Smoothing the Extrapolated Midpoint Rule*

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Summary. The extrapolated midpoint rule is a popular way to solve the initial value problem for a system of ordinary differential equations. As originally formulated by Gragg, the results are smoothed to remove the weak instability of the midpoint rule. It is shown that this smoothing is not necessary. A cheaper smoothing scheme is proposed. A way to exploit smoothing to increase the robustness of extrapolation codes is formulated.

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1. Introduction

In his dissertation [4] and later in [5], W.B. Gragg proposed that the explicit midpoint rule with special starting procedure serve as the fundamental formula for the solution by $h^2$-extrapolation of the initial value problem for a system of ordinary differential equations (ODEs). The idea was implemented by Bulirsch and Stoer [2] who showed the approach to be an effective one for non-stiff problems.

It seems to have been considered obvious that smoothing is necessary, or at least highly desirable, when the midpoint rule is used for extrapolation. In the extrapolation methods one integrates repeatedly from $x_n$ to $x_n + H$ with successively smaller (fixed) step sizes $h$. The results at $x_n + H$ of the various subintegrations are combined in a linear (polynomial extrapolation) or non-linear (rational extrapolation) way to yield a high order result at $x_n + H$. The midpoint rule is well known to have no region of absolute stability. These successive integrations with a weakly stable formula appear to be dangerous. Milne and Reynolds [7] successfully smoothed the results of integrations with Milne's formula to eliminate a similar instability. In view of this, Gragg

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proposed a smoothing scheme for his extrapolation procedure and justified it with the asymptotic expansion he developed for the error.

For nearly 20 years Gragg’s approach to solving ODEs has been used without questioning if smoothing is really necessary. In a preliminary study [11], we showed it is not. Here we report our findings along with important new insight. First we shall observe that the analogy with the work of Milne and Reynolds is false. Gragg’s scheme is intended to estimate and then eliminate a weakly stable component of the error expansion. It is easiest to understand what is happening if one considers an “ideal” smoothing which removes exactly this term. The remarkable result then is that polynomial extrapolation gives precisely the same numerical results with and without ideal smoothing. There is a rather tricky point about the effect of smoothing on the algorithms for accepting a step which we shall explain.

Recently Bader and Deuflhard [1] have been studying an extrapolated semi-implicit midpoint rule for the solution of stiff problems. The method generalizes the explicit midpoint rule in a natural way. Bader invented a smoothing scheme for the semi-implicit midpoint rule which resembles Gragg’s scheme. We shall point out that in contrast to the situation for non-stiff problems, Bader’s scheme is quite important for stiff problems. The schemes of Gragg and Bader suggest a family of schemes for non-stiff problems which we explore. Shampine invented a cheap smoothing scheme as an alternative to Gragg’s which will be explained.

We propose a way to exploit smoothing which we believe will significantly increase the robustness of extrapolation codes.

Finally we consider the merits of the various smoothing schemes as compared to each other and to not smoothing at all.

2. Preliminaries

First it will be useful to explain why one might not need to smooth the midpoint rule as it is used to solve non-stiff ODEs. There are two distinct ways one might use the idea of extrapolation – local and global. In global extrapolation one begins an integration with step size \( h \) at the initial point of the interval of integration \( a \) and advances all the way to the final point \( b \). One then reduces \( h \) and integrates again from \( a \) to \( b \). (In practice the integrations might be done simultaneously.) Extrapolation is done at mesh points of interest, common to both integrations, so as to obtain accurate results there. A virtue of this approach is that one obtains global, or true, error estimates. For this reason we have been studying the possibility of writing a code of this kind. This approach is analogous to that of Milne and Reynolds. Smoothing must be done occasionally in each integration to remove the weakly stable component of the error, else meaningless results or overflow may result.

As implemented by Bulirsch and Stoer first and in all succeeding codes for non-stiff problems, extrapolation is done locally. The integrations with the midpoint rule are done from a solution at a mesh point \( x_n \) to the next mesh point \( x_{n+1} = x_n + H \). The results of the various subintegrations are smoothed at