Theory and Practice ;
Pride and Precudice

Pure Mathematical Theory

Theory of integration, Theory of differential equations,
Unsolved integrals and diff. eqs., Unsolvable equations
Problems from Physics, Chemistry etc.

Construction of Numerical Methods

Quadrature formulas, Runge-Kutta methods,
Multistep methods, Extrapolation methods
Linear Algebra, Iteration methods etc.

↓

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Theory of integration, Theory of differential equations,
Unsolved integrals and diff. eqs., Unsolvable equations
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Theory of Numerical Methods
Stability theory, Order theory,
Convergence theory, Order Barriers
Contractivity, A-stability, B-stability, etc.

↓

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Indeed, since my first academic steps, my scientific guideline has been and still is that ‘good’ mathematical theory should have a palpable influence on the construction of algorithms, while ‘good’ algorithms should be as firmly as possible backed by a transparently underlying theory. Only on such a basis, algorithms will be efficient enough . . . (P. Deuflhard 2004)

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Theory without practice cannot survive and dies as quickly as it lives. (Leonardo da Vinci 1452-1519)

He who loves practice without theory is like the sailor who boards ship without a rudder and compass and never knows where he may be cast. (Leonardo da Vinci 1452-1519)

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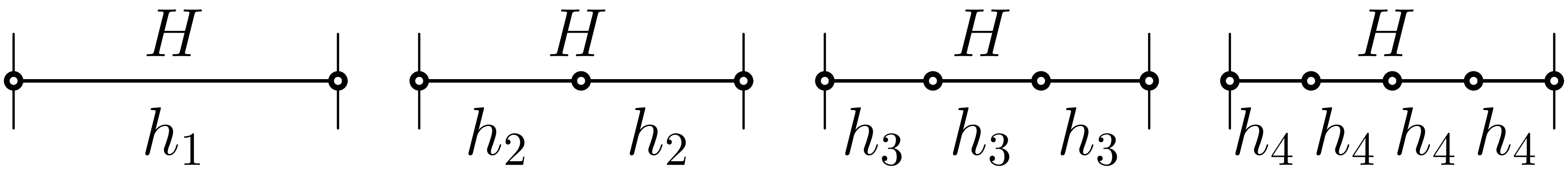
(For Saint Boniface, see the Conclusion.)

1. Convergence Theory of Extrapolation Methods.

$$n_1 < n_2 < n_3 < \ldots \quad \Rightarrow \quad h_1 > h_2 > h_3 > \ldots, \qquad h_i = H/n_i$$



$$y_{h_i}(x) =: T_{i,1} = y(x) - e_1 h_i - e_2 h_i^2 - \ldots \quad \Rightarrow \quad \begin{array}{cccc} T_{11} & & & \\ T_{21} \to & T_{22} & & \\ T_{31} \to & T_{32} \to & T_{33} & \\ T_{41} \to & T_{42} \to & T_{43} \to & T_{44} \end{array}$$

Theorem (Laurent 1963, Bauer–Rutishauser–Stiefel 1963)

$$\liminf_{i\to\infty} \frac{h_{i+1}}{h_i} \le \alpha < 1 \qquad \Rightarrow \qquad \lim_{k\to\infty} T_{kk} = \lim_{k\to\infty} T_{k1}.$$

Examples.

Romberg sequence (1955) : $1, 2, 4, 8, 16, 32, 64, 128, 256, 512,$

Bulirsch sequence : $1, 2, 3, 4, 6, 8, 12, 16, 24, 32, 48, 64 \ldots$

Mein Verzicht auf das Restglied war leichtsinnig. F.L. Bauer bewies es mit der Euler-Maclaurin-Summenformel *mit* Restglied. (W. Romberg, handwritten notice to P. Dd., 1979)

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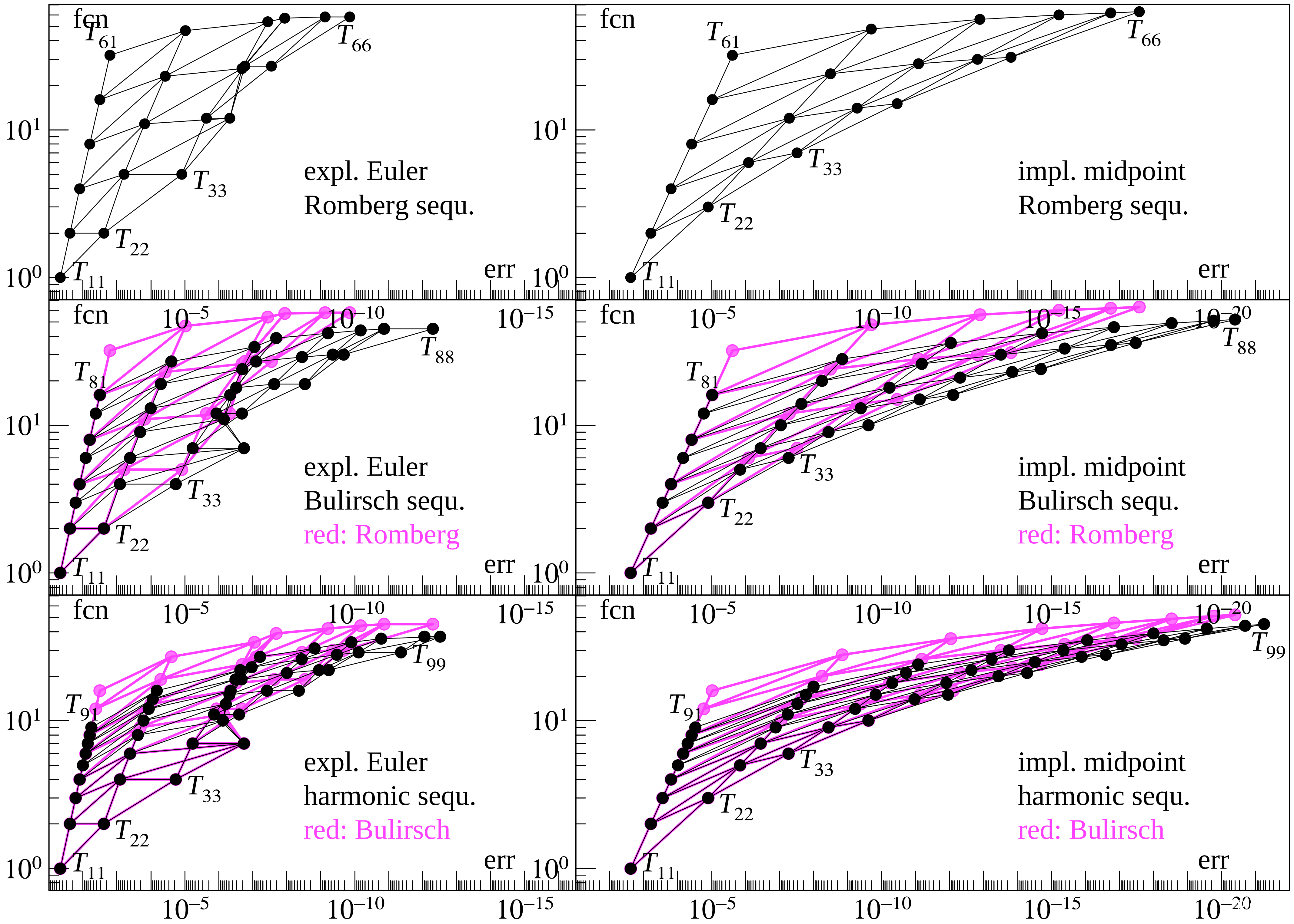
But the harmonic sequence : $1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, \ldots$

(Deuflhard 1983) is numerically the best ! (“Surprisingly, the harmonic sequence $\mathcal{F}_H$ occurs”, code DIFEX1).

Numerical Example.



fcn
err
expl. Euler
Romberg sequ.
impl. midpoint
Romberg sequ.
expl. Euler
Bulirsch sequ.
red: Romberg
impl. midpoint
Bulirsch sequ.
red: Romberg
expl. Euler
harmonic sequ.
red: Bulirsch
impl. midpoint
harmonic sequ.
red: Bulirsch

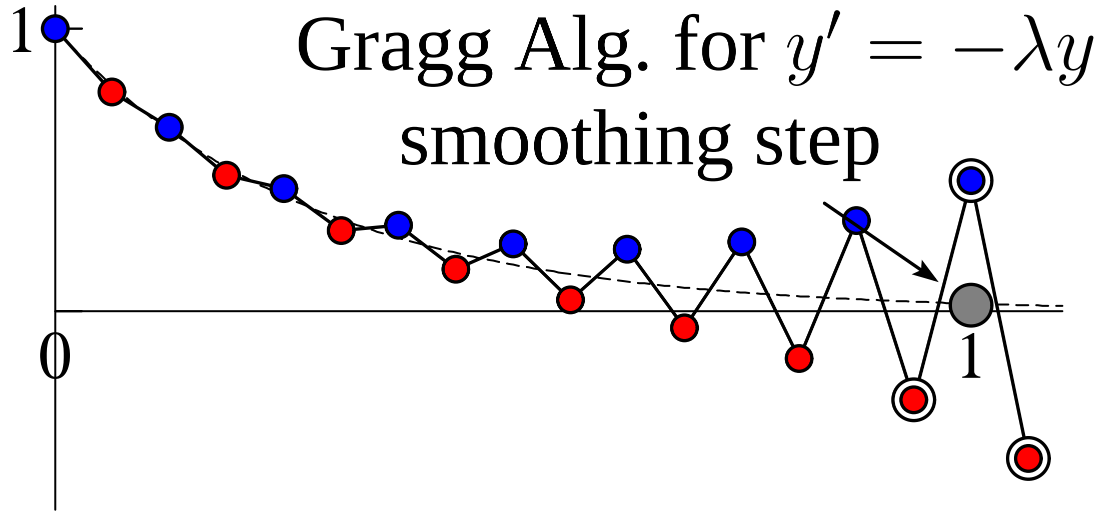
Gragg Algorithm (Gragg 1964).

$$y_1 = y_0 + hf(x_0, y_0)$$

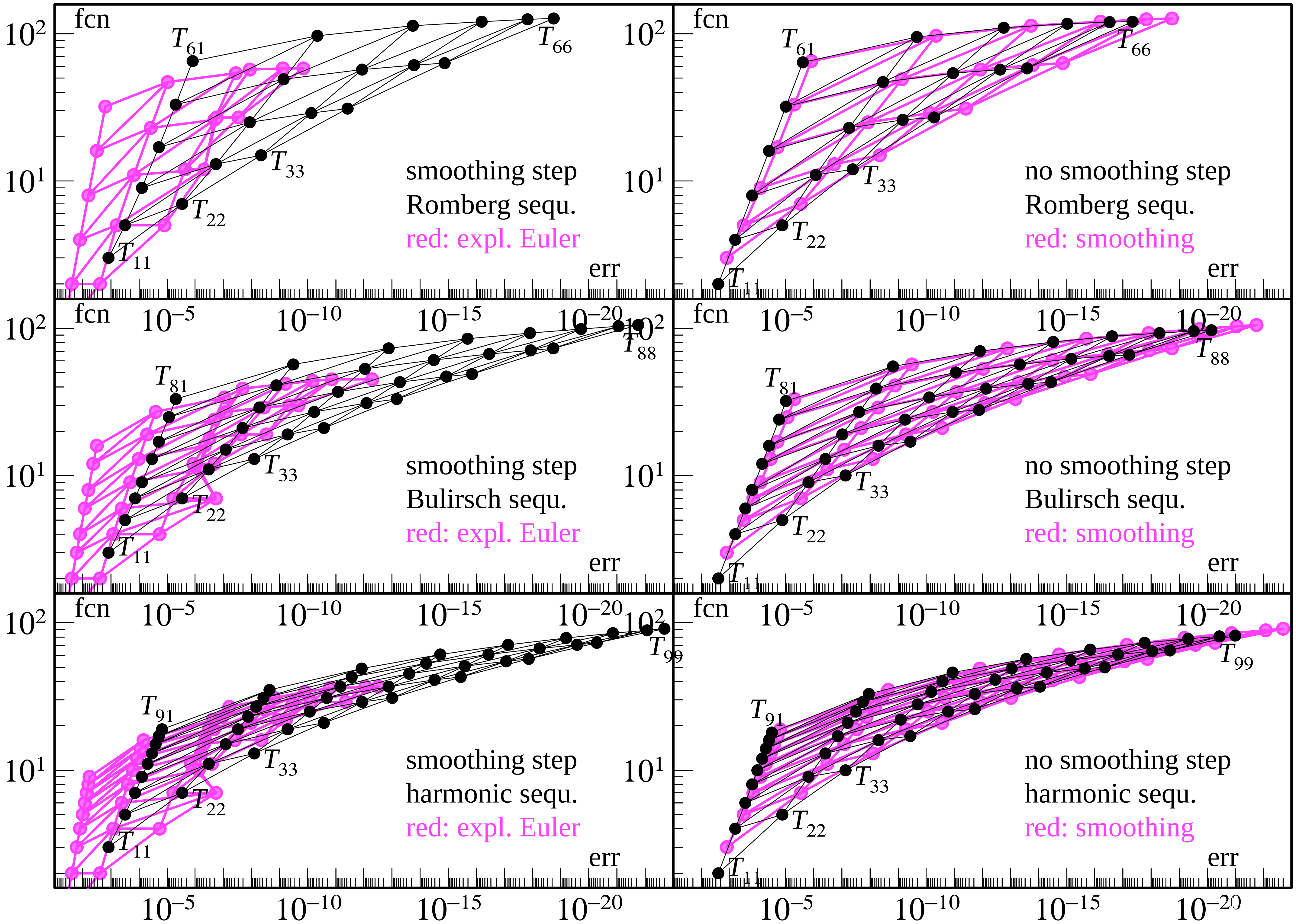
$$y_{i+1} = y_{i-1} + 2hf(x_i, y_i)$$

$$S_h = \frac{1}{4}\left(y_{2n-1} + 2y_{2n} + y_{2n+1}\right)$$

(smoothing step)



Is the smoothing step necessary ? (Shampine & Baca 1983).
H.–N.–W. (93) : “ However, since the method is anyway followed by extrapolation, this step is not of great importance . . . the differences are seen to be tiny.”



