

Stochastic Discrete Hamiltonian Variational Integrators

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Stochastic Hamiltonian systems

□ Mechanical systems:

- subject to random perturbations
- whose parameters are not precisely known
- stochastic landmarks, dissipation phenomena, particle storage rings

$$\begin{aligned}dq_a &= \frac{\partial H}{\partial p_a} dt + \sum_{i=1}^M \frac{\partial h_i}{\partial p_a} \circ dW_t^i \\ dp_a &= -\frac{\partial H}{\partial q_a} dt - \sum_{i=1}^M \frac{\partial h_i}{\partial q_a} \circ dW_t^i\end{aligned}$$



Plan

1. Geometric and variational integration
2. Stochastic variational principle in phase space
3. Stochastic Galerkin variational integrators
4. Examples and numerical tests

Why geometric integration?

- Preserving the geometric properties of the flow of a differential equation
- Symplectic and variational integrators
- Long-time integration – excellent behavior (provable by *backward error analysis*)
- Applications in astronomy, molecular dynamics, mechanics, theoretical physics, etc.

Hamiltonian systems

□ Phase space T^*Q with coordinates (q^μ, p_μ)

□ Hamiltonian

$$H : T^*Q \longrightarrow \mathbb{R}$$

□ Hamiltonian equations

$$\begin{aligned}\dot{q}^\mu &= \frac{\partial H}{\partial p_\mu}, \\ \dot{p}_\mu &= -\frac{\partial H}{\partial q^\mu}.\end{aligned}$$

Hamiltonian systems

- Symplectic form

$$\Omega = -d\Theta = dq^\mu \wedge dp_\mu$$

- Symplecticity of the flow

$$(F_t^H)^* \Omega = \Omega$$

- Conservation of energy

$$H \circ F_t^H = H$$

Symplectic integrators

- Numerical scheme

$$F_h : T^*Q \longrightarrow T^*Q$$

$$(q_{k+1}, p_{k+1}) = F_h(q_k, p_k)$$

- Symplectic integrator

$$(DF_h)^T \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} DF_h = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

Symplectic integrators

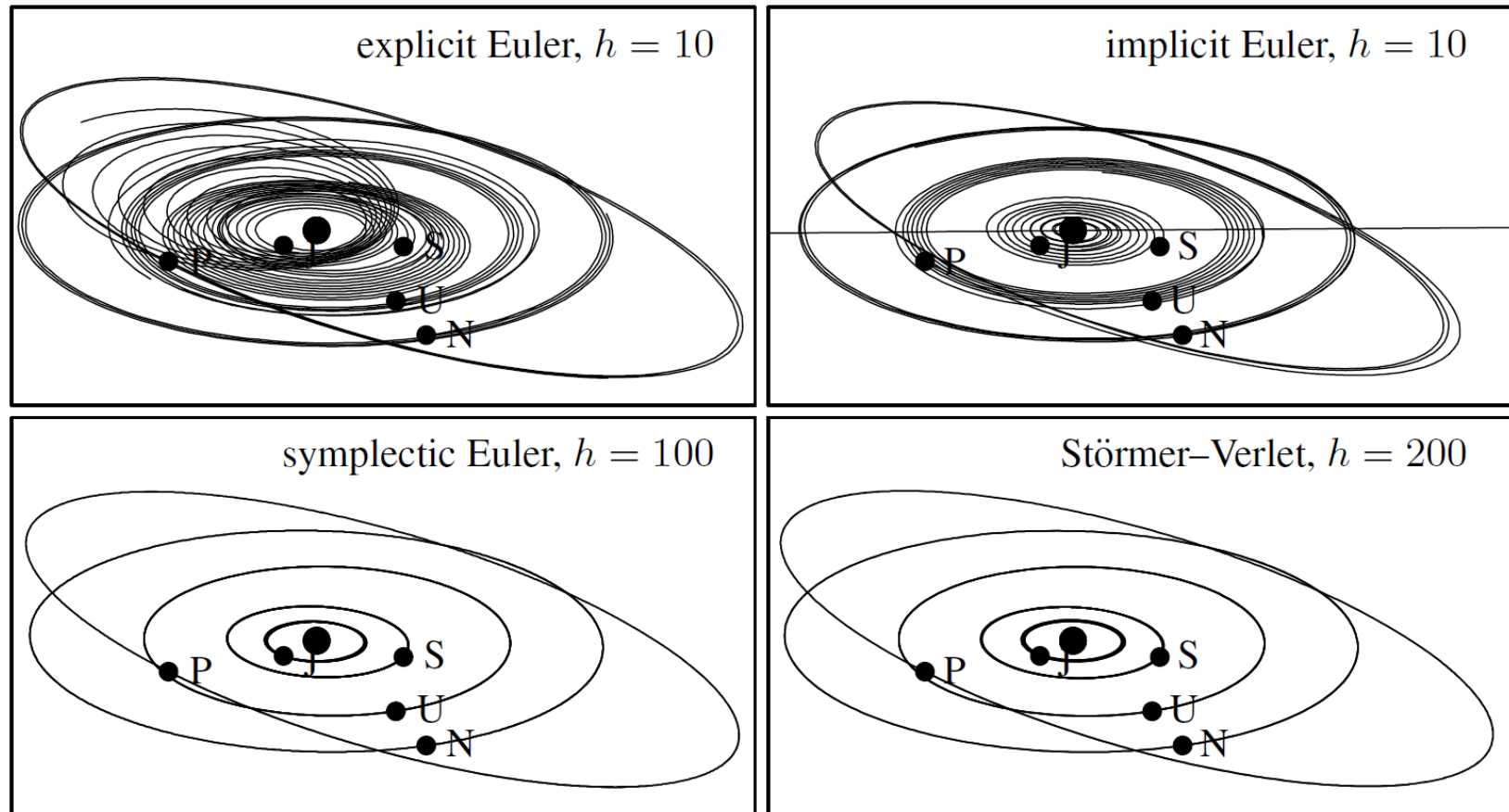
□ Symplectic Euler scheme

$$\begin{aligned}q_{k+1} &= q_k + h \frac{\partial H}{\partial p}(q_{k+1}, p_k), \\p_{k+1} &= p_k - h \frac{\partial H}{\partial q}(q_{k+1}, p_k).\end{aligned}$$

