General linear methods

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Our finishing point will be some completely new methods.

Contents

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- Generalizations of Linear Multistep Methods
  - Hybrid methods
  - Cyclic composite methods

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Contents

Contents

- Generalizations of Linear Multistep Methods
  - Hybrid methods
  - Cyclic composite methods
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  - Reuse of past values
  - Pseudo Runge-Kutta methods
  - ARK methods
  - Effective Order
- General Linear Methods

Contents

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Generalizations of Linear Multistep Methods

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- Variable stepsize and variable order are complicated.
- Their performance is limited by the Dahlquist barrier.
- For stiff problems where A-stability is desirable, order is limited to 2.
- We will look at two possible generalizations which retain the general nature of linear multistep methods but overcome some of the handicaps.

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we can include an “off-step point” as an additional predictor:

$$y_{n-\frac{1}{2}}^* = y_{n-2} + \tfrac{9}{8}hf_{n-1} + \tfrac{3}{8}hf_{n-2}$$
$$y_n^* = \tfrac{28}{5}y_{n-1} - \tfrac{23}{5}y_{n-2} + \tfrac{32}{15}hf_{n-\frac{1}{2}}^* - 4hf_{n-1} - \tfrac{26}{15}hf_{n-2}$$
$$y_n = \tfrac{32}{31}y_{n-1} - \tfrac{1}{31}y_{n-2} + \tfrac{5}{31}hf_n^* + \tfrac{64}{93}hf_{n-\frac{1}{2}}^* + \tfrac{4}{31}hf_{n-1} - \tfrac{1}{93}hf_{n-2}$$

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Below is a selected bibliography

Butcher J. C. (1965) A modified multistep method for the numerical integration of ordinary differential equations, *J. Assoc. Comput. Mach.*, 12: 124–135.

Gear C. W. (1965) Hybrid methods for initial value problems in ordinary differential equations, *SIAM J. Numer. Anal.*, 2: 69–86.

Gragg W. B. and Stetter H. J. (1964) Generalized multistep predictor–corrector methods, *J. Assoc. Comput. Mach.* 11: 188–209.

Cyclic composite methods

Given m linear multistep methods

$$y_n = \sum_{i=1}^{k} \alpha_i^{[j]} y_{n-i} + \sum_{i=0}^{k} \beta_i^{[j]} h f_{n-i}, \quad j = 1, \dots, m$$

apply them cyclically.

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apply them cyclically.

By careful choice of the m constituent methods, many limitations of single methods can be overcome.

As a trivial example, consider the following two methods based on (open) Newton-Cotes formulae:

$$y_n = y_{n-2} + 2hf_{n-1} \qquad (*)$$

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That is, if n is odd then (*) is used and if n is even then (**) is used.

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For example:

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$$y_n = \frac{449}{240}y_{n-1} + \frac{19}{30}y_{n-2} - \frac{361}{240}y_{n-3} + \frac{251}{720}hf_n + \frac{19}{30}hf_{n-1} - \frac{449}{240}hf_{n-2} - \frac{35}{72}hf_{n-3}$$

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The corresponding cyclic method has perfect stability.

To verify these remarks, analyse stability using $y' = 0$

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The difference equation for $y_n - y_{n-1}$ is

$$\begin{bmatrix} y_n - y_{n-1} \\ y_{n-1} - y_{n-2} \end{bmatrix} = X \begin{bmatrix} y_{n-1} - y_{n-2} \\ y_{n-2} - y_{n-3} \end{bmatrix}$$

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Neither matrix is power-bounded but their product is nilpotent.

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J. Donelson, and E. Hansen (1971) ‘Cyclic composite multistep predictor-corrector methods’. *SIAM J. Numer. Anal.* **8** 137–157.

T. A. Bickart and Z. Picel (1973) ‘High order stiffly stable composite multistep methods for numerical integration of stiff differential equations’, *BIT* **13** 272–286.

Generalizations of Runge-Kutta Methods

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- Although such methods are A-stable, they have many disadvantages.
- For example, they have low stage-order.
- And they are very expensive to implement.
- For both explicit and implicit RK methods, it is very difficult to estimate errors for variable h and p.

From one of Kutta's fourth order families:

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & c_2 & & & \\
\frac{1}{2} & \frac{1}{2}-\frac{1}{8c_2} & \frac{1}{8c_2} & & \\
1 & \frac{1}{2c_2}-1 & -\frac{1}{2c_2} & 2 & \\
\hline
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If $c_2 = -1$:

$$\begin{array}{c|cccc} 0 & & & & \\ -1 & -1 & & & \\ \frac{1}{2} & \frac{5}{8} & -\frac{1}{8} & & \\ 1 & -\frac{3}{2} & \frac{1}{2} & 2 & \\ \hline & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{array}$$

We can interpret the abscissa at -1 as reuse of the derivative found as the beginning of the previous step.

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We then have the method

$$Y_1 = y_{n-1} + \tfrac{5}{8}hf(y_{n-1}) - \tfrac{1}{8}hf(y_{n-2}), \qquad F_1 = f(Y_1)$$

$$Y_2 = y_{n-1} - \tfrac{3}{2}hf(y_{n-1}) + \tfrac{1}{2}hf(y_{n-2}) + 2hF_1, \quad F_2 = f(Y_2)$$

