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GLOBAL EXTRAPOLATION OF A FIRST ORDER SPLITTING METHOD

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Global extrapolation of a first order splitting method *)

by

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ABSTRACT

This note deals with the numerical solution of multi-space dimensional parabolic partial differential equations and advocates classic global Richardson extrapolation for splitting methods. The paper concentrates on the first order locally one-dimensional splitting method. This robust, low order splitting method is known to possess two favourable properties. It rapidly damps high frequency components, which is of importance for problems having non-smooth initial data, and it possesses excellent stability properties for non-linear problems. Global extrapolation to higher order leaves these properties invariant. In addition, global extrapolation is easy to implement. A comparison is made with a local extrapolation procedure which has been proposed by Lawson and Morris (SIAM J. Numer. Anal. 15 (1978), pp. 1212-1224). A few numerical results are reported.

KEY WORDS & PHRASES: *Numerical analysis, Parabolic partial differential equations, Splitting methods, Method of lines, Global extrapolation*

*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

In the numerical solution of parabolic partial differential equations with non-smooth initial data, it is desirable to employ a time discretization which, in a sufficient manner, simulates the rapid exponential decay of high frequency components. For example, when a discontinuity exists between the initial function and the boundary conditions. Within the class of splitting methods for multi-space dimensional problems, the first order locally one-dimensional method (LOD method, cf. [16]) possesses this damping property. A disadvantage of this method is its low accuracy in time. To increase the accuracy, Lawson and Morris [8] have proposed a local extrapolation of the LOD method to order two which maintains the rapid damping of high frequency components (see also [3]). This locally extrapolated LOD scheme requires twice as many operations per step as the basic LOD scheme. However, a numerical experiment [8] on a model heat equation in two space dimensions with a discontinuity between the initial and boundary conditions, has shown that local extrapolation may pay off. In particular, for such problems the Lawson-Morris scheme will perform better than the second order Peaceman-Rachford scheme due to a lack of damping of high frequency components in the latter one.

We advocate an alternative extrapolation of the LOD method, viz. global Richardson extrapolation. This type of Richardson extrapolation, which is classic in the numerical solution of ordinary differential equations ([4], p. 81), involves parallel integration with the same basic scheme on different time grids, but completely separated. Consequently, all stability and damping properties of the basic scheme are left invariant by global extrapolation, contrary to local extrapolation. Global extrapolation is easy to implement. For the LOD method it is also less expensive than the Lawson-Morris extrapolation. Global extrapolation to order two requires one and a half as many operations per step as the basic scheme. For global extrapolation to order three this factor is equal to $7/4$ or 2, depending on the implementation.

Recent alternative approaches to increasing the accuracy of splitting methods include the application of defect correction techniques [6, 7, 13]. A common property of these techniques with the local extrapolation technique

of Lawson and Morris [8], is that the accuracy is increased by some local procedure. For splitting methods such local procedures always seem to interfere with the requirement of unconditional stability and, particularly, with rapid damping of high frequency components. In this respect, the present approach differs in principle. By global extrapolation the accuracy is increased in a global way and by no means the stepwise stability of the solution process is influenced. This latter point is our main motive to advocate global extrapolation. Furthermore, the technique is simple and can be applied to any one-step splitting method for time dependent, multi-space dimensional problems.

In this note we concentrate on the LOD method. Apart from its well-known damping properties, this method also possesses excellent stability properties for nonlinear problems [14]. Global extrapolation does not interfere with these nonlinear stability properties either.

2. THE LOD METHOD

In this section we briefly recall the LOD method [16]. By following the method of lines approach, the LOD method can be formulated in a very compact way (cf. [5]). Let the initial value problems for the ordinary differential system

$$(2.1) \quad \dot{y}(t) = f(t, y(t)), \quad t > 0, \quad y(0) = y_0,$$

represent a semi-discrete version of a given initial-boundary value problem for a partial differential equation. For the moment it will not be necessary to be specific about the partial differential equation and the space discretization. We only assume that the vector function $f(t, y)$ can be written as

