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Global extrapolation procedures for linear partial differential equations.

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ABSTRACT

Global extrapolation procedures, in space and time are considered for the numerical Solution of linear partial differential equations. Global extrapolation procedures in time only are reviewed.

The procedures are tested on three problems from the literature, one of which has a nonlinear source term.

INTRODUCTION

Consider the linear partial differential equation (PDE)

$$\frac{\partial^{v} u}{\partial t^{v}} - A_{\Omega} u + f_{\Omega}(\underline{x}, t,) , \underline{x} \in \Omega, 0 < t \leq T < \infty \tag{1}$$

in which v=1 ,2, $u = u(\underline{x}, t), \Omega$, is a spatial domain in R, R^2 or R^3 with boundary $\partial\Omega$, and A_{Ω} denotes a linear differential operator of order q which differentiates the function u with respect to the space variables. Obviously, equation (1) describes a first order hyperbolic equation when v=1 and q=1, a second order hyperbolic equation when v=2 and q=2, a second order parabolic equation when v=1 and q=2, and a fourth order parabolic equation when v=2 and q=4.

Associated with the PDE (1) are the initial conditions

$$\frac{\partial^{r} u}{\partial t^{r}} (\underline{x}, 0) = u_0^{(r)} , r = 0(1)(v-1) , \underline{x} \varepsilon \Omega \cup \partial\Omega \tag{2}$$

and the boundary conditions

$$A_{\partial\Omega} u = f_{\partial\Omega}(t), \underline{x} \varepsilon \partial\Omega , \quad 0 < t < T, \tag{3}$$

where $A_{\partial\Omega}$ is a linear differential operator of order less than q , which also differentiates u with respect to the space variables and acts on the boundary $\partial\Omega$. It must be noted that A_{Ω}, f_{Ω}, $A_{\partial\Omega}$ and $A_{\partial\Omega}$ may all depend on $\underline{x}$.

A popular method (*cf* [1 ,3,4,5,7,8,9,10,13,14,15,16,17]) of solving the initial-boundary value problem {(1),(2),(3)} is the so-called *method of lines* (MOL) in which the space domain Ω is discretized in some way and, *via* some finite difference or finite element approximation to A_{Ω}, the PDE is transformed into a time-continuous system of ordinary differential equations (ODEs) of order v , which has the form

$$D^{v}\underline{U}_h(t) = A_h\underline{U}_h(t) + \underline{f}_h(t), \quad 0 < t < T, \tag{4}$$

with the associated initial conditions

$$D^{r}\underline{U}_h(0) = \underline{u}_0^{(r)}, \; r = 0(1)(v-1). \tag{5}$$

In (4) and (5), upper case U has been introduced to distinguish the theoretical solution of an approximating method from the theoretical solution (lower case u) of the initial-boundary value problem, h is the parameter of a grid in $\Omega \cup \partial\Omega$ $\underline{U}_h(t)$ is an N-dimensional vector the elements of which are the approximations to the unknown dependent variable u at the grid points, the N-dimensional vector $\underline{f}_h(t)$ arises from f_Ω and $f_{\partial\Omega}$, the N-vector(s) $\underline{u}_0^{(r)}$ $(r = 0\ (1)(v-1))$ arise from (2), A_h is a time-independent matrix of order N which arises from A_Ω and $A_{\partial\Omega}$, and D = diag{d/dt} is of order N. The MOL approach then solves the initial value problem {(4), (5)} by dividing the time-interval 0 < t < T into Q subintervals (time-steps) each of length ℓ , say, so that $Q\ell = T$, and then employing a k→step (k>v) ODE solver to integrate from t=0 to t=T. In the case of PDEs with v=2, the initial conditions are used to determine an approximation to $\underline{U}_h(\ell)$, thus providing enough starting values for a two-step ODE solver. The MOL thus determines the solution in a recursive manner on a grid G_1 in $[\Omega \cup \partial\Omega] \times [0 < t < T]$ which has a total of Q+l time levels.

Under conditions such as those detailed in [11,Th.4.1] the full global error at each of the N grid points of G_1 at time t=T=Qℓ is given by the quantity E_1, which has the form

$$E_1 = h^s C + \ell^P B + K \tag{6}$$

In (6), p is the order of the ODE solver and s is the order of the approximations to A_Ω and $A_{\partial\Omega}$ (the reader is referred to the work in [11] on order reduction and to [2,12,18] for the reduction in the accuracy of the time integration in the presence of time-dependent boundary conditions). The quantities C and B are independent of h, ℓ and T and the quantity K is $0(h^{s*} + \ell^{P*})$ where p* > p and s* > s are integers.

