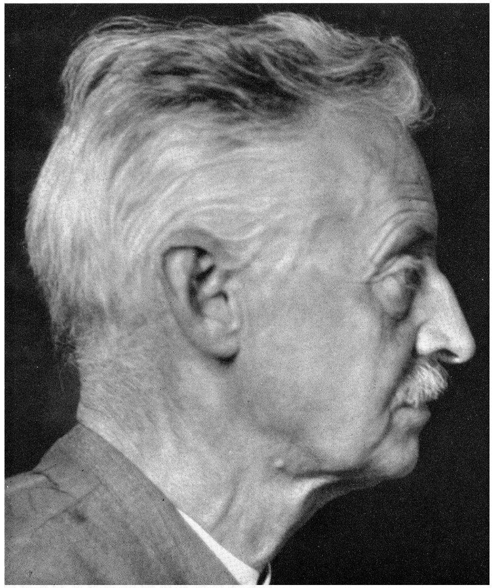
Upon this ROCK I will build my ...

Upon this ROCK I will build my ...
Stiff Integrators

Upon this ROCK I will build my ...
Stiff Integrators

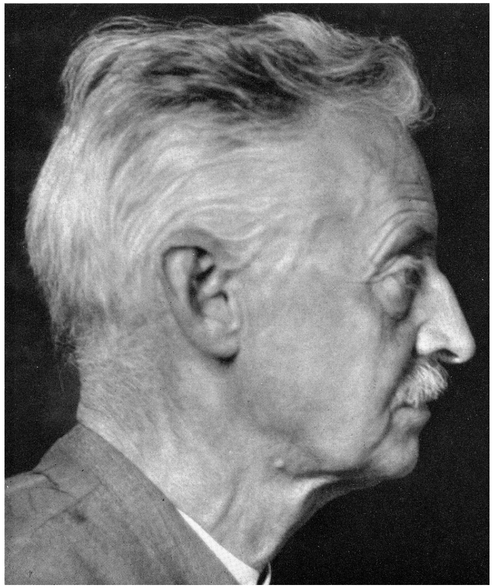
standing on the shoulders of great people ...



Runge

Upon this ROCK I will build my ...
Stiff Integrators

standing on the shoulders of great people ...



Runge

Kutta

Upon this ROCK I will build my ...
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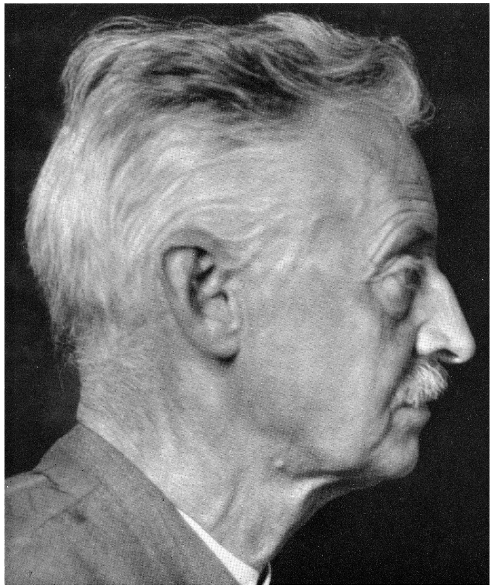
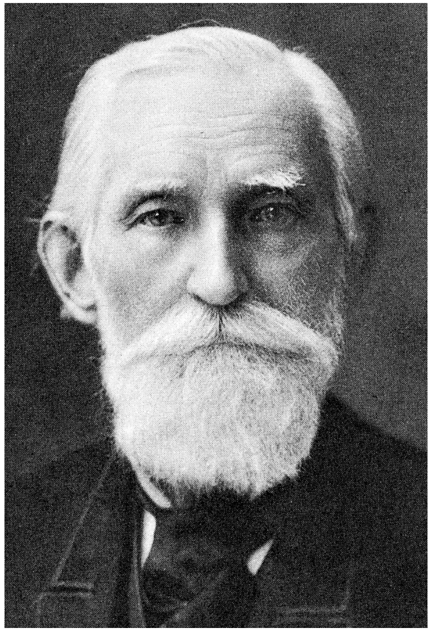


Runge



Chebyshev

Kutta

Upon this ROCK I will build my ...
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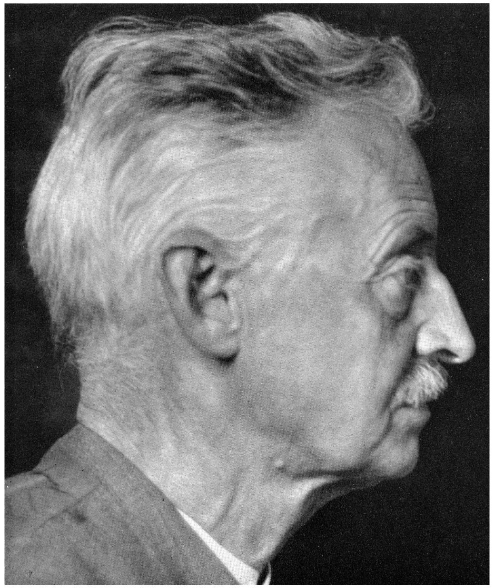
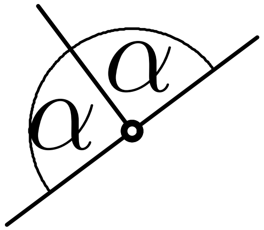
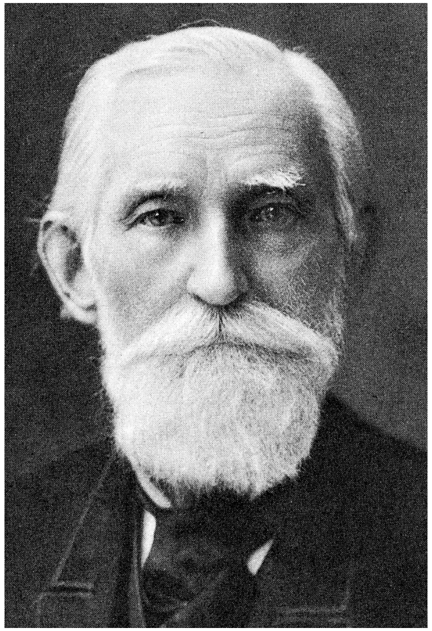
standing on the shoulders of great people ...



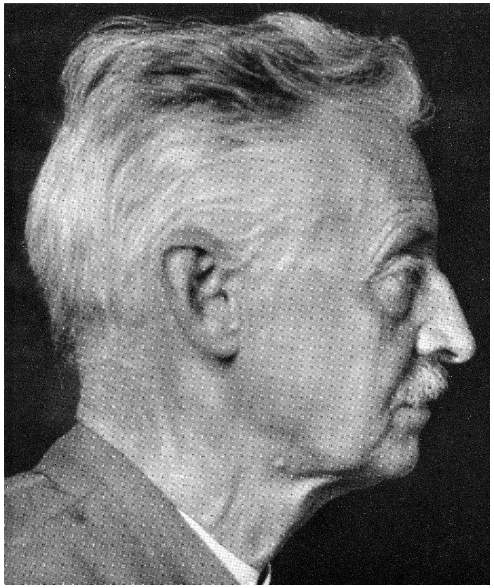


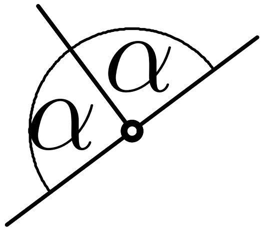


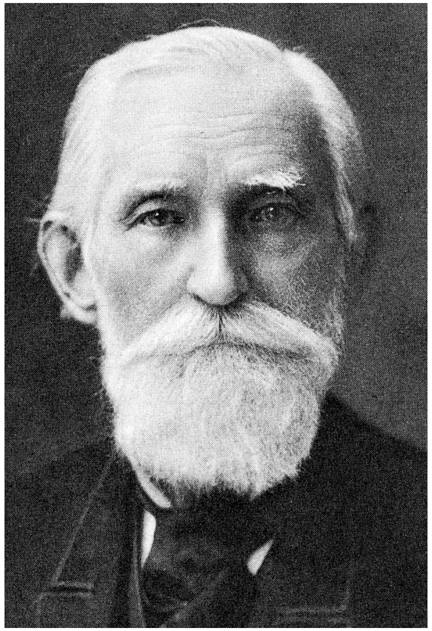
Runge Orthog. Chebyshev Kutta

Upon this ROCK I will build my ...
Stiff Integrators

standing on the shoulders of great people ...



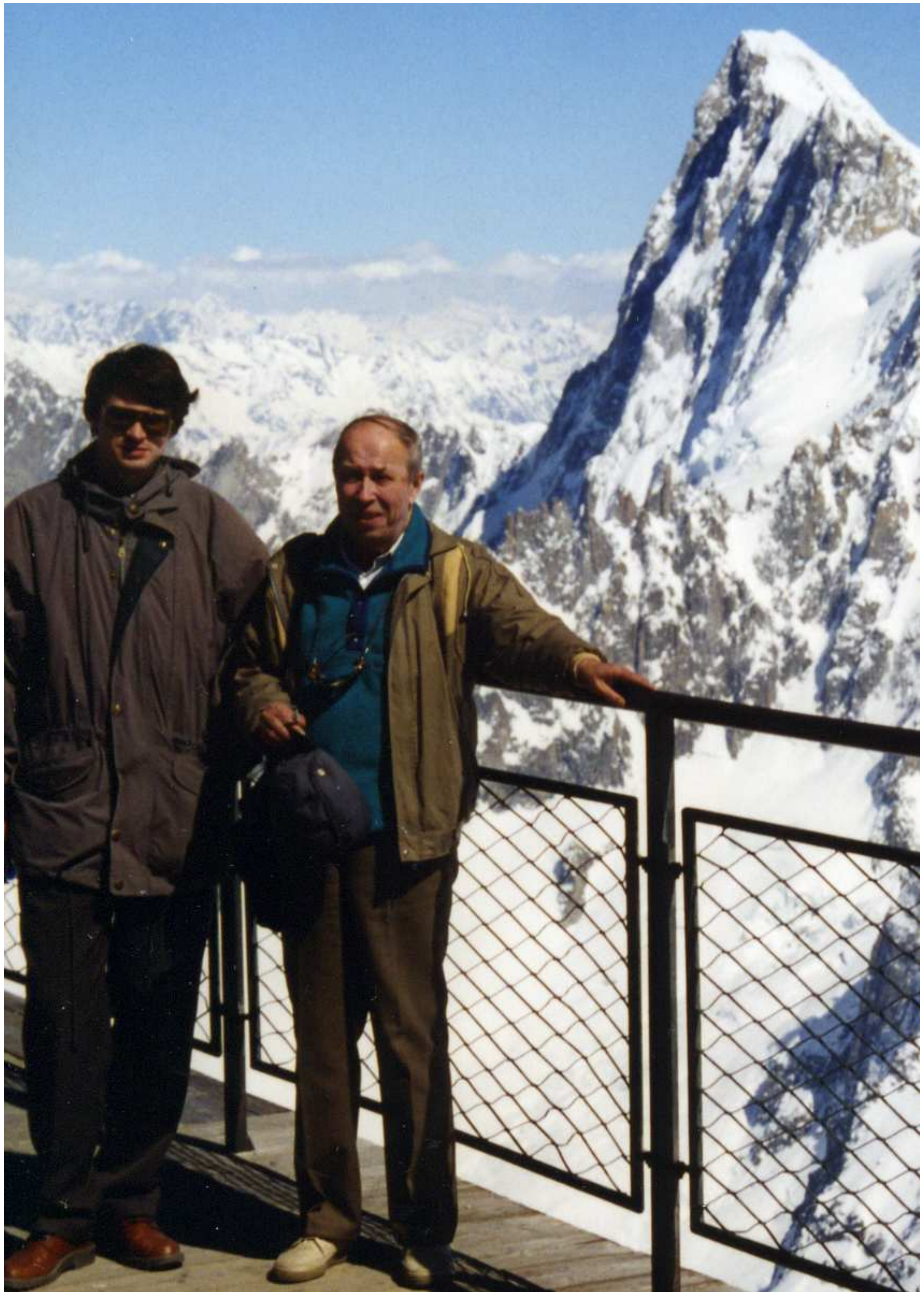




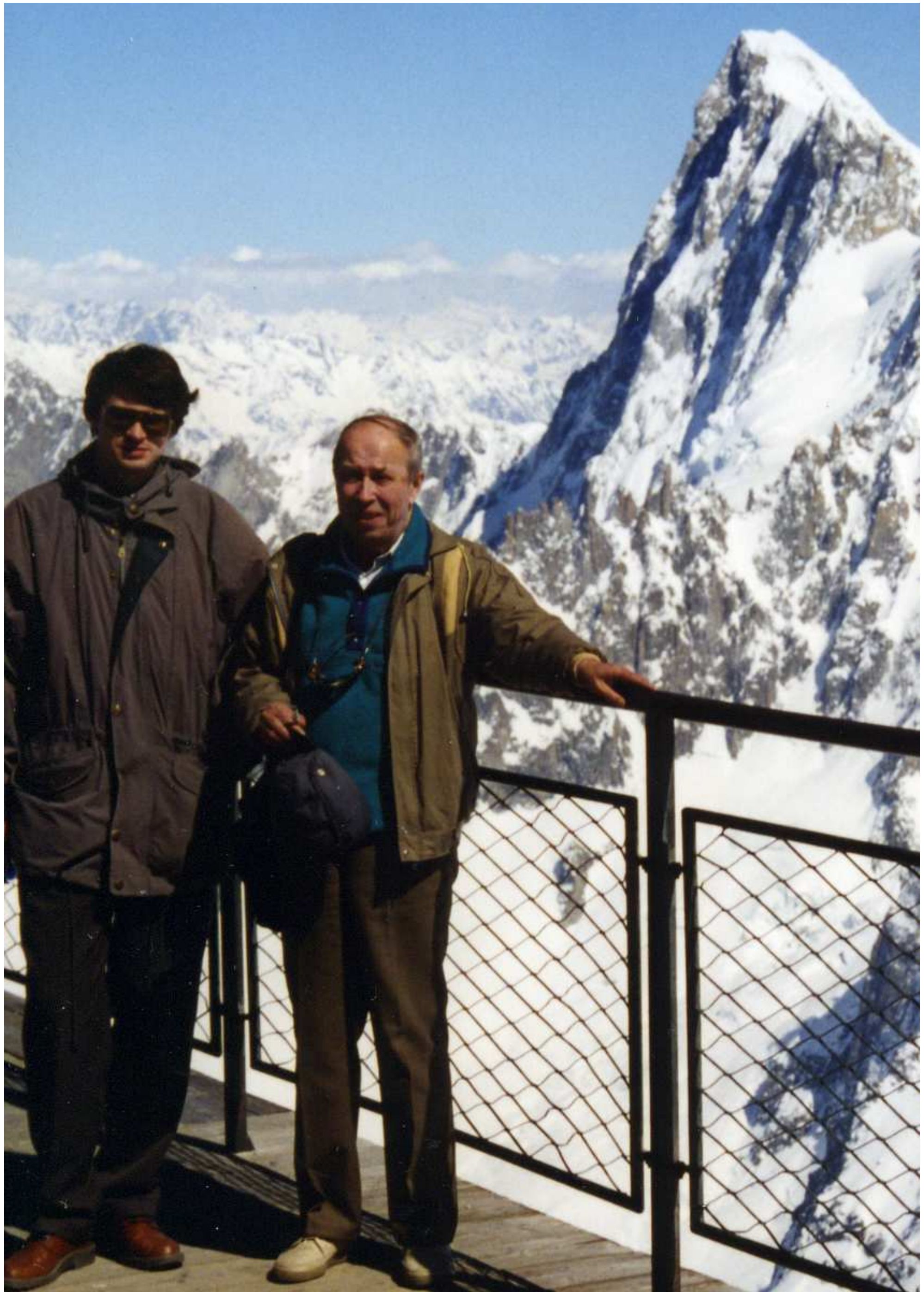
Runge Orthog. Chebyshev Kutta

Yuan Chzao Din, Saul’ev, Guillou-Lago, Verwer-Sommeijer ...