fcn
err
smoothing step
Romberg sequ.
red: expl. Euler
no smoothing step
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no smoothing step
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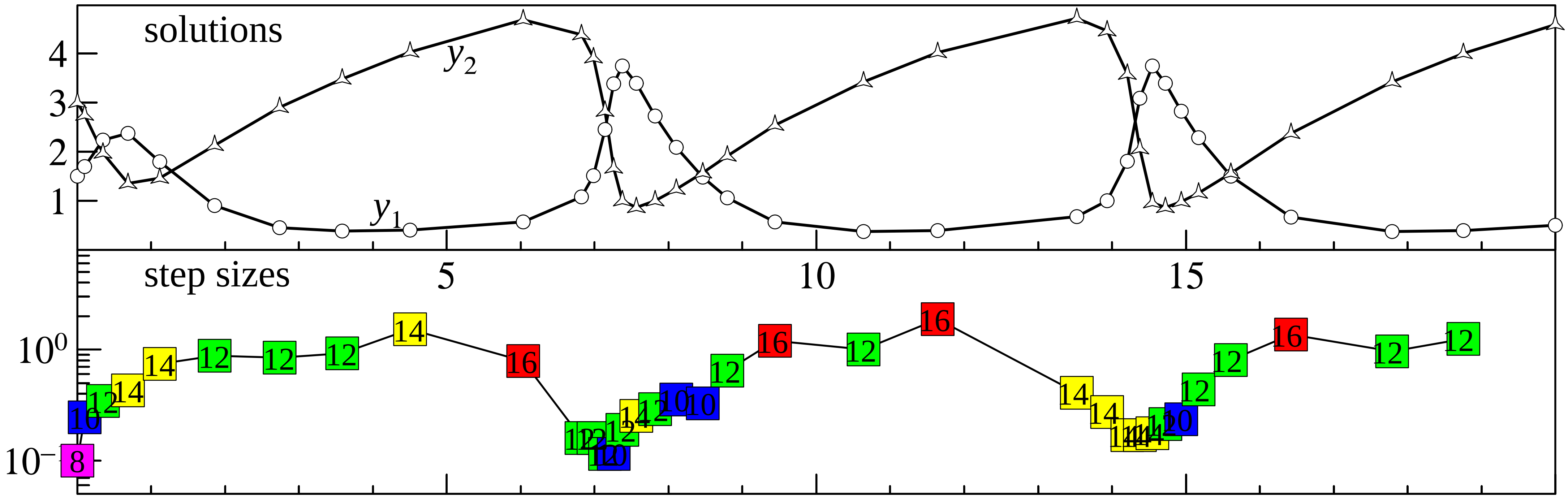
smoothing step
harmonic sequ.
red: expl. Euler
no smoothing step
harmonic sequ.
red: smoothing
T_{11}
T_{22}
T_{33}
T_{61}
T_{66}
T_{81}
T_{88}
T_{91}
T_{99}
10^{1}
10^{2}
10^{-5}
10^{-10}
10^{-15}
10^{-20}

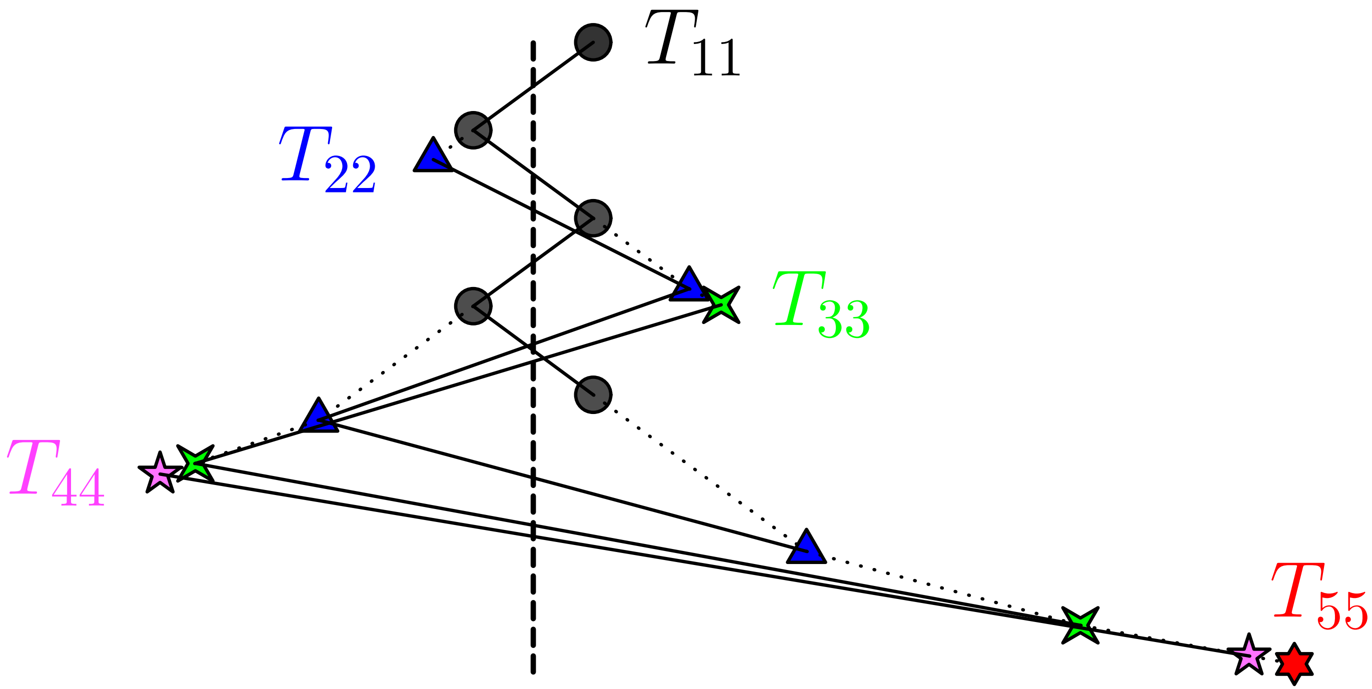
Order and Stepsize Control.

- Bulirsch–Stoer (1966): use of interpolation error formula ;
- Deuflhard (1983): Work min. + Information Theor. Model ;
- H.–N.–W. (1987): Work minimization only (ODEX) ;



Rounding Errors

Since the sensitivity to round-off of the extrapolation process increases with the order of extrapolation . . . the program computes only $T_k^{(i)}$ for $k \leq 6$ which has proved reasonable for machine accuracy of 40 bits . . . . (Bulirsch–Stoer, *Num. Math.* 1966, p. 8)



Clever trick: T. Fukushima (*Astron. J.* 1996), extrapolating the *increments* and not the T-values.

Theory of rational extrapolation (Bulirsch–Stoer 1964).

> Beispiele zeigen die Überlegenheit dieses Verfahrens, das . . . in allen untersuchten Fällen nicht schlechter, meistens sogar erheblich besser konvergierte als entsprechende Polynom-Verfahren. (Bulirsch–Stoer, *Num. Math.* 1963, p. 414)

> Moreover, polynomial extrapolation turned out to be slightly preferable to rational extrapolation . . .. (Deuflhard, *Num. Math.* 1983, p. 413)

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2. Order Theory of Runge-Kutta Methods

> Not being a pure mathematician I was never quite sure of what I was talking about. It is difficult to keep a cool head when discussing the various derivatives of one variable with respect to another and I think this would justify a solid attack by a pure mathematician to put everything on a sound basis. I did however see the one-one correspondence between the trees and the "basic operators" . . . (Dr. S. Gill, in a discussion 1956)

Classical Runge-Kutta Theory

- order 2 and 3 by Runge (1895) and Heun (1900) ;
- order 4 by Kutta (1901) ;
- order 5 by Nyström (1925) ;
- order 6 by Hut'a (1956) ;

hopeless for higher orders.

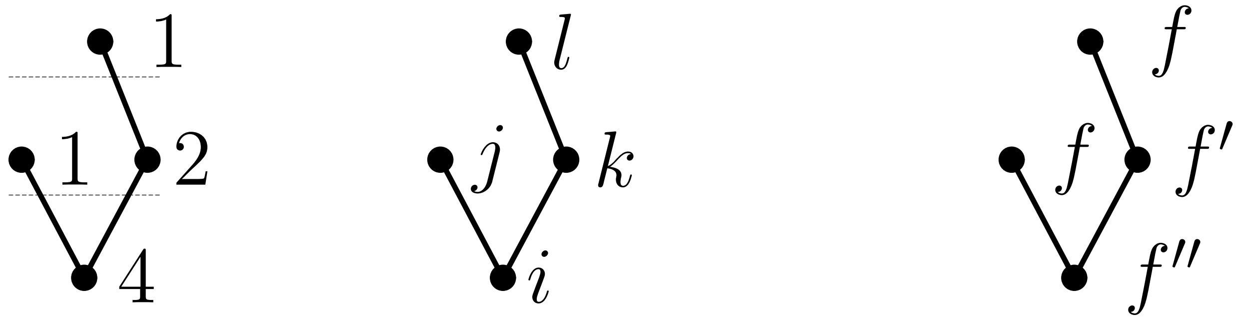
Butcher's First Theorem (Butcher 1963).

Numerical solution :

$$y_1 = y_0 + \ldots + \frac{h^4}{4!}(\ldots + \text{CE} + \ldots) + \ldots$$

$$\text{CE} = 3 \cdot \quad 4 \cdot 2 \quad \cdot \sum_{i,j,k,l} b_i\, a_{ij}\, a_{ik}\, a_{kl} \quad \cdot f''(f, f'(f))_0$$

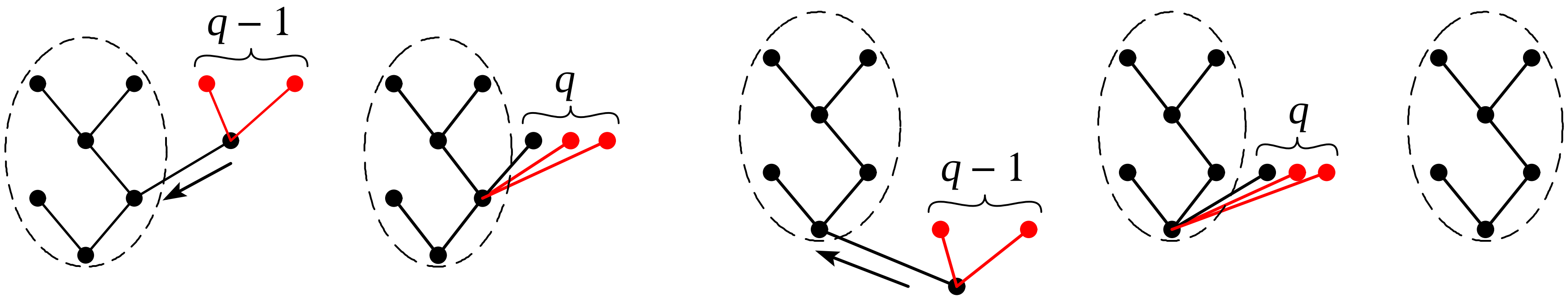
$\uparrow \qquad\qquad\qquad \uparrow \qquad\qquad\qquad \uparrow$



$\Rightarrow$ **order conditions** $\qquad \displaystyle\sum_{i,j,k,l} b_i\, a_{ij}\, a_{ik}\, a_{kl} = \frac{1}{4 \cdot 2}$

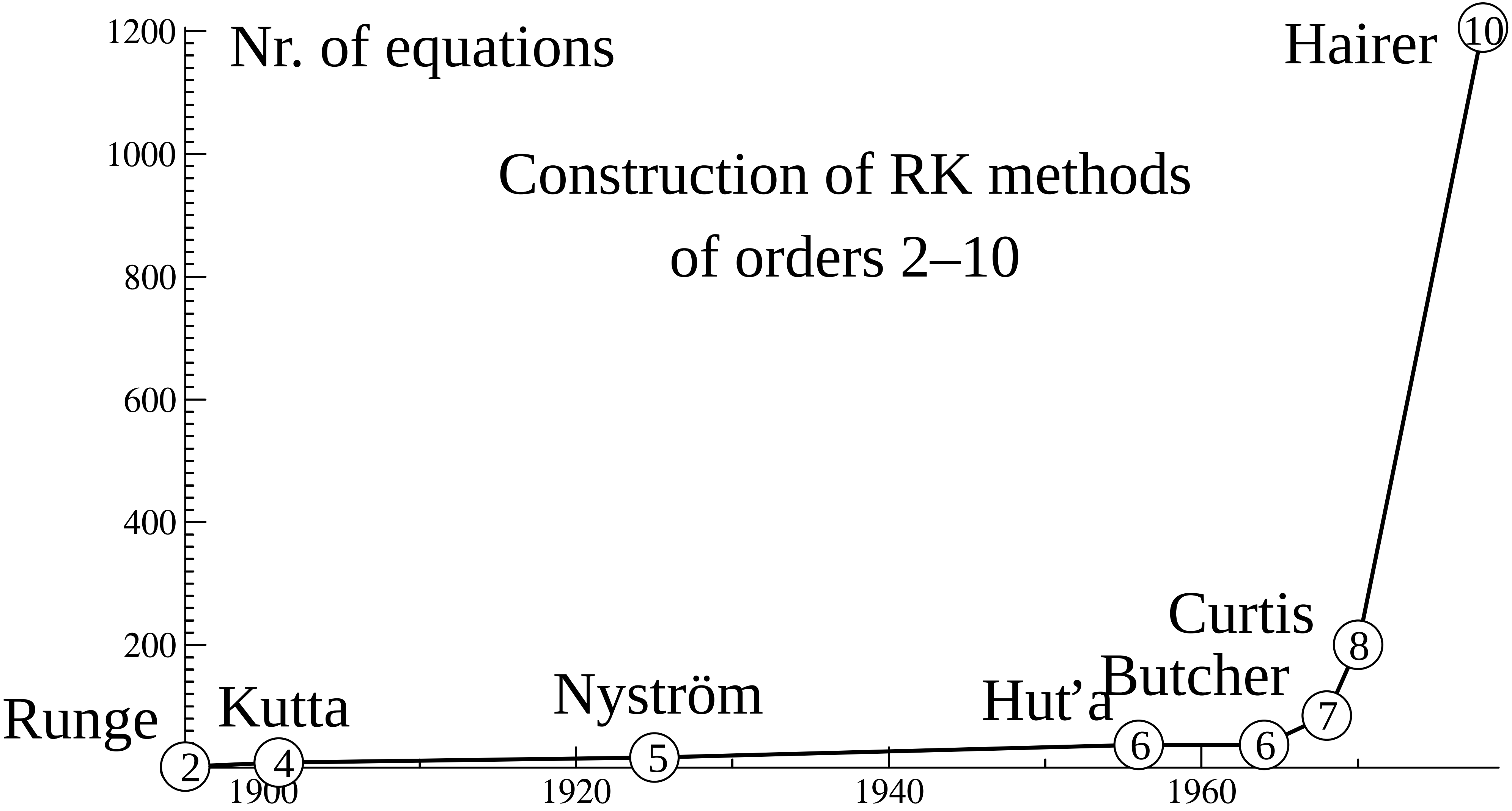
$$\sum_{i,j,k,l} b_i \, a_{ij} \, a_{ik} \, a_{kl} = \sum_{i,k} b_i \, c_i \, a_{ik} \, c_k = \frac{1}{4 \cdot 2}$$

