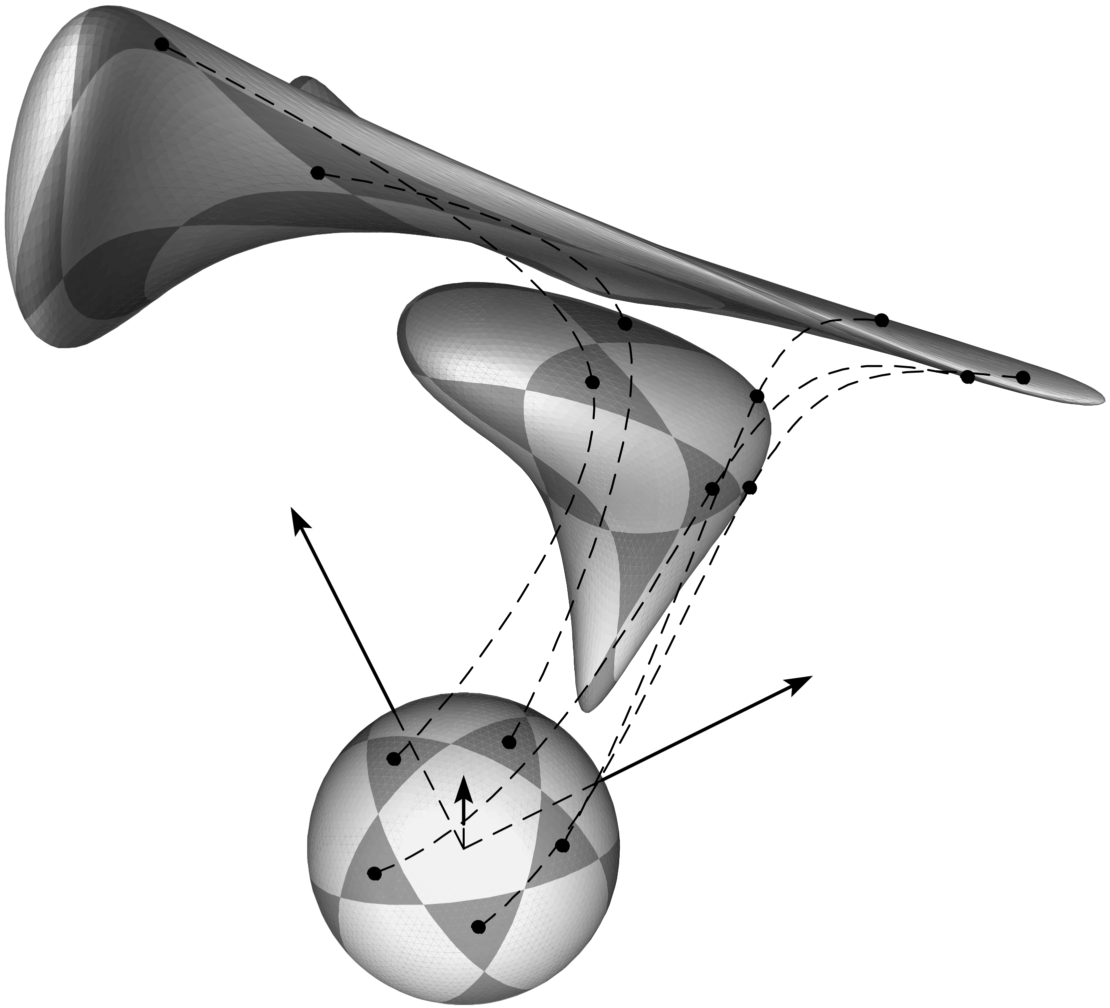
To preserve dynamics of some pictures visualize with Adobe Reader not in full screen mode.

From Geometry to Geometric Integration

Chr. Lubich, E. Hairer, G. Wanner



From where come the words?

"Geometry"

First written evidence on the door of Plato's Academy (4th century B.C.):

$$\boxed{M\eta\delta\epsilon\acute{\iota}\varsigma\ \text{'}\alpha\gamma\epsilon\omega\mu\acute{\epsilon}\tau\rho\eta\tau o\varsigma\ \text{'}\epsilon\acute{\iota}\sigma\acute{\iota}\tau\omega}$$

English translation:

> Those not knowing Geometry stay out!

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$$\boxed{M\eta\delta\epsilon\acute{\iota}\varsigma\ \ ^{\backprime}\alpha\gamma\epsilon\omega\mu\acute{\epsilon}\tau\rho\eta\tau o\varsigma\ \ ^{\backprime}\epsilon\acute{\iota}\sigma\acute{\iota}\tau\omega}$$

English translation:

$$\boxed{\text{Those not knowing Geometry stay out!}}$$

Nowadays, we are less demanding ; we recommend to any

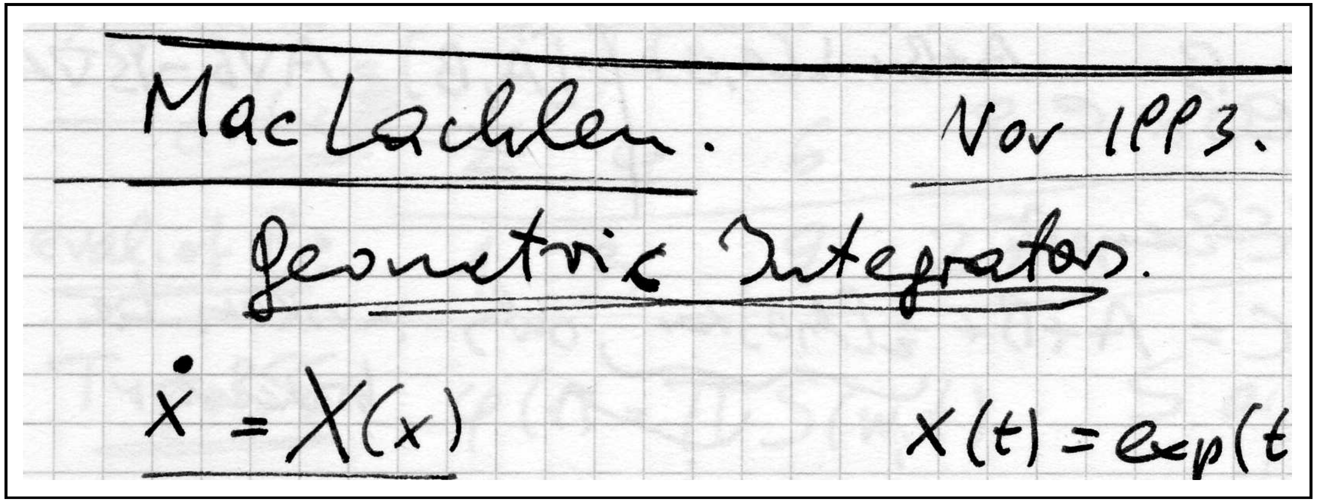
$$^{\backprime}\alpha\gamma\epsilon\omega\mu\acute{\epsilon}\tau\rho\eta\tau o\varsigma$$

to read an excellent forthcoming book.

From where come the expression

“Geometric Integration” ?

First written evidence in Codex Gerhardicus



MacLachlan. Nov 1993.

Geometric Integrators.

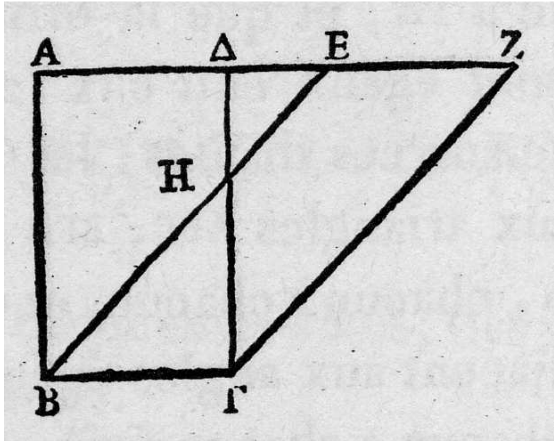
$\dot{x} = X(x)$ $x(t) = \exp(t$

asking McLachlan: “Perhaps from discussions with Sanz-Serna.”

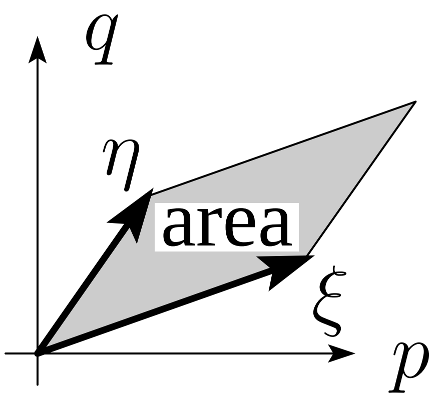
asking Sanz-Serna: “Perhaps in discussions with McLachlan, or perhaps found it myself.”

Euclid, Book I, Prop. 35:

Area of parallelogram :



Euler 1769, Grassmann (1844/62): Exterior product



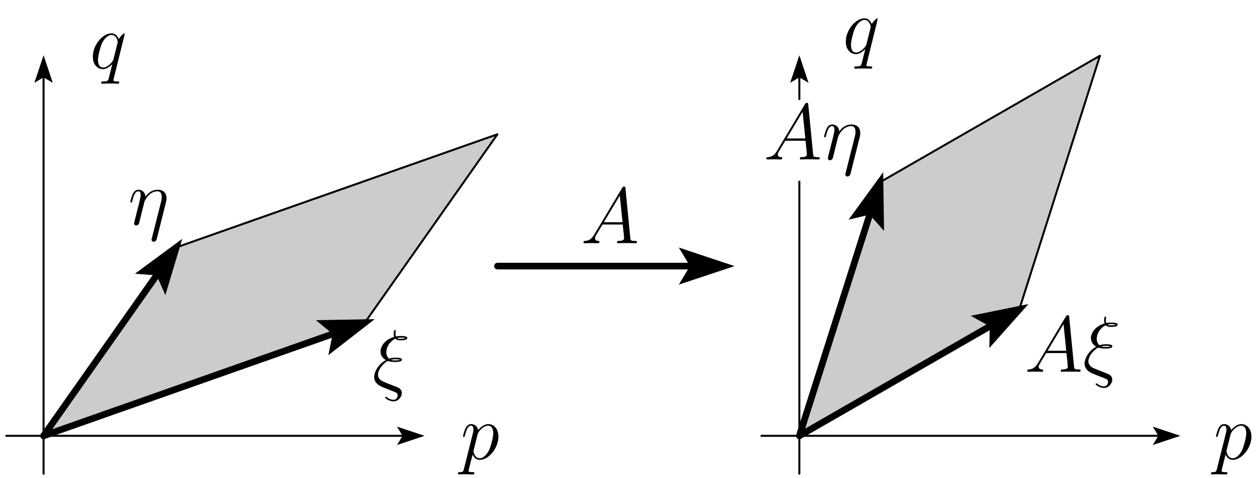
$$= \xi^p \eta^q - \xi^q \eta^p = (\xi^p \ \ \xi^q) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix}$$

In higher dimensions $\Rightarrow$ sum of projected areas:

$$\omega(\xi,\eta) := \sum_{i=1}^{d} (\xi_i^p \eta_i^q - \xi_i^q \eta_i^p) = \xi^T J \eta \quad \text{with} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

Symplectic linear mappings: $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is symplectic if

$$\boxed{A^T J A = J}$$



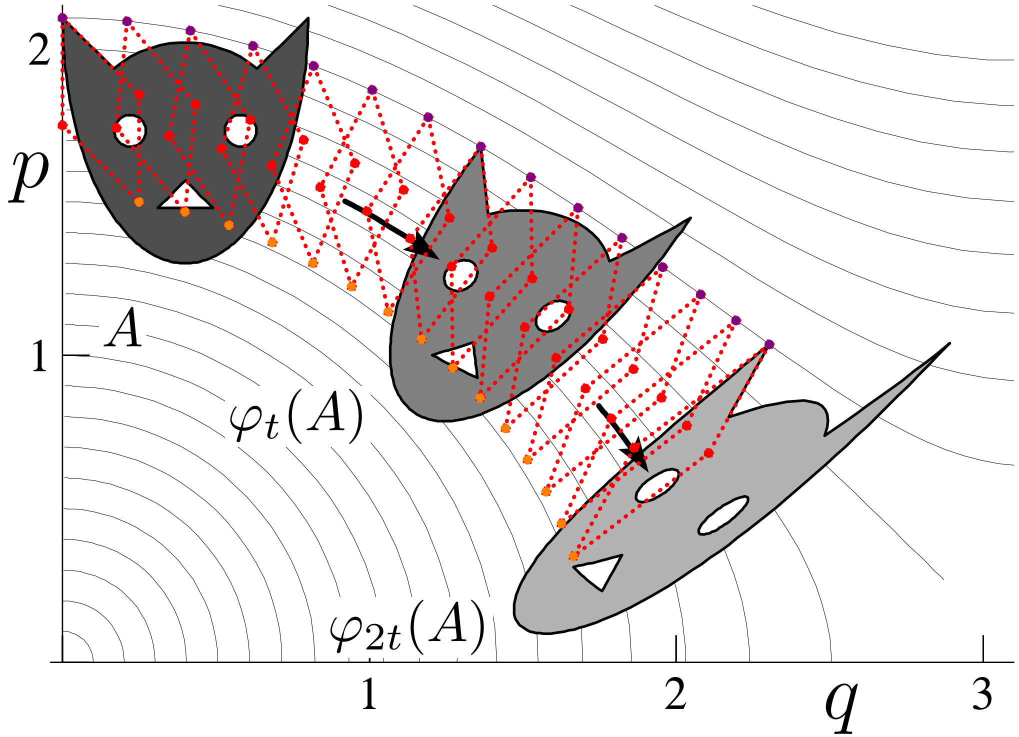
i.e., if $\omega(A\xi, A\eta) = \omega(\xi,\eta)$.

Hamiltonian Systems (Hamilton 1834)

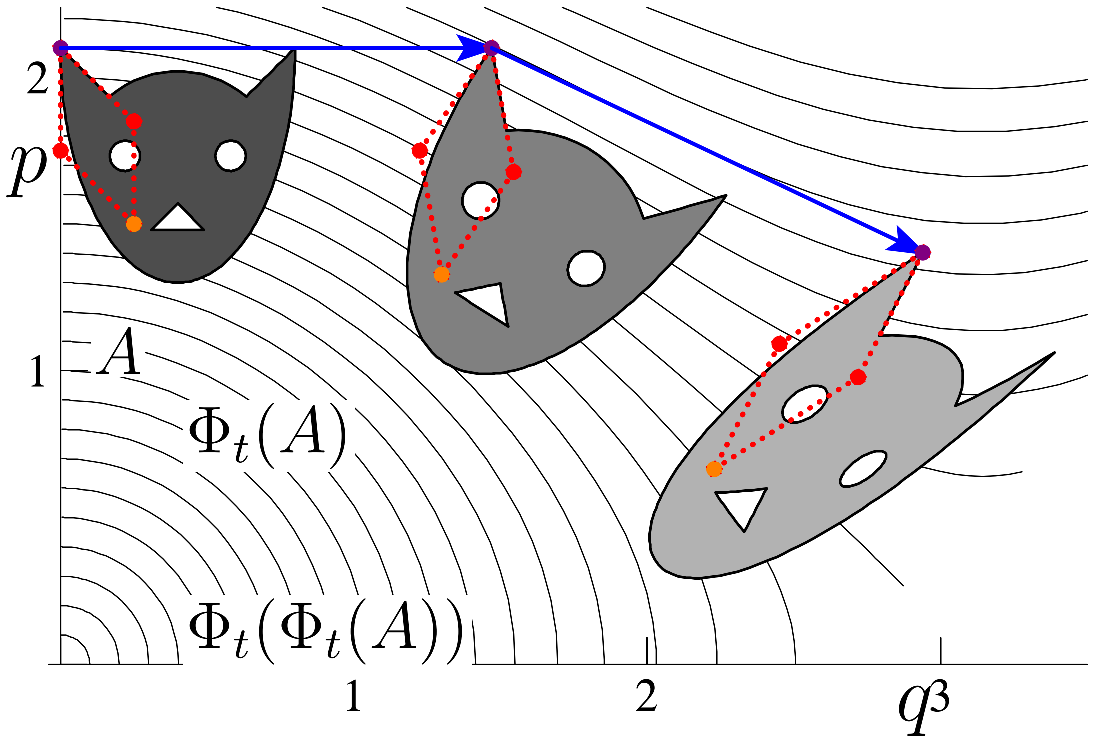
$$\dot p_k = -\frac{\partial H}{\partial q_k}(p,q), \qquad \dot q_k = \frac{\partial H}{\partial p_k}(p,q), \qquad \text{or} \qquad \dot y = J^{-1}\nabla H(y)$$

Theorem (Poincaré 1899). The flow of a Hamiltonian system is symplectic, i.e., the Jacobian of the flow map satisfies

$$\Big(\frac{\partial \varphi_t}{\partial y_0}\Big)^T J \,\Big(\frac{\partial \varphi_t}{\partial y_0}\Big) = J$$



Example: Explicit Euler method is not symplectic:



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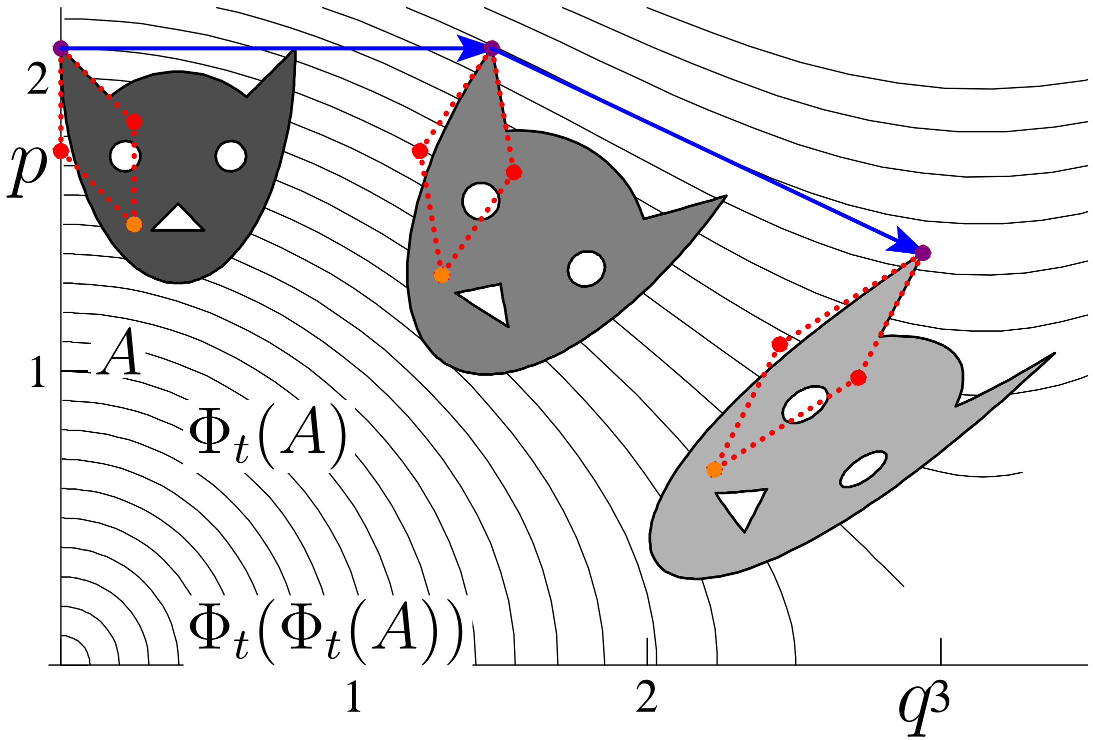


Great and Glorious Names:

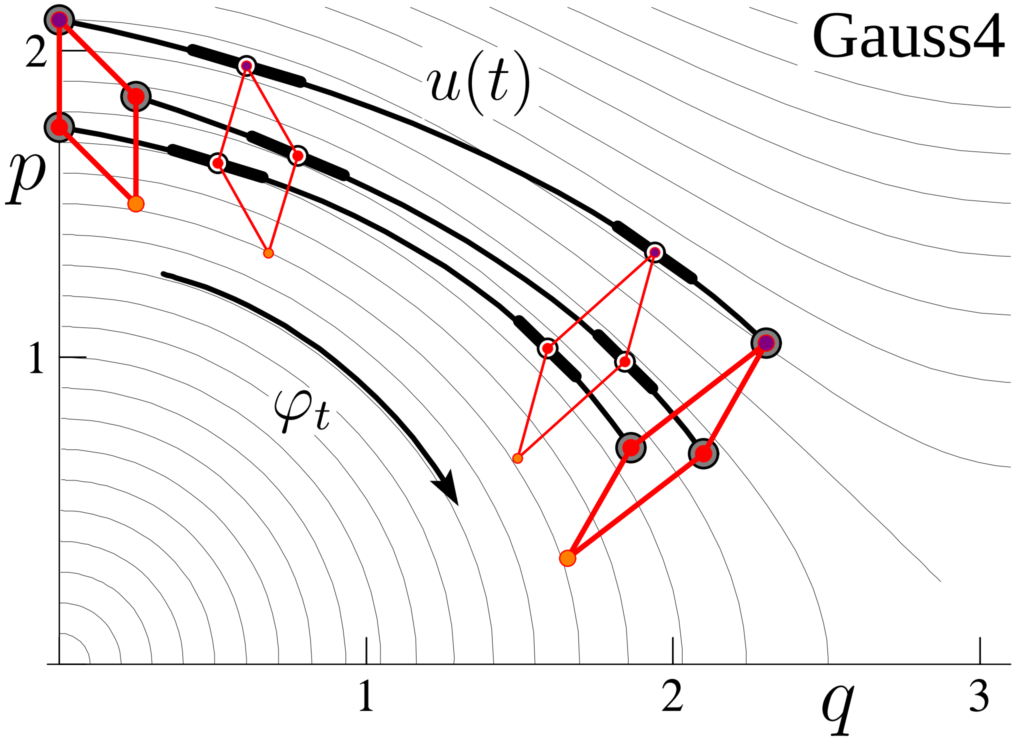
de Vogelaere 1956, Ruth 1983, Feng Kang 1985...,
Sanz-Serna, Suris, Lasagni 1988...,
Channell, Scovel, Suzuki, Yoshida 1990...,
MacKay, Marsden, Miesbach, Pesch, Skeel 1992...,
Murua, Calvo, Abia, McLachlan, Reich, Sun, Hairer, Lubich 1993... . . .

Examples of Symplectic 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.