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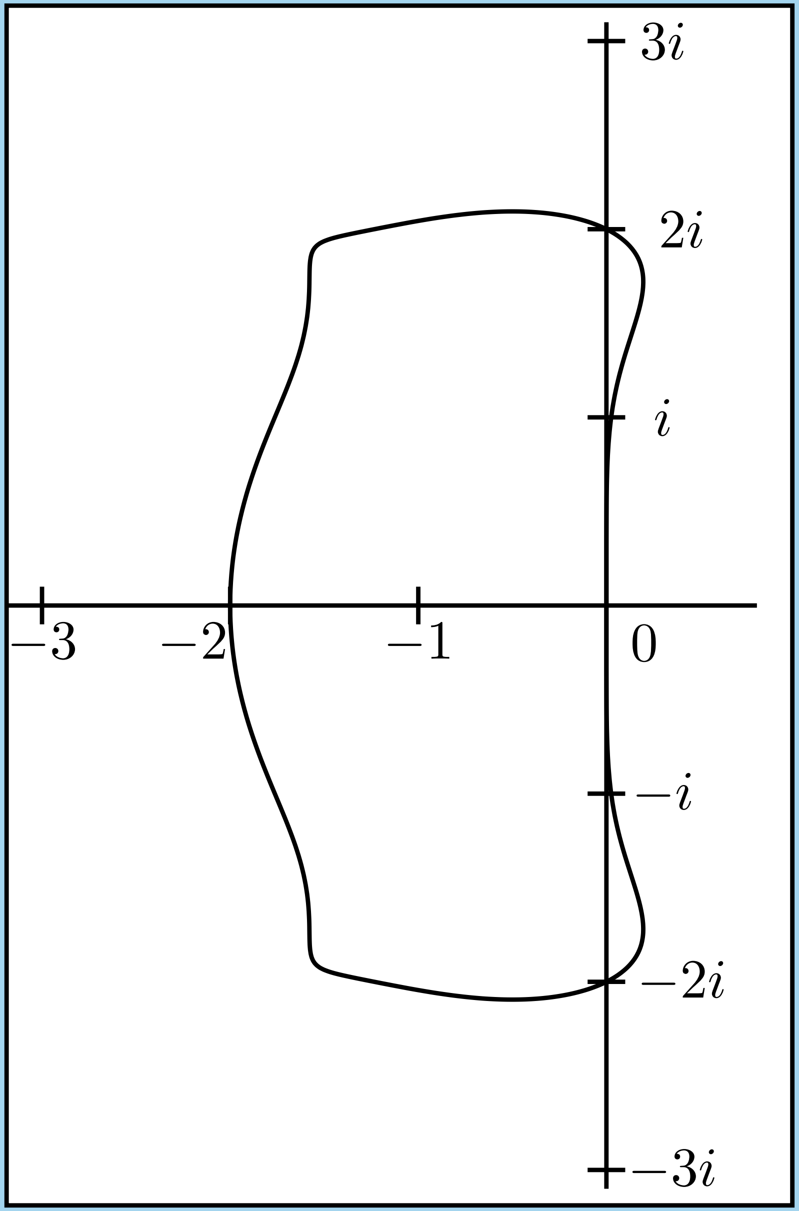
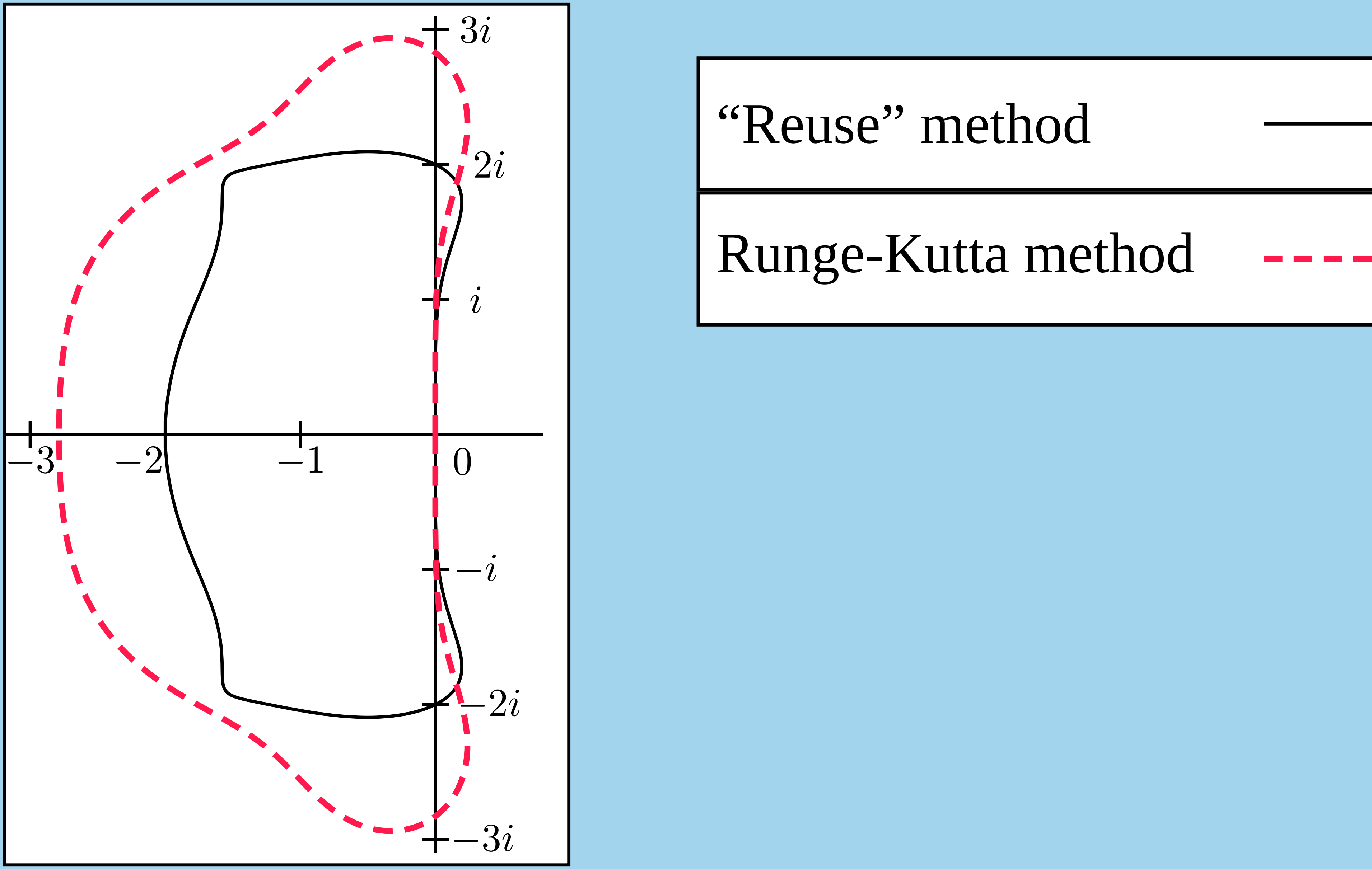
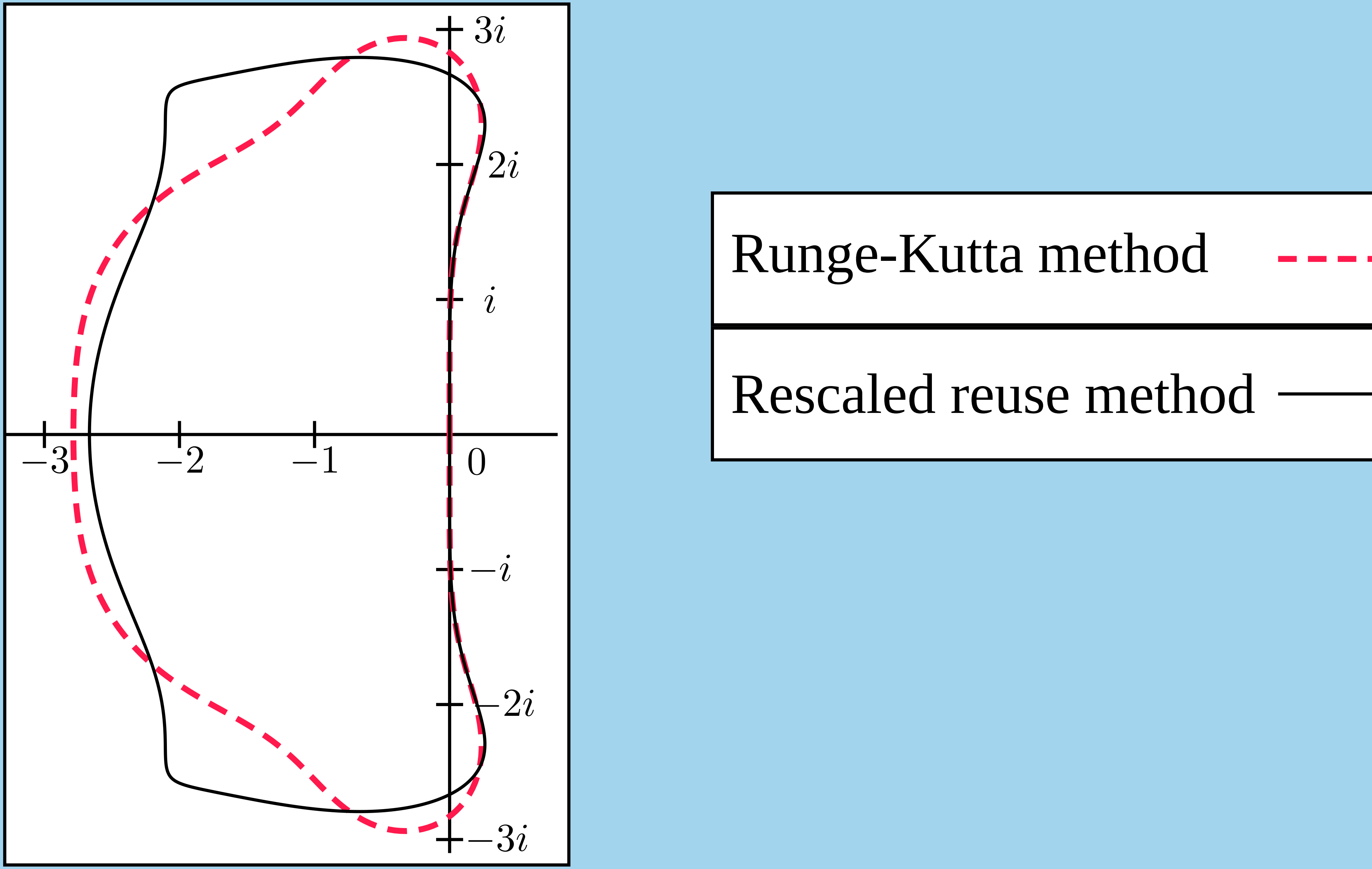
We can understand something about the behaviour of the new method by plotting its stability region.



"Reuse" method


3i
2i
i
−i
−2i
−3i
−3
−2
−1
0
“Reuse” method
Runge-Kutta method


3i
2i
i
−i
−2i
−3i
−3
−2
−1
0
Runge-Kutta method
Rescaled reuse method

Pseudo RK methods

Recall the conditions for a Runge-Kutta method to have order p.

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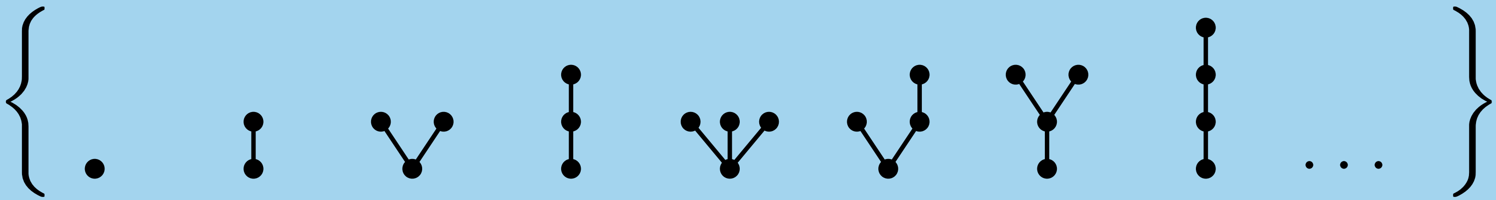
Let T denote the set of rooted trees:



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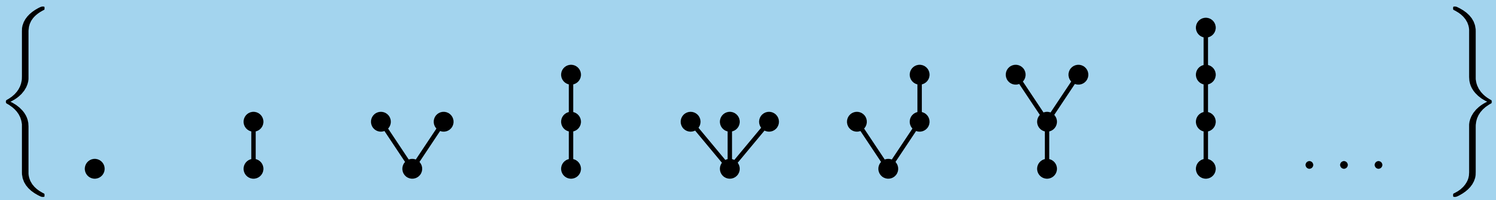

Associated with each $t \in T$ is an equation

$$\Phi(t) = \frac{1}{\gamma(t)}$$

where the “elementary weight” is a function of the coefficients of the method.

