Multiscale computation of oscillatory ODEs with more than two separated time scales

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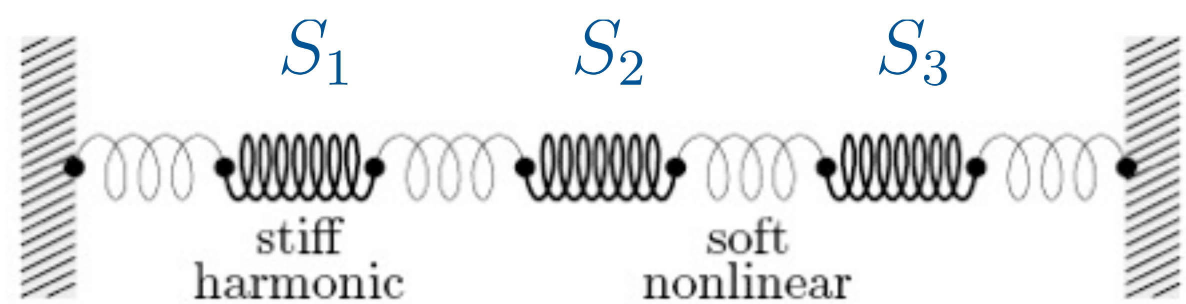
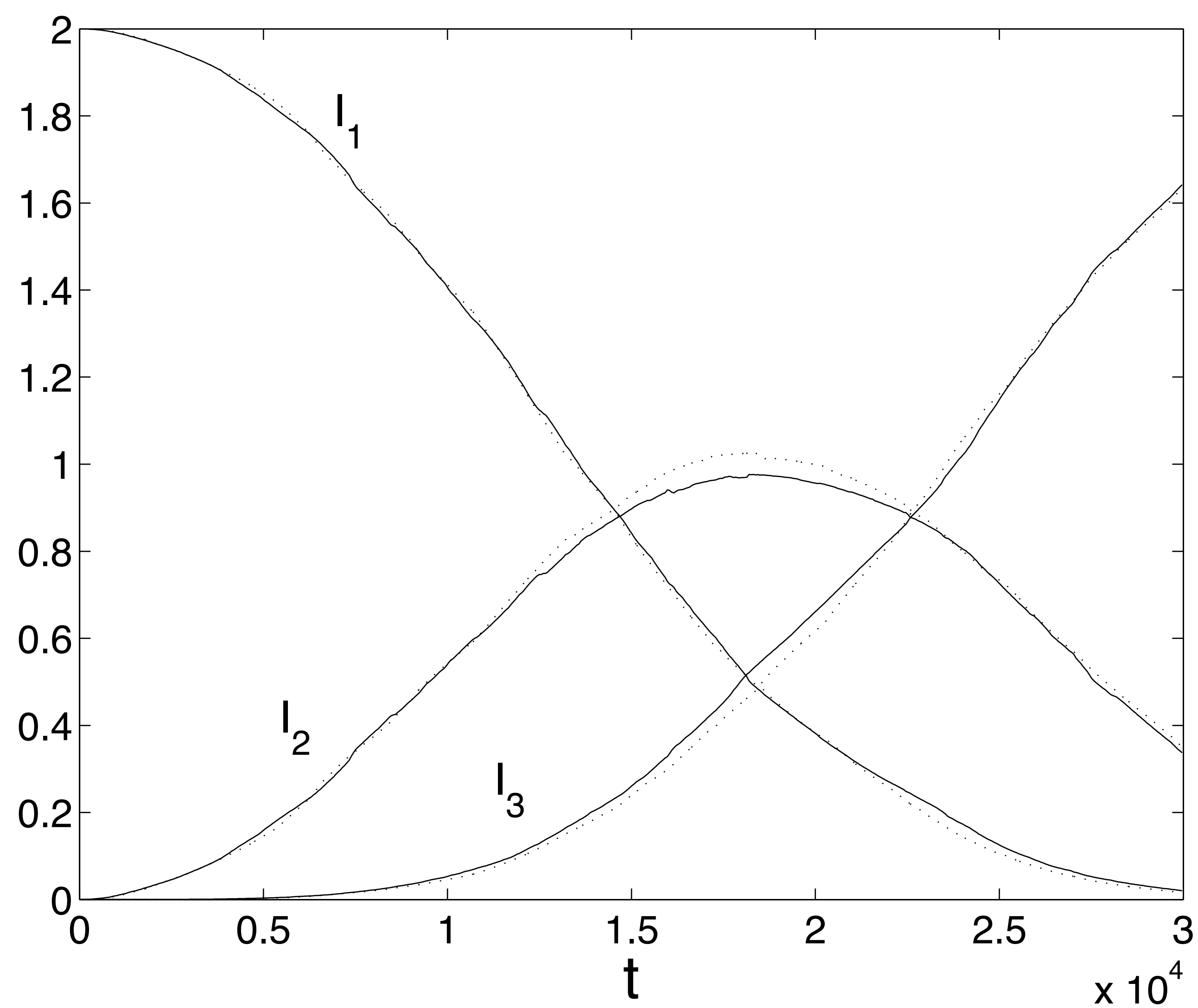
Dahlquist's alarm clock

- Mechanical alarm clock on a hard surface
- Fast vibrations lead "slow" drift path
- Drift seems to be deterministic

- Fast vibrations too costly to compute for the time scale of interest.
  Conventional stiff methods damps out oscillations.
- Is it possible to compute the drift path
  without resolving the fast vibrations for all time?

Fermi-Pasta-Ulam Problem





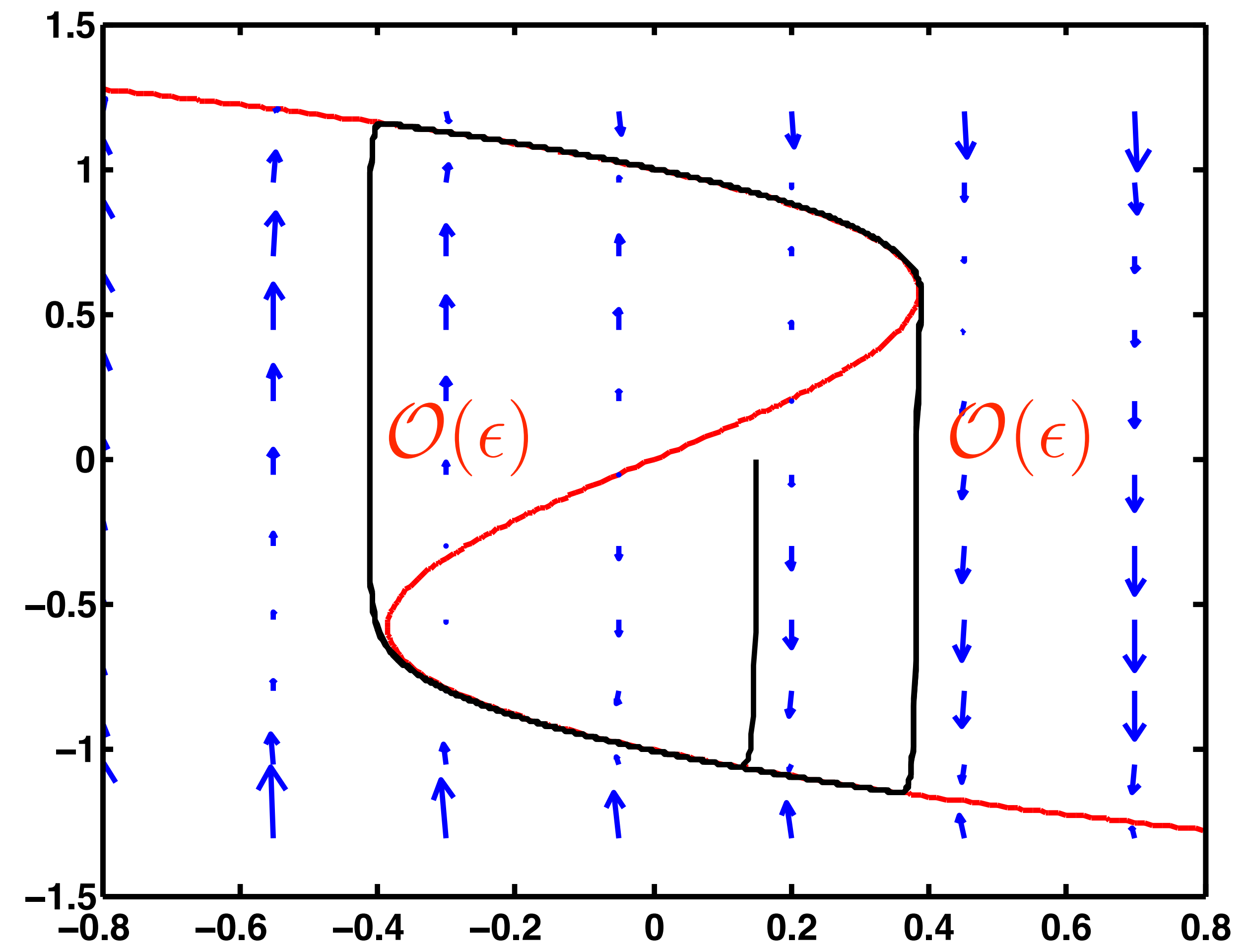
Fast oscillations:
- costly computation
- accumulation of error

$\epsilon = 10^{-4}, H = 0.02$

Relaxation oscillators

[Dahlquist et al]

$$\begin{aligned}\dot{x}_1 &= -1 - x_1 + 8y_1^3 \\ \dot{y}_1 &= \frac{1}{\epsilon}(-x_1 + y_1 - y_1^3)\end{aligned}$$



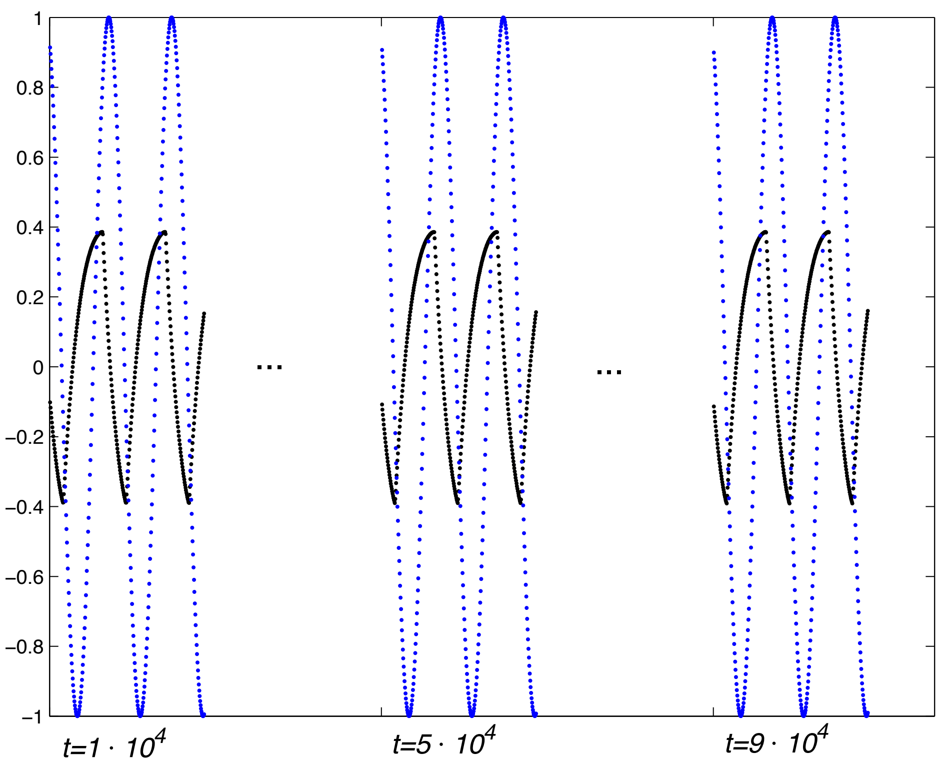
- Solutions quickly approach the periodic limit cycle.

