A Retrospective Survey on Deriving Explicit Runge-Kutta Pairs[†*]

Jim Verner

PIMS & Department of Mathematics
Simon Fraser University, Canada
jverner@pims.math.ca
http://www.math.sfu.ca/∼jverner

Abstract: Techniques for solving the order conditions for explicit Runge–Kutta methods have evolved in the past five decades. Even now new methods are being found. This presentation reviews some of the approaches that have been exploited.

[†] Thanks to G.J. Cooper, J.C. Butcher, P.W. Sharp, M. Zennaro, Z. Jackiewicz, A. Kværnø

July 13, 2011

Jan Verwer in Dundee, 1991

Jan Verwer in Washington, 1991

MOTIVATION

- Explicit Runge–Kutta pairs form an accepted basis for developing software to solve non-stiff initial value problems
- Order conditions for Runge–Kutta methods can be generalized to other methods for IVPs, and to other problems
- Approaches to solving RK order conditions can be generalized to solving the analogs for other methods or other problems
- CONSIDERATIONS:
  - minimizing the number of f-evaluations
  - optimizing the region of absolute stability
  - minimizing a norm of the error coefficients
  - providing a robust error estimator for stepsize control
  - obtaining interpolants as continuous approximations

OVERVIEW

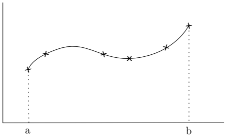
- Deriving methods arises by generalizing numerical quadrature
- Characteristics of early methods
- Identifying order conditions by rooted trees and algebraic theory
- Approaches to solving order conditions
- Error estimation using RK pairs
- DETEST results with XEPS
- Predicting the quality of RK formulas
- Classification of efficient explicit pairs
- Recent derivations
- RK interpolants
- Related problems with analogous methods

NUMERICAL INTEGRATION

A definite integral is approximated by the average height times the width, written as

$$\int_a^b f(x)dx = \sum_{k=1}^{s} b_k f(c_k) + Cf^{(\overline{k+1})}(b-a)^{\overline{k+1}}$$

Profile of a Quadrature Rule



This leads to the approximate solution of

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

on $[x_0, \overline{x}]$ by quadrature, namely

$$y(\overline{x}) = y_0 + \int_{x_0}^{\overline{x}} f(x)dx \tag{2}$$

$$\approx y_0 + \sum_{k=1}^{s} b_k f(c_k), \quad c_k \in [x_o, \overline{x}]. \tag{3}$$

Initial Value Problems

If f is Lipschitz, and $\mathrm{y(x)}$ is the unique solution to

$$y' = f(x, y(x)), \qquad y(x_0) = y_0, \tag{4}$$

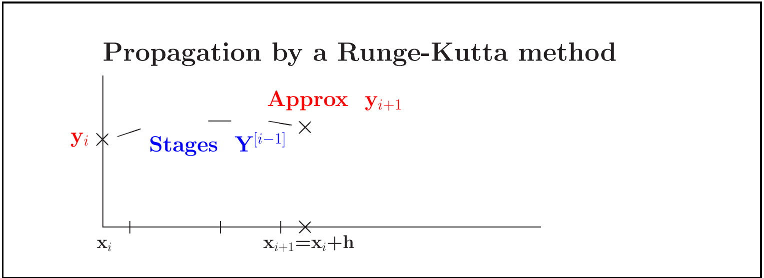
a Runge–Kutta method for (4) is defined for each $x_i = x_0 + ih$ by cascading numerical integrations within $[x_i, x_{i+1}]$

$$\mathrm{Y}_j^{[i]} = \mathrm{y}_i + h\left\{\sum_{k=1}^{j-1} \mathbf{a_{jk}} f(x_i + h\,\mathbf{c_k}, \mathrm{Y}_k^{[i]})\right\}, \qquad j = 1, .., s, \tag{5}$$