$$(2.2) \quad f(t, y) = \sum_{i=1}^k f_i(t, y),$$

where f_i corresponds to a one-space dimensional partial differential operator. The following time integration formula

$$\begin{aligned}
 y_{n+1}^{(0)} &= y_n, \\
 (2.3) \quad y_{n+1}^{(i)} &= y_{n+1}^{(i-1)} + \tau f_i(t_{n+1}^{(i)}, y_{n+1}^{(i)}), \quad i = 1, \dots, k, \\
 y_{n+1} &= y_{n+1}^{(k)},
 \end{aligned}$$

then defines the LOD step $y_n \rightarrow y_{n+1}$. Here, y_n is the approximation to $y(t)$, the exact solution of (2.1), at time $t = t_n$, and $\tau = t_{n+1} - t_n$ is the time-step. Further, we suppose $t_n \leq t_{n+1}^{(i)} \leq t_{n+1}$, $i = 1, \dots, k$.

The order of consistency of (2.3) is equal to one for all splitting functions f_i , $i = 1, \dots, k$, satisfying (2.2). Observe that (2.3) consists of k consecutive backward Euler steps, each of which applied with a different function f_i . The computation of the vectors $y_{n+1}^{(i)}$ from the implicit backward Euler relations can be performed cheaply using a Newton type iteration, because we assumed that f_i stands for a semi-discrete, one-space dimensional partial differential operator.

The LOD method is known to be unconditionally stable for the linear model problem

$$(2.4) \quad u_t = \sum_{i=1}^k u_{x_i x_i},$$

where the second order derivative has been replaced by the central difference operator. Furthermore, the method possesses excellent damping properties for high frequent solution components (see e.g. [8]). In addition to these linear stability properties, the LOD method can also be shown to be unconditionally stable for non-linear parabolic problems of the form

$$(2.5) \quad u_t = \sum_{i=1}^k F_i(t, x, u, \frac{\partial}{\partial x_i} (p_i(t, x) \frac{\partial u}{\partial x_i})), \quad x \in \Omega \subset \mathbb{R}^k.$$

This non-linear stability result can be shown by exploiting the intimate relation with the backward Euler scheme. For details we refer to [14].

To conclude our description of the LOD method we have to recall two possible sources of inaccuracies, viz. non-constant boundary values and non-constant inhomogeneous terms [2, 11, 15]. These inaccuracies will also

be noticeable for globally extrapolated results (see experiment 2⁰ of section 5). Other splitting methods, such as ADI, also suffer from these phenomena, although to a somewhat lesser extent.

3. GLOBAL RICHARDSON EXTRAPOLATION

The LOD method (2.3) may be considered as a particular one-step integration method of order of consistency $p = 1$ for the ordinary differential system (2.1). Suppose that a p -th order one-step method is applied from $t_0 = 0$ up to $t_N = T$, using a time grid G_N . This grid does not need to be uniform. It is only assumed that for N sufficiently large, the minimal and maximal stepsizes τ behave like $O(N^{-1})$. If this natural assumption is satisfied, we are assured of the existence of an asymptotic expansion in the maximal stepsize, τ_N say, for the global error [12]

$$(3.1) \quad \varepsilon_N = y_N - y(t_N).$$

If we let f be M times differentiable, in some neighbourhood of the exact solution (2.1), then functions e_j , $j = p, \dots, M$, exist, independent of τ_N , such that

$$(3.2) \quad \varepsilon_N = \sum_{j=p}^M \tau_N^j e_j(t_N) + O(\tau_N^{M+1}), \quad \tau_N \rightarrow 0.$$

The existence of this asymptotic expansion for ε_N forms the basis for global Richardson extrapolation.

The use of this technique for estimating the global error of one-step integration methods for ordinary differential equations is classic (see [4], p. 81 and [12], p. 157), although it is not very often applied [1, 9, 10]. As far as we know, the possibility of using this technique for increasing the accuracy of low order splitting methods has not yet been discussed in the literature.