- Oscillations induced by stiffness

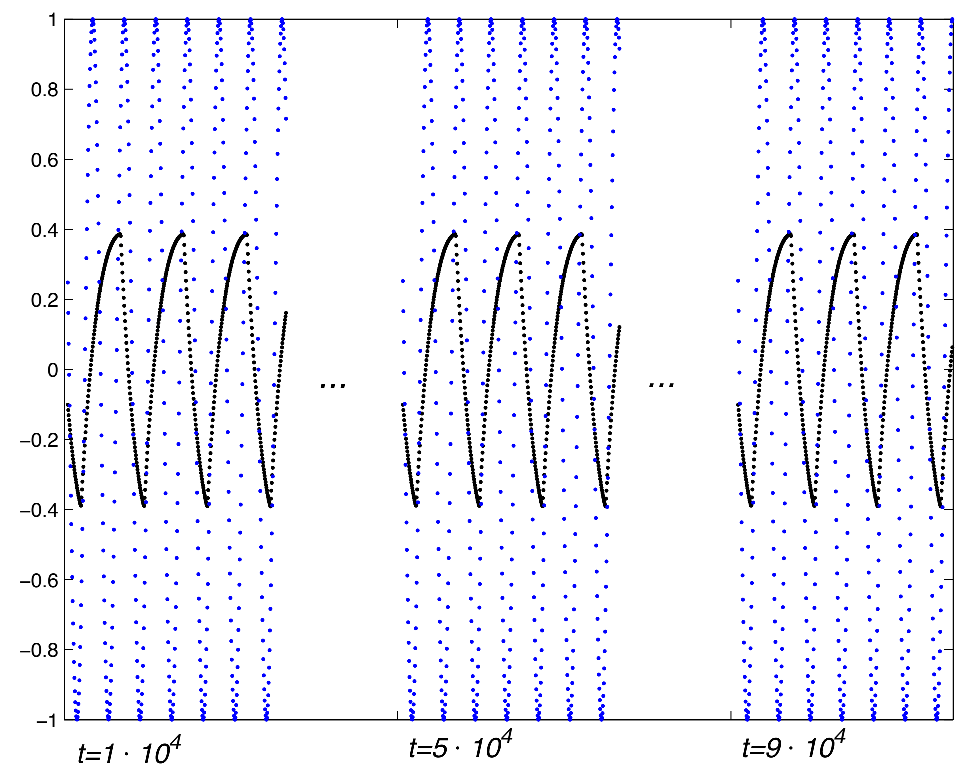
Synchronization

$$\begin{aligned}\dot{x}_1 &= -1 - x_1 + 8y_1^3 + \epsilon\lambda x_2 \\ \dot{y}_1 &= \frac{1}{\epsilon}(-x_1 + y_1 - y_1^3)\end{aligned}$$

$$\begin{aligned}\dot{x}_2 &= (\mu\omega_0 + \epsilon\omega_1)y_2 \\ \dot{y}_2 &= -(\mu\omega_0 + \epsilon\omega_1)x_2\end{aligned}$$



$\mu = 1$



$\mu = 2$

$$\epsilon = 10^{-4}, H = 2500, T = \mathcal{O}(\frac{1}{\epsilon})$$

Systems in near resonance

$$\frac{d}{dt}z_1 = i\frac{1}{\epsilon}z_1 + f_1(z_1, z_2),$$
$$\frac{d}{dt}z_2 = i\frac{\lambda}{\epsilon}z_2 + f_2(z_1, z_2).$$

$$\lambda = 1 + \delta, \quad |\delta| \in \mathbb{R} \setminus \mathbb{Q} \ll 1$$

- trajectories are ergodic on invariant tori, but in which time scale?
- $\delta = \epsilon^p, p > 1$: in O(1) time, problem effectively in resonance. Effect takes place at a longer time scale.
- $\delta = \epsilon^{1/q}, q > 1$: deal with an intermediate time scale

$$\frac{d}{dt}z_2 = i\frac{1}{\epsilon}z_2 + \frac{\delta}{\epsilon}z_2 + f_2(z_1, z_2).$$

Effective properties in longer time scale

- Diffusion (noise, chaotic fast scales)
- Dispersion (wave equation): Engquist, Holst, Runborg
- Not all systems "thermalize":

  FPU:

  - Energy among springs do not equilibrate
  - Interesting phenomena appear in very long time scale

Objectives

Longtime slow phenomena "driven" by fast oscillations:

$$\begin{aligned} v' &= h(v, w, z, t) \\ w' &= \frac{1}{\epsilon} g(w, v, z, t) \\ z' &= \frac{1}{\epsilon^2} f_\epsilon(z, v, w, t) \end{aligned}$$

- Compute v & w at a cost sublinear to $\mathcal{O}(\epsilon^{-1})$
- A method that applies to a wide class of systems.

Our approach

- Characterize the slow behavior by slow variables (effective behavior)

- Numerically sample how they are driven by the fast oscillations

(Temporarily back to the two-scale setting.)

- Give up full resolution of oscillations by averaging:

$$\xi' = f(\xi, \frac{t}{\epsilon}) \quad \longrightarrow \quad \bar{\xi}' = \bar{f}(\bar{\xi})$$

- Evolve the effective behavior of the system at a large time scale.

$$\xi = \bar{\xi} + \mathcal{O}(\epsilon)$$

A "stellar" problem

An example from [Kevorkian,Cole] $\begin{cases} r_1'' + a^2 r_1 &= \epsilon r_2^2 \\ r_2'' + b^2 r_2 &= 2\epsilon r_1 r_2 \end{cases}$

$$X = [x_1, x_2, x_3, x_4]^T = [r_1, r_1'/a, r_2, r_2'/b]^T, t = \epsilon\tilde{t}$$

$$X' = \frac{1}{\epsilon}\begin{pmatrix} 0 & a & 0 & 0 \\ -a & 0 & 0 & 0 \\ 0 & 0 & 0 & b \\ 0 & 0 & -b & 0 \end{pmatrix} X + \begin{pmatrix} 0 \\ x_3^2/a \\ 0 \\ 2x_1x_3/b \end{pmatrix}, X_0(0,\epsilon) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Nonlinear interactions.
Nontrivial O(1) effects

Slow variables

$$X' = \frac{1}{\epsilon}\begin{pmatrix} 0 & a & 0 & 0 \\ -a & 0 & 0 & 0 \\ 0 & 0 & 0 & b \\ 0 & 0 & -b & 0 \end{pmatrix} X + \begin{pmatrix} 0 \\ x_3^2/a \\ 0 \\ 2x_1x_3/b \end{pmatrix}, X_0(0,\epsilon) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Slow variables obtained by a numerical algorithm [Ariel-Engquist-T]

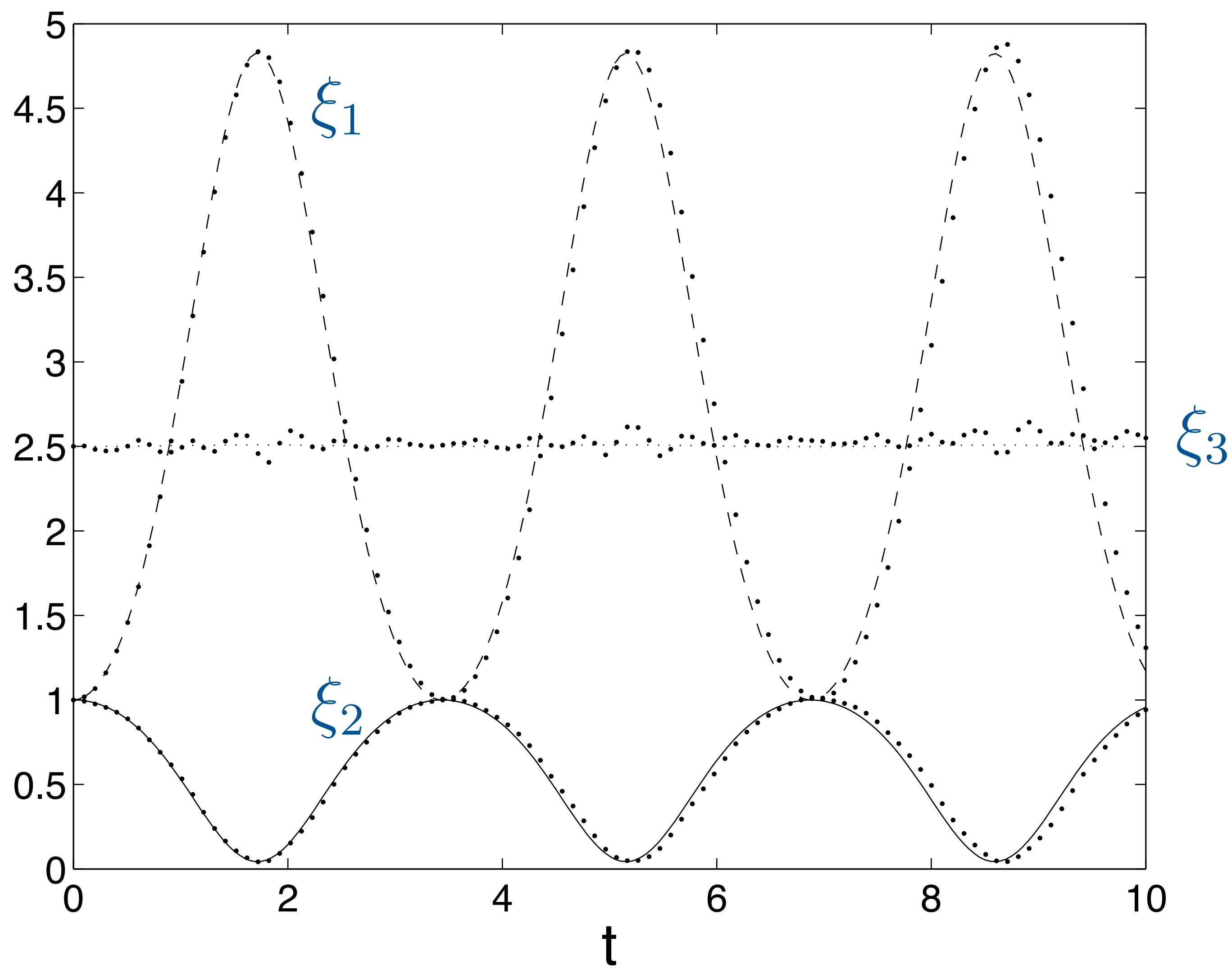
Energy of the oscillators

Relative phase of the two oscillators.