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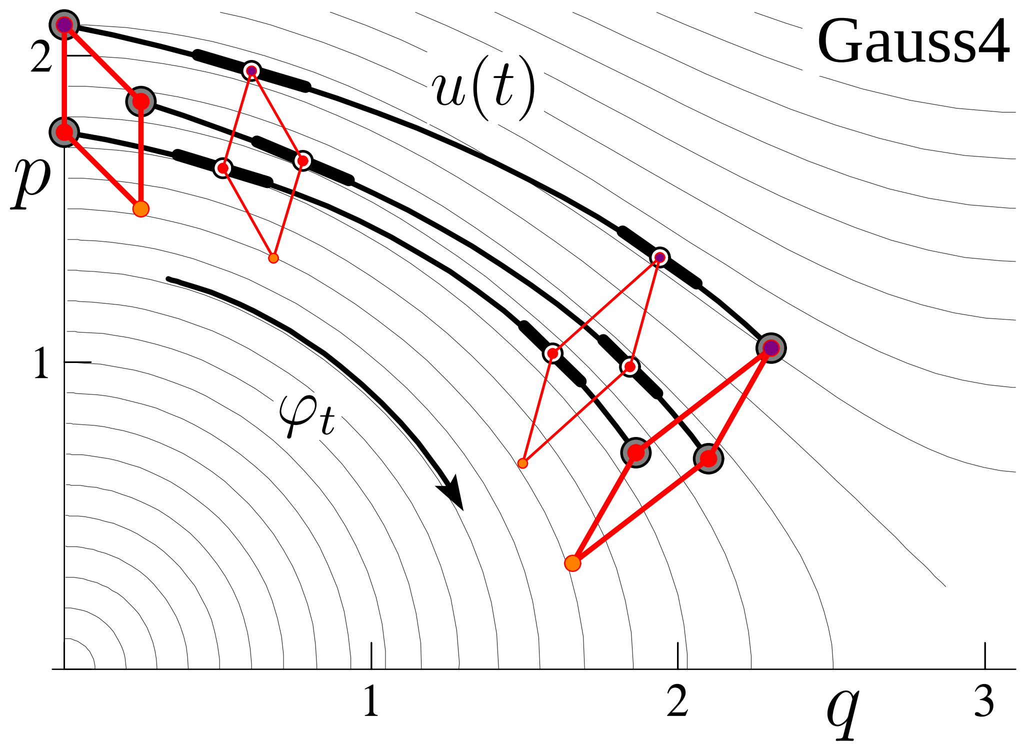
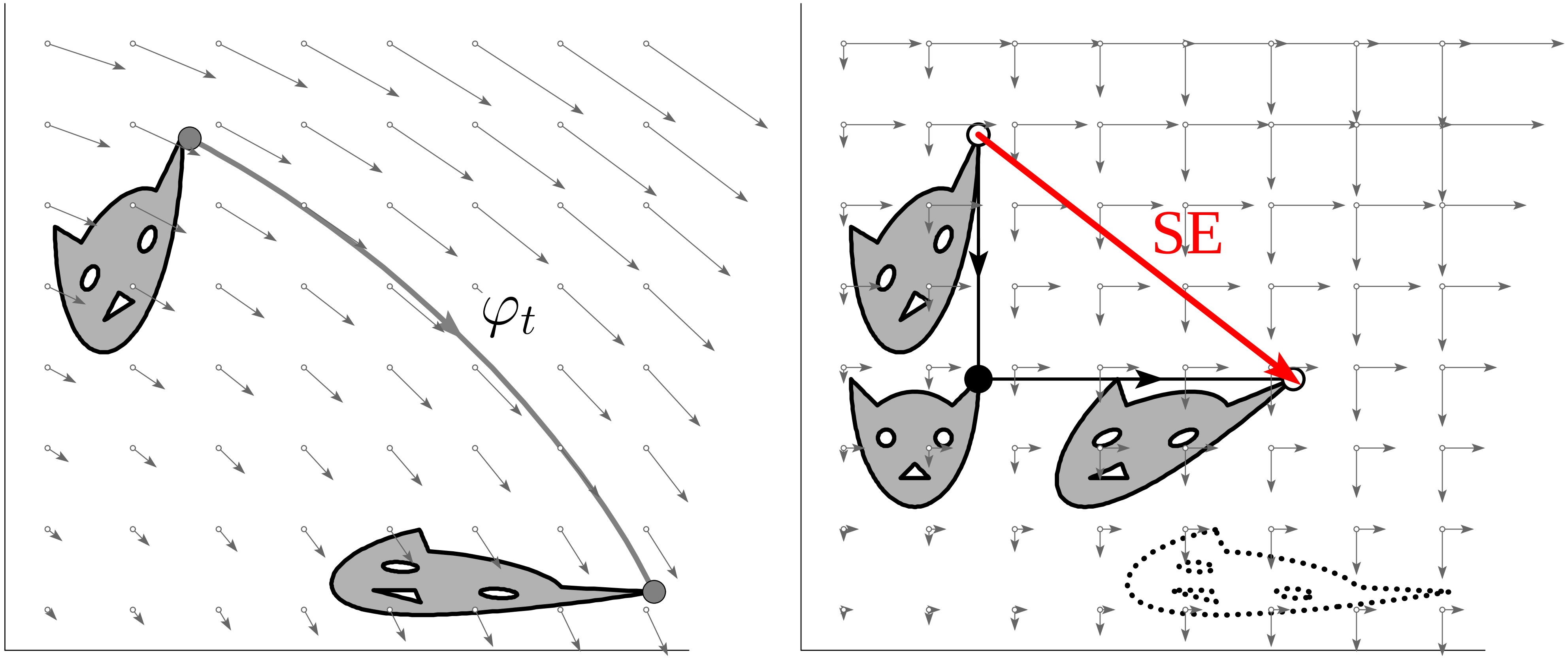


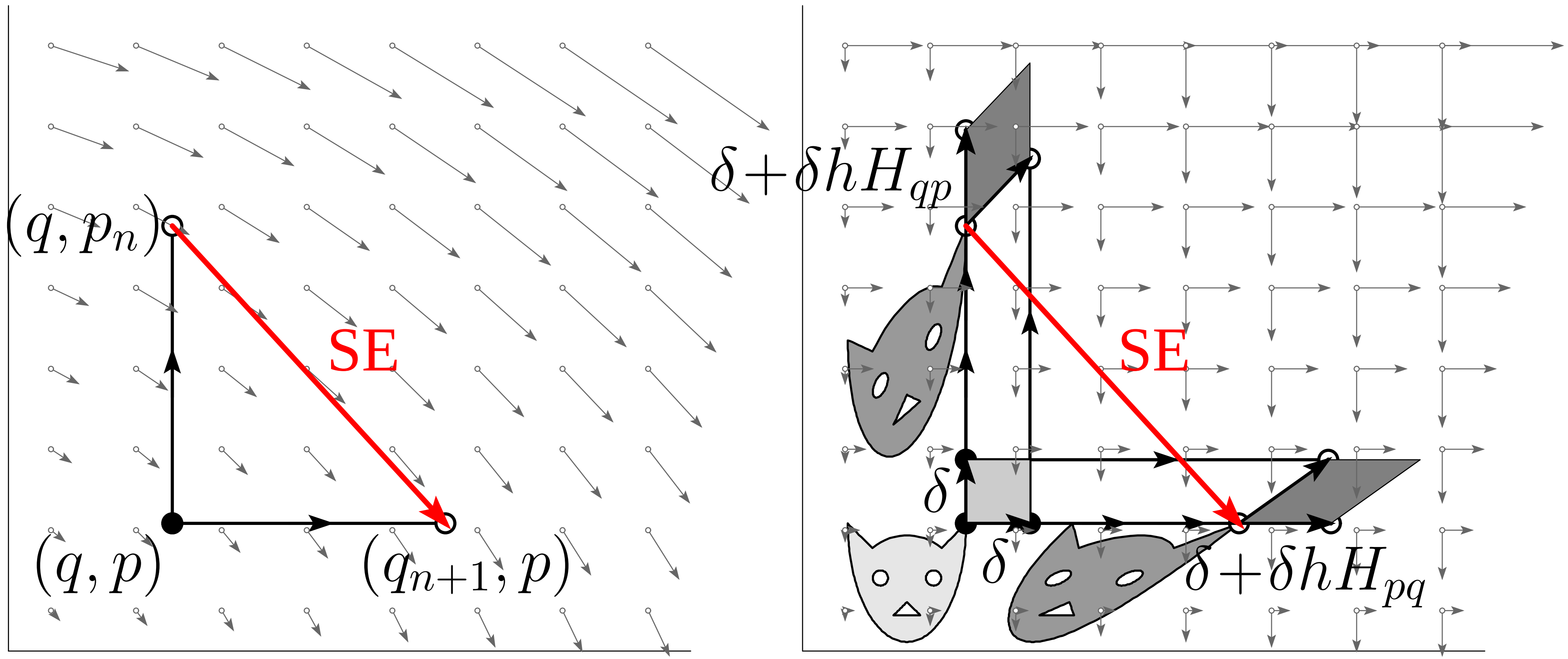
Demonstratio elegantissima: Along the collocation polynomial, the area is of degree $2s$, it's derivative is of degree $2s-1$ and zero at the Gauss points. Apply Gaussian quadrature formula.

The Symplectic Euler Method. (de Vogelaere 1956)



$$\dot p - hH_q(p,q) \qquad\qquad p_{n+1} = p_n - hH_q(p_{n+1}, q_n)$$
$$\Rightarrow$$
$$\dot q = hH_p(p,q) \qquad\qquad q_{n+1} = q_n + hH_p(p_{n+1}, q_n)$$

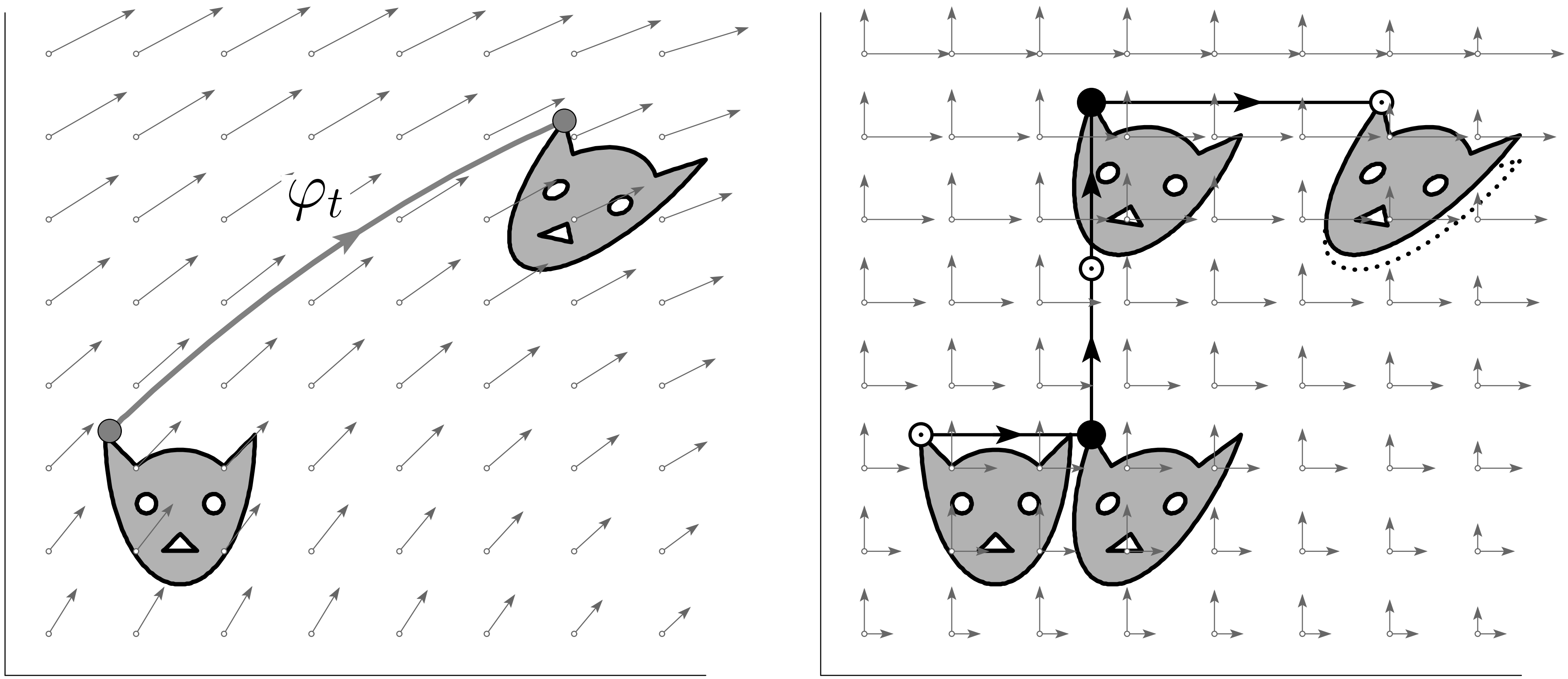
Proof of Symplecticity (in 2D): imagine (q,p) given, and obtain (q_{n+1},p) as well as (q,p_n) by 2 expl. Euler steps :



$$p_n = p + hH_q(p,q)$$
$$q_{n+1} = q + hH_p(p,q)$$

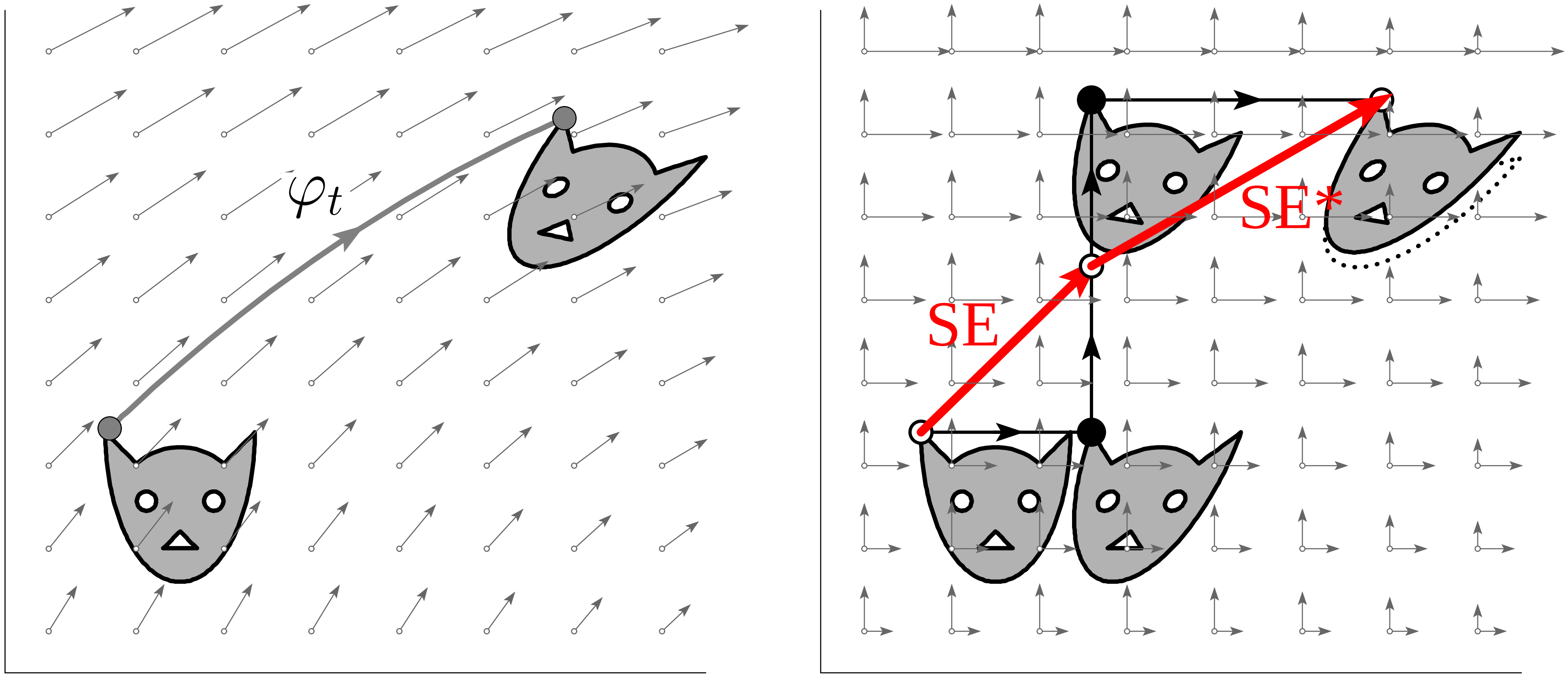
$\Rightarrow$ two dark parallelograms have same basis and same height, hence, by Eucl. I.35, same area.

The Störmer-Verlet Method. (Störmer 1907, Verlet 1967)



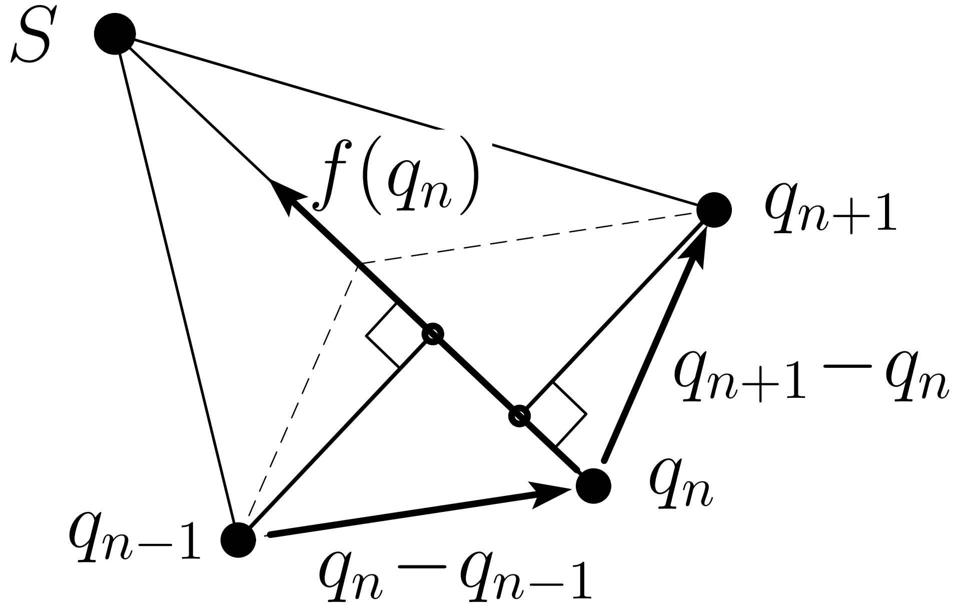
- Strang splitting :

The Störmer-Verlet Method. (Störmer 1907, Verlet 1967)



- Strang splitting :
- Composition of SE and SE* $\Rightarrow$ symplectic.

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



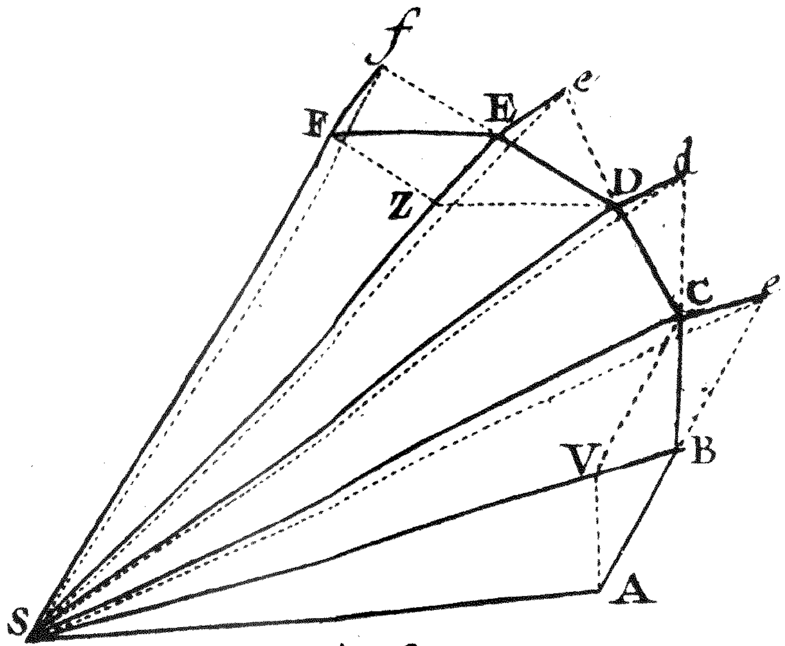


Fig.13.

The “Verlet” method was used by

I. Newton, *Philosophia Naturalis Principia Mathematica* 1687

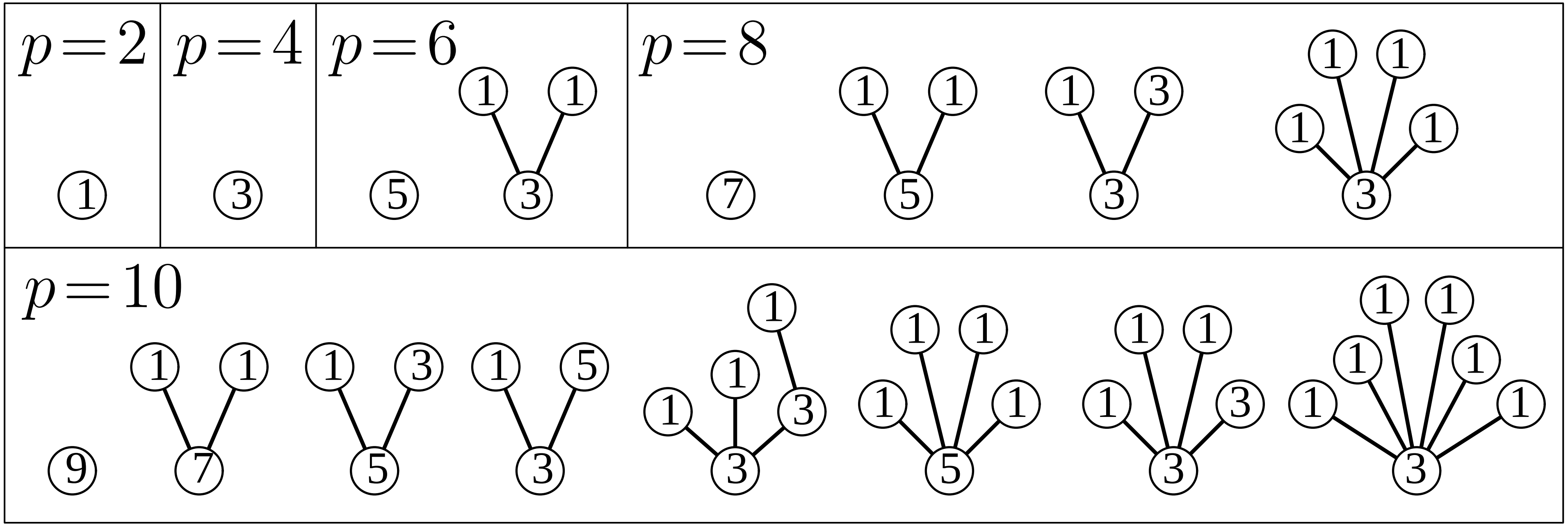
for a geometric proof of the preservation of $L = q_1 p_2 - q_2 p_1$
(Kepler’s second law) .

Higher Orders.

- Either higher order Gauss methods or
- Composition meth. (Suzuki, Yoshida, McLachlan, ...)

$$\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}.$$

Order theory based on B_∞-series (Murua & Sanz-Serna 1999):

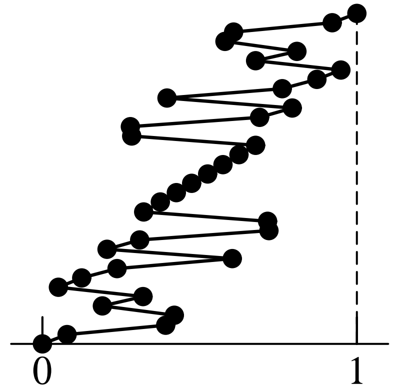


(if Φ and the γ_i are symmetric).

