# Numerical Study of Cauchy Problems for Parabolic Differential Equations with a Lagrangian Multiplier Method

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**Abstract**

A Cauchy problem for a parabolic differential equation of standard typ is stated in a weak form by means of a Lagrange multiplier technic. It is shown that a numerical finite element method results in a formally simple system of differential–algebraic equations (DAE). However, the pencil of the DAE is (in a sense given) practically singular showing the known ill–posed character of the Cauchy problem. Therefore, a regularization (e.g. of Tychonov type) of the DAE is discussed. The general results are illustrated throughout the paper by an example.

## 1. Introduction

There are several methods of treating Cauchy problems for second order elliptic and parabolic differential equations, see e.g. [2], [9], [10]. In this paper the numerical solution of problems of this type by means of finite elements based on a variational formulation with Lagrangian multipliers is investigated. To be specific, we consider a bounded open region $\Omega \subset \mathbb{R}^n, n = 2$ or $3$, with sufficiently smooth boundary $\Gamma$ which ist decomposed into two non empty parts $\Gamma_0$ and $\Gamma_1$ such that $\Gamma = \Gamma_0 \cup \Gamma_1$ and $\Gamma_0 \cap \Gamma_1 = \emptyset$. Furthermore, let $\gamma_1$ be a non empty subset of $\Gamma_1$, $\gamma_1 \subset \Gamma_1$. With these preliminaries we define formally the two Cauchy problems in more than one space dimension:

**Problem** $P1_{ell}$ : Find $u: \Omega \to \mathbb{R}$ such that

$$- div(a_0\, grad\, u) + b_0 u = f \quad \text{on} \quad \Omega \tag{1}$$

$$u = 0 \quad \text{on } \gamma_1 \tag{2}$$

$$g + a_0 \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_1. \tag{3}$$

**Problem** $P1_{par}$ : Find $u: \Omega \times (0,T) \to \mathbb{R}$ such that

$$\frac{\partial u}{\partial t} - div(a_0\, grad\, u) + b_0 u = f \quad \text{on } \Omega \times (0,T), \quad T > 0, \tag{4}$$

$$u = 0 \quad \text{on } \gamma_1 \times (0,T) \tag{5}$$

$$g + a_0 \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_1 \times (0,T) \tag{6}$$

$$u = u_0 \quad \text{on } \Omega \quad \text{for } t = 0. \tag{7}$$

In either case $u$ must be thought of as element of a suitable linear space (see the weak formulation below where spaces are specified). The given data $a_0$, $b_0$, $g$ and $f$ are assumed to be independent of $u$ and sufficiently smooth. Furthermore, let $u_0$ be given and $a_0 > 0,\ b_0 \geq 0$. $\partial/\partial n$ on a surface part means the derivative with respect to the outer normal. As usual, in $P1_{par}$ we also assume the compatibility of the initial function $u_0$ in (7) with the boundary condition (5).

There are many applications of the above problems. Especially, we mention the electrocardiology, see e.g. [6], where problem $P1_{ell}$ is a mathematical model of the electric potential $u$ of the heart.

With the given expositions, $P1_{ell}$ is the classical formulation of an elliptic Cauchy problem while $P1_{par}$ describes the corresponding parabolic Cauchy problem. Note that on the surface part $\Gamma_0$ no boundary condition is given. On $\gamma_1$ two boundary conditions must hold. As is well known these problems are (in the sense of Hadamard) improperly posed [9]. There is a large literature about these. Especially we mention the work of Burggraf [4] which discusses the question of the unique solution of the one dimensional analogue of problem $P1_{par}$.

In [8] problem $P1_{ell}$ has been considered in a weak formulation which is now the starting point. For details we refer to [8]. Using standard notation [5], we introduce the space

$$V = H^1(\Omega) \times H^{-1/2}(\Gamma) \tag{8}$$

with norm

$$\| (v,\mu) \|_V = \left( \| v \|^2_{H^1(\Omega)} + \| \mu \|^2_{H^{-1/2}(\Gamma)} \right)^{1/2} \tag{9}$$

and the bilinear resp. linear forms

$$a(u,v) \;=\; \int_\Omega \left( a_0 \sum_{i=1}^{n} \frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_i} + b_0 uv \right) dx\,, \qquad dx = dx_1 ... dx_n, \tag{10}$$

$$B(u,\lambda;v,\mu) \;=\; a(u,v) + \int_{\Gamma_0} \lambda v \, ds + \int_{\gamma_1} u\mu \, ds \tag{11}$$

$$F(v,\mu) \equiv F(v) = \int_\Omega fv \, dx - \int_{\Gamma_1} gv \, ds \tag{12}$$

