

Stochastic parameterizations of deterministic dynamical systems: Theory, applications and challenges

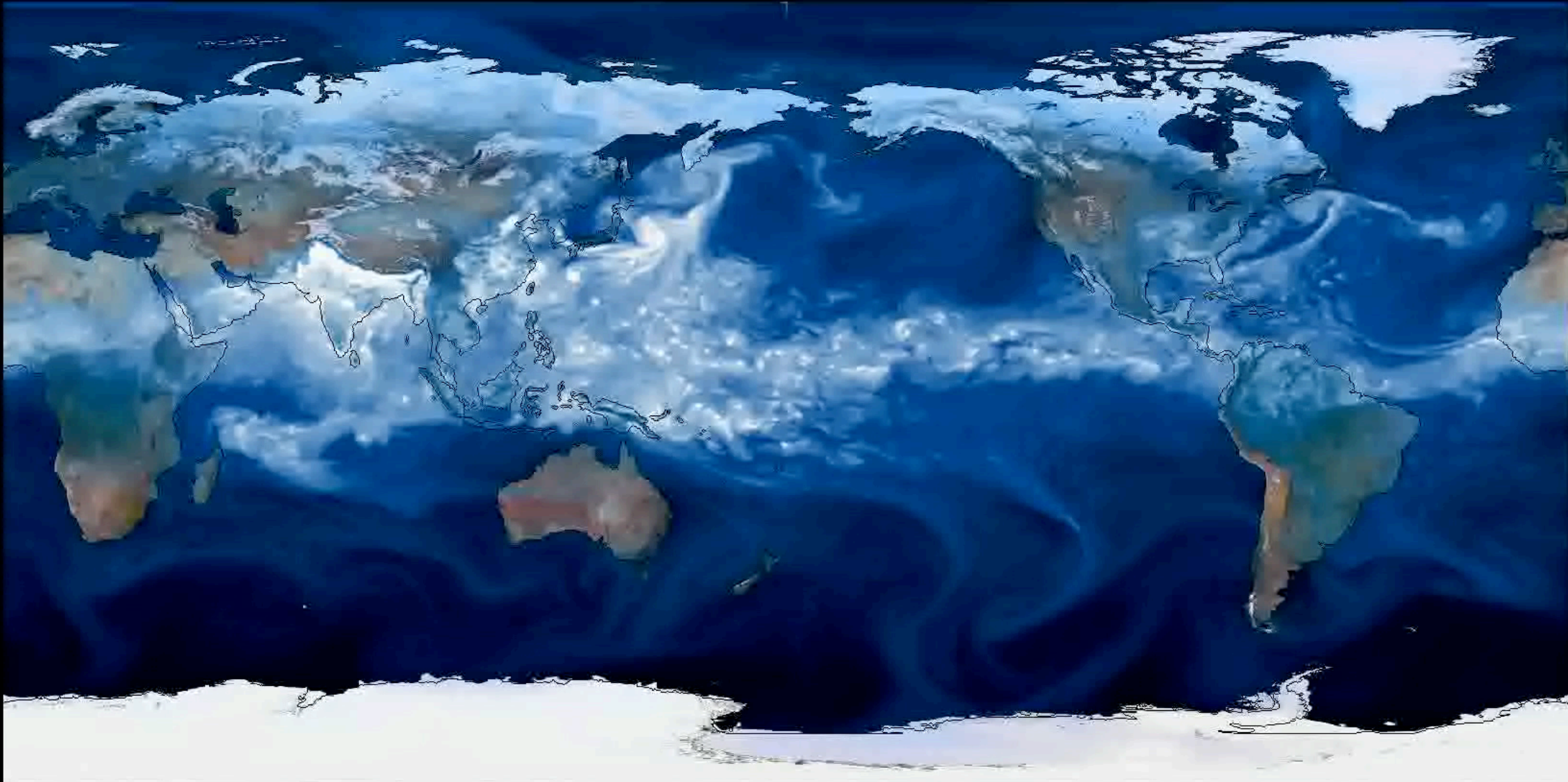
Georg Gottwald

joint work with Jeroen Wouters, Ian Melbourne, Jason Frank



THE UNIVERSITY OF
SYDNEY

Geneva, January 30, 2017



Pseudocolor
Var: TMQ
Units: kg/m2
100.0
31.62
10.00
3.162
1.000
Max: 89.88
Min: 0.04105

August 3 1979

small scale dynamics effecting large scales

Pseudocolor
Var: TMQ
Units: kg/m²
100.0
31.62
10.00
3.162
1.000
Max: 87.98
Min: 0.1053

October 29 1979

Motivation for stochastic parametrisation:

- prediction: computational cost in running model

$$\left. \begin{aligned} \dot{x} &= f(x, y) \\ \dot{y} &= \frac{1}{\varepsilon} g(x, y) \\ x &\in \mathbb{R}^n \\ y &\in \mathbb{R}^m \\ \varepsilon &\ll 1 \end{aligned} \right\}$$

stiff high-dimensional deterministic
multi-scale problem

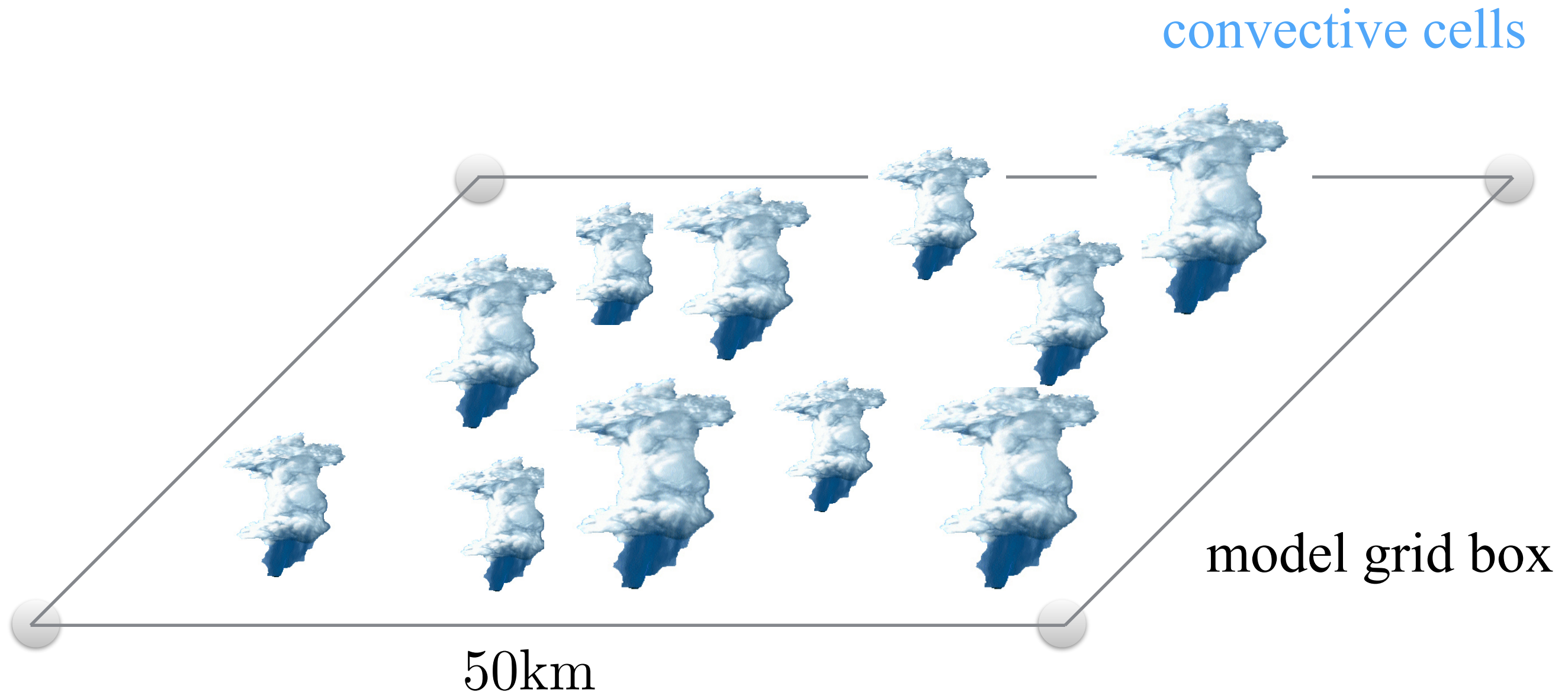
$$dX = F(X)dt + \Sigma dW_t$$

$$X \in \mathbb{R}^n$$

lower-dimensional stochastic problem

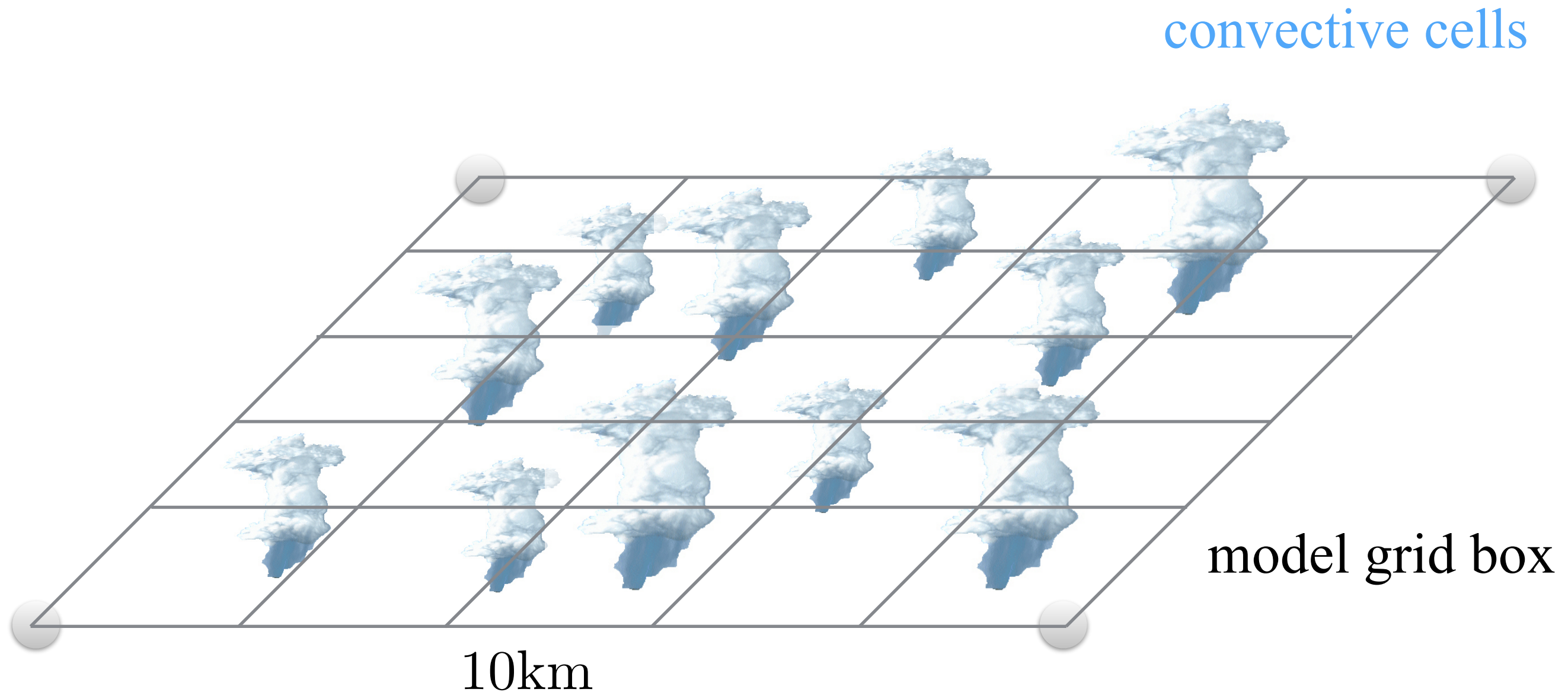
Motivation for stochastic parametrisation:

- prediction: computational cost in running model
- increase of resolution necessitates stochastic approach



Motivation for stochastic parametrisation:

- prediction: computational cost in running model
- increase of resolution necessitates stochastic approach



Motivation for stochastic parametrisation:

- prediction: computational cost in running model
- increase of resolution necessitates stochastic approach
- data assimilation/ensemble filters: use the reduced stochastic model as your forecast model (Mitchell and GAG, JAS (2012), GAG & Harlim, Proc Roy Soc A (2014))

combine limited observations with our knowledge of the laws of physics for optimal state estimation

Observations

Forecast

Analysis

Optimal state estimate



Motivation for stochastic parametrisation:

- prediction: computational cost in running model
- increase of resolution necessitates stochastic approach
- data assimilation/ensemble filters: use the reduced stochastic model as your forecast model (Mitchell and GAG, JAS (2012), GAG & Harlim, Proc Roy Soc A (2014))

combine limited observations with our knowledge of the laws of physics for optimal state estimation

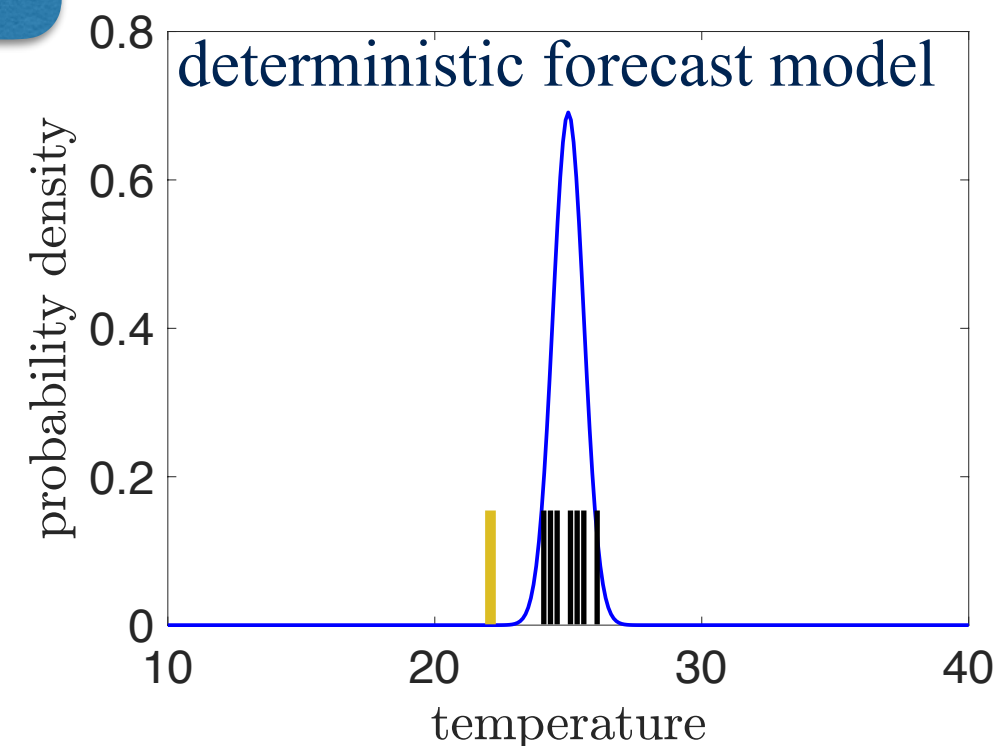
Observations

Forecast

Analysis

Optimal state estimate

What can go wrong?



