Order and stability for general linear methods

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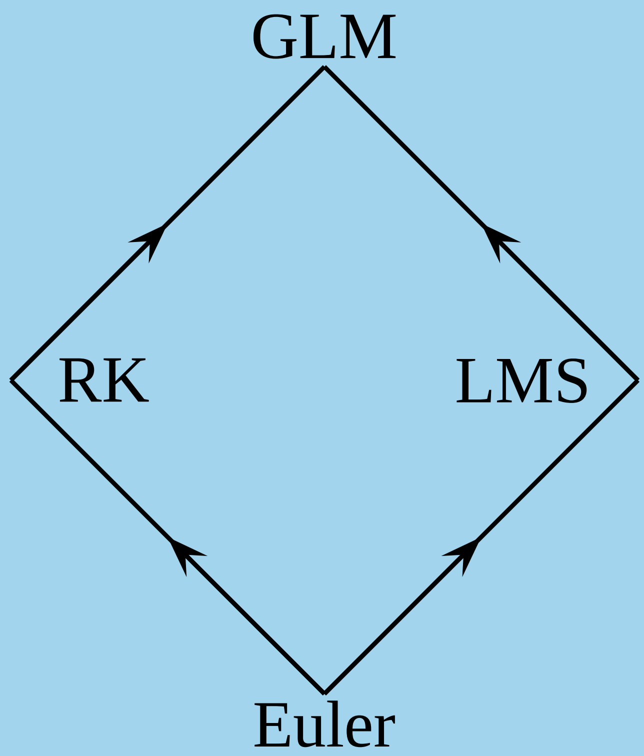

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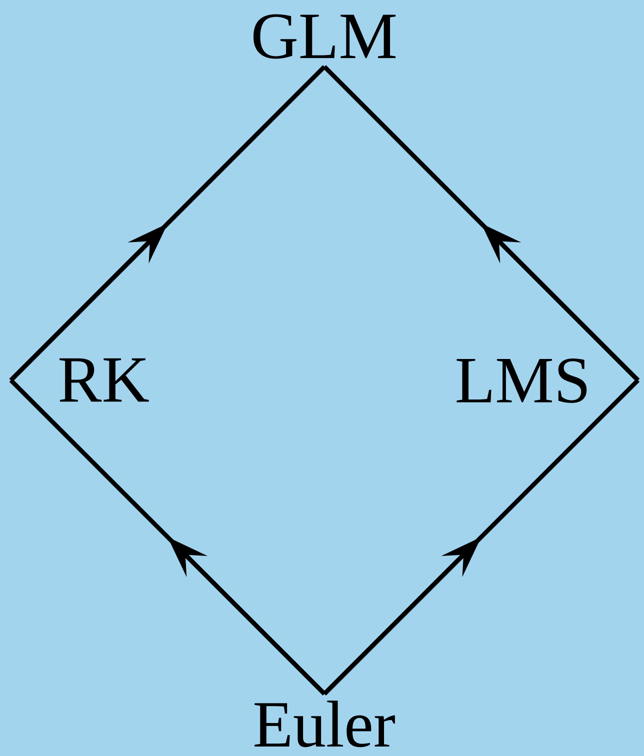

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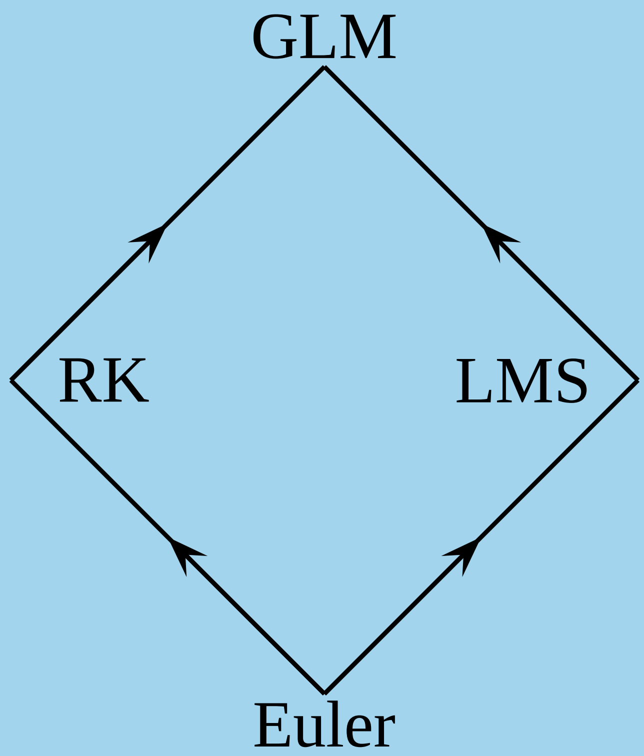

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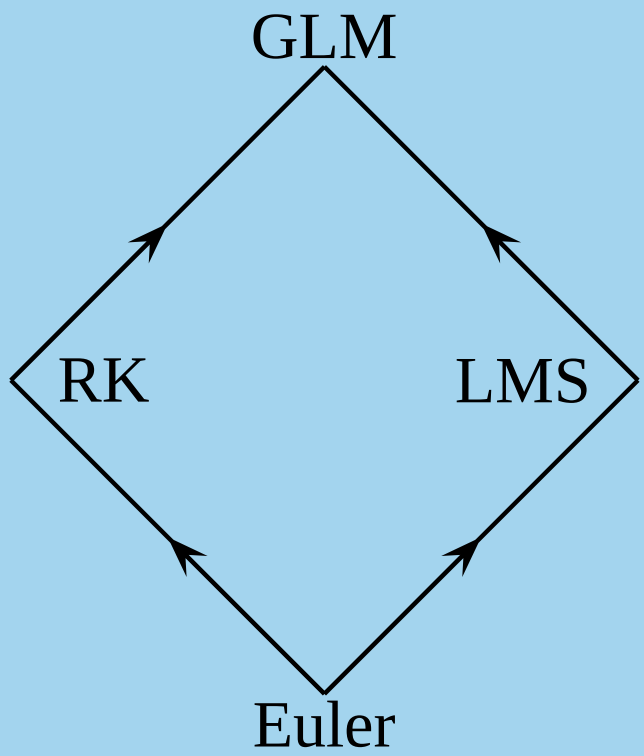
A second characteristic feature is that, within the step, s stages are computed, together with the corresponding s stage derivatives.



Denote the output approximations from step number n by $y_i^{[n]}$, $i = 1, 2, \dots, r$, the stage values by Y_i, $i = 1, 2, \dots, s$ and the stage derivatives by F_i, $i = 1, 2, \dots, s$.

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For convenience, write

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

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It is assumed that Y and F are related by a differential equation.

The computation of the stages and the output from step number n is carried out according to the formulae

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

$$y_i^{[n]} = \sum_{j=1}^{s} b_{ij} h F_j + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \qquad i = 1, 2, \dots, r,$$

where the matrices $A = [a_{ij}]$, $U = [u_{ij}]$, $B = [b_{ij}]$, $V = [v_{ij}]$ are characteristic of a specific method.

We can write these relations more compactly in the form

$$\begin{bmatrix} Y \\ y^{[n]} \end{bmatrix} = \begin{bmatrix} A \otimes I & U \otimes I \\ B \otimes I & V \otimes I \end{bmatrix} \begin{bmatrix} hF \\ y^{[n-1]} \end{bmatrix}$$

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which we can simplify by making a harmless abuse of notation in the form

$$\begin{bmatrix} Y \\ y^{[n]} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hF \\ y^{[n-1]} \end{bmatrix}$$

A Runge-Kutta method

The famous fourth order Runge-Kutta method is simply written as a general linear method

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \longrightarrow \left[\begin{array}{cc} A & U \\ B & V \end{array}\right] = \left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & 1 \\ \frac{1}{2} & 0 & 0 & 0 & 1 \\ 0 & \frac{1}{2} & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ \hline \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & 1 \end{array}\right]$$

Like all Runge-Kutta methods, $r = 1$.

Linear multistep methods

The 2-step Adams-Bashforth and Adams-Moulton methods are, respectively,

$$y_n = y_{n-1} + \tfrac{3}{2}hy'_{n-1} - \tfrac{1}{2}hy'_{n-2},$$

$$y_n = y_{n-1} + \tfrac{5}{12}hy'_n + \tfrac{2}{3}hy'_{n-1} - \tfrac{1}{12}hy'_{n-2}.$$

The $r = 3$ inputs are y_{n-1}, hy'_{n-1}, hy'_{n-2} with outputs y_n, hy'_n, hy'_{n-1}.

The general linear formulations are respectively,

$$\left[\begin{array}{c|ccc} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right] \quad \text{and} \quad \left[\begin{array}{c|ccc} \frac{5}{12} & 1 & \frac{2}{3} & -\frac{1}{12} \\ \hline \frac{5}{12} & 1 & \frac{2}{3} & -\frac{1}{12} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right].$$

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

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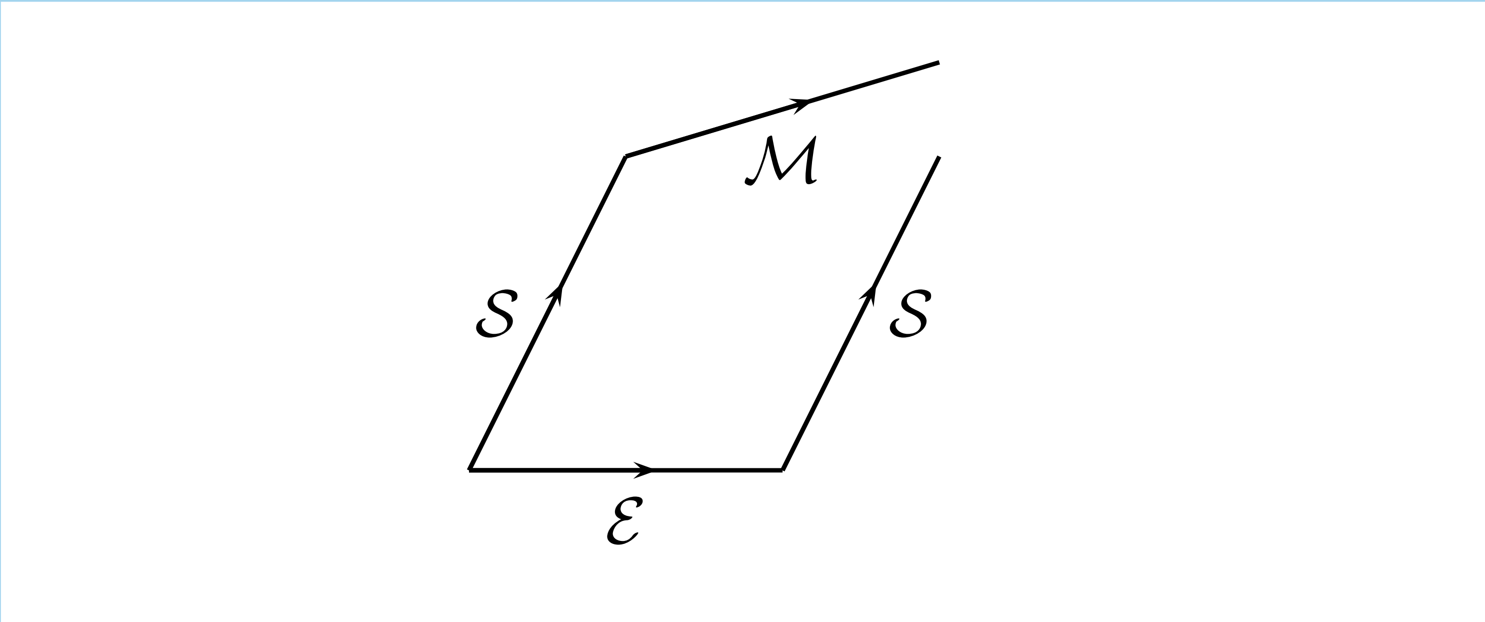

