Towards practical general linear methods

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Our starting point will be the classical methods and some mild generalizations.

Our finishing point will be some completely new methods and steps towards their practical implementation.

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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.

Rather than methods like Adams-Bashforth

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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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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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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 & \\
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 & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6}
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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 & \\
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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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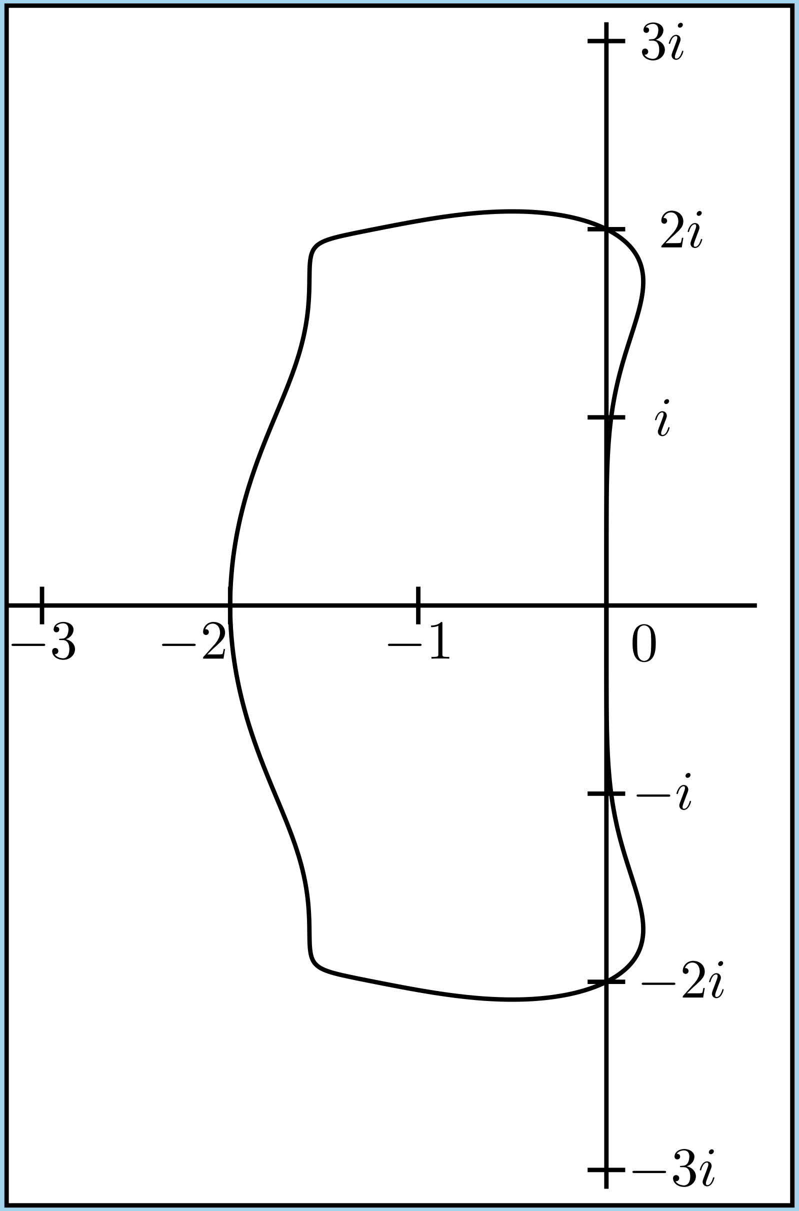
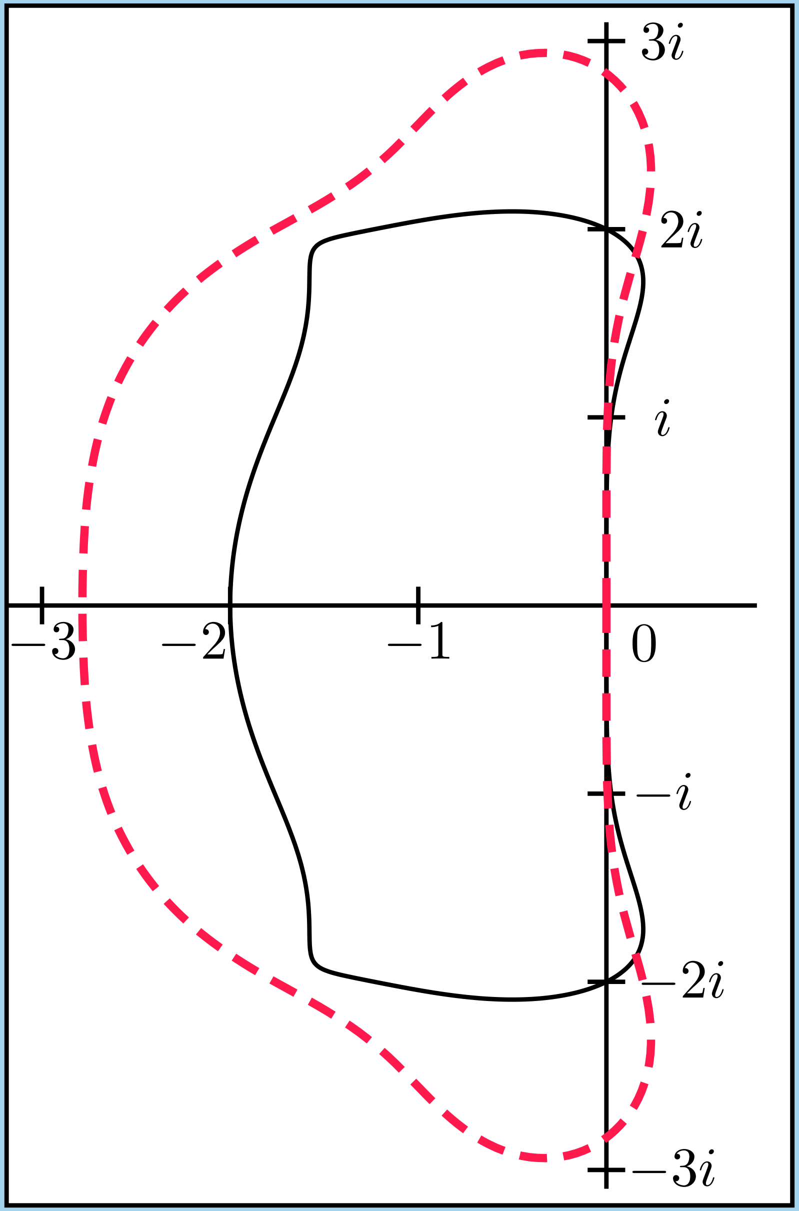
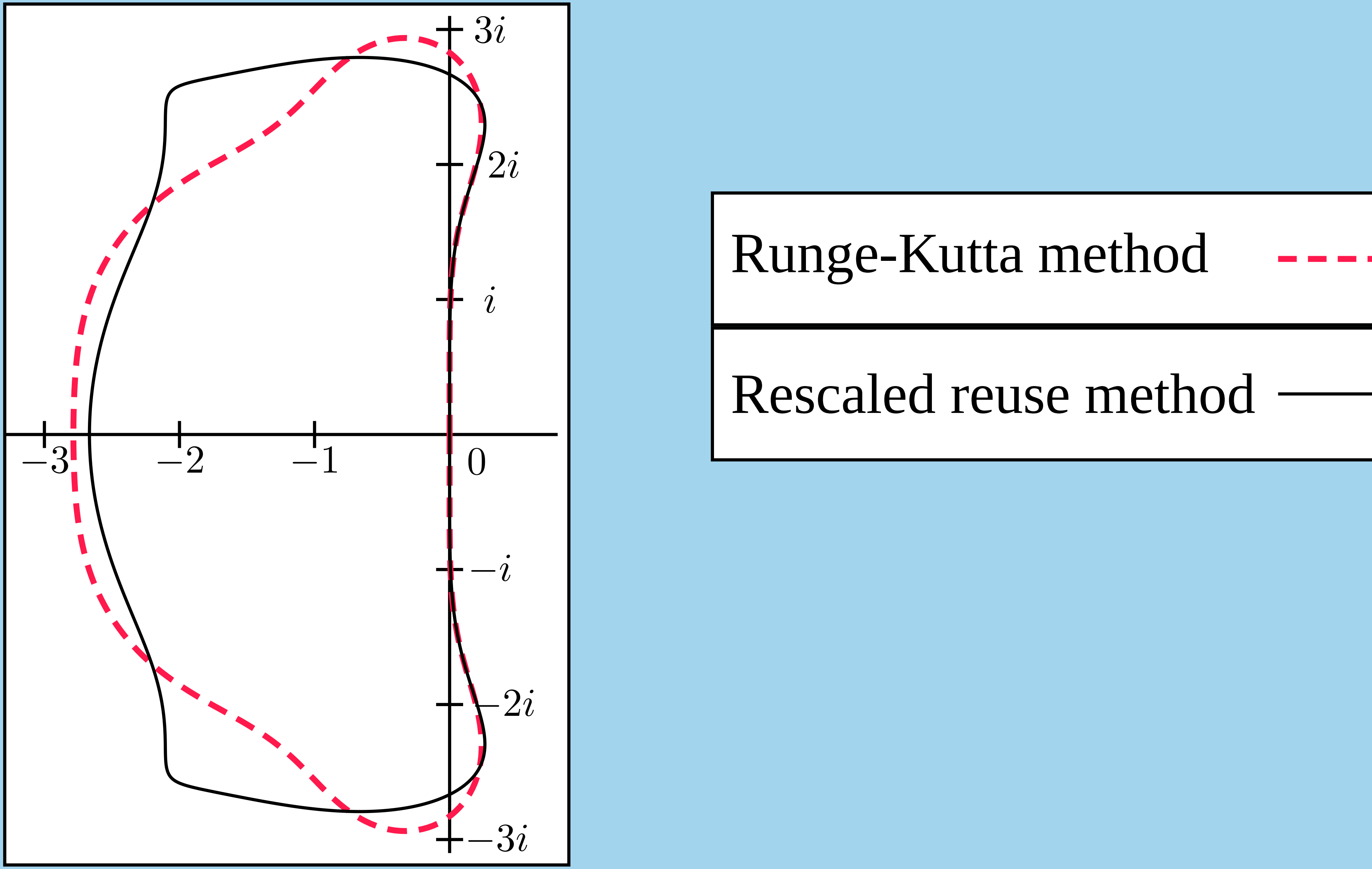
We can understand something about the behaviour of the new method by plotting its stability region.



