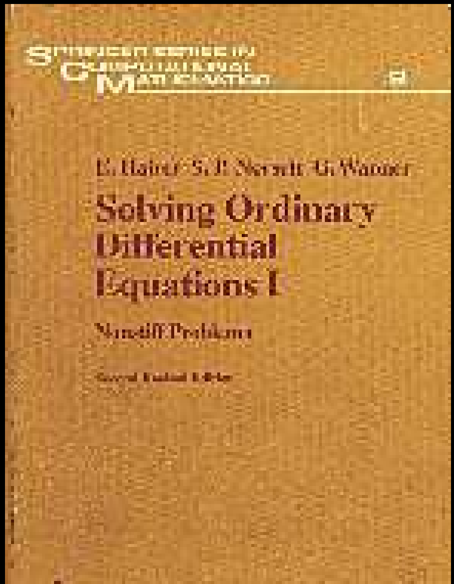
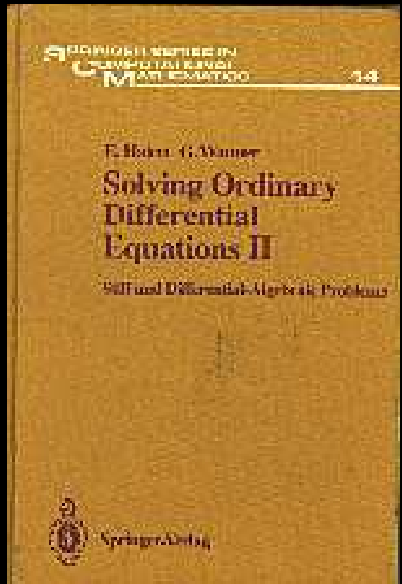
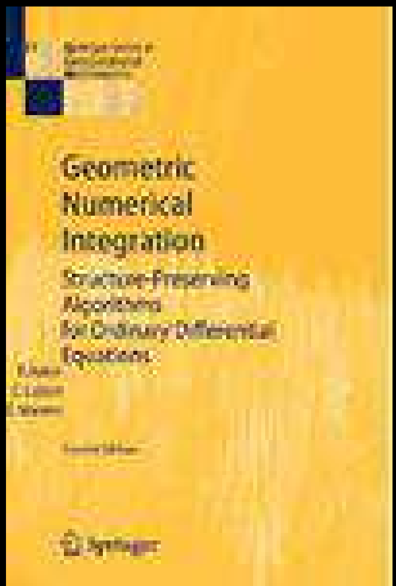
Nonstiff, Stiff and Geometric Integration

Nonstiff, Stiff and Geometric Integration







E. Hairer, Chr. Lubich, S.P. Nørsett, G. Wanner

From where come Differential Equations ??

Kepler

Newton

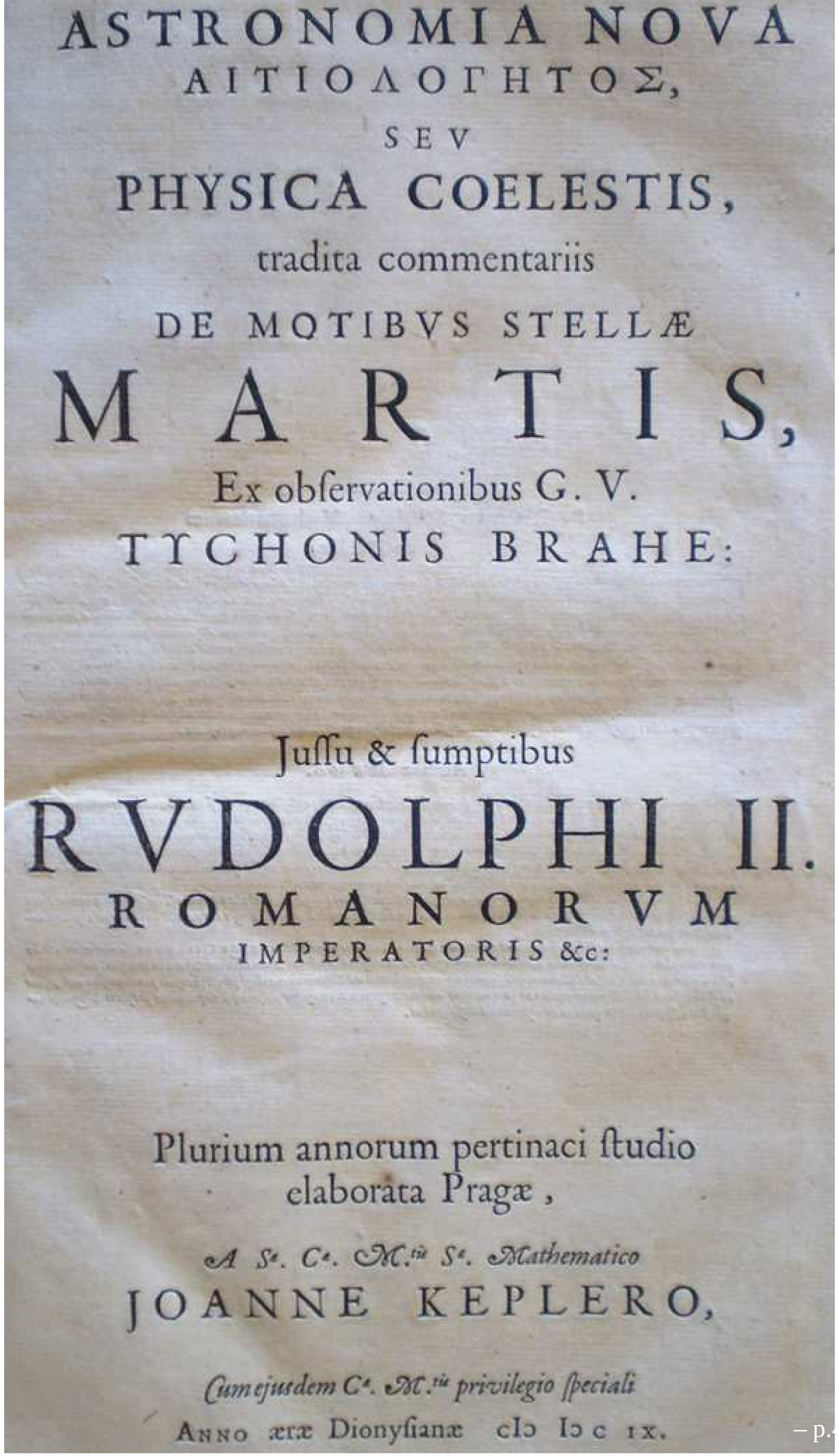
Euler

... from heaven !!

Astronomy is older than physics. In fact, it got physics started by showing the beautiful simplicity of the motion of the stars and planets, the understanding of which was the beginning of physics.

(R. Feynman 1963)

Johannes Kepler (1609): Astronomia Nova



ASTRONOMIA NOVA
ΑΙΤΙΟΛΟΓΗΤΟΣ,
SEV
PHYSICA COELESTIS,
tradita commentariis
DE MOTIBVS STELLÆ
MARTIS,
Ex obſervationibus G. V.
TYCHONIS BRAHE:

Juſſu & ſumptibus
RVDOLPHI II.
ROMANORVM
IMPERATORIS &c:

Plurium annorum pertinaci ſtudio
elaborata Pragæ,

A S^e. C^e. M.^tis S^e. Mathematico
JOANNE KEPLERO,

Cum ejusdem C^e. M.^tis privilegio ſpeciali
Anno æræ Dionyſianæ clɔ Iɔ c ix.

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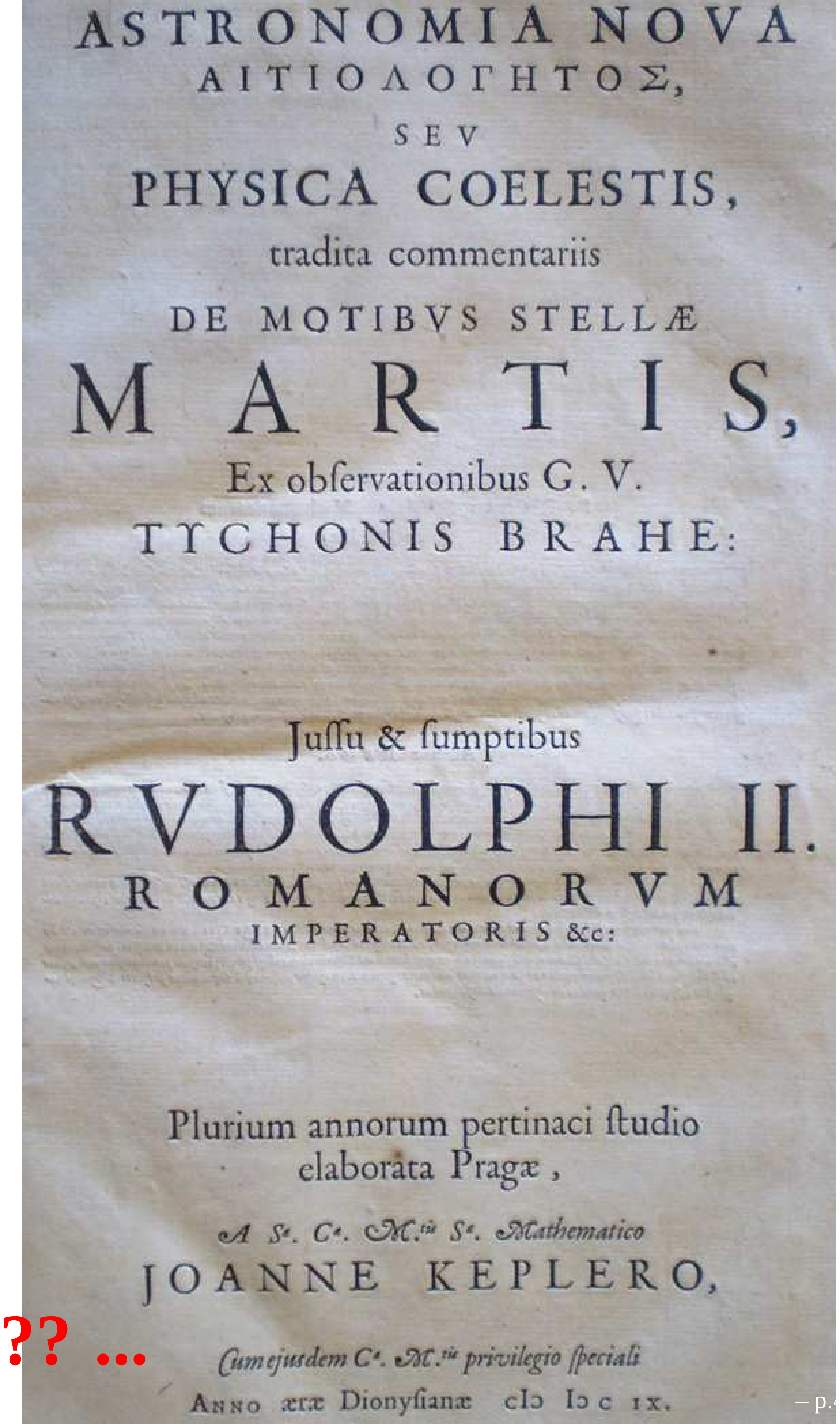

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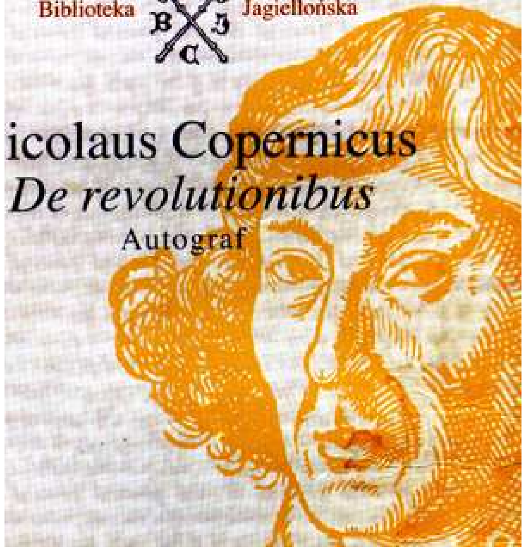
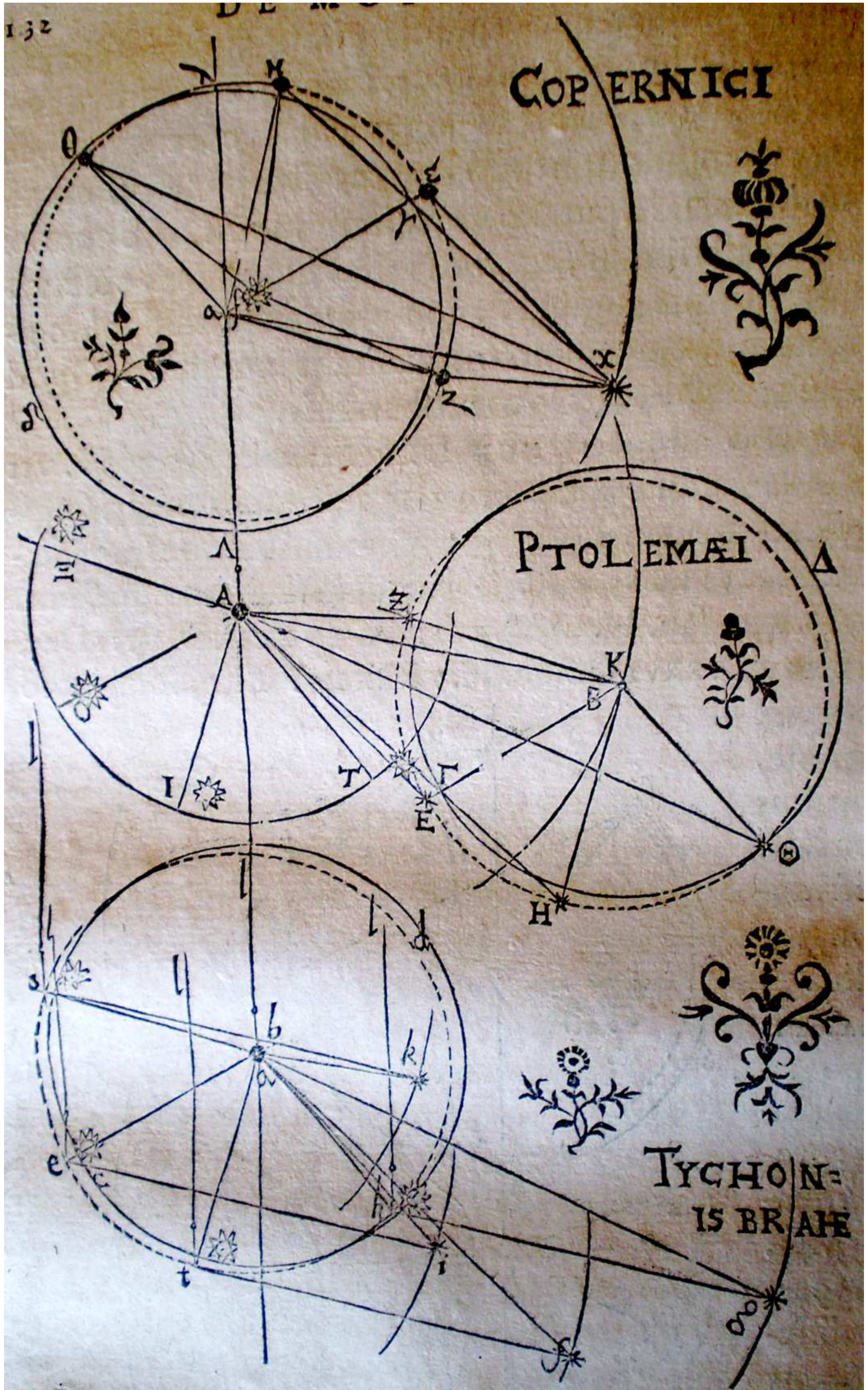
What was the old astronomy ?? ...


Biblioteka Jagiellońska
icolaus Copernicus
De revolutionibus
Autograf


RVDER
VLESTANDER


132
COPERNICI
PTOLEMÆI
TYCHONIS BRAHE

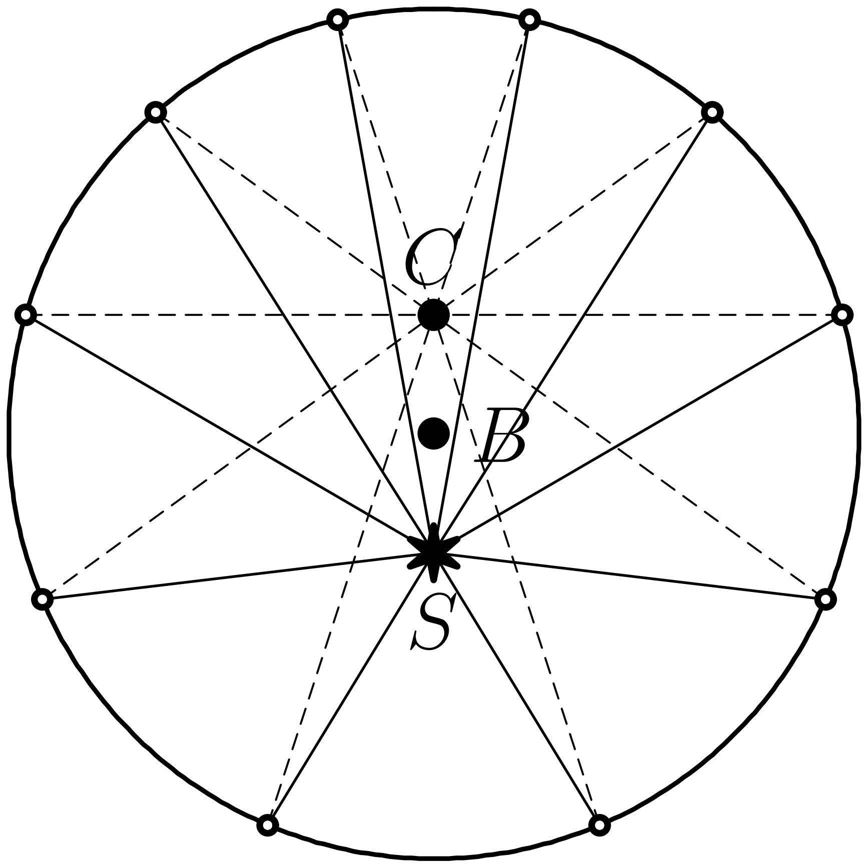
Ptolemy – Copernicus – Brahe ::

geometrically all equivalent:

orbits are excentric circles !!
(Inaequalitatis primae)

rotation speed governed by
"punctum aequans" C
with $CB = BS$
(Inaequalitatis secundae)

Thousands of data
to adapt parameters



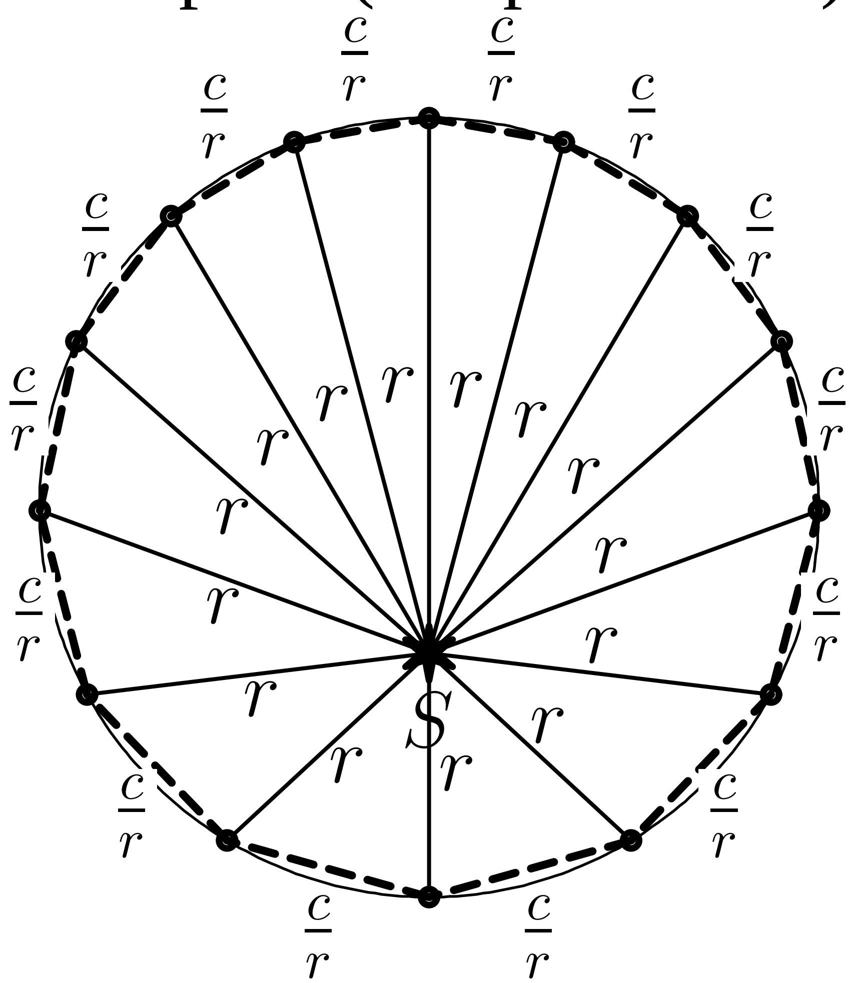
S: Sun,
B: "Mean" Sun,
C: punctum aequans.

Did not work for Mars !!

Astronomia Nova: Search first law for speed (Chap. 32 – 39):

Long discussions,
attractive forces, magnetism,
the planets have a “Soul” ;
the planets “wish” to move;
the planets “look” at the Sun and
see diameter inv. prop. to r

⇒ Speed inversely prop. to r !!



No good ...
arc length
requires Pythagoras
and $\sqrt{\ldots}$

Chap. 40: End of Pars Tertia : Simplified model:

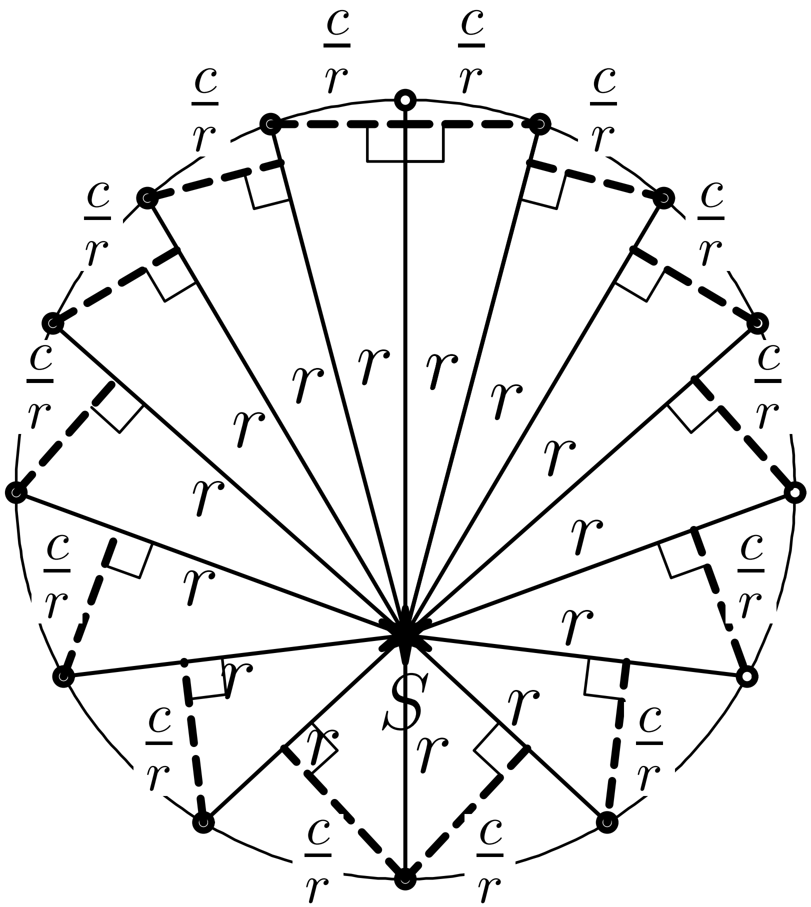
CAPVT XL.

Methodus imperfecta æquationes ex Phyſica hypotheſi computandi, quæ tamen ſufficit theoriæ SOLIS vel TERRÆ.

Above model too complicated ...

$\Rightarrow$ Inspired by Archimedes

diſtantias omnes ineſſe. Nam memineram, ſic olim & ARCHIMEDEM, cum circumferentiæ proportionem ad diametrum quæreret, circulum in infinita triangula diſſecuiſſe. nam hæc vis occulta eſt ejus demon-

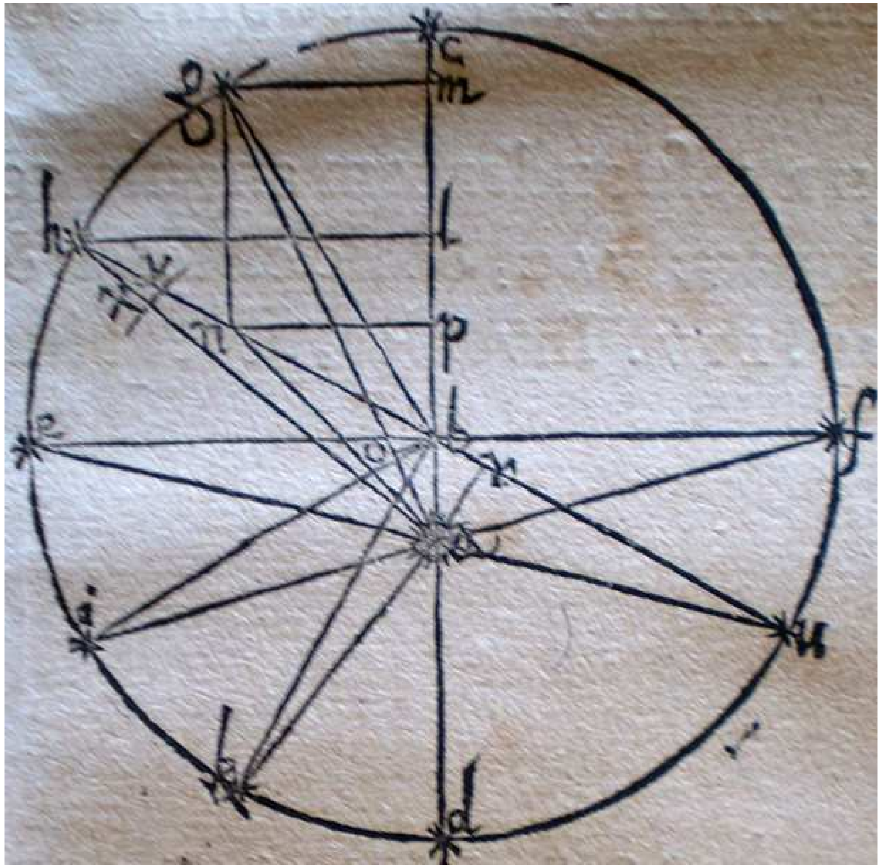


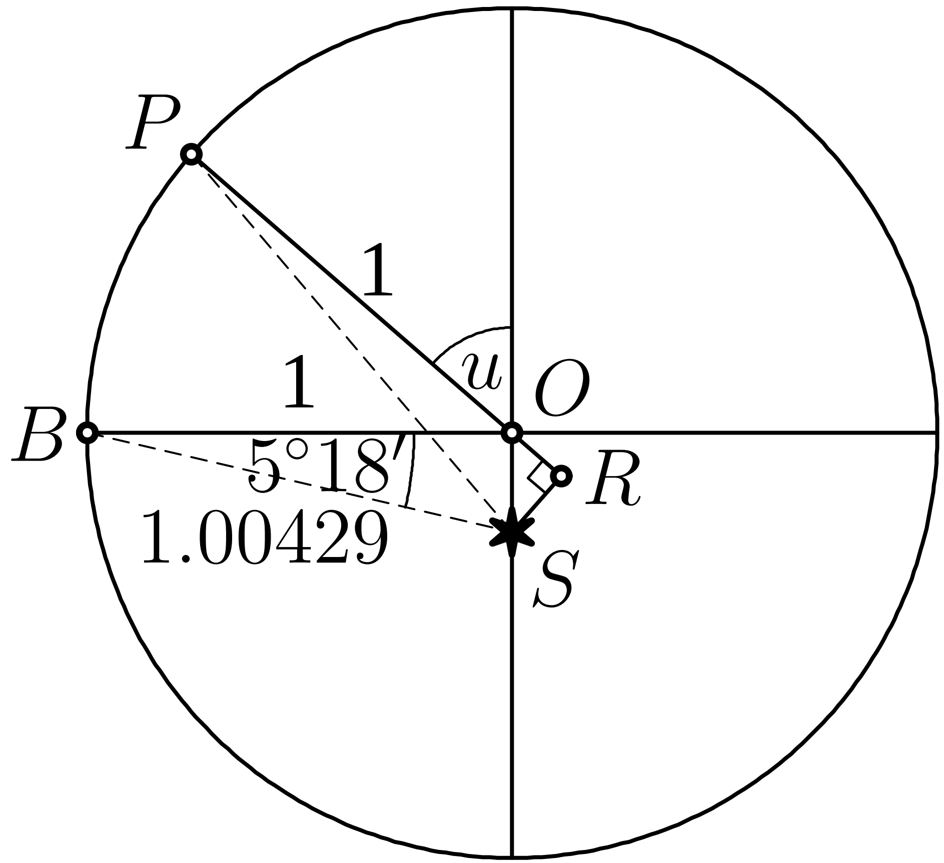
Kepler 2:

all triangles have same area !!

