Principles of stochastic geometric numerical integration

Part II: stochastic Hamiltonian problems

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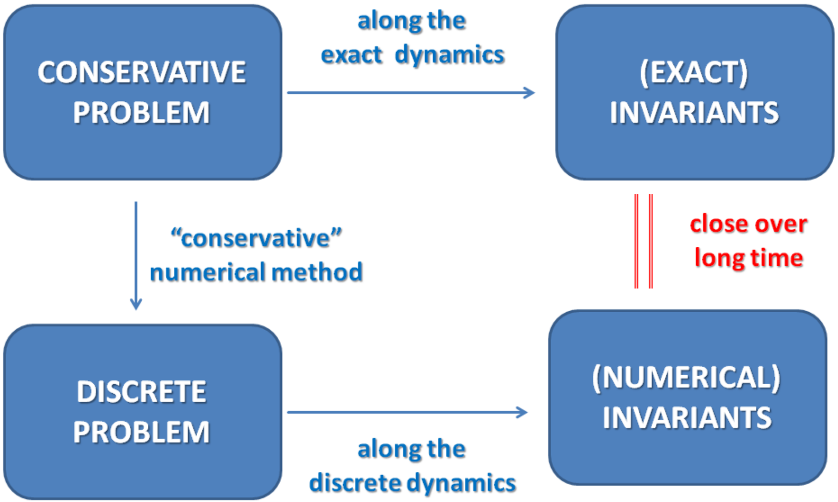
Zoom, May 6, 2021

The numerics of preserving structures



Deterministic Hamiltonians: *memorandum*

$$\dot{y}(t) = J\,\nabla\mathcal{H}(y(t)), \quad t \geq 0, \qquad J = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}.$$
$$y(0) = y_0,$$

- $y(t) = \begin{bmatrix} p(t) \\ q(t) \end{bmatrix} \in \mathbb{R}^{2d}$, generalized moments and coordinates;
- the Hamiltonian function

$$\mathcal{H} : \mathbb{R}^{2d} \to \mathbb{R}$$

  is a first integral of the problem:

$$\mathcal{H}(y(t)) = \mathcal{H}(y_0), \qquad t \geq 0.$$

  Indeed,

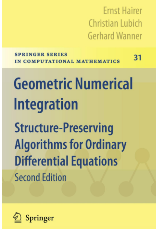
$$\frac{d}{dt}\mathcal{H}(y(t)) = \nabla\mathcal{H}(y(t))^{\intercal}\dot{y}(t) = \nabla\mathcal{H}(y(t))^{\intercal}J^{-1}\nabla\mathcal{H}(y(t)) = 0.$$

Conservative integrators

- **Symplectic Runge-Kutta** methods exactly preserve quadratic Hamiltonians;
- if the solution, computed by a Runge-Kutta method of order p, lays in a **compact set**, then

$$\mathcal{H}(y_n) = \mathcal{H}(y_0) + \mathcal{O}(h^p),$$

  over exponentially long times (Benettin-Giorgilli, 1994);



- nearly preserving **linear multistep methods** over long times (Hairer-Lubich, 2004);
- nearly preserving **multivalue methods** (Butcher, D'Ambrosio, 2017; D'Ambrosio, Hairer, 2013, 2014).

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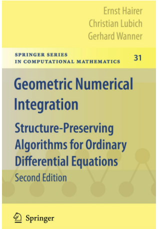
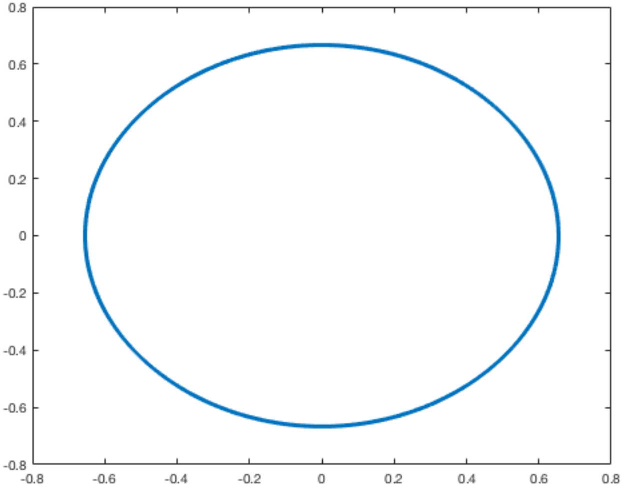