Generalizations of Runge-Kutta Methods

Pseudo RK methods

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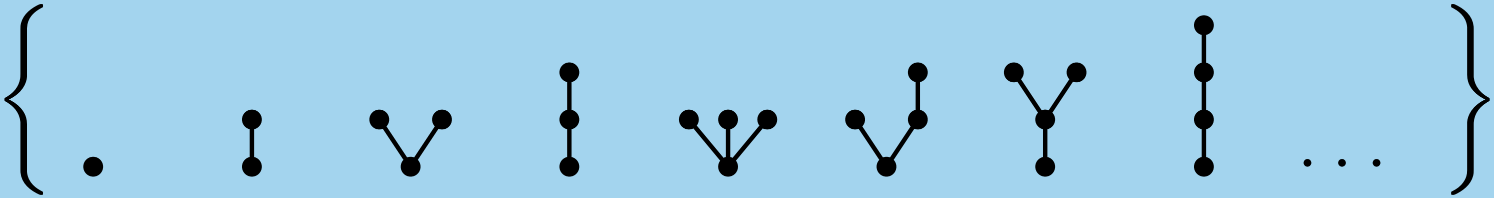

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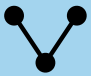
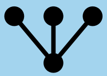
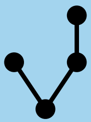
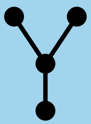
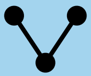
Expressions for Φ and γ are given on the next slide.

t	$\Phi(t)$	$\gamma(t)$
	$\sum b_i$	1
	$\sum b_i c_i$	2
	$\sum b_i c_i^2$	3
	$\sum b_i a_{ij} c_j$	6
	$\sum b_i c_i^3$	4
	$\sum b_i c_i a_{ij} c_j$	8
	$\sum b_i a_{ij} c_j^2$	12
	$\sum b_i a_{ij} a_{jk} c_k$	24

t	$\Phi(t)$	$\gamma(t)$
	$\sum b_i$	1
	$\sum b_i c_i$	2
	$\sum b_i c_i^2$	3
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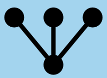
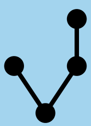
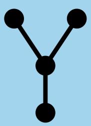
	$\sum b_i c_i^3$	4
	$\sum b_i c_i a_{ij} c_j$	8
	$\sum b_i a_{ij} c_j^2$	12
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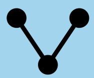
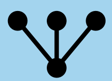
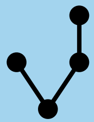
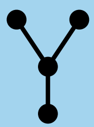
We will now introduce an additional column $\widehat{\Phi}(t)$

t	$\Phi(t)$	$\gamma(t)$	$\widehat{\Phi}(t)$
	$\sum b_i$	1	$\sum \widehat{b}_i$
	$\sum b_i c_i$	2	$\sum \widehat{b}_i (c_i - 1)$
	$\sum b_i c_i^2$	3	$\sum \widehat{b}_i (c_i - 1)^2$
	$\sum b_i a_{ij} c_j$	6	$\sum \widehat{b}_i (a_{ij} c_j - c_i + \frac{1}{2})$
	$\sum b_i c_i^3$	4	$\sum \widehat{b}_i (c_i - 1)^3$
	$\sum b_i c_i a_{ij} c_j$	8	$\sum \widehat{b}_i (c_i - 1)(a_{ij} c_j - c_i + \frac{1}{2})$
	$\sum b_i a_{ij} c_j^2$	12	$\sum \widehat{b}_i (a_{ij}(c_j^2 - 2c_j) + c_i - \frac{1}{3})$
	$\sum b_i a_{ij} a_{jk} c_k$	24	$\sum \widehat{b}_i (a_{ij}(a_{jk} c_k - c_j) + \frac{1}{2} c_i - \frac{1}{6})$

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$$\widehat{\Phi}(t) + \Phi(t) = \frac{1}{\gamma(t)}$$

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The order conditions thus become

$$\widehat{\Phi}(t) + \Phi(t) = \frac{1}{\gamma(t)}$$

A third order method can be constructed with two stages:

$$F_1^{[n]} = f(y_{n-1})$$

$$F_2^{[n]} = f(y_{n-1} + hF_1^{[n]})$$

$$y_n = y_{n-1} - \tfrac{1}{12}hF_1^{[n-1]} - \tfrac{5}{12}hF_2^{[n-1]} + \tfrac{13}{12}hF_1^{[n]} + \tfrac{5}{12}hF_2^{[n]}$$

The idea of using information from a previous step can be taken much further.

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Basic references on pseudo RK methods are given below

G. D. Byrne and R. J. Lambert (1966) ‘Pseudo-Runge-Kutta methods involving two points’, *J. Assoc. Comput. Mach* **13** 114–123.

R. Caira, C. Costabile and F. Costabile (1990) ‘A class of pseudo Runge-Kutta methods’, *BIT* **30** 642–649.

ARK methods

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\begin{aligned}
Y_1 &= y_{n-1} + \tfrac{5}{8}hf(y_{n-1}) - \tfrac{1}{8}hf(y_{n-2}), & F_1 &= hf(Y_1)\\
Y_2 &= y_{n-1} - \tfrac{3}{2}hf(y_{n-1}) + \tfrac{1}{2}hf(y_{n-2}) + 2hF_1, & F_2 &= f(Y_2)\\
y_n &= y_{n-1} + \tfrac{1}{6}hf(y_{n-1}) + \tfrac{2}{3}hF_1 + \tfrac{1}{6}hF_2
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$$\boldsymbol{y_n \longrightarrow y_1^{[n]}}, \qquad \boldsymbol{hf(y_n) \longrightarrow y_2^{[n]}}$$

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Y_2 &= y_1^{[n-1]} - y_2^{[n-1]} - \tfrac{1}{2}(y_2^{[n-1]} - y_2^{[n-2]}) + 2hF_1, \quad F_2 = f(Y_2) \\
y_1^{[n]} &= y_1^{[n-1]} + \tfrac{1}{6} y_2^{[n-1]} + \tfrac{2}{3} hF_1 + \tfrac{1}{6} hF_2 \\
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Y_2 &= y_1^{[n-1]} - y_2^{[n-1]} - \tfrac{1}{2} y_3^{[n]} + 2hF_1, & F_2 &= f(Y_2)\\
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y_2^{[n]} &= hf(y_1^{[n]})\\
y_3^{[n]} &= y_2^{[n]} - y_2^{[n-1]}
\end{aligned}
$$

Note that in this formulation there are three quantities passed from step to step and three derivative computations within each step.
The three input and output quantities approximate scaled derivatives as follows

$$
\begin{aligned}
y_1^{[n-1]} &\approx y(x_{n-1}) & \qquad y_1^{[n]} &\approx y(x_n)\\
y_2^{[n-1]} &\approx hy'(x_{n-1}) & \qquad y_2^{[n]} &\approx hy'(x_n)\\
y_3^{[n-1]} &\approx h^2y''(x_{n-1}) & \qquad y_3^{[n]} &\approx h^2y''(x_n)
\end{aligned}
$$

Even though the method has order 4, the third output quantity is accurate only to order 2.

We now extend this idea by restoring a fourth stage and making $y_3^{[n]}$ depend on quantities computed in the step.

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$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ \hline y_1^{[n]} \\ y_2^{[n]} \\ y_3^{[n]} \end{bmatrix} = \left[\begin{array}{cccc|ccc} 0 & 0 & 0 & 0 & 1 & 1 & \frac{1}{2} \\ \frac{1}{16} & 0 & 0 & 0 & 1 & \frac{7}{16} & \frac{1}{16} \\ -\frac{4}{3} & 2 & 0 & 0 & 1 & -\frac{3}{4} & -\frac{1}{4} \\ 0 & \frac{2}{3} & \frac{1}{6} & 0 & 1 & \frac{1}{6} & 0 \\ \hline 0 & \frac{2}{3} & \frac{1}{6} & 0 & 1 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & -\frac{2}{3} & 2 & 0 & -1 & 0 \end{array}\right] \begin{bmatrix} hF_1 \\ hF_2 \\ hF_3 \\ hF_4 \\ \hline y_1^{[n-1]} \\ y_2^{[n-1]} \\ y_3^{[n-1]} \end{bmatrix}$$

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- A possible starting method is

$$y_1^{[0]} = y_0, \quad y_2^{[0]} = hf(y_1^{[0]}), \quad y_3^{[0]} = hf(y_0 + y_2^{[0]}) - y_2^{[0]}$$

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- Stepsize change $h \to rh$ can be achieved without loss of order by

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- A method like this is an “Almost Runge-Kutta method” (ARK method).

Basic references on ARK methods are given below

J. C. Butcher (1997b) ‘An introduction to “Almost Runge–Kutta" methods’, *Appl. Numer. Math.* **24** 331–342.

J. C. Butcher (1998) ‘ARK methods up to order five’, *Numer. Algorithms*, **17** 193–221.

J. C. Butcher and N. Moir (2003) ‘Experiments with a new fifth order method’, *Numer. Algorithms*, **33** 137–151.

N. Moir (2005) ‘ARK methods: some recent developments’, *J. Comput. Appl. Math.*, **175** 101–111.

Effective Order

Developing the ideas on Runge-Kutta and pseudo Runge-Kutta methods, we introduce a group G whose elements are mappings on the set of trees to real numbers

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We will write H_p as the normal subgroup whose members are characterized by $t \mapsto 0$ if t has less than or equal to p vertices.

