Numerical calculations in a problem with heat conduction and heat production

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Numerical calculations in a problem with heat conduction and heat production

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Abstract

The temperature u of an exothermic reacting chemical in a vessel, governed by the equation

$$u_t = \Delta u + Ae^u ,$$

is studied. With the initial condition $u(\underline{x},0) = u_0$ and the boundary condition $u(\underline{x},t) = 0$ at the wall of the vessel, a critical initial value u_0^* is calculated such that if $u_0 < u_0^*$, the temperature remains bounded and otherwise, if $u_0 > u_0^*$, an explosion occurs. The cases that the vessel is a slab, an infinite cylinder, or a sphere are considered. The possible steady states, together with the questions of their stability are studied; this study should be considered as a personal presentation of some results, which, in principle, can be extracted from the literature.
The problem is solved numerically, using standard techniques for solving partial differential equations (Crank Nicolson).
A number of numerical results are presented in order to justify the suppositions that are fundamental for the algorithm.

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0. Statement of the problem

A vessel is filled with a chemical having the homogeneous temperature u_0. An exothermic reaction takes place. The wall of the vessel is kept at constant temperature. Therefore the temperature of the reacting mass changes by heat conduction to the wall and by heat production due to the reaction. The problem is to determine a critical value u_0^* such that, if $u_0 < u_0^*$, the temperature of the chemical remains bounded and that, if $u_0 > u_0^*$, the temperature tends to infinity (explosion).
The cases that the vessel is a slab, an infinite cylinder, or a sphere are considered.

1. Mathematical model

The temperature of the reacting mass is governed by the equation ([1, ch. 2])

$$u_t = \operatorname{div}(k \operatorname{grad} u) + W(u)/(\rho C_v) \ , \tag{1.1}$$

where

- t time
- k coefficient of thermal conductivity
- ρ density
- C_v specific heat at constant volume
- W heat production per unit time and per unit volume.

The heat production term W has the following form (Arrhenius' law)

$$W(u) = A_0 e^{-E/(Ru)} \ , \tag{1.2}$$

where

- E internal energy
- R gas constant
- A_0 constant depending on the reacting mass.

The linearization of (1.2) around u_0, supposing that k is a constant and choosing suitable dimensionless quantities, transforms (1.1) into

$$u_t = \Delta u + Ae^u \ . \tag{1.3}$$

Hence, the problem can be formulated as follows. Let V be the reactant and let S denote the wall. Let u be the solution of

$$\left.\begin{aligned} u_t &= \Delta u + Ae^u , && \underline{x} \in V,\ t > 0 \\ u(\underline{x},0) &= u_0 , && \underline{x} \in V \\ u(\underline{x},t) &= 0 , && \underline{x} \in S,\ t > 0 . \end{aligned}\right\} \qquad (1.4)$$

Determine u_0^* such that, if $u_0 < u_0^*$, $u(x,t)$ remains bounded; otherwise, if $u_0 > u_0^*$, $u(x,t)$ tends to infinity.

If V is a slab, an infinite cylinder, or a sphere, (1.4) transforms (after appropriate scaling and because of symmetry) into

$$\left.\begin{aligned} u_t &= u_{xx} + \frac{n}{x} u_x + Ae^u , && 0 < x < 1,\ t > 0 \\ u(x,0) &= u_0 , && 0 < x < 1 \\ u(1,t) &= 0,\ u_x(0,t) = 0, && t > 0 , \end{aligned}\right\} \qquad (1.5)$$

where $n = 0$ if V is a slab, $n = 1$ if V is a cylinder, $n = 2$ if V is a sphere.

2. Some properties of the model

In this section some - for our purpose essential - properties of the model will be discussed.

In principle, one can extract these properties from the literature ([1, ch. 3 + references], [2]).

The following should be considered as a result of the study of the literature, with a personal presentation.

2.1. First, we study the steady state solutions of equation (1.5).

These satisfy

$$\left.\begin{aligned} &\frac{d^2v}{dx^2} + \frac{n}{x}\frac{dv}{dx} + Ae^v = 0 , \quad 0 < x < 1 \\ &\left.\frac{dv}{dx}\right|_{x=0} = 0 \\ &v(1) = 0 . \end{aligned}\right\} \qquad (2.1)$$

We write the solutions of (2.1), if any, as

$$\left.\begin{aligned} v(x) &= v(0) + f(y) \ , \\ \text{where} & \\ y &= \sqrt{A}e^{v(0)/2}x \ . \end{aligned}\right\} \tag{2.2}$$

It follows that f satisfies

$$\left.\begin{aligned} &\frac{d^2f}{dy^2} + \frac{n}{y}\frac{df}{dy} + e^f = 0 \\ &\left.\frac{df}{dy}\right|_{y=0} = 0 \\ &f(0) = 0 \ . \end{aligned}\right\} \tag{2.3}$$

The relation between v(0) and A follows from the boundary condition for $x = 1$

$$f(\sqrt{A}e^{v(0)/2}) = -v(0) \ . \tag{2.4}$$

Lemma. (2.4), considered as equation in A with v(0) fixed, has exactly one solution.