“Reuse” method



"Reuse" method	——
Runge-Kutta method	- - - -


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

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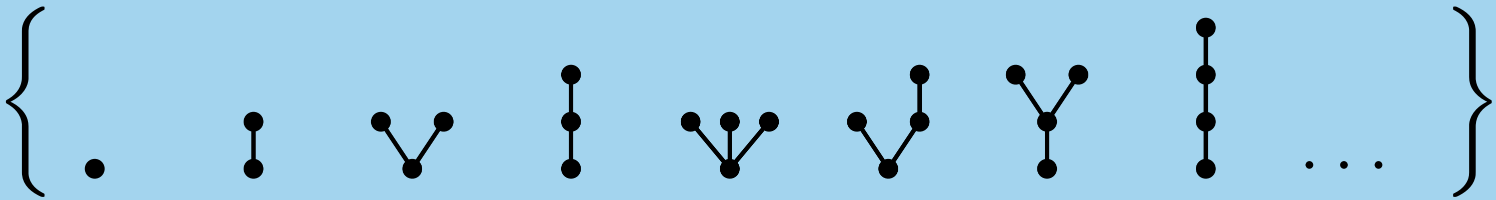

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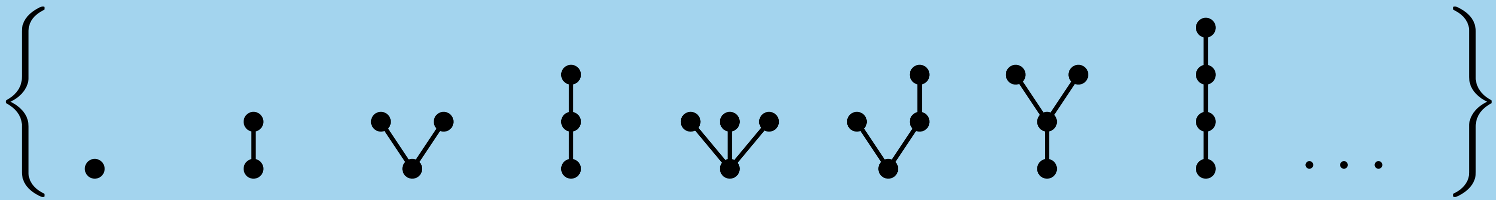


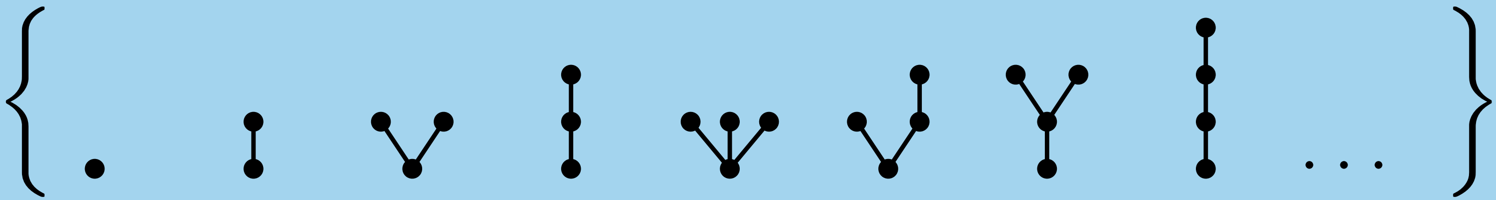
Associated with each $t \in T$ is an equation

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

where the "elementary weight" is a function of the coefficients of the method.

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

Let T denote the set of rooted trees:

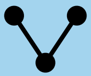
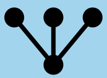
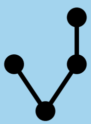
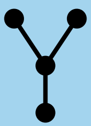


Associated with each $t \in T$ is an equation

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

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

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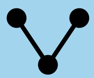
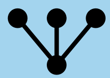
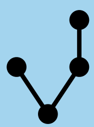
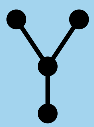
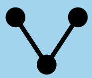
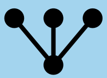
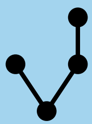
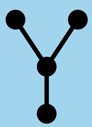
	$\sum b_i c_i^2$	3
	$\sum b_i a_{ij} c_j$	6
	$\sum b_i c_i^3$	4
	$\sum b_i c_i a_{ij} c_j$	8
	$\sum b_i a_{ij} c_j^2$	12
	$\sum b_i a_{ij} a_{jk} c_k$	24

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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The order conditions thus become

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

A third order method can be constructed with two stages:

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

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

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

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One possible generalization is known as “Two Step Runge-Kutta” methods in which all quantities computed in one step are available for the evaluation of the stages and the output value in the following step.

