Towards practical general linear methods

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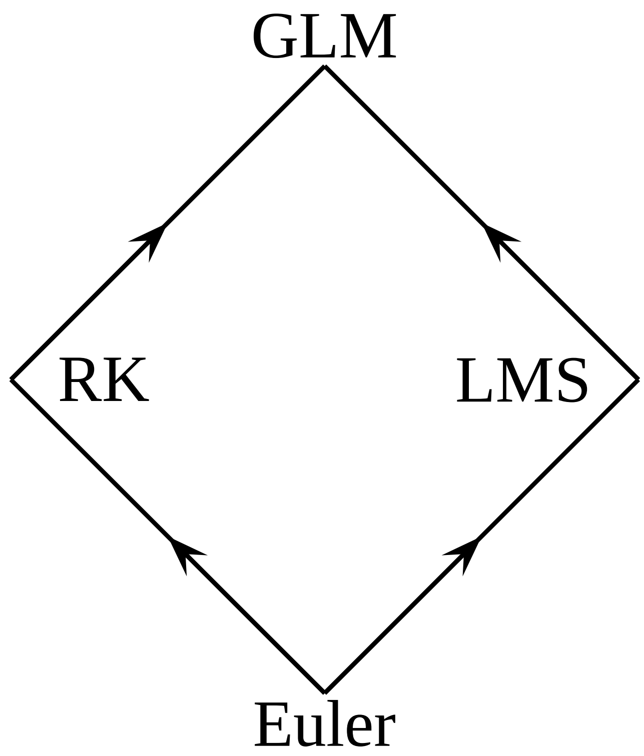

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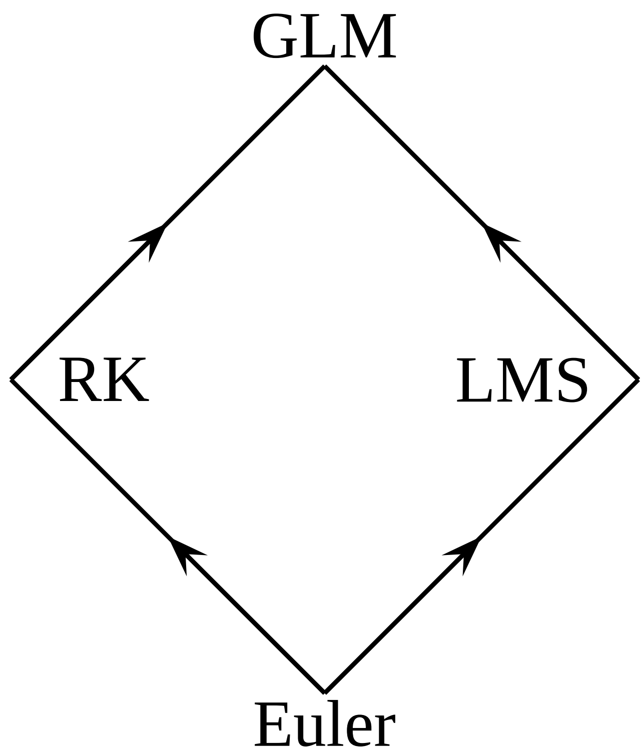