Proof. Multiply (2.3) by y^n to find

$$y^n \frac{d^2f}{dy^2} + ny^{n-1}\frac{df}{dy} + y^n e^f = 0 \ ,$$

or

$$\frac{d}{dy}\left(y^n \frac{df}{dy}\right) = -y^n e^f \ .$$

Since $\left.\frac{df}{dy}\right|_{y=0} = 0$, we obtain

$$\frac{df}{dy} = -\frac{1}{y^n}\int_0^y t^n e^{f(t)}\,dt \ .$$

We conclude that $\frac{df}{dy} < 0$, so f is decreasing and, clearly, $\lim_{y\to\infty} f(y) = -\infty$.

Thus, with v(0) fixed, there is exactly one value of A satisfying (2.4).□

Conversely, considering (2.4) as equation in $v(0)$ with A fixed, it turns out that (2.4) has one or more solutions if $A \leq A_{cr}$ and no solution if $A > A_{cr}$. We now develop this assertion for $n = 0$, 1 or 2.

(i) $n = 0$.

The solution f of (2.3) is given by

$$f(y) = -2 \log(\cosh(y/\sqrt{2})) \; . \qquad (2.5)$$

Hence, (2.4) reduces to

$$\sqrt{\frac{A}{2}} \cosh(S) = S \; ,$$

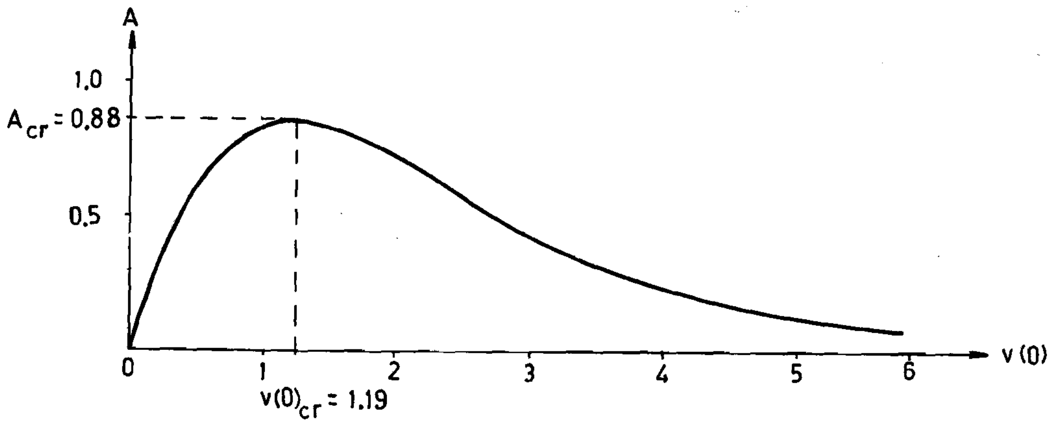
where $S = \sqrt{\frac{A}{2}}\, e^{v(0)/2}$.

Consequently, $A_{cr} = 2/(\sinh^2(S_{cr}))$, where S_{cr} satisfies $S \tanh(S) = 1$.

Numerical values:

$$A_{cr} \doteq 0.88 \; , \quad v(0)_{cr} \doteq 1.19 \; .$$

The dependence of A on $v(0)$ is illustrated in the following diagram.



(ii) $n = 1$.

The solution f of (2.3) is now given by

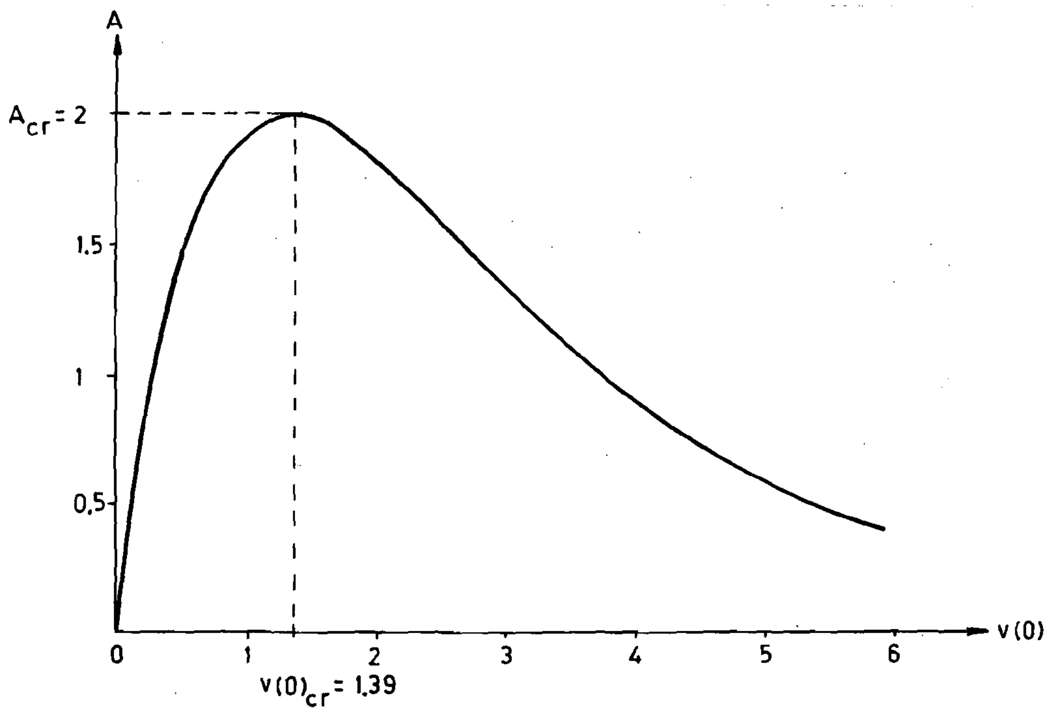
$$f(y) = -2 \log(1 + y^2/8) \; . \qquad (2.6)$$