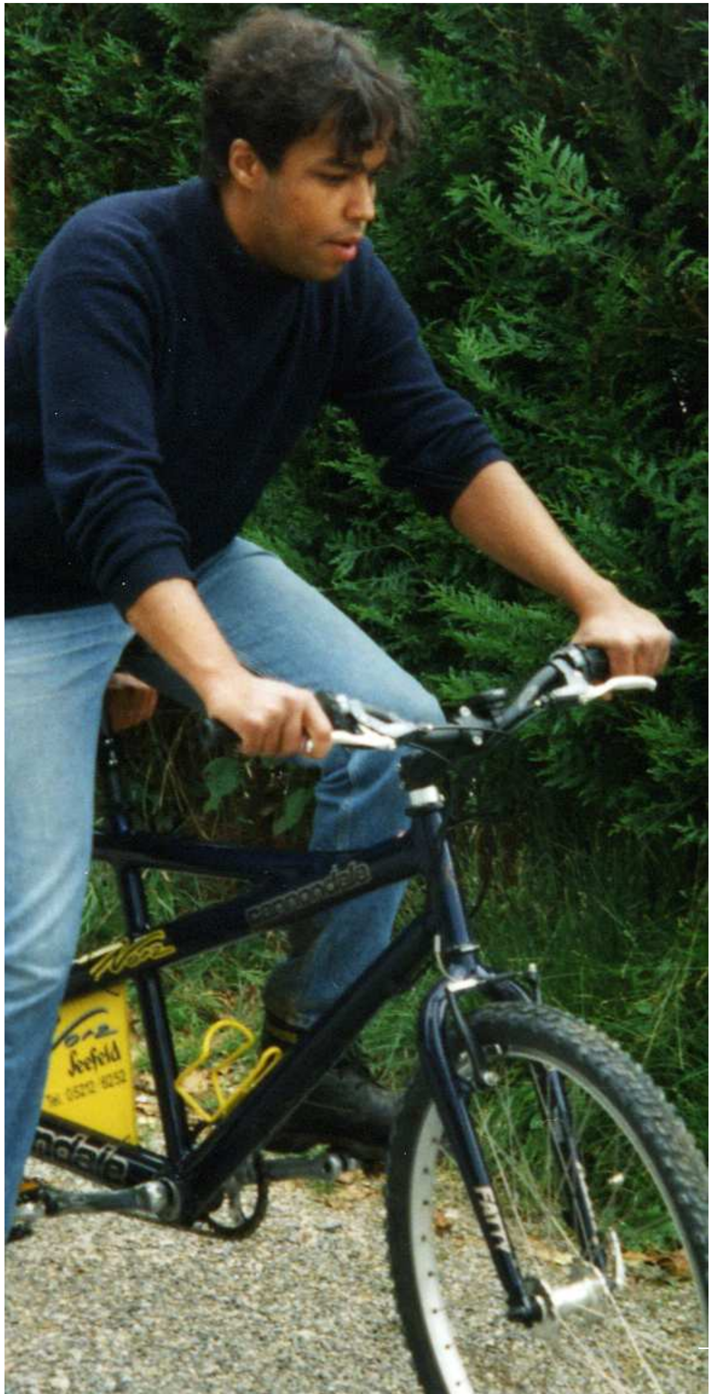
...Lebedev, Medovikov



...Lebedev, Medovikov



... and Assyr Abdulle

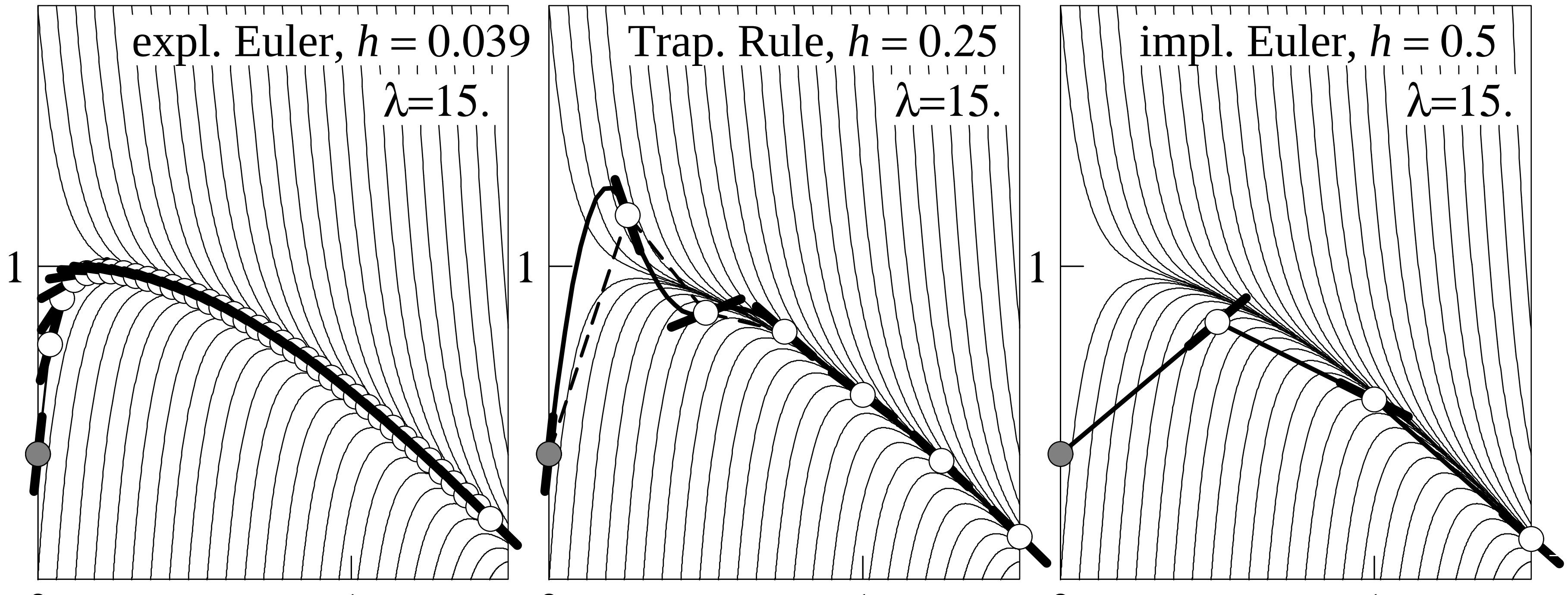


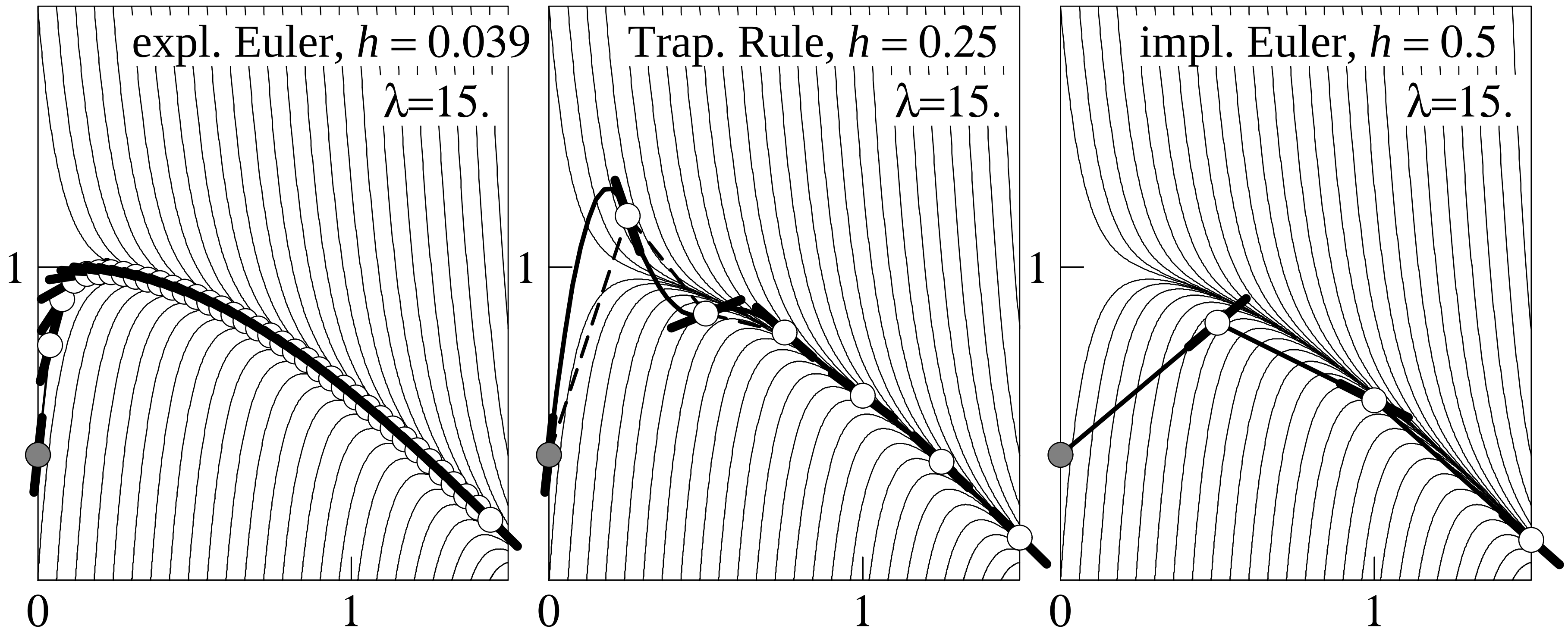
Stiff Equations

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

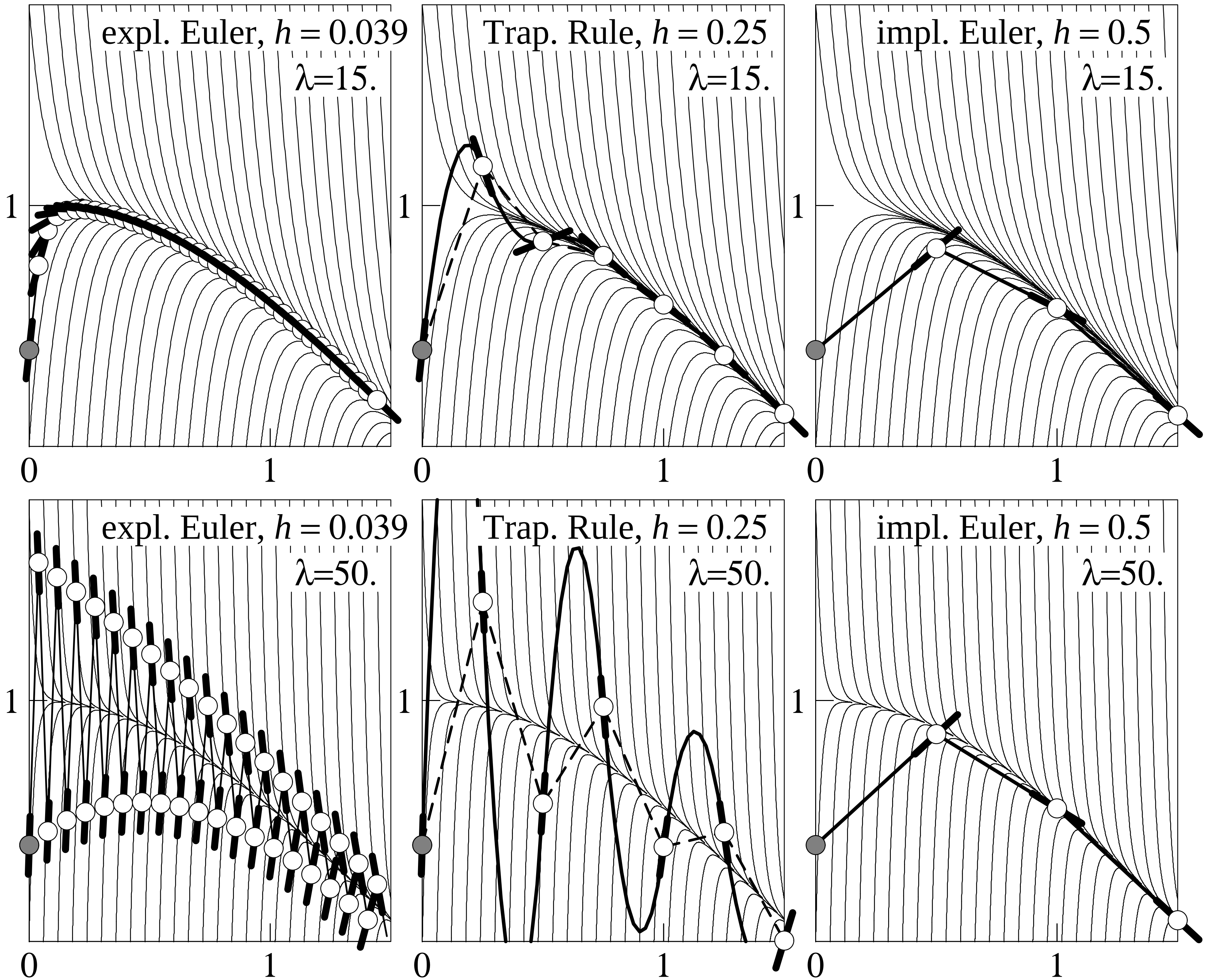
Stiff Problem
= search for a quiet life inside a turbulent world ...