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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

The idea of reuse of stage derivatives can be taken further to produce "Almost Runge-Kutta" methods (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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$$Y_2 = y_{n-1} - \tfrac{3}{2}hf(y_{n-1}) + \tfrac{1}{2}hf(y_{n-2}) + 2hF_1, \quad F_2 = hf(Y_2)$$

$$y_n = y_{n-1} + \tfrac{1}{6}hf(y_{n-1}) + \tfrac{2}{3}hF_1 + \tfrac{1}{6}hF_2$$

$$\boldsymbol{y_n \longrightarrow y_1^{[n]}}, \qquad \boldsymbol{hf(y_n) \longrightarrow y_2^{[n]}}$$

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$$Y_1 = y_1^{[n-1]} + \tfrac{1}{2}y_2^{[n-1]} + \tfrac{1}{8}(y_2^{[n-1]} - y_2^{[n-2]}), \qquad F_1 = f(Y_1)$$

$$Y_2 = y_1^{[n-1]} - y_2^{[n-1]} - \tfrac{1}{2}(y_2^{[n-1]} - y_2^{[n-2]}) + 2hF_1, \quad F_2 = f(Y_2)$$

$$y_1^{[n]} = y_1^{[n-1]} + \tfrac{1}{6}y_2^{[n-1]} + \tfrac{2}{3}hF_1 + \tfrac{1}{6}hF_2$$

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

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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

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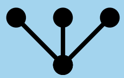
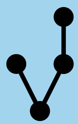
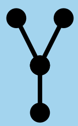
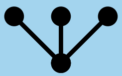
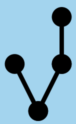
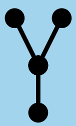
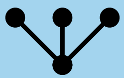
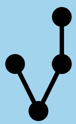
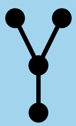
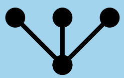
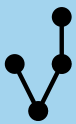
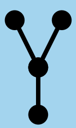
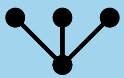
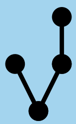
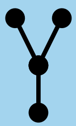
We will illustrate the group operation in a table where we also give values of E.

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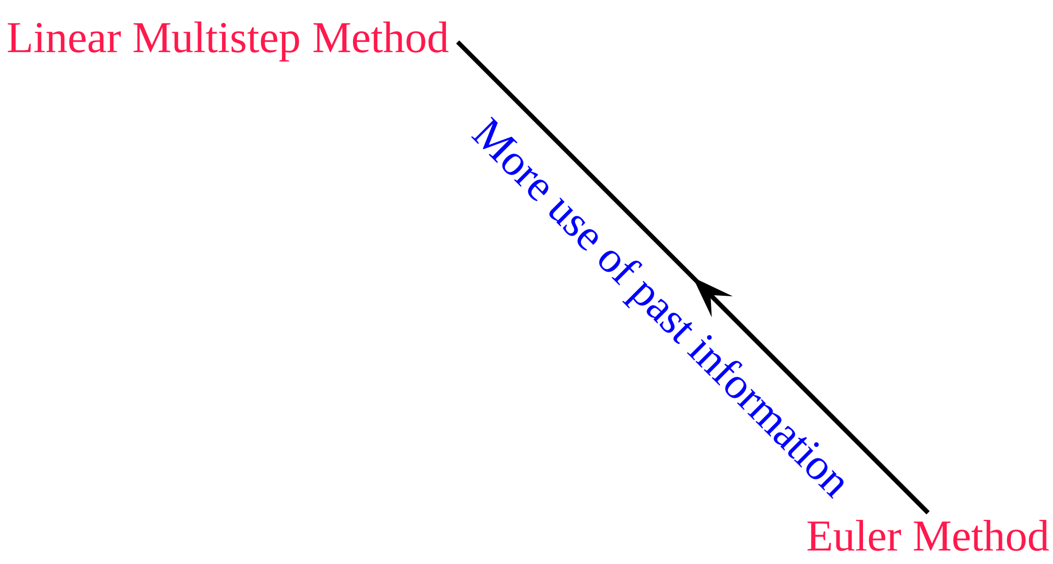
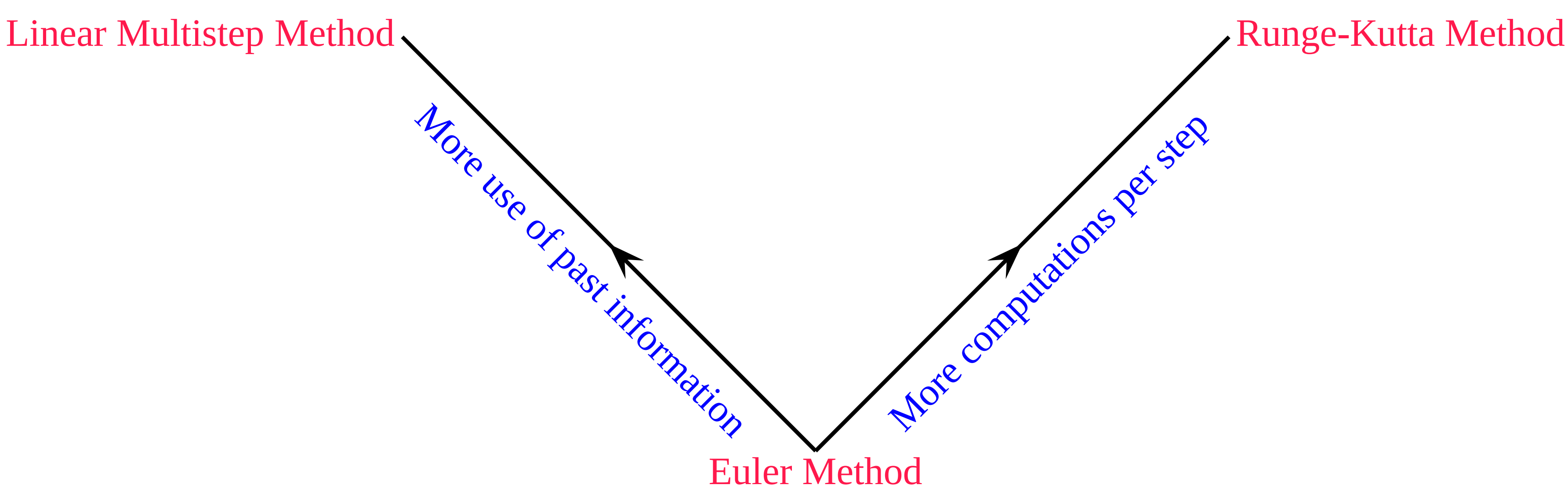
We will summarize this in the diagram on the next slide.