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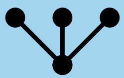
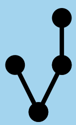
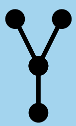
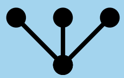
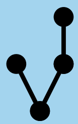
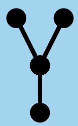
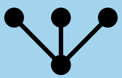
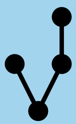
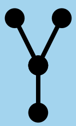
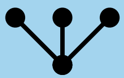
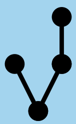
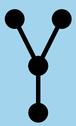
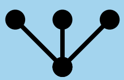
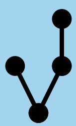
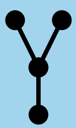
We will illustrate the group operation in a table where we also give values of E.

i	t_i
1	
2	
3	
4	
5	
6	
7	
8	

$r(t_i)$	i	t_i
1	1	
2	2	
3	3	
3	4	
4	5	
4	6	
4	7	
4	8	

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$
1	1		α_1	β_1
2	2		α_2	β_2
3	3		α_3	β_3
3	4		α_4	β_4
4	5		α_5	β_5
4	6		α_6	β_6
4	7		α_7	β_7
4	8		α_8	β_8

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$	$(\alpha\beta)(t_i)$
1	1		α_1	β_1	$\alpha_1 + \beta_1$
2	2		α_2	β_2	$\alpha_2 + \alpha_1\beta_1 + \beta_2$
3	3		α_3	β_3	$\alpha_3 + \alpha_1^2\beta_1 + 2\alpha_1\beta_2 + \beta_3$
3	4		α_4	β_4	$\alpha_4 + \alpha_2\beta_1 + \alpha_1\beta_2 + \beta_4$
4	5		α_5	β_5	$\alpha_5 + \alpha_1^3\beta_1 + 3\alpha_1^2\beta_2 + 3\alpha_1\beta_3 + \beta_5$
4	6		α_6	β_6	$\alpha_6 + \alpha_1\alpha_2\beta_1 + (\alpha_1^2 + \alpha_2)\beta_2 + \alpha_1(\beta_3 + \beta_4) + \beta_6$
4	7		α_7	β_7	$\alpha_7 + \alpha_3\beta_1 + \alpha_1^2\beta_2 + 2\alpha_1\beta_4 + \beta_7$
4	8		α_8	β_8	$\alpha_8 + \alpha_4\beta_1 + \alpha_2\beta_2 + \alpha_1\beta_4 + \beta_8$

$r(t_i)$	i	t_i	$\alpha(t_i)$	$\beta(t_i)$	$(\alpha\beta)(t_i)$	$E(t_i)$
1	1		α_1	β_1	$\alpha_1+\beta_1$	1
2	2		α_2	β_2	$\alpha_2+\alpha_1\beta_1+\beta_2$	$\frac{1}{2}$
3	3		α_3	β_3	$\alpha_3+\alpha_1^2\beta_1+2\alpha_1\beta_2+\beta_3$	$\frac{1}{3}$
3	4		α_4	β_4	$\alpha_4+\alpha_2\beta_1+\alpha_1\beta_2+\beta_4$	$\frac{1}{6}$
4	5		α_5	β_5	$\alpha_5+\alpha_1^3\beta_1+3\alpha_1^2\beta_2+3\alpha_1\beta_3+\beta_5$	$\frac{1}{4}$
4	6		α_6	β_6	$\alpha_6+\alpha_1\alpha_2\beta_1+(\alpha_1^2+\alpha_2)\beta_2$ $+\alpha_1(\beta_3+\beta_4)+\beta_6$	$\frac{1}{8}$
4	7		α_7	β_7	$\alpha_7+\alpha_3\beta_1+\alpha_1^2\beta_2+2\alpha_1\beta_4+\beta_7$	$\frac{1}{12}$
4	8		α_8	β_8	$\alpha_8+\alpha_4\beta_1+\alpha_2\beta_2+\alpha_1\beta_4+\beta_8$	$\frac{1}{24}$

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Thus, the benefits of high order can be enjoyed by high effective order.

We analyse the conditions for effective order 4.

Without loss of generality assume $\beta(t_1) = 0$.

i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
1	α_1	1
2	$\beta_2 + \alpha_2$	$\frac{1}{2} + \beta_2$
3	$\beta_3 + \alpha_3$	$\frac{1}{3} + 2\beta_2 + \beta_3$
4	$\beta_4 + \beta_2\alpha_1 + \alpha_4$	$\frac{1}{6} + \beta_2 + \beta_4$
5	$\beta_5 + \alpha_5$	$\frac{1}{4} + 3\beta_2 + 3\beta_3 + \beta_5$
6	$\beta_6 + \beta_2\alpha_2 + \alpha_6$	$\frac{1}{8} + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
7	$\beta_7 + \beta_3\alpha_1 + \alpha_7$	$\frac{1}{12} + \beta_2 + 2\beta_4 + \beta_7$
8	$\beta_8 + \beta_4\alpha_1 + \beta_2\alpha_2 + \alpha_8$	$\frac{1}{24} + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$

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The 5 order conditions, written in terms of the Runge-Kutta tableau, are

$$\begin{aligned}
\sum b_i &= 1\\
\sum b_i c_i &= \tfrac{1}{2}\\
\sum b_i a_{ij} c_j &= \tfrac{1}{6}\\
\sum b_i a_{ij} a_{jk} c_k &= \tfrac{1}{24}\\
\sum b_i c_i^2(1-c_i) + \sum b_i a_{ij} c_j (2c_i - c_j) &= \tfrac{1}{4}
\end{aligned}$$

General linear methods

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4. Output quantities are computed corresponding to the input quantities in step 1.
5. These output quantities are also linear combinations of the stage derivatives and the input quantities.

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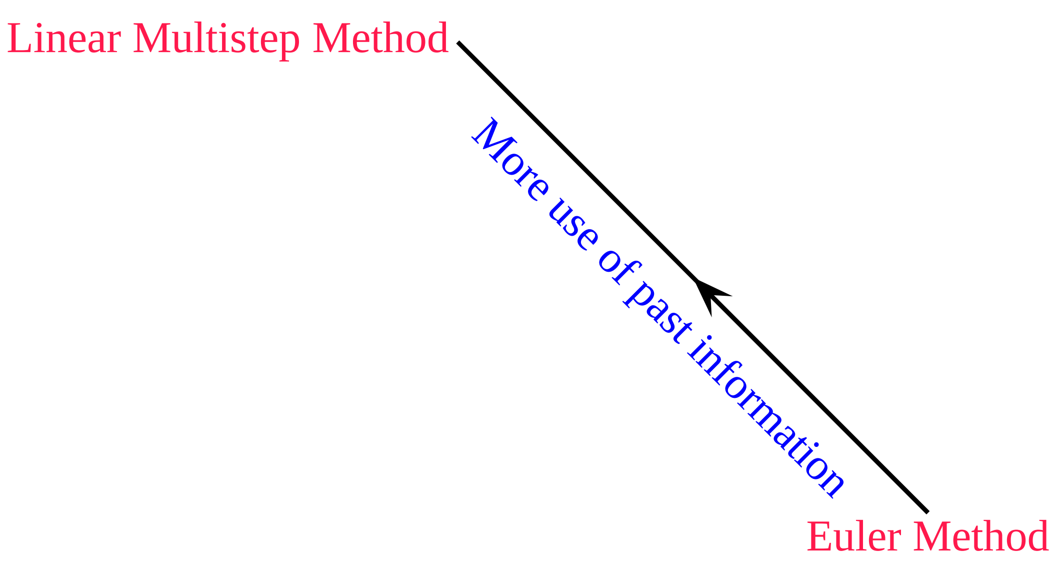
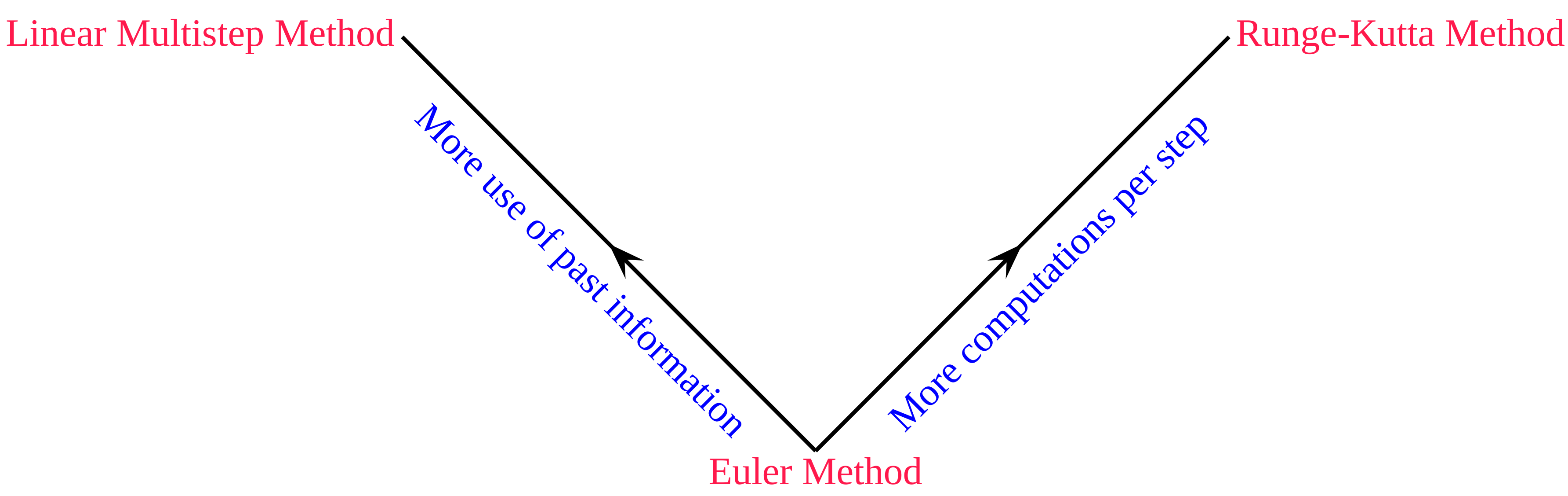
We will summarize this in the diagram on the next slide.