Motivation for stochastic parametrisation:

- prediction: computational cost in running model
- increase of resolution necessitates stochastic approach
- data assimilation/ensemble filters: use the reduced stochastic model as your forecast model (Mitchell and GAG, JAS (2012), GAG & Harlim, Proc Roy Soc A (2014))

combine limited observations with our knowledge of the laws of physics for optimal state estimation

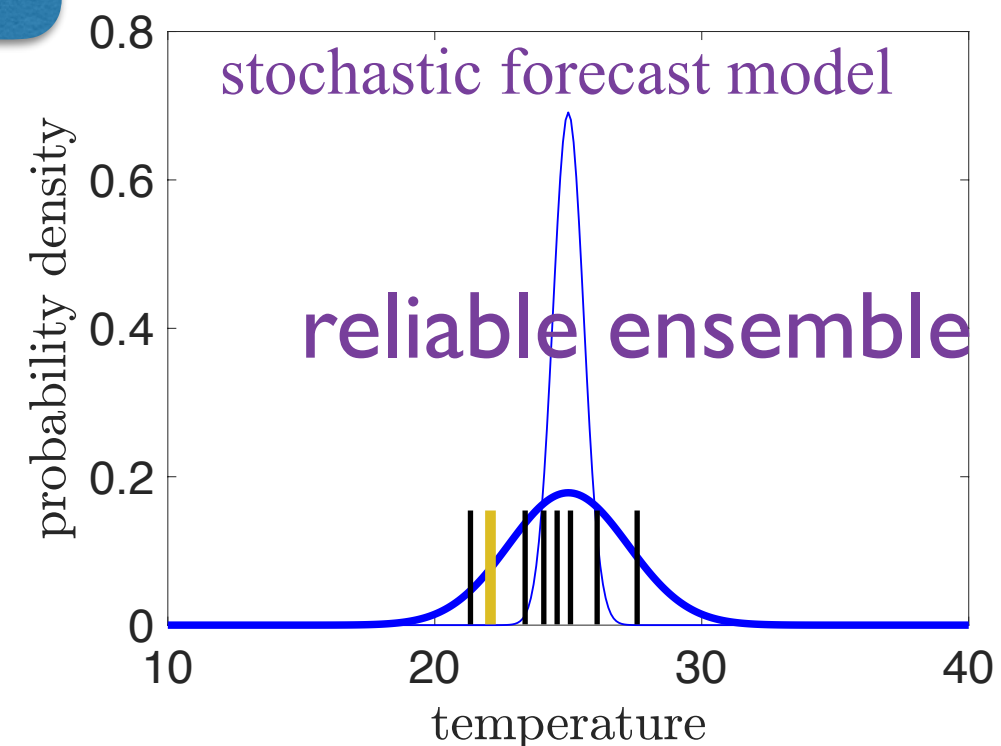
Observations

Forecast

Analysis

Optimal state estimate

What can go wrong?



Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \int_0^t f(x^{(\varepsilon)}, y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon}} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{n} \int_0^{nt} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \int_0^t f(x^{(\varepsilon)}, y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon}} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{n} \int_0^{nt} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Invoking Birkhoff's **Ergodic** Theorem

$$X(t) = X(0) + \int_0^t F(X(s)) ds$$

$$F(X) = \int f(x, y) \mu(dy)$$

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \int_0^t f(x^{(\varepsilon)}, y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon}} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{n} \int_0^{nt} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Invoking Birkhoff's **Ergodic** Theorem

$$X(t) = X(0) + \int_0^t F(X(s)) ds$$

$$F(X) = \int f(x, y) \mu(dy)$$

Averaged deterministic dynamics

law of large numbers

Heuristics for why the fast process can be replaced by noise

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

Integrate the slow equation

$$\begin{aligned}x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \int_0^t f(x^{(\varepsilon)}, y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon}} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{n} \int_0^{nt} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau\end{aligned}$$

Invoking Birkhoff's **Ergodic** Theorem

$$\begin{aligned}X(t) &= X(0) + \int_0^t F(X(s)) ds \\ F(X) &= \int f(x, y) \mu(dy)\end{aligned}$$

Averaged deterministic dynamics

law of large numbers

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \int_0^t f(x^{(\varepsilon)}, y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon}} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{n} \int_0^{nt} f(x^{(\varepsilon)}, y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Invoking Birkhoff's **Ergodic** Theorem

$$X(t) = X(0) + \int_0^t F(X(s)) ds$$

$$F(X) = \int f(x, y) \mu(dy)$$

Averaged deterministic dynamics

law of large numbers

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = f(x^{(\varepsilon)}, y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon} g(y^{(\varepsilon)}) dt + \frac{1}{\sqrt{\varepsilon}} \sigma dW_t$$

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = \frac{1}{\varepsilon} f(y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon^2} g(y^{(\varepsilon)}) dt + \frac{1}{\varepsilon} \sigma dW_t$$

 **go to long *diffusive* time scale**

Heuristics for why the fast process can be replaced by noise

$$dx^{(\varepsilon)} = \frac{1}{\varepsilon} f(y^{(\varepsilon)}) dt$$

$$dy^{(\varepsilon)} = \frac{1}{\varepsilon^2} g(y^{(\varepsilon)}) dt + \frac{1}{\varepsilon} \sigma dW_t$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \frac{1}{\varepsilon} \int_0^t f(y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f(y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{\sqrt{n}} \int_0^{nt} f(y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Heuristics for why the fast process can be replaced by noise

$$\begin{aligned}dx^{(\varepsilon)} &= \frac{1}{\varepsilon} f(y^{(\varepsilon)}) dt \\ dy^{(\varepsilon)} &= \frac{1}{\varepsilon^2} g(y^{(\varepsilon)}) dt + \frac{1}{\varepsilon} \sigma dW_t\end{aligned}$$

Integrate the slow equation

$$\begin{aligned}x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \frac{1}{\varepsilon} \int_0^t f(y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f(y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{\sqrt{n}} \int_0^{nt} f(y^{(\varepsilon=1)}(\tau)) d\tau\end{aligned}$$

Assuming $\int f_0(y) \mu(dy) = 0$ and invoking the Central Limit Theorem

$$X(t) = X(0) + W_t$$

$$dX = dW_t$$

Heuristics for why the fast process can be replaced by noise

$$\begin{aligned}dx^{(\varepsilon)} &= \frac{1}{\varepsilon} f(y^{(\varepsilon)}) dt \\ dy^{(\varepsilon)} &= \frac{1}{\varepsilon^2} g(y^{(\varepsilon)}) dt + \frac{1}{\varepsilon} \sigma dW_t\end{aligned}$$

Integrate the slow equation

$$\begin{aligned}x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \frac{1}{\varepsilon} \int_0^t f(y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f(y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{\sqrt{n}} \int_0^{nt} f(y^{(\varepsilon=1)}(\tau)) d\tau\end{aligned}$$

Assuming $\int f_0(y) \mu(dy) = 0$ and invoking the Central Limit Theorem

$$X(t) = X(0) + W_t$$

$$dX = dW_t$$

Homogenised stochastic equation

central limit theorem

Heuristics for why the fast process can be replaced by noise

$$\begin{aligned} dx^{(\varepsilon)} &= \frac{1}{\varepsilon} f(y^{(\varepsilon)}) dt \\ dy^{(\varepsilon)} &= \frac{1}{\varepsilon^2} g(y^{(\varepsilon)}) dt + \frac{1}{\varepsilon} \sigma dW_t \end{aligned}$$

Integrate the slow equation

$$\begin{aligned} x^{(\varepsilon)}(t) &= x^{(\varepsilon)}(0) + \frac{1}{\varepsilon} \int_0^t f(y^{(\varepsilon)}(s)) ds \\ &= x^{(\varepsilon)}(0) + \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f(y^{(\varepsilon=1)}(\tau)) d\tau \\ &= x^{(\varepsilon)}(0) + \frac{1}{\sqrt{n}} \int_0^{nt} f(y^{(\varepsilon=1)}(\tau)) d\tau \end{aligned}$$

Assuming $\int f_0(y) \mu(dy) = 0$ and invoking the Central Limit Theorem

$$X(t) = X(0) + W_t$$

$$dX = dW_t$$

Homogenised stochastic equation

central limit theorem

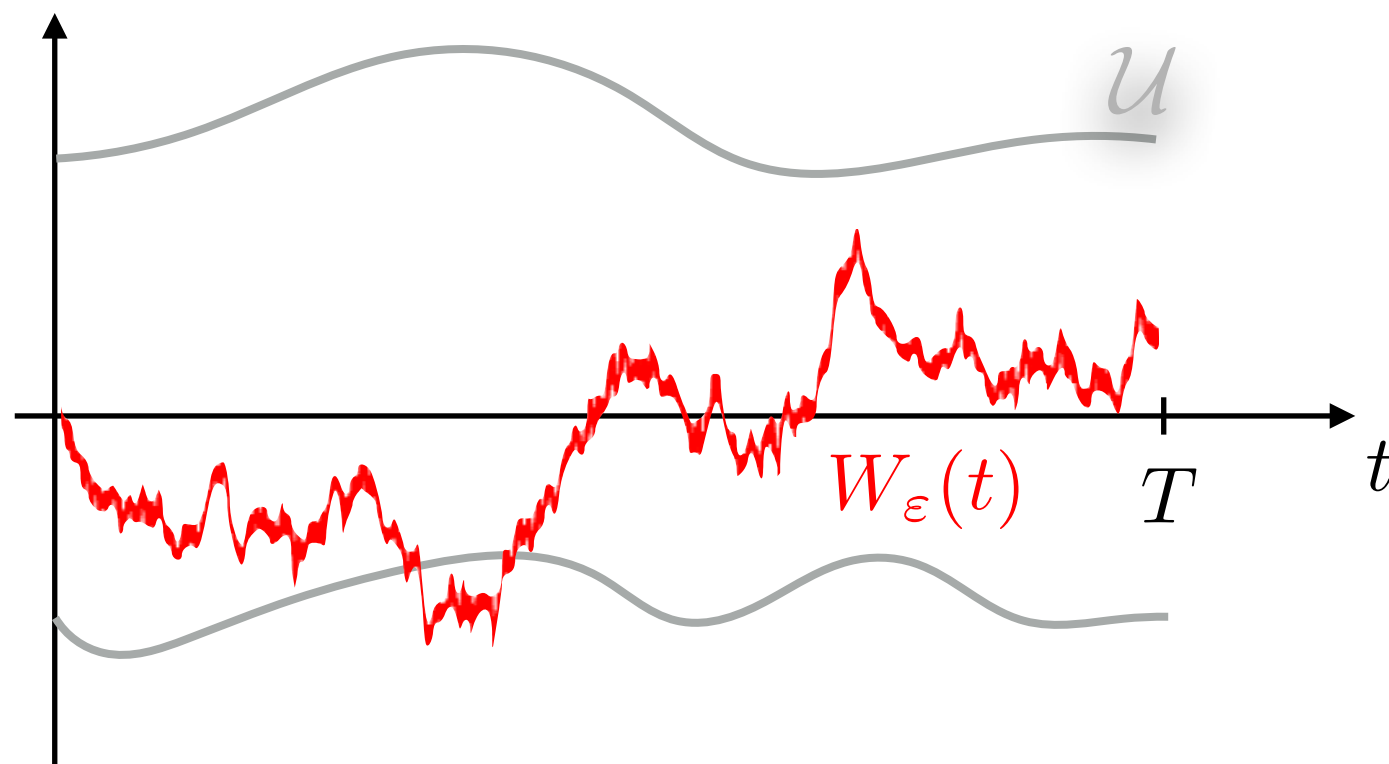
The Weak Invariance Principle

$$W_\varepsilon(t) = \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f_0(y(s)) ds \longrightarrow_w W(t) \quad \text{as } \varepsilon \rightarrow 0$$

weak convergence in $C([0, T], \mathbb{R})$

$$\mathbb{P}(W_\varepsilon \in \mathcal{U}) \longrightarrow \mathbb{P}(W \in \mathcal{U})$$

for suitable subsets of open collection of sample paths $\mathcal{U} \subset C([0, T], \mathbb{R})$



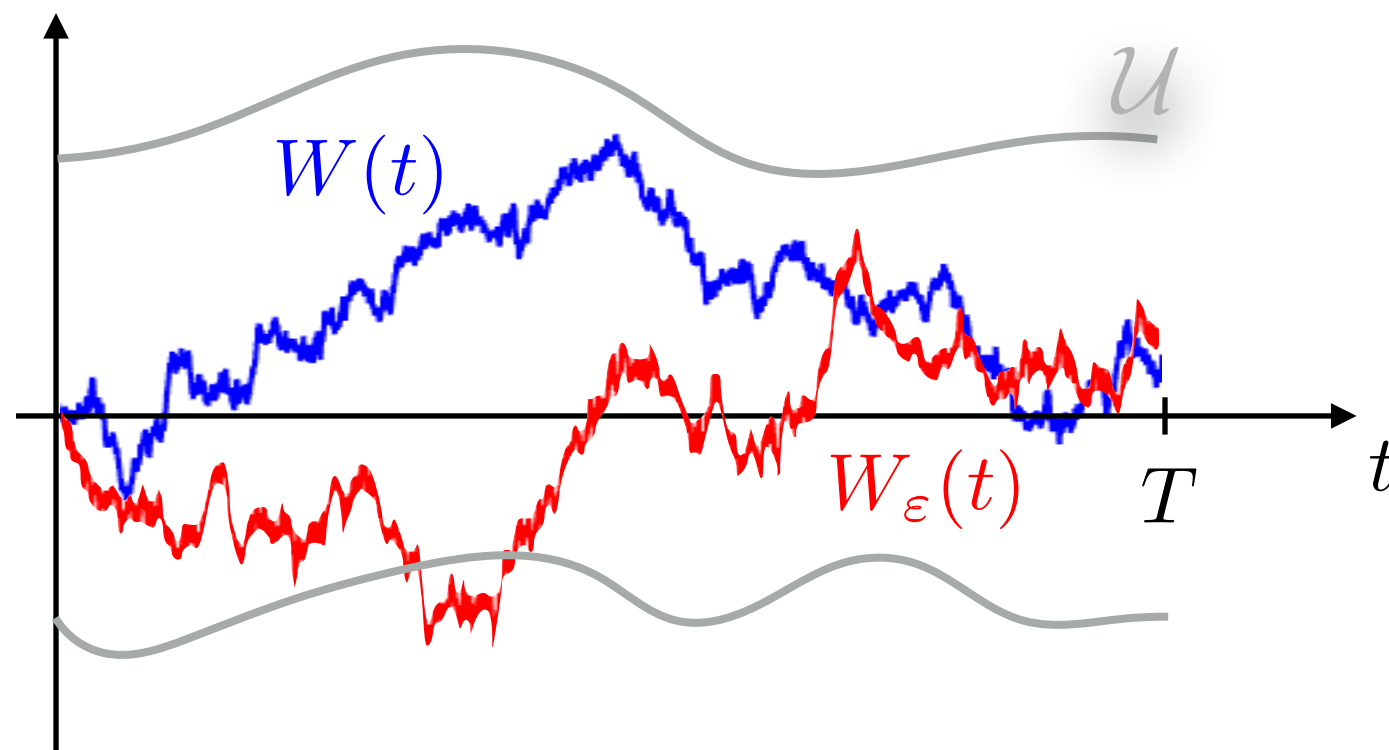
The Weak Invariance Principle

$$W_\varepsilon(t) = \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f_0(y(s)) ds \longrightarrow_w W(t) \quad \text{as } \varepsilon \rightarrow 0$$

weak convergence in $C([0, T], \mathbb{R})$

$$\mathbb{P}(W_\varepsilon \in \mathcal{U}) \longrightarrow \mathbb{P}(W \in \mathcal{U})$$

for suitable subsets of open collection of sample paths $\mathcal{U} \subset C([0, T], \mathbb{R})$