Simplifying assumptions :



$$\sum_{j=1}^{s} a_{ij} c_j^{q-1} = \frac{c_i^q}{q} \qquad\qquad \sum_{i=1}^{s} b_i c_i^{q-1} a_{ij} = \frac{b_j}{q} \left(1 - c_j^q\right)$$

Achievements :



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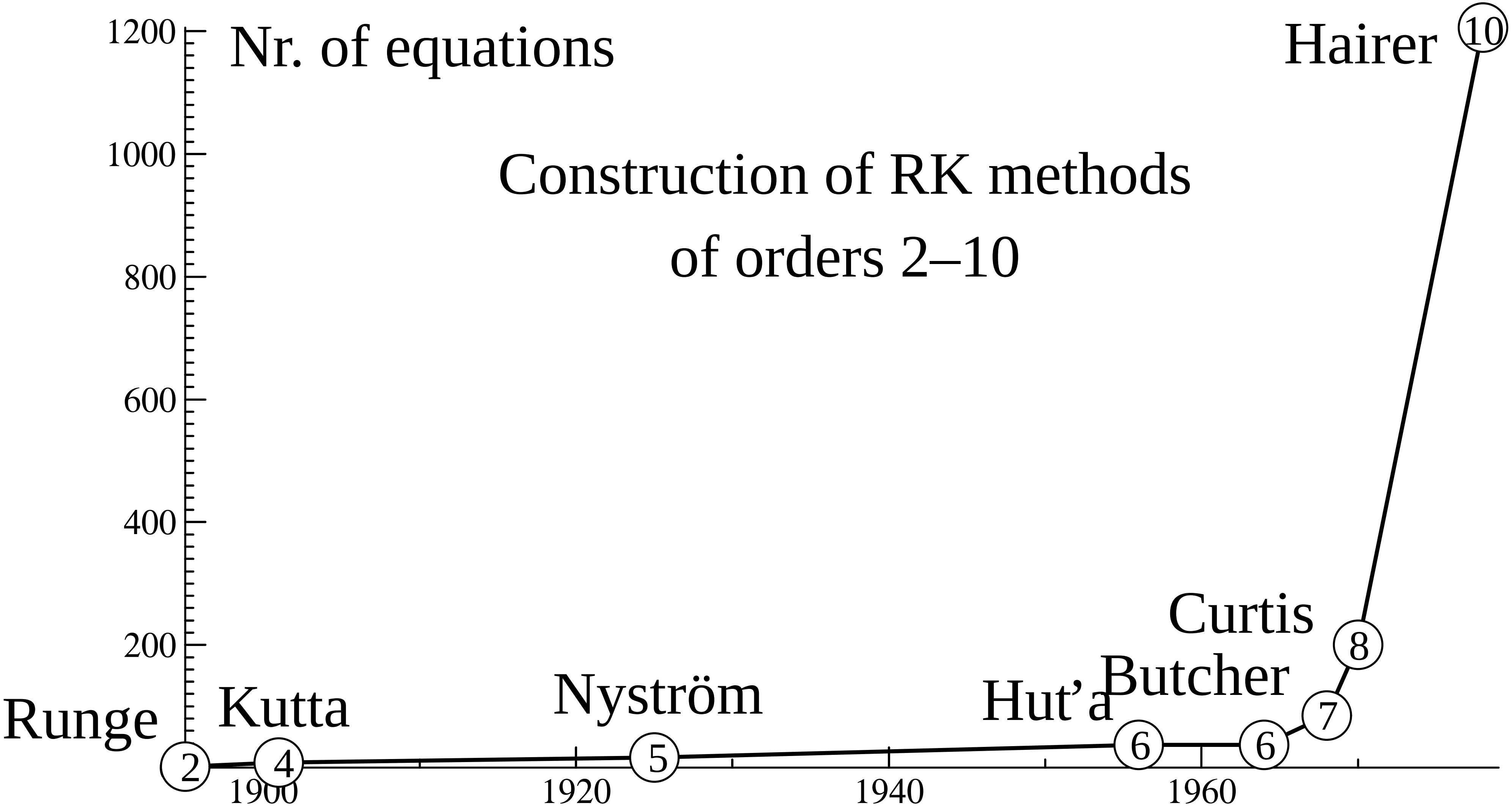


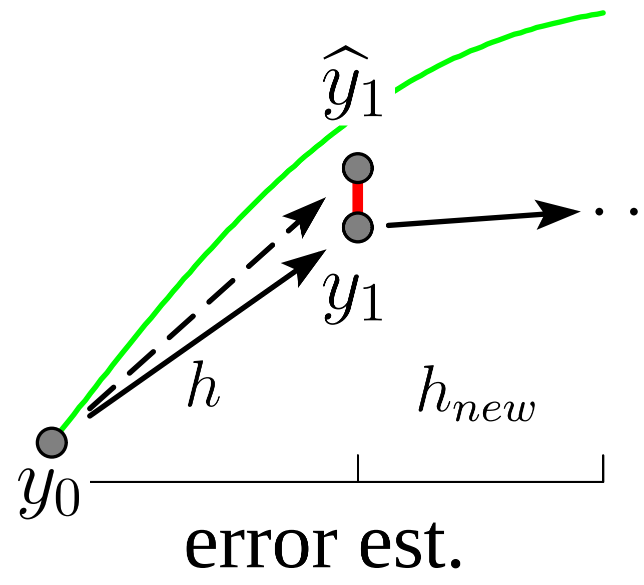
None of these methods is actually in use . . .

Error Estimation and Step-Size Control

Das besondere Schmerzenskind sind die
Fehlerabschätzungen. (L. Collatz 1950)

1. Error estimation with embedded method (Merson 1957, Ceschino 1961, Fehlberg 1969) : $\widehat{y}_1$ higher order result used for error estimation.

- returns 'bad' numerical result;
- if y_1 optimized $\Rightarrow$ dangerous underestimation.

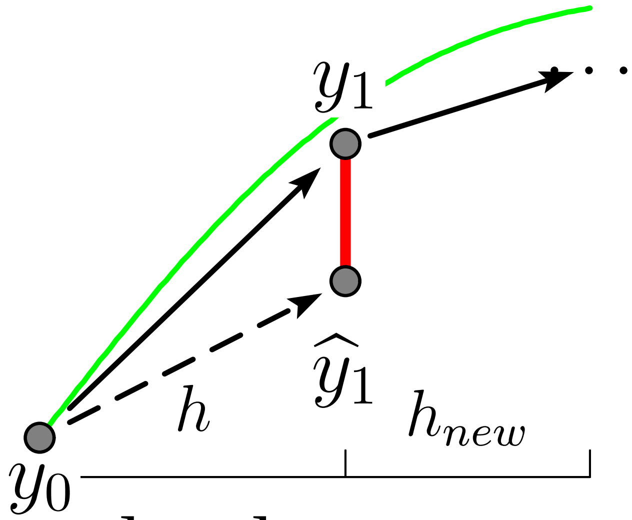


2. Local extrapolation

To start with, recall the well-known *dilemma* of error estimation: once a good error estimate is computed, one will certainly add it to the associated approximation – thus obtaining a *refined* approximation, which then, however, does *not* have an associated error estimate ! (P. Deuflhard, *Num. Math.* 1983, p. 403)

(Dormand & Prince 1980, 1989, Dd 1983). Optimize y_1:

- excellent numerical result;
- save error and step-size handling.

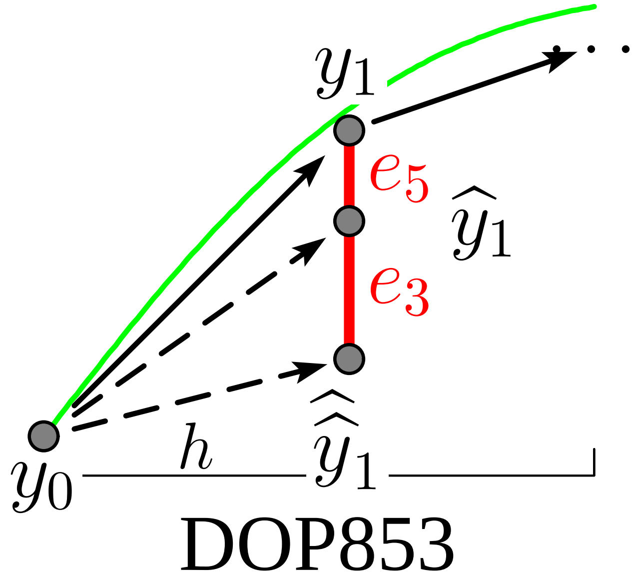


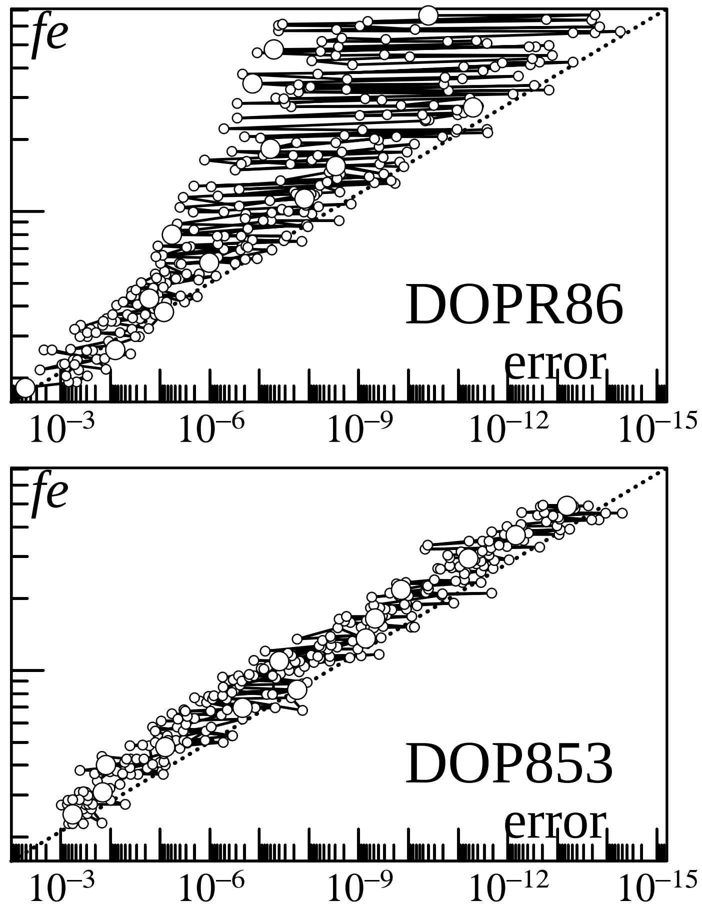
local extrap.

3. ‘Stretched’ error estimator (Hairer 1993).

In DOPR86 necessarily $b_{12} = \widehat{b}_{12}$, error insensitive at $t = t_1$:
$\Rightarrow$ DOP853 with two error estimators e_5, e_3

$$\text{err} = \frac{e_5^2}{e_3}.$$

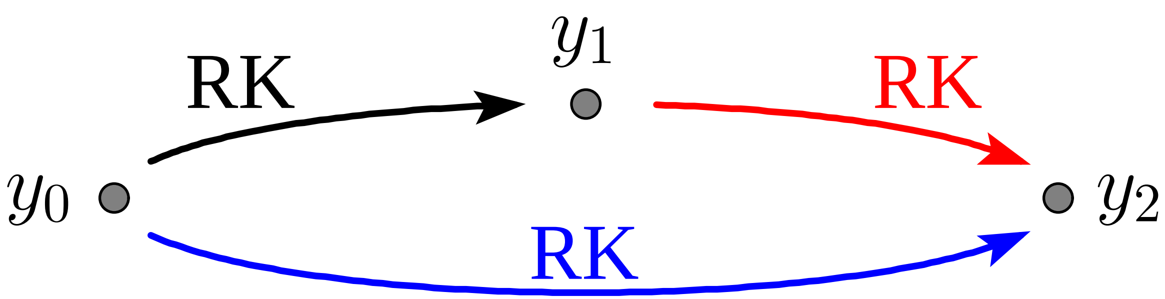




Remark. ‘Smoothing step in Gragg alg. $\Rightarrow$ ‘Stretched’ error est.

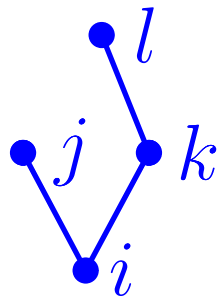
3. Butcher's Second Theorem (Butcher 1969, 1972).