“Equal times — equal areas”

Kepler's Pars IV : The Great Idea in Chap. 56:

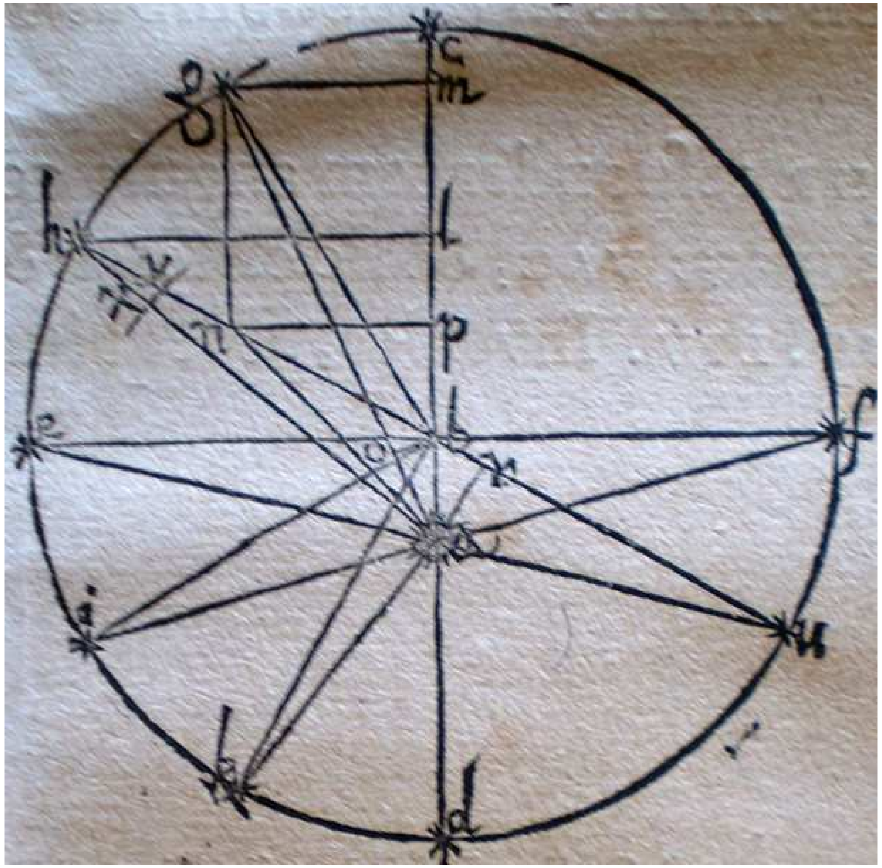


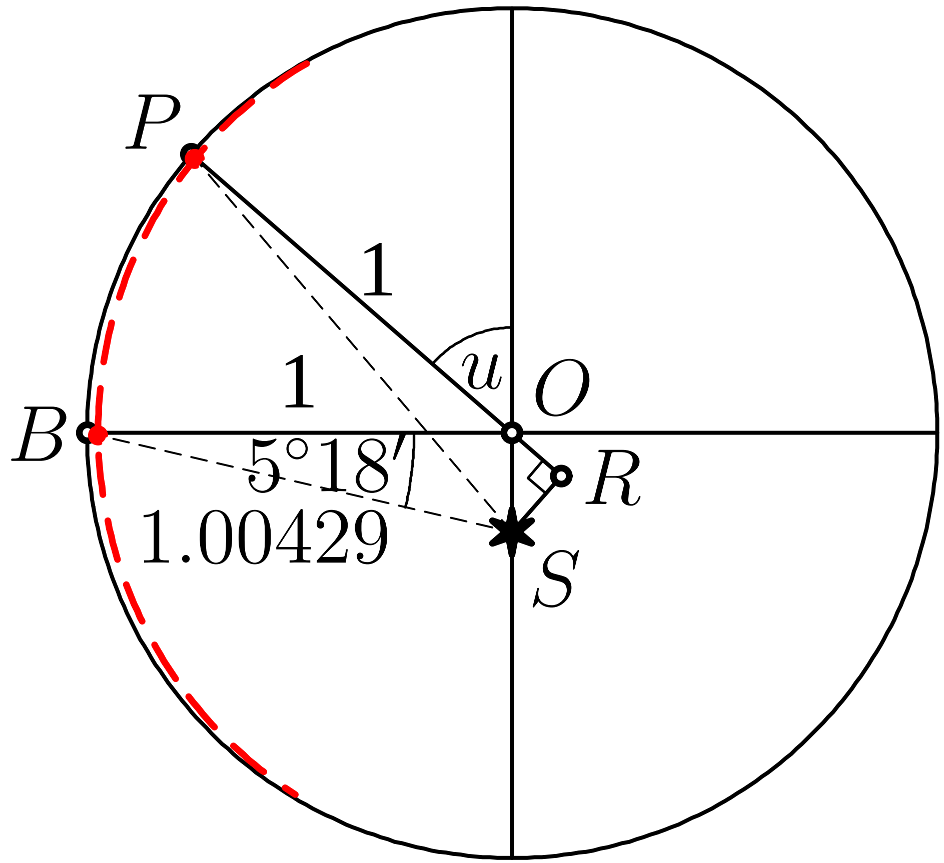


Obs.: Dist. BS of Tycho's circle by factor 1.00429 too large;
This value is (by chance) $1/\cos 5°18'$;

plane nihil dictum esse, itaque futilem fuisse meum de Marte triumphum; forte fortuito incido in secantem anguli 5. 18. quæ est mensura æquationis Opticæ maximæ. Quem cum viderem esse 100429, hic quasi e somno expergefactus, & novam lucem intuitus, sic cœpi ratio-

Kepler's Pars IV : The Great Idea in Chap. 56:



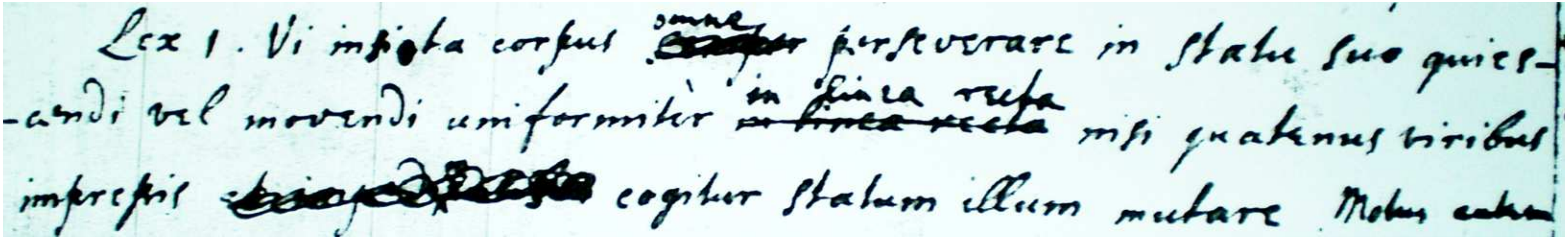


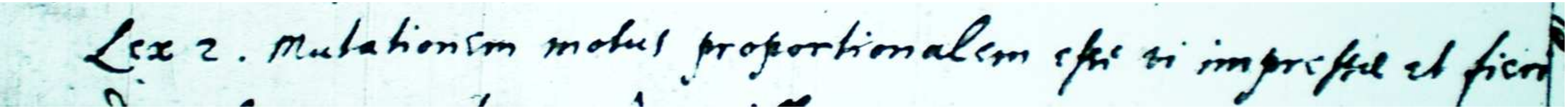
Idea: Replace 'hypoth.' by 'legs', $BS = BO$, $PS = PR$,...
and "I awoke from sleep & new light broke on me"!!!

$$PS = PR = 1 + e\cos u$$

Kepler 1: **Planet moves on ellipse !!**

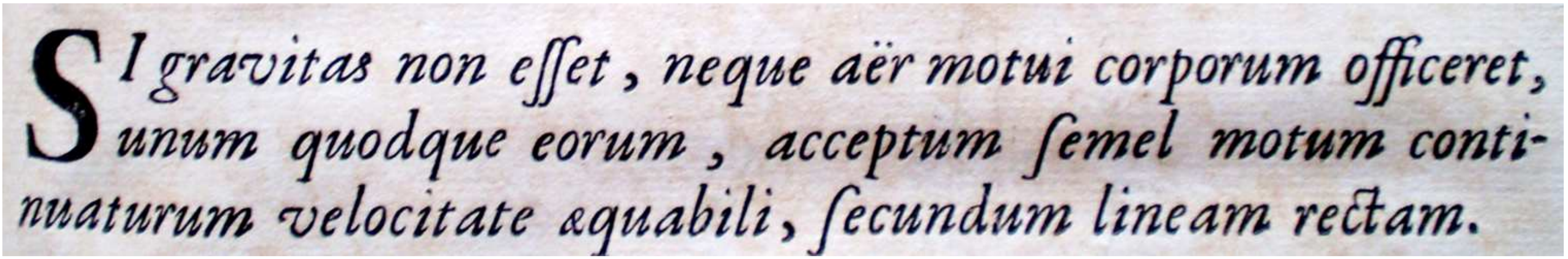
Newton: Manuscript (1684), **Principia** (1687)


Lex 1. Vi insita corpus omne perseverare in statu suo quiescendi vel movendi uniformiter in linea recta nisi quatenus viribus impressis cogitur statum illum mutare. Motus autem


Lex 2. Mutationem motus proportionalem esse vi impressae et fieri

(Newton, Cambridge Univ. Lib. manuscript Add. 3965^{7a} from 1684)

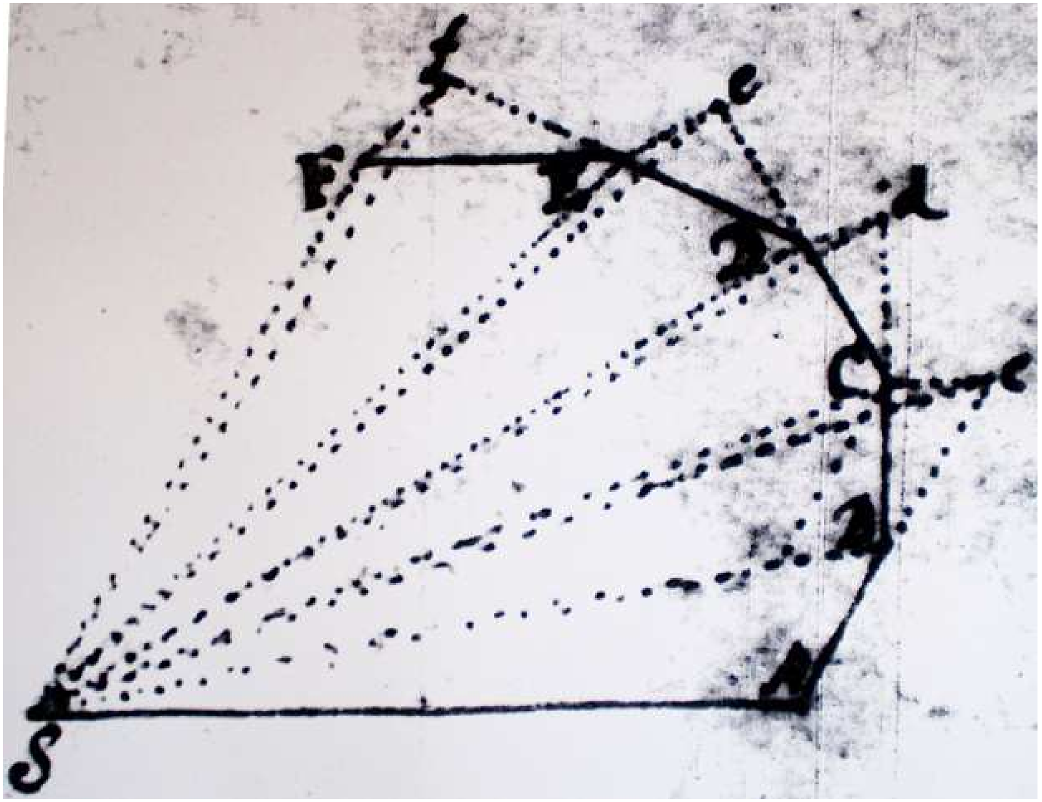
Huygens (Horologium 1673)


SI gravitas non eſſet, neque aër motui corporum officeret, unumquodque eorum, acceptum ſemel motum continuaturum velocitate æquabili, ſecundum lineam rectam.

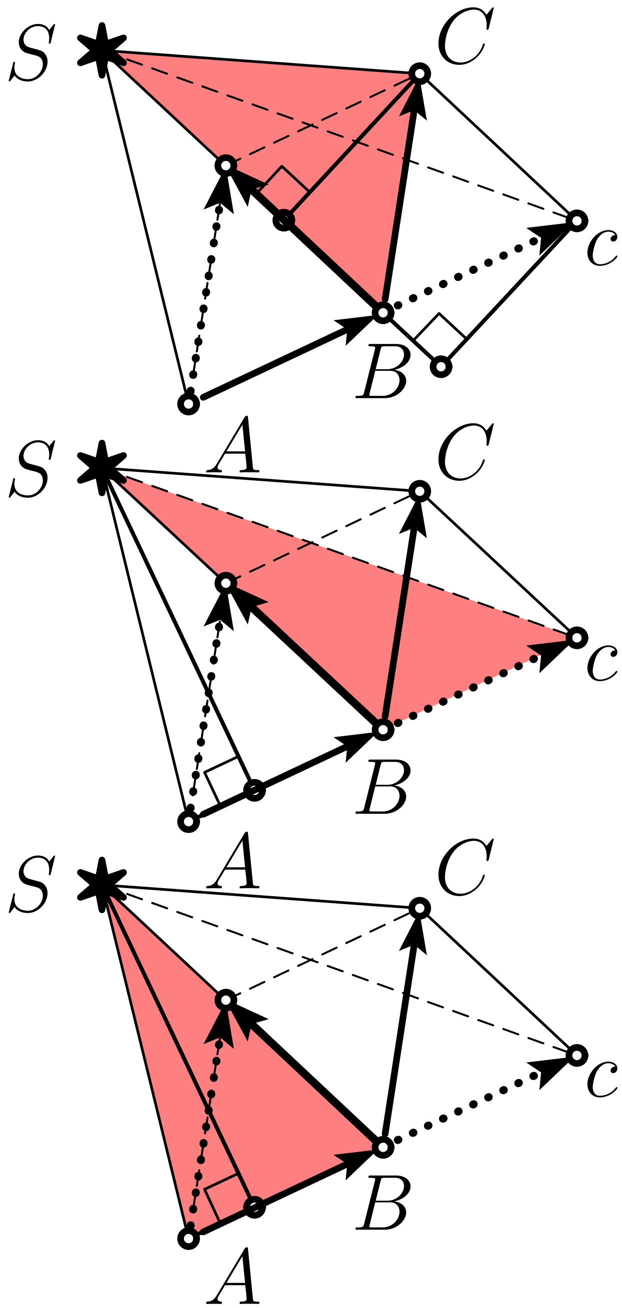
Proof of Kepler 2:

at end of time step Δt

one force impulse $f \cdot \Delta t$



(Picture from ms. Add. 3965^{7a})

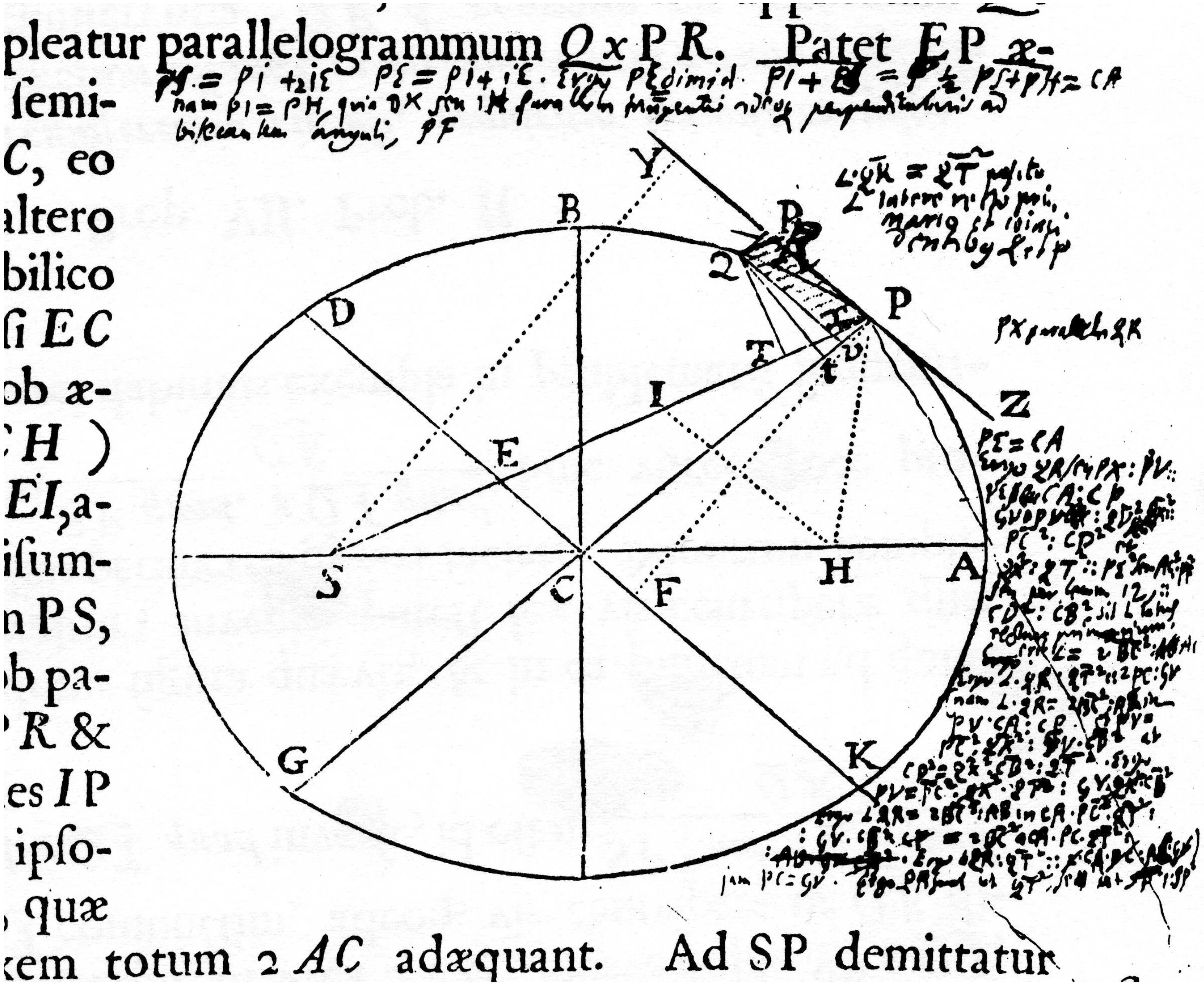


Eucl. I.41: All triangles have same area !

This became the "Theorema 1" of the *Principia* (1687).

Newton's Discovery of Gravitation Law from Kepler 1 & 2.

... i libri di Apollonio, ... delle quali sole siamo bisogni nel presente trattato. (Galilei 1638, giornata quarta)



(Newton's Princ. 1687, Leibniz' handwriting)

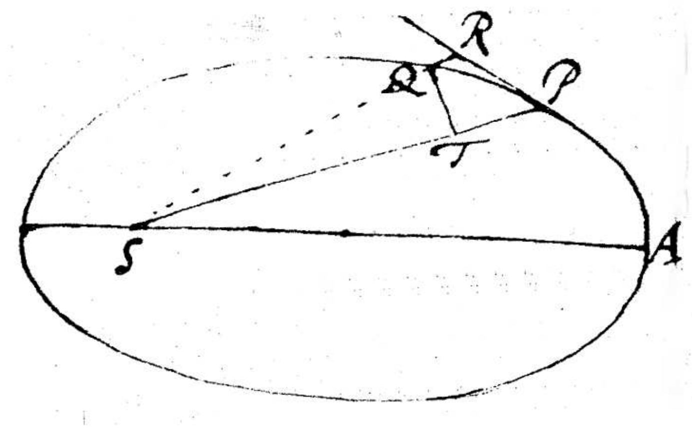
Conj. diam. $\parallel$ tang.
(Apoll. II.6+Eucl. II.14)
$\Rightarrow PV = \text{Const} \cdot QV^2$

Tangents $\alpha = \alpha$
(Apoll. III.48)

$SP + HP = 2a$
(Apoll. III.52)
$\Rightarrow EP = a$

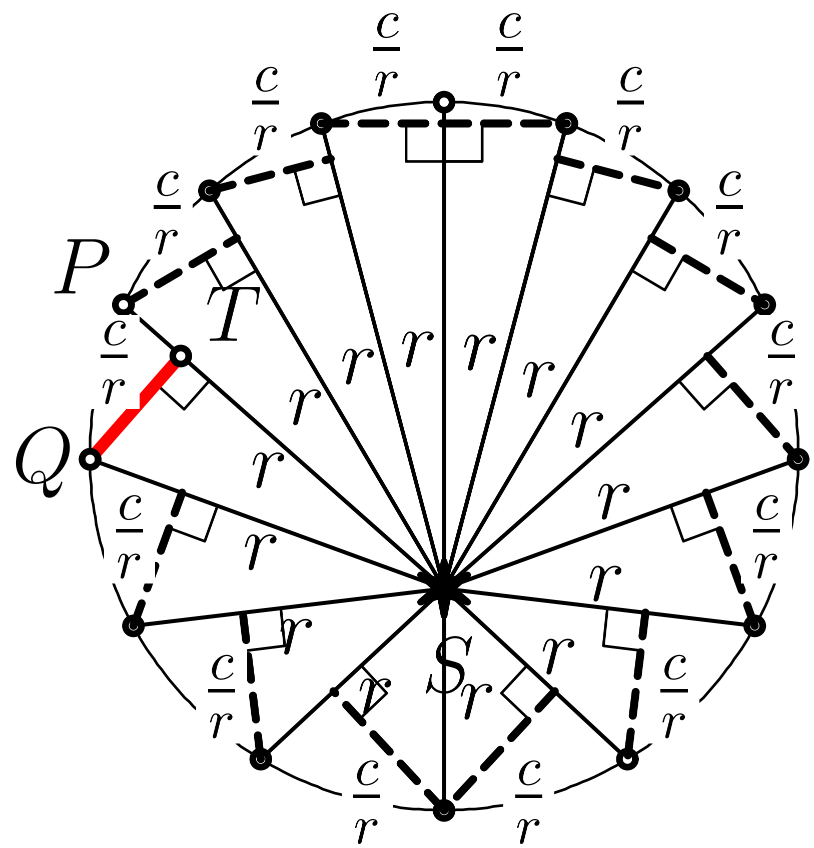
$\Rightarrow$ $\boxed{RQ = \text{Const} \cdot QT^2}$
(Thales)

The Law of Gravitation.



RQ prop. QT^2

(Newton's Lemma)



QT prop. $\frac{1}{r}$

(Kepler 2)

hence: **force is proportional to $\frac{1}{r^2}$**

(Prop. XI of the Principia).

L. Euler (E122, 1747): **Differential Eqs. for Mechanics.**

$$\text{I. } \frac{2\,ddx}{dt^2} = \frac{X}{M}; \quad \text{II. } \frac{2\,ddy}{dt^2} = \frac{Y}{M}; \quad \text{III. } \frac{2\,ddz}{dt^2} = \frac{Z}{M}$$

"While physicists call these
"Newton's equations",
they occur nowhere in the work of Newton
or of anyone else prior to 1747."
**"... such is the universal ignorance
of the true history of mechanics."**

(C. Truesdell, *Essays in the*
History of Mechanics, 1968)

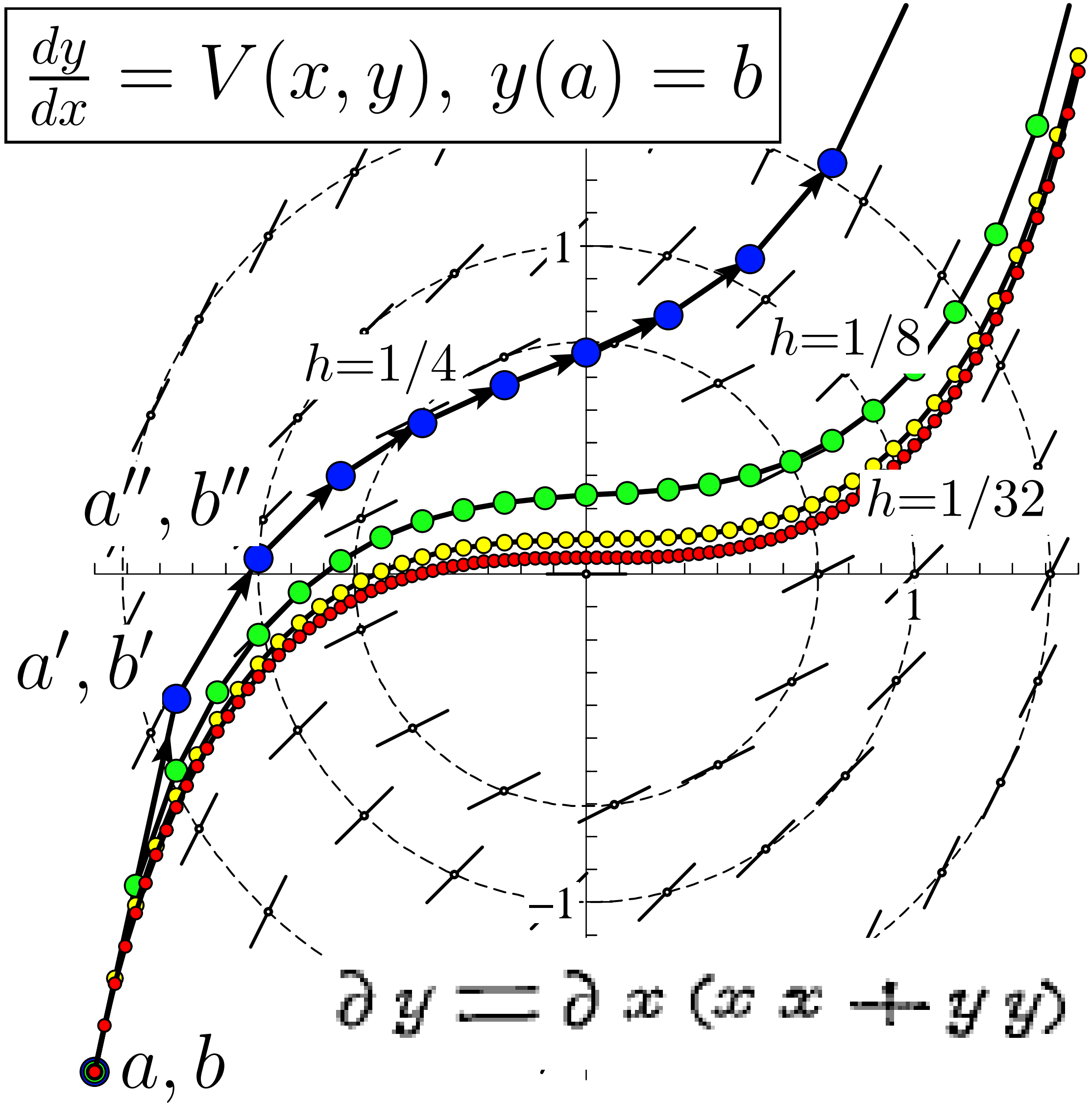
L.Euler (E342), Inst. Calc. Integralis 1768, §650:

$b' = b + A(a' - a)$

$b'' = b' + A'(a'' - a')$

$b''' = b'' + A''(a''' - a'')$

Ipsius	valores successiui
x	a ; a' ; a'' ; a''' ; a^{IV} ; . . . . $'x$; x
y	b ; b' ; b'' ; b''' ; b^{IV} ; . . . . $'y$; y
V	A ; A' ; A'' ; A''' ; A^{IV} ; . . . . $'V$; V.



1. Taylor Method (Londini MDCCXV) 300 years !!!

METHODUS
Incrementorum
Directa & Inversa.

AUCTORE
BROOK TAYLOR, LL.D. &

PROP. VII. THEOR. III.

$$x + x\frac{v}{1z} + x\frac{v\dot{v}}{1.2z^2} + x\frac{v\dot{v}\ddot{v}}{1.2.3z^3} + \&c.$$

(Euler E342, ICI 1768, §656):

$$y = b + \frac{(x-a)\,db}{da} + \frac{(x-a)^2\,ddb}{1.2\,da^2} + \frac{(x-a)^3\,d^3b}{1.2.3\,da^3} + \text{etc.}$$

$$\frac{dy}{dx} = V(x,y) \quad \Rightarrow \quad \frac{ddy}{dx^2} = \left(\frac{dV}{dx}\right) + V\left(\frac{dV}{dy}\right)$$

$$\frac{d^3y}{dx^3} = \left(\frac{ddV}{dx^2}\right) + \left(\frac{dV}{dx}\right)\left(\frac{dV}{dy}\right) + 2V\left(\frac{ddV}{dx\,dy}\right) + V\left(\frac{dV}{dy}\right)^2 + VV\left(\frac{ddV}{dy^2}\right).$$

Exemplum 2.

662. *Aequationis differentialis* $\partial y = \partial x\,(xx + yy)$ *integrale completum proxime investigare.*

Cum hic sit $\frac{\partial y}{\partial x} = V = xx + yy$, erit continuo differentiando

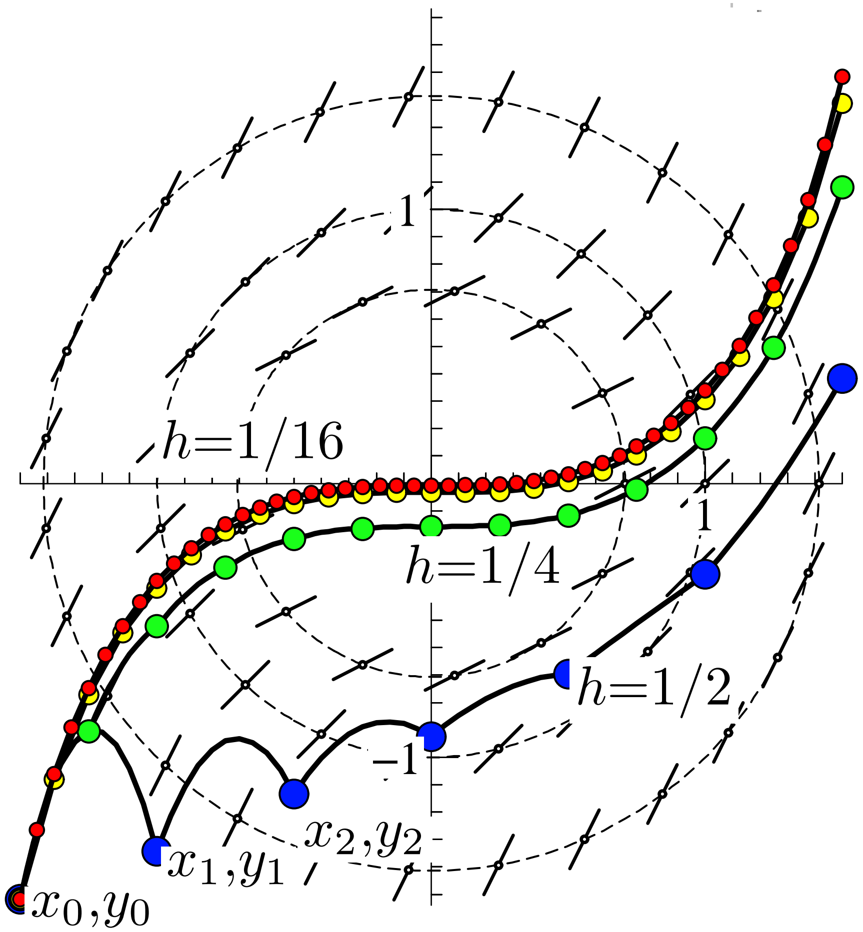
$$\frac{\partial\partial y}{\partial x^2} = 2x + 2xxy + 2y^3 \text{ et}$$

$$\frac{\partial^3 y}{\partial x^3} = 2 + 4xy + 2x^4 + 8xxyy + 6y^4$$

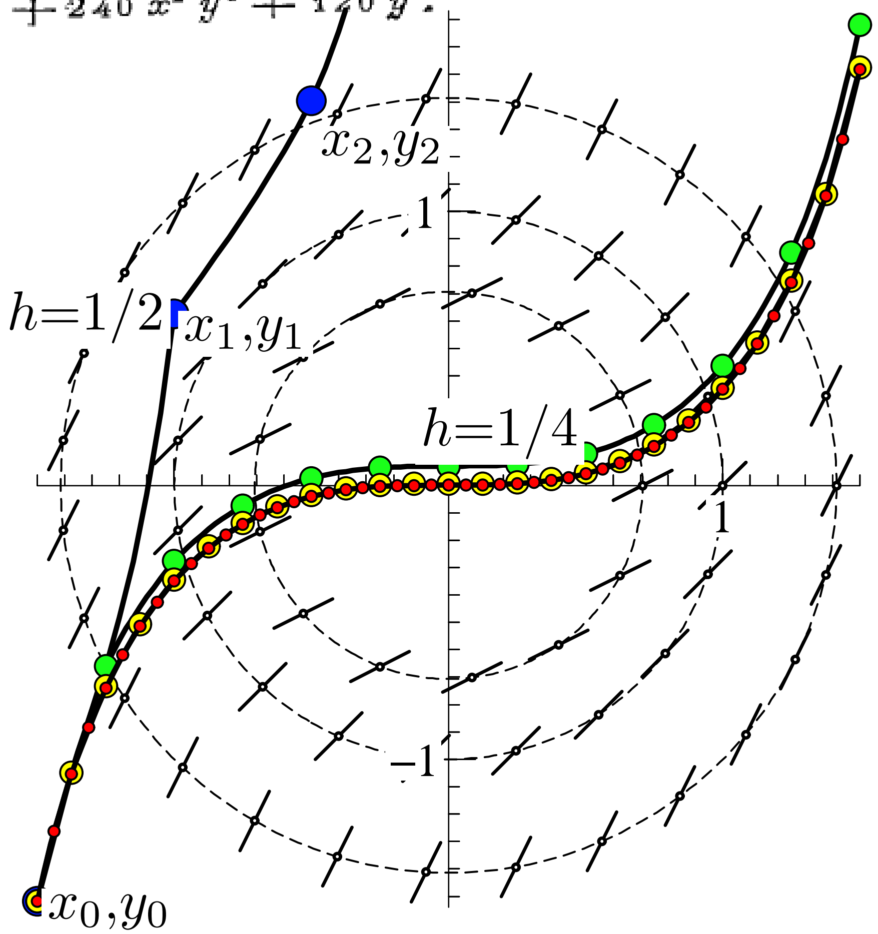
$$\frac{\partial^4 y}{\partial x^4} = 4y + 12x^3 + 20xyy + 16x^4y + 40xxy^3 + 24y^5$$

$$\frac{\partial^5 y}{\partial x^5} = 40x^2 + 24y^2 + 104x^3y + 120xy^3 + 16x^6 + 136x^4y^2 + 240x^2y^4 + 120y^6.$$