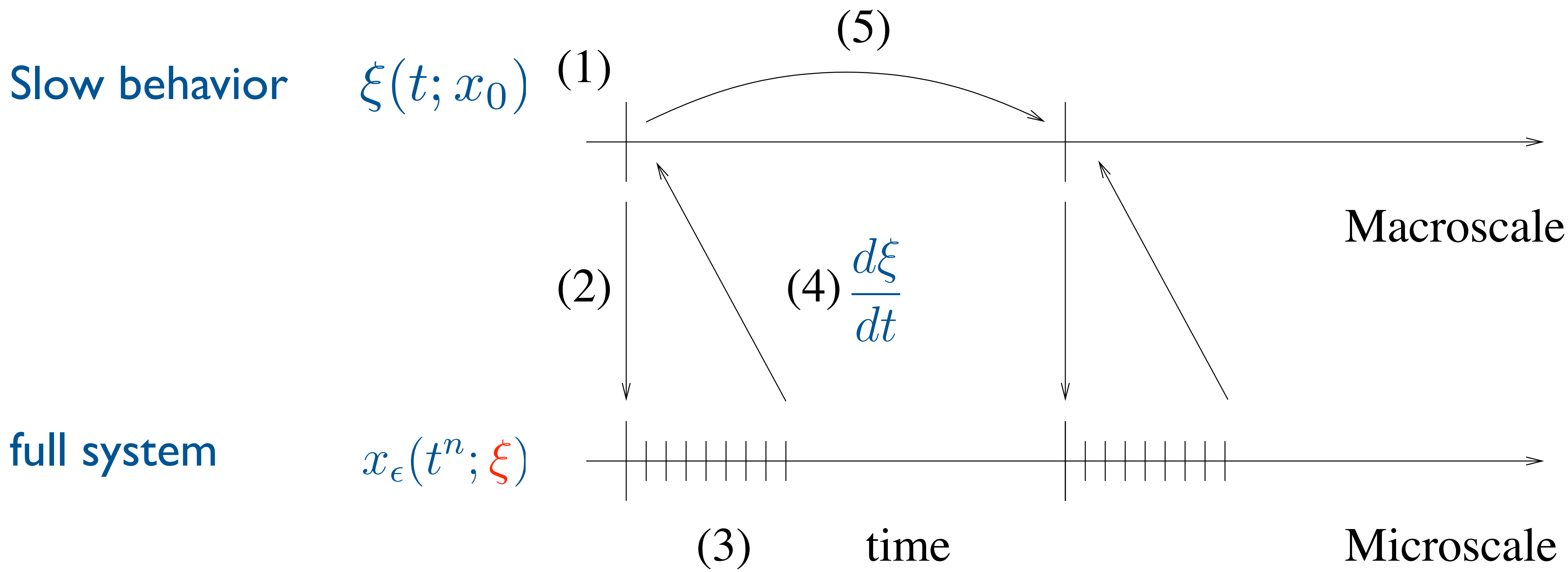
(These are resonant modes when a=2b)

$$\begin{aligned} \xi_1 &= x_1^2 + x_2^2 \\ \xi_2 &= x_3^2 + x_4^2 \\ \xi_3 &= b^2 x_1 x_3^2 + x_2 x_3 x_4 - x_1 x_4^2 \end{aligned}$$

Evolutions of the slow variables (Stellar problem)



$$\epsilon = 10^{-5}, H = 0.1$$



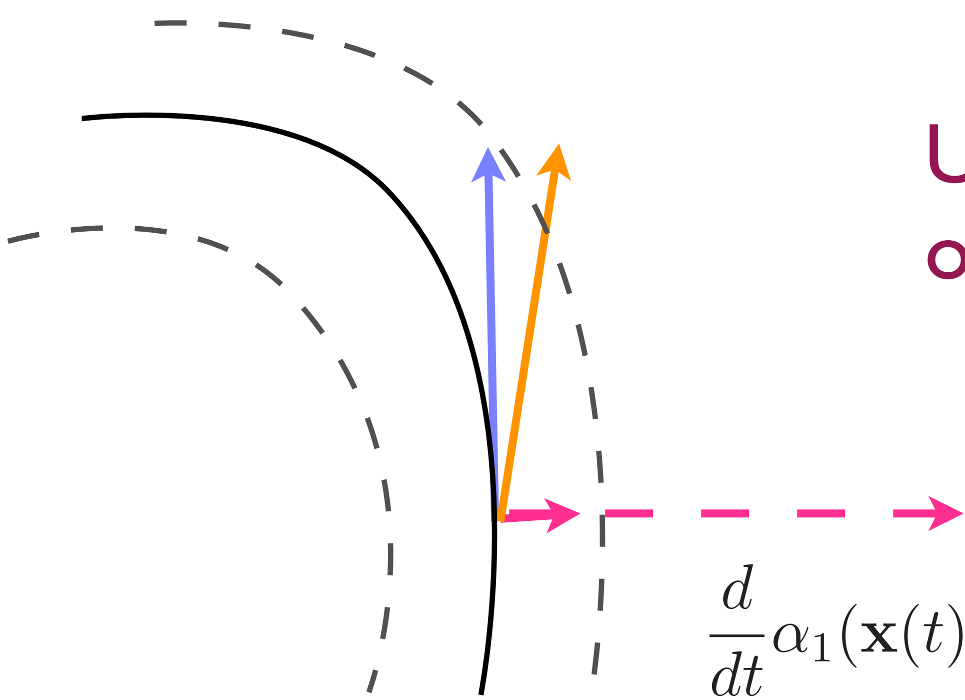
- Compute with consistent initial data $\quad \xi \iff x_\epsilon$
- Closure problem: $\quad \dfrac{d\xi}{dt} = F(\xi)$

- Assume widely separated time scales.
- Efficiency lies in how long (3) is run.

Slow variables

Definition: $\mathbf{x} \in \mathcal{D}_0 \mapsto \alpha(\mathbf{x}) \in \mathbb{R}$ $\quad \frac{d}{dt}\mathbf{x} = f_\epsilon(\mathbf{x})$ highly oscillatory.

$$\left| \frac{d}{dt}\alpha(\mathbf{x}) \right| \leq C_0, \quad 0 \leq t \leq T, \quad 0 < \epsilon < \epsilon_0.$$



Use slow variables to analyze the structure of the vector field.

$$\frac{d}{dt}\alpha_1(\mathbf{x}(t)) = \nabla\alpha_1((x) \cdot f_\epsilon(\mathbf{x})$$

$\{\alpha_1 = \text{constant}\}$

Observations

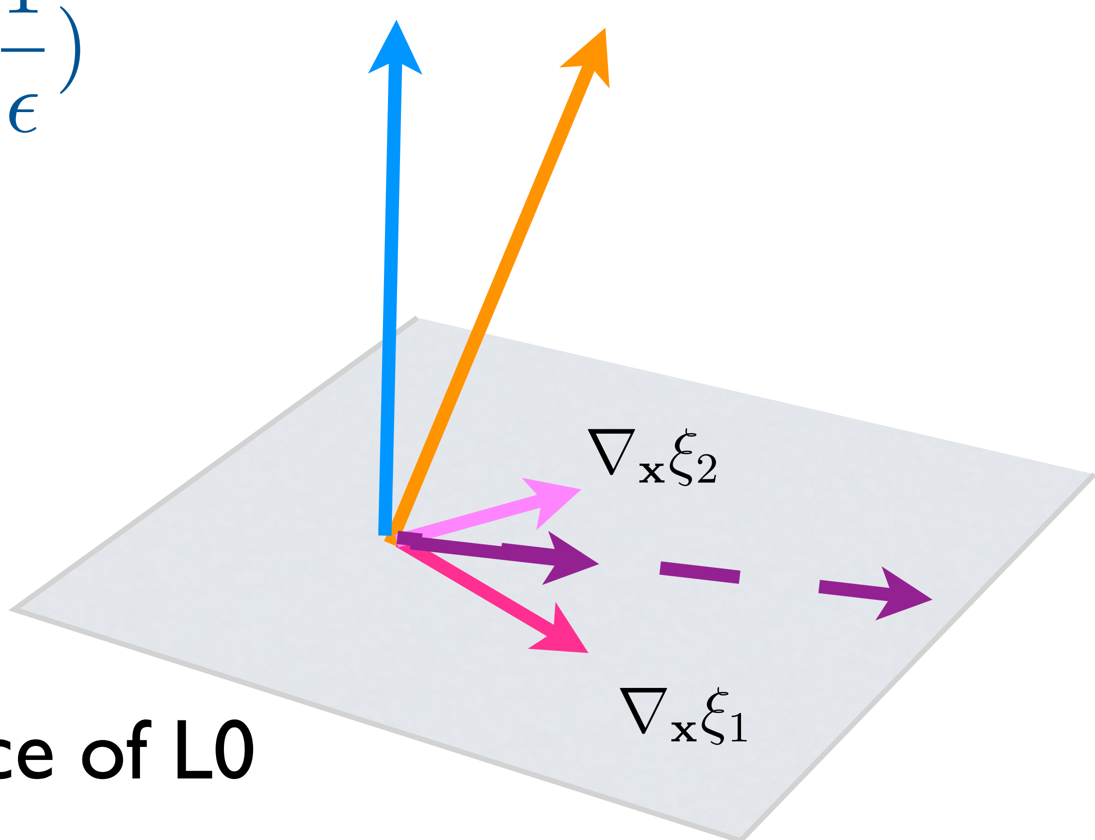
In d dimensions:

- At most $d-1$ slow directions/coordinates
- At most $d-1$ slow variables are needed
- Maximal slow chart: $(\xi_1, \cdots, \xi_{d-1}, \phi)$

$$\frac{d}{dt}\xi_j = \mathcal{O}(1) \qquad \frac{d}{dt}\phi = \mathcal{O}(\frac{1}{\epsilon})$$

- If A(x) is slow and non-constant,

$$A = A(\xi_1, \cdots, \xi_{d-1})$$



- Slow variables lie in the null space of L0

Averaging

$$\frac{d\mathbf{x}_\epsilon}{dt} = f_\epsilon(\mathbf{x}_\epsilon, t) \quad \xleftrightarrow[\text{diffeo.}]{} \quad \begin{cases} \dot{\xi} &= F(\xi, \phi) \\ \dot{\phi} &= \epsilon^{-1}\Omega(\xi) + G(\xi, \phi) \end{cases}$$

$$\dot{\zeta} = \bar{F}(\zeta) = \int_{S^1} F(\zeta, \sigma) d\sigma \quad \textbf{(closure)}$$

$$\Longrightarrow \ |\xi(t) - \zeta(t)| \leq C\epsilon$$

ζ captures the effective behavior of $\mathbf{x}_\epsilon$!

More general averaging theorems by Bogoliubov, Sanders, Verhulst, etc.

Averaging and approximations

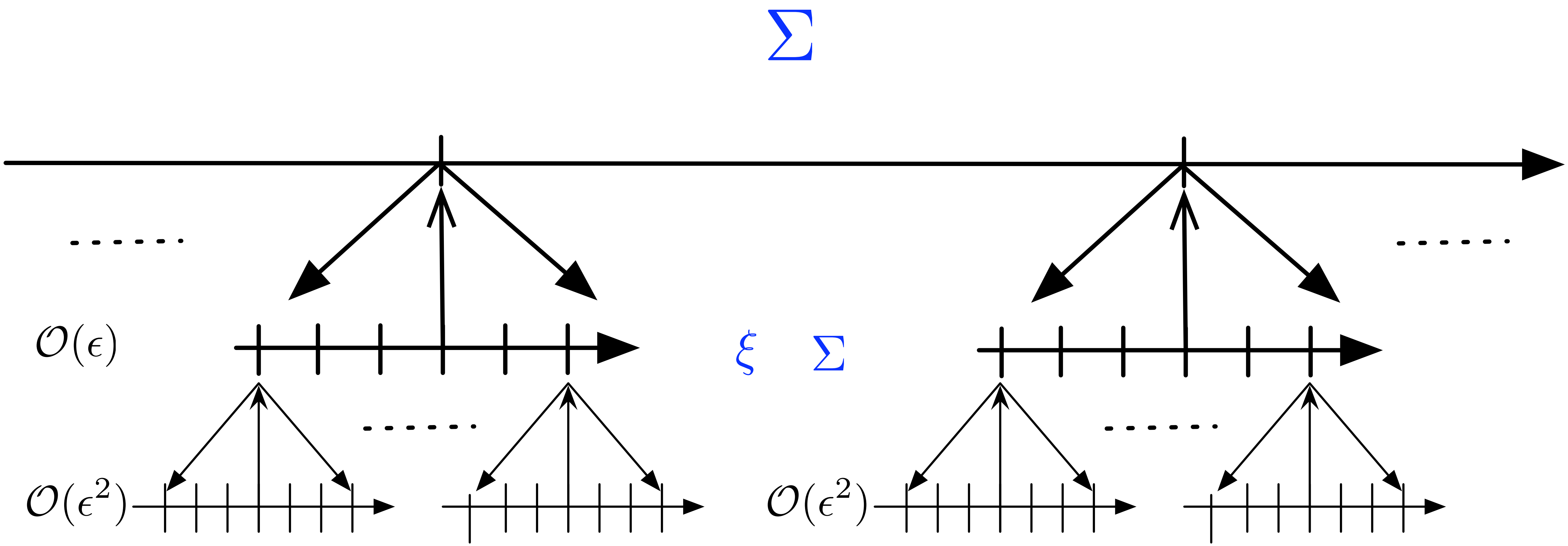
Averaging over a circle ~ averaging with a suitable kernel.

$$\bar{F}(\zeta(t)) = \int_{S^1} F(\zeta, \sigma) d\sigma \simeq \tilde{K}_\eta * \zeta(t)$$

Diffeomorphism $\Phi : U \subset \mathbb{R}^n \mapsto (\xi, \phi) \subset \mathbb{R}^{n-r} \times \mathbb{R}^r$
such that $\xi(x)$ are slow and ϕ fast.

$|\frac{d}{dt}\alpha(x)| \leq C_0 \implies \alpha(\mathbf{x}) = \tilde{\alpha}(\xi, \phi) = \tilde{\alpha}(\xi)$(closure)

HMM involving three scales



$$\frac{d}{dt}x = \epsilon^{-2} f_\epsilon(x,t)$$

Interaction among scales

$$\mathcal{O}(1): \qquad \Sigma(\xi), \qquad |\frac{d}{dt}\Sigma(\xi(t))| \leq C_0$$

$$|\frac{d}{dt}\Sigma(\xi(t))| = \mathcal{O}(1) \quad \updownarrow$$

$$\mathcal{O}(\epsilon): \qquad \xi(x(t)), \qquad |\frac{d}{dt}\xi(x(t))| \leq C_0\epsilon^{-1}$$

$$|\frac{d}{dt}\xi(x(t))| = \mathcal{O}(\epsilon^{-1}) \quad \updownarrow$$

$$\mathcal{O}(\epsilon^2): \qquad x(t), \qquad \frac{d}{dt}x(t) = \epsilon^{-2}f(x,t)$$

Complete set of slow variables: (d-2) or (d-1)?

Interaction among scales

$$\mathcal{O}(1): \qquad \Sigma(\xi), \qquad |\frac{d}{dt}\Sigma(\xi(t))| \leq C_0$$

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$$\mathcal{O}(\epsilon): \qquad \xi(x(t)), \qquad |\frac{d}{dt}\xi(x(t))| \leq C_0\epsilon^{-1}$$

$$\mathcal{O}(\epsilon^2): \qquad x(t), \qquad \frac{d}{dt}x(t) = \epsilon^{-2}f(x,t)$$

Complete set of slow variables: (d-2) or (d-1)?

(d-1) ==> new type of slow variables

Interaction among scales

$$\mathcal{O}(1) : \qquad \Sigma(\xi), \qquad |\frac{d}{dt}\Sigma(\xi(t))| \leq C_0$$

$$|\frac{d}{dt}\Sigma(x(t))| = \mathcal{O}(1)$$

$$\mathcal{O}(\epsilon) : \qquad \xi(x(t)), \qquad |\frac{d}{dt}\xi(x(t))| \leq C_0\epsilon^{-1}$$

$$\mathcal{O}(\epsilon^2) : \qquad x(t), \qquad \frac{d}{dt}x(t) = \epsilon^{-2} f(x,t)$$

Computation in the intermediate scale necessary
for efficiency of averaging: $\Sigma(x(t)) = \Sigma(t, t/\epsilon, t/\epsilon^2)$

Averaging

$$\frac{d\mathbf{x}_\epsilon}{dt} = f_\epsilon(\mathbf{x}_\epsilon, t)$$

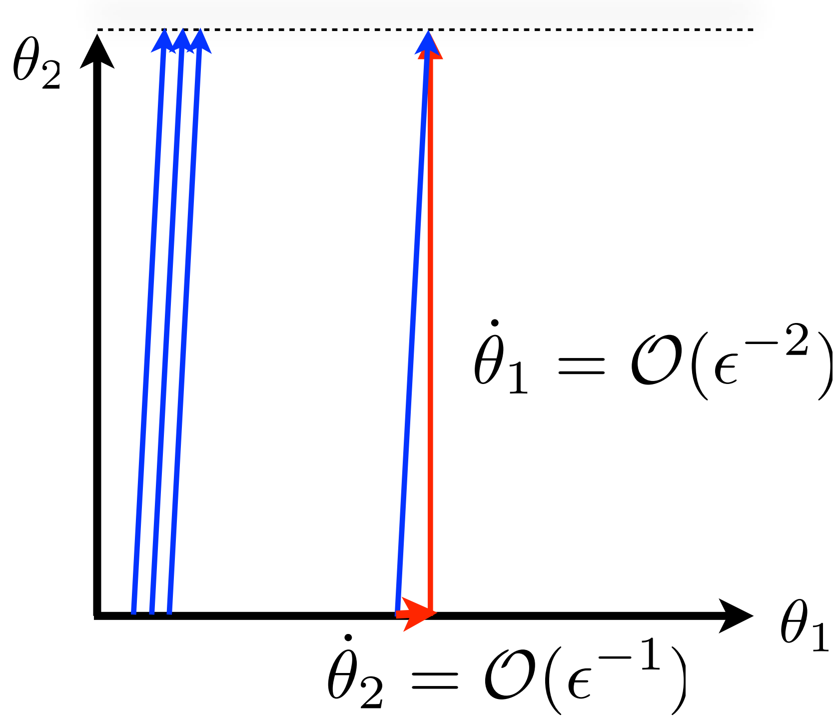
diffeo.

$$\begin{cases} \dot{\xi} &= F(\xi, \phi) \\ \dot{\phi} &= \epsilon^{-1}\Omega(\xi) + G(\xi, \phi) \end{cases}$$

$$\dot{\zeta} = \bar{F}(\zeta) = \int_{\mathbb{S}^1} F(\zeta, \sigma) d\sigma$$ **(closure)**

$$\dot{\zeta} = \bar{F}(\zeta) = \int_{\mathbb{T}^2} F(\zeta, \sigma) d\sigma$$

$$\Longrightarrow \; |\xi(t) - \zeta(t)| \leq C\epsilon$$



Development of efficient averaging algorithms.

A simple example

$$\begin{aligned}\dot{x}_1 &= \frac{1}{\epsilon^2}x_2 + \frac{1}{\epsilon} + x_1 \\ \dot{x}_2 &= -\frac{1}{\epsilon^2}x_1 + x_2\end{aligned}$$

$$I = x_1^2 + x_2^2$$

$$\frac{d}{dt}I = 2\epsilon^{-1}x_1 + 2I$$

$$I(t) = A^2 e^{2t} + \mathcal{O}(\epsilon)$$

New type of slow variables!