At the Dundee Conference in 1969, a paper by J. Butcher was read which contained a surprising result. (H.J. Stetter 1971)



$$
\begin{array}{|cccc}
a_{11} & a_{12} & & \\
a_{21} & a_{22} & & \\
b_1 & b_2 & \color{red}{a_{11}} & \color{red}{a_{12}} \\
b_1 & b_2 & \color{red}{a_{21}} & \color{red}{a_{22}} \\
\hline
b_1 & b_2 & \color{red}{b_1} & \color{red}{b_2}
\end{array}
\quad = \quad
\color{blue}{
\begin{array}{|cccc}
a_{11} & a_{12} & \multicolumn{2}{c}{\mathbf{0}} \\
a_{21} & a_{22} & & \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44} \\
\hline
b_1 & b_2 & b_3 & b_4
\end{array}}
$$

$$\sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{k=1}^{4}\sum_{l=1}^{4} b_i\, a_{ij}\, a_{ik}\, a_{kl} = \dots$$



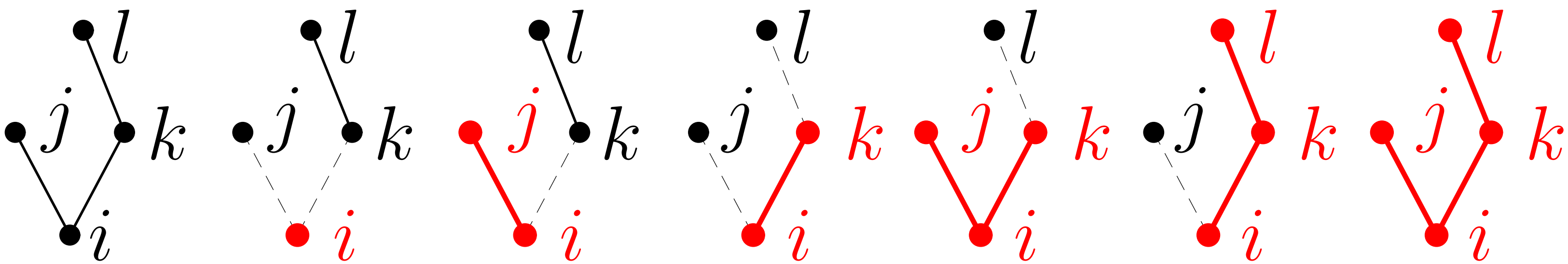
(separating black and red index sets)

$$= \sum_i \sum_j \sum_k \sum_l \,./.\, + \sum_i \sum_j \sum_k \sum_l \,./.\, + \sum_i \sum_j \sum_k \sum_l \,./.\, + \dots$$

$$= \sum b_i\, a_{ij}\, a_{ik}\, a_{kl} + \sum b_i \sum b_j \sum b_k\, a_{kl} + \sum b_i\, a_{ij} \sum b_k\, a_{kl}$$

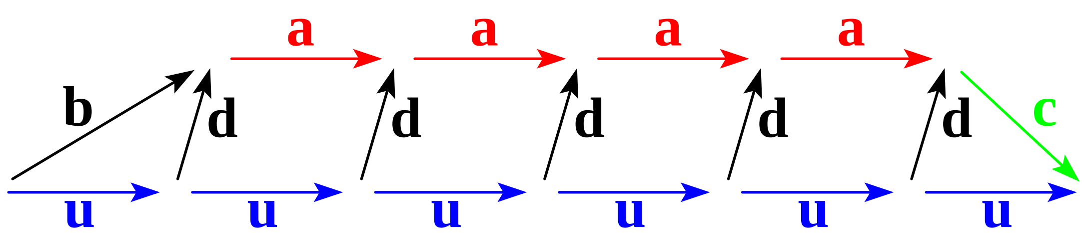
$$+ \sum b_i a_{ik} \sum b_j \sum b_l + \sum b_i a_{ij} a_{ik} \sum b_l + \sum b_i a_{ik} a_{kl} \sum b_j + \sum b_i a$$

(all other combinations disappear because of the big 0)



Applications.

- Butcher's "effective order" $RK5 \circ RK5 \circ RK5 = \text{order } 5$;



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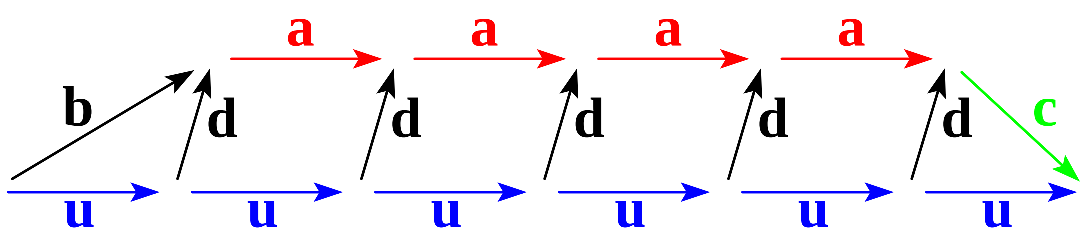

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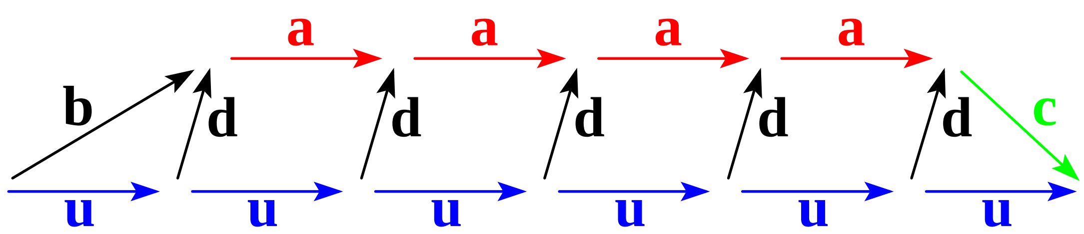
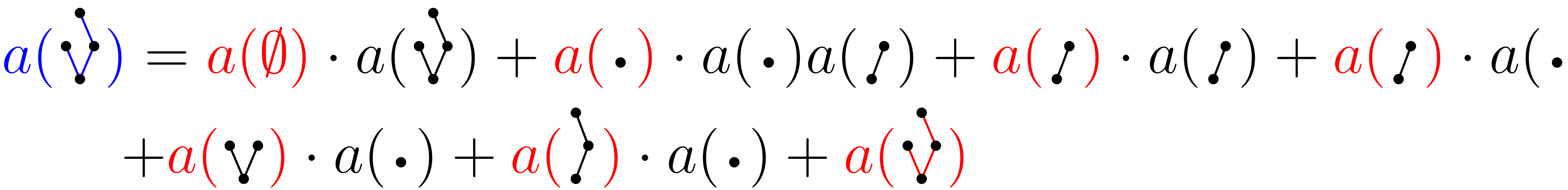


- compos. of B-series $B(a, B(a, y_0)) = B(aa, y_0) = B(a, y_0), ;$



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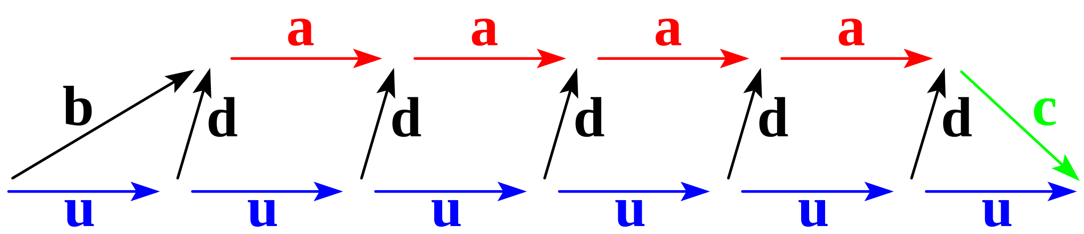

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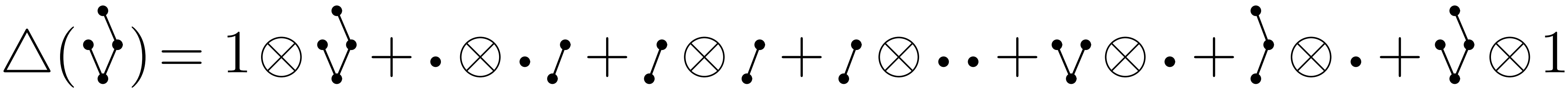
$$a(\mathring{\vee}) = a(\emptyset)\cdot a(\mathring{\vee}) + a(\bullet)\cdot a(\bullet)a(\bullet\!\!-\!\!\bullet) + a(\bullet\!\!-\!\!\bullet)\cdot a(\bullet\!\!-\!\!\bullet) + a(\bullet\!\!-\!\!\bullet)\cdot a(\bullet$$
$$+a(\vee)\cdot a(\bullet) + a(\wr)\cdot a(\bullet) + a(\mathring{\vee})$$

- General Multivalue Methods (K. Burrage and P. Moss 1980) ;
- General Linear Methods (Burrage and Butcher 1980) ;
- Rosenbrock methods (Nørsett, Wolfbrandt, Kaps, Rentrop) ;
- Multiderivative RK methods (Kastlunger 1972) ;

- Partitioned ODE's, P-series (Hairer 1981) ;
- Volterra Integral Eq's, V-series (Brunner-Hairer-Nørsett 1982) ;
- Index 1 DAE's and Singular Pert. Pr., (Roche 1988, HLR 1988) ;
- Index 2 DAE's (A. Kværno 1990, Hairer-Lubich-Roche 1989) ;
- Manifolds (Crouch-Grossmann 1993, Owren and Martinsen 1997
- Equations on Lie Groups (Munthe-Kaas 1995, 1997) ;
- Stochastic Diff. Eq. (K. and P.M. Burrage 2000, Cirilli 2002) ;
- ROCK Methods for PDE's. Abdulle–Medovikov 1999) ;
- Hamiltonian Syst., Sympl. B-series. (Calvo and Sanz-Serna 1994
- Sympl. Integrators ; Backward Error Anal. (Hairer and Lubich 19
- B_∞-series for Composition Meth. (Murua and Sanz-Serna 1999).

Connection with Hopf Algebras and Quantum Field Theory

The algebraic structure of the above Butcher Group leads to a mapping $\triangle : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$, for example

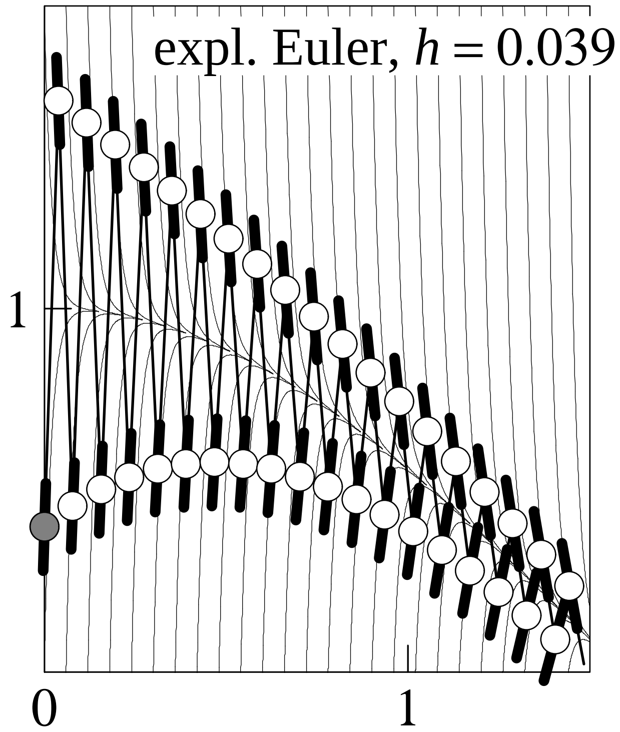


which defines a *coproduct* on the algebra generated by families of rooted trees, and has proved to be extremely useful in Theoretical Physics for simplifying the intricate combinatorics of renormalization (Connes, Kreimer 1998), (Brouder 2000). An unexpected connection. ...and a nice citation :

> We regard Butcher's work on the classification of numerical integration methods as an impressive example that concrete problem-oriented work can lead to far-reaching conceptual results. (A. Connes, cited from Chr. Brouder, talk in Trondheim 2003)

4. Stiff Equations ; Dahlquist's Second Barrier

. . . Around 1960, things became completely different and everyone became aware that the world was full of stiff problems. (G. Dahlquist in 1985)



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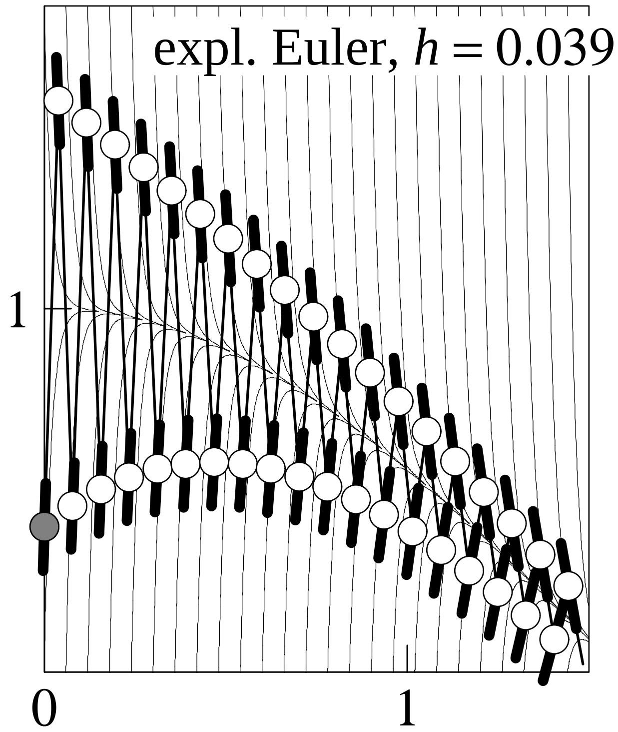

Theorem (Dq 1963).

Multistep method A-stable $\Rightarrow$ $p \leq 2$.

For $p = 2$ best error constant by Trap. Rule.

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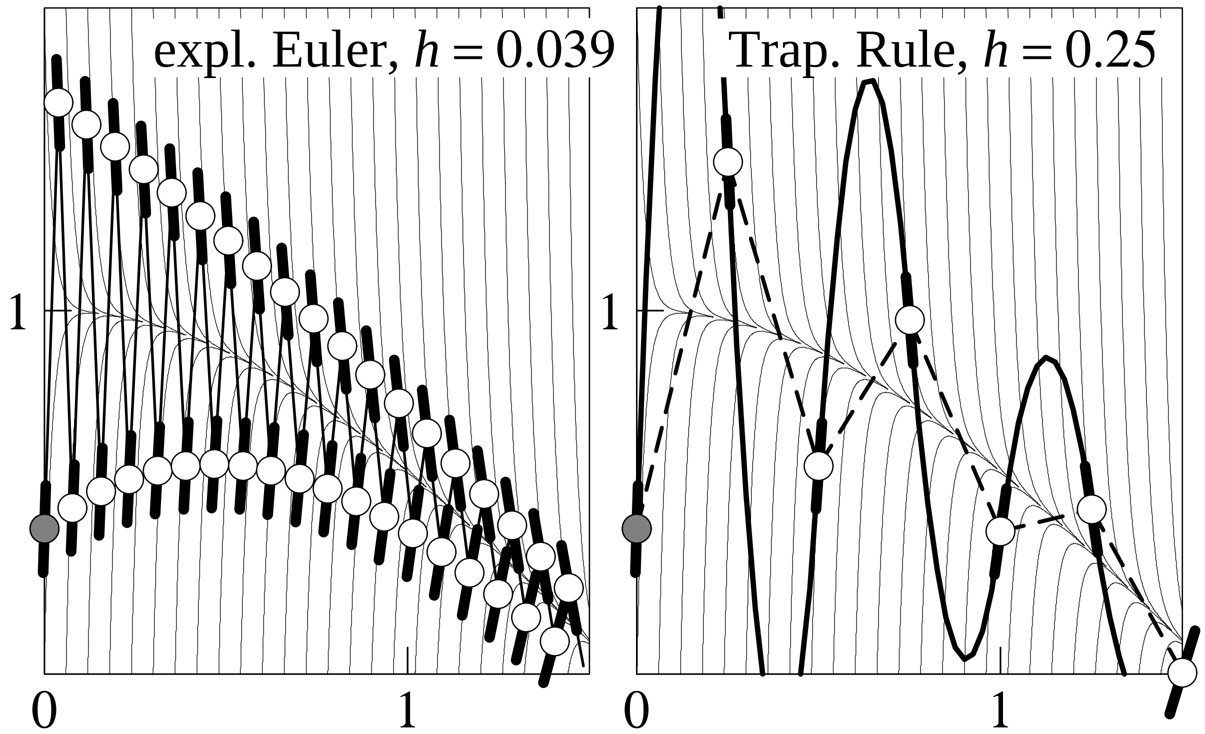

