Structure preserving homogenization of stiff (possibly stochastic) Hamiltonian systems.

Houman Owhadi

Molei Tao, Jerry Marsden

$$\frac{du^\epsilon}{dt} = G(u^\epsilon) + \frac{1}{\epsilon} F(u^\epsilon)$$

Assumptions **1. Hidden slow and fast variables**

$$\eta \ : \ \mathbb{R}^d \longrightarrow \mathbb{R}^{d-p} \times \mathbb{R}^p$$

$$u \longrightarrow \big(\eta^x(u), \eta^y(u)\big)$$

diffeomorphism independent from ϵ, uniformly bounded C^1, C^2 derivatives.

$$(x_t^\epsilon, y_t^\epsilon) := (\eta^x(u_t^\epsilon), \eta^y(u_t^\epsilon))$$

$$\begin{cases} \dot{x}^\epsilon = g(x^\epsilon, y^\epsilon), \\ \dot{y}^\epsilon = \frac{1}{\epsilon} f(x^\epsilon, y^\epsilon) \end{cases}$$

Assumptions

2. Hidden fast variables are locally ergodic

$$\begin{cases} \dot{x}^\epsilon = g(x^\epsilon, y^\epsilon), \\ \dot{y}^\epsilon = \frac{1}{\epsilon} f(x^\epsilon, y^\epsilon) \end{cases}$$

$$\dot{Y}_t = f(x_0, Y_t) \qquad Y_0 = y_0$$

$$\left| \frac{1}{T} \int_0^T \varphi(Y_s) - \int \varphi(y) \mu(x_0, dy) \right| \leq \chi\big(\|(x_0, y_0)\|\big) E(T) (\|\varphi\|_{L^\infty} + \|\nabla \varphi\|_{L^\infty})$$

$\lim_{T\to\infty} E(T) = 0$

$\mu(x, dy)$: Family of probability measures indexed by x_0

$r \to \chi(r)$: bounded on compact sets

$$\frac{du^\epsilon}{dt} = G(u^\epsilon) + \frac{1}{\epsilon} F(u^\epsilon)$$

Legacy code/simulator

$$\bar{u}_{t+h} = \Phi_h^{\frac{1}{\epsilon}}(\bar{u}_t)$$

For $h \leq h_0 \min(\frac{1}{\alpha}, 1)$

$$\left|\Phi_h^\alpha(u) - u - hG(u) - \alpha h F(u)\right| \leq Ch^2(1+\alpha)^2$$

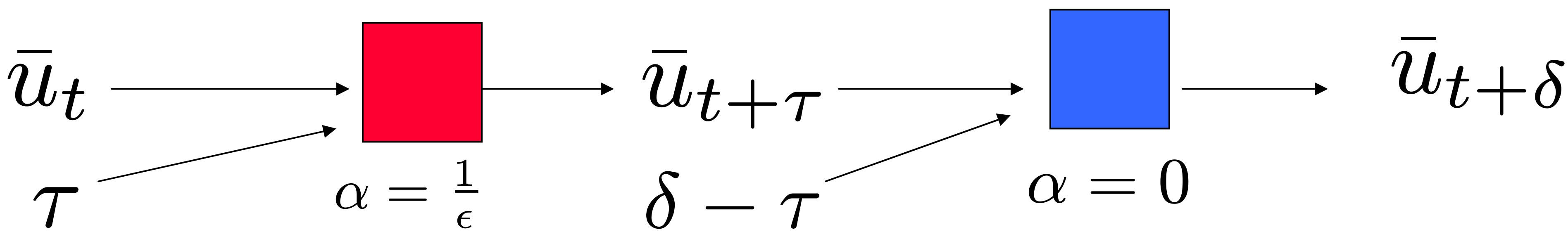
Direct simulation requires

$$h \ll \epsilon$$

$$\left|\Phi_h^{\alpha}(u) - u - hG(u) - \alpha h F(u)\right| \leq Ch^2(1+\alpha)^2$$

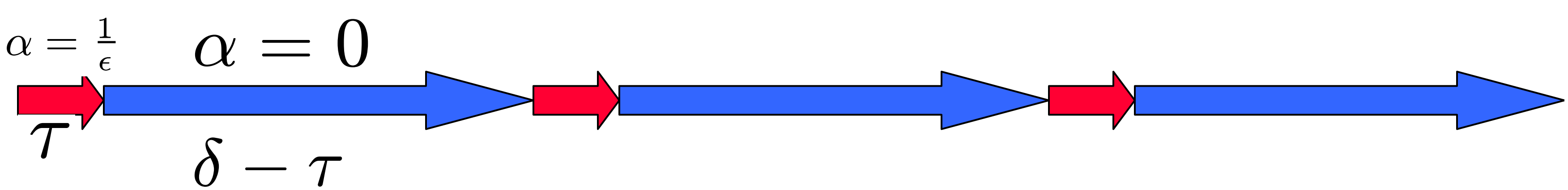
Flow Averaging Integrator

$$\bar{u}_t = \left(\Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_{\tau}\right)^k (u_0) \quad \text{for} \quad k\delta \leq t < (k+1)\delta$$



$$\epsilon \ll \delta \ll h_0, \; \tau \ll \epsilon \text{ and } \left(\frac{\tau}{\epsilon}\right)^2 \ll \delta \ll \frac{\tau}{\epsilon}.$$

Rule of thumb $\delta \sim 0.1\frac{\tau}{\epsilon}$



Two scale flow convergence

$(\xi_t^\epsilon)_{t\in\mathbb{R}^+}$: a sequence of processes on $\mathbb{R}^d$ indexed by $\epsilon > 0$.

$(X_t)_{t\in\mathbb{R}^+}$: a process on $\mathbb{R}^m$ $(m \leq d)$

$\nu(x, dy)$: A function from $\mathbb{R}^m$ onto the space of measures of probability on $\mathbb{R}^d$.

Definition. *We say that the process ξ^ϵ F-converges towards $\nu(X, dy)$ as $\epsilon \downarrow 0$ and write $\xi^\epsilon \xrightarrow[\epsilon\to 0]{F} \nu(X, dy)$ if and only if for all function φ bounded and uniformly Lipshitz-continuous on $\mathbb{R}^d$, and for all $t > 0$*

$$\lim_{h\to 0} \lim_{\epsilon\to 0} \frac{1}{h} \int_t^{t+h} \varphi(\xi_s^\epsilon)\, ds = \int_{\mathbb{R}^d} \varphi(y)\nu(X_t, dy)$$

$$\frac{du^\epsilon}{dt} = G(u^\epsilon) + \frac{1}{\epsilon} F(u^\epsilon)$$

$$\bar{u}_{k\delta} = \left(\Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_{\tau}\right)^k (u_0)$$

Theorem

$$u^\epsilon_t \xrightarrow[\epsilon \to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\lim_{h\to 0} \lim_{\epsilon\to 0} \frac{1}{h} \int_t^{t+h} \varphi(u^\epsilon_s)\, ds = \int_{\mathbb{R}^p} \varphi(\eta^{-1}(X_t, y))\mu(X_t, dy)$$

$$\dot{X}_t = \int g(X_t, y)\, \mu(X_t, dy) \qquad X_0 = x_0$$

$$\bar{u}_t \xrightarrow[\epsilon \to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$\frac{\tau}{\epsilon} \downarrow 0$, $\frac{\epsilon}{\tau}\delta \downarrow 0$ and $(\frac{\tau}{\epsilon})^2 \frac{1}{\delta} \downarrow 0$.

$$\epsilon \ll \delta \ll h_0,\ \tau \ll \epsilon \text{ and } \left(\frac{\tau}{\epsilon}\right)^2 \ll \delta \ll \frac{\tau}{\epsilon}.$$

Proof

$$(\bar{x}_t, \bar{y}_t) := \eta(\bar{u}_t)$$

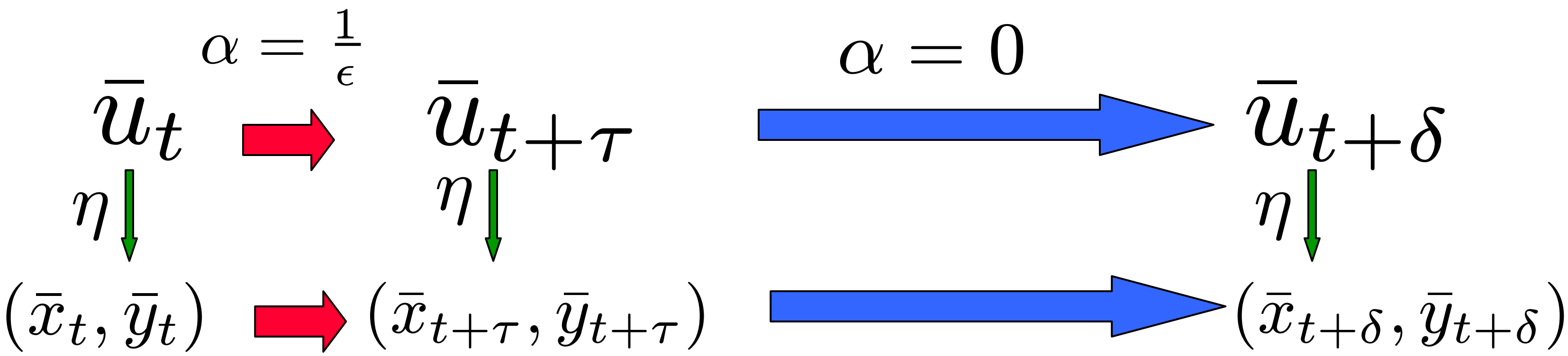
$$\bar{u}_t \xrightarrow[\epsilon \to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\Updownarrow$$

$$(\bar{x}_t, \bar{y}_t) \xrightarrow[\epsilon \to 0]{F} \delta_{X_t} \otimes \mu(X_t, dy)$$

Proof

$$(\bar{x}_t, \bar{y}_t) := \eta(\bar{u}_t)$$

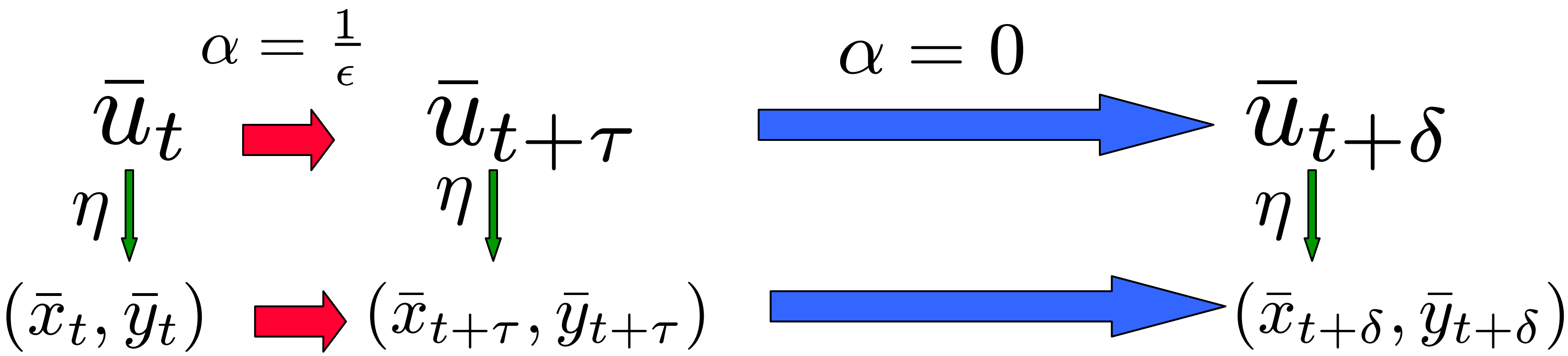


$$(\bar{x}_{t+\delta}, \bar{y}_{t+\delta}) = \Psi^0_{\delta-\tau} \circ \Psi^{\frac{1}{\epsilon}}_{\tau}(\bar{x}_t, \bar{y}_t)$$

$$\Psi^\alpha_h = \eta \circ \Phi^\alpha_h \circ \eta^{-1}$$

Proof

$$(\bar{x}_t, \bar{y}_t) := \eta(\bar{u}_t)$$



$$(\bar{x}_{t+\delta}, \bar{y}_{t+\delta}) = \Psi^{0}_{\delta-\tau} \circ \Psi^{\frac{1}{\epsilon}}_{\tau}(\bar{x}_t, \bar{y}_t)$$

$$\Psi^{\alpha}_{h} = \eta \circ \Phi^{\alpha}_{h} \circ \eta^{-1}$$

Assume $\Phi_h^{\frac{1}{\epsilon}}(u) = u + hG(u) + \frac{1}{\epsilon} hF(u)$

$$\Psi_\tau^{\frac{1}{\epsilon}}(x,y) - (x,y) - \tau\big(g(x,y),0\big) - \frac{\tau}{\epsilon}\big(0, f(x,y)\big)$$

$$= \int_0^1 v^T \operatorname{Hess} \eta(u+sv) v \, ds$$

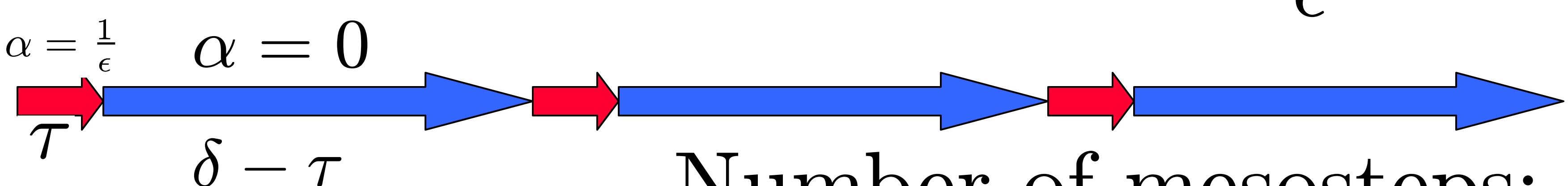
$$u = \eta^{-1}(x,y)$$

$$v = \tau G(u) + \frac{\tau}{\epsilon} F(u)$$

$$(\bar{x}_{t+\delta}, \bar{y}_{t+\delta}) = \Psi^{0}_{\delta-\tau} \circ \Psi^{\frac{1}{\epsilon}}_{\tau}(\bar{x}_t, \bar{y}_t)$$

$$\Psi^{\frac{1}{\epsilon}}_{\tau}(x,y) - (x,y) - \tau\big(g(x,y),0\big) - \frac{\tau}{\epsilon}\big(0, f(x,y)\big)$$
$$= \int_0^1 v^T \,\mathrm{Hess}\,\eta(u+sv)v\,ds$$

$$v = \tau G(u) + \frac{\tau}{\epsilon} F(u)$$



Number of mesosteps: $\frac{1}{\delta}$

$\mathcal{O}(1)$-timescale

Number of microsteps: $\frac{1}{\delta}$

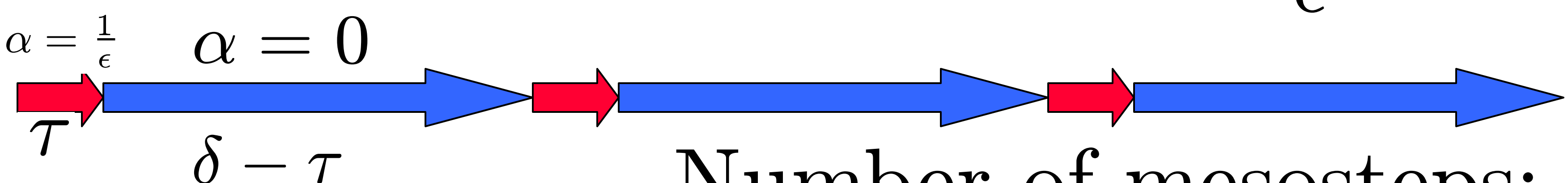
Averaging $\Leftrightarrow$ y-clock time $>> 1$

y-clock time: $\frac{\tau}{\epsilon}\frac{1}{\delta} >> 1 \Leftrightarrow \delta << \frac{\tau}{\epsilon}$

$$(\bar{x}_{t+\delta}, \bar{y}_{t+\delta}) = \Psi^{0}_{\delta-\tau} \circ \Psi^{\frac{1}{\epsilon}}_{\tau}(\bar{x}_t, \bar{y}_t)$$

$$\Psi^{\frac{1}{\epsilon}}_{\tau}(x,y) - (x,y) - \tau\big(g(x,y),0\big) - \frac{\tau}{\epsilon}\big(0, f(x,y)\big)$$
$$= \int_0^1 v^T \,\mathrm{Hess}\,\eta(u+sv)v\,ds$$

$$v = \tau G(u) + \frac{\tau}{\epsilon} F(u)$$



Number of mesosteps: $\frac{1}{\delta}$

$\mathcal{O}(1)$-timescale

Number of microsteps: $\frac{1}{\delta}$

Error accumulation on x

$$\frac{1}{\delta}\left(\frac{\tau}{\epsilon}\right)^2 << 1 \Leftrightarrow \left(\frac{\tau}{\epsilon}\right)^2 << \delta$$

A simple example: a stiff ODE with hidden slow and fast variables

$$\begin{cases} \dot{r} = \frac{1}{\epsilon}(r\cos\theta + r\sin\theta - \frac{1}{3}r^3\cos^3\theta)\cos\theta - \epsilon\, r\cos\theta\sin\theta \\ \dot{\theta} = -\epsilon\, cos^2\theta - \frac{1}{\epsilon}(\cos\theta + \sin\theta - \frac{1}{3}r^2\cos^3\theta)\sin\theta \end{cases}$$

The system is characterized by hidden slow and fast variables

$$[x, y] = [r\cos\theta, r\sin\theta]$$

$$\begin{cases} \dot{x} = \frac{1}{\epsilon}(y + x - \frac{1}{3}x^3) \\ \dot{y} = -\epsilon x \end{cases}$$

$$\ddot{x} + x = \frac{1}{\epsilon}(1 - x^2)\dot{x}$$

Van der Pol oscillator

FLow AVeraging integratORS

$$\begin{cases} \dot{r} = \frac{1}{\epsilon}(r\cos\theta + r\sin\theta - \frac{1}{3}r^3\cos^3\theta)\cos\theta - \epsilon\, r\cos\theta\sin\theta \\ \dot{\theta} = -\epsilon\, cos^2\theta - \frac{1}{\epsilon}(\cos\theta + \sin\theta - \frac{1}{3}r^2\cos^3\theta)\sin\theta \end{cases}$$

Legacy integrator: Forward Euler

$$\Phi_h^{\alpha,\epsilon}(r,\theta) := \begin{pmatrix} r \\ \theta \end{pmatrix} + \alpha h \begin{pmatrix} (r\cos\theta + r\sin\theta - \frac{1}{3}r^3\cos^3\theta)\cos\theta \\ -(\cos\theta + \sin\theta - \frac{1}{3}r^2\cos^3\theta)\sin\theta \end{pmatrix} - \epsilon h \begin{pmatrix} r\cos\theta\sin\theta \\ cos^2\theta \end{pmatrix}$$

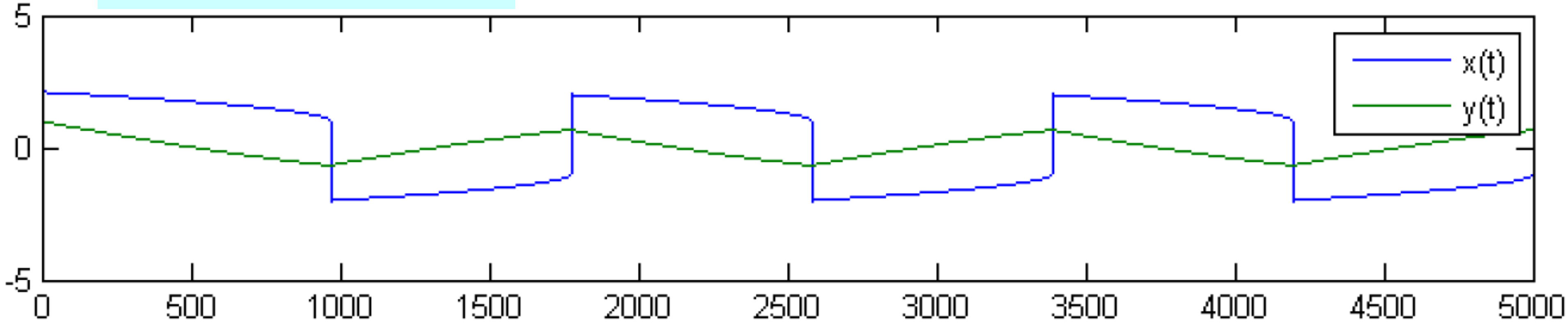
Proposed method

Non intrusive FLAVOR

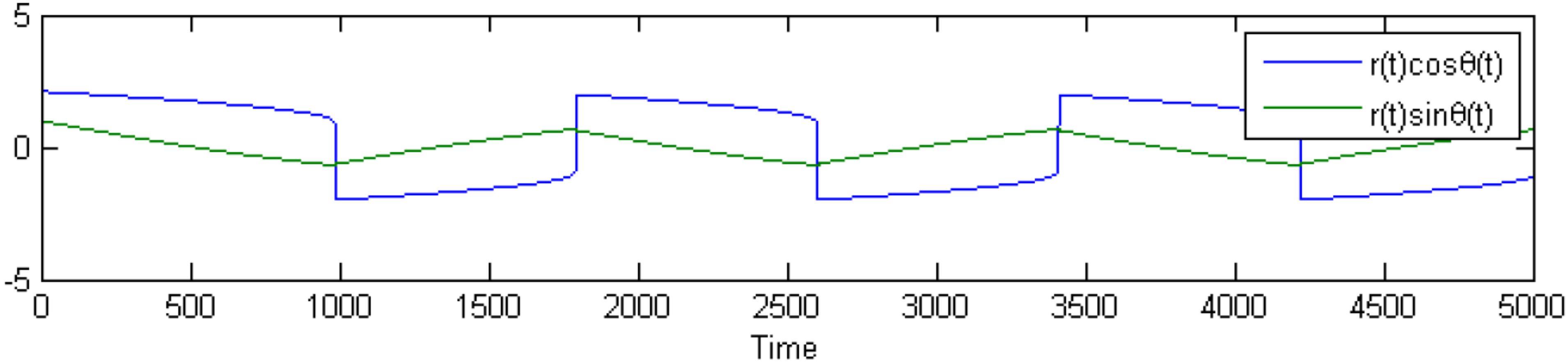
$$(\bar{r}_t, \bar{\theta}_t) = \left(\Phi_{\delta-\tau}^{0,\epsilon} \circ \Phi_{\tau}^{\frac{1}{\epsilon},\epsilon}\right)^k (r_0, \theta_0) \quad \text{for} \quad k\delta \le t < (k+1)\delta$$

$T = 5/\epsilon$ $[x, y] = [r\cos\theta, r\sin\theta]$

Forward Euler $h = 5 \cdot 10^{-5}$



FLAVOR $\delta = 10^{-2} \quad \tau = 5 \cdot 10^{-5}$



ODEs derived from Hamiltonian Systems

$$\dot{p} = -\partial_q H(p,q) \quad \dot{q} = \partial_p H(p,q)$$

$$H(q,p) := \frac{1}{2} p^T M^{-1} p + V(q) + \frac{1}{\epsilon} U(q)$$

Symplectic with quadratic stiff potentials

- Impulse and mollified impulse methods. [Skeel et Al, 1999]
- Hamilton-Jacobi homogenization method [Legoll, Lebris, 2007]
- IMEX (implicit for non-quadratic stiff potentials) (Stern, Grinspun, 2009)

Time reversible methods (enforced as an optimization constraint by tracking slow variables) for stiff potentials of the form $\frac{1}{\epsilon}\sum_{j=1}^{\nu} g_j(q)^2$

- HMM [Ariel, Engquist, Tsai, 2009]
- HMM [Sanz-Serna, Ariel, Tsai, 2009]

$$\dot{p} = -\partial_q H(p,q) \quad \dot{q} = \partial_p H(p,q)$$

$$H(q,p) := \frac{1}{2} p^T M^{-1} p + V(q) + \frac{1}{\epsilon} U(q)$$

on the tangent bundle $T^*\mathcal{M}$ of a configuration manifold $\mathcal{M}$

Legacy integrator

$$\left| \Phi_h^\alpha(q,p) - (q,p) - h\big(M^{-1}p, -V(q) - \alpha U(q)\big) \right| \leq C h^2 (1+\alpha)$$

FLAVOR $\left(q_{(n+1)\delta}, p_{(n+1)\delta}\right) := \Theta_\delta(q_{n\delta}, p_{n\delta})$

$$\Theta_\delta := \Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_\tau$$

$\tau \ll \sqrt{\epsilon} \ll \delta$ and $\frac{\tau^2}{\epsilon} \ll \delta \ll \frac{\tau}{\sqrt{\epsilon}}$ Rule of thumb $\delta \sim 0.1 \frac{\tau}{\sqrt{\epsilon}}$

If the legacy integrator is symmetric under a group action then FLAVOR is symmetric under the same group action.