It will be assumed that the space and time increments h and ℓ satisfy any restriction of the form

$$\ell < \lambda h^{a} , a = q / v , \quad (7)$$

where λ is a fixed positive constant, which must be imposed for stability.

2. GLOBAL EXTRAPOLATION IN TIME

A number of authors (*cf* [3,4,5,7,8,9]) have used local extrapolation methods to integrate (4) (with v=l) and (5) from time t to time t+2ℓ, t+3ℓ or t+4ℓ. The merits of local extrapolation in time were shown in [17] to be overshadowed somewhat by those of global extrapolation in time. Using a half-time step of length $\frac{1}{2}\ell$, the time interval 0 < t < T is divided into 2Q subintervals and, if the same space step h is retained, a new grid G_2 is constructed which has N interior grid points of G_2 at time $t = T = 2Q(\frac{1}{2}\ell)$ is given by the quantity E_2 which has the form

$$E_2 = h^{s}C + 2^{-P}\ell^{P}B + K . \quad (8)$$

The grid parameters h and $\frac{1}{2}\ell$ of G_2 clearly satisfy (7) if the parameters h and ℓ of G_1 do so.

Introducing some new notation, suppose that $\underline{U}_{h,1}(T)$ denotes the computed solution vector at time T on G_1, and that $\underline{U}_{h,2}(T)$ is the associated vector on G_2. Consider now the approximation

$$\underline{V}(T) = \alpha \underline{U}_{h,2}(T) + (1-\alpha)\underline{U}_{h,1}(T) \quad (9)$$

and the associated error E_v defined by

$$E_V = \alpha E_2 + (1-\alpha)E_1 . \quad (10)$$

It is easy to show that the term in ℓP in (10) vanishes when the parameter α takes the value

$$\alpha = 2^{P}/(2-1) \text{ with } 1-\alpha = -1/(2^{P}-1) . \quad (11)$$

This global extrapolation in time only using grids G_1 and G_2 has thus produced an approximation $\underline{V}(T)$ defined by (9) which is $0(h^{s} + \ell P^{*})$ provided α takes the

(4)

value given in (11).

3. GLOBAL EXTRAPOLATION IN SPACE AND TIME

Suppose now, that, in addition to halving the time step ℓ , the space parameter h is also halved. In the special case where Ω is an interval XεR with N interior points on Grids 1 and 2, X is now divided into 2N+2 subintervals. A third grid G_3 is thus constructed which has 2N+1 grid points at each of its 2Q+1 time levels.

The full global error at the 2N+1 grid points of G_3 at time $t=T=2Q(\frac{1}{2}\ell)$ is given by the quantity E_3 which has the form

$$E_3 = 2^{-s} h^s c + 2^{-p} \ell^p B + K . \tag{12}$$

Replacing ℓ and h in (7) by $\frac{1}{2}$ and $\frac{1}{2}$h, respectively, gives

$$\ell < \lambda h^a / 2^{a-1} \ , \quad a = q / v \tag{13}$$

so that in a space-time global extrapolation procedure the parameters h and ℓ used on G_1, must satisfy (13) instead of (7).

Suppose, now, that $\underline{U}_{\frac{1}{2}h,3}(T)$ denotes the computed solution vector at time T on G_3, then $\underline{U}_{\frac{1}{2}h,3}(T)$ has 2N+1 elements. Let $I^h_{\frac{1}{2}h}$ be an operator which isolates the N elements of $\underline{U}_{\frac{1}{2}h,3}(T)$ corresponding to the N elements of $\underline{U}_{h,1}(T)$ and $\underline{U}_{h,2}(T)$: that is, $I^h_{\frac{1}{2}h}\ \underline{U}_{\frac{1}{2}h,3}(T)$ has N elements. Consider, next, the approximation

$$\underline{W}(T) = \beta I^h_{\frac{1}{2}h} \underline{U}_{\frac{1}{2}h,3}(T) \ + \gamma \underline{U}_{h,2}(T) + (1-\beta-\gamma)\underline{U}_{h,1}(T) \tag{14}$$