□ Backward error analysis

$$\tilde{H}(q, p) = H(q, p) + hH_2(q, p) + h^2H_3(q, p) + \dots$$

Example: Outer Solar System



(Hairer, Lubich, Wanner, 2002)

Lagrangian systems

□ Configuration space TQ with coord. (q^μ, \dot{q}^μ)

□ Lagrangian

$$L : TQ \longrightarrow \mathbb{R}$$

□ Action functional

$$S[q(t)] = \int_a^b L(q^\mu(t), \dot{q}^\mu(t)) dt$$

Lagrangian systems

- Hamilton's principle

$$dS[q(t)] \cdot \delta q(t) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} S[q_\epsilon(t)] = 0$$

- Euler-Lagrange equations

$$\frac{\partial L}{\partial q^\mu} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^\mu} = 0$$

- Symplectic structure on TQ

Variational integrators

□ Discrete state space $Q \times Q$ with coord. (q^μ, \bar{q}^μ)

□ Discrete Lagrangian

$$L_d : Q \times Q \longrightarrow \mathbb{R}$$

□ Discrete action for a discrete path (q_0, q_1, \dots, q_N)

$$S = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}).$$

Variational integrators

□ Discrete Euler-Lagrange equations

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0$$

$$F_{L_d} : Q \times Q \longrightarrow Q \times Q \quad F_{L_d}(q_{k-1}, q_k) = (q_k, q_{k+1})$$

□ Position-momentum formulation

$$\begin{aligned} p_k &= -D_1 L_d(q_k, q_{k+1}), \\ p_{k+1} &= D_2 L_d(q_k, q_{k+1}). \end{aligned}$$

$$\tilde{F}_{L_d} : T^*Q \longrightarrow T^*Q$$

Variational integrators

- Variational integrators are symplectic
- Discrete Noether's theorem
- Example: symplectic Euler scheme

$$L_d(q, \bar{q}) = hL\left(\bar{q}, \frac{\bar{q} - q}{h}\right)$$

- (*Marsden & West, 2001*)

Stochastic Hamiltonian systems

$$\begin{aligned} dq &= \frac{\partial H}{\partial p} dt + \frac{\partial h}{\partial p} \circ dW(t) \\ dp &= -\frac{\partial H}{\partial q} dt - \frac{\partial h}{\partial q} \circ dW(t) \end{aligned}$$

□ Assumptions:

- $Q \cong \mathbb{R}^N$, $T^*Q = Q \times Q^* \cong \mathbb{R}^N \times \mathbb{R}^N$, $TQ = Q \times Q \cong \mathbb{R}^N \times \mathbb{R}^N$
- $H : T^*Q \longrightarrow \mathbb{R}$, $h : T^*Q \longrightarrow \mathbb{R}$
- $(\Omega, \mathcal{F}, \mathbb{P})$, $\{\mathcal{F}_t\}_{t \geq 0}$

Stochastic symplectic flow

- Pathwise unique stochastic flow

$$F_{t,t_0} : \Omega \times T^*Q \longrightarrow T^*Q$$

- Mean-square differentiable and almost surely a diffeomorphism
- Symplectic

$$F_{t,t_0}^* \Omega_{T^*Q} = \Omega_{T^*Q}$$

where $\Omega_{T^*Q} = \sum_{i=1}^N dq^i \wedge dp^i$

Stochastic variational principle

□ Function vector space

$$C([t_a, t_b]) = \{(q, p) : \Omega \times [t_a, t_b] \longrightarrow T^*Q \mid q, p \text{ a.s. cont. } \mathcal{F}_t\text{-adapted semimartingales}\}$$

□ Action functional $\mathcal{B} : \Omega \times C([t_a, t_b]) \longrightarrow \mathbb{R}$

$$\mathcal{B}[q(\cdot), p(\cdot)] = p(t_b)q(t_b) - \int_{t_a}^{t_b} \left[p \circ dq - H(q(t), p(t)) dt - h(q(t), p(t)) \circ dW(t) \right]$$

Stochastic variational principle

- Noise in the action functional (for Lagrangian systems)
 - *Bismut 1982*
 - *Bou-Rabee & Owhadi 2009*

- Zero noise limit
 - *Leok & Zhang 2011*

Stochastic variational principle

Theorem 1 (Stochastic Variational Principle in Phase Space). *Suppose that $H(q, p)$ and $h(q, p)$ are C^2 functions of their arguments with globally Lipschitz derivatives. If the curve $(q(t), p(t))$ in T^*Q satisfies the stochastic Hamiltonian system for $t \in [t_a, t_b]$, where $t_b \geq t_a > 0$, then the pair $(q(\cdot), p(\cdot))$ is a critical point of the stochastic action functional, that is,*

$$\delta \mathcal{B}[q(\cdot), p(\cdot)] \equiv \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{B}[q(\cdot) + \epsilon \delta q(\cdot), p(\cdot) + \epsilon \delta p(\cdot)] = 0$$

almost surely for all variations $(\delta q(\cdot), \delta p(\cdot)) \in C([t_a, t_b])$ such that almost surely $\delta q(t_a) = 0$ and $\delta p(t_b) = 0$.