FLAVOR $\left(q_{(n+1)\delta}, p_{(n+1)\delta}\right) := \Theta_\delta\left(q_{n\delta}, p_{n\delta}\right)$

Theorem

$$\Phi_h^\alpha \text{ symplectic} \Rightarrow \Theta_\delta := \Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_{\tau} \text{ is symplectic}$$

$$\Phi_h^* := \left(\Phi_{-h}\right)^{-1}$$

$$\Phi_h^\alpha \text{ symplectic} \Rightarrow \quad \Theta_\delta := \Phi^{\frac{1}{\epsilon},*}_{\frac{\tau}{2}} \circ \Phi^{0,*}_{\frac{\delta-\tau}{2}} \circ \Phi^0_{\frac{\delta-\tau}{2}} \circ \Phi^{\frac{1}{\epsilon}}_{\frac{\tau}{2}}$$

is symplectic and time-reversible

An example of symplectic FLAVOR

$$\Theta_\delta := \Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_{\tau}$$

$$\Phi_h^\alpha(q,p) = \begin{pmatrix} q \\ p \end{pmatrix} + h \begin{pmatrix} M^{-1}\Big(p - h\big(V(q) + \alpha U(q)\big)\Big) \\ -V(q) - \alpha U(q) \end{pmatrix}$$

An example of symplectic, time reversible FLAVOR

$$\Theta_\delta := \Phi^{\frac{1}{\epsilon},*}_{\frac{\tau}{2}} \circ \Phi^{0,*}_{\frac{\delta-\tau}{2}} \circ \Phi^0_{\frac{\delta-\tau}{2}} \circ \Phi^{\frac{1}{\epsilon}}_{\frac{\tau}{2}}$$

$$\Phi_h^{\alpha,*}(q,p) = \begin{pmatrix} q \\ p \end{pmatrix} + h \begin{pmatrix} M^{-1}p \\ -V(q + hM^{-1}p) - \alpha U(q + hM^{-1}p) \end{pmatrix}$$

FLAVORS based on variational legacy integrators are variational

$$L_{d_h}^{1/\epsilon}(q_k, q_{k+1}) = h\left[\frac{1}{2}\left(\frac{q_{k+1}-q_k}{h}\right)^2 - \left(V(q_k) + \frac{1}{\epsilon}U(q_k)\right)\right]$$

$$\begin{array}{ccc}
Singlescale\ L_d & \xrightarrow{FLAVORization} & Multiscale\ L_d \\
\downarrow{\scriptstyle variational\ principle} & & \downarrow{\scriptstyle variational\ principle} \\
Singlescale\ DEL & \xrightarrow{FLAVORization} & Multiscale\ DEL
\end{array}$$

$$\begin{cases} p_{k+1} & = p_k - h[\nabla V(q_k) + \frac{1}{\epsilon}\nabla U(q_k)] \\ q_{k+1} & = q_k + h p_{k+1} \end{cases}$$

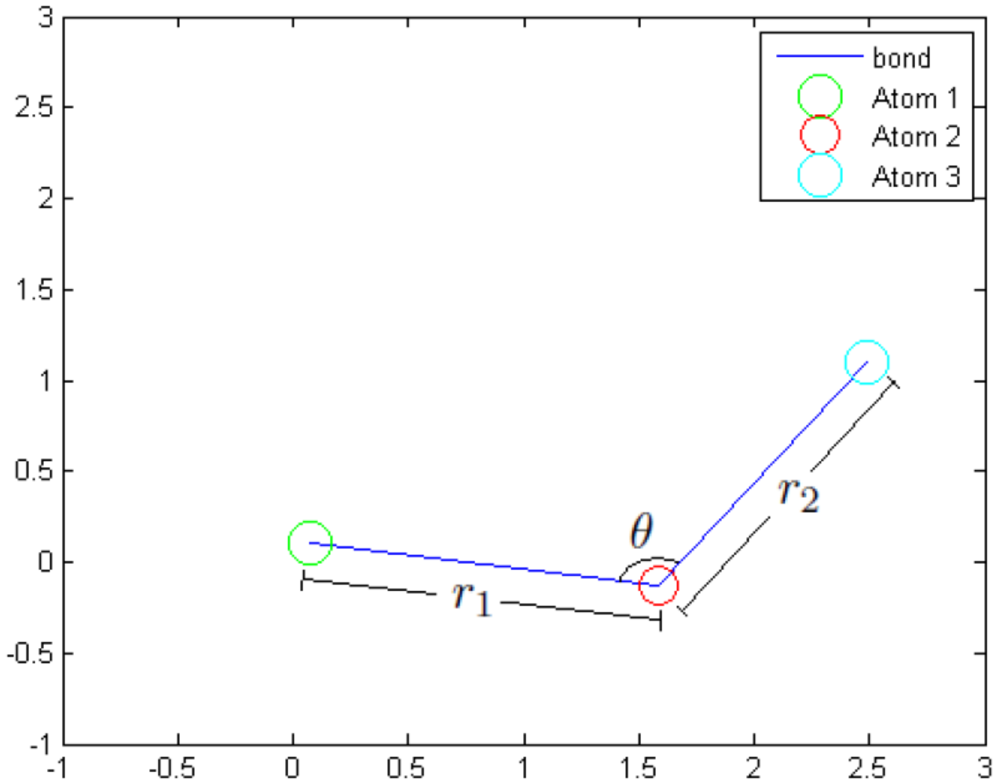
FLAVORS based on variational legacy integrators are variational

$$L_{d\delta}(q_k, q_k', q_{k+1}) = L_{d_\tau}^{1/\epsilon}(q_k, q_k') + L_{d_{\delta-\tau}}^{0}(q_k', q_{k+1})$$
$$= \tau\left[\frac{1}{2}\left(\frac{q_k'-q_k}{\tau}\right)^2 - \left(V(q_k)+\frac{1}{\epsilon}U(q_k)\right)\right] + (\delta-\tau)\left[\frac{1}{2}\left(\frac{q_{k+1}-q_k'}{\delta-\tau}\right)^2 - V(q_k')\right]$$

$$\begin{array}{ccc} Singlescale\ L_d & \xrightarrow{FLAVORization} & Multiscale\ L_d \\ \downarrow{\scriptstyle variational\ principle} & & \downarrow{\scriptstyle variational\ principle} \\ Singlescale\ DEL & \xrightarrow{FLAVORization} & Multiscale\ DEL \end{array}$$

$$\begin{cases} p_k' & = p_k - \tau[\nabla V(q_k) + \frac{1}{\epsilon}\nabla U(q_k)] \\ q_k' & = q_k + \tau p_k' \\ p_{k+1} & = p_k' - (\delta-\tau)\nabla V(q_k') \\ q_{k+1} & = q_k' + (\delta-\tau)p_{k+1} \end{cases}$$

Nonlinear 2D molecular clipper



$$H = K.E. + P.E.$$

$$K.E. = \frac{1}{2}m_1(\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2}m_2(\dot{x}_2^2 + \dot{y}_2^2) + \frac{1}{2}m_3(\dot{x}_3^2 + \dot{y}_3^2)$$

$$P.E. = V_{bond} + V_{angle}$$

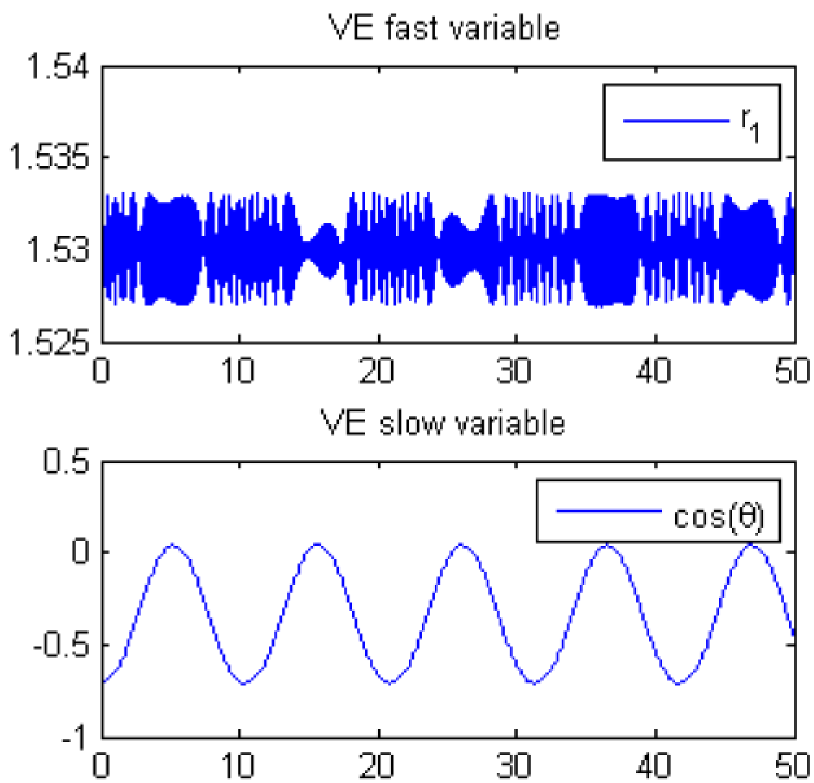
$$V_{bond} = \frac{1}{2}K_r[(r_1 - r_0)^2 + (r_2 - r_0)^2]$$

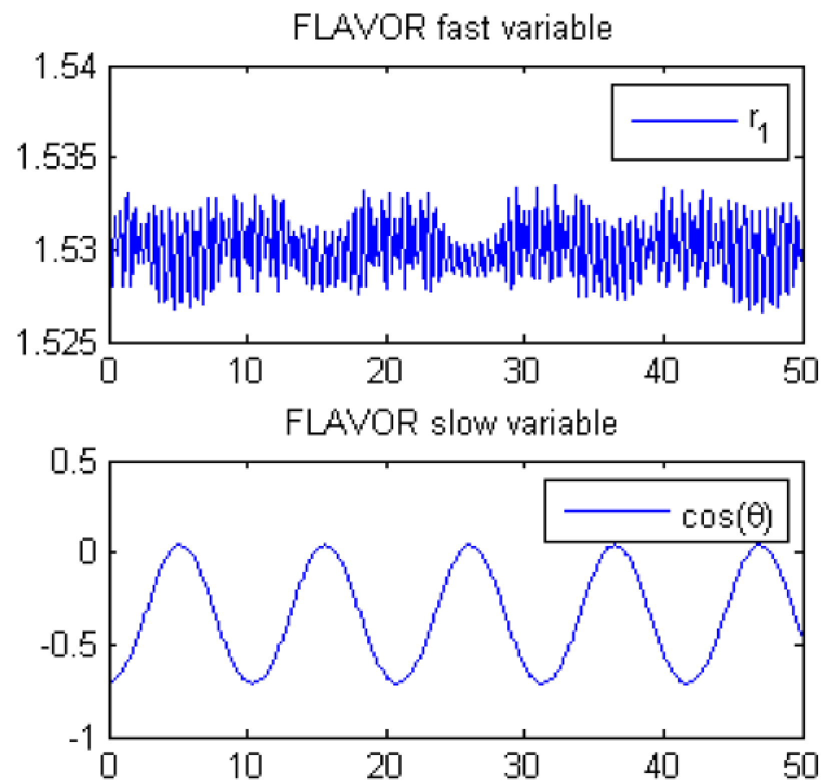
$$V_{angle} = \frac{1}{2}K_\theta(\cos(\theta) - \cos(\theta_0))^2$$

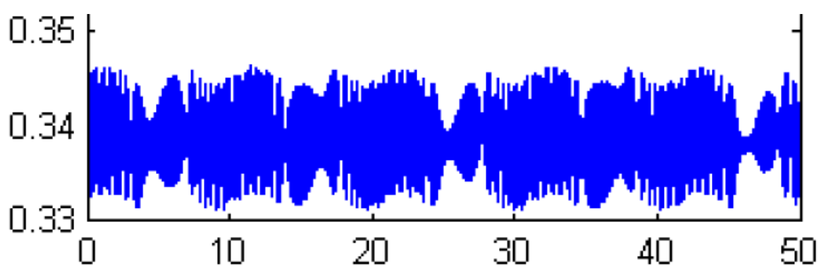
Nonlinear 2D molecular clipper

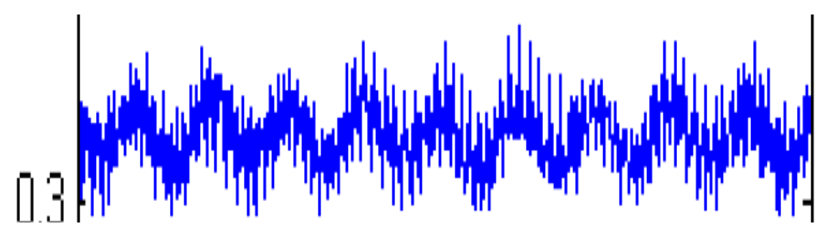
Velocity Verlet $h = 0.001$

FLAVOR $\delta = 0.1 \quad \tau = 0.001$

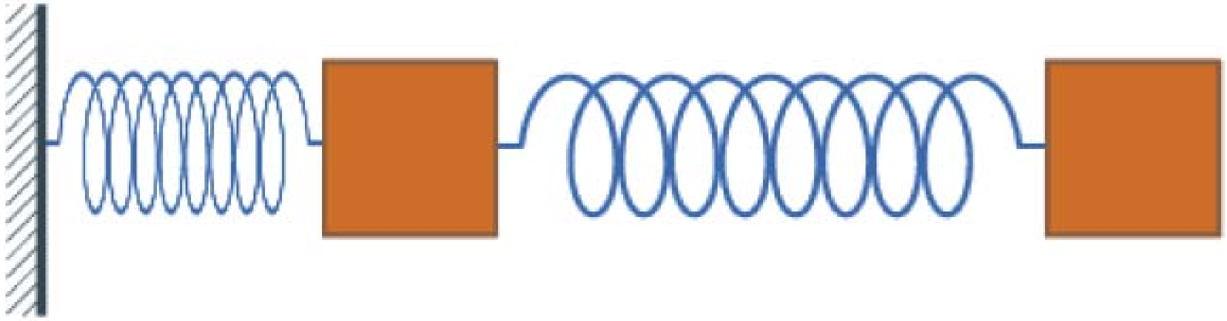




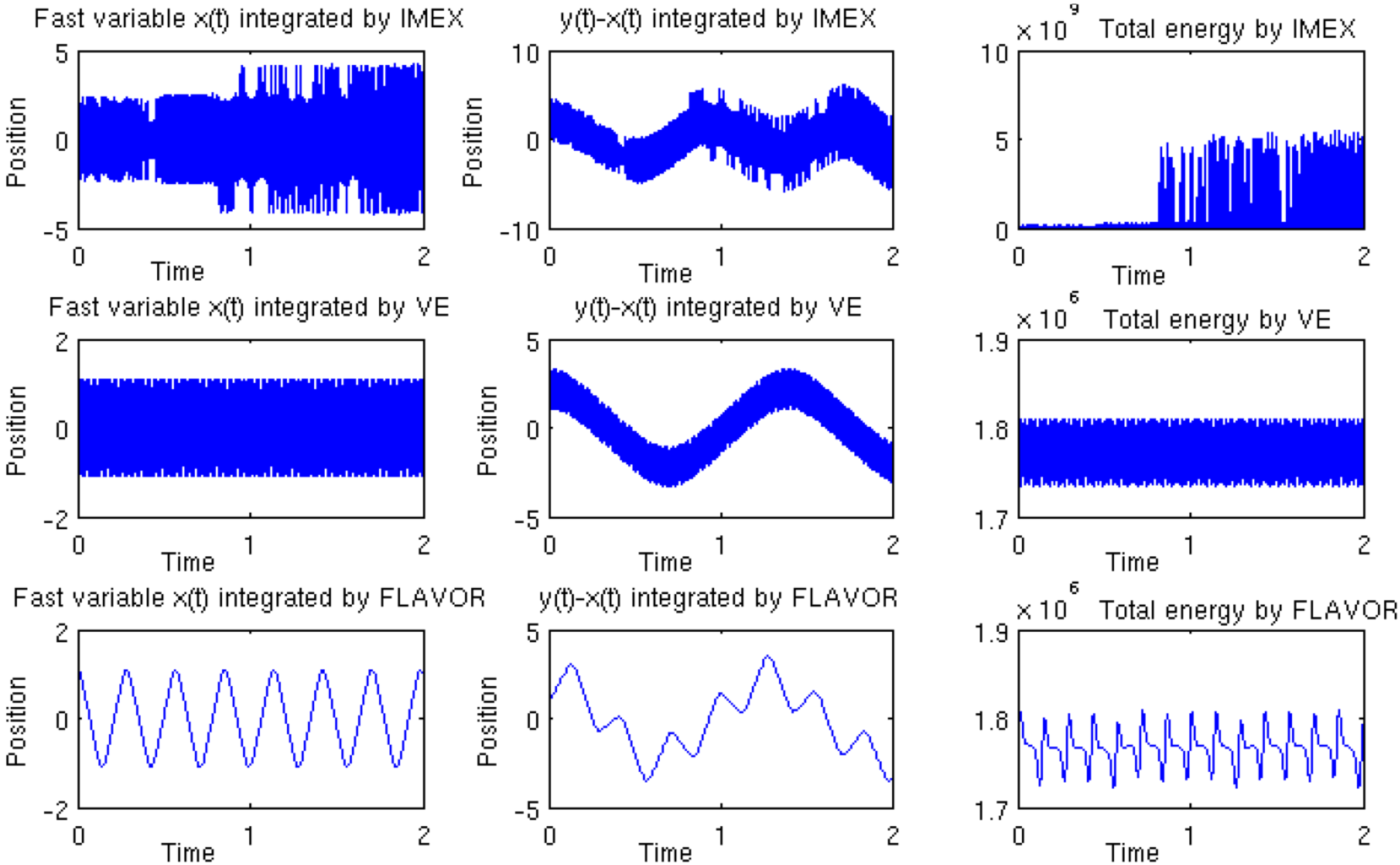




Nonlinear stiff and soft potentials



$$H(x,y,p_x,p_y) := \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \epsilon^{-1}x^6 + (y-x)^4$$



$$\epsilon = 10^{-6}$$

FLAVOR

$$\delta = 10^{-3}$$

$$\tau = 10^{-5}$$

IMEX

$$\delta = 10^{-3}$$

VE

$$h = 10^{-5}$$

Forced non-autonomous mechanical system: Kapitza's Inverted Pendulum.

$$l\ddot{\theta} = [g + \omega^2 \sin(2\pi\omega t)] \sin\theta$$

Variational Euler+
D'Alembert

$$\begin{cases} f_i = \omega^2 \sin(2\pi\omega i h) \\ p_{i+1} = p_i + h[g + f_i] \sin\theta_i \\ \theta_{i+1} = \theta_i + h p_{i+1} \end{cases}$$

FLAVOR

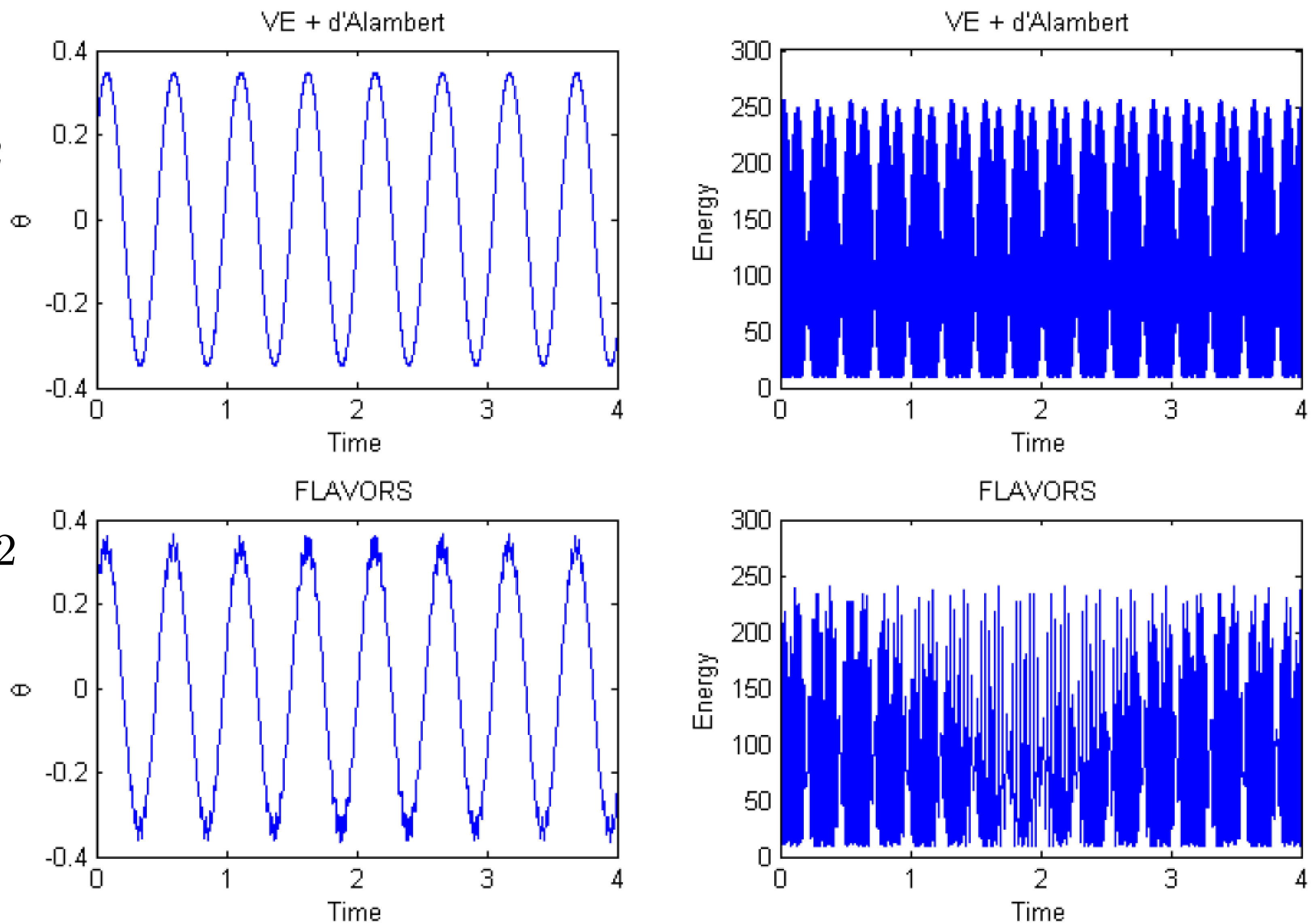
$$\begin{cases} q_{n\delta+\tau} = q_{n\delta} + \tau p_{n\delta} \\ p_{n\delta+\tau} = p_{n\delta} + \tau g \sin(q_{n\delta+\tau}) + \omega^2 \sin(2\pi\omega n\tau) \\ q_{(n+1)\delta} = q_{n\delta+\tau} + (\delta - \tau) p_{n\delta+\tau} \\ p_{(n+1)\delta} = p_{n\delta+\tau} + (\delta - \tau) g \sin(q_{(n+1)\delta}) \end{cases}$$

Forced non-autonomous mechanical system: Kapitza's Inverted Pendulum.