Global extrapolation is easy to implement. It involves parallel integration with the same method on different grids G_N . Let us consider the coherent grids G_N , G_{2N} and G_{3N} depicted in Fig. 1. G_{2N} is obtained from G_N by halving all stepsizes, etc. . Because of this coherence between

the grids, expansion (3.2) holds for τ_N , $\tau_{2N} = \tau_N/2$ and $\tau_{3N} = \tau_N/3$, at all common gridpoints, i.e. on the whole of G_N . Let $y_{n,i}$ denote the approximation

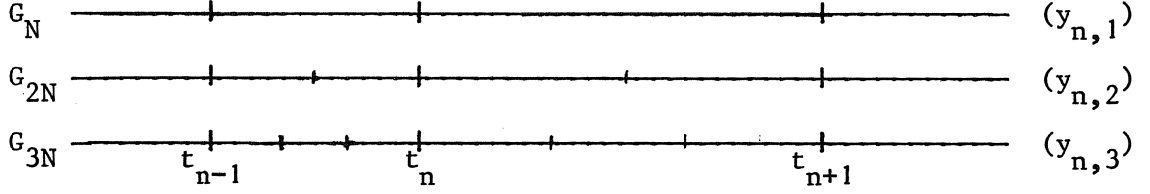


Fig. 1 Three coherent grids.

to $y(t_n)$ at the grid G_{iN} . Then, at all common points,

$$(3.3) \quad \varepsilon_{n,i} \equiv y_{n,i} - y(t_n) = \sum_{j=1}^M (\tau_N/i)^j e_j(t_n) + O(\tau_N^{M+1}), \quad \tau_N \rightarrow 0,$$

if $p = 1$. Next suppose M sufficiently large and compute

$$(3.4) \quad \begin{aligned} y_n^{[2]} &\equiv 2y_{n,2} - y_{n,1}, \\ y_n^{[3]} &\equiv \frac{9}{2}y_{n,3} - 4y_{n,2} + \frac{1}{2}y_{n,1}. \end{aligned}$$

Then

$$(3.5) \quad \begin{aligned} y_n^{[2]} &= y(t_n) - \frac{1}{2}\tau_N^2 e_2(t_n) + O(\tau_N^3), \\ y_n^{[3]} &= y(t_n) + \frac{1}{6}\tau_N^3 e_3(t_n) + O(\tau_N^4), \end{aligned}$$

showing that $y_n^{[2]}$ and $y_n^{[3]}$ are of order of convergence two and three, respectively.

It is emphasized that the extrapolation is passive, i.e. the integrations are performed independent of each other. This trivially implies that global extrapolation cannot interfere with the stability of the basic scheme.

Observe that it is theoretically possible to extrapolate to arbitrarily high order of convergence. We restrict ourselves to order two and three, assuming that this is sufficiently high for partial differential equations. When compared with the result $y_{n,2}$ computed at the grid G_{2N} , the computation

of $y_n^{[2]}$ requires an additional computational effort of 50 %. Global extrapolation to order three requires twice as many operations per step as the basic scheme on G_{3N} . When using the grids G_N , G_{2N} and G_{4N} , the corresponding factor is equal to 7/4. We prefer to use G_N , G_{2N} and G_{3N} in order to avoid a too large difference between the stepsizes.

4. A COMPARISON WITH THE LAWSON-MORRIS SCHEME

Consider the LOD scheme (2.3). Let, for convenience, $k = 2$. Introduce the formal notation $y_{n+1} = E[\tau, t_n, y_n, f_1, f_2]$ for the LOD scheme. The second order, locally extrapolated LOD scheme of Lawson & Morris [8] then can be written as

$$\begin{aligned}
 (4.1) \quad & z_0 = E[\tau, t_n, y_n, f_1, f_2], \quad z_1 = E[\tau, t_n + \tau, z_0, f_2, f_1], \\
 & z_2 = E[2\tau, t_n, y_n, f_1, f_2], \quad z_3 = E[2\tau, t_n, y_n, f_2, f_1], \\
 & y_{n+2} = 2z_1 - \frac{1}{2}(z_2 + z_3).
 \end{aligned}$$

This scheme performs the step $y_n \rightarrow y_{n+2}$ over an interval of length 2τ by performing four basic LOD steps. Hence, per interval of length τ , it requires twice as many operations as the basic scheme. Lawson and Morris have defined their extrapolation in such a way that, for the linear model (2.4), (i) the scheme is unconditionally stable, and (ii) the damping of the basic scheme is maintained. In fact, the preservation of damping has been their main concern.