($ds$ means the surface element). These definitions give the weak form of the two problems

**Problem** $P2_{ell}$ : Find $(u,\lambda) \equiv (u(x),\lambda(x)) \in V$ such that

$$B(u,\lambda;v,\mu) = F(v,\mu) \qquad \forall (v,\mu) \in V. \tag{13}$$

**Problem** $P2_{par}$ : Find for all $t \in (0,T)$ $(u(x,t),\lambda(x,t)) \in V$ such that

$$\int_\Omega \frac{\partial u}{\partial t} v \, dx \;+\; B(u,\lambda;v,\mu) = F(v,\mu) \qquad \forall (v,\mu) \in V \tag{14}$$

and

$$u(x,0) \;=\; u_0(x)\,, \quad x \in \Omega. \tag{15}$$

$\lambda$ can be interpreted as a Lagrangian multiplier. It is easy to see that the variational problem (13) reproduces eqs. (1) – (3) and in addition

$$\lambda + a_0 \frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_0. \tag{16}$$

Thus the Lagrange multiplier is (up to the factor $-a_0$) the normal derivative of $u$ on $\Gamma_0$. The same is true for the variational problem (14). It yields

formally eqs. (4) – (6) and again eq. (16). This can be proved by standard arguments (using partial integration of the first term in the bilinearform $a(u,v)$ and taking into account that eqs. (13) resp. (14) must be valid on the whole space $V$).
Using a theorem of Babuška [1] it can be shown [8] there is a unique solution of problem $P2_{ell}$ in the space $V$. Furthermore, an inequality of the form

$$\| (u,\lambda) \|_V \leq \; const. \| F \|_{V'}, \qquad const. > 0,$$

is valid for the solution $(u,\lambda) \in V$. ($V'$ denotes the dual space of $V$.)
The introduction of the bilinearform $B(\cdot,\cdot)$ which ist not symmetric (because of the surface terms) enables us to incorporate the non-standard boundary conditions of the problems $P1_{ell}$ and $P1_{par}$ into a variational formulation. Note further that the space $V = H^1(\Omega) \times H^{-1/2}(\Gamma)$ is free of constraints caused by boundary conditions. This simplifies the construction of $V$ which is necessary in finite dimensional approximations (e.g. finite element solutions). On the other hand, according to the definition of the space $V$ it requires the approximate representation of the two spaces $H^1(\Omega)$ and $H^{-1/2}(\Gamma)$.

In the next section a typical two dimensional case for the elliptic problem is considered. We generate a finite element approximation of $u \in V$. The corresponding finite system of equations is ill–conditioned what is discussed. In the third section the same example is the basis for investigating the parabolic case $P2_{par}$. It is shown that this problem results in a system of differential–algebraic equations (DAE's). The specific properties of this system are represented. In either case for a numerical solution a regularization is necessary.

## 2. The elliptic Cauchy problem

In order to demonstrate the numerical difficulties of the two Cauchy problems we consider first the elliptic case $P2_{ell}$. For concretness let $\Omega \subset \mathbb{R}^2$ be of the type shown in the Figure.

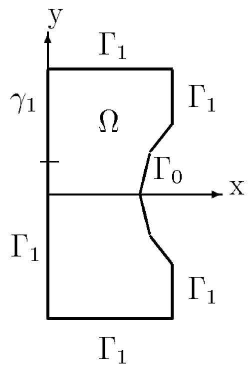


Fig.
The bounded open set $\Omega$ used in a typical example (see also section 2.1.).
$\Gamma = \Gamma_0 \cup \Gamma_1, \quad \gamma_1 \subset \Gamma_1$.