$h = 0.0002$

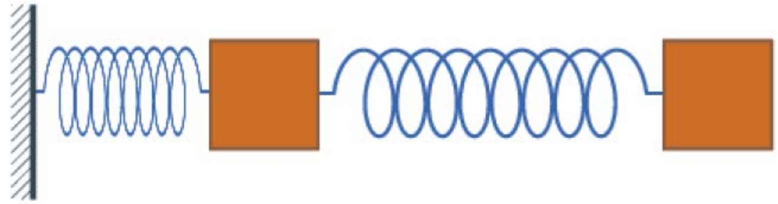
$\tau = 0.0002$

$\delta = 0.002$

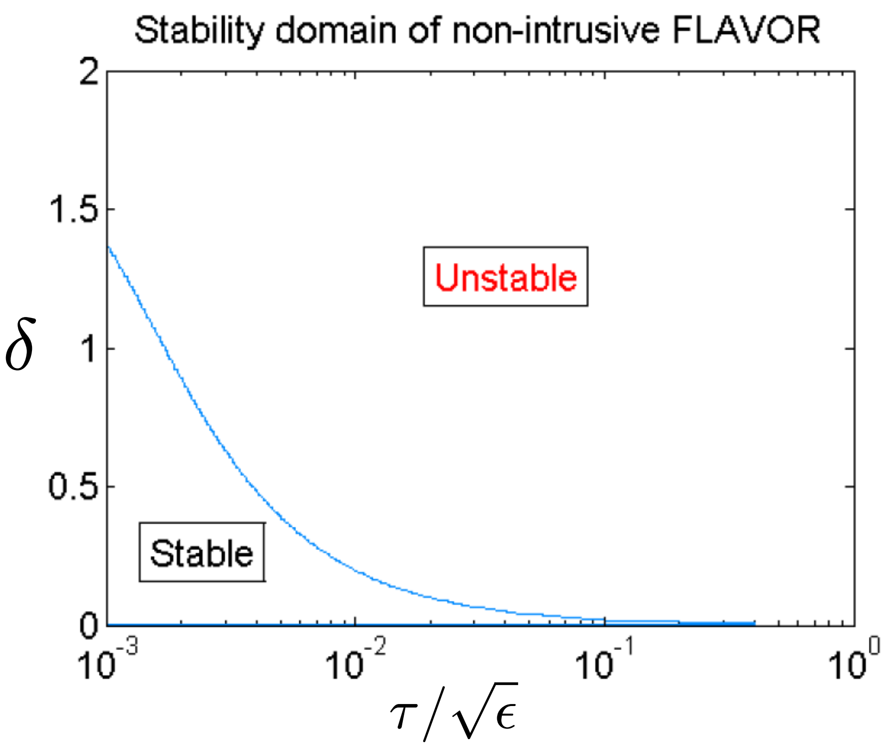


$\omega = 1000$

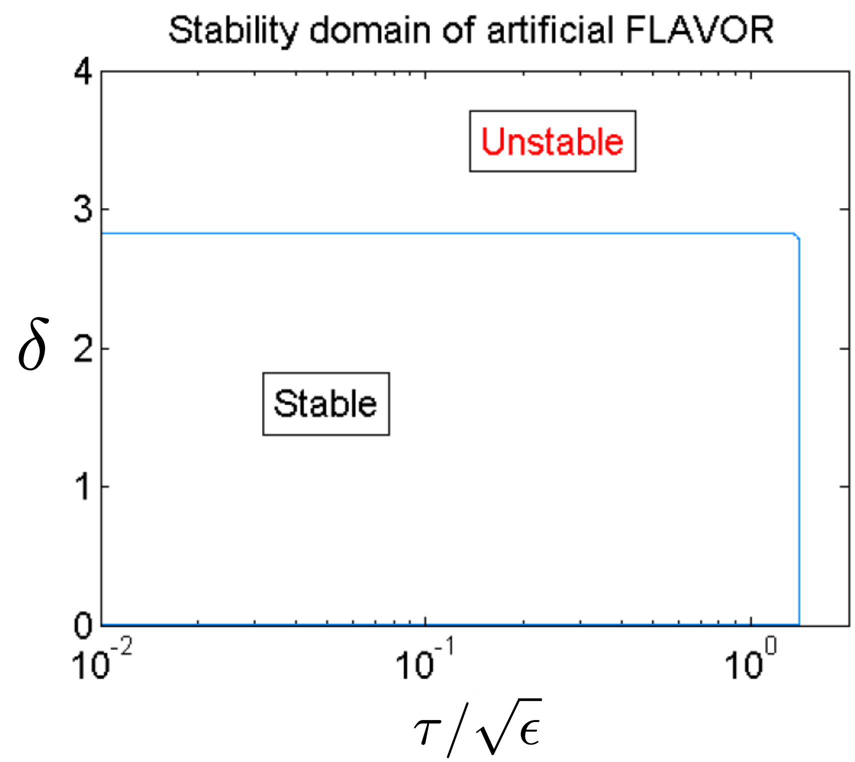
Stability domain



$$H(x,y,p_x,p_y) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}(y-x)^2$$

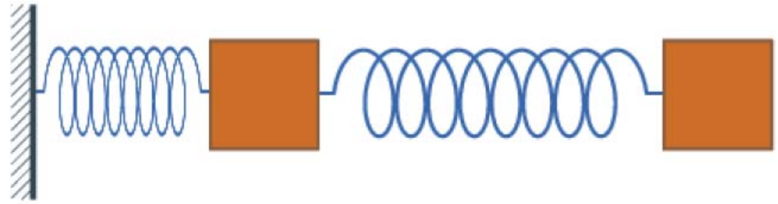


(a) ***Non-intrusive FLAVOR***



(b) ***Artificial FLAVOR***

Stability



$$H(x,y,p_x,p_y) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}(y-x)^2$$

Theorem

Non intrusive FLAVOR

$$\Theta_\delta := \Phi^0_{\delta-\tau} \circ \Phi^{\omega^2}_\tau$$

$$\Phi^\alpha_h(q,p) = \begin{pmatrix} q \\ p \end{pmatrix} + h \begin{pmatrix} M^{-1}\Big(p - h\big(V(q) + \alpha U(q)\big)\Big) \\ -V(q) - \alpha U(q) \end{pmatrix}$$

with $1/\tau \gg \omega \gg 1$ is stable for $\delta \in (0, \sqrt{2})$

Artificial FLAVOR

$$\Theta_\delta := \theta^{tr}_{\delta-\tau} \circ \theta^\epsilon_\tau \circ \theta^V_\delta$$

with $1/\tau \gg \omega \gg 1$ is stable for $\delta \in (0, 2)$

FLAVOR $(q_{(n+1)\delta}, p_{(n+1)\delta}) := \Theta_\delta(q_{n\delta}, p_{n\delta})$

Artificial FLAVOR

$$\Theta_\delta := \theta^{tr}_{\delta-\tau} \circ \theta^{\epsilon}_{\tau} \circ \theta^{V}_{\delta}$$

$$H^{slow}(q,p) := V(q)$$

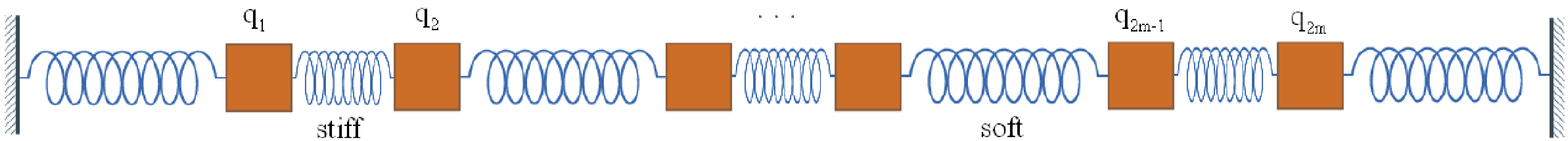
$$\theta^V_h(q,p) = (q, p - h\nabla V(q))$$

$$H^{fast}(q,p) := \frac{1}{2}p^T M^{-1} p + \frac{1}{\epsilon}U(q)$$

$$\theta^{\epsilon}_{\tau}(q,p) = \left(q + \tau M^{-1}p, p - \frac{\tau}{\epsilon}\nabla U(q + tM^{-1}p)\right)$$

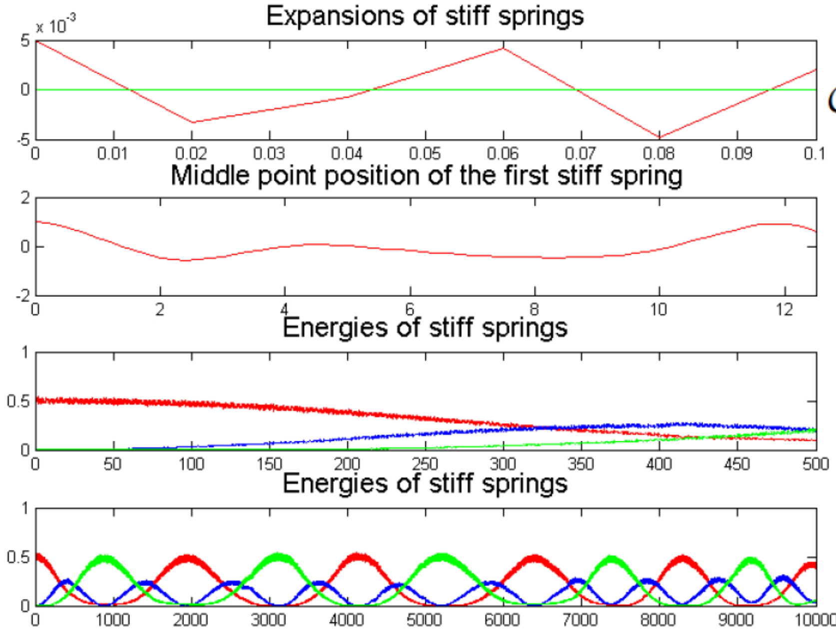
$\theta^{tr}_{\delta-\tau}$ is a map approximating the flow of the Hamiltonian $H^{free}(q,p) := \frac{1}{2}p^T M^{-1} p$ under holonomic constraints imposing the freezing of stiff bonds. Velocities along the direction of constraints have to be stored and set to be 0 before the constrained dynamics, i.e. freezed, and the stored velocities should be restored after the constrained dynamics, i.e. un-freezed

Fermi-Pasta-Ulam problem



$$H(q,p) := \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4$$

4 orders of magnitudes of time scales

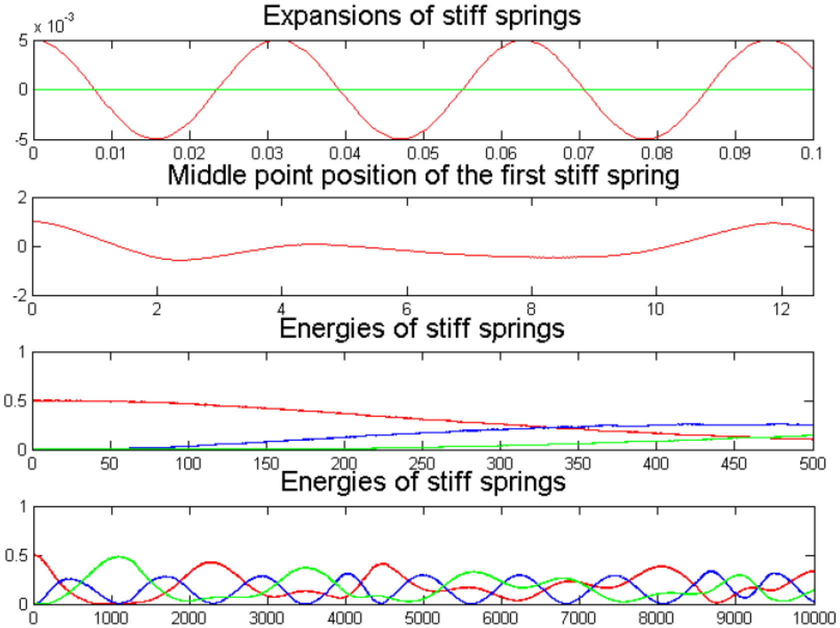


$\mathcal{O}(\omega^{-1})$

$\mathcal{O}(1)$

$\mathcal{O}(\omega)$

$\mathcal{O}(\omega^2)$



FLAVOR

$$\omega = 200$$

Velocity Verlet

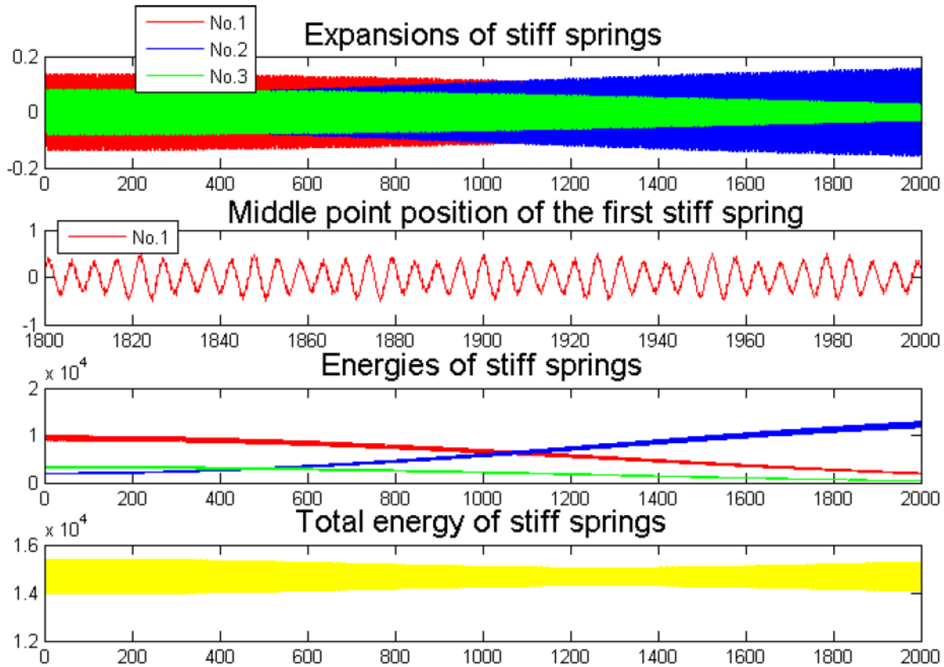
$$\delta = 0.002$$

$$\tau = 0.0005$$

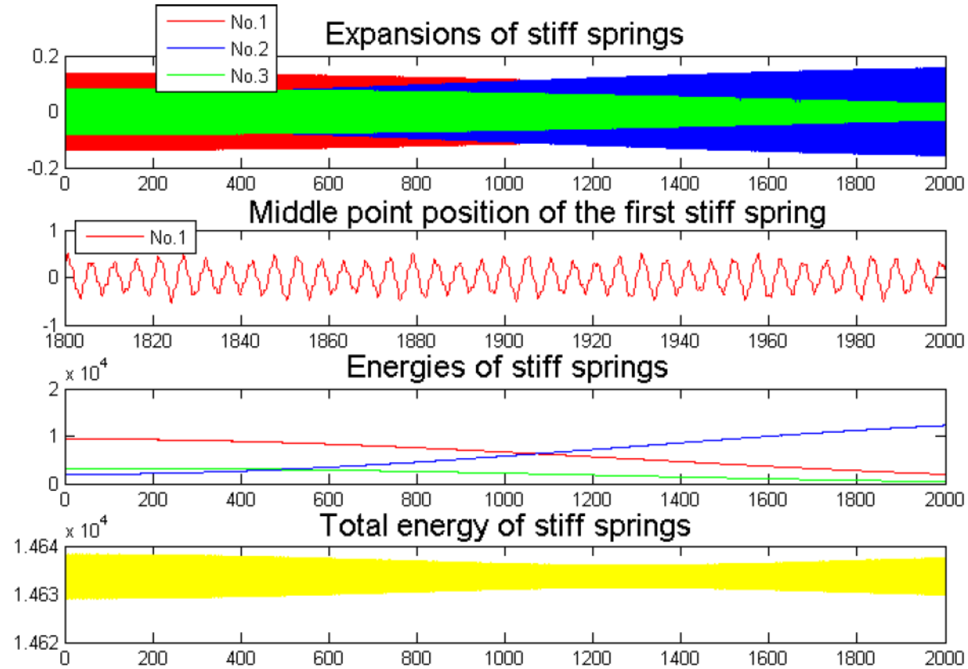
200 fold acceleration

$$h = 10^{-5}$$

$O(\omega)$ time scale



FLAVOR



Velocity Verlet

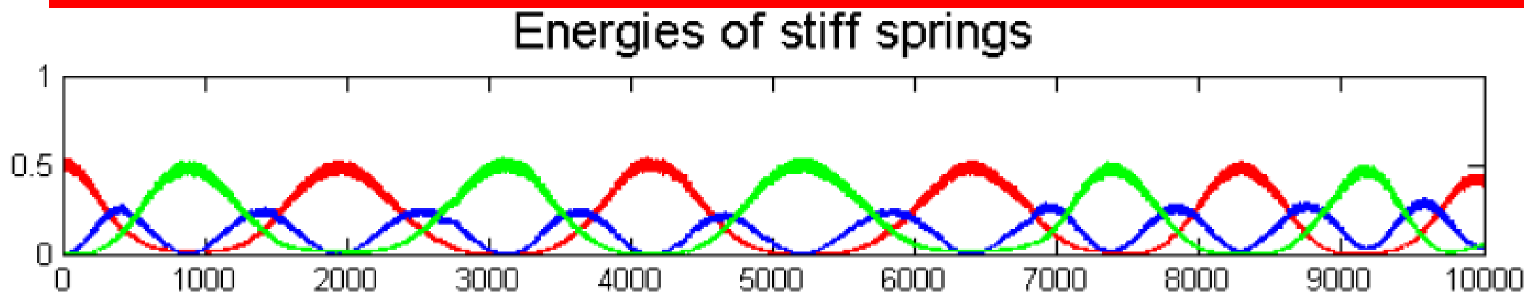
$$\delta = 0.002, \tau = 0.0001$$

$$h = 0.00005$$

$$\omega = 1000$$

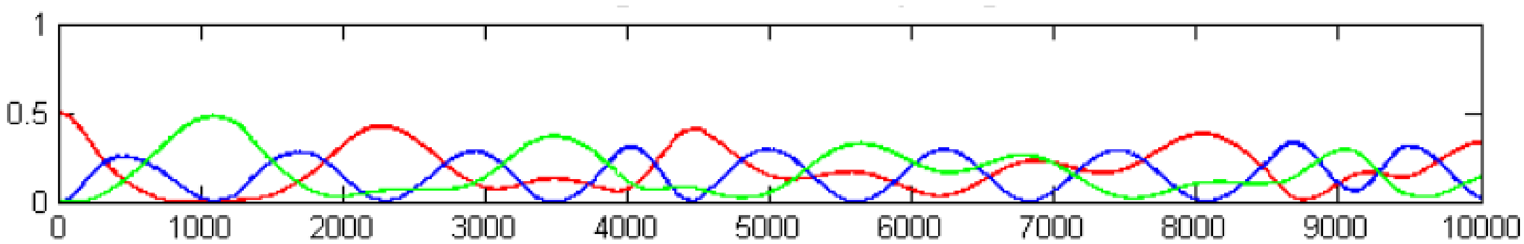
FLAVORS are not equivalent to rescaling ω, i.e. ϵ