To demonstrate their scheme, Lawson & Morris [8] computed the solution to the problem

$$\begin{aligned}
 (4.2) \quad & U_t = U_{x_1 x_1} + U_{x_2 x_2}, \quad t > 0, \quad 0 < x_1, x_2 < 2, \\
 & U(0, x_1, x_2) = \sin(\frac{1}{2}\pi x_2), \quad 0 \leq x_1, x_2 \leq 2, \\
 & U(t, x_1, x_2) = 0, \quad t > 0, \quad x_1, x_2 \text{ on the boundary.}
 \end{aligned}$$

The Fourier solution of this problem is given by

$$(4.3) \quad U(t, x_1, x_2) = \sin\left(\frac{\pi}{2}x_2\right) \sum_{n=1}^{\infty} [1 - (-1)^n] \frac{2}{n\pi} \sin\left(\frac{n\pi x_1}{2}\right) \exp\left(\frac{-\pi^2}{4}(n^2+1)t\right).$$

Because of the discontinuity between the initial function and the boundary function, this problem should be integrated with a method which rapidly damps high frequency components.

Following Lawson & Morris [8], we also compute the solution to this problem, at $t = 1$, using the first order LOD scheme, the second order Lawson-Morris scheme, the second order ADI scheme of Peaceman-Rachford, and global extrapolation to order two and three applied to the LOD scheme. The spatial discretization is based on the standard 5-point finite difference operator on a uniform grid of stepsize h . In Table 2 we show the maximum of the absolute errors for some values of τ and h . It should be noted that at $t = 1$ the theoretical solution has a maximum value of approximately 0.01. The values of τ given in the table belong to the finest time grids. In the column "Work" we have expressed the total computational effort per τ -interval into the computational effort of the LOD scheme.

Method	Work	$\tau=1/12$			$\tau=1/24$		
		$h=0.1$	$h=0.05$	$h=0.025$	$h=0.1$	$h=0.05$	$h=0.025$
LOD	1	$5.3_{10^{-3}}$	$5.2_{10^{-3}}$	$5.2_{10^{-3}}$	$2.5_{10^{-3}}$	$2.5_{10^{-3}}$	$2.5_{10^{-3}}$
Peaceman-Rachford	$\frac{3}{2}$	$2.3_{10^{-3}}$	$1.8_{10^{-2}}$	$4.1_{10^{-2}}$	$3.4_{10^{-5}}$	$2.3_{10^{-3}}$	$1.8_{10^{-2}}$
Lawson-Morris	2	$7.5_{10^{-4}}$	$6.9_{10^{-4}}$	$6.7_{10^{-4}}$	$3.0_{10^{-4}}$	$2.4_{10^{-4}}$	$2.3_{10^{-4}}$
Global extrapolation (2)	$\frac{3}{2}$	$8.4_{10^{-4}}$	$9.0_{10^{-4}}$	$9.2_{10^{-4}}$	$1.8_{10^{-4}}$	$2.3_{10^{-4}}$	$2.5_{10^{-4}}$
Global extrapolation (3)	2	$5.5_{10^{-5}}$	$1.1_{10^{-4}}$	$1.2_{10^{-4}}$	$5.9_{10^{-5}}$	$3.1_{10^{-6}}$	$1.1_{10^{-5}}$

Table 2 Maximum absolute errors in solving problem (4.5) at $t=1$.

It can be concluded that for problem (4.1), which serves as a test example for problems with non-smooth initial data, the third order global extrapolation scheme is to be preferred to the other schemes. Note that the ADI scheme yields relatively large errors when h decreases. This is caused by a lack of damping of high frequency components. The LOD type schemes do not suffer from this phenomenon.