Example: $y' = -\lambda(y - \cos x)$

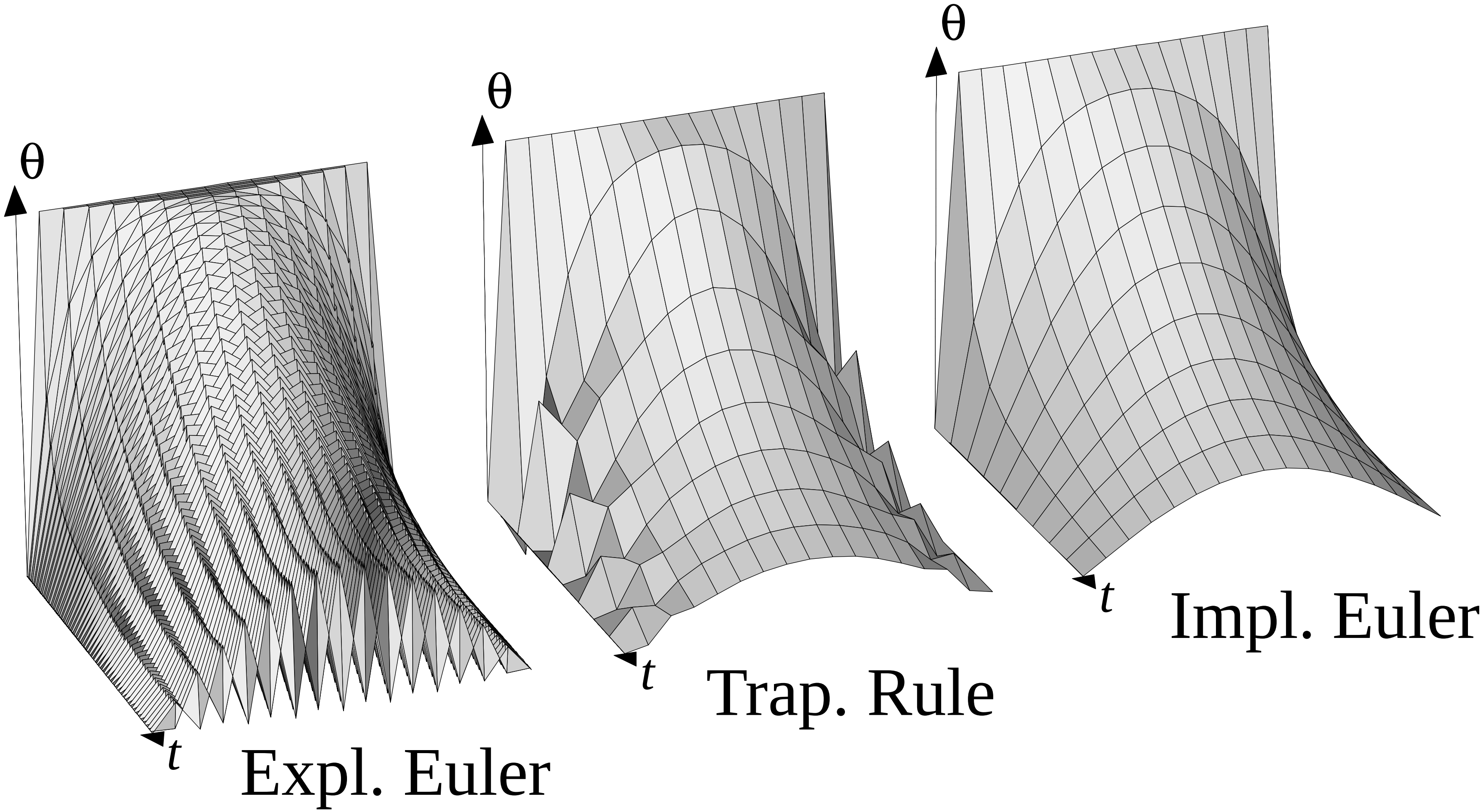




expl. Euler, $h = 0.039$
λ=15.
Trap. Rule, $h = 0.25$
λ=15.
impl. Euler, $h = 0.5$
λ=15.
1
0
1


expl. Euler, $h = 0.039$
λ=15.
Trap. Rule, $h = 0.25$
λ=15.
impl. Euler, $h = 0.5$
λ=15.
expl. Euler, $h = 0.039$
λ=50.
Trap. Rule, $h = 0.25$
λ=50.
impl. Euler, $h = 0.5$
λ=50.
1
0
1

Another Example. The heat equation $\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}$



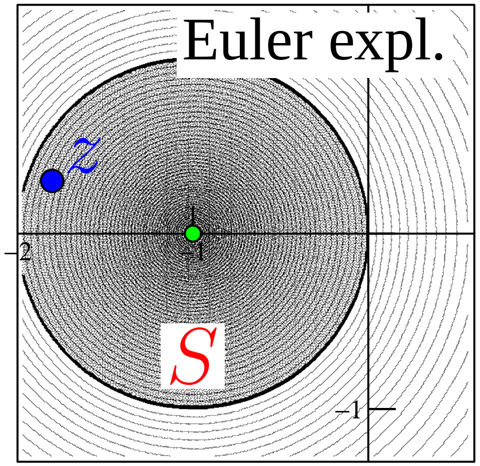
Stability Analysis:

$$y' = \lambda y \qquad \Rightarrow \qquad y_{n+1} = R(z) y_n \quad z = h\lambda;$$

Examples:

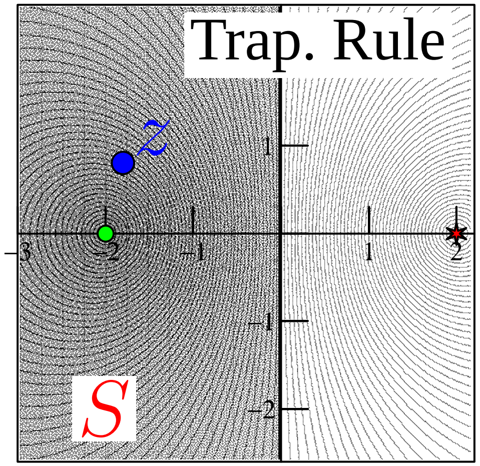
Expl. Euler

$$R(z) = 1 + z$$



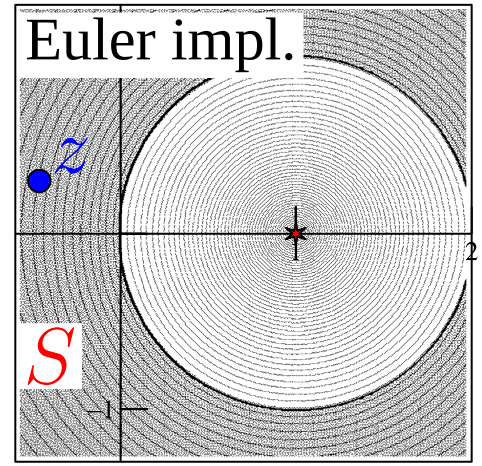
Trap. Rule

$$R(z) = \frac{1 + \frac{z}{2}}{1 - \frac{z}{2}}$$

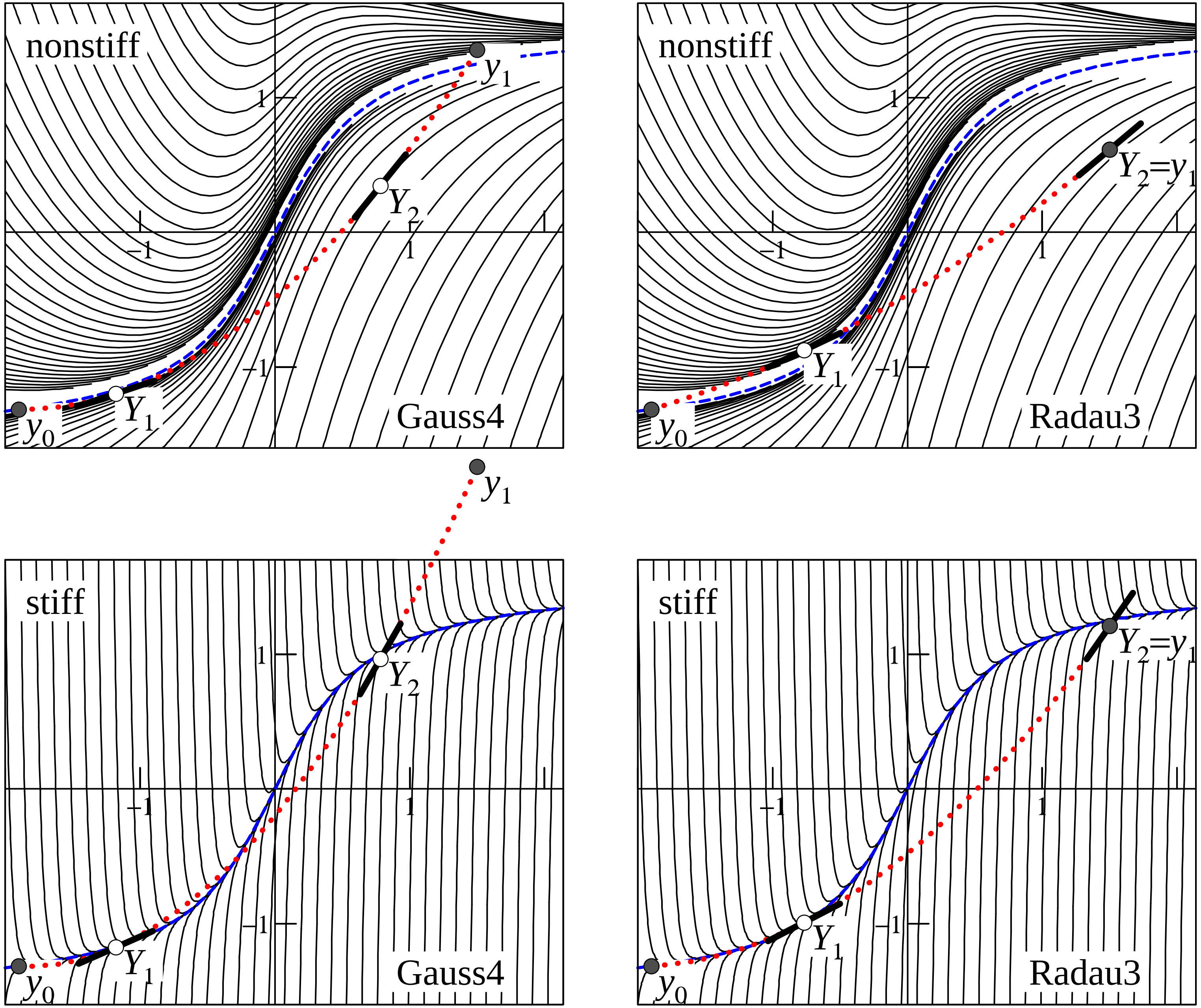


Impl. Euler

$$R(z) = \frac{1}{1 - z}$$



More general methods (Kuntzmann, Butcher 1964, Ehle 1968)



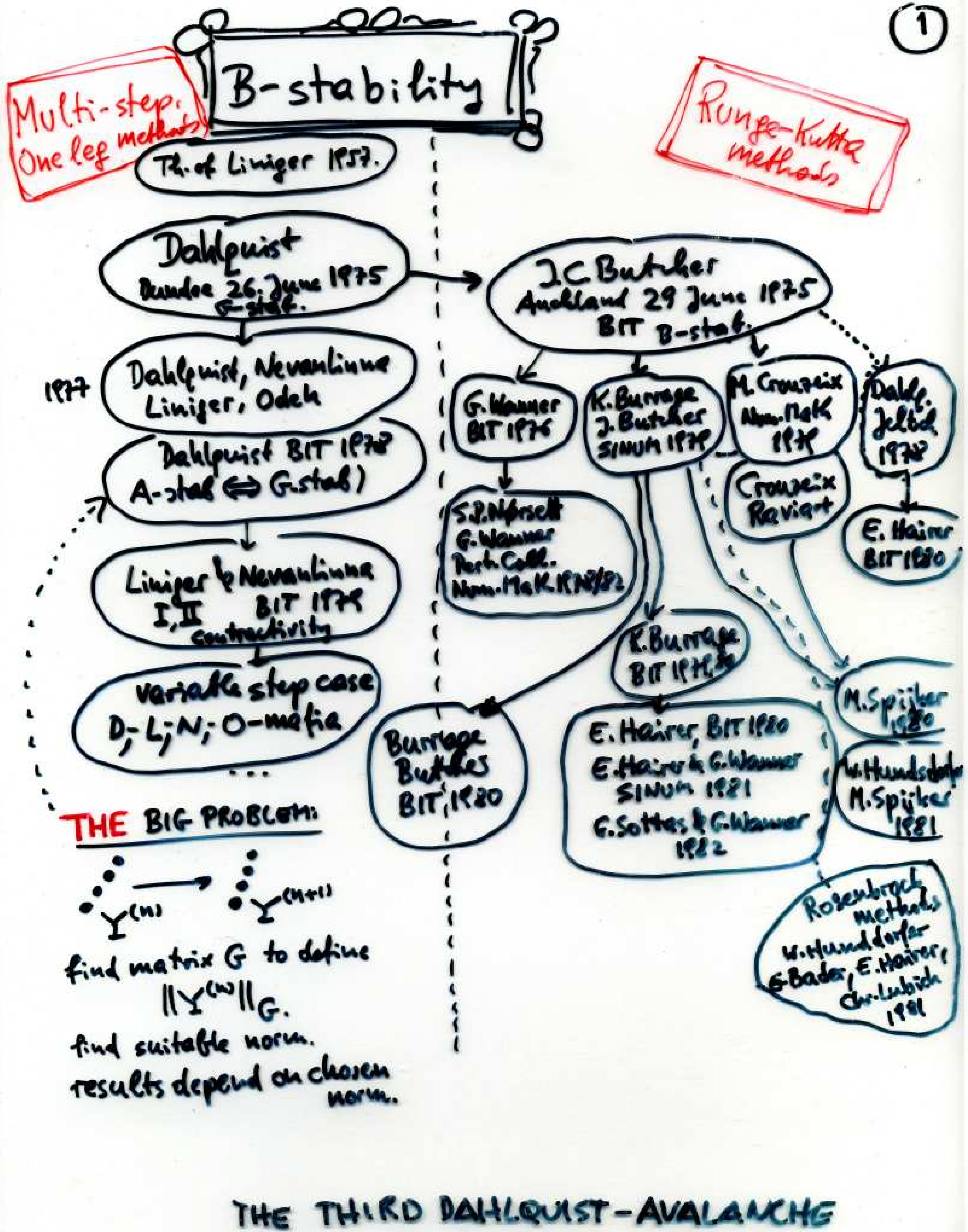
Theories

STABILITÄTSTHEORIEN
FÜR STEIFE DIFFERENTIALGLEICHUNGEN

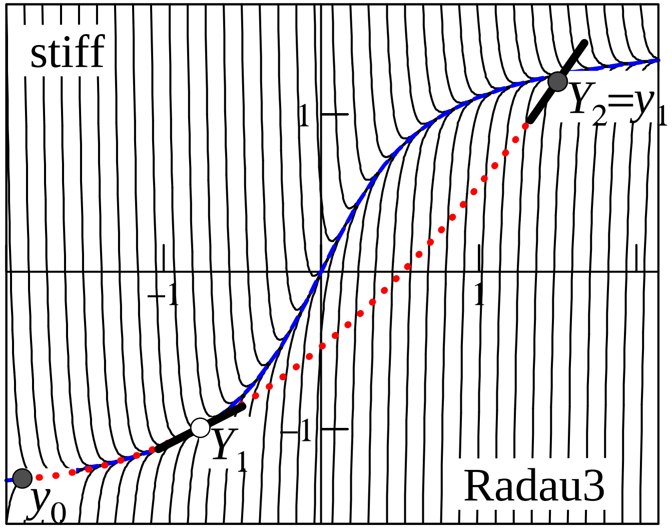
INHALT:

A-stable
A(α)-stable
A(0)-stable
A_0-stable
Å-stable
AN-stable
A_D-stable
algebraically stable
B-stable, B-consistent, B-convergent
BN-stable
BS-stable
BSI-stable ← C-stable
circle contractive
D-stable
D-stable
G-stable (A-contr.)
I-stable
internally stable
L-stable
internally L-stable
multiplyers
O-stable
P-stable, stable, R-stable, S-stable, stiffly stable, variable Schritte, splitting Methoden, W-methoden ...