Euler Method


Linear Multistep Method
More use of past information
Euler Method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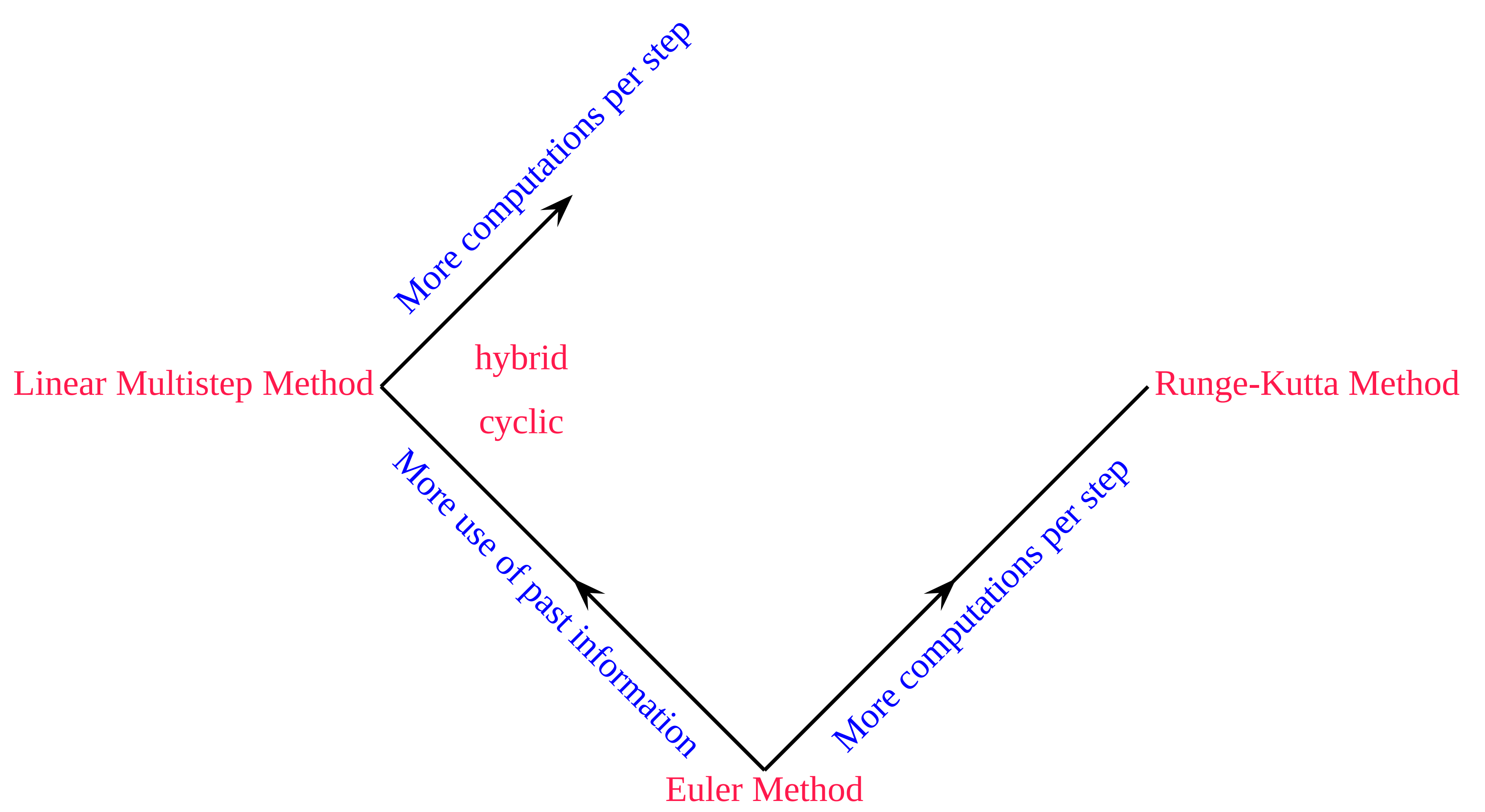
More computations per step
hybrid
Linear Multistep Method
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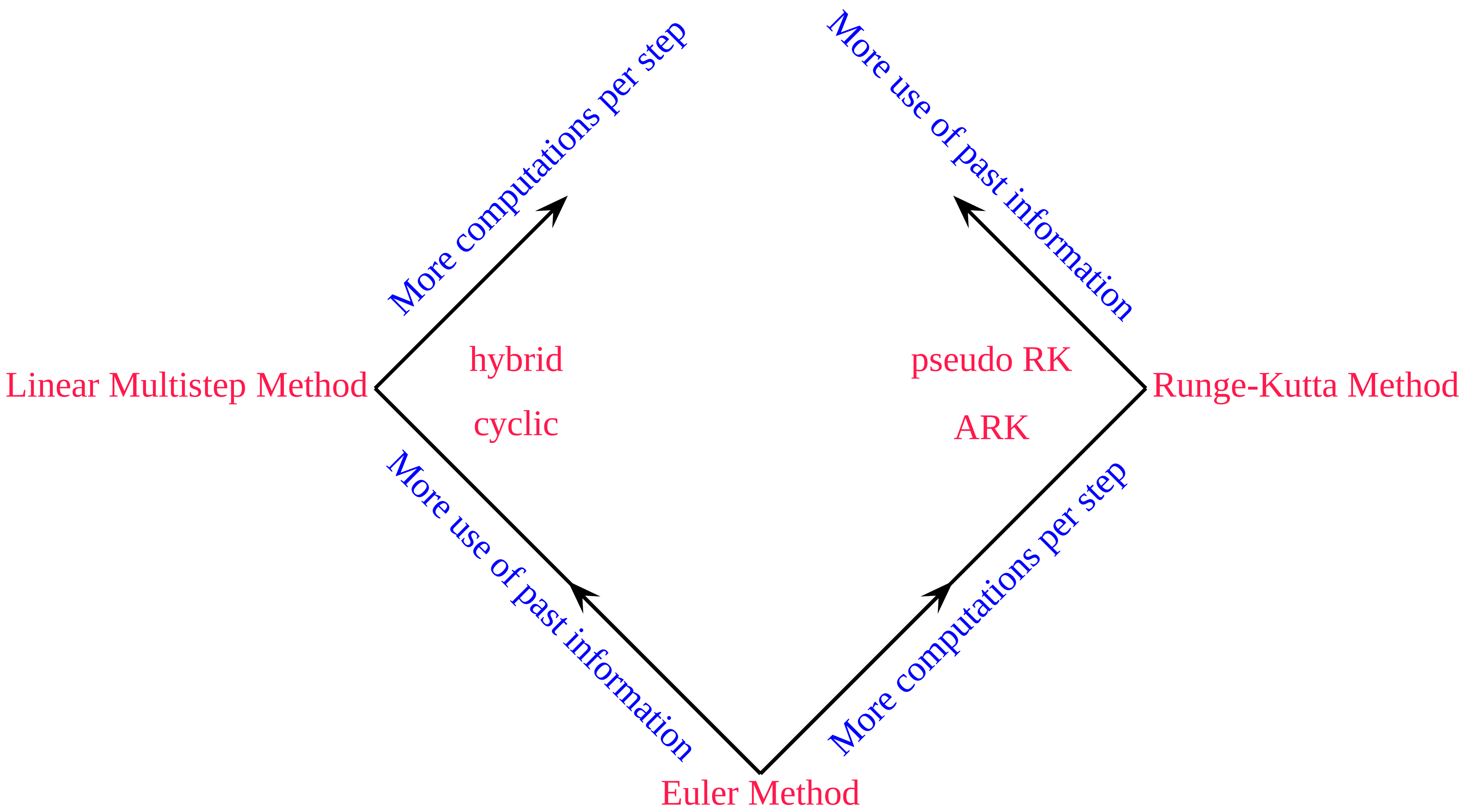
More computations per step
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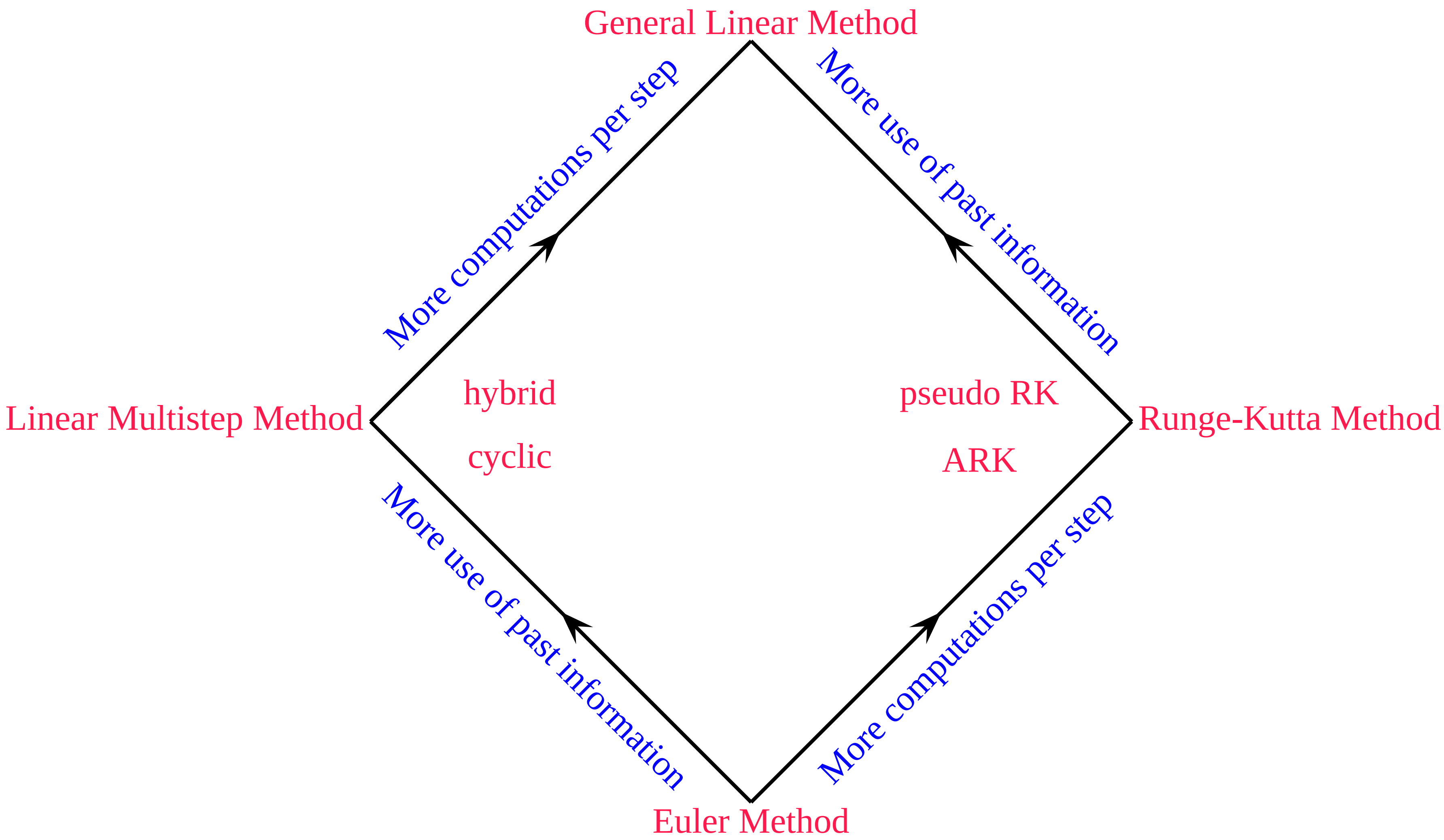
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$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}$$