and the associated error E_W defined by

$$E_W = \beta E_3 + \gamma E_2 + (1-\beta-\gamma) E_1 . \tag{15}$$

It may be shown that the terms in h^s and ℓP in (15) vanish when the parameters β and γ take the values

$$\beta = 2^s / (2^s - 1) \, , \gamma = (2^s - 2^p) / [(2^s - 1)(2^p - 1)] \tag{16}$$

so that

$$1-\beta-\gamma=-1/(2^{p}-1)\,. \tag{17}$$

This global extrapolation in both space and time using grids G_1 ,G_2 and G_3 has thus produced an approximation $\underline{W}(T)$ which is $0(h^{s^*}+\ell P^{*})$ provided the parameters β and γ take the values given in (16). In special cases when s=p the parameter γ vanishes and thus only two grids, G_1 and G_3, are needed to obtain the global space-time extrapolation. A notable example of this is the Crank-Nicolson method, for which s=p=2, for solving second order parabolic equations (v=l,q=2)(see Problem 2, in §4).

As noted in [17] it is of course theoretically possible to extrapolate to arbitrarily high orders: this remark is applicable to space-time extrapolation as well as time only [17]. However, in the belief that the extra orders achieved in §§2 and 3 of the present paper are high enough for PDE's, no further extrapolations will be considered.

The economics of the extrapolations are easy to compare. When compared with the result $\underline{U}_{h,2}(T)$ computed on grid G_2, the computation of the time-only extrapolation vector $\underline{V}$ defined by (9) requires an additional computation effort of 50%. When compared with the result $\underline{U}_{\frac{1}{2}h,3}(T)$ computed on grid G_3, the computation of the space-time extrapolation vector $\underline{W}$ defined by (14) requires 1.75 times as many operations. This factor is reduced to 1.25 when s=p, for then γ=0 and grid G_2 is not required.

4. NUMERICAL RESULTS

The global extrapolation algorithms outlined in Sections 2 and 3 were tested on three problems from the literature, two from the literature on linear second order parabolic equations and one from the literature on nonlinear second order hyperbolic equations. (The last problem is not, of course, of the type described by (1), but the authors feel that the results obtained were sufficiently interesting to report in the present paper.)

Problem 1 (Lawson and Morris [9], Gourlay and Morris [3], Twizeli and Khaliq [15]).

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}\,,\ \ 0<x<2\,,\ \ t>0\,,$$

with boundary conditions $u(0,t) = u(2,t) = 0$, $t > 0$ and initial conditions $u(x,0) = 1$, $0 \le x \ge 2$. This problem is of continuing interest because it has a discontinuity between initial and boundary conditions. The theoretical solution is given by

$$u(x,t) = \sum_{s=1}^{\infty} \left[1-(-1)^s\right] \frac{2}{s\pi} \sin\ (\frac{1}{2}s\pi x) \exp\ (-\frac{1}{4}s^2\pi^2 t)\ .$$

Lawson and Morris [9] transformed this problem into the system

$$d\underline{U}(t)/dt = A_h \underline{U}(t)$$

by the MOL, where

$$A_h = h^{-2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} , \tag{18}$$

and then used the fully implicit, L_0-stable method

$$(I - \ell A_h)\ \underline{U}(t+\ell) = \underline{U}(t) \tag{19}$$

to obtain a numerical solution; for (19), p=l and s=2.

The behaviour of (19) and comparisons of it with other methods are well documented (see, for instance, [3,9,15,17]). The purpose of the present paper is to show that the global extrapolation procedures described in Sections 2 and 3 improve accuracy.

Four numerical experiments were carried out in which the space and time increments on grid G_1, were given by

$(h, \ell) = (0.1,0.1), (0.1,0.05), (0.05,0.002), (0.05,0.05)$,

respectively, the increments on G_2 and G_3 following in an obvious manner. It was observed in [9] that (19) produces a smooth solution to Problem 1, with maximum errors occurring where x=l. The errors at this point at time t=1.0 using (19) on grids G_1, G_2 and G_3 individually, the time-only global extrapolation of (18) on G_1, and G_2 (defined by (9) with $\alpha=2$), and the space time global extrapolation of (19) on G_1, G_2 and G_3 (defined by (14) with $\beta={}^4/3$ and $\gamma={}^2/3$), are given in Table 1. It is easy to see from Table 1 that the two extrapolation procedures produce the improved accuracy predicted in Sections 2 and 3.