B-Stability


B-stability
Multi-step, One leg methods
Runge-Kutta methods
Th. of Liniger 1957.
Dahlquist Dundee 26. June 1975 G-stab.
J.C. Butcher Auckland 29 June 1975 BIT B-stab.
1977 Dahlquist, Nevanlinna Liniger, Odeh
Dahlquist BIT 1978 (A-stab ⇔ G-stab)
Liniger & Nevanlinna I, II BIT 1979 contractivity
variable step case D; L; N; O-mafia
G. Wanner BIT 1976
K. Burrage J. Butcher SINUM 1979
M. Crouzeix Num. Math. 1979
Dahlq. Jeltsch 1979
S.P. Nørsett G. Wanner Perth Coll. Num. Math. 1979/82
Crouzeix Raviart
E. Hairer BIT 1980
K. Burrage BIT 1978
Burrage Butcher BIT 1980
E. Hairer, BIT 1980
E. Hairer & G. Wanner SINUM 1981
G. Söttes & G. Wanner 1982
M. Spijker 1980
W. Hundsdorfer M. Spijker 1981
Rosenbrock methods W. Hundsdorfer, G. Bader, E. Hairer, Chr. Lubich 1981
THE BIG PROBLEM:
find matrix G to define
find suitable norm.
results depend on chosen norm.
THE THIRD DAHLQUIST-AVALANCHE

RADAU (General purpose code for stiff problems, E. Hairer):



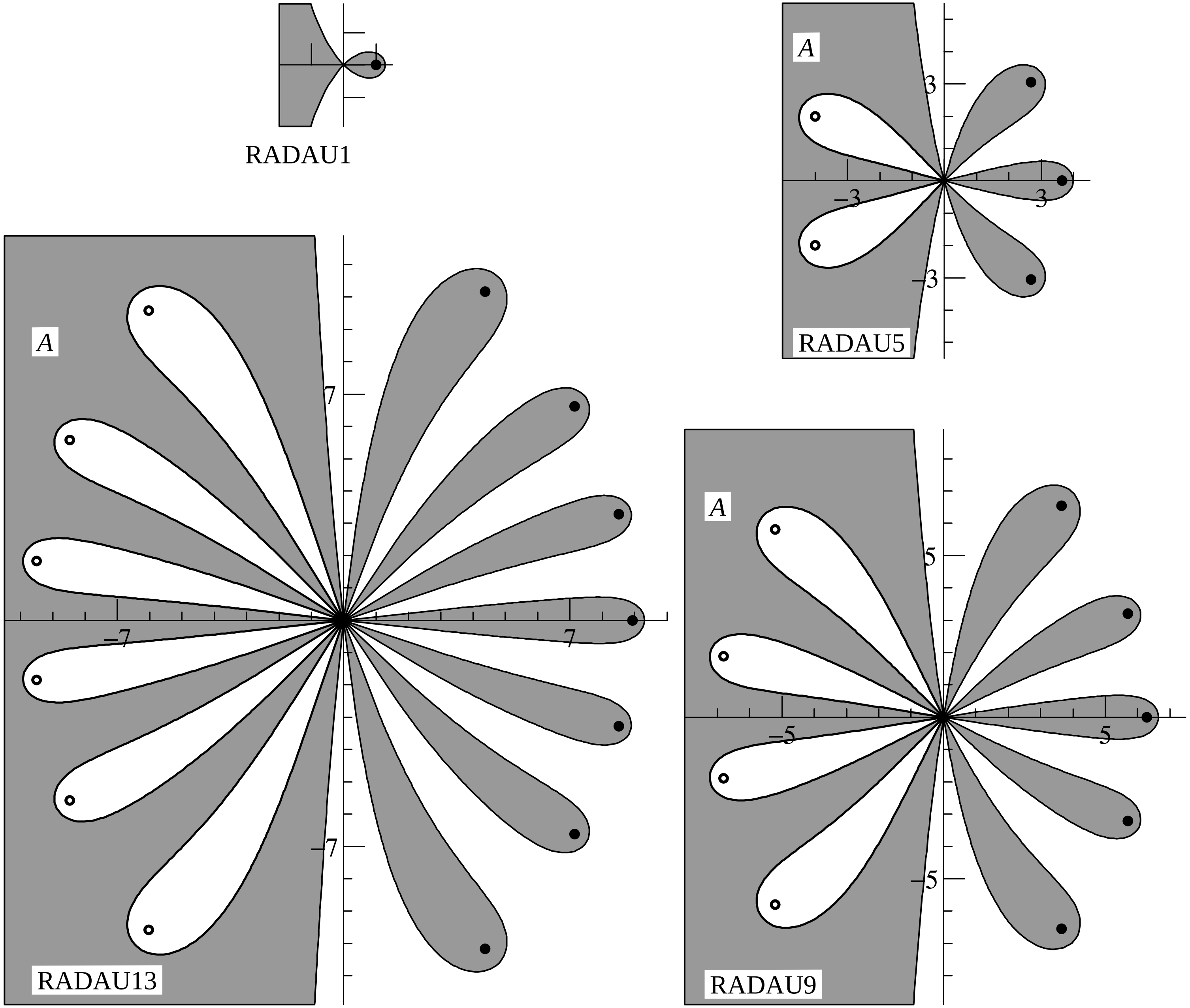
$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & \frac{-1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

Radau3

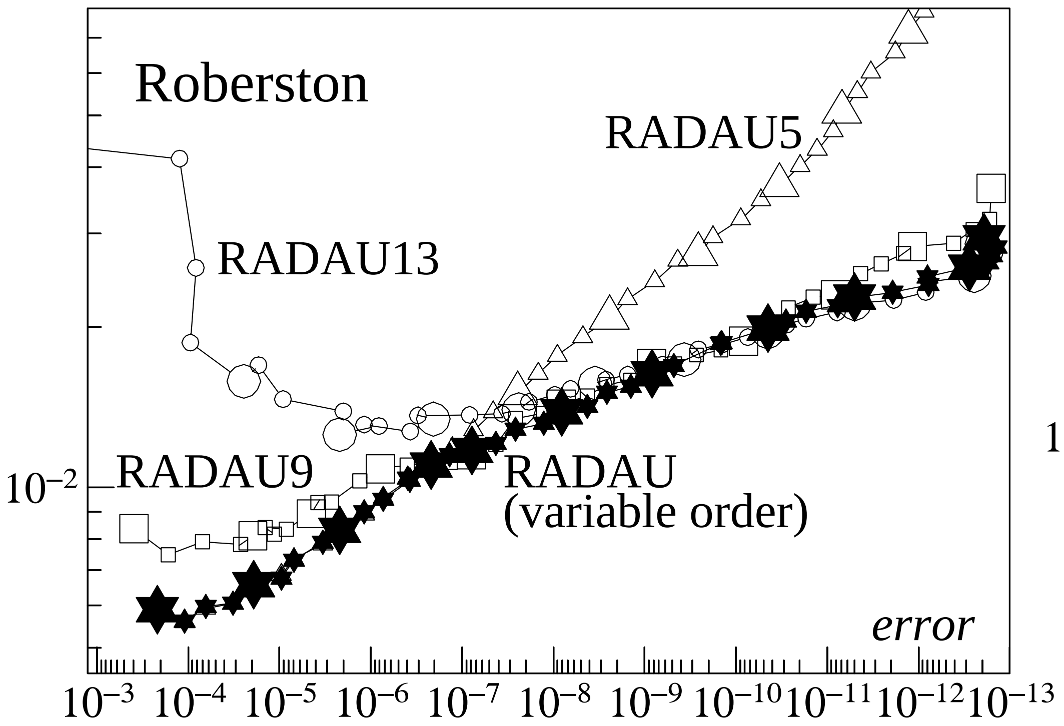
$$\begin{array}{c|ccc} \frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\ \frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\ 1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

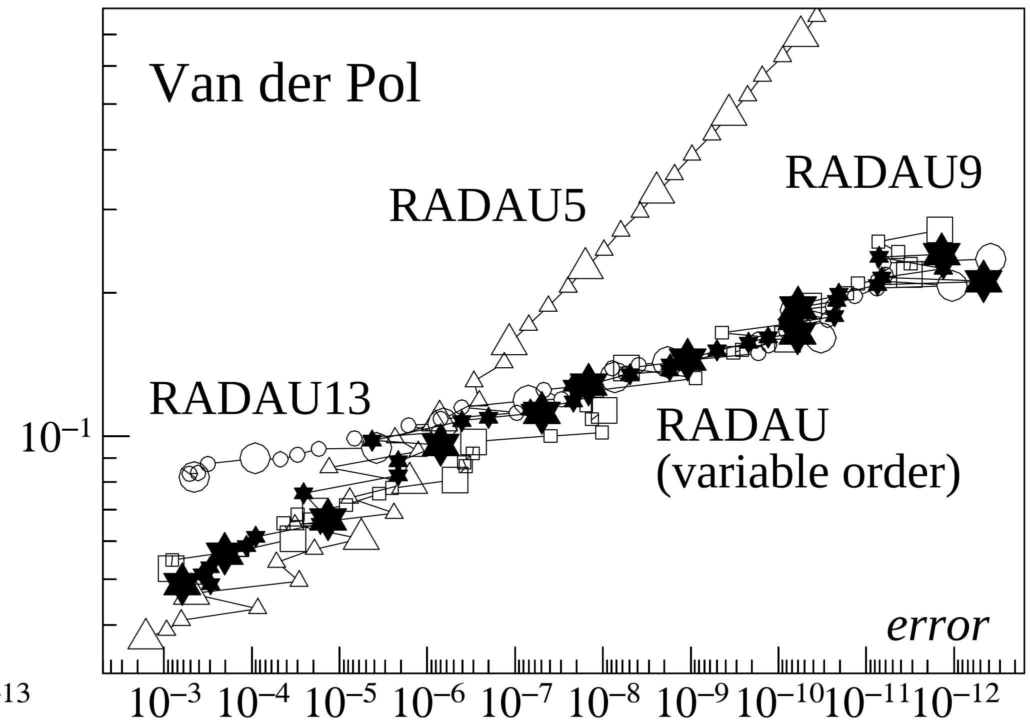
Radau5

Their order stars:

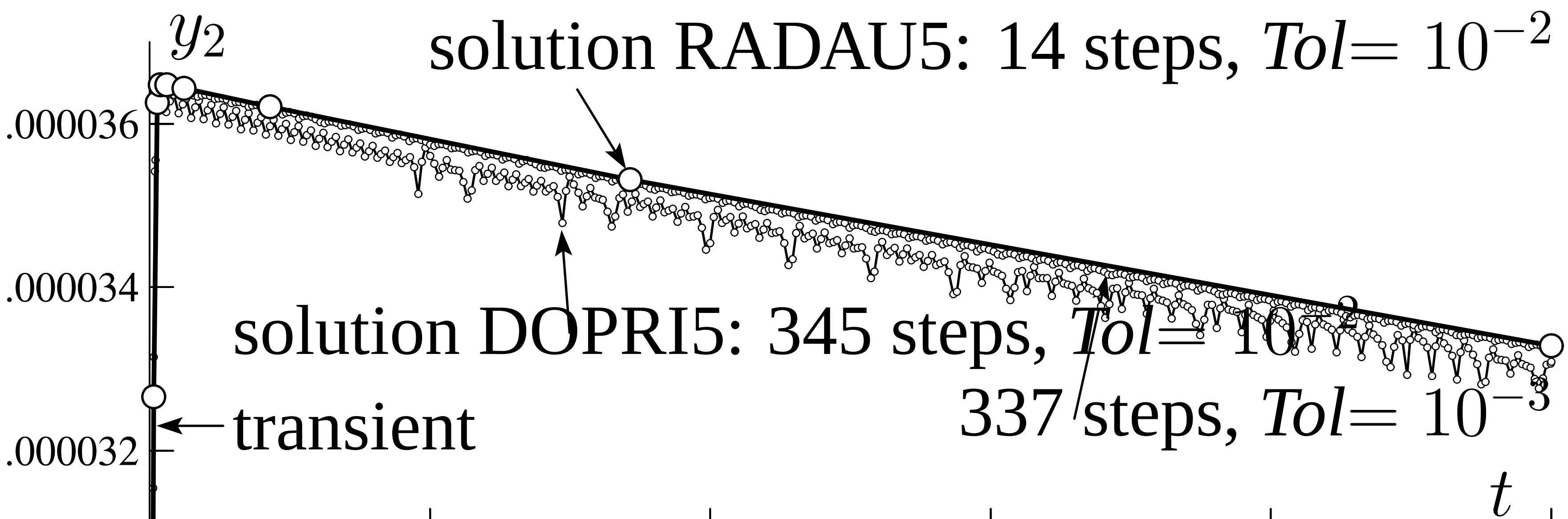


Variable order RADAU code:





Robertson reaction:



The Price to Pay: Fully Implicit Method..

The Price to Pay: Fully Implicit Method..

Explicit Methods ..?

The Controversy between Multistep and Runge-Kutta

> 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...
>
> (Dr. J.M. Bennett, Sydney, in a discussion 1956)

> 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)

Circle Theorems (Jeltsch, Nevanlinna)

19.10.78

I) Kreis Sätze

$$D_r = \{\mu \mid |\mu + r| \le r\}$$

Möchte $D_r \subset S$, r so gross wie möglich.