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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.

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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".

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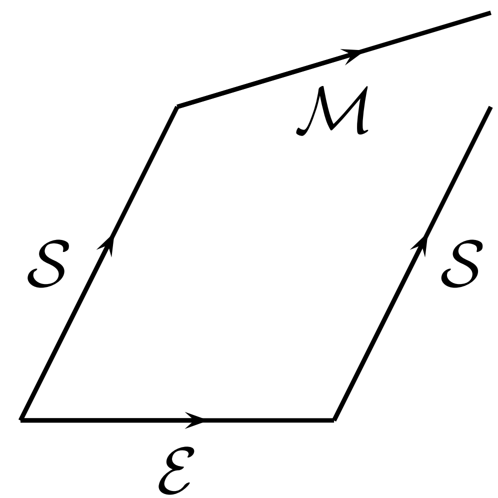

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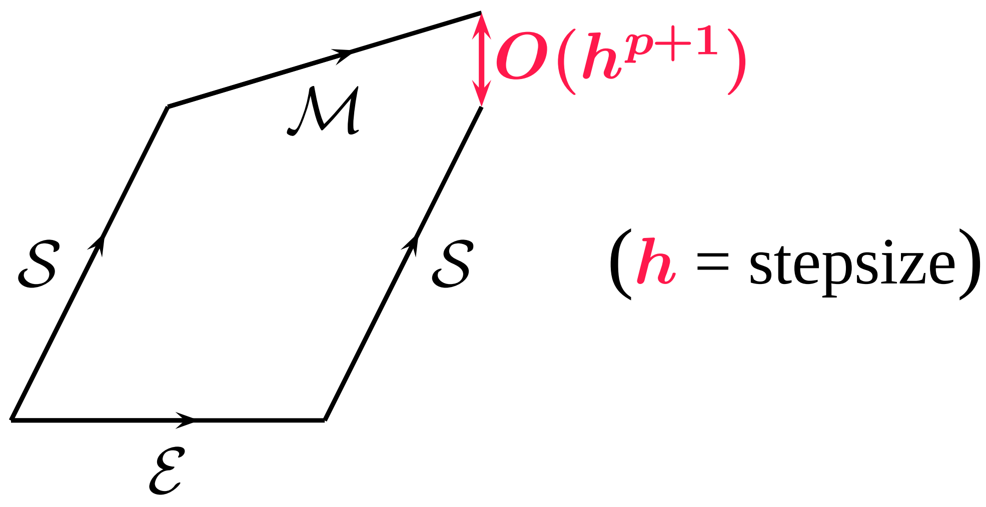

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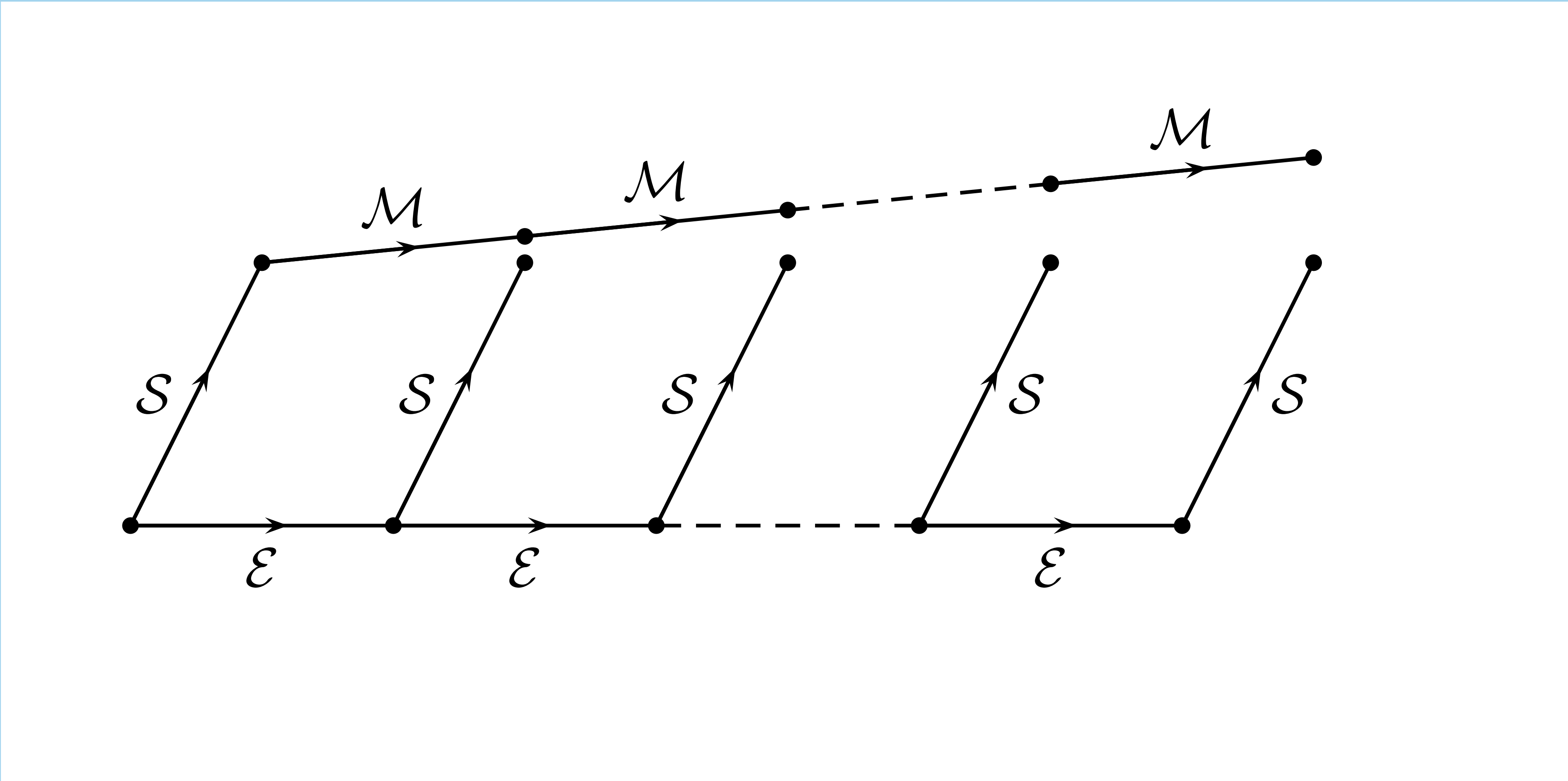