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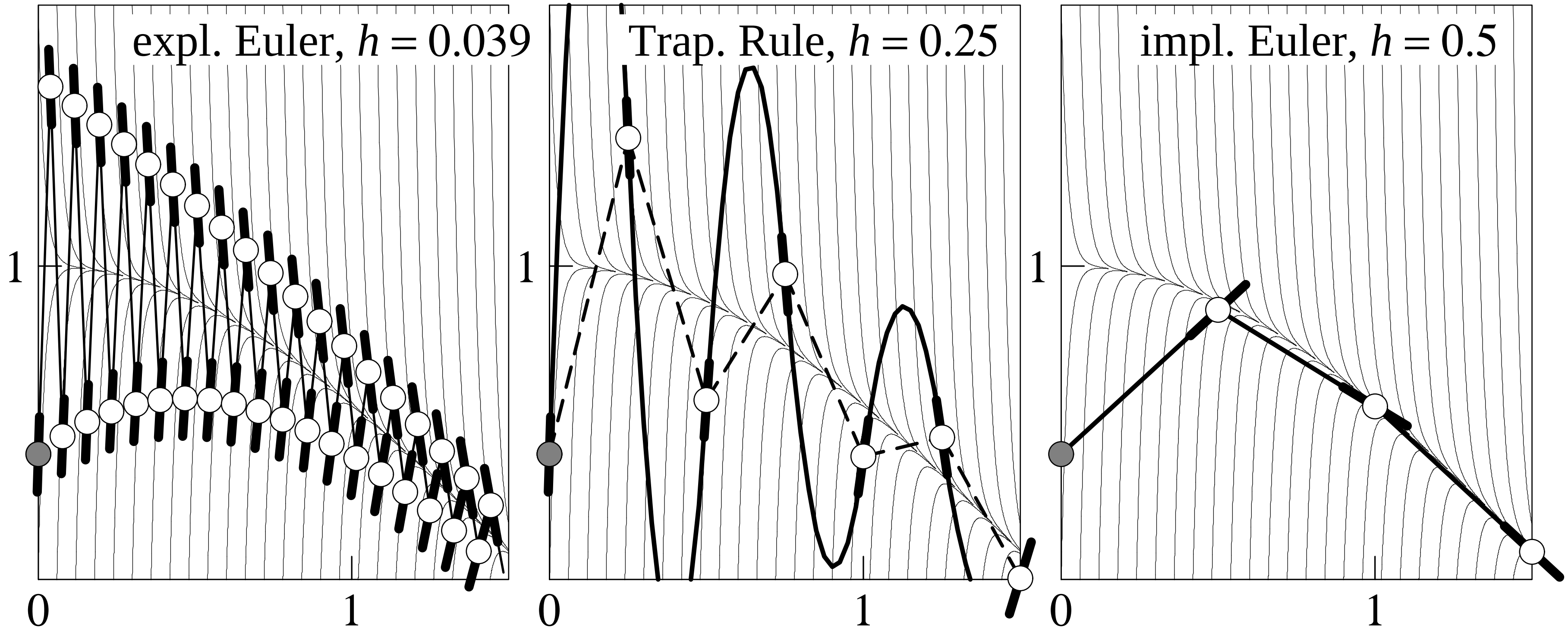


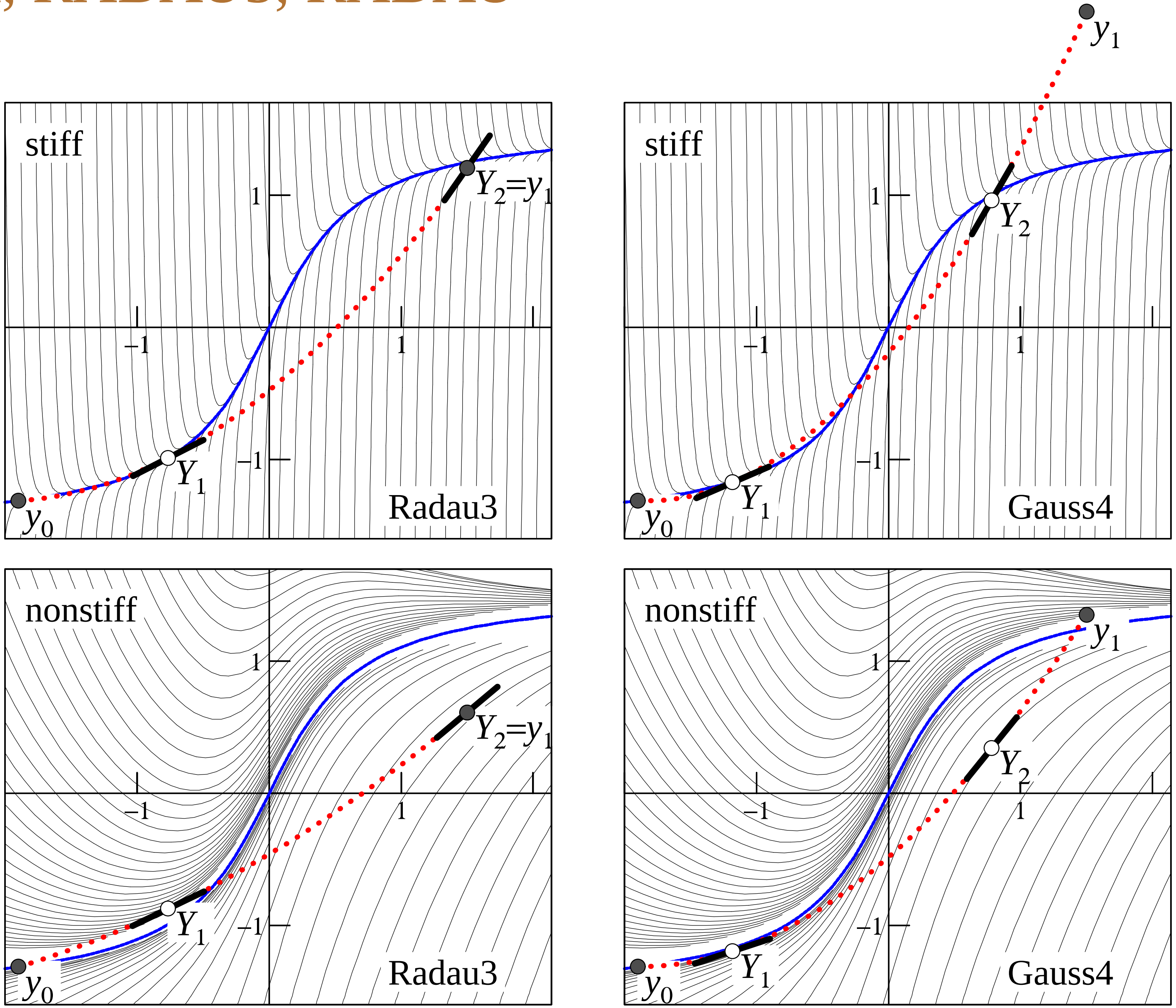
Prothero-Robinson 1974 : *A*-stability is not enough !

Method must be stiffly accurate.

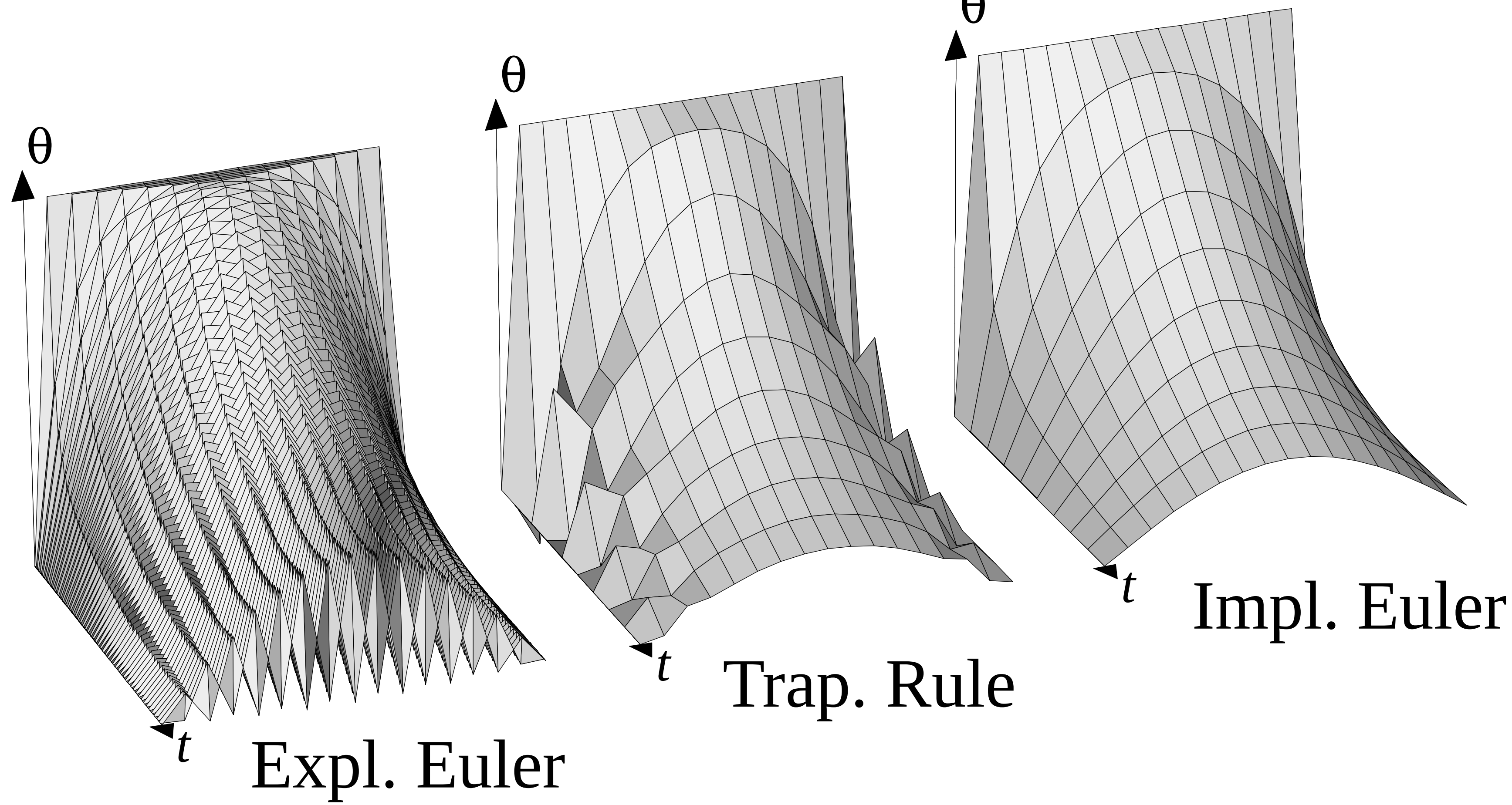
$\Rightarrow$ excellent codes METAN1, LARKIN,

$\Rightarrow$ excellent codes METAN1, LARKIN, LSODE, DASSL,

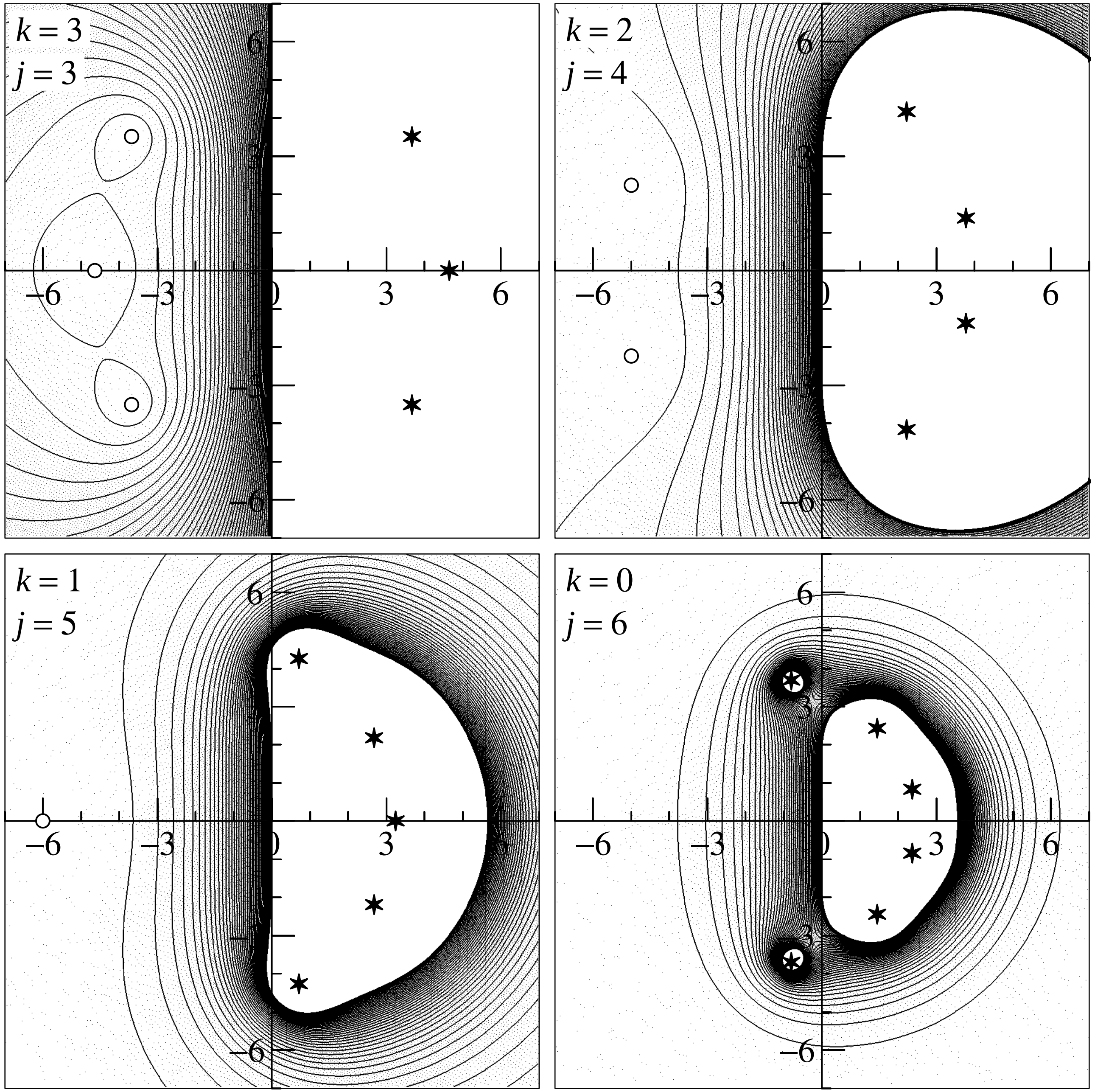
⇒ excellent codes METAN1, LARKIN, LSODE, DASSL, SODEX, RADAU5, RADAU