Order 2

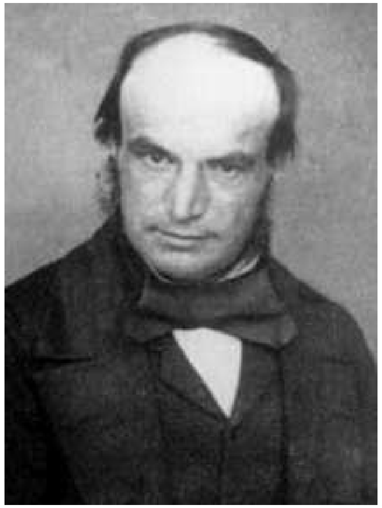


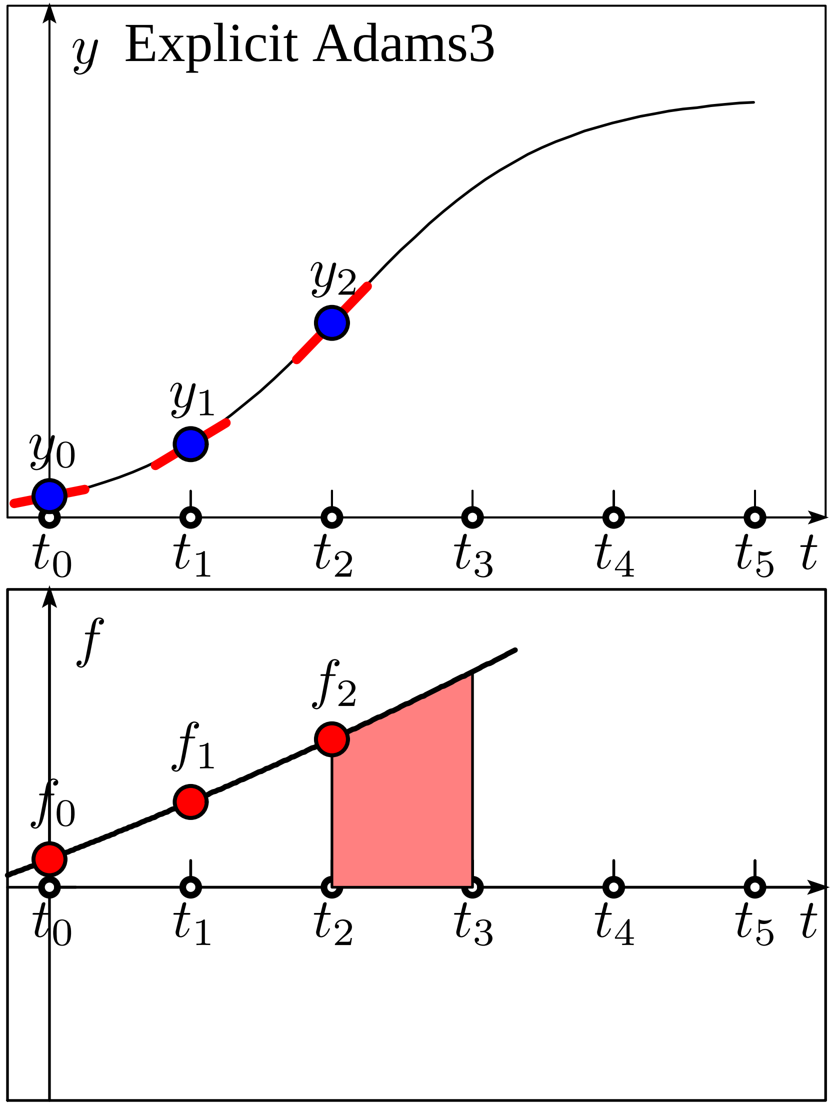
Order 3



2. Multistep methods (J.C. Adams-F. Bashforth 1883)

$$y_1 - y_0 = \omega\left\{q_0 + \frac{1}{2}\Delta q_0 + \frac{5}{12}\Delta^2 q_0 + \frac{3}{8}\Delta^3 q_0 + \frac{251}{720}\Delta^4 q_0 + \frac{95}{288}\Delta^5 q_0 + \frac{19087}{60480}\Delta^6 q_0 + \frac{5257}{17280}\Delta^7 q_0 + \frac{1070017}{3628800}\Delta^8 q_0 + \frac{2082753}{7257600}\Delta^9 q_0 + \&c.\right\}.$$





- Initial values $y_0, , \dots, y_{k-1}$ approximating solution $y(t_i)$;
- Initialize slopes $f_0, \dots, f_{k-1}$ $f_i = f(t_i, y_i)$;
- Interpolate $f_n, \dots, f_{n+k-1}$, find area $\int_{t_{n+k-1}}^{t_{n+k}} p(t)\,dt$;
- Compute new y value $y_{n+k} = y_{n+k-1} +$ area;
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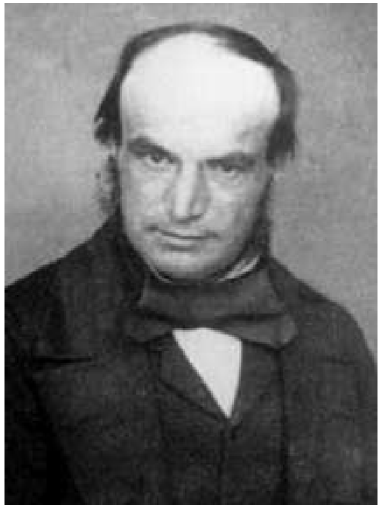

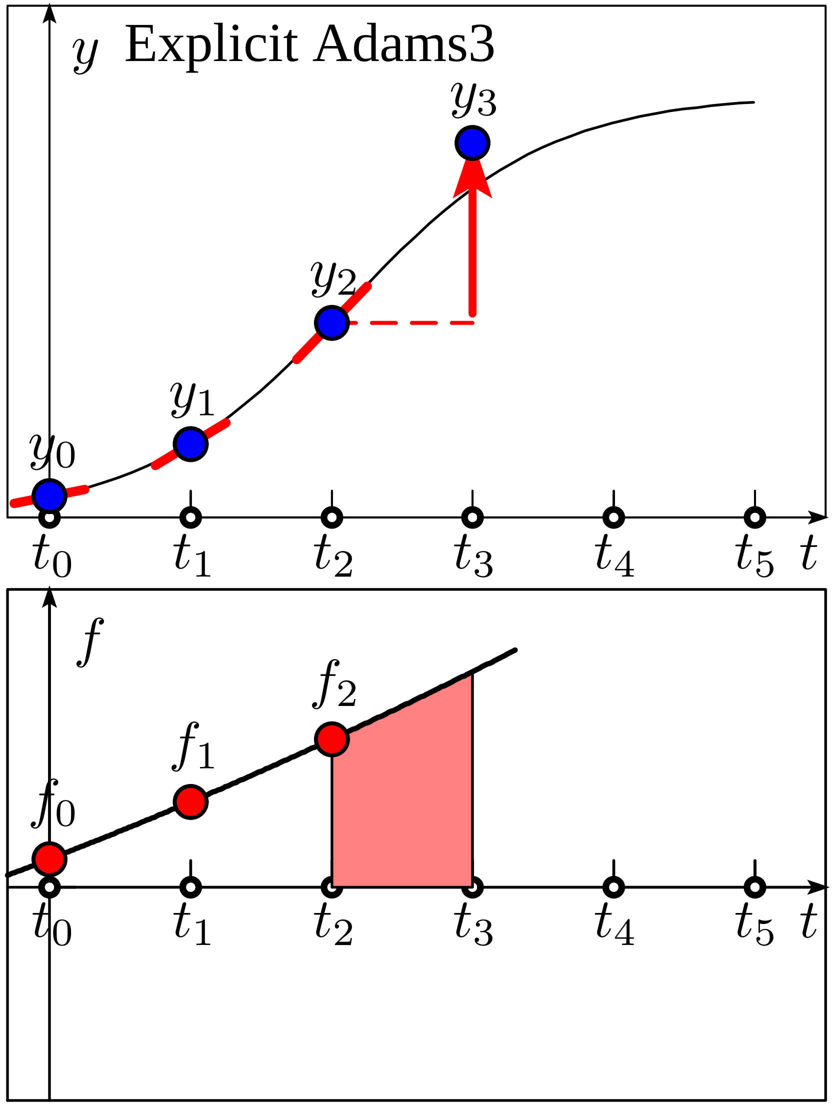

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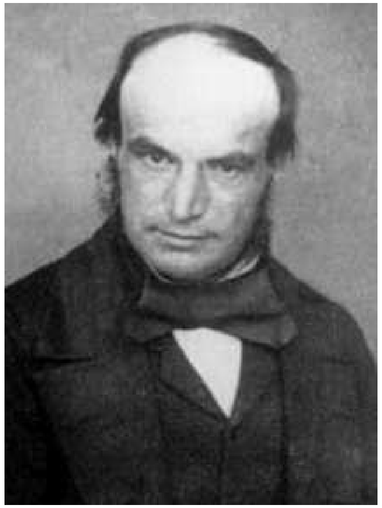

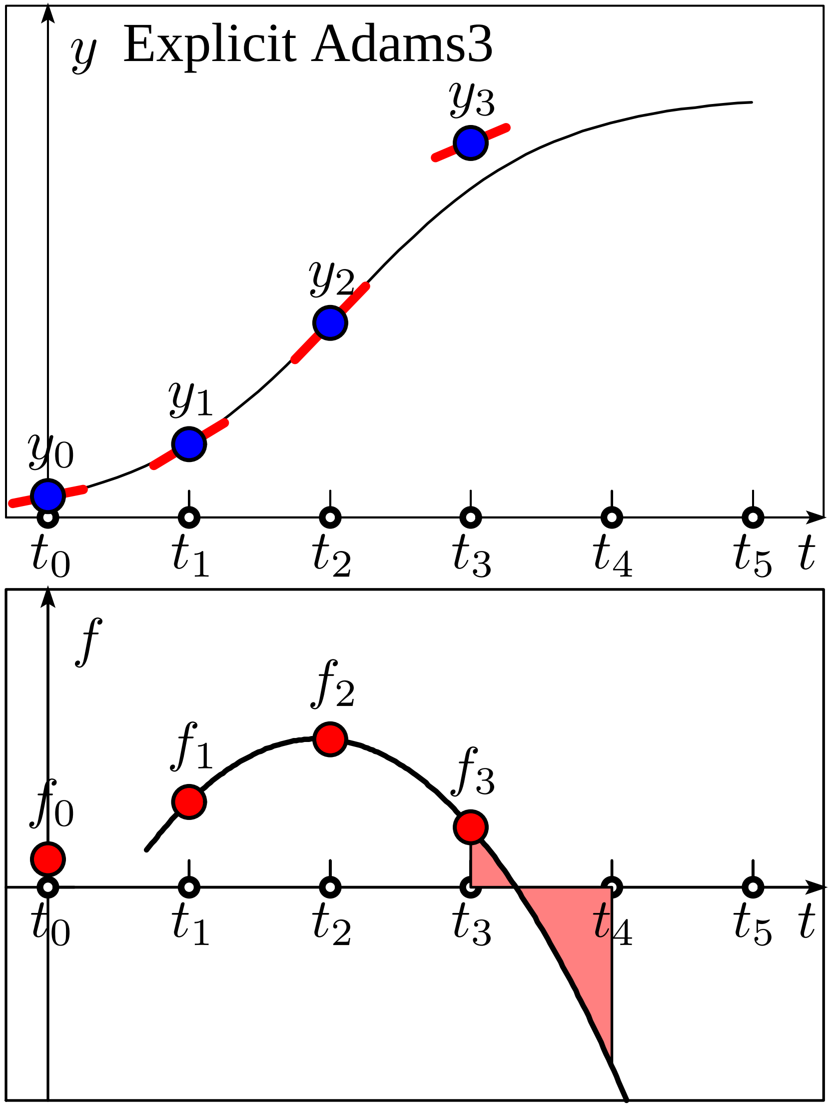

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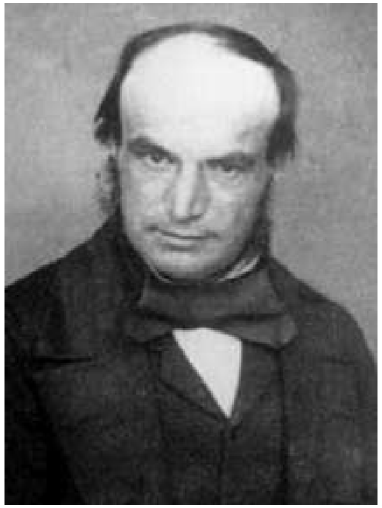

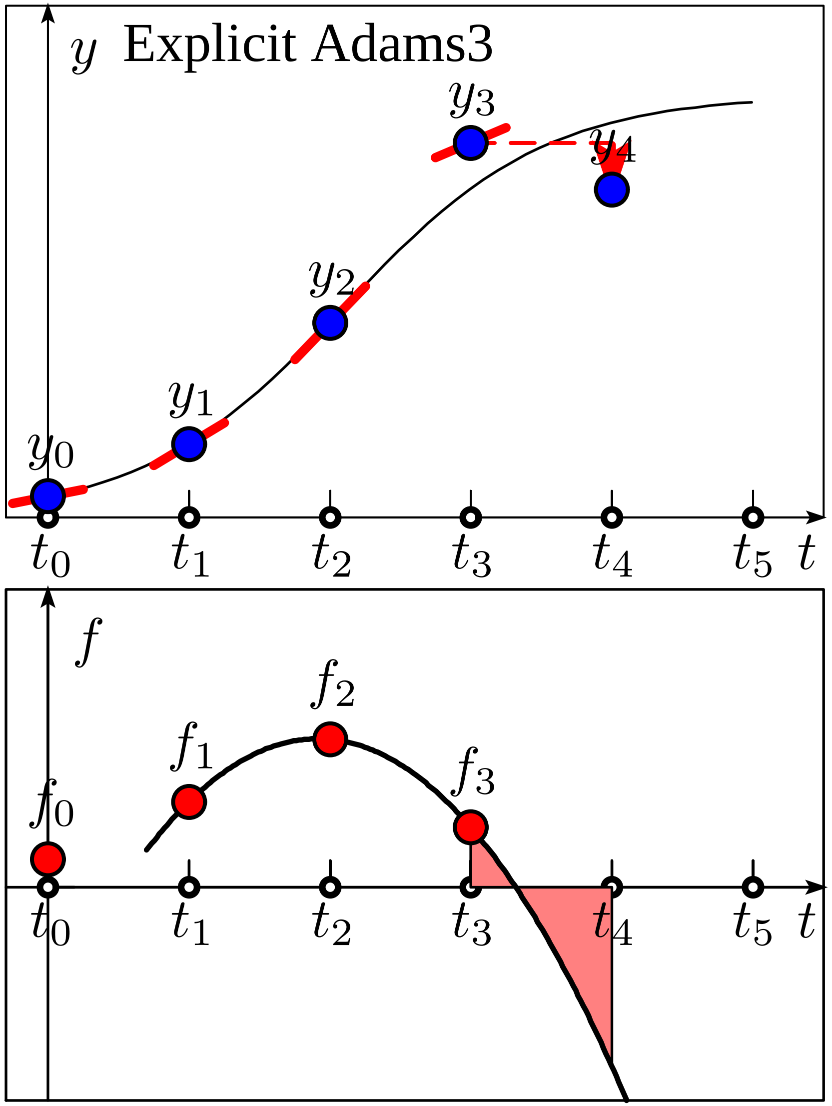

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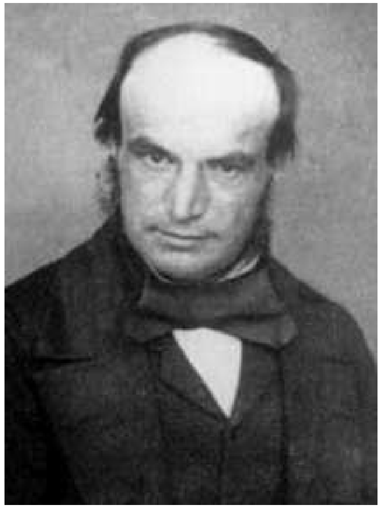

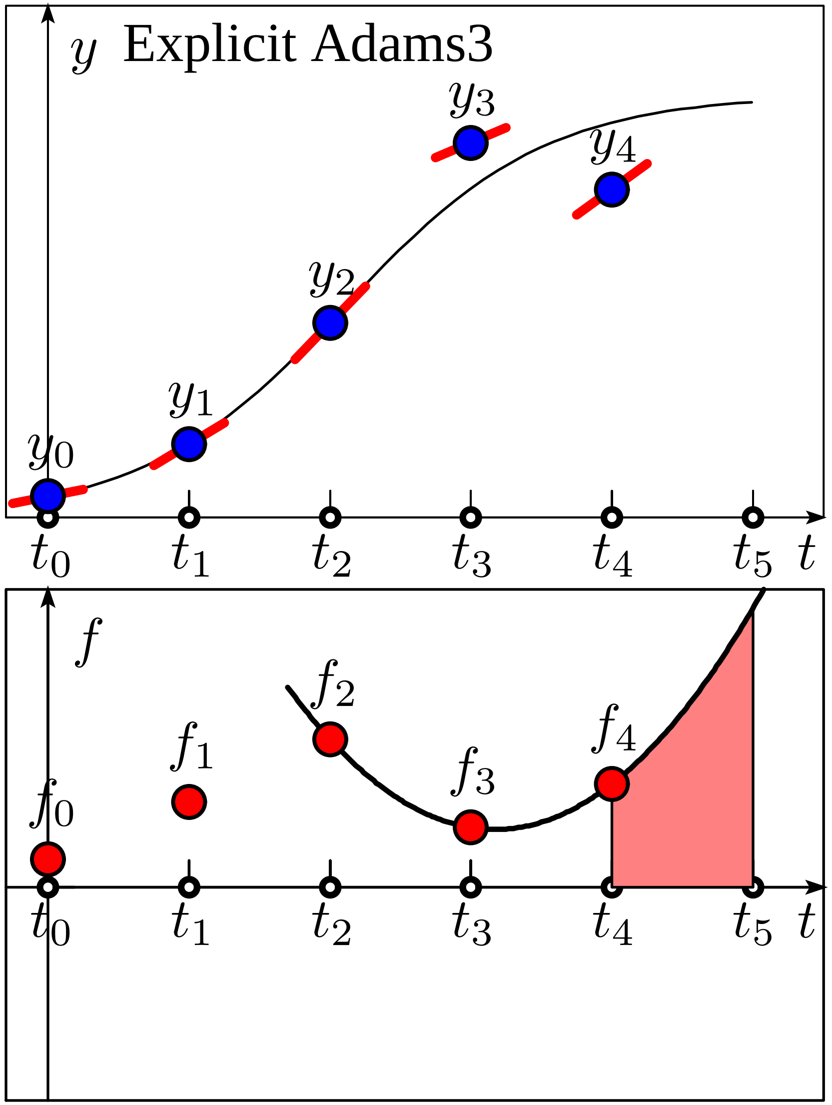

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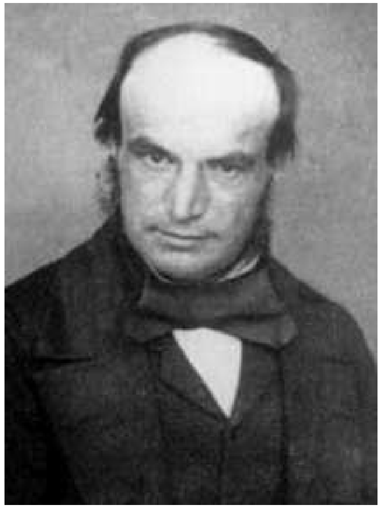
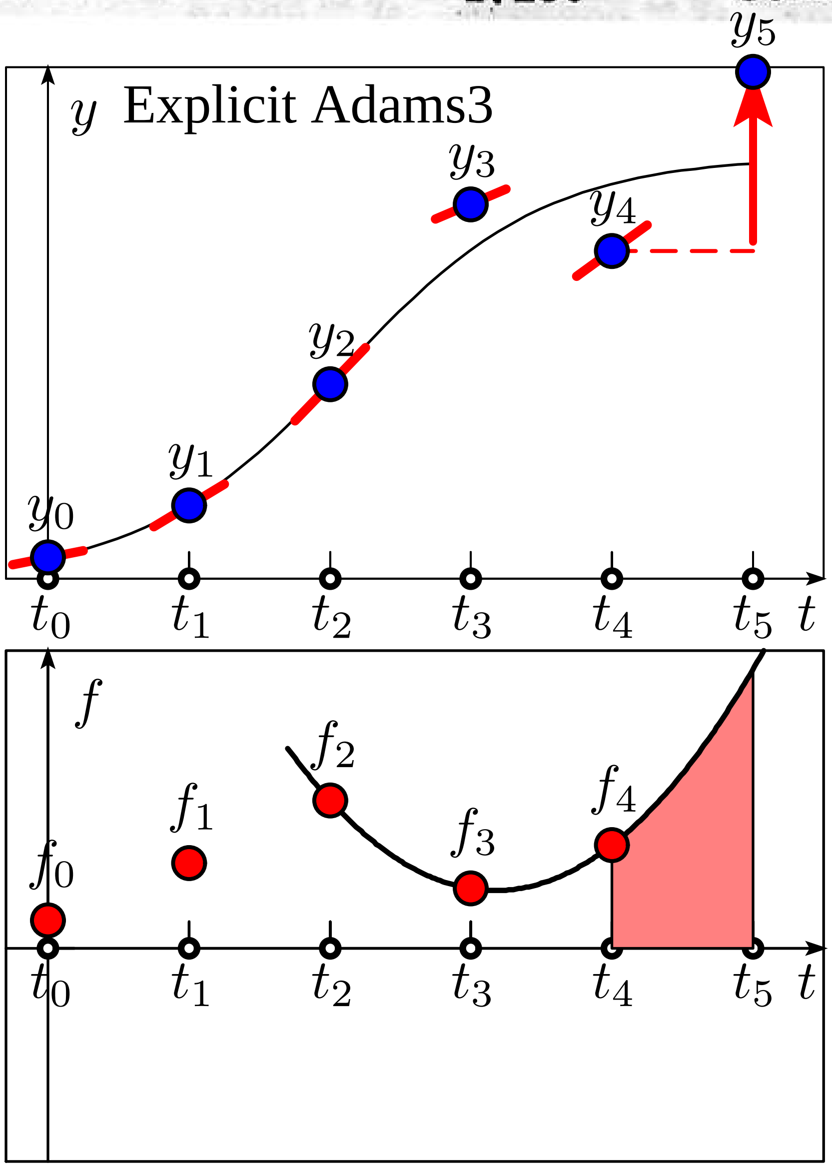
- Interpolate $f_n, \dots, f_{n+k-1}$, find area $\int_{t_{n+k-1}}^{t_{n+k}} p(t)\, dt$;
- Compute new y value $y_{n+k} = y_{n+k-1} +$ area;
- Evaluate new derivative $f_{n+k} = f(t_{n+k}, y_{n+k})$ and continue from item 3;

2. Multistep methods (J.C. Adams-F. Bashforth 1883)

$$y_1 - y_0 = \omega \left\{ q_0 + \frac{1}{2}\Delta q_0 + \frac{5}{12}\Delta^2 q_0 + \frac{3}{8}\Delta^3 q_0 + \frac{251}{720}\Delta^4 q_0 + \frac{95}{288}\Delta^5 q_0 + \frac{19087}{60480}\Delta^6 q_0 + \frac{5257}{17280}\Delta^7 q_0 + \frac{1070017}{3628800}\Delta^8 q_0 + \frac{2082753}{7257600}\Delta^9 q_0 + \&c. \right\}.$$





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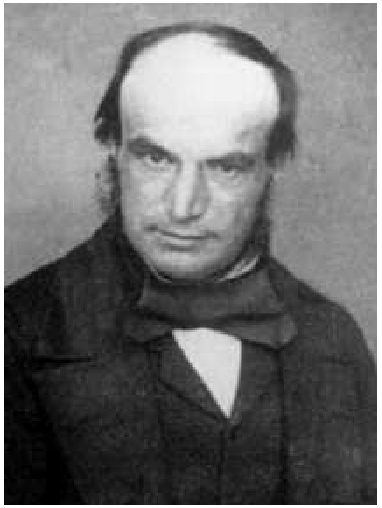

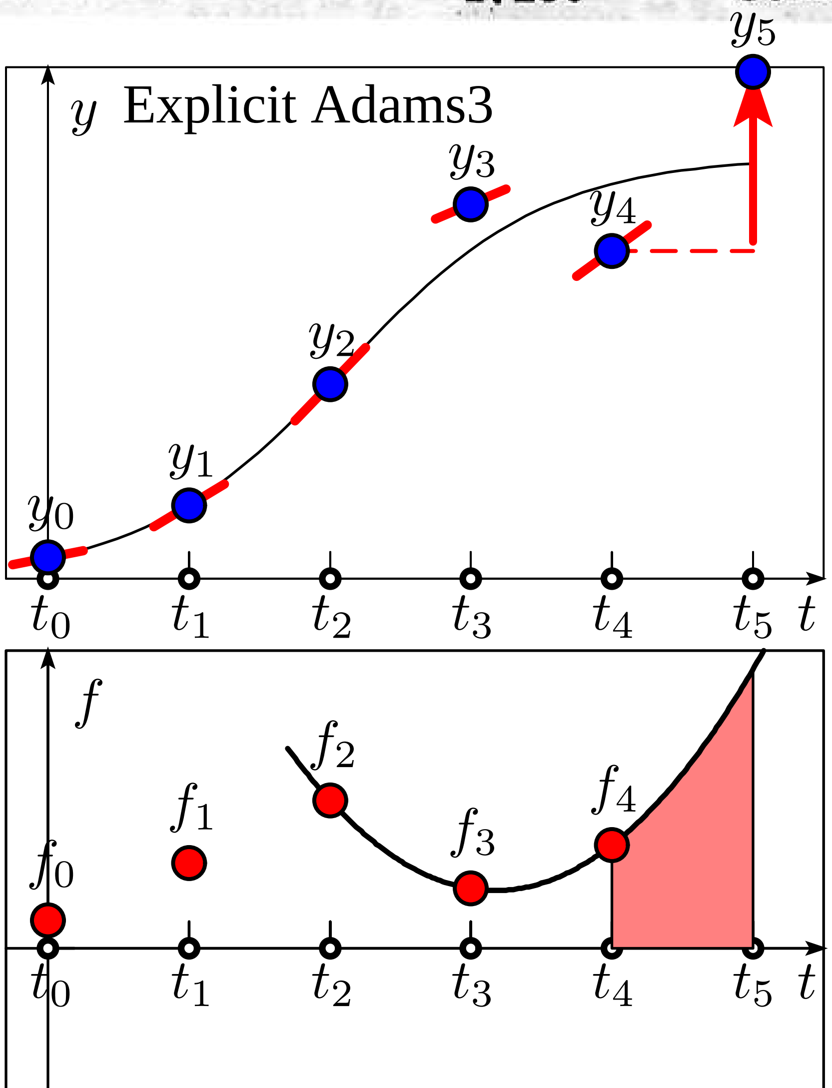

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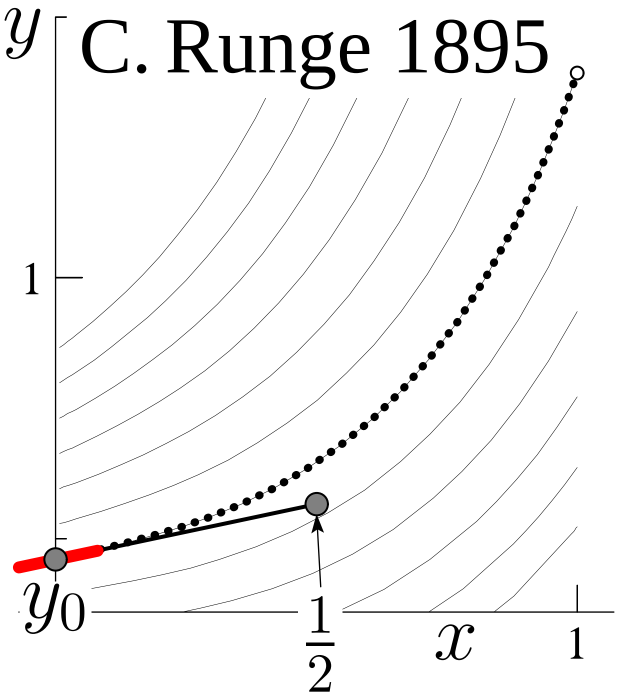
etc.

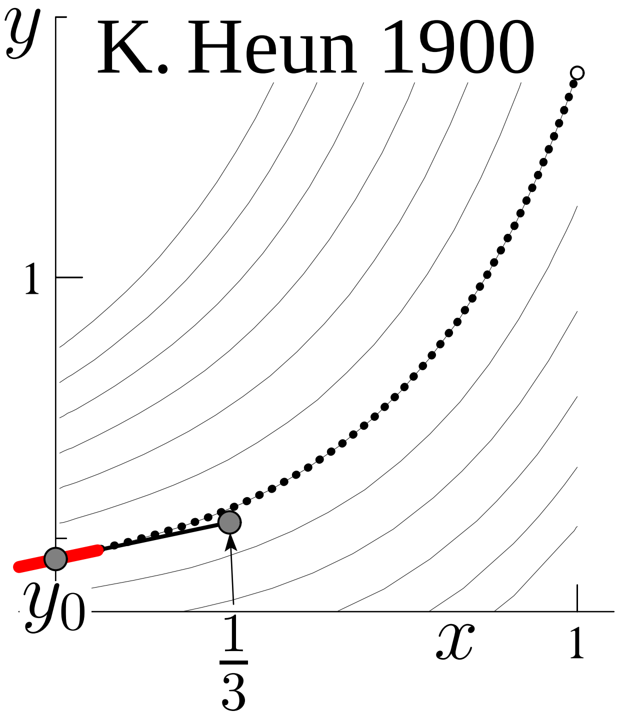
Codes LSODE, DEABM, ...