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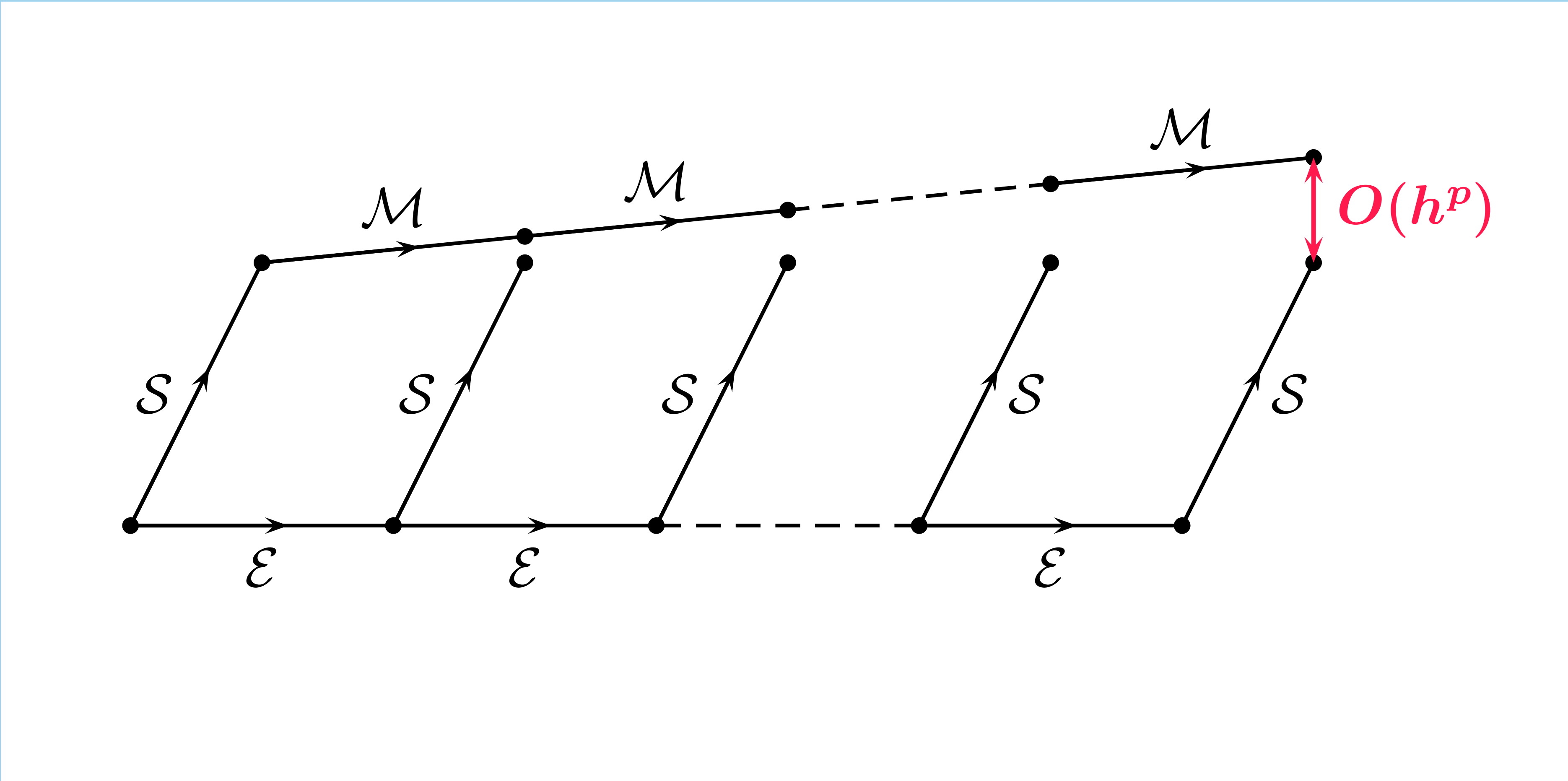

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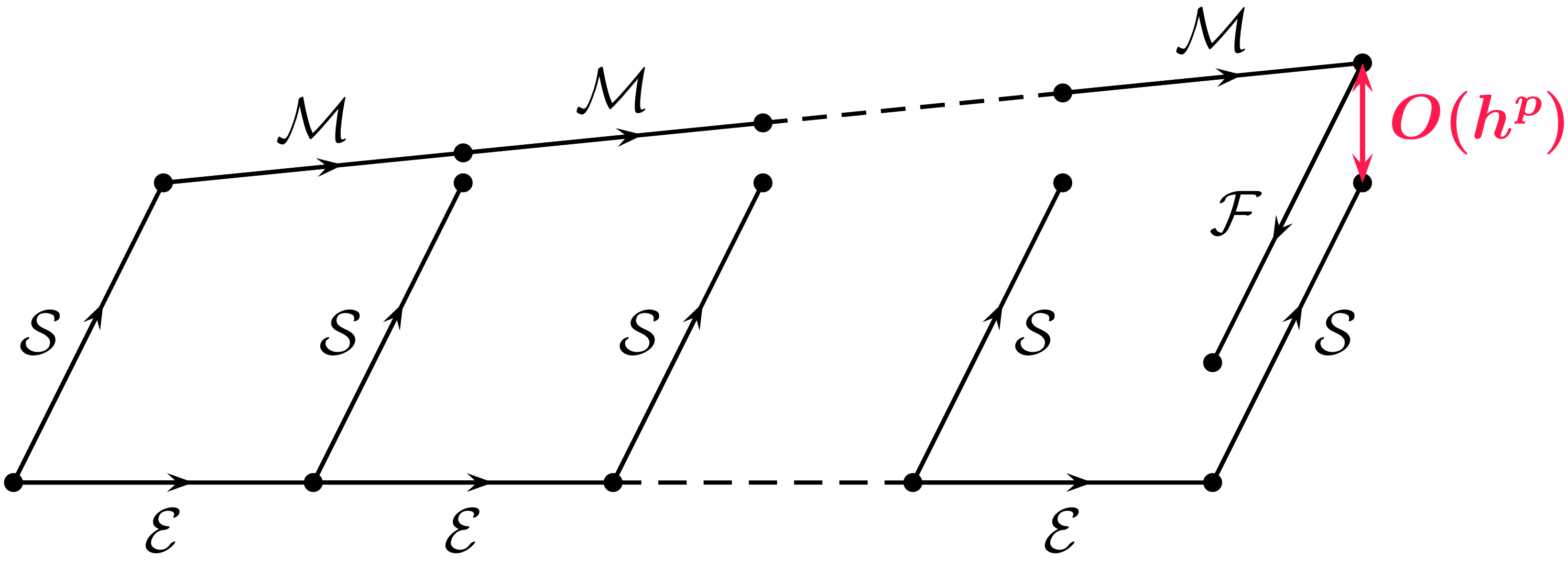