$O(\omega^2)$ time scale



FLAVOR

$\mathcal{O}(\omega^2)$



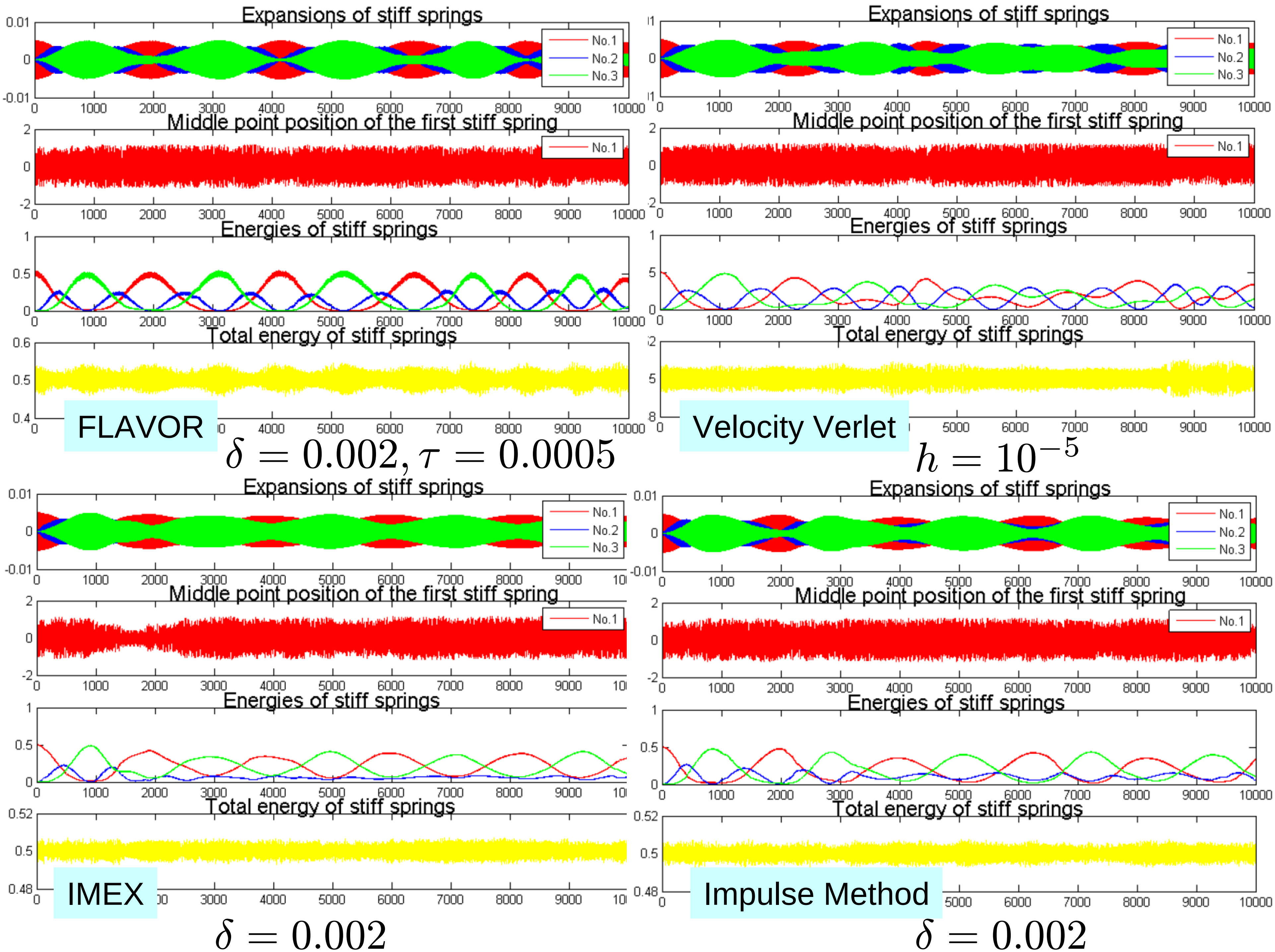
Velocity Verlet

$$\omega = 200$$

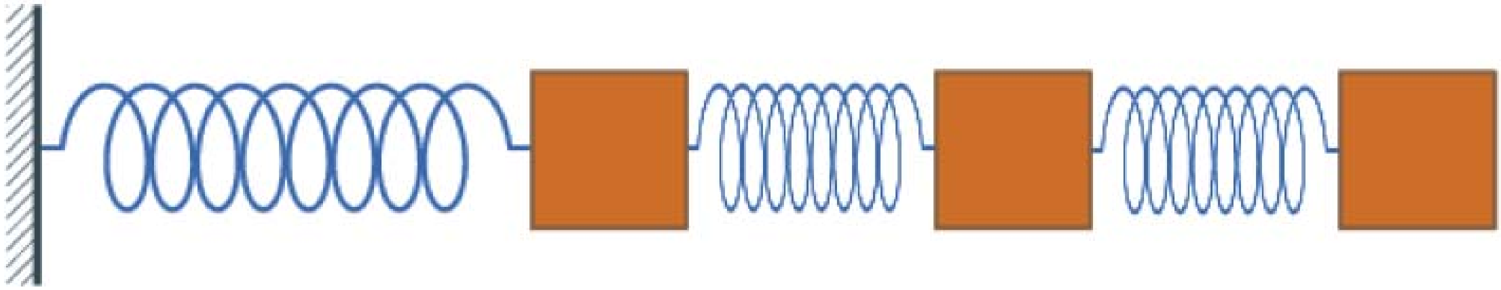
$$\delta = 0.002$$
$$\tau = 0.0005$$

200 fold acceleration

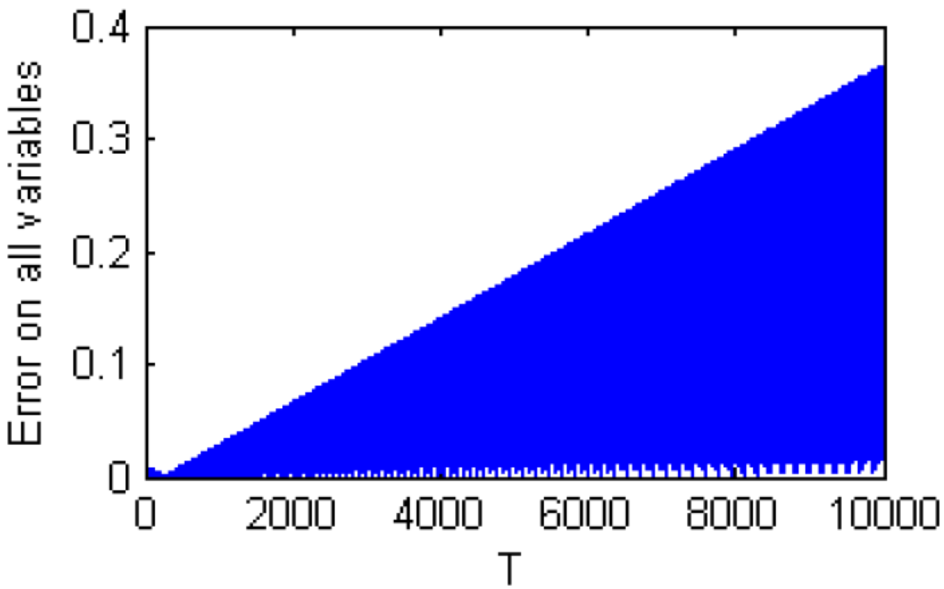
$$h = 10^{-5}$$

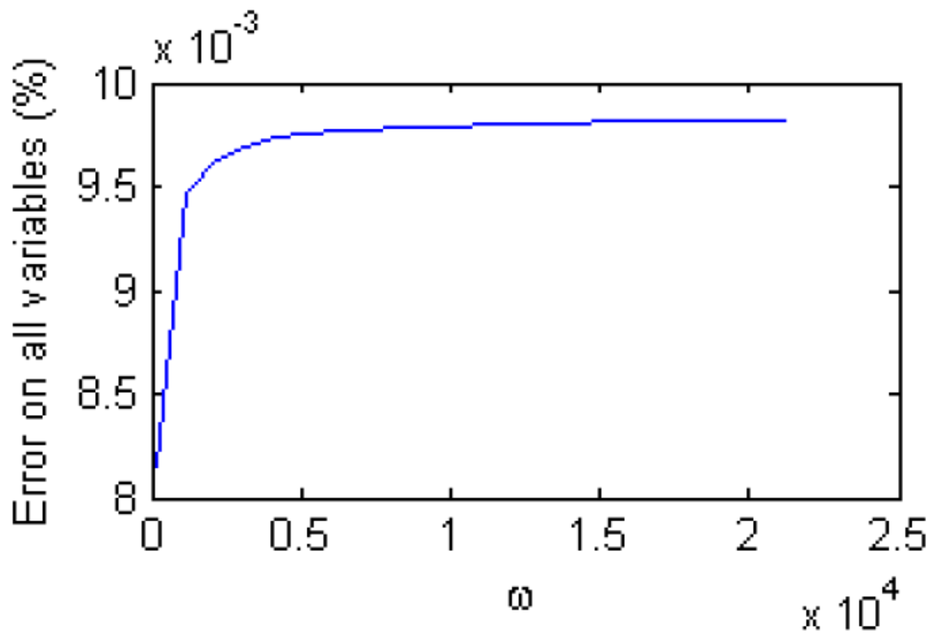

Expansions of stiff springs
Middle point position of the first stiff spring
Energies of stiff springs
Total energy of stiff springs
No.1
No.2
No.3
FLAVOR
$\delta = 0.002, \tau = 0.0005$
Velocity Verlet
$h = 10^{-5}$
IMEX
$\delta = 0.002$
Impulse Method
$\delta = 0.002$

Numerical error analysis



$$H(x,y,z,p_x,p_y,p_z) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}p_z^2 + x^4 + \epsilon^{-1}\frac{\omega_1}{2}(y-x)^2 + \epsilon^{-1}\frac{\omega_2}{2}(z-y)^2$$

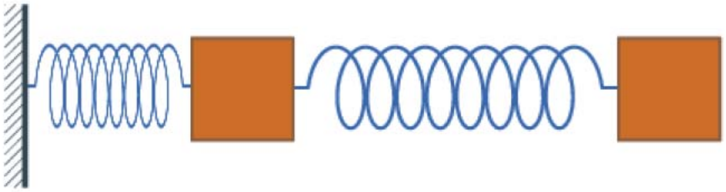




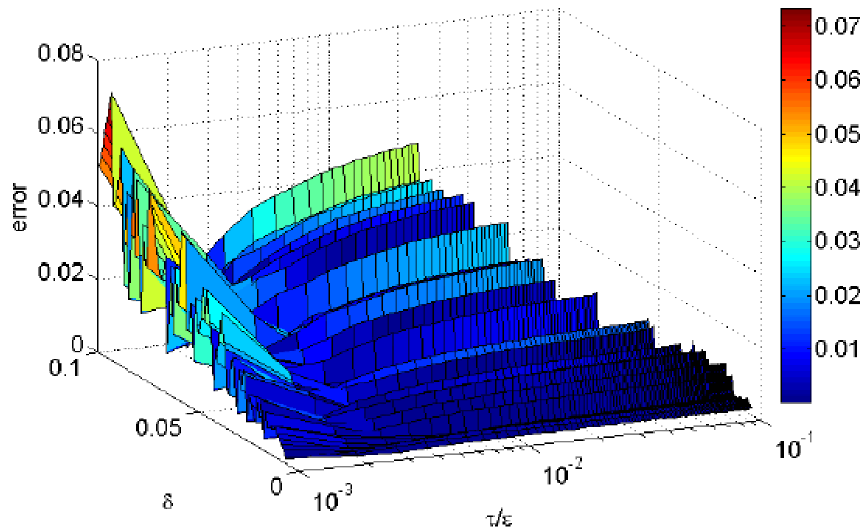
Error grows linearly with total simulation time

Error asymptotically independent from stiff parameter

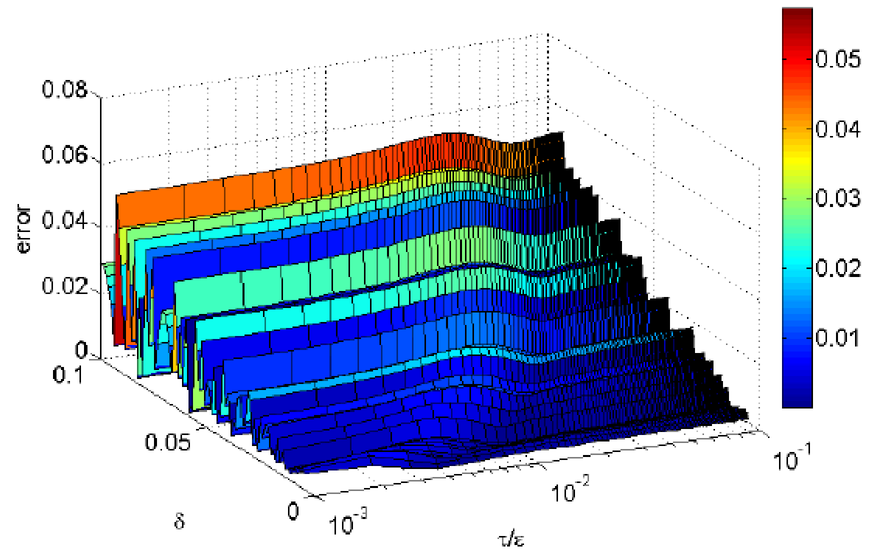
Numerical error analysis



$$H(x, y, p_x, p_y) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}x^2 + \frac{\omega^2}{2}(y - x)^2$$

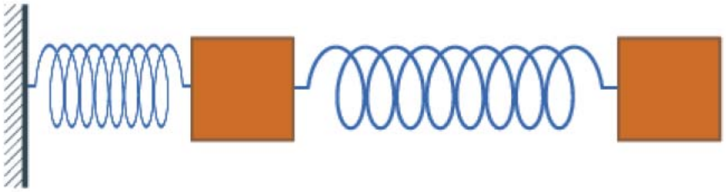


(a) *Error of non-intrusive FLAVOR as a function of δ and τ/ϵ*

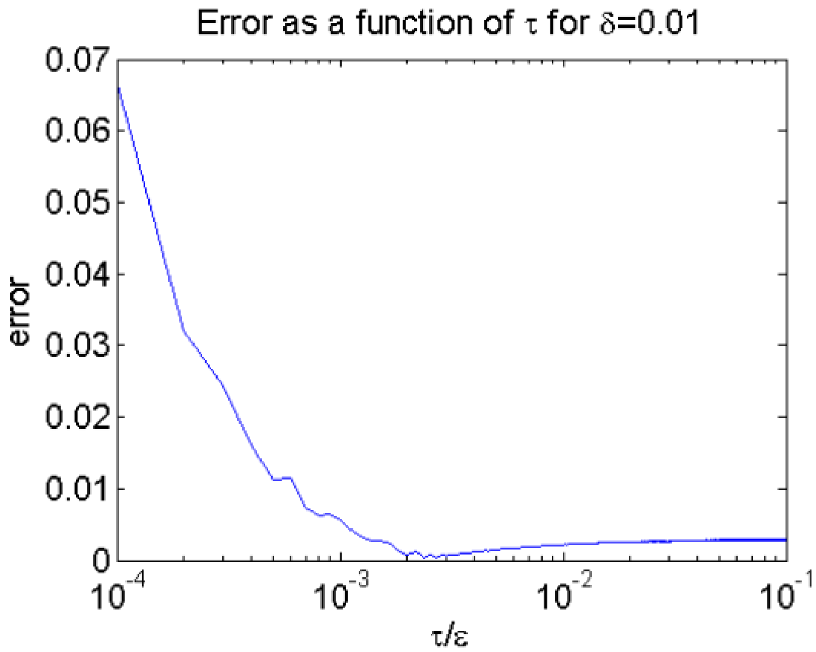


(b) *Error of artificial FLAVOR as a function of δ and τ/ϵ*

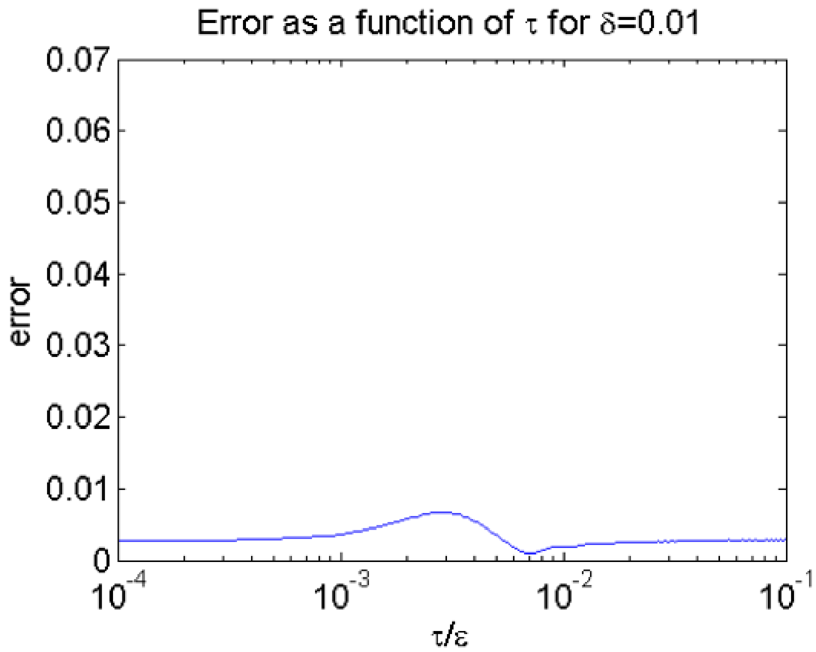
Numerical error analysis



$$H(x,y,p_x,p_y) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}x^2 + \frac{\omega^2}{2}(y-x)^2$$

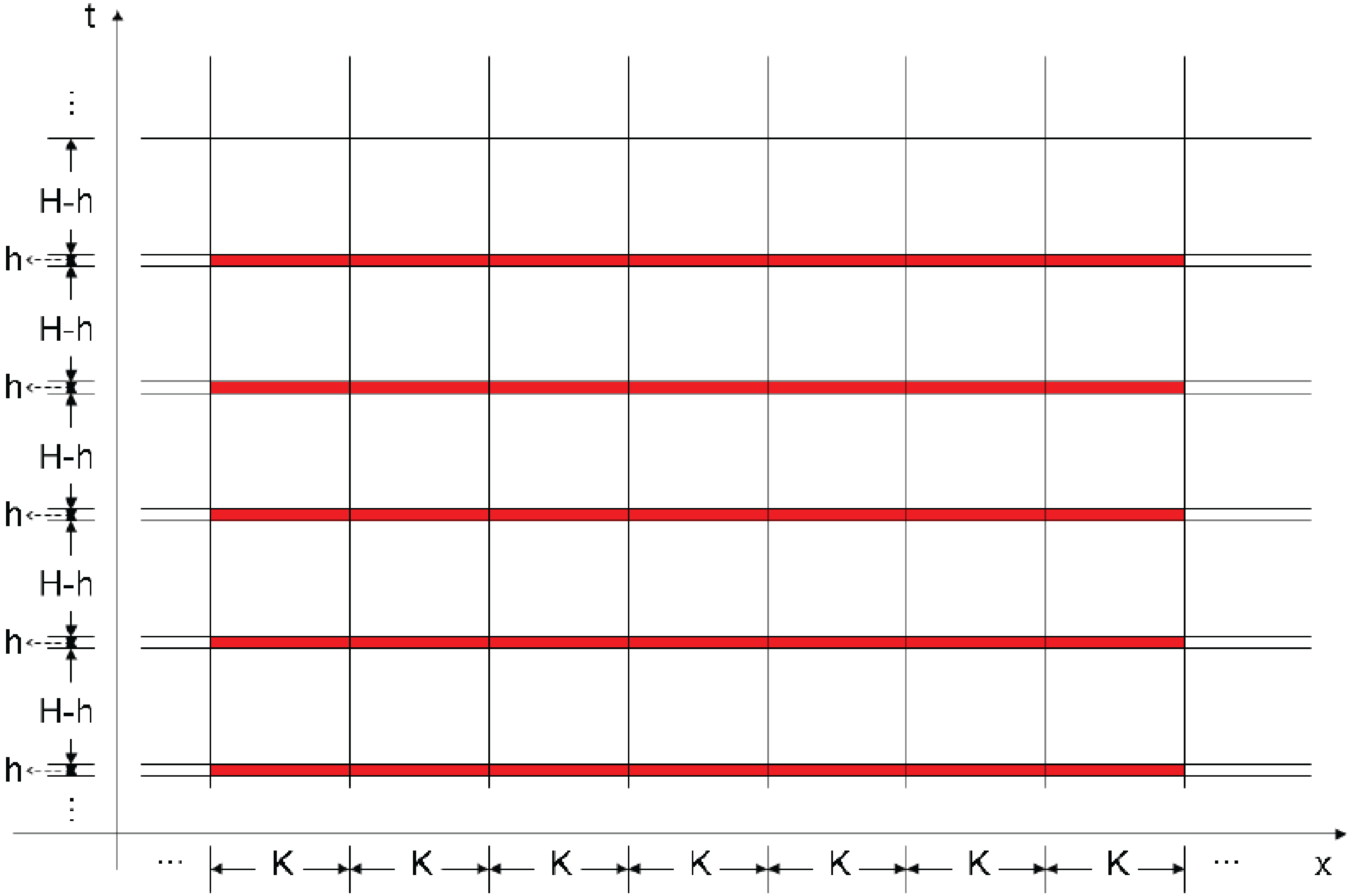


(e) ***Error dependence on τ/ϵ for a given δ: non-intrusive FLAVOR***



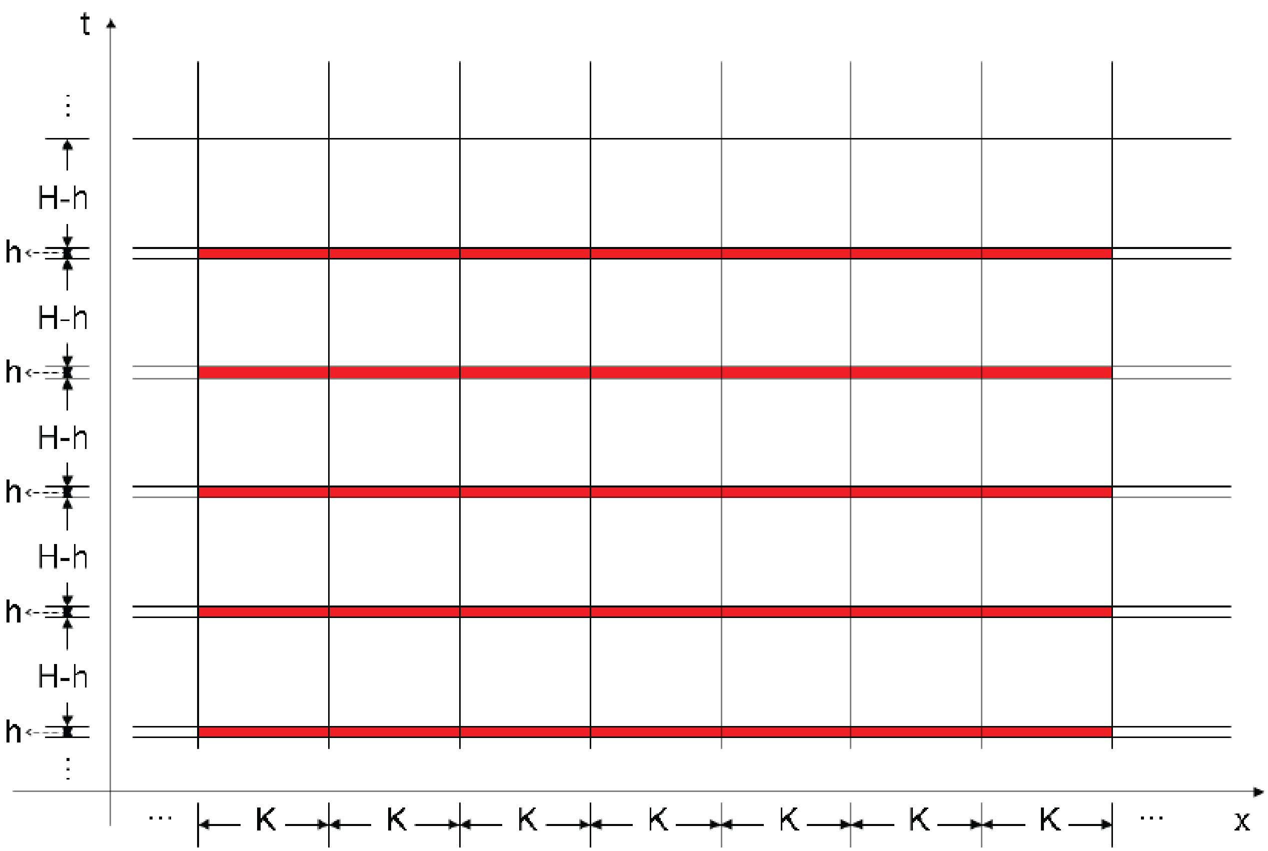
(f) ***Error dependence on τ/ϵ for a given δ: artificial FLAVOR***