In this section our aim is the solution of problem $P2_{ell}$ by a finite element method with second order elements. By standard methods [5] finite dimensional spaces $H_h^1(\Omega) \subset H^1(\Omega)$, $H_h^{-1/2}(\Gamma) \subset H^{-1/2}(\Gamma)$ and $V_h = H_h^1(\Omega) \times H_h^{-1/2}(\Gamma) \subset V$ are constructed. With these definitions we have the following problem for an approximation $(u_h, \lambda_h)$:

**Problem** $P2_{ell}^h$ : Find $(u_h, \lambda_h) \in V_h$ such that

$$a(u_h, v_h) + \int_{\Gamma_0} \lambda_h v_h ds = F(v_h) \quad \forall\, v_h \in H_h^1(\Omega) \tag{17}$$

and

$$\int_{\gamma_1} u_h \mu_h ds = 0 \quad \forall\, \mu_h \in H_h^{-1/2}(\Gamma). \tag{18}$$

Note that we determine $\lambda \in H_h^{-1/2}(\Gamma)$ without any condition on $\Gamma_1$.
The triangulation (by triangles) of $\overline{\Omega}$ is supposed to have $M$ knots. On each of the boundary parts $\gamma_1$ and $\Gamma_0$ $p$ knots $(2p < M)$ may be situated. The knots on $\gamma_1$ are numbered by $P_1, P_2, ..., P_p$ and on $\Gamma_0$ by $P_{p+1}, P_{p+2}, ..., P_{2p}$. We assume that the points $P_1, P_p$ and $P_{p+1}, P_{2p}$ are on the border of $\gamma_1$ and $\Gamma_0$, respectively. The basis functions (second order elements) to build $H_h^1(\Omega)$ and $H_h^{-1/2}(\Gamma)$ are denoted by $\{w_j\}$ and $\{t_i\}$, respectively. Thus the unknown functions $u_h$ on $\overline{\Omega}$ and $\lambda_h$ on $\Gamma_0$ can be represented in the form

$$u_h = \sum_{i=1}^{M} u_i w_i \qquad \text{in } \overline{\Omega} \tag{19}$$

and

$$\lambda_h = \sum_{i=p+1}^{2p} \lambda_i t_i \qquad \text{on } \Gamma_0 \tag{20}$$

where the coefficients $u_i$ and $\lambda_i$ must be determined. Now it is observed that the second finite dimensional equation (18) is a linear homogeneous system with a quadratic regular matrix which gives $u = 0$ on $\gamma_1$, i.e. $u_i = 0$ for

$i = 1, 2, ..., p$. Therefore, this equation need not be considered further and the index $i$ in the sum in eq. (19) can be chosen to run from $p+1$ (instead of 1).
Because of the last result, we introduce a new vector $X$ with $M$ components

$$X_i = \lambda_{p+i} \quad \text{for} \quad i = 1, ..., p \qquad \text{and} \qquad X_i = u_i \quad \text{for} \quad i = p+1, ..., M. \quad (21)$$

From this it follows that the finite dimensional system (17) can be written

$$\begin{pmatrix} O_1 & B_1 \\ S & B_2 \\ O_3 & B_3 \end{pmatrix} X = b \qquad \text{or for short} \qquad BX = b. \qquad (22)$$

$b$ is a vector with components

$$b_j = \int_\Omega f w_j dx - \int_{\Gamma_1} g w_j ds, \qquad j = 1, ..., M. \qquad (23)$$

$O_1$ and $O_3$ are $(p,p)-$ and $(M-2p, p)-$matrices with zero elements, respectively. $S$ is a $(p,p)-$matrix with elements

$$s_{i,j} = \int_{\Gamma_0} t_j w_i ds \qquad (24)$$

The matrices $B_1$, $B_2$ and $B_3$ are of the form $(p, M-p)$, $(p, M-p)$ and $(M-2p, M-p)$, respectively, with elements

$$B_{k;i,j} = a(w_j, w_i), \qquad k = 1, 2, 3. \qquad (25)$$

For each $k$ the range of the indices $(i,j)$ can be read off from eq. (22).
For later use (especially in the parabolic case) we write eq. (22) also in a different form, namely

$$B\,X \equiv \begin{pmatrix} O_1 & B_1 \\ S_{21} & B_{22} \end{pmatrix} X = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} \qquad (26)$$

where now $S_{21}$ is a $(M-p, p)-$matrix and $B_{22}$ a $(M-p, M-p)-$matrix. The vectors $F_1$ and $F_2$ with $p$ and $M-p$ components, respectively, are given by the corresponding components of the vector $b$.
It appears that for Cauchy problems the matrix $B$ is extremely ill–conditioned, for elliptic Cauchy problems see also [8]. Furthermore, in the parabolic case

we get a differential algebraic system of equations. This is discussed in section 3.