Iterated averaging

$$\Sigma' = \frac{1}{\epsilon} f(\Sigma, \xi, \frac{t}{\epsilon^2}) + g(\Sigma, \xi, \frac{t}{\epsilon^2})$$

f,g 1-periodic in the last variable.

$$X' = \bar{\bar{F}}(x) := \int \bar{F}(x,y) d\mu^x$$
$$X(0) = \Sigma(0)$$

$$\sup_{0 \le t \le T} |\Sigma(t) - X(t)| \le C\epsilon$$

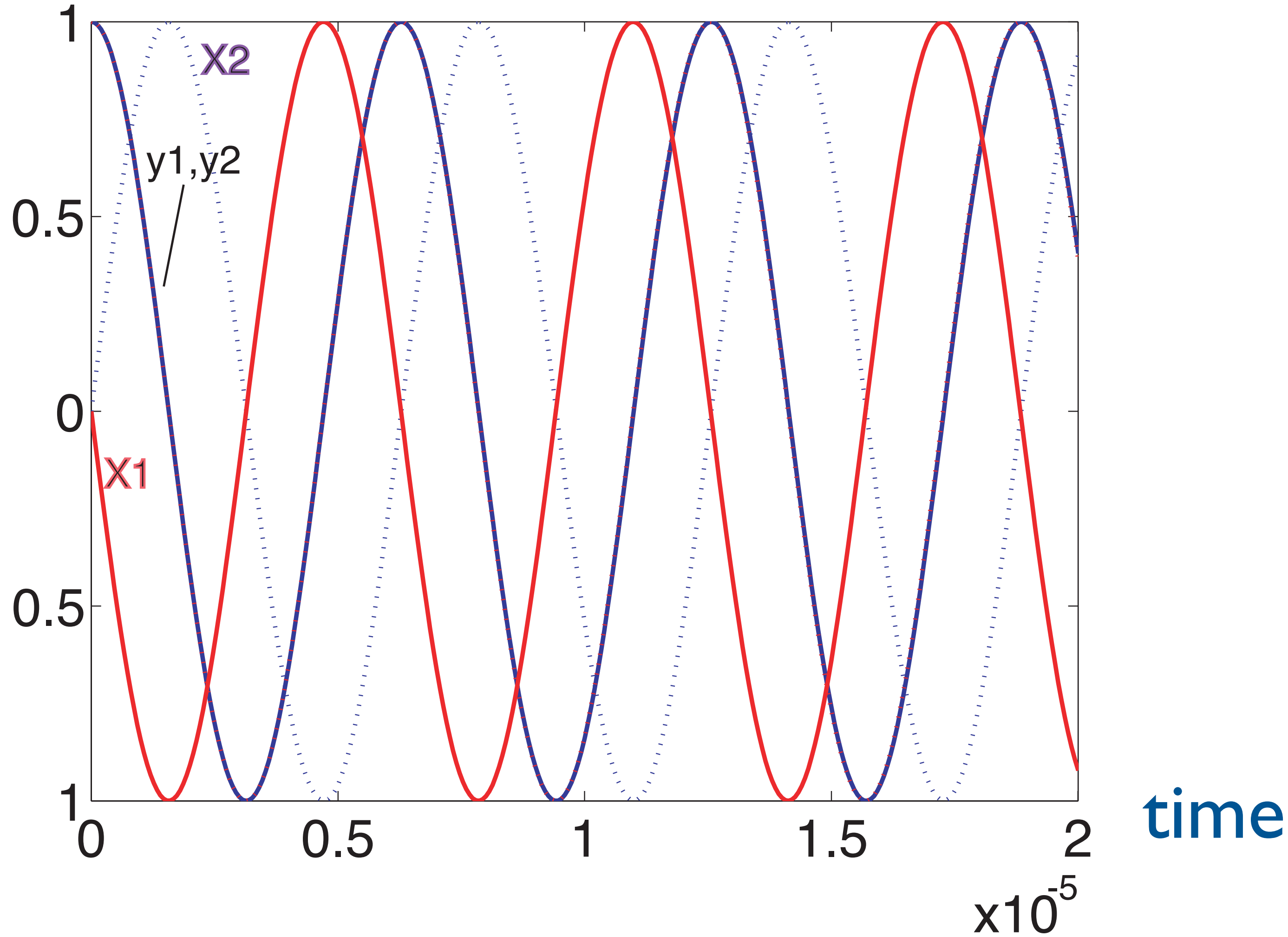
$$\bar{F}(x,y) = \bar{g}(x,y) + \bar{\gamma}(x,y)$$

$$\bar{g}(x,y) = \int_0^1 g(x,y,s) ds$$

corrector depending on

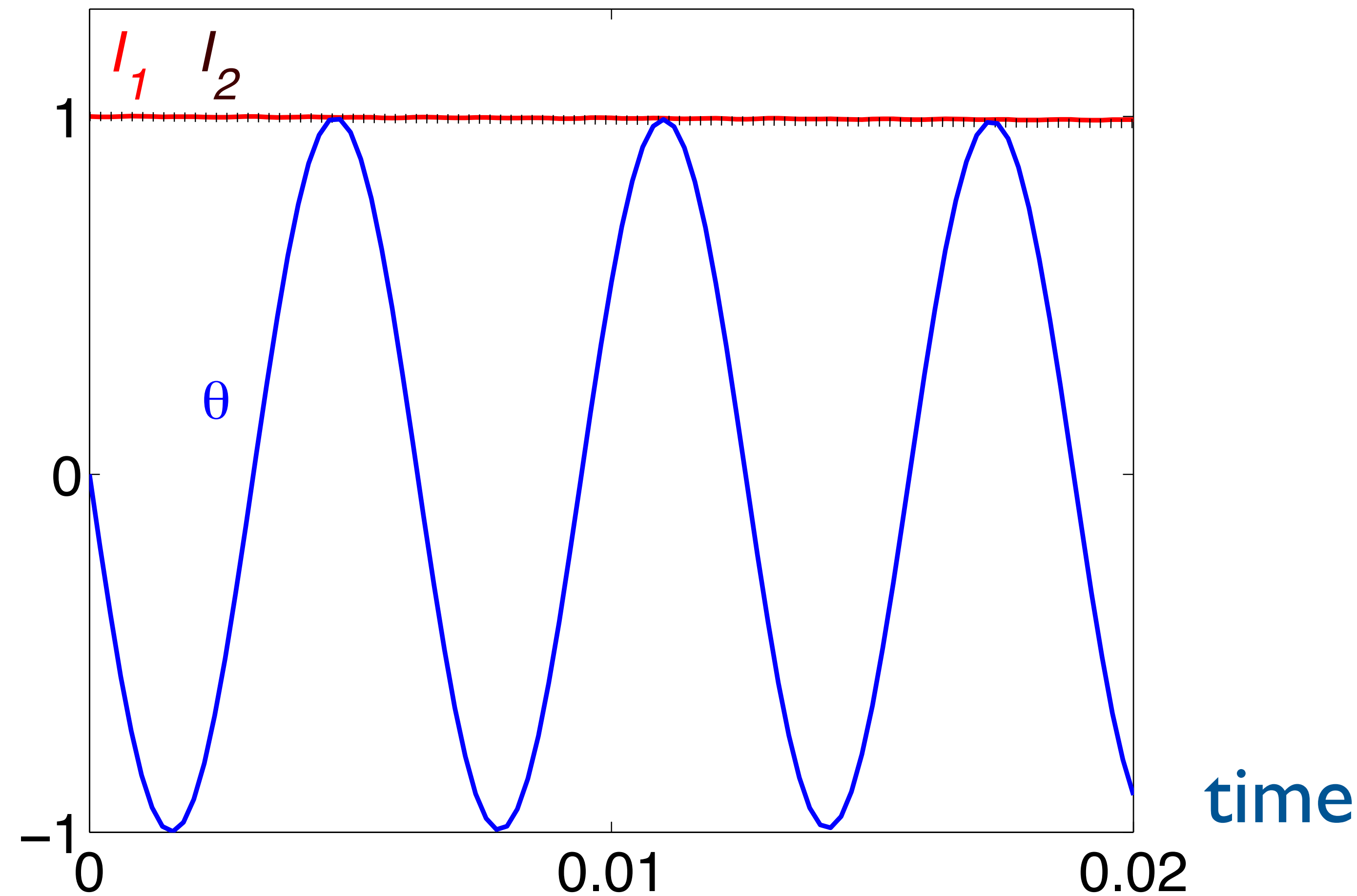
$$h(x,y,t) = \int_0^t f(x,y,\epsilon^{-1} s) ds - t\bar{f}(x,y)$$

$$\begin{cases} \dot{x}_1 &= -\frac{1}{\epsilon^2} y_1 + \frac{1}{\epsilon} y_2^2 - 3x_1 x_2^2 \\ \dot{y}_1 &= \frac{1}{\epsilon^2} x_1 + \frac{1}{2} y_1 \\ \dot{x}_2 &= -\left(\frac{1}{\epsilon^2} + \frac{1}{\epsilon}\right) y_2 - x_2 \\ \dot{y}_2 &= \left(\frac{1}{\epsilon^2} + \frac{1}{\epsilon}\right) x_2 - y_2 + 2x_1^2 y_2 \end{cases}$$

