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)

\[
\frac{\partial^v u}{\partial t^v} - A_\Omega u + f_\Omega (x,t), \quad x \in \Omega, \quad 0 < t \leq T < \infty
\]  

(1)

in which \( v = 1, 2 \), \( u = u(x,t), \Omega \) is a spatial domain in \( \mathbb{R}, \mathbb{R}^2 \) or \( \mathbb{R}^3 \) with boundary \( \partial \Omega \), and \( A_\Omega \) 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

\[
\frac{\partial^r u}{\partial t^r} (x, 0) = u_0^{(r)}, \quad r = 0(1)(v - 1), \quad x \in \Omega \cup \partial \Omega
\]  

(2)

and the boundary conditions

\[
A_{\partial \Omega} u = f_{\partial \Omega} (t), \quad x \in \partial \Omega, \quad 0 < t < T,
\]  

(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 \( A_\Omega, f_\Omega, A_{\partial \Omega} \) and \( A_{\partial \Omega} \) may all depend on \( x \).

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 \( \Omega \) is discretized in some way and, via some finite difference or finite element approximation to \( A_\Omega \), the PDE is transformed into a time-continuous system of ordinary differential equations (ODEs) of order \( v \), which has the form
with the associated initial conditions
\[
D^r U_h(0) = u_0^{(r)}, \quad r = 0(1)(v-1).
\]

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 \( \Omega \cup \partial \Omega \), \( U_h(t) \) 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 \( f_h(t) \) arises from \( f_{\Omega} \) and \( f_{\partial \Omega} \), the \( N \)-vector(s) \( u_0^{(r)} \) \( (r = 0(1)(v-1)) \) arise from (2), \( A_h \) is a time-independent matrix of order \( N \) which arises from \( A_{\Omega} \) and \( A_{\partial \Omega} \), and \( D = \text{diag}\{d/dt\} \) 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 \( \ell \), say, so that \( Q\ell = T \), and then employing a \( k \rightarrow \) 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 \( U_h(\ell) \), 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 \( Q+1 \) 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 \( t=T=Q \ell \) is given by the quantity \( E_1 \), which has the form
\[
E_1 = h^s C + \ell^p B + K
\]

In (6), \( p \) is the order of the ODE solver and \( s \) is the order of the approximations to \( A_{\Omega} \) 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 \( h, \ell \) 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 $\ell$ satisfy any restriction of the form

$$\ell < \lambda h^a, \quad a = q/v,$$  \hspace{1cm} (7)

where $\lambda$ 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 $v=1$) and (5) from time $t$ to time $t+2\ell$, $t+3\ell$ or $t+4\ell$. 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 $G_1$ at time $t = T = 2Q(\frac{1}{2}\ell)$ is given by the quantity $E_2$ which has the form

$$E_2 = h^8C + 2^{-P}\ell^PB + K.$$  \hspace{1cm} (8)

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

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

and the associated error $E_v$ defined by

$$E_v = \alpha E_2 + (1-\alpha)E_1.$$  \hspace{1cm} (10)

It is easy to show that the term in $\ell P$ in (10) vanishes when the parameter $\alpha$ takes the value

$$\alpha = 2^p / (2-1) \quad \text{with} \quad 1-\alpha = -1 / (2^p -1).$$  \hspace{1cm} (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 $0(h^8 + \ell^P)$ provided $\alpha$ takes the
value given in (11).

3. GLOBAL EXTRAPOLATION IN SPACE AND TIME

Suppose now, that, in addition to halving the time step $\ell$, the space parameter $h$ is also halved. In the special case where $\Omega$ is an interval $X \subset \mathbb{R}$ 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 $t=T=2Q(\ell_2/\ell_1)$ is given by the quantity $E_3$ which has the form

$$E_3 = 2^{-a}h^c + 2^{-p}\ell^pB + K.$$  \hspace{1cm} (12)

Replacing $\ell$ and $h$ in (7) by $\ell_2/\ell_1$ and $h/2$, respectively, gives

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

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

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

$$W(T) = \beta I^{(1)}_{2h} U^{(1)}_{2h,3}(T) + \gamma U_{h,2}(T) + (1-\beta-\gamma) U_{h,1}(T)$$ \hspace{1cm} (14)

and the associated error $E_W$ defined by

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

It may be shown that the terms in $h^s$ and $\ell^p$ in (15) vanish when the parameters $\beta$ and $\gamma$ take the values

$$\beta = 2^s / (2^s - 1), \quad \gamma = (2^s - 2^p) / [(2^s - 1)(2^p - 1)]$$ \hspace{1cm} (16)
so that
\[ 1 - \beta - \gamma = -1/(2^p - 1). \] (17)

This global extrapolation in both space and time using grids \( G_1, G_2 \) and \( G_3 \) has thus produced an approximation \( W(T) \) which is \( 0(h^{s^*} + \ell P^*) \) provided the parameters \( \beta \) and \( \gamma \) take the values given in (16). In special cases when \( s = p \) the parameter \( \gamma \) 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 \((v = 1, q = 2)\) (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 \( U_{h,2}(T) \) computed on grid \( G_2 \), the computation of the time-only extrapolation vector \( V \) defined by (9) requires an additional computation effort of 50%. When compared with the result \( U_{1/2h,3}(T) \) computed on grid \( G_3 \), the computation of the space-time extrapolation vector \( W \) defined by (14) requires 1.75 times as many operations. This factor is reduced to 1.25 when \( s = p \), for then \( \gamma = 0 \) 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]).