Using (2.6), (2.4) can be written as

$$8S = A(1 + S)^2 \; ,$$

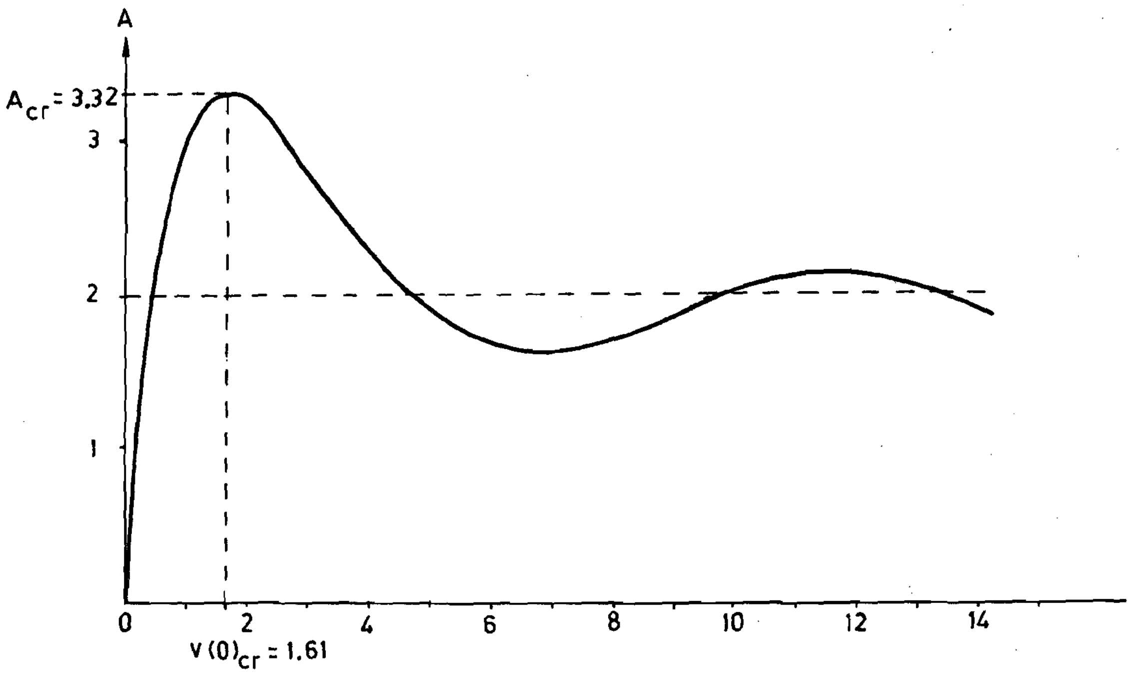
where $S = \frac{A}{8}\, e^{v(0)}$.

Consequently, $A_{cr} = 2$, $v(0)_{cr} = \log 4 \doteq 1.39$.
The dependence of A on v(0) is illustrated in the following diagram.



iii) n = 2.

In this case the solution of (2.3) is not analytically known. From numerical calculations it follows that $A_{cr} \doteq 3.32$, $v(0)_{cr} \doteq 1.61$ and the following diagram.



2.2. We are now going to investigate how a small perturbation of a steady state solution varies with time.
Let

$$u(x,t) = v(x) + \varphi(x,t) \tag{2.7}$$

be a solution of

$$\left.\begin{aligned} & u_t = u_{xx} + \frac{n}{x} u_x + Ae^u \\ & u_x(0,t) = 0 , \quad u(1,t) = 0 , \end{aligned}\right\} \tag{2.8}$$

where v(x) is a steady state solution and φ a small perturbation of it. Substituting (2.7) in (2.8) and linearizing we obtain

$$\left.\begin{aligned} & \varphi_t = \varphi_{xx} + \frac{n}{x} \varphi_x + Ae^{v(x)} \varphi = 0 \\ & \varphi_x(0,t) = 0 , \quad \varphi(1,t) = 0 . \end{aligned}\right\} \tag{2.9}$$

We look for non-trivial solutions of (2.9) by applying the technique of separation of variables.
Supposing that

$$\varphi(x,t) = F(x).G(t)$$

we find

$$\frac{dG}{dt} = -\lambda G, \text{ so } G(t) = e^{-\lambda t} \tag{2.10}$$

$$\left.\begin{aligned} & \frac{d^2F}{dx^2} + \frac{n}{x}\frac{dF}{dx} + (Ae^{v(x)} + \lambda)F = 0 \\ & \left.\frac{dF}{dx}\right|_{x=0} = 0 , \quad F(1) = 0 , \end{aligned}\right\} \tag{2.11}$$

where λ is a constant such that (2.11) has solutions that are not identically zero. λ is called an eigenvalue and F(x) the eigenfunction belonging to it.
From the theory of Sturm-Liouville we have

a) The eigenvalues are real and can be numbered such that

$$\lambda_0 < \lambda_1 < \lambda_2, \ldots ,$$

with $\lambda_n \to \infty$.

b) The eigenfunction $F_i(x)$ belonging to λ_i has exactly i zeros in (0,1).

c) The functions $F_n(x)$ form a complete set, so $\varphi(x,t)$ can be written as

$$\varphi(x,t) = \sum_{n=0}^{\infty} a_n F_n(x) e^{-\lambda_n t} .$$

Consequently, if $\lambda_0 > 0$, the perturbation φ decreases ($v(x)$ is stable); otherwise, if $\lambda_0 < 0$, φ increases ($v(x)$ is unstable).