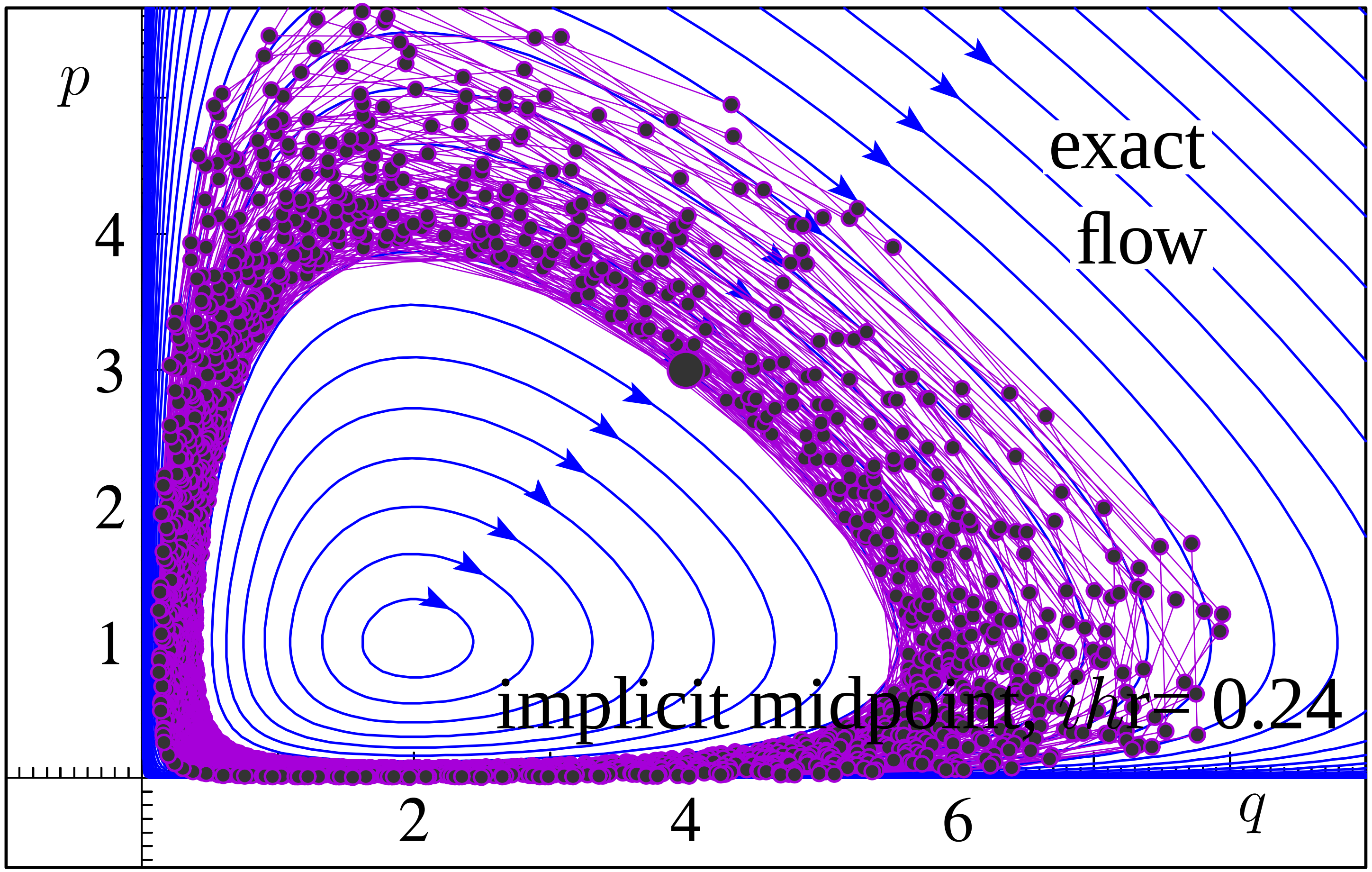
10th order solution (Sofroniou & Spaletta 2004)

$$
\begin{aligned}
\gamma_1 = \gamma_{35} &= 0.07879572252168641926390768\\
\gamma_2 = \gamma_{34} &= 0.31309610341510852776481247\\
\gamma_3 = \gamma_{33} &= 0.02791838323507806610952027\\
\gamma_4 = \gamma_{32} &= -0.22959284159390709415121340\\
\gamma_5 = \gamma_{31} &= 0.13096206107716486317465686\\
\gamma_6 = \gamma_{30} &= -0.26973340565451071434460973\\
\gamma_7 = \gamma_{29} &= 0.07497334315589143566613711\\
\gamma_8 = \gamma_{28} &= 0.11199342399981020488957508\\
\gamma_9 = \gamma_{27} &= 0.36613344954622675119314812\\
\gamma_{10} = \gamma_{26} &= -0.39910563013603589787862981\\
\gamma_{11} = \gamma_{25} &= 0.10308739852747107731580277\\
\gamma_{12} = \gamma_{24} &= 0.41143087395589023782070412\\
\gamma_{13} = \gamma_{23} &= -0.00486636058313526176219566\\
\gamma_{14} = \gamma_{22} &= -0.39203335370863990644808194\\
\gamma_{15} = \gamma_{21} &= 0.05194250296244964703718290\\
\gamma_{16} = \gamma_{20} &= 0.05066509075992449633587434\\
\gamma_{17} = \gamma_{19} &= 0.04967437063972987905456880\\
\gamma_{18} &= 0.04931773575959453791768001
\end{aligned}
$$

$p10\,s35$



Other Structures: Lotka-Volterra Model and impl. Midpoint



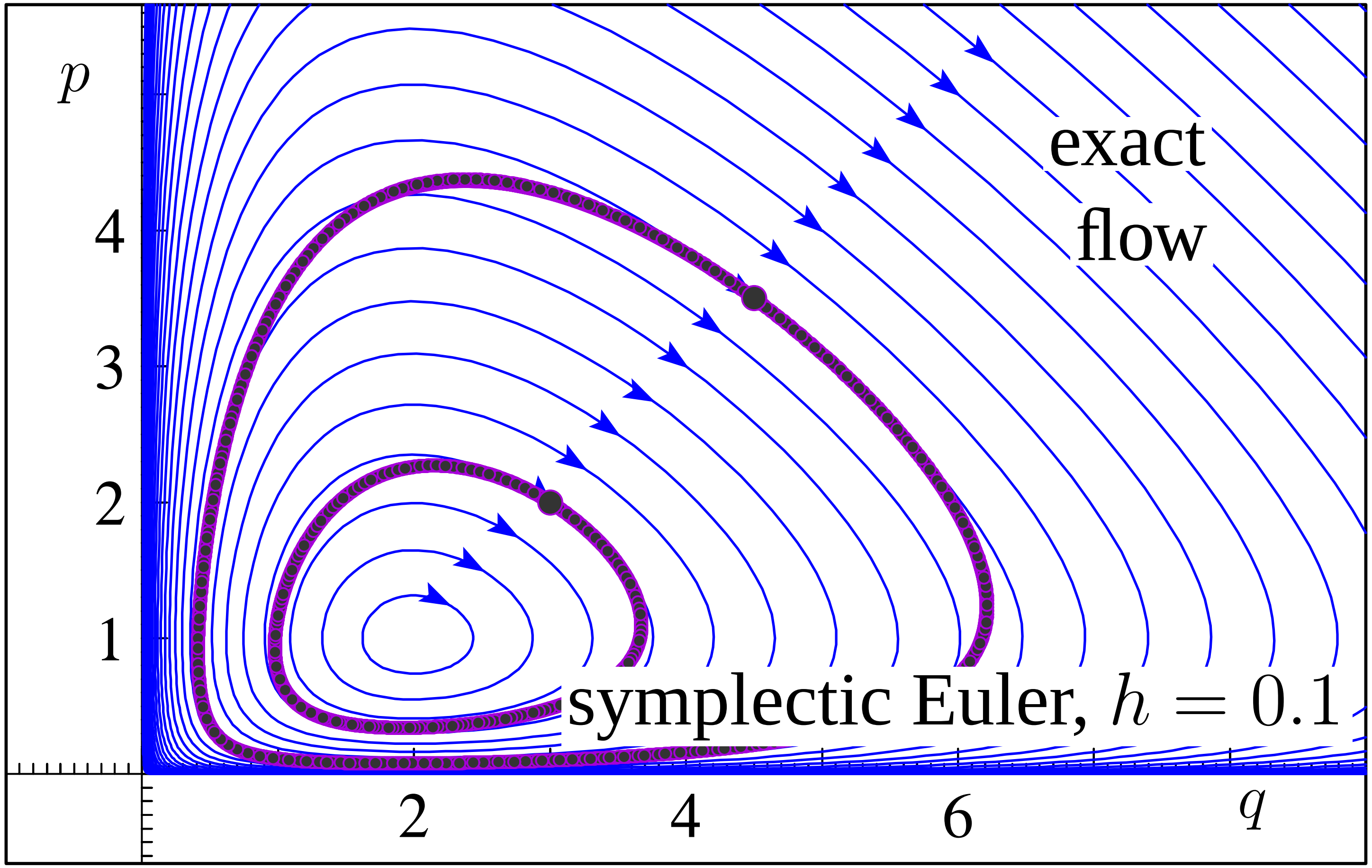
$$\dot{q} = q(p-1)$$
$$\dot{p} = -p(q-2)$$

or

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & uv \\ -uv & 0 \end{pmatrix} \nabla H(u,v),$$

is a Poisson System. Method is sympl., but not Poisson integr.

Lotka-Volterra Model and sympl. Euler



$$\dot{q} = q(p-1) \qquad \text{or} \qquad \begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & uv \\ -uv & 0 \end{pmatrix} \nabla H(u,v),$$
$$\dot{p} = -p(q-2)$$

Method is Poisson integrator (for separable Hamiltonians).

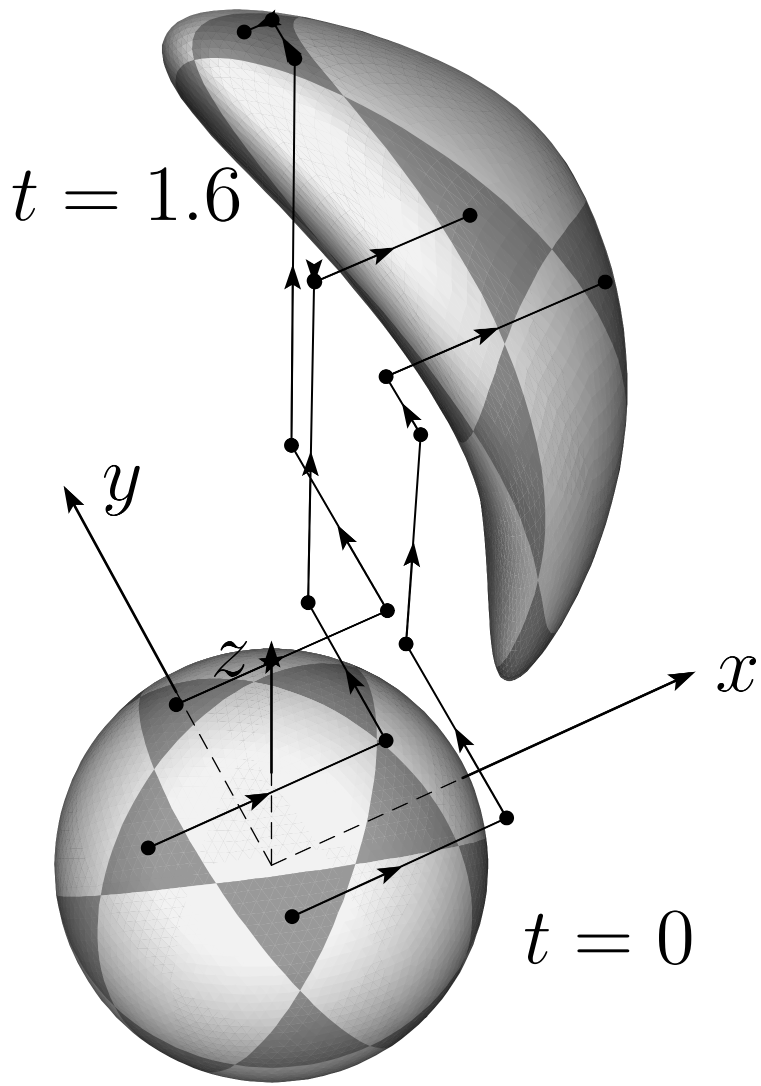
Volume Preservation of (modif.) Störmer-Verlet

$$\dot{x} = a(y, z),$$

$$\dot{y} = b(x, z),$$

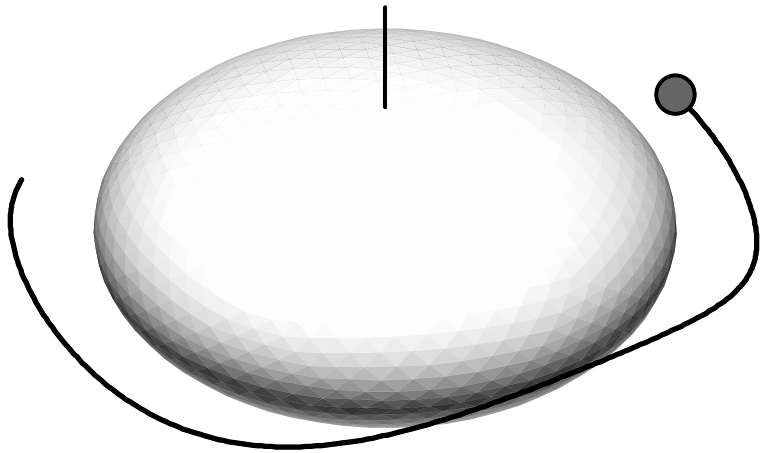
$$\dot{z} = c(x, y)$$

S.-V. volume preserving
for separable
div.-free systems.



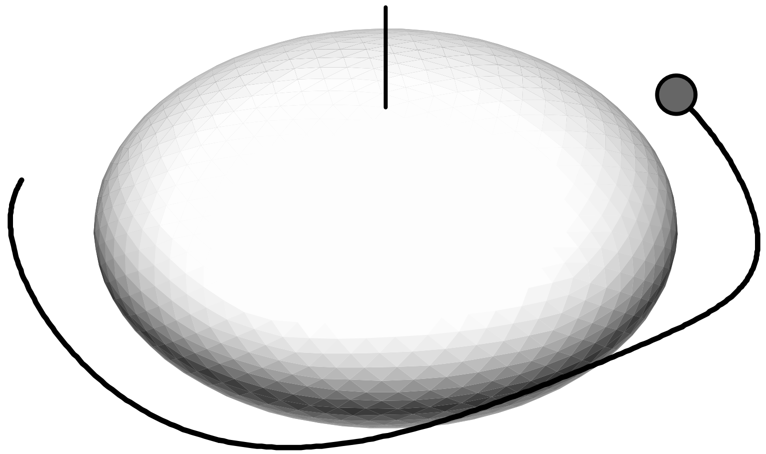
For general div.-free systems : more compl. (Feng-Shang 1995).

Numerical Example. The Hénon-Heiles Model (1964).



Problem. Does there exist, for astr. motion in cylindrical symmetry, besides H and L, a 3rd analytical integral ?

Numerical Example. The Hénon-Heiles Model (1964).



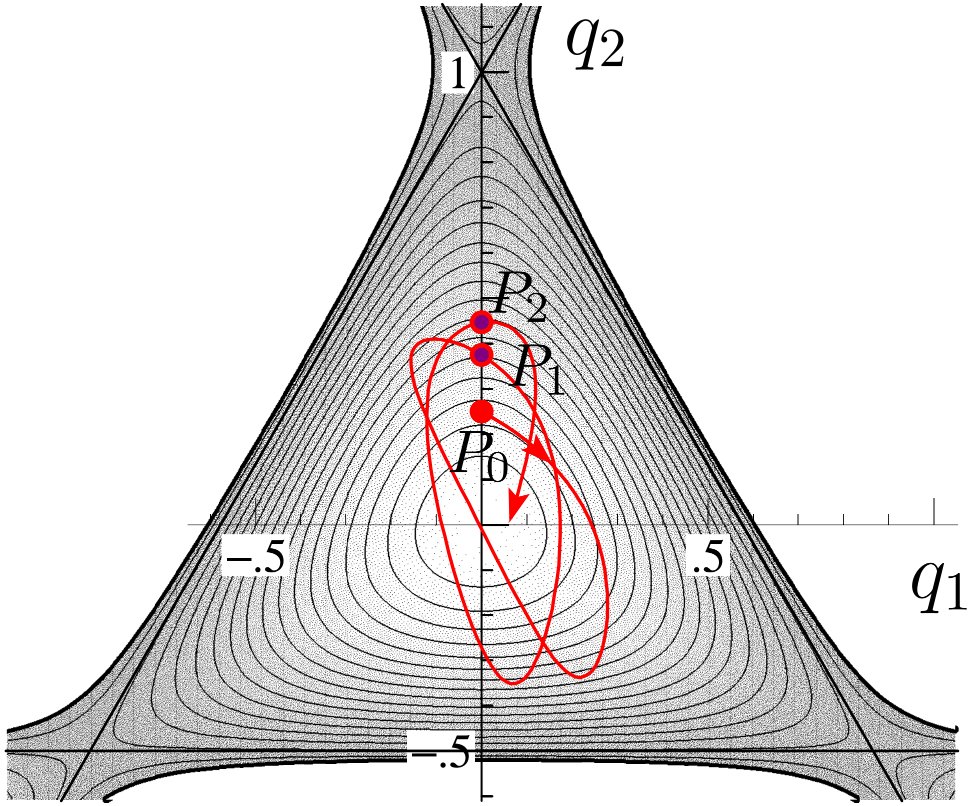
Problem. Does there exist, for astr. motion in cylindrical symmetry, besides H and L, a 3rd analytical integral ?

After a century of fruitless analytical calculations (starting with Poisson, Hamilton, Jacobi, Liouville, Poincaré, Wintner,...), Hénon and Heiles decided to perform numerical tests:

- eliminate φ with the help of the integral $L \Rightarrow$ Problem in 2D
- forget astronomy, choose simple "artificial" potential $U \quad \Rightarrow$

Numerical Example. The Hénon-Heiles Model (1964).

$$H(p,q) = \frac{1}{2}(p_1^2 + p_2^2) + U(q) \qquad U(q) = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3$$



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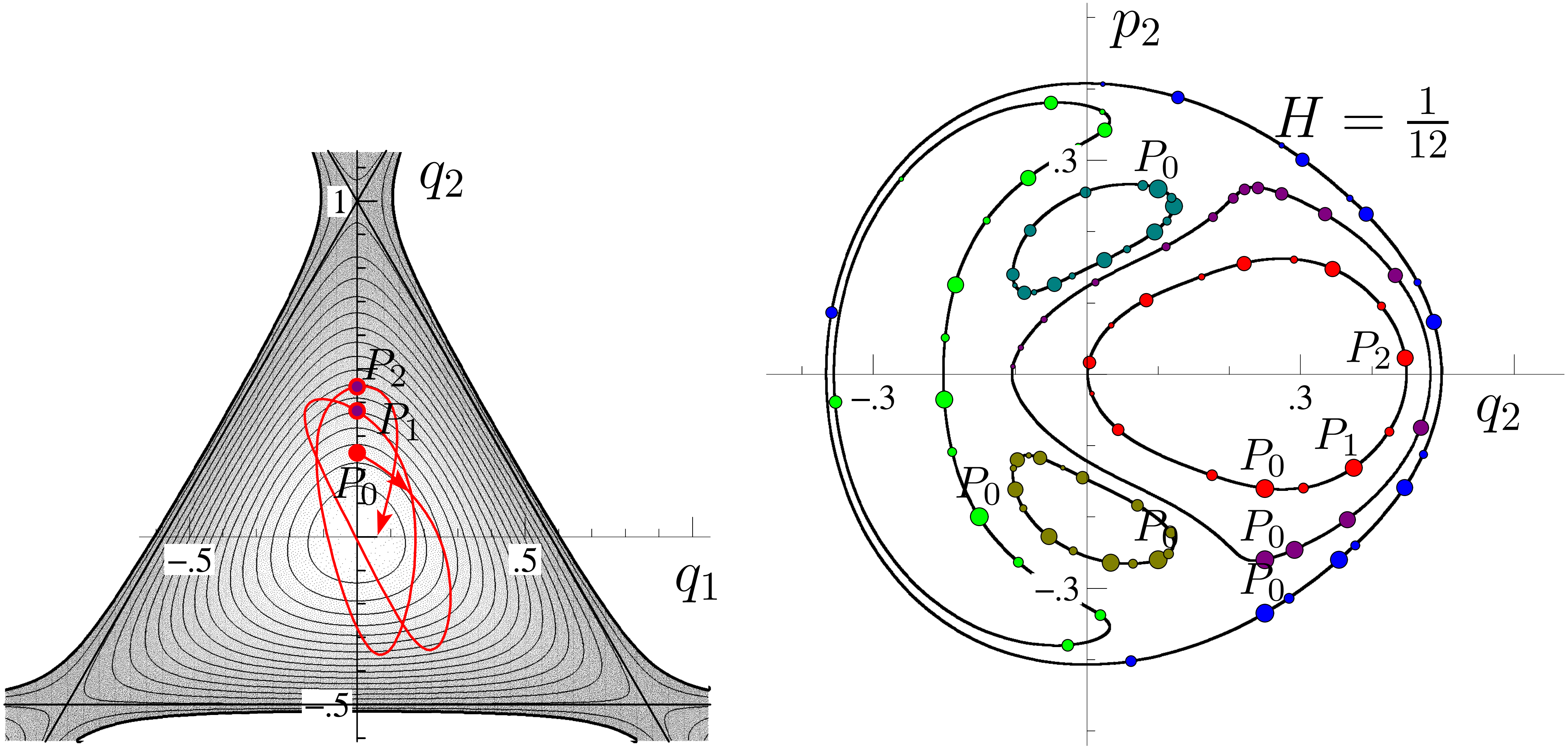
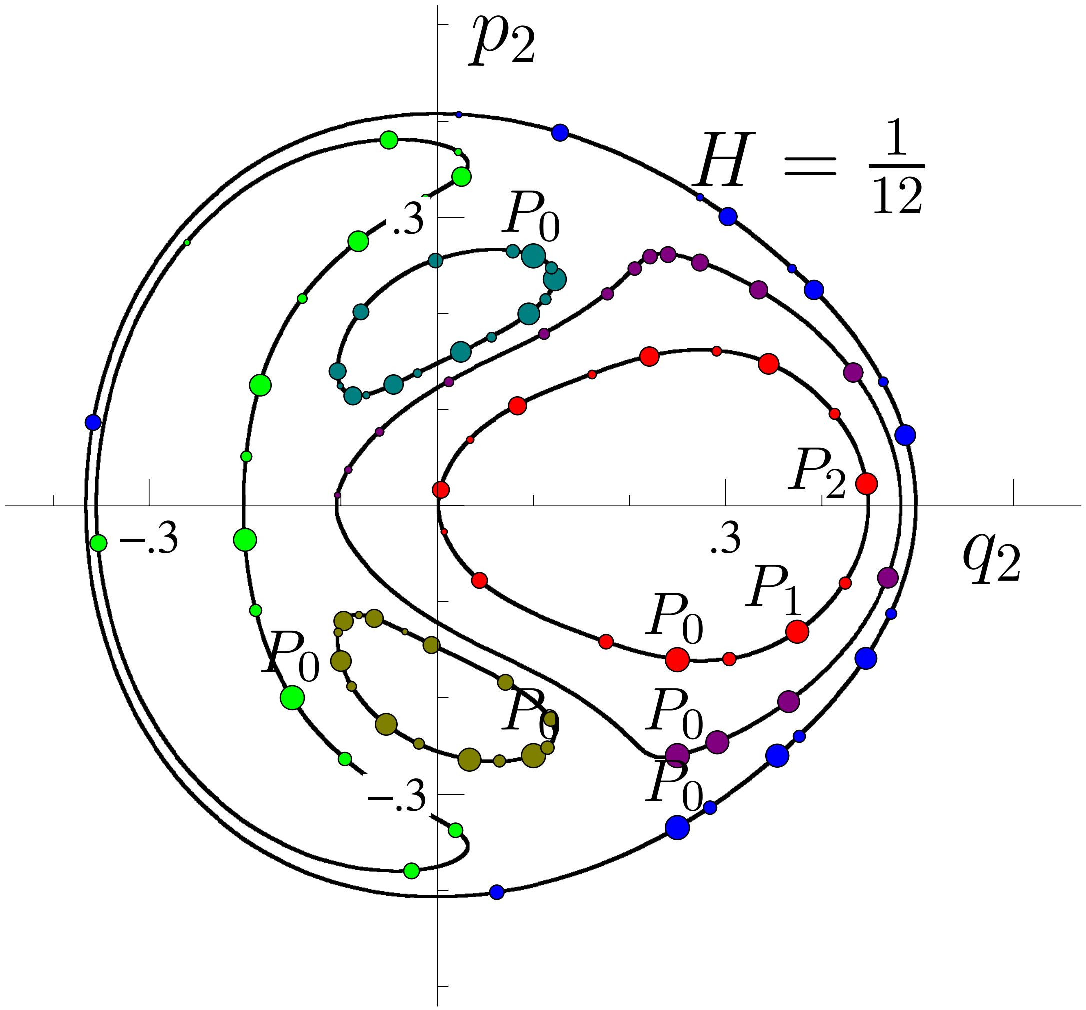
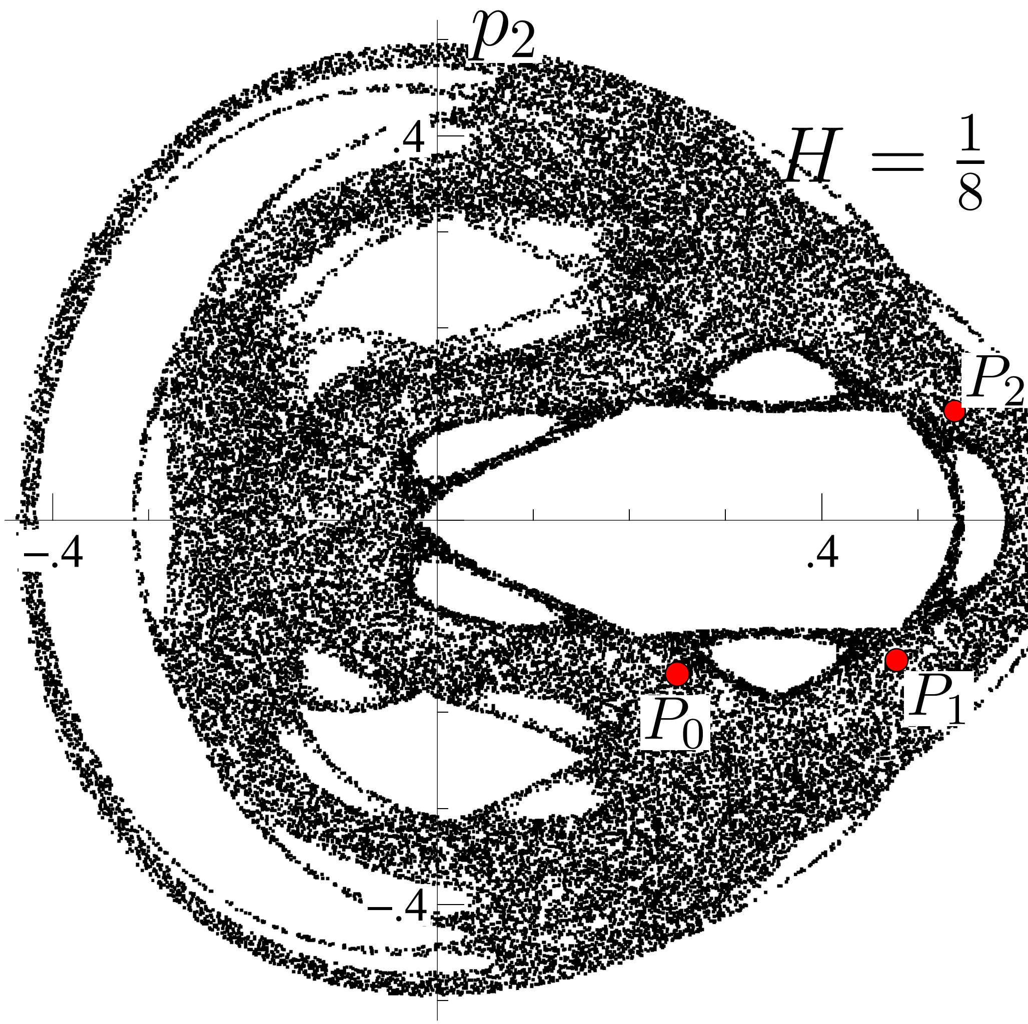