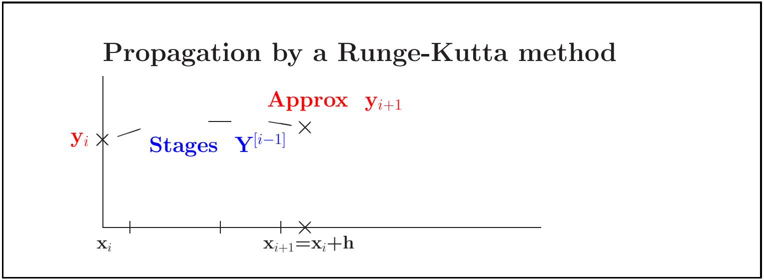
to yield a new approximation at $x_i + h$:

$$\mathrm{y}_{i+1} = \mathrm{y}_i + h\left\{\sum_{j=1}^{s} \mathbf{b_j}\, f(x_i + h\,\mathbf{c_j}, \mathrm{Y}_j^{[i]})\right\}. \tag{6}$$

Profile of an RK step



Profile of an RK step



$$\mathrm{Y}_j^{[i]} = \mathrm{y}_i + h\left\{\sum_{k=1}^{j-1} \mathbf{a_{jk}} f(x_i + h\,\mathbf{c_k}, \mathrm{Y}_k^{[i]})\right\}, \qquad j = 1, .., s, \qquad (5)$$

$$\mathrm{y}_{i+1} = \mathrm{y}_i + h\left\{\sum_{j=1}^{s} \mathbf{b_j}\, f(x_i + h\,\mathbf{c_j}, \mathrm{Y}_j^{[i]})\right\}, \quad x_i = x_0 + ih, \qquad (6)$$

approximates $\mathrm{y}(\mathrm{x_i} + \mathrm{h})$ at $x_{i+1} = x_i + h, \quad i = 1, ..$

Achieving order p

Parameters $\{\mathbf{b}_j,\ \mathbf{a}_{j,k},\ \mathbf{c}_k\}$ are selected primarily to satisfy a system of **polynomial equations** so that the global error is a multiple of $\mathbf{h}^p$ when the solution $\mathrm{y(x)}$ is sufficiently smooth.

- N **linear equations** in $N-k$ unknowns can easily be solved "exactly" when the matrix of coefficients has rank $N-k$.
- **In contrast**, **these polynomial systems** may be solved using
  - Direct elimination of variables ("brute force") for p small
  - Exploiting simplifying conditions which allow for cascading subsets of equations to be solved
  - Computing homogeneous polynomials as an intermediate step
  - Iteration by Newton-like methods (maybe on a restricted subset)
  - Algebraic tools which characterize families of methods
  - Linear subspaces of algebraic order expressions which lead to cascading solutions

Equations up to Order 5 (Solved by Kutta - 1901)

No.	Equation	p	No.	Equation	p
1.	$\mathbf{b}^t\mathbf{e} = 1$	1	9.	$5\mathbf{b}^t\mathbf{C}^4\mathbf{e} = 1$	5
2.	$2\mathbf{b}^t\mathbf{C}\mathbf{e} = 1$	2	10.	$10\mathbf{b}^t\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{e} = 1$	5
3.	$3\mathbf{b}^t\mathbf{C}^2\mathbf{e} = 1$	3	11.	$20\mathbf{b}^t \cdot (\mathbf{A}\mathbf{C}\mathbf{e})^2\mathbf{e} = 1$	5
4.	$6\mathbf{b}^t\mathbf{A}\mathbf{C}\mathbf{e} = 1$	3	12.	$15\mathbf{b}^t\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{e} = 1$	5
5.	$4\mathbf{b}^t\mathbf{C}^3\mathbf{e} = 1$	4	13.	$30\mathbf{b}^t\mathbf{C}\mathbf{A}^2\mathbf{C}\mathbf{e} = 1$	5
6.	$8\mathbf{b}^t\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{e} = 1$	4	14.	$20\mathbf{b}^t\mathbf{A}\mathbf{C}^3\mathbf{e} = 1$	5
7.	$12\mathbf{b}^t\mathbf{A}\mathbf{C}^2\mathbf{e} = 1$	4	15.	$40\mathbf{b}^t\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{e} = 1$	5
8.	$24\mathbf{b}^t\mathbf{A}^2\mathbf{C}\mathbf{e} = 1$	4	16.	$60\mathbf{b}^t\mathbf{A}^2\mathbf{C}^2\mathbf{e} = 1$	5
			17.	$120\mathbf{b}^t\mathbf{A}^3\mathbf{C}\mathbf{e} = 1$	5

Table 1: 17 equations in 21 variables
Left side of equation i is a polynomial of order p.