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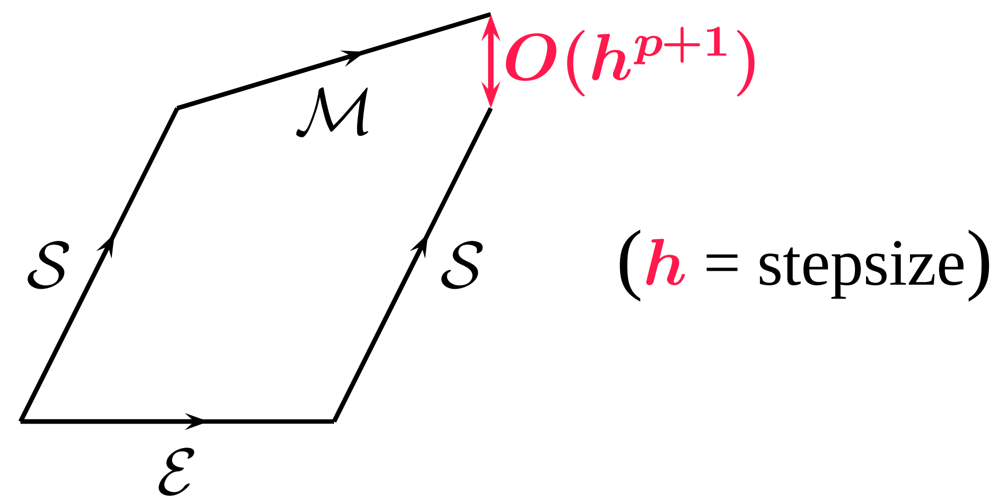

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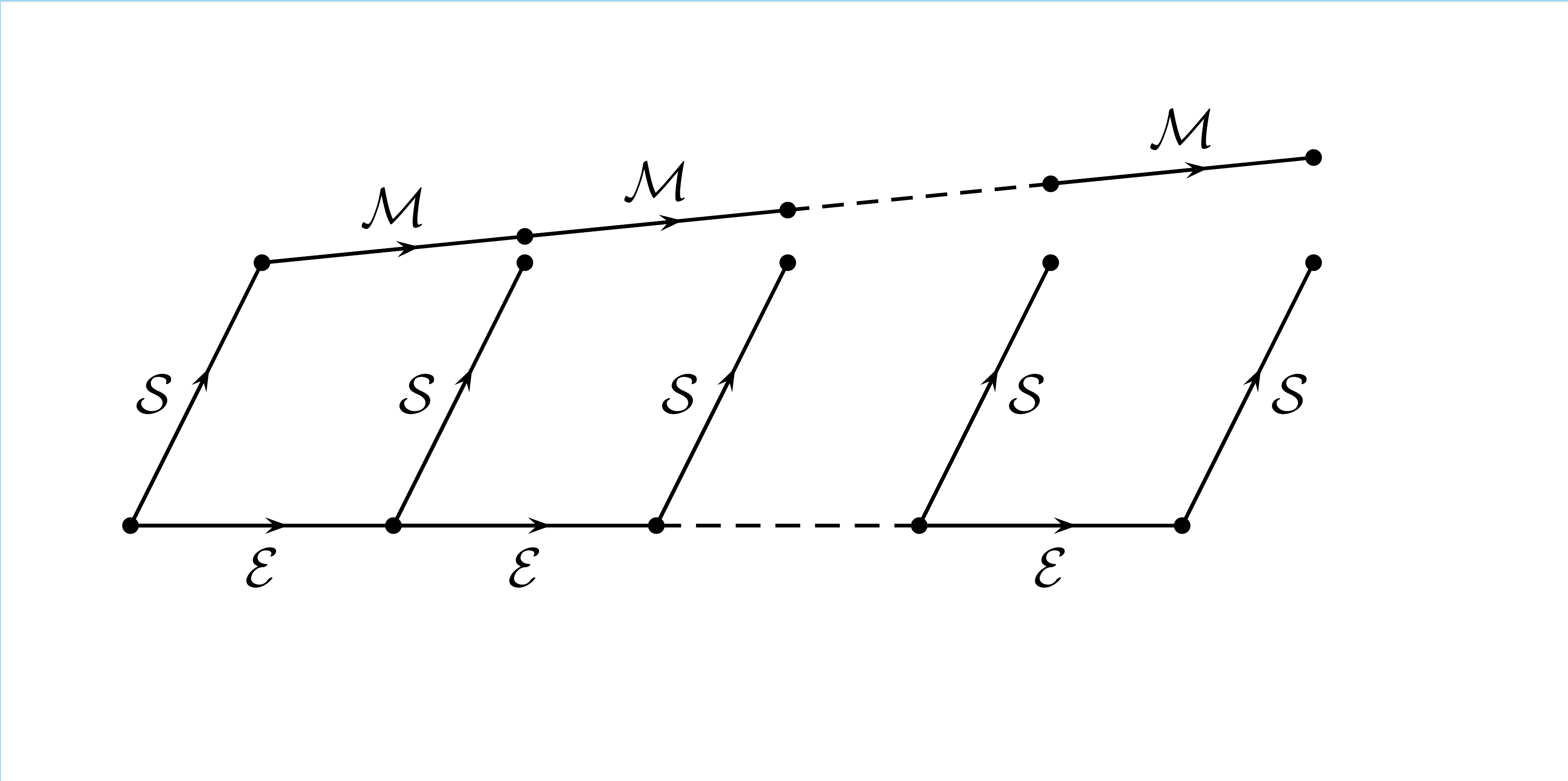

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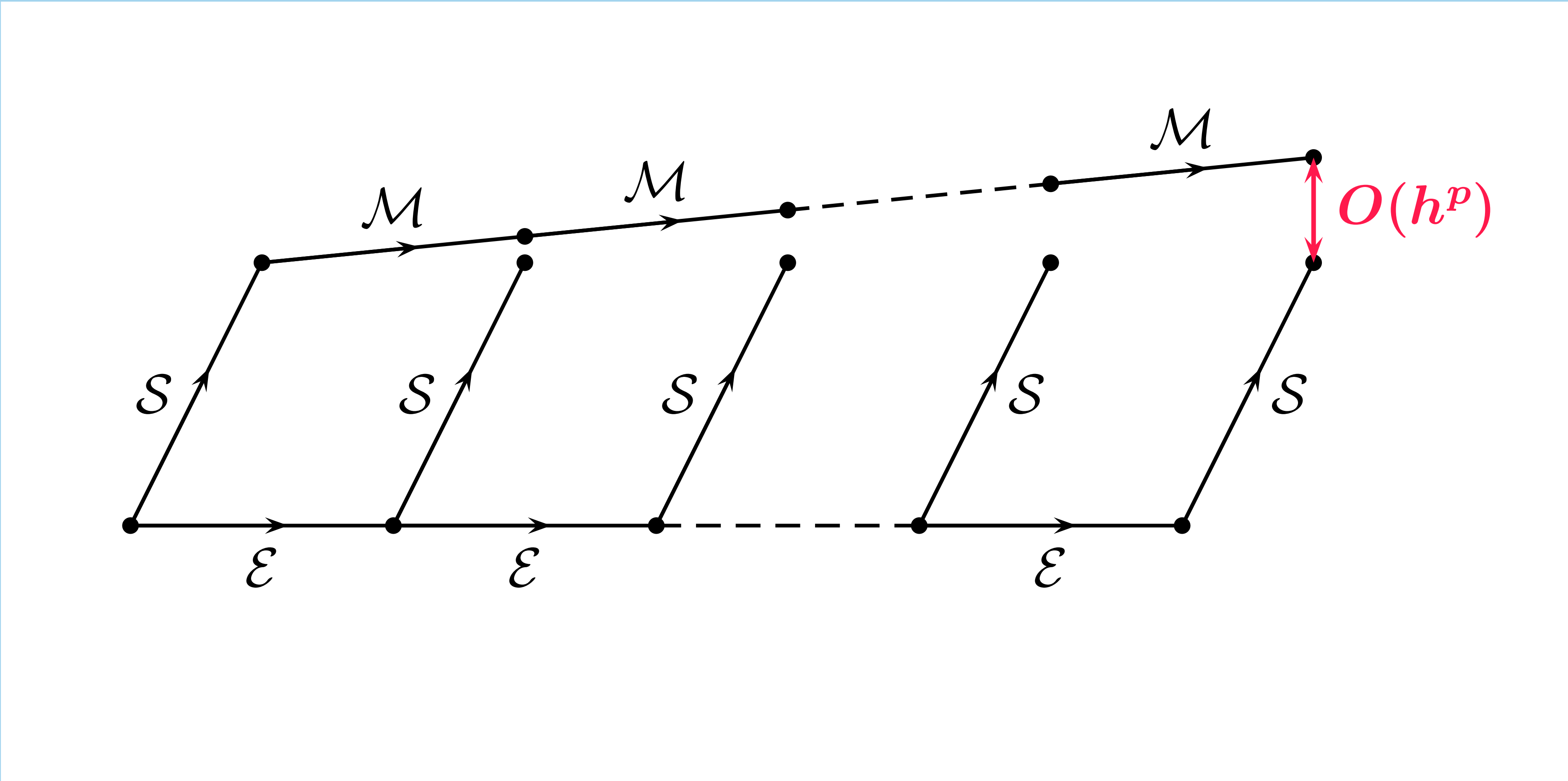