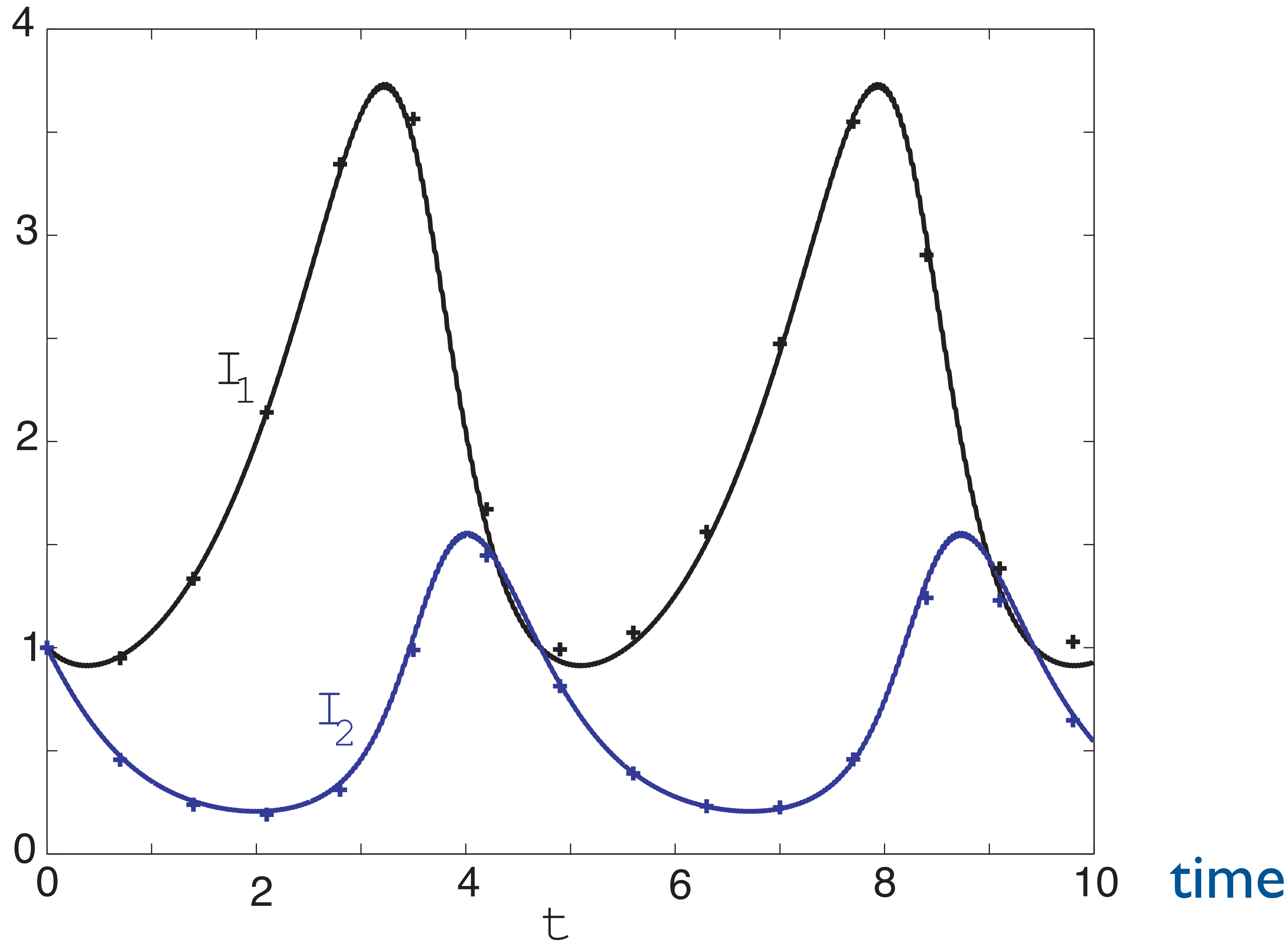


$$\varepsilon = 10^{-3}$$

$$I_1 = x_1^2 + y_1^2$$
$$I_2 = x_2^2 + y_2^2$$
$$\theta = x_1 x_2 + y_1 y_2.$$



$$\dot{I}_1 = \frac{2}{\epsilon} x_1 y_2^2 - 3x_1 x_2^2 + y_1^2$$
$$\dot{I}_2 = 2x_2 y_2 - 2x_2^2 - 2y_2^2 + 4x_1^2 x_2 y_2$$
$$\dot{\theta} = \frac{1}{\epsilon}(x_2 y_2^2 + y_1 x_2 - x_1 y_2) + (y_1 x_2 - x_1 x_2 - 3x_1 x_2^3 + 2x_1^2 y_1 y_2).$$

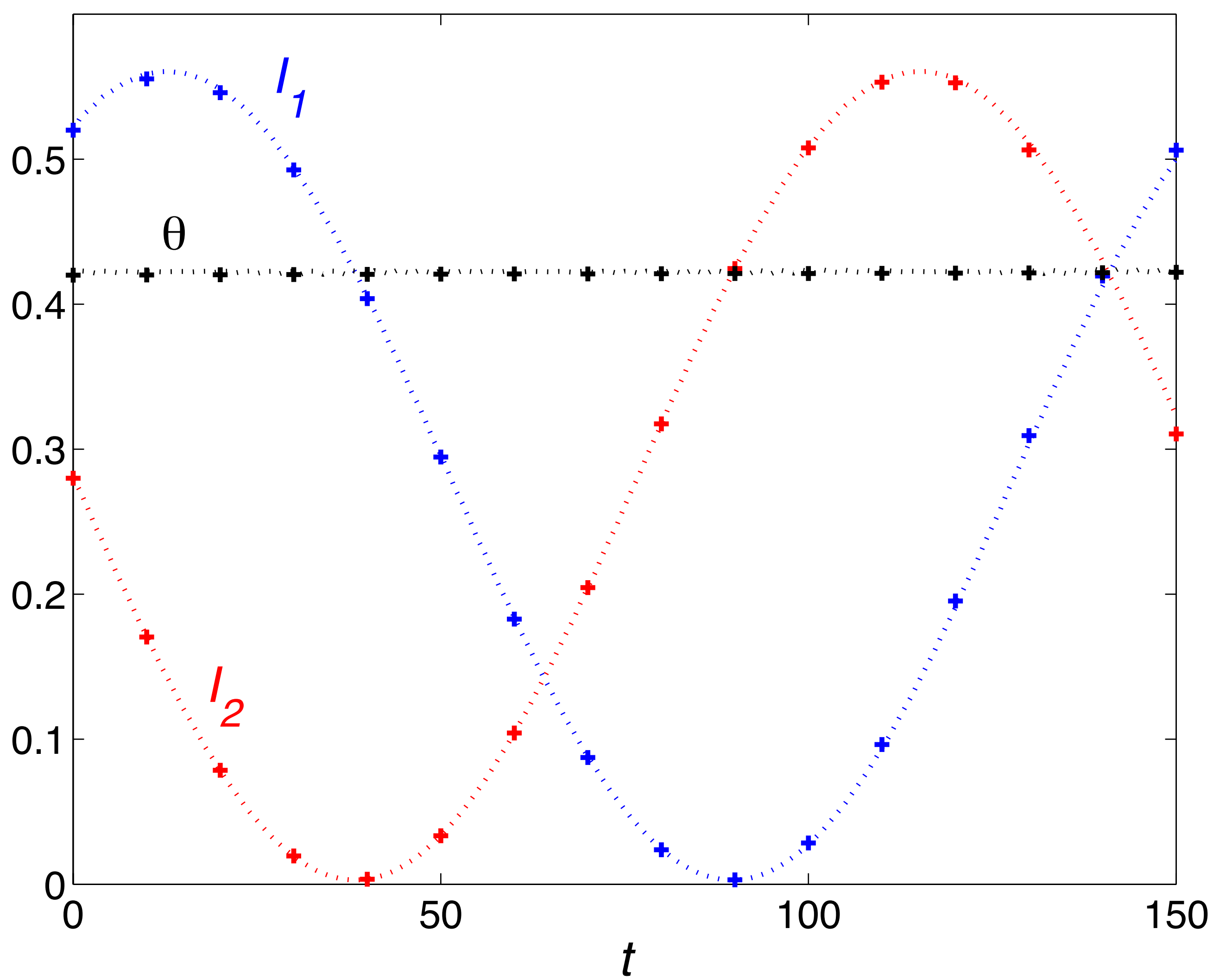


Plus signs are results computed by a 2-tier HMM with RK4 on all scales.

Long time scale

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{3} p_i^2 + \sum_{i=1}^{3}\left[\frac{1}{2}(q_{i+1}-q_i)^2 + \frac{\epsilon}{3}(q_{i+1}-q_i)^3\right] \qquad q_0 = q_3,\ q_4 = q_1$$

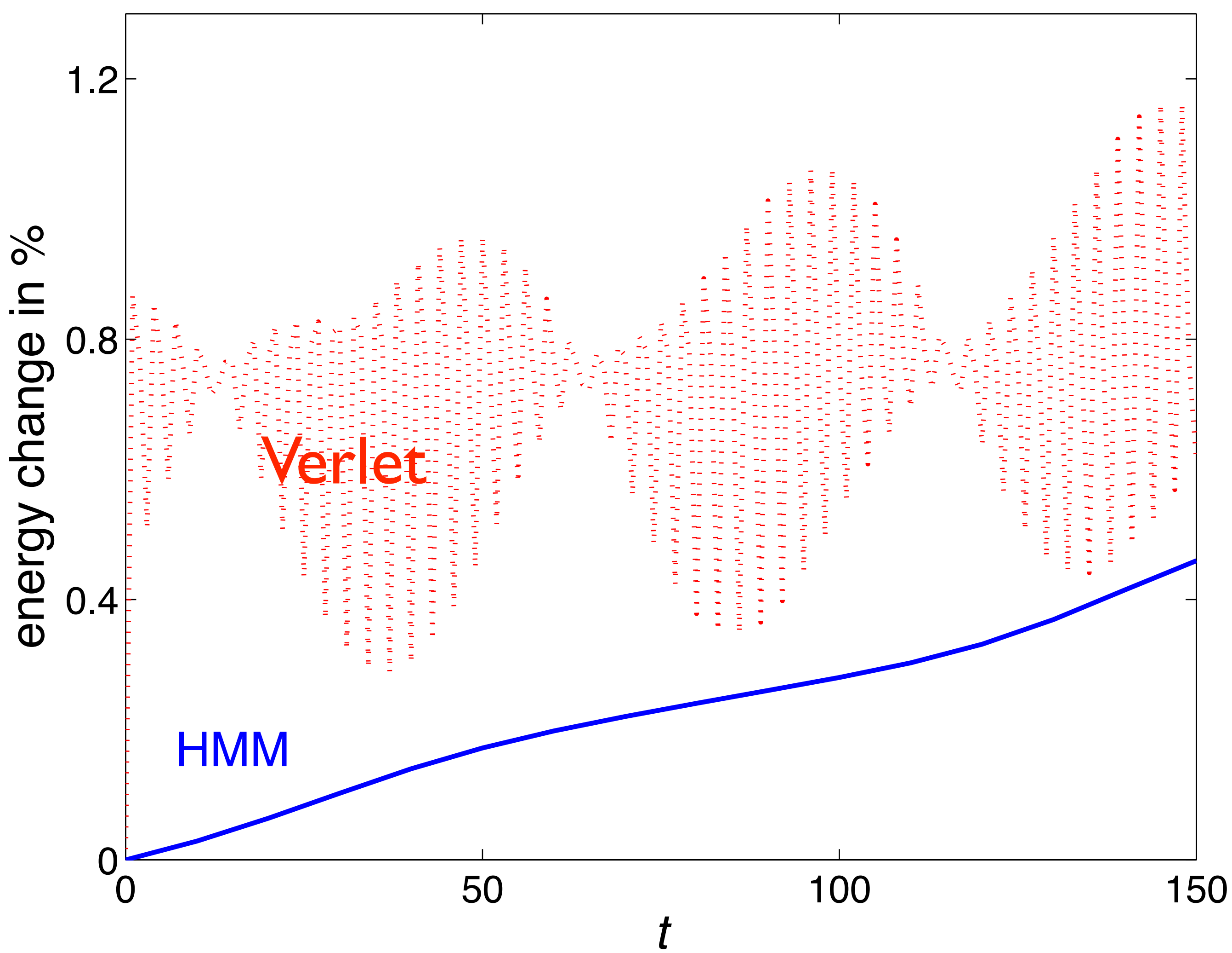
Rescaling time, $s = \epsilon^2 t$, and denoting $[\cdot]' = (d/ds)$