Extension to PDEs



Conservation law with Ginzburg-Landau source

$$u_t + f(u)_x = \epsilon^{-1} u(1 - u^2)$$



$$u_{i+1,j+1} = u_{i+1,j} - h\Big(f_u(u_{i+1,j}) \frac{u_{i+1,j} - u_{i,j}}{k} + \epsilon^{-1} u_{i+1,j}(1 - u_{i+1,j}^2) \Big)$$

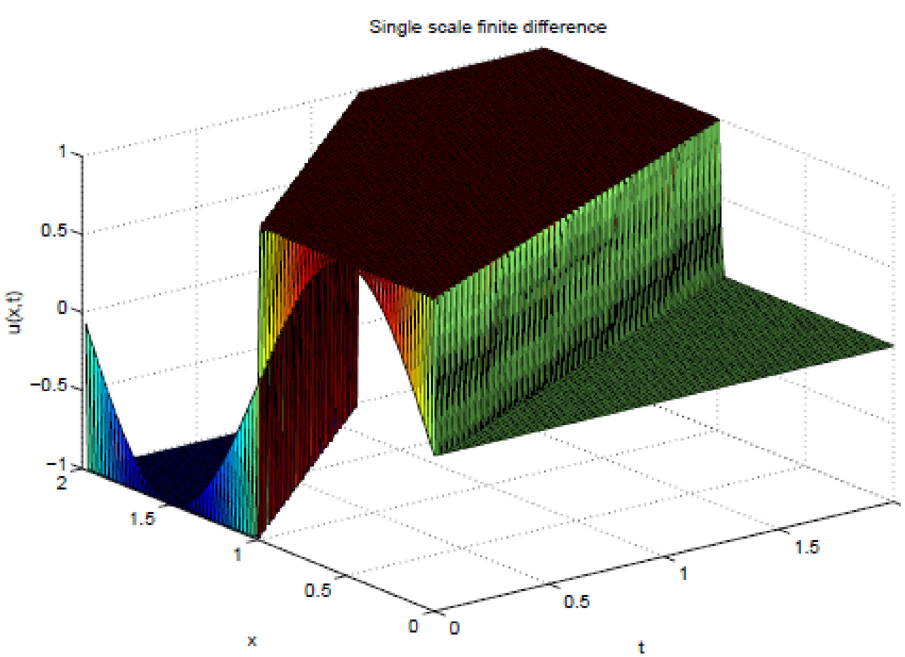
Conservation law with Ginzburg-Landau source

$$u_t + f(u)_x = \epsilon^{-1} u(1 - u^2)$$

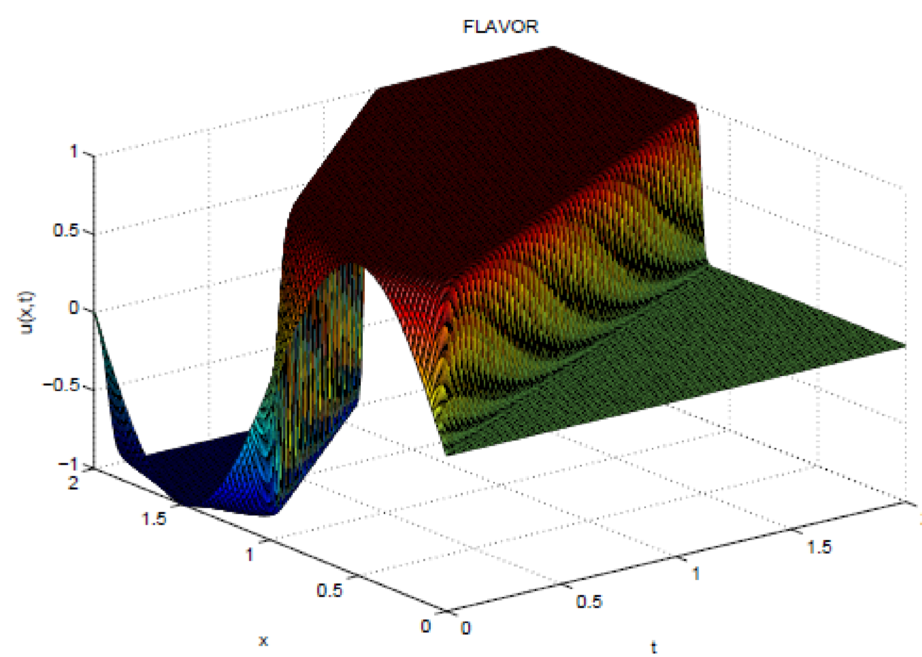
$\epsilon = 2.10^{-3}$

$\frac{HK}{2hk} = 312.5 \text{ acceleration}$

Single scale finite difference



FLAVOR



Multisymplectic (Hamiltonian) PDEs

A PDE is said to be multisymplectic if it can be written as

$$\mathcal{M} z_t + \mathcal{K} z_x = \nabla_z H(z)$$

$z(x,t) \in \mathbb{R}^n$

$\mathcal{M}$, $\mathcal{K}$: $n \times n$ skew symmetric matrices on $\mathbb{R}^n$

$H \; : \; \mathbb{R}^n \to \mathbb{R}$ smooth function of z

$$(x,t) \in \mathbb{R}^2$$

Ex: Non linear Wave equation

$$u_{tt} - u_{xx} + V'(u) = 0$$

$\Updownarrow$

$$z = (u, v, w)^T \qquad \begin{cases} -v_t + w_x = & V'(u) \\ -u_x = & -w \\ u_t = v \end{cases}$$

$\Updownarrow$

$$\boxed{\mathcal{M} z_t + \mathcal{K} z_x = \nabla_z H(z)} \qquad H(z) = V(u) + \tfrac{1}{2}v^2 - \tfrac{1}{2}w^2$$

$$\mathcal{M} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \mathcal{K} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Multisymplectic structure

$$\mathcal{M} z_t + \mathcal{K} z_x = \nabla_z H(z)$$

$\mathcal{M}$, $\mathcal{K}$: skew symmetric matrices on $\mathbb{R}^n$

$H : \mathbb{R}^n \to \mathbb{R}$ smooth function

The solution preserves the multisymplectic structure

$$\partial_t \langle \mathcal{M} U, V \rangle + \partial_x \langle \mathcal{K} U, V \rangle = 0$$

U, V arbitrary pair of solutions to the variational problem

$$\mathcal{M}\, dz_t + \mathcal{K}\, dz_x = D_{zz} H(z)\, dz, \quad dz \in \mathbb{R}^n$$

Multisymplectic integrator for Hamiltonian PDEs

$$\mathcal{M} z_t + \mathcal{K} z_x = \nabla_z H(z)$$

Obtained as the extremizers of the following action

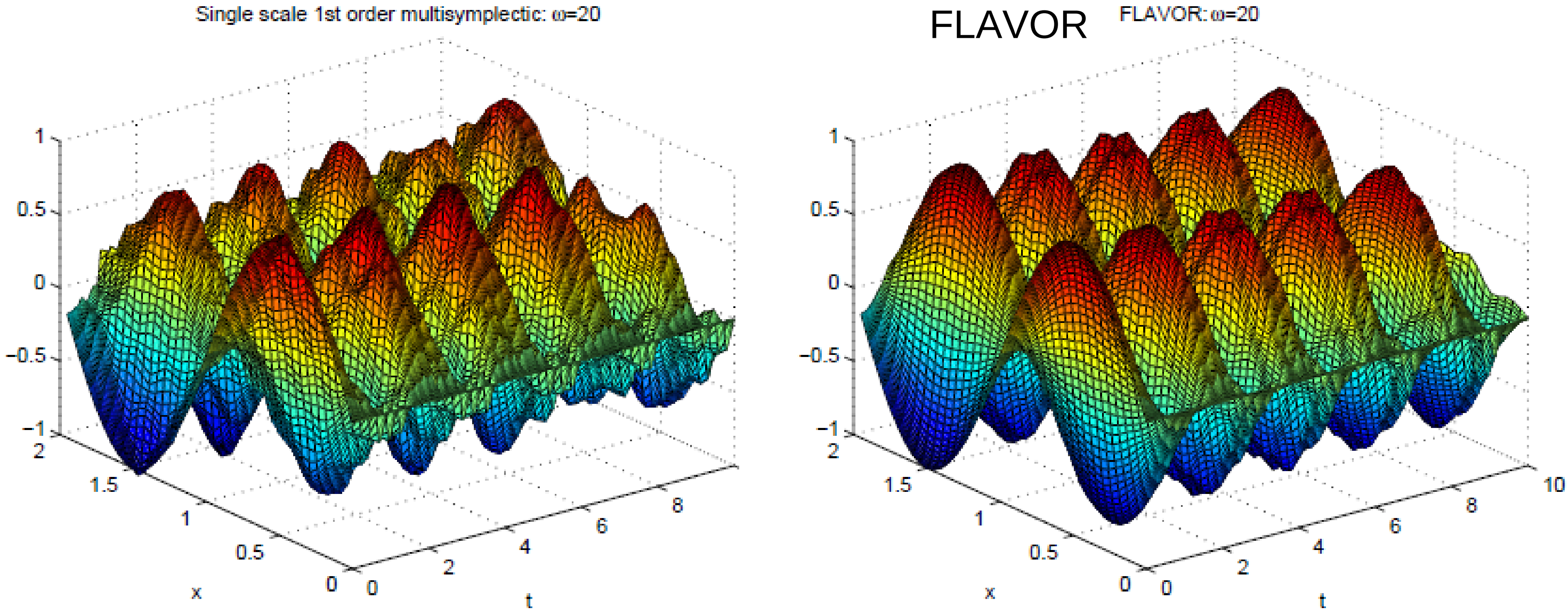
$$\mathcal{S}\big(z(.,.)\big) = \int\int \mathcal{L}(z, z_t, z_x)\, dt\, dx$$

$$\mathcal{L}(z, z_t, z_x) = \tfrac{1}{2} < \mathcal{M} z_t, z > + \tfrac{1}{2} < \mathcal{K} z_x, z > - H(z)$$

FLAVORIZATION

Turn on and off $\frac{1}{\epsilon}$ in the discrete variational formulation

Sine Gordon Wave equation

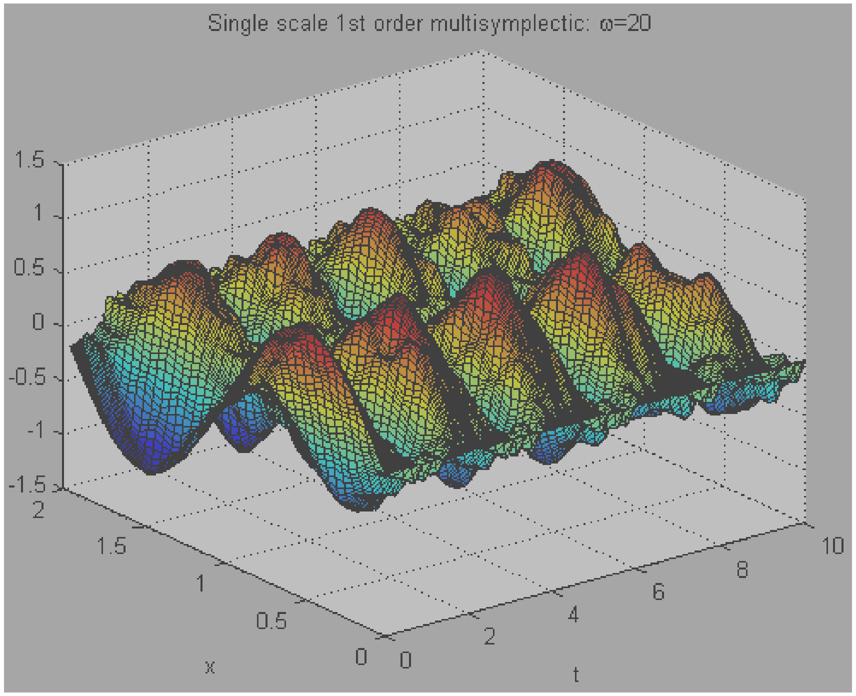


$$u_{tt} - u_{xx} = \omega \sin(\omega u) + \sin(u)$$

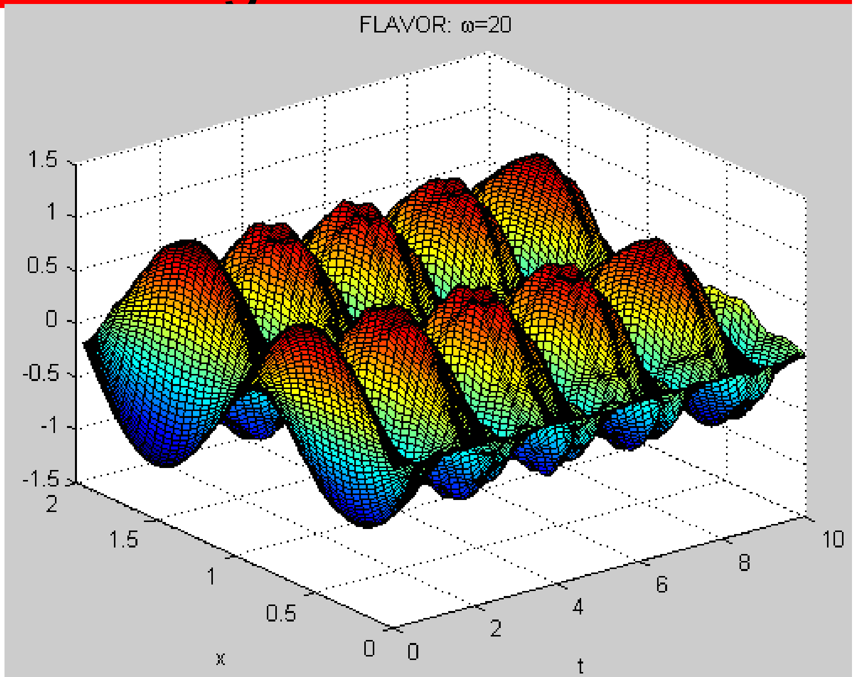
$$\begin{cases} u(x,t) = u(x+2,t) \\ u(x,0) = \sin(\pi x) \\ u_t(x,0) = 0 \end{cases}$$

50x acceleration

FLAVORS are more than softening the stiffness



50x



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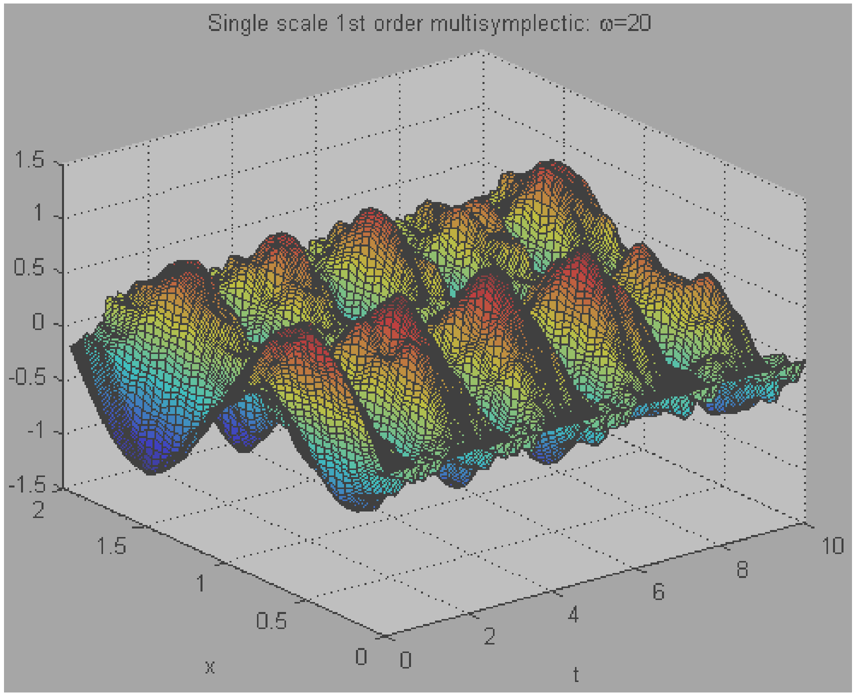
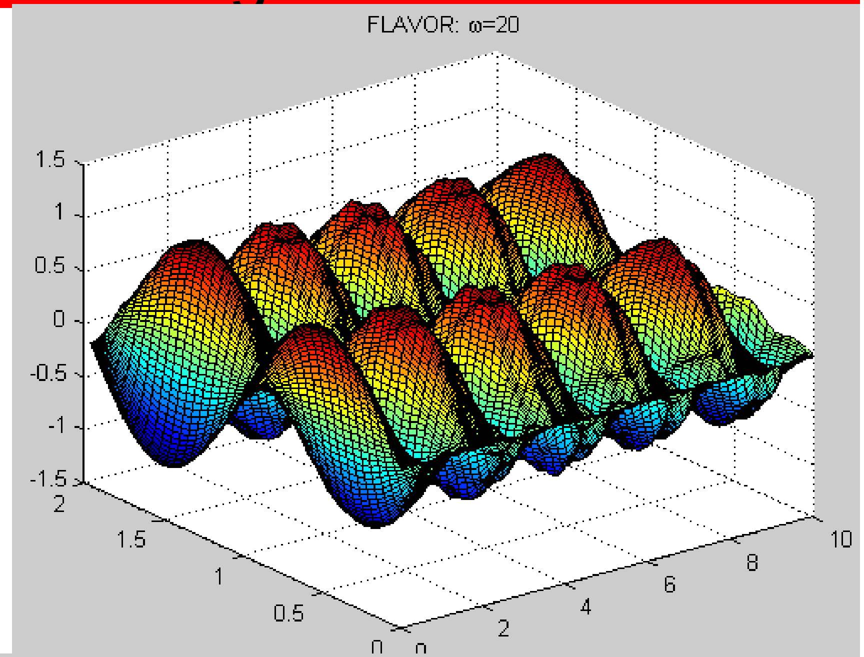
$$h = 0.05/\omega, H = 0.025$$

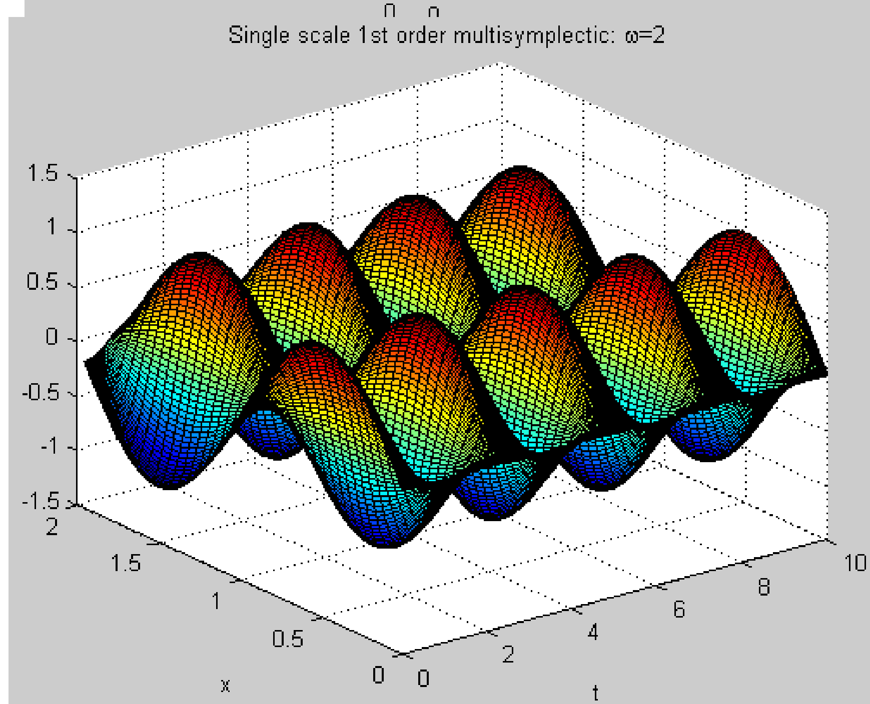
Equivalent to softened stiffness $\omega = 2$?

FLAVORS are more than softening the stiffness



50x





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$$h = 0.05/\omega, H = 0.025$$

Equivalent to softened stiffness $\omega = 2$?