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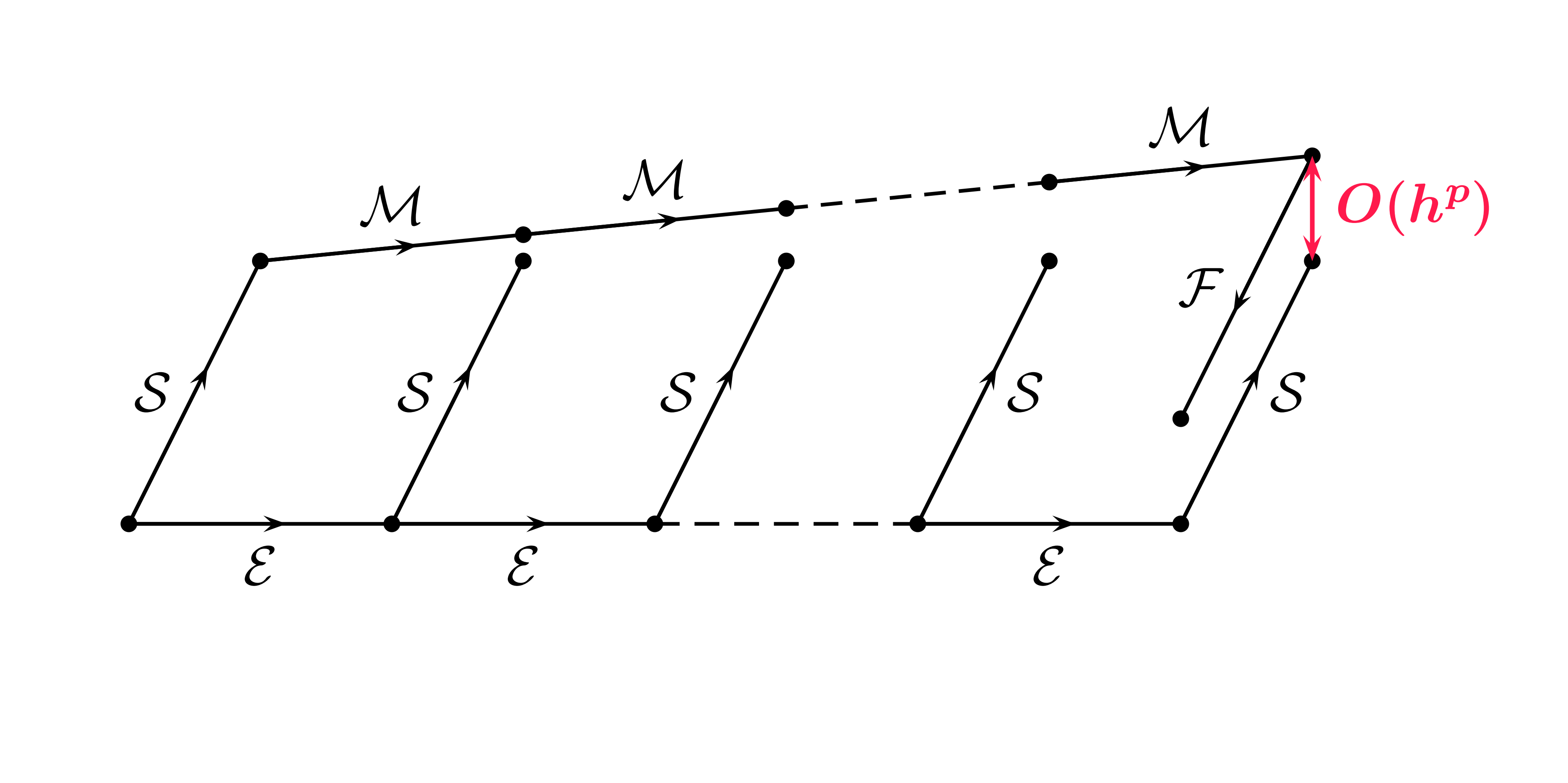

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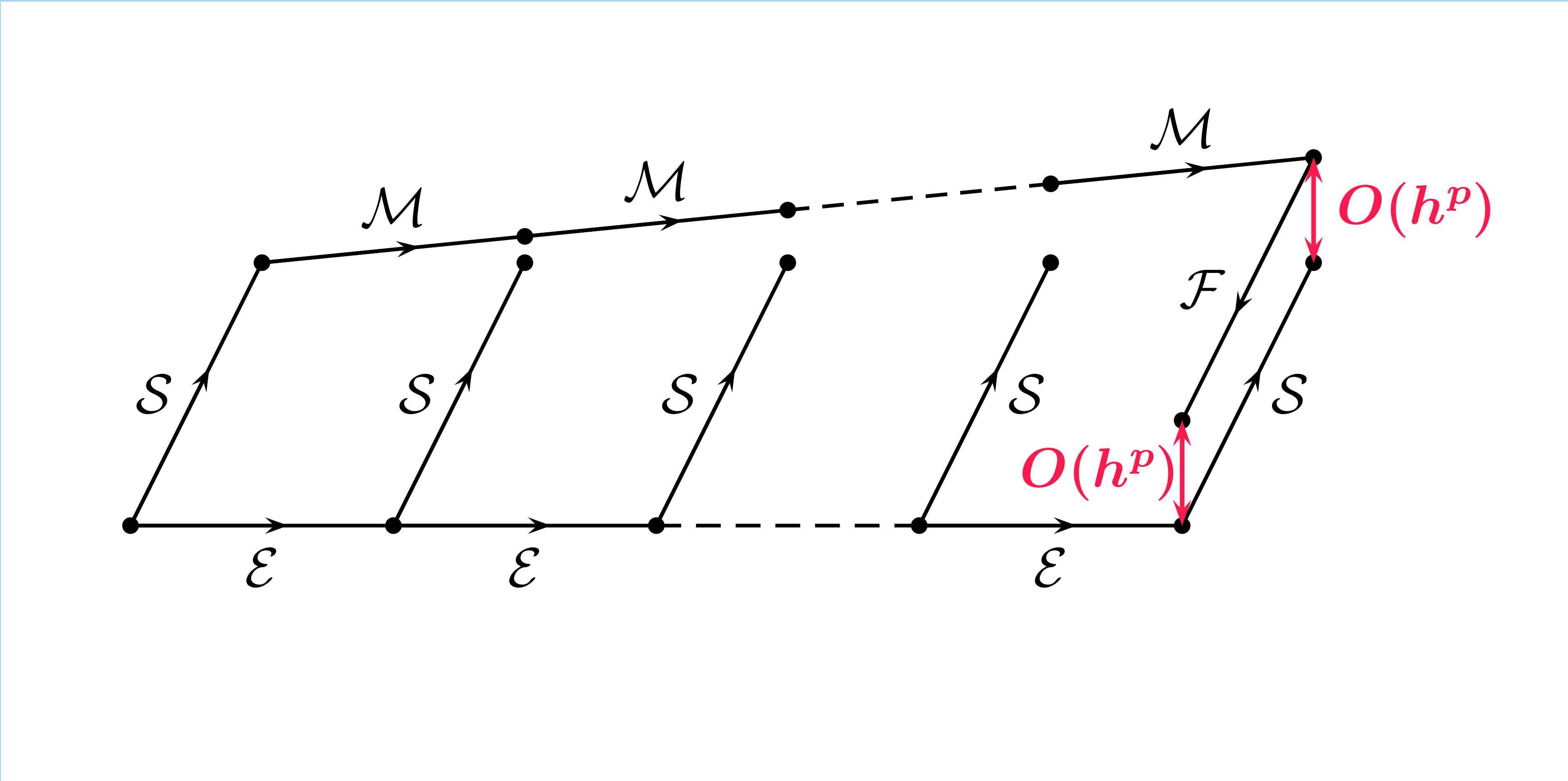

To represent $\mathcal{S}$ and turn the definition of order into a practical algorithm for analysing a specific method, operations on the set of mappings $T^{\#} \to \mathbb{R}$ can be used, where $T^{\#}$ is the set of rooted trees, together with the empty tree.

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The conditions are

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

$$E\eta = B\xi D + V\eta,$$

where $\eta \in X^r$ represents $y^{[n-1]}$ and $\xi \in X_1^s$ represents Y.

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To understand the operations ξD (or the operation for a single component $\xi_i D$) and $E\eta$ (or a single component $E\eta_i$) we need to use what I call the Runge-Kutta space (equivalent to the concept of B-series).

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Before we show the details, we note that

$$(\alpha\beta)(t) = \alpha(t)\beta(\emptyset) + \sum_{u \in T} \phi(t, u, \alpha)\beta(u)$$

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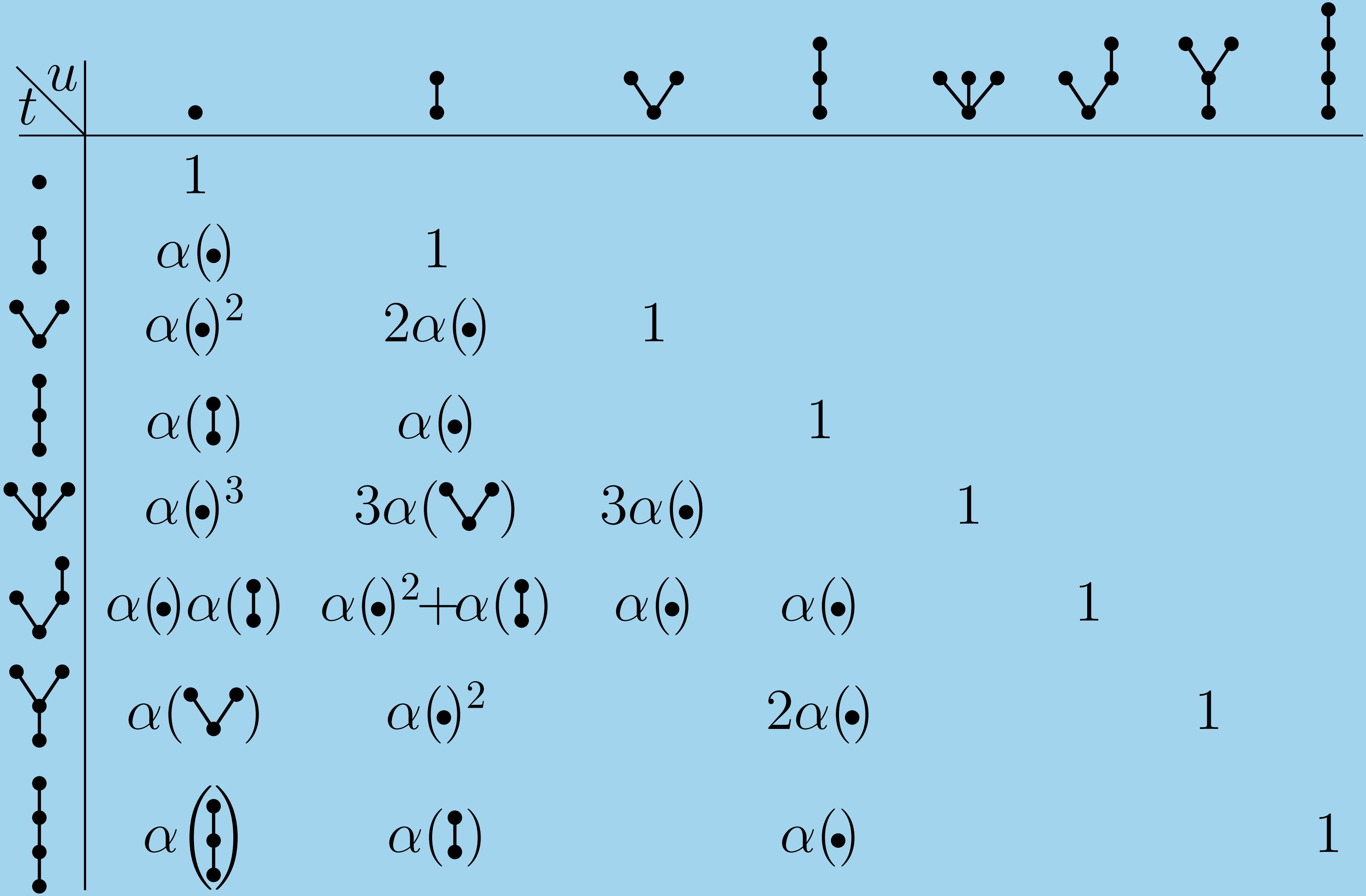
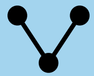
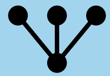
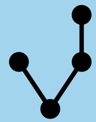
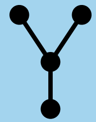
A table of ϕ up to t of order 4 is shown on the next slide.