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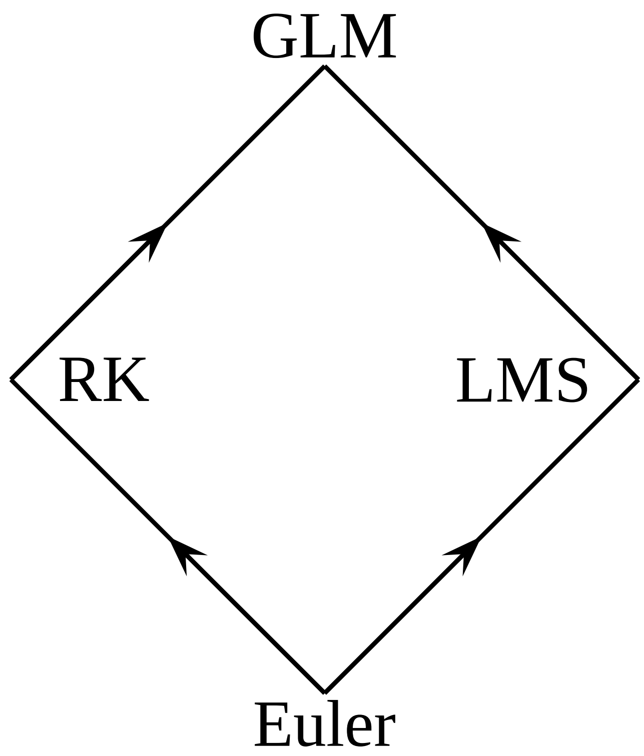

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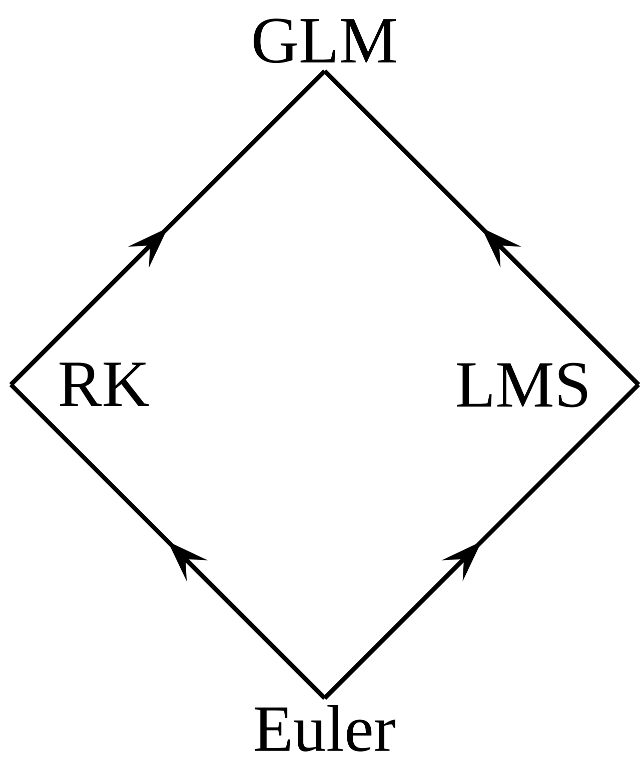
A second characteristic feature is that, within the step, s stages are computed, together with the corresponding s stage derivatives.



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

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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

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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 $\mathcal{F} \circ \mathcal{S} = \text{id}$.

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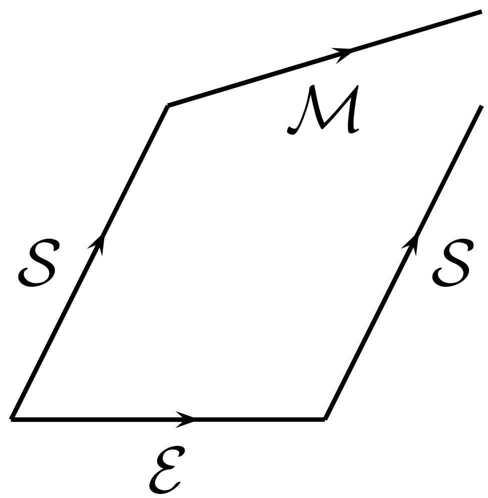