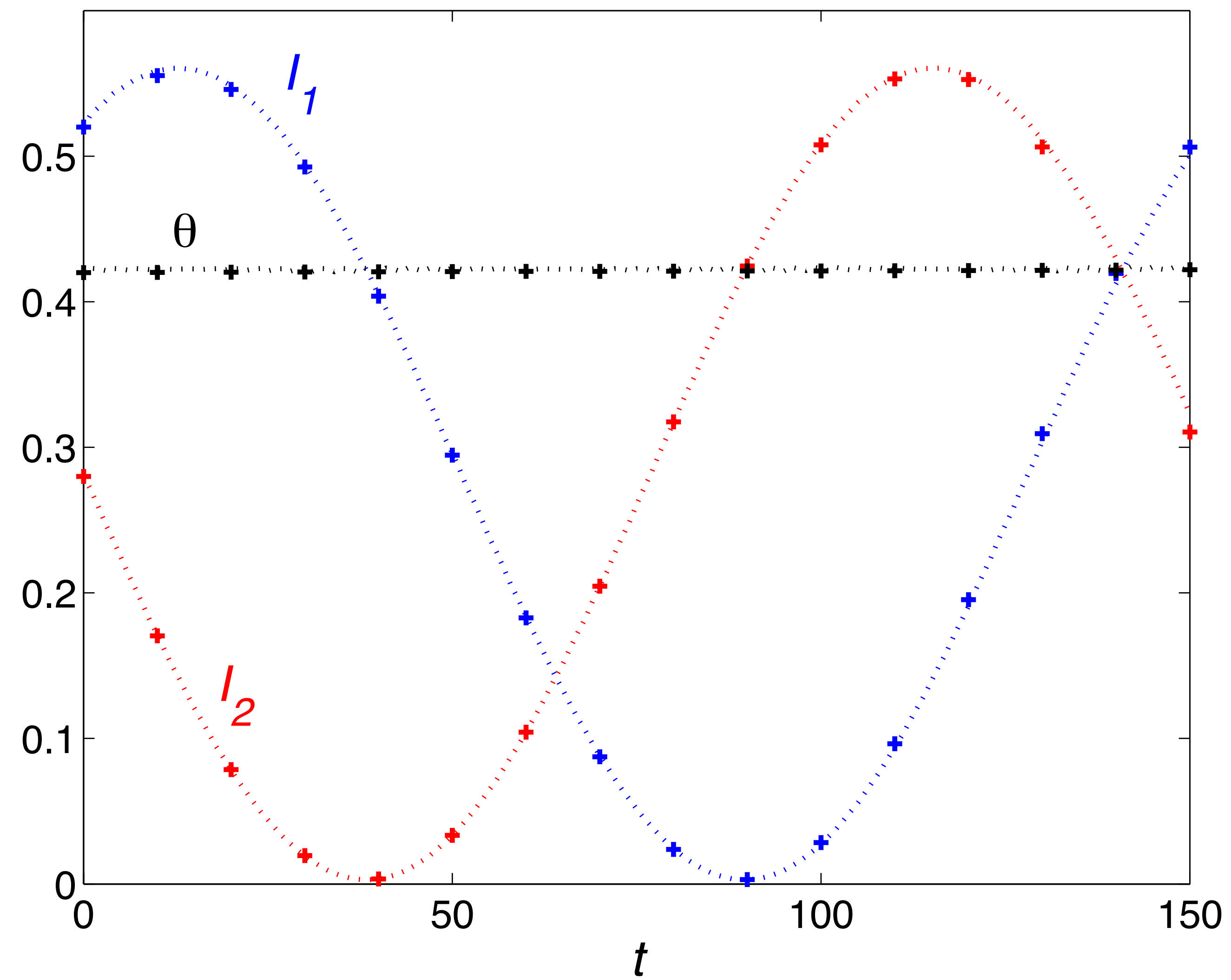


“new” type of slow variables:

$$\begin{aligned} I_1' &= \frac{18}{\epsilon} p_2 q_2 (2q_3 + q_2) \\ I_2' &= -\frac{18}{\epsilon} p_3 q_3 (2q_3 + q_2) \\ \theta' &= \frac{3}{\epsilon}(p_2 q_2 - p_3 q_3)(2q_3 + q_2) \end{aligned}$$

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{3} p_i^2 + \sum_{i=1}^{3}\left[\frac{1}{2}(q_{i+1}-q_i)^2 + \frac{\epsilon}{3}(q_{i+1}-q_i)^3\right]$$