Pseudo-Spectral Methods

$$u_t(x,t) = \mathcal{L}u(x,t)$$

$$u(x,t) = u(x+L,t)$$

$$u_N(x,t) = \sum_{|n|\leq N/2} a_n(t) e^{in2\pi x/L}$$

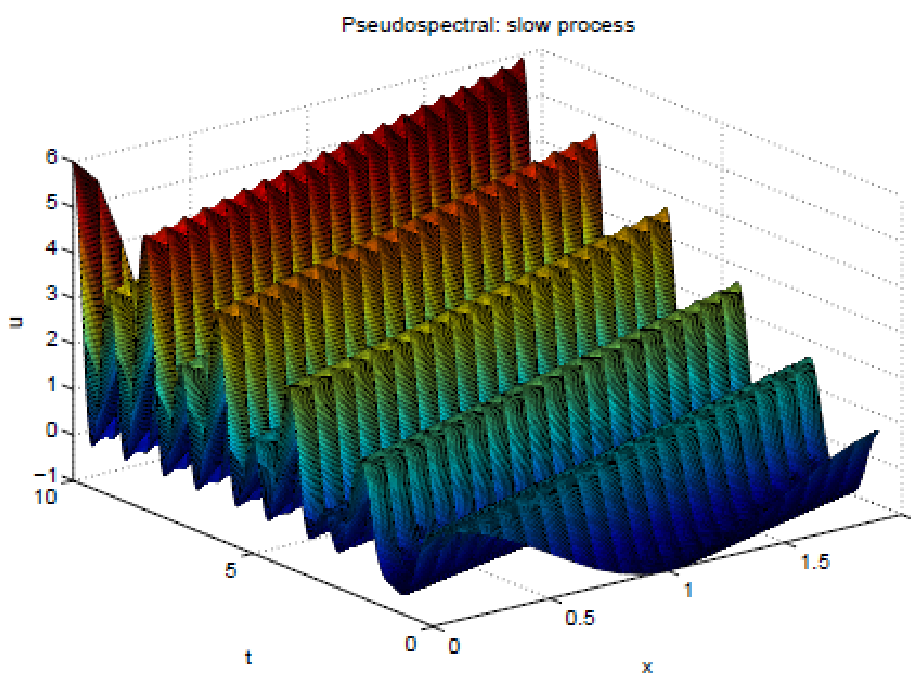
$$u_t(y_j,t) = \mathcal{L}u(y_j,t)$$

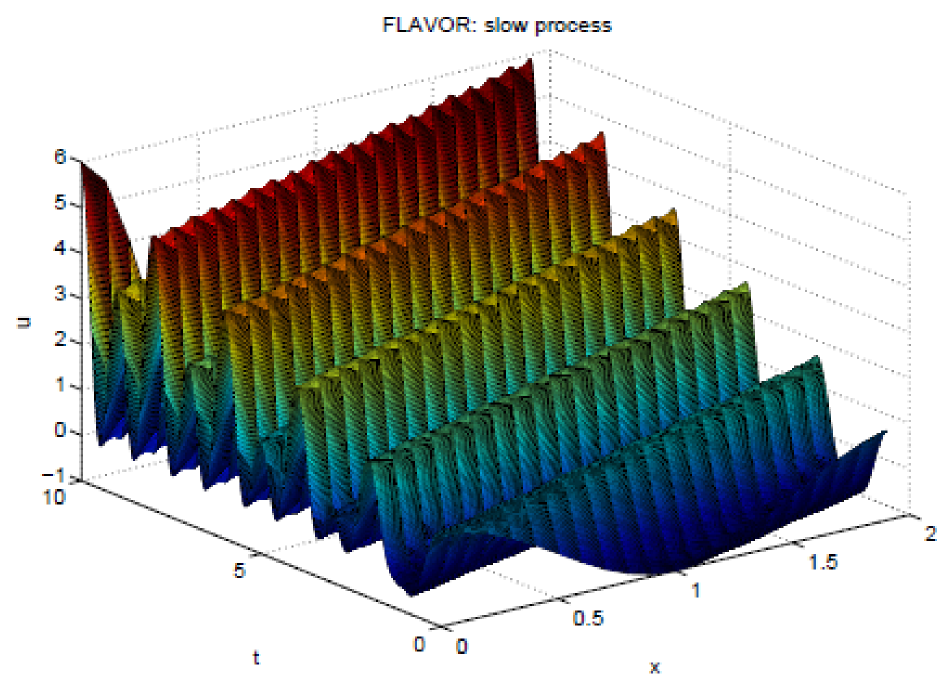
$$y_j = Lj/N,\ j = 0,\ldots,N-1$$

Slow process driven by a non Dirac fast process

$$\begin{cases} u_t + u_x - q^2 = 0 \\ q_t + q_x - p = 0 \\ p_t + p_x + \omega^2 q = 0 \end{cases}$$

50x acceleration

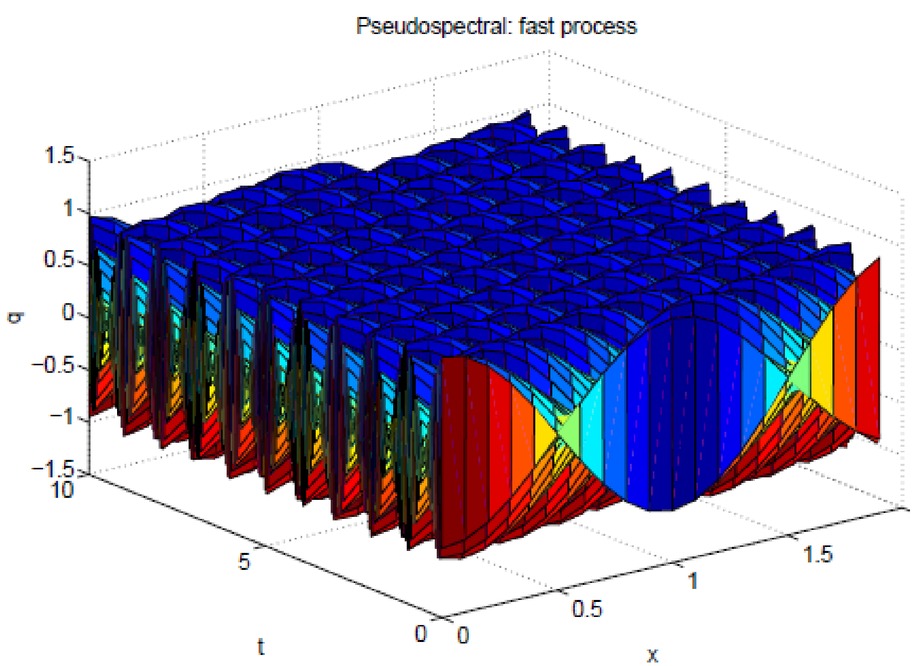


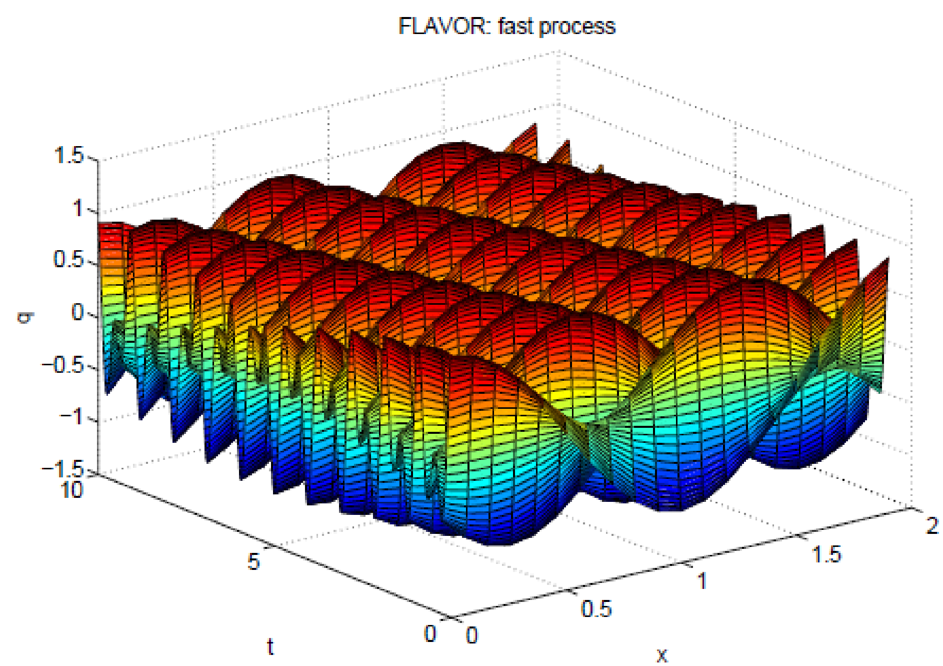


Slow process driven by a non Dirac fast process

$$\begin{cases} u_t + u_x - q^2 = 0 \\ q_t + q_x - p = 0 \\ p_t + p_x + \omega^2 q = 0 \end{cases}$$

50x acceleration





$$du^{\frac{1}{\epsilon},\epsilon} = F(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dt + K(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dW_t$$

$(W_t)_{t\geq 0}$ is a d-dimensional Brownian Motion

$u \to F(u, \alpha, \epsilon)$ is uniformly Lipschitz continuous in $\mathbb{R}^d$

$u \to K(u, \alpha, \epsilon)$ is uniformly Lipschitz continuous in $\mathbb{R}^d$

$\epsilon \to F(u, \alpha, \epsilon)$ is uniformly continuous in the neighborhood of 0

$\epsilon \to K(u, \alpha, \epsilon)$ is uniformly continuous in the neighborhood of 0

$$du^{\alpha,\epsilon} = F(u^{\alpha,\epsilon}, \alpha, \epsilon)\, dt + K(u^{\alpha,\epsilon}, \alpha, \epsilon)\, dW_t$$

$$\begin{aligned} \eta\ :\ \mathbb{R}^d &\longrightarrow \mathbb{R}^{d-p} \times \mathbb{R}^p \\ u &\longrightarrow \left(\eta^x(u), \eta^y(u)\right) \end{aligned}$$

η is a diffeomorphism independent from ϵ, with uniformly bounded C^1, C^2, C^3 derivatives.

$$(x_t^\alpha, y_t^\alpha) = (\eta^x(u_t^{\alpha,0}), \eta^y(u_t^{\alpha,0}))$$

$$dx^\alpha = g(x^\alpha, y^\alpha)\, dt + \sigma(x^\alpha, y^\alpha)\, dW_t$$

g is $d-p$ dimensional vector field, σ is a $(d-p)\times d$-dimensional matrix field, g and σ are uniformly bounded and Lipschitz continuous in x and y.

The system is characterized by **hidden** Slow and Fast variables

$$du^{\alpha,\epsilon} = F(u^{\alpha,\epsilon}, \alpha, \epsilon)\, dt + K(u^{\alpha,\epsilon}, \alpha, \epsilon)\, dW_t$$

$$dx^{\alpha} = g(x^{\alpha}, y^{\alpha})\, dt + \sigma(x^{\alpha}, y^{\alpha})\, dW_t$$

There exists a family of probability measures $\mu(x, dy)$ on $\mathbb{R}^p$, $r \to \chi(r)$ bounded on compact sets, a positive function $T \to E_1(T)$ such that $\lim_{T\to 0} E_1(T) = 0$, a positive function $T \to E_2(T)$ such that $\lim_{T\to\infty} E_2(T) = 0$, and such that for all x_0, y_0, T and φ

$$\left|\frac{1}{T}\int_0^T \mathbb{E}[\varphi(y_s^{\alpha})]\, ds - \int \varphi(y)\mu(x_0, dy)\right| \leq \chi\big(\|(x_0, y_0)\|\big)\big(E_1(T) + E_2(T\alpha^{\nu})\big) \max_{r\leq 3} \|\varphi\|_{C^r}$$

For all u_0, $T > 0$, $\sup_{0\leq t\leq T} \mathbb{E}\Big[\chi\big(\|u_t^{\alpha,0}\|\big)\Big]$ is uniformly bounded in $\alpha \geq 1$.

Hidden fast variables are locally ergodic

For all u_0, $T > 0$, $\sup_{0\leq n\leq T/\delta} \mathbb{E}\Big[\chi\big(\|\bar{u}_{n\delta}\|\big)\Big]$ is uniformly bounded in ϵ, $0 < \delta \leq h_0$, $\tau \leq \min(\tau_0\epsilon, \delta)$.

$$du^{\frac{1}{\epsilon},\epsilon} = F(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dt + K(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dW_t$$

Legacy numerical integrator

There exists a constant $h_0 > 0$ and a normal random vector $\xi(\omega)$ such that for for $h \leq h_0 \min(\frac{1}{\alpha^\nu}, 1)$, $0 < \epsilon \leq 1 \leq \alpha$

$$\left(\mathbb{E}\Big[\big|\Phi_h^{\alpha,\epsilon}(u) - u - hF(u,\alpha,\epsilon) - \sqrt{h}\xi(\omega)K(u,\alpha,\epsilon)\big|^2\Big)\right)^{\frac{1}{2}} \leq Ch^{\frac{3}{2}}(1+\alpha^{\frac{3\nu}{2}})$$

Flow Averaging Integrators (FLAVORS)

$$\begin{cases} \bar{u}_0 = u_0 \\ \bar{u}_{(k+1)\delta} = \Phi^{0,\epsilon}_{\delta-\tau}(.,\omega'_k) \circ \Phi^{\frac{1}{\epsilon},\epsilon}_{\tau}(\bar{u}_{k\delta},\omega_k) \\ \bar{u}_t = \bar{u}_{k\delta} \quad \text{for} \quad k\delta \leq t < (k+1)\delta \end{cases}$$

$$\epsilon \ll \delta \ll h_0,\ \tau \ll \epsilon^\nu \text{ and } \left(\frac{\tau}{\epsilon^\nu}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\epsilon^\nu}$$

Rule of thumb $\delta \sim 0.1\frac{\tau}{\epsilon^\nu}$

Two scale flow convergence

$(\xi^\epsilon_t)_{t\in\mathbb{R}^+}$: a sequence of (progressively measurable) stochastic processes on $\mathbb{R}^d$ indexed by $\epsilon > 0$.

$(X_t)_{t\in\mathbb{R}^+}$: a progressively measurable stochastic process on $\mathbb{R}^m$ $(m \le d)$

$\nu(x, dy)$: A function from $\mathbb{R}^m$ onto the space of measures of probability on $\mathbb{R}^d$.

Definition. *We say that the process ξ^ϵ F-converges towards $\nu(X, dy)$ as $\epsilon \downarrow 0$ and write $\xi^\epsilon \xrightarrow[\epsilon\to 0]{F} \nu(X, dy)$ if and only if for all function φ bounded and uniformly Lipshitz-continuous on $\mathbb{R}^d$, and for all $t > 0$*

$$\lim_{h\to 0}\lim_{\epsilon\to 0}\frac{1}{h}\int_t^{t+h}\mathbb{E}\big[\varphi(\xi^\epsilon_s)\big]\,ds = \mathbb{E}\Big[\int_{\mathbb{R}^d}\varphi(y)\nu(X_t, dy)\Big]$$

$$du^{\frac{1}{\epsilon},\epsilon} = F(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dt + K(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dW_t$$

Legacy code/simulator

There exists $\nu, h_0 > 0$ and a Gaussian normal random vector $\xi(\omega)$ such that for for $h \leq h_0 \min(\frac{1}{\alpha^\nu}, 1)$, $0 < \epsilon \leq 1 \leq \alpha$

$$\left(\mathbb{E}\Big[\Big|\Phi_h^{\alpha,\epsilon}(u) - u - hF(u,\alpha,\epsilon) - \sqrt{h}\xi(\omega)K(u,\alpha,\epsilon)\Big|^2\Big]\right)^{\frac{1}{2}} \leq Ch^{\frac{3}{2}}(1+\alpha^{\frac{3\nu}{2}})$$

Direct simulation requires

$$h \ll \epsilon^\nu$$

$$du^{\frac{1}{\epsilon},\epsilon} = F(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dt + K(u^{\frac{1}{\epsilon},\epsilon}, \frac{1}{\epsilon}, \epsilon)\, dW_t$$

Theorem

$$u_t^{\frac{1}{\epsilon},\epsilon} \xrightarrow[\epsilon\to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\lim_{h\to 0} \lim_{\epsilon\to 0} \frac{1}{h} \int_t^{t+h} \mathbb{E}\big[\varphi(u_s^{\epsilon})\big]\, ds = \mathbb{E}\big[\int_{\mathbb{R}^p} \varphi(\eta^{-1}(X_t, y))\mu(X_t, dy)\big]$$

$$dX_t = \int g(X_t, y)\, \mu(X_t, dy)\, dt + \bar{\sigma}(X_t)\, dB_t \qquad X_0 = x_0$$

$$\bar{\sigma}\bar{\sigma}^T = \int \sigma\sigma^T(x, y)\, \mu(x, dy)$$

$$\begin{cases} \bar{u}_0 = u_0 \\ \bar{u}_{(k+1)\delta} = \Phi^{0,\epsilon}_{\delta-\tau}(.,\omega'_k) \circ \Phi^{\frac{1}{\epsilon},\epsilon}_{\tau}(\bar{u}_{k\delta},\omega_k) \\ \bar{u}_t = \bar{u}_{k\delta} \quad \text{for} \quad k\delta \le t < (k+1)\delta \end{cases}$$

Theorem

$$\bar{u}_t \xrightarrow[\epsilon\to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\frac{\tau}{\epsilon^\nu} \downarrow 0,\ \frac{\epsilon^\nu}{\tau}\delta \downarrow 0 \text{ and } \left(\frac{\tau}{\epsilon^\nu}\right)^{\frac{3}{2}}\frac{1}{\delta} \downarrow 0.$$

$$\epsilon^\nu \ll \delta \ll h_0,\ \tau \ll \epsilon^\nu \text{ and } \left(\frac{\tau}{\epsilon^\nu}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\epsilon^\nu}.$$

Proof

Use the convergence of generators

Skorokhod 1987

Let $\xi_n(t)$ be a sequence of stochastic processes.

If the sequence of generators of ξ_n
is converging towards a generator L
then ξ_n is converging in distrubution
towards the stochastic process generated by L.

For n large enough,

$$\mathbb{E}\Big[\varphi\big(\xi_n(t+h)\big) - \varphi\big(\xi_n(t)\big) - hL\varphi\big(\xi_n(t)\big)\Big] = o(h)$$

SDE with hidden slow and fast variables

$$\begin{cases} du = \frac{4}{3(u+v)^2}\left(-\frac{1}{2}\left(\frac{v-u}{2}\right)^2 + 5\sin(2\pi t)\right)dt - \frac{1}{\epsilon}\left(\left(\frac{u+v}{2}\right)^3 + c - \frac{v-u}{2}\right)dt - \sqrt{\frac{2}{\epsilon}}dW_t \\ dv = \frac{4}{3(u+v)^2}\left(-\frac{1}{2}\left(\frac{v-u}{2}\right)^2 + 5\sin(2\pi t)\right)dt + \frac{1}{\epsilon}\left(\left(\frac{u+v}{2}\right)^3 + c - \frac{v-u}{2}\right)dt + \sqrt{\frac{2}{\epsilon}}dW_t \end{cases}$$

Hidden slow and fast variables

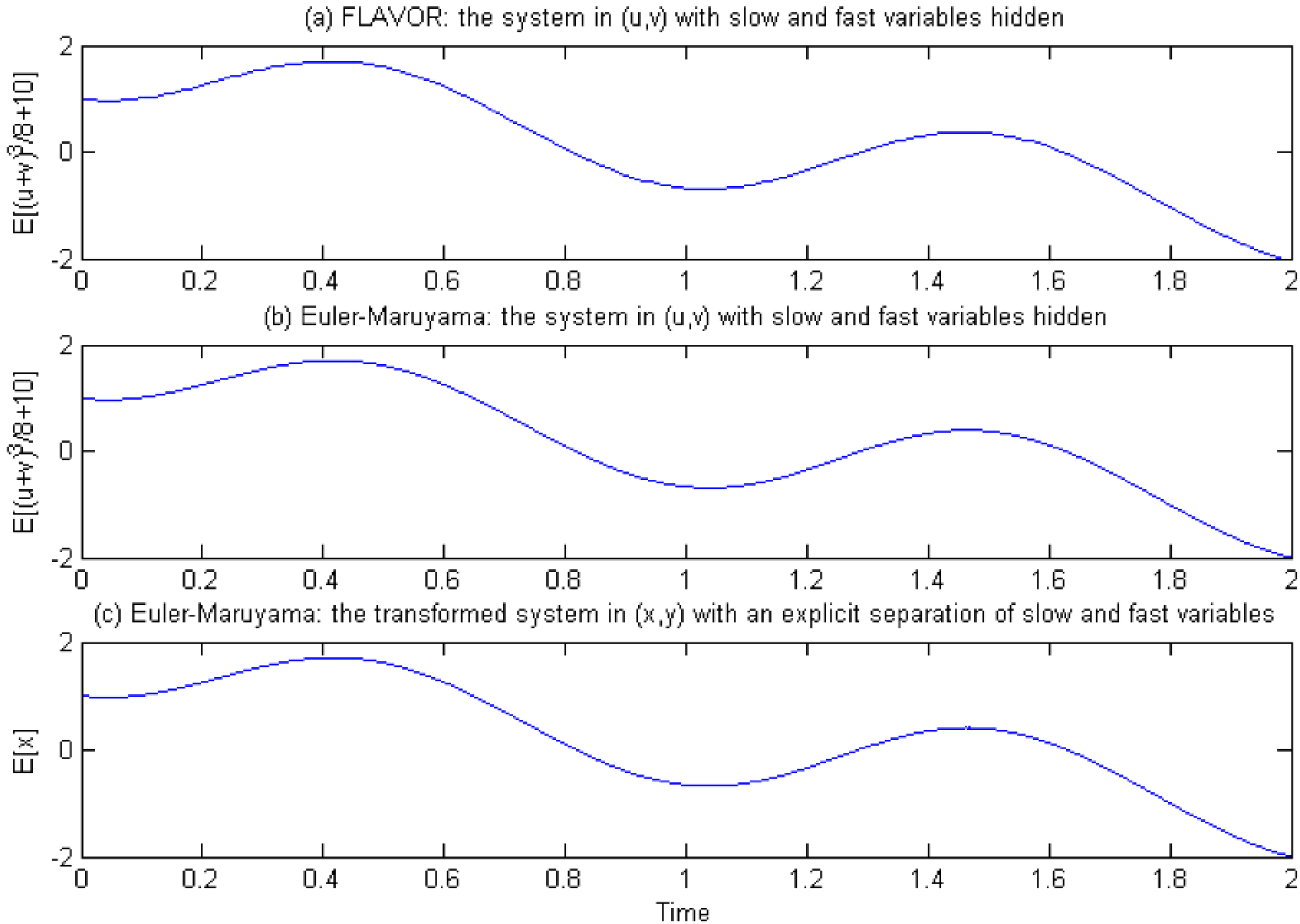
$$\begin{cases} u = (x-c)^{1/3} - y \\ v = (x-c)^{1/3} + y \end{cases}$$

$$\begin{cases} dx = -\frac{1}{2}y^2 dt + 5\sin(2\pi t)dW_t \\ dy = \frac{1}{\epsilon}(x-y)dt + \sqrt{\frac{2}{\epsilon}}dW_t \end{cases}$$

Proposed Method (FLAVORS)

Average the flow of the Legacy integrator for the stiff SDE
With hidden slow and fast processes
by turning on and off stiff parameters

SDE with hidden slow and fast variables



FLAVOR with hidden

$\delta = 0.01$

$\tau = 10^{-4}$

E-M hidden

$h = 10^{-4}$

E-M explicit

$h = 10^{-4}$

Langevin Equations, i.e. Stochastic Hamiltonian systems on manifolds

$$\begin{cases} dq = M^{-1}p \\ dp = -\nabla V(q)\,dt - \frac{1}{\epsilon}\nabla U(q)\,dt - Cp\,dt + \sqrt{2\beta^{-1}}C^{\frac{1}{2}}dW_t \end{cases}$$

Legacy symplectic integrator for the Hamiltonian part

$$H(q,p) := \frac{1}{2}p^T M^{-1}p + V(q) + \frac{1}{\epsilon}U(q)$$

$$\left|\Phi_h^\alpha(q,p) - (q,p) - h\big(M^{-1}p, -V(q) - \alpha U(q)\big)\right| \le Ch^2(1+\alpha)$$

$$\Phi_h^\alpha(q,p) = \begin{pmatrix} q \\ p \end{pmatrix} + h\begin{pmatrix} M^{-1}\Big(p - h\big(V(q) + \alpha U(q)\big)\Big) \\ -V(q) - \alpha U(q) \end{pmatrix}$$

Ornstein-Uhlenbeck part

$$\begin{cases} dq = M^{-1}p \\ dp = -\nabla V(q)\,dt - \frac{1}{\epsilon}\nabla U(q)\,dt - Cp\,dt + \sqrt{2\beta^{-1}}C^{\frac{1}{2}}\,dW_t \end{cases}$$