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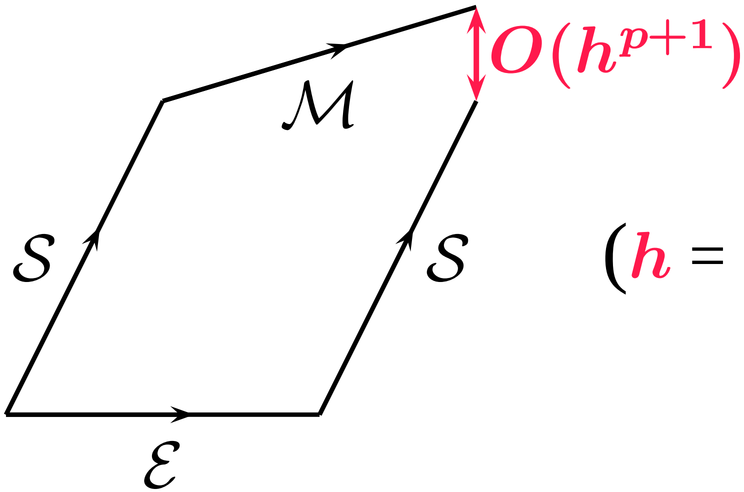

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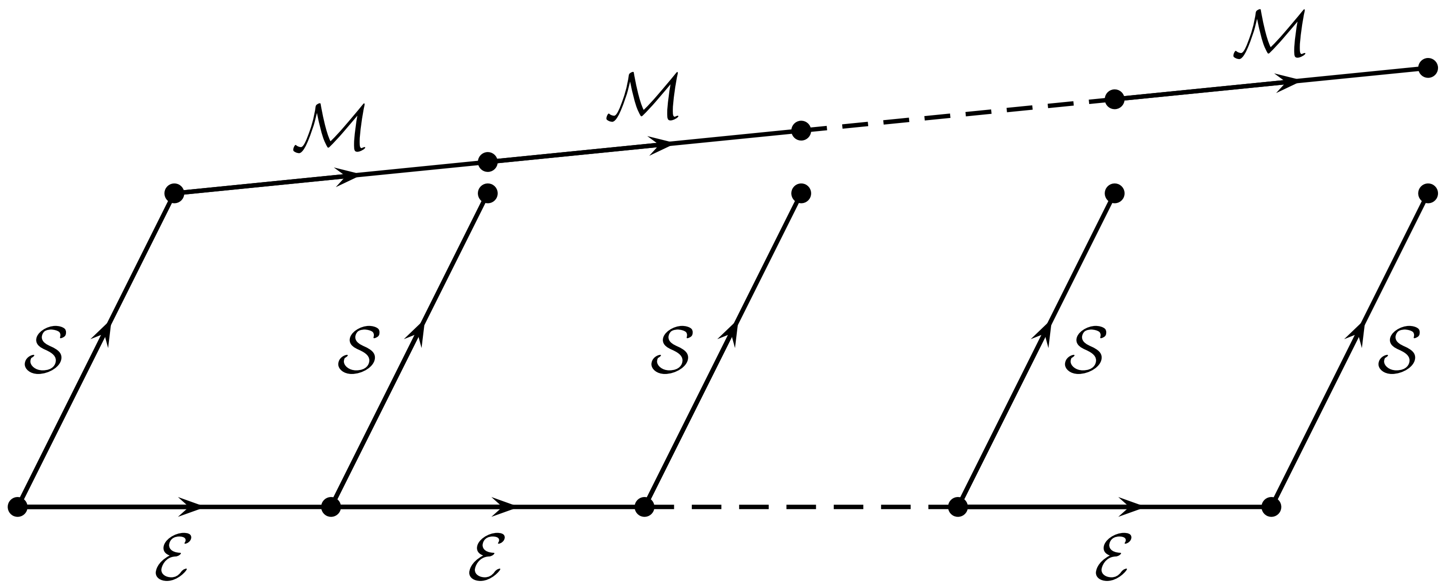