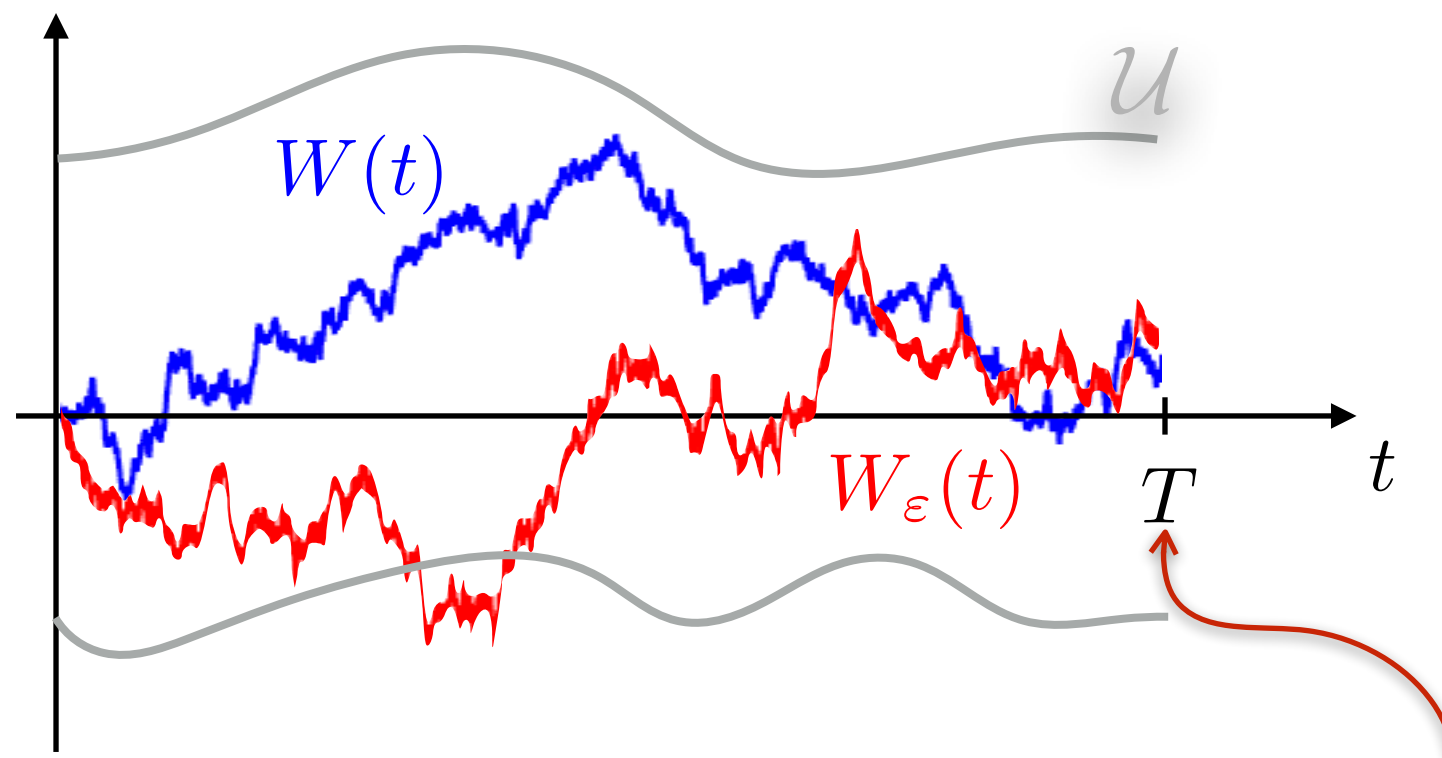
The Weak Invariance Principle

$$W_\varepsilon(t) = \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f_0(y(s)) ds \longrightarrow_w W(t) \quad \text{as } \varepsilon \rightarrow 0$$

weak convergence in $C([0, T], \mathbb{R})$

$$\mathbb{P}(W_\varepsilon \in \mathcal{U}) \longrightarrow \mathbb{P}(W \in \mathcal{U})$$

for suitable subsets of open collection of sample paths $\mathcal{U} \subset C([0, T], \mathbb{R})$



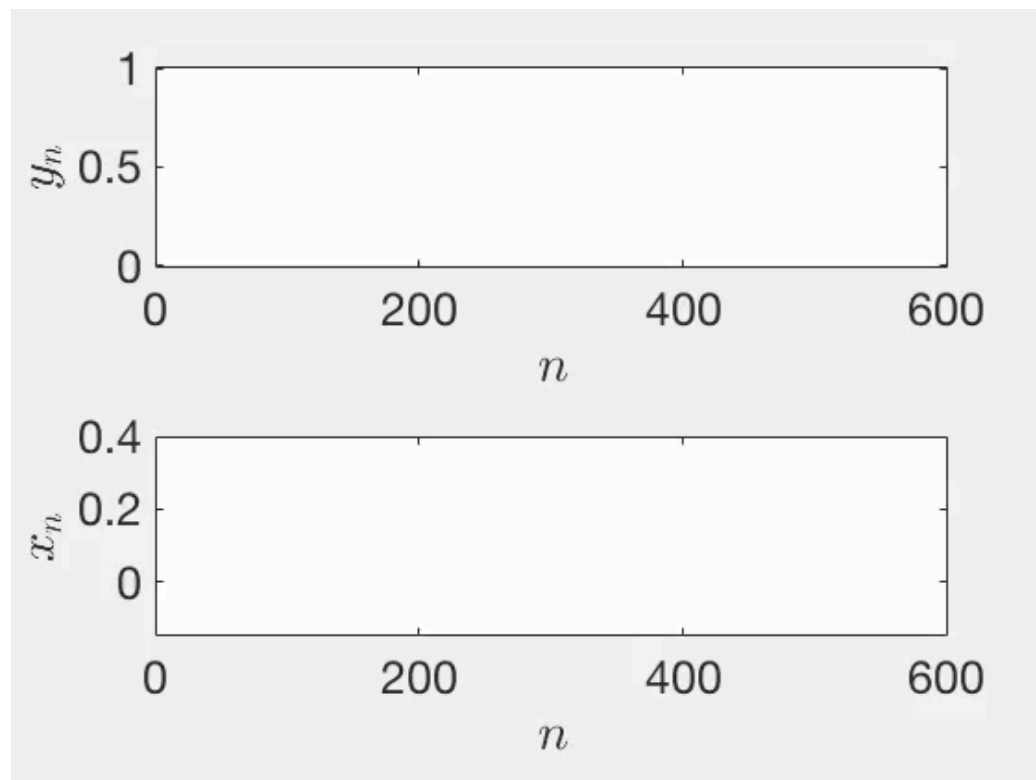
this implies the **Central Limit Theorem**
at all times $t \in [0, T]$

Homogenisation in action

$$x_{n+1} = x_n + \varepsilon(y_n - \tfrac{1}{2})$$

$$y_{n+1} = 4y_n(1 - y_n)$$

strong chaos



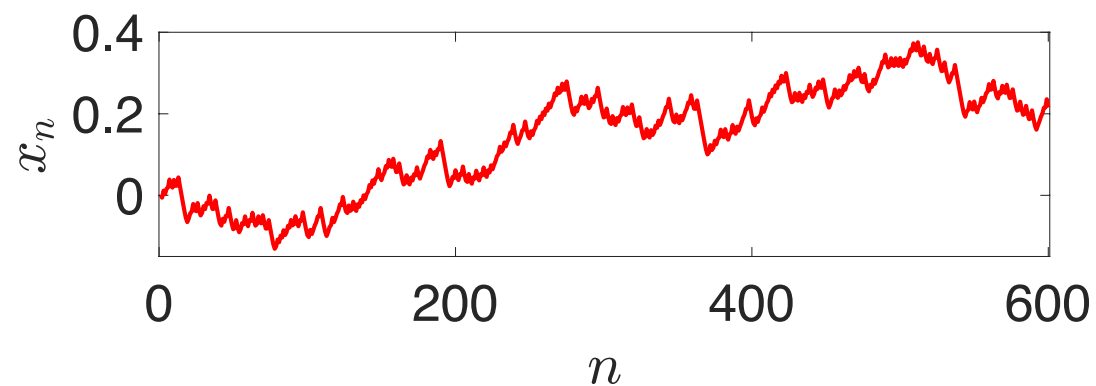
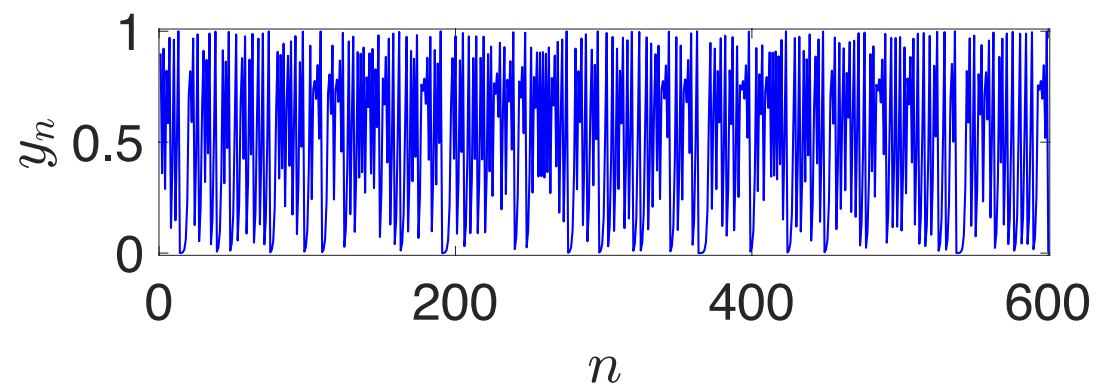
Brownian motion

Homogenisation in action

$$x_{n+1} = x_n + \varepsilon(y_n - \tfrac{1}{2})$$

$$y_{n+1} = 4y_n(1 - y_n)$$

strong chaos

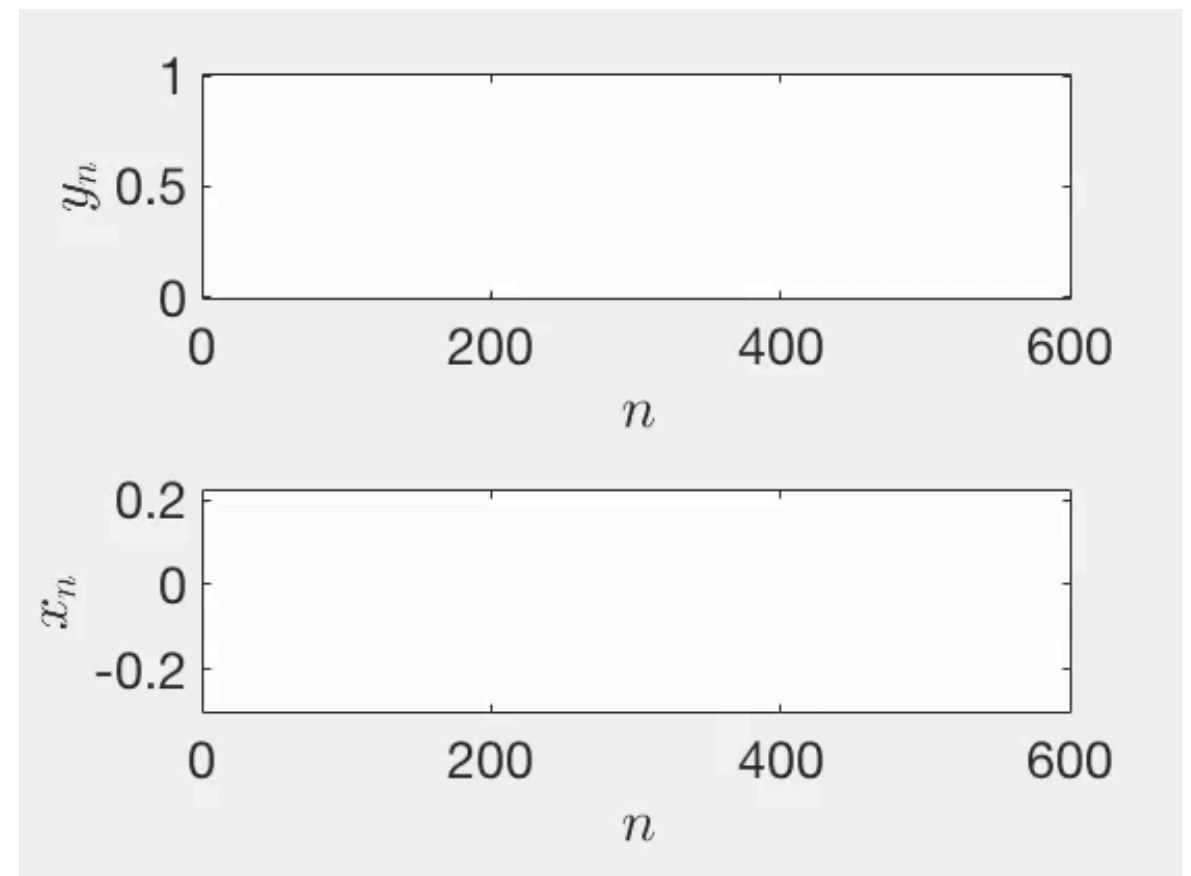


Brownian motion

$$x_{n+1} = x_n + \varepsilon(y^* - y_n)$$

$$y_{n+1} = \begin{cases} y_n(1 + 2^\gamma y_n^\gamma) & 0 \leq y_n \leq \frac{1}{2} \\ 2y_n - 1 & \frac{1}{2} \leq y_n \leq 1 \end{cases}$$

weak chaos

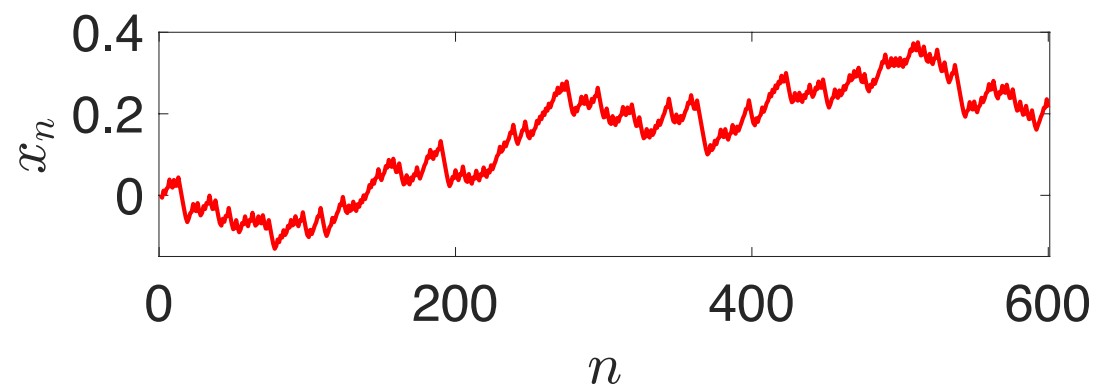
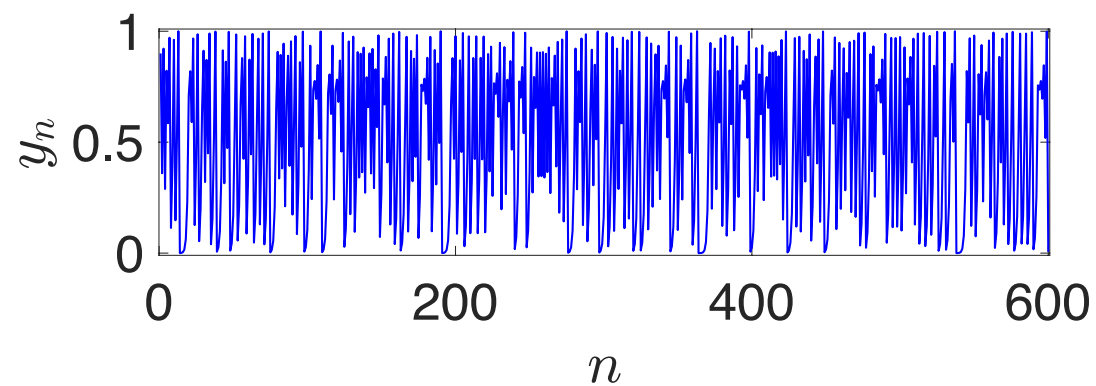