Equations up to Order 5 (Solved by Kutta - 1901)

No.	Equation	p	No.	Equation	p
1.	$\mathbf{b}^t\mathbf{e} = 1$	1	9.	$5\mathbf{b}^t\mathbf{C}^4\mathbf{e} = 1$	5
2.	$2\mathbf{b}^t\mathbf{C}\mathbf{e} = 1$	2	10.	$10\mathbf{b}^t\mathbf{C}^2\mathbf{A}\mathbf{C}\mathbf{e} = 1$	5
3.	$3\mathbf{b}^t\mathbf{C}^2\mathbf{e} = 1$	3	11.	$20\mathbf{b}^t \cdot (\mathbf{A}\mathbf{C}\mathbf{e})^2\mathbf{e} = 1$	5
4.	$6\mathbf{b}^t\mathbf{A}\mathbf{C}\mathbf{e} = 1$	3	12.	$15\mathbf{b}^t\mathbf{C}\mathbf{A}\mathbf{C}^2\mathbf{e} = 1$	5
5.	$4\mathbf{b}^t\mathbf{C}^3\mathbf{e} = 1$	4	13.	$30\mathbf{b}^t\mathbf{C}\mathbf{A}^2\mathbf{C}\mathbf{e} = 1$	5
6.	$8\mathbf{b}^t\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{e} = 1$	4	14.	$20\mathbf{b}^t\mathbf{A}\mathbf{C}^3\mathbf{e} = 1$	5
7.	$12\mathbf{b}^t\mathbf{A}\mathbf{C}^2\mathbf{e} = 1$	4	15.	$40\mathbf{b}^t\mathbf{A}\mathbf{C}\mathbf{A}\mathbf{C}\mathbf{e} = 1$	5
8.	$24\mathbf{b}^t\mathbf{A}^2\mathbf{C}\mathbf{e} = 1$	4	16.	$60\mathbf{b}^t\mathbf{A}^2\mathbf{C}^2\mathbf{e} = 1$	5
			17.	$120\mathbf{b}^t\mathbf{A}^3\mathbf{C}\mathbf{e} = 1$	5

Table 1: 17 equations in 21 variables

Left side of equation i is a polynomial of order p.

Subtract: Linearity shows $\mathbf{b}^t$ is orthogonal to 16 s-Vectors.

Parameters of Kutta 5a

Table 2a: An Incorrect Kutta 5a method of order 5

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & \\
\frac{2}{5} & 0 & \frac{2}{5} & & & & \\
1 & \frac{9}{4} & -5 & \frac{15}{4} & & & \\
\frac{3}{5} & -\frac{19}{25} & \frac{9}{5} & -\frac{13}{25} & \frac{2}{25} & & \\
\frac{4}{5} & -\frac{6}{25} & \frac{4}{5} & \frac{2}{15} & \frac{8}{75} & 0 & \\
\hline
\mathbf{b} & \frac{17}{144} & 0 & \frac{25}{48} & \frac{1}{72} & -\frac{25}{72} & \frac{25}{48}
\end{array}
$$

Parameters of Kutta 5a

Table 2b: The corrected Kutta 5a method of order 5

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & \\
\frac{2}{5} & 0 & \frac{2}{5} & & & & \\
1 & \frac{9}{4} & -5 & \frac{15}{4} & & & \\
\frac{3}{5} & -\frac{63}{100} & \frac{9}{5} & -\frac{13}{20} & \frac{2}{25} & & \\
\frac{4}{5} & -\frac{6}{25} & \frac{4}{5} & \frac{2}{15} & \frac{8}{75} & 0 & \\
\hline
\mathbf{b} & \frac{17}{144} & 0 & \frac{25}{48} & \frac{1}{72} & -\frac{25}{72} & \frac{25}{48}
\end{array}
$$

(HNW: in 1925 Nyström found such errors in Kutta 5b.)

I will return to these methods later.