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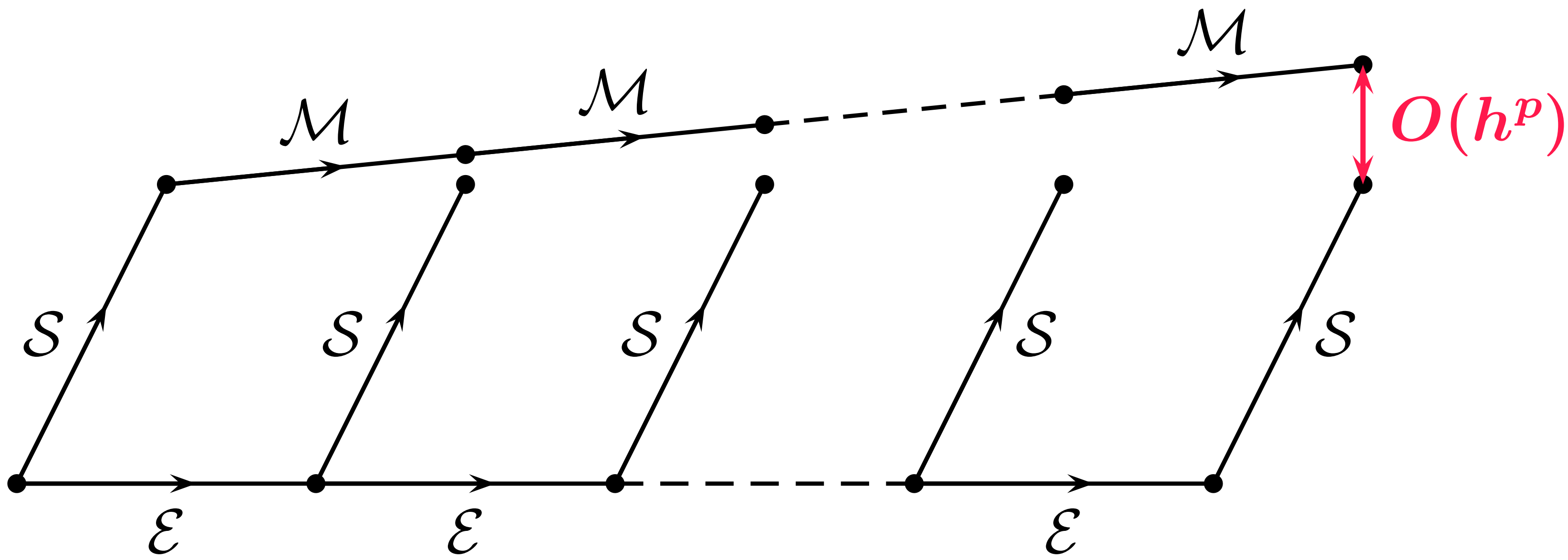