Homogenisation in action

$$x_{n+1} = x_n + \varepsilon(y_n - \tfrac{1}{2})$$

$$y_{n+1} = 4y_n(1 - y_n)$$

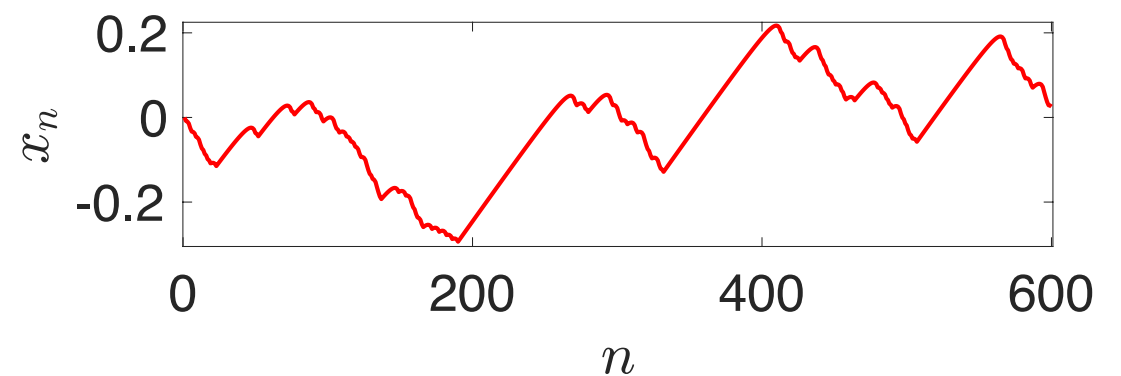
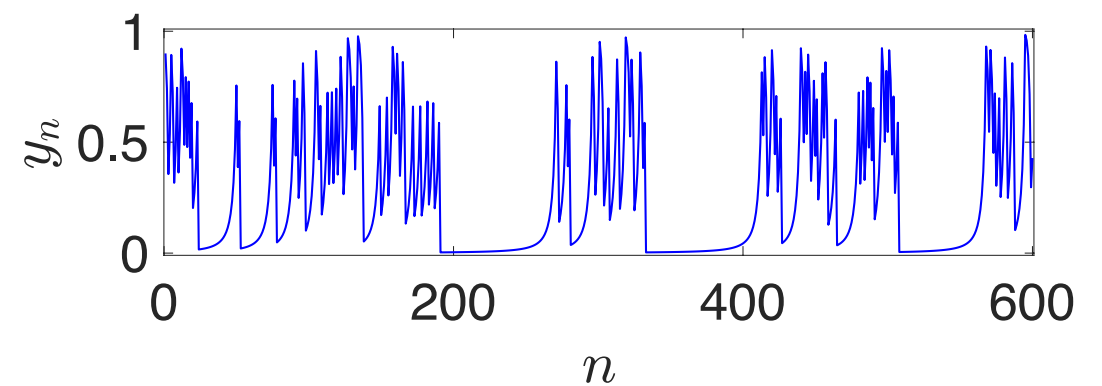
strong chaos



$$x_{n+1} = x_n + \varepsilon(y^* - y_n)$$

$$y_{n+1} = \begin{cases} y_n(1 + 2^\gamma y_n^\gamma) & 0 \leq y_n \leq \frac{1}{2} \\ 2y_n - 1 & \frac{1}{2} \leq y_n \leq 1 \end{cases}$$

weak chaos



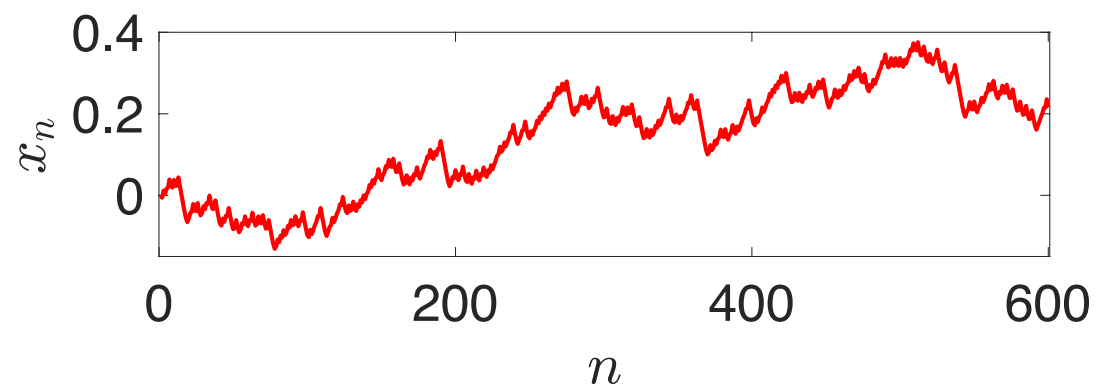
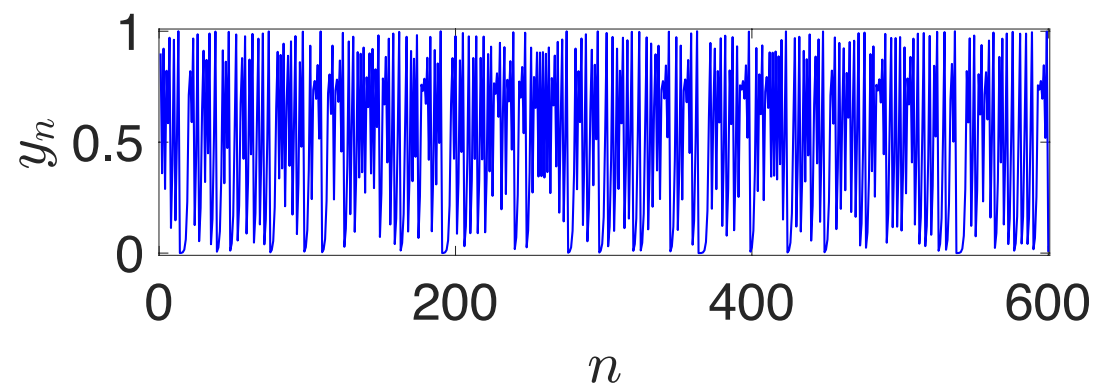
Brownian motion

Homogenisation in action

$$x_{n+1} = x_n + \varepsilon(y_n - \tfrac{1}{2})$$

$$y_{n+1} = 4y_n(1 - y_n)$$

strong chaos

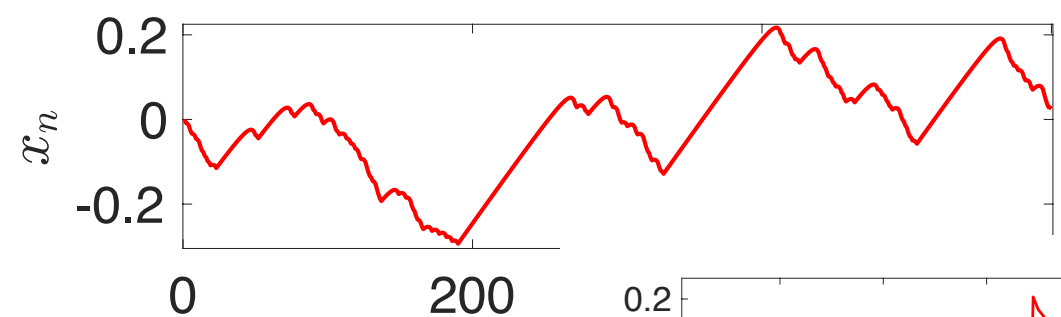
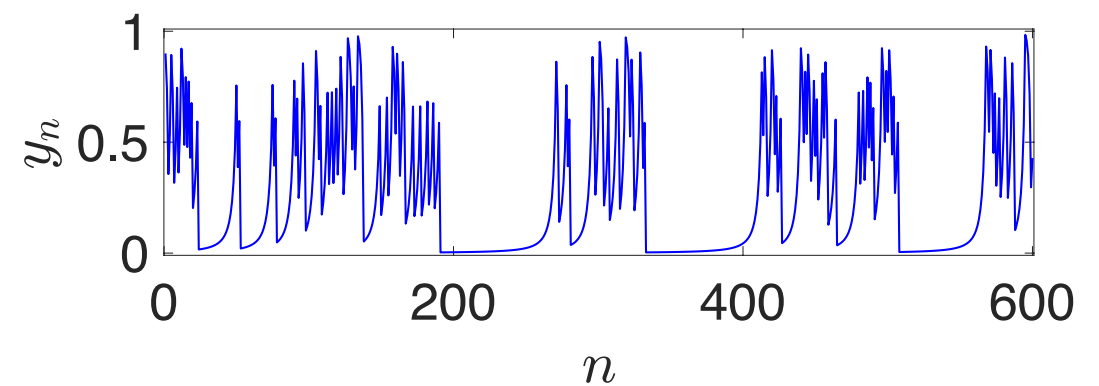


Brownian motion

$$x_{n+1} = x_n + \varepsilon(y^* - y_n)$$

$$y_{n+1} = \begin{cases} y_n(1 + 2^\gamma y_n^\gamma) & 0 \leq y_n \leq \frac{1}{2} \\ 2y_n - 1 & \frac{1}{2} \leq y_n \leq 1 \end{cases}$$

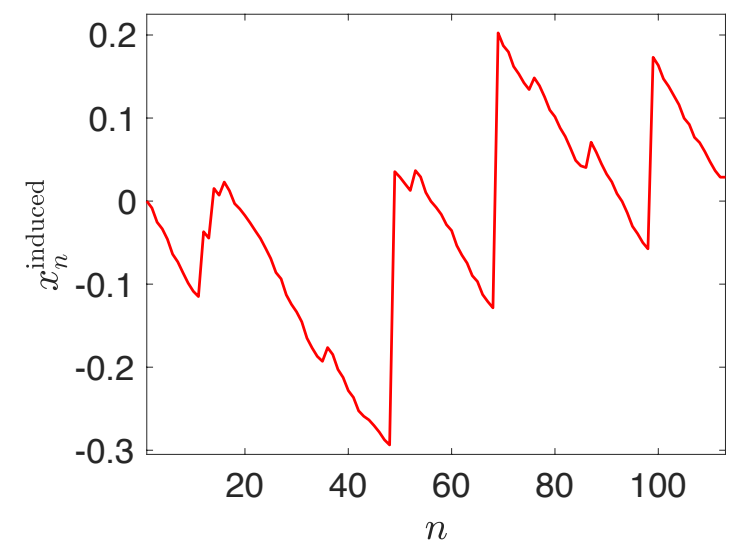
weak chaos



inducing

α -stable noise

$$S(\alpha, \beta, \eta, \mu)$$



Homogenisation

resolved/slow: $dx = \frac{1}{\varepsilon} f_0(x, y) dt + f_1(x, y) dt$

unresolved/fast: $dy = \frac{1}{\varepsilon^2} g(x, y) dt + \frac{1}{\varepsilon} \sigma(x, y) dW_t$

Assumptions:

- fast y -process is ergodic with measure μ_x (mild chaoticity assumptions)
- $\int f_0(x, y) d\mu_x = 0$

Then, in the limit of $\varepsilon \rightarrow 0$, the statistics of the slow x -dynamics is approximated by

$$dX = F(X) dt + \Sigma(X) dW_t$$

where the diffusion matrix is given by a Green-Kubo formula

$$\frac{1}{2} \Sigma \Sigma^T = \int_0^\infty C(s) ds$$

with the auto-correlation matrix $C(t) = \mathbb{E}^{\mu_x} [f_0(x, y) f_0(x, y(t))]$ and

$$F(X) = \int f_1(x, y) d\mu_x + \int_0^\infty \int \nabla_x f_0(x, y(s)) \otimes f_0(x, y) d\mu_x ds$$

What is known rigorously and what are the challenges?

- stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:
skew product structure

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:

skew product structure

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

1. $f_0 = f_0(y)$  additive noise $dX = F(X)dt + \sigma dW$

Melbourne & Stuart (2011)

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:
skew product structure

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

1. $f_0 = f_0(y)$  additive noise $dX = F(X)dt + \sigma dW$
Melbourne & Stuart (2011)

2. $f_0 = f_0(x, y)$  multiplicative noise $dX = \tilde{F}(X)dt + \sigma(X)dW$
GAG & Melbourne (2013)

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:
skew product structure

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

1. $f_0 = f_0(y)$  additive noise $dX = F(X)dt + \sigma dW$

Melbourne & Stuart (2011)

2. $f_0 = f_0(x, y)$  multiplicative noise $dX = \tilde{F}(X)dt + \sigma(X)dW$

GAG & Melbourne (2013)

Restrictions: $x \in \mathbb{R}^1$ or restrictive class of functions $f_0(x, y)$

What type of noise? * strongly chaotic fast dynamics: Brownian noise

* weakly chaotic fast dynamics: α -stable noise

► continuous time: Stratonovich/Marcus

(Wong-Zakai Theorem)

► discrete time: Ito or “neither”  later

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:
skew product structure

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

1. $f_0 = f_0(y)$  additive noise $dX = F(X)dt + \sigma dW$

Melbourne & Stuart (2011)

3. $f_0 = f_0(x, y)$  multiplicative noise $dX = \tilde{F}(X)dt + \sigma(X)dW$

Melbourne & Kelly (2015)

No restriction on dimension of x

only the strongly chaotic case

leading to Stratonovich noise in line with the Wong-Zakai Theorem

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:

skew product structure

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$

$$\dot{y} = \frac{1}{\varepsilon^2} g_0(x, y)$$

↑

back-coupling

What is known rigorously and what are the challenges?

● stochastic fast dynamics: *Khasminsky '66, Kurtz '73, Papanicolaou '76*

● deterministic fast dynamics:

skew product structure

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$

$$\dot{y} = \frac{1}{\varepsilon^2} g_0(x, y) \text{ back-coupling}$$

strongly chaotic case

weakly chaotic fast dynamics with $x \in \mathbb{R}^n$

allowing for multi-dimensional α -stable noise

Open problems from a modelling perspective

- slow dynamics couples back into the fast dynamics

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

What can go wrong?

If the fast invariant measure μ_x does not depend smoothly on x (“no linear response”) even averaging does not “work”

$$F(X) = \underbrace{\int f_1(x, y) \mu_x(dy)}$$

non-Lipschitz
uniqueness of solutions not guaranteed

Open problems from a modelling perspective

- slow dynamics couples back into the fast dynamics

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g_0(x, y)\end{aligned}$$

What can go wrong?

If the fast invariant measure μ_x does not depend smoothly on x (“no linear response”) even averaging does not “work”

$$F(X) = \underbrace{\int f_1(x, y) \mu_x(dy)}_{\text{non-Lipschitz}}$$

How to detect failure
of linear response in
time series?

*GAG, Wormell & Wouters
(2016)*

non-Lipschitz
uniqueness of solutions not guaranteed

Open problems from a modelling perspective

- slow dynamics couples back into the fast dynamics
- finite time scale separation

Theory works in the limit $\varepsilon \rightarrow 0$

but in many physical applications ε is not so small

Where do we need the limit?