Stochastic variational principle

□ Sketch of proof

- $\int_{t_a}^{t_b} p(t) \circ d\delta q(t) = p(t_b)\delta q(t_b) - p(t_a)\delta q(t_a) - \int_{t_a}^{t_b} \delta q(t) \circ dp(t)$
- $$\begin{aligned} \delta \mathcal{B}[q(\cdot), p(\cdot)] = & \int_{t_a}^{t_b} \delta q(t) \left[\circ dp(t) + \frac{\partial H}{\partial q}(q(t), p(t)) dt + \frac{\partial h}{\partial q}(q(t), p(t)) \circ dW(t) \right] \\ & - \int_{t_a}^{t_b} \delta p(t) \left[\circ dq(t) - \frac{\partial H}{\partial p}(q(t), p(t)) dt - \frac{\partial h}{\partial p}(q(t), p(t)) \circ dW(t) \right] \end{aligned}$$

Stochastic variational principle

□ Converse theorem

- proved in case $h = h(q)$ for Lagrangian systems
(*Bou-Rabee & Owhadi, 2009*)
- may not be true in general
(*Lazaro-Cami & Ortega, 2008*)

Stochastic type-II generating function

- Generating function

$$S(q_a, p_b) = \mathcal{B}[\bar{q}(\cdot; q_a, p_b), \bar{p}(\cdot; q_a, p_b)]$$

where (\bar{q}, \bar{p}) is the exact solution such that

$$\bar{q}(t_a; q_a, p_b) = q_a, \bar{p}(t_b; q_a, p_b) = p_b$$

Stochastic type-II generating function

Theorem 2. *The function $S(q_a, p_b)$ is a type-II stochastic generating function for the stochastic mapping F_{t_b, t_a} , that is, $F_{t_b, t_a} : (q_a, p_a) \longrightarrow (q_b, p_b)$ is implicitly given by the equations*

$$q_b = D_2 S(q_a, p_b), \quad p_a = D_1 S(q_a, p_b),$$

where the derivatives are understood in the mean-square sense.

Stochastic type-II generating function

□ Sketch of proof

$$\begin{aligned} \frac{\partial S}{\partial q_a}(q_a, p_b) = \bar{p}(t_a) &+ \int_{t_a}^{t_b} \frac{\partial \bar{q}(t)}{\partial q_a} \left[\circ d\bar{p} + \frac{\partial H}{\partial q}(\bar{q}(t), \bar{p}(t)) dt + \frac{\partial h}{\partial q}(\bar{q}(t), \bar{p}(t)) \circ dW(t) \right] \\ &+ \int_{t_a}^{t_b} \frac{\partial \bar{p}(t)}{\partial q_a} \left[\circ d\bar{q} - \frac{\partial H}{\partial p}(\bar{q}(t), \bar{p}(t)) dt - \frac{\partial h}{\partial p}(\bar{q}(t), \bar{p}(t)) \circ dW(t) \right] = \bar{p}(t_a) \end{aligned}$$

Stochastic Noether's theorem

Theorem 3 (Stochastic Noether's theorem). *Suppose that the Hamiltonians $H : T^*Q \longrightarrow \mathbb{R}$ and $h : T^*Q \longrightarrow \mathbb{R}$ are invariant with respect to the cotangent lift action $\Phi^{T^*Q} : G \times T^*Q \longrightarrow T^*Q$ of the Lie group G , that is,*

$$H \circ \Phi_g^{T^*Q} = H, \quad h \circ \Phi_g^{T^*Q} = h,$$

*for all $g \in G$. Then the cotangent lift momentum map $J : T^*Q \longrightarrow \mathfrak{g}^*$ associated with Φ^{T^*Q} , in coordinates given by*

$$J_\xi(q, p) = p \cdot \xi_Q(q),$$

is almost surely preserved along the solutions of the stochastic Hamiltonian system.

Stochastic Galerkin Variational Integrator

- Generating function

$$S(q_a, p_b) = \underset{\substack{(q,p) \in C([t_a, t_b]) \\ q(t_a) = q_a, p(t_b) = p_b}}{\text{ext}} \mathcal{B}[q(\cdot), p(\cdot)]$$

- Step 1 – extremize over a subspace
- Step 2 – approximate integrals with quadrature rules

Stochastic Galerkin Variational Integrator

- Discrete set of times

$$t_k = k \cdot \Delta t, \quad k = 0, 1, \dots, K, \quad \Delta t = T/K$$

- Discrete curve $\{(q_k, p_k)\}_{k=0, \dots, K}$

$$(q_{k+1}, p_{k+1}) \approx F_{t_{k+1}, t_k}(q_k, p_k)$$

Stochastic Galerkin Variational Integrator

□ Approximation space

$$C^s([t_k, t_{k+1}]) = \{(q, p) \in C([t_k, t_{k+1}]) \mid q \text{ is a polynomial of degree } s\}$$

□ Lagrange polynomials for $0 = d_0 < d_1 < \dots < d_s = 1$

$$q_d(t_k + \tau \Delta t; q^\mu) = \sum_{\mu=0}^s q^\mu l_{\mu,s}(\tau), \quad \dot{q}_d(t_k + \tau \Delta t; q^\mu) = \frac{1}{\Delta t} \sum_{\mu=0}^s q^\mu \dot{l}_{\mu,s}(\tau)$$