Problem 2

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - e^{-t}\ (x^2+2);\ 0 < x < 1\ ,\ t > 0$$

with initial conditions $u(x,0) = 1 + x^2$, $0 \le x \le 1$, and boundary conditions $u(0,t) = 1$, $u(1\,,t) = 1+e^{-t}$, $t > 0$. The theoretical solution is given by $u(x,t) = 1 + e^{-t}x^2$. This problem is the one-space dimensional form of Problem (5.2) in Verwer and de Vries [17].

Using the MOL, Problem 2 may be transformed into the equivalent first order initial value problem

$$d\underline{U}(t)/dt = A_h \underline{U}(t) + \underline{w}_h(t)$$

in which A_h is as defined by (18) and

$$\underline{w}_h(t) = [\, w_{1,h}(t),\, w_{2,h}(t), \ldots, w_{N,h}(t)]^T$$

(T, here, denoting transpose) with

$$w_{1,h}(t) = h^{-2} - e^{-t}(h^2+2),$$

$$w_{m,h}(t) = -e^{-t}(m^2h^2+2), \quad m = 2,3,\ldots,N-1$$

$$w_{N,h}(t) = h^{-2}(1+e^{-t}) - e^{-t}(N^2h^2+2).$$

The A_0 -stable implicit method

$$(I - \frac{1}{2}\ell A_h)\underline{U}(t+\ell) = (I + \frac{1}{2}A_h)\,\underline{U}(t) + \frac{1}{2}\ell\left[\, I - \frac{1}{2}\ell A_h)\,\underline{W}_h(t+\ell) + (\,I + \frac{1}{2}\ell A_h)\,\underline{w}_h(t)\right], \qquad (20)$$

for which p=s=2, was used to compute the solution at time t=l .0. Six numerical experiments were carried out for which the space and time steps on grid G_1 were taken to be

h, ℓ) = (0.1,0.1), (0.1,0.05), (0.1,0.002), (0.05,0.1), (0.05,0,05) and (0.05,0.02)

(respectively. The errors at the grid points where x = 0.3,0.6,0,9 are given in Table 2 for grids G_1 and G_3 individually and for the space-time global extrapolation of (20) on G_1 and G_3 (defined by (14) with $\beta={}^4/_3$ and $\gamma=0$). The errors on G_2 were found to be similar to those on G_1, and, consequently, the errors for the time-only extrapolation to be similar to those for the space-time extrapolation experiments (because $\alpha=\beta={}^4/_3$ and $\gamma=0$). It may be seen from Table 2 that errors were larger in modulus near the time-dependent boundary where some of the errors on G_1, had a dominant effect on the errors after extrapolation.

Problem 3

$$\frac{\partial^2 u}{\partial t^2} = gd(x)\ \frac{\partial^2 u}{\partial x^2} + \frac{1}{4}\lambda^2(x,u)u, \quad 0 \le x \le b, \quad t \ge 0$$

with boundary conditions

$$\frac{\partial u}{\partial x}(x,0) = \frac{\partial u}{\partial t}(b,0) = 0\ , t > 0$$

and initial conditions

$$u(x,0) = \sin(\pi x/b)\ , \frac{\partial u}{\partial t}(x,0) = -\pi(gd)^{\frac{1}{2}} \cos(\pi x/b)\ ,\ 0 \le x \le b\ . \tag{21}$$

In this problem (which does not conform to the type described by equation (1)), d(x) is a depth function given by d(x) = d*[2+cos(2πx/b)], g is the acceleration due to gravity, and λ(x,u) is the coefficient of bottom friction defined by $\lambda = g\ |\ u\ |/(C^2 d)$, C being the Chezy coefficient.

Using the MOL, this second order hyperbolic problem may be converted into the second order initial value problem

$$\frac{d^2 \underline{U}(t)}{dt^2} = gMB_h \underline{U}(t) + [g^2/(4C^4)]\, M^{-2} \underline{\varphi}(\underline{U}(t)) \equiv \underline{f}(t, \underline{U}(t))\ , t > 0 \tag{22}$$

with initial conditions $\underline{U}(0)$ and $d\underline{U}(0)/dt$ derived from (21). In (22), M = diag$\{d_i\}$ is a diagonal matrix in which $d_i = d(x_i)$ for i=0,1,...,N, and x_i=ih with h=b/N. The matrix B_h is of order N+l and is given by

$$B_h = h^{-2} \begin{bmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{bmatrix} ;$$

the vectors $\underline{U}(t) = [U_0(t), U_,(t), \ldots U_N(t)]^T$, $\underline{\varphi} = [\varphi_0, \varphi_1, \ldots, \varphi N]^T$ with $\varphi_i = \varphi_i(\underline{U}(t)) = |U_i(t)|^2 U_i(t)$, i=0,l,...,N, and $\underline{f} = [f_0, f, , f_2, \ldots, f_N]^T$ are of order N+l.