u
t

The values of D and E are shown in the following table

t	$\emptyset$								
$D(t)$	0	1	0	0	0	0	0	0	0
$E(t)$	1	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{12}$	$\frac{1}{24}$

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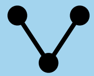
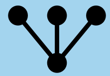
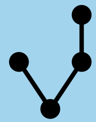
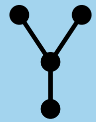
t	$\emptyset$								
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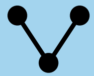
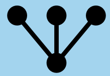
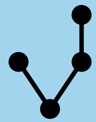
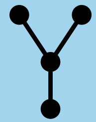
t	$\emptyset$								
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Note than D denotes differentiation and E represents flow through a single time step.
If we are interested in order not exceeding p, then we will interpret such expressions as η, $E\eta$, ξ and ξD as mappings restricted to trees of order not exceeding p.

With these interpretations we look at the order criteria again:

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To within order p, this states that the output values are equal to the composition of the flow and the starting process.

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If α denotes the mapping from trees to elementary weights for a specific method,

$$\alpha = E,$$

up to trees of order p.

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A particular consequence is that, although 5 stage explicit Runge-Kutta methods cannot have order 5, they can 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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$$y_i^{[n-1]} = \alpha_{i1}y(x_{n-1}) + \alpha_{i2}hy'(x_{n-1}) + \cdots + \alpha_{i,p+1}h^p y^{(p)}(x_{n-1})$$

and where

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

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We will consider only methods which are strongly zero-stable, so that only the principal eigenvalue of V lies on the unit circle.

By formulating the method appropriately, that is by making a simple change of basis transformation:

$$\left[\; A,\;\; U,\;\; B,\;\; V \;\right] \rightarrow \left[\; A,\;\; UT,\;\; T^{-1}B,\;\; T^{-1}VT \;\right]$$

we can assume that V has the form

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

where

$$\rho(\dot{V}) < 1.$$

Stability matrix and stability function

By considering the linear test problem $y' = qy$ and defining $z = hq$, we arrive at the stability matrix

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We define the “stability region” as the set of points in the complex plane such that $M(z)$ is power bounded.

We also define the “stability function” as

$$\Phi(w, z) = \det(wI - M(z)).$$

Finding new methods from stability

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- The second approach is to decide first what its stability function should be and then search for methods with this stability function.

Before going on to look at examples based on modifying classical methods, we look briefly at some ramifications of the second approach.

Generalized Padé approximations

The following function represents an approximation of order 3 to $\exp$:

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It happens to be the stability function of the rather contrived general linear method:

$$\left[\begin{array}{cc|cc} \frac{2}{7} & -\frac{2}{7} & 1 & 0 \\ \frac{3}{7} & \frac{4}{7} & 1 & \frac{\sqrt{7}}{7} \\ \hline \frac{6-\sqrt{7}}{7} & \frac{1+\sqrt{7}}{7} & 1 & 0 \\ \frac{343-131\sqrt{7}}{98} & -\frac{\sqrt{7}}{49} & 0 & \frac{1}{7} \end{array}\right]$$

It is also the stability function of the Obreshkov method

$$y(x_n) \approx \frac{6}{7} h y'(x_n) - \frac{2}{7} h^2 y''(x_n) + \frac{8}{7} y(x_{n-1}) - \frac{1}{7} y(x_{n-2})$$

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The function $\Phi(w,z)$ is an order 2 approximation to $\exp$ because

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or alternatively because one of the solutions to the quadratic equation in w is

$$\begin{aligned} w &= \tfrac{4+\sqrt{9+6z-2z^2}}{7-6z+2z^2} \\ &= 1 + z + \tfrac{1}{2}z^2 + \tfrac{1}{6}z^3 - \tfrac{1}{72}z^4 + \cdots \\ &= \exp(z) - \tfrac{1}{18}z^4 - \cdots \end{aligned}$$

For any sequence of integers $[d_0, d_1, \ldots, d_n]$ such that

$$d_0 \geq 0, d_n \geq 0, \quad d_j \geq -1, j = 1, 2, \ldots, n-1,$$

there exists polynomials P_j of degree d_j, $j = 0, 1, \ldots, n$ such that

$$\sum_{j=0}^{n} \exp((n-j)z) P_j(z) = O(z^{p+1})$$

where the "order" p is

$$p = \sum_{j=0}^{n} (d_j + 1) - 1.$$

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If generalized Padé approximations are going to be used as a starting point in the search for A-stable general linear methods, it is appropriate to ask which approximations have acceptable stability functions.

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If generalized Padé approximations are going to be used as a starting point in the search for A-stable general linear methods, it is appropriate to ask which approximations have acceptable stability functions.

That is, we want to know which approximations have the property that there do not exist (w, z) such that

$$\Phi(w, z) = 0, \quad |w| > 1, \quad \text{Re}(z) < 0.$$

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Quick review of order stars and order arrows

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Quick review of order stars and order arrows

Stability results such as the Ehle barrier and the Daniel-Moore barrier can be conveniently proved using order stars.
Order arrows are an alternative tool for deriving these and similar results and sometimes give a slightly different emphasis.

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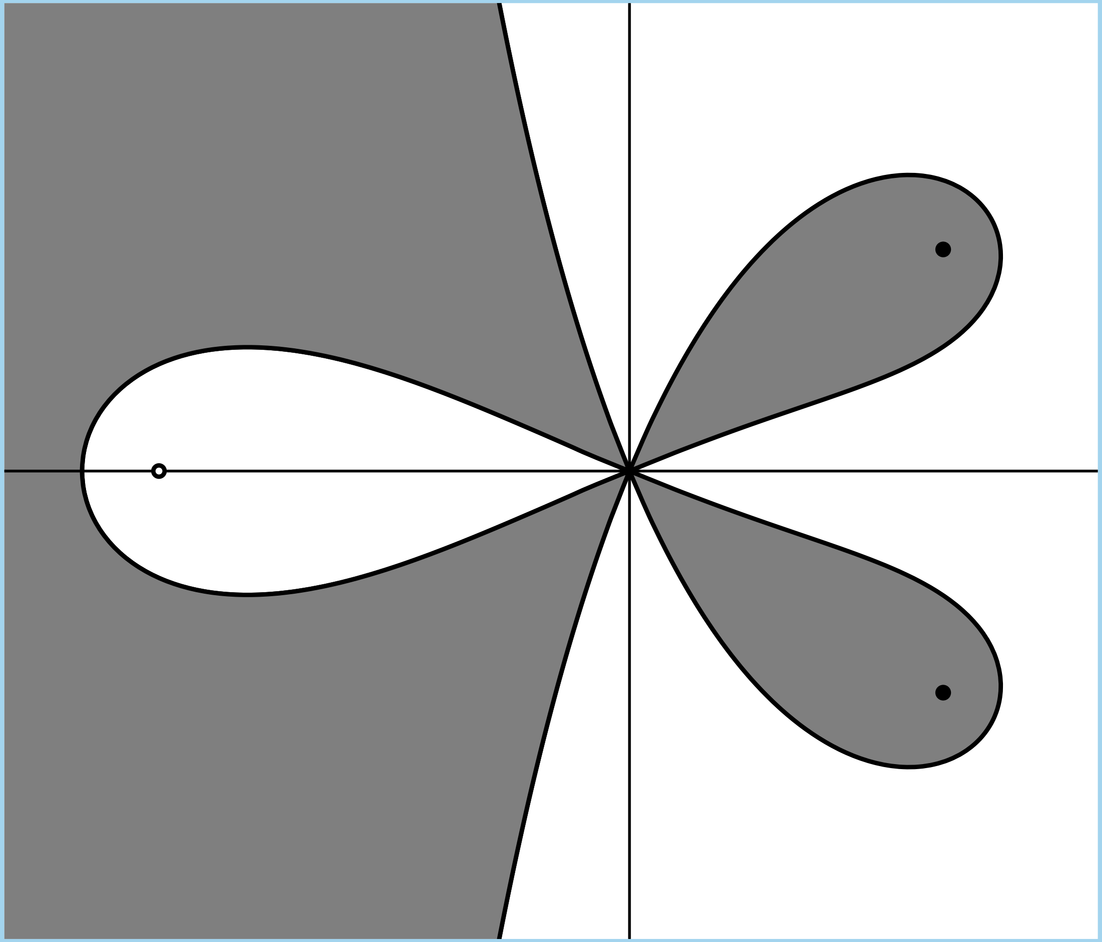