## 2.1. An example

In order to demonstrate the ill–conditioness we consider an example where $\Omega$ and the boundary parts are given as indicated in the Figure. We take (compare problem $P1_{ell}$)

$$a_0 = a_0(x,y) = 0.5 + 0.1(\mid x - 0.5 \mid + \mid y \mid)/(1 + x + \mid y \mid),$$

$$b_0 = 0.01, \quad g = 0.05, \quad f = 1, \quad p = 9 \quad \text{and} \quad M = 80,$$

i.e. eqs. (22) and (26) are systems of 80 equations.
In detail the boundary parts $\Gamma_0$, $\Gamma_1$ and $\gamma_1 \subset \Gamma_1$ are given by the straight lines between the following points (compare the Figure)

$$\Gamma_0 : \quad (5,-3), \quad (2.8727,-2.1213), \quad (2,0), \quad (2.8727,2.1213), \quad (5,3),$$

$$\Gamma_1 : \quad (5,3), \quad (5,5), \quad (0,5), \quad (0,-5), \quad (5,-5), \quad (5,-3),$$

$$\gamma_1 : \quad (0,5), \quad (0,1).$$

To obtain a numerical solution we use a second order finite element method for both spaces $H^1(\Omega)$ and $H^{-1/2}(\Gamma)$. This gives in the standard way the $(80,80)-$matrix $B$. Let the condition number of a square matrix $A$ and the rank be denoted by $\kappa(A) = \parallel A \parallel \parallel A^{-1} \parallel$ with a specified norm and $rank(A)$, respectively. Then one finds the values shown in Table 1 (all numerical results in this paper are computed in FORTRAN double precision arithmetic).

Tab. 1

| matrix | $\kappa(\cdot) \approx$ | $rank(\cdot)$ |
|---|---|---|
| $B$ | $3 \cdot 10^{16}$ | 78 |
| $S$ | 4 | 9 |
| $B_{22}$ | $8 \cdot 10^{02}$ | 71 |

We get the result that problem $P2_{ell}$ is practically an ill–conditioned one. Thus to obtain a numerical solution a regularization procedure is necessary.

## 3. The parabolic Cauchy problem as a DAE

In this section the finite element solution of the parabolic problem $P2_{par}$ is investigated. For each $t \in (0,T)$ we consider

**Problem** $P2^h_{par}$ : Find $(u_h, \lambda_h) \in V_h = H^1_h(\Omega) \times H_h^{-1/2}(\Gamma)$ such that

$$\int_\Omega \frac{\partial u_h}{\partial t} v_h dx + a(u_h, v_h) + \int_{\Gamma_0} \lambda_h v_h ds = F(v_h) \quad \forall v_h \in H^1_h(\Omega), \tag{27}$$

$$\int_{\gamma_1} u_h \mu_h ds = 0 \quad \forall \mu_h \in H_h^{-1/2}(\Gamma), \tag{28}$$

$$u_h(x,0) - u_0(x) \quad \text{small}, \quad x \in \overline{\Omega}. \tag{29}$$

The representations in the parabolic case are analogous to eqs. (19) and (20). However, now the coefficients $u_i$ and $\lambda_i$ depend on the time $t$, i.e. (suppressing the x-dependence again) for each $t \in (0,T)$

$$u_h(t) = \sum_{i=p+1}^{M} u_i(t) w_i \qquad \text{in } \overline{\Omega}, \tag{30}$$

$$\lambda_h(t) = \sum_{i=p+1}^{2p} \lambda_i(t) t_i \qquad \text{on } \Gamma_0. \tag{31}$$

(Note here that $t_i$ has nothing to do with $t$. $t_i$ is a basis function associated with the knot $a_i \in \Gamma_0$.) Since eq. (28) is identical with eq. (18) we immediately get from eq. (27) the system of equations

$$A\frac{d}{dt}X(t) + BX(t) = F, \quad t \in (0,T), \tag{32}$$

where the vector $X$ is defined in eq. (21) and $F = (F_1, F_2)^T$ (here $T$ means transposition). The matrix $B$ is given in eqs. (22) or (26). $A$ is a (M,M)–matrix which can be written

$$A = \begin{pmatrix} O_1 & A_1 \\ O_{21} & A_{22} \end{pmatrix}. \tag{33}$$

Its structure is like that of $B$ in eq. (26). $O_1$ and $O_{21}$ are zero matrices of the form $(p,p)$ and $(M-p,p)$, respectively. $A_1$ and $A_{22}$ are $(p, M-p)-$ and

$(M-p, M-p)-$matrices, respectively. The elements of the last two matrices are defined by

$$A_{k;i,j} = \int_\Omega w_j w_i dx, \quad k = 1,\ 22. \tag{34}$$

By inspection for both $k$ the range of the indices $i, j$ follows easily from eq. (33).