□ Quadrature rules

$$(\alpha_i, c_i)_{i=1}^r, \quad (\beta_i, c_i)_{i=1}^r, \quad 0 \leq c_1 < \dots < c_r \leq 1$$

Stochastic Galerkin Variational Integrator

□ Discrete stochastic Hamiltonian

$$H_d^+(q_k, p_{k+1}) = \underset{\substack{q^1, \dots, q^s \in Q \\ P_1, \dots, P_r \in Q^* \\ q^0 = q_k}}{\text{ext}} \left\{ p_{k+1} q^s - \Delta t \sum_{i=1}^r \alpha_i \left[P_i \dot{q}_d(t_k + c_i \Delta t) - H(q_d(t_k + c_i \Delta t), P_i) \right] \right. \\ \left. + \Delta W \sum_{i=1}^r \beta_i h(q_d(t_k + c_i \Delta t), P_i) \right\}$$

where $P_i \equiv p(t_k + c_i \Delta t)$

□ Discrete flow

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \quad p_k = D_1 H_d^+(q_k, p_{k+1})$$

Stochastic Galerkin Variational Integrator

□ System defining the integrator

$$\begin{aligned} -p_k &= \sum_{i=1}^r \alpha_i \left[P_i \dot{l}_{0,s}(c_i) - \Delta t \frac{\partial H}{\partial q}(t_k + c_i \Delta t) l_{0,s}(c_i) \right] - \Delta W \sum_{i=1}^r \beta_i \frac{\partial h}{\partial q}(t_k + c_i \Delta t) l_{0,s}(c_i) \\ 0 &= \sum_{i=1}^r \alpha_i \left[P_i \dot{l}_{\mu,s}(c_i) - \Delta t \frac{\partial H}{\partial q}(t_k + c_i \Delta t) l_{\mu,s}(c_i) \right] - \Delta W \sum_{i=1}^r \beta_i \frac{\partial h}{\partial q}(t_k + c_i \Delta t) l_{\mu,s}(c_i) \\ p_{k+1} &= \sum_{i=1}^r \alpha_i \left[P_i \dot{l}_{s,s}(c_i) - \Delta t \frac{\partial H}{\partial q}(t_k + c_i \Delta t) l_{s,s}(c_i) \right] - \Delta W \sum_{i=1}^r \beta_i \frac{\partial h}{\partial q}(t_k + c_i \Delta t) l_{s,s}(c_i) \\ \alpha_i \dot{q}_d(t_k + c_i \Delta t) &= \alpha_i \frac{\partial H}{\partial p}(t_k + c_i \Delta t) + \beta_i \frac{\Delta W}{\Delta t} \frac{\partial h}{\partial p}(t_k + c_i \Delta t) \\ q_{k+1} &= q^s \end{aligned}$$

where $H(t_k + c_i \Delta t) \equiv H(q_d(t_k + c_i \Delta t), p(t_k + c_i \Delta t))$

Discrete flow

□ Symplecticity

$$(F_{t_{k+1}, t_k}^+)^* \Omega_{T^*Q} = \Omega_{T^*Q}$$

□ Proof:

$$0 = ddH^+(q_k, p_{k+1}) = \sum_{i=1}^N dq_{k+1}^i \wedge dp_{k+1}^i - \sum_{i=1}^N dq_k^i \wedge dp_k^i = (F_{t_{k+1}, t_k}^+)^* \Omega_{T^*Q} - \Omega_{T^*Q}$$

Discrete stochastic Noether's theorem

- Action of a Lie group

$$\Phi : G \times Q \longrightarrow Q$$

- Equivariance of the interpolating polynomial

$$\Phi_g^{TQ} \left(q_d(t; q^\mu), \dot{q}_d(t; q^\mu) \right) = \left(q_d(t; \Phi_g(q^\mu)), \dot{q}_d(t; \Phi_g(q^\mu)) \right)$$

Discrete stochastic Noether's theorem

Theorem 4 (Discrete stochastic Noether's theorem). *Suppose that the Hamiltonians $H : T^*Q \rightarrow \mathbb{R}$ and $h : T^*Q \rightarrow \mathbb{R}$ are **invariant with respect to the cotangent lift action** $\Phi^{T^*Q} : G \times T^*Q \rightarrow T^*Q$ of the Lie group G , that is,*

$$H \circ \Phi_g^{T^*Q} = H, \quad h \circ \Phi_g^{T^*Q} = h,$$

*for all $g \in G$, and suppose the interpolating polynomial $q_d(t; q^\mu)$ is **equivariant with respect to G** . Then the cotangent lift momentum map J associated with Φ^{T^*Q} is almost surely preserved, i.e., a.s.*

$$J(q_{k+1}, p_{k+1}) = J(q_k, p_k).$$

Example: Stochastic midpoint method

- Polynomials of degree $s = 1$
- Midpoint rule $r = 1, c_1 = 1/2, \alpha_1 = \beta_1 = 1$

$$\begin{aligned} q_{k+1} &= q_k + \frac{\partial H}{\partial p} \left(\frac{q_k + q_{k+1}}{2}, \frac{p_k + p_{k+1}}{2} \right) \Delta t + \frac{\partial h}{\partial p} \left(\frac{q_k + q_{k+1}}{2}, \frac{p_k + p_{k+1}}{2} \right) \Delta W \\ p_{k+1} &= p_k - \frac{\partial H}{\partial q} \left(\frac{q_k + q_{k+1}}{2}, \frac{p_k + p_{k+1}}{2} \right) \Delta t - \frac{\partial h}{\partial q} \left(\frac{q_k + q_{k+1}}{2}, \frac{p_k + p_{k+1}}{2} \right) \Delta W \end{aligned}$$