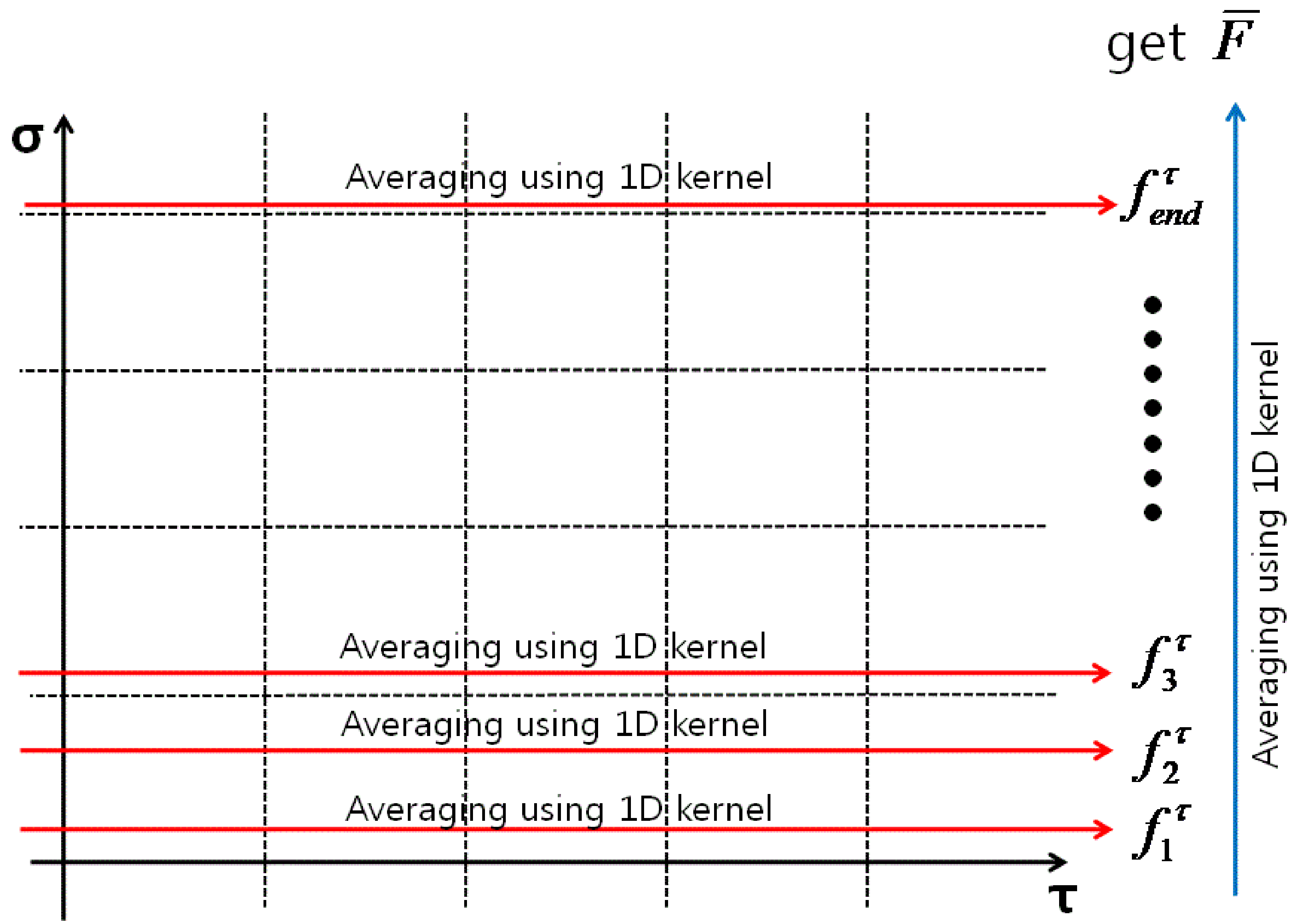


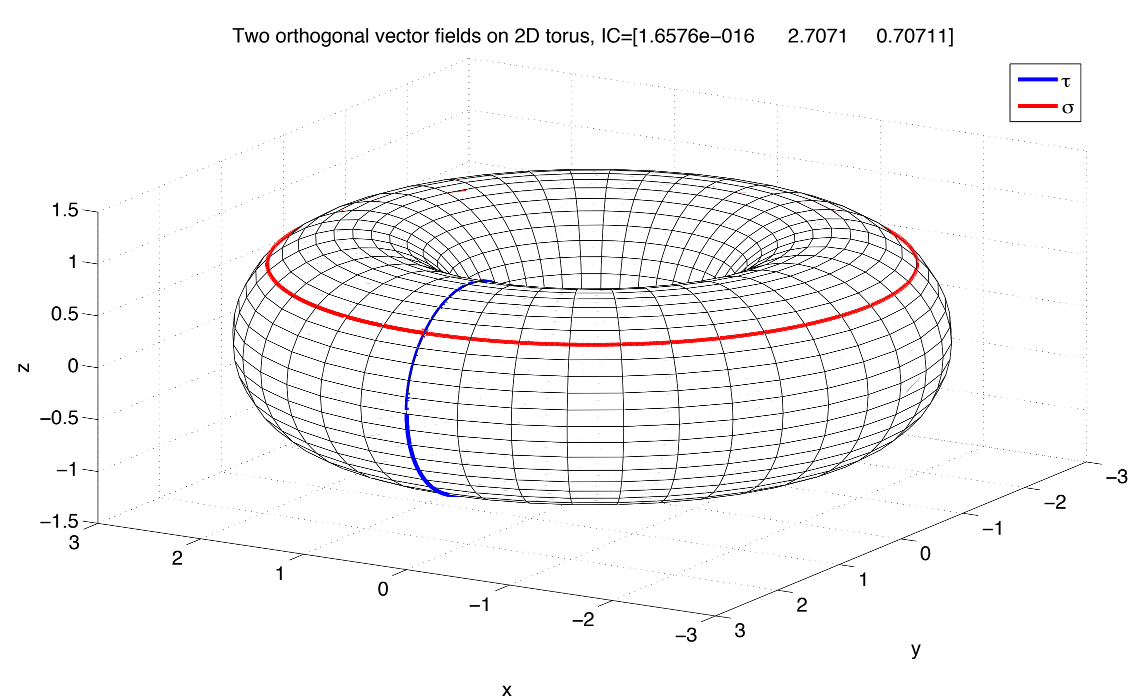


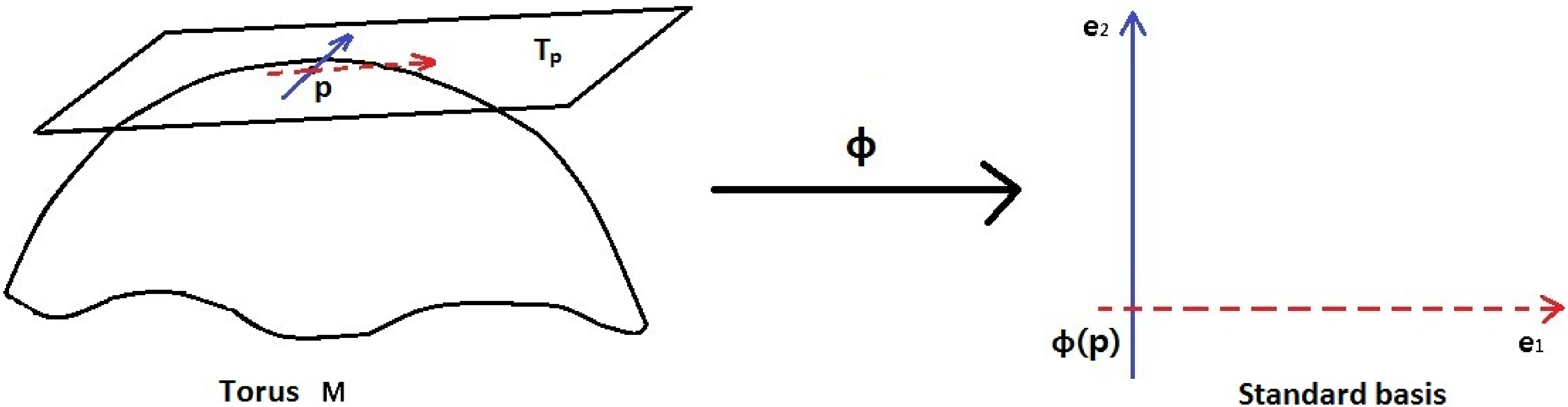
$$\epsilon = 10^{-4}, H = 10$$

With similar errors, HMM is many digits faster than Verlet.

Averaging over a torus


get $\overline{F}$
σ
τ
Averaging using 1D kernel
f_{end}^{τ}
Averaging using 1D kernel
f_{3}^{τ}
Averaging using 1D kernel
f_{2}^{τ}
Averaging using 1D kernel
f_{1}^{τ}
Averaging using 1D kernel


Two orthogonal vector fields on 2D torus, IC=[1.6576e−016 2.7071 0.70711]
τ
σ
z
x
y


T_p
p
Torus M
ϕ
e_2
$\phi(p)$
e_1
Standard basis

Consider a pair of harmonic oscillators for $\mathbf{x} = [x_1, v_1, x_2, v_2, x_3, v_3]^T$,

$$\dot{\mathbf{x}} = \mathbf{F}_\epsilon(\mathbf{x}) = \frac{1}{\epsilon}\begin{bmatrix} v_1 \\ -x_1 \\ \lambda_1 v_2 \\ -\lambda_1 x_2 \\ \lambda_2 v_3 \\ -\lambda_2 x_3 \end{bmatrix}, \quad \mathbf{x}(0) = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \tag{8}$$

where $\lambda_1 = 1 + \delta\sqrt{2}$, $\lambda_2 = 1 + \delta\sqrt{3}$ and $\delta = \epsilon^{\frac{1}{q}}$ with $q = 2, 3, \cdots$.

- $\mathbb{T}^3$ is defined by three functions $\xi_i : \mathbb{R}^6 \to \mathbb{R}^1$, $i = 1, 2, 3$;

$$\xi_1 = x_1^2 + v_1^2,\ \xi_2 = x_2^2 + v_2^2,\ \xi_3 = x_3^2 + v_3^2. \tag{9}$$

- Need to find $\tau : \mathbb{R}^6 \to \mathbb{R}^6$ and $\sigma : \mathbb{R}^6 \to \mathbb{R}^6$

$\to \{\mathbf{F}, \tau, \sigma, \nabla\xi_1, \nabla\xi_2, \nabla\xi_3\}$ forms a set of orthogonal vector fields over $\mathbb{T}^3$

Two orthogonal vector fields

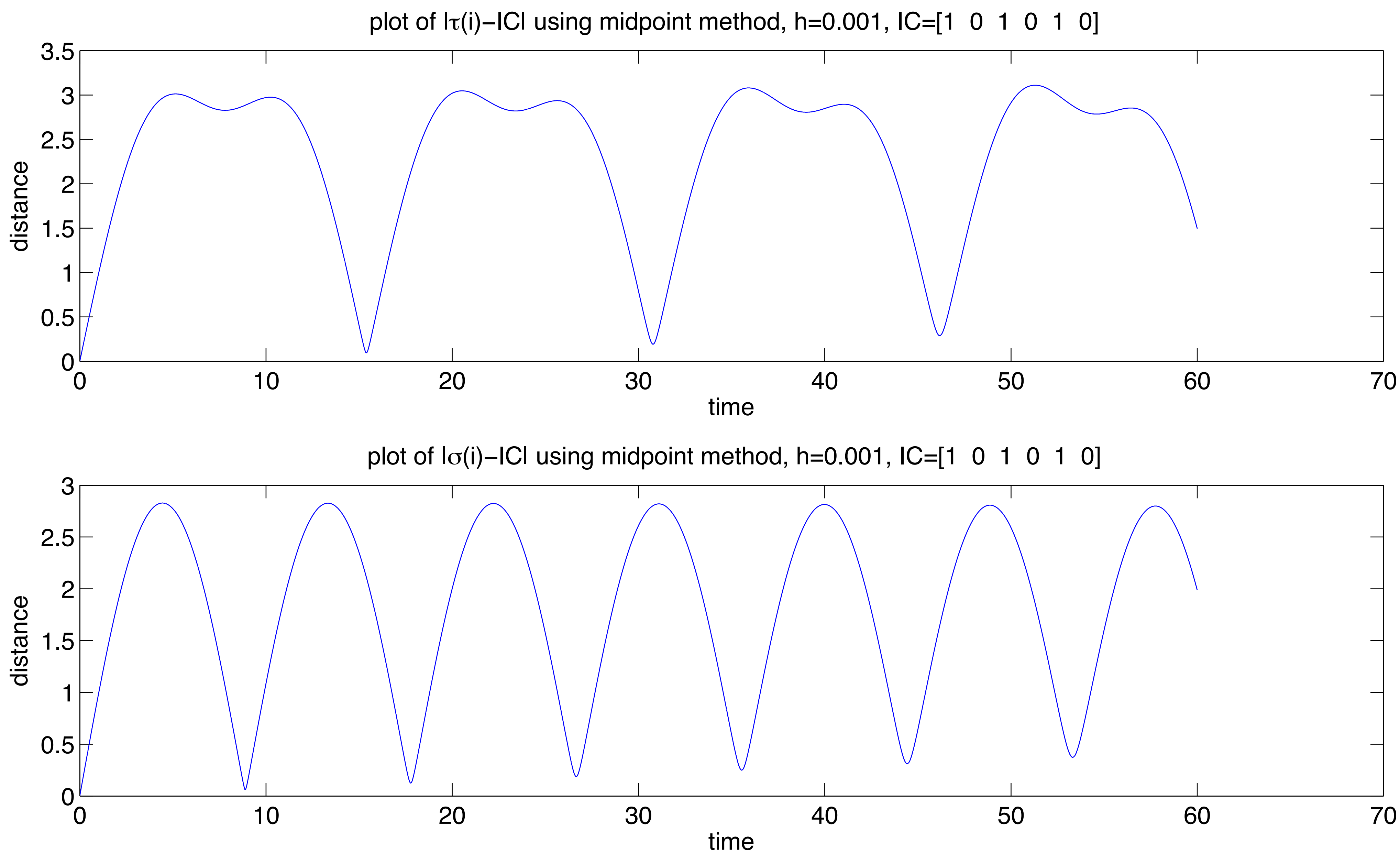


Figure: plot of $|\tau(t){-}\mathrm{IC}|$ and $|\sigma(t){-}\mathrm{IC}|$; this show that two integral curves are almost periodic.

Exact averaged force $\bar{\mathbf{f}} = \frac{1}{\mu(\mathbb{T}^3)} \int_{\mathbb{T}^3} \mathbf{f}\, d\mu = \mathbf{0}$

η	our method	time	time	$\frac{1}{T}\int_0^T \mathbf{f}(\varphi_t \mathbf{x})dt$	T
20ϵ	0.0131	29.71	0.731	0.0131	152
30ϵ	0.0026	43.51	9.75	0.0026	521.6
40ϵ	7.81e-04	57.56	46.01	7.80e-04	2550
50ϵ	2.14e-04	70.92	146.0	2.42e-04	8000
60ϵ	3.45e-05	85.62	29069	3.90e-05	50000

Table: comparison of approximated $||\bar{\mathbf{f}}||_{L^\infty}$, time=sec, $H = 1$, $h = \frac{\epsilon}{5}$

Summary

- Issues in designing an HMM algorithm
- Characterizing effective behavior by slow variables

- Issues with longer time scales
  - interactions between scales
  - detection of new type of slow variables
  - averaging