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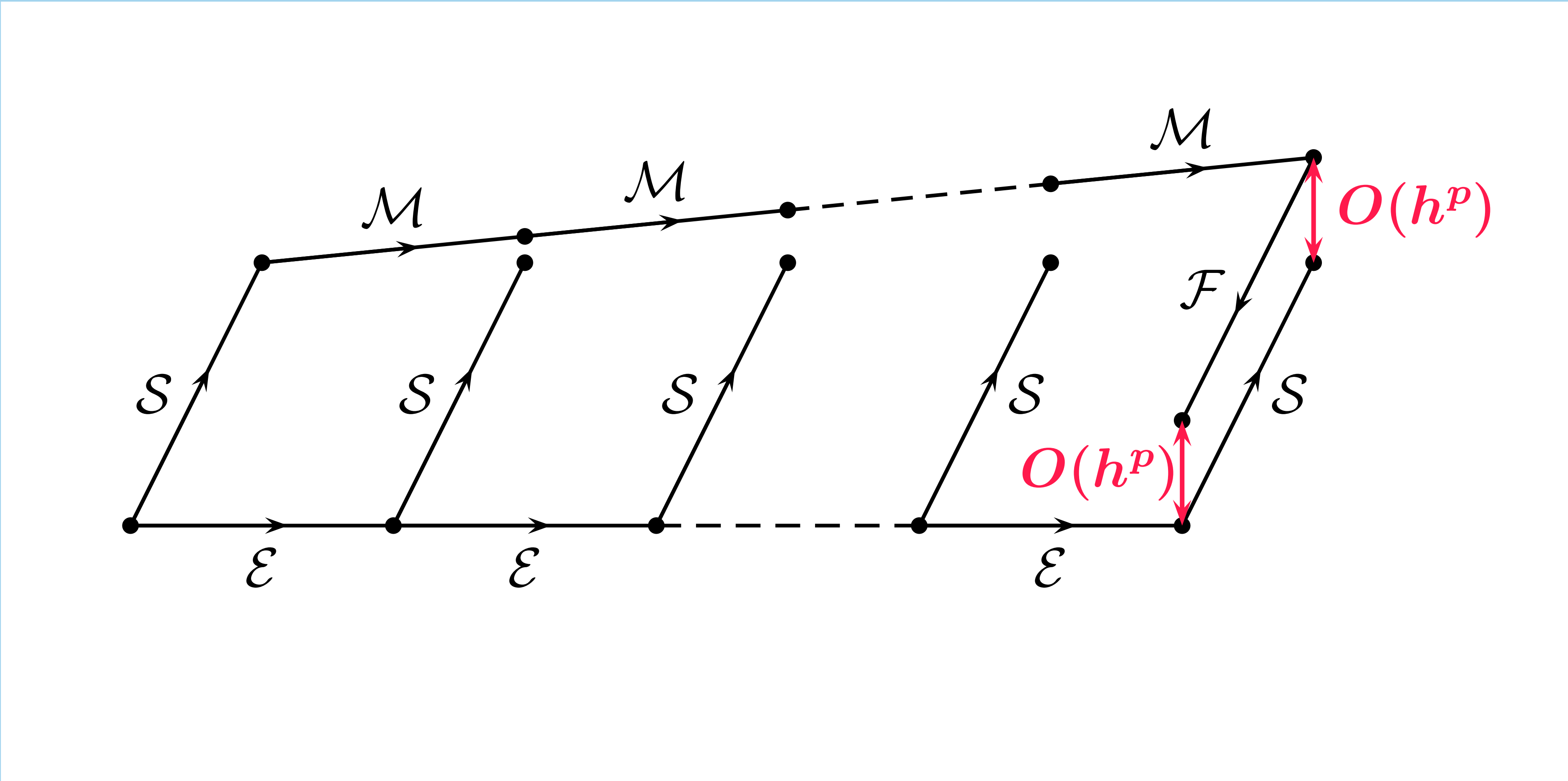

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It is possible for a Runge–Kutta method with 5 stages to have effective order 5.

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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:

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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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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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- Information on the structure of V

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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

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

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

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where we have assumed that $s = p + 1$.

It follows that

$$N(z) = (\alpha(z) + \xi(z))\beta(z) + O(z^{p+2})$$

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and ξ is easily found from

$$\xi(z) = N(z)\beta(z)^{-1} - \alpha(z)$$

From the equations

$$\begin{aligned} \exp(cz) &= zA\exp(cz) + U\phi(z) + O(z^{p+1}), \\ \exp(z)\phi(z) &= zB\exp(cz) + V\phi(z) + O(z^{p+1}), \end{aligned}$$

we deduce, in the Nordsieck case, that

$$\begin{aligned} U &= C - ACK, \\ V &= E - BCK, \end{aligned}$$

where

$$K = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \qquad E = \exp(K), \qquad C_{ij} = \frac{c_i^{j-1}}{(j-1)!}$$

To see how the value of ξ_{p+1}, related to the error constant, comes into the derivation of actual methods, look at the consequences of the formulae

$$BA = XB, \tag{1}$$

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Remarkably, this reduces to an equation of the form $BCv = w$, where v and w are vectors.

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

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

Implementation questions

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- Initial stepsize
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- Evaluation of stages

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- Initial stepsize
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The naive method of achieving variable stepsize ($h \to rh$) is to rescale the Nordsieck vector by a matrix

$$D(r) = \text{diag}(1, r, r^2, \ldots, r^p).$$

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If r is constrained to lie in an interval $I = [r_{\text{min}}, r_{\text{max}}]$ then zero-stability generalizes to the existence of a uniform bound on

$$\|D(r_n)VD(r_{n-1})V \cdots D(r_2)VD(r_1)V\|$$

when $r_1, r_2, \dots, r_n \in I$.

For implicit methods, we might also want "infinity-stability" by requiring a uniform bound on

$$\|D(r_n)\widehat{V}D(r_{n-1})\widehat{V}\cdots D(r_2)\widehat{V}D(r_1)\widehat{V}\|,$$

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This naive approach is very unsatisfactory from the stability point of view and it has other disadvantages, as we will see.

Less naive is to modify the rescaled Nordsieck vector by adding quantities computed from $hF_1, hF_2, \dots, hF_{p+1}, y_2^{[n-1]}, y_3^{[n-1]}, \dots, y_{p+1}^{[n-1]}$, such that the order remains p

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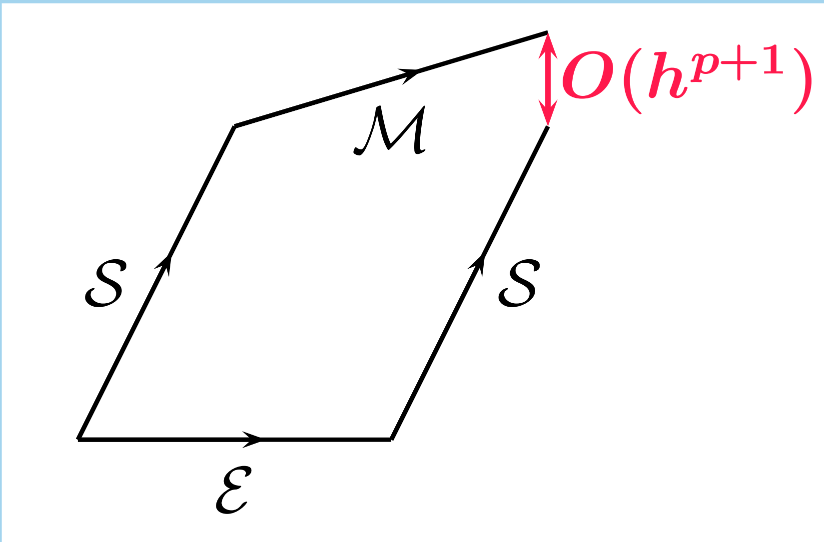
We introduce these ideas in the context of the underlying one-step method.