The simple explicit method

$$\underline{U}(t+\ell) = 2\underline{U}(t) - \underline{U}(t-\ell) + \ell^2 \underline{f}(t,\underline{U}(t))\ ;\ t=\ell, 2\ell, \ldots \tag{23}$$

for which p=s=2, was used to compute the solution on grid G_1. In using (23) $\underline{U}(0)$, derived from (21), and $\underline{U}(\ell) = \underline{U}(0) + \ell^2 \underline{f}(0,\underline{U}(0))$ were used as starting values. Following van der Houwen and Sommeijer [6], the various parameters associated with the problem were given the values

$$h = 10, \quad \ell = \frac{1}{3} \text{ (grid } G_1\text{) ; } b= 100, \quad g=9.81. \; d^*=10, \; C=50$$

and the solution was computed to time t=3600.

Taking as reference solution that used by van der Houwen and Sommeijer [6], the second order Runge-Kutta-Nystrdm method given by their equation (3.14), the solution in the interval $3567 \le t \le 3600$ at the point x=80 is depicted in Figure 1. The graphs in Figure 1 refer to the reference solution, the solution obtained on G_1 using (23), the time-only extrapolation defined by (9) with $\alpha={}^4/_3$, and the space-time extrapolation defined by (14) with $\beta={}^4/_3$ and $\gamma=0$.

It is seen from Figure 1 that the extrapolation procedures clearly improve accuracy, as predicted in §§2 and 3, a marked reduction in phase-lag being evident (*cf* van der Houwen and Sommeijer [6]).

5. SUMMARY

This paper has considered global extrapolation procedures, in time only and in space and time, for the numerical solution of linear partial differential equations.

The procedures were tested on three problems from the literature, one of which was nonlinear. It was seen that the extrapolation procedure involving both space and time produced notable reductions in error.

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Table1. Errors U-u where x=1.0 at time t=1.0 for the four experiments of Problem 1.

Increments on G_1		Errors on grids				
h	ℓ	G_1	G_2	G_3	G_1,G_2	G_1,G_2,G_3
0.1	0.1	0.33E-1	0.17E-1	0.16E-1	0.37E-3	0.31E-3
0.1	0.05	0.17E-1	0.85E-2	0.83E-2	0.14E-3	0.73E-4
0.05	0.002	0.66E-2	0.34E-2	0.33E-2	0.29E-4	0.87E-5
0.05	0.05	0.16E-1	0.83E-2	0.82E-2	0.82E-2	0.62E-4

Table 2. Errors U-u at the points where x=0.3,0.6,0.9 at time t=1.0 for the six experiments of Problem 2.

Increments on G_1			Errors on grids		
h	ℓ	x	G_1	G_3	G_1,G_3
0.1	0.1	0.3	0.16E-2	0.45E-3	0.77E-4
		0.6	0.47E-2	0.36E-3	-0.11E-2
		0.9	-0.54E-1	-0.27E-1	-0.18E-1
0.1	0.05	0.3	0.46E-3	0.11E-3	0.30E-6
		0.6	0.41E-3	0.11E-3	0.15E-4
		0.9	-0.22E-1	-0.83E-4	0.73E-2
0.1	0.002	0.3	0.73E-4	0.18E-4	0.30E-7
		0.6	0.73E-4	0.18E-4	0.60E-7
		0.9	-0.36E-2	0.18E-4	0.12E-2
0.05	0.1	0.3	0.15E-2	0.45E-3	0.10E-3
		0.6	0.54E-2	0.35E-3	-0.13E-2
		0.9	-0.19E+0	-0.16E-1	0.43E-1
0.05	0.05	0.3	0.45E-3	0.11E-3	0.17E-5
		0.6	0.36E-3	0.11E-3	0.30E-4
		0.9	-0.27E-1	0.30E-2	0.13E-1
0.05	0.02	0.3	0.73E-4	0.18E-4	-0.64E-6
		0.6	0.73E-4	0.18E-4	-0.77E-6
		0.9	0.64E-3	0.14E-3	-0.33E-4