Euler Method


Linear Multistep Method
More use of past information
Euler Method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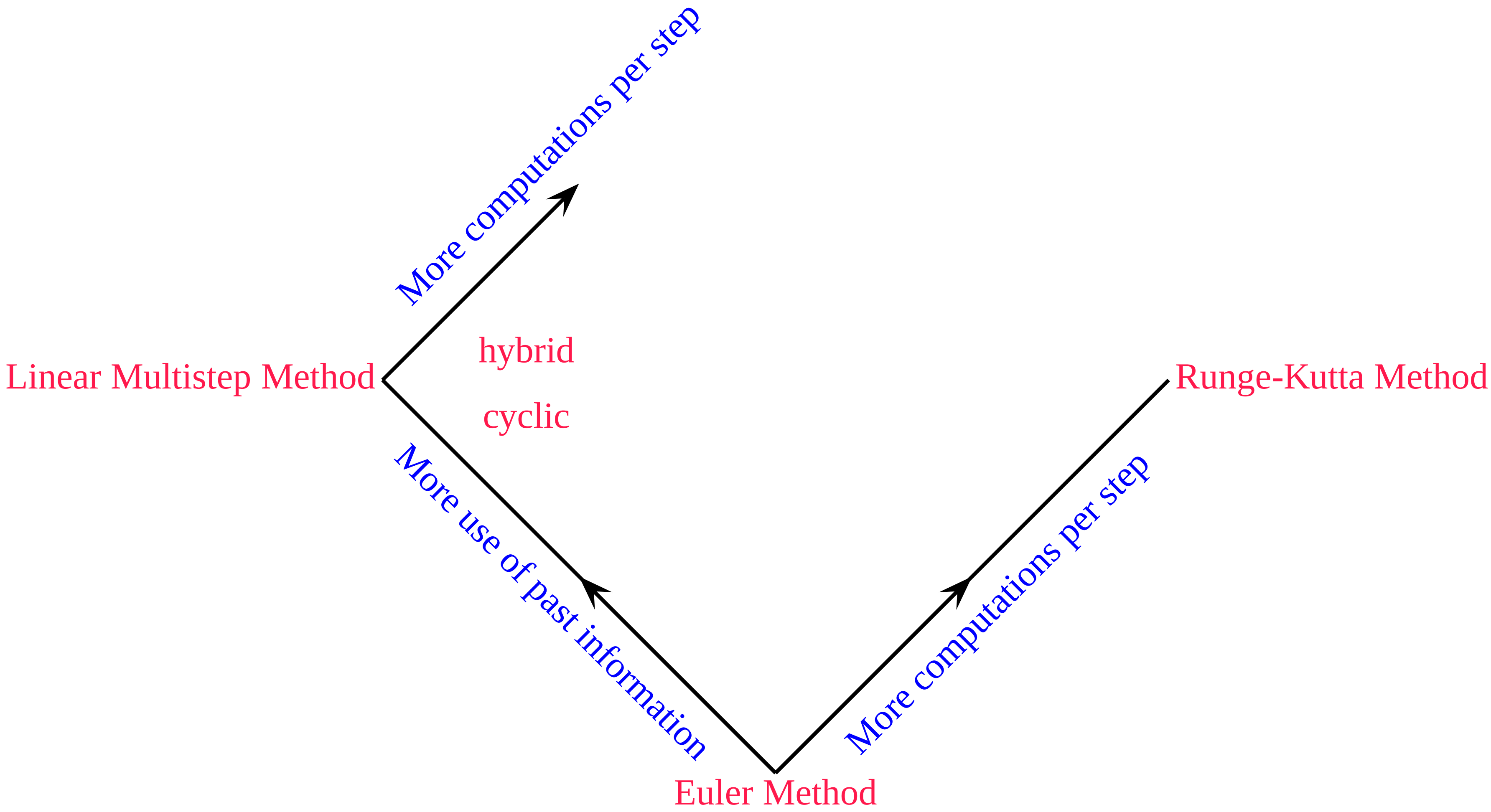
More computations per step
hybrid
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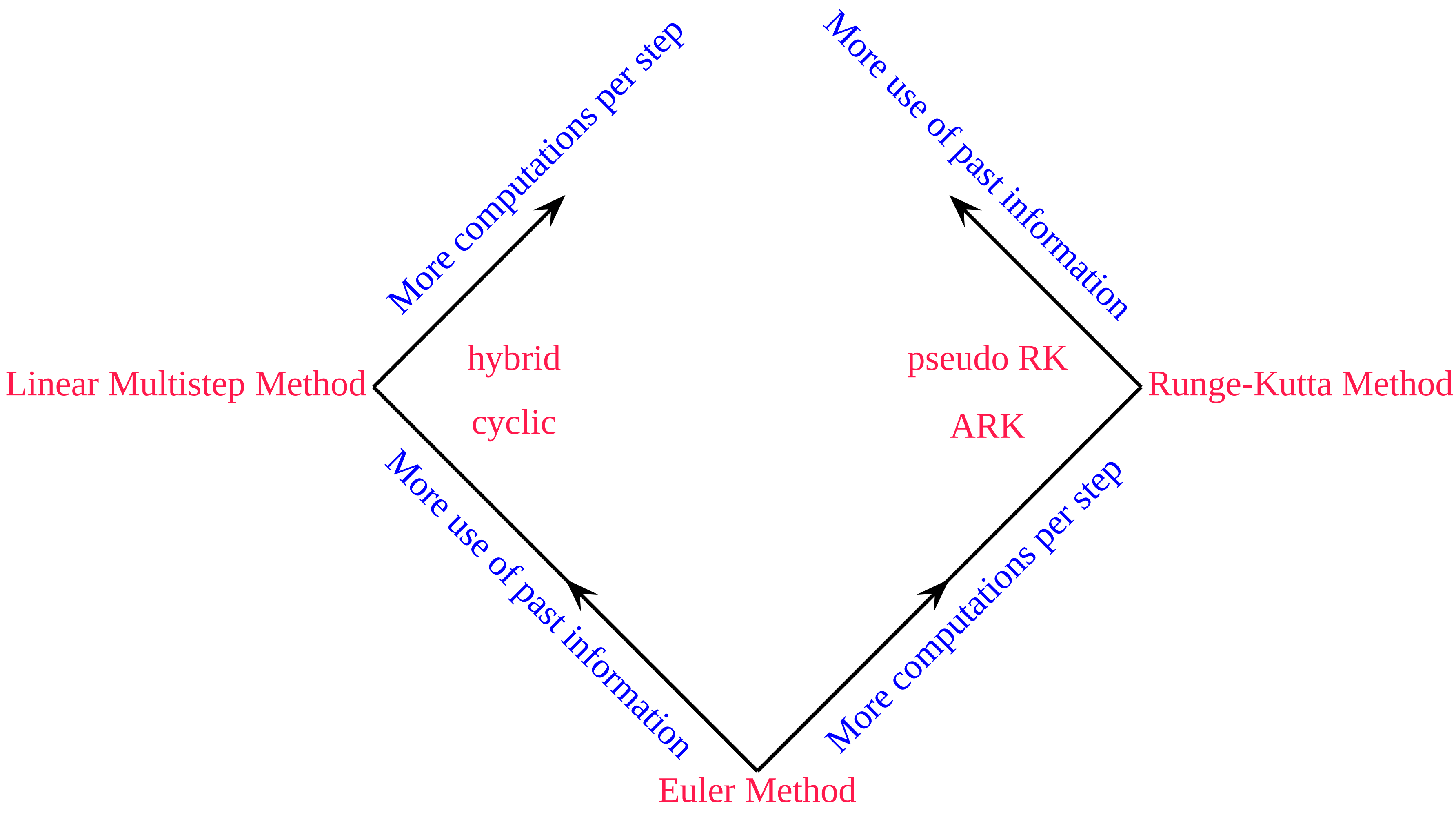
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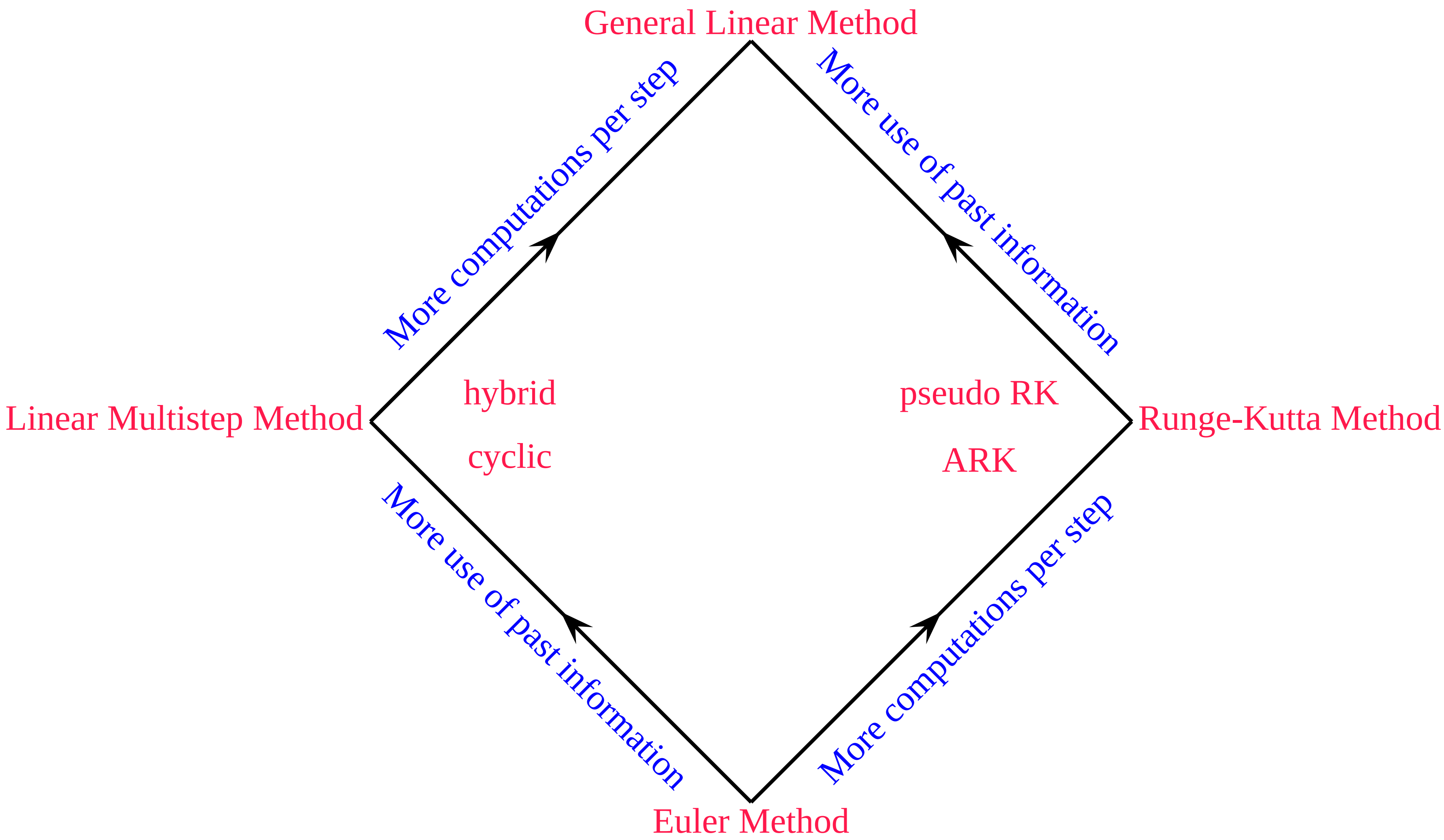
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The quantities exported at the end of step n will be denoted by $y_i^{[n]}$, $i = 1, 2, \dots, r$.

