Study of numerical methods for evolutionary equations and construction of the corresponding software for sequential and parallel computers

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The research, coordinated by Professor D. Trigiante, has been done in collaboration with the Bari unit coordinated by Professor G. Di Lena. It has regarded the study of numerical methods for approximating the solution of differential equations. In particular, it has been considered the class of BVMs (Boundary Value Methods), introduced by this group of research (see [11]). These are difference methods based on LMF, which are used so as to overcome Dahlquist's order barriers. The discrete problem defined by a BVM is generally a boundary value problem. The basic themes developed have been:

1. the study of the theoretical properties of the methods,
2. the study of the implementation techniques for BVMs, both on sequential and parallel computers,
3. the construction of numerical codes based on such methods.

The researches carried out so far have clearly evidenced the good potentialities of BVMs in their block implementation (block BVMs). In such implementation, the additional conditions for the discrete problem have been implicitly imposed through suitable "additional methods". In the light of this implementation, it has been necessary to reconsider the convergence and stability properties of the methods. In [7], the framework of General Linear Methods (GLMs) has been considered for this purpose: this because a block BVM can be reformulated in such a form. In particular, the study of the linear stability theory has been carried out for some block GAMs (Generalized Adams Methods), namely the block BVMs which have been used in the construction of the code, called GAM, described below.

An ulterior theoretical aspect that has been deepening object regards the conditions for the numerical methods in order to be efficiently applicable to Hamiltonian problems [1]. In fact, for such problems the usual linear stability analysis turns out to be insufficient. This because the test equation, on which it is based, is a prototype of dissipative system, while an Hamiltonian system is conservative. For such systems, it is necessary for the numerical method to satisfy an additional condition, called "time reversal symmetry". Such a condition is needed in order the discrete solution to be time isotropic, thus satisfying the same property of the continuous one. In particular, the analysis in [1] has been done for block BVMs, showing that only the symmetric schemes, in such class [11], satisfy the "time reversal symmetry" property.

The application of block BVMs for the numerical solution of DAEs (differential algebraic equations) has been considered in [3]. In particular, some properties of GBDF (Generalized BDF) have been studied, which allow the determination of the consistent initial conditions needed for determining the discrete solution. The proposed technique has been tested on problems of index 1, 2 and 3 in Hessemberg form.

The implementation of block BVMs, both on sequential and parallel computers, has been carefully studied.

Concerning the implementation on sequential computers, in [6] it has been shown how efficiently solve the linear and nonlinear systems deriving by the application of the methods. The problem of getting an estimate of the local error has been also considered and solved. It is connected to the problem of the automatic variation

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of both the stepsize and the order of the method. For the solution of the nonlinear equations, it has been developed a nonlinear splitting, which has very good convergence properties. As matter of fact, the linear analysis shows that the iteration corresponding to the block GAMs of order 3, 5, and 7 is A-convergent, whereas that corresponding to the method of order 9 is $A(\alpha)$-convergent with $\alpha \approx \pi/2$. The estimate of the local error is obtained by a modification of the technique called "deferred correction", by taking advantage of the natural feature of block BVMs of having higher order methods within the same family. This allows an efficient stepsize variation and, moreover, an additional comparative cost analysis permits to derive a strategy for the dynamic variation of the order of the method. A wide experimentation has proved such strategies to be very effective. The results have been used in the construction of the computational code called GAM [9], which turns out to be competitive with the currently best available codes (such as MEBDFDAE [10] and RADAU5 [12]), both for robustness and efficiency.

For the implementation of block BVMs on parallel computers, two possibilities have been considered.

One of these consists in the parallelization of the procedure used in the sequential code GAM [8]. In such a case, the parallelization essentially concerns the solution of the nonlinear system deriving at each step from the application of the methods (parallelism "across the method"). In order to obtain a better parallel performance, the nonlinear splitting has been replaced by a block diagonalization of the coefficient matrix of the method: each diagonal block is then assigned to a distinct processor. The numerical experiments confirm the theoretical analysis, even though the code is not yet in its final version.

A different strategy taken in consideration consists instead in the simultaneous approximation of several consecutive time steps of the same method (parallelism "across the steps"). Such a strategy proved to be very promising for linear problems, when a uniform mesh is used (see, for example, [11]). Nevertheless, its application to nonlinear problems requires the solution of the following related problems:

- the selection of a suitable mesh,
- the convergence of the nonlinear iteration over the whole considered interval,
- the determination of an initial point for the iteration itself.

In order to solve such problems, in [5] it has been proposed a two-phase procedure: in the first phase, a modification of the trapezoidal rule is used in a sequential fashion, in order to determine a suitable mesh and an initial profile for the solution. Then, in the second phase, the simplified Newton method is applied, over a suitable "window" of the integration interval, for solving the discrete problem. The latter is generated by using a higher order block GAM on the previously determined mesh. Such phase, on the contrary of the first one, is highly parallelizable. The window of integration is dynamically determined in the first phase of the procedure, through the estimate of a couple of parameters which, in a sense, measure the speed of convergence of the Newton iteration in the second phase. Such two-phase strategy has been used in [2] to develop a parallel code. Nevertheless, in its original version such code turned out to be relatively expensive, in terms of number of operations and memory requirement, when used on large sized continuous problems. This drawback derives from the Newton iteration used in the second phase of the procedure, which requires the computation (and the factorization) of the Jacobian matrix relative to the whole window of integration. This is, indeed, computationally expensive, even though such a matrix is lower block bidiagonal and distinct processors handle each block row. In order to overcome such drawback, in [4] a new family of block methods have been proposed. Such methods, called blended block BVMs, should be used in the second phase of the procedure. They are obtained by combining two different block BVMs, which naturally define a nonlinear splitting for solving the corresponding discrete problem. By carefully choosing the block BVMs, the resulting splitting turns out to generate an A-convergent iteration. Moreover, since the matrices defining the splitting are Toeplitz lower bidiagonal, a considerable reduction of both memory requirements and number of operations is obtained. A family of such methods, called hybrid block GAMs (HB_2GAMs) has then been used in the second phase of the parallel procedure, thus generating a more efficient code. However, the sequential nature of the first phase still needs further investigations.

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