Other early methods

Early designs provided a basis for study:

Hŭta (1957), Ceschino and Kuntzman (1959), Merson(1957), Butcher (1963), Cassity (1965, 1967), Konen and Luther (1967)

Butcher's

- Simplifying conditions to reduce the number of equations
- Explicit and implicit methods with Gaussian nodes
- Rooted trees to identify and tabulate order conditions
- Algebraic theory of integration methods

and B-series by **Hairer, Nørsett and Wanner** gave new impetus to a search for better methods

For detailed derivations and extensive bibliographies, I recommend

- Extensive monographs by Butcher, and by
- Hairer, Nørsett, Wanner, and later Lubich

Error Estimation

- Two approximations per step led to **Runge–Kutta pairs**

Some *early RK pairs* were derived by

- Merson (1957) - Order 3,4
- England (1969) - Order 4,5
- Fehlberg (1968, 1969) - Orders 4,5 to 8,9

Other new **high-order methods** motivated the derivation of *RK pairs*:

- Curtis (1970): 11-stage order 8
- Cooper and V. (1972): 11-stage order 8
- Hairer (1976): 17-stage order 10

Their Butcher tableaus have "stepped" designs and require Lobatto nodes.

Hull's Plea

T.E. Hull with colleagues and students developed DETEST in 1972 for assessing the quality of various methods when applied in a uniform test to 25 problems carefully selected to represent IVPs using adaptive stepsize implementations.

They found RK pairs of orders$>$5 developed by **Fehlberg had merit, but** were deficient because **the error estimate for quadrature problems failed** to be reliable.

About February, 1974, his group sent out a request for RK pairs of orders 5 and 6 that would overcome this particular problem.

Responses with New Pairs - 1974 and later

- **Butcher** quickly derived a 9*-stage *FSAL pair* (Only eight stages per step were required to propagate the method of order 5.)
- **Shampine** proposed numerical detection of a quadrature problem, and then estimation of the error in a different way.
- **V.** With a contrast of order 5 and 6 methods using the same nodes already *in progress*, construction of an 8-stage pair of orders 5 and 6 quickly followed.
- The latter pair was implemented by the Toronto group as the IMSL software program DVERK.
- Later pairs by Dormand-Prince improved on the efficiency of this first 5-6 pair.

Order Conditions for Methods

Now I want to consider aspects of solving the order conditions. We have seen that 6-stage methods of order 5 are obtained by solving 17 polynomial equations in 21 variables.

For higher order methods, we can do better:

Table 3a: Order Conditions and Variables for Methods:

Order	1	2	3	4	5	6	7	8	9	10
Stages	1	2	3	4	6	7	9	11	≤ 15	≤ 17
Equations	1	2	4	8	17	37	85	200	486	1205
Variables	1	2	6	10	21	28	45	66	118	151

We observe that for $s > 5$, fewer variables than equations are needed for a solution.

Order Conditions for Pairs

Now I want to consider aspects of solving the order conditions. We have seen that 6-stage methods of order 5 are obtained by solving 17 polynomial equations in 21 variables.

For higher order **pairs**, we need **more stages**:

Table 3b: Order Conditions and Variables for Pairs:

Order	2(1)	3(2)	4(3)	5(4)	6(5)	7(6)	8(7)	9(8)	10(9)
Stages	2	3	5	6	8	10	13	16	?
Equations	3	6	12	25	54	122	285	686	1691
Variables	3	8	19	26	35	54	90	135	?

We observe that for $s > 5$, fewer variables than equations are needed for a solution.

Tools for solving Order Conditions:

Simplifying conditions

Butcher observed from the order conditions that the numbers of equations were reduced by **assuming**:

$$B(p): \qquad \sum_{i=1}^{s} b_i {c_i}^{k-1} = \int_0^1 c^{k-1}\, dc, \qquad k = 1, ..., p. \qquad (7)$$

For known nodes, **some** b_i may be computed by linearity.

If only p components of $\mathbf{b}$ are selected to be non-zero, the weights $\mathbf{b}^t$ are uniquely determined.