Example. The heat equation

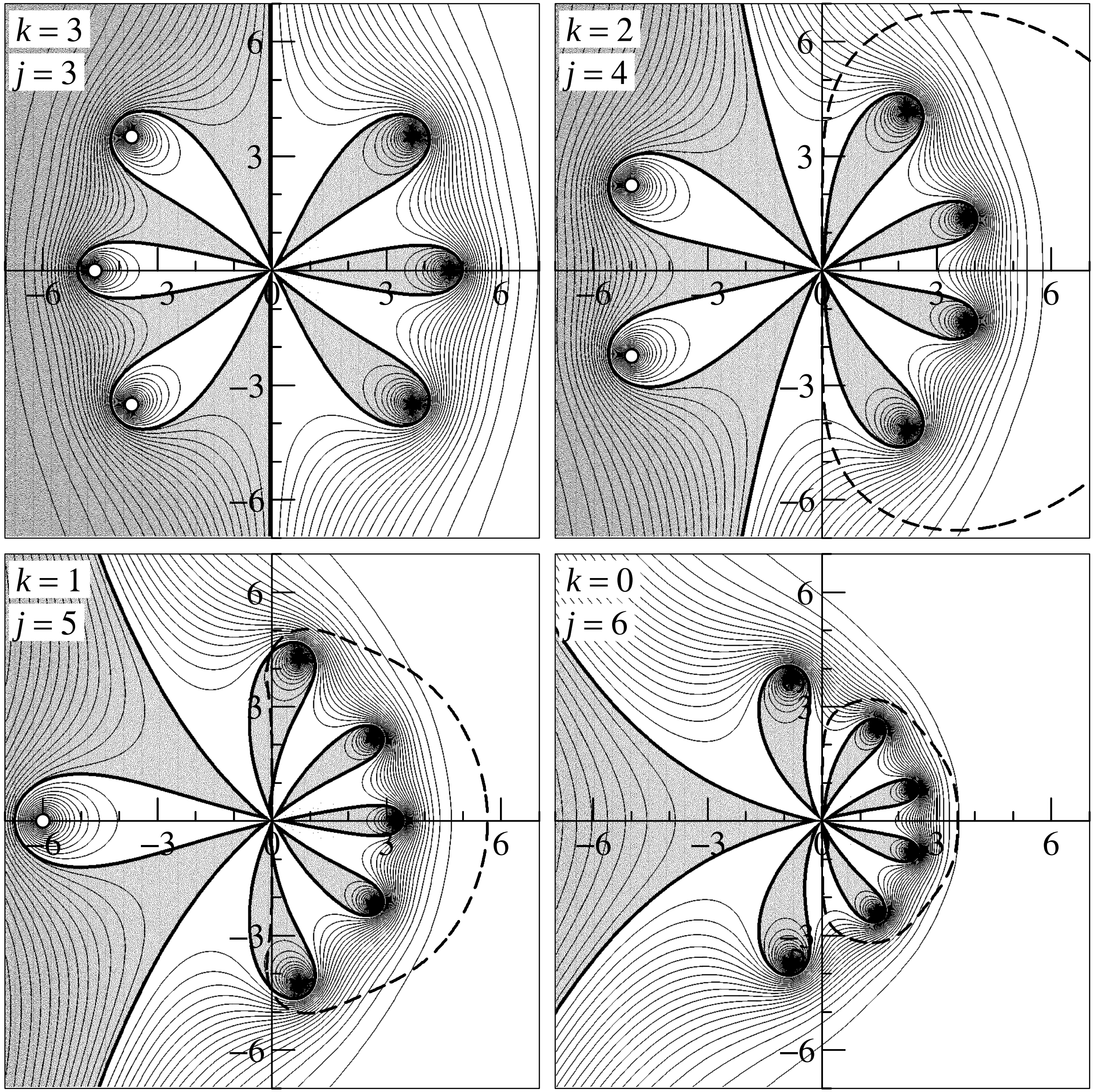


Ehle's Conjecture ; Order Stars



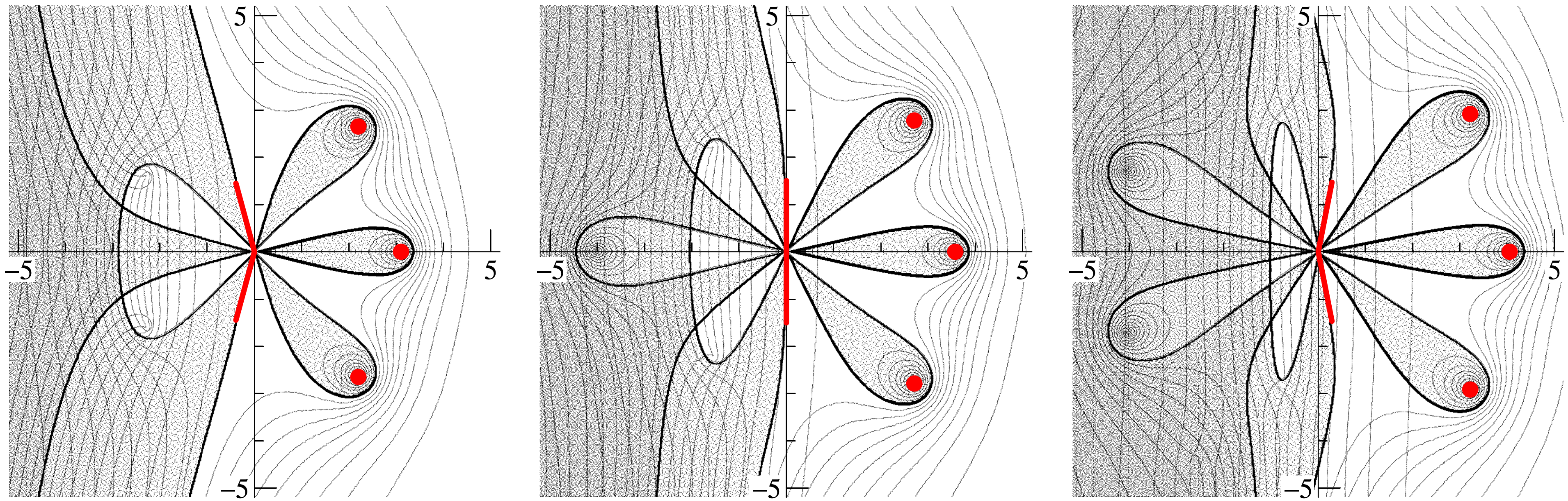
Conjecture. A-stable $\Leftrightarrow$ $k \le j \le k+2.$

Ehle's Conjecture ; Order Stars



Theorem. A-stable $\Leftrightarrow$ $k \leq j \leq k+2$.

The Daniel–Moore Conjecture

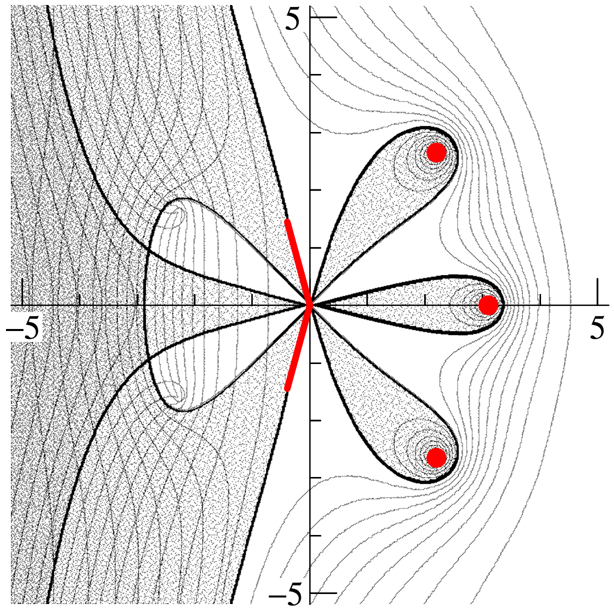


order 5 order 6 order 7

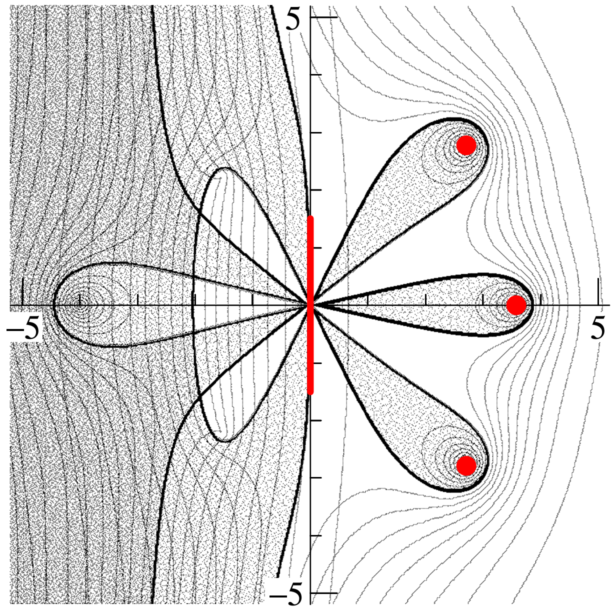
Theorem. *A-stable method with s poles* $\Rightarrow$ $p \le 2s$.

For $s = 1$ this is Dahlquist's second barrier.

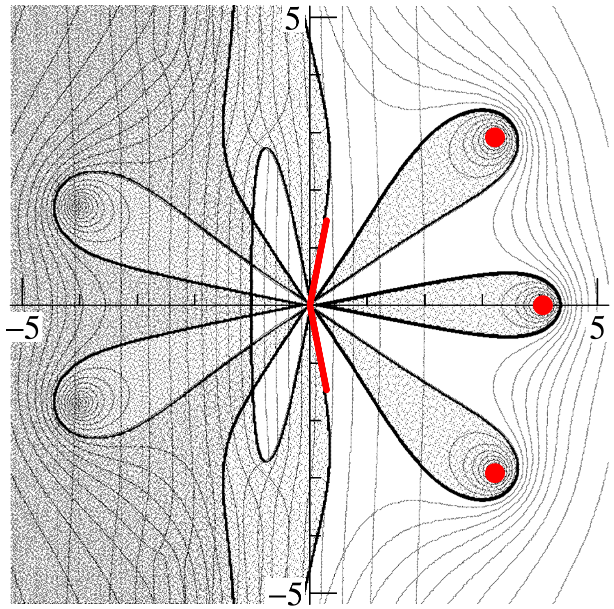
The Daniel–Moore Conjecture



order 5

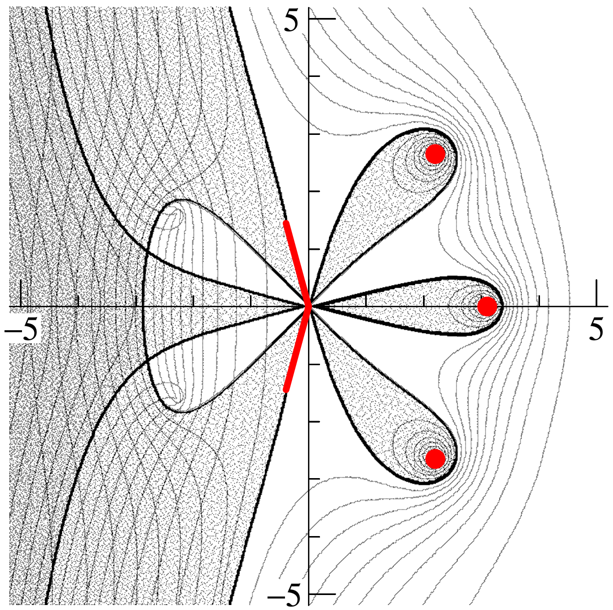


order 6

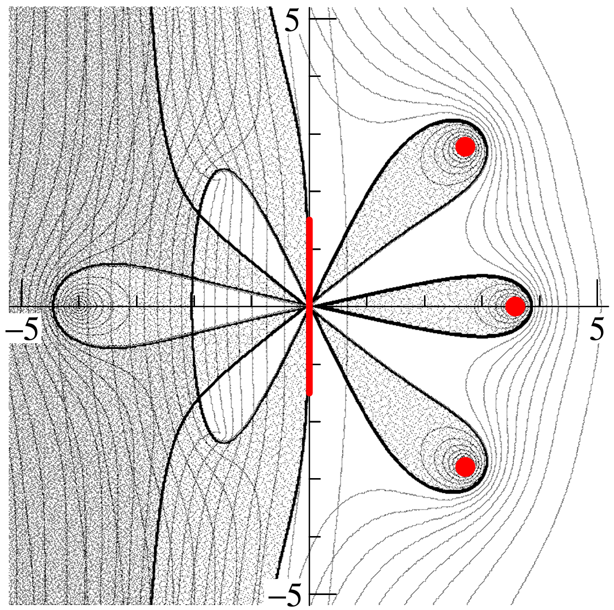


order 7

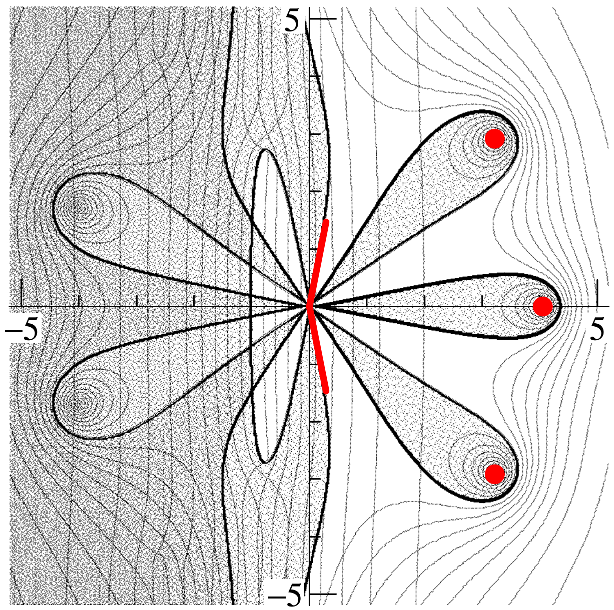
The Daniel–Moore Conjecture



order 5



order 6



order 7

There is a sort of ‘Conservation Law of Misery’ in Numerical Analysis. (H. van der Vorst, in a talk 2000)