For convenience we will write:

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}$$

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We now go through the process of carrying out a step in terms of this notation.

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The matrices of coefficients in step 3 are A and U and those in step 5 are B and V.

The formulae for the various steps are

$$Y_i = \sum_{j=1}^{s} a_{ij} h F_j + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \qquad i = 1, 2, \ldots s$$

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or, using a compact notation,

$$Y = (A \otimes I) hF + (U \otimes I) y^{[n-1]}$$
$$y^{[n]} = (B \otimes I) hF + (V \otimes I) y^{[n-1]}$$

Consistency, Stability, Convergence

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and we will discuss the meaning of this result in the next few slides.

Introduce two vectors $u, v \in \mathbb{R}^r$, known as the pre-consistency and consistency vectors respectively.

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We will require that the GL method with inputs

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By Taylor's theory these requirements can be written

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$$\begin{aligned} Uu &= \mathbf{1} \\ Vu &= u \qquad \text{(*)} \\ B\mathbf{1} + Vv &= u + v \qquad \text{(**)} \end{aligned}$$

Note that (*) and (**) are related to the ability of the numerical method to solve the problem

$$y'(x) = 1$$

exactly, for an arbitrary initial value.

Stability refers to the ability of a method to generate a convergent sequence of approximations to the problem

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This in turn is equivalent to the requirement that the minimal polynomial of V has all its zeros in the closed unit disc with only simple zeros on the boundary.

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We will refer to the calculation which produces $y^{[n-1]}$ from $y(x_{n-1})$ as a "starting method".

Let S denote the "starting method", that is a mapping from $\mathbb{R}^N$ to $\mathbb{R}^{rN}$ and a corresponding finishing method $F : \mathbb{R}^{rN} \to \mathbb{R}^N$ such that $F \circ S = \mathrm{id}$.

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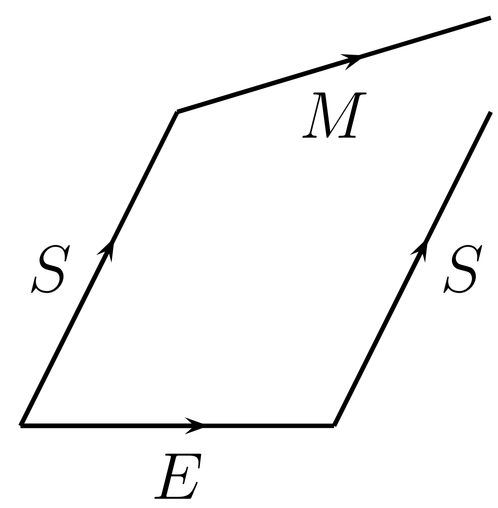

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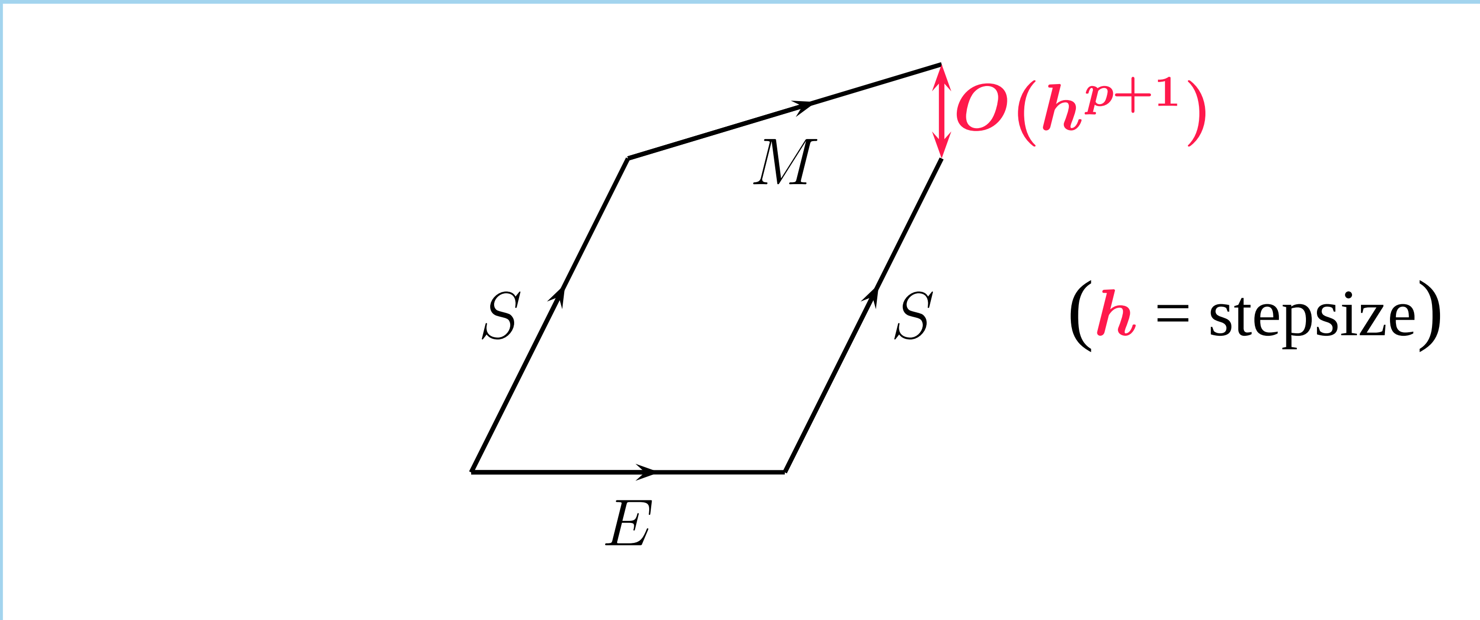

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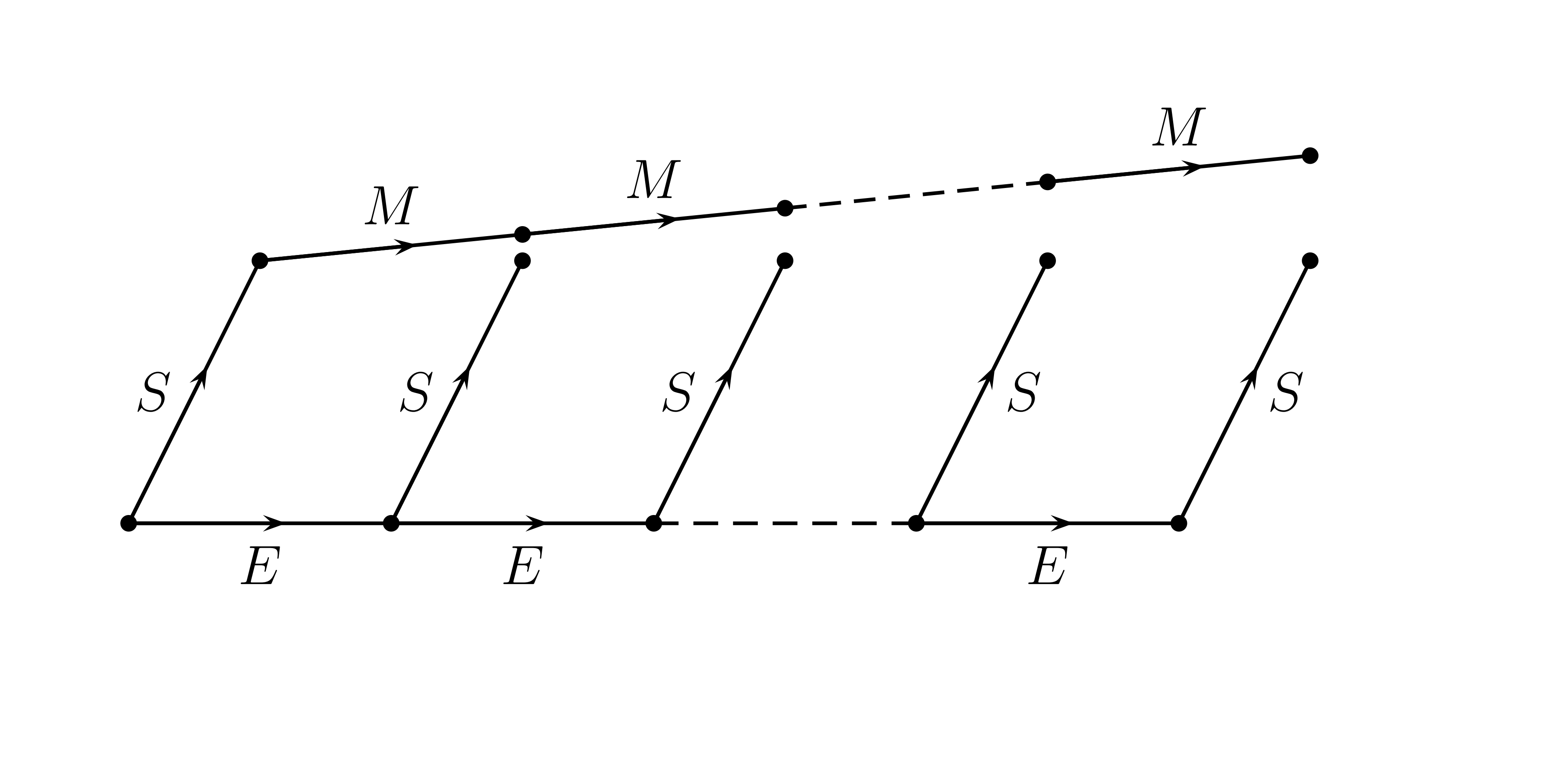