Therefore, to investigate whether $v(x)$ is stable or unstable we try to determine the sign of λ_0.

For this purpose we look at the following problem that arises if we drop the condition $F(1) = 0$ in (2.11) and put $\lambda = 0$. Hence,

$$\left.\begin{aligned} &\frac{d^2F}{dx^2} + \frac{n}{x}\frac{dF}{dx} + Ae^{v(x)}F = 0 \\ &\left.\frac{dF}{dx}\right|_{x=0} = 0 \ . \end{aligned}\right\} \qquad (2.12)$$

The solutions of (2.12) can be written as $F(x) = CH(x)$, with $H(0) = 1$ and C a constant.

Let ξ be the first zero of $H(x)$. Then it follows from the properties a) and b) that zero is the smallest eigenvalue of

$$\left.\begin{aligned} &\frac{d^2F}{dx^2} + \frac{n}{x}\frac{dF}{dx} + (Ae^{v(x)} + \lambda)F = 0 \\ &\left.\frac{dF}{dx}\right|_{x=0} = 0 \ , \quad F(\xi) = 0 \ . \end{aligned}\right\}$$

Therefore,

- if $\xi > 1$, then (2.11) has only positive eigenvalues;
- if $\xi < 1$, then (2.11) has at least one negative eigenvalue.

This follows from the fact that, according to the theory of Sturm-Liouville, the smallest eigenvalue of

$$\left.\begin{aligned} &\frac{d^2F}{dx^2} + \frac{n}{x}\frac{dF}{dx} + (Ae^{v(x)} + \lambda)F = 0 \\ &\left.\frac{dF}{dx}\right|_{x=0} = 0 \ , \quad F(\alpha) = 0 \ , \end{aligned}\right\}$$

is a decreasing function of α.

□ Summarizing, the problem of investigating whether $v(x)$ is stable or unstable reduces to the location of the first zero ξ from the solutions of

$$\left.\begin{aligned} &\frac{d^2F}{dx^2} + \frac{n}{x}\frac{dF}{dx} + Ae^{v(x)}F = 0 \\ &\left.\frac{dF}{dx}\right|_{x=0} = 0 \ , \end{aligned}\right\} \qquad (2.13)$$

- if $\xi > 1$, then $v(x)$ is stable,
- if $\xi < 1$, then $v(x)$ is unstable. □

The solutions of (2.13) are

$$F(x) = C\left(x \frac{dv}{dx} + 2\right) \ , \qquad (2.14)$$

where C is a constant.
From (2.2) it follows that

$$F(x) = C\left(y \frac{df}{dy} + 2\right) \ ,$$

where $y = \sqrt{A}e^{v(0)/2}x$.
For the first zero ξ of $F(x)$ we have

$$\xi = \frac{y_0}{\sqrt{A}e^{v(0)/2}} \ , \qquad (2.15)$$

where y_0 is the smallest root of

$$y \frac{df}{dy} + 2 = 0 \ . \qquad (2.16)$$

The function f is decreasing so it follows from (2.4) that $\sqrt{A}e^{v(0)/2}$ is an increasing and ξ in (2.15) is a decreasing function of $v(0)$.
Let $v^*(0)$ be the value of $v(0)$ such that $\xi = 1$, then it follows that

- if $v(0) < v^*(0)$ then $v(x)$ is stable,
- if $v(0) > v^*(0)$ then $v(x)$ is unstable.

$v^*(0)$ is determined from

$$\left.\begin{aligned} &1 = y_0/(\sqrt{A^*}e^{v^*(0)/2}) \\ &f(\sqrt{A^*}e^{v^*(0)/2}) = -v^*(0) \end{aligned}\right\}$$

or

$$\left.\begin{aligned} &v^*(0) = -f(y_0) \\ \text{and}\quad &A^* = y_0^2/e^{v^*(0)} \ . \end{aligned}\right\} \tag{2.17}$$

Finally we show that A, considered as a function of v(0) given by (2.4), has its first extreme value in $v^*(0)$.
From (2.4) it follows that the extreme values of A considered as a function of v(0) satisfy

$$f(\sqrt{A}e^{v(0)/2}) = -v(0) \tag{2.4}$$

$$\sqrt{A}e^{v(0)/2} \left.\frac{df}{dy}\right|_{y = \sqrt{A}e^{v(0)/2}} + 2 = 0 \ . \tag{2.18}$$

So we find $\sqrt{A}e^{v(0)/2} = y_i$, where y_i is a root of (2.16). Using (2.4) we obtain

$$v(0) = -f(y_i) \ .$$

The smallest value, $v(0)_{cr}$, introduced in section 2.1, where A is extreme, equals