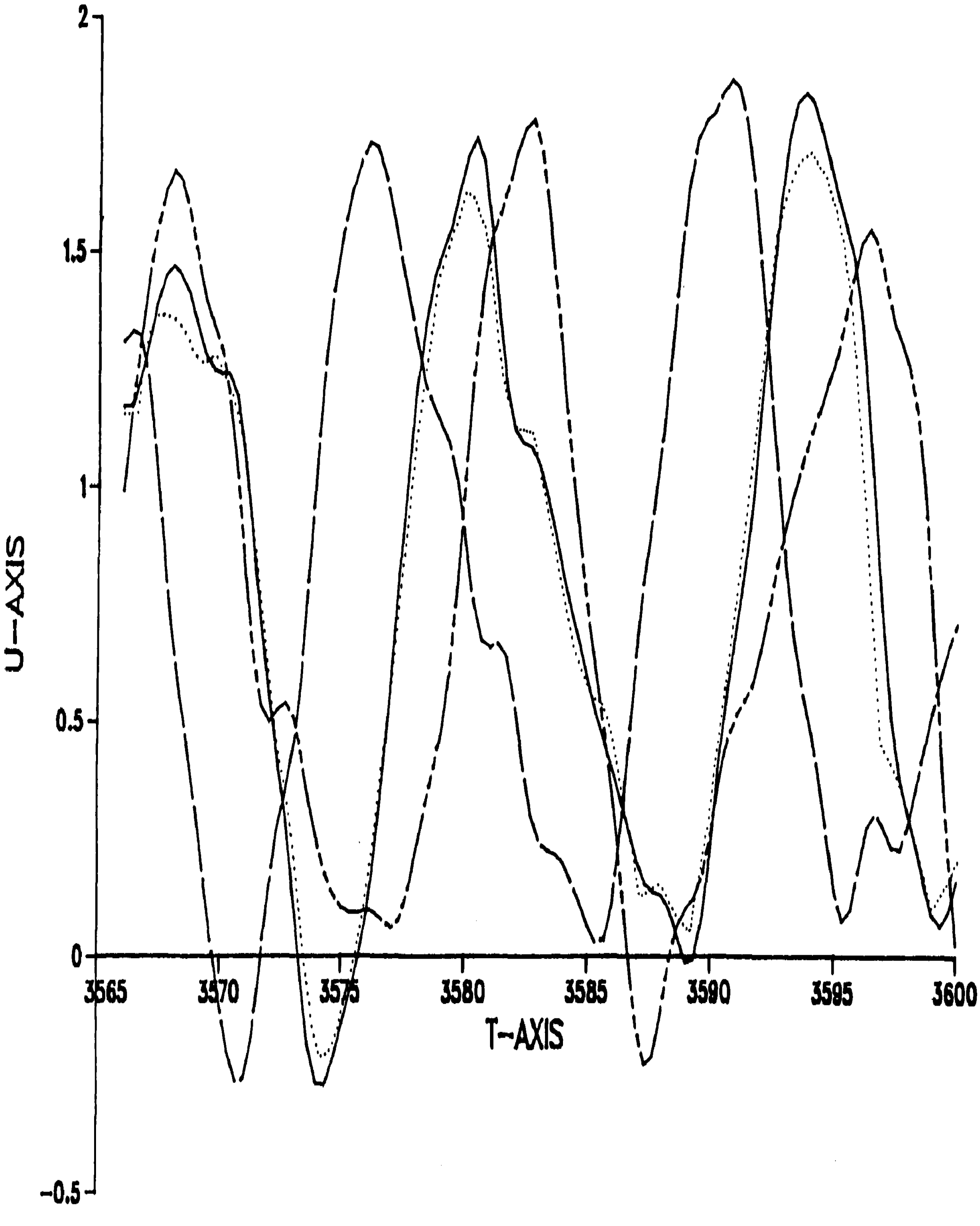

Figure 1: Numerical solutions of Problem 3 with h =10, $\ell = \frac{1}{3}$ on grid G_1.

.... Reference solution on G_1. Method (23) on G_1.

– – —Time-only extrapolation of (23).

_____ Space-time extrapolation of (23).