Ornstein-Uhlenbeck equations

$$dp = -\alpha Cp\,dt + \sqrt{\alpha}\sqrt{2\beta^{-1}}C^{\frac{1}{2}}\,dW_t$$

Exact stochastic evolution map

$$\Psi^{\alpha}_{t_1,t_2}(q,p) = \left(q, e^{-C\alpha(t_2-t_1)}p + \sqrt{2\beta^{-1}\alpha}C^{\frac{1}{2}}\int_{t_1}^{t_2} e^{-C\alpha(t_2-s)}dW_s\right)$$

Quasi/conformally symplectic FLAVORS

$$\begin{cases} dq = M^{-1}p \\ dp = -\nabla V(q)\,dt - \frac{1}{\epsilon}\nabla U(q)\,dt - Cp\,dt + \sqrt{2\beta^{-1}}C^{\frac{1}{2}}dW_t \end{cases}$$

FLAVOR

$$\begin{cases} (\bar{q}_0, \bar{p}_0) = (q_0, p_0) \\ (\bar{q}_{(k+1)\delta}, \bar{p}_{(k+1)\delta}) = \Phi^0_{\delta-\tau} \circ \Psi^1_{k\delta+\tau,(k+1)\delta} \circ \Phi^{\frac{1}{\epsilon}}_{\tau} \circ \Psi^1_{k\delta,k\delta+\tau}(q,p) \end{cases}$$

$\tau \ll \sqrt{\epsilon} \ll \delta$ and $\left(\frac{\tau}{\sqrt{\epsilon}}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\sqrt{\epsilon}}$ Rule of thumb $\delta \sim 0.1\frac{\tau}{\sqrt{\epsilon}}$

Quasi-Symplectic

Conformally-Symplectic $\quad \Theta^*_\delta \Omega = e^{-c\delta}\Omega$

Quasi/conformally symplectic and symmetric FLAVORS

$$\begin{cases} dq = M^{-1}p \\ dp = -\nabla V(q)\,dt - \frac{1}{\epsilon}\nabla U(q)\,dt - Cp\,dt + \sqrt{2\beta^{-1}}C^{\frac{1}{2}}dW_t \end{cases}$$

FLAVOR

$$(\bar{q}_{(k+1)\delta}, \bar{p}_{(k+1)\delta}) = \Psi^1_{k\delta+\frac{\delta}{2},(k+1)\delta} \circ \Phi^{\frac{1}{\epsilon},*}_{\frac{\tau}{2}} \circ \Phi^{0,*}_{\frac{\delta-\tau}{2}} \circ \Phi^{0}_{\frac{\delta-\tau}{2}} \circ \Phi^{\frac{1}{\epsilon}}_{\frac{\tau}{2}} \circ \Psi^1_{k\delta,k\delta+\frac{\delta}{2}}(q,p)$$

$\tau \ll \sqrt{\epsilon} \ll \delta$ and $\left(\frac{\tau}{\sqrt{\epsilon}}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\sqrt{\epsilon}}$ Rule of thumb $\delta \sim 0.1\frac{\tau}{\epsilon}$

Quasi-Symplectic

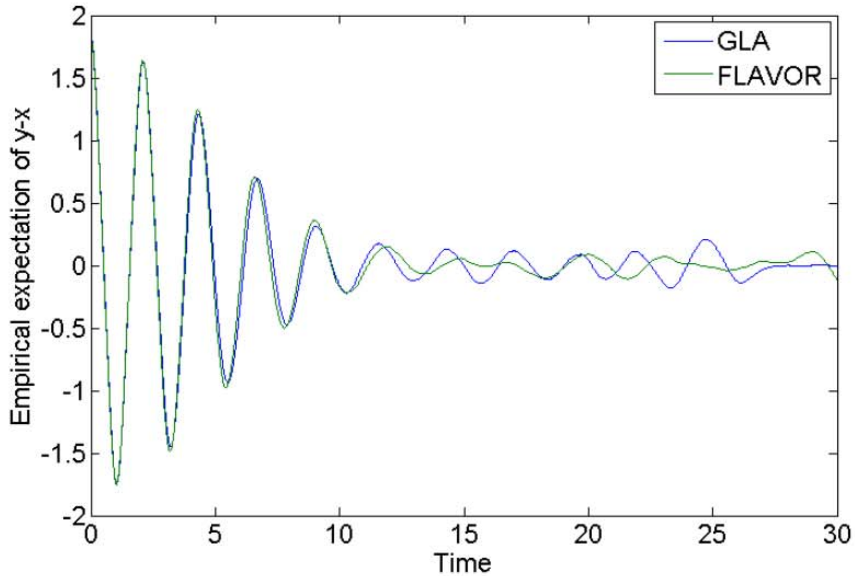
Conformally-Symplectic

Time-reversible

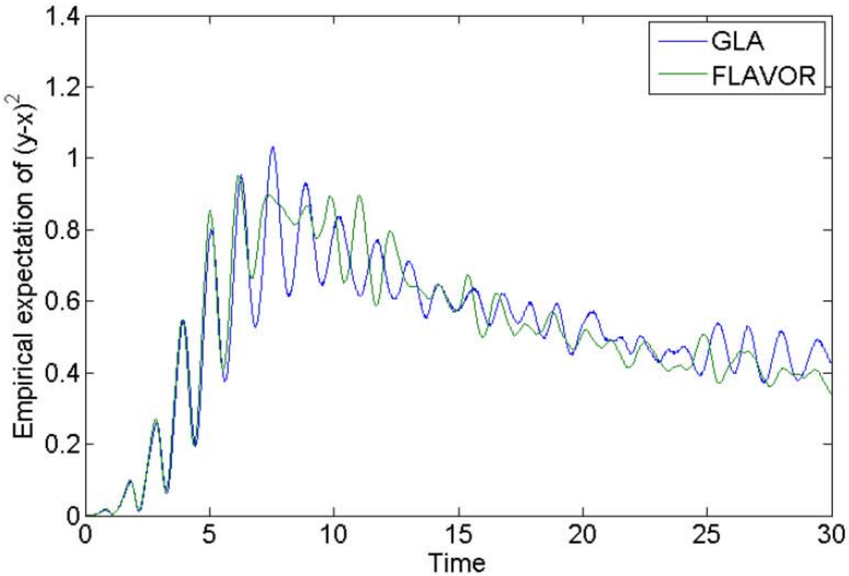
$$\Theta^*_\delta \Omega = e^{-c\delta}\Omega$$

Langevin. Slow noise and friction.

$$\begin{cases} dx = dp_x \\ dy = dp_y \\ dp_x = -\epsilon^{-1}x^3dt - 4(x-y)^3dt - cp_xdt + \sigma dW_t^1 \\ dp_y = -4(y-x)^3dt - cp_ydt + \sigma dW_t^2 \end{cases}$$



(a) $\mathbb{E}\big(y(t) - x(t)\big)$



(b) $\mathbb{E}\big((y(t) - x(t))^2\big)$

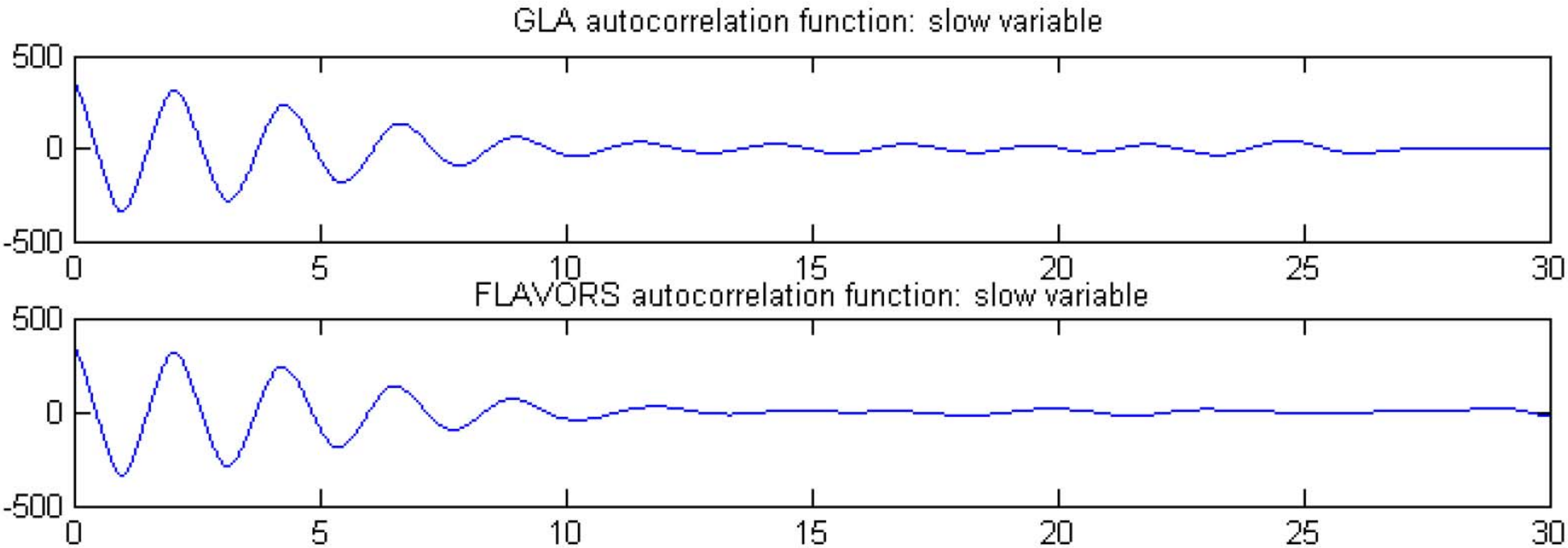
100 samples

GLA $h = 0.001$

FLAVOR $\delta = 0.01$ $\tau = 0.001$

Langevin. Slow noise and friction.

$$\mathbb{E}\Big[\big(y(t) - x(t)\big)\big(y(0) - x(0)\big)\Big]$$



100 samples

Langevin equations on manifolds with fast noise and friction

$$\begin{cases} dq = M^{-1}p \\ dp = -\nabla V(q)\,dt - \frac{1}{\epsilon}\nabla U(q)\,dt - \frac{C}{\epsilon}p\,dt + \sqrt{2\beta^{-1}}\frac{C^{\frac{1}{2}}}{\sqrt{\epsilon}}dW_t \end{cases}$$

Structure preserving FLAVOR

$$\begin{cases} (\bar{q}_0, \bar{p}_0) = (q_0, p_0) \\ (\bar{q}_{(k+1)\delta}, \bar{p}_{(k+1)\delta}) = \Phi^0_{\delta-\tau} \circ \Phi^{\frac{1}{\epsilon}}_{\tau} \circ \Psi^{\frac{1}{\epsilon}}_{k\delta, k\delta+\tau}(q,p) \end{cases}$$

$$\tau \ll \sqrt{\epsilon} \ll \delta \text{ and } \left(\frac{\tau}{\sqrt{\epsilon}}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\sqrt{\epsilon}}$$

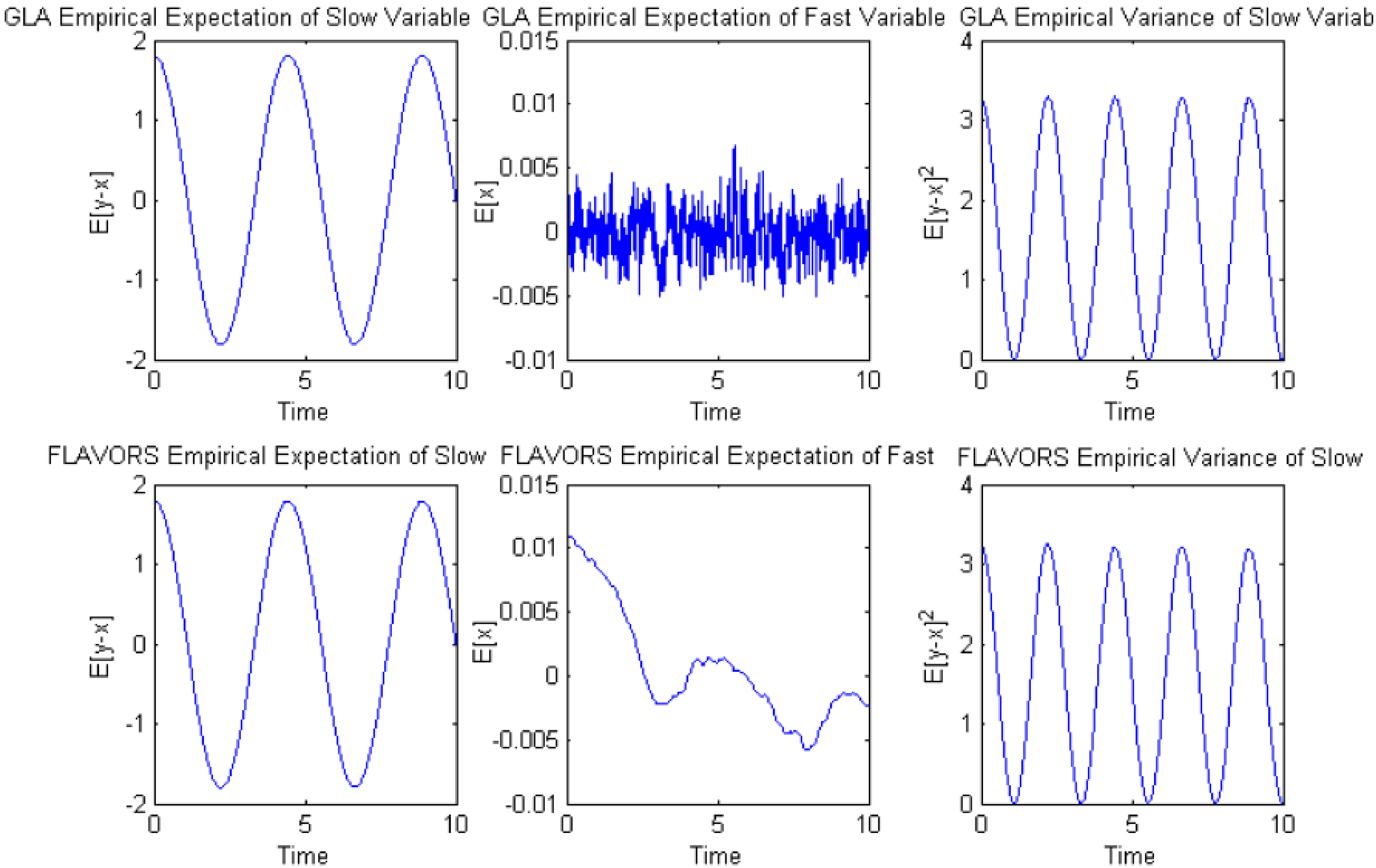
$$\text{Rule of thumb } \delta \sim 0.1\frac{\tau}{\sqrt{\epsilon}}$$

Langevin. Fast noise and friction.

$$\begin{cases} dx = dp_x \\ dy = dp_y \\ dp_x = -\omega^4 x^3 dt - (2 + x - y)(x - y)e^x dt - \omega^2 c p_x dt + \omega\sigma dW^t \\ dp_y = -2(y - x)e^x dt \end{cases}$$

$$H(x, y, p_x, p_y) = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2/2 + \frac{1}{4}\omega^4 x^4 + e^x(y - x)^2$$

$$\omega = 100$$



100 samples

GLA

$h = 10^{-4}$

FLAVOR

$\delta = 0.01$

$\tau = 10^{-4}$

Connections with Current methods

$$\frac{du^\epsilon}{dt} = G(u^\epsilon) + \frac{1}{\epsilon}F(u^\epsilon)$$

Two distinct classes of integrators

Stiff systems with fast transience

- Chebychev methods [Lebedev, Abdulle]

Construct high order explicit scheme using explicit Runge-Kutta-Chebyshev formulas

Stiff systems with rapid oscillations

- Poincare map techniques. [Gear, Petzold]
- Geometric Integrators [Lubich et al]
- Filtering techniques [Skeel et al]

Projection/Averaging methods

Equation free methods

I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and K. Theodoropoulos (2003)

C. W. Gear and I. G. Kevrekidis (2003)

I. G. Kevrekidis, C. W. Gear and G. Hummer (2004)

Identify slow variables

Use the legacy code as a microsolver **to Average the instantaneous drift of slow variables** and use a **macro-solver** to update slow variables with the estimated average drift

Convergence

Dror Givon, Ioannis G. Kevrekidis and Raz Kupferman (2006)

Projection/Averaging methods

Equation free methods

Current evolution

Young measure approach to convergence

Zvi Artstein, Jasmine Linshiz, and Edriss S. Titi (2007). Young Measure Approach to Computing Slowly Advancing Fast Oscillations

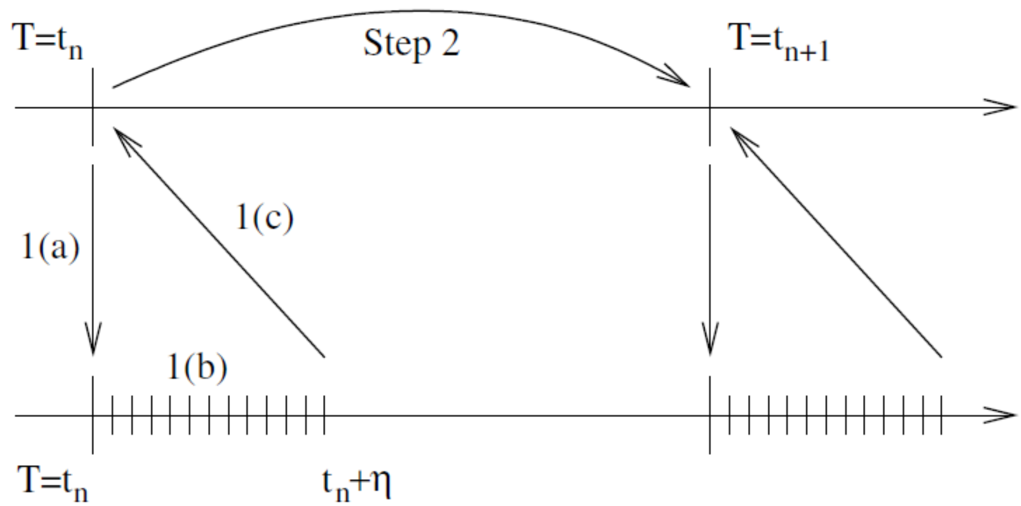
Zvi Artstein, Ioannis G Kevrekidis, Marshall Slemrod and Edriss S Titi (2007)

Artstein, Zvi; Gear, C. William; Kevrekidis, Ioannis G.; Slemrod, Marshall; Titi, Edriss S. (2009). KDV-Burgers type equation with fast dispersion and slow diffusion.

The limit behavior of singularly perturbed systems which may not possess a natural coordinate split into slow and fast dynamics is **depicted as an invariant measure of the fast component drifted by the slow part of the system**

Young measures are used to identify slow observables and evaluate their slow derivatives by numerical differencing.

HMM
Original version



Identify slow variables

Perform M micro-steps with a micro-solver to average the instantaneous drift of slow variables with respect to fast variables

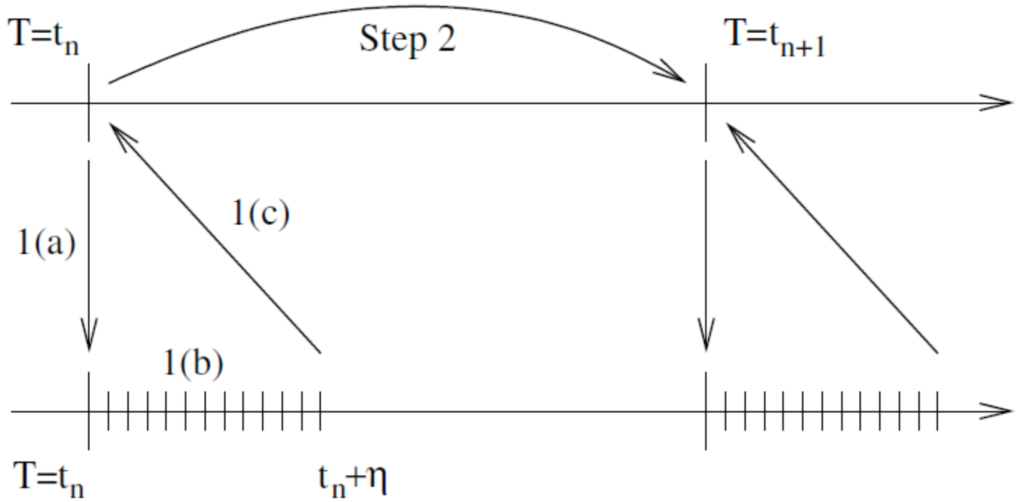
Update slow variables with a macro-solver and the estimated average drift

Weinan E and Bjorn Engquist. The heterogeneous multiscale methods. Commun. Math. Sci., 1(1):87132, 2003

Weinan E, Di Liu, and Eric Vanden-Eijnden (2003). Analysis of multiscale techniques for stochastic dynamical systems.

Eric Vanden-Eijnden. Numerical techniques for multiscale dynamical systems with stochastic effects. Comm. Math. Sci., 1(2):385391, 2003.

HMM: evolution



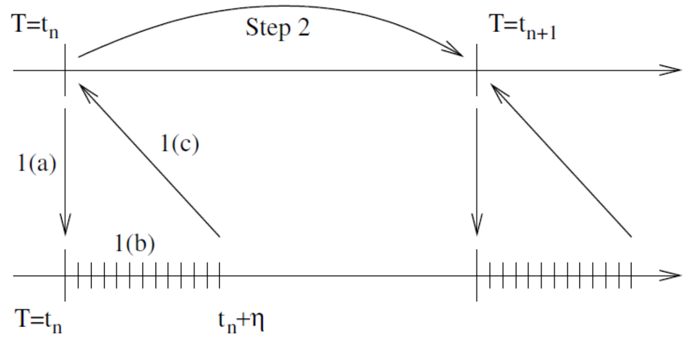
Bjorn Engquist , Richard Tsai (2005) Heterogeneous multiscale methods for stiff ordinary differential equations. Math. Comp., 74(252):1707174.