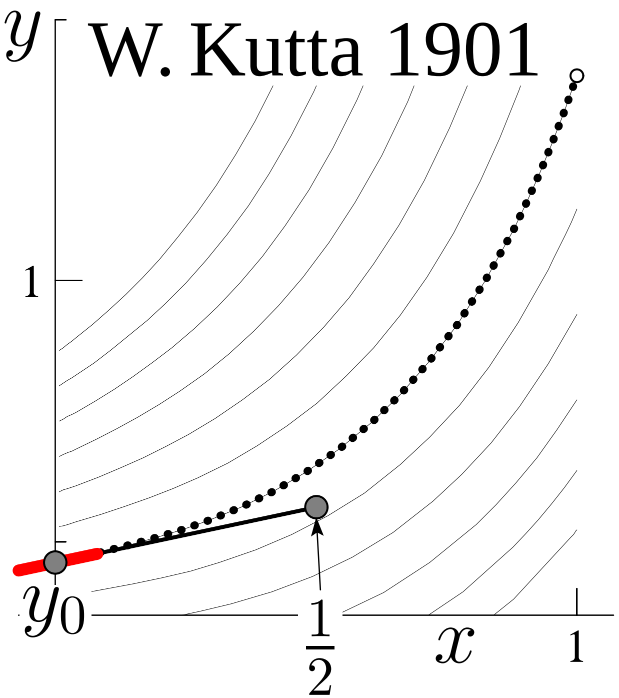
3. Runge-Kutta

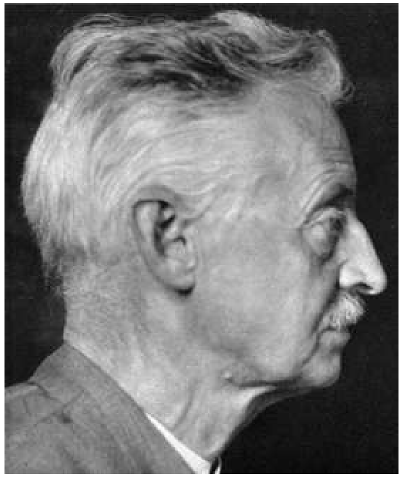
durch gesetzmäſsige polygonale Linienzüge

(Kutta 1901)









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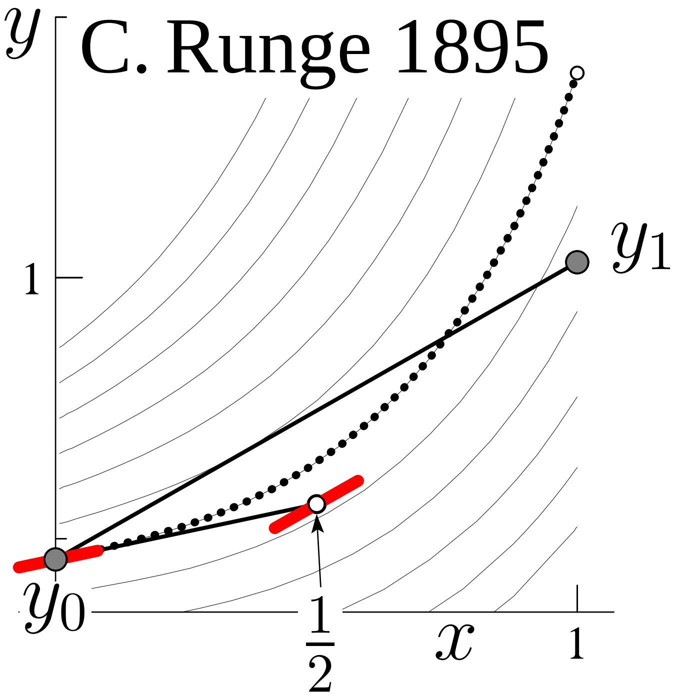

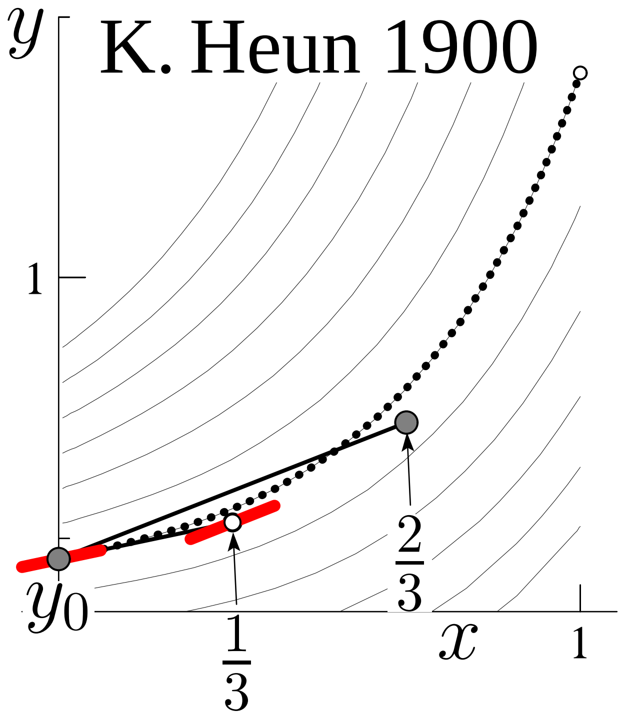

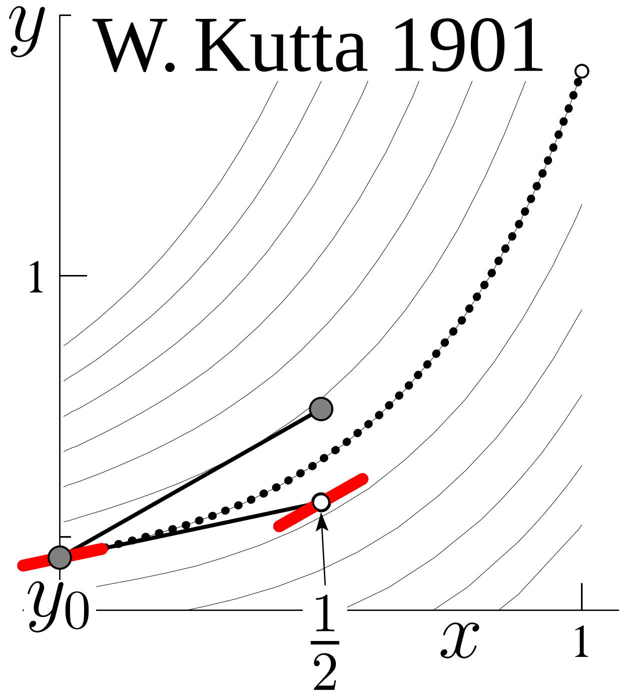

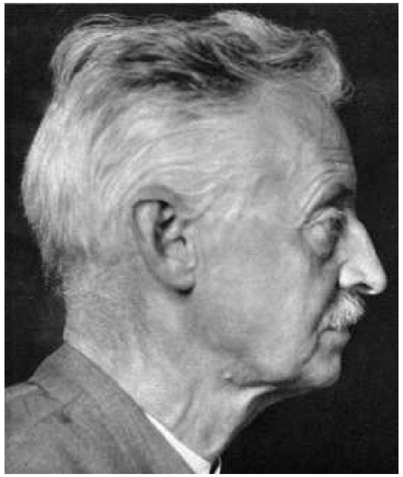

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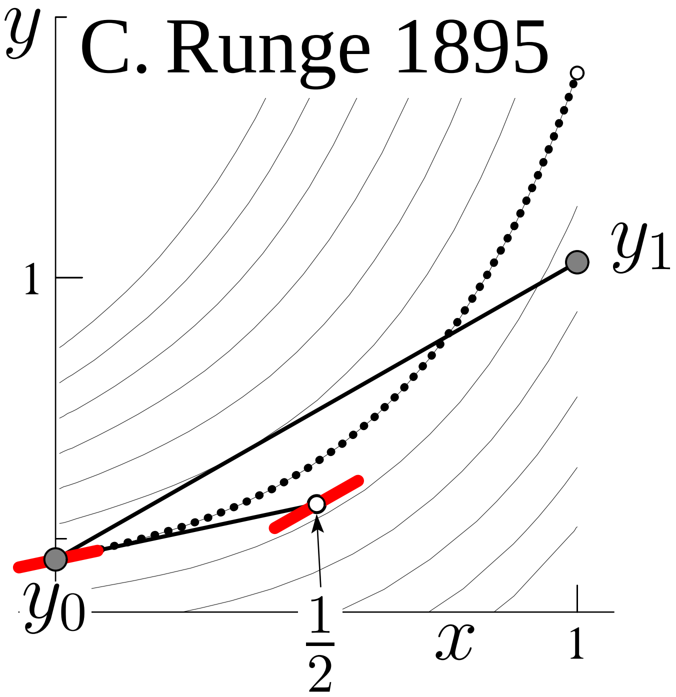

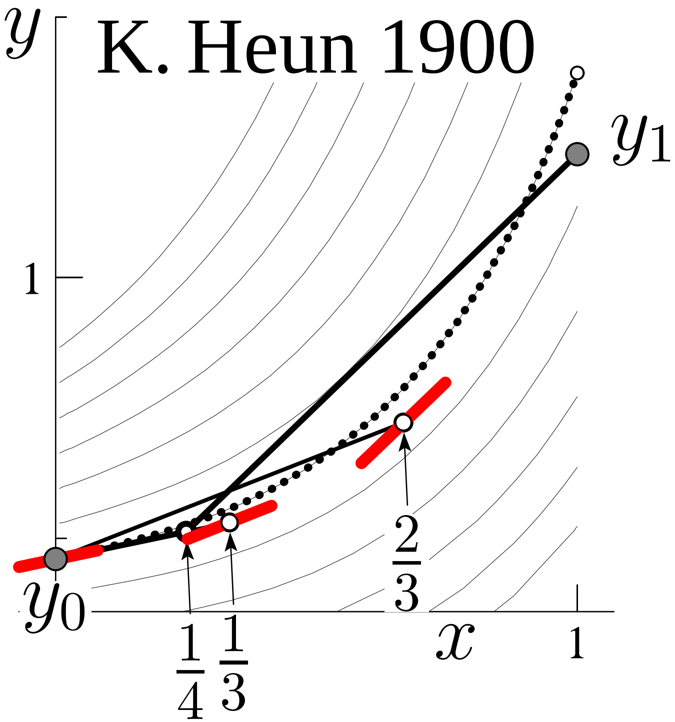

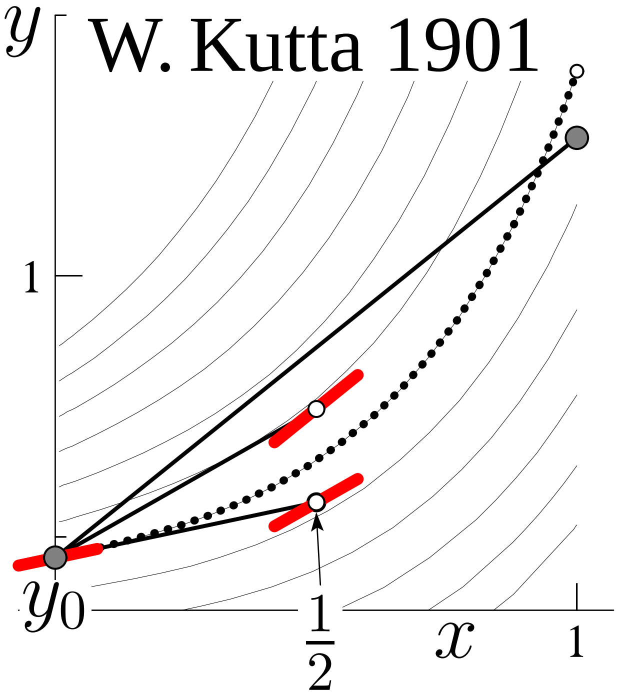

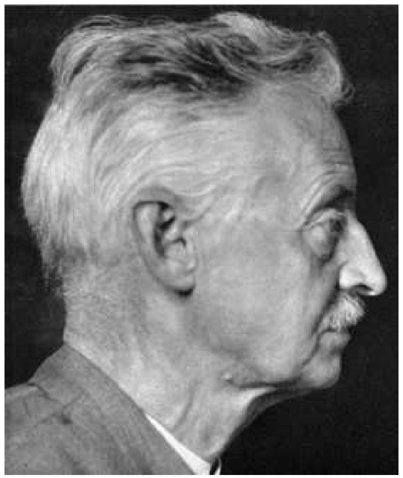

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durch gesetzmäfsige polygonale Linienzüge

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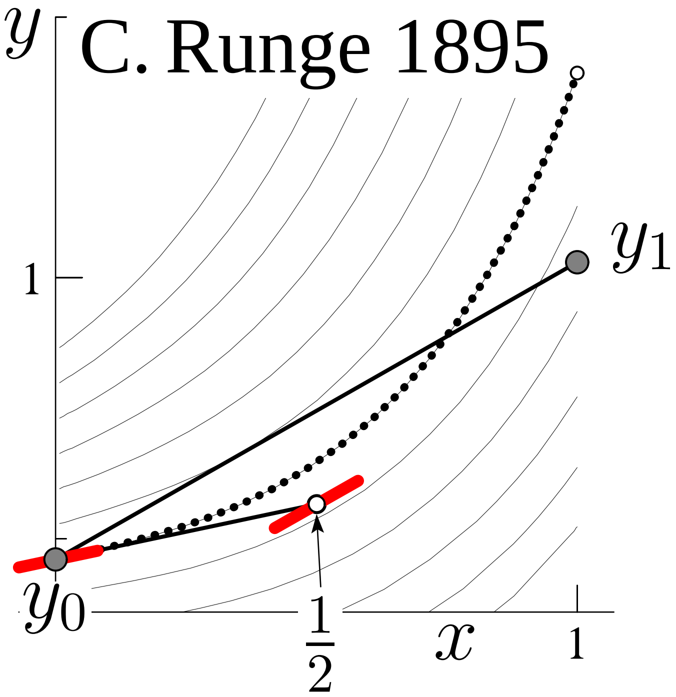
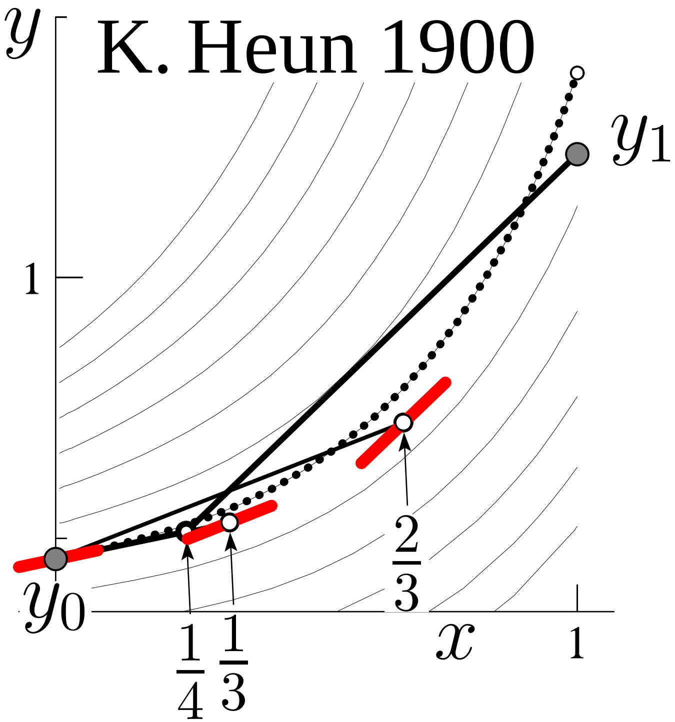
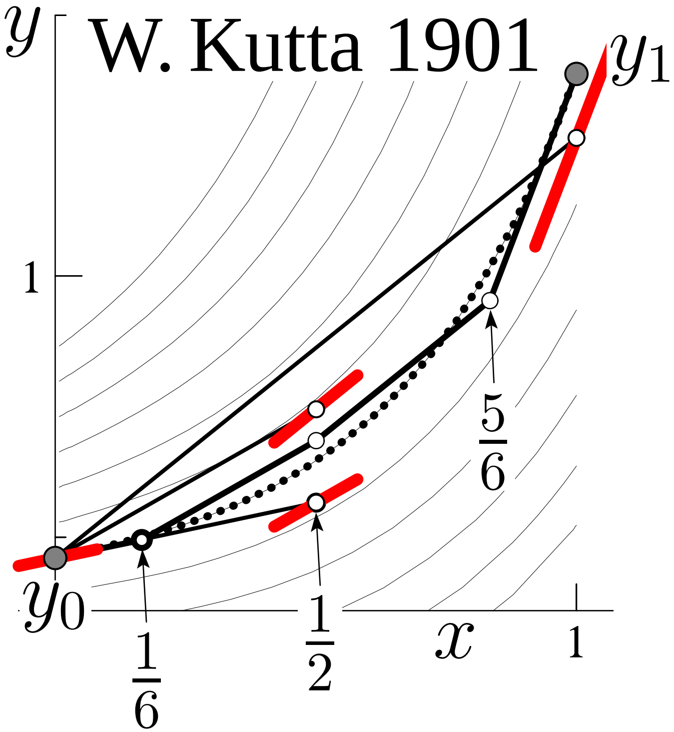
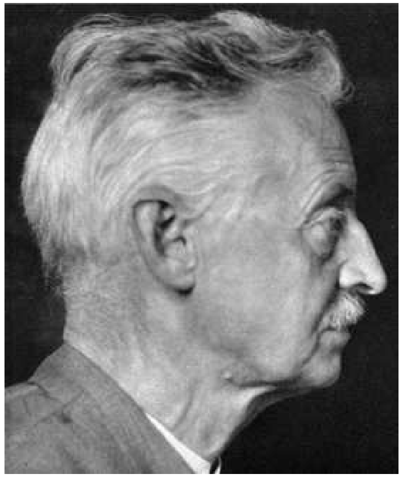








... nice pictures — but the theory became...

... soon very ugly (A. Hut’a 1956, Order 6):

$$
\begin{aligned}
&+ 60(\varphi_1^2\beta_1^2\zeta_2 + \varphi_1^2\gamma_1^2\zeta_3 + \varphi_2^2\gamma_2^2\zeta_3 + \varphi_1^2\delta_1^2\zeta_4 + \varphi_2^2\delta_2^2\zeta_4 + \varphi_3^2\delta_3^2\zeta_4 +\\
&+ \varphi_1^2\varepsilon_1^2\zeta_5 + \varphi_2^2\varepsilon_2^2\zeta_5 + \varphi_3^2\varepsilon_3^2\zeta_5 + \varphi_4^2\varepsilon_4^2\zeta_5 + 2\varphi_1\varphi_2\gamma_1\gamma_2\zeta_3 +\\
&+ 2\varphi_1\varphi_2\delta_1\delta_2\zeta_4 + 2\varphi_1\varphi_3\delta_1\delta_3\zeta_4 + 2\varphi_2\varphi_3\delta_2\delta_3\zeta_4 +\\
&+ 2\varphi_1\varphi_2\varepsilon_1\varepsilon_2\zeta_5 + 2\varphi_1\varphi_3\varepsilon_1\varepsilon_3\zeta_5 + 2\varphi_1\varphi_4\varepsilon_1\varepsilon_4\zeta_5 + 2\varphi_2\varphi_3\varepsilon_2\varepsilon_3\zeta_5 +\\
&+ 2\varphi_2\varphi_4\varepsilon_2\varepsilon_4\zeta_5 + 2\varphi_3\varphi_4\varepsilon_3\varepsilon_4\zeta_5 + 2\varphi_1^2\beta_1\zeta_1\zeta_2 + 2\varphi_1^2\gamma_1\zeta_1\zeta_3 +\\
&+ 2\varphi_1^2\delta_1\zeta_1\zeta_4 + 2\varphi_1^2\varepsilon_1\zeta_1\zeta_5 + 2\varphi_2^2\gamma_2\zeta_2\zeta_3 + 2\varphi_2^2\delta_2\zeta_2\zeta_4 + 2\varphi_2^2\varepsilon_2\zeta_2\zeta_5 +\\
&+ 2\varphi_3^2\delta_3\zeta_3\zeta_4 + 2\varphi_3^2\varepsilon_3\zeta_3\zeta_5 + 2\varphi_4^2\varepsilon_4\zeta_4\zeta_5 + 2\varphi_1\varphi_2\gamma_2\zeta_1\zeta_3 +\\
&+ 2\varphi_1\varphi_2\delta_2\zeta_1\zeta_4 + 2\varphi_1\varphi_2\varepsilon_2\zeta_1\zeta_5 + 2\varphi_1\varphi_2\beta_1\zeta_2^2 + 2\varphi_1\varphi_2\gamma_1\zeta_2\zeta_3 +\\
&+ 2\varphi_1\varphi_2\delta_1\zeta_2\zeta_4 + 2\varphi_1\varphi_2\varepsilon_1\zeta_2\zeta_5 + 2\varphi_1\varphi_3\delta_1\zeta_1\zeta_4 + 2\varphi_1\varphi_3\varepsilon_3\zeta_1\zeta_5 +\\
&+ 2\varphi_1\varphi_3\beta_1\zeta_2\zeta_3 + 2\varphi_1\varphi_3\gamma_1\zeta_3^2 + 2\varphi_1\varphi_3\delta_1\zeta_3\zeta_4 + 2\varphi_1\varphi_3\varepsilon_1\zeta_3\zeta_5 +\\
&+ 2\varphi_2\varphi_3\delta_3\zeta_2\zeta_4 + 2\varphi_2\varphi_3\varepsilon_3\zeta_2\zeta_5 + 2\varphi_2\varphi_3\gamma_2\zeta_3^2 + 2\varphi_2\varphi_3\delta_2\zeta_3\zeta_4 +\\
&+ 2\varphi_2\varphi_3\varepsilon_2\zeta_3\zeta_5 + 2\varphi_1\varphi_4\varepsilon_4\zeta_1\zeta_5 + 2\varphi_1\varphi_4\beta_1\zeta_2\zeta_4 + 2\varphi_1\varphi_4\gamma_1\zeta_3\zeta_4 +\\
&+ 2\varphi_1\varphi_4\delta_1\zeta_4^2 + 2\varphi_1\varphi_4\varepsilon_1\zeta_4\zeta_5 + 2\varphi_2\varphi_4\varepsilon_4\zeta_2\zeta_5 + 2\varphi_2\varphi_4\gamma_2\zeta_2\zeta_4 +\\
&+ 2\varphi_2\varphi_4\delta_2\zeta_4^2 + 2\varphi_2\varphi_4\varepsilon_2\zeta_4\zeta_5 + 2\varphi_3\varphi_4\varepsilon_4\zeta_3\zeta_5 + 2\varphi_3\varphi_4\delta_3\zeta_4^2 +\\
&+ 2\varphi_3\varphi_4\varepsilon_3\zeta_4\zeta_5 + 2\varphi_1\varphi_5\beta_1\zeta_2\zeta_5 + 2\varphi_1\varphi_5\gamma_1\zeta_3\zeta_5 + 2\varphi_1\varphi_5\delta_1\zeta_4\zeta_5 +\\
&+ 2\varphi_1\varphi_5\varepsilon_1\zeta_5^2 + 2\varphi_2\varphi_5\gamma_2\zeta_3\zeta_5 + 2\varphi_2\varphi_5\delta_2\zeta_4\zeta_5 + 2\varphi_2\varphi_5\varepsilon_2\zeta_5^2 +\\
&+ 2\varphi_2\varphi_5\delta_3\zeta_4\zeta_5 + 2\varphi_3\varphi_5\varepsilon_3\zeta_5^2 + 2\varphi_4\varphi_5\varepsilon_4\zeta_5^2)f_1f_2(Df)^2]\,h^5 + \dots
\end{aligned}
$$

$$
\begin{aligned}
m_7 = f &+ \varphi_7 Df\,.\,h + \frac{1}{2}[\varphi_7^2D^{(2)}f + 2(\varphi_1\eta_1 + \varphi_2\eta_2 + \varphi_3\eta_3 + \varphi_4\eta_4 +\\
&+ \varphi_5\eta_5 + \varphi_6\eta_6)f_1Df]\,h^2 + \frac{1}{6}[\varphi_7^3D^{(3)}f + 3(\varphi_1^2\eta_1 + \varphi_2^2\eta_2 + \varphi_3^2\eta_3 +\\
&+ \varphi_4^2\eta_4 + \varphi_5^2\eta_5 + \varphi_6^2\eta_6)f_1D^{(2)}f + 6(\varphi_1\varphi_7\eta_1 + \varphi_2\varphi_7\eta_2 + \varphi_3\varphi_7\eta_3 +\\
&+ \varphi_4\varphi_7\eta_4 + \varphi_5\varphi_7\eta_5 + \varphi_6\varphi_7\eta_6)Df_1Df + 6(\varphi_1\beta_1\eta_2 + \varphi_1\gamma_1\eta_3 +\\
&+ \varphi_2\gamma_2\eta_3 + \varphi_1\delta_1\eta_4 + \varphi_2\delta_2\eta_4 + \varphi_3\delta_3\eta_4 + \varphi_1\varepsilon_1\eta_5 + \varphi_2\varepsilon_2\eta_5 +\\
&+ \varphi_3\varepsilon_3\eta_5 + \varphi_4\varepsilon_4\eta_5 + \varphi_1\zeta_1\eta_6 + \varphi_2\zeta_2\eta_6 + \varphi_3\zeta_3\eta_6 + \varphi_4\zeta_4\eta_6 +\\
&+ \varphi_5\zeta_5\eta_6)f_1^2Df]\,h^3 + \frac{1}{24}[\varphi_7^4D^{(4)}f + 4(\varphi_1^3\eta_1 + \varphi_2^3\eta_2 + \varphi_3^3\eta_3 + \varphi_4^3\eta_4 +\\
&+ \varphi_5^3\eta_5 + \varphi_6^3\eta_6)f_1D^{(3)}f + 12(\varphi_1^2\varphi_7\eta_1 + \varphi_2^2\varphi_7\eta_2 + \varphi_3^2\varphi_7\eta_3 + \varphi_4^2\varphi_7\eta_4 +\\
&+ \varphi_5^2\varphi_7\eta_5 + \varphi_6^2\varphi_7\eta_6)Df_1D^{(2)}f + 12(\varphi_1\varphi_7^2\eta_1 + \varphi_2\varphi_7^2\eta_2 + \varphi_3\varphi_7^2\eta_3 +\\
&+ \varphi_4\varphi_7^2\eta_4 + \varphi_5\varphi_7^2\eta_5 + \varphi_6\varphi_7^2\eta_6)D^{(2)}f_1Df + 12(\varphi_1\eta_1 + \varphi_2\eta_2 + \varphi_3\eta_3 +\\
&+ \varphi_4\eta_4 + \varphi_5\eta_5 + \varphi_6\eta_6)^2f_2(Df)^2 + 24(\varphi_1\varphi_2\beta_1\eta_2 + \varphi_1\varphi_3\gamma_1\eta_3 +\\
&+ \varphi_2\varphi_3\gamma_2\eta_3 + \varphi_1\varphi_4\delta_1\eta_4 + \varphi_2\varphi_4\delta_2\eta_4 + \varphi_3\varphi_4\delta_3\eta_4 + \varphi_1\varphi_5\varepsilon_1\eta_5 +\\
&+ \varphi_2\varphi_5\varepsilon_2\eta_5 + \varphi_3\varphi_5\varepsilon_3\eta_5 + \varphi_4\varphi_5\varepsilon_4\eta_5 + \varphi_1\varphi_6\zeta_1\eta_6 + \varphi_2\varphi_6\zeta_2\eta_6 +\\
&+ \varphi_3\varphi_6\zeta_3\eta_6 + \varphi_4\varphi_6\zeta_4\eta_6 + \varphi_5\varphi_6\zeta_5\eta_6 + \varphi_1\varphi_7\beta_1\eta_2 + \varphi_1\varphi_7\gamma_1\eta_3 +\\
&+ \varphi_2\varphi_7\gamma_2\eta_3 + \varphi_1\varphi_7\delta_1\eta_4 + \varphi_2\varphi_7\delta_2\eta_4 + \varphi_3\varphi_7\delta_3\eta_4 + \varphi_1\varphi_7\varepsilon_1\eta_5 +\\
&+ \varphi_2\varphi_7\varepsilon_2\eta_5 + \varphi_3\varphi_7\varepsilon_3\eta_5 + \varphi_4\varphi_7\varepsilon_4\eta_5 + \varphi_1\varphi_7\zeta_1\eta_6 + \varphi_2\varphi_7\zeta_2\eta_6 +\\
&+ \varphi_3\varphi_7\zeta_3\eta_6 + \varphi_4\varphi_7\zeta_4\eta_6 + \varphi_5\varphi_7\zeta_5\eta_6)f_1Df_1Df + 12(\varphi_1^2\beta_1\eta_2 + \varphi_1^2\gamma_1\eta_3 +\\
&+ \varphi_2^2\gamma_2\eta_3 + \varphi_1^2\delta_1\eta_4 + \varphi_2^2\delta_2\eta_4 + \varphi_3^2\delta_3\eta_4 + \varphi_1^2\varepsilon_1\eta_5 + \varphi_2^2\varepsilon_2\eta_5 +\\
&+ \varphi_3^2\varepsilon_3\eta_5 + \varphi_4^2\varepsilon_4\eta_5 + \varphi_1^2\zeta_1\eta_6 + \varphi_2^2\zeta_2\eta_6 + \varphi_3^2\zeta_3\eta_6 + \varphi_4^2\zeta_4\eta_6 +\\
&+ \varphi_5^2\zeta_5\eta_6)f_1^2D^{(2)}f + 24(\varphi_1\beta_1\gamma_2\eta_3 + \varphi_1\beta_1\delta_2\eta_4 + \varphi_1\gamma_1\delta_3\eta_4 + \varphi_2\gamma_2\delta_3\eta_4 +
\end{aligned}
$$

$$
\begin{aligned}
&+ \varphi_1\beta_1\varepsilon_2\eta_5 + \varphi_1\gamma_1\varepsilon_3\eta_5 + \varphi_2\gamma_2\varepsilon_3\eta_5 + \varphi_1\delta_1\varepsilon_4\eta_5 + \varphi_2\delta_2\varepsilon_4\eta_5 +\\
&+ \varphi_3\delta_3\varepsilon_4\eta_5 + \varphi_1\beta_1\zeta_2\eta_6 + \varphi_1\gamma_1\zeta_3\eta_6 + \varphi_2\gamma_2\zeta_3\eta_6 + \varphi_1\delta_1\zeta_4\eta_6 +\\
&+ \varphi_2\delta_2\zeta_4\eta_6 + \varphi_3\delta_3\zeta_4\eta_6 + \varphi_1\varepsilon_1\zeta_5\eta_6 + \varphi_2\varepsilon_2\zeta_5\eta_6 + \varphi_3\varepsilon_3\zeta_5\eta_6 +\\
&+ \varphi_4\varepsilon_4\zeta_5\eta_6)f_1^3Df]\,h^4 + \frac{1}{120}\{\varphi_7^5D^{(5)}f + 5(\varphi_1^4\eta_1 + \varphi_2^4\eta_2 + \varphi_3^4\eta_3 +\\
&+ \varphi_4^4\eta_4 + \varphi_5^4\eta_5 + \varphi_6^4\eta_6)f_1D^{(4)}f + 20(\varphi_1^3\varphi_7\eta_1 + \varphi_2^3\varphi_7\eta_2 + \varphi_3^3\varphi_7\eta_3 +\\
&+ \varphi_4^3\varphi_7\eta_4 + \varphi_5^3\varphi_7\eta_5 + \varphi_6^3\varphi_7\eta_6)Df_1D^{(3)}f + 30(\varphi_1^2\varphi_7^2\eta_1 + \varphi_2^2\varphi_7^2\eta_2 +\\
&+ \varphi_3^2\varphi_7^2\eta_3 + \varphi_4^2\varphi_7^2\eta_4 + \varphi_5^2\varphi_7^2\eta_5 + \varphi_6^2\varphi_7^2\eta_6)D^{(2)}f_1D^{(2)}f + 20(\varphi_1\varphi_7^3\eta_1 +\\
&+ \varphi_2\varphi_7^3\eta_2 + \varphi_3\varphi_7^3\eta_3 + \varphi_4\varphi_7^3\eta_4 + \varphi_5\varphi_7^3\eta_5 + \varphi_6\varphi_7^3\eta_6)D^{(3)}f_1Df +\\
&+ 60(\varphi_1\eta_1 + \varphi_2\eta_2 + \varphi_3\eta_3 + \varphi_4\eta_4 + \varphi_5\eta_5 + \varphi_6\eta_6)(\varphi_1^2\eta_1 + \varphi_2^2\eta_2 +\\
&+ \varphi_3^2\eta_3 + \varphi_4^2\eta_4 + \varphi_5^2\eta_5 + \varphi_6^2\eta_6)f_2D^{(2)}fDf + 60(\varphi_1\eta_1 + \varphi_2\eta_2 +\\
&+ \varphi_3\eta_3 + \varphi_4\eta_4 + \varphi_5\eta_5 + \varphi_6\eta_6)^2\,.\,\varphi_7\,.\,Df_2\,(Df)^2 + 60(\varphi_1^2\varphi_2\beta_1\eta_2 +\\
&+ \varphi_1^2\varphi_3\gamma_1\eta_3 + \varphi_2^2\varphi_3\gamma_2\eta_3 + \varphi_1^2\varphi_4\delta_1\eta_4 + \varphi_2^2\varphi_4\delta_2\eta_4 + \varphi_3^2\varphi_4\delta_3\eta_4 +\\
&+ \varphi_1^2\varphi_5\varepsilon_1\eta_5 + \varphi_2^2\varphi_5\varepsilon_2\eta_5 + \varphi_3^2\varphi_5\varepsilon_3\eta_5 + \varphi_4^2\varphi_5\varepsilon_4\eta_5 + \varphi_1^2\varphi_6\zeta_1\eta_6 +\\
&+ \varphi_2^2\varphi_6\zeta_2\eta_6 + \varphi_3^2\varphi_6\zeta_3\eta_6 + \varphi_4^2\varphi_6\zeta_4\eta_6 + \varphi_5^2\varphi_6\zeta_5\eta_6 + \varphi_1^2\varphi_7\beta_1\eta_2 +\\
&+ \varphi_1^2\varphi_7\gamma_1\eta_3 + \varphi_2^2\varphi_7\gamma_2\eta_3 + \varphi_1^2\varphi_7\delta_1\eta_4 + \varphi_2^2\varphi_7\delta_2\eta_4 + \varphi_3^2\varphi_7\delta_3\eta_4 +\\
&+ \varphi_1^2\varphi_7\varepsilon_1\eta_5 + \varphi_2^2\varphi_7\varepsilon_2\eta_5 + \varphi_3^2\varphi_7\varepsilon_3\eta_5 + \varphi_4^2\varphi_7\varepsilon_4\eta_5 + \varphi_1^2\varphi_7\zeta_1\eta_6 +\\
&+ \varphi_2^2\varphi_7\zeta_2\eta_6 + \varphi_3^2\varphi_7\zeta_3\eta_6 + \varphi_4^2\varphi_7\zeta_4\eta_6 + \varphi_5^2\varphi_7\zeta_5\eta_6)f_1Df_1D^{(2)}f +\\
&+ 60(\varphi_1\varphi_2^2\beta_1\eta_2 + \varphi_1\varphi_3^2\gamma_1\eta_3 + \varphi_2\varphi_3^2\gamma_2\eta_3 + \varphi_1\varphi_4^2\delta_1\eta_4 + \varphi_2\varphi_4^2\delta_2\eta_4 +\\
&+ \varphi_3\varphi_4^2\delta_3\eta_4 + \varphi_1\varphi_5^2\varepsilon_1\eta_5 + \varphi_2\varphi_5^2\varepsilon_2\eta_5 + \varphi_3\varphi_5^2\varepsilon_3\eta_5 + \varphi_4\varphi_5^2\varepsilon_4\eta_5 +\\
&+ \varphi_1\varphi_6^2\zeta_1\eta_6 + \varphi_2\varphi_6^2\zeta_2\eta_6 + \varphi_3\varphi_6^2\zeta_3\eta_6 + \varphi_4\varphi_6^2\zeta_4\eta_6 + \varphi_5\varphi_6^2\zeta_5\eta_6 +\\
&+ \varphi_1\varphi_7^2\beta_1\eta_2 + \varphi_1\varphi_7^2\gamma_1\eta_3 + \varphi_2\varphi_7^2\gamma_2\eta_3 + \varphi_1\varphi_7^2\delta_1\eta_4 + \varphi_2\varphi_7^2\delta_2\eta_4 +\\
&+ \varphi_3\varphi_7^2\delta_3\eta_4 + \varphi_1\varphi_7^2\varepsilon_1\eta_5 + \varphi_2\varphi_7^2\varepsilon_2\eta_5 + \varphi_3\varphi_7^2\varepsilon_3\eta_5 + \varphi_4\varphi_7^2\varepsilon_4\eta_5 +\\
&+ \varphi_1\varphi_7^2\zeta_1\eta_6 + \varphi_2\varphi_7^2\zeta_2\eta_6 + \varphi_3\varphi_7^2\zeta_3\eta_6 + \varphi_4\varphi_7^2\zeta_4\eta_6 +\\
&+ \varphi_5\varphi_7^2\zeta_5\eta_6)f_1D^{(2)}f_1Df + 120(\varphi_1\varphi_2\varphi_7\beta_1\eta_2 + \varphi_1\varphi_3\varphi_7\gamma_1\eta_3 +\\
&+ \varphi_2\varphi_3\varphi_7\gamma_2\eta_3 + \varphi_1\varphi_4\varphi_7\delta_1\eta_4 + \varphi_2\varphi_4\varphi_7\delta_2\eta_4 + \varphi_3\varphi_4\varphi_7\delta_3\eta_4 +\\
&+ \varphi_1\varphi_5\varphi_7\varepsilon_1\eta_5 + \varphi_2\varphi_5\varphi_7\varepsilon_2\eta_5 + \varphi_3\varphi_5\varphi_7\varepsilon_3\eta_5 + \varphi_4\varphi_5\varphi_7\varepsilon_4\eta_5 +\\
&+ \varphi_1\varphi_6\varphi_7\zeta_1\eta_6 + \varphi_2\varphi_6\varphi_7\zeta_2\eta_6 + \varphi_3\varphi_6\varphi_7\zeta_3\eta_6 + \varphi_4\varphi_6\varphi_7\zeta_4\eta_6 +\\
&+ \varphi_5\varphi_6\varphi_7\zeta_5\eta_6)(Df_1)^2Df + 20(\varphi_1^3\beta_1\eta_2 + \varphi_1^3\gamma_1\eta_3 + \varphi_2^3\gamma_2\eta_3 + \varphi_1^3\delta_1\eta_4 +\\
&+ \varphi_2^3\delta_2\eta_4 + \varphi_3^3\delta_3\eta_4 + \varphi_1^3\varepsilon_1\eta_5 + \varphi_2^3\varepsilon_2\eta_5 + \varphi_3^3\varepsilon_3\eta_5 + \varphi_4^3\varepsilon_4\eta_5 +\\
&+ \varphi_1^3\zeta_1\eta_6 + \varphi_2^3\zeta_2\eta_6 + \varphi_3^3\zeta_3\eta_6 + \varphi_4^3\zeta_4\eta_6 + \varphi_5^3\zeta_5\eta_6)f_1^2D^{(3)}f +\\
&+ 120(\varphi_1\varphi_2\beta_1\gamma_2\eta_3 + \varphi_1\varphi_3\beta_1\gamma_2\eta_3 + \varphi_1\varphi_2\beta_1\delta_2\eta_4 + \varphi_1\varphi_3\gamma_1\delta_3\eta_4 +\\
&+ \varphi_2\varphi_3\gamma_2\delta_3\eta_4 + \varphi_1\varphi_4\beta_1\delta_2\eta_4 + \varphi_1\varphi_2\gamma_1\delta_3\eta_4 + \varphi_2\varphi_4\gamma_2\delta_3\eta_4 +\\
&+ \varphi_1\varphi_2\beta_1\varepsilon_2\eta_5 + \varphi_1\varphi_3\gamma_1\varepsilon_3\eta_5 + \varphi_2\varphi_3\gamma_2\varepsilon_3\eta_5 + \varphi_1\varphi_4\delta_1\varepsilon_4\eta_5 +\\
&+ \varphi_2\varphi_4\delta_2\varepsilon_4\eta_5 + \varphi_3\varphi_4\delta_3\varepsilon_4\eta_5 + \varphi_1\varphi_5\beta_1\varepsilon_2\eta_5 + \varphi_1\varphi_5\gamma_1\varepsilon_3\eta_5 +\\
&+ \varphi_2\varphi_5\gamma_2\varepsilon_3\eta_5 + \varphi_1\varphi_5\delta_1\varepsilon_4\eta_5 + \varphi_2\varphi_5\delta_2\varepsilon_4\eta_5 +\\
&+ \varphi_3\varphi_5\delta_3\varepsilon_4\eta_5 + \varphi_1\varphi_2\beta_1\zeta_2\eta_6 + \varphi_1\varphi_3\gamma_1\zeta_3\eta_6 + \varphi_2\varphi_3\gamma_2\zeta_3\eta_6 +\\
&+ \varphi_1\varphi_4\delta_1\zeta_4\eta_6 + \varphi_2\varphi_4\delta_2\zeta_4\eta_6 + \varphi_3\varphi_4\delta_3\zeta_4\eta_6 + \varphi_1\varphi_5\varepsilon_1\zeta_5\eta_6 +\\
&+ \varphi_2\varphi_5\varepsilon_2\zeta_5\eta_6 + \varphi_3\varphi_5\varepsilon_3\zeta_5\eta_6 + \varphi_4\varphi_5\varepsilon_4\zeta_5\eta_6 + \varphi_1\varphi_6\beta_1\zeta_2\eta_6 +\\
&+ \varphi_1\varphi_6\gamma_1\zeta_3\eta_6 + \varphi_2\varphi_6\gamma_2\zeta_3\eta_6 + \varphi_1\varphi_6\delta_1\zeta_4\eta_6 + \varphi_2\varphi_6\delta_2\zeta_4\eta_6 +\\
&+ \varphi_3\varphi_6\delta_3\zeta_4\eta_6 + \varphi_1\varphi_6\varepsilon_1\zeta_5\eta_6 + \varphi_2\varphi_6\varepsilon_2\zeta_5\eta_6 + \varphi_3\varphi_6\varepsilon_3\zeta_5\eta_6 +
\end{aligned}
$$

Towards a New Era:

Autonomous syst.