Averaging: Large deviation principle: $|\frac{1}{T} \int_0^T f_1(x, y(s)) ds - F(x)|$

Homogenisation: Central Limit Theorem (Weak Invariance Principle)

$$W_\varepsilon(t) = \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f_0(y(s)) ds \rightarrow_w W(t) \quad \text{as } \varepsilon \rightarrow 0$$

Finite ε effects are finite size effects

The Central Limit Theorem and the Edgeworth expansion

The Central Limit Theorem

Assume X_i are *i.i.d.* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n (X_j - \mu) \rightarrow_d \mathcal{N}(0, 1)$$

where $\mu = \mathbb{E}[X_i]$ and $\sigma^2 = \mathbb{E}[X_i^2]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0,\sigma^2}(x) \times \left(1 + \frac{1}{6\sqrt{n}} \frac{\gamma}{\sigma^3} H_3(x/\sigma) \right) + o\left(\frac{1}{\sqrt{n}}\right)$$

where $H_3(x) = x^3 - 3x$ is the third Hermite polynomial

and γ/σ^3 is the skewness of X_i

The Central Limit Theorem and the Edgeworth expansion

The Central Limit Theorem

Assume X_i are *i.i.d.* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n (X_j - \mu) \rightarrow_d \mathcal{N}(0, 1)$$

where $\mu = \mathbb{E}[X_i]$ and $\sigma^2 = \mathbb{E}[X_i^2]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0,\sigma^2}(x) \times \left(1 + \frac{1}{6\sqrt{n}} \frac{\gamma}{\sigma^3} H_3(x/\sigma) \right) + o\left(\frac{1}{\sqrt{n}}\right)$$

where $H_3(x) = x^3 - 3x$ is the third Hermite polynomial

and γ/σ^3 is the skewness of X_i **this is not a density!**

The Central Limit Theorem and the Edgeworth expansion

The Central Limit Theorem

Assume X_i are *i.i.d.* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n (X_j - \mu) \rightarrow_d \mathcal{N}(0, 1)$$

where $\mu = \mathbb{E}[X_i]$ and $\sigma^2 = \mathbb{E}[X_i^2]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0,\sigma^2}(x) \times \left(1 + \frac{1}{6\sqrt{n}} \frac{\gamma}{\sigma^3} H_3(x/\sigma) \right) + o\left(\frac{1}{\sqrt{n}}\right)$$

where $H_3(x) = x^3 - 3x$ is the third Hermite polynomial

and γ/σ^3 is the skewness of X_i

**can be pushed to any order
involving higher-order moments**

The Central Limit Theorem and the Edgeworth expansion

The Central Limit Theorem

Assume X_i are stationary *weakly dependent* random variables

$$S_n := \frac{1}{\sigma\sqrt{n}} \sum_{j=1}^n (X_j - \mu) \rightarrow_d \mathcal{N}(0, 1)$$

where $\mu = \mathbb{E}[X_i]$ and $\sigma^2 = \mathbb{E}[X_i^2] + 2 \sum_{j=1}^{\infty} \mathbb{E}[X_1 X_{j+1}]$

For finite n there are *deviations* to the CLT

These are described by the **Edgeworth expansion**

$$\rho_n(x) = \Phi_{0, \sigma^2 + \delta\sigma^2/n}(x) \times \left(1 + \frac{1}{\sqrt{n}} \delta\kappa H_3(x/\sigma) \right) + o\left(\frac{1}{\sqrt{n}}\right)$$

where H_3 is the third Hermite polynomial and $\delta\sigma^2$ and $\delta\kappa$ are integrals of correlation functions of X_i (Götze & Hipp (1983))

Stochastic Parametrisation using the Edgeworth expansion

Given a multi-scale dynamical system

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

- (I) determine the Edgeworth expansion coefficients σ_{GK}^2 , $\delta\kappa$ associated with $f_0(x, y)$

Stochastic Parametrisation using the Edgeworth expansion

Given a multi-scale dynamical system

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

- (I) determine the Edgeworth expansion coefficients σ_{GK}^2 , $\delta\kappa$ associated with $f_0(x, y)$
- (II) model the multi-scale system by the surrogate stochastic process

$$\begin{aligned}\dot{X} &= \frac{1}{\varepsilon} A(\eta) + F(X) \\ d\eta &= -\frac{1}{\varepsilon^2} \gamma \eta dt + \frac{1}{\sqrt{\varepsilon}} dW_t\end{aligned}\quad \begin{array}{l} \text{with } A(\eta) = a\eta^2 + b\eta + c \\ \text{Id Ornstein-Uhlenbeck process} \end{array}$$

where the parameters a , b , c , γ are determined such that the Edgeworth expansion coefficients associated with $A(\eta)$ match σ_{GK}^2 , $\delta\kappa$

Stochastic Parametrisation using the Edgeworth expansion

Given a multi-scale dynamical system

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

- (I) determine the Edgeworth expansion coefficients σ_{GK}^2 , $\delta\kappa$ associated with $f_0(x, y)$
- (II) model the multi-scale system by the surrogate stochastic process

$$\begin{aligned}\dot{X} &= \frac{1}{\varepsilon} A(\eta) + F(X) \\ d\eta &= -\frac{1}{\varepsilon^2} \gamma \eta dt + \frac{1}{\sqrt{\varepsilon}} dW_t\end{aligned}\quad \text{with } A(\eta) = a\eta^2 + b\eta + c$$

Id Ornstein-Uhlenbeck process

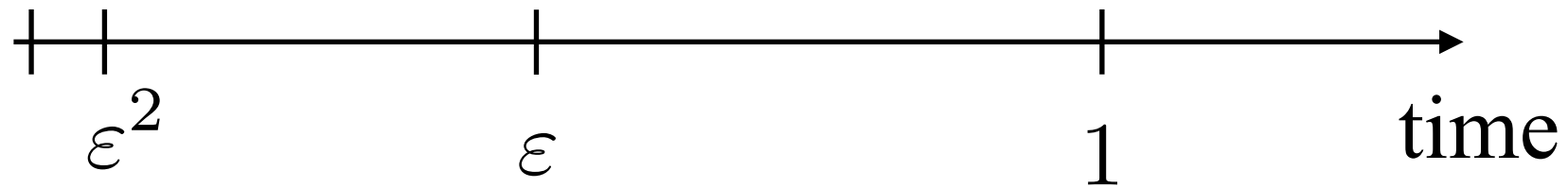
where the parameters a , b , c , γ are determined such that the Edgeworth expansion coefficients associated with $A(\eta)$ match σ_{GK}^2 , $\delta\kappa$

Remark: By construction the homogenized limit system of the original and the surrogate system are the same!

How to calculate the Edgeworth coefficients?

The three time scales of multi-scale systems

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$



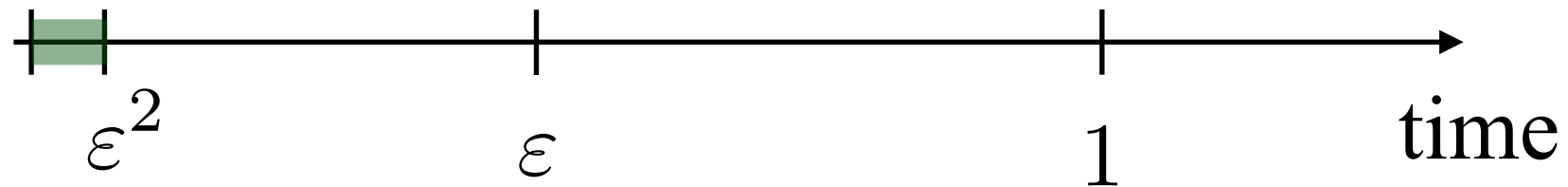
How to calculate the Edgeworth coefficients?

The three time scales of multi-scale systems

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$
$$\dot{y} = \frac{1}{\varepsilon^2} g(y)$$

nontrivial fast dynamics

trivial slow dynamics $x(t) = x_0$



How to calculate the Edgeworth coefficients?

The three time scales of multi-scale systems

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

nontrivial fast dynamics

trivial slow dynamics $x(t) = x_0$



fast dynamics has equilibrated

trivial slow dynamics $x(t) = x_0$

How to calculate the Edgeworth coefficients?

The three time scales of multi-scale systems

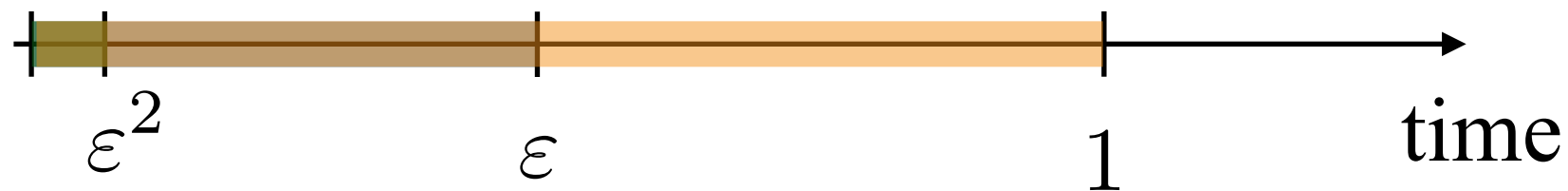
$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

nontrivial fast dynamics

trivial slow dynamics $x(t) = x_0$

diffusive time scale: CLT

$$dX = F(X) dt + \sigma(X) \circ dW_t$$



fast dynamics has equilibrated

trivial slow dynamics $x(t) = x_0$

How to calculate the Edgeworth coefficients?

The three time scales of multi-scale systems

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y) \\ \dot{y} &= \frac{1}{\varepsilon^2} g(y)\end{aligned}$$

nontrivial fast dynamics

trivial slow dynamics $x(t) = x_0$

diffusive time scale: CLT

$$dX = F(X) dt + \sigma(X) \circ dW_t$$



fast dynamics has equilibrated

trivial slow dynamics $x(t) = x_0$

expect deviations of CLT on timescale $t = \varepsilon$

$$\frac{x(t) - x_0}{\sqrt{t}} \rightarrow \sigma(x_0) W_t$$

How to calculate the Edgeworth coefficients?

Consider $\rho_t(x(t)|x(0) = x_0) = \int dx dy e^{\mathcal{L}t} \delta_{x_0}(x) \mu(dy)$ for $t = \varepsilon$

 transfer operator

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$

$$\dot{y} = \frac{1}{\varepsilon^2} g(y)$$

$$\mathcal{L} = \frac{1}{\varepsilon^2} \mathcal{L}_0 + \frac{1}{\varepsilon} \mathcal{L}_1 + \mathcal{L}_2$$

$$\mathcal{L}_0 \rho = -\partial_y (g(y) \rho), \quad \mathcal{L}_1 \rho = -\partial_x (f_0(x, y) \rho), \quad \mathcal{L}_2 \rho = -\partial_x (f_1(x, y) \rho)$$

How to calculate the Edgeworth coefficients?

Consider $\rho_t(x(t)|x(0) = x_0) = \int dx dy e^{\mathcal{L}t} \delta_{x_0}(x) \mu(dy)$ for $t = \varepsilon$

transfer operator

$$\dot{x} = \frac{1}{\varepsilon} f_0(x, y) + f_1(x, y)$$

$$\mathcal{L} = \frac{1}{\varepsilon^2} \mathcal{L}_0 + \frac{1}{\varepsilon} \mathcal{L}_1 + \mathcal{L}_2$$

$$\dot{y} = \frac{1}{\varepsilon^2} g(y)$$

$$\mathcal{L}_0 \rho = -\partial_y (g(y) \rho), \quad \mathcal{L}_1 \rho = -\partial_x (f_0(x, y) \rho), \quad \mathcal{L}_2 \rho = -\partial_x (f_1(x, y) \rho)$$

Calculate asymptotically, using successive applications of the Duhamel-Dyson formula, up to $\mathcal{O}(\varepsilon^n)$:

$$\frac{\mathbb{E}[x(\varepsilon) - x_0]}{\sqrt{\varepsilon}} = \sqrt{\varepsilon} \xi = \sqrt{\varepsilon} \langle f_1(x_0) \rangle$$

$$\frac{\mathbb{E}[\hat{x}^2]}{\varepsilon} = \sigma_{\text{GK}}^2 - 2\varepsilon \int_0^{\frac{t}{\varepsilon^2}} ds (s \langle f_0 e^{\mathcal{L}_0 s} f_0 \rangle - \langle f_0 e^{\mathcal{L}_0 s} f_1 \rangle) + \dots$$

$\hat{x} = x - \mathbb{E}[x]$

$$\frac{\mathbb{E}[\hat{x}^3]}{\varepsilon^{\frac{3}{2}}} = \sqrt{\varepsilon} \int_0^{\frac{t}{\varepsilon^2}} ds_1 ds_2 \langle f_0 e^{\mathcal{L}_0 s_1} f_0 e^{\mathcal{L}_0 s_2} f_0 \rangle$$

Example I Diffusive limit of a deterministic multi-scale system

$$\begin{aligned}x_{j+1}^{(\varepsilon)} &= x_j^{(\varepsilon)} + \varepsilon f_0(y_j) + \varepsilon^2 f_1(x_j^{(\varepsilon)}) \\y_{j+1} &= p y_j \pmod{1}\end{aligned}$$

Homogenisation

$$dX = f(X)dt + \sigma_{\text{GK}} dW$$

GAG & Melbourne (2013)

Edgeworth expansion

$$X_{j+1}^{(\varepsilon)} = X_j^{(\varepsilon)} + \varepsilon A(\eta_j) + \varepsilon^2 f_1(X_j^{(\varepsilon)})$$

$$A(\eta) = a_s \eta^2 + b_s \eta + c_s$$

$$\eta_{j+1} = \phi \eta_j + N_j \quad N_j \sim \mathcal{N}(0, 1)$$

$$\sigma_{\text{GK}}^2 \text{ and } \delta \kappa_3$$

Example I Diffusive limit of a deterministic multi-scale system

$$\begin{aligned}x_{j+1}^{(\varepsilon)} &= x_j^{(\varepsilon)} + \varepsilon f_0(y_j) + \varepsilon^2 f_1(x_j^{(\varepsilon)}) \\y_{j+1} &= p y_j \pmod{1}\end{aligned}$$

Homogenisation

$$dX = f(X)dt + \sigma_{\text{GK}} dW$$

GAG & Melbourne (2013)

$$\begin{aligned}p &= 3 \\f_0(y) &= y^5 + y^4 + y^3 + y^2 + y - \frac{29}{20} \\f_1(x) &= -x(x^2 + x - 1)\end{aligned}$$