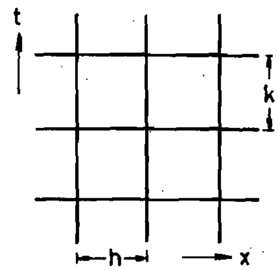
$$v(0)_{cr} = -f(y_0) = v^*(0) \ .$$

2.3. We conclude by making some suppositions that are useful for the algorithm which we shall describe in the next section.
Only those cases are examined where an unstable steady state solution exists.
Let $u(x,t,u_0)$ denote the solution of (1.5). We suppose that, if at some time t_0 $u(x,t_0,u_0) > v_\ell(x)$ $(0 < x < 1)$, then $u_0 > u_0^*$; otherwise if at some time t_0 $u(x,t_0,u_0) < v_\ell(x)$ $(0 < x < 1)$, then $u_0 < u_0^*$.
Indeed, in all cases that were examined there was a time t_0 where either $u(x,t_0,u_0) > v_\ell(x)$ or $u(x,t_0,u_0) < v_\ell(x)$.
With this supposition u_0^* can be determined by successive halving the interval $(0,v_\ell(0))$.

3. Numerical method

To solve the problem numerically, we start by replacing (1.5) by a finite difference approximation (Crank Nicolson).

We introduce a rectilinear grid with sides parallel to the x- and t-axes, h and k being the grid spacings in the x- and t-directions respectively.



The grid points are:

$$x_i = i * h,\ i = 0,1,\dots,M,\ Mh = 1$$

$$t_j = j * k,\ j = 0,1,\dots .$$

We write down the differential equation of (1.5) for the points

$$x_i = i * h,\ i = 0,1,\dots,M-1$$

$$t_{j+\frac{1}{2}} = (j + \tfrac{1}{2})k,\ j = 0,1,\dots .$$

We have, denoting $f(x_i,t_j)$ by $f_{i,j}$,

$$(u_t)_{i,j+\frac{1}{2}} = \frac{u_{i,j+1} - u_{i,j}}{k} + O(k^2)\ ,\quad k \downarrow 0 \tag{3.1}$$

$$(u_{xx})_{i,j+\frac{1}{2}} =$$

$$= \tfrac{1}{2}\left[\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h^2}\right] +$$

$$+ O(h^2) + O(k^2),\ h \downarrow 0,\ k \downarrow 0 \tag{3.2}$$

if $i \neq 0$

$$(\tfrac{n}{x}\, u_x)_{i,j+\frac{1}{2}} = \frac{n}{ih}\ \tfrac{1}{2}\left[\frac{u_{i+1,j} - u_{i-1,j}}{2h} + \frac{u_{i+1,j+1} - u_{i-1,j+1}}{2h}\right] +$$

$$+ O(h^2) + O(k^2),\ h \downarrow 0,\ k \downarrow 0 . \tag{3.3}$$

If $i = 0$, then we have, because $u_x(0,t) = 0$,

$$(\tfrac{n}{x}\, u_x)_{0,j+\frac{1}{2}} = (nu_{xx})_{0,j+\frac{1}{2}} . \tag{3.4}$$

Furthermore,

$$e^{u_{i,j+\frac{1}{2}}} = \tfrac{1}{2}[e^{u_{i,j+1}} + e^{u_{i,j}}] + O(k^2) =$$

$$= e^{u_{i,j}}[1 + \tfrac{1}{2}(u_{i,j+1} - u_{i,j})] + O(k^2),\ k \downarrow 0\ . \qquad (3.5)$$

It follows from the boundary conditions that

$$\left.\begin{aligned} & u_{i,0} = u_0 \\ & u_{M,j} = 0 \\ & (u_x)_{0,j} = 0 = \frac{u_{1,j} - u_{-1,j}}{2h} + O(h^2),\ h \downarrow 0\ . \end{aligned}\right\} \qquad (3.6)$$

If the order terms are neglected the finite difference approximation of (1.5) arises by substituting (3.1) to (3.5) incl. in the differential equation of (1.5) for the points

$$(x_i, t_{j+\frac{1}{2}}),\ i = 0,1,\ldots,M-1,\ j = 0,1,\ldots\ .$$

$u_{-1,j}$ and $u_{M,j}$ are eliminated by means of (3.6).
We formulate the above with matrices as follows.
We introduce the M-dimensional vectors

$$\underline{U}_0 = \begin{pmatrix} u_0 \\ u_0 \\ \vdots \\ u_0 \end{pmatrix} \qquad \underline{U}_j = \begin{pmatrix} U_{0,j} \\ U_{1,j} \\ \vdots \\ U_{M-1,j} \end{pmatrix} \qquad j = 0,1,\ldots$$

$$\underline{f}(\underline{U}_j) = kA \begin{pmatrix} e^{U_{0,j}} \\ e^{U_{1,j}} \\ \vdots \\ e^{U_{M-1,j}} \end{pmatrix}$$

the tridiagonal M × M-matrices B and C

$$B = \begin{pmatrix} \alpha_0 & \beta_0 & & & & \\ \gamma_1 & \alpha_1 & \beta_1 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \beta_{M-2} \\ & & & & \gamma_{M-1} & \alpha_{M-1} \end{pmatrix}$$

