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Accurate and stable time integrators

Butcher, J.C[1]

[1]*Department of Mathematics,The University of Auckland, Auckland, New Zealand,*
Email: butcher@math.auckland.ac.nz

Abstract: In method of lines solutions to partial differential equations, the selection of a suitable time integrator is often a limiting factor on the performance of the overall computation. A survey will be given of some known approaches to the construction of appropriate time integrators to perform this role. Amongst the attributes that have to be taken into account are the numerical order of the method, its stability characteristics and its implementation cost. As a starting point, methods based on Gauss or Radau quadrature will be considered. A-stable methods in these families exist for arbitrarily high orders and they would seem to be excellent choices. However, in a practical context, stage order can be as important as order and there seems to be little advantage in the use of Gauss or Radau points in an attempt to obtain super-convergence. Furthermore, the implementation costs for these methods are unreasonably high. The search for methods which overcome these deficiencies will be investigated through the use of alternative one-step and multistep methods.

Ordinary differential equation systems arising from the method of lines are invariably stiff, and this means that stability is one of the basic requirements for a practical integrator. Although $A(\alpha)$ – stable methods can be satisfactory for many problems, full A-stability is usually required. This means that linear multistep methods have to be completely ruled out of contention, unless low order is acceptable. Hence, Runge–Kutta methods or possibly some other multi-stage methods, come under consideration. The choice between competing A-stable Runge–Kutta methods hinges on the balance between accuracy and computational cost. We will look at these two issues separately in the choice of suitable numerical methods.

Methods based on Gaussian or Radau quadrature are ideal in terms of stability. They are also attractive because of their super-convergence. This means that, because of the underlying quadrature formula, the order is much higher than might otherwise be expected. However, this high order comes at the cost of order reduction. This means that the stepsize required to observe asymptotic behaviour of the theoretical order is often too small to have practical significance. This phenomenon almost completely nullifies the benefits of high theoretical order. Equally serious is the fact that these methods come with high implementation costs, sufficiently high to make them completely impractical for many problems.

If any attempt to obtain super-convergence is abandoned, but a collocation structure is retained, there remains complete freedom in the choice of distinct abscissae for the method. How then should the abscissae be chosen for computational advantage? One answer to this question is to place them at points chosen in proportion to zeros of the Laguerre polynomial. This choice has a dramatic effect on the numerical cost and makes the method practical when, for example, Gauss or Radau methods would not be. Methods based on Laguerre polynomials do, however, have their own shortcomings. This paper will discuss these disadvantages and explain how to overcome them.

Abstract only