RUNGE-KUTTA RESEARCH AT NATIONAL TECHNICAL UNIVERSITY OF ATHENS

G. PAPAGEORGIOU

Dept. of Applied Mathematical & Physical Sciences, Natl. Technical Univ. Athens, Zografou Campus, GR-15780 Athens, GREECE

CH. TSITOURAS[†*]

Dept. of Applied Sciences, TEI of Chalkis, GR-34400 Psahna, GREECE

Abstract: The main purpose of this presentation is to review the work on Runge-Kutta (RK) methods at the National Technical University of Athens (NTUA) during the last twenty years. More than thirty papers on this subject, due to the team of RK research at NTUA, consisting of G. Papageorgiou, Ch. Tsitouras, S. N. Papakostas and I. Th. Famelis are briefly presented and referred.

1. First years

G. Papageorgiou, the founder of RK research team at NTUA, received his Ph. D. degree from University of Essex back in 1979. His supervisor was J. Oliver. Coming in Greece he continued the research on Numerical ordinary differential equations (ODEs) and especially in the area of the Runge-Kutta methods [1-2].

Later in the decade of 80's the group of G. Papageorgiou, T. Kalvouridis (from Mechanics section of our department) and T. E. Simos, evolved in the application of RK methods in celestial mechanics problems [3-5]. Ch. Tsitouras participated that group after coming at NTUA as Ph. D. student of G. Papageorgiou [6-7].

Also in the 80's a large number of papers appeared in the literature considering continuous extensions for RK methods. We contributed that research presenting such extensions for classical RK [8], and for Runge-Kutta-Nystrom (RKN) methods [9-10]. The most interesting proposal of us on this subject was the use of two-step interpolants [11], which are costless and keep the truncation error of the underlying formula low. Since then, we have also dealt with this subject once [12].

2. The period 1992-1999

At the beginning of 90's, S. N. Papakostas, a new Ph. D. student of G. Papageorgiou joined with Dr Ch. Tsitouras a group which was to be dealing with the study and derivation of new RK and RKN methods. In a series of five articles published mainly in SIAM journals, the core of our research that period was presented.

First we gave new families of RK pairs of orders 5(4) [13], and 6(5) [14]. In these families we avoided the use of the simplifying assumption

$$Ac^2 = \frac{c^3}{3}$$

gaining a free parameter more. Theoretical justification of the orders attained is given and some new pairs derived, that proved by extended numerical tests to outperform other pairs of the same order.

A variable step stability analysis of Runge-Kutta-Nordsieck methods is actually studied in [15]. Later a number of new efficient RK pairs from families of orders 4(2), 6(4), 8(6), 8(4), 10(6) were given along with a new step-size control algorithm that keeps tolerance proportionality [16]. The RK8(6) pair is suggested for tolerances from 10^{-5} to 10^{-11}, since it seems to have better performance than every other pair appeared in the literature.

Studying properties of methods scheduled for problems with oscillatory solutions we consider the test problem

$$y^{(k)} = (-i\omega)^k y, i = \sqrt{-1}, \omega \in \Re .$$

The concepts of dissipation and phase errors and P-Stability are used for derivation of better methods for such problems. Compact forms of the dissipation order conditions for RK methods and phase-lag order conditions for RKN pairs are proved in [17]. Many RK(-N) pairs with reduced phase-lag are constructed and tested numerically.

Before that, equations in closed form for phase-lag order conditions for RK methods were proved in [18]. RK(-N) interpolants with reduced phase errors were constructed in [19]. Zero dissipative RKN pair of orders 8(6) is presented in [20], while very high dissipative order RK8(7) pair was derived in [21].

Order conditions of symplectic RKN methods are studied in [22], and a particular method of tenth order is given which is, as expected, by far less efficient than the conventional RKN methods when applied in the two body problem. Another interesting paper of that period [23], deals with a RK family of orders 6(5).

I. Famelis was the new member of our team by the mid 90's. He was dealt with delay differential equations (DDE) as a M. Sc. Student of D. Higham. Part of his RK research was in DDE direction [24], and part in deriving P-stable Diagonally Implicit RKN methods [25].