Example: pendulum

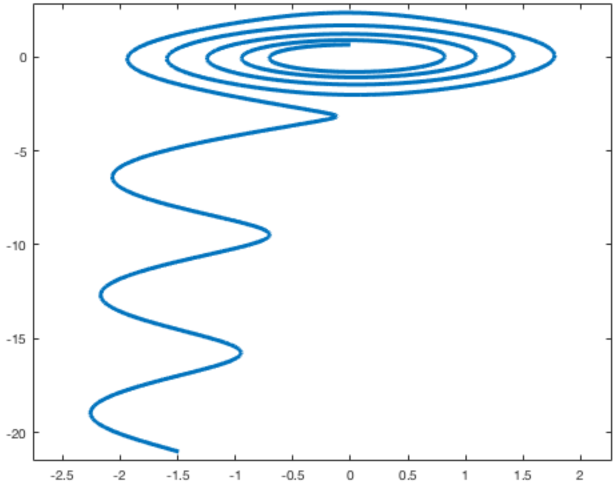
$$\mathcal{H}(y) = \frac{p^2}{2} - \cos q.$$

Simple pendulum



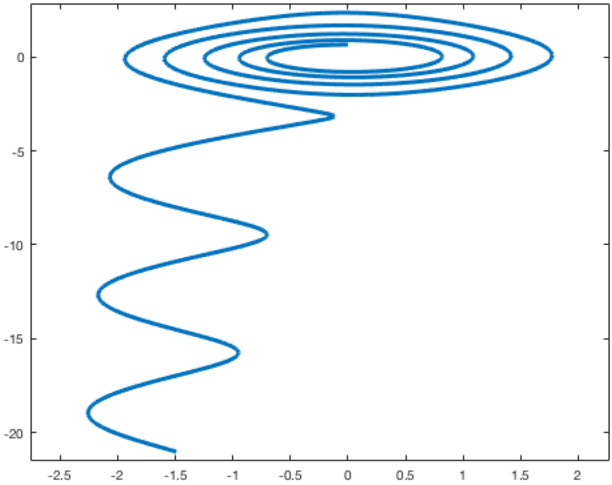
2-stage Gaussian Runge-Kutta method (symplectic)

Simple pendulum (ctd.)



Explicit Euler method (non-symplectic)

Simple pendulum (ctd.)



Explicit Euler method (non-symplectic)

Uri M. Ascher, Surprising computations, Appl. Numer. Math. (2012).

Stochastic differential equations

Itō problem:

$$\mathrm{d}X(t) = f(X(t))\mathrm{d}t + g(X(t))\,\mathrm{d}W(t), \quad t \geq 0,$$

$f : \mathbb{R}^d \to \mathbb{R}^d$ (drift), $g : \mathbb{R}^d \to \mathbb{R}^{d\times m}$ (diffusion),

$W(t)$ m-dimensional Wiener process.
Integral form:

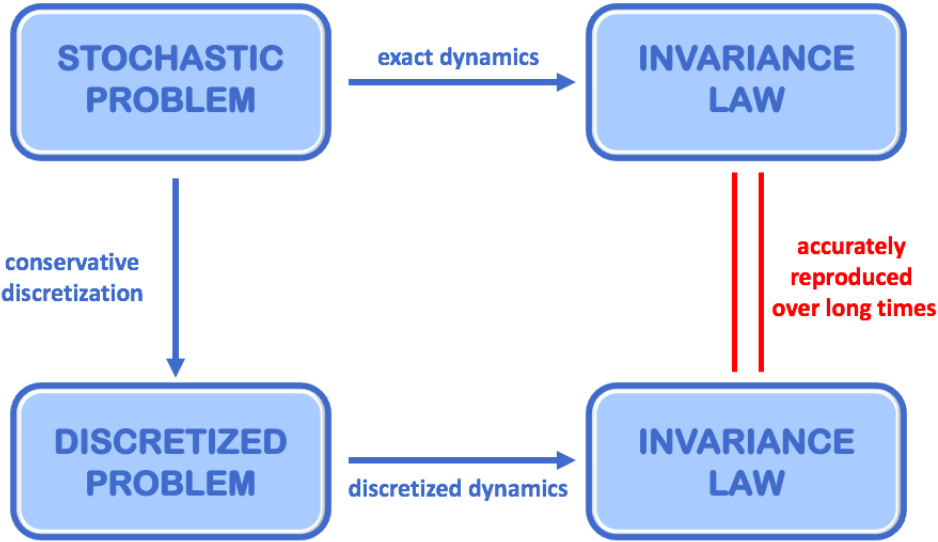
$$X(t) = X(0) + \int_0^t f(X(s))ds + \underbrace{\int_0^t g(X(s))dW(s)}_{\text{Itō integral*}}.$$

*On a uniform grid $\{0 < t_1 < t_2 < \cdots \leq t_n\}$, it is defined as

$$\lim_{n\to\infty} \sum_{j=1}^{n} g(X(t_j))(W(t_{j+1}) - W(t_j)).$$

Wiener increments are $\sqrt{h} \cdot \mathcal{N}(0,1) - \textit{distributed}$, where $h = t_{j+1} - t_j$.

Stochastic geometric numerical integration



Stochastic geometric numerical integration

- Invariance of asymptotic laws in the discretization of **linear systems** (Schurz, 1999);
- long-term conservation of stationary densities for **stochastic linear oscillators** (Melbo, Higham, 2004; Burrage, Lythe, 2007, 2009; Welfert, 2017; D'Ambrosio, Moccaldi, Paternoster, 2018) and **nonlinear oscillators** (D'Ambrosio, Scalone, 2020);
- stochastic **Runge-Kutta** per separable Hamiltonians (Burrage 2012, 2014).
- energy-preserving methods for **stochastic Hamiltonian problems**.

C. Chen, D. Cohen, R. D'Ambrosio, A. Lang, *Drift-preserving numerical integrators for stochastic Hamiltonian systems*, Adv. Comput. Math. 46, article number 27 (2020).

R. D'Ambrosio, G. Giordano, B. Paternoster, A. Ventola, *Perturbative analysis of stochastic Hamiltonian problems under time discretizations*, Appl. Math. Lett. 120, article number 107223 (2021).

Stochastic Hamiltonian problems

For Hamiltonians of the form

$$\mathcal{H}(p(t), q(t)) = \frac{1}{2} p^{\mathsf{T}} p + V(q), \quad t \geq 0,$$

with $V \colon \mathbb{R}^d \to \mathbb{R}$ sufficiently smooth potential, we consider

$$\begin{aligned} \mathrm{d}q(t) &= p(t)\,\mathrm{d}t \\ \mathrm{d}p(t) &= -V'(q(t))\,\mathrm{d}t + \Sigma\,\mathrm{d}W(t). \end{aligned}$$

with $\Sigma \in \mathbb{R}^{d \times m}$.

Stochastic Hamiltonian problems

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Invariance trace law (Burrage, 2014)

$$\mathbb{E}\left[\mathcal{H}(p(t), q(t))\right] = \mathbb{E}\left[\mathcal{H}(p(t_0), q(t_0))\right] + \frac{1}{2} \mathrm{Tr}\left(\Sigma^{\top} \Sigma\right) t$$

Linear drift in the expected Hamiltonian.

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Linear drift in the expected Hamiltonian.

Is this property naturally preserved along discretizations?

Augmented stochastic Runge-Kutta methods

Consider a general scalar ($d = 1$) additive noise problem

$$\mathrm{d}y = f(y)\,\mathrm{d}t + \varepsilon\, r\,\mathrm{d}W,$$

$y, r \in \mathbb{R}^2$, $\varepsilon \in \mathbb{R}$, $W(t)$ a scalar Wiener process.