(Gill, Ferranti Ltd.)

"It is difficult to keep a cool head
when discussing the various derivatives ..."

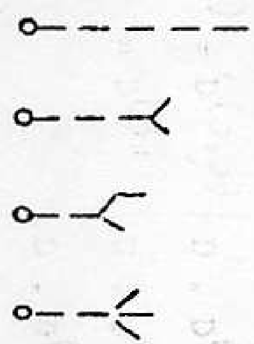
Term $\left(f_i^j = \left(\frac{\partial f_i}{\partial y_j}\right)_X\right)$	Coef	
	$y_i(X+h) - y_i(X)$	δy_i from (12)
hf_i	1	$a+b+c+d$
$h^2 f_j f_i^j$	$\frac{1}{2}$	$bm+cn+dp$
$h^3 f_j f_k f_i^{jk}$	$\frac{1}{6}$	$\frac{1}{2}(bm^2+cn^2+dp^2)$
$h^3 f_j f_k^j f_i^k$	$\frac{1}{6}$	$crm+d(sm+tn)$
$h^4 f_j f_k f_l f_i^{jkl}$	$\frac{1}{24}$	$\frac{1}{6}(bm^3+cn^3+dp^3)$
$h^4 f_j f_k f_l^k f_i^{jl}$	$\frac{1}{8}$	$crmn+d(sm+tn)p$
$h^4 f_j f_k f_l^{jk} f_i^l$	$\frac{1}{24}$	$\frac{1}{2}\{crm^2+d(sm^2+tn^2)\}$
$h^4 f_j f_k^j f_l^k f_i^l$	$\frac{1}{24}$	$dtrm$

... cool the head down

with the use of Trees...

(Merson 1957)

Standard Notation	Tree
$f_i f_j^i f_k^j f_\ell^k f_m^\ell (\,)^m$	
$f_i f_j f_k^{ij} f_\ell^k f_m^\ell (\,)^m$	
$f_i f_j^i f_k f_\ell^{jk} f_m^\ell (\,)^m$	
$f_i f_j f_k f_\ell^{ijk} f_m^\ell (\,)^m$	



... and an elegant notation

for the coefficients

$$a_{ij},\, b_i,\, c_i = \sum a_{ij}$$

(Kuntzmann 1959)

$$y_{i,\alpha} = y_{i,0} + h \sum_{\beta=0}^{\alpha-1} A_{\alpha,\beta} Y_{i,\beta}$$

$$z_{i,\alpha} = z_{i,0} + h \sum_{\beta=0}^{\alpha-1} A_{\alpha,\beta} Z_{i,\beta}$$

$$t_{i,\alpha} = t_i + h\,\theta_\alpha \qquad (\theta_q = 1)$$

$$Y_{i,\beta} = Y(y_{i,\beta},\, z_{i,\beta},\, t_{i,\beta})$$

Les θ_α, $A_{\alpha,\beta}$ sont des constantes convenables.

J. BUTCHER, Austral. Math. Soc. 1963

COEFFICIENTS FOR THE STUDY OF RUNGE-KUTTA INTEGRATION PROCESSES

J. C. BUTCHER

(received 21 May 1962)

Introduction

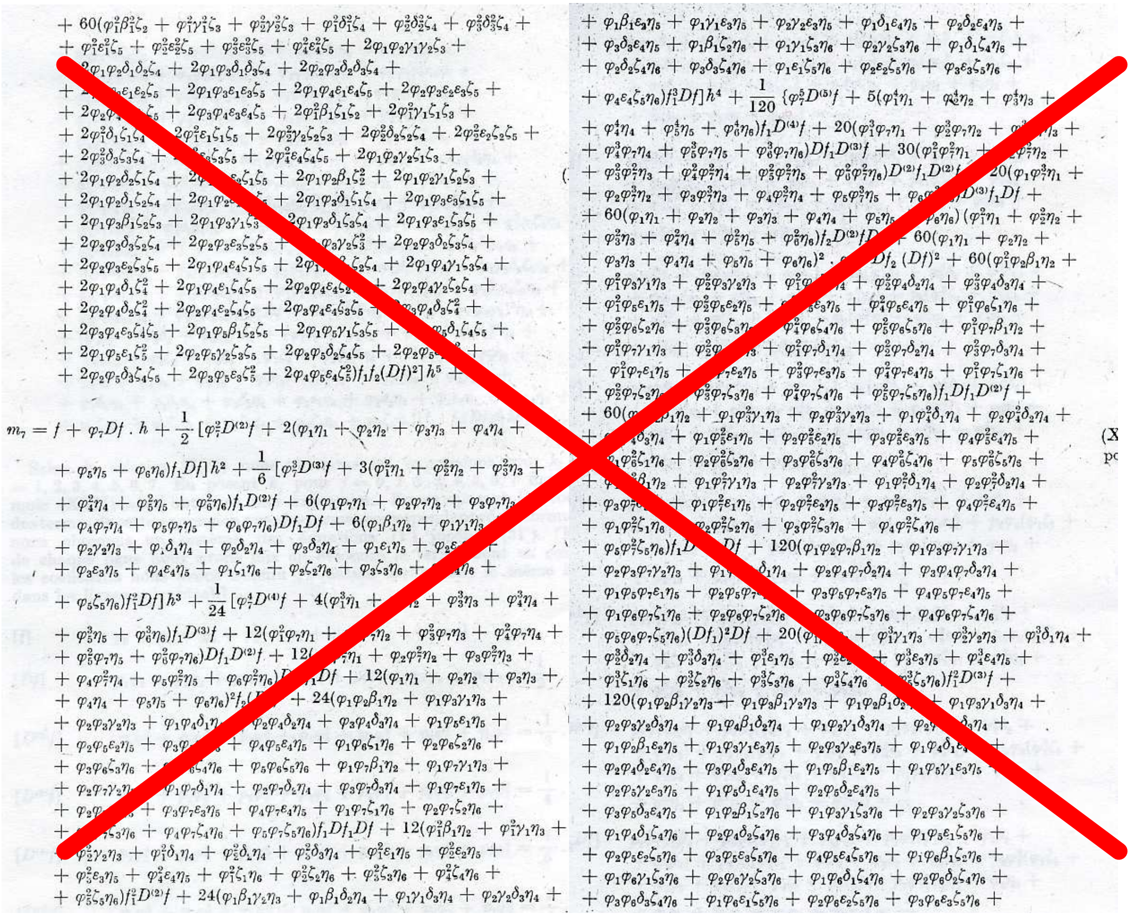
We consider a set of n first order simultaneous differential equations in the dependent variables $y_1, y_2, \cdots, y_n$ and the independent variable x

$$(1)\qquad \begin{aligned} \frac{dy_1}{dx} &= f_1(y_1, y_2, \cdots, y_n), \\ \frac{dy_2}{dx} &= f_2(y_1, y_2, \cdots, y_n), \\ &\vdots \\ \frac{dy_n}{dx} &= f_n(y_1, y_2, \cdots, y_n). \end{aligned}$$

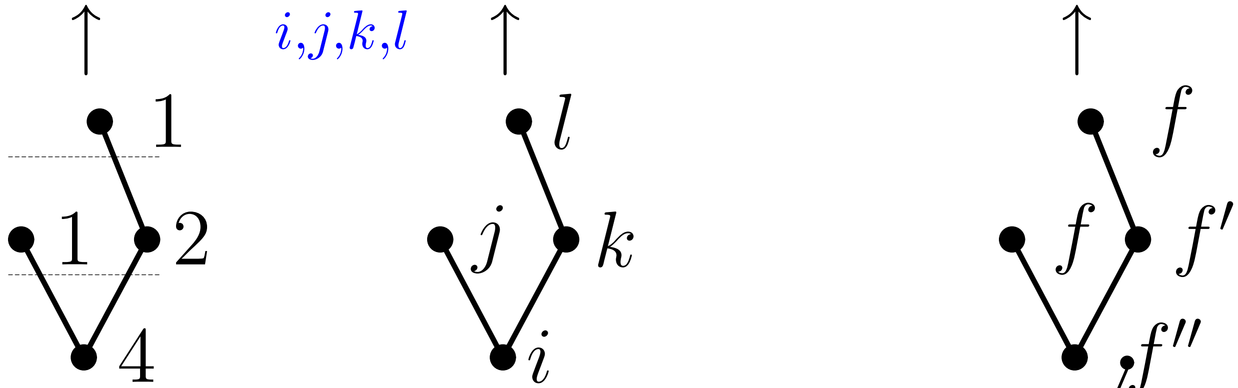
J. C. Butcher

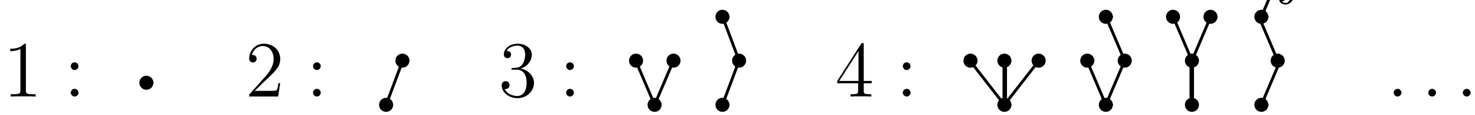
$$g^{(I)} = f(y_0 + h \sum_{J=1}^{\nu} a_{IJ} g^{(J)}),$$

$$\hat{y} = y_0 + h \sum_{I=1}^{\nu} b_I g^{(I)},$$



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

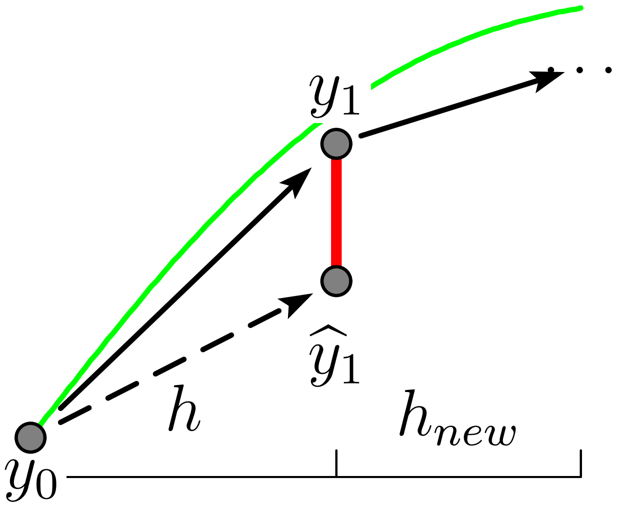




Butcher's Classical Achievements :

- 1963: Simplifying assumptions $B(\eta), C(\mu), D(\nu)$;
- 1963: Implicit method of order 5.
- 1964: Implicit RK processes order $2s$ (Gauss);
- 1964: Radau I, Radau II, Lobatto III methods;
- 1964: Explicit methods of high order; 6th order, 7 stages;
- 1965: Order barriers for explicit methods (5-5 and 7-8 impossible);
- 1966: towards general linear methods;
- 1968: ERK 7-9 constructed;
- 1969: Composition laws; effective order;
- 1972: Algebraic theory, "my" Group;
- 1975, 1979: B-stability, algebraic stability (with Burrage);
- 1976: Implementation of IRK (tensor structure);
  $\Rightarrow$ SIRK methods, code STRIDE;
- 1985: Non-existence of ERK 8-10;

Step-Size Control (Merson, Ceschino, Zonneveld,....)



Ex. Restr. 3-body problem:

$$\mu = 0.012277471$$

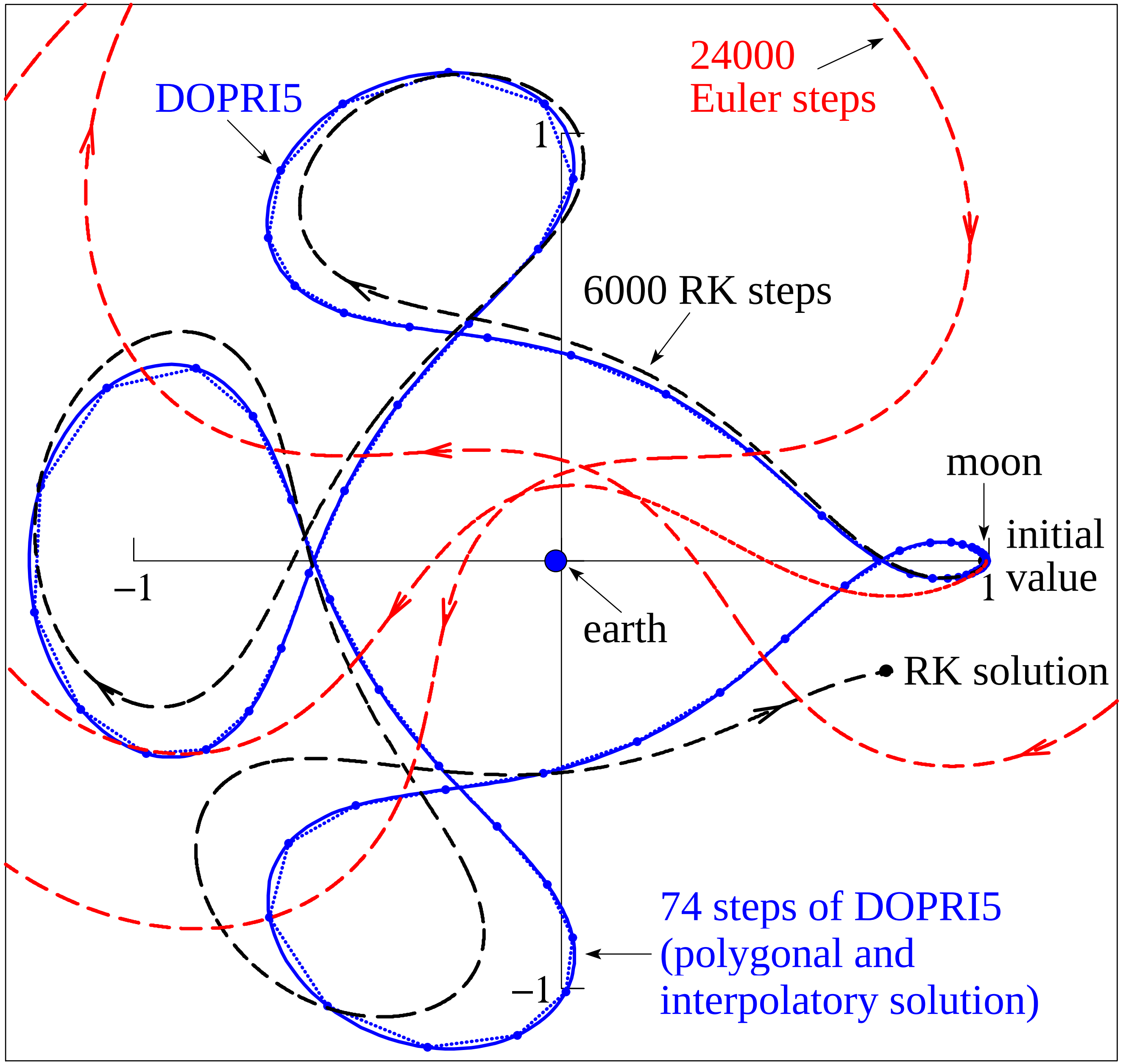
$$y_1(0) = 0.994$$

$$\dot{y}_1(0) = 0$$

$$y_2(0) = 0$$

$$\dot{y}_2 = -2.00158510637908252240$$

$$T = 17.0652165601579625588$$



Codes: **DOPRI5**, **DOP86** (Dormand-Prince) **DOP853** (E.Hairer).

4. Stiff Equations

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

Recent Example:

Asymptotical computations for a model of flow in saturated porous media

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[b] *Mathematical Sciences, University of Bath, Bath BA2 7AY, United Kingdom*
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ARTICLE INFO

Keywords:
Flow in concrete
Interface problem
Adaptive mesh selection
Asymptotic theory

ABSTRACT

We discuss an initial value problem for an implicit second order ordinary differential equation which arises in models of flow in saturated porous media such as concrete. Depending on the initial condition, the solution features a sharp interface with derivatives which become numerically unbounded. By using an integrator based on finite difference methods and equipped with adaptive step size selection, it is possible to compute the solution on highly irregular meshes. In this way it is possible to verify and predict asymptotical theory near the interface with remarkable accuracy.

1. Introduction and problem statement

A model for the time dependent flow of water through a variably saturated porous medium with exponential diffusivity, such as soil, rock or concrete is given by

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right), \quad x \in [0, \infty), \quad t > 0, \tag{1}$$

solution for exponential diffusivity (3)–(5) below is derived. In [18], an iterative approach to solving this problem is developed. The paper [6] gives an asymptotic series expansion for the similarity solution under certain simplifying assumptions. Further asymptotic analysis of the similarity solution is developed in [16,17]. However, there has been a lack both of sharp asymptotic results and of convincing numerical calculations.

In the present paper we adopt a sophisticated numerical approach to investigate the asymptotical behavior of such self-similar solutions of Eqs. (1) and (2). These are stable attractors and take the form

$$u(x,t) = \psi(y), \quad y = x/t^{1/2}, \quad 0 < y < \infty.$$

If we set

$$\theta(y) = e^{\beta(\psi(y) - u_i)},$$

it then follows that $\theta(y)$ satisfies the boundary value problem

$$\theta(y)\theta_{yy}(y) = -y\theta_y(y), \quad y > 0, \tag{3}$$

$$\theta(0) = 1, \quad \theta(\infty) = \theta_\infty \equiv e^{\beta(u_o - u_i)}. \tag{4}$$

It is convenient, for both the analysis and computation of this system to consider instead the initial value problem

$$\theta_y(0) = -\gamma < 0, \quad \theta(0) = 1. \tag{5}$$

and to determine the value of γ corresponding to θ_∞. The purpose of this paper is to make a numerical study of the solutions of (3)–(5) in the limit of large γ which corresponds to a problem with large diffusion with $\beta \gg 1$ when u is not small. The motivation for this investigation is to study a series of refined asymptotic estimates developed in [9] which significantly improve the earlier estimates. A second motivation is that the extreme nature of the problem and the existence of true asymptotical results give an important test and validation of the numerical method described in this paper.

A plot of the solution $\theta(y)$ of (3)–(5) for $\gamma = 3$ is given in Fig. 1. In this plot we can see that for smaller values of y the solution $\theta(y)$ decreases almost linearly, coming close to zero at the point $y \sim 1/\gamma$. As θ approaches zero it follows from solution for exponential diffusivity (3)–(5) below is derived. In [18], an iterative approach to solving this problem is developed. The paper [6] gives an asymptotic series expansion for the similarity solution under certain simplifying assumptions. Further asymptotic analysis of the similarity solution is developed in [16,17]. However, there has been a lack both of sharp asymptotic results and of convincing numerical calculations.

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... is simply stiff equation with steady state solution

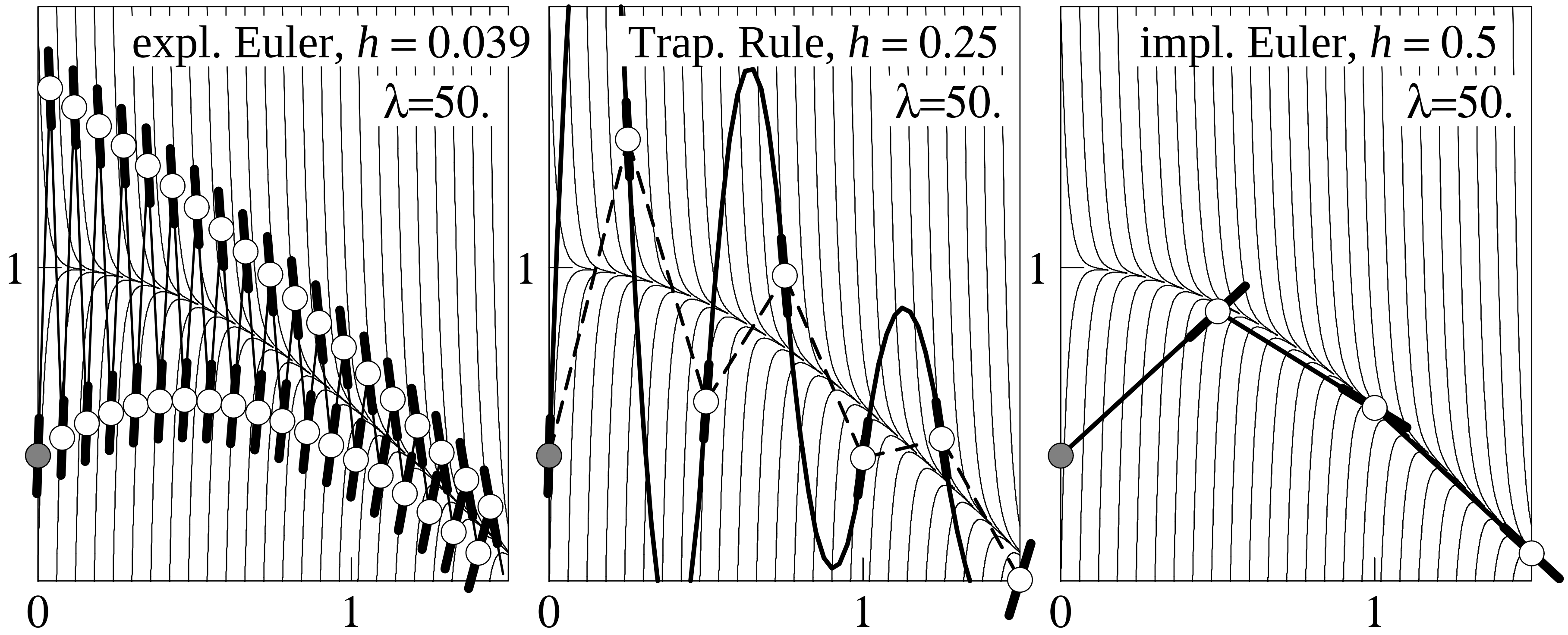
$$y' = p \qquad y(0) = 1$$

$$p' = -\frac{x}{y} \cdot p \qquad p(0) = -\gamma\,, \qquad \Rightarrow \qquad \boxed{p = c - a \log y}$$

4. Stiff Equations

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

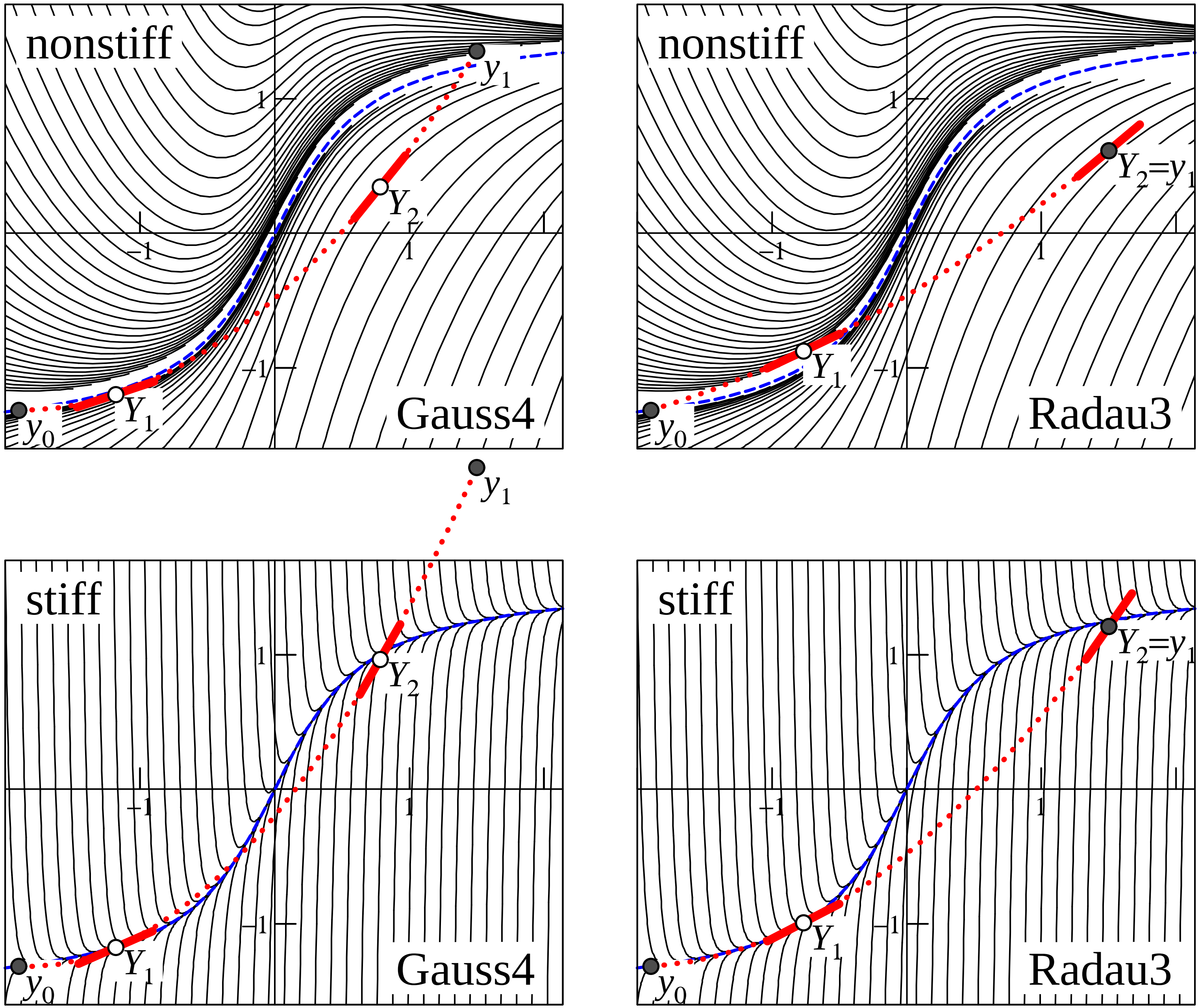
Explicit methods don't work ... Example: $y' = -\lambda(y - \cos x)$



Remedy: implicit methods (Euler E342 §656)

$$y = b + \frac{(x-a)dy}{dx} - \frac{(x-a)^2 ddy}{1 \cdot 2\, dx^2} + \frac{(x-a)^3 d^3y}{1 \cdot 2 \cdot 3\, dx^3} - \frac{(x-a)^4 d^4y}{1 \cdot 2 \cdot 3 \cdot 4\, dx^4} + \text{etc.}$$

IRK (Gauss-Kuntzmann-Butcher 1963, Radau-Ehle 1968)



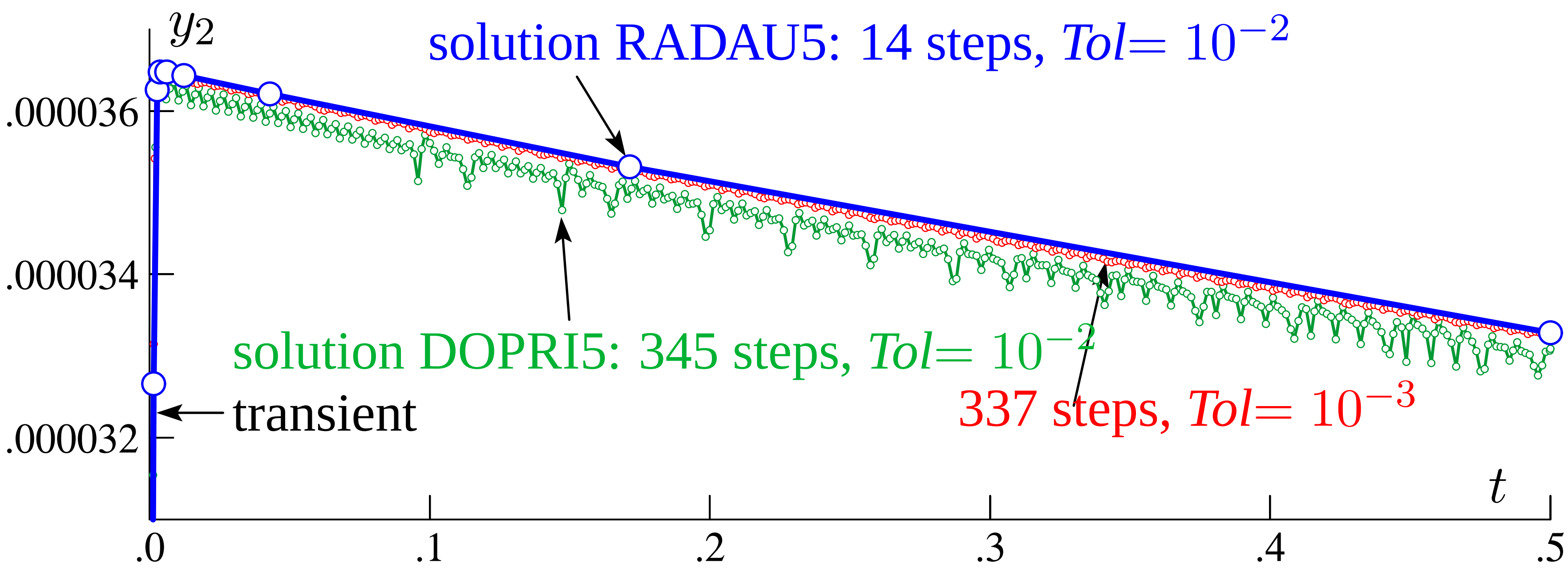
highest order ↑ best stability ↑

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

Example: (Robertson 1966)

$$
\begin{array}{ccccl}
A & \xrightarrow{0.04} & B & & \text{(slow)} \\
B+B & \xrightarrow{3\cdot 10^7} & C+B & & \text{(very fast)} \\
B+C & \xrightarrow{10^4} & A+C & & \text{(fast)}
\end{array}
$$

$$
\begin{array}{llr}
\text{A:} \quad y_1' = -0.04 y_1 + 10^4 y_2 y_3 & & y_1(0) = 1 \\
\text{B:} \quad y_2' = 0.04 y_1 - 10^4 y_2 y_3 - 3\cdot 10^7 y_2^2 & & y_2(0) = 0 \\
\text{C:} \quad y_3' = 3\cdot 10^7 y_2^2 & & y_3(0) = 0.
\end{array}
$$



Stability Analysis: (CFL 1928, Dahlquist 1963)

the famous definition of A-stability ...