Since $A$ is a singular matrix eq. (32) is a differential–algebraic system of equations (DAE). This is a direct consequence of the fact that problem $P1_{par}$ is a Cauchy problem. In the following this DAE is considered. For this we introduce the two vectors $\Lambda$ and $U$ with $p$ and $M-p$ components, respectively:

$$\Lambda = (\lambda_{p+1}, ..., \lambda_{2p})^T, \qquad U = (u_{p+1}, ..., u_M)^T.$$

Thus the vector $X$, eq. (21), can be written $X = (\Lambda, U)^T$. From this we get

**Lemma 1:** Assume $A_{22}$ to be a regular matrix. Then the DAE (32) can be represented in the semi explicite form ($U' = dU/dt$)

$$U' = f(\Lambda, U) := M_2\Lambda + M_1 U + M_0, \qquad t \in (0, T), \tag{35}$$

$$0 = g(\Lambda, U) := C_2\Lambda + C_1 U + C_0 \tag{36}$$

where the matrices $M_i$ and $C_i$, $i = 0, 1, 2$, are characterized in Table 2.

Tab. 2

| matrix | definition | structure |
|---|---|---|
| $M_0$ | $A_{22}^{-1}F_2$ | $(M-p, 1)$ |
| $M_1$ | $-A_{22}^{-1}B_{22}$ | $(M-p, M-p)$ |
| $M_2$ | $-A_{22}^{-1}S_{21}$ | $(M-p, p)$ |
| $C_0$ | $-A_1A_{22}^{-1}F_2 + F_1$ | $(p, 1)$ |
| $C_1$ | $A_1A_{22}^{-1}B_{22} - B_1$ | $(p, M-p)$ |
| $C_2$ | $A_1A_{22}^{-1}S_{21}$ | $(p, p)$ |

**Proof:** We insert $A$ and $B$ (from eqs. (33) and (26)) into eq. (32). So we get the two equations

$$A_{22}U' + S_{21}\Lambda + B_{22}U = F_2,$$

$$A_1U' + B_1U = F_1.$$

The first equation is directly equivalent to eq. (35). To obtain eq. (36) we multiply the first equation from the left by $A_1 A_{22}^{-1}$. Subtracting then the second equation from the first gives eq. (36).
The assumption of the Lemma (regularity of $A_{22}$) is realistic since the basis functions are linearly independent, see also definition (34). (In passing we mention that the corresponding example of section 2.1. in the parabolic case leads to a matrix $A_{22}$ with condition number $\kappa(A_{22}) \approx 26$.)
The DAE (35), (36) needs initial conditions. From eq. (29) these must be

$$u_i = u_0(a_i), \quad i = p+1, ..., M, \quad \text{or for short} \quad U(0) = u_0. \tag{37}$$

The points $a_i \in \overline{\Omega}$ are knots introduced by the finite element method. Furthermore we assume consistent initial conditions $\Lambda(0)$ satisfying

$$g(\Lambda(0), U(0)) = 0. \tag{38}$$

Theoretically the matrix $C_2$ in eq. (36) is regular. This follows from the general existence and uniqueness theorem [8] and is confirmed by computer experiments. Under this assumption, the DAE is of differential index one, see e.g. [3]. However, practically the matrix $C_2$ is ill–conditioned. Using the example represented in section 2.1. also in the parabolic case we find the condition number

$$\kappa(C_2) \approx 7 \cdot 10^{18}. \tag{39}$$

The matrix $C_2$ is practically singular, i.e. eq. (36) cannot be solved for $\Lambda$ in an ordinary sense. But this means the differential index of the DAE is practically at least two. The following Lemma shows that a time differentiation of eq. (36) leads to a new system which is again of the structure (35), (36) and which, in general, cannot be solved for $\Lambda$ with sufficient accuracy.