Surprise by increasing the energy:



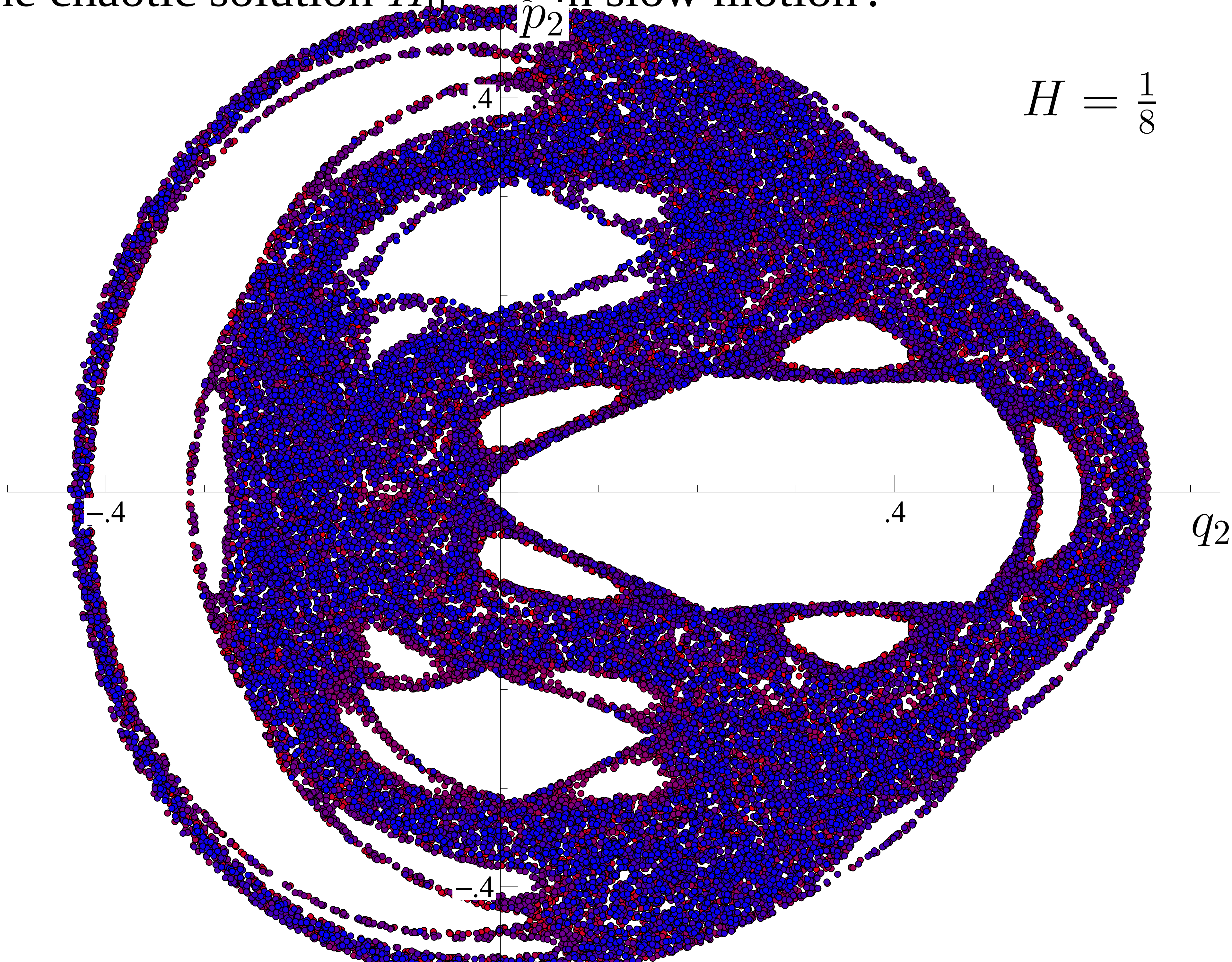
six orbits



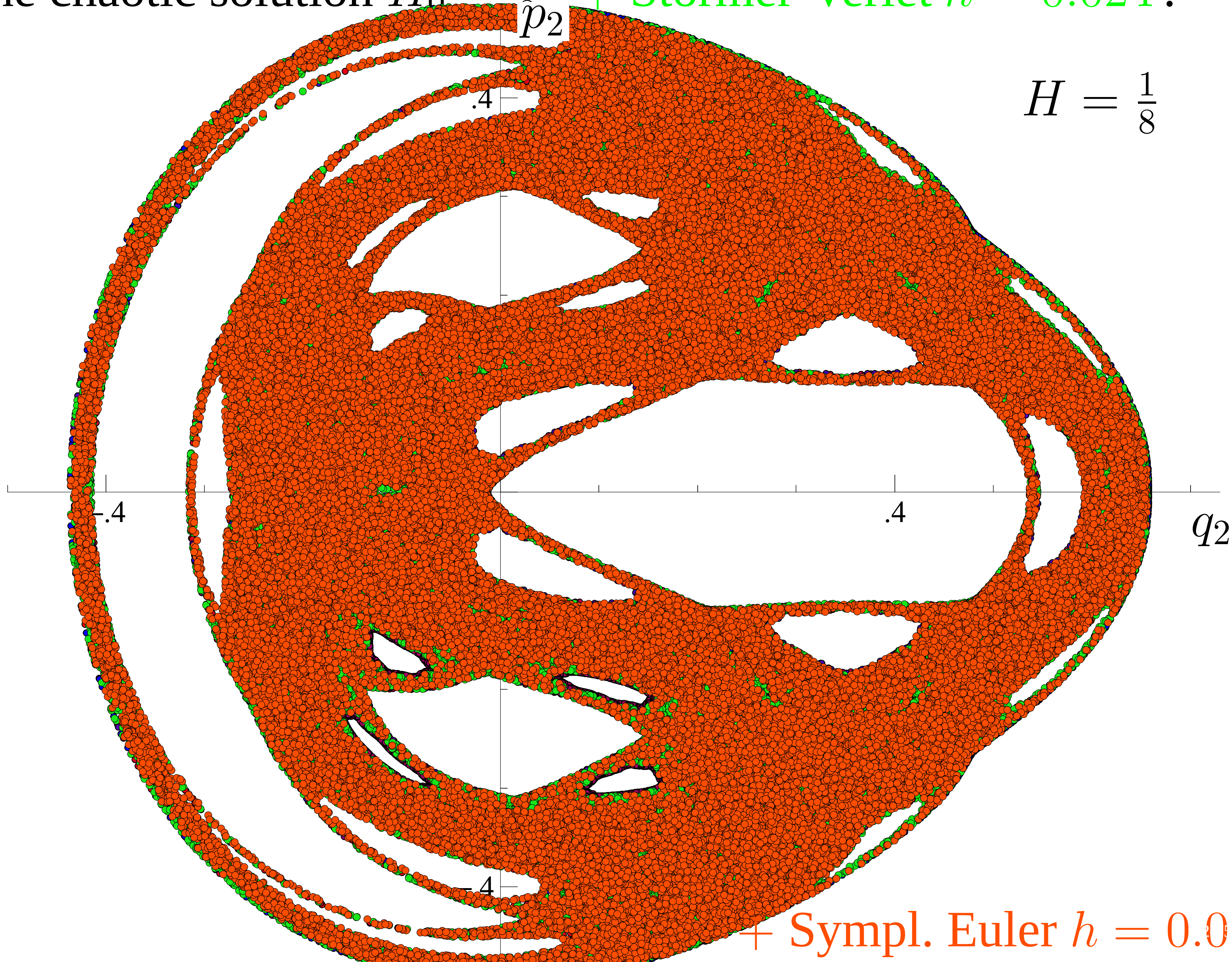
one orbit

Lasciate ogni speranza for a second analytical integral ...!

The chaotic solution $H_0 = \frac{1}{8}$ in slow motion:

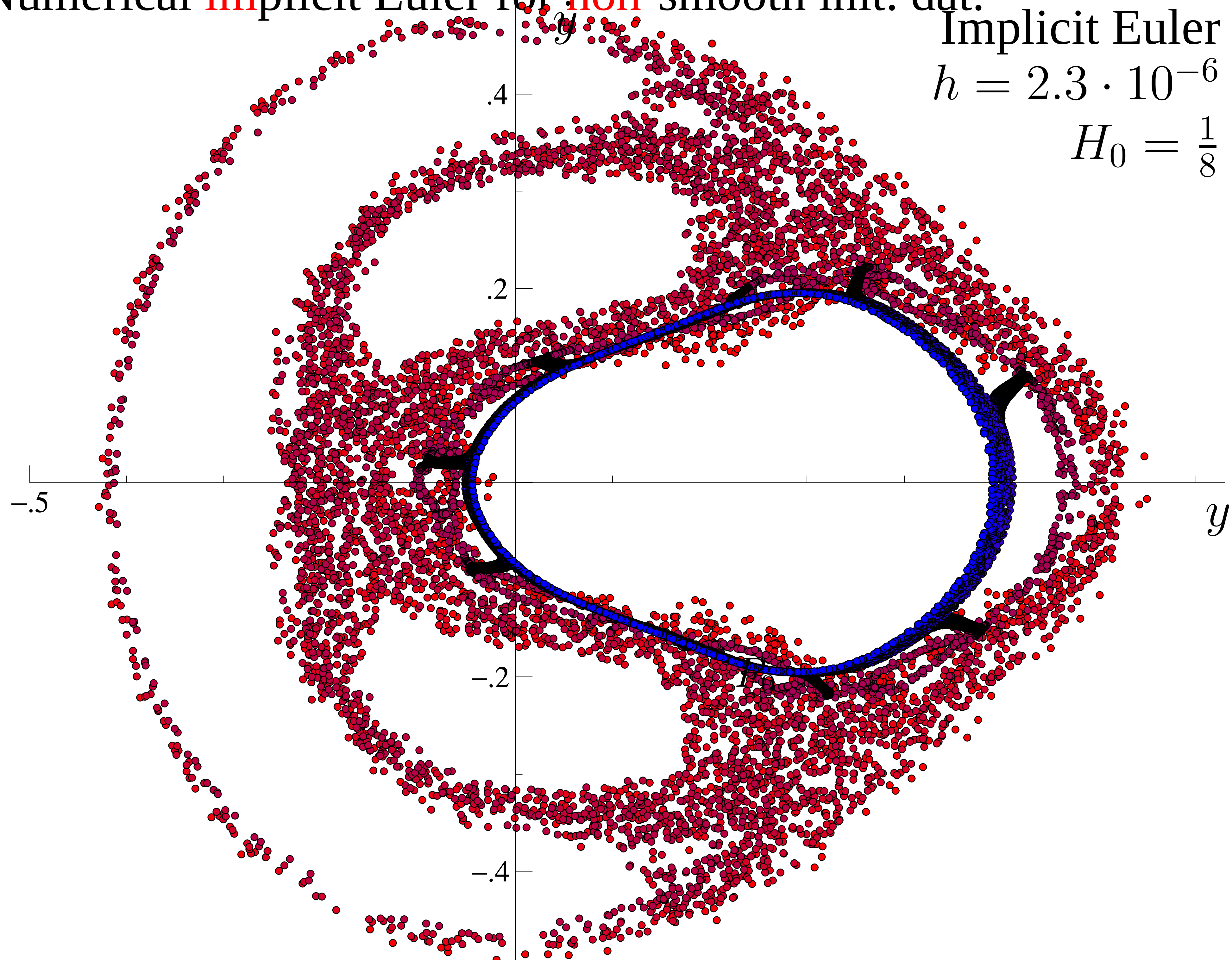


The chaotic solution $H_0 = \frac{1}{8}$ + Störmer-Verlet $h = 0.024$:



+ Sympl. Euler $h = 0.012$:

Numerical implicit Euler for non-smooth init. dat.

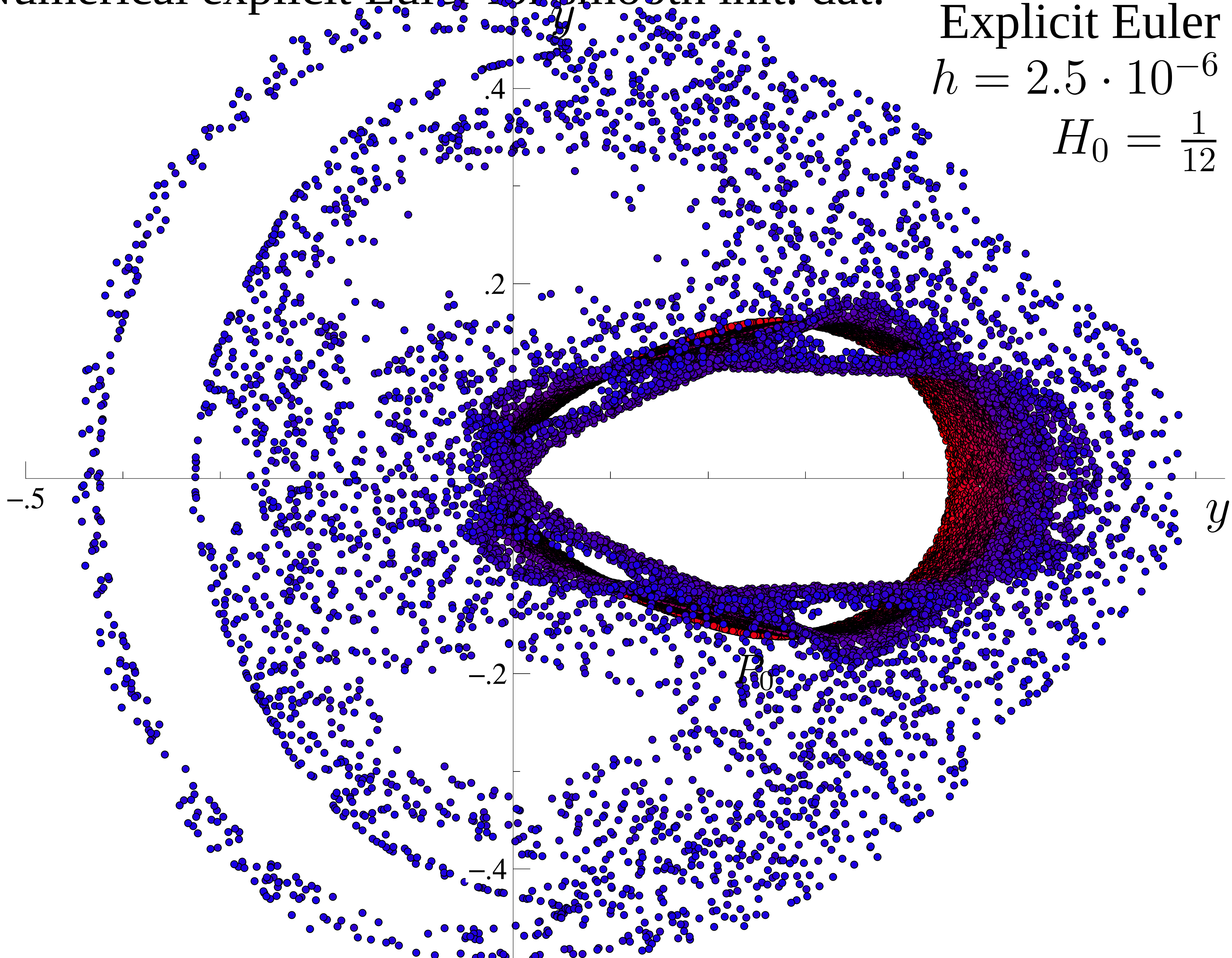


Numerical explicit Euler for smooth init. dat.