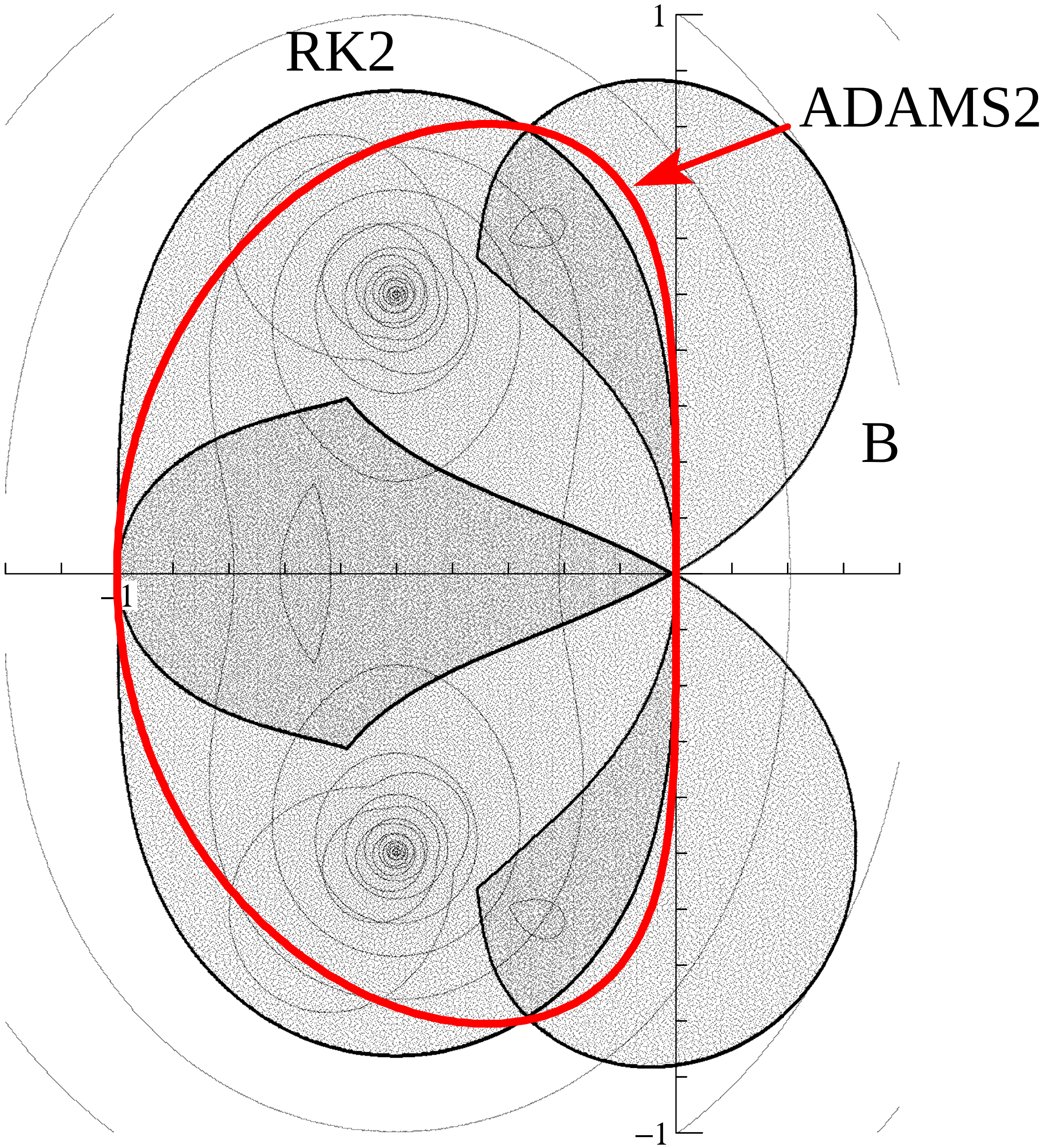
(Warum $D_r \subset S$, stabilitäts Resultat kann für nicht lineare Fall auch gezeigt werden

Satz 3 m-stufig, $P(\mu)$ irreduzibel

$$\Rightarrow D_m \not\subset S \quad \text{oder} \quad P(\mu) = \left(1 + \frac{\mu}{m}\right)^m$$

Bem. 1–4 Siehe 1.13.1 – 1.13.4

Jeltsch-Nevanlinna Theorem.



$$|\zeta_{\text{adams}}(\mu)| > |R_{\text{rk}}(\mu)|$$

$$\Rightarrow \qquad S_1^{scal} \not\supset S_2^{scal}$$

and $\qquad S_1^{scal} \not\subset S_2^{scal}$

there is no overall good explicit method !

Is there really no hope ...?

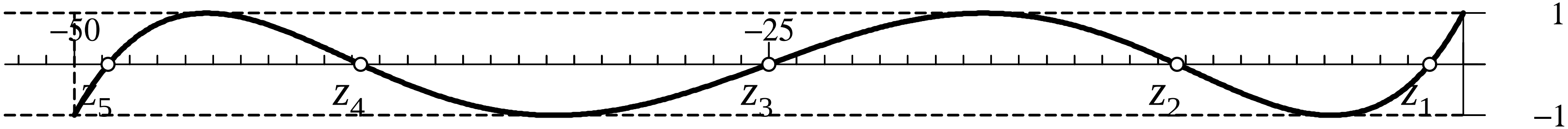
Yes, if, e.g., we know that eigenvalues are real.

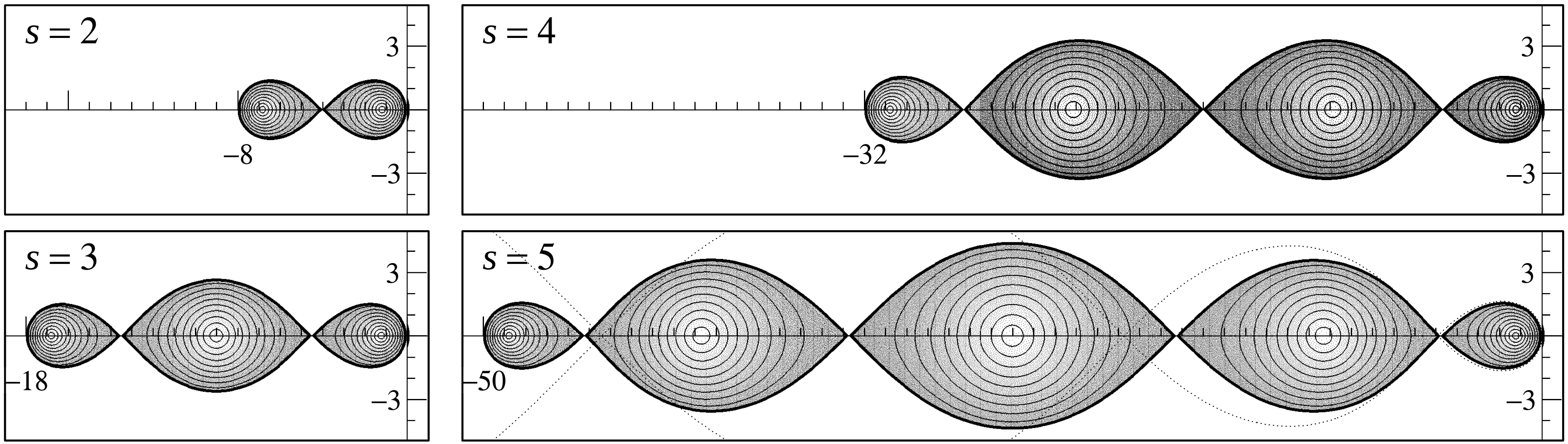
Problem. Find $R(z) = 1 + z + a_2 z^2 + \ldots + a_s z^s$ as stable as long as possible for $z \to -\infty$.

Yes, if, e.g., we know that eigenvalues are real.

Problem. Find $R(z) = 1 + z + a_2 z^2 + \ldots + a_s z^s$ as stable as long as possible for $z \to -\infty$.

Answer. $R(z) = T_s(1 + z/s^2)$ (Chebyshev polynomial)





Yes, if, e.g., we know that eigenvalues are real.

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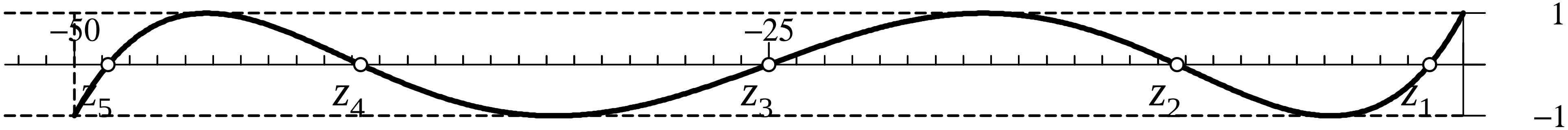


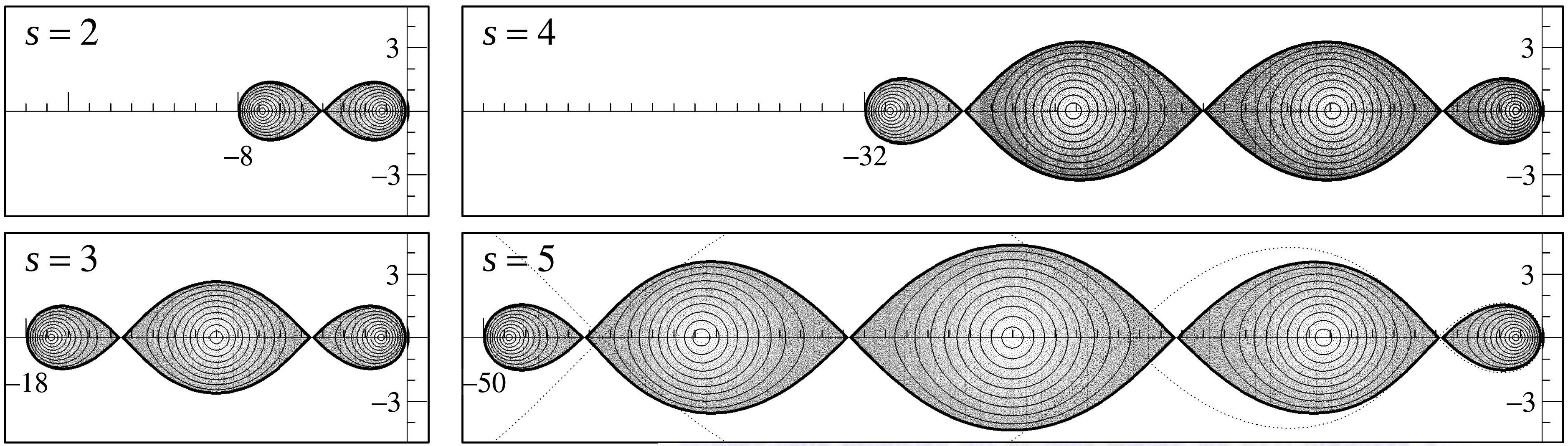
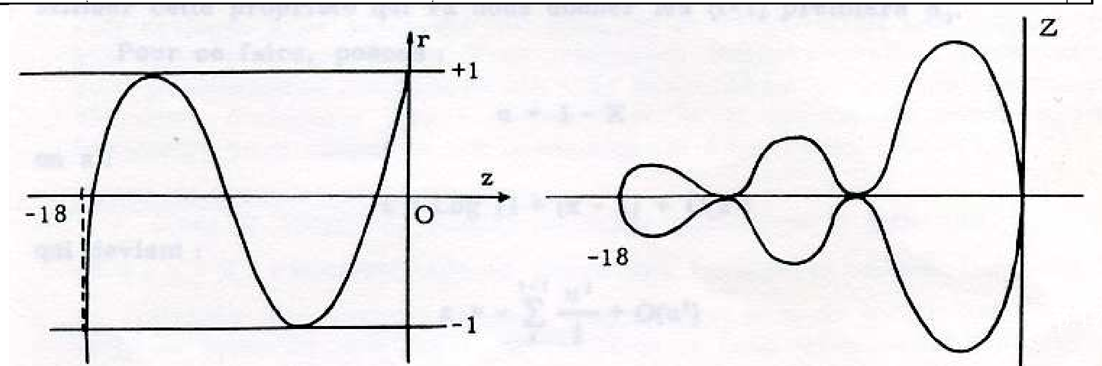


Illustration from Guillou-Lago (1961):

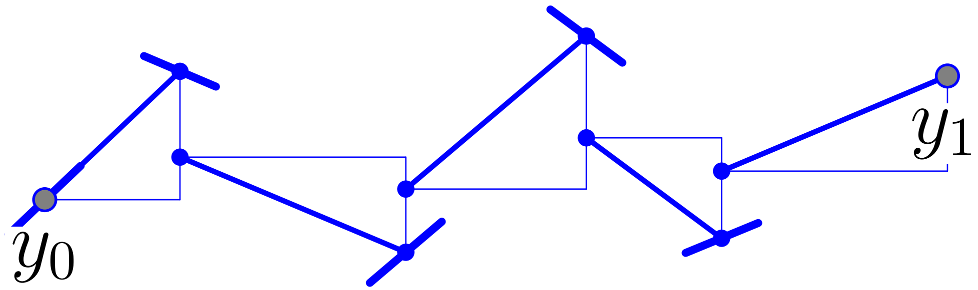


Realization for nonlinear problems:

Guillou-Lago, Saul'ev, Lebedev:

$$R_s(z) = \prod_{i=1}^{s} (1 + \delta_i z) \quad \Rightarrow \quad \text{composition of Euler steps.}$$

Van der Houwen-Sommeijer: Three term recursion for T_n $\Rightarrow$

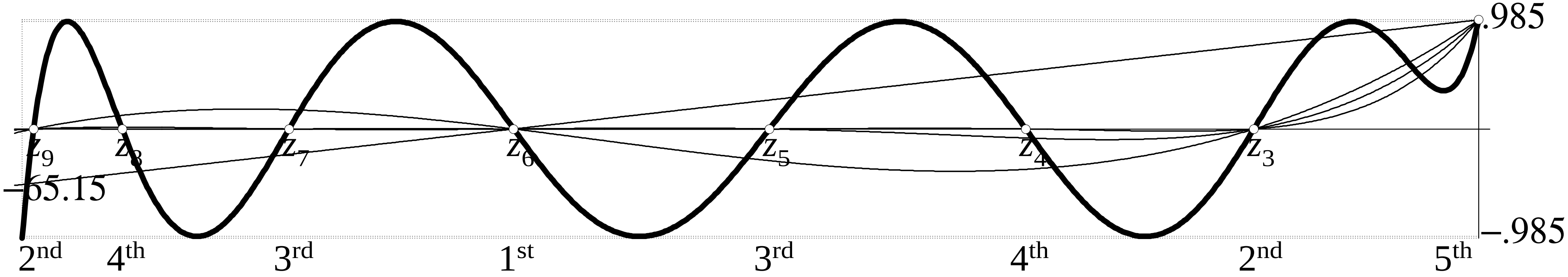


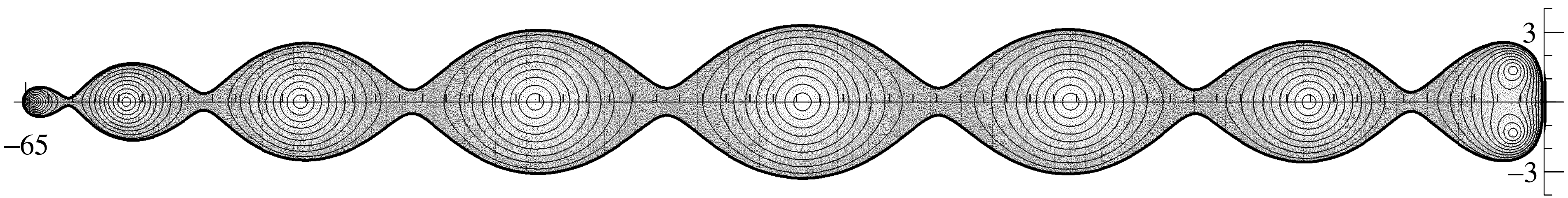
composition of 2-step formulas.

