UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

DIPARTIMENTO DI INFORMATICA

PhD Program in Computer Science and Mathematics
XXXIV **cycle**

Research Project

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1 Research title:

CONTINUOUS BLOCK METHODS FOR SOLVING BOUNDARY AND INITIAL VALUE PROBLEMS IN ODEs.

2 Research area:

Numerical methods for the solution of differential equations.

3 Research motivation and objectives:

This research work will consider the derivation of new numerical methods for the solution of boundary and initial value problems in ordinary differential equations (ODEs). Continuous linear multistep methods will be generated by interpolating and collocating at grid and off-grid points the approximate solution. We will use several basis functions, one example is given by Laguerre polynomials, the generated methods will be implemented in block mode. The basic properties of the proposed methods will be discussed. The efficiency and accuracy of the new methods shall be tested for some real world problems and in particular, optimal control problems solved with indirect methods, SI Models, SIR Models, the Lane–Emden singular perturbed, Troesch's and Bratu's problems, Prothero-Robinson, Bessel's equation, nonlinear Fehlberg problems, oscillatory problems, simple harmonic motion and critically damped motion problems and highly stiff oscillatory problems. The results of the proposed block methods shall be adequately discussed and analysed graphically, and its numerical results have to yield better accuracy by numerical testing. This will be done by updating the testset websites available at the INDAM unit of the University of BARI Aldo Moro:Testset for IVP solvers (www.dm.uniba.it/ testset/testsetivpsolvers/) and Testset for BVP solvers (www.dm.uniba.it/ testset/testsetbvpsolvers/) and the R-packages deTestSet (https://cran.r-project.org/web/packages/deTestSet/index.html) and bvpSolve (https://cran.r-project.org/web/packages/bvpSolve/index.html).
This thesis work will be motivated by the needs to address various shortcomings associated with some of the existing numerical methods by deriving new numerical methods that will be more cost-effective, time-saving, highly efficient in term of accuracy and error terms with better rates of convergence.

4 State of the art

4.1 Introduction

Numerical problems can be found in different disciplines, for example, they may be found in mathematical modelling, physical and social sciences, engineering design, manufacturing systems, economics among other disciplines. In order to examine the utility of the numerical problems, there is a need for an efficient and robust computational algorithm which can be used to solve numerical problems arising in various fields of application. Different models had been developed to help in solving some real world problems. These models frequently result in equations that contain derivatives of an unknown function of one or more variables. We do not only encounter such equations in physical sciences but also in the diverse fields like Medicine, Psychology, Operation Research, Biology and

Anthropology. Realistically, the theoretical solutions of equations arising from modelling of some real world situations might not be easily obtainable. This necessitates the need for an approximate solution by the application of numerical methods. To that extent, many algorithms had been presented in the literature based on the nature and the type of the differential equations to be solved. Some of these methods are the Euler forward and Euler backwards methods, Adams-Moulton and Adams-Bashforth methods, Runge-Kutta method, Spectral method, Galerkin method, finite element method, finite volume method, finite difference method, backwards difference method and so on.

4.2 Definition of the problems and related literature

In this section, we will review the numerical solution of

- general first order initial value problems of ordinary differential equations

$$y' = f(x, y),\ y(x_0) = y_0; \tag{1}$$

- second order systems

$$y'' = f(x, y, y'), \tag{2}$$

  subject to initial values

$$y(x_0) = y_0,\ y'(x_0) = y_0',$$

  or boundary values

$$y(a) = y_L,\ y(b) = y_R, \quad \text{or} \quad y(a) = y_0,\ y'(b) = y_R';$$

- third order systems

$$y''' = f(x, y, y', y''), \tag{3}$$

  subject to initial values

$$y(x_0) = \ y_0,\ y'(x_0) = y_0',\ y''(x_0) = y_0'',$$

  or boundary values,

$$y(a) = y_L,\ y'(a) = y_L',\ y(b) = y_R, \quad \text{or} \quad y(a) = y_L,\ y'(a) = y_L',\ y'(b) = y_R,$$

  where x_0 represents initial point, $a, b, y_0, y_0', y_0'', y_L, y_R, y_L', y_R', y_S$ are constants and f is a continuous function that satisfies the Lipchitz's condition that assures the uniqueness and existence theorem.