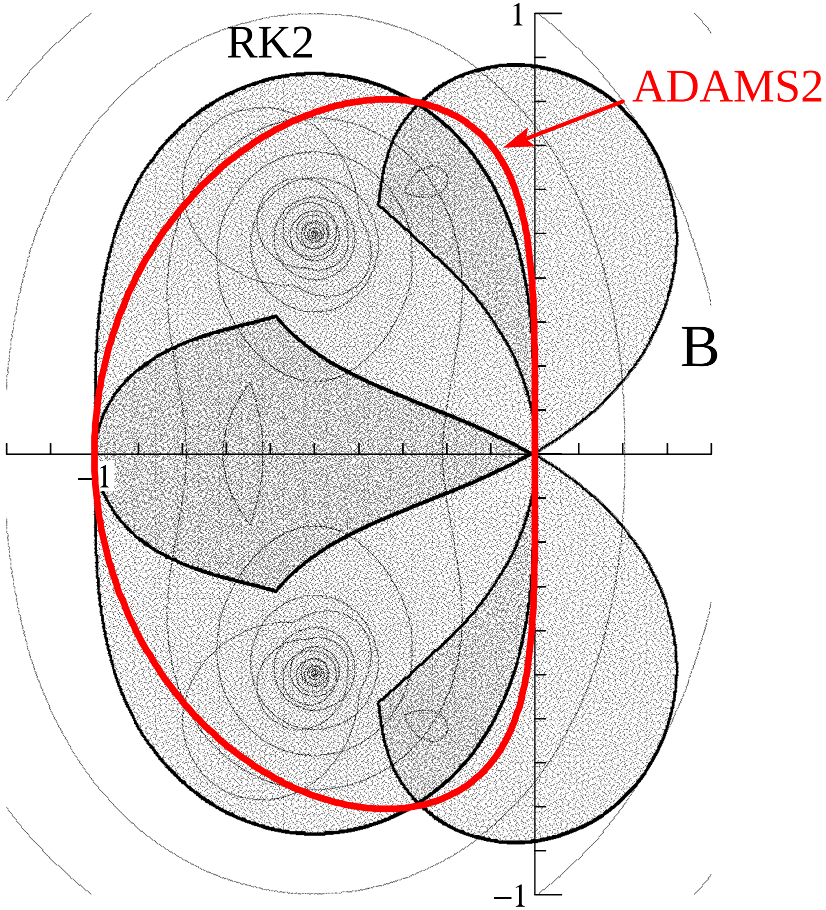
5. The Controversy between Multistep and Runge-Kutta

The greater accuracy and the error-estimating ability of predictor-corrector methods make them desirable for systems of any complexity. . . . Runge-Kutta methods still find applications in starting the computation . . . (A. Ralston, *Math. Comput.* 1962)

But surely the predictor-corrector techniques (Milne's for example) will result in one getting an answer to the same accuracy in a shorter time simply because information outside a single interval is used. You can choose formulae so that the theoretical truncation error is of any order you wish. (Dr. J.M. Bennett, Sydney, in a discussion 1956)

Theorem of Jeltsch–Nevanlinna.

Two explicit methods
with comparable numerical work
. . . have also comparable
stability domains.



In answer to Dr. Bennett's first question, I have found that the predictor-corrector formulae do not have the wide stability range of R. Kutta processes. (Mr. R.H. Merson (In Reply))

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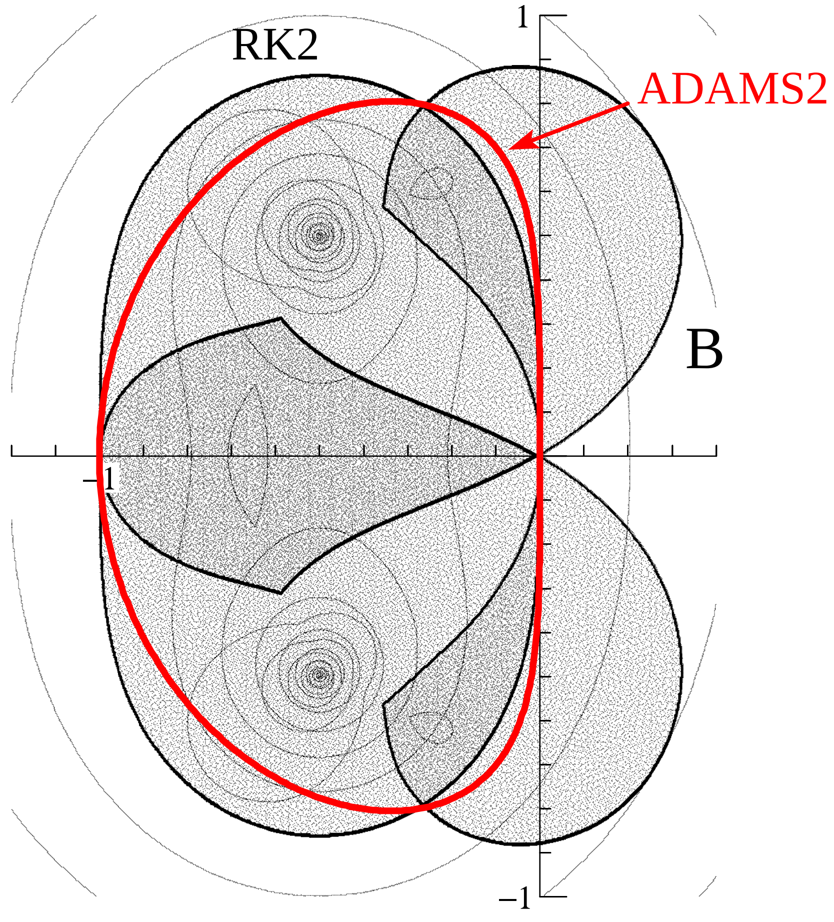
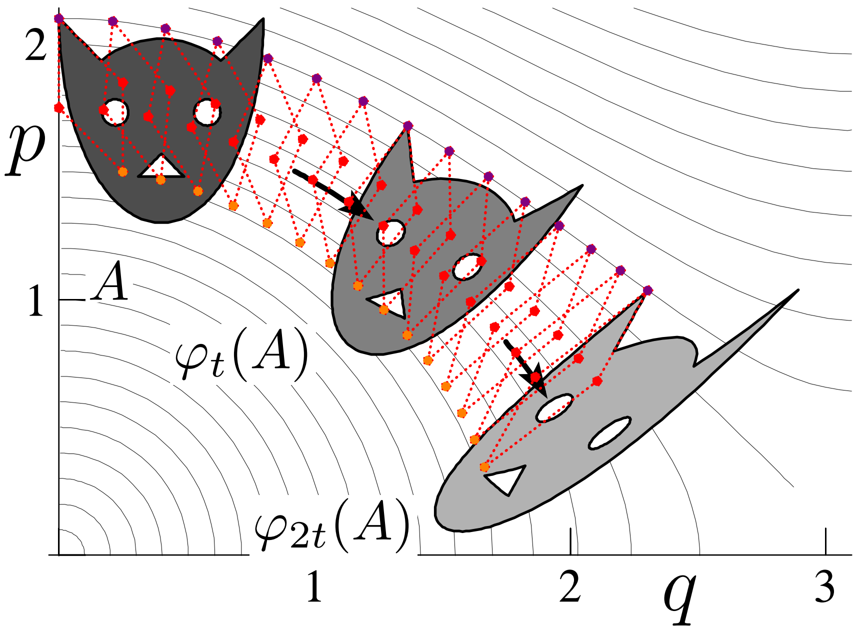
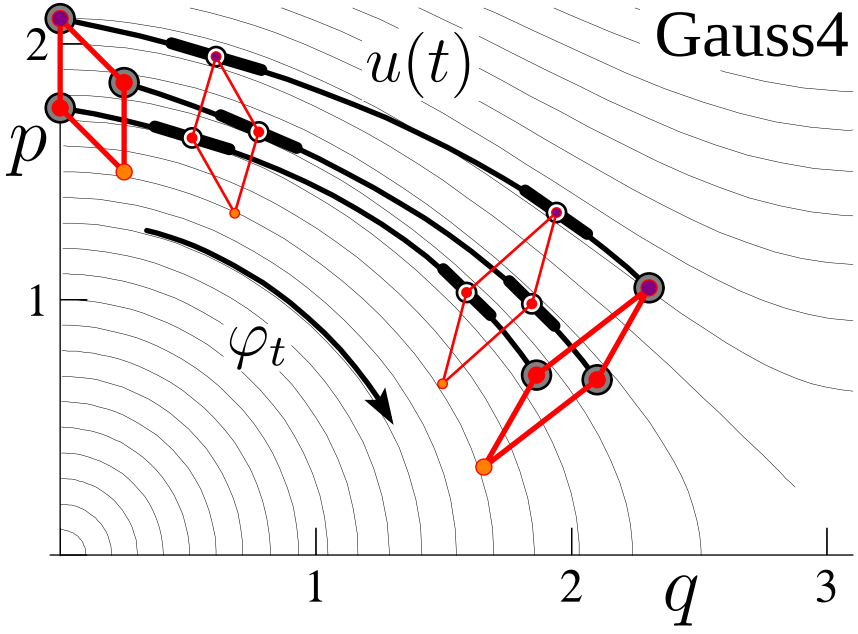


In answer to Dr. Bennett's first question, I have found that the predictor-corrector formulae do not have the wide stability range of R. Kutta processes. (Mr. R.H. Merson (In Reply))