3. The new millenium

G. Papageorgiou, Ch. Tsitouras and I. Famelis formed a stable team at late 90's and increased the rate of their publications. A new family of 9(8) pairs studied in [26] and a particular pair suggested that outperforms any other RK pair at stringent tolerances, say lower than 10^{-11}. Papageorgiou and Famelis extent the idea in [19] to higher order RKN pairs [27], and Tsitouras presented high phase-lag order RK pairs suitable for engineering applications [28].

Neural Networks and Numerical Analysis are combined in [29]. RK theory is useful for introducing learning algorithms with vector transfer functions. Back propagating in the direction of minimizing principal truncation error of the underlying numerical scheme is proposed and even FSAL became LLAF (Last Layer As First).

The RK order conditions for the scalar autonomous problem are studied in [30] where a 5 stages 5th order pair of orders 5(4) is constructed. Tsitouras and Simos [31], propose families of trigonometric and phase fitted RK pairs of orders 5(4). Our last accepted article [32], implements an old symbolic algorithm of us for producing RK order conditions. This method derives the RK truncation error coefficients based on their combinatorial attributes and the powerful programming abilities of the symbolic algebra package Mathematica.

Of course many other articles have been published from NTUA group in the area of Numerical ODEs and do not involve RK(-N) methods [33-41].

We have to notice here, that another NTUA group, dealing mainly with modifications of Numerov method, applied to ODEs with oscillatory solutions, was active at the decade of 80's. Namely A. D. Raptis and his Ph. D. student T. E. Simos. The later author is now very active in the same area, but not working with NTUA.

4. Influences and inspirations

Our group was an isolated research team at NTUA. No collaborations out of Greece have been done and we have participated in very few international conferences due to economical reasons. Nevertheless we have accepted many influences and inspired from many other researchers even if we have never met them.

First, Fehlberg's NASA reports were the technical bible for someone who wanted to derive new RK(-N) pairs [42-44]. Shampine papers were fruitful of ideas and included very helpful discussions. We refer report [45] containing the code RKF45, and [46] which helped a lot at the first "interpolation" years. Then Butcher published his book [47], so many fundamental issues became clear (it took some years of course) and raised new interesting questions.

Statistics on papers [1-41] shows more objectively the connection of our work with other researchers. So, we observe that Dormand and Prince received 45 references, Enright 43, Fehlberg 41, Shampine 36, Butcher 32, Hairer 31, Chawla 30 and Verner 26.

Journals in descending order according to the number of references received are: SIAM Journal on

Numerical Analysis with 103 references, Journal of Computational and Applied Mathematics 74, SIAM Journal on Scientific Computing 37, Mathematics of Computation 34, ACM Transactions on Mathematical Software 30, and IMA Journal on Numerical Analysis 25.

The book of Hairer, Norsett, Wanner [48] is the most referent item since it appears 22 times in our bibliographies. Hull et. al. [49] paper on DETEST follows with 16, Houwen & Sommeijer article [50] on RK phase-lag analysis with 14, and Dormand & Prince classical article on their FSAL 5(4) pair with 13. Tsitouras and Papakostas [16] have also received 13 self-references in the most representative article of our team.

In spite of the above-mentioned numbers, Fehlberg reports had many explanations and were more useful to us than Dormand & Prince papers that explained very little. The influence of the Butcher book was much more significant but Hairer et. al. is always a standard reference. It is peculiar that Runge's original article [51] and Marquardt [52] work on nonlinear least squares minimization does not exist on our papers while Riordan [53] is hardly referent on 2003 for the first time.

Combinatorial analysis, tree theory, constraint optimization and solutions of systems of nonlinear equations are back up mathematical fields for our research. Among other subjects of interest are interpolation, semi-discretization of partial differential equations, symbolic computation, linear algebra, celestial mechanics and neural networks.

Most of the members of the team were actually unemployed for long periods during the difficult decade of 90's but we managed to stay in business because of the following reasons. At late 80's, some books were printed that put the things together and focused the evolution of the subject for the next years. The symbolic manipulation package Mathematica [54] appeared, which is very well suited for the kind of research we conduct [32], and it was used, in some degree, in all of our papers after 1992.

Finally we owe much to Internet because it changed the flow of information. Fifteen years ago, we had access only on some papers that were at best 4-5 years old already. Now we earn almost everything at the time of submission but in many cases we do not prevent to read them.

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