5. TWO MORE NUMERICAL EXPERIMENTS

In addition to the previous experiment, we discuss two more experiments in order to give some more insight in the use of the extrapolation procedures. For that purpose we consider the first initial-boundary value problem for the simple linear problems

$$(5.1) \quad \begin{aligned} U_t &= \frac{x_1^2 - x_1^2}{4} U_{x_1 x_1} + \frac{x_2^2 - x_2^2}{4} U_{x_2 x_2}, \quad t > 0, \quad 0 < x_1, x_2 < 1, \\ U(t, x_1, x_2) &= 1 - e^{-t(x_1^2 - x_1^2)(x_2^2 - x_2^2)}, \quad t \geq 0, \quad 0 \leq x_1, x_2 \leq 1, \end{aligned}$$

and

$$(5.2) \quad \begin{aligned} U_t &= U_{x_1 x_1} + U_{x_2 x_2} - e^{-t(x_1^2 + x_2^2 + 4)}, \quad t > 0, \quad 0 < x_1, x_2 < 1, \\ U(t, x_1, x_2) &= 1 + e^{-t(x_1^2 + x_2^2)}, \quad t \geq 0, \quad 0 \leq x_1, x_2 \leq 1. \end{aligned}$$

For the space discretization we use again standard finite differences on a uniform grid with mesh width h . Note that, due to the solutions selected, the space discretization is exact. So we can illustrate the effect of the extrapolations without interference of space discretization errors. Note also that the selected solutions are smooth, i.e. free of high frequency components. This implies that here the ADI scheme could also successfully be applied, possibly in combination with global extrapolation.

We have applied

- (i) The first order LOD scheme

$$(5.3) \quad y^* = y_n + \tau f_1(t_n + \tau, y^*), \quad y_{n+1} = y^* + \tau f_2(t_n + \tau, y_{n+1}).$$

- (ii) Global extrapolation on this scheme to order three.
- (iii) The Lawson-Morris scheme (4.1), where E now represents (5.3).
- (iv) The second order Peaceman-Rachford ADI scheme

$$(5.4) \quad \begin{aligned} y^* &= y_n + \frac{\tau}{2} f_1(t_n + \frac{1}{2}\tau, y^*) + \frac{\tau}{2} f_2(t_n, y_n), \\ y_{n+1} &= y^* + \frac{\tau}{2} f_1(t_n + \frac{1}{2}\tau, y^*) + \frac{\tau}{2} f_2(t_{n+1}, y_{n+1}). \end{aligned}$$

- (v) Global extrapolation on this ADI scheme to order four using the grids of Fig. 1. The extrapolation formula reads

$$y_n^{[4]} = \frac{27}{12} y_{n,3} - \frac{4}{3} y_{n,2} + \frac{1}{12} y_{n,1}.$$

Experiment 1. This experiment deals with the homogeneous problem (5.1). We emphasize that the solution is constant at the boundary. Space discretization leads to the splitting functions

$$(5.5) \quad f_1(t, y) = A_1 y + B_1, \quad f_2(t, y) = A_2 y + B_2,$$

where B_1 and B_2 are sparse vectors containing the constant boundary values. The meaning of A_1 and A_2 should be self-evident.

Table 3 shows maximum absolute errors at $t = 1$ for three values of τ using $h = \frac{1}{40}$. The τ -values correspond to the finest grid. We emphasize that the LOD scheme (5.3) and the ADI scheme (5.4) were applied using half the value of τ given in the table. The column "Work" has the same meaning as in Table 2.

Method	Work	$\tau=1/6$	$\tau=1/12$	$\tau=1/24$
LOD (applied with $\frac{\tau}{2}$)	2	4.7_{10}^{-4}	2.4_{10}^{-4}	1.2_{10}^{-4}
Lawson-Morris	2	8.0_{10}^{-5}	2.3_{10}^{-5}	6.2_{10}^{-6}
Global Extrap. LOD (3)	2	4.9_{10}^{-6}	6.9_{10}^{-7}	9.2_{10}^{-8}
ADI (applied with $\frac{\tau}{2}$)	3	3.3_{10}^{-6}	8.3_{10}^{-7}	2.1_{10}^{-7}
Global Extrap. ADI (4)	3	2.3_{10}^{-8}	1.4_{10}^{-9}	8.8_{10}^{-11}

Table 3 Maximum absolute errors in solving problem (5.1) at $t = 1$.