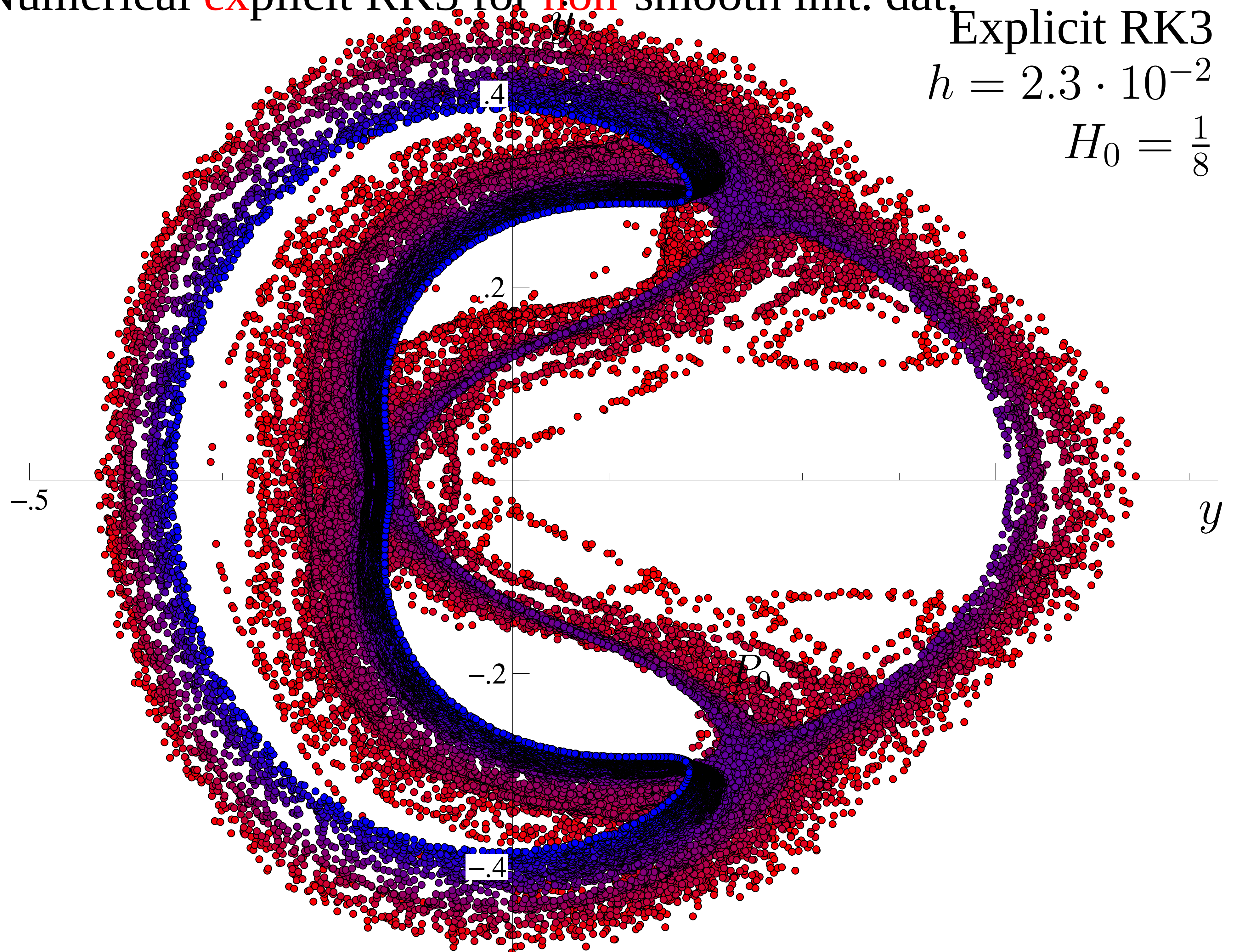
Explicit Euler

$h = 2.5 \cdot 10^{-6}$

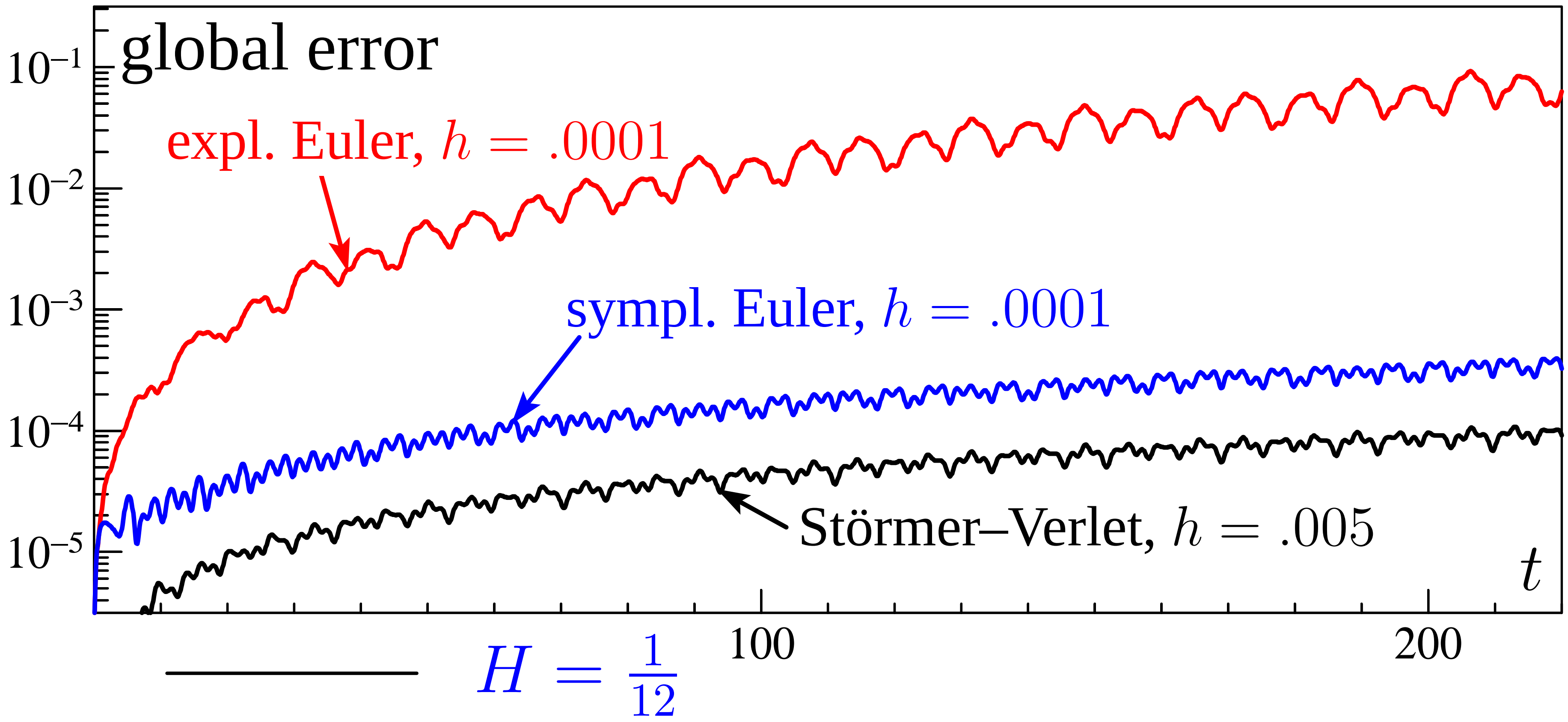
$H_0 = \frac{1}{12}$



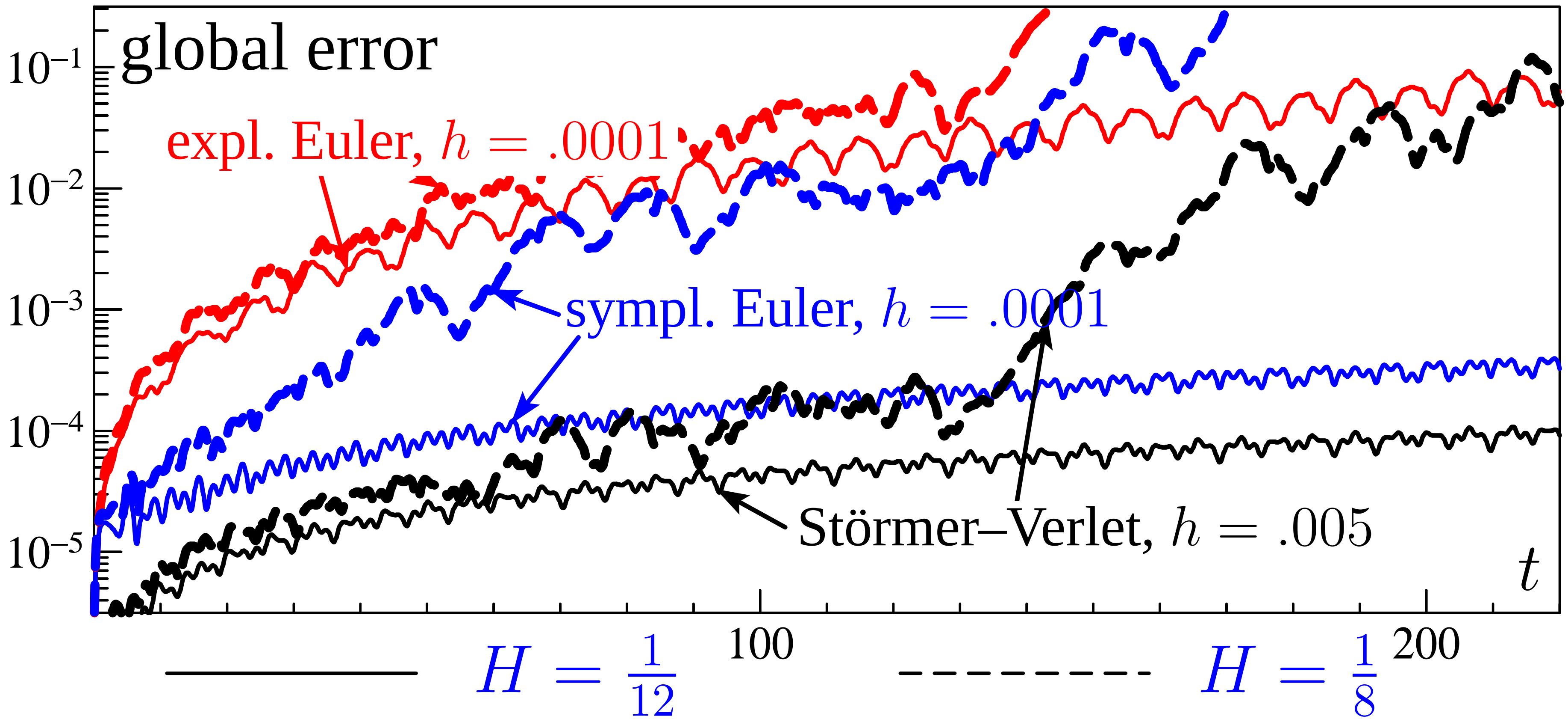
Numerical explicit RK3 for non-smooth init. dat.



Global error of numerical methods for smooth initial data $H = 1/12$:



Global error of numerical methods for smooth initial data $H = 1/12$ and non-smooth data $H = 1/8$:



R. Skeel, *Sympl. Integr. for Macromolecular Dynamics*, 1992:

“There is increasing empirical evidence favoring symplectic integrators, but the role of symplecticness is not well understood”

“Most popular is the symplectic Störmer/leapfrog/Verlet method”.

but also ... (Beijing , Sept. 2, 1992)

the evidence for using symplectic methods is not so strong.

“Possibly, it is some consequence of being symplectic that is important”.

The Answer : Backward Error Analysis.

Idea around for a while (Ruth 1983), Griffiths, Sanz-Serna 1986; for Hamiltonian problems Sanz-Serna, Yoshida, Eirola, Hairer; Feng Kang (Beijing , Sept. 1, 1992):

Numerical Approx: wrong sol of right equation $\dot{a}=a$
right sol of wrong equation $\dot{x}=at$.

Idea. Interpret numerical solution as exact solution of a modified problem:

$$
\begin{array}{ccc}
 & \xrightarrow{\text{exact}} & \boxed{\varphi_t(y_0)} \\
\boxed{\dot{y} = f(y)} & & \\
 & \xrightarrow{\text{numerical}} & \boxed{y_{n+1} = \Phi_h(y_n)} \\
\boxed{\dot{\widetilde{y}} = f_h(\widetilde{y})} & \xrightarrow{\text{exact}} &
\end{array}
$$

Great News :

- The modified equation is an expansion of the form

$$\dot{\widetilde{y}} = f(\widetilde{y}\,) + hf_2(\widetilde{y}\,) + h^2 f_3(\widetilde{y}\,) + \ldots,$$

which can be computed recursively from the error term.

- The whole artillery of theoretical results (Perturbation Theory, Poincaré-Lindstedt series, KAM Theory ...) can now be applied to the study of numerical methods.

Flow Maps and Vector Fields developped in B-series:

$$\Phi\{a\} = a(\emptyset)\mathrm{Id} + h a(\bullet) f + h^2 a([\bullet]) f' f + \ldots$$

$$\text{exact sol.:} \quad e(\tau) = \frac{1}{\gamma(\tau)}$$

$$\mathcal{VF}\{b\} \sim b(\bullet) f + h b([\bullet]) f' f + h^2 b([\bullet,\bullet]) f''(f,f) + \ldots$$

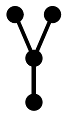
$$\text{exact } \mathcal{VF}\text{:} \quad u(\bullet) = 1, \quad u(\tau) = 0 \text{ else}$$

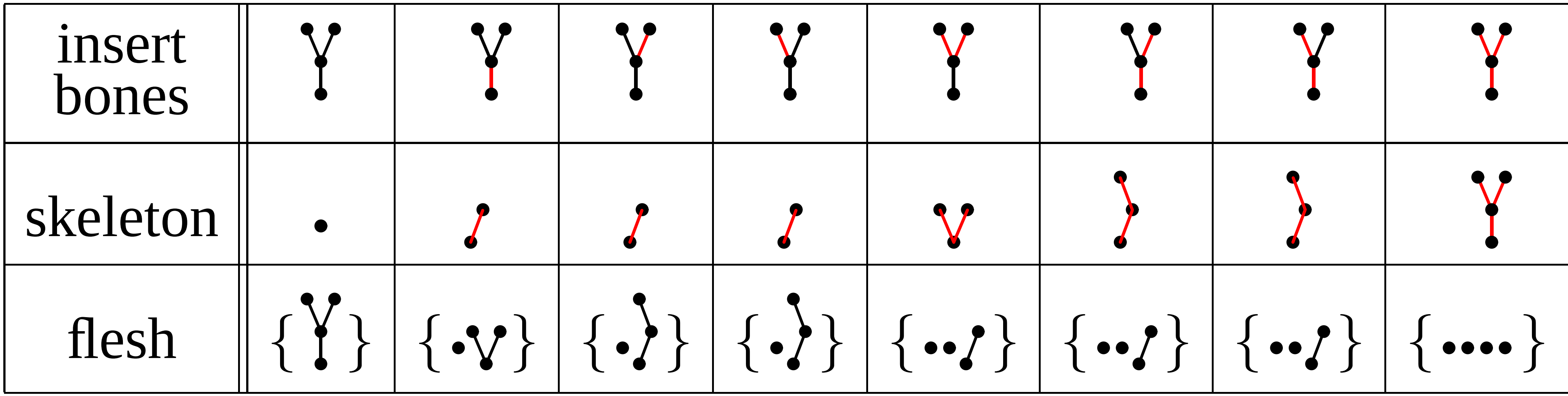
Theorem. (Chartier, Hairer, Vilmart 2006)

$$\begin{tikzcd}
\boxed{\mathcal{VF}\{u\}} \arrow[dr, "\Phi\{b\star a\}"] & \\
 & \boxed{\text{num. sol.}} \\
\boxed{\mathcal{VF}\{b\}} \arrow[uu, Rightarrow] \arrow[ur, "\Phi\{a\}"'] &
\end{tikzcd}$$

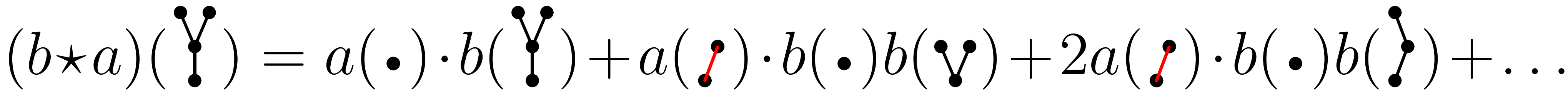
if ...

The Substitution Law for Tree-Maps:

Take a tree, for ex. , then ...

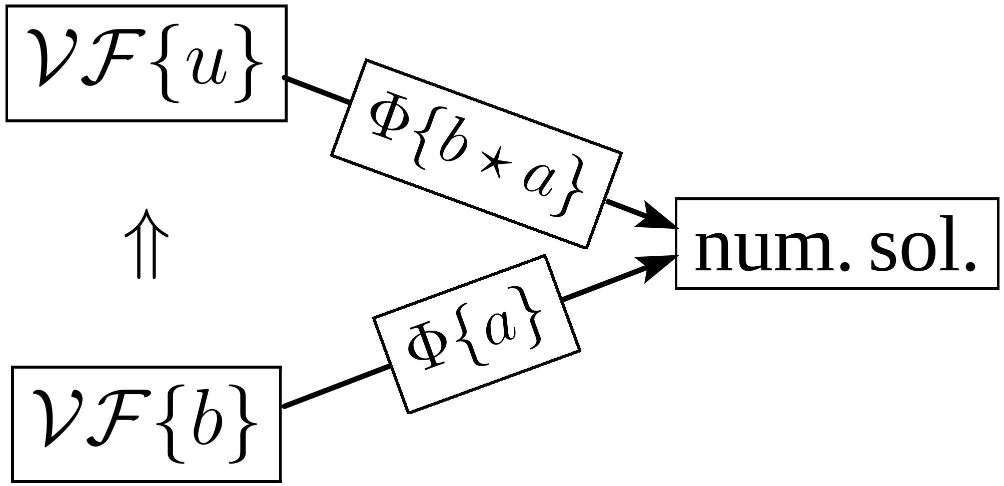


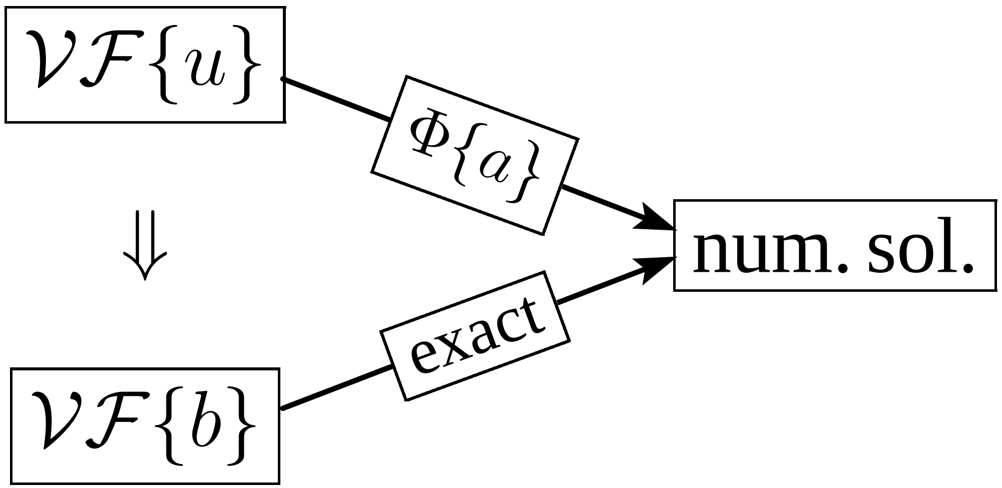
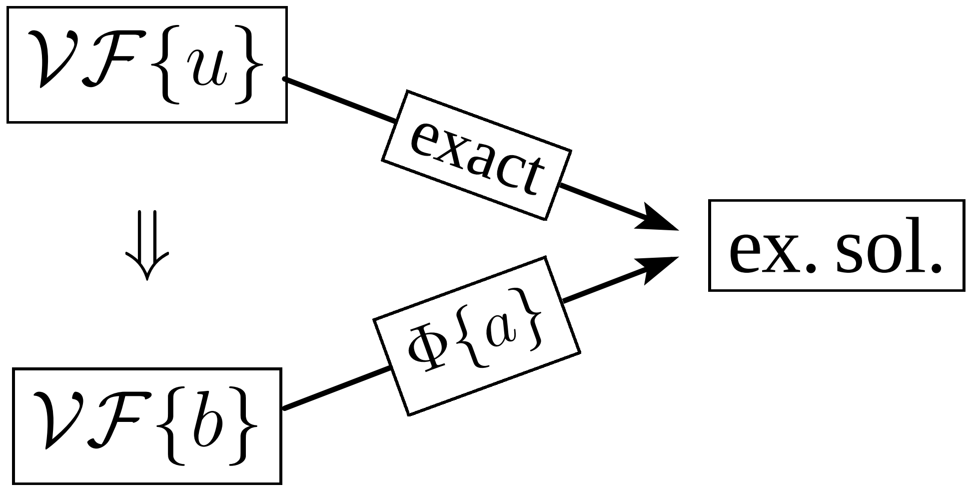
then define



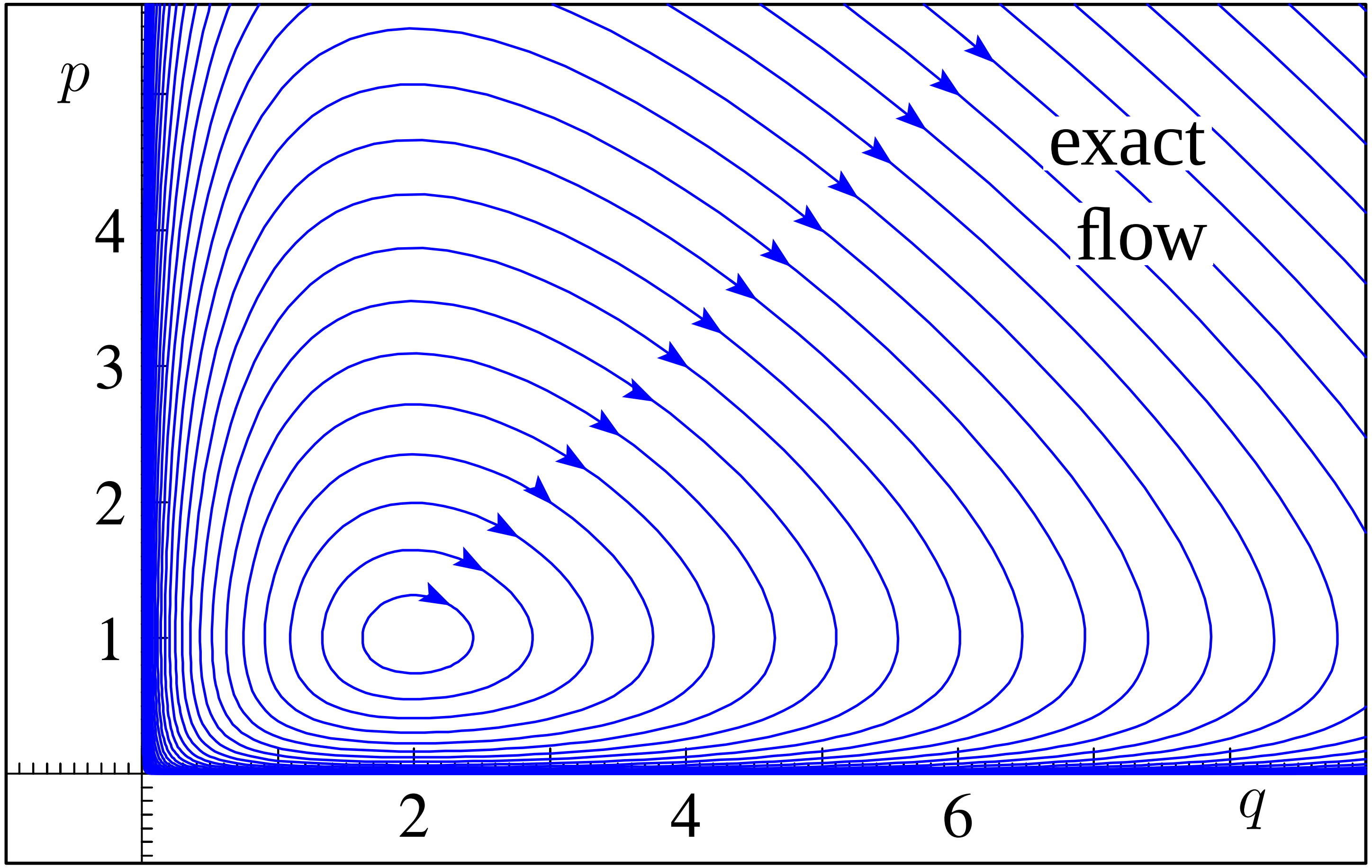
(in the a goes the skeleton, in the b goes the flesh...)