- Burrage (2012): **a single Wiener increment** per step does not permit the preservation of the stochastic Hamiltonian structure;
- Burrage (2014): consider $s+1$ independent samples per step

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij}\, f(Y_j) + \varepsilon \sum_{j=1}^{i} z_j\, r,$$

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_j\, f(Y_j) + \varepsilon \sum_{j=1}^{s+1} z_j\, r,$$

$z_i = W(t_n + hc_i) - W(t_n + hc_{i-1}) = \sqrt{c_i - c_{i-1}}\,\Delta W_i$, $i = 1, \ldots, s+1$, $c_0 = 0, c_{s+1} = 1$.

Example: augmented midpoint rule

The augmented midpoint rule (Burrage, 2012)

$$Y = y_n + \frac{h}{2} f(Y) + \frac{\sqrt{2}}{2} \Delta W_1 \varepsilon r,$$

$$y_{n+1} = y_n + h f(Y) + \frac{\sqrt{2}}{2} \left(\Delta W_1 + \Delta W_2 \right) \varepsilon r.$$

applied to the linear problem

$$\mathrm{d}y = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y \, \mathrm{d}t + \varepsilon \, r \, \mathrm{d}W,$$

exactly preserves the expected value of the Hamiltonian $\mathcal{H}(p,q) = \frac{1}{2}(p^2 + q^2)$, given by

$$\mathbb{E}[\mathcal{H}(p(t), q(t))] = \mathbb{E}[\mathcal{H}(p(t_0), q(t_0))] + \frac{\varepsilon^2}{2}(t - t_0).$$

Hence, after one single step, denoting by $\mathcal{H}_n \approx \mathcal{H}(p(t_n), q(t_n))$,

$$\mathbb{E}[\mathcal{H}_n] = \mathbb{E}[\mathcal{H}_{n-1}] + \frac{\varepsilon^2}{2} h.$$

Nonlinear case

Double well potential with Hamiltonian

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{1}{2}q^2, \quad t \in [0, 40].$$

- MQ: $y_{n+1} = y_n + \frac{h}{6}\left(f(y_n) + 4f\left(\frac{y_n+y_{n+1}}{2}\right) + f(y_{n+1})\right)$. Preserves deterministic quartic Hamiltonians (Celledoni, 2013); energy-preserving B-series method (Chartier, 2006);
- L: Lobatto IIIA (symmetric, non-symplectic);
- IM: augmented implicit midpoint rule

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Table 1 Errors in $E(H(40))$ for the three methods

ϵ	h	MQ	L	IM
0	0.05	9.5(−15)	7.9(−7)	4.3(−4)
0	0.2	5.6(−14)	2.1(−4)	6.1(−3)
0.001	0.1	8.4(−6)	2.1(−5)	1.6(−3)
0.01	0.1	1.5(−5)	4.7(−6)	1.2(−4)
0.01	0.2	4.3(−5)	1.5(−4)	6.0(−3)
0.5	0.05	1.5(−2)	8.0(−3)	1.2(−2)
0.5	0.2	1.6(−2)	6.5(−3)	6.9(−2)

ε-expansions

- Classical idea in the deterministic setting (e.g. singularly perturbed problems; see Hairer, Wanner monographs).
- A toy example:

$$x^2 + 2\varepsilon x - 1 = 0, \quad \varepsilon \ll 1.$$

Ansatz: $x = \sum_{n=0}^{\infty} x_n \varepsilon^n$. Replacing the ansatz in the equation and collecting the powers of ε we get

$$\begin{aligned} \varepsilon^0 : &\quad x_0^2 - 1 = 0 \\ \varepsilon^1 : &\quad 2x_0(x_1 + 1) = 0 \\ \varepsilon^2 : &\quad x_1^2 + 2x_0 x_2 + 2x_1 = 0 \end{aligned}$$

$$\boxed{x \approx x_\varepsilon = \pm 1 - \varepsilon \pm \frac{\varepsilon^2}{2}}$$