Problems $(1), (2), (3)$ emerge from several application areas, such as Mathematical Biology and Epidemiology, Engineering, Physics, Economics, Classical Mechanics, Celestial Mechanics, Quantum Mechanics and Social Sciences. It is commonly known that many first order ordinary differential equations of the form (1) do not admit a solution in closed form, hence looking for the numerical solution is very important. Equation (1) is used in simulating the growth of population, the trajectory of a particle, epidemiology models like SI model, SIR model, Prothero-Robinson oscillatory problems and highly stiff oscillatory problems and other related models can be transformed into the equation (1). Numerous numerical approaches including higher derivative multistep methods, Runge-Kutta methods, Runge-Kutta-Nystrom methods and hybrid block methods have been developed for solving oscillatory initial and boundary value problems see [1], [2], and [3]. In most cases, reduction methods were mostly adopted by scholars for the solution of higher order initial and boundary value problems of ODEs. One standard procedure is to reduce high order IVPs and BVPs to an equivalent system of first order ODEs of the form (1). The resulting system is solved using appropriate methods for first order ODEs, see for example [4] and [5].

Equations $((2),(3))$ occur in obstacle problems see [6], thin film flow see [7], sandwich boundary layer and laminar flow beam problems see [8] and in fluid mechanics and dynamics see [9]. Many real life problems in Economics, Applied Chemistry, Physics and Engineering have been modelled mathematically by first and higher order ordinary differential equations(ODEs). Dynamic problems, simple harmonic motion problems, nonlinear Duffing equation and critically damped motion problems are modelled using second Newton's law of motion and the results obtained lead to a system of second order ODEs, see [10] and the reference therein. The majority of these models in ODEs do not admit the theoretical solutions, thus approximate solutions and numerical approaches are often employed to solve many of them. Notable researchers like [[11],[12], [13], [14], [15]] among other have applied different numerical methods to give solutions to first order and higher order IVPs and BVPs of ODEs.

Recently, Higinio Ramos et al. [16] proposed an efficient variable step-size rational Falkner-type method for solving the special second-order IVPs, Li and Wu [17] have adopted Falkner block methods to give a direct solution to second order IVPs, Nazan and Hikmet [18] presented B-spline approach for solving linear system of second orders BVPs, but their accuracy is not encouraging. Fidele and Samuel [19], implemented trigonometrically-fitted second derivative method for solving oscillatory problems but their solutions have lower order of accuracy. Regardless of the improvement of prominent researchers in developing numerical methods that solve first order and higher order of ODEs, there are still drawbacks of less accuracy in their result, especially for higher order problems. As a result of this, the main aim of my work will be to develop new block methods for the numerical solution of ODEs.

5 Problem approach

5.1 General research objectives

First of all we will review some existing methods for the numerical solution of first order and higher order in ordinary differential equations that also uses high order derivative in the scheme. We shall study their advantages and disadvantages and derive efficient new methods for solving initial and boundary values problems.

5.1.1 Specific objectives

The specific objectives are:

1. to develop new numerical methods via collocation and interpolation approach at an appropriate set of grid and off-grid points,
2. to derive a family of continuous implicit schemes that give solutions to first, second and third order differential equations,
3. to analyse the basic properties of the developed block methods which include consistency, convergence, zero-stability, linear-stability, order and local truncation errors,
4. to write powerful computer codes that implement the new methods,
5. to test and compare the accuracy of the methods, via some numerical samples of initial and boundary value problems with the existing methods,
6. to improve the testset for IVP and BVP solvers adding new codes and test problems.

5.2 Research methodology

One class of method that will be considered will be based on the use of Laguerre polynomial as basis function, an approximate solution of the differential problem is written, for first order ODEs, in the form:

$$Y(x) = \sum_{j=0}^{((i+c)-1)} \frac{a_j \left(-1\right)^j \left(i+c-1\right)! \, x^j}{\left(j!\right)^2 \left(\left(i+c-1\right)-j\right)!} \tag{4}$$

where c represents the number of collocation points and i is the number of interpolation points. x^j represents polynomial basis function and a_j $'s \in \Re$ are coefficients to be determined.
One way to determine the unknown coefficients is given by looking at schemes that uses the second and third derivative of the solution of the following form:

$$y_{n+2} = y_n + h \sum_{j=0}^{k} \alpha_j f_{n+j} + h^2 \sum_{j=0}^{k} \beta_j g_{n+j} + h^3 \delta_j e_{n+2}, \tag{5}$$

where

$$\begin{aligned} y_{n+j} &\approx y(x_n + jh), \\ f_{n+j} &\equiv f(x_n + jh, y(x_n + jh)) \\ g_{n+j} &= \frac{df(x,y(x))}{dx}\Big|_{\substack{x=x_{n+j} \\ y=y_{n+j}}}, \\ e_{n+j} &= \frac{dg(x,y(x))}{dx}\Big|_{\substack{x=x_{n+j} \\ y=y_{n+j}}}, j = 0,1,2 \end{aligned}$$

x_n represents a discrete point at n, α_j, β_j , δ_j represent unknown constants.
These methods need additional schemes of the form;

$$y_{n+1} = y_n + h \sum_{j=0}^{k} \alpha_j f_{n+j} + h^2 \sum_{j=0}^{k} \beta_j g_{n+j} + h^3 \delta_j e_{n+2}, \tag{6}$$

These methods differs from the standard one, because uses higher derivative for the computation of the solution. We will analyze both methods in which the higher derivatives are exactly computed and methods in which they are numerically approximated. Convergence and stability will be studied. Suitable error estimation techniques and step variation strategy will be analyzed for both initial and boundary value problems. In particular special care will be taken for the solution of non-linear boundary value problem, that need robust step-variation strategies and non linear solvers.

6 Expected results

The following contributions will be made to the body of knowledge:

1. family of new methods with additional derivatives for solving first, second, and third order ODEs will be constructed,

2. the numerical methods that will be derived in this thesis work will be tested for the solutions to SI and SIR Models problems, Prothero-Robinson problems, Troesch's and Bratu's problems, nonlinear Fehlberg problems, oscillatory problems, simple harmonic motion and critically damped motion problems and highly stiff oscillatory problems,

3. powerful and efficient codes will be written using high level programming languages (Mathematica, Matlab, R or python), in order to compare these methods with the well know general purpose codes available in the Test Set for IVP problems in the packages deTestSet and bvpSolve, the numerical test will be inserted in the related website,

4. if the resulting are encouraging a Fortran or C implementation will be provided,

5. the expected results of the new proposed methods have to be motivated and yield better accuracy by numerical testing.

7 Phases of the project

Table 1: This table shows the schedule of the research work

S/N	Description of Work	Duration
1	State of the art and derivation of the family of methods	Six months
2	Analyzing the basic properties of the new methods	Four months
3	Implementing the proposed methods for solving first order ODEs of IVPs	Four months
4	Implementing the new proposed methods for solving second order ODEs both IVPs and BVPs	Five months
5	Implementing the new methods for solving third order ODEs both IVPs and BVPs	Five months
6	Developing computer programs to implement the new proposed methods	Six months
7	Compilation of the Thesis	Six months

8 Result evaluation

The accuracy and performance of the new proposed methods will be tested on some numerical examples ranging from non-linear, linear and systems of first, second and third order initial and boundary value problems in ODEs. The maximum absolute errors of the approximate solutions would be computed and compared with the results of other researchers in the area of Numerical Analysis and of general purpose codes for first order ODEs and BVPs presented in the R-packages deSolve, deTestSet and bvpSolve. In particular, the comparison will be done with BS and BS2 methods in [20, 21], explicit Runge-Kutta methods presented by Mazzia and Nagy [22], the block approach proposed by Jator et al. [23], non-polynomial spline technique proposed by Al-Said and Noor [24]. By the end of this research work, the new proposed modified block methods will give solutions to first, second and third order boundary and initial value problems directly without reducing to a system of first-order ordinary differential equations. We will use our new developed methods to solve some numerical problems in form of equations (1), (2), (3). We will also apply the proposed methods to solve real world problems in industries, physical sciences, medicine, engineering and population dynamics.

9 Possible reference persons external to the department

Professor Higinio Ramos Calle, Department of Applied Mathematics, Scientific Computing Group, Universidad de Salamanca, Plaza de la Merced, Salamanca 37008, Spain.

Prof. Dr. Caren Tischendorf, Chair for Applied Mathematics, Institute of Mathematics Humboldt University of Berlin Unter den Linden 6 10099 Berlin, Germany.

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