Applications:



postmodified VF	premodified VF
	
$b \star e = a$	$b \star a = e$
(Backward error an.)	(Ch.,H.,Vilmart 2006)

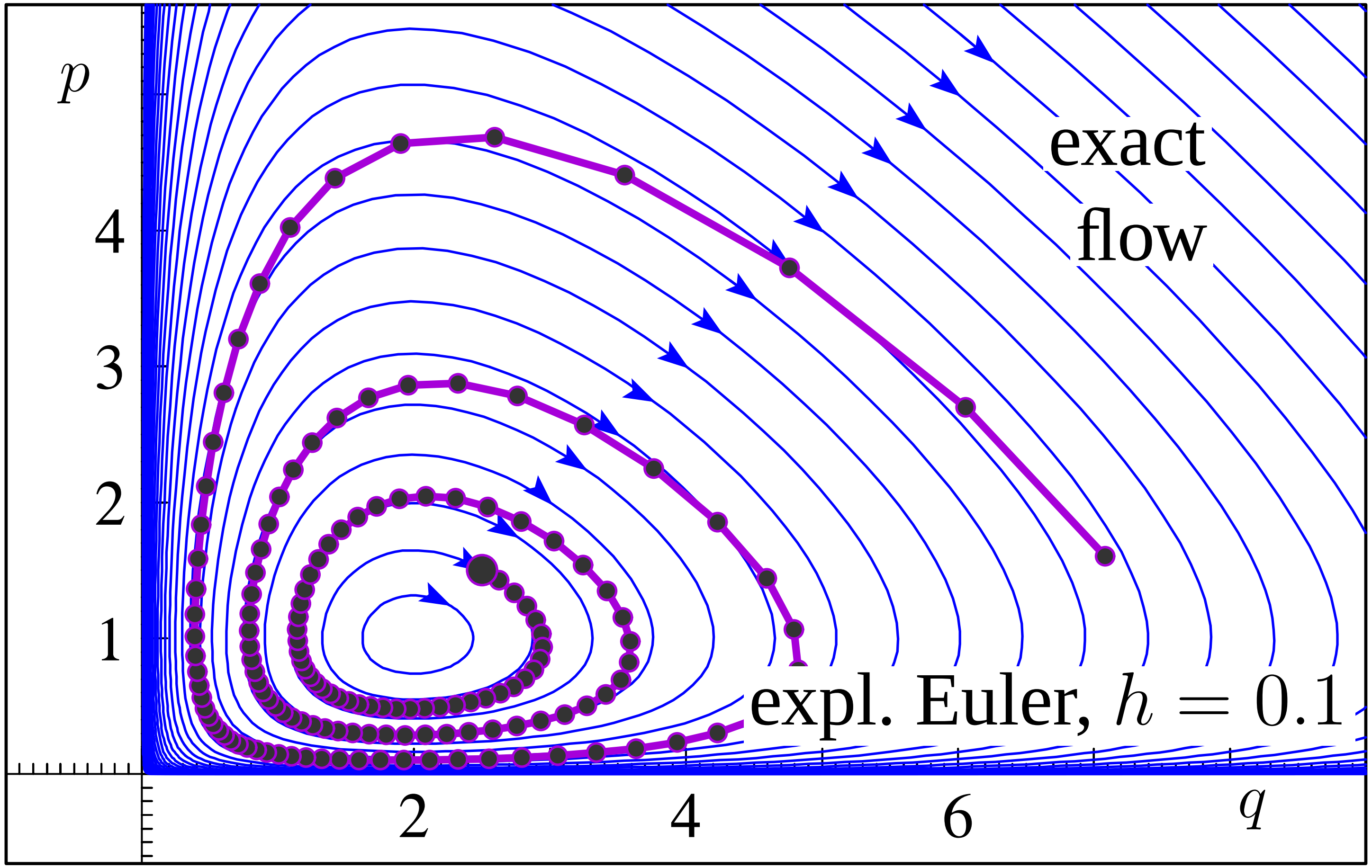
Example. The Lotka-Volterra Model



$$\dot{q} = q(p-1)$$

$$\dot{p} = -p(q-2)$$

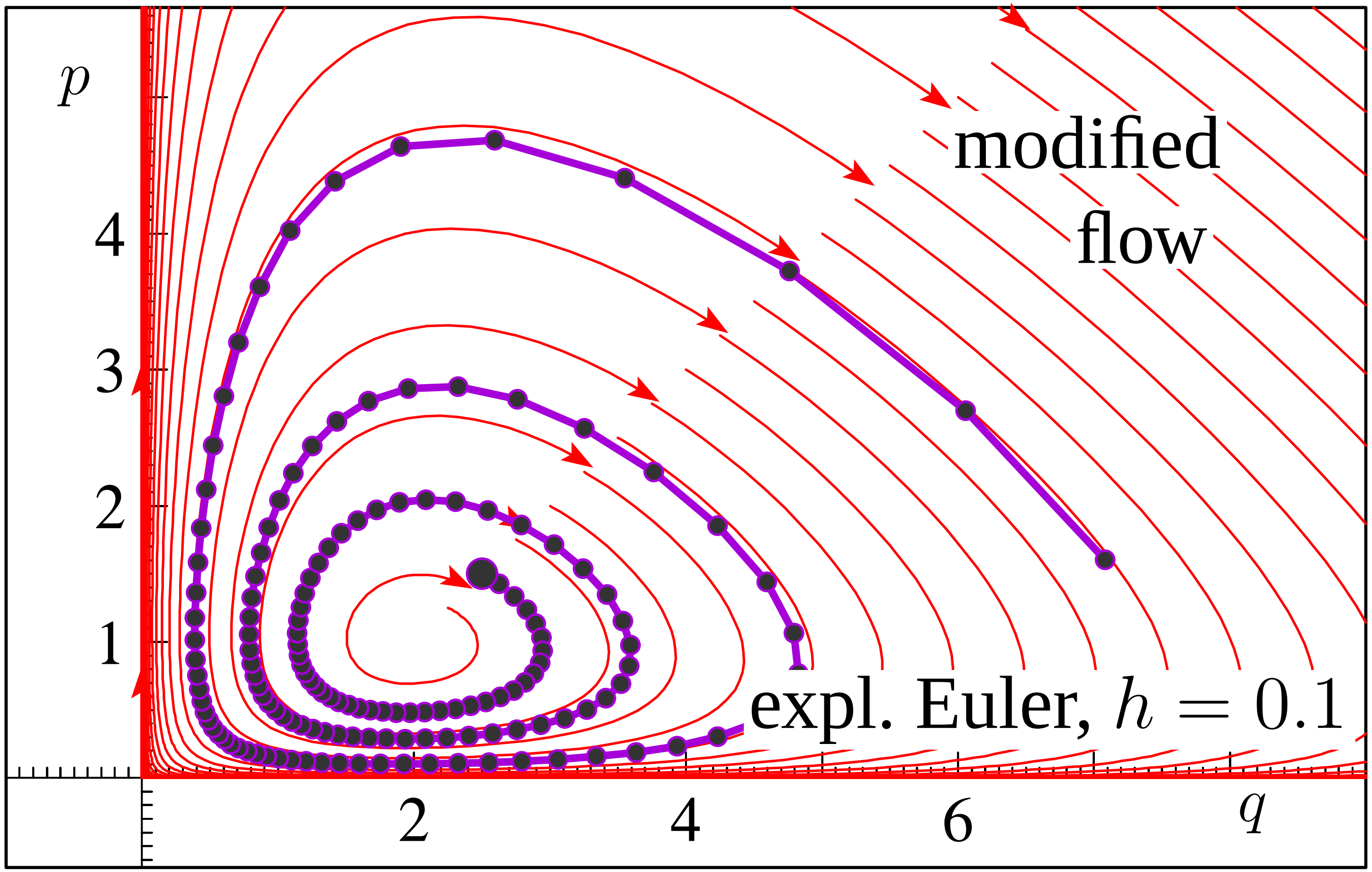
Example. The Lotka-Volterra Model and Euler's method



$$\dot{q} = q(p-1)$$

$$\dot{p} = -p(q-2)$$

Example. The Modified Model and Euler's method



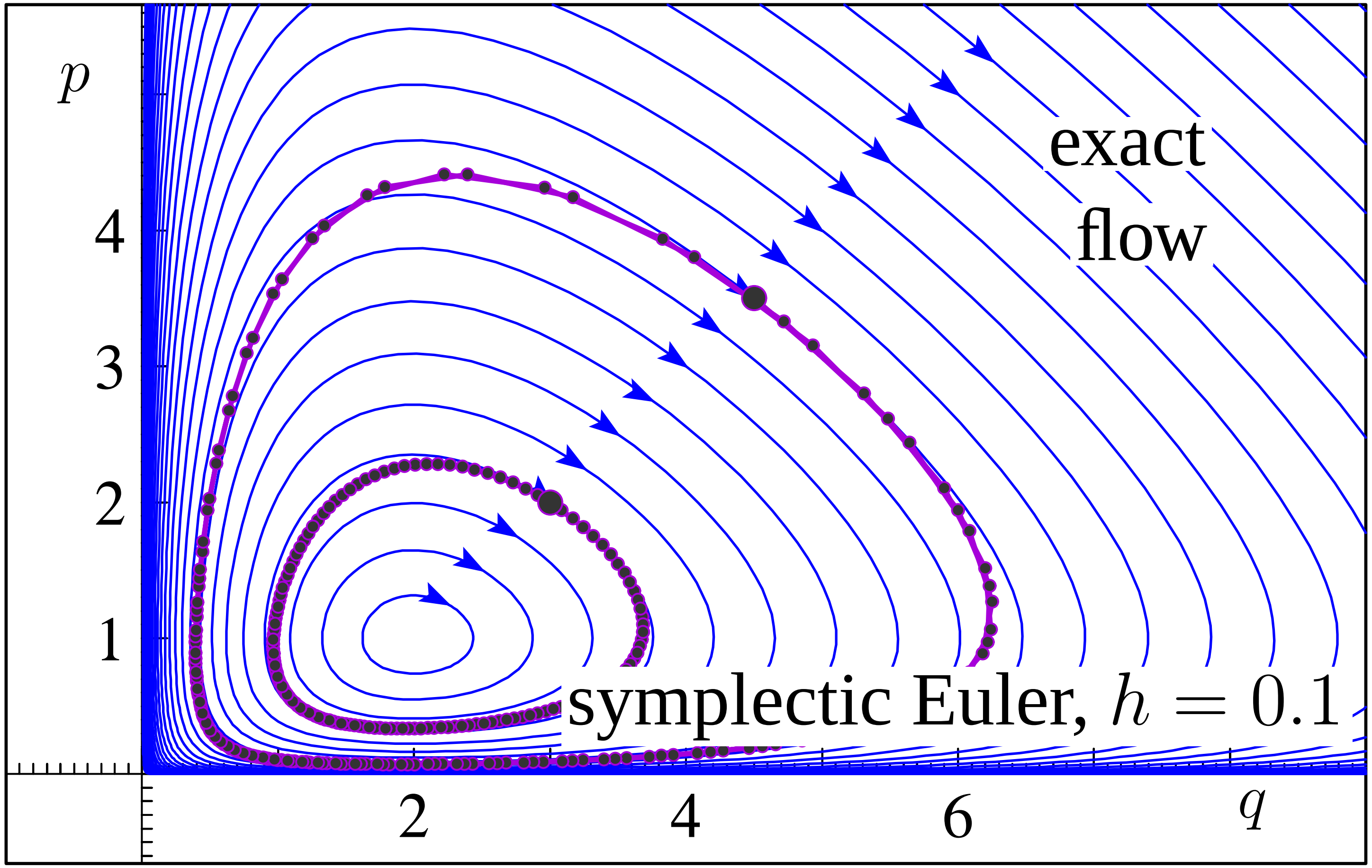
$$\dot{q} = q(p-1) - \frac{h}{2}\,q(p^2 - pq + 1) + \mathcal{O}(h^2),$$

$$\dot{p} = -p(q-2) - \frac{h}{2}\,p(q^2 - pq - 3q + 4) + \mathcal{O}(h^2)$$

Second Great News :

- If the original problem has some structure (symplectic, symmetric, Poisson, volume preserving, first integrals ...)
- and if the numerical method is structure preserving ...
- then the modified problem has the same structure !!

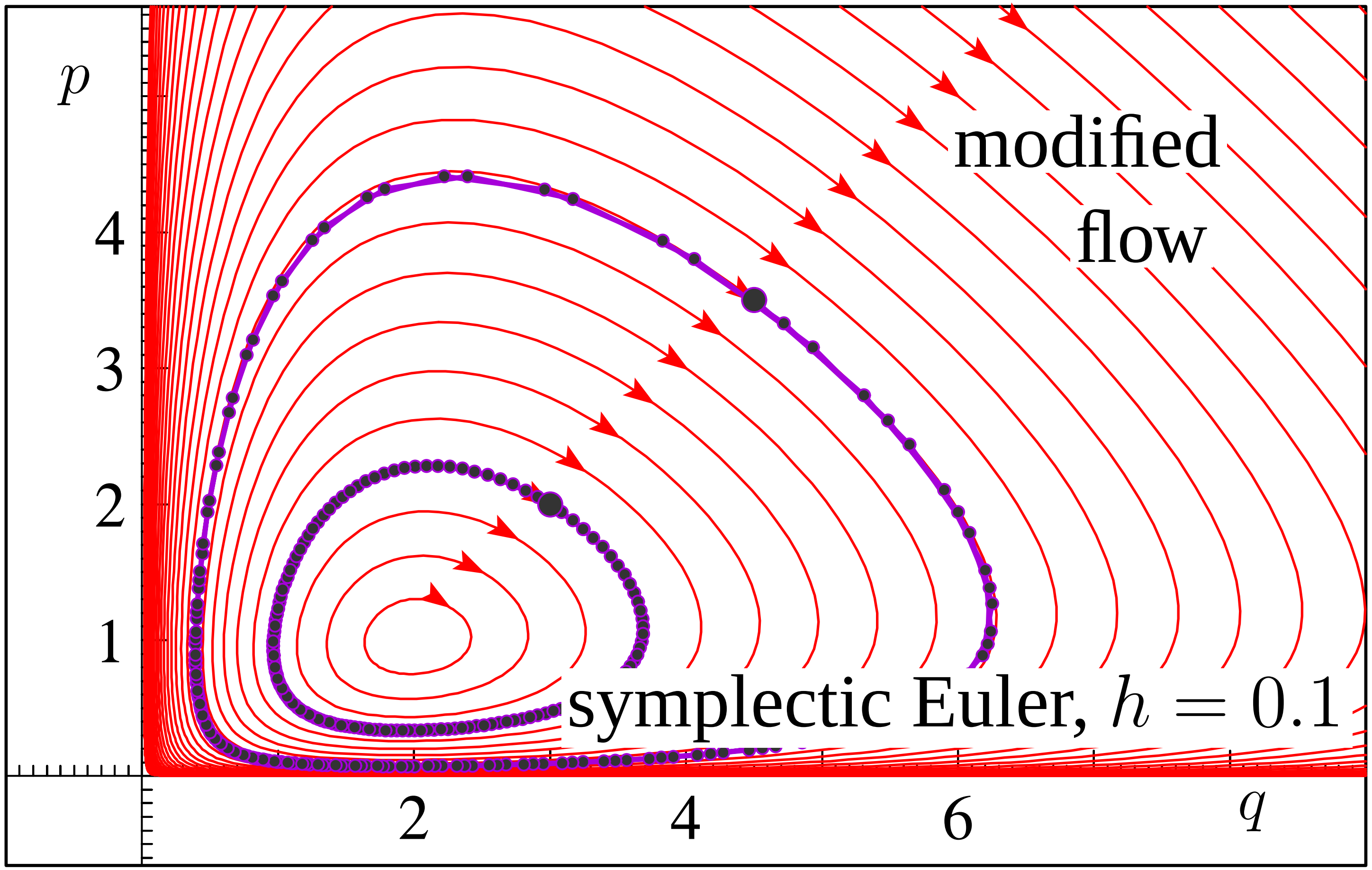
Example. The Lotka-Volterra Model and symplectic Euler



$$\dot{q} = q(p-1)$$

$$\dot{p} = -p(q-2)$$

Example. **The Modified Model** and symplectic Euler



$$\dot{q} = q(p-1) - \frac{h}{2}\,q(p^2 + pq - 4p + 1) + \mathcal{O}(h^2),$$

$$\dot{p} = -p(q-2) + \frac{h}{2}\,p(q^2 + pq - 5q + 4) + \mathcal{O}(h^2)$$

$$\dot{q} = q(p-1) - \frac{h}{2}\,q(p^2 + pq - 4p + 1) + \mathcal{O}(h^2),$$
$$\dot{p} = -p(q-2) + \frac{h}{2}\,p(q^2 + pq - 5q + 4) + \mathcal{O}(h^2)$$

$$\dot{q} = q(p-1) - \frac{h}{2}\, q(p^2 + pq - 4p + 1) + \mathcal{O}(h^2),$$
$$\dot{p} = -p(q-2) + \frac{h}{2}\, p(q^2 + pq - 5q + 4) + \mathcal{O}(h^2)$$

$$\dot{q} = qp\left[1 - \frac{1}{p} - \frac{h}{2}\left(p + q - 4 + \frac{1}{p}\right)\right] + \mathcal{O}(h^2)$$
$$\dot{p} = -qp\left[1 - \frac{2}{q} - \frac{h}{2}\left(q + p - 5 + \frac{4}{q}\right)\right] + \mathcal{O}(h^2))$$

is Poisson with $H =$

$$p - \ln p + q - 2\ln q - \frac{h}{2}\left(\frac{p^2}{2} + pq + \frac{q^2}{2} - 4p - 5q + \ln p + 4\ln q\right).$$

Very Bad News :

The expansion

$$\dot{\widetilde{y}} = f(\widetilde{y}\,) + hf_2(\widetilde{y}\,) + h^2 f_3(\widetilde{y}\,) + \ldots,$$

is (nearly always) diverging for $N \to \infty$!!

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Need rigorous Error Estimations
(Benettin & Giorgilli 1994, Hairer & Lubich 1997, Reich 1999)

$\Rightarrow$ Optimal choice of N ;

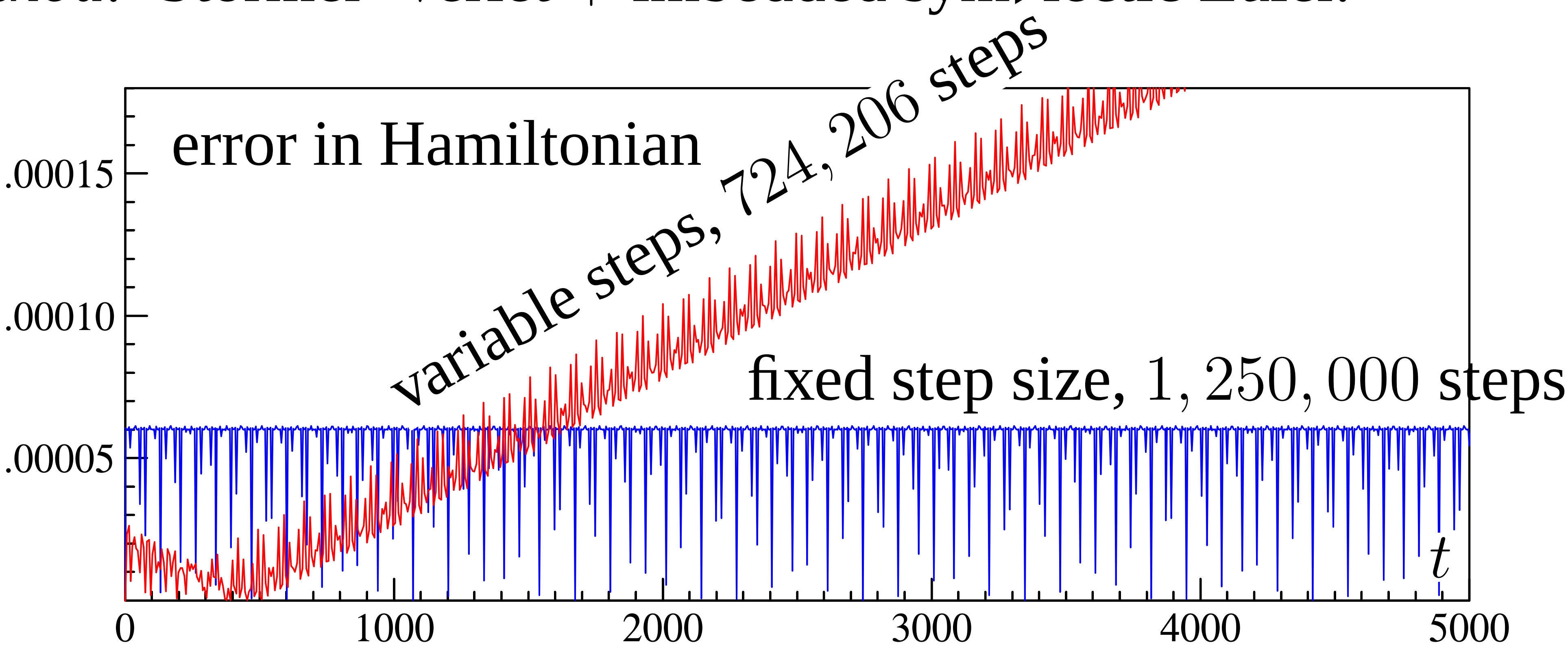
$\Rightarrow$ Exponentially long estimates for the numerical solution.

However, Symplecticity is not everything !!

Counter-Example.

(Sanz-Serna, Calvo 1992, Gladman, Duncan, Candy 1991) : Kepler problem with eccentricity $e = 0.6$.

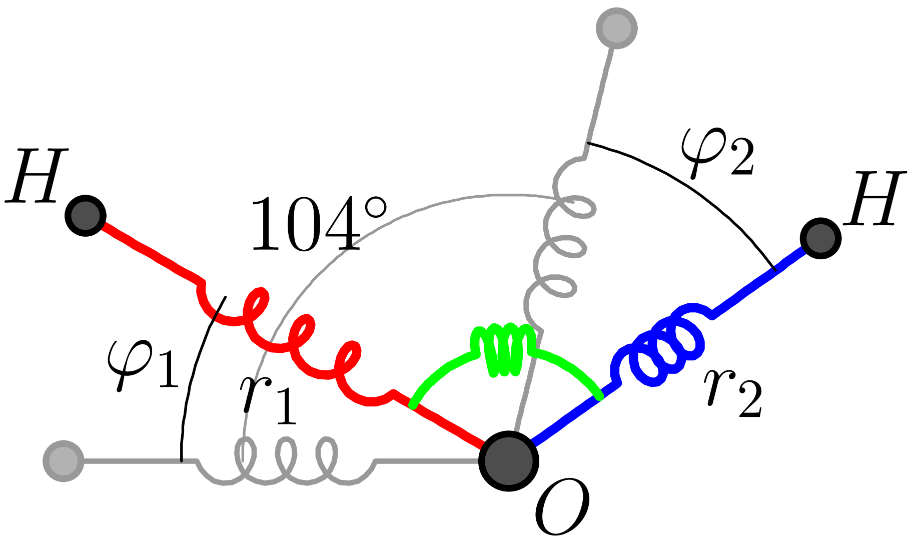
Method: Störmer–Verlet + imbedded symplectic Euler.

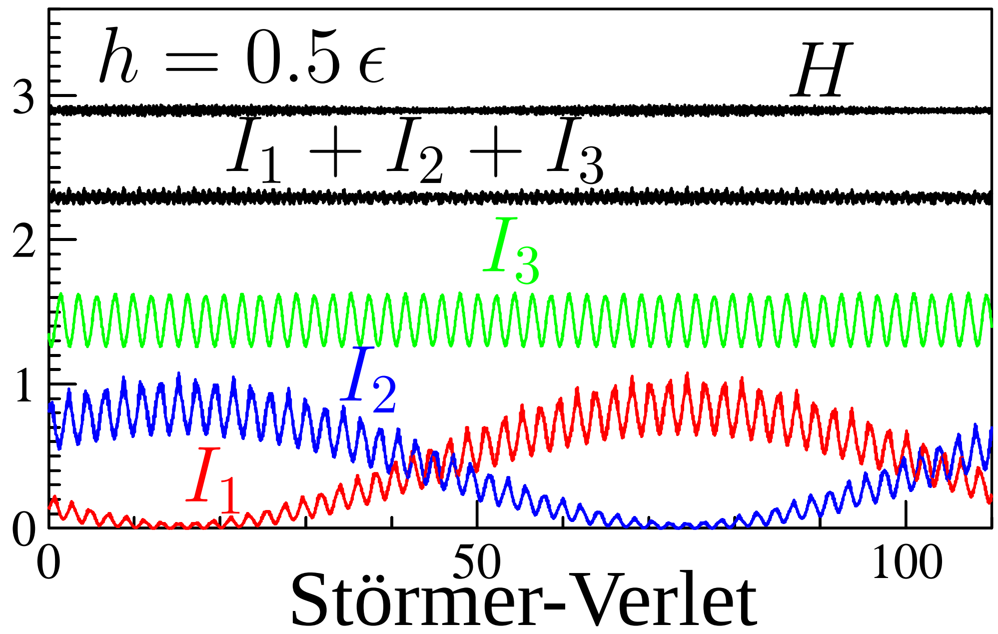


Method theoretically symplectic, but must be applied carefully!

(⇒ Stoffer 1988, Huang, Leimkuhler 1997, Hairer, Söderlind 2004).