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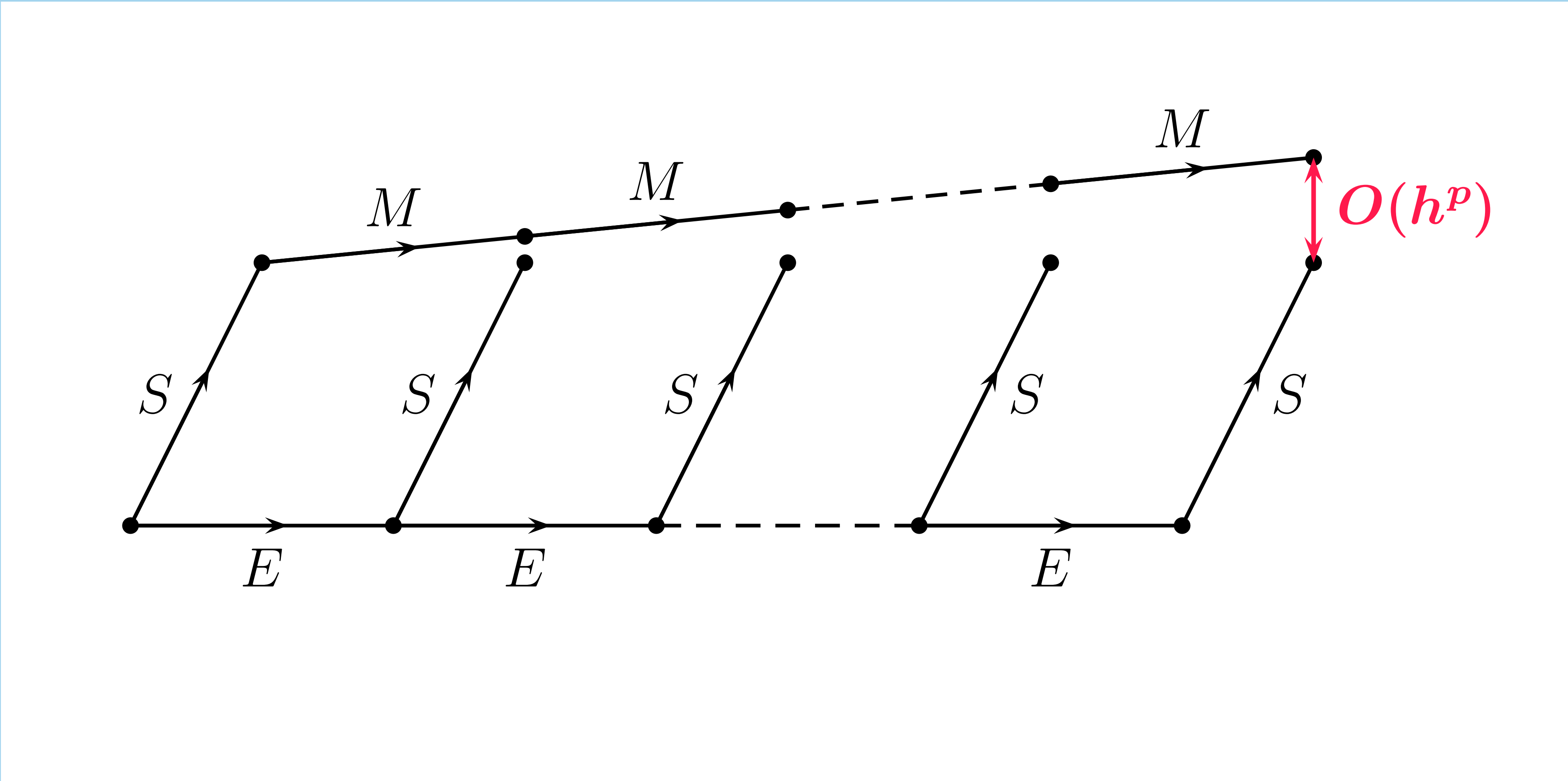

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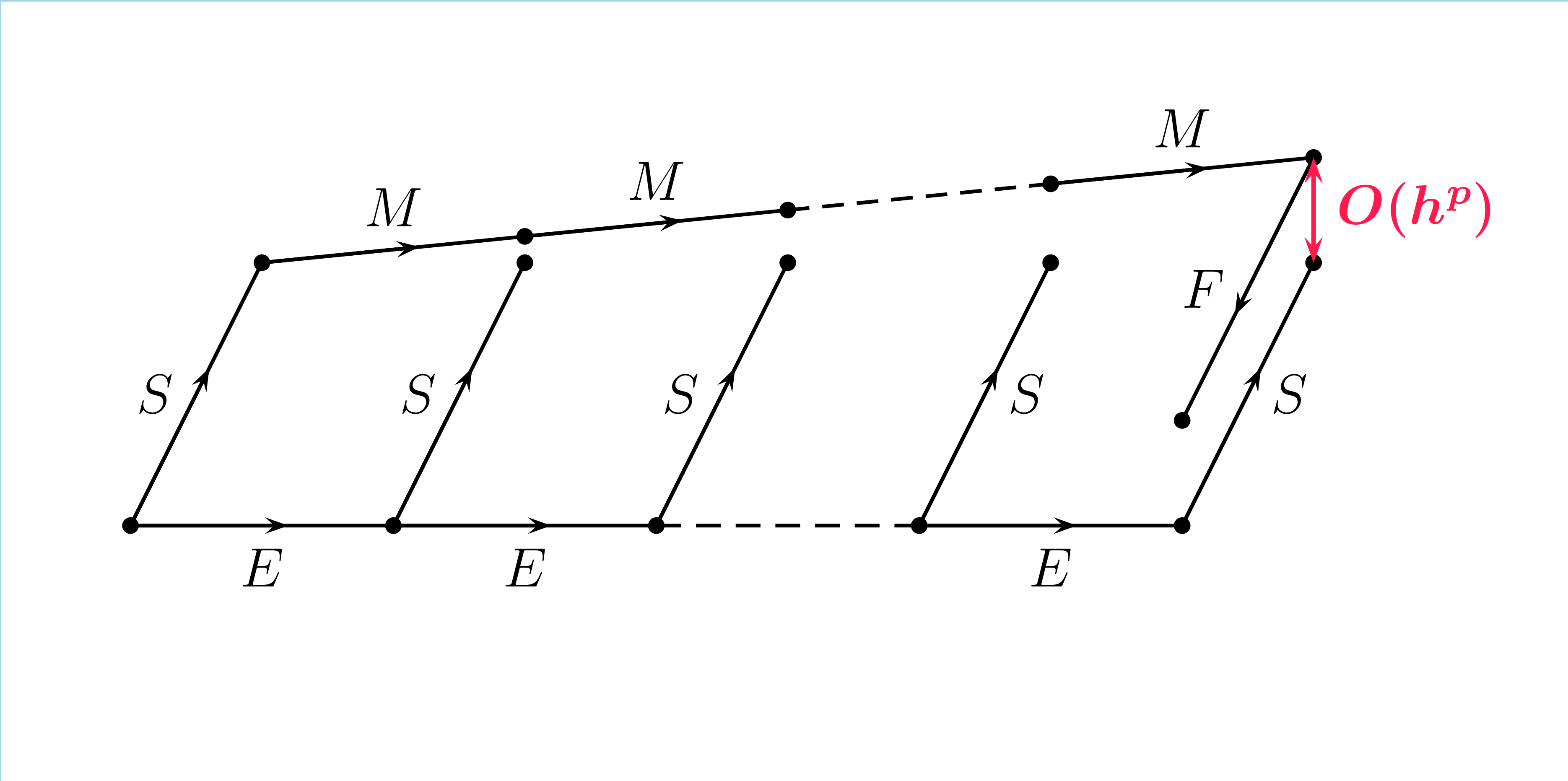