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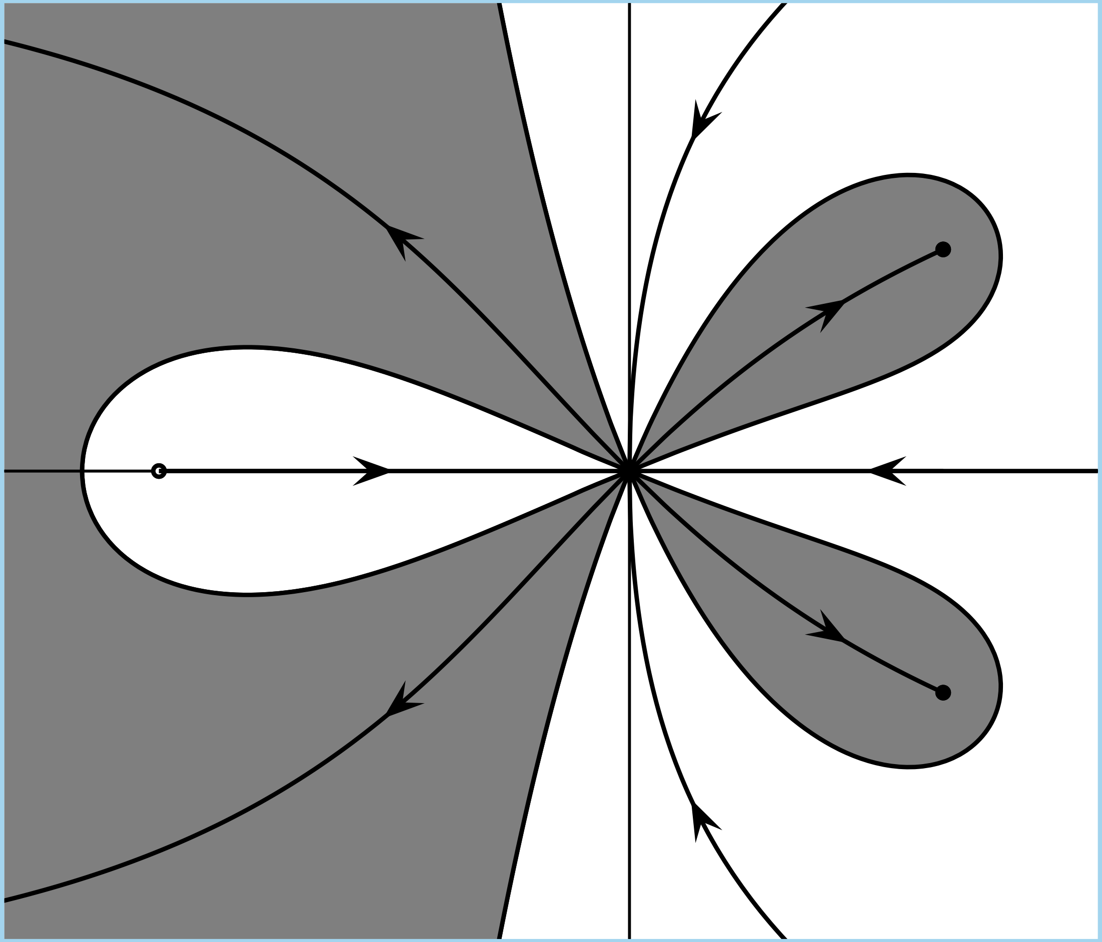

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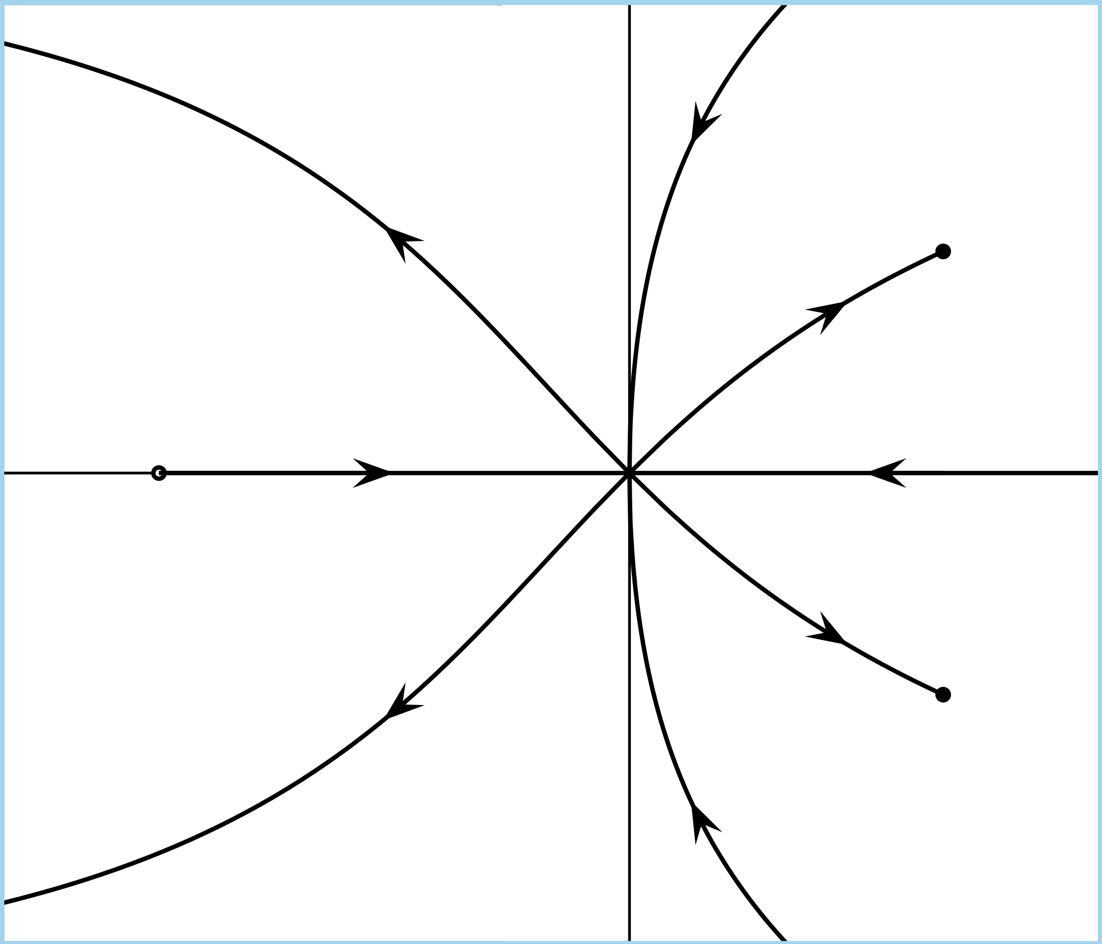

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Criterion for A-stability

If a rational approximation is A-stable then

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Note

Although these properties are necessary, they do not appear to be sufficient for A-stability.

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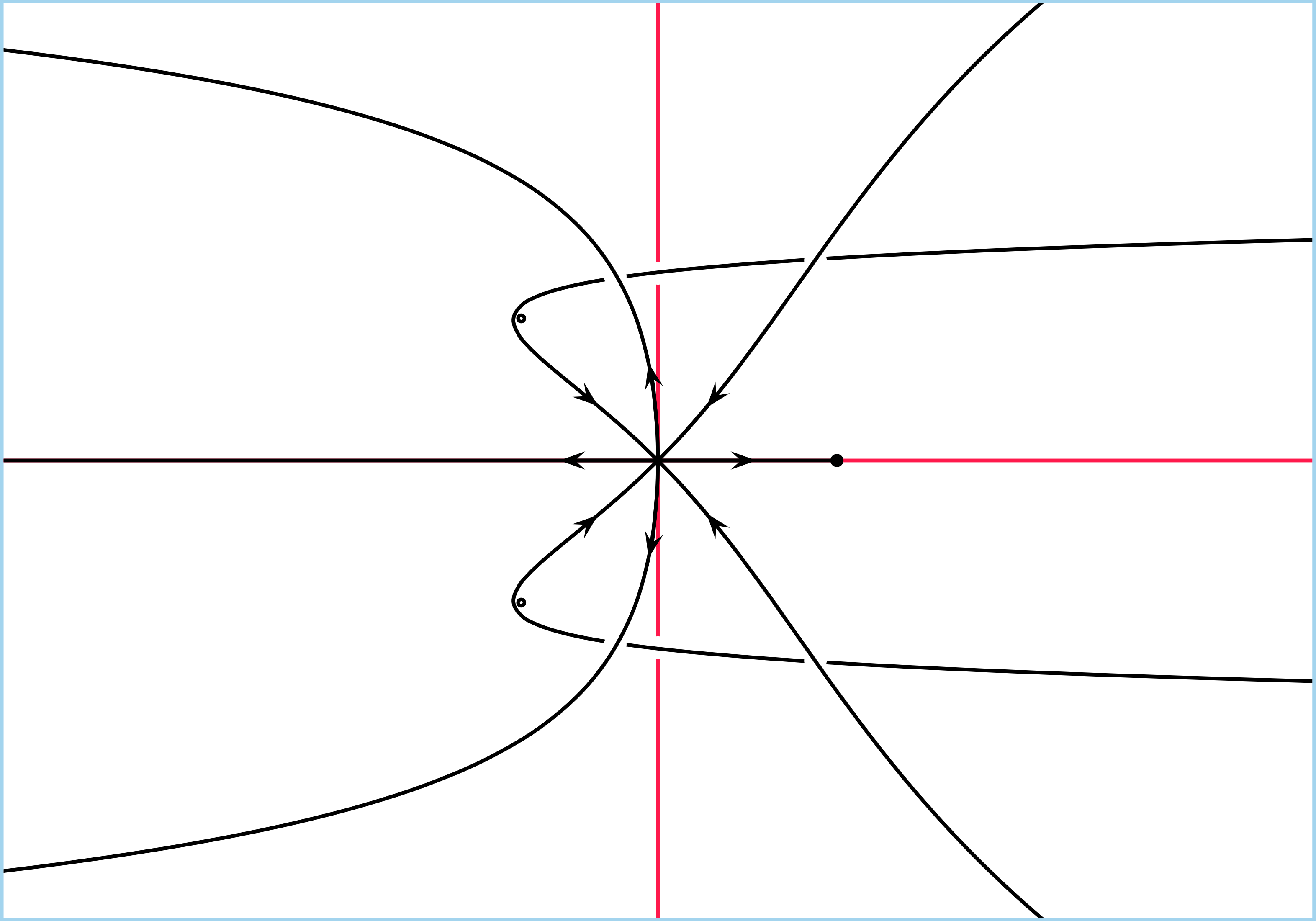
Hence

$$2s + 2 > p + 1$$

and the result follows.