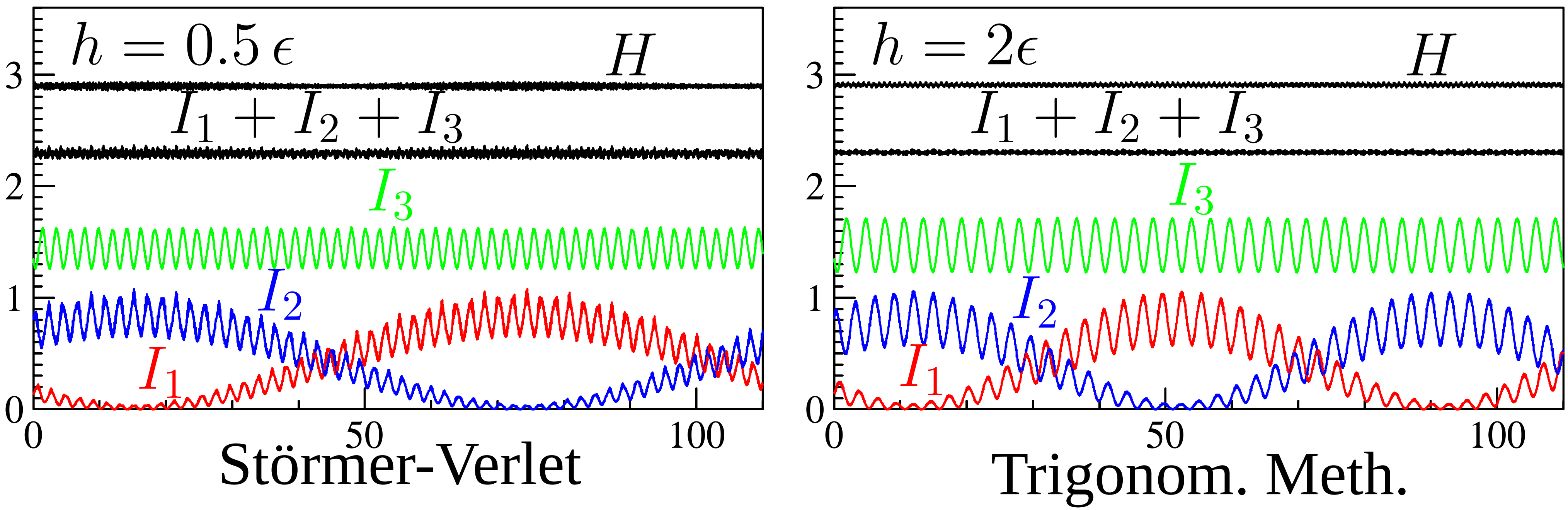
Highly Oscillatory Problem : The water molecule ($\epsilon = 0.01$)





The symplectic method is not good....

Highly Oscillatory Problem : Special trigonometric meth.:



Major instrument of analysis:

Modulated Fourier Expansions

(Gautschi, García, Sanz-Serna, Skeel, Hochbruck, Lubich, Hairer, Cohen).

Multistep Methods.

Theorem (Tang 1993, Hairer–Leone 1997).

(True) Multi-value methods are never symplectic.

Multistep Methods.

Theorem (Tang 1993, Hairer–Leone 1997).

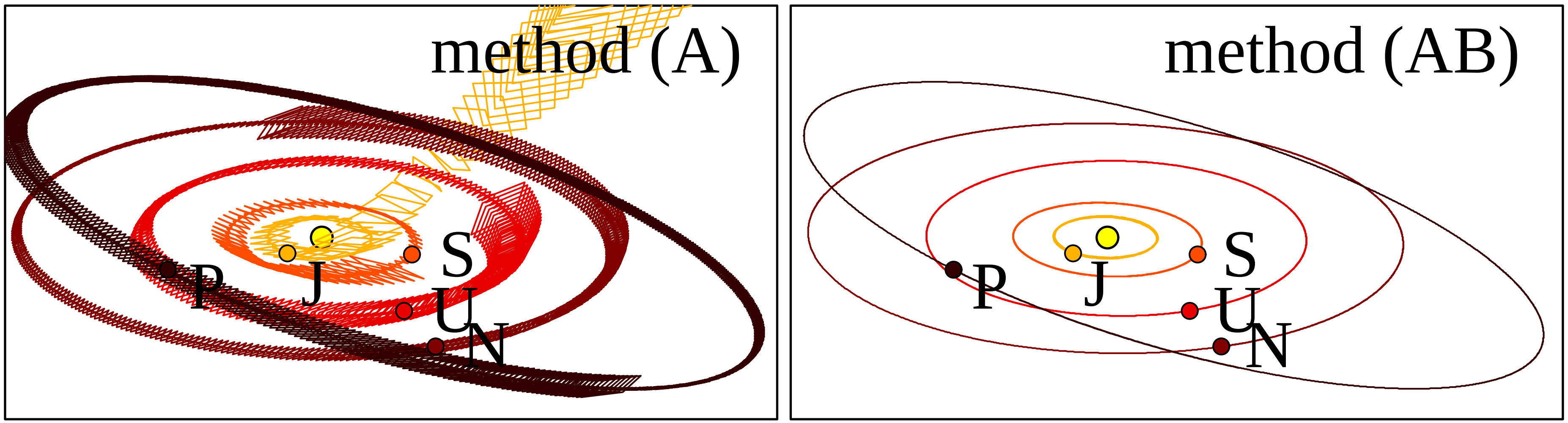
(True) Multi-value methods are never symplectic.

Surprise : (Quinlan–Tremaine) Can be excellent !

Example.

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

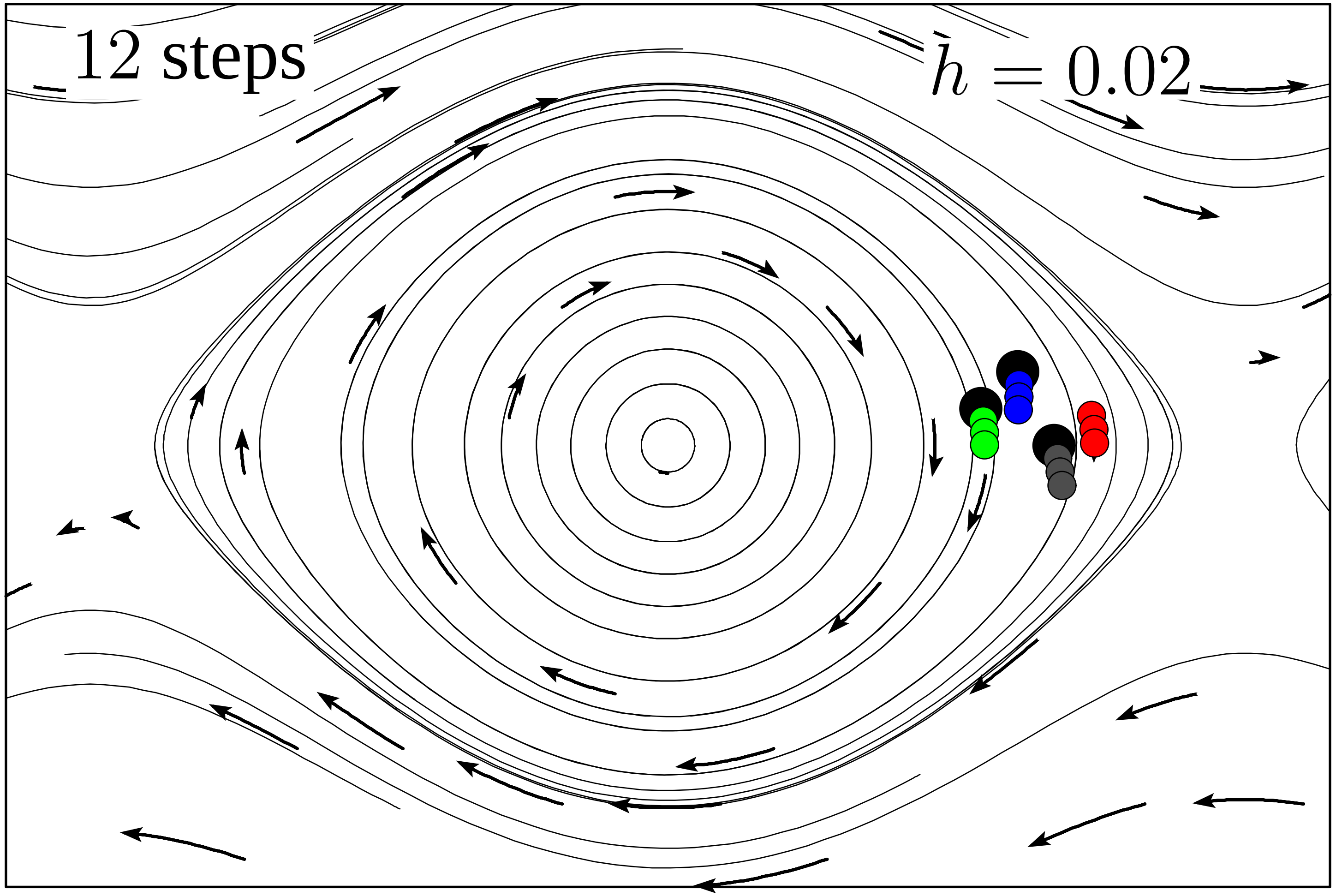
$$(B) : \quad z_{n+3} - z_{n+1} = 2hg_{n+2}.$$



Analysis: Modulated “Root Power series” (E. Hairer).

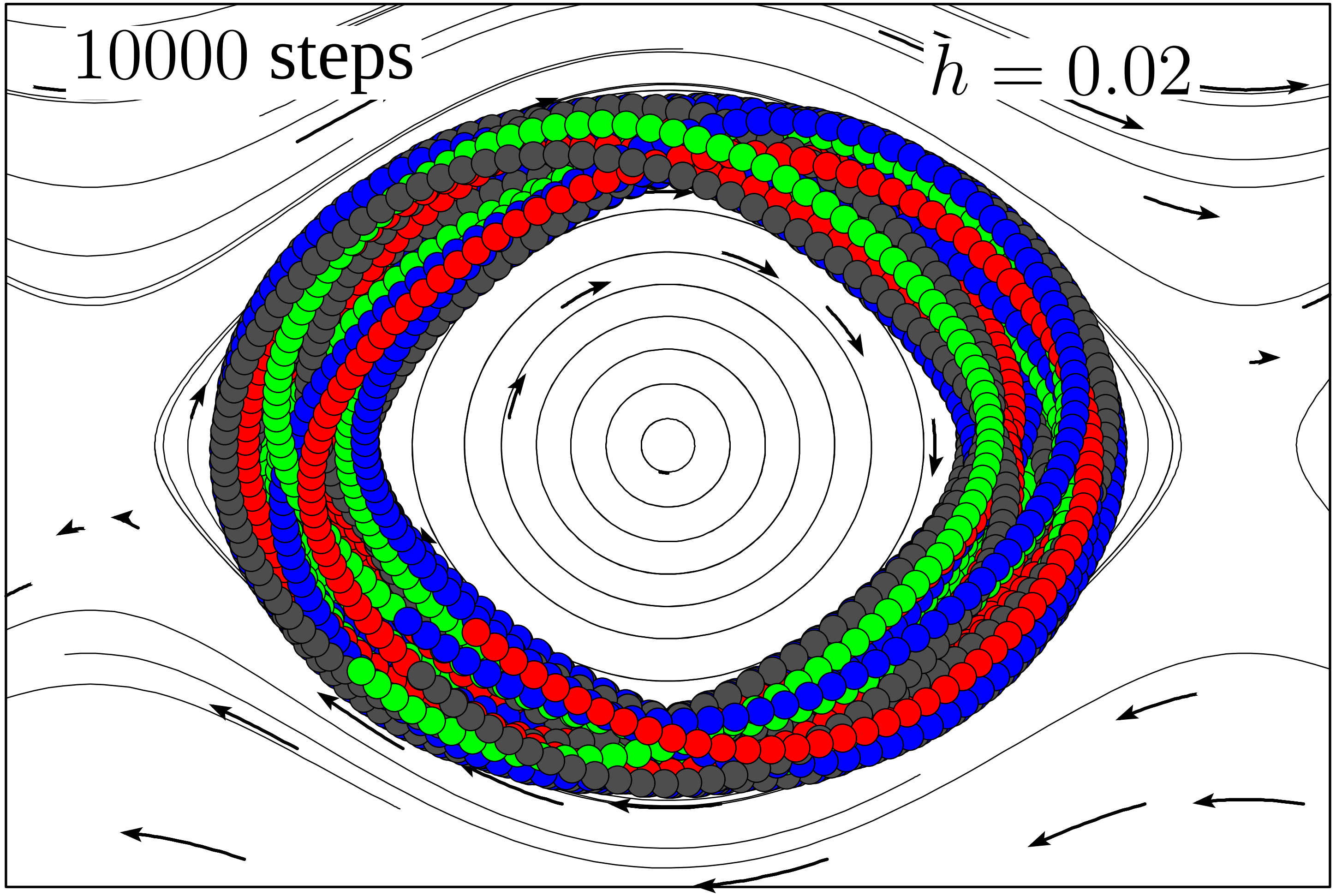
Method (A) alone at pendulum equation:

$$\text{(A)}: \quad y_{n+3} - y_{n+2} + y_{n+1} - y_n = h(f_{n+2} + f_{n+1})$$



Method (A) alone at pendulum equation:

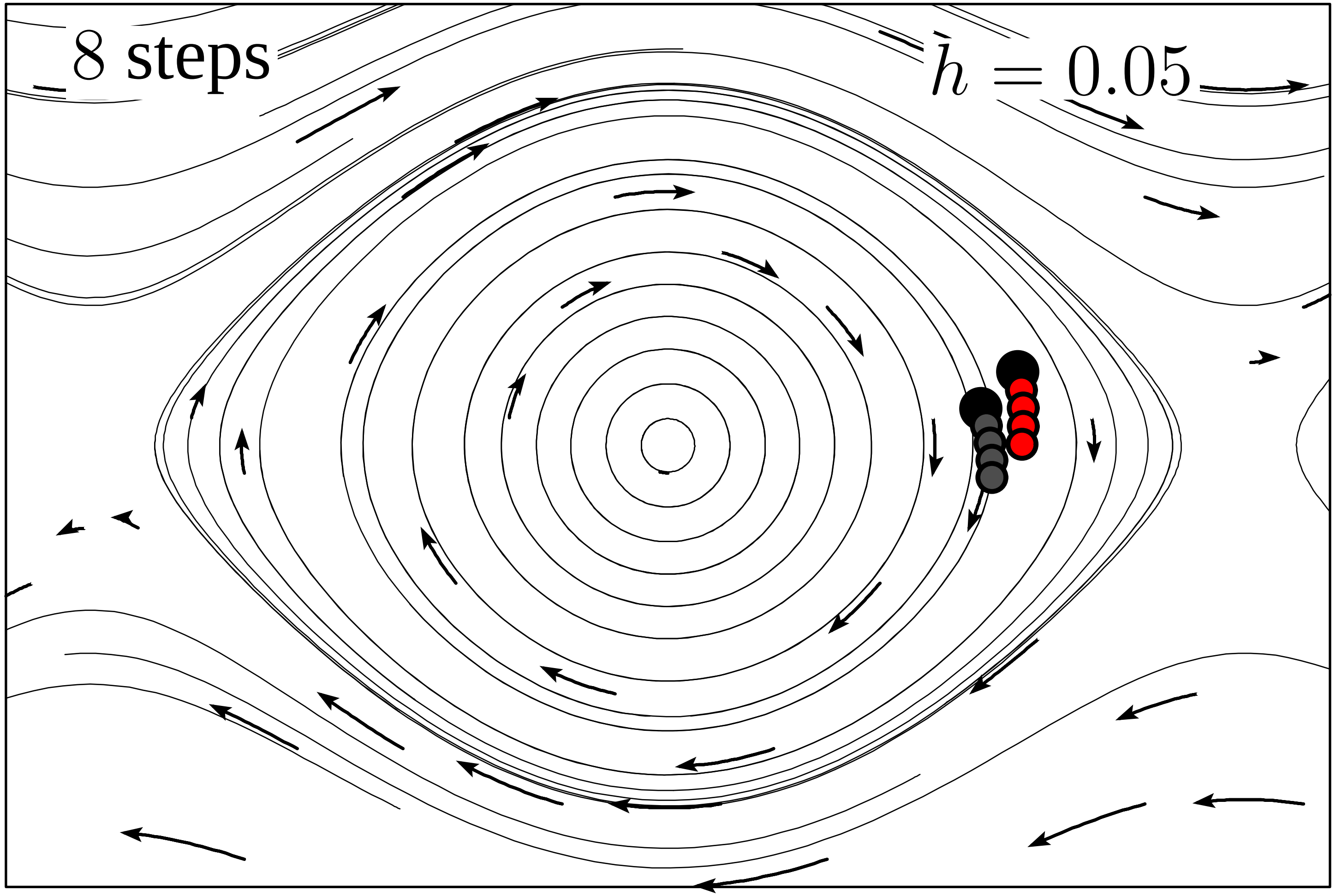
$$(\mathrm{A}) \; : \quad y_{n+3} - y_{n+2} + y_{n+1} - y_n = h(f_{n+2} + f_{n+1})$$



Behaves stable — but stability not understood (proof ??).

Method (B) alone at pendulum equation:

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



Method (B) alone at pendulum equation:

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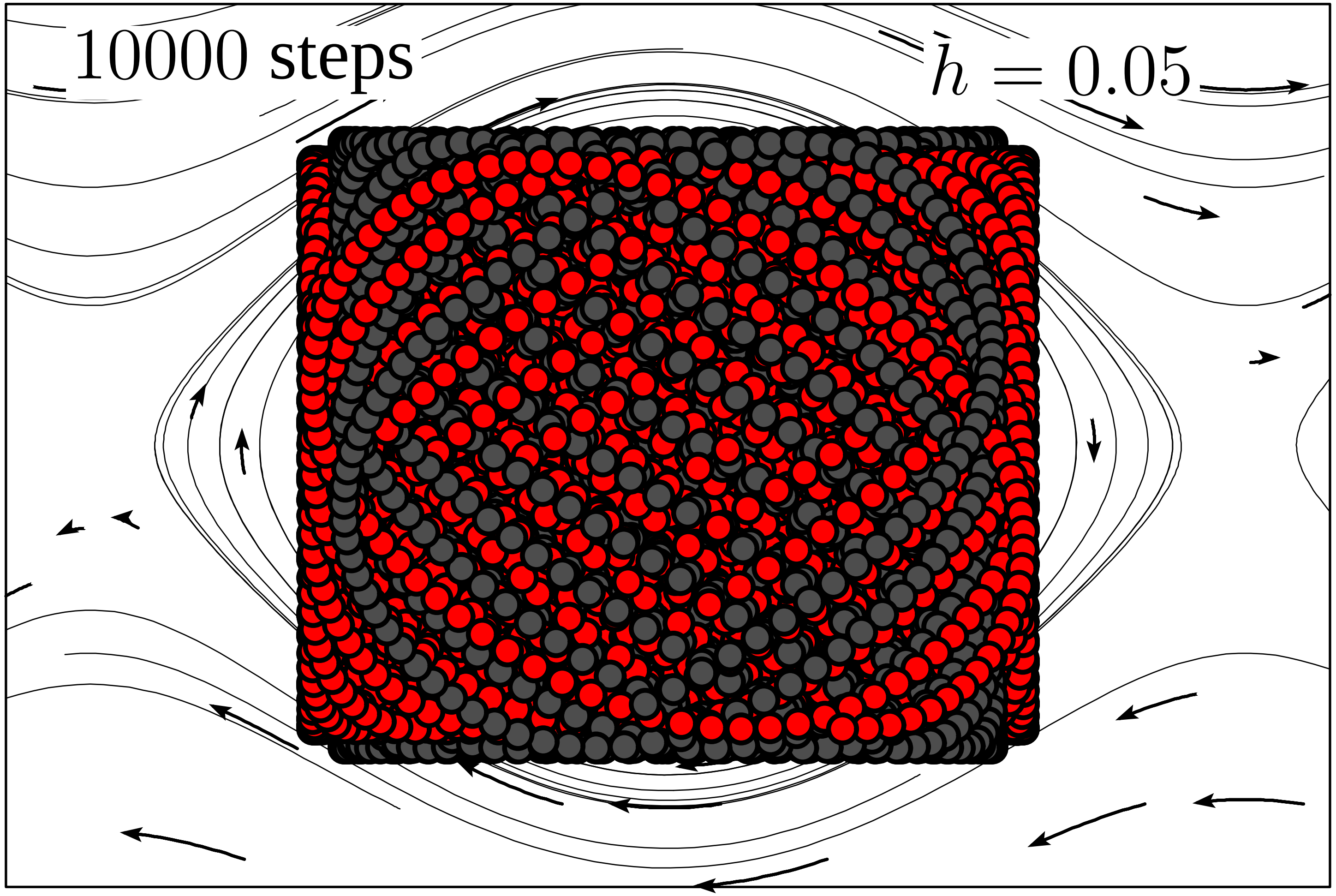


Behaves unstable.

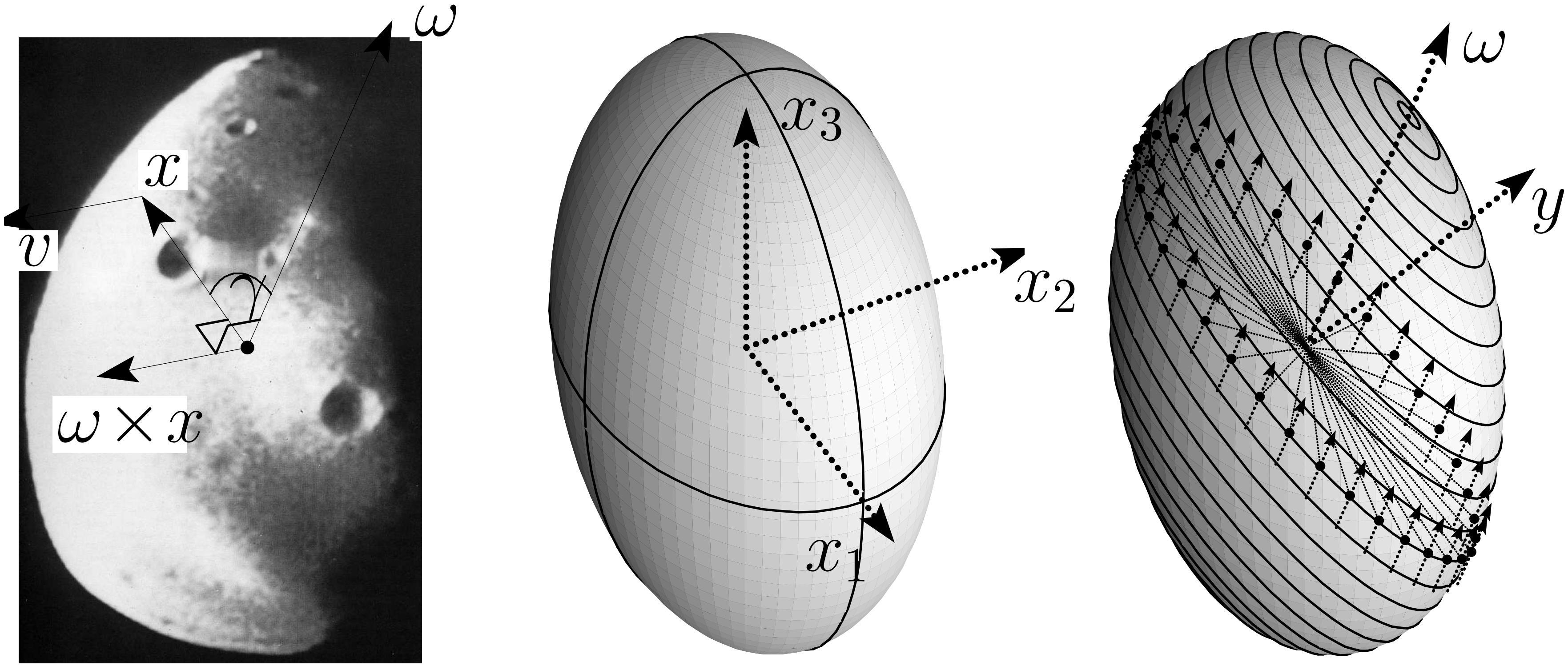
Some Images for the Rigid Body: Euler 1758:

$$dx + \frac{cc - bb}{aa} \cdot yz\,dt = \frac{2gP\,dt}{Maa}$$

$$dy + \frac{aa - cc}{bb} \cdot xz\,dt = \frac{2gQ\,dt}{Mbb}$$

$$dz + \frac{bb - aa}{cc} \cdot xy\,dt = \frac{2gR\,dt}{Mcc}$$

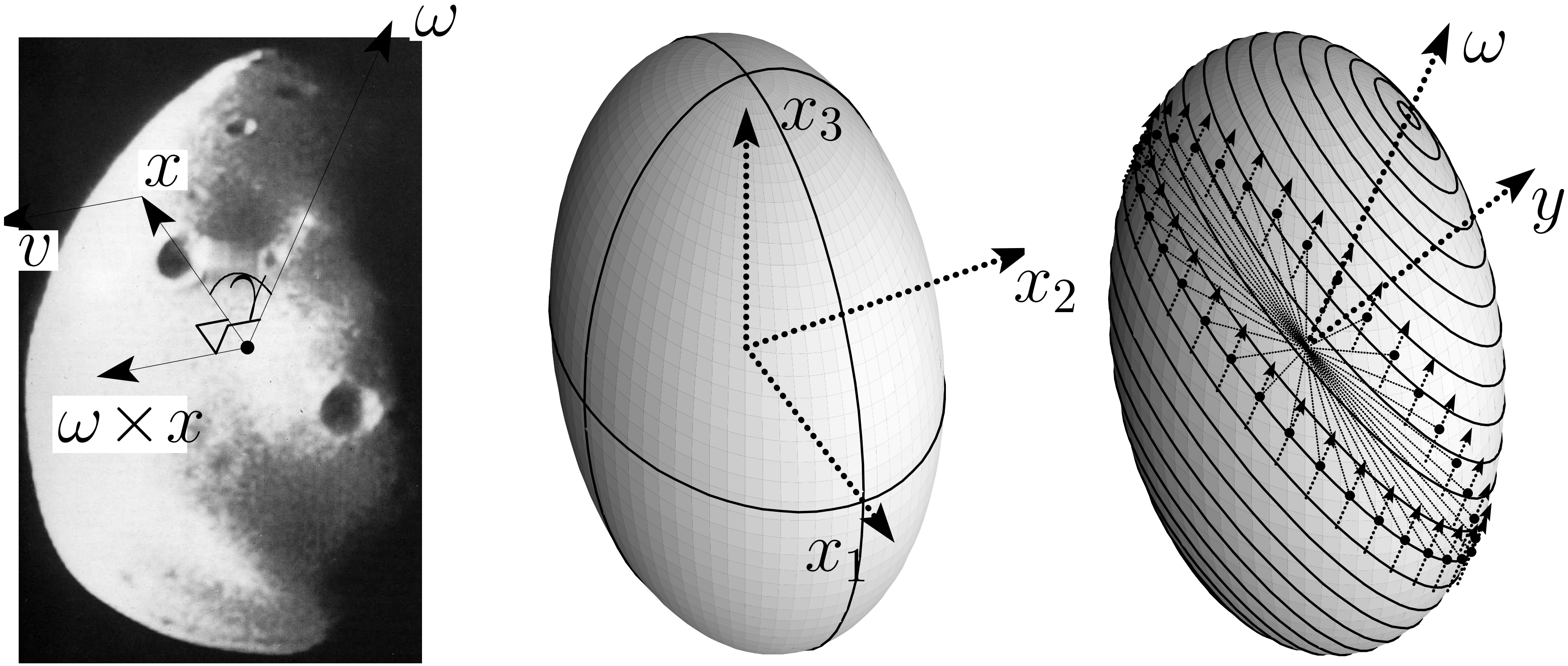
Kinetic Energy:



$$v = \omega \times x = \begin{pmatrix} \omega_2 x_3 - \omega_3 x_2 \\ \omega_3 x_1 - \omega_1 x_3 \\ \omega_1 x_2 - \omega_2 x_1 \end{pmatrix} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$T = \frac{1}{2} \int_{\mathcal{B}} \|\omega \times x\|^2 \, dm = \frac{1}{2} \omega^T \Theta \omega = \frac{1}{2} (I_1 \omega_1^2 + I_2 \omega_2^2 + I_3 \omega_3^2) \; .$$