- (*Milstein, Repin & Tretyakov, 2002*)

Example: Stochastic Störmer-Verlet method

□ Polynomials of degree $s = 2$

□ Trapezoidal rule

$$r = 2, \quad c_1 = 0, \quad c_2 = 1, \quad \alpha_1 = \beta_1 = 1/2, \quad \alpha_2 = \beta_2 = 1/2$$

$$\begin{aligned} P_1 &= p_k - \frac{1}{2} \frac{\partial H}{\partial q}(q_k, P_1) \Delta t - \frac{1}{2} \frac{\partial h}{\partial q}(q_k, P_1) \Delta W \\ q_{k+1} &= q_k + \frac{1}{2} \frac{\partial H}{\partial p}(q_k, P_1) \Delta t + \frac{1}{2} \frac{\partial H}{\partial p}(q_{k+1}, P_1) \Delta t + \frac{1}{2} \frac{\partial h}{\partial p}(q_k, P_1) \Delta W + \frac{1}{2} \frac{\partial h}{\partial p}(q_{k+1}, P_1) \Delta W \\ p_{k+1} &= P_1 - \frac{1}{2} \frac{\partial H}{\partial q}(q_{k+1}, P_1) \Delta t - \frac{1}{2} \frac{\partial h}{\partial q}(q_{k+1}, P_1) \Delta W \end{aligned}$$

□ (*Ma & Ding, 2015*)

Example: Stochastic trapezoidal method

□ Polynomials of degree $s = 1$

□ Trapezoidal rule

$$r = 2, \quad c_1 = 0, \quad c_2 = 1, \quad \alpha_1 = \beta_1 = 1/2, \quad \alpha_2 = \beta_2 = 1/2$$

$$p_k = \frac{1}{2}(P_1 + P_2) + \frac{1}{2} \frac{\partial H}{\partial q}(q_k, P_1) \Delta t + \frac{1}{2} \frac{\partial h}{\partial q}(q_k, P_1) \Delta W$$

$$p_{k+1} = \frac{1}{2}(P_1 + P_2) - \frac{1}{2} \frac{\partial H}{\partial q}(q_{k+1}, P_2) \Delta t - \frac{1}{2} \frac{\partial h}{\partial q}(q_{k+1}, P_2) \Delta W$$

$$q_{k+1} = q_k + \frac{\partial H}{\partial p}(q_k, P_1) \Delta t + \frac{\partial h}{\partial p}(q_k, P_1) \Delta W$$

$$q_{k+1} = q_k + \frac{\partial H}{\partial p}(q_{k+1}, P_2) \Delta t + \frac{\partial h}{\partial p}(q_{k+1}, P_2) \Delta W$$

Numerical tests: convergence

- Kubo oscillator

$$H(q, p) = p^2/2 + q^2/2 \qquad h(q, p) = \beta(p^2/2 + q^2/2)$$

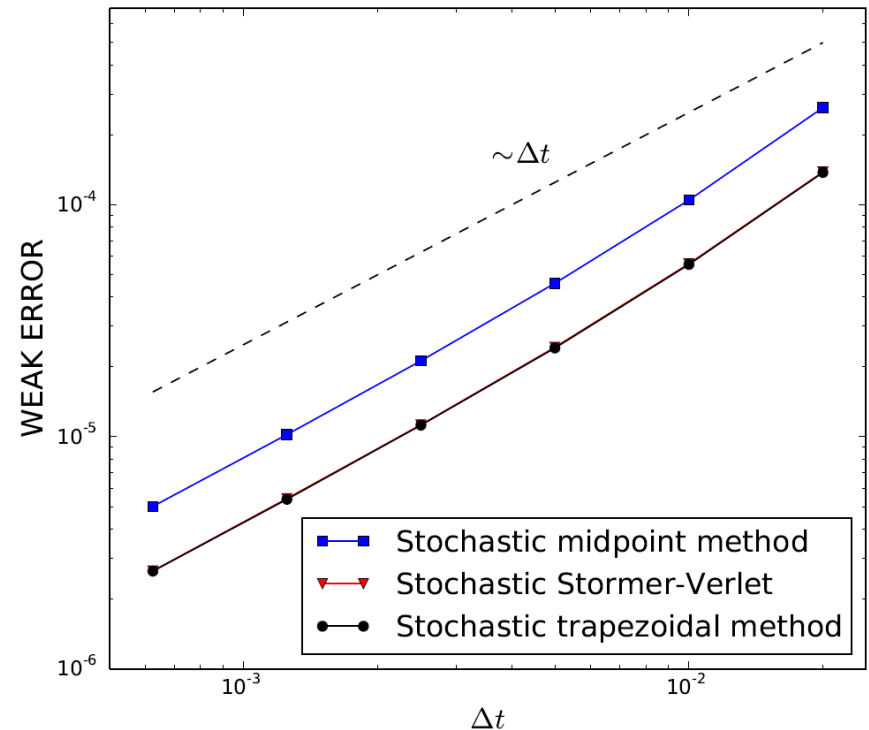
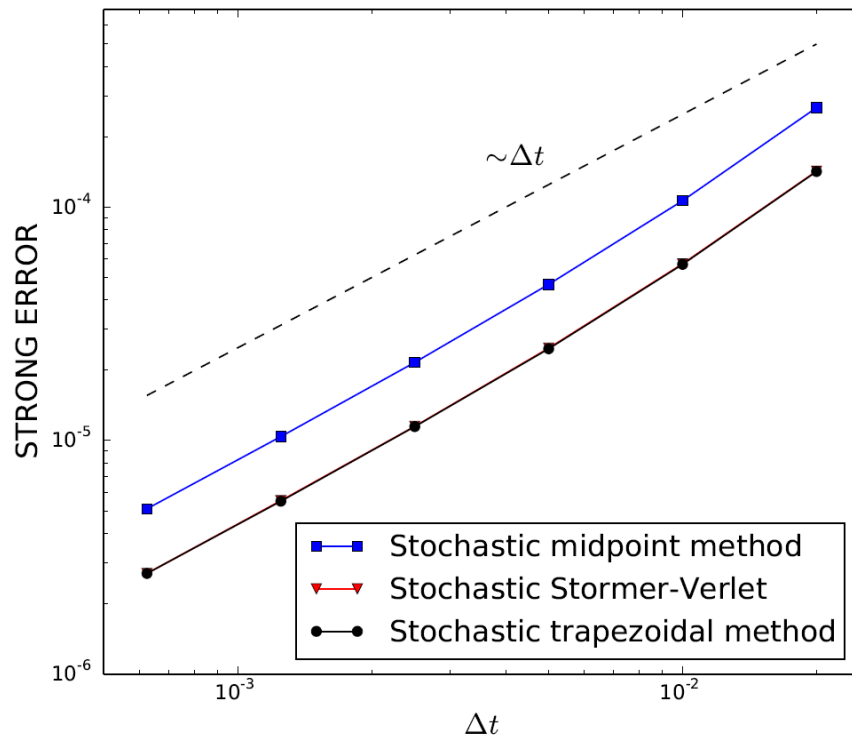
- Exact solution