**Lemma 2:** Let $W, K_0$ and $W_0$ be defined by

$$W := U - M_2 C_2 \Lambda, \quad K_0 := C_1 U(0) + C_2 \Lambda(0), \quad W_0 := U(0) - M_2 C_2 \Lambda(0).$$

Then the DAE (35), (36) can be transformed into the new DAE

$$W' = \overline{f}(\Lambda, W) := \overline{M}_2 \Lambda + \overline{M}_1 W + \overline{M}_0, \tag{40}$$

$$0 = \overline{g}(\Lambda, W) := \overline{C}_2 \Lambda + \overline{C}_1 W + \overline{C}_0 \tag{41}$$

with $W(0) = W_0$.

Especially the $(p,p)-$matrix $\overline{C}_2$ is given by

$$\overline{C}_2 = (I_p + C_1 M_2) C_2 \tag{42}$$

where $I_p$ is the $(p,p)-$unit matrix. (The other matrices $\overline{M}_i$ and $\overline{C}_j$ are not further used.)

**Proof:** For short we only sketch the proof. It has the following steps. First differentiate eq. (36) with respect to $t$. Solve it for $-C_2\Lambda'$. Multiply the resulting equation with $M_2$ from the left. To this add eq. (35). Introducing now the definition of $W$ we get eq. (40). To obtain eq. (41) we multiply eq. (35) from the left with $C_1$ and combine it with the equation $0 = dg(\Lambda, U)/dt$ where $U'$ is eliminated by means of eq. (35). This yields the equation $C_1 U' + C_2 \Lambda' = 0$ which can be integrated. One can see that the integration constant must be $K_0$ given above. Into the integrated form of the equation we introduce $W$ giving at once eq. (41) with $\overline{C}_2$ defined in eq. (42). The initial condition $W(0) = W_0$ follows directly from the definition of $W$ in terms of $U$ and $\Lambda$. This proves Lemma 2.

We emphasize that to prove this Lemma no matrix inverses are used. The new DAE (40), (41) with eq. (42) shows that $\overline{C}_2$ is ill–conditioned again since $C_2$ is ill–conditioned. Thus compared with the system (35), (36) we do not obtain a new qualitative situation. (For instance the example in section 2.1. gives $\kappa(\overline{C}_2) \approx 3 \cdot 10^{18}$.) This procedure can be continued further but in all generated DAE's the coefficient matrix of $\Lambda$ is ill–conditioned.
The stated difficulties can be seen also from another point of view. We consider the question of regularity of the pencil $[A, B]$ of the DAE (32). As is known [3] the DAE is solvable if and only if $[A, B]$ is regular. This is easily illustrated. Suppose we wish to solve eq. (32) by the implicit Euler method with a constant stepsize $h$. Let $t_n = nh$ and $X^n$ be the estimate for $X(t_n)$. Then the numerical method for given $X^0$ is

$$A\frac{X^n - X^{n-1}}{h} + BX^n = F \quad \text{or} \quad (A + hB)X^n = AX^{n-1} + hF, \quad n = 1, 2, ...$$

In order to uniquely determine $X^n$ the regularity of the matrix $A + hB$ for small $h$ is needed. But for the Cauchy problem $P2_{par}$ this matrix is

Tab. 3

| $h$ | $\kappa(A+hB) \approx$ |
|---|---|
| 0.2 | $2 \cdot 10^{16}$ |
| 0.1 | $10^{17}$ |
| $10^{-2}$ | $2 \cdot 10^{18}$ |
| $10^{-6}$ | $2 \cdot 10^{18}$ |
| $10^{-10}$ | $4 \cdot 10^{18}$ |
| $10^{-14}$ | $3 \cdot 10^{19}$ |
| $10^{-15}$ | $\infty$ |

ill–conditioned (nearly singular). For illustration we give in Table 3 the corresponding condition number $\kappa$ for the example of section 2.1.
The ill–conditioness of the pencil $[A, B]$ is reflected in numerical computations. In fact, the direct application of the code RADAU5 [7] to solve the DAE (32) of the example in section 2.1. shows that it does not work. The pencil $[A, B]$ is practically singular in the interval of $h$ used in the table.