Methods of Order 2:

$$R_s(z) = 1 + z + \frac{z^2}{2} + a_3 z^3 + \ldots + a_s z^s$$

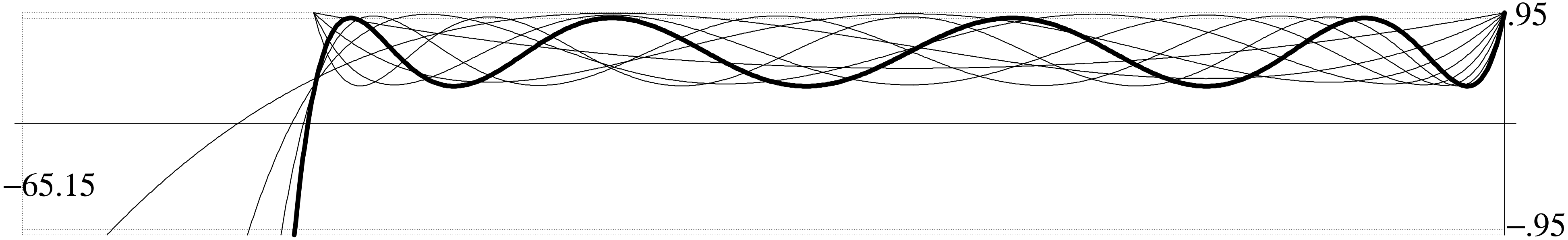
Lebedev: Zolotarev polynomials:

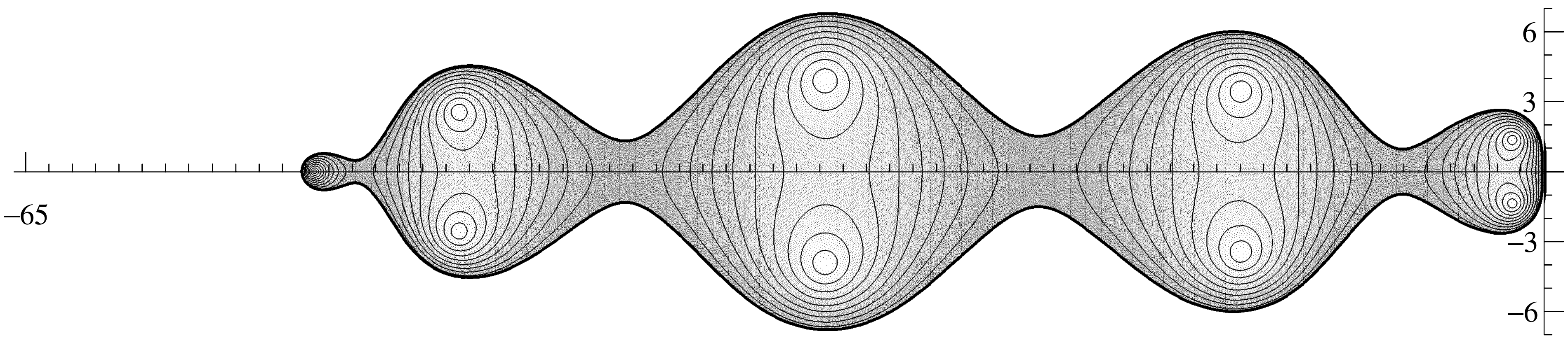




Van der Houwen-Sommeijer-Verwer:

Shift and scaling of T_n to produce 2nd order:





$\Rightarrow$ some loss of stability, but three term recursion preserved.

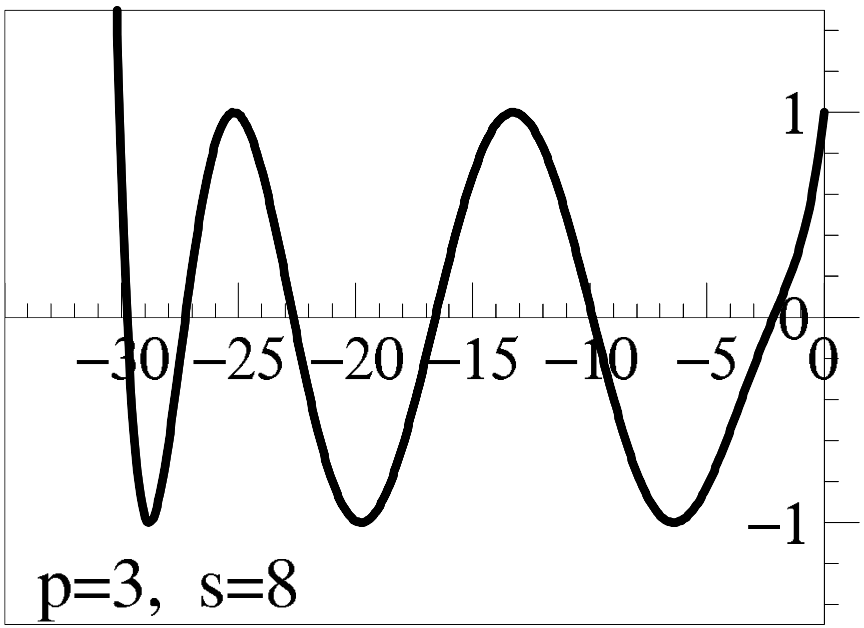
Higher Orders.

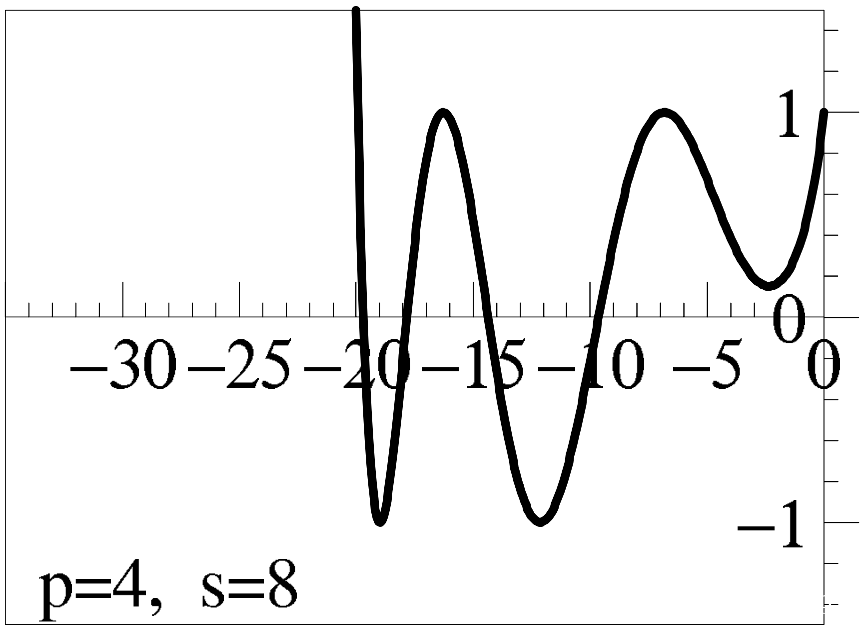
$$R_s^p(z) = 1 + z + \ldots + \frac{z^p}{p!} + a_{p+1}z^{p+1} + \ldots + a_s z^s$$

Problem (Lebedev 1995) **Theorem (Abdulle 2000)**

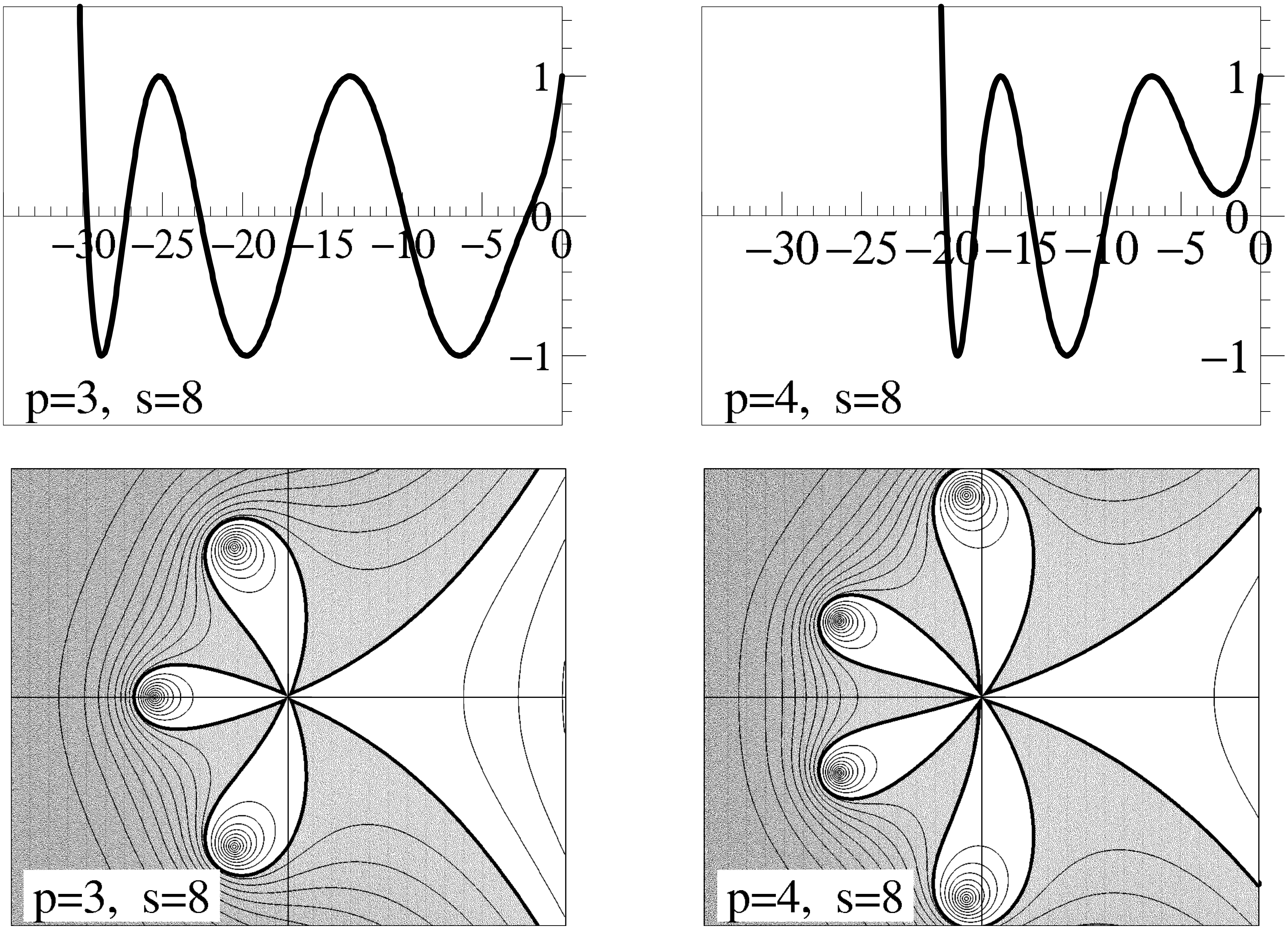
$R_s^p(z)$ possesses exactly p complex zeros if p is even and exactly $p-1$ complex zeros if p is odd. Remaining real zeros distinct $\in (-l_s^p, 0)$.

Error constants: for p given $C_{p+1}^p > C_{p+2}^p > \ldots > 0.$



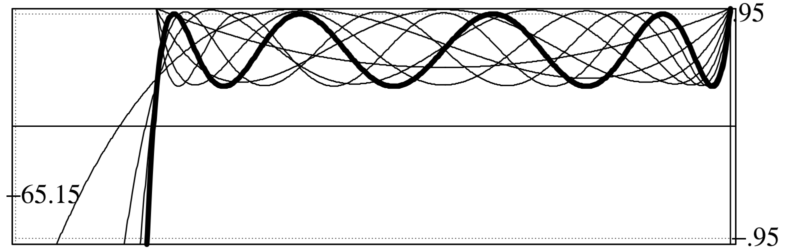


Proof by Order-Stars.

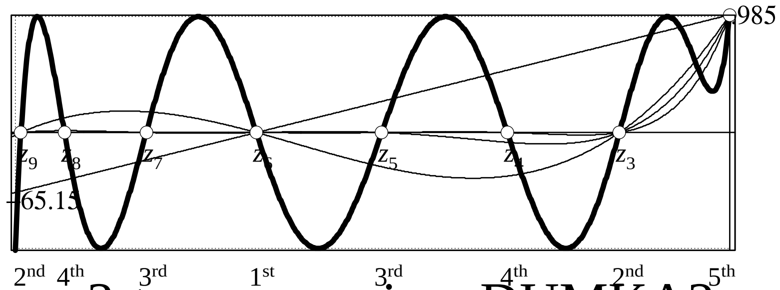


Towards ROCK : (Abdulle-Medovikov 1999, Abdulle 2002):

van der Houwen-Sommeijer 1980



Lebedev 1993

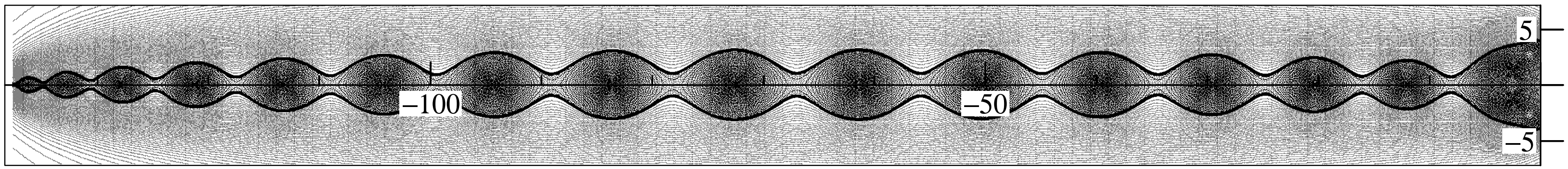


no 3-term recursion, DUMKA2

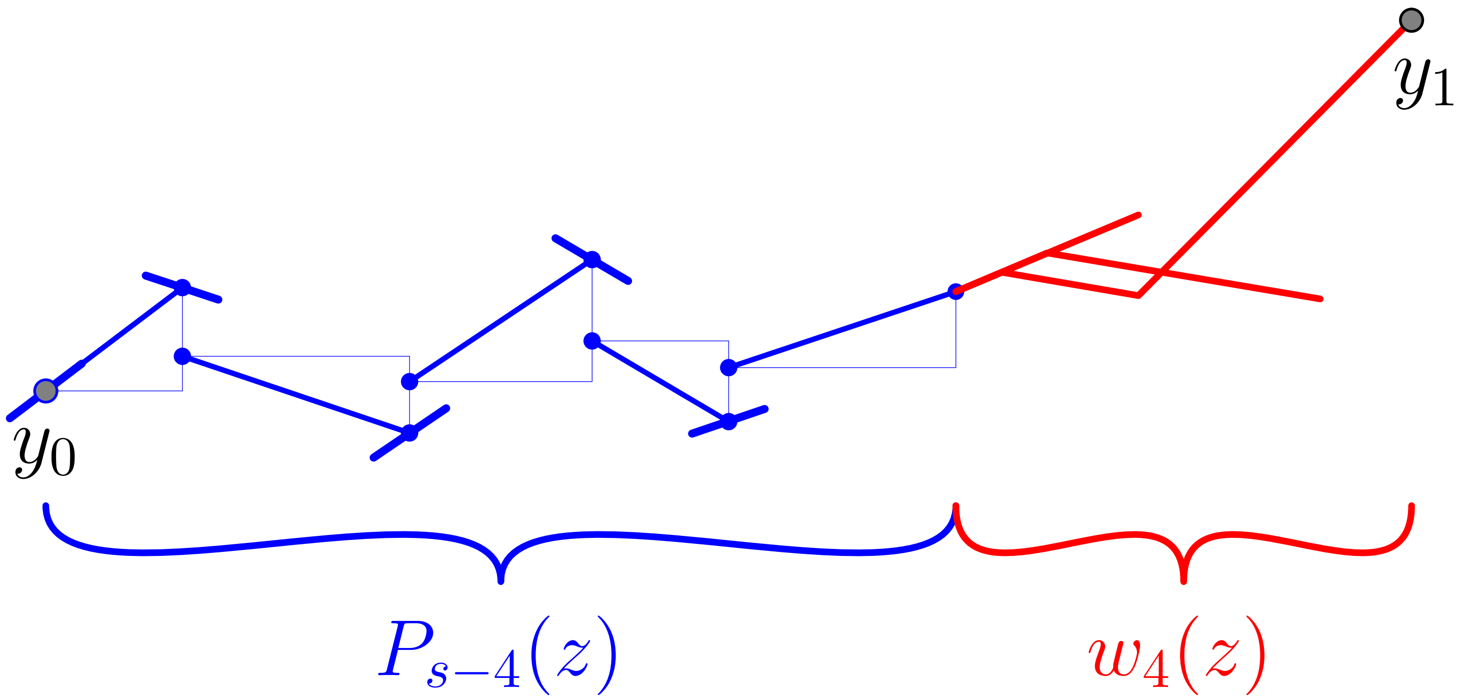
find approx. of order 4 to e^z

$$R_s(z) = w_4(z) P_{s-4}(z), \quad P_j(x) \text{ orthog. w.r.} \frac{w_4^2(x)}{\sqrt{1-x^2}}$$

Thm. Bernstein (1930): $\Rightarrow$ $R_s(z)$ 'nearly' optimal;
orthogonality: $\Rightarrow$ 3-term recursion .