$$q(t) = p_0 \sin(t + \beta W(t)) + q_0 \cos(t + \beta W(t))$$

$$p(t) = p_0 \cos(t + \beta W(t)) - q_0 \sin(t + \beta W(t))$$

- Hamiltonian is preserved

Numerical tests: convergence



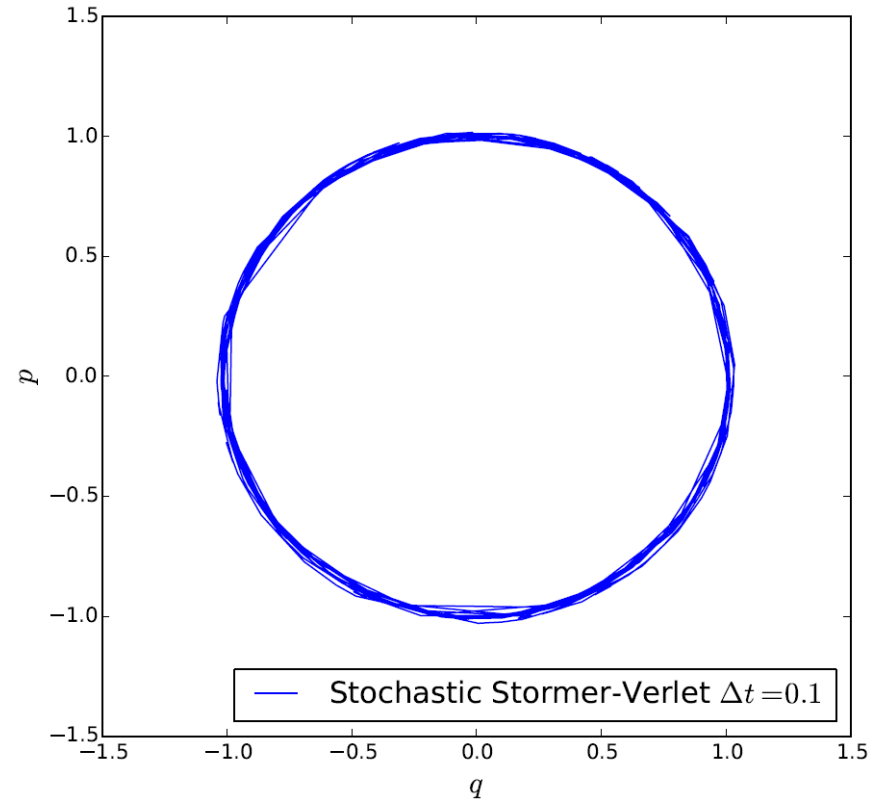
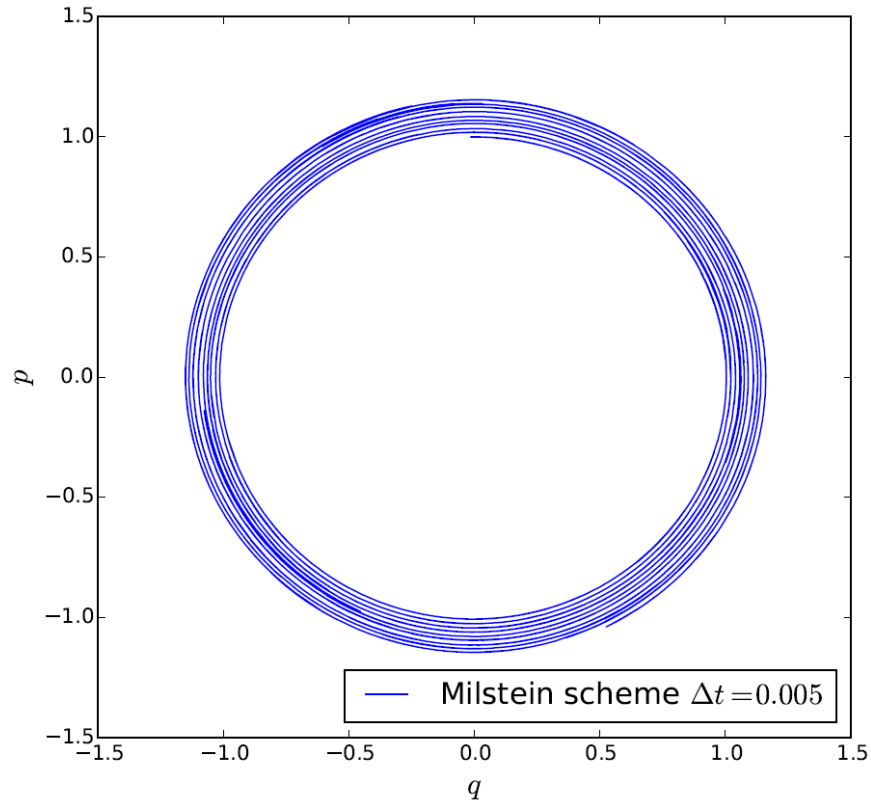
Strong error $E(\|z_K - \bar{z}(T)\|)$