## 4. Regularization

After the discussion of the difficulties of the DAE (32) we consider in this section the regularization of the system of equations. One possibility is the following regularized form of eq. (32)

$$B^T A \frac{d}{dt} X_\alpha(t) + (B^T B + \alpha I) X_\alpha(t) = B^T F, \quad t \in (0, T), \tag{43}$$

with a small parameter $\alpha > 0$. If $A$ is the zero matrix then it is the well known Tychonov regularization.
If consistent initial values $\Lambda_\alpha(0)$ are assumed, system (43) can be solved for $\alpha$ not to small. To compute consistent initial values eq. (43) can be written

$$D_3 U'_\alpha + D_2(\alpha)\Lambda_\alpha + D_1 U_\alpha = D_0,$$

$$G_3 U'_\alpha + G_2 \Lambda_\alpha + G_1(\alpha) U_\alpha = G_0$$

where the matrices $D_i, G_i$, $i = 0, .., 3$, are given in Table 4. Especially, as can be seen by its definition the matrix $G_3$ (which does not depend on $\alpha$) is of moderate regularity and condition. (In the example of section 2.1. it is $\kappa(G_3) \approx 3 \cdot 10^3$.) Therefore the last equation can be solved for $U_\alpha$ :

$$U'_\alpha = f^r_\alpha(\Lambda_\alpha, U_\alpha) := M^r_2 \Lambda_\alpha + M^r_1(\alpha) U_\alpha + M^r_0, \qquad U_\alpha(0) = U_{\alpha 0}. \tag{44}$$

Furthermore, we multiply the second equation from the left by $D_3 G_3^{-1}$ and subtract it from the first. The result is the regularized equation of constraints

$$0 = g^r_\alpha(\Lambda_\alpha, U_\alpha) := C^r_2(\alpha)\Lambda_\alpha + C^r_1(\alpha) U_\alpha + C^r_0. \tag{45}$$

The matrices $M^r_i$ and $C^r_i$, $i = 0, 1, 2$, are defined in Table 4.

Tab. 4

| matrix | definition | structure |
|---|---|---|
| $D_0$ | $S_{21}^T F_2$ | (p,1) |
| $D_1$ | $S_{21}^T B_{22}$ | (p,M-p) |
| $D_2(\alpha)$ | $S_{21}^T S_{21} + \alpha I_p$ | (p,p) |
| $D_3$ | $S_{21}^T A_{22}$ | (p,M-p) |
| $G_0$ | $B_1^T F_1 + B_{22}^T F_2$ | (M-p,1) |
| $G_1(\alpha)$ | $B_1^T B_1 + B_{22}^T B_{22} + \alpha I_{M-p}$ | (M-p,M-p) |
| $G_2$ | $B_{22}^T S_{21}$ | (M-p,p) |
| $G_3$ | $B_1^T A_1 + B_{22}^T A_{22}$ | (M-p,M-p) |
| $M^r_0$ | $G_3^{-1} G_0$ | (M-p,1) |
| $M^r_1(\alpha)$ | $-G_3^{-1} G_1(\alpha)$ | (M-p,M-p) |
| $M^r_2$ | $-G_3^{-1} G_2$ | (M-p,p) |
| $C^r_0$ | $D_3 G_3^{-1} G_0 - D_0$ | (p,1) |
| $C^r_1(\alpha)$ | $-D_3 G_3^{-1} G_1(\alpha) + D_1$ | (p,M-p) |
| $C^r_2(\alpha)$ | $-D_3 G_3^{-1} G_2 + D_2(\alpha)$ | (p,p) |

Accepting the regularization, the equation of constraints (45) can be solved for $\Lambda_\alpha$. Hence given $U_\alpha(0)$ the consistent initial value $\Lambda_\alpha(0)$ can be calculated. In Table 5 we again computed for the example of section 2.1. the condition number of $C^r_2(\alpha)$ for some values of $\alpha$.

For $\alpha = 0$ the matrix $C^r_2$ is nearly singular. Besides eqs. (44), (45) for $t \in (0, T)$ the singular perturbation problem

Tab. 5

| $\alpha$ | $\kappa(C_2^r(\alpha)) \approx$ |
|---|---|
| $10^{-1}$ | 1.4 |
| $10^{-2}$ | 6 |
| $10^{-3}$ | 87 |
| $10^{-4}$ | 2000 |
| $10^{-8}$ | $9 \cdot 10^6$ |
| $10^{-14}$ | $4 \cdot 10^{12}$ |
| 0 | $10^{14}$ |

$$U'_{\alpha,\epsilon} = f^r_\alpha(\Lambda_{\alpha,\epsilon}, U_{\alpha,\epsilon}), \quad U_{\alpha,\epsilon}(0) = U_{\alpha 0}, \tag{46}$$

$$\epsilon\Lambda'_{\alpha,\epsilon} = -g^r_\alpha(\Lambda_{\alpha,\epsilon}, U_{\alpha,\epsilon}), \quad \Lambda_{\alpha,\epsilon}(0) = \Lambda_{\alpha 0}, \tag{47}$$

is considered. $\epsilon > 0$ is also a small parameter being in general different from $\alpha$.
The idea is to choose a fixed $\alpha$ such that the matrix $C_2^r(\alpha)$ has a reasonable condition. Then we solve the singular perturbation problem (46), (47) where, of course, the limit $\epsilon \to 0$ is of interest. Singular perturbation theory gives the following result :