Analogs for the interior stage approximations $Y_j^{[i]}$ require

$$C(q_i): \qquad \sum_{j=1}^{i-1} a_{ij} {c_j}^{k-1} = \int_0^{c_i} c^{k-1}\, dc, \qquad k = 1, ..., q_i. \tag{8}$$

To identify different *types* of pairs, we define the **Dominant Stage-Order** of a method as

$$DSO = min\{q_i,\ b_i \neq 0\}$$

Other simplifying conditions have the form:

$$D(r_j): \qquad \sum_{i=j+1}^{s} b_i c_i^{k-2} a_{ij} = b_j \int_{c_j}^{1} c^{k-2}\, dc, \qquad k = 2, .., r_j. \tag{9}$$

Integrals emphasize (i) IVP link to numerical quadrature
(ii) the equations are homogeneous

Tools developed using Rooted Trees

- In 1968, Cooper - V. derived precisely 12 methods of order 8 requiring 11 stages
- During a visit to Kingston in 1969, Butcher dictated an algorithm to numerically test the order of an RK method.
- After coding it in APL, this algorithm verified the order of such 11-stage methods.
- Independently, A.R. Curtis found a parametric family of 11-stage methods of order 8.
- Thereafter, Butcher attempted to determine the **possible existence of 10-stage methods of order 8**, but it took 15 years to determine a **negative** result. (The proof was intricate!)
- In the interim, I have utilized this algorithm in various computing languages, and now use it as a MAPLE tool to verify orders, and to determine the relative efficiency of various RK methods and pairs.

Kutta 1901 Pairs!

I said I would return to the Kutta formulas of 1901.

- Recall order equations are linear in b_i.
- For any RK *method* with coefficients $b_i,\ a_{ij},\ c_i$, a different set $\hat{b}_i$ of weights provides an embedded method.
- For either CORRECT Kutta method, by choosing $\hat{b}_2 = \hat{b}_6 = 0$, and the four remaining weights to satisfy the quadrature equations (7), we obtain two order 5(4) pairs.

Here is one connected with the formula above:

Parameters of a Kutta 5a Pair

Table 2c: A 5(4) pair that might have been obtained by Kutta (1901)

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{5} & \frac{1}{5} & & & & & \\
\frac{2}{5} & 0 & \frac{2}{5} & & & & \\
1 & \frac{9}{4} & -5 & \frac{15}{4} & & & \\
\frac{3}{5} & \frac{63}{100} & \frac{9}{5} & -\frac{13}{20} & \frac{2}{25} & & \\
\frac{4}{5} & -\frac{6}{25} & \frac{4}{5} & \frac{2}{15} & \frac{8}{75} & 0 & \\
\hline
\mathbf{b} & \frac{17}{144} & 0 & \frac{25}{48} & \frac{1}{72} & -\frac{25}{72} & \frac{25}{48} \\
\hat{\mathbf{b}} & \frac{11}{72} & 0 & \frac{25}{72} & \frac{11}{72} & \frac{25}{72} & 0
\end{array}
$$

How effective is this pair?

Contrast of Kutta (1901) pairs with RKF45

Leading non-zero truncation error coefficients indicate the relative effectiveness of pairs:

We want norms of A_q small, and B_q, C_q near to 1, D_∞ small:

Table 4: Characteristic Properties of selected RK Pairs

Pair	p	s	$A_{p+1,2}$	$\hat{B}_{p+1,2}$	$\hat{C}_{p+1,2}$	$\hat{A}_{p,2}$	D_∞
Kutta5a	5(4)	6	4.04(-3)	1.26	1.30	1.07(-2)	5.00
Kutta5b	5(4)	6	3.84(-3)	1.27	1.33	8.53(-3)	3.75
RKF45	5(4)	6	3.36(-3)	3.16	1.36	1.84(-3)	8.00
DOPRI5	5(4)	6	3.99(-4)	1.54	1.67	1.18(-3)	9.82
DVERK56	6	8	2.07(-3)	3.75	1.48	6.96(-4)	9.17
IIIXb-6(5)	6	9*	1.44(-6)	1.72	1.72	2.25(-3)	207.9
IIb-6(5)	6	8	5.17(-5)	1.31	1.32	1.48(-3)	26.3

Implementation of **(p-1)p** Pairs

- Initially, the RK approximation of order **p-1** was propagated
- This ensured reliable error estimates, but with restricted efficiency
- XEPS (and EPUS): Shampine showed by requiring

  Error Per Step $<$**TOL**

  propagation of the high-order approximation (eXtrapolation) makes the global error proportional to TOL. (Hence, by reducing a selected TOL, the global error would be reduced correspondingly.
- Dormand and Prince (1980-86) obtained some (FSAL) formulas in which the error coefficients of the higher-order formula were (nearly) minimal. Using the (XEPS) implementation, the DOPRI5 formula became a popular choice.

