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VARIABLE STEP-SIZE SELECTION METHODS FOR IMPLICIT INTEGRATION SCHEMES FOR ODES

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Abstract. Implicit integration schemes for ODEs, such as Runge-Kutta and Runge-Kutta-Nyström methods, are widely used in mathematics and engineering to numerically solve ordinary differential equations. Every integration method requires one to choose a step-size, h, for the integration. If h is too large or too small the efficiency of an implicit scheme is relatively low. As every implicit integration scheme has a global error inherent to the scheme, we choose the total number of computations in order to achieve a prescribed global error as a measure of efficiency of the integration scheme. In this paper, we propose the idea of choosing h by minimizing an efficiency function for general Runge-Kutta and Runge-Kutta-Nyström integration routines. This efficiency function is the critical component in making these methods variable step-size methods. We also investigate solving the intermediate stage values of these routines using both Newton's method and Picard iteration. We then show the efficacy of this approach on some standard problems found in the literature, including a well-known stiff system.

Key Words. Runge-Kutta, implicit integration methods, variable step-size methods, solving stiff systems

1. Introduction

Recently, there has been interest in the literature concerning the use of geometric integration methods, which are numerical methods that preserve some geometric quantities. For example, the symplectic area of a Hamiltonian system is one such concern in recent literature [1, 2, 3, 4]. Tan [5] explores this concept using implicit Runge-Kutta integrators. Hamiltonian systems are of particular interest in applied mathematics, and in fact we test our variable step-size selection method on a well-known Hamiltonian system in Section 4.2. Furthermore, Hairer and Wanner [6, 7] showed that although implicit Runge-Kutta methods can be difficult to implement, they possess the strongest stability properties. These properties include A-stability and A-contractivity (algebraic stability). These are the main reasons we choose to investigate variable integration step-size selection using Runge-Kutta methods.

First order ordinary differential equations are solved numerically using many different integration routines. Among the most popular methods are Runge-Kutta methods, multistep methods and extrapolation methods. Hull, Enright, Fellen and Sedgwick [8] have written an excellent comparison of these types of methods. They test a number of Runge-Kutta methods against multistep methods based on Adams formulas and an extrapolation method due to Bulirsch and Stoer [9]. A goal of that paper was to compare these different types of methods as to how

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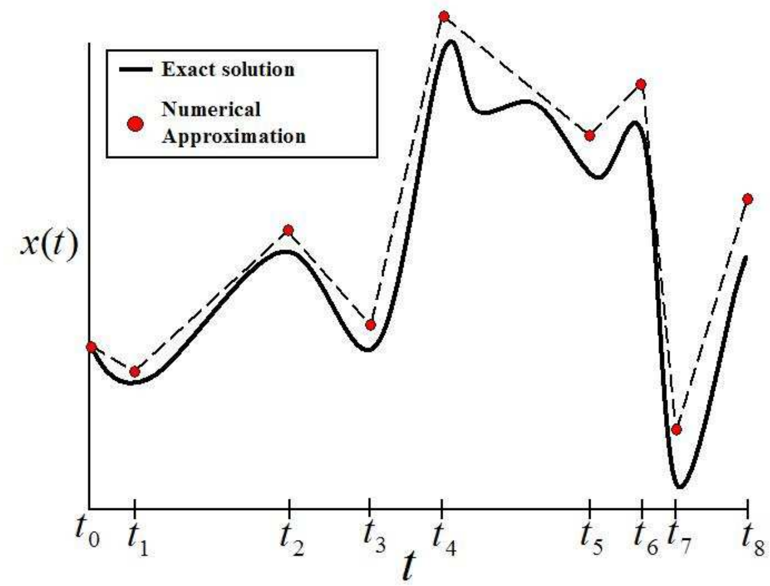

FIGURE 1.0.1. Illustration of variable step-sizes and error propagation in numerical integration

they handle routine integration steps under a variety of accuracy requirements. Implicit or explicit integration methods require one to choose a step-size, h, for the integration. One of the questions Bulirsch and Stoer investigate is a strategy for deciding what step-size h to use as the methods progress from one step to another. Others have investigated this very same problem in the past [8, 10, 11, 12].

In this paper, we propose the idea of choosing variable step-sizes by minimizing an efficiency function for general Runge-Kutta and Runge-Kutta-Nyström integration routines. As every implicit integration scheme has a global error inherent to the scheme, we choose the total number of computations in order to achieve a prescribed global error as a measure of efficiency of the integration scheme. For illustration purposes, consider Figure 1.0.1, referring to the solution of (2). Let $\tilde{x}(t_k)$ be our approximation to $x(t_k)$. We determine the variable step-sizes $h_1, h_2, \ldots, h_8$, where $h_k = t_k - t_{k-1}$, so that we minimize an efficiency function that minimizes the sum of the total number of computations to compute $\tilde{x}(t_k)$ for $k = 1, 2, \ldots, 8$ and the global error that propagates from the local truncation errors at each step of integration. To the best of our knowledge, our proposed method is novel.

The paper that most closely parallels the spirit of our optimization is that of Gustafsson and Söderlind [13]. They arrive at a function very similar to (31) using approximations while optimizing convergence rates, α, for a fixed-point iteration. They conclude that $\alpha_{\text{opt}} = e^{-1} = h_{\text{opt}}\overline{L}\|A\|$. They do not carry the argument further and include the global error in calculating the step-size, h, as we have done here.

One of the most important benefits of using a variable step-size numerical method is it's effectiveness at solving stiff initial value problems when combined with an implicit integration routine. Stiff systems are found in the description of atmospheric phenomena, chemical reactions occurring in living species, chemical kinetics (e.g. explosions), engineering control systems, electronic circuits, lasers, mechanics, and