Example of Daniel-Moore barrier: BDF3 method



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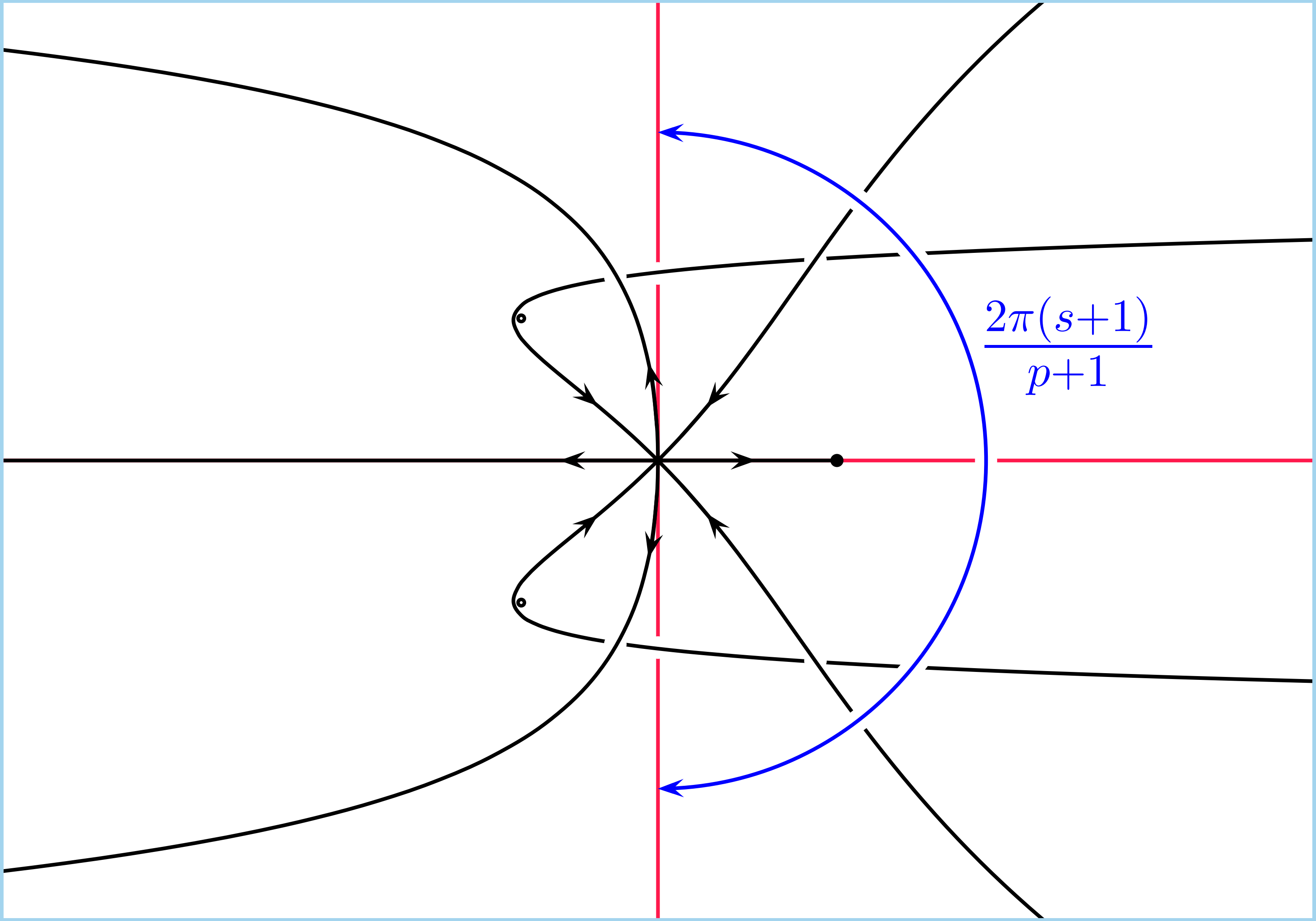

Example methods

We will give the following examples;

1. “Reuse” modifications of a Runge–Kutta method
2. Pseudo Runge-Kutta methods
3. ARK (“Almost Runge-Kutta”) methods
4. Hybrid methods
5. Cyclic composite methods

Reuse modifications of a Runge-Kutta method

From one of Kutta's fourth order families, we substitute $c_2 = -1$:

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & c_2 & & & \\
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1 & \frac{1}{2c_2} - 1 & -\frac{1}{2c_2} & 2 & \\
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We can interpret the abscissa at -1 as reuse of the derivative found as the beginning of the previous step.

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

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

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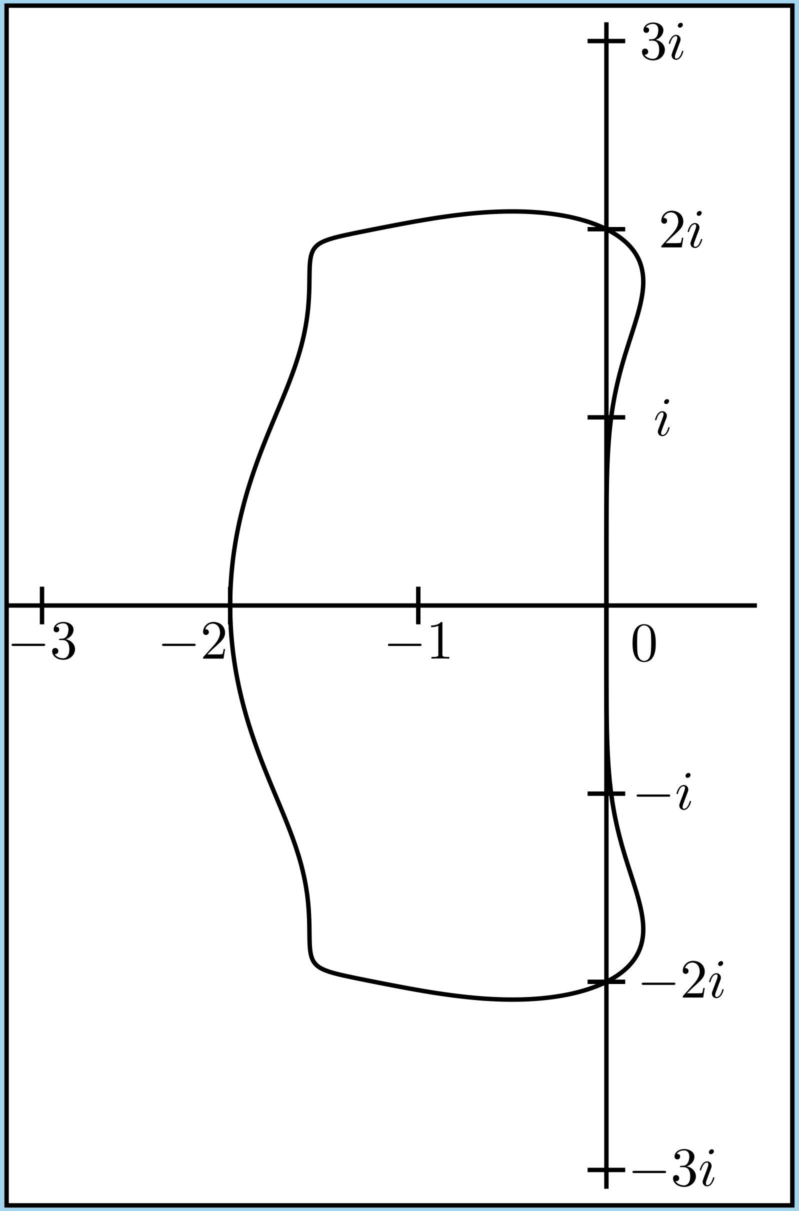
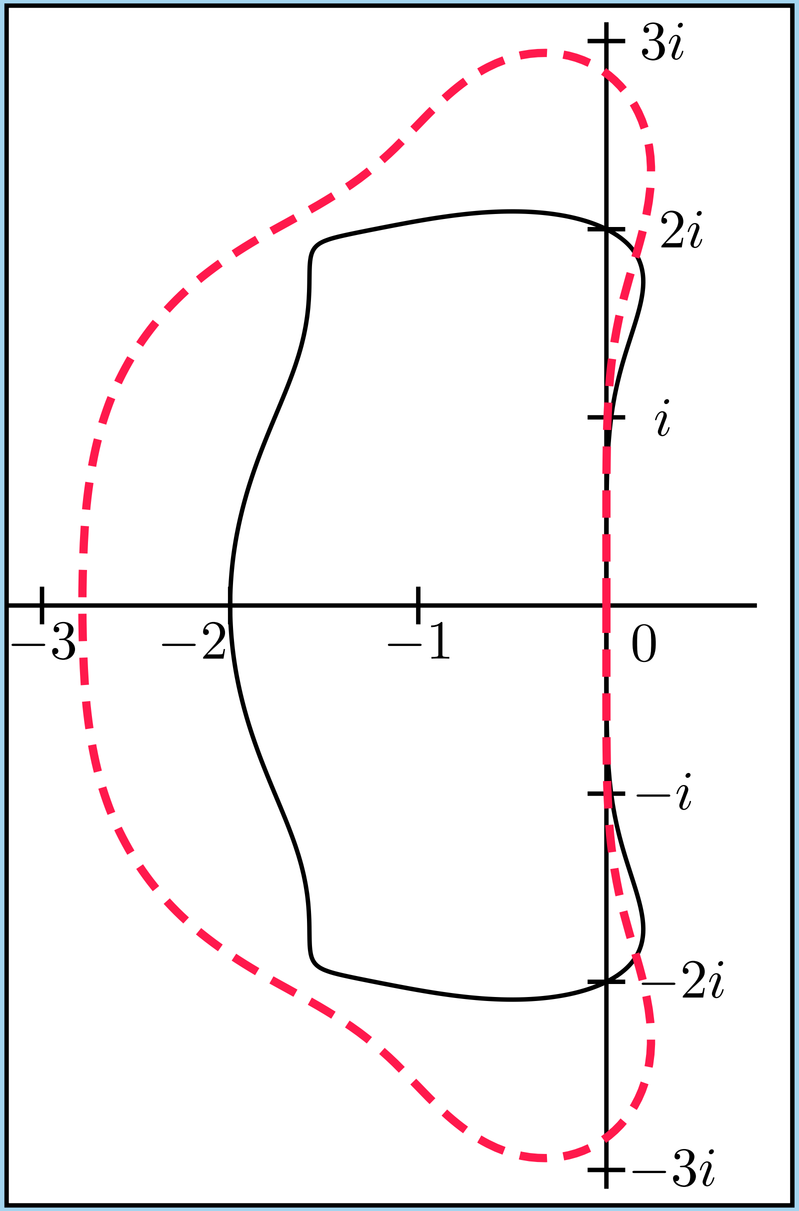
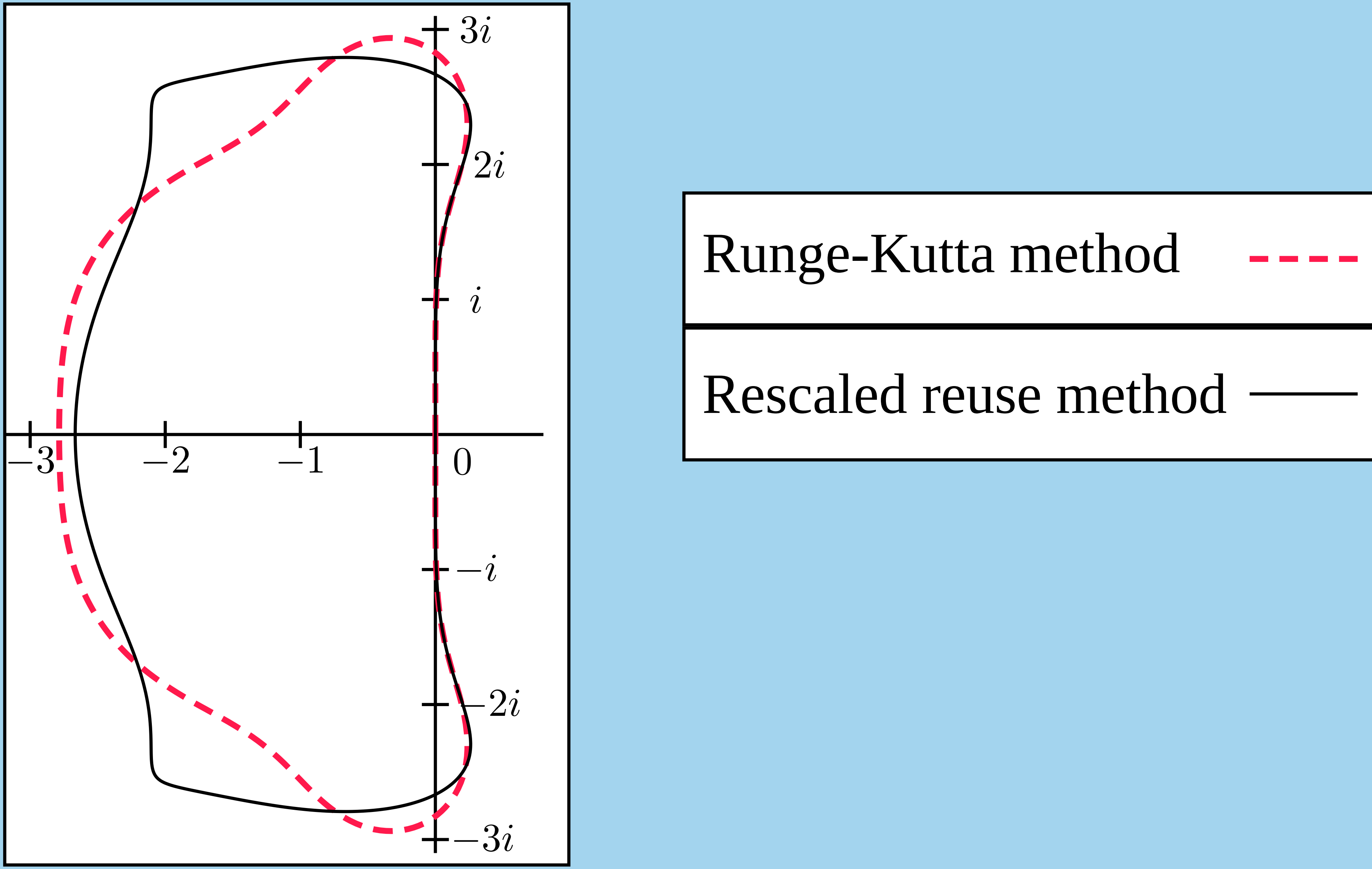
We can understand something about the behaviour of the new method by plotting its stability region.