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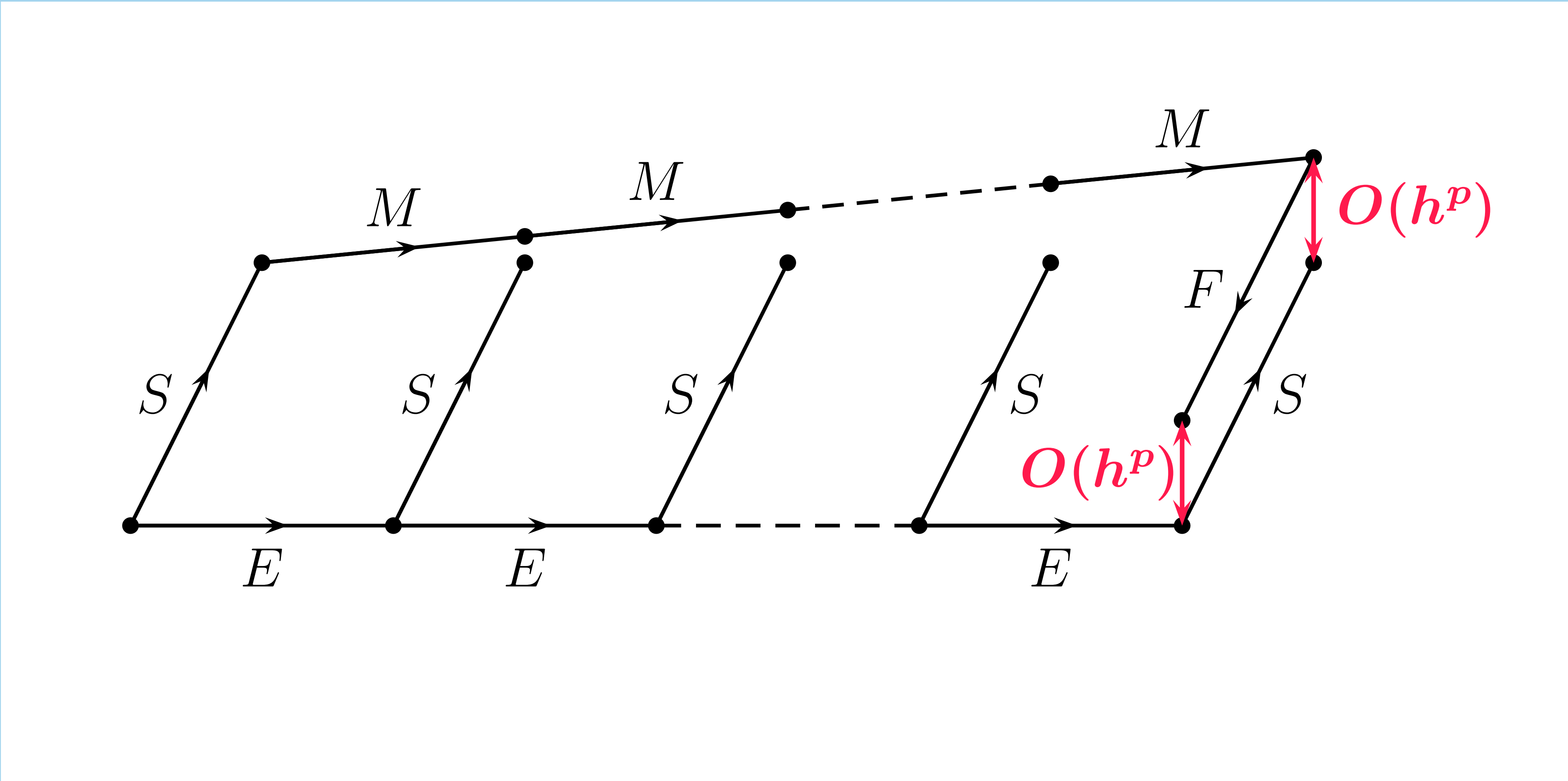

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To represent S and turn the definition of order into a practical algorithm for analysing a specific method, operations on the set of mappings $T \rightarrow \mathbb{R}$ can be used. Without considering the details, the conditions are

$$\xi = A\xi D + U\eta$$

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It is possible for a Runge–Kutta method with 5 stages to have effective order 5.

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$$y_i^{[n-1]} = \alpha_{i1}y(x_{n-1}) + \alpha_{i2}hy'(x_{n-1}) + \cdots + \alpha_{i,p+1}h^p y^{(p)}(x_{n-1})$$

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$$\phi_i(z) = \alpha_{i1} + \alpha_{i2}z + \cdots + \alpha_{i,p+1}z^p$$

Methods with inherent Runge-Kutta stability

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If $s \geq r = p + 1$, it is possible to construct the methods in a systematic way by imposing a condition known as “Inherent Runge-Kutta Stability”.

Doubly companion matrices

Matrices like the following are “companion matrices” for the polynomial

$$z^n + \alpha_1 z^{n-1} + \cdots + \alpha_n$$

$$\begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \cdots & -\alpha_{n-1} & -\alpha_n \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

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respectively:

$$\begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \cdots & -\alpha_{n-1} & -\alpha_n \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & -\beta_n \\ 1 & 0 & 0 & \cdots & 0 & -\beta_{n-1} \\ 0 & 1 & 0 & \cdots & 0 & -\beta_{n-2} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\beta_2 \\ 0 & 0 & 0 & \cdots & 1 & -\beta_1 \end{bmatrix}$$

Their characteristic polynomials can be found from $\det(I - zA) = \alpha(z)$ or $\beta(z)$, respectively, where,

$$\alpha(z) = 1+\alpha_1 z+\cdots+\alpha_n z^n, \quad \beta(z) = 1+\beta_1 z+\cdots+\beta_n z^n.$$

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$\alpha(z) = 1+\alpha_1 z+\cdots+\alpha_n z^n, \quad \beta(z) = 1+\beta_1 z+\cdots+\beta_n z^n.$
A matrix with both α and β terms:

$$X = \begin{bmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \cdots & -\alpha_{n-1} & -\alpha_n - \beta_n \\ 1 & 0 & 0 & \cdots & 0 & -\beta_{n-1} \\ 0 & 1 & 0 & \cdots & 0 & -\beta_{n-2} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\beta_2 \\ 0 & 0 & 0 & \cdots & 1 & -\beta_1 \end{bmatrix},$$

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$$\Psi^{-1} = \begin{bmatrix} 1 & \lambda+\alpha_1 & \lambda^2+\alpha_1\lambda+\alpha_2 & \cdots \\ 0 & 1 & 2\lambda+\alpha_1 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

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We have a similar expression for Ψ:

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- Information on the structure of V

Consider only methods for which the step n outputs approximate the "Nordsieck vector"

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$$\begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ y_3^{[n]} \\ \vdots \\ y_{p+1}^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ h^2y''(x_n) \\ \vdots \\ h^py^{(p)}(x_n) \end{bmatrix}$$

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For such methods, V has the form

$$V = \begin{bmatrix} 1 & v^T \\ 0 & \dot{V} \end{bmatrix}$$

Such a method has the IRKS property if a doubly companion matrix X exists so that for some vector ξ,

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$$M(z) \sim V + ze_1\xi^T(I - zX)^{-1}$$

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$$R(z) = \frac{N(z)}{(1-\lambda z)^s}$$

The following third order method is explicit and suitable for the solution of non-stiff problems

$$
\begin{bmatrix} AU \\ BV \end{bmatrix} = \left[\begin{array}{cccc|cccc}
0 & 0 & 0 & 0 & 1 & \frac{1}{4} & \frac{1}{32} & \frac{1}{384} \\
-\frac{176}{1885} & 0 & 0 & 0 & 1 & \frac{2237}{3770} & \frac{2237}{15080} & \frac{2149}{90480} \\
-\frac{335624}{311025} & \frac{29}{55} & 0 & 0 & 1 & \frac{1619591}{1244100} & \frac{260027}{904800} & \frac{1517801}{39811200} \\
-\frac{67843}{6435} & \frac{395}{33} & -5 & 0 & 1 & \frac{29428}{6435} & \frac{527}{585} & \frac{41819}{102960} \\
\hline
-\frac{67843}{6435} & \frac{395}{33} & -5 & 0 & 1 & \frac{29428}{6435} & \frac{527}{585} & \frac{41819}{102960} \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{82}{33} & -\frac{274}{11} & \frac{170}{9} & -\frac{4}{3} & 0 & \frac{482}{99} & 0 & -\frac{161}{264} \\
-8 & -12 & \frac{40}{3} & -2 & 0 & \frac{26}{3} & 0 & 0
\end{array}\right]
$$

The following fourth order method is implicit, L-stable, and suitable for the solution of stiff problems

$$
\left[\begin{array}{ccccc|ccccc}
\frac{1}{4} & 0 & 0 & 0 & 0 & 1 & \frac{3}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\
-\frac{513}{54272} & \frac{1}{4} & 0 & 0 & 0 & 1 & \frac{27649}{54272} & \frac{5601}{27136} & \frac{1539}{54272} & -\frac{459}{6784} \\
\frac{3706119}{69088256} & -\frac{488}{3819} & \frac{1}{4} & 0 & 0 & 1 & \frac{15366379}{207264768} & \frac{756057}{34544128} & \frac{1620299}{69088256} & -\frac{4854}{454528} \\
\frac{32161061}{197549232} & -\frac{111814}{232959} & \frac{134}{183} & \frac{1}{4} & 0 & 1 & -\frac{32609017}{197549232} & \frac{929753}{32924872} & \frac{4008881}{32924872} & \frac{174981}{3465776} \\
-\frac{135425}{2948496} & -\frac{641}{10431} & \frac{73}{183} & \frac{1}{2} & \frac{1}{4} & 1 & -\frac{367313}{8845488} & -\frac{22727}{1474248} & \frac{40979}{982832} & \frac{323}{25864} \\
\hline
-\frac{135425}{2948496} & -\frac{641}{10431} & \frac{73}{183} & \frac{1}{2} & \frac{1}{4} & 1 & -\frac{367313}{8845488} & -\frac{22727}{1474248} & \frac{40979}{982832} & \frac{323}{25864} \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{2255}{2318} & -\frac{47125}{20862} & \frac{447}{122} & -\frac{11}{4} & \frac{4}{3} & 0 & -\frac{28745}{20862} & -\frac{1937}{13908} & \frac{351}{18544} & \frac{65}{976} \\
\frac{12620}{10431} & -\frac{96388}{31293} & \frac{3364}{549} & -\frac{10}{3} & \frac{4}{3} & 0 & -\frac{70634}{31293} & -\frac{2050}{10431} & -\frac{187}{2318} & \frac{113}{366} \\
\frac{414}{1159} & -\frac{29954}{31293} & \frac{130}{61} & -1 & \frac{1}{3} & 0 & -\frac{27052}{31293} & -\frac{113}{10431} & -\frac{491}{4636} & \frac{161}{732}
\end{array}\right]
$$

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