Weak error $\|E(z_K) - E(\bar{z}(T))\|$

$$z = (q, p)$$

Numerical tests: Hamiltonian behavior

□ Kubo oscillator $0 \leq t \leq 60$



Numerical tests: Hamiltonian behavior

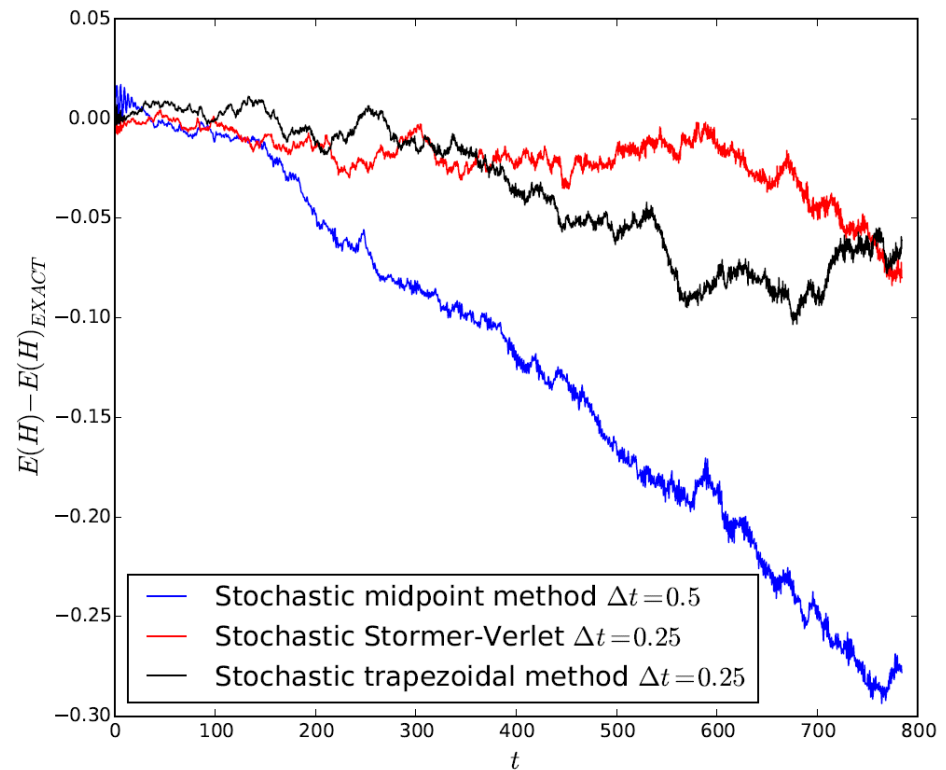
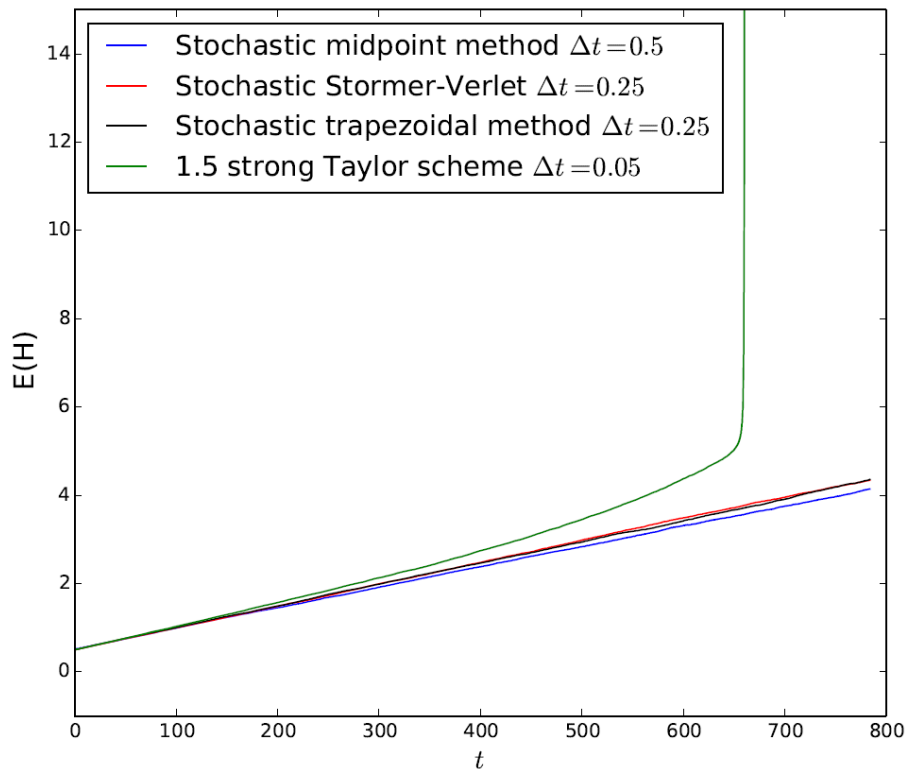
- Anharmonic oscillator