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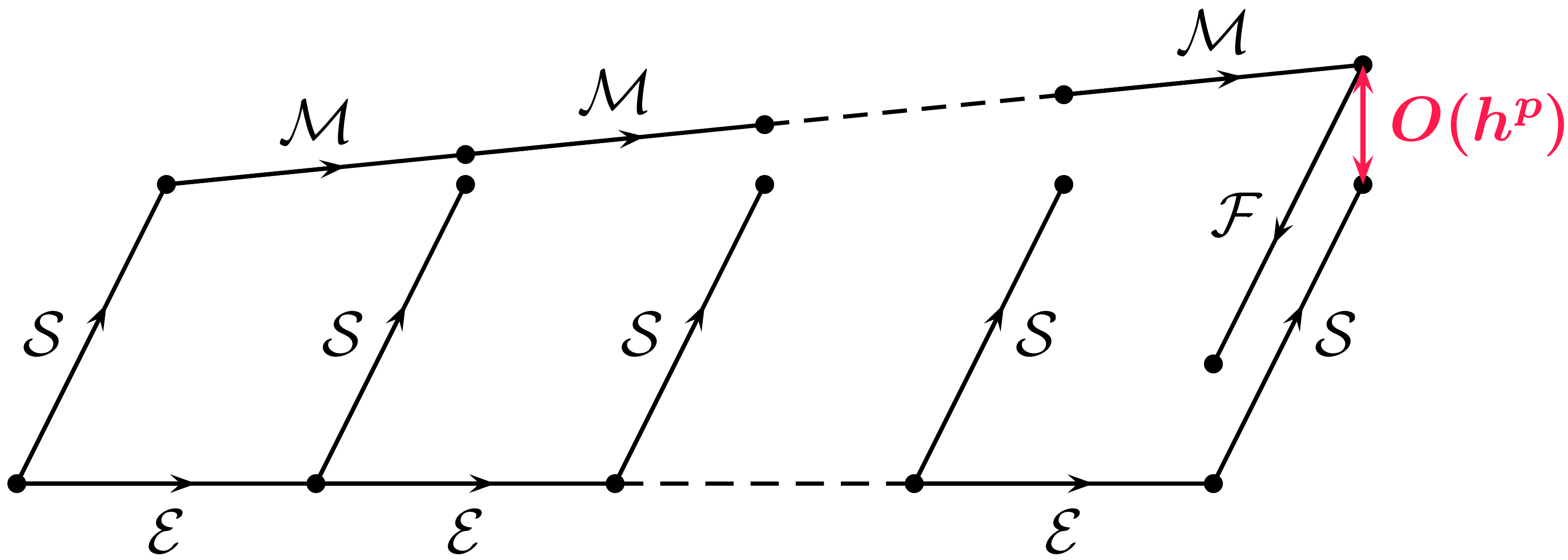

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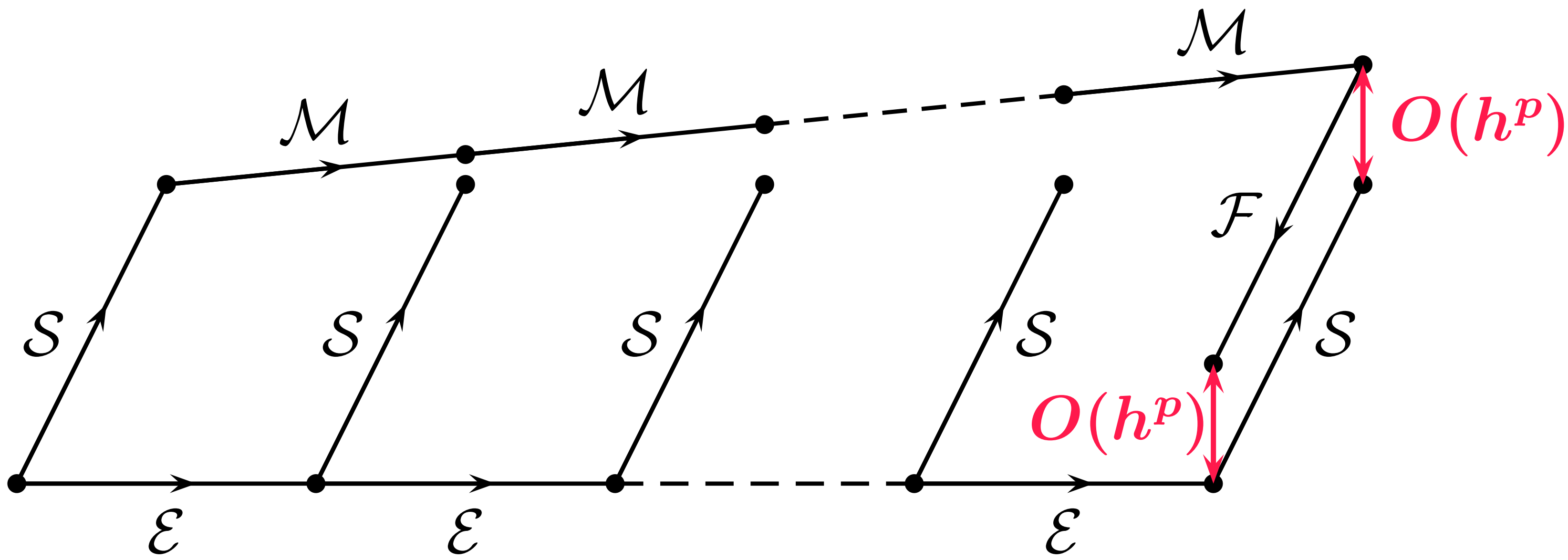