DEFINITION. *A k-step method is called A-stable, if all solutions of* (1.2) *tend to zero, as* $n \to \infty$, *when the method is applied with fixed positive h to any differential equation of the form,*

$$dx/dt = qx\,, \qquad (1.8)$$

where q is a complex constant with negative real part.

stable for $y' = \lambda y$, $\Re\lambda \leq 0$, $\Rightarrow$A-stable;

... and "Dahlquist's second barrier"

THEOREM 2.2. *The order, p, of an A-stable linear multistep method cannot exceed* 2. *The smallest error constant,* $c^* = \frac{1}{12}$, *is obtained for the trapezoidal rule,* $k = 1$, *with the generating polynomials* (2.2).

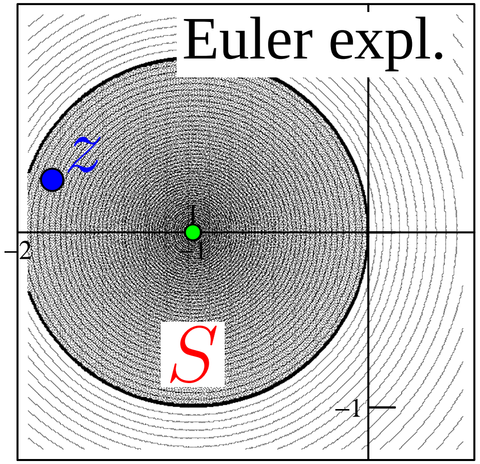
A-stable MSM $\Rightarrow$ $\boxed{p \leq 2}$.

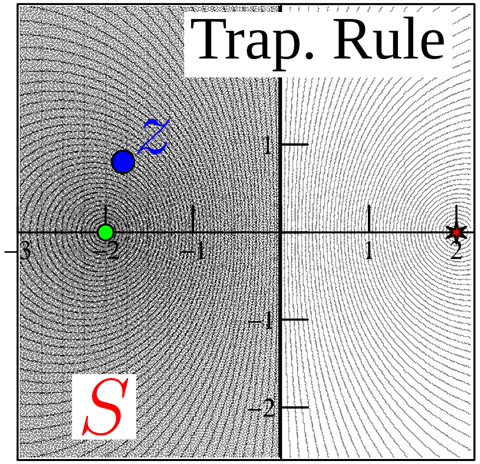
"I searched for a long time, finally Professor Lax showed me the Riesz-Herglotz theorem and I knew that I had my theorem." (G. Dahlquist in 1979)

Stability Analysis for IRK methods: (Ehle 1968)

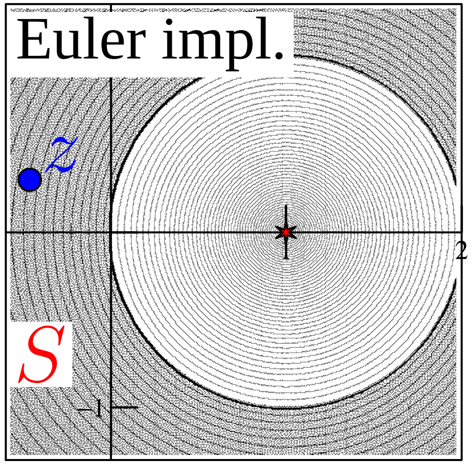
$y' = \lambda y \Rightarrow y_{n+1} = R(z) y_n \quad z = h\lambda;$ Stab. Cond. $|R(z)| \leq 1$

Expl. Euler	Trap. Rule	Impl. Euler
$R(z) = 1 + z$	$R(z) = \frac{1+\frac{z}{2}}{1-\frac{z}{2}}$	$R(z) = \frac{1}{1-z}$



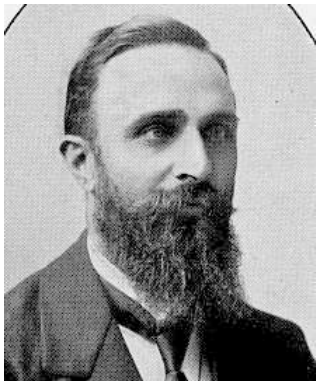


A-stable



A-stable

Padé approx. to e^z



$$R(z) = P_k(z)/Q_j(z)$$

$$P_k(z) = 1 + \frac{k}{j+k} z + \ldots + \frac{k(k-1)\ldots 1}{(j+k)\ldots(j+1)} \cdot \frac{z^k}{k!}$$

$$Q_j(z) = 1 - \frac{j}{k+j} z + \ldots \pm \frac{j(j-1)\ldots 1}{(k+j)\ldots(k+1)} \cdot \frac{z^j}{j!}$$

Padé Table for e^z:

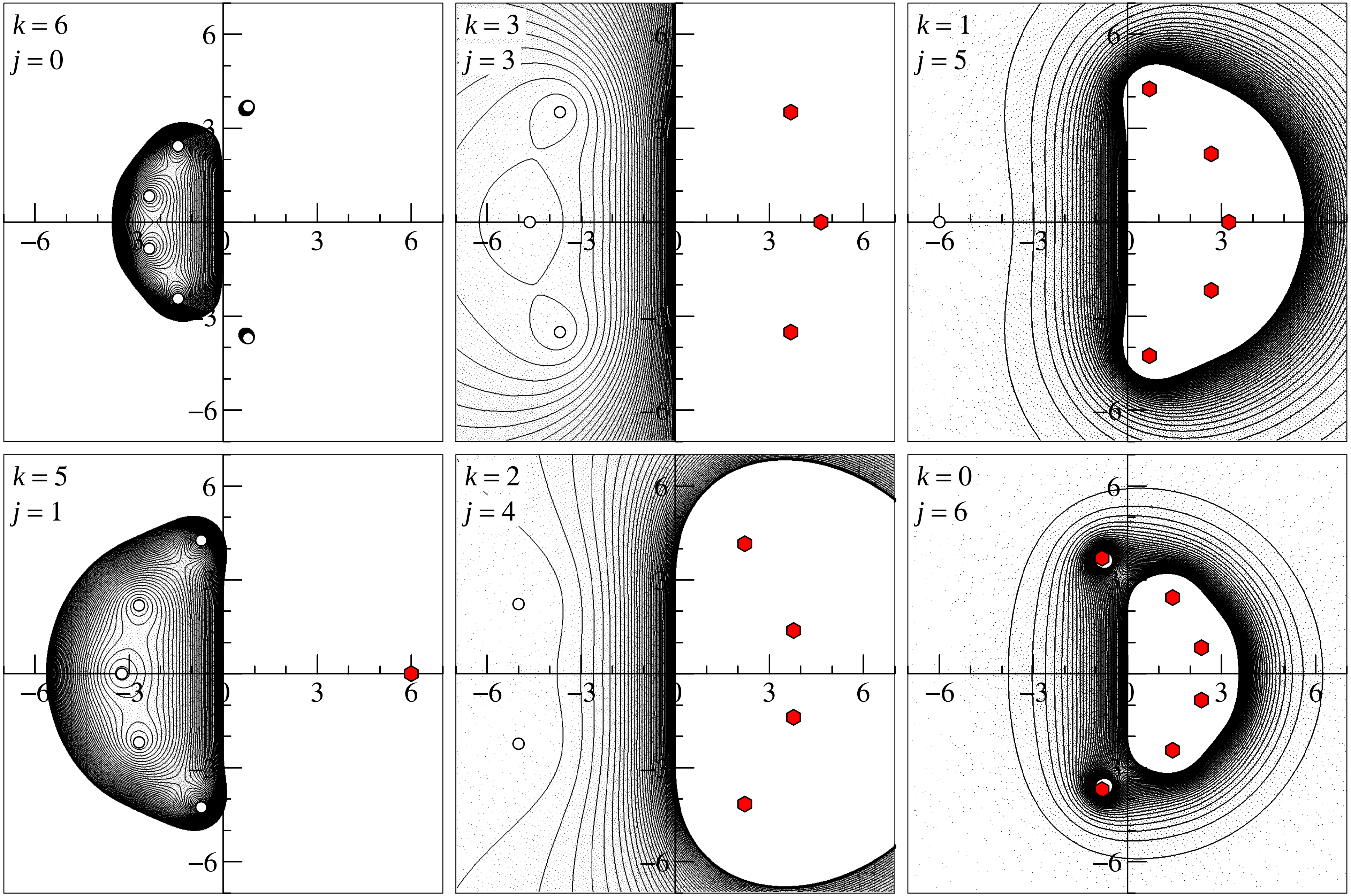
$\frac{1}{1}$	$\frac{1+z}{1}$	$\frac{1+z+\frac{z^2}{2!}}{1}$
$\frac{1}{1-z}$	$\frac{1+\frac{1}{2}z}{1-\frac{1}{2}z}$	$\frac{1+\frac{2}{3}z+\frac{1}{3}\frac{z^2}{2!}}{1-\frac{1}{3}z}$
$\frac{1}{1-z+\frac{z^2}{2!}}$	$\frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{3}\frac{z^2}{2!}}$	$\frac{1+\frac{1}{2}z+\frac{1}{6}\frac{z^2}{2!}}{1-\frac{1}{2}z+\frac{1}{6}\frac{z^2}{2!}}$
$\frac{1}{1-z+\frac{z^2}{2!}-\frac{z^3}{3!}}$	$\frac{1+\frac{1}{4}z}{1-\frac{3}{4}z+\frac{1}{2}\frac{z^2}{2!}-\frac{1}{4}\frac{z^3}{3!}}$	$\frac{1+\frac{2}{5}z+\frac{1}{10}\frac{z^2}{2!}}{1-\frac{3}{5}z+\frac{3}{10}\frac{z^2}{2!}-\frac{1}{10}\frac{z^3}{3!}}$

Birkhoff-Varga (1965): **Thm.:** Entire Diagonal A-stable.

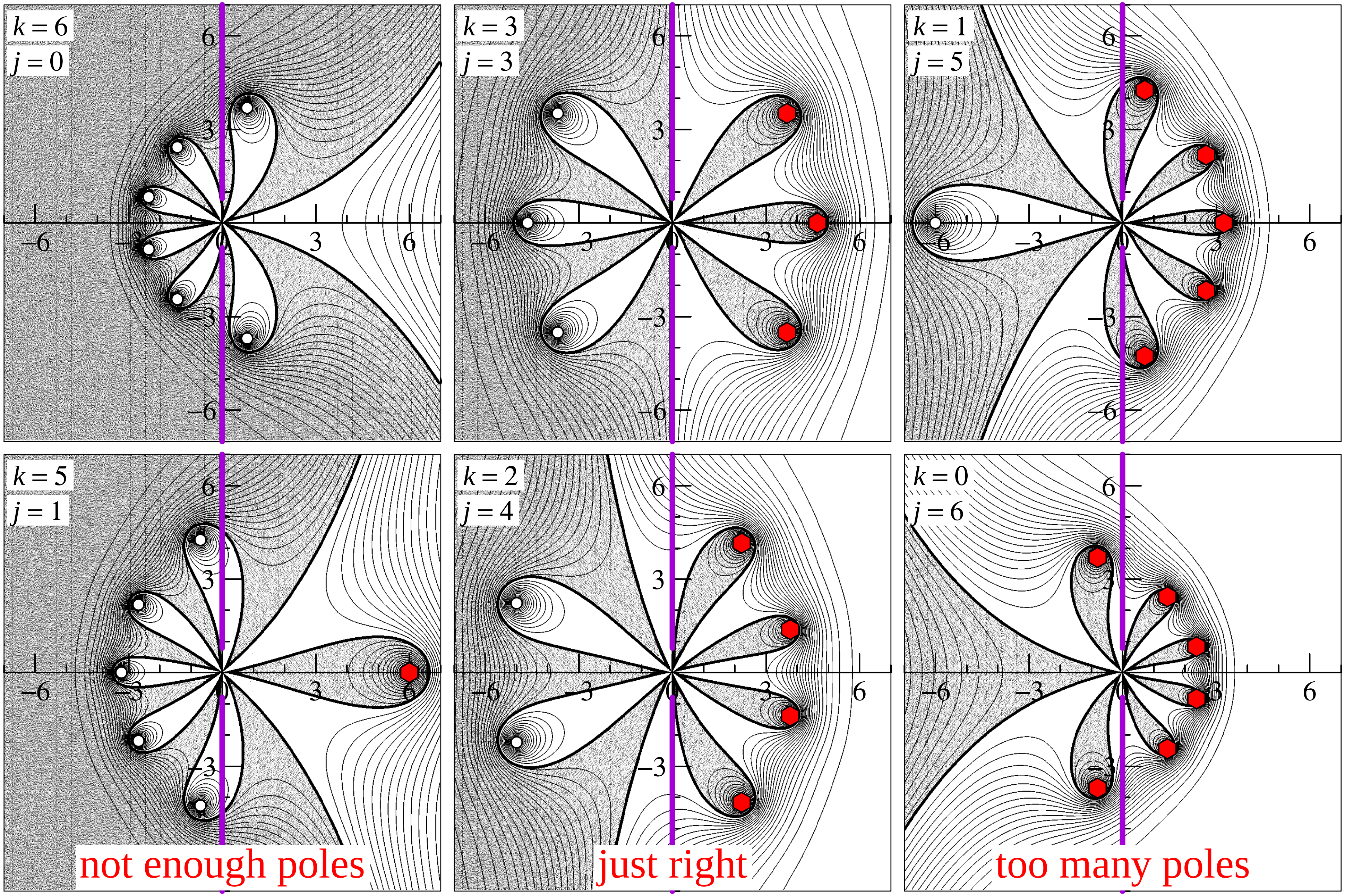
Ehle (1968): **Thm.:** 1^{st} and 2^{nd} Subdiagonal A-stable.

Ehle (1968): **Conj.:** All others **not** A-stable.

Why ??



Order Stars (1978). Idea: $|R(z)| \le 1 \;\Rightarrow\; |R(z)| > |e^z|$

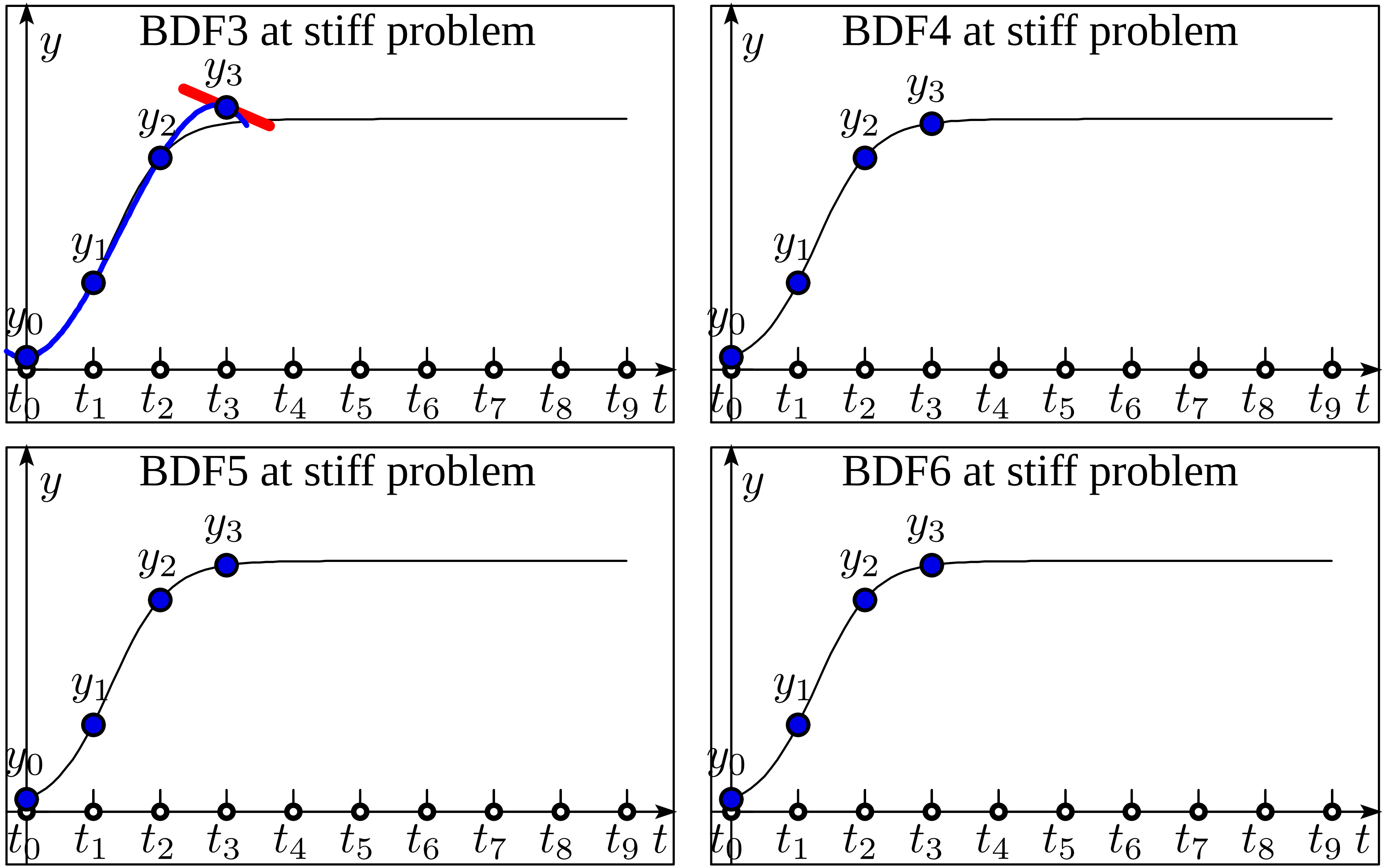


Proof of B-V-Ehle's theorem and Ehle's conjecture.

BDF methods (Curtiss-Hirschfelder 1952, Gear 1971)

"BDF is so beautiful that it is hard to imagine something else could be better." (L. Petzold 1988, heard by P. Deuflhard)

Polyn. collocation at t_{n+1} : $\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = h f_{n+1}$



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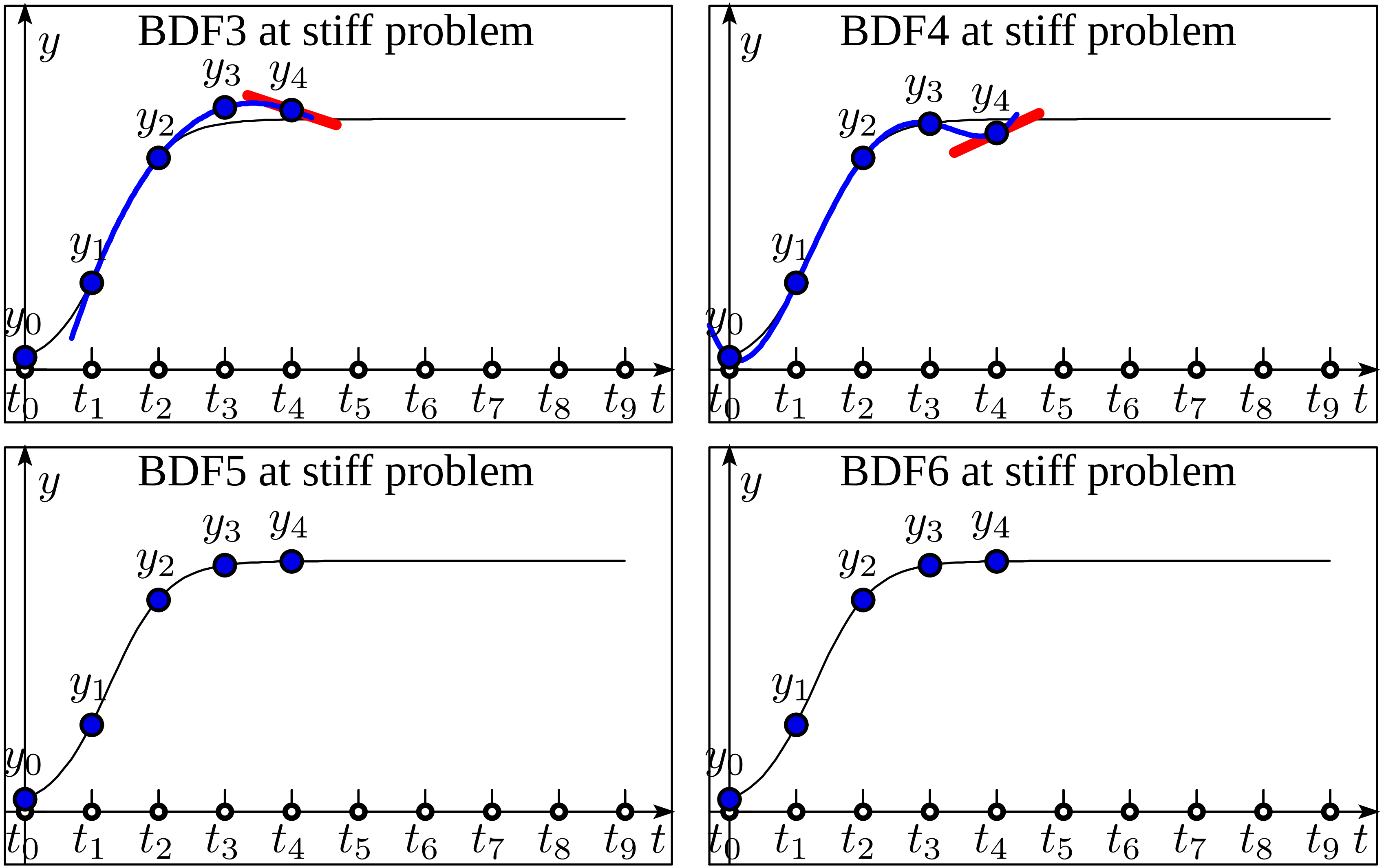

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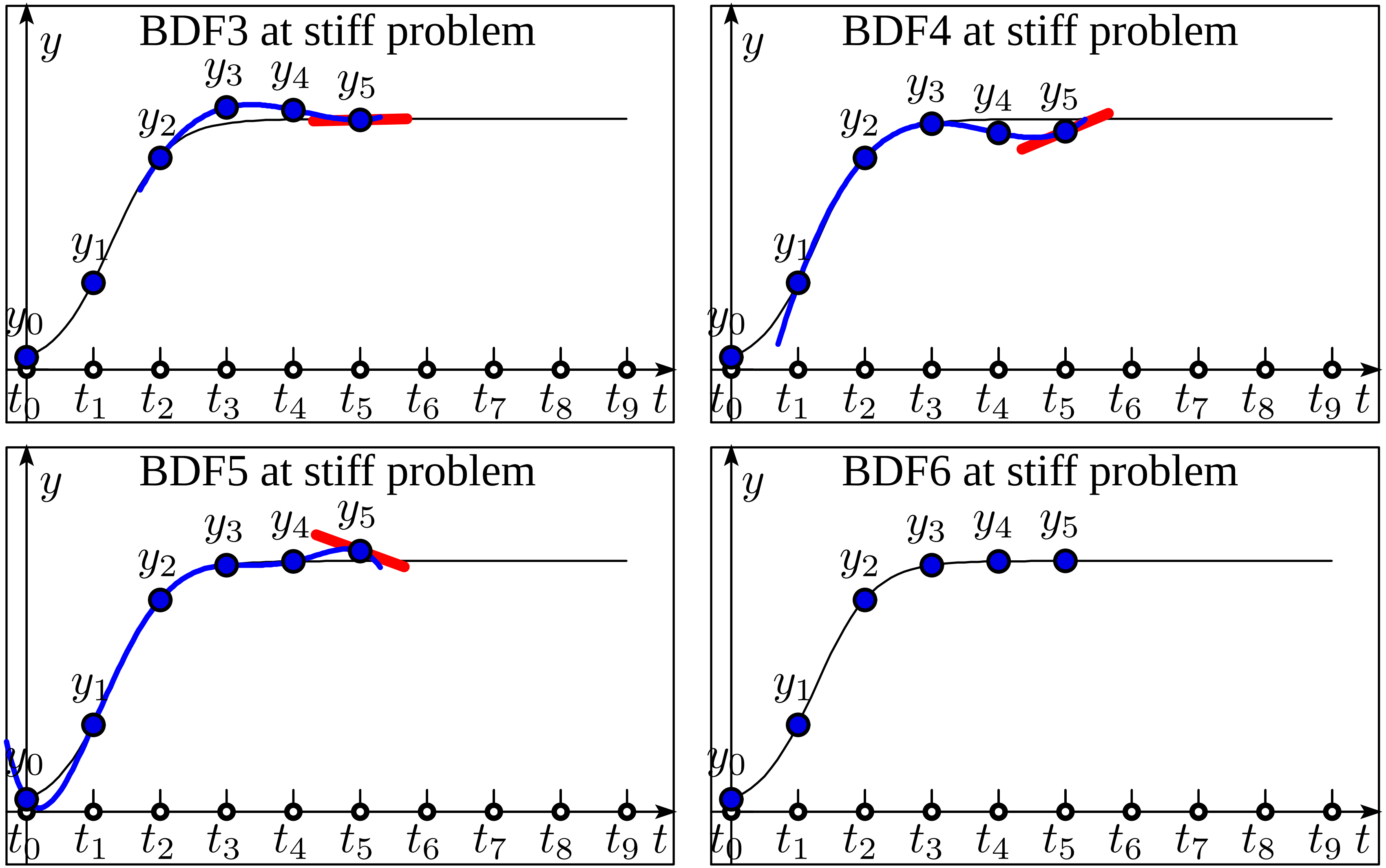

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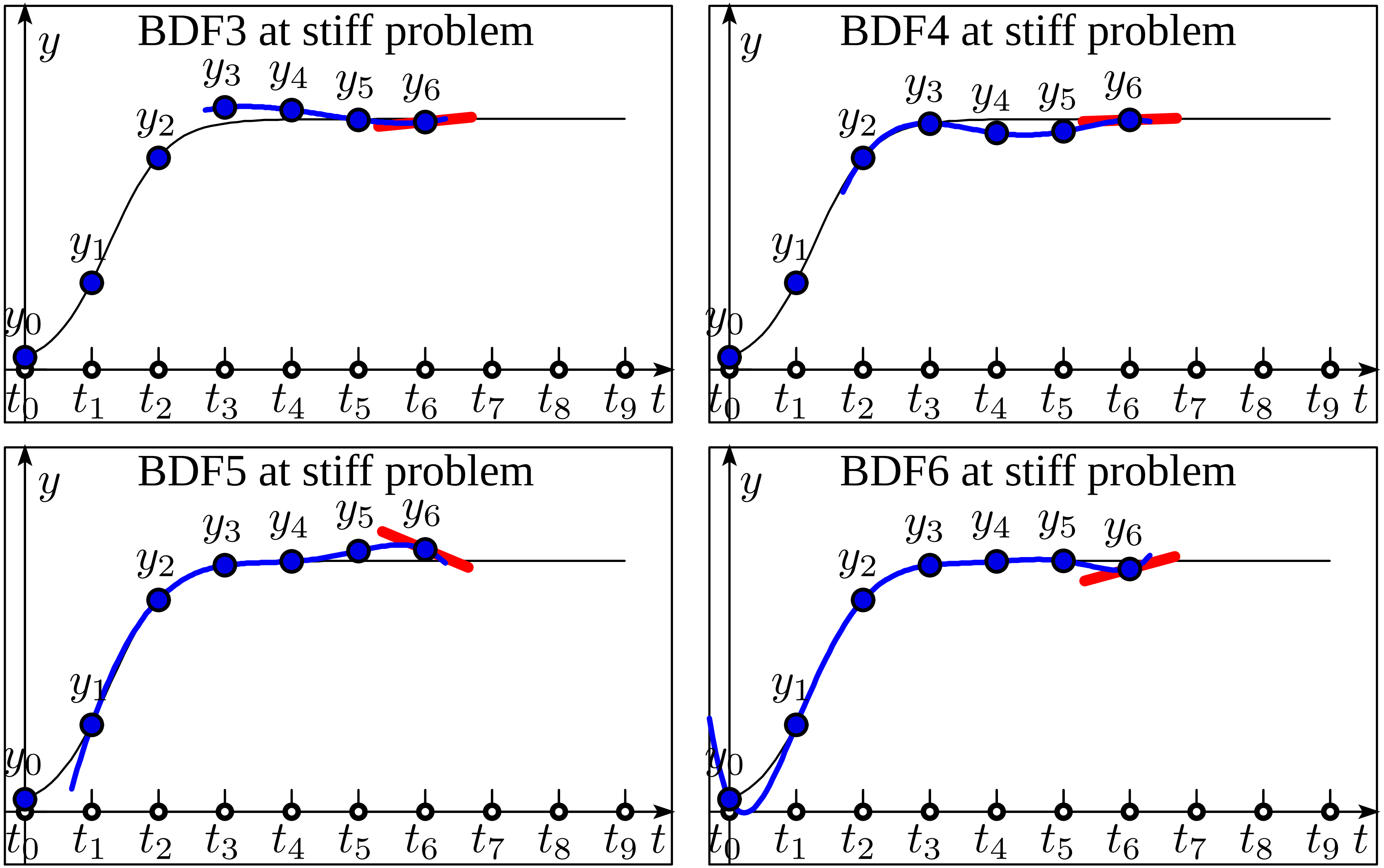

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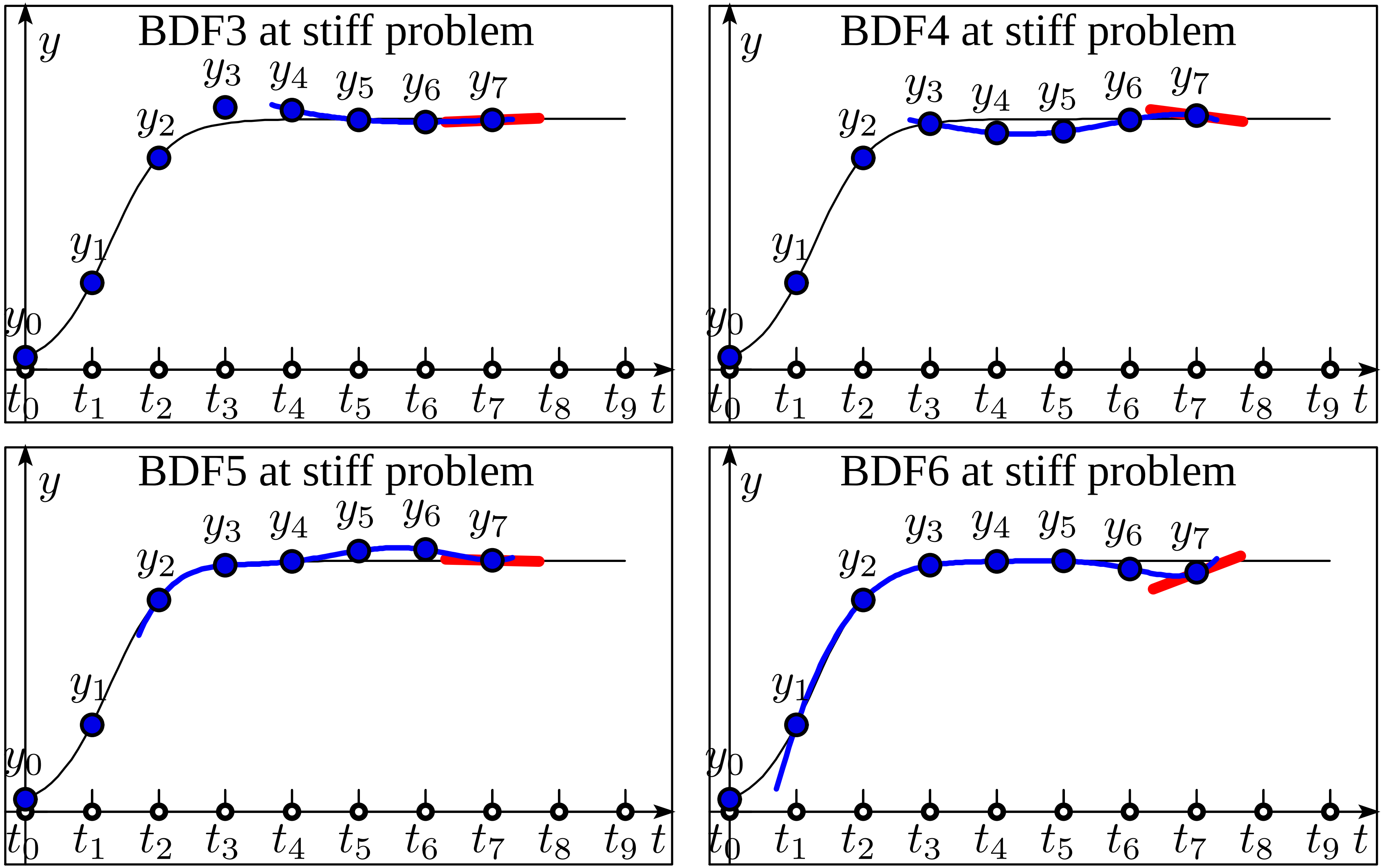