To introduce the underlying one-step method, consider a modification of the diagram relating the starting method and a single step of the method.



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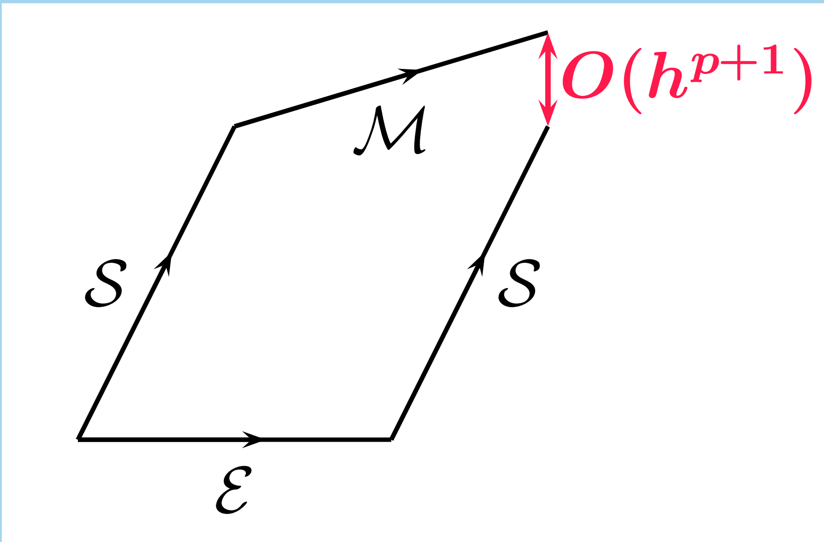

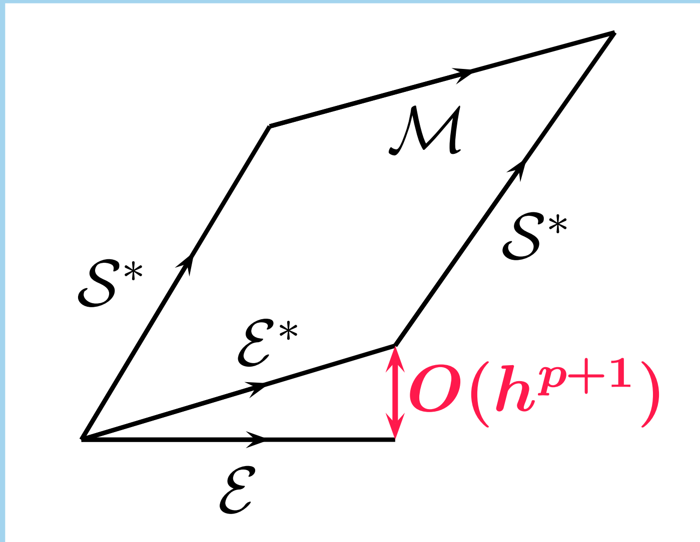

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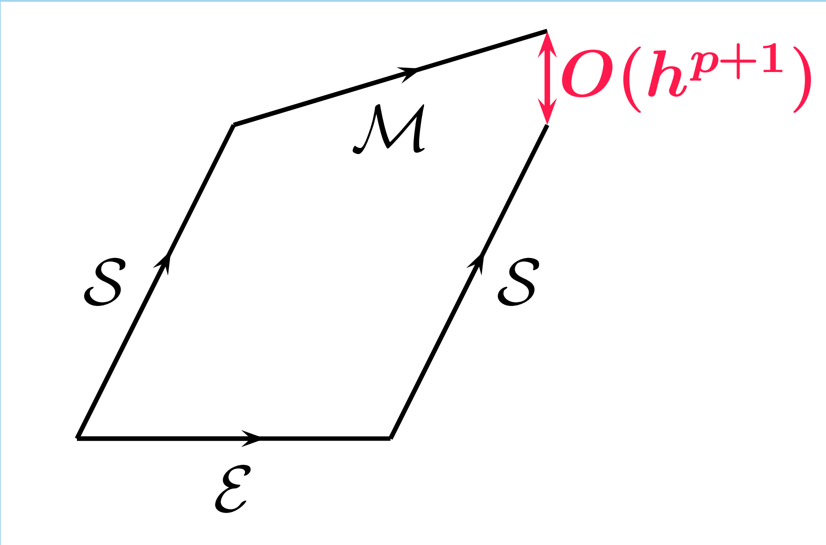

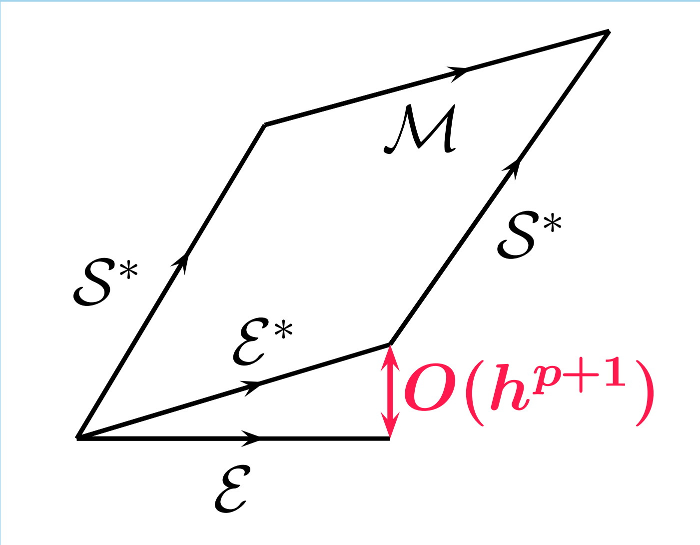

In the modified diagram, the perturbed starting method, shown as $\mathcal{S}^*$, is chosen to obtain a commutative diagram if $\mathcal{E}$ is replaced by the underlying one-step method $\mathcal{E}^*$.

If $\mathcal{S}$ maps $y(x)$ to

$$\begin{bmatrix} y(x) \\ hy'(x) \\ \vdots \\ h^p y^{(p)}(x) \end{bmatrix}$$

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then $\mathcal{S}^*$ maps $y(x)$ to

$$\begin{bmatrix} y(x) \\ hy'(x) - \theta_1 h^{p+1} y^{(p+1)}(x) - \phi_1 h^{p+2} y^{(p+2)}(x) - \psi_1 h^{p+2} \frac{\partial f}{\partial y} y^{(p+1)}(x) + O(h^{p+3}) \\ \vdots \\ h^p y^{(p)}(x) - \theta_p h^{p+1} y^{(p+1)}(x) - \phi_p h^{p+2} y^{(p+2)}(x) - \psi_p h^{p+2} \frac{\partial f}{\partial y} y^{(p+1)}(x) + O(h^{p+3}) \end{bmatrix}$$

Values of the coefficients θ_i, ϕ_i, ψ_i $(i = 1, 2, \ldots, p)$ are known.

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We now know how to do this so that behaviour is stabilised and so that at least the θ values effectively retain their constant values.

It is now possible to estimate

- The value of $h^{p+1}y^{(p+1)}(x_n)$ to within $O(h^{p+2})$.

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- Hence the local truncation error of a contending method of order $p+1$.

We believe we now have the ingredients for constructing a variable order, variable stepsize code based on the new methods.

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