	$\varepsilon = 10^{-1}$	$\varepsilon = 10^{-3}$
$\lvert x^+ - x_\varepsilon^+ \rvert$	1.24e-5	1.25e-13

ε-expansions

Consider the linear scalar test problem

$$\begin{bmatrix} \mathrm{d}q \\ \mathrm{d}p \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y \, \mathrm{d}t + \begin{bmatrix} \sigma \\ 0 \end{bmatrix} \mathrm{d}W,$$

corresponding to the second order problem

$$\ddot{q} = -q + \sigma\xi(t),$$

where $\xi(t)$ is a Gaussian white noise. Generally, the literature considers as test problem

$$\boxed{\ddot{q} = -q + \varepsilon\sqrt{t}}$$

with $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. Ansatz:

$$\boxed{q(t) = q_0(t) + \varepsilon q_1(t) + \varepsilon^2 q_2(t) + \dots}$$

ε-expansions (ctd.)

Replace the ansatz in the equation and collect in powers of ε, leads to

$$\begin{aligned} \varepsilon^0 : &\quad \ddot{q}_0 + q_0 = 0 \\ \varepsilon^1 : &\quad \ddot{q}_1 + q_1 = \sqrt{t} \\ &\quad \vdots \end{aligned}$$

We have

$$q(t) = \cos(t) + \sin(t) - \varepsilon \left(\sqrt{\frac{\pi}{2}}\, C\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\cos(t) + \sqrt{\frac{\pi}{2}}\, S\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\sin(t) + \sqrt{t} \right) + \dots$$

$$p(t) = \cos(t) - \sin(t) + \varepsilon \sqrt{\frac{\pi}{2}} \left(C\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\sin(t) - S\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\cos(t) \right) + \dots$$

where S e C are the Fresnel integrals

$$S(x) = \int_0^x \sin\left(\frac{\pi}{2}\, t^2\right) dt,$$

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}\, t^2\right) dt.$$

ε-expansions (ctd.)

$$q(t) = \cos(t) + \sin(t) - \varepsilon \left(\sqrt{\frac{\pi}{2}}\, C\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\cos(t) + \sqrt{\frac{\pi}{2}}\, S\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\sin(t) + \sqrt{t} \right) + \dots$$

$$p(t) = \cos(t) - \sin(t) + \varepsilon \sqrt{\frac{\pi}{2}} \left(C\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\sin(t) - S\left(\sqrt{\frac{2}{\pi}}\sqrt{t}\right)\cos(t) \right) + \dots$$

- $\sqrt{t}$: secular term;
- in the long-term integration, the secular term becomes dominant;
- in the long-term integration, the modified Hamiltonian (arising from the ε-solution) significantly differs from the original one;
- energy-drift preservation is not a characteristic property of stochastic methods.

R. D'Ambrosio, G. Giordano, B. Paternoster, A. Ventola, *Perturbative analysis of stochastic Hamiltonian problems under time discretizations*, Appl. Math. Lett. 120, article number 107223 (2021).

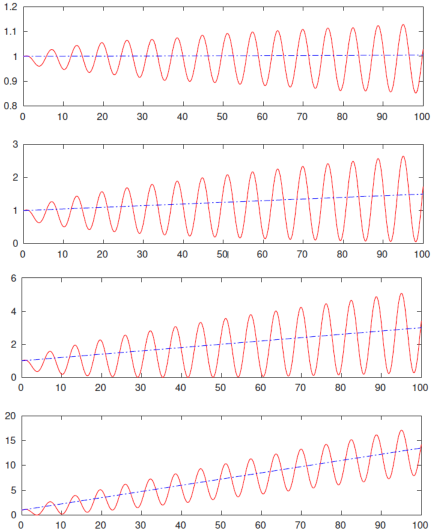


Figure: Comparison between the expectation of the modified Hamiltonian (red) and the original Hamiltonian (blue) for $\varepsilon = 0.01; 0.1; 0.2; 0.5$.