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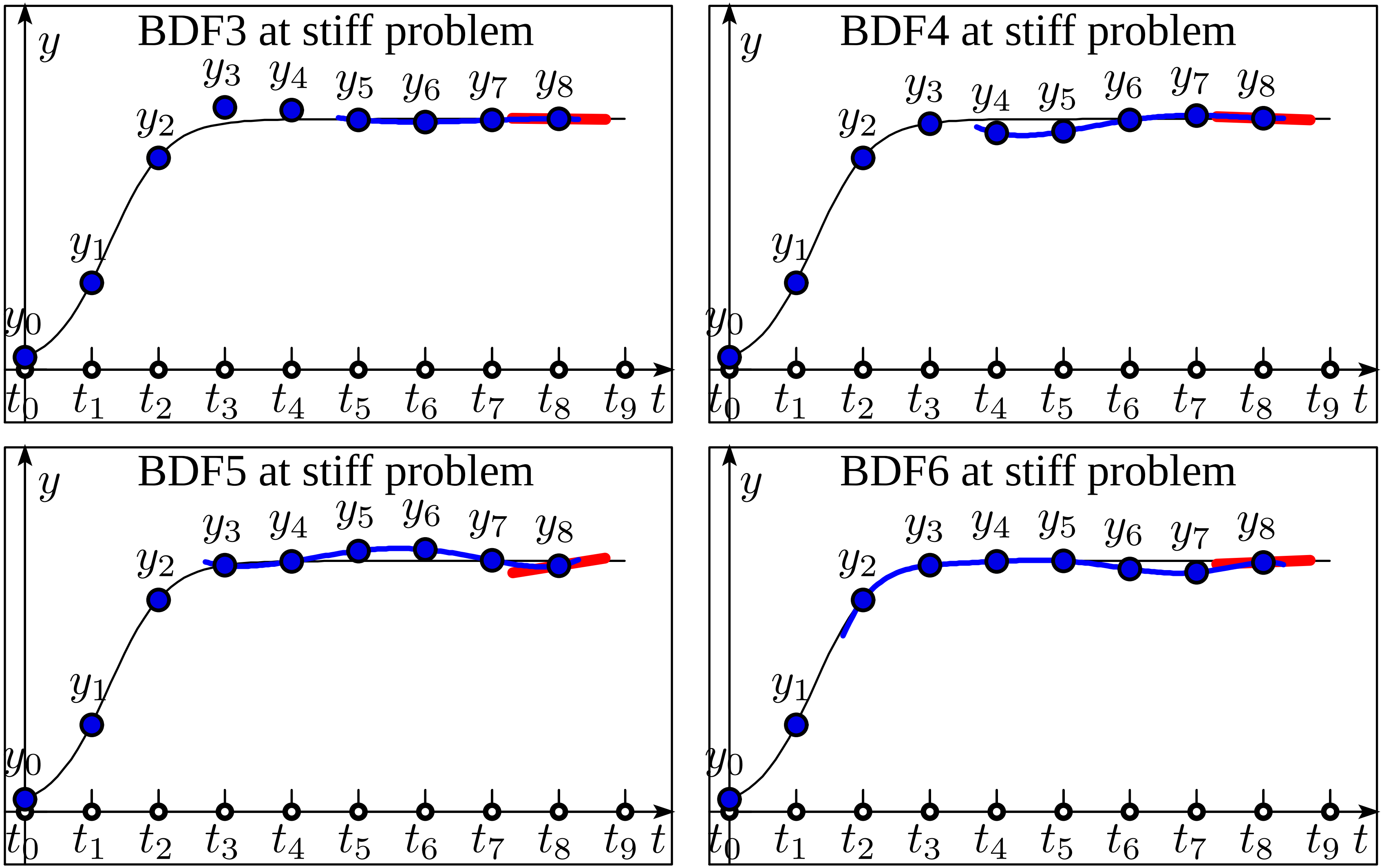

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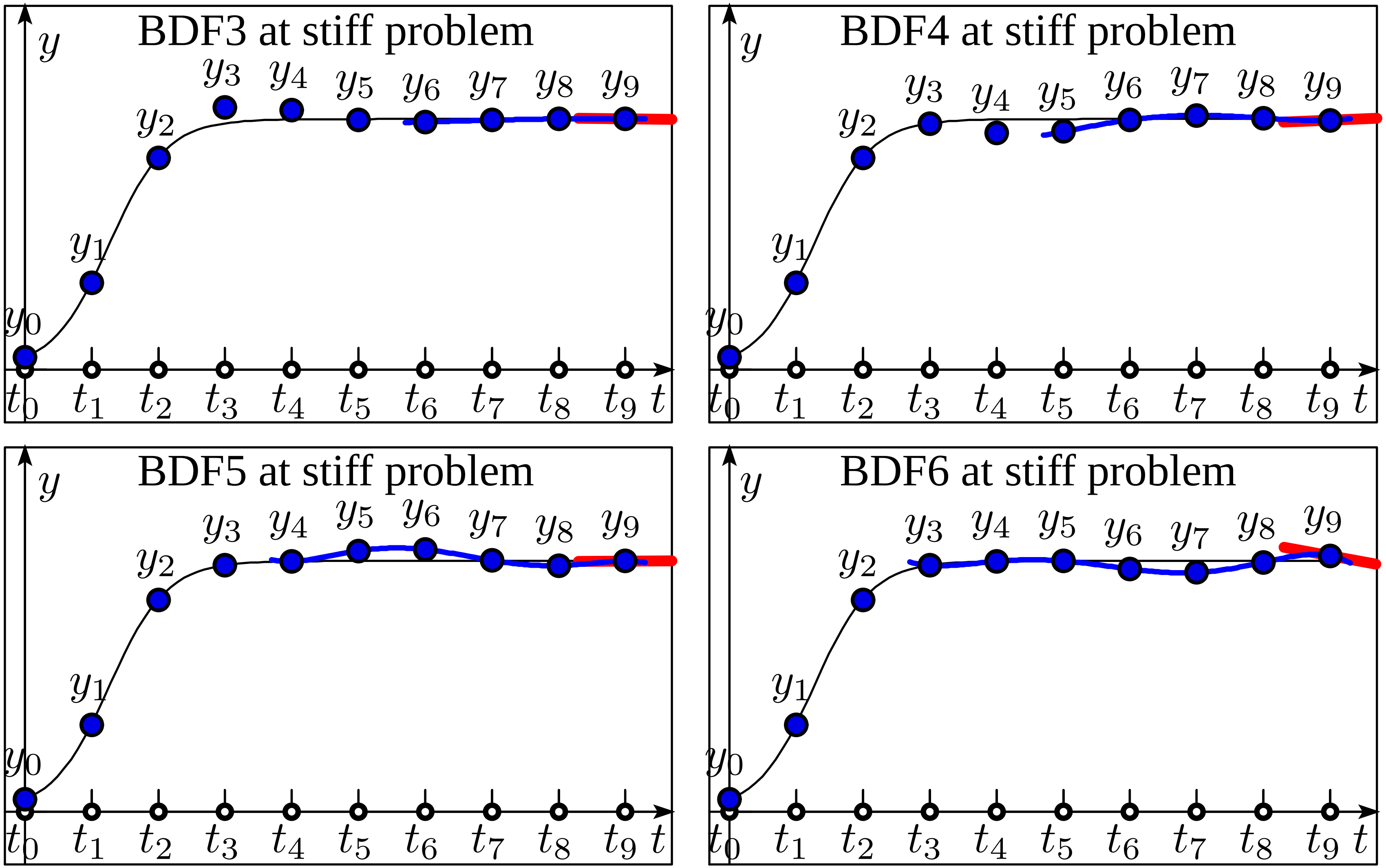

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Polyn. collocation at t_{n+1} : $\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = h f_{n+1}$

Codes:

LSODE (MF=21, Hindmarsh),
DEBDF (Shampine & Watts),
VODE (Brown, Byrne & Hindmarsh),
MEBDF (Cash & Considine),
DASSL (Petzold; for DAE-systems),...

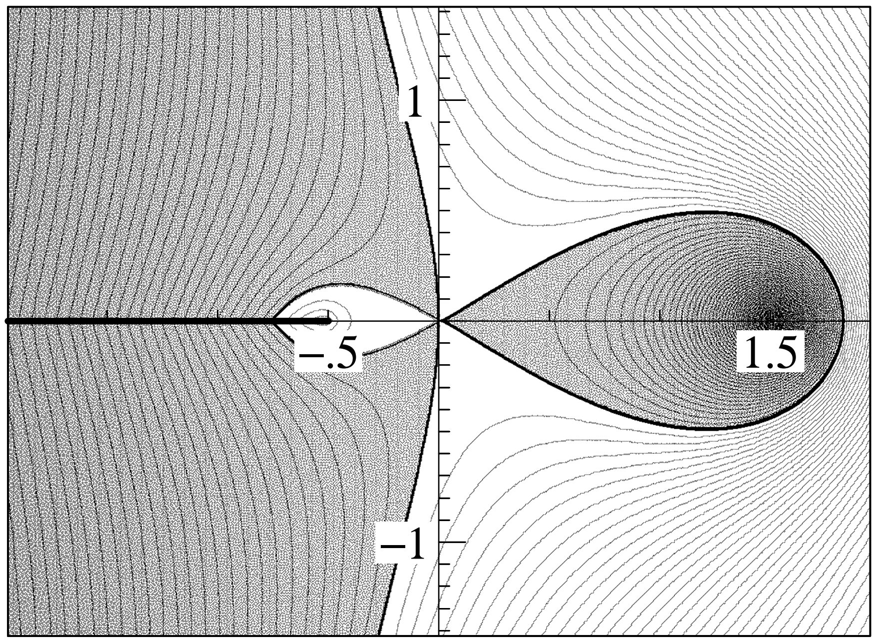
Stability Analysis for BDF.

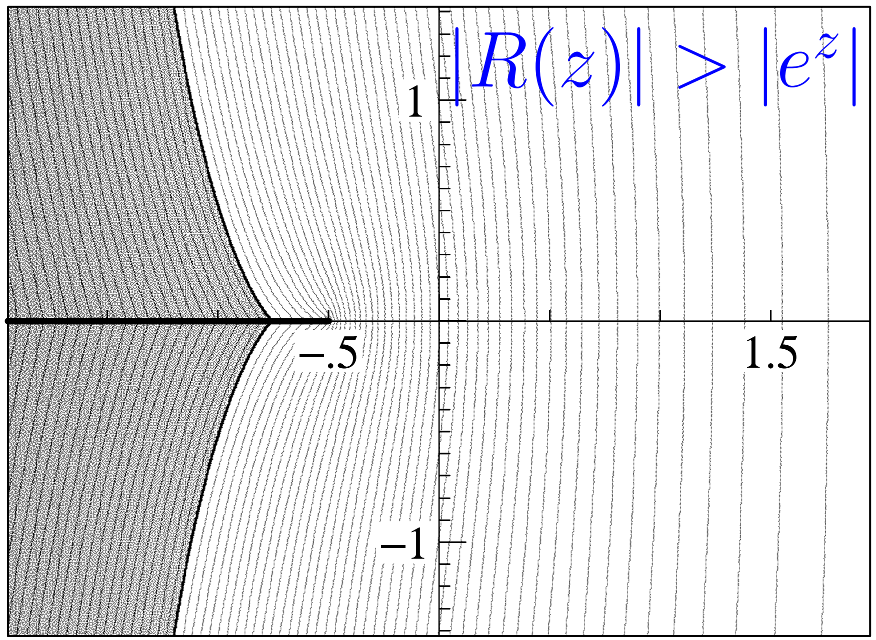
$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = hf_{n+1} \left| \begin{matrix} f = \lambda y \\ h\lambda = z \end{matrix} \right| (\frac{3}{2} - z)y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = 0.$$

Lagrange opus 2 (1759):

$$y_n = c_1 \cdot R_1^n + c_2 \cdot R_2^n \quad \text{where} \quad (\frac{3}{2} - z)R^2 - 2R + \frac{1}{2} = 0.$$

with solutions $R_{1,2}(z) = \dfrac{2 \pm \sqrt{1 + 2z}}{3 - 2z}$





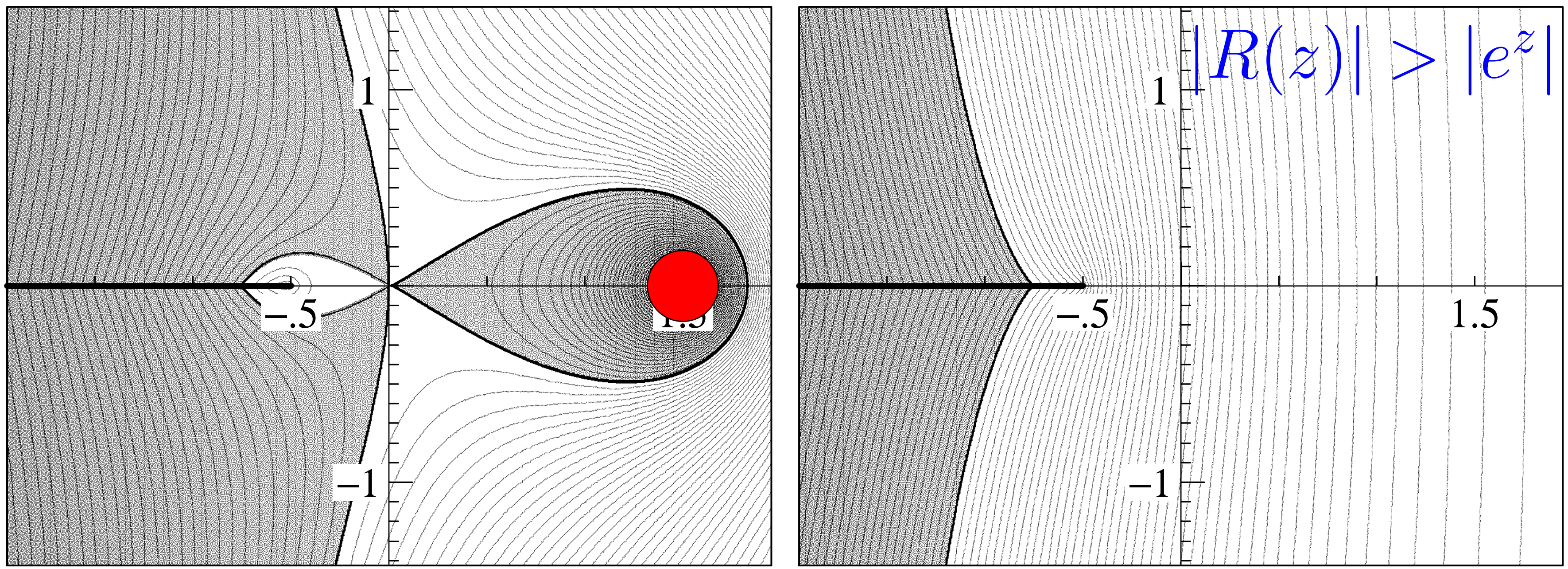
Multistep Methods. Example: BDF2.

- 1 Implicit stage

$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = hf_{n+1}$$

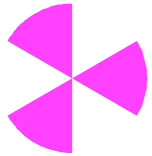
$$\left(\frac{3}{2} - z\right)R^2 - 2R + \frac{1}{2} = 0.$$

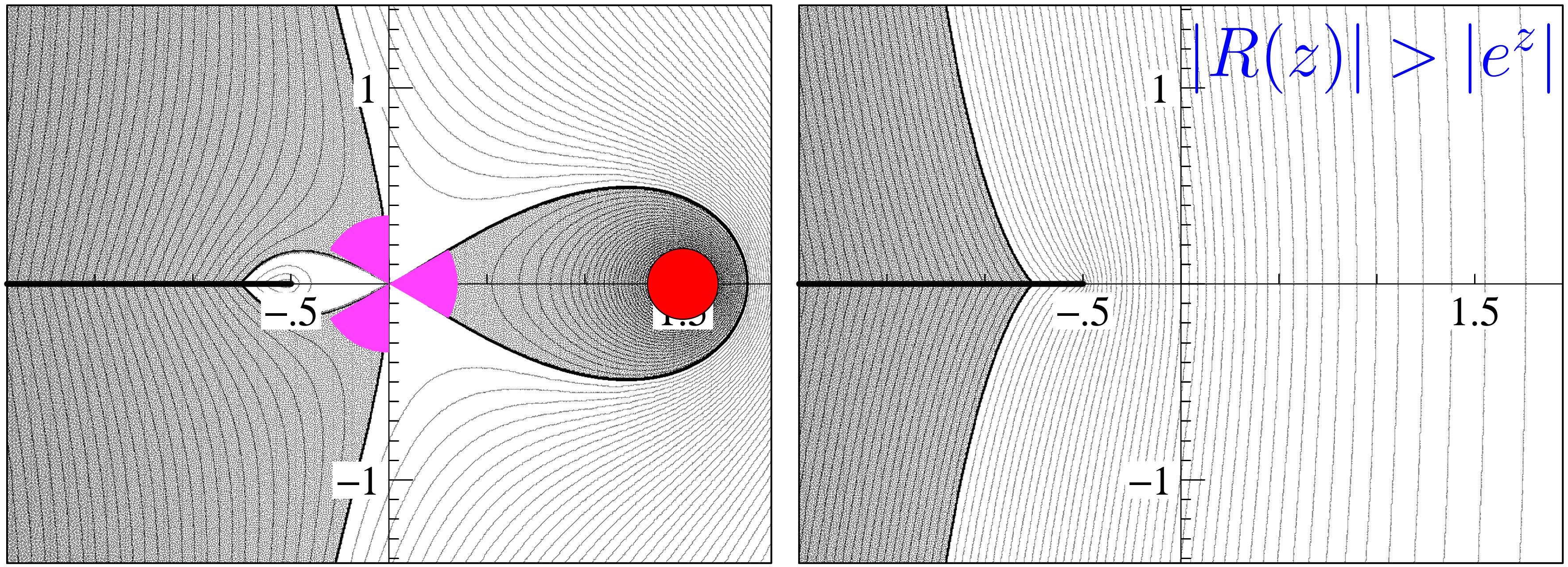
$$R_{1,2}(z) = \frac{2 \pm \sqrt{1+2z}}{3-2z} \quad \Rightarrow \quad \text{1 Pole of } R$$



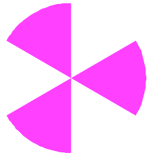
Multistep Methods. Example: BDF2.

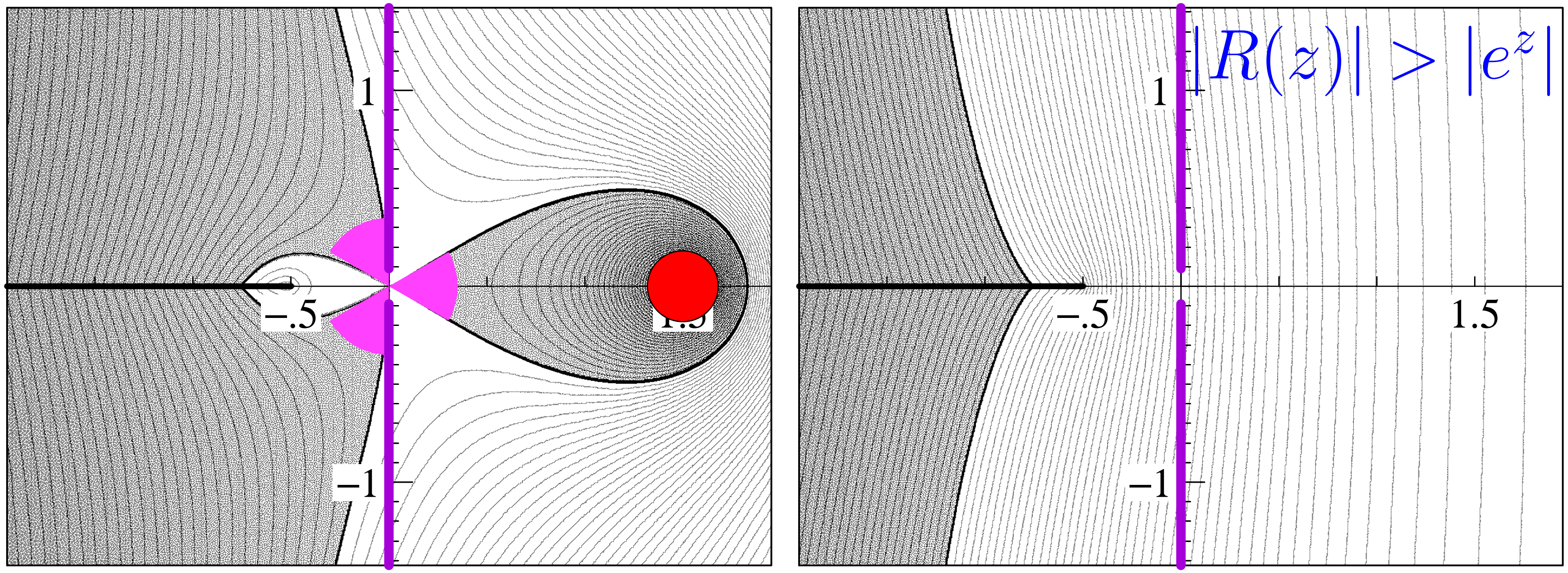
- Implicit stage $\Rightarrow$ Pole of R

- Order 2 $\Rightarrow$ $e^z - R_1(z) = C \cdot z^3 + \ldots$ 



Multistep Methods. Example: BDF2.

- Implicit stage $\Rightarrow$ Pole of R
- Order $\Rightarrow$ $e^z - R_1(z) = C \cdot z^3 + \dots$ 
- A-stable $\Rightarrow$ order star away from imag. axis.



Numerical properties $\Leftrightarrow$ Geometrical properties

Dahlquist's second barrier:

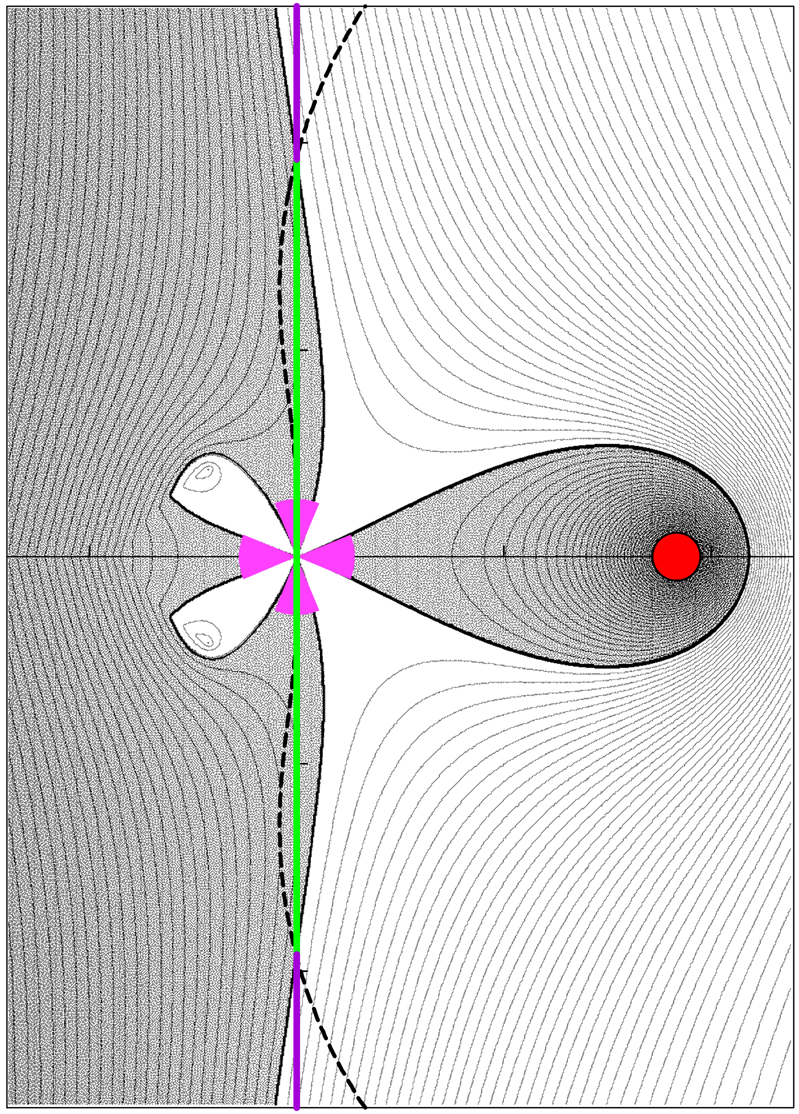
Example BDF3:

$$\frac{11}{6}y_{n+1} - 3y_n + \frac{3}{2}y_{n-1} - \frac{1}{3}y_{n-2}$$

$$= hf_{n+1}$$

$$\left(\frac{11}{6} - z\right)R^3 - 3R^2 + \frac{3}{2}R - \frac{1}{3} = 0.$$

A-stable MSM $\Rightarrow$ $\boxed{p \leq 2}$.



Daniel-Moore Conj.: A-stable MDM with j poles $\Rightarrow$ $\boxed{p \leq 2j}$.

Similar proof.

The Controversy Runge-Kutta ⇔ Adams

Thus, the greater accuracy and the error-estimating ability of predictor-corrector methods make them desirable for systems of any complexity.

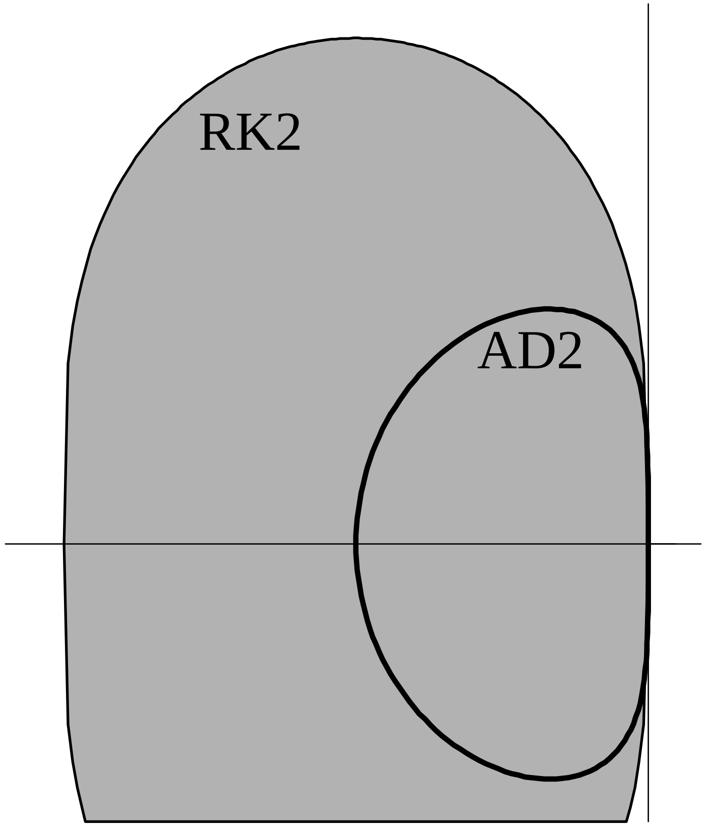
A. Ralston 1962

A careful trial of the method in comparison with others convinces me that it possesses distinct advantages in ease, speed, and simplicity.

W.E. Milne, Oregon 1926

I think the essential point is the maximum amount of information one can derive from the number of function values calculated.

T.E. Cherry, Melbourne 1957

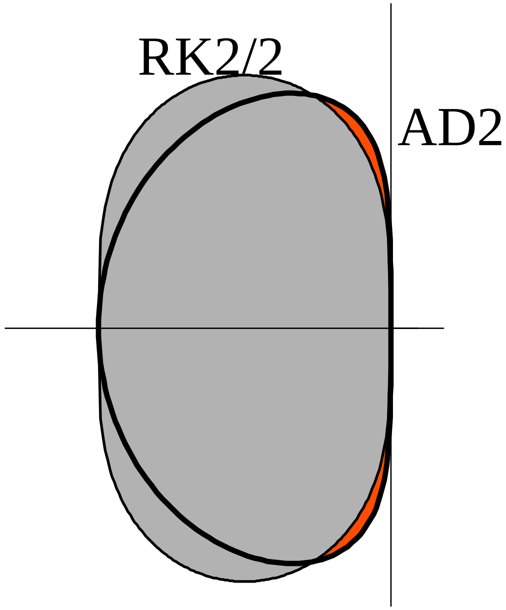


R.H. Merson (1957):

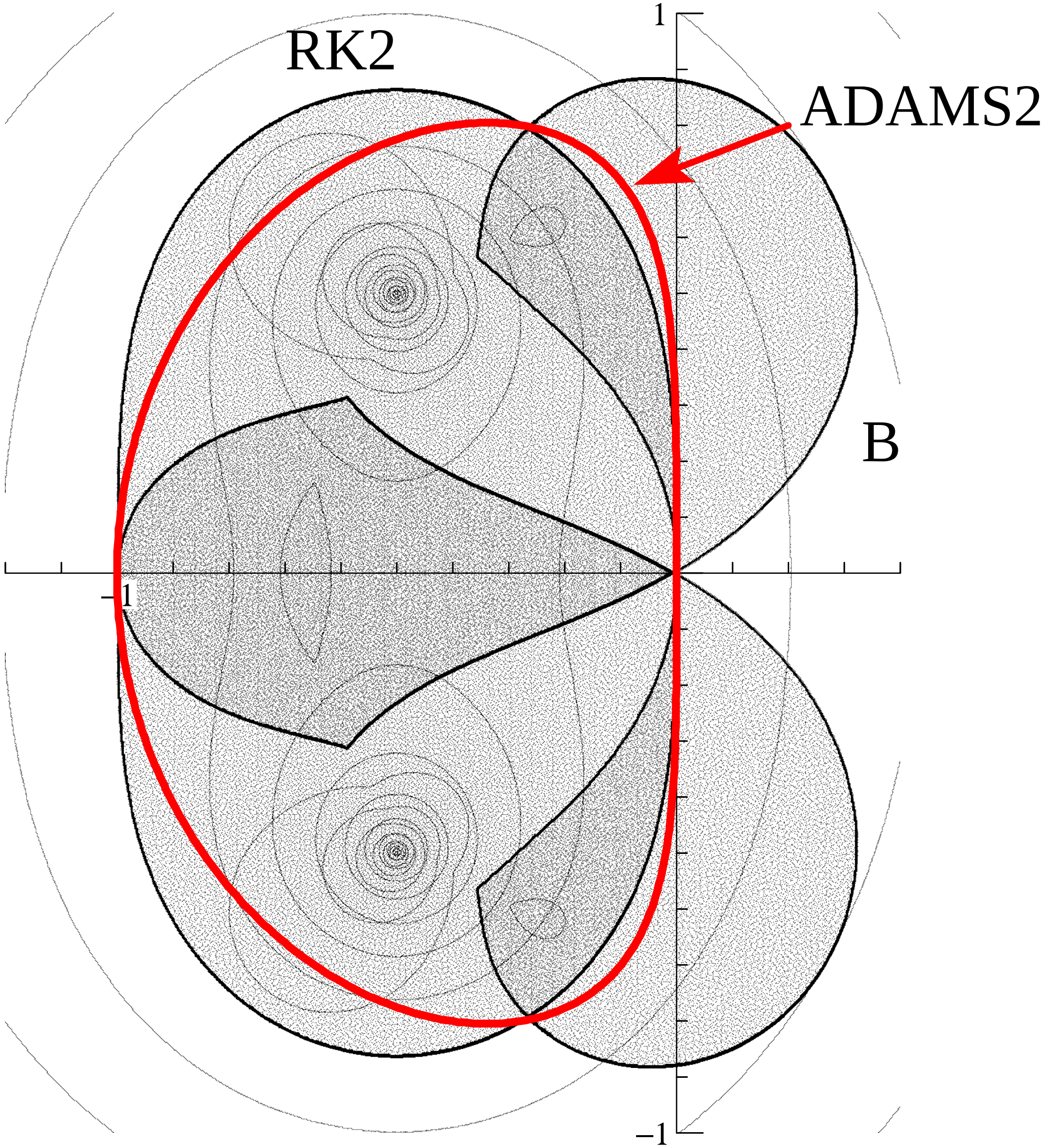
"I am talking about the stability !!"