**Lemma 3:** Assume that eqs. (44), (45) have a solution, and that the real parts of the eigenvalues $\mu_i(\alpha)$ of the matrix $-\partial g^r_\alpha/\partial\Lambda_\alpha = -C_2^r(\alpha)$ are negative:

$$Re\{\mu_i(\alpha)\} < 0 \qquad \text{for} \quad i = 1, ..., p.$$

Then the solution of (46), (47) converges to that of (44), (45) as $\epsilon \to 0^+$.

**Proof:** Since a similar result is discussed in [3, p. 59] we only sketch the proof. Let the solution be written in the form (the index $\alpha$ is suppressed here)

$$U(t) = \overline{U}^0(t) + \epsilon\widetilde{U}^1(t) + \overline{U}(\tau) + \epsilon\widetilde{U}(\tau) \tag{48}$$

$$\Lambda(t) = \overline{\Lambda}^0(t) + \epsilon\widetilde{\Lambda}^1(t) + \overline{\Lambda}(\tau) + \epsilon\widetilde{\Lambda}(\tau) \tag{49}$$

where $\tau = t/\epsilon$. $\overline{U}^0(t)$ and $\overline{\Lambda}^0(t)$ are assumed to satisfy the reduced problem (44), (45). The terms with a tilde are bounded uniformly in $\epsilon$, $t$ for $0 \le t \le$

$T, \quad 0 \leq \epsilon \leq \epsilon_0, \quad \epsilon_0 > 0$. We insert (48), (49) into eqs. (46), (47) and consider for $\epsilon \to 0^+$ the leading terms (these are for $\epsilon^{-1}$ and $\epsilon^0$). This gives the differential equations for $\overline{U}(\tau)$ and $\overline{\Lambda}(\tau)$ :

$$\frac{d}{d\tau}\overline{U}(\tau) = 0, \qquad \frac{d}{d\tau}\overline{\Lambda}(\tau) = -C_2^r(\alpha)\overline{\Lambda}(\tau) - C_1^r(\alpha)\overline{U}(\tau), \quad \tau \in (0, T/\epsilon).$$

Using now the assumption on the eigenvalues of $-C_2^r(\alpha)$ we see that $\overline{\Lambda}(\tau)$ goes to zero for $\epsilon \to 0^+$ ($t$ fixed). This proves Lemma 3.

The essential requirement in our context is the assumption on $-C_2^r(\alpha)$. From the analytical form of $C_2^r$, see Table 4, it is expected that for $\alpha$ not to small all real parts $Re\{\mu_i(\alpha)\}$ are negative while for $\alpha \to 0$ this matrix may also have eigenvalues with positive real parts. This is confirmed by numerical experiments. In the example of section 2.1. we observe the following:

$$Re\{\mu_i(\alpha)\} < 0 \quad \text{for} \quad \alpha \geq 10^{-5}, \quad i = 1, ..., p.$$

However, for $\alpha \lesssim 10^{-5}$ one or more of the quantities $Re\{\mu_i(\alpha)\}$ are positive. In the first case ($\alpha \geq 10^{-5}$) the assumptions of Lemma 3 are fulfilled. In this case the solution of (46), (47) follows by standard theory [7].

## 4. Conclusion

The application of a Lagrange multiplier method enabled us to incorporate the boundary conditions of the Cauchy problem into the variational equation (eq.(14)). This formulation is the reason that the ill–posed Cauchy problem can be transformed into a system of DAE (eq. (32)). Theoretically, this system is of a simple form. Especially it is of index one. However, it is (practically) extremely ill–conditioned. This can be seen, e. g., if the system is written in the semi explicit form (eqs. (35), (36)). The reason of the ill–conditioness is the ill–posed nature of the Cauchy problem. Therefore, for a numerical solution a regularization is necessary. One such possibility has been discussed. After regularization the problem can be solved by known software.

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