6. Symplectic Integration of Hamiltonian Systems



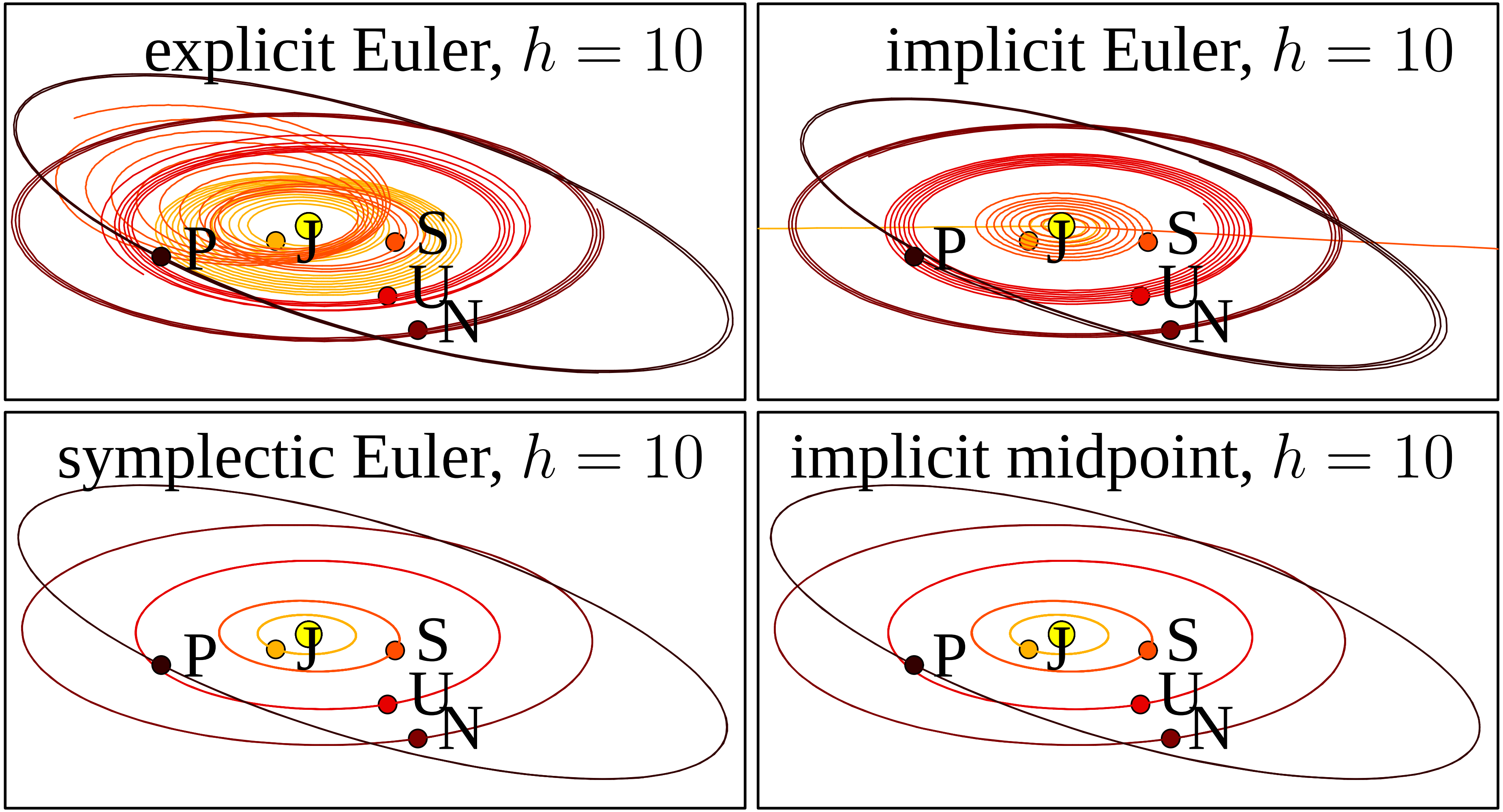


Geometric Numerical Integration

Structure-Preserving Algorithms for Ordinary Differential Equations

E. Hairer, C. Lubich, G. Wanner, Springer 2002

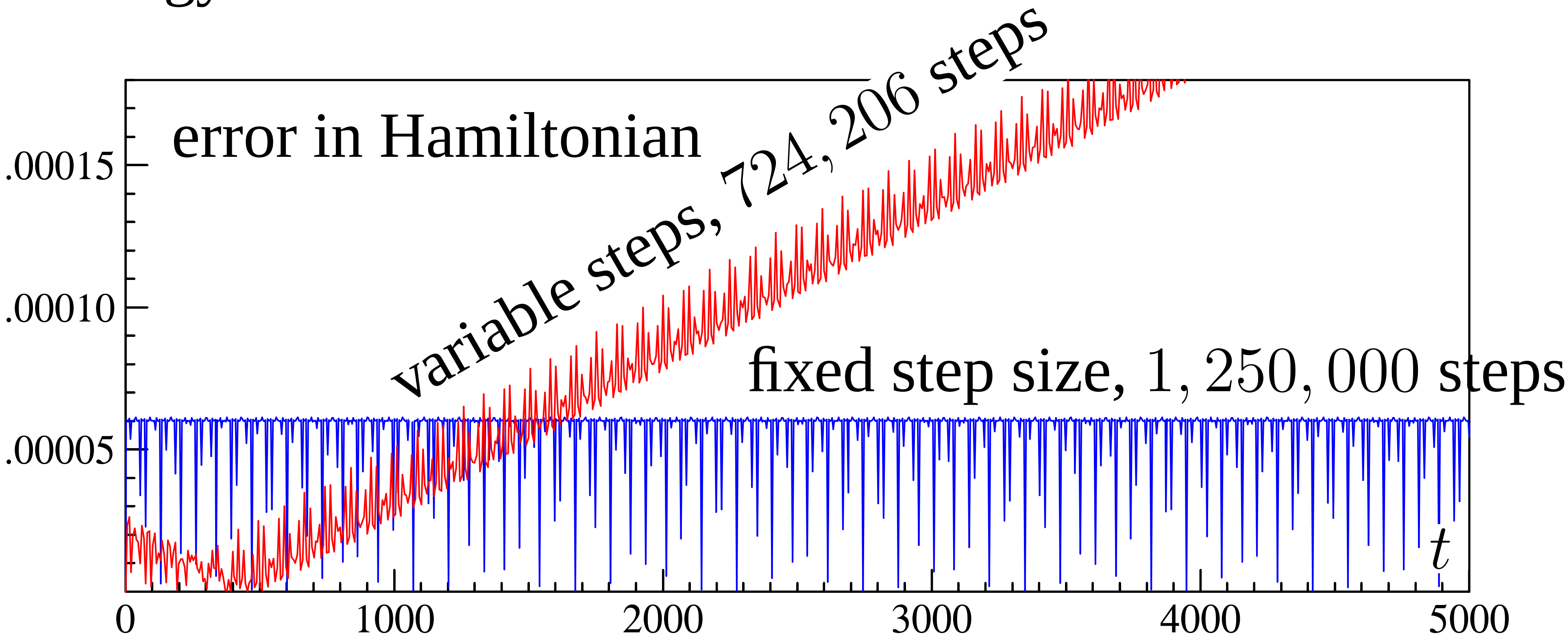
Example. The outer solar system.



Counter-Example. (Sanz-Serna, Calvo) :
The Kepler with eccentricity $e = 0.6$.

Method: Störmer–Verlet

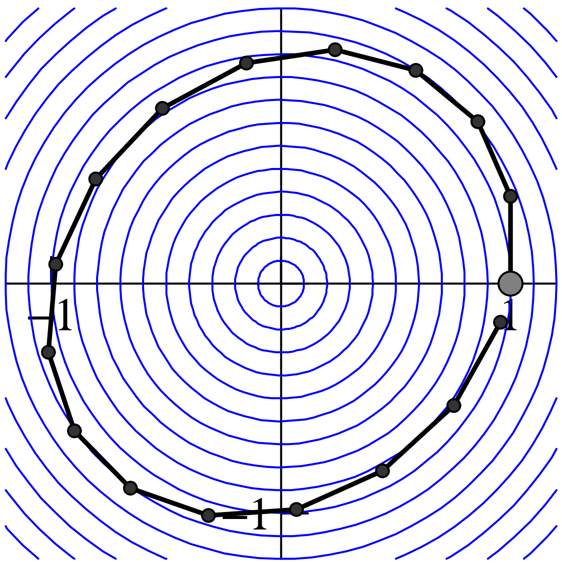
Error estimator: imbedded symplectic Euler and standard step size strategy



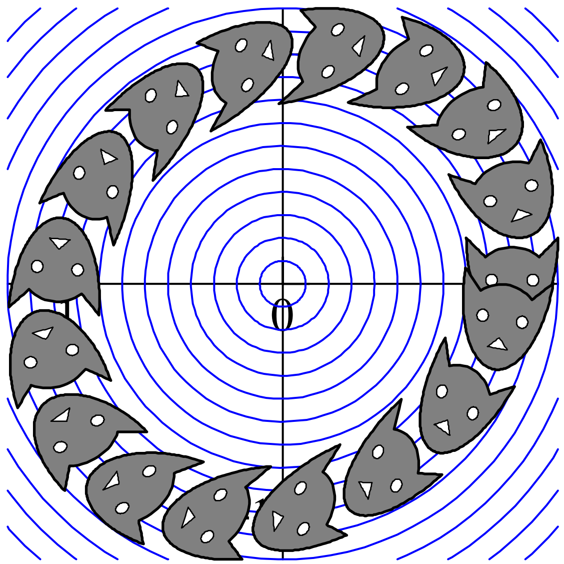
Counter-Example : a symplectic method which is bad.

For the harmonic oscillator $\dot{p} = -q, \; \dot{q} = p$ we put (EH)

$$
\begin{aligned}
p_{n+1} &= p_n - h q_n \\
q_{n+1} &= q_n + h p_{n+1}
\end{aligned}
$$



$h = .38$



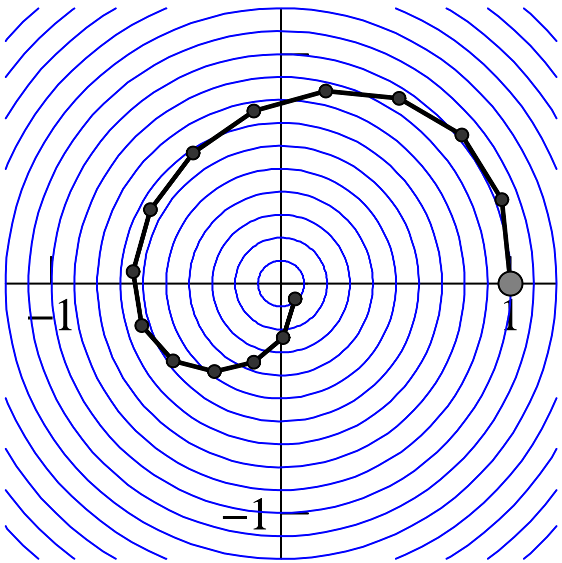
$h = .38$

Counter-Example : a symplectic method which is bad.

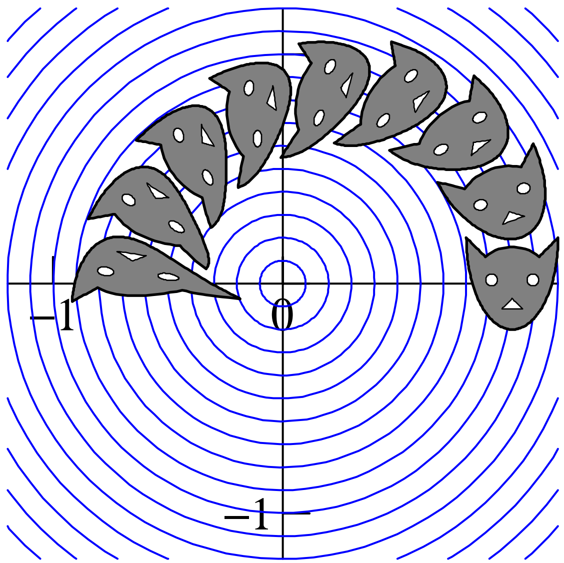
For the harmonic oscillator $\dot p = -q,\ \dot q = p$ we put (EH)

$$\begin{aligned} p_{n+1} &= p_n - hq_n - h^2\gamma\, p_{n+1}, \\ q_{n+1} &= q_n + hp_{n+1} - h^2\gamma\, q_n \end{aligned}$$

where $\gamma = 0.25/(p_{n+1}^2 + q_n^2)$.



$h = .38$



$h = .38$

This curious method is *symplectic*, but is of no use anyway !

"I'll tell you in **two** words : im**poss**ible !" (Laurel & Hardy)

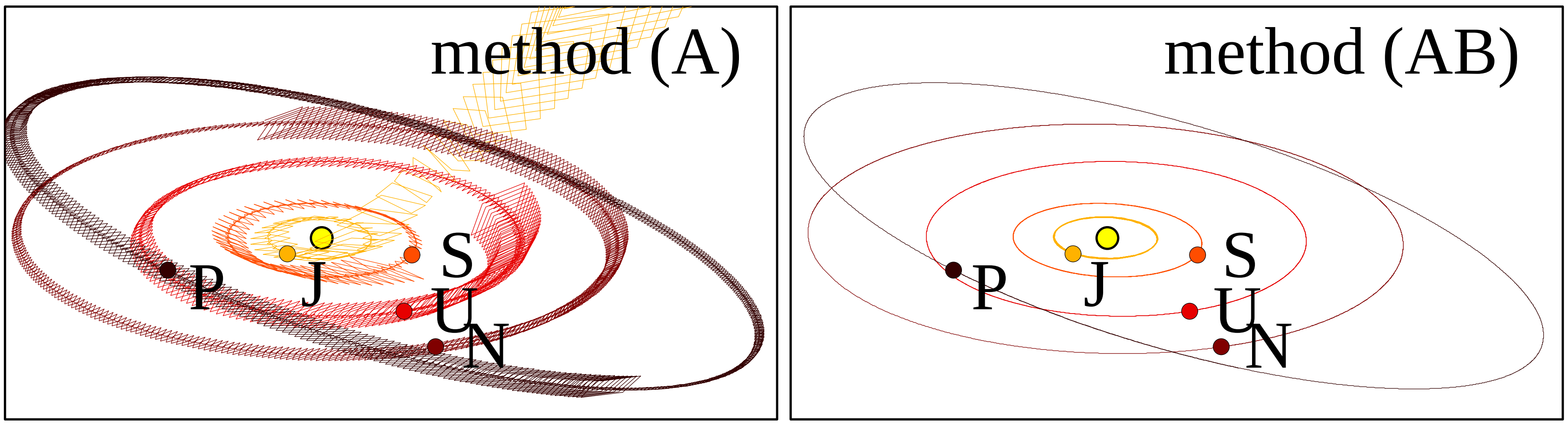
Theorem (Tang 1993, Hairer–Leone 1997).

Symplectic (true) multi-value methods are impossible.

Discovery : (Quinlan–Tremaine) Multistep methods can be excellent !

Example. (A) : $y_{n+3} - y_{n+2} + y_{n+1} - y_n = h(f_{n+2} + f_{n+1})$

(B) : $z_{n+3} - z_{n+1} = 2hg_{n+2}.$



Explication : new paper by E. Hairer and C. Lubich.

Conclusion.

“Ora et Labora”

(The *Regula Benedicti* promoted by Saint Boniface)

Conclusion.

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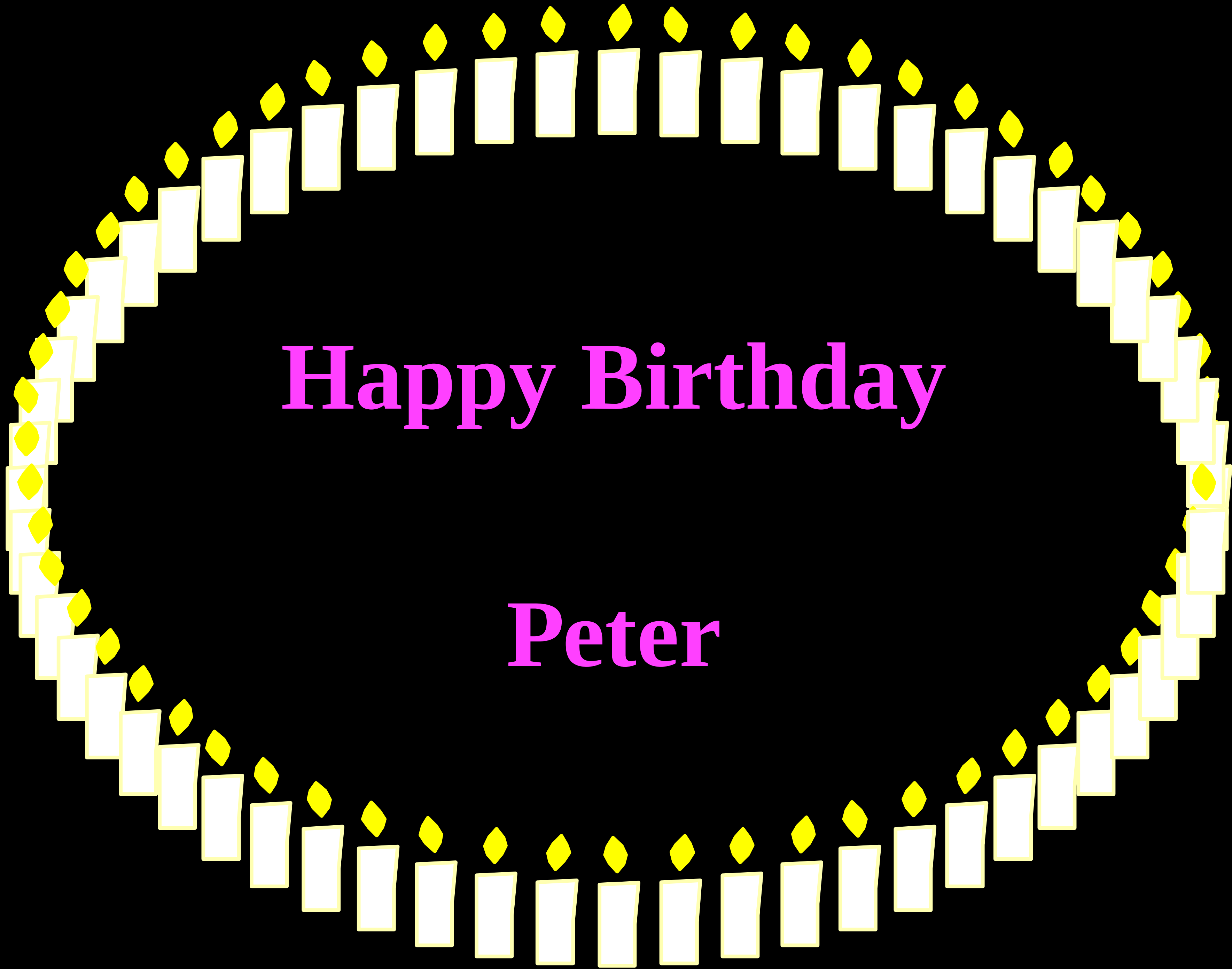
Thanks to E. Hairer and C. Lubich

thanks to Martin Hairer.



Happy Birthday

Peter