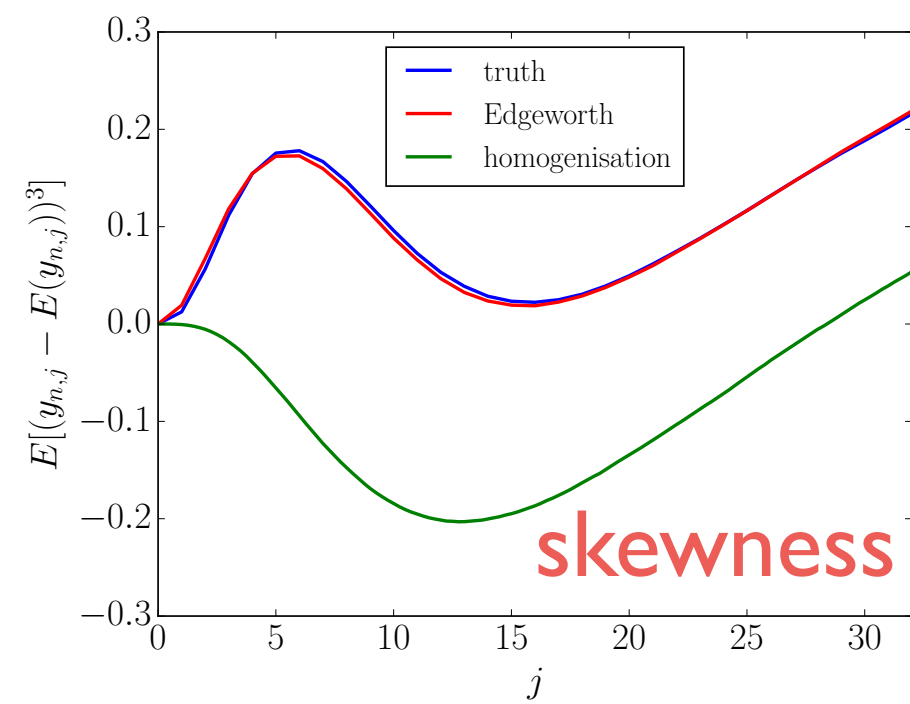
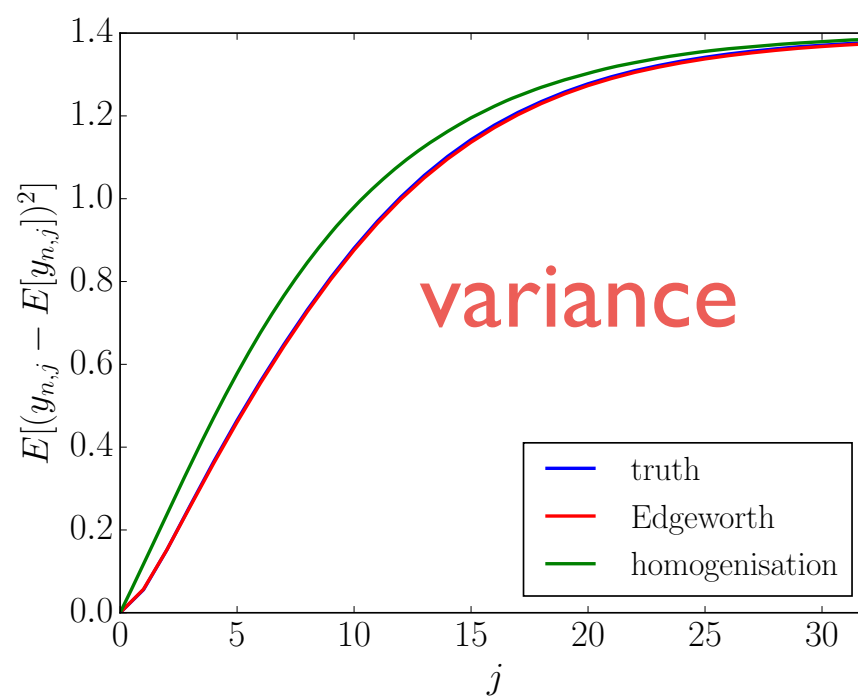
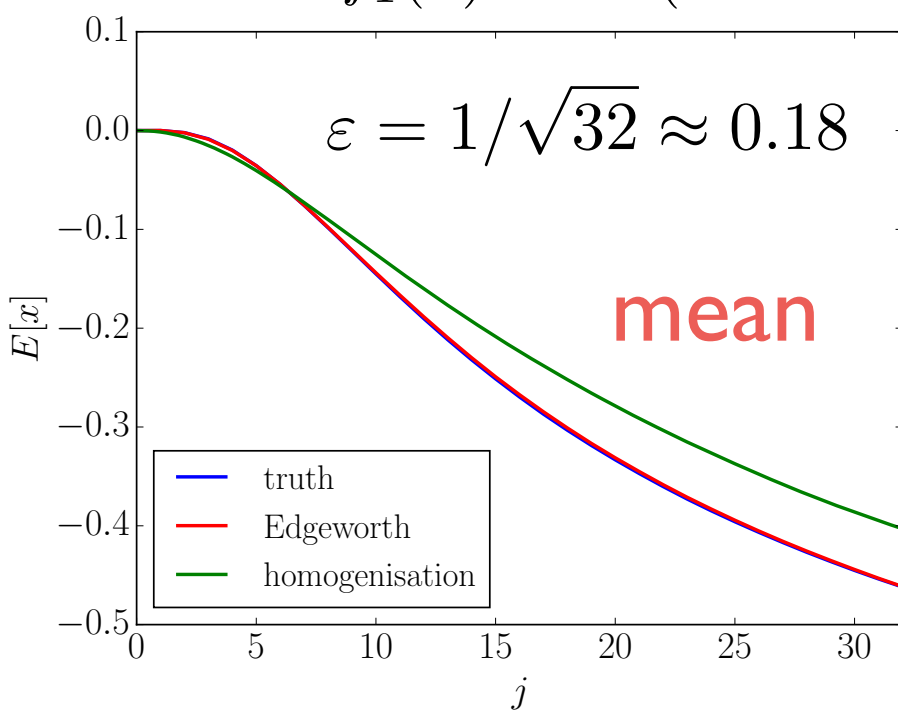
Edgeworth expansion

$$X_{j+1}^{(\varepsilon)} = X_j^{(\varepsilon)} + \varepsilon A(\eta_j) + \varepsilon^2 f_1(X_j^{(\varepsilon)})$$

$$A(\eta) = a_s \eta^2 + b_s \eta + c_s$$

$$\eta_{j+1} = \phi \eta_j + N_j \quad N_j \sim \mathcal{N}(0, 1)$$

$$\sigma_{\text{GK}}^2 \text{ and } \delta \kappa_3$$



Example I Diffusive limit of a deterministic multi-scale system

$$\begin{aligned}x_{j+1}^{(\varepsilon)} &= x_j^{(\varepsilon)} + \varepsilon f_0(y_j) + \varepsilon^2 f_1(x_j^{(\varepsilon)}) \\ y_{j+1} &= p y_j \pmod{1}\end{aligned}$$

Homogenisation

$$dX = f(X)dt + \sigma_{\text{GK}} dW$$

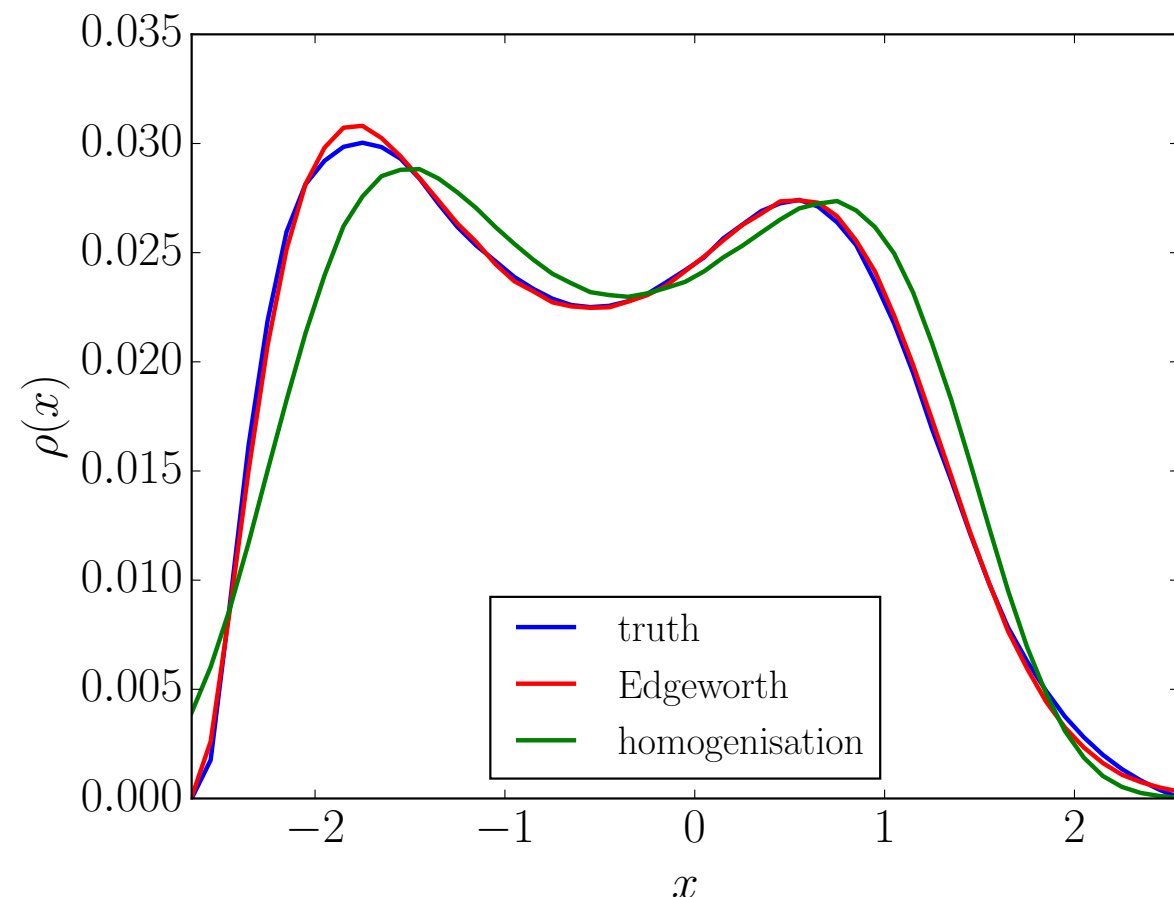
GAG & Melbourne (2013)

Edgeworth expansion

$$X_{j+1}^{(\varepsilon)} = X_j^{(\varepsilon)} + \varepsilon A(\eta_j) + \varepsilon^2 f_1(X_j^{(\varepsilon)})$$

$$A(\eta) = a_s \eta^2 + b_s \eta + c_s$$

$$\begin{aligned}\eta_{j+1} &= \phi \eta_j + N_j & N_j &\sim \mathcal{N}(0, 1) \\ &\sigma_{\text{GK}}^2 \text{ and } \delta \kappa_3\end{aligned}$$



empirical density

Example II Diffusive limit of a triad system

$$\begin{aligned}\dot{x} &= \frac{1}{\varepsilon} B_0 y_1 y_2 \\ \dot{y}_1 &= \frac{1}{\varepsilon} B_1 x y_2 - \frac{1}{\varepsilon^2} \gamma_1 y_1 - \frac{1}{\varepsilon} \sigma_1 \dot{W}_1 \\ \dot{y}_2 &= \frac{1}{\varepsilon} B_2 x y_1 - \frac{1}{\varepsilon^2} \gamma_2 y_2 - \frac{1}{\varepsilon} \sigma_2 \dot{W}_2\end{aligned}$$

Triad system

Majda et al (2001)

backcoupling

$$\dot{X} = \frac{1}{\varepsilon} A(\eta)$$

$$\dot{\eta} = \frac{1}{\varepsilon} \alpha X - \frac{1}{\varepsilon^2} \eta - \frac{1}{\varepsilon} \sigma \dot{W}$$

$$A(\eta) = a_s \eta^2 + b_s \eta + c_s$$

Example II Diffusive limit of a triad system

$$\sigma_{\text{GK}}^2 = \int_0^\infty C(\tau) d\tau = \frac{B_0^2 \sigma_{1\infty}^2 \sigma_{2\infty}^2}{\gamma_1 + \gamma_2}$$

$$\delta\kappa_3 = 0$$

$$\mu = \int_0^\infty R(\tau) d\tau = x \frac{B_0}{\gamma_1 + \gamma_2} (B_1 \sigma_{2\infty}^2 + B_2 \sigma_{1\infty}^2)$$

$$\delta\mu = \int_0^\infty \tau R(\tau) d\tau = x \frac{B_0}{(\gamma_1 + \gamma_2)^2} (B_1 \sigma_{2\infty}^2 + B_2 \sigma_{1\infty}^2)$$

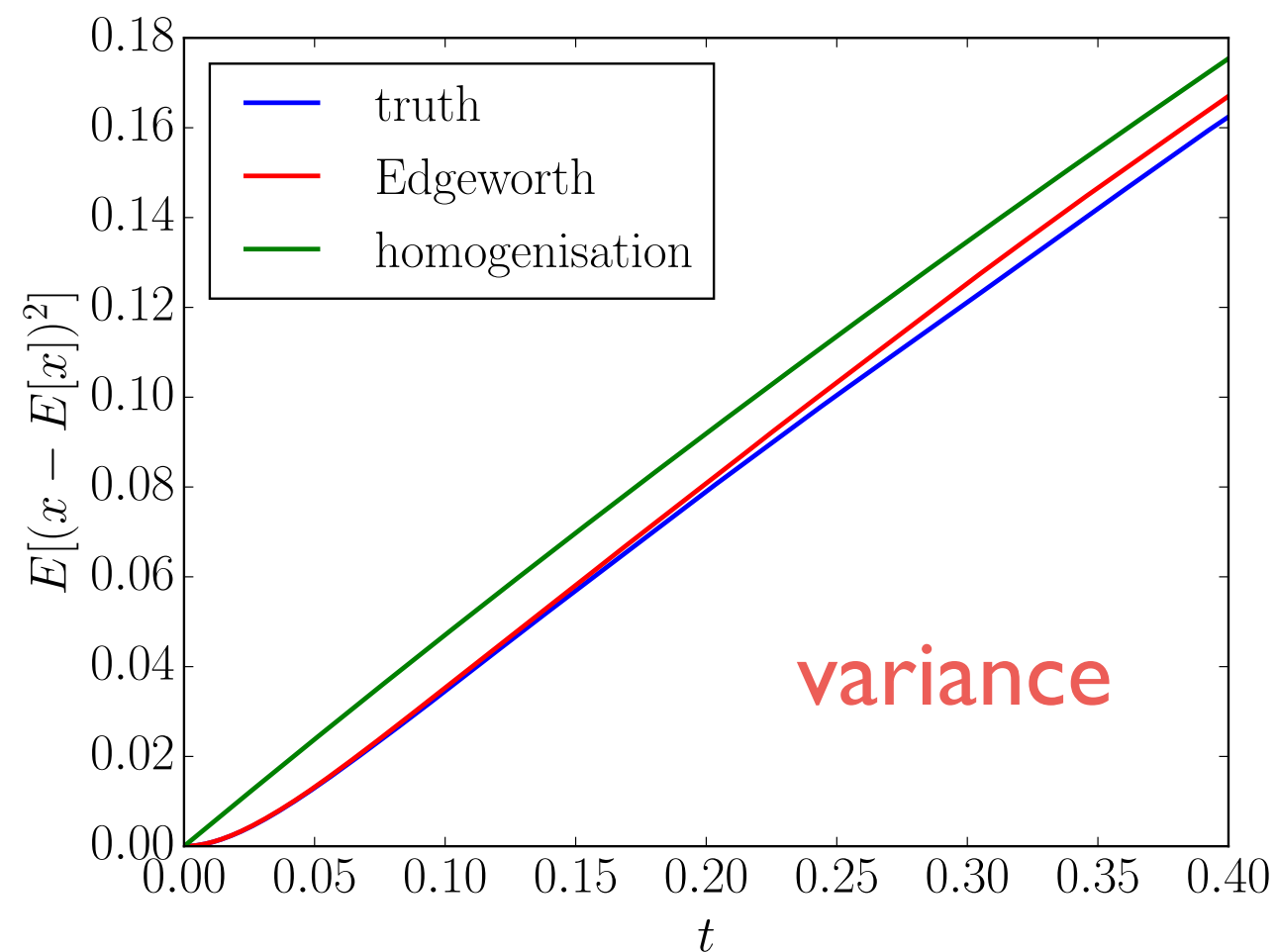
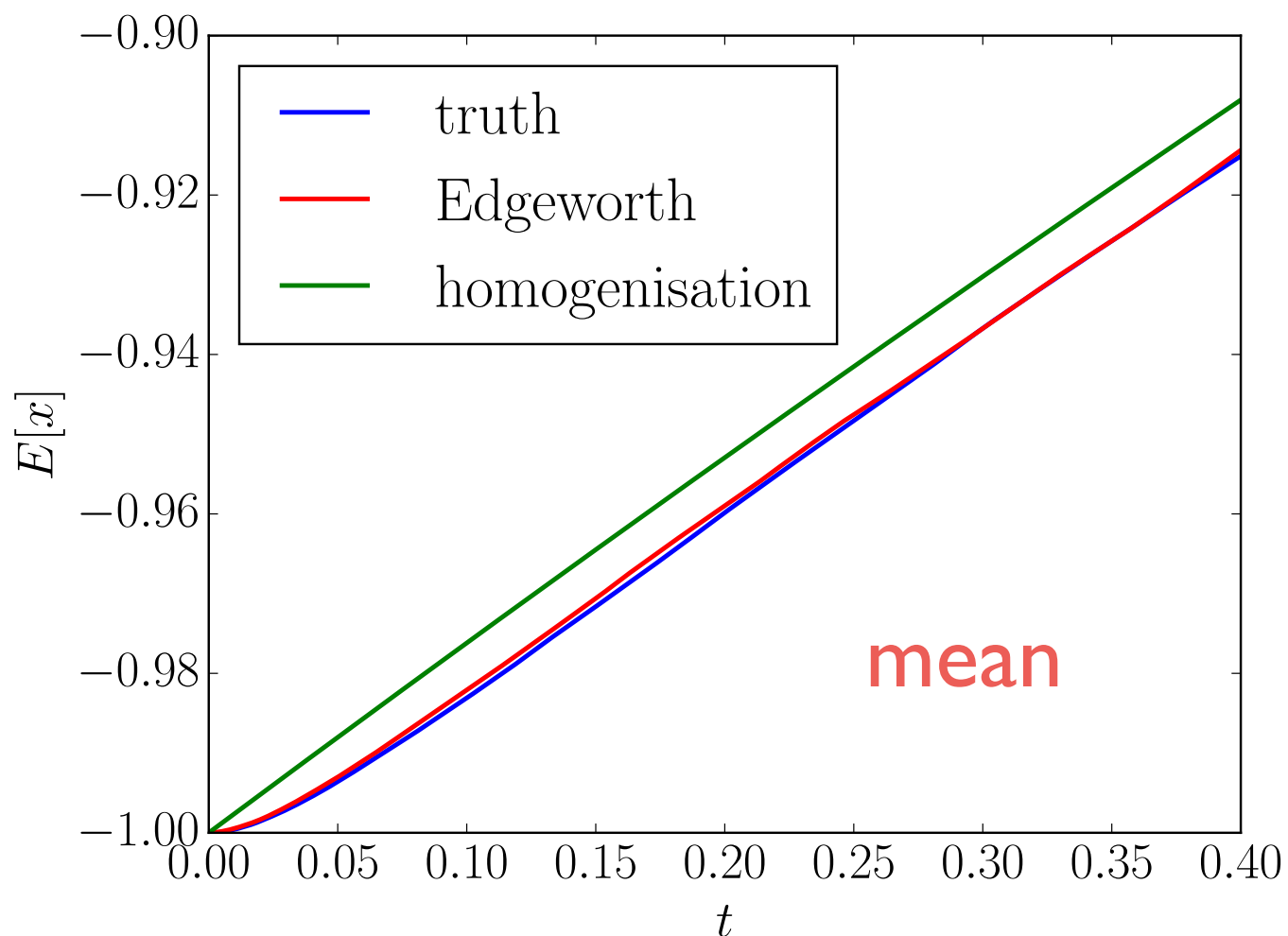
Triad system

$$\int_0^\infty C(\tau) d\tau = \frac{\sigma_\infty^2}{\gamma} (a^2 \sigma_\infty^2 + b^2)$$

$$\int_0^\infty R(\tau) d\tau = x \frac{\alpha b}{\gamma}$$

$$\int_0^\infty \tau R(\tau) d\tau = x \frac{\alpha b}{\gamma^2}$$

Surrogate system



Statistical consistency of numerical integrators for deterministic multi-scale systems

Question:

How does the numerical time integrator affect the statistical behaviour of the simulation?