where

$$\alpha_0 = 1 + \lambda(n+1) - \tfrac{1}{2}Ake^{U_{0,j}}, \quad \lambda = \frac{k}{h^2}$$

$$\alpha_i = 1 + \lambda - \tfrac{1}{2}Ake^{U_{i,j}}, \quad i = 1,\ldots,M-1$$

$$\beta_0 = -\lambda(n+1), \quad \beta_i = -\tfrac{1}{2}\lambda(1 + \frac{n}{2i}), \quad i = 1,\ldots,M-2$$

$$\gamma_i = -\tfrac{1}{2}\lambda(1 - \frac{n}{2i}), \quad i = 1,\ldots,M-1 .$$

The matrix C is found from B by replacing λ by $-\lambda$.

As an approximation of $u_{i,j}$ in (1.5) we take $U_{i,j}$ which satisfies

$$\left.\begin{aligned} &B\underline{U}_{j+1} = C\underline{U}_j + \underline{f}(\underline{U}_j), \quad j = 0,1,\ldots \\ &\underline{U}_0 = \begin{pmatrix} u_0 \\ u_0 \\ \vdots \\ u_0 \end{pmatrix} . \end{aligned}\right\} \qquad (3.7)$$

Given $\underline{U}_j$ we can calculate $\underline{U}_{j+1}$ from (3.7) solving the tridiagonal system. If we look at the approximation in a fixed point (x,t), we expect, because of (3.1) - (3.7), that

$$U(x,t) = u(x,t) + C_1(x,t)h^2 + C_2(x,t)k^2 + $$
$$+ o(h^2) + o(k^2), \quad h \downarrow 0, \ k \downarrow 0 . \qquad (3.8)$$

We make the following suppositions (cf. section 2.3), which in all cases examined appeared to be satisfied.

(i) The difference equation in (3.7) has (with appropriate A and h) at least two steady state solutions, a stable one $\underline{U}^s$ and an unstable one $\underline{U}^\ell$.

(ii) Successive solving of (3.7) with u_0, h, k and A given, we find a j_0 such that either $\underline{U}_{j_0} < \underline{U}^\ell$ or $\underline{U}_{j_0} > \underline{U}^\ell$.

Let $U_0^*(h,k,A)$ be defined so that, if $u_0 < U_0^*(h,k,A)$, we find when solving (3.7) successively, a $\underline{U}_{j_0} < \underline{U}^\ell$, and if $u_0 > U_0^*(h,k,A)$, a $\underline{U}_{j_0} > \underline{U}^\ell$ respectively.
$U_0^*(h,k,A)$ is taken as an approximation of u_0^*.

Remark. $\underline{U}^1 > \underline{U}^2$ stands for $(\underline{U}^1)_i > (\underline{U}^2)_i$, $i = 0,1,\ldots,M-1$.

Now $U_0^*(h,k,A)$ can be calculated by successive halving of the interval $I := (0,(U^\ell)_0)$.

Given h, k and A, we use the following algorithm to calculate $U_0^*(h,k,A)$.

1) Calculate $\underline{U}^\ell$.
2) Determine u_0 by halving I.
3) Solve (3.7) successively; then it follows that either $u_0 > U_0^*(h,k,A)$ or $u_0 < U_0^*(h,k,A)$.
4) Adapt I and go back to 2.

Sub 1. To calculate $\underline{U}^\ell$ we proceed as follows:
A steady state solution of (3.7) satisfies

$$(B - C)\underline{U} = \underline{f}(\underline{U}) \ .$$

To solve this non-linear system we use Newton's method

$$(E - \frac{\partial \underline{g}}{\partial \underline{U}}\bigg|_{\underline{U}=\underline{U}^n})\underline{U}^{n+1} = \underline{g}(\underline{U}^n) - (\frac{\partial \underline{g}}{\partial \underline{U}}\bigg|_{\underline{U}=\underline{U}^n})\underline{U}^n, \quad n = 0,1,2,\ldots \ , \qquad (3.9)$$

where

$$E = \frac{1}{k}\,(B - C) \ , \quad \underline{g}(\underline{U}) = \frac{1}{k}\,\underline{f}(\underline{U}) \ ,$$

$$(\frac{\partial \underline{g}}{\partial \underline{U}})_{i,j} = \frac{\partial g_i}{\partial (\underline{U})_j} \ .$$

If $\underline{U}_0$ is appropriate, we have $\lim_{n\to\infty} \underline{U}^n = \underline{U}^\ell$. As $\underline{U}_0$ we take the unstable steady state solution of the differential equation in (1.5). If n = 0 or n = 1, then this solution is analytically known. If n = 2, we determine it numerically.

We expect that, analogously to (3.8),

$$U_0^*(h,k,A) = u_0^* + C_1 h^2 + C_2 k^2 + o(h^2) + o(k^2), \; h \downarrow 0, \; k \downarrow 0. \quad (3.10)$$

Numerical experimentation has supported this supposition and thus we can apply extrapolation, if desired so.

4. Numerical results

As an illustration of the numerical method we present some intermediate results for the case n = 0, A = 0.5.