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where it is assumed the input is

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

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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

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We also define the "stability function" as

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

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

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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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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".

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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.

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For such methods, V has the form

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which has all except one of its eigenvalues zero. The non-zero eigenvalue has the role of stability function

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$$BA = XB, \quad BU = XV - VX + e_1\xi^T, \quad \rho(\dot{V}) = 0$$

It can be shown that, for such methods, the stability matrix satisfies

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

which has all except one of its eigenvalues zero. The non-zero eigenvalue has the role of stability function

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

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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

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

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

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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 $\widetilde{B}C \begin{bmatrix} \beta_p & \beta_{p-1} & \cdots & \beta_1 & 1 \end{bmatrix}^T$ 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

$$
\begin{aligned}
A &= \widetilde{B}^{-1}(J + \lambda I)\widetilde{B}, \\
U &= C - ACK, \\
B &= \Psi \widetilde{B}, \\
V &= E - BCK.
\end{aligned}
$$

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

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

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

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 $r_1, r_2, \ldots, r_n \in I$.

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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where

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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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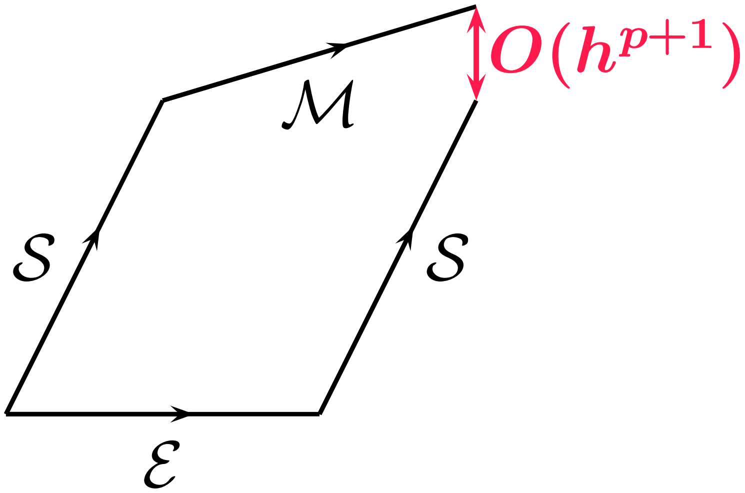
In particular we need to consider the effect of variable h on the error constants in incoming approximations.

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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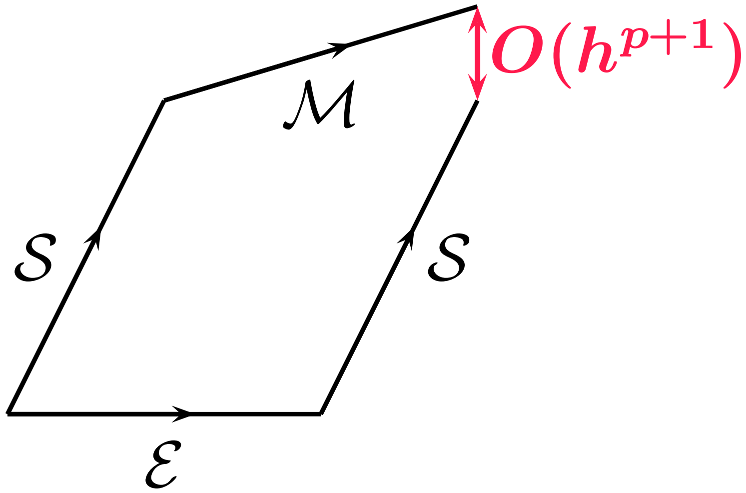