“Reuse” method —



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


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

As a General Linear Method, the reuse method has the following matrices:

$$\left[\begin{array}{cc} A & U \\ B & V \end{array}\right] = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 0 \\ \frac{5}{8} & 0 & 0 & 1 & -\frac{1}{8} \\ -\frac{3}{2} & 2 & 0 & 1 & \frac{1}{2} \\ \hline \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{array}\right]$$

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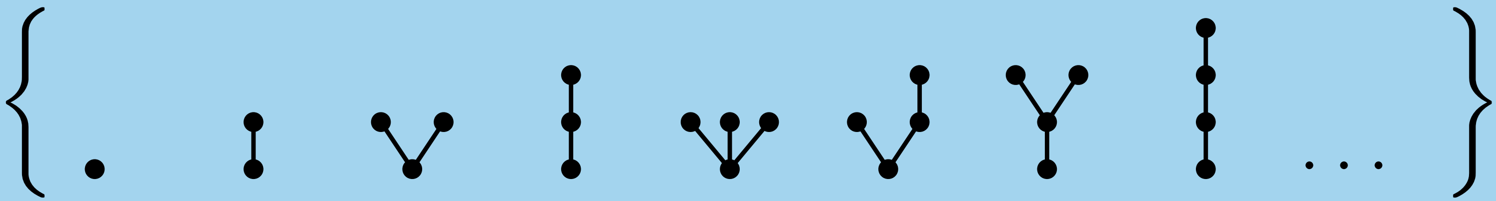

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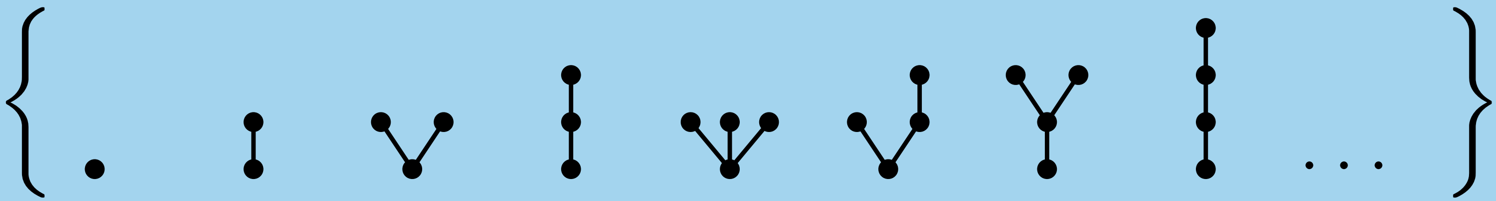

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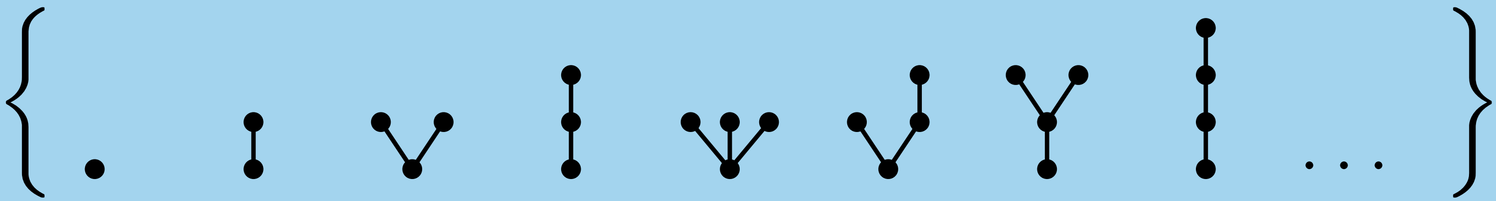

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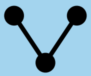
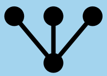
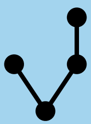
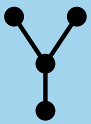
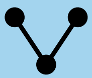
Expressions for Φ and γ are given on the next slide.

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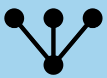
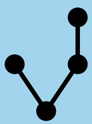
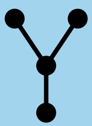
	$\sum b_i c_i^3$	4
	$\sum b_i c_i a_{ij} c_j$	8
	$\sum b_i a_{ij} c_j^2$	12
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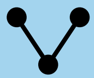
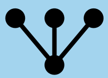
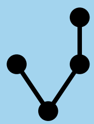
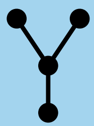
We will now introduce an additional column $\widehat{\Phi}(t)$

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

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A third order method can be constructed with two stages:

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

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

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

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

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

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

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

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Y_2 &= y_1^{[n-1]} - y_2^{[n-1]} - \tfrac{1}{2} y_3^{[n-1]} + 2hF_1, & 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 \\
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

$$y_1^{[n-1]} \approx y(x_{n-1}) \qquad y_1^{[n]} \approx y(x_n)$$

$$y_2^{[n-1]} \approx hy'(x_{n-1}) \qquad y_2^{[n]} \approx hy'(x_n)$$

$$y_3^{[n-1]} \approx h^2y''(x_{n-1}) \qquad y_3^{[n]} \approx h^2y''(x_n)$$

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

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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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The defining matrices are as follows:

$$\left[\begin{array}{cc} A & U \\ B & V \end{array}\right] = \left[\begin{array}{ccc|cccc} 0 & 0 & 0 & 0 & 1 & \frac{9}{8} & \frac{3}{8} \\ \frac{32}{15} & 0 & 0 & \frac{28}{5} & -\frac{23}{5} & -4 & -\frac{26}{15} \\ \frac{64}{93} & \frac{5}{31} & 0 & \frac{32}{31} & -\frac{1}{31} & \frac{4}{31} & -\frac{1}{93} \\ \hline \frac{64}{93} & \frac{5}{31} & 0 & \frac{32}{31} & -\frac{1}{31} & \frac{4}{31} & -\frac{1}{93} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array}\right]$$

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Methods like this exist up to $k = 7$ with order $2k + 1$.

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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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.

To put this method into general linear formulation, treat each pair of steps as a single step

$$\left[\begin{array}{cc} A & U \\ B & V \end{array}\right] = \left[\begin{array}{cc|ccc} 0 & 0 & 1 & 1 & 0 \\ \frac{3}{2} & 0 & 1 & \frac{3}{4} & \frac{3}{4} \\ \hline 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{array}\right]$$

The desirable stability of the cyclic method is seen from the fact that V has eigenvalues $\{1, 0, 0\}$.

Cycles of explicit methods can be constructed which overcome the first Dahlquist barrier.

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For example:

$$
\begin{aligned}
y_n &= -\frac{8}{11}y_{n-1} + \frac{19}{11}y_{n-2} \\
&\qquad + \frac{10}{11}hf_n + \frac{19}{11}hf_{n-1} + \frac{8}{11}hf_{n-2} - \frac{1}{33}hf_{n-3} \\
y_n &= \frac{449}{240}y_{n-1} + \frac{19}{30}y_{n-2} - \frac{361}{240}y_{n-3} \\
&\qquad + \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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Each of these methods has order 5 and each is unstable.

The corresponding cyclic method has perfect stability.