*Example: Influence of conservation laws on invariant measure in Hamiltonian systems
Dubinkina & Frank (2007)*

Statistical consistency of numerical integrators for deterministic multi-scale systems

Question:

How does the numerical time integrator affect the statistical behaviour of the simulation?

*Example: Influence of conservation laws on invariant measure in Hamiltonian systems
Dubinkina & Frank (2007)*

What are minimal requirements for a numerical scheme to assure that the statistics of the numerical simulations match those of the original continuous-time system?

Take Home Message:

Avoid first-order time-stepping when simulating deterministic multi-scale systems

Statistical consistency of numerical integrators for deterministic multi-scale systems

Question:

How does the numerical time integrator affect the statistical behaviour of the simulation?

*Example: Influence of conservation laws on invariant measure in Hamiltonian systems
Dubinkina & Frank (2007)*

What are minimal requirements for a numerical scheme to assure that the statistics of the numerical simulations match those of the original continuous-time system?

Take Home Message:

Avoid first-order time-stepping when simulating deterministic multi-scale systems

Tools:

- ★ Homogenisation
- ★ Backward error analysis

Homogenisation

The statistical behaviour of deterministic multi-scale systems is well described by **homogenisation** (modulo Edgeworth corrections)

The statistical behaviour of the slow dynamics of the deterministic multi-scale system

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$\begin{aligned}x &\in \mathbb{R}^n \\ y &\in \mathbb{R}^m, m \geq 3\end{aligned}$$

with chaotic fast dynamics and fast invariant measure μ , and $\int_{\Lambda} f_0 d\mu = 0$

is (in the limit $\varepsilon \rightarrow 0$) described by the homogenised SDE

$$dX = F(X) dt + \sigma h(X) \circ dW_t$$

Melbourne & Stuart (2011)
GAG & Melbourne (2013)
Kelly & Melbourne (2015)

where

$$F(X) = \int_{\Lambda} f(X, y) d\mu$$

$$\frac{1}{2}\sigma^2 = \int_0^\infty \mathbb{E}[f_0(y) f_0(\varphi^t y)] dt$$

Green-Kubo formula

flow map of fast dynamics

Homogenisation

The statistical behaviour of deterministic multi-scale systems is well described by **homogenisation** (modulo Edgeworth corrections)

The statistical behaviour of the slow dynamics of the deterministic multi-scale system

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$\begin{aligned}x &\in \mathbb{R}^n \\ y &\in \mathbb{R}^m, m \geq 3\end{aligned}$$

with chaotic fast dynamics and fast invariant measure μ , and $\int_{\Lambda} f_0 d\mu = 0$
is (in the limit $\varepsilon \rightarrow 0$) described by the homogenised SDE

$$dX = F(X) dt + \sigma h(X) \circ dW_t$$

★ noise is **Stratonovich** á la Wong-Zakai Theorem:
“approximate a rough noise by smooth functions”

$$W_{\varepsilon}(t) = \varepsilon \int_0^{\frac{t}{\varepsilon^2}} f_0(y(s)) ds \longrightarrow_w W(t)$$

The **forward Euler scheme** for the slow variables of

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

is

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

The **forward Euler scheme** for the slow variables of

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

is

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

This map has the homogenised limit system

GAG & Melbourne (2013)

$$dX = \left(F(X) - \frac{1}{2} \Delta t h(X) h'(X) \mathbb{E}[f_0^2] \right) dt + \sqrt{\Delta t} \hat{\sigma} h(X) \circ d\tilde{W}_t$$

where

$$F(X) = \int_{\Lambda} f(X, y) d\mu$$

$$\hat{\sigma}^2 = \mathbb{E}[f_0^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[f_0(y) f_0(\Phi^n y)]$$

Discretisation



$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

Discretisation

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

Homogenisation

$$\begin{aligned}dX &= F(X) dt + \sigma h(X) \circ dW_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \frac{1}{2} \sigma^2 &= \int_0^\infty \mathbb{E}[f_0(y) f_0(\varphi^t y)] dt\end{aligned}$$

Homogenisation

$$\begin{aligned}dX &= \left(F(X) - \frac{1}{2} \Delta t h(X) h'(X) \mathbb{E}[f_0^2] \right) dt + \sqrt{\Delta t} \hat{\sigma} h(X) \circ d\tilde{W}_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \hat{\sigma}^2 &= \mathbb{E}[f_0^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[f_0(y) f_0(\Phi^n y)]\end{aligned}$$

Discretisation

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

Homogenisation

$$\begin{aligned}dX &= F(X) dt + \sigma h(X) \circ dW_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \frac{1}{2} \sigma^2 &= \int_0^\infty \mathbb{E}[f_0(y) f_0(\varphi^t y)] dt\end{aligned}$$

Homogenisation

$$\begin{aligned}dX &= \left(F(X) - \frac{1}{2} \Delta t h(X) h'(X) \mathbb{E}[f_0^2] \right) dt + \sqrt{\Delta t} \hat{\sigma} h(X) \circ d\tilde{W}_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \hat{\sigma}^2 &= \mathbb{E}[f_0^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[f_0(y) f_0(\Phi^n y)]\end{aligned}$$

Remarks: $\hat{\sigma}^2 \Delta t \rightarrow \sigma^2$ for $\Delta t \rightarrow 0$

Discretisation

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

$$x_{n+1} = x_n + \Delta t \varepsilon h(x_n) f_0(y_n) + \Delta t \varepsilon^2 f(x_n, y_n)$$

Homogenisation

$$\begin{aligned}dX &= F(X) dt + \sigma h(X) \circ dW_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \frac{1}{2} \sigma^2 &= \int_0^\infty \mathbb{E}[f_0(y) f_0(\varphi^t y)] dt\end{aligned}$$

Homogenisation

$$\begin{aligned}dX &= \left(F(X) - \frac{1}{2} \Delta t h(X) h'(X) \mathbb{E}[f_0^2] \right) dt + \sqrt{\Delta t} \hat{\sigma} h(X) \circ d\tilde{W}_t \\ F(X) &= \int_{\Lambda} f(X, y) d\mu \\ \hat{\sigma}^2 &= \mathbb{E}[f_0^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[f_0(y) f_0(\Phi^n y)]\end{aligned}$$

Remarks: $\hat{\sigma}^2 \Delta t \rightarrow \sigma^2$ for $\Delta t \rightarrow 0$

noise is neither Stratonovich nor Itô

$$\mathbf{E} := -\frac{1}{2} \Delta t h(\mathbf{X}) h'(\mathbf{X}) \mathbb{E}[f_0^2]$$

for *i.i.d.* fast dynamics, i.e. $\hat{\sigma}^2 = \mathbb{E}[f_0^2]$, the noise is Itô
(dynamics is already rough on time scale of $\mathcal{O}(\Delta t)$)

but it is never Stratonovich!

Question:

The only difference between the two homogenised equations is

$$\mathbf{E} := -\frac{1}{2}\Delta t \mathbf{h}(\mathbf{X})\mathbf{h}'(\mathbf{X}) \mathbb{E}[\mathbf{f}_0^2]$$

How can we interpret this extra drift term in the homogenised equation of the discretisation?

Can the extra term be significant? It is only $\mathcal{O}(\Delta t)$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \cdots$$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$z(t + \Delta t) = z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3)$$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$\begin{aligned} z(t + \Delta t) &= z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3) \\ &= z(t) + \Delta t b + \Delta t^2 \left[b_1 + \frac{1}{2} D b b \right] + \mathcal{O}(\Delta t^3) \end{aligned}$$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$\begin{aligned} z(t + \Delta t) &= z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3) \\ &= z(t) + \Delta t b + \Delta t^2 \left[b_1 + \frac{1}{2} D b b \right] + \mathcal{O}(\Delta t^3) \end{aligned}$$

Example I: Forward Euler $z_{n+1} = z_n + \Delta t b(z_n)$

consistency up to $\mathcal{O}(\Delta t^2)$  first-order scheme

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$\begin{aligned} z(t + \Delta t) &= z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3) \\ &= z(t) + \Delta t b + \Delta t^2 \left[b_1 + \frac{1}{2} D b b \right] + \mathcal{O}(\Delta t^3) \end{aligned}$$

Example 1: Forward Euler $z_{n+1} = z_n + \Delta t b(z_n)$

consistency up to $\mathcal{O}(\Delta t^2)$  first-order scheme

However, it would be a second-order scheme for the modified equation

$$\dot{z} = b - \frac{\Delta t}{2} D b b$$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$\begin{aligned} z(t + \Delta t) &= z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3) \\ &= z(t) + \Delta t b + \Delta t^2 \left[b_1 + \frac{1}{2} D b b \right] + \mathcal{O}(\Delta t^3) \end{aligned}$$

Example II: Second-order Runge-Kutta method

$$z_{n+1} = z_n + \frac{\Delta t}{2} [b(z_n) + b(z_n + \Delta t b(z_n))]$$

Backward error analysis

Hairer, Lubich & Wanner

A numerical integrator $z_{n+1} = \Phi(z_n)$ does not approximate solutions of the original system $\dot{z} = b(z)$ but the solution of a so called *modified equation*

$$\dot{z} = \tilde{b}(z) = b(z) + \Delta t b_1(z) + \Delta t^2 b_2(z) + \dots$$

Solutions of the modified equation can be Taylor expanded as

$$\begin{aligned} z(t + \Delta t) &= z(t) + \Delta t \tilde{b} + \frac{\Delta t^2}{2} D\tilde{b} \tilde{b} + \mathcal{O}(\Delta t^3) \\ &= z(t) + \Delta t b + \Delta t^2 \left[b_1 + \frac{1}{2} D b b \right] + \mathcal{O}(\Delta t^3) \end{aligned}$$

Example II: Second-order Runge-Kutta method

$$\begin{aligned} z_{n+1} &= z_n + \frac{\Delta t}{2} [b(z_n) + b(z_n + \Delta t b(z_n))] \\ &= z_n + \frac{\Delta t}{2} [b(z_n) + b(z_n) + \Delta t D b(z_n) b(z_n) + \mathcal{O}(\Delta t^2)] \end{aligned}$$

so it approximates the modified equation $\dot{z} = b(z) + \mathcal{O}(\Delta t^2)$ ($b_1 \equiv 0$)

Backward error analysis

Back to our deterministic multi-scale system

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

The forward Euler discretisation of the slow dynamics yields as a **modified equation**

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ &\quad - \frac{\Delta t}{2} \left(\varepsilon^2 \partial_x h(x) h(x) f_0^2(y) + \varepsilon h(x) \partial_y f_0(y) g(y) \right) + \mathcal{O}(\varepsilon^3 \Delta t)\end{aligned}$$

Backward error analysis

Back to our deterministic multi-scale system

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

The forward Euler discretisation of the slow dynamics yields as a **modified equation**

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ &\quad - \frac{\Delta t}{2} \left(\varepsilon^2 \partial_x h(x) h(x) f_0^2(y) + \varepsilon h(x) \partial_y f_0(y) g(y) \right) + \mathcal{O}(\varepsilon^3 \Delta t)\end{aligned}$$

which has the same **homogenisation limit** as the forward Euler map ✓

Backward error analysis

Back to our deterministic multi-scale system

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ \dot{y} &= g(y)\end{aligned}$$

The **forward Euler discretisation** of the slow dynamics yields as a **modified equation**

$$\begin{aligned}\dot{x} &= \varepsilon h(x) f_0(y) + \varepsilon^2 f(x, y) \\ &\quad - \frac{\Delta t}{2} \left(\varepsilon^2 \partial_x h(x) h(x) f_0^2(y) + \varepsilon h(x) \partial_y f_0(y) g(y) \right) + \mathcal{O}(\varepsilon^3 \Delta t)\end{aligned}$$

which has the same **homogenisation limit** as the forward Euler map ✓

Remark: The additional drift term $E := -\frac{1}{2} \Delta t h(x) \partial_x h(x) f_0^2$ would be absent in a numerical scheme of at least second order

For a second-order time-stepping method the homogenized modified equation therefore agrees with the homogenized equation of the full multi-scale system up to $\mathcal{O}(\Delta t^3)$

Numerical results

$$\begin{cases} \dot{x} = \varepsilon \sqrt{x} y + \varepsilon^2 b(c - x) y^2 \\ \dot{\xi} = -\eta - \zeta \\ \dot{\eta} = \xi + r\eta \\ \dot{\zeta} = s + (\xi - u)\zeta \end{cases} \quad \begin{matrix} y = \eta + \zeta \\ \text{Rössler system} \\ r = s = 0.25 \\ u = 7 \end{matrix}$$

discretise



Second-order Runge-Kutta

discretise



First-order forward Euler

Numerical results

$$\begin{cases} \dot{x} = \varepsilon \sqrt{x} y + \varepsilon^2 b(c - x) y^2 \\ \dot{\xi} = -\eta - \zeta \\ \dot{\eta} = \xi + r\eta \\ \dot{\zeta} = s + (\xi - u)\zeta \end{cases} \quad \begin{array}{l} y = \eta + \zeta \\ \text{Rössler system} \\ r = s = 0.25 \\ u = 7 \end{array}$$

discretise

Second-order Runge-Kutta

homogenisation

discretise

First-order forward Euler

$$\begin{aligned} \sigma^2 &= 2 \int_0^\infty \mathbb{E}[(\varphi^t y) y] dt \\ \beta &= c + \frac{\sigma^2 a^2}{8\alpha b} \end{aligned}$$