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 2, \quad t > 0, \]
with boundary conditions \( u(0,t) = u(2,t) = 0, \ t > 0 \) and initial conditions \( u(x,0) = 1, \ 0 \leq x \leq 2 \). This problem is of continuing interest because it has a discontinuity between initial and boundary conditions. The theoretical solution is given by

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

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

\[
d\mathbf{U}(t)/dt = \mathbf{A}_h \mathbf{U}(t)
\]

by the MOL, where

\[
\mathbf{A}_h = h^{-2} \begin{bmatrix}
  -2 & 1 & 1 & 0 \\
  1 & -2 & 1 & -1 \\
  0 & 1 & -2 & 1 \\
  0 & 0 & 1 & -2
\end{bmatrix}, \tag{18}
\]

and then used the fully implicit, \( \text{L}_0 \)-stable method

\[
(I-\ell \mathbf{A}_h) \mathbf{U}(t+\ell) = \mathbf{U}(t) \tag{19}
\]

to obtain a numerical solution; for (19), \( p=1 \) 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 \( x=1 \). 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 \( u(x,0) = 1 + x^2, \ 0 \leq x \leq 1 \), and boundary conditions \( u(0,t) = 1, u(l ,t) = 1+e^{-t}, \ t > 0 \). 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
\[
dU(t)/dt = A_h U(t) + w_h(t)
\]
in which \( A_h \) is as defined by (18) and
\[
w_h(t) = [w_{1,h}(t), w_{2,h}(t), \ldots, w_{N,h}(t)]^T
\]
(T, here, denoting transpose) with
\[
w_{1,h}(t) = h^2 - e^{-t}(h^2 + 2),
\]
\[
w_{m,h}(t) = -e^{-t}(m^2h^2 + 2), \ m = 2,3, \ldots, N-1
\]
\[
w_{N,h}(t) = h^2(1+e^{-1}) - e^{-t}(N^2h^2 + 2).
\]
The \( A_0 \)-stable implicit method
\[
(I-\frac{1}{2}A_h) U(t+\ell) = (I+\frac{1}{2}A_h) U(t)
\]
\[
+ \frac{1}{2} \ell \left[ (I-\frac{1}{2}A_h) W_h(t+\ell) + (I+\frac{1}{2}A_h) W_h(t) \right], \tag{20}
\]
for which \( p=s=2 \), was used to compute the solution at time \( t=1.0 \). Six numerical experiments were carried out for which the space and time steps on grid \( G_1 \) were taken to be
\[
h, \ell = (0.1,0.1), (0.1,0.05), (0.1,0.002), (0.05,0.1), (0.05,0.05) \text{ and } (0.05,0.02)
\]
(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 \( \beta=\frac{4}{3} \) 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 \( \alpha=\beta=\frac{4}{3} \) 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

\( \frac{\partial^2 u}{\partial t^2} = g d(x) \frac{\partial^2 u}{\partial x^2} + \frac{1}{4} \lambda^2(x,u) u, \quad 0 \leq x \leq b, \quad t \geq 0 \)

with boundary conditions

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

and initial conditions

\[ u(x,0) = \sin(\pi x/b), \quad \frac{\partial u}{\partial t}(x,0) = -\pi (gd)^{\frac{1}{2}} \cos(\pi x/b), \quad 0 \leq x \leq b. \] (21)

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

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

\[ \frac{d^2 U(t)}{dt^2} = g M B_h U(t) + \left[ g^2 / (4C^4) \right] M^{-2} \varphi(U(t)) = f(t, U(t)), \quad t > 0 \] (22)

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

\[ B_h = h^{-2} \begin{bmatrix} -2 & 2 \\ 1 & -2 & 1 \\ -2 & 1 & -2 \\ 2 & -2 \end{bmatrix} \];

the vectors \( U(t) = [U_0(t), U_1(t), \ldots, U_N(t)]^T \), \( \varphi = [\varphi_0, \varphi_1, \ldots, \varphi_N]^T \) with \( \varphi_i = \varphi_i(U(t)) = |U_i(t)|^2 U_i(t), \quad i = 0, 1, \ldots, N \), and \( f = [f_0, f_1, f_2, \ldots, f_N]^T \) are of order \( N+1 \).

The simple explicit method

\[ U(t + \ell) = 2U(t) - U(t-\ell) + \ell^2 f(t, U(t)) ; \quad t = \ell, 2\ell, \ldots \] (23)

for which \( p = s = 2 \), was used to compute the solution on grid \( G_1 \). In using (23) \( U(0) \), derived from (21), and \( U(\ell) = U(0) + \ell^2 f(0, U(0)) \) were used as starting values. Following van der Houwen and Sommeijer [6], the various parameters associated with the problem were given the values
Taking as reference solution that used by van der Houwen and Sommeijer [6], the second order Runge-Kutta-Nyström method given by their equation (3.14), the solution in the interval $3567 \leq t \leq 3600$ 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 $\alpha=\frac{4}{3}$, and the space-time extrapolation defined by (14) with $\beta=\frac{4}{3}$ 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.

REFERENCES


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

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<th>ℓ</th>
<th>G_1</th>
<th>G_2</th>
<th>G_3</th>
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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.

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<td>0.6</td>
<td>0.73E-4</td>
<td>0.18E-4</td>
<td>-0.77E-6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.9</td>
<td>0.64E-3</td>
<td>0.14E-3</td>
<td>-0.33E-4</td>
</tr>
</tbody>
</table>
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).