$$H(q, p) = \frac{1}{2}p^2 + \gamma q^4 \qquad h(q, p) = \beta q$$

- Expected value of the Hamiltonian

$$E(H) = H_0 + \frac{1}{2}\beta^2 t$$

Numerical tests: Hamiltonian behavior



Stochastic symplectic Runge-Kutta methods

□ s -stage Runge-Kutta method (*Ma & Ding, 2015*)

$$Q_i = q_k + \Delta t \sum_{j=1}^s a_{ij} \frac{\partial H}{\partial p}(Q_j, P_j) + \Delta W \sum_{j=1}^s b_{ij} \frac{\partial h}{\partial p}(Q_j, P_j), \quad i = 1, \dots, s$$

$$P_i = p_k - \Delta t \sum_{j=1}^s \bar{a}_{ij} \frac{\partial H}{\partial q}(Q_j, P_j) - \Delta W \sum_{j=1}^s \bar{b}_{ij} \frac{\partial h}{\partial q}(Q_j, P_j), \quad i = 1, \dots, s$$

$$q_{k+1} = q_k + \Delta t \sum_{i=1}^s \alpha_i \frac{\partial H}{\partial p}(Q_i, P_i) + \Delta W \sum_{i=1}^s \beta_i \frac{\partial h}{\partial p}(Q_i, P_i)$$

$$p_{k+1} = p_k - \Delta t \sum_{i=1}^s \alpha_i \frac{\partial H}{\partial q}(Q_i, P_i) - \Delta W \sum_{i=1}^s \beta_i \frac{\partial h}{\partial q}(Q_i, P_i)$$

□ Symplecticity conditions

$$\alpha_i \bar{a}_{ij} + \alpha_j a_{ji} = \alpha_i \alpha_j$$

$$\beta_i \bar{a}_{ij} + \alpha_j b_{ji} = \beta_i \alpha_j$$

$$\alpha_i \bar{b}_{ij} + \beta_j a_{ji} = \alpha_i \beta_j$$

$$\beta_i \bar{b}_{ij} + \beta_j b_{ji} = \beta_i \beta_j$$

Stochastic Galerkin methods as SPRK

Theorem 5. Let $\mathbf{r} = \mathbf{s}$ and let $\bar{l}_{i,s-1}(\tau)$ for $i = 1, \dots, s$ denote the Lagrange polynomials of degree $s-1$ associated with the quadrature points $0 \leq c_1 < \dots < c_s \leq 1$. Moreover, let the weights α_i be given by

$$\alpha_i = \int_0^1 \bar{l}_{i,s-1}(\tau) d\tau,$$

and assume $\alpha_i \neq 0$ for $i = 1, \dots, s$. Then *the stochastic Galerkin Hamiltonian variational integrator is equivalent to the stochastic partitioned Runge-Kutta method with the coefficients*

$$a_{ij} = \int_0^{c_i} \bar{l}_{j,s-1}(\tau) d\tau$$

$$\bar{a}_{ij} = \frac{\alpha_j(\alpha_i - a_{ji})}{\alpha_i}$$

$$b_{ij} = \frac{\beta_j a_{ij}}{\alpha_j}$$

$$\bar{b}_{ij} = \frac{\beta_j(\alpha_i - a_{ji})}{\alpha_i}$$

for $i, j = 1, \dots, s$.

Methods of strong order 3/2

- Must include $\Delta Z = \int_{t_k}^{t_{k+1}} \int_{t_k}^t dW(\xi) dt$
- For separable Hamiltonians $H(q, p) = T(p) + U(q)$

$$H_d^+(q_k, p_{k+1}) = \underset{\substack{q^1, \dots, q^s \in Q \\ P_1, \dots, P_r \in Q^* \\ q^0 = q_k}}{\text{ext}} \left\{ p_{k+1} q^s - \Delta t \sum_{i=1}^r \left[\bar{\alpha}_i P_i \dot{q}_d(t_k + c_i \Delta t) - \bar{\alpha}_i U(q_d(t_k + c_i \Delta t)) - \alpha_i T(P_i) \right] \right. \\ \left. + \Delta W \sum_{i=1}^r \bar{\beta}_i h(q_d(t_k + c_i \Delta t)) + \frac{\Delta Z}{\Delta t} \sum_{i=1}^r \bar{\gamma}_i h(q_d(t_k + c_i \Delta t)) \right\}$$

where $\Delta W = \chi \sqrt{\Delta t}$ $\Delta Z = \frac{1}{2} \Delta t^{\frac{3}{2}} \left(\chi + \frac{1}{\sqrt{3}} \eta \right)$

- For $r = s$ one gets a type of Runge-Kutta methods
- *Milstein, Repin, Tretyakov, 2002* – method of order 3/2



THANK YOU!