Realization for nonlinear problems:

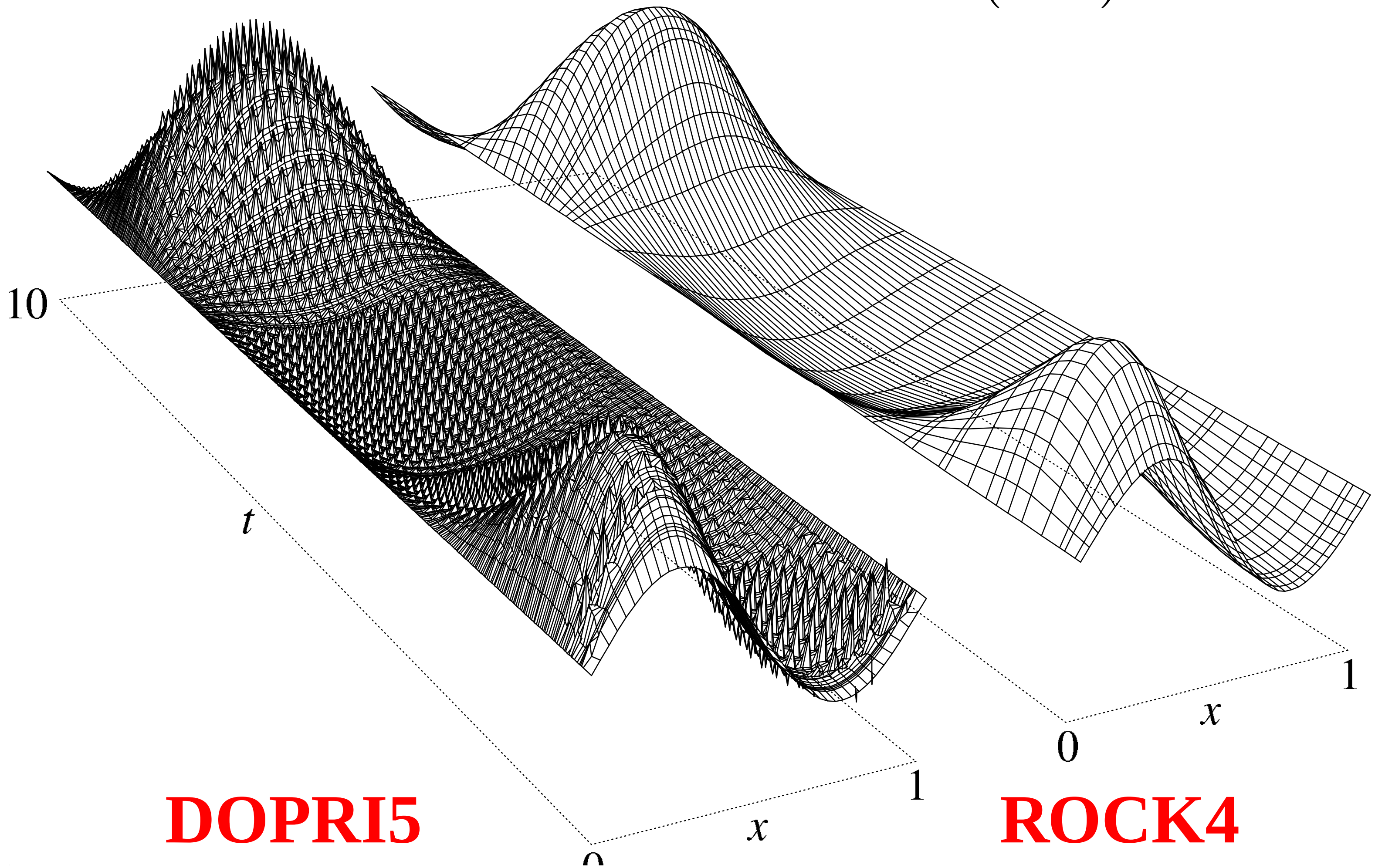


blue method given (from 3-term recursion), compose with red classical 4-stage RK method and achieve order 4 with the help of the **Butcher Group**

$\Rightarrow$ code **ROCK4**.

Example. Reaction-Diffusion (Brusselator with 1D diffusion).

$$\frac{\partial c}{\partial t} + f(c) = D\Delta c, \qquad \text{CFL:} \quad \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2D}$$



DOPRI5

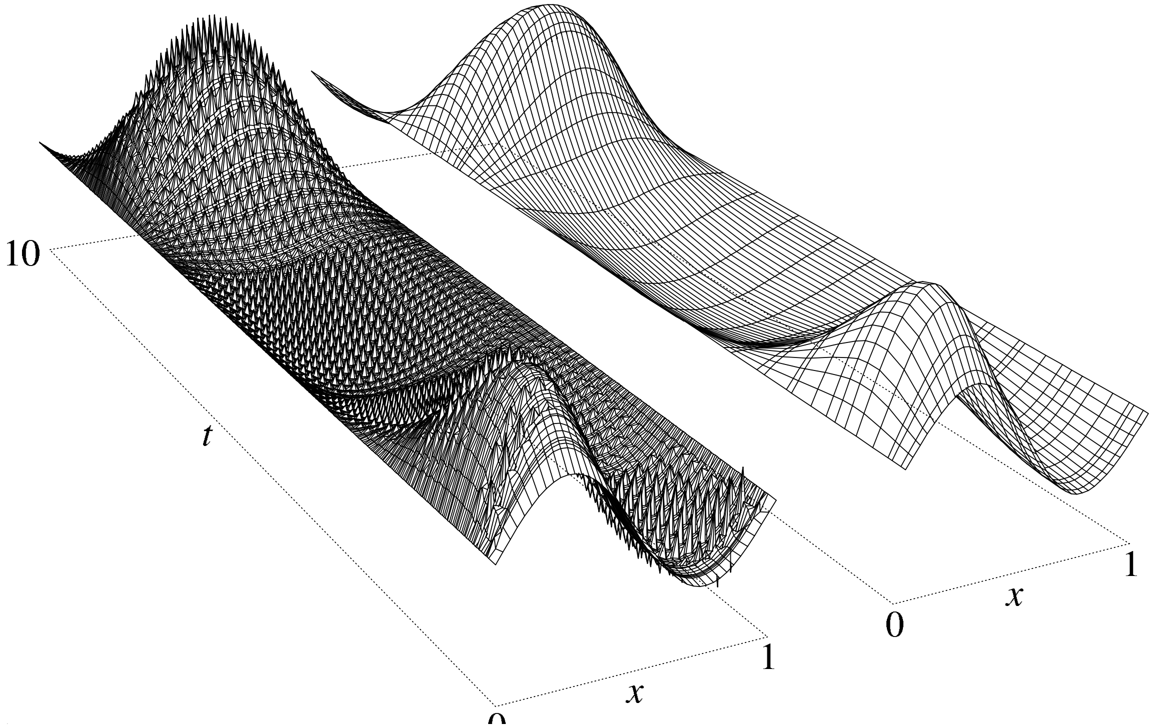
406 steps

Fcn. evaluation $C/(\Delta x)^2$

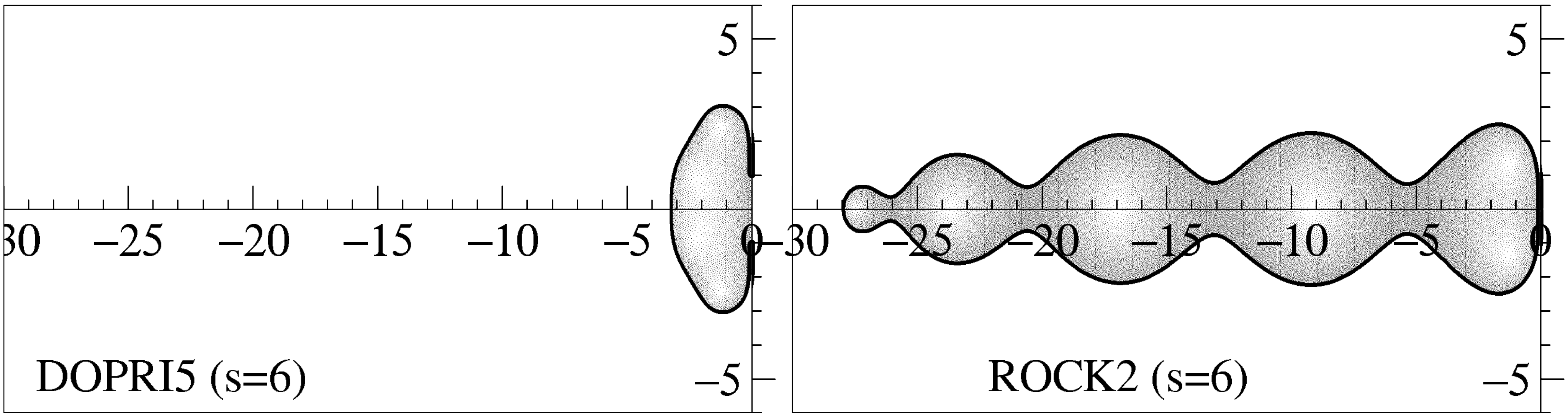
ROCK4

23 steps

Fcn. evaluation $\bar{C}/(\Delta x)$



Comparison of Stability Domains



Other Applications. (advection-diffusion-reaction)

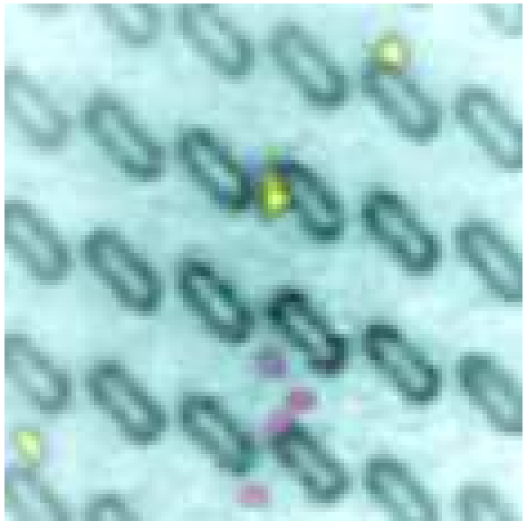
Nanoscale Tunneling Devices, Stiff biogeochemical models, Aggregation processes of molecules, Quantum problem, Competition between Protein Folding and Aggregation, Soft Tissue Simulation, Simulation of the Saint-Venant System, Modelisation of High Current Arc, etc.

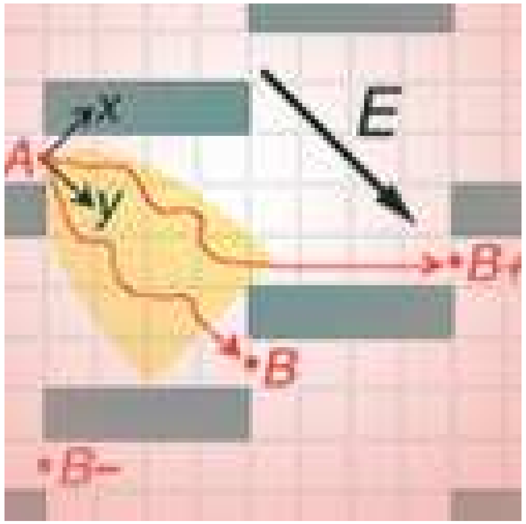
Other Applications. (advection-diffusion-reaction)

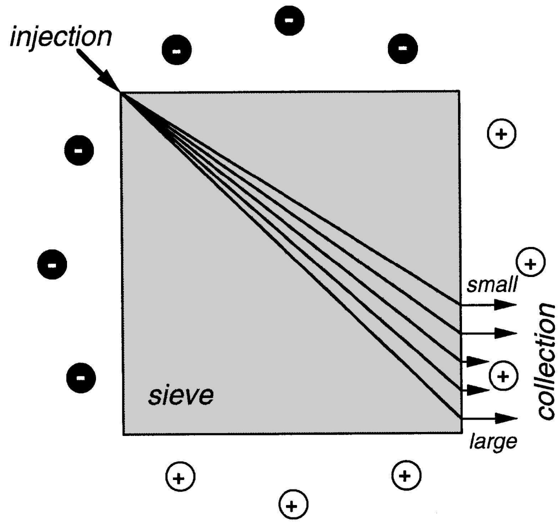
Nanoscale Tunneling Devices, Stiff biogeochemical models, Aggregation processes of molecules, Quantum problem, Competition between Protein Folding and Aggregation, Soft Tissue Simulation, Simulation of the Saint-Venant System, Modelisation of High Current Arc, etc.

More detailed Application. (Transport in microarray)

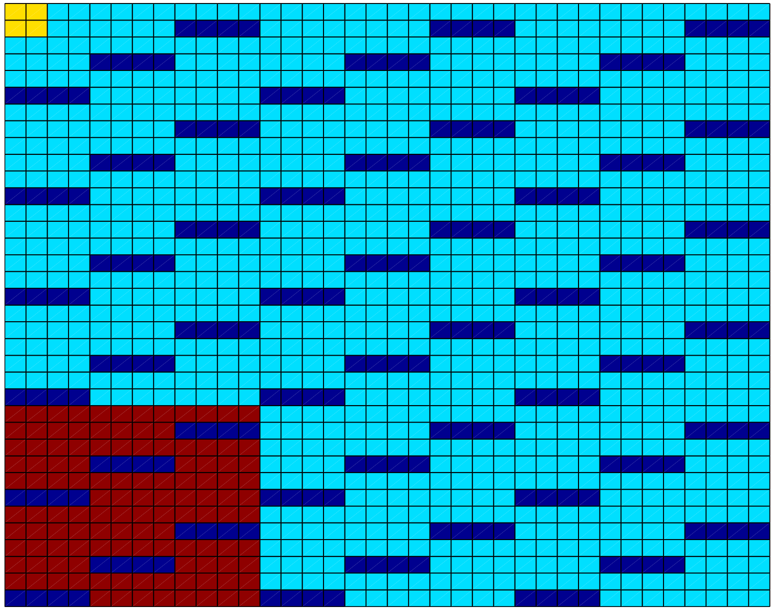
DNA separation in heterogeneous media (Duke and Austin, Ertas 1998-2003)







Multiscale transport modeling (Abdulle-Attinger).