← unfair

fair →



Jeltsch-Nevanlinna Theorem (for explicit methods):



For **scaled** stability domains

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

and

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

there is no overall
best explicit method !

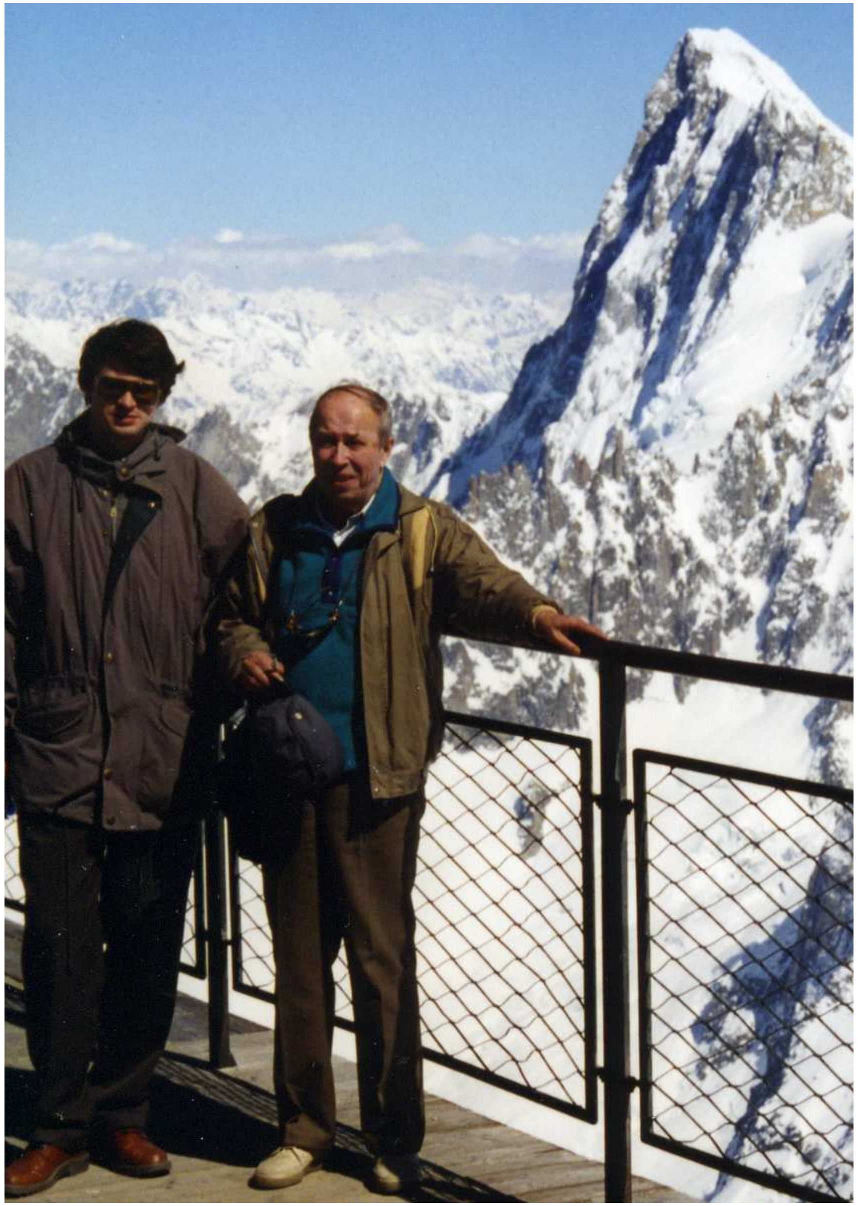
Proof by order stars

$$|R_{\text{adams}}(z)| > |R_{\text{rk}}(z)|.$$

There is a sort of 'Conservation Law of Misery' in Numerical Analysis. (H. van der Vorst, in a talk, Sydney 2003)

5. Чебышев **Methods.**

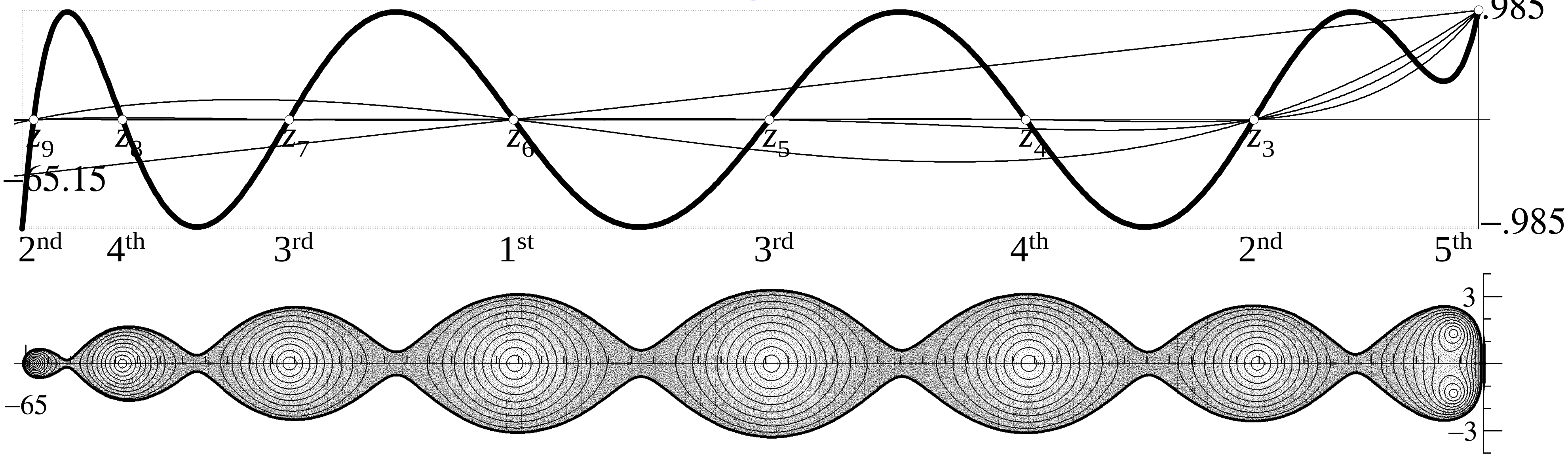
Yuan Chzao Din 1958
Медовиков, Лебедев...



van der Houwen
Sommeijer...

and Assyr Abdulle

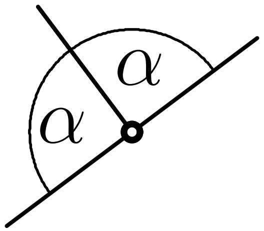
Чебышев - Золотарев **Polynomials.**



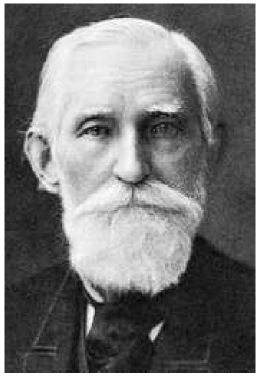
Codes are good for **real neg. eigenvalues**:

DUMKA (Russian), **RKC** (Dutch), **ROCK4** (Swiss)

Runge



Orthog.

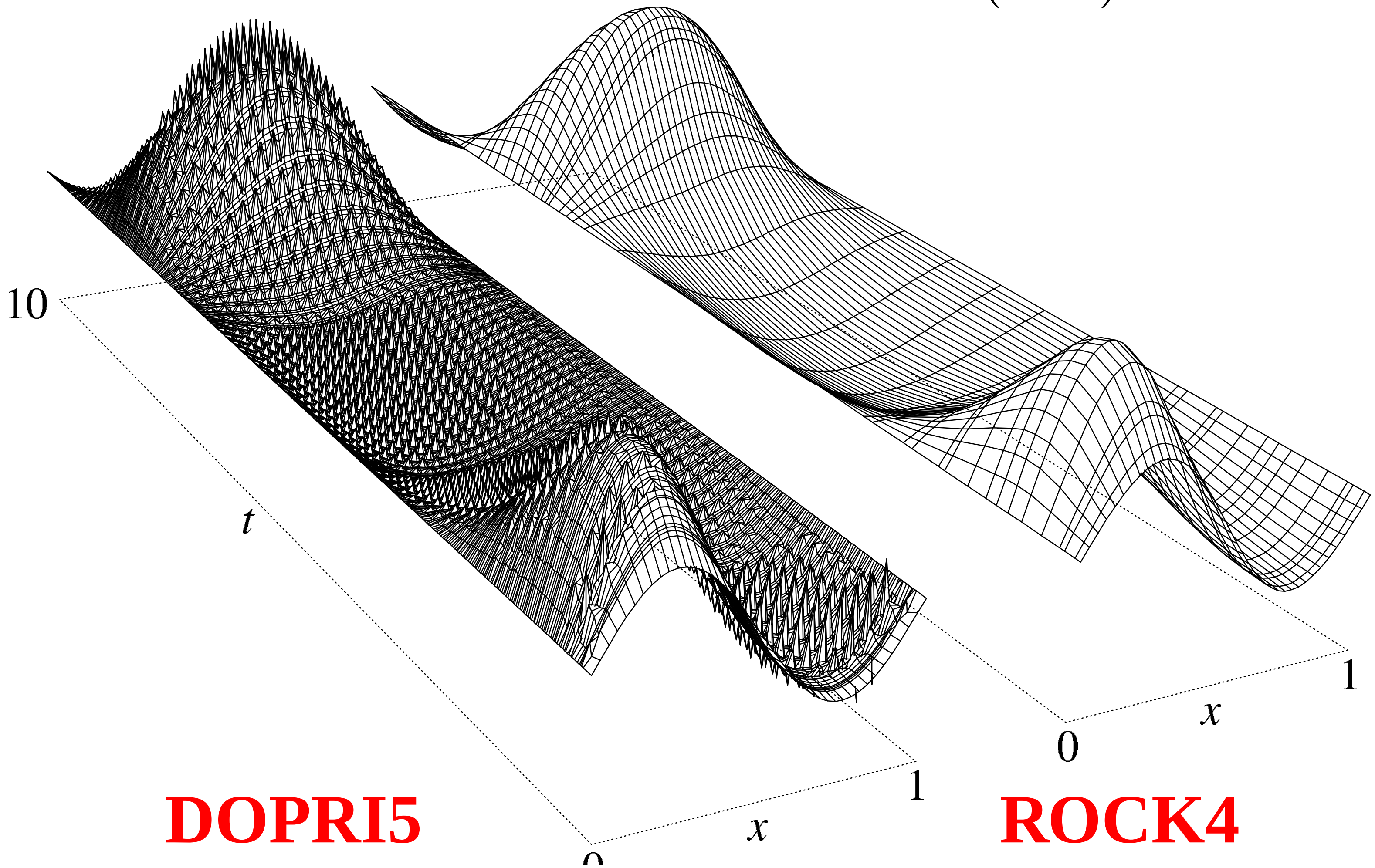


Chebyshev

Kutta

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

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

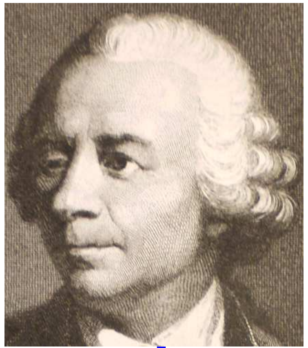


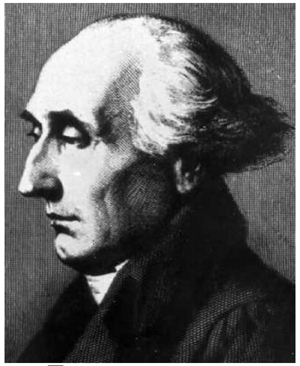
DOPRI5 406 steps Fcn. evaluation $C/(\Delta x)^2$

ROCK4 23 steps Fcn. evaluation $\bar{C}/(\Delta x)$

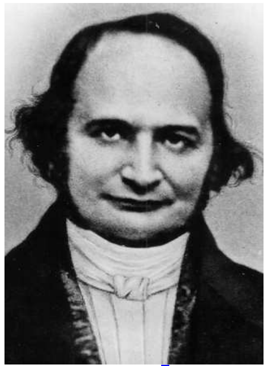
6. Geometric Numerical Integration.


Newton


Euler

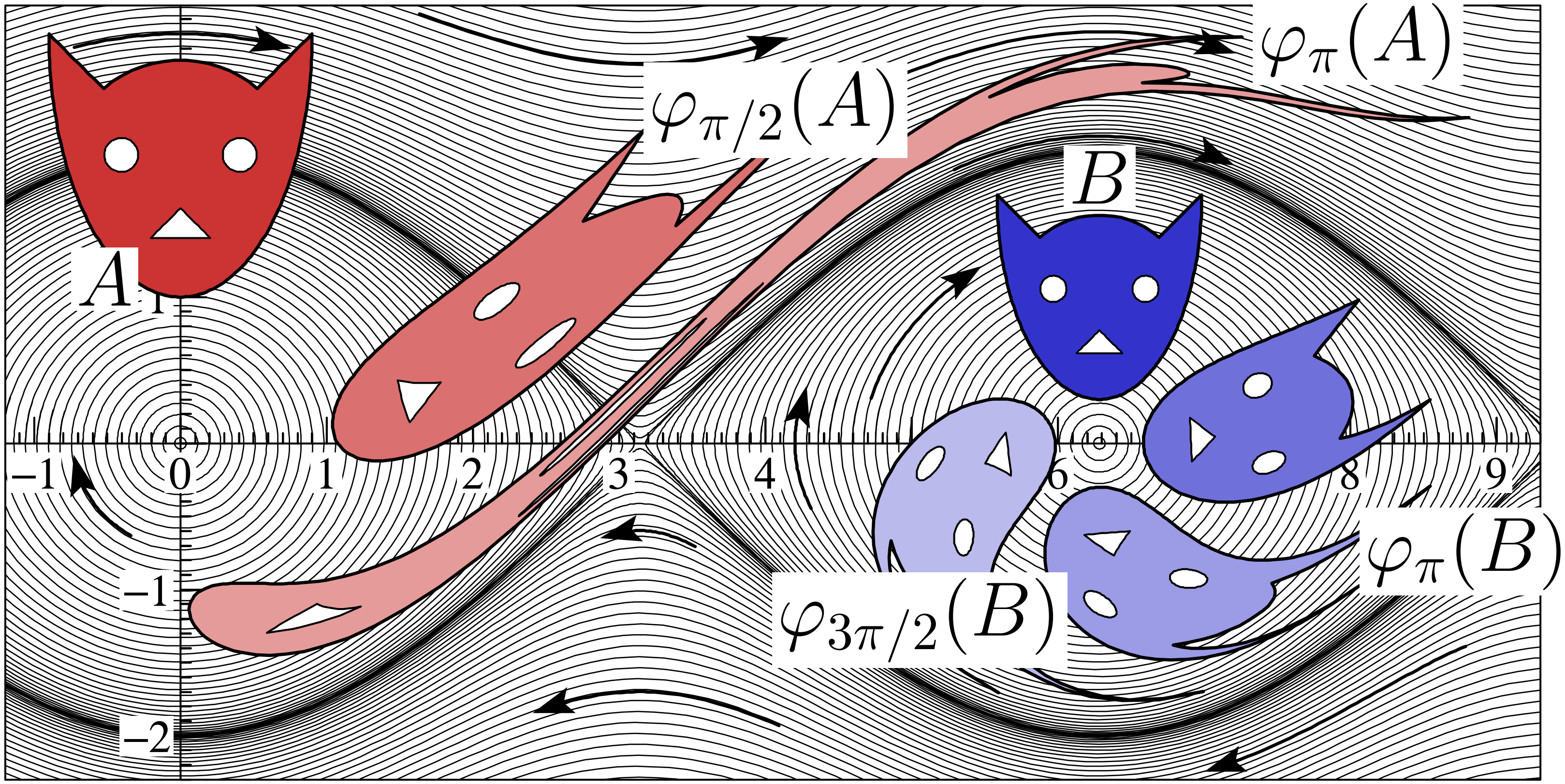

Lagrange


Hamilton


Jacobi


Poincaré


冯康



$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p,q),$$

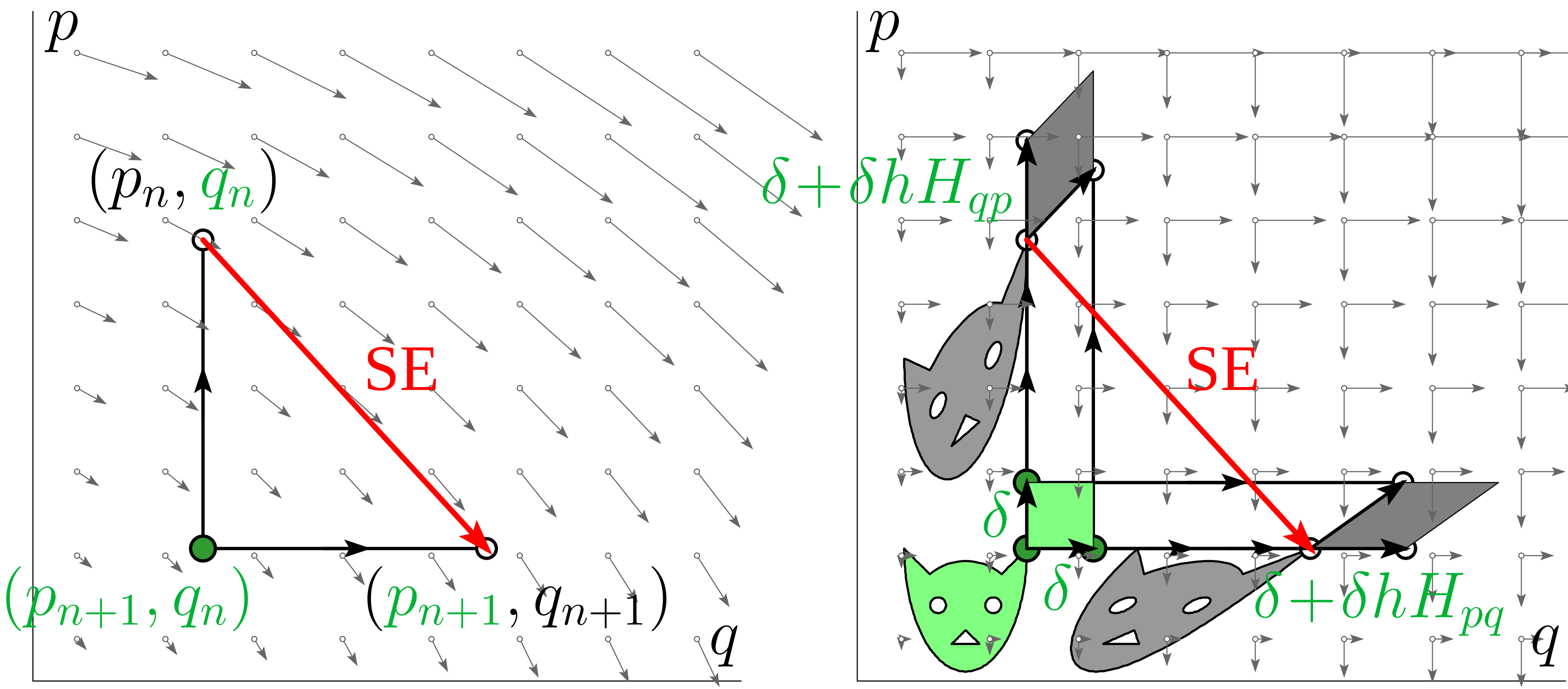
$$\dot{q}_k = \frac{\partial H}{\partial p_k}(p,q)$$

$$\dot{q} = p$$

$$\dot{p} = -\sin q$$

Poincaré (1899): Flow σύμπλεκτος, i.e. pres. 2-dim. areas.

The Symplectic Euler Method. (de Vogelaere 1956)



$$\begin{aligned}\dot p &= -H_q \\ \dot q &= H_p\end{aligned} \quad \Rightarrow \quad \begin{aligned}p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n)\end{aligned} \quad \Rightarrow \quad \begin{aligned}p_n &= p_{n+1} + hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n)\end{aligned}$$

Strang splitting $\Rightarrow$ **Störmer-Verlet Method (order 2)**

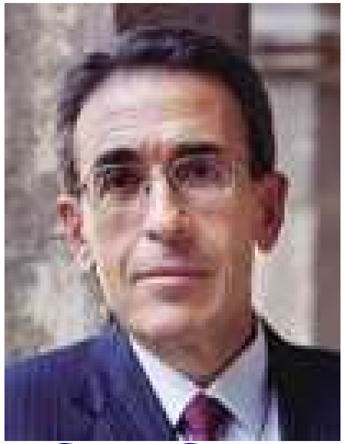
(Principal battle horse for calculations in mol. dynamics).

Symplectic Runge-Kutta Methods:

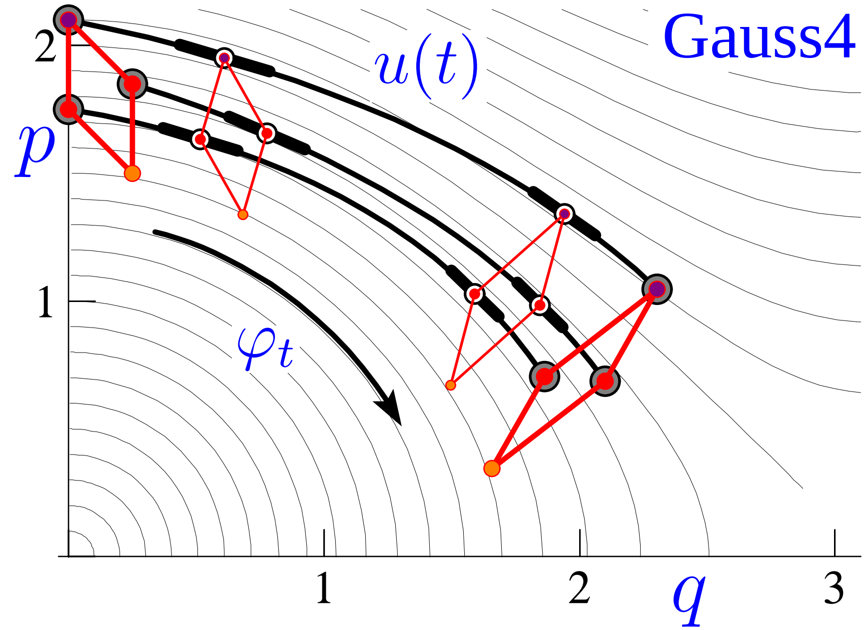
Theorem (Sanz-Serna, Suris, Lasagni 1988).

A Runge-Kutta method is symplectic, if $b_i a_{ij} + b_j a_{ji} = b_i b_j$.

In particular, Runge-Kutta-Gauss methods are symplectic.



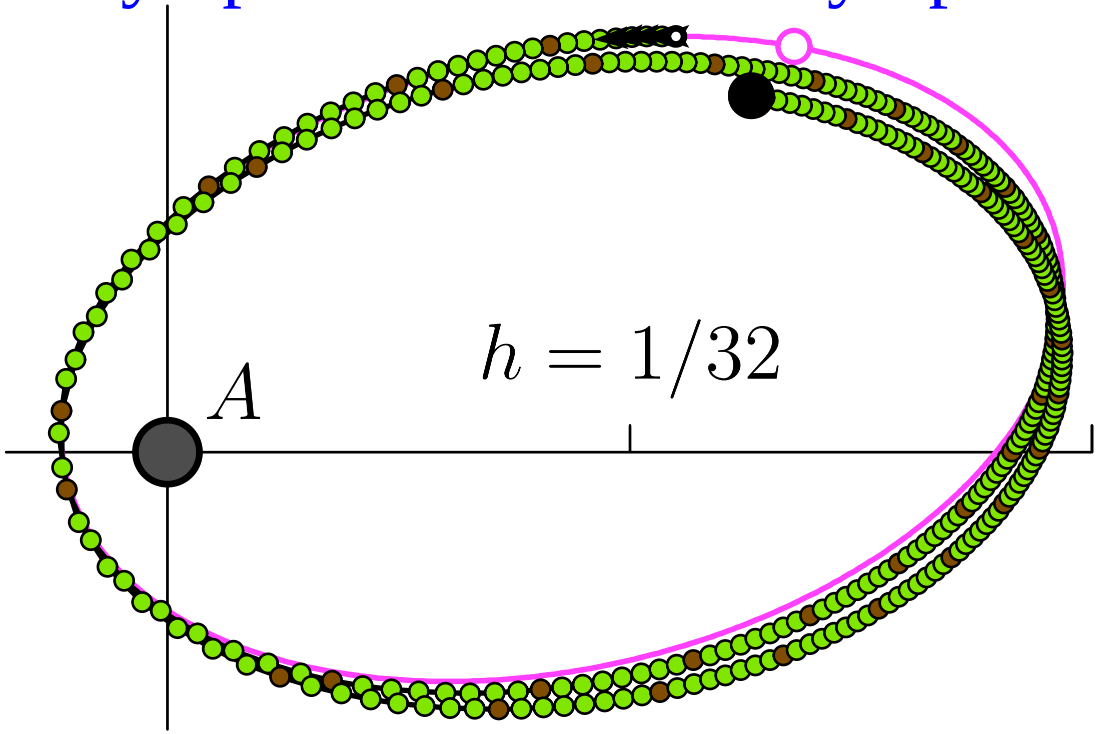
Sanz-Serna



Elegant proof: Along the collocation polynomial, the area is of degree $2s$, it's derivative is of degree $2s - 1$ and zero at the Gauss points. Apply Gaussian quadrature formula.

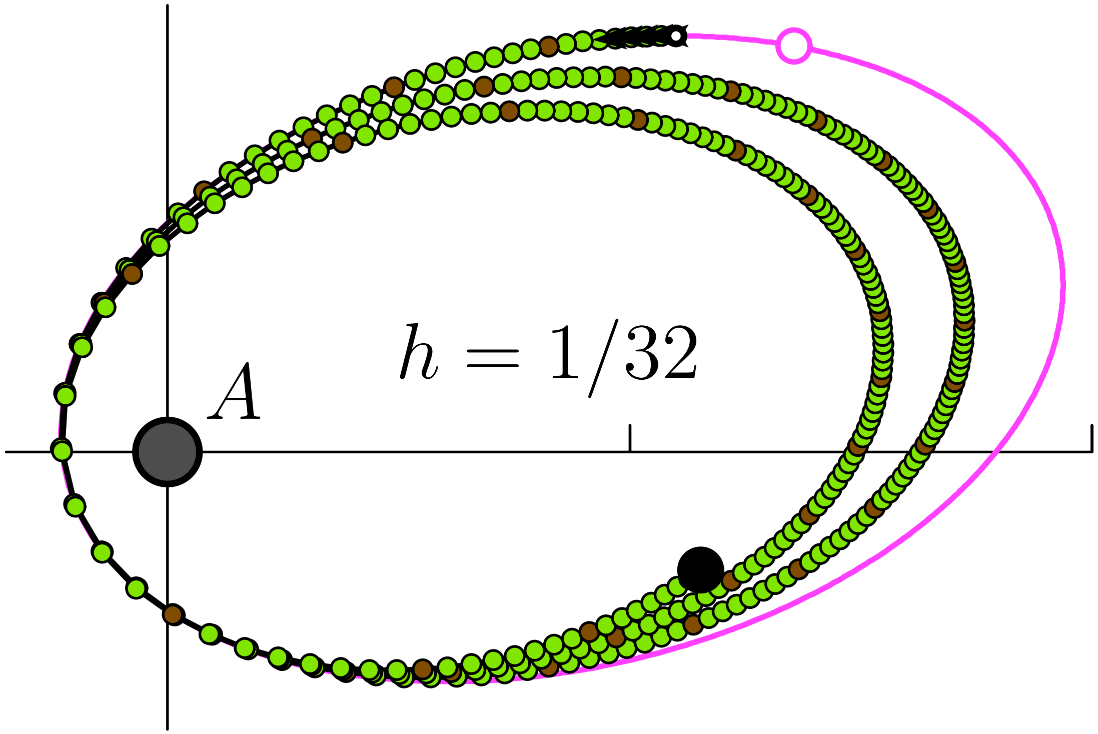
GNI_CODES (Runge Kutta, Composition, Multistep); (E. Hairer and Martin Hairer 2002).

Symplectic versus not symplectic (at Kepler problem):



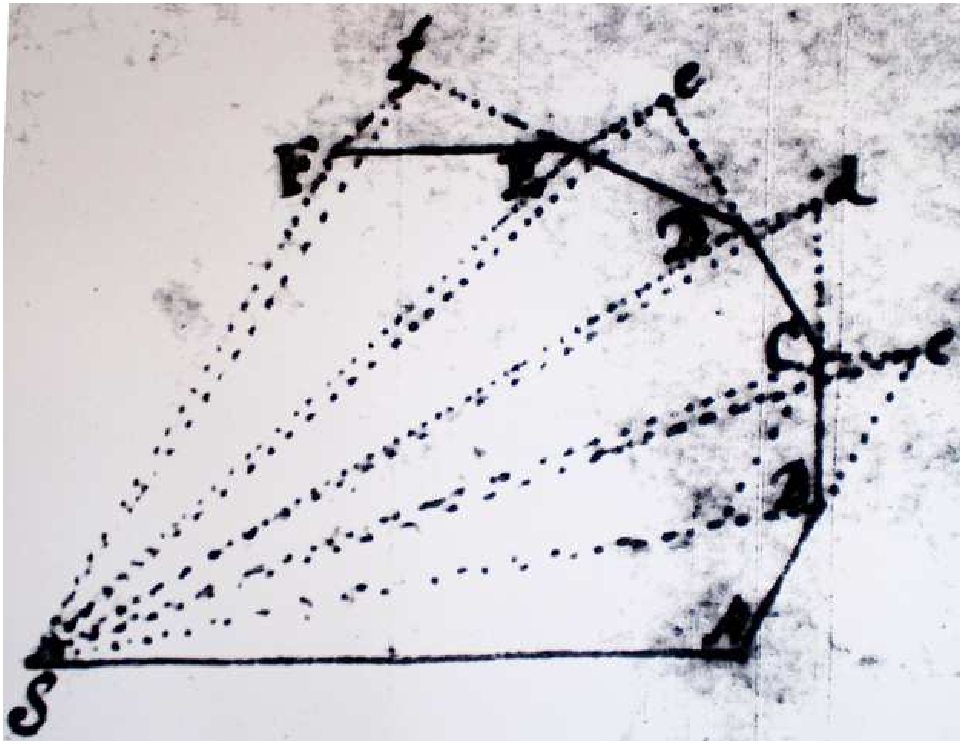
$y_1(0) = 1.1, \quad \dot{y}_1(0) = -1$
$y_2(0) = 0.9, \quad \dot{y}_2(0) = 0.$
$m_A = 2, \quad T = 10.$

symplectic Euler
(order 1).

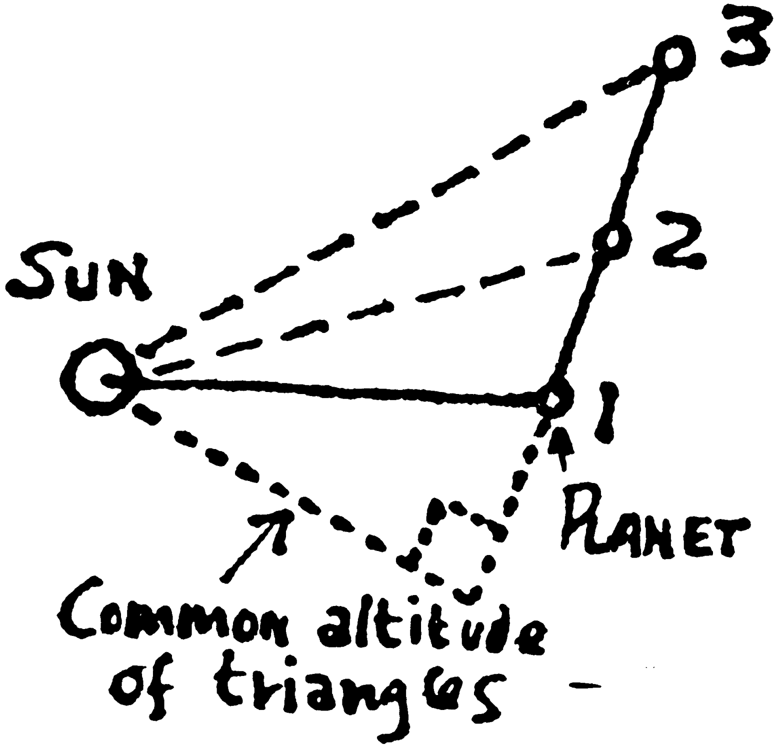


order 3 Taylor method
(for long time integration worse than symplectic order 1 method)

Surprise. (L. Verlet , priv. comm. 2002)



Newton's drawing 1684



Drawing by R. Feynman 1964

Symplectic Euler method used by I. Newton, *Principia* **1687**

Funny:

"Newton's equations"	are due to Euler...
"Symplectic Euler method"	is due to Newton.

Thank you.