Identify slow variables on the fly (numerically)

Compute effective drift convolution with a compactly supported kernel

Balancing the different error contributions yields an explicit stable integration method having the **order of the macro scheme**

HMM: evolution



E, Liu, Vanden-Eijnden 2005. J. Chem. Phys. 123, 194107. Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates,

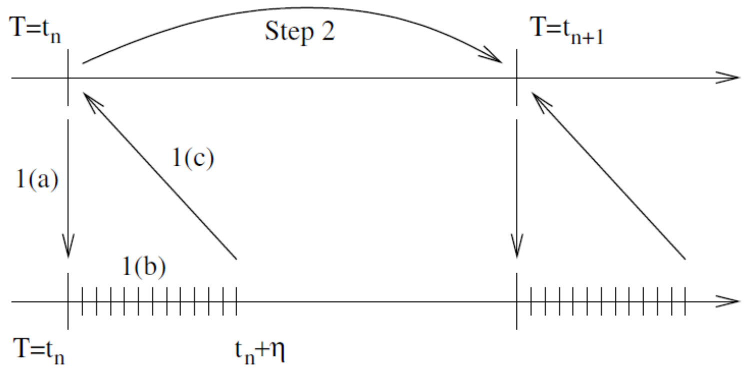
E, Liu, Vanden-Eijnden 2007. J. Comp. Phys. Nested stochastic simulation algorithm for chemical kinetic systems with multiple time scales,

Eric-Vanden-Eijnden (2007) Commun. Math. Sci. Volume 5, Issue 2, 495-505. ON HMM-like integrators and projective integration methods for systems with multiple time scales

If slow variables are hidden via an arbitrary permutation (decomposition u=(x,y)), it is not necessary to explicitly identify them

It is worthwhile to emphasize that, as we will see in Section 3, the algorithm proposed in [7] is quite general and seamless. In particular, it makes no explicit mentioning of the fast and slow variables. At a first sight, this might seem surprising, since there are counterexamples showing that algorithms of the same spirit do not work for deterministic ODEs with separated time scales [8] if the slow variables are not explicitly identified and made use of. But in the present context, the slow variables are linear functions of the original variables, as a consequence of the fact that the state change vectors $\{v_j\}$s are constant vectors, and this is the reason why the seamless algorithm works.

HMM: evolution



E, Liu, Vanden-Eijnden 2005. Comm. Pure App. Math. 58, 1544-1585. Analysis of multiscale methods for stochastic differential equations

Initialize the micro-solver at macro-step n+1 using the last point of the micro-solver at macro-step n

The method is convergent with M=1

Weinan E, Wiqing Ren, Eric-Vanden-Eijnden (2009) A general strategy for designing seamless multiscale methods

- Run the micro-solver using its own time step τ
- Run the macro-solver using its own time step δ
- Exchange data between the micro and macro solvers at every step

High-dimensional Hamiltonian systems with slowly varying quadratic stiff potentials

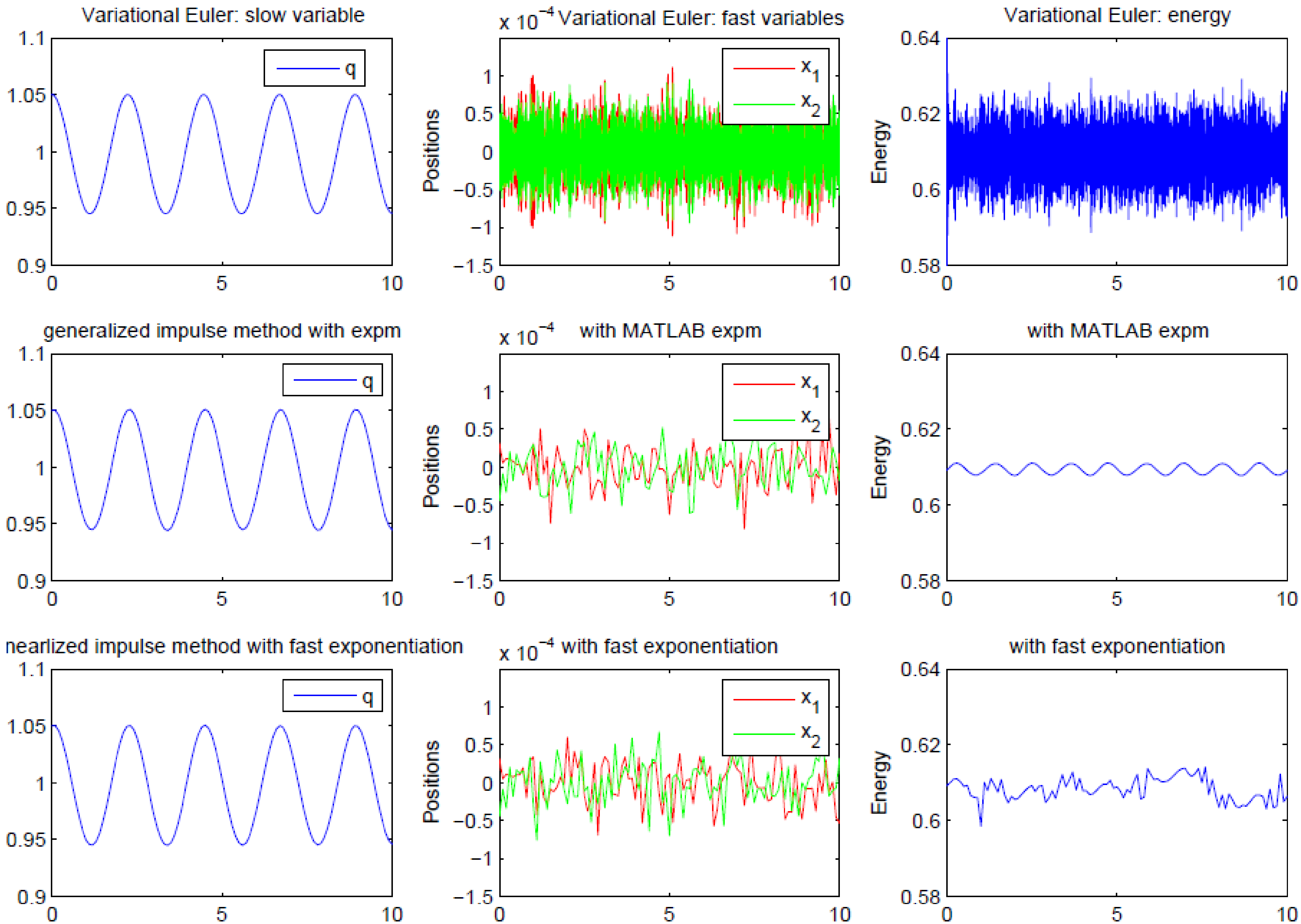
$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}y^T y + (x^T x + q^2 - 1)^2 + \frac{1}{2}\omega^2 x^T T(q) x$$

$q, p \in \mathbb{R}$: Slow variables $\quad \hat{q} = q/10$

$x, y \in \mathbb{R}^d$: Fast variables $\quad d = 200$

$$T(q) = \begin{bmatrix} 1 & \hat{q}^2 & \hat{q}^3 & \dots & \hat{q}^d \\ \hat{q}^2 & 1 & \hat{q}^2 & \dots & \hat{q}^{d-1} \\ \hat{q}^3 & \hat{q}^2 & 1 & \dots & \hat{q}^{d-2} \\ & & \vdots & & \\ \hat{q}^d & \hat{q}^{d-1} & \hat{q}^{d-2} & \dots & 1 \end{bmatrix}$$

h=0.00005 H=0.1 VE->1282s exp->445s fastexp->72s



$$du_t^\epsilon = \big(G(u_t^\epsilon) + \frac{1}{\epsilon}F(u_t^\epsilon)\big)\, dt + \big(H(u_t^\epsilon) + \frac{1}{\sqrt{\epsilon}}K(u_t^\epsilon)\big)\, dW_t$$

$$\eta \,:\, \mathbb{R}^d \longrightarrow \mathbb{R}^{d-p} \times \mathbb{R}^p$$

$$u \longrightarrow \big(\eta^x(u), \eta^y(u)\big)$$

$$(x_t, y_t) := (\eta^x(u_t^\epsilon), \eta^y(u_t^\epsilon))$$

η is a diffeomorphism independent from ϵ, with uniformly bounded C^1, C^2, C^3 derivatives.

$$\begin{cases} dx^\epsilon = g(x^\epsilon, y^\epsilon)\, dt + \sigma(x^\epsilon, y^\epsilon) dW_t, \\ dy^\epsilon = \frac{1}{\epsilon} f(x^\epsilon, y^\epsilon)\, dt + \frac{1}{\sqrt{\epsilon}} Q(x^\epsilon, y^\epsilon) dW_t \end{cases}$$

The system is characterized by hidden Slow and Fast variables

$$du_t^\epsilon = \left(G(u_t^\epsilon) + \frac{1}{\epsilon}F(u_t^\epsilon)\right)dt + \left(H(u_t^\epsilon) + \frac{1}{\sqrt{\epsilon}}K(u_t^\epsilon)\right)dW_t$$

$$\begin{cases} dx^\epsilon = g(x^\epsilon, y^\epsilon)\,dt + \sigma(x^\epsilon, y^\epsilon)dW_t, \\ dy^\epsilon = \frac{1}{\epsilon}f(x^\epsilon, y^\epsilon)\,dt + \frac{1}{\sqrt{\epsilon}}Q(x^\epsilon, y^\epsilon)dW_t \end{cases}$$

$$dY_t = f(x_0, Y_t)\,dt + Q(x_0, Y_t)\,dW_t \qquad Y_0 = y_0$$

There exists a family of probability measures $\mu(x, dy)$ on $\mathbb{R}^p$, $r \to \chi(r)$ bounded on compact sets, a positive function $T \to E(T)$ such that $\lim_{T\to\infty} E(T) = 0$ and such that for all x_0, y_0, T and φ

$$\left|\frac{1}{T}\int_0^T \mathbb{E}\big[\varphi(Y_s)\big] - \int \varphi(y)\mu(x_0, dy)\right| \le \chi\big(\|(x_0, y_0)\|\big)E(T)\max_{r\le 3}\|\varphi\|_{C^r}$$

For all u_0, $T > 0$, $\sup_{0\le t\le T}\mathbb{E}\Big[\chi\big(\|u_t^\epsilon\|\big)\Big]$ is uniformly bounded in ϵ

Hidden fast variables are ergodic

$$du_t^\epsilon = \Big(G(u_t^\epsilon) + \frac{1}{\epsilon}F(u_t^\epsilon)\Big)\,dt + \Big(H(u_t^\epsilon) + \frac{1}{\sqrt{\epsilon}}K(u_t^\epsilon)\Big)\,dW_t$$

Legacy numerical integrator

There exists a constant $h_0 > 0$ and a normal random vector $\xi(\omega)$ such that for for $h \le h_0 \min(\frac{1}{\alpha}, 1)$

$$\left(\mathbb{E}\Big[\big|\Phi_h^\alpha(u,\omega) - u - hG(u) - \alpha h F(u) - \sqrt{h}H(u)\xi(\omega) - \sqrt{\alpha h}K(u)\xi(\omega)\big|^2\Big]\right)^{\frac{1}{2}} \le C h^{\frac{3}{2}}(1+\alpha)^{\frac{3}{2}}$$

Flow Averaging Integrators (FLAVORS)

$$\begin{cases} \bar{u}_0 = u_0 \\ \bar{u}_{(k+1)\delta} = \Phi^0_{\delta-\tau}(.,\omega_k') \circ \Phi^{\frac{1}{\epsilon}}_{\tau}(\bar{u}_{k\delta},\omega_k) \\ \bar{u}_t = \bar{u}_{k\delta} \quad \text{for} \quad k\delta \le t < (k+1)\delta \end{cases}$$

$$\epsilon \ll \delta \ll h_0,\ \tau \ll \epsilon \text{ and } \left(\frac{\tau}{\epsilon}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\epsilon}.$$

Rule of thumb $\delta \sim 0.1\frac{\tau}{\epsilon}$

$$du_t^\epsilon = \left(G(u_t^\epsilon) + \frac{1}{\epsilon}F(u_t^\epsilon)\right) dt + \left(H(u_t^\epsilon) + \frac{1}{\sqrt{\epsilon}}K(u_t^\epsilon)\right) dW_t$$

Theorem

$$u_t^\epsilon \xrightarrow[\epsilon\to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\lim_{h\to 0} \lim_{\epsilon\to 0} \tfrac{1}{h} \int_t^{t+h} \mathbb{E}\big[\varphi(u_s^\epsilon)\big]\, ds = \mathbb{E}\big[\int_{\mathbb{R}^p} \varphi(\eta^{-1}(X_t, y))\mu(X_t, dy)\big]$$

$$dX_t = \int g(X_t, y)\, \mu(X_t, dy)\, dt + \bar\sigma(X_t)\, dB_t \qquad X_0 = x_0$$

$$\bar\sigma\bar\sigma^T = \int \sigma\sigma^T(x, y)\, \mu(x, dy)$$

$$\begin{cases} \bar{u}_0 = u_0 \\ \bar{u}_{(k+1)\delta} = \Phi^0_{\delta-\tau}(., \omega'_k) \circ \Phi_\tau^{\frac{1}{\epsilon}}(\bar{u}_{k\delta}, \omega_k) \\ \bar{u}_t = \bar{u}_{k\delta} \quad \text{for} \quad k\delta \leq t < (k+1)\delta \end{cases}$$

Theorem

$$\bar{u}_t \xrightarrow[\epsilon \to 0]{F} \eta^{-1} * \left(\delta_{X_t} \otimes \mu(X_t, dy)\right)$$

$$\frac{\tau}{\epsilon} \downarrow 0, \ \frac{\epsilon}{\tau}\delta \downarrow 0 \text{ and } \left(\frac{\tau}{\epsilon}\right)^{\frac{3}{2}} \frac{1}{\delta} \downarrow 0.$$

$$\epsilon \ll \delta \ll h_0, \ \tau \ll \epsilon \text{ and } \left(\frac{\tau}{\epsilon}\right)^{\frac{3}{2}} \ll \delta \ll \frac{\tau}{\epsilon}.$$

Chemical kinetic (Bayati-Koumoutsakos-Owhadi)

$$S_1 \overset{1/\epsilon}{\longleftrightarrow} S_2 \overset{1}{\longleftrightarrow} S_3$$

Legacy Integrator: stochastic simulation algorithm

Huge literature: HMM, Equation-free, tau-leaping (7400 entries), slow-scale tau-leaping (Petzold), r-Leaping (Bayati-Koumoutsakos)

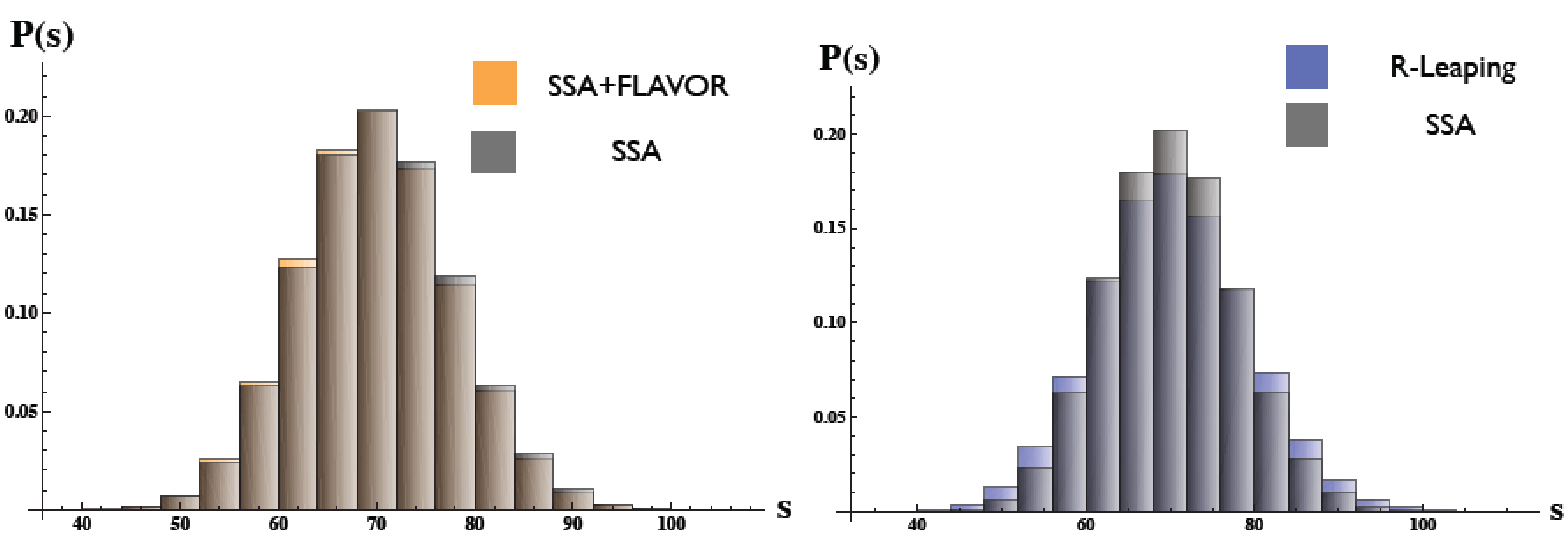


Figure 5: Discrete probability density functions for the species s_2.

Chemical kinetic (Bayati-Koumoutsakos-Owhadi)

$$S_1 \overset{1/\epsilon}{\longleftrightarrow} S_2 \overset{1}{\longleftrightarrow} S_3$$

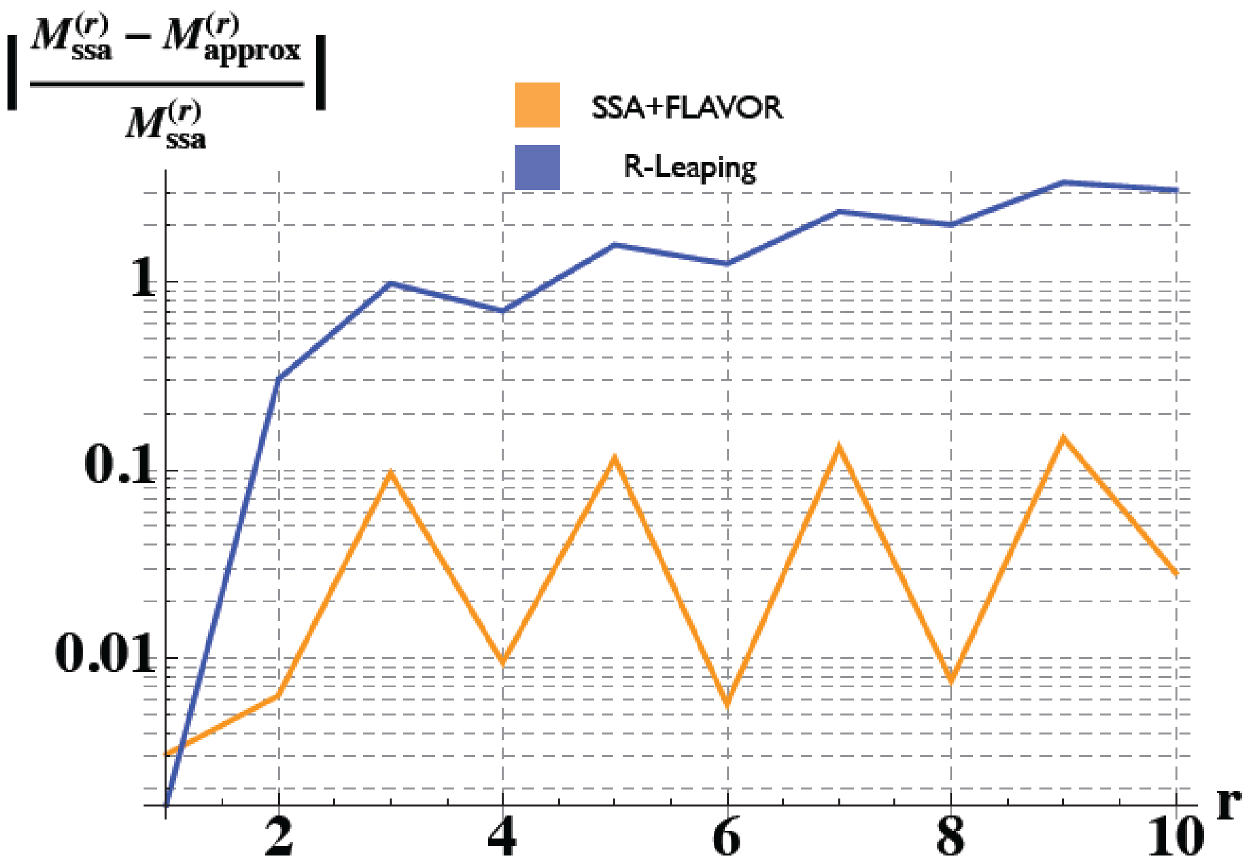


Figure 6: Relative errors of the moments of the stochastic processes.

Chemical kinetic (Bayati-Koumoutsakos-Owhadi)

$$S_1 \overset{1}{\longleftrightarrow} S_2$$

$$S_1 \overset{1}{\longleftrightarrow} S_3$$

$$2S_2 + S_3 \overset{2}{\longleftrightarrow} 3S_4$$

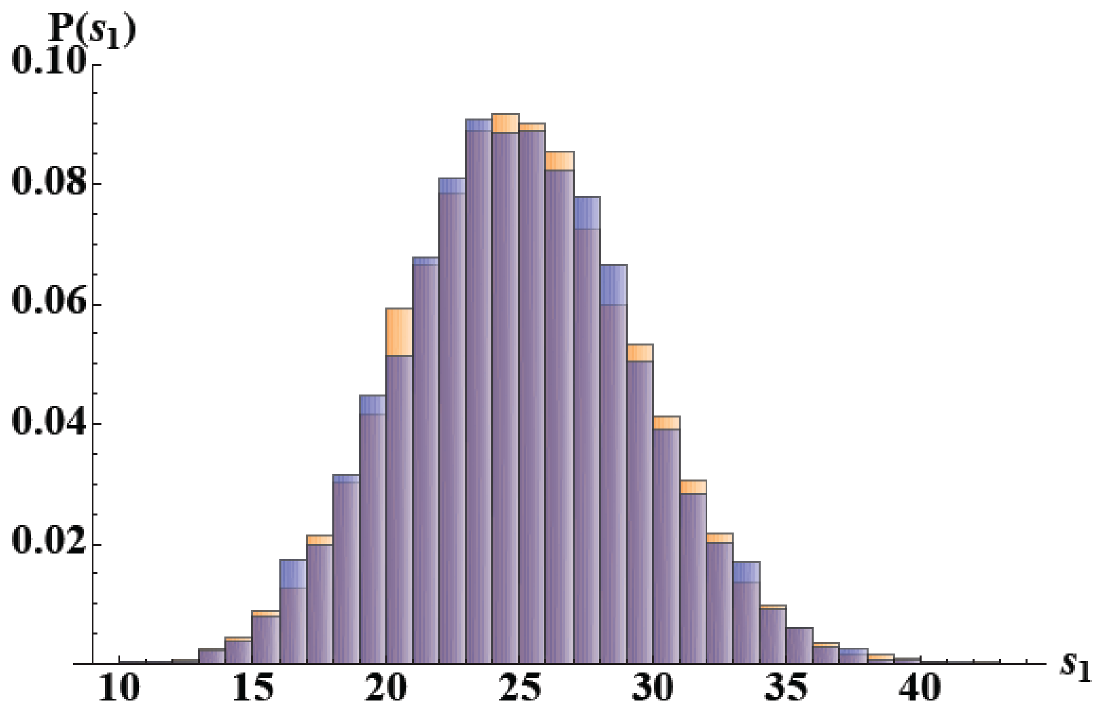


Figure 9: Discrete probability density functions for the species s_1. Orange, SSA; blue, SSA+FLAVOR.

Error vs Speed-up

$$S_1 \longleftrightarrow S_2,$$
$$S_1 \longleftrightarrow S_3,$$
$$2S_2 + S_3 \longleftrightarrow 3S_4.$$