Efficient methods for special second–order ODEs

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Many physical problems arising from celestial mechanics, molecular dynamics, seismology and so on are modelled by the special second order Differential Equation

$$y'' = f(t, y(t)), \qquad y, f, \in R^d \tag{1}$$

in which the first derivative does not appear explicitly. Systems of ODEs (1) may be of large dimension and highly stiff, and can present a right hand side which is very expensive to evaluate. Therefore it is appropriate to derive parallel numerical methods with high stability properties to obtain efficient solutions.

Most of ODEs (1) have periodic or oscillatory solutions. Classical methods may need to use a small stepsize to track the oscillations and only methods which take advantage of some previous knowledge about the solution have hope to integrate by using quite large stepsize. Therefore, in the case of oscillatory soutions, efficiency can also be obtained by using numerical methods in which the informations *a priori* available on the solution can be embedded such as, for example, a good estimate of the period or of the dominant frequency.

For stiff problems we derived [2] iterative methods which consist of the modified Newton method in which the linear Newton systems are solved by a second iteration process which is based on the approximate factorization of the system matrix associated with the linear Newton system. These methods are effective in cases where the Jacobian of the right–hand side can be split into a sum of matrices with simple structure.

For nonstiff problems we constructed high–order parallel Störmer–Cowell type methods [5], which are the second order ODEs analogue of the parallel Adams methods for first order ODEs proposed in [3]. In each step these methods compute blocks of k approximate solution values at k different points by using the whole previous block of solution values. The k stage values can be computed in parallel, so that on a k–processor computer system such methods effectively perform as a one–value method.

For the special second order ODEs (1) having periodic solution with frequencies lying in the interval $[\omega, \bar{\omega}]$, we constructed methods based on the classical Störmer–Cowell methods and the Parallel Störmer–Cowell methods [4, 5], by *tuning* the method parameters to the interval $[\omega, \bar{\omega}]$, that we suppose to be known, through a minimax technique. The derived methods possess stage order at least equal to the number of stages.

As far as the linear stability analysis is concerned, we also studied the modification of the stability properties of a numerical method with constant coefficients when it is reformulated in such a way to fit one frequency exactly. To this purpose we derived the *exponential–fitting* version of a P–stable multistep algorithm with an order greater than two and showed that this version is conditionally P–stable and can be used for stiff problems [6].

The results derived in [6] helped us in understanding how to apply an exponential–fitting technique to methods which seemed still resistent to it, such as Runge–Kutta methods. Indeed, assuming that good estimate of the frequency k of the periodic solution can be known in advance, we were able to derive Runge–Kutta–Nyström methods which are based on trigonometric polynomials [8], with parameters depending on the predicted frequency k. We defined the *trigonometric order* of these methods and analyse their algebraic order.

Computer algebra has been very useful not only to prove order bounds [7], but especially to derive methods with high linear stability properties [1, 9]. We derived two symbolic–numerical packages for this purpose, which are freely available on `netlib`.

References

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