Steady state solutions of the difference equation (3.7).

h = 1/8.

x_i	Stable solution $\underline{U}^s$	Unstable solution $\underline{U}^\ell$
0	0.329 301 216 8	2.891 333 774
0.125	0.323 871 543 1	2.820 953 600
0.25	0.307 641 324 7	2.619 379 233
0.375	0.280 784 442 1	2.310 561 119
0.5	0.243 582 495 9	1.922 992 386
0.625	0.196 413 271 8	1.481 975 217
0.75	0.139 736 002 8	1.006 570 302
0.875	0.074 074 591 7	0.509 788 821
1	0	0

Solving (3.7) successively, $h = \frac{1}{8}$, $k = \frac{1}{64}$.

We find with $u_0 = 2.272\ 672\ 213\ 04$

$$\underline{U}_{30} = \begin{pmatrix} 2.889\ 856\ 0 \\ 2.819\ 574\ 4 \\ 2.618\ 258\ 3 \\ 2.309\ 770\ 7 \\ 1.922\ 516\ 7 \\ 1.481\ 740\ 8 \\ 1.006\ 483\ 6 \\ 0.509\ 768\ 6 \\ 0 \end{pmatrix}$$

and with $u_0 = 2.273\ 705\ 115\ 69$ we find

$$\underline{U}_{21} = \begin{pmatrix} 2.892\ 422\ 8 \\ 2.822\ 482\ 1 \\ 2.622\ 006\ 1 \\ 2.314\ 421\ 5 \\ 1.927\ 668\ 0 \\ 1.486\ 669\ 1 \\ 1.010\ 365\ 8 \\ 0.511\ 907\ 0 \end{pmatrix}$$

Approximations of u_0^*.

$k = h^2$

h	$U_0^*(h,k,A)$	Extrapolated values
1/4	2.28612	
1/6	2.27592	2.26776
1/8	2.27283	2.26886
1/10	2.27154	2.26925
1/12	2.27089	2.26941
1/16	2.27029	2.26952

$k = h$

h	$U_0^*(h,k,A)$	Extrapolated values
1/6	2.32287	
1/8	2.30475	2.28145
1/12	2.28844	2.27539
1/16	2.28145	2.27246

To choose a value of k, when h is given, we have to take into account a number of contradictory demands. On the one hand we want a large k to reach quickly the time t_0, whereupon either $\underline{U}_{j_0} > \underline{U}^{\ell}$ or $\underline{U}_{j_0} < \underline{U}^{\ell}$. On the other hand, it appears from the table that a large k leads to a bad approximation of u_0. This means that $|C_2| >> |C_1|$ in (3.10).
An optimum value of k is about $\frac{|C_1|}{|C_2|}$ h.
In this case we have $\frac{|C_2|}{|C_1|} \sim 10$.
As an illustration we tabulate the approximations u_0^* for $k = \frac{1}{3}h$.

$k = \frac{1}{3} h$

h	$U_0^*(h,k,A)$	Extrapolated values
1/4	2.29147	
1/6	2.28146	2.27345
1/8	2.27702	2.27131
1/12	2.27331	2.27034
1/16	2.27184	2.26995

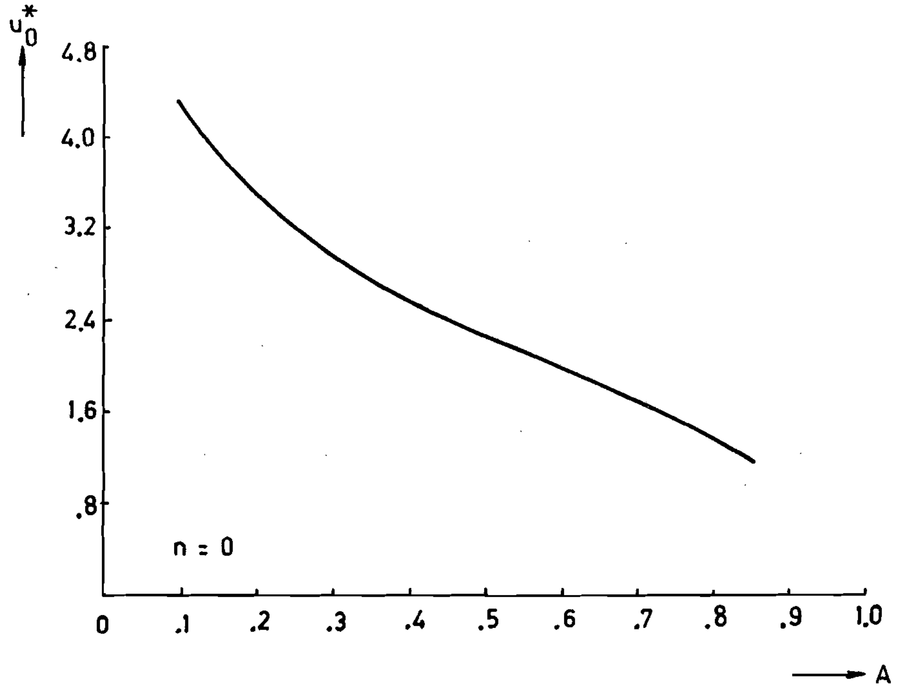
For practical reasons we have dropped the idea of trying to determine an optimum value of k in all cases. We always took $k = h^2$.
Finally, we present a table and a plot of u_0^*. The tabulated values were obtained by extrapolation and have a relative error of at most approx. 0.001. Our algorithm was not applicable to small values of A for n = 2. These cases were not further examined because there was no need for them.