For the present problem it can be concluded that, due to the smooth solution, the homogeneity, and the constant boundary values, all methods perform relatively accurate. In particular, it pays to apply extrapolation.

Experiment 2. The second experiment deals with the inhomogeneous problem (5.2), whose solution has time dependent boundary values. This experiment serves to illustrate the effect of the extrapolation procedures in the presence of time dependent boundary values and time dependent source terms. For all splitting methods these dependencies are known to reduce the accuracy of the time integration [2, 11, 15]. Space discretization yields the splitting functions

$$(5.6) \quad f_1(t, y) = A_1 y(t) + B_1(t) + \frac{1}{2}V(t), \quad f_2(t, y) = A_2 y(t) + B_2(t) + \frac{1}{2}V(t),$$

where $V(t)$ originates from the source term of (5.2) and A_1 , A_2 and $B_1(t)$, $B_2(t)$ have the same meaning as in Experiment 1. The results for $h = \frac{1}{40}$ are given in Table 4.

Method	Work	$\tau=1/6$	$\tau=1/12$	$\tau=1/24$
LOD (applied with $\frac{\tau}{2}$)	2	1.2_{10}^{-2}	7.8_{10}^{-3}	4.5_{10}^{-3}
Lawson-Morris	2	2.3_{10}^{-2}	1.5_{10}^{-2}	8.7_{10}^{-3}
Global Extrap. LOD (3)	2	9.8_{10}^{-3}	4.7_{10}^{-3}	2.0_{10}^{-3}
ADI (applied with $\frac{\tau}{2}$)	3	2.6_{10}^{-6}	6.6_{10}^{-7}	1.6_{10}^{-7}
Global Extrap. ADI (4)	3	3.8_{10}^{-6}	2.2_{10}^{-7}	1.3_{10}^{-8}

Table 4 Maximum absolute errors in solving problem (5.2) at $t = 1$.

It is striking that all LOD methods are significantly less accurate than in the previous experiment, although the solution of problem (5.2) has the same "smoothness properties" as the solution of problem (5.1). As pointed out before, this is caused by the time dependent boundary function and source term. Here we must conclude that the extrapolation procedures are hardly more efficient than their respective basic schemes. The Lawson-Morris errors are even larger than the LOD ($\frac{\tau}{2}$) errors. For this problem the basic ADI scheme is considerably more accurate than all LOD methods. We note that for the present problem the ADI errors are strongly sensitive to the splitting of the source term. This is not the case for the LOD scheme.

The inaccuracy caused by the time dependent boundary function can be removed by applying the Fairweather-Mitchell boundary-value correction (see [2, 11, 15] for details). This is clearly illustrated by the results shown in Table 5, although the influence of the source term is still visible. The gain in accuracy of the extrapolated LOD schemes is again beyond our expectations. The accuracy of the ADI scheme (5.4) is not improved by applying the boundary-value correction. On the other hand, the global extrapolation of the ADI scheme is benefited by this correction technique.

Method	Work	$\tau=1/6$	$\tau=1/12$	$\tau=1/24$
LOD (applied with $\frac{\tau}{2}$)	2	$2.2_{10^{-3}}$	$1.3_{10^{-3}}$	$7.0_{10^{-4}}$
Lawson-Morris	2	$2.2_{10^{-3}}$	$1.1_{10^{-3}}$	$5.0_{10^{-4}}$
Global Extrapol. LOD (3)	2	$1.3_{10^{-3}}$	$4.5_{10^{-4}}$	$1.1_{10^{-4}}$
ADI (applied with $\frac{\tau}{2}$)	3	$2.7_{10^{-6}}$	$6.6_{10^{-7}}$	$1.6_{10^{-7}}$
Global Extrapol. ADI (4)	3	$1.3_{10^{-6}}$	$8.3_{10^{-8}}$	$4.7_{10^{-9}}$

Table 5 Maximum absolute errors in solving problem (5.2) at $t=1$ when using the boundary-value correction technique.

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