Charged particles advected by electrical potential

$$v^{\varepsilon} = -\rho a^{\varepsilon} \nabla u \; , \qquad a^{\varepsilon} = a(x/\varepsilon)$$

Elliptic Equ. $\nabla \cdot (a^{\varepsilon} \nabla u^{\varepsilon}) = 0, \; u_{|\partial\Omega} = u_0$

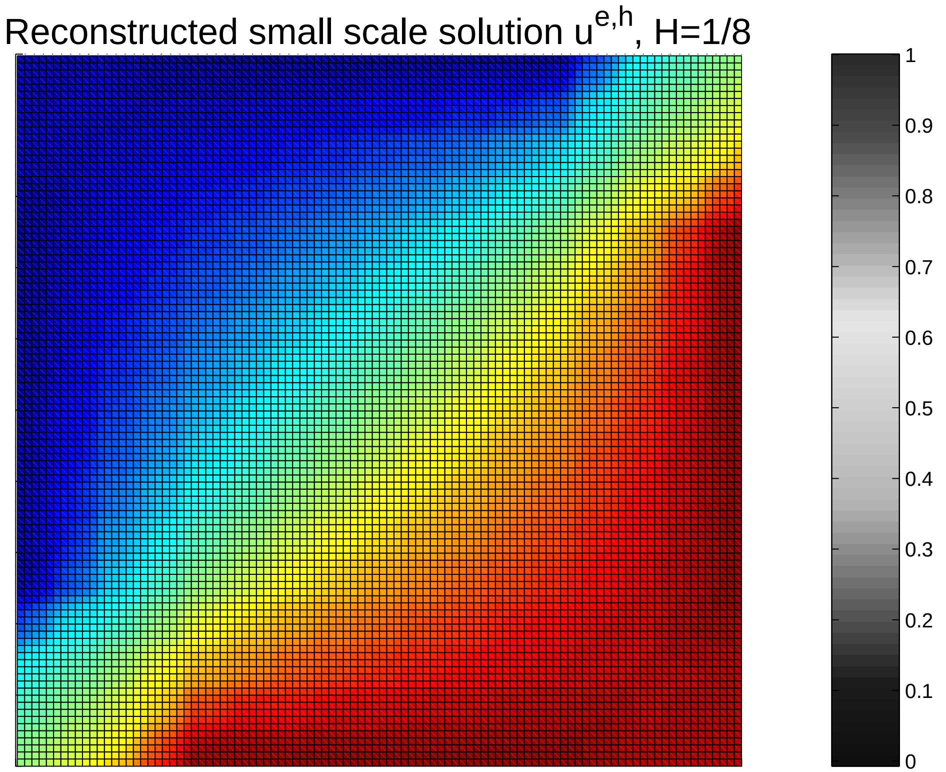
Adv.-Diff. $\dfrac{\partial c^{\varepsilon}}{\partial t} + v^{\varepsilon} \cdot \nabla c^{\varepsilon} = D \Delta c^{\varepsilon},$ with I. & B. cond.

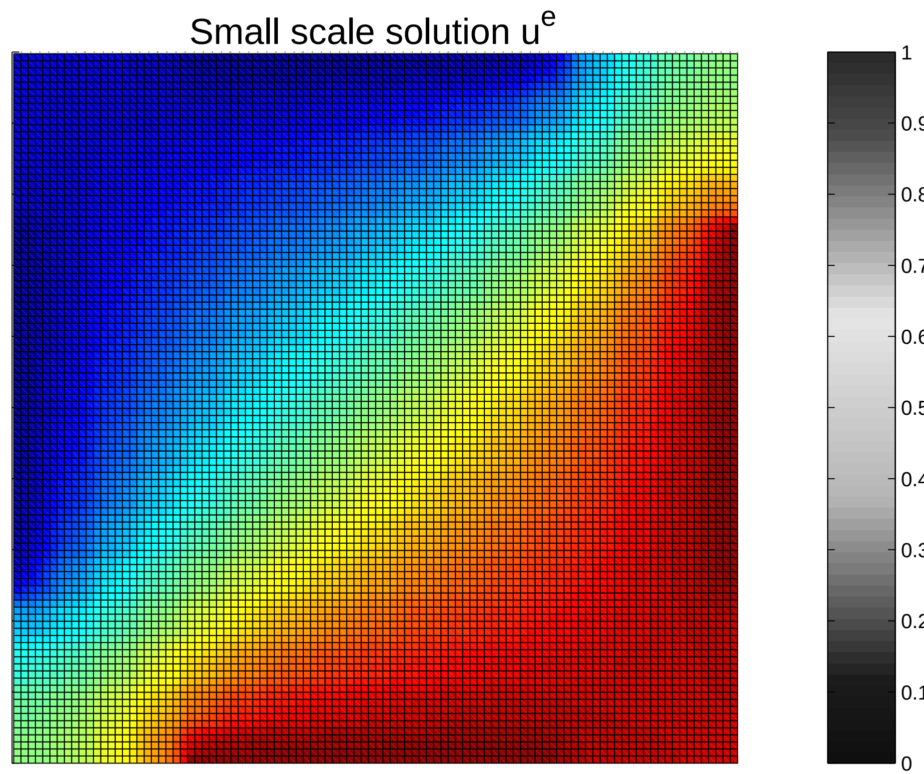
Multiscale:

Obstacles $\sim$ micrometer $\ll$ Device $\sim$ centimeter

Computational Simulation:

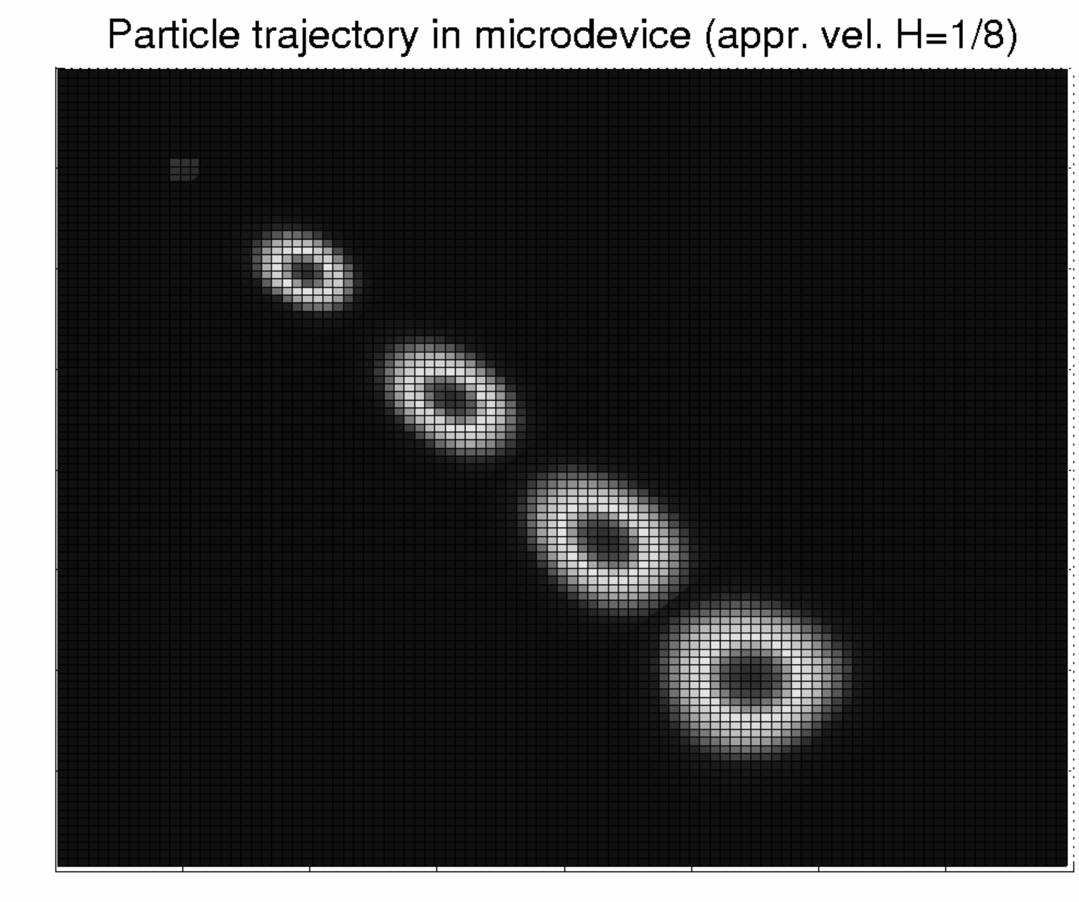
use finite element multiscale method (FE-HMM, Abdulle, E ...) for the multiscale elliptic problem ...

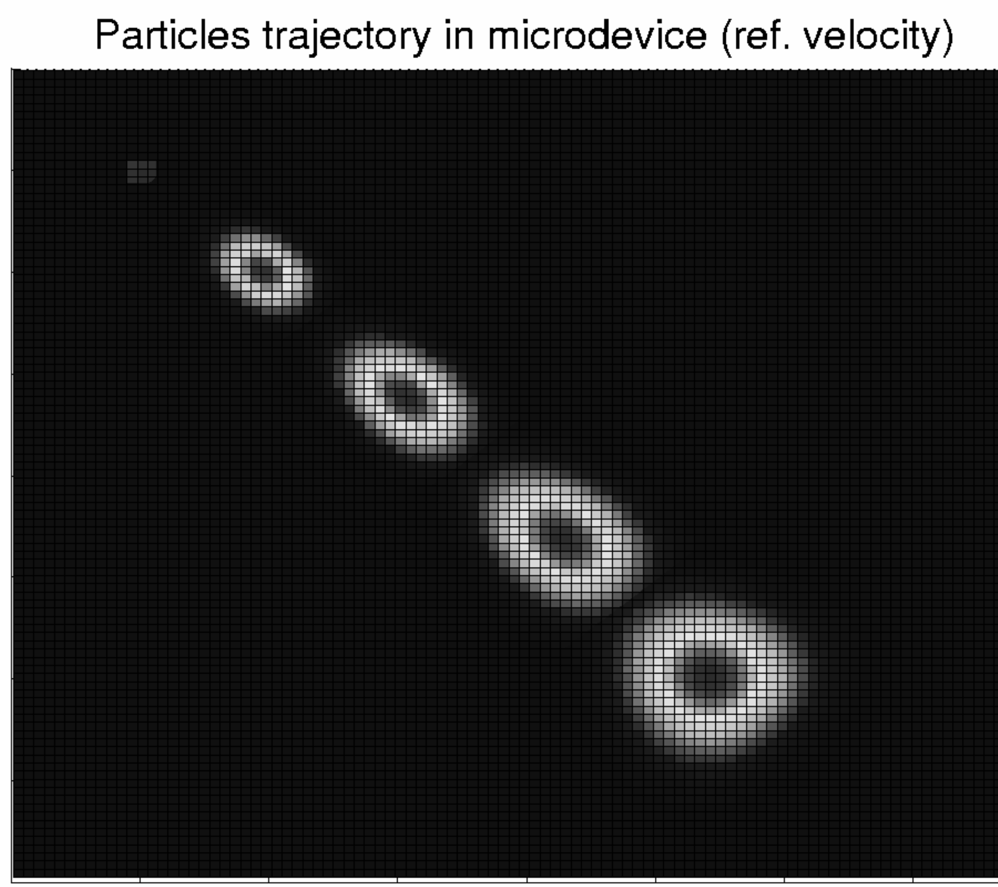




FE-HMM DOF$\sim 10^3$ FEM DOF$\sim 10^6$

... and ROCK for the transport problem:

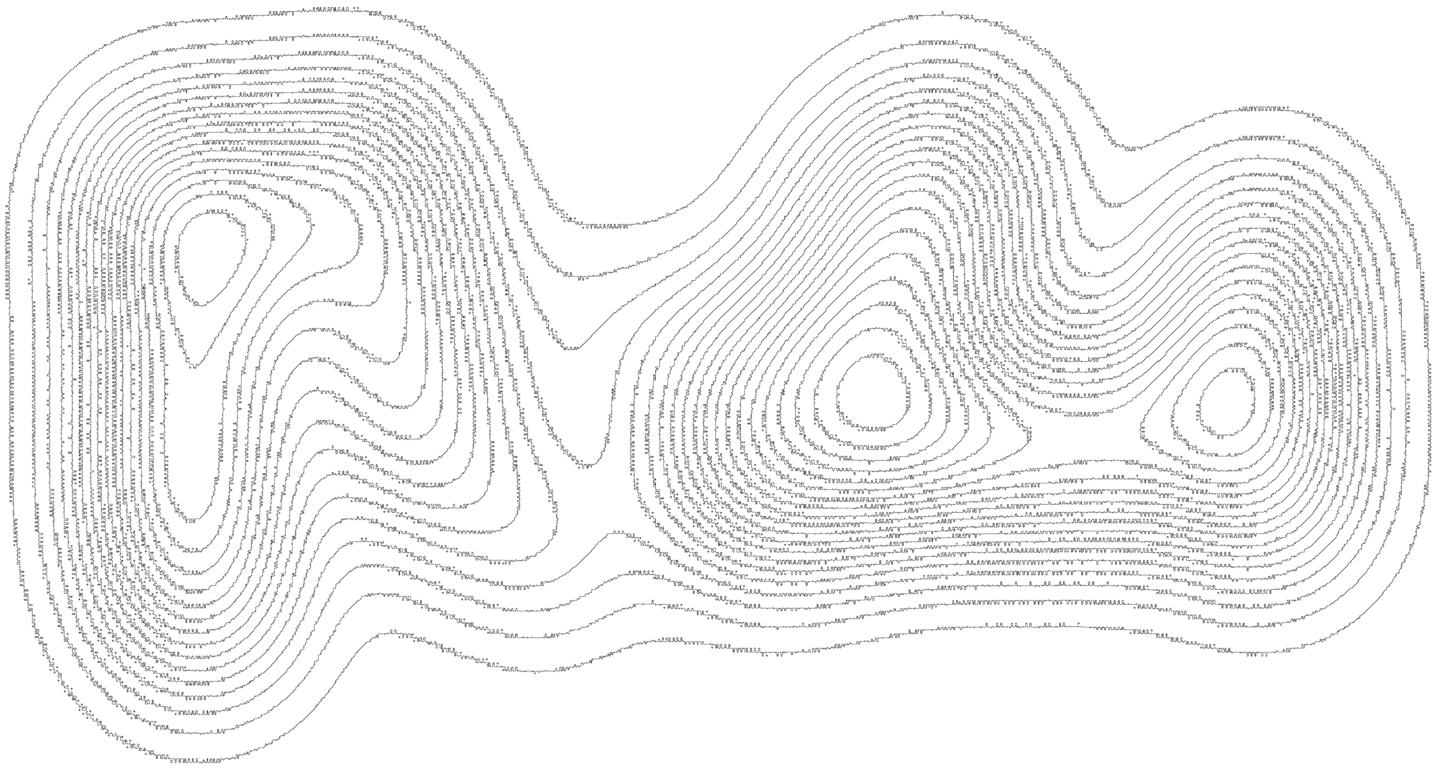




Cordiales félicitations et nos meilleurs voeux !!

Michel

What is ROCK doing with you?



Good Bye !! **Au revoir !!** **Do svidaniia !!**

Tot ziens !! **Uff wiederluege !!**

Auf Wiedersehen !!