Numerical preservation of the trace law (ctd.)

C. Chen, D. Cohen, R. D'Ambrosio, A. Lang, Drift-preserving numerical integrators for stochastic Hamiltonian systems, Adv. Comp. Math. (2020).

$$\begin{aligned} \Psi_{n+1} &= p_n + \Sigma\Delta W_n - \frac{h}{2}\int_0^1 V'(q_n + sh\Psi_{n+1})\mathrm{d}s, \\ q_{n+1} &= q_n + h\Psi_{n+1}, \qquad\qquad (\star) \\ p_{n+1} &= p_n + \Sigma\Delta W_n - h\int_0^1 V'(q_n + sh\Psi_{n+1})\,\mathrm{d}s. \end{aligned}$$

Theorem

If $V \in \mathcal{C}^1(\mathbb{R}^d)$, the scheme $(\star)$ satisfies the trace law

$$\mathbb{E}\left[\mathcal{H}(p_n, q_n)\right] = \mathbb{E}\left[\mathcal{H}(p(t_0), q(t_0))\right] + \frac{1}{2}\mathrm{Tr}\left(\Sigma^\top\Sigma\right)t_n,$$

for any grid point $t_n = nh$.

Numerical preservation of the trace law (ctd.)

Theorem

If V' is Lipschitz continuous, then there exists $h^* > 0$ such that, for any $0 < h \leq h^*$, the scheme $(\star)$ converges with order 1 in the mean-square sense, i.e.,

$$\left(\mathbb{E}\left[|q(t_n) - q_n|^2\right]\right)^{1/2} + \left(\mathbb{E}\left[|p(t_n) - p_n|^2\right]\right)^{1/2} \leq Ch,$$

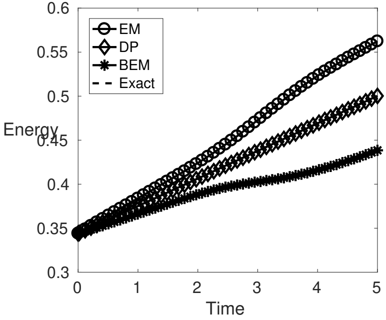
where the constant C is independent on h and n.

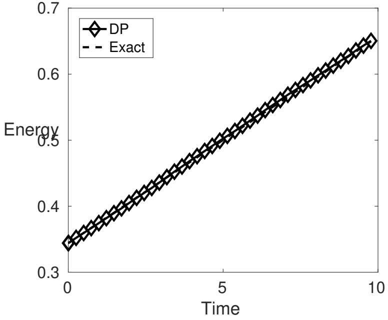
Other properties

- Error analysis in the strong and weak senses;
- error analysis in dependence on the estimation of the expected value (Monte Carlo, Monte Carlo multilevel, ...);
- long-term analysis of the Hamiltonian error.

Numerical test (stochastic pendulum)

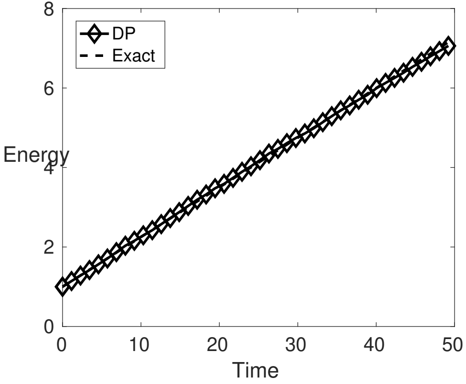
$$H(p,q) = \frac{1}{2}p^2 - \cos(q), \quad \sigma = 0.25, \quad (p_0, q_0) = (1, \sqrt{2}).$$





Numerical test (double-well potential)

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{1}{2}q^2, \quad \sigma = 0.5, \quad (p_0, q_0) = (\sqrt{2}, \sqrt{2}).$$



Numerical test (Hénon-Heiles with double noise)

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

$$\Sigma = \begin{pmatrix} 0.2 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad p_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad q_0 = \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}, \quad \alpha = 1/16.$$