Table of u_0^*.

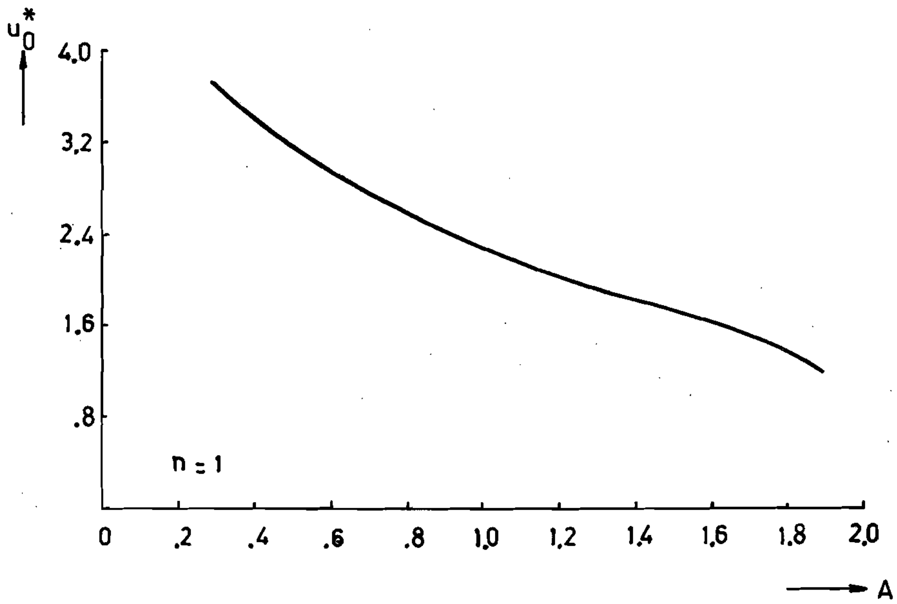
$n = 0$	A	u_0^*
	0.1	4.30
	0.2	3.48
	0.3	2.976
	0.4	2.591
	0.5	2.270
	0.6	1.979
	0.7	1.700
	0.8	1.395
	0.85	1.197

$n = 1$	A	u_0^*
	0.3	3.726
	0.5	3.143
	0.7	2.742
	0.9	2.429
	1.1	2.162
	1.3	1.923
	1.5	1.697
	1.7	1.467
	1.9	1.194

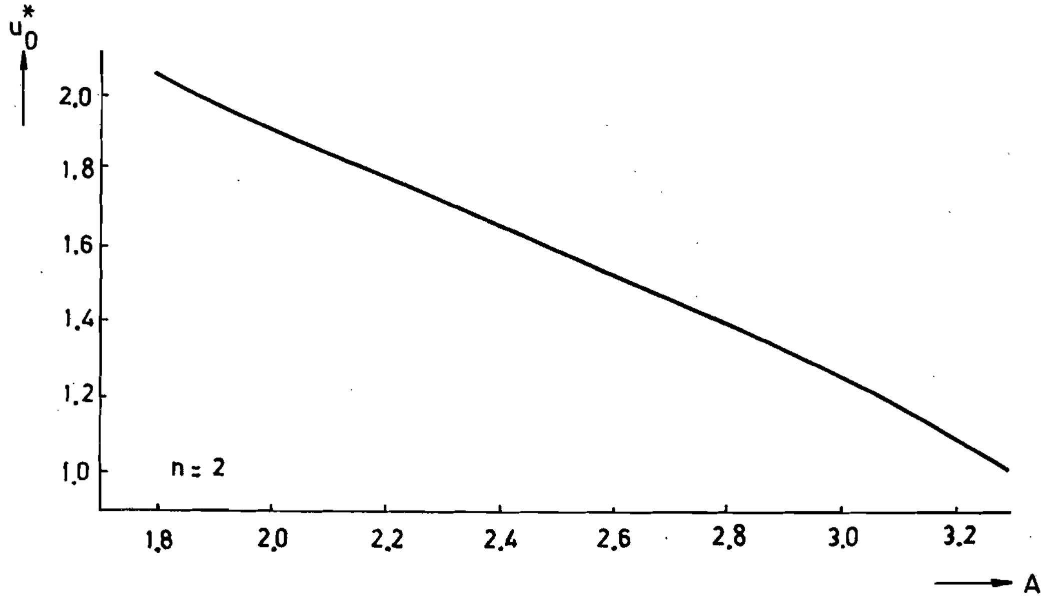
$n = 2$	A	u_0^*
	1.8	2.039
	1.9	1.970
	2.0	1.900
	2.2	1.771
	2.4	1.645
	2.5	1.583
	2.6	1.520
	2.8	1.392
	3.0	1.254
	3.2	1.082
	3.25	1.025



u_0^*
4.8
4.0
3.2
2.4
1.6
.8
n = 0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
A



u_0^*
4.0
3.2
2.4
1.6
.8
n = 1
0
.2
.4
.6
.8
1.0
1.2
1.4
1.6
1.8
2.0
A



u_0^*
2.0
1.8
1.6
1.4
1.2
1.0
n = 2
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
A

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