} e_{m+1} \\ e_m \end{bmatrix} \in R^{2n}, \quad G_m = \begin{bmatrix} (I - 2\Theta\tau A)^{-1}R_m \\ 0 \end{bmatrix} \in R^{2n}$$

and the block Frobenius matrix

$$\begin{aligned} \Phi(\tau A) = & \\ = & \begin{bmatrix} 2(1 - 2\Theta)(I - 2\Theta\tau A)^{-1}\tau A & (I - 2\Theta\tau A)^{-1}(I + 2\Theta\tau A) \\ I & 0 \end{bmatrix} \end{aligned}$$

The eigenvalues of $\Phi(\tau A)$ coincide with the zeros of the characteristic polynomial of (39). Recursion (40) takes the form

$$(42) \quad E_{m+1} = \Phi(\tau A)E_m + G_m \quad (m = 0, 1, \dots)$$

with the solution

$$(43) \quad E_m = [\Phi(\tau A)]^m E_0 + \sum_{i=0}^{m-1} [\Phi(\tau A)]^{m-i-1} G_i \quad (m \geq 0).$$

The triangle inequality implies

$$(44) \quad \|E_m\| \leq \|\Phi(\tau A)\|^m \|E_0\| + \sum_{i=0}^{m-1} \|\Phi(\tau A)\|^{m-i-1} \|G_i\|.$$

The term G_i may be estimated as follows

$$\|G_i\| = \|(I - 2\Theta\tau A)^{-1}R_i\| \leq \|(I - 2\Theta\tau A)^{-1}\|(2\tau L\|E_i\| + \|T_i\|).$$

Assume that there exists a constant $\gamma > 0$ such that for every $\tau > 0$ the inequality

$$(45) \quad \|(I - 2\Theta\tau A)^{-1}\| \leq \gamma$$

holds. It is also supposed that A is diagonalizable, that is $A = X^{-1}\Lambda X$ with $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. Then we have

$$(46) \quad \Phi(\tau A) = \begin{bmatrix} X^{-1} & 0 \\ 0 & X^{-1} \end{bmatrix} \Phi(\tau \Lambda) \begin{bmatrix} X & 0 \\ 0 & X \end{bmatrix}$$

which implies

$$(47) \quad \Phi(\tau A)^m = \begin{bmatrix} X^{-1} & 0 \\ 0 & X^{-1} \end{bmatrix} \Phi(\tau \Lambda)^m \begin{bmatrix} X & 0 \\ 0 & X \end{bmatrix}$$

Since in the spectral norm $\|\cdot\|_2$ we have

$$(48) \quad \|\Phi(\tau \Lambda)^m\|_2 = \max_{1 \leq \mu \leq n} \|\Phi(\tau \lambda_\mu)^m\|_2$$

and the method (25) is A -stable we can use the uniform boundedness theorem of Gekeler [5]. This result guarantees the existence of constant $K > 0$ such that

$$(49) \quad \sup_{\xi \in \mathbb{C}^-} \sup_{m \in \mathbb{N}} \|\Phi(\xi)^m\| \leq K.$$

From (49) the estimations $\|\Phi(\tau \Lambda)^m\|_2 \leq K$ and

$$(50) \quad \|\Phi(\tau A)^m\|_2 \leq K k_2(X) \quad (m \geq 0)$$

follow, where $k_2(X) = \|X^{-1}\|_2 \|X\|_2$ is the condition number of the matrix X . Using (50) and (45) we have

$$(51) \quad \begin{aligned} \|E_m\| &\leq K k_2(X) (\|E_0\| + \gamma \sum_{i=0}^{m-1} \|T_i\|) + \\ &+ \sum_{i=0}^{m-1} 2K k_2(X) \gamma \tau L \|E_i\|. \end{aligned}$$

We need a discrete version of the Gronwall-Bellman lemma : if $z(j) \geq 0$ ($j \geq 0$) and $x(i) \leq y(i) + \sum_{j=0}^{i-1} z(j)x(j)$ $i = 0, 1, \dots, m$; $n \in \mathbf{N}$ then

$$(52) \quad x(m) \leq y(m) + \sum_{i=0}^{m-1} z(i)y(i) \prod_{j=i+1}^{m-1} [1 + z(j)] \quad (m \in \mathbf{N}).$$

In our case we can chose

$$(53) \quad \begin{aligned} x(i) &= \|E_i\| \\ y(i) &= Kk_2(X)(\|E_0\| + \gamma \sum_{j=1}^{i-1} \|T_j\|) \\ z(i) &= 2Kk_2(x)\gamma\tau L = z^*. \end{aligned}$$

Using the monotonicity of $y(i)$ and the lemma we obtain

$$\|E_m\| \leq Kk_2(X)(\|E_0\| + \gamma \sum_{j=0}^{m-1} \|T_j\|)(1 + \sum_{i=0}^{m-1} z^*(1 + z^*)^{m-i-1}).$$

The inequality $1 + z^* \leq e^{z^*}$ implies that

$$1 + \sum_{i=0}^{m-1} z^*(1 + z^*)^{m-i-1} = (1 + z^*)^m \leq e^{mz^*}.$$

Hence we have proven

Theorem 3. *If the matrix A is diagonalizable, $\sigma(A) \in \mathbf{C}^-$ and (45) is satisfied then*

$$(54) \quad \|E_m\| \leq c_1 e^{c_2 m \tau} (\|E_0\| + \gamma \sum_{j=1}^{m-1} \|T_j\|),$$

where

$$(55) \quad c_1 = Kk_2(X), \quad c_2 = 2c_1\gamma L.$$

First we remark that the exponential part of the error constant is due to the nonlinear part of (11)-(12). Consequently for vanishing nonlinear part ($L = 0$) we obtain a sharp estimation (see [5]). In our application $\sigma(A) \in \mathbb{C}^-$ (condition (iv)) and what is more $\sigma(A) \subset \mathbb{R}^-$. If A is diagonalizable, then

$$(I - 2\Theta\tau A)^{-1} = X^{-1}(I - 2\Theta\tau\Lambda)^{-1}X$$

and

$$\|(I - 2\Theta\tau A)^{-1}\|_2 \leq k_2(X)\|(I - 2\Theta\tau\Lambda)^{-1}\|_2.$$

For $\Theta > \frac{1}{4}$ $\|(I - 2\Theta\tau\Lambda)^{-1}\|_2 \leq 1$. Hence one can choose $\gamma = k_2(X)$. If A is Hermitian, then $k_2(X) = 1$.

The convergence of (25) clearly follows from the inequality (54) and the fact that the methods under consideration are of order 2.

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I. FARAGÓ

A. GALÁNTAI

*University of Agriculture
Institute of Mathematics
H-2103, Gödöllő*

HUNGARY