Cox-Ingersoll-Ross model

$$dX = \sigma a \sqrt{X} dW + 2\alpha b(\beta - X) dt$$

$$\alpha = \frac{1}{2} \mathbb{E}[y^2]$$

Numerical results

$$\begin{cases} \dot{x} = \varepsilon \sqrt{x} y + \varepsilon^2 b(c - x) y^2 \\ \dot{\xi} = -\eta - \zeta \\ \dot{\eta} = \xi + r\eta \\ \dot{\zeta} = s + (\xi - u)\zeta \end{cases} \quad \begin{matrix} y = \eta + \zeta \\ \text{Rössler system} \\ r = s = 0.25 \\ u = 7 \end{matrix}$$

discretise

Second-order Runge-Kutta

homogenisation

$$\begin{aligned} \sigma^2 &= 2 \int_0^\infty \mathbb{E}[(\varphi^t y) y] dt \\ \beta &= c + \frac{\sigma^2 a^2}{8\alpha b} \end{aligned}$$

discretise

First-order forward Euler

homogenisation

$$\begin{aligned} \hat{\sigma}^2 &= \mathbb{E}[y^2] + 2 \sum_{n=1}^\infty \mathbb{E}[(\Phi^n y) y] \\ \beta &= c + \frac{\Delta t \hat{\sigma}^2 a^2}{8\alpha b} - \frac{a^2 \Delta t}{4b} \end{aligned}$$

Cox-Ingersoll-Ross model

$$\begin{aligned} dX &= \sigma a \sqrt{X} dW + 2\alpha b(\beta - X) dt \\ \alpha &= \frac{1}{2} \mathbb{E}[y^2] \end{aligned}$$

Numerical results

parameters for
discrete-time map

$$\hat{\sigma}^2 = \mathbb{E}[y^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[(\Phi^n y)y]$$
$$\beta = c + \frac{\Delta t \hat{\sigma}^2 a^2}{8\alpha b} - \frac{a^2 \Delta t}{4b}$$

parameters for
continuous-time ODE

$$\sigma^2 = 2 \int_0^{\infty} \mathbb{E}[(\varphi^t y)y] dt$$
$$\beta = c + \frac{\sigma^2 a^2}{8\alpha b}$$

Cox-Ingersoll-Ross model

$$dX = \sigma a \sqrt{X} dW + 2\alpha b(\beta - X) dt$$

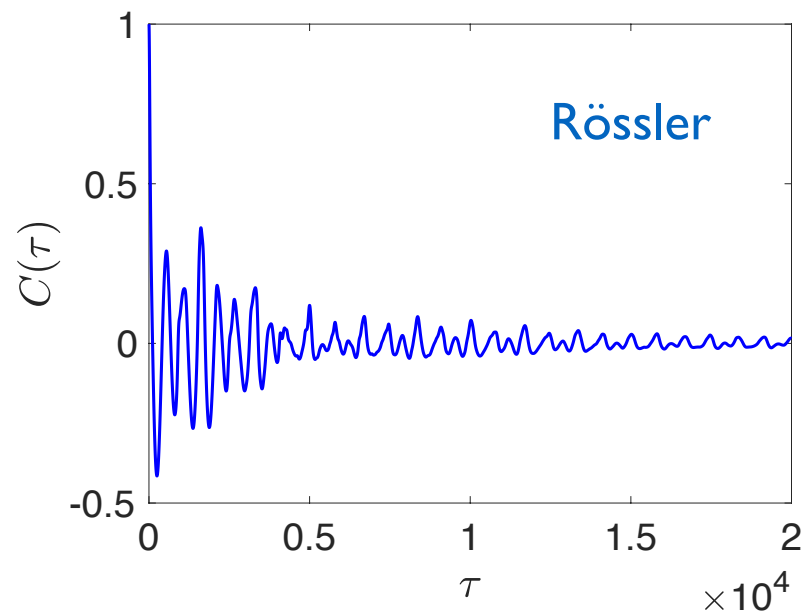
$$\alpha = \frac{1}{2} \mathbb{E}[y^2]$$

Numerical results

When is the difference significant?

$$a^2/b \gg 1$$

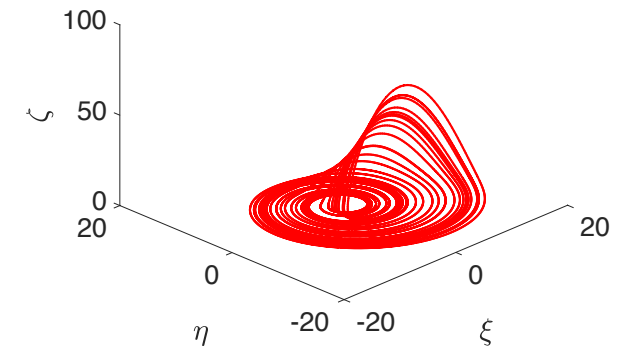
$$\sigma^2/4\alpha = \frac{\int_0^\infty \mathbb{E}[y(\varphi^t y)] dt}{\mathbb{E}[y^2]} \ll 1$$



parameters for
discrete-time map

$$\hat{\sigma}^2 = \mathbb{E}[y^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[(\Phi^n y)y]$$

$$\beta = c + \frac{\Delta t \hat{\sigma}^2 a^2}{8\alpha b} - \frac{a^2 \Delta t}{4b}$$



parameters for
continuous-time ODE

$$\sigma^2 = 2 \int_0^\infty \mathbb{E}[(\varphi^t y)y] dt$$

$$\beta = c + \frac{\sigma^2 a^2}{8\alpha b}$$

Cox-Ingersoll-Ross model

$$dX = \sigma a \sqrt{X} dW + 2\alpha b(\beta - X) dt$$

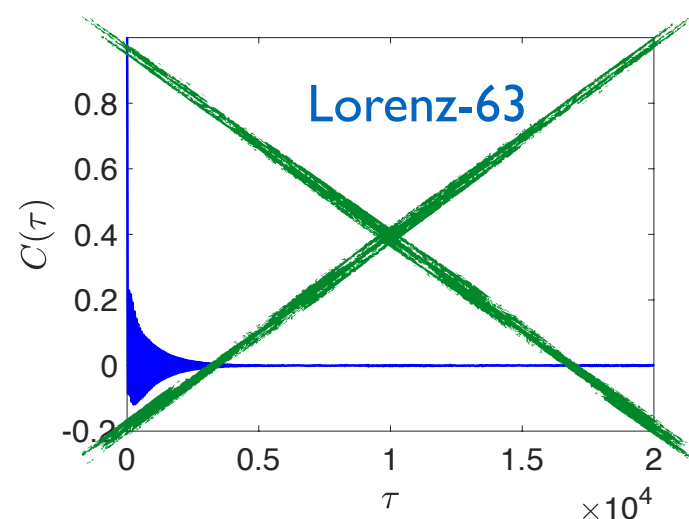
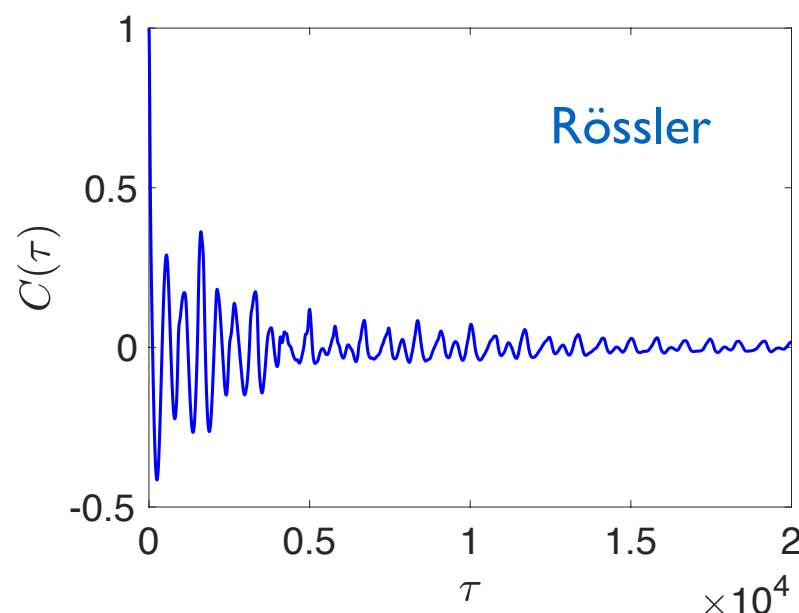
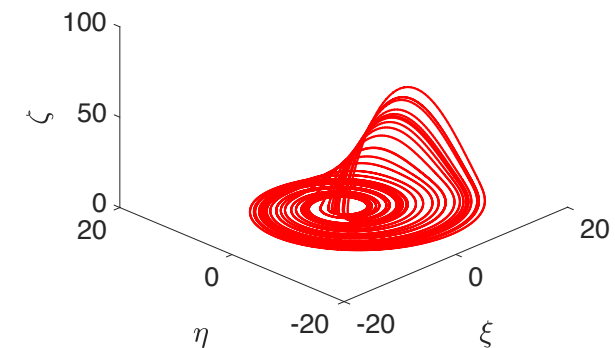
$$\alpha = \frac{1}{2} \mathbb{E}[y^2]$$

Numerical results

When is the difference significant?

$$a^2/b \gg 1$$

$$\sigma^2/4\alpha = \frac{\int_0^\infty \mathbb{E}[y(\varphi^t y)] dt}{\mathbb{E}[y^2]} \ll 1$$



parameters for
continuous-time ODE

$$\sigma^2 = 2 \int_0^\infty \mathbb{E}[(\varphi^t y)y] dt$$

$$\beta = c + \frac{\sigma^2 a^2}{8\alpha b}$$

parameters for
discrete-time map

$$\hat{\sigma}^2 = \mathbb{E}[y^2] + 2 \sum_{n=1}^{\infty} \mathbb{E}[(\Phi^n y)y]$$

$$\beta = c + \frac{\Delta t \hat{\sigma}^2 a^2}{8\alpha b} - \frac{a^2 \Delta t}{4b}$$

Cox-Ingersoll-Ross model

$$dX = \sigma a \sqrt{X} dW + 2\alpha b(\beta - X) dt$$

$$\alpha = \frac{1}{2} \mathbb{E}[y^2]$$

The Cox-Ingersoll-Ross model has an exact solution

$$X(t) = c(t)H(t) \quad \text{with} \quad c(t) = \frac{\sigma^2}{4\alpha}(1 - e^{-\alpha t})$$

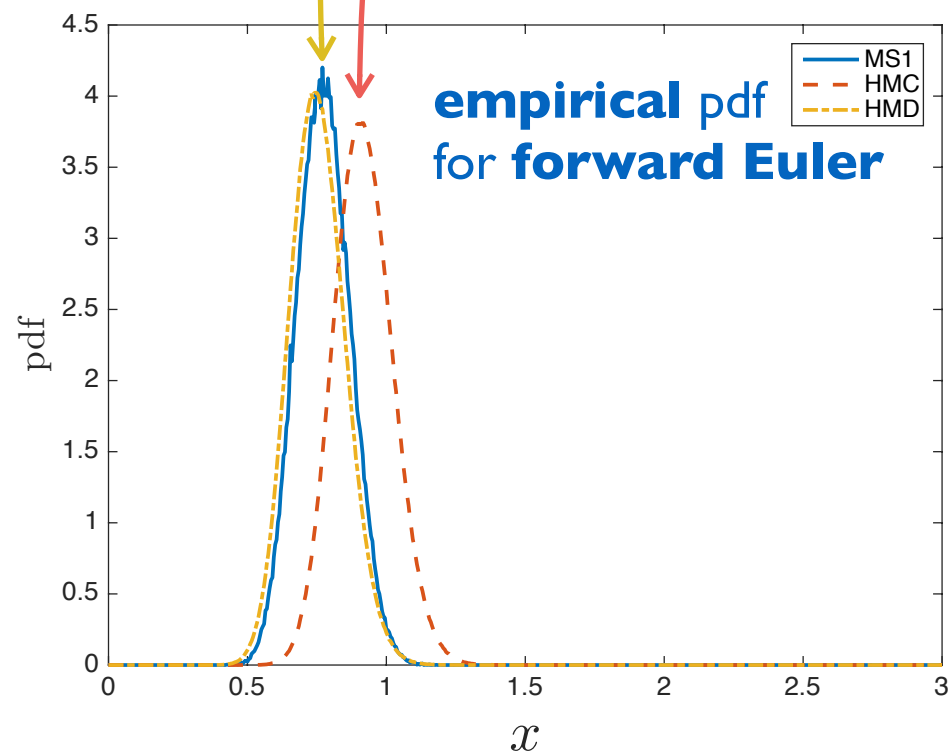
noncentral χ -squared distribution

$4\alpha\beta/\sigma^2$ degrees of freedom

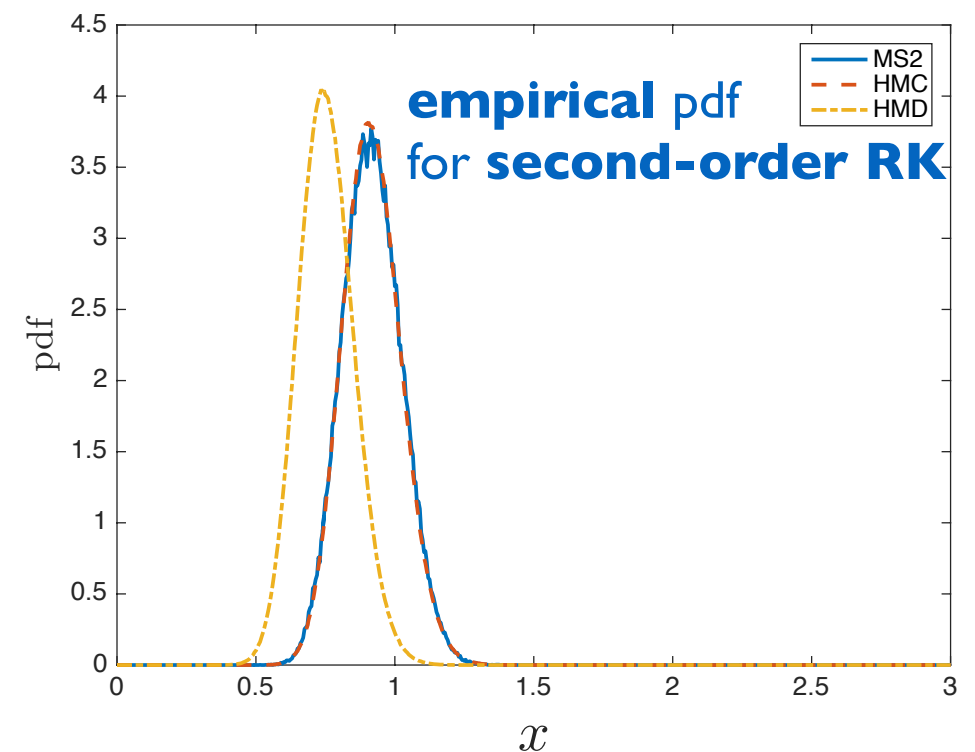
noncentrality parameter $c(t)^{-1}e^{-\alpha t}\xi$

analytical pdf of homogenised equation
for full **discrete**-time multi-scale system

analytical pdf of homogenised equation
for full **continuous**-time multi-scale system



$$\varepsilon = 0.1$$



15.6% error in mean!

Summary

We have used the Edgeworth expansion to **push stochastic model reduction past the limit of infinite time scale separation**, going beyond the Central Limit Theorem

We have developed a **machinery to calculate the Edgeworth corrections** for continuous time deterministic systems

The fast dynamics are replaced by a stochastic surrogate process, the parameters of which are tuned to match the Edgeworth expansion corrections of the full multi-scale system

Summary

We have used the Edgeworth expansion to **push stochastic model reduction past the limit of infinite time scale separation**, going beyond the Central Limit Theorem

We have developed a **machinery to calculate the Edgeworth corrections** for continuous time deterministic systems

The fast dynamics are replaced by a stochastic surrogate process, the parameters of which are tuned to match the Edgeworth expansion corrections of the full multi-scale system

Outlook:

- * Use the strategy for the triad system to apply Edgeworth expansion to the barotropic vorticity equation
- * Use Edgeworth expansions in a data-driven approach
- * Prove the corrections rigorously (start with stochastic fast dynamics)

Summary

- We have resolved the discrepancy between the homogenized equations for a continuous-time fast-slow system and its first-order discretization using backward error analysis

Take Home Message:

Avoid first-order time-stepping when simulating deterministic multi-scale systems

In particular, when the system is far from *i.i.d.*