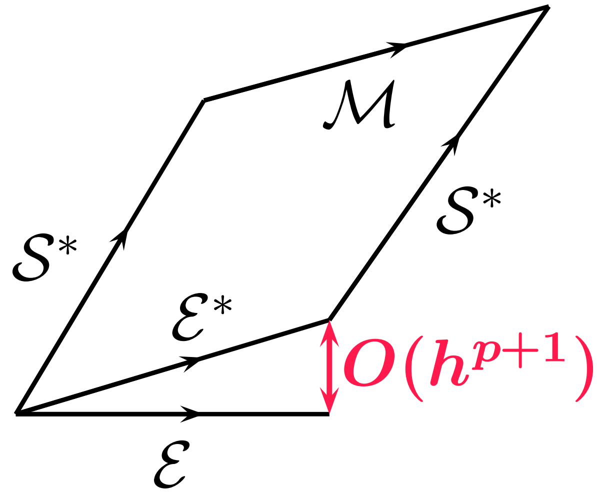

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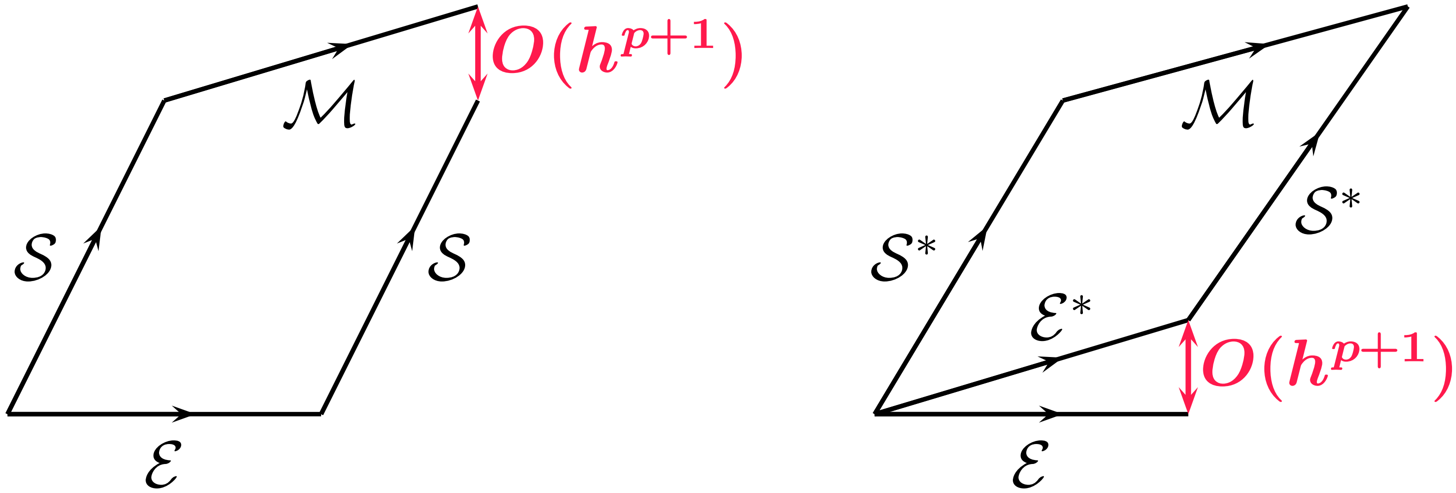

In the modified diagram, the perturbed starting method, shown as $\mathcal{S}^*$, is chosen to obtain a commutative diagram if $\mathcal{E}$ is replaced by the underlying one-step method $\mathcal{E}^*$.

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

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

then $\cdots$

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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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- 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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