Angular Momentum:

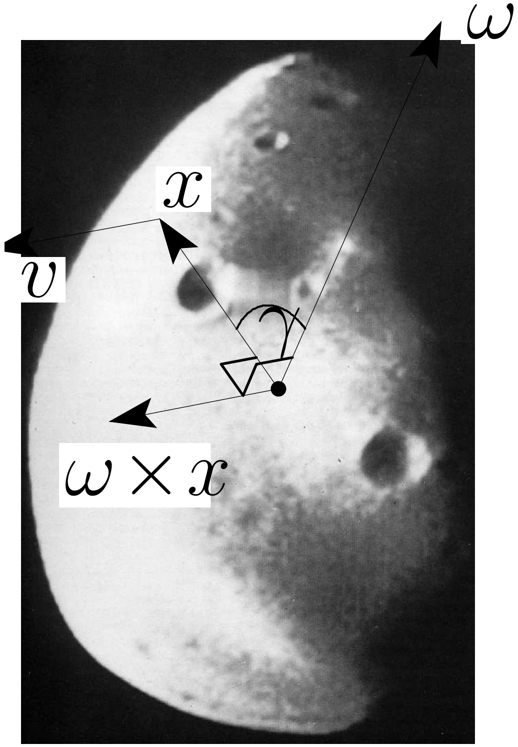


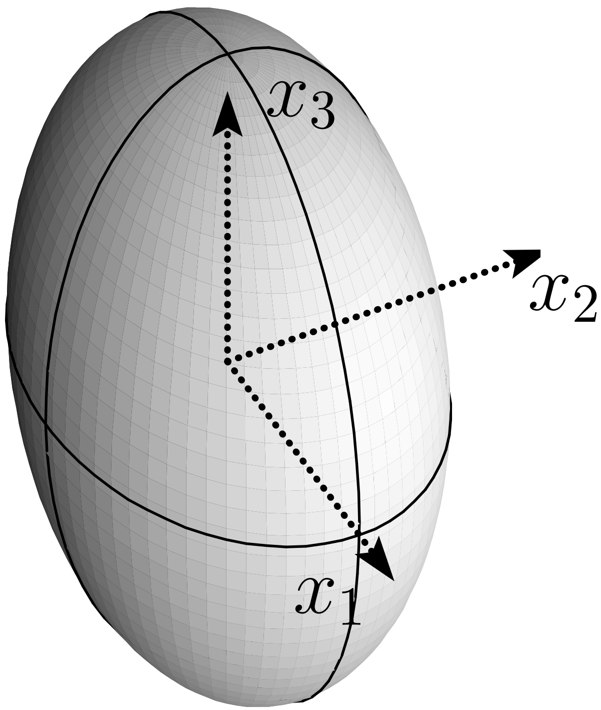
$$y = \int_{\mathcal{B}} (x \times v)\, dm = \int_{\mathcal{B}} (x \times (\omega \times x))\, dm \; = \Theta\, \omega,$$

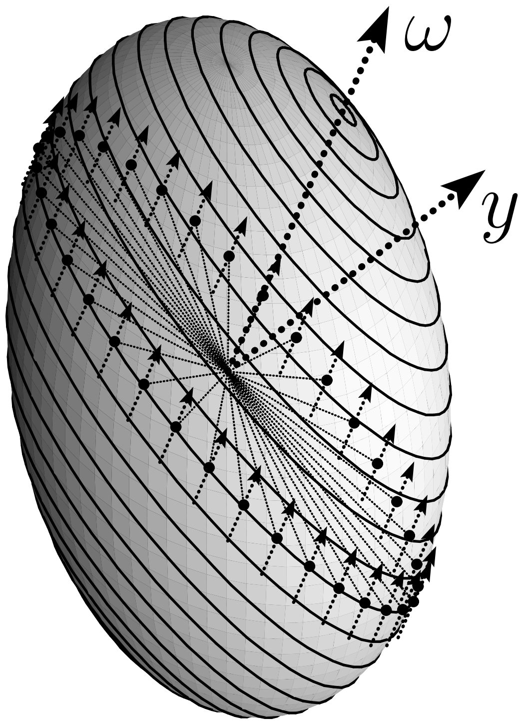
or, in the principal axes coordinates,

$$y_k = I_k\, \omega_k \, .$$

Elegant Idea: (Hayward 1856)







In absence of exterior forces, the angular momentum, seen from the fixed space, is a constant vector. Thus, seen from the body's coordinates, y rotates around ω in the other direction i.e.,

$$v = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad \to \quad \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

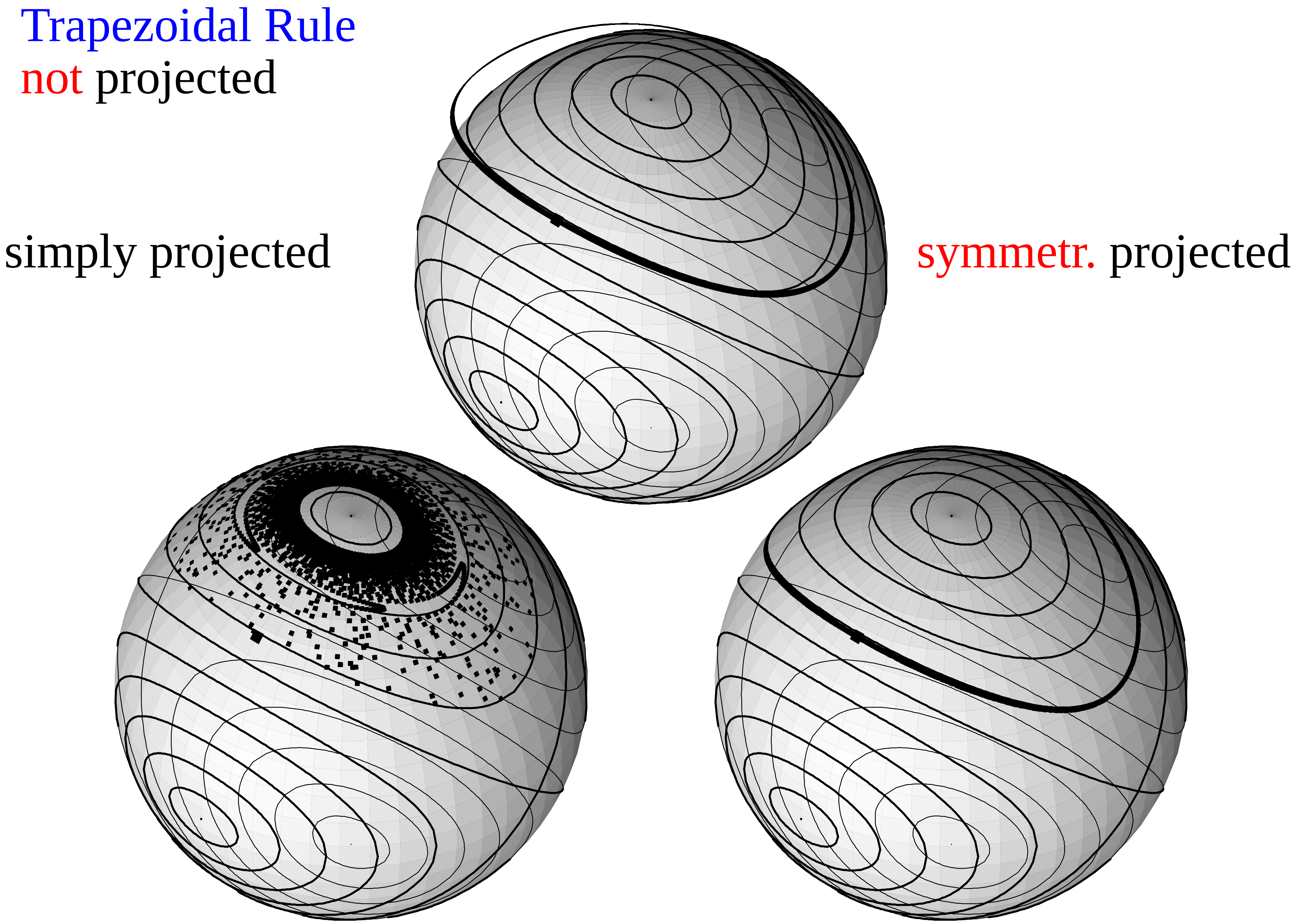
Inserting $y_k = I_k\omega_k$, i.e., $\omega_k = y_k/I_k$, this gives

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & y_3/I_3 & -y_2/I_2 \\ -y_3/I_3 & 0 & y_1/I_1 \\ y_2/I_2 & -y_1/I_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} (I_3^{-1} - I_2^{-1})\, y_3 y_2 \\ (I_1^{-1} - I_3^{-1})\, y_1 y_3 \\ (I_2^{-1} - I_1^{-1})\, y_2 y_1 \end{pmatrix}$$

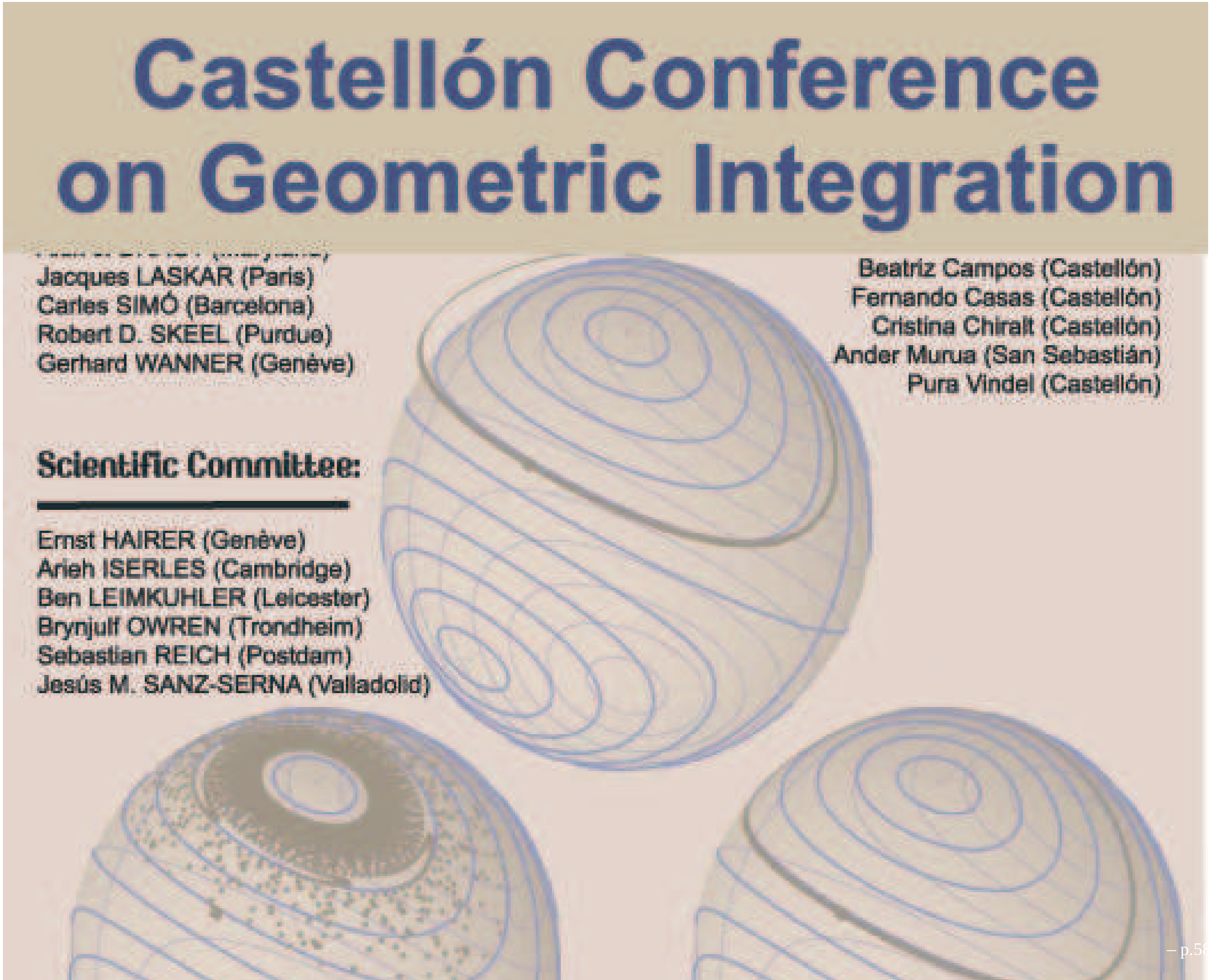
or

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix} \begin{pmatrix} y_1/I_1 \\ y_2/I_2 \\ y_3/I_3 \end{pmatrix},$$

two ways of writing the Euler equations as a Poisson system, once with the sphere, once with an ellipsoid, as first integral, whose intersections determine the solution curves.



Trapezoidal Rule
not projected
simply projected
symmetr. projected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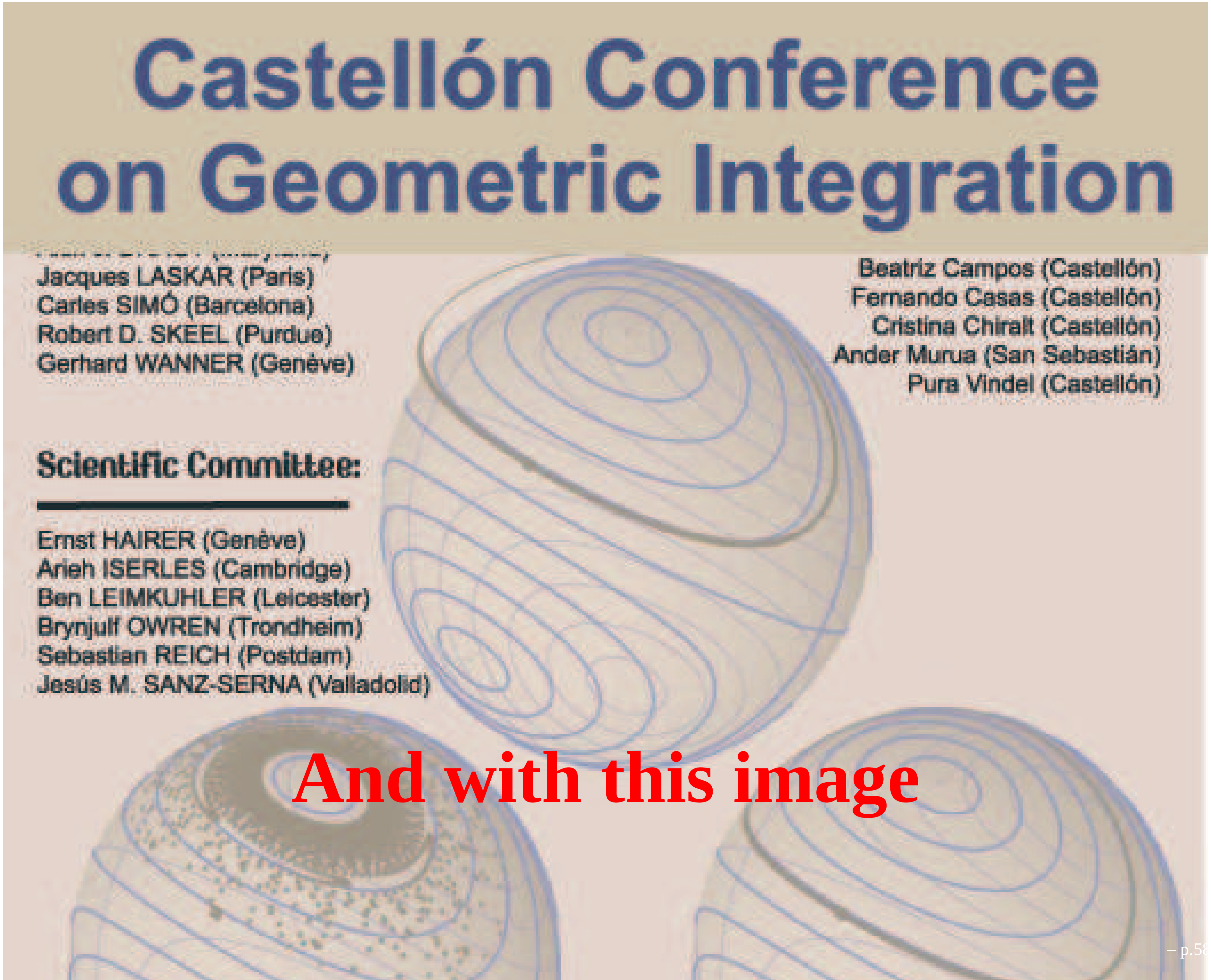

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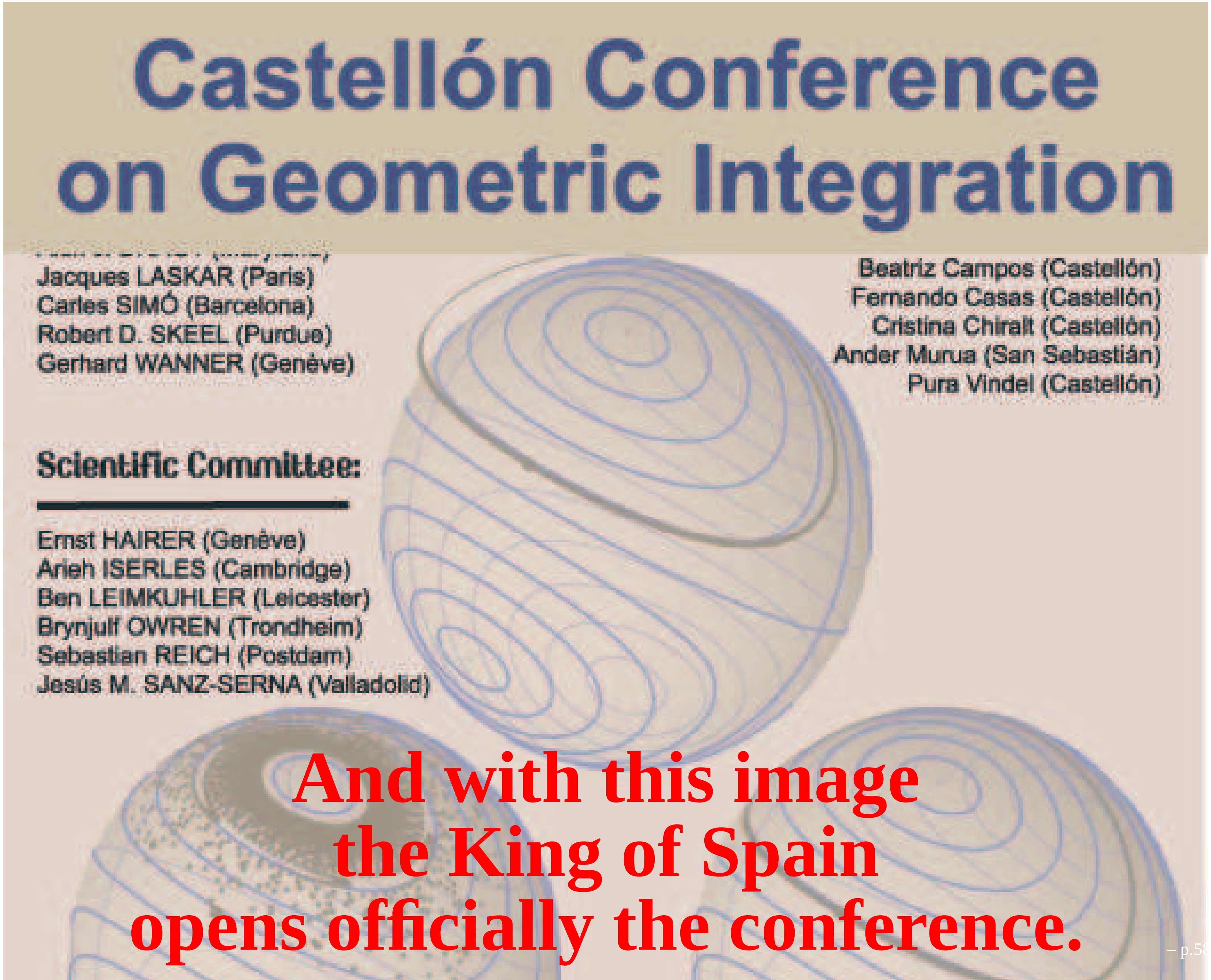

**And with this image
the King of Spain
opens officially the conference.**