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

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Neither matrix is power-bounded but their product is nilpotent.
We omit the exercise of writing this method in GL form.

Methods with the RK stability property

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Although methods exist with this property with $r = s = p = q$, it is difficult to construct them.

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 matrics

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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or

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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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is known as a “doubly companion matrix” and has characteristic polynomial defined by

$$\det(I - zX) = \alpha(z)\beta(z) + O(z^{n+1})$$

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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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$$\Psi^{-1}X\Psi = \begin{bmatrix} \lambda & 0 & \cdots & 0 & 0 \\ 1 & \lambda & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda & 0 \\ 0 & 0 & \cdots & 1 & \lambda \end{bmatrix}$$

Construction of methods

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Apart from exceptional cases, (in which certain matrices are singular), we characterize the method with $r = s = p + 1 = q + 1$ by several parameters.

Parameters for construction of methods

- λ single eigenvalue of lower triangular matrix A

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

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where

$$C = \begin{bmatrix} 1 & c_1 & \frac{1}{2}c_1^2 & \cdots & \frac{1}{p!}c_1^p \\ 1 & c_2 & \frac{1}{2}c_2^2 & \cdots & \frac{1}{p!}c_2^p \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & c_s & \frac{1}{2}c_s^2 & \cdots & \frac{1}{p!}c_s^p \end{bmatrix}, \quad K^T = J = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Substitute these formulae for U and V into $BU = XV - VX + e_1\xi^T$ and, after some simplification, we find

$$\dot{B}C \begin{bmatrix} \beta_p \\ \beta_{p-1} \\ \vdots \\ \beta_1 \\ 1 \end{bmatrix} = \begin{bmatrix} \beta_{p-1} + \frac{1}{2!}\beta_{p-2} + \cdots + \frac{1}{p!} \\ \beta_{p-2} + \frac{1}{2!}\beta_{p-3} + \cdots + \frac{1}{(p-1)!} \\ \vdots \\ \beta_1 + \frac{1}{2!} \\ 1 \end{bmatrix},$$

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where $\dot{B}$ denotes the last p rows of B.

By taking account of the error constant prescribed for the method, we can find a similar formula involving the first row of B.

To simplify the construction we introduce a matrix $\widetilde{B} = \Psi^{-1}B$, assumed to be non-singular.
Because

$$\widetilde{B}A = (\lambda I + J)\widetilde{B},$$

we know that $\widetilde{B}$ is lower triangular.
Using the known value for $\widetilde{B}C \left[\begin{array}{ccccc} \beta_p & \beta_{p-1} & \cdots & \beta_1 & 1 \end{array}\right]^T$ and the fact that the $\rho(\dot{V}) = 0$, where

$$V = E - \Psi\widetilde{B}CK,$$

we can find a suitable value of $\widetilde{B}$.

Once $\widetilde{B}$ is known, we find the defining matrices for the method from

$$A = \widetilde{B}^{-1}(J + \lambda I)\widetilde{B},$$

$$U = C - ACK,$$

$$B = \Psi\widetilde{B},$$

$$V = E - BCK.$$

Collaboration with Will Wright

When two people work together, it is often hard to untangle the contributions that each makes.

Will's contributions include, but are not confined to,

- Showing how to extend the original formulation of stiff IRKS methods to explicit non-stiff methods.
- Showing how to use doubly companion matrices in the formulation of IRKS methods.
- Relating the principal error coefficients to the β values.

Example methods

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 for IRKS methods

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- Initial stepsize
- Starting method

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

If r is constrained to lie in an interval $I = [r_{\min}, r_{\max}]$ 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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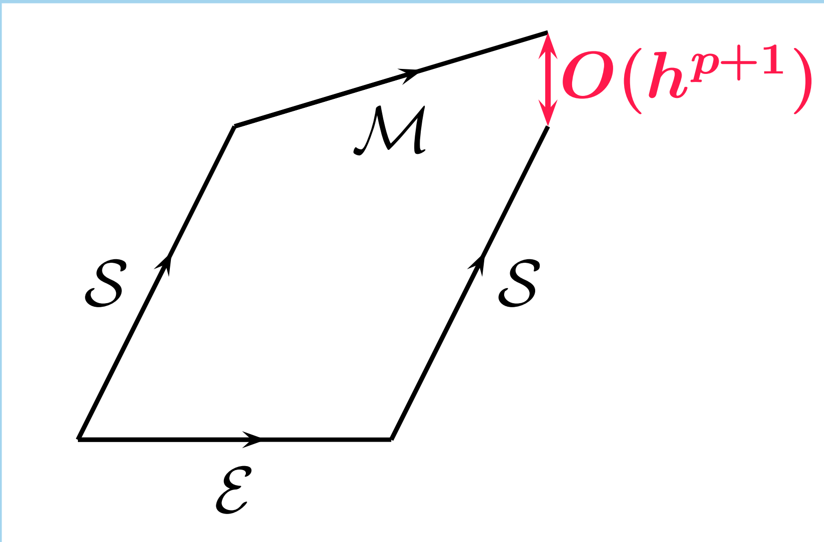
We introduce these ideas in the context of the underlying one-step method.

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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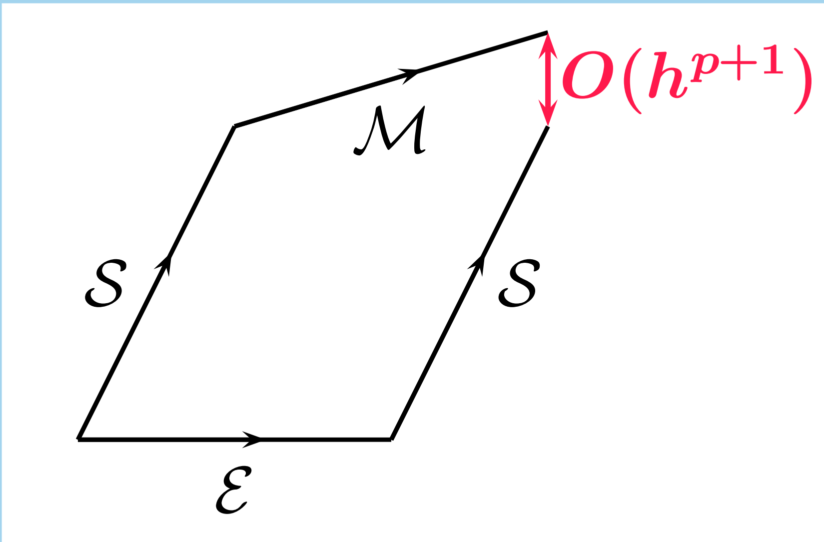

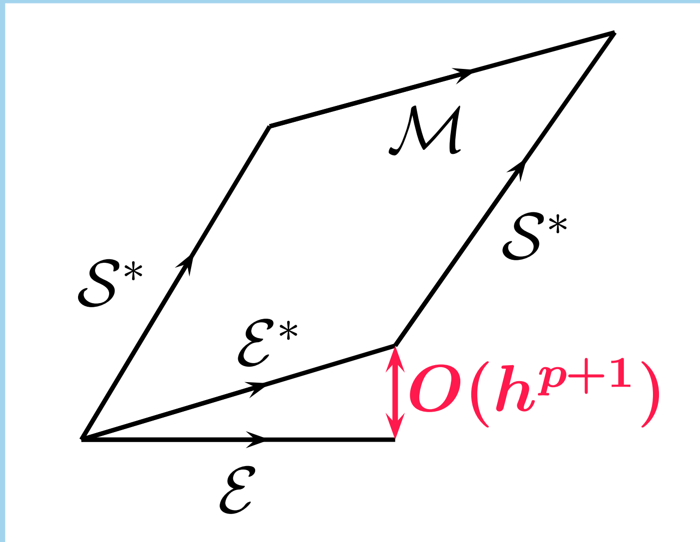

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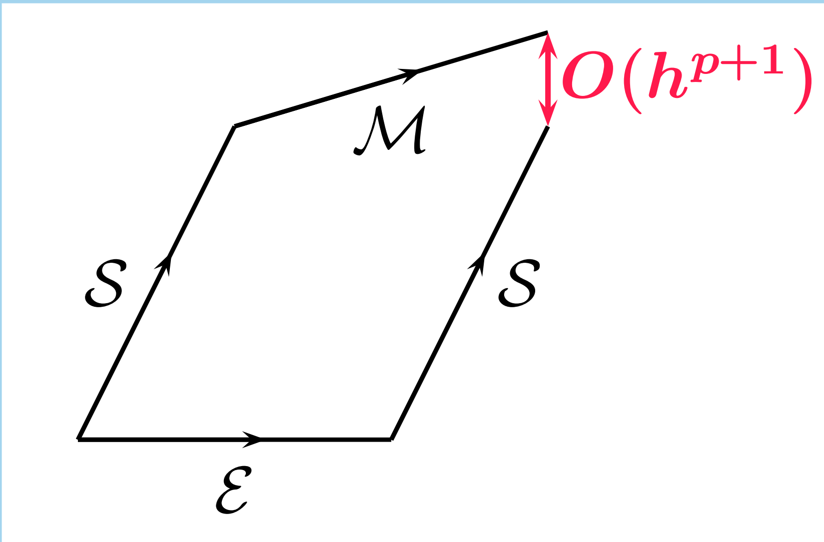

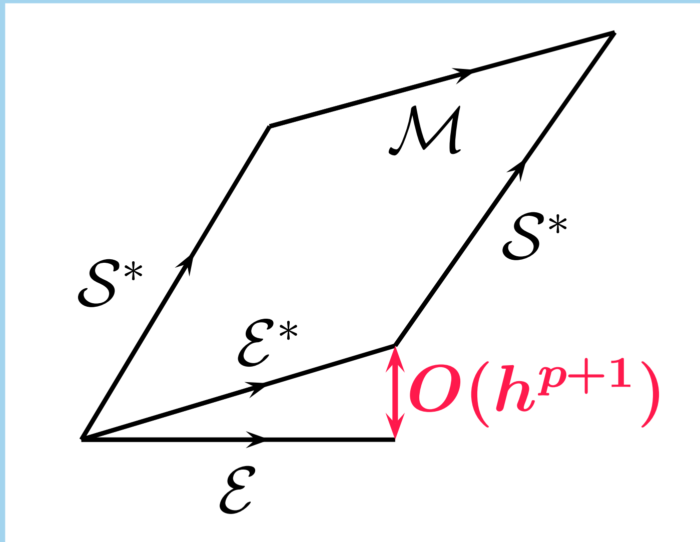

In the modified diagram, the perturbed starting method, shown as $\mathcal{S}^*$, is chosen to obtain a commutative diagram if $\mathcal{E}$ is replaced by the underlying one-step method $\mathcal{E}^*$.

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

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

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

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