Progress in the 1980s

- Dormand and Prince: Higher-order pairs and RK-triples
- Cash: Block methods
- Butcher , Cooper: General Linear Methods

RK methods were generalized to give continuous approximations:

- Enright et. al.: Interpolatory family of order 6
- Owren and Zennaro: Order 5 continuous methods

Enright utilized continuous methods to control stepsize by defect correcdtion.

More Progress in the 1990s

Some new pairs were explored

- Calvo, Montijano & Randez, A 5-6 pair
- Papakostas, Tsitouras & Papageorgiou: 6(5) pairs
- Sharp and V.: DSO=p-3 pairs
- V.: A classification of RK pairs
- V.: subspace derivations of new pairs

V.: Differentiable Interpolants of high orders

Some related explicit methods began to appear:

- Jackiewicz, Tracogna, Butcher, Welfert, V.: Two-step Runge–Kutta
- Rattenbury, Butcher: ARK

Some Extreme Methods of Interest

- V: (1976): 29-stage RK method of order 12
- Ono: (2005): 25 stage RK method of order 12
- Feagin: (2006): 25 stage RK method of orders 12 (& 14)

- Most new pairs and methods are providing a better understanding of algorithms for IVPs.
- **Most formulas** obtained after the problem encountered with Fehlberg's formulas **are fairly robust for well-behaved problems.**
- V. (2010): From (*some* families), I extracted the best formulas I could find. I found that minimizing the error coefficients led to formulas that were most efficient and coefficients for these now reside on the web.
- The various techniques developed in pursuit of these RK pairs are exploitable in searching for other methods, and for treating related types of problems.

Other Methods and Other Problems

- In the 1990's, Sharp suggested we develop some (Bel'tukov) methods for integral equations of the second kind.
- Approaches developed are applicable to studying both special and general Nystöm methods for second order differential equations.
- In 2000, Jackiewicz and V. used these techniues to derive TSRK pairs up to order 8.
- In 2000, I worked with Philippe Chartier in applying these approaches to the construction of pseudo-symplectic methods.
- Recently, A. Kvaerno and I have constructed a unified derivation of order conditions for TSRK methods.
- I have found some order 5 SDIRK pairs with all nodes inside [0,1]

Why is this problem so fascinating?

In our early mathematical training, we put a lot of effort into understanding that a system of N well-behaved linear equations in N unknowns has one solution.

While *some* non-linear problems have no solutions: the algebraic order conditions in a large number of variables, and (often) a LARGER number of unknowns often have SEVERAL FAMILIES of PARAMETRIC SOLUTIONS.

Initially, we established existence by finding methods and pairs of low orders. Detailed study of these simple examples led to characterizations of a variety of families of high orders: observing their basic structures have advanced our tools to allow the derivation of some very intricate algorithms.

Recall approaches to DERIVING METHODS/PAIRS

Parameters $\{\mathbf{b}_j,\ \mathbf{a}_{j,k},\ \mathbf{c}_k\}$ are selected by

- Direct elimination of variables ("brute force") for p small
- Exploiting simplifying conditions $\Sigma a_{ij} c_j = c_i^2/2$, etc. to collapse some subsets of equations
- Computing homogeneous polynomials $\Sigma b_i a_{ij} a_k$ etc.
- Iteration by Newton-like methods (maybe on a restricted subset)
- Algebraic tools which characterize families of methods
- Make (other) interior (sub)quadrature expressions such as $a_{i2}(\Sigma a_{2j} c_j - c_2^2/2) = K(\Sigma a_{ij} c_j^2 = c_i^3/3)$ to be orthogonal to $b_i,\ b_i a_{ij}$, etc.

Suggestions

- Determine whether currently available ODE codes {ODE45 in Matlab, DVERK78 in MAPLE} use (nearly) optimal algorithms available for non-stiff problems
- Determine if we found all (families of) the best RK methods and pairs.
- Apply derivation techniques available for explicit RK methods to characterize complete families of **other types of methods**, and methods for **other types of problems**.