Stochastic modeling of diffusion in dynamical systems: three examples

R. Klages

School of Mathematical Sciences, Queen Mary University of London

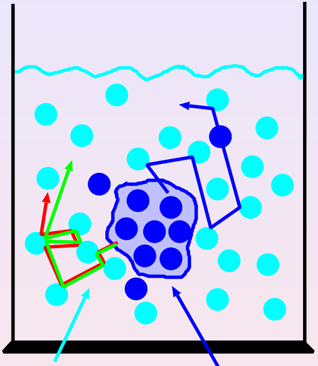
Climate Fluctuations and Non-equilibrium Statistical Mechanics: An Interdisciplinary Dialogue
MPIPKS Dresden, 14th July 2017

Queen Mary
University of London

Outline

1. **Motivation:**
   dynamical systems, diffusion and stochastic modeling
2. **Diffusion in three random walk-like examples:**
   1. non-chaotic ‘slicer’ map
   2. dissipative randomly perturbed standard map
   3. a simple random dynamical system
3. **Conclusion:**
   pitfalls when relating the above three layers to each other

Microscopic chaos in a glass of water?



- dispersion of a droplet of ink by diffusion
- chaotic collisions between billiard balls
- **chaotic hypothesis:**

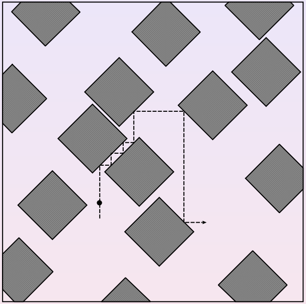
microscopic chaos
⇓
macroscopic diffusion

Gallavotti, Cohen (1995)

P.Gaspard et al. (1998): experiment on small colloidal particle in water; diffusion due to microscopic chaos based on positive *pattern entropy per unit time* $h(\epsilon, \tau) \leq h_{KS} = \sum_{\lambda_i > 0} \lambda_i$

The random wind tree model

counterexample:



Ehrenfest, Ehrenfest (1959)

no positive Lyapunov exponent, hence non-chaotic dynamics

Dettmann et al. (1999): generates trajectories and $h(\epsilon, \tau)$ *indistinguishable from the colloidal particle dynamics*

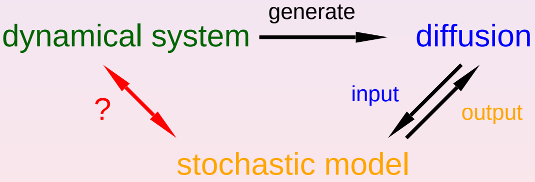
Microscopic models, diffusion and stochastic modeling

conclusion:

- **theory:** (chaotic) model $\rightarrow$ diffusion
- **experiment:** diffusion $\rightarrow$ (chaotic) model?

$\Rightarrow$ non-trivial interplay microscopic model $\leftrightarrow$ diffusion

theme of this talk:
add yet a third layer of stochastic modeling



two questions:

1. what type of diffusion is generated by a dynamical system?
2. can it be reproduced by some stochastic model?

Basic diffusive setup

- in the following only diffusion in one dimension
- key quantity: **mean square displacement**

$$< x^2 >:= \int dx\, x^2 \rho(x,t) \sim t^\gamma$$

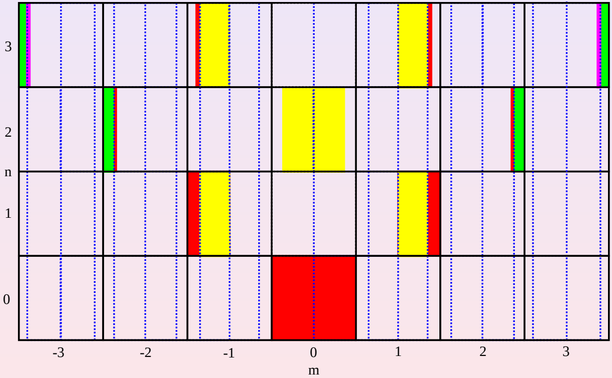
- **note:** three basic types of diffusion
  1. there is not only 'Brownian' (normal) diffusion with $\gamma = 1$
     but also anomalous diffusion:
  2. subdiffusion with $\gamma < 1$
     and
  3. superdiffusion with $\gamma > 1$

(plus more exotic types)

I. The slicer map

Pictorial construction

a one-dimensional ‘random walk-like’ but fully deterministic system; diffusion of a density of points from uniform initial density in **space (m) - discrete time (n) diagram**:



‘slicers’ at points (of Lebesgue measure zero) split the density
no stretching, hence zero Lyapunov exponent: **no chaos!**

Formal definition

- consider a chain of intervals $\widehat{M} := M \times \mathbb{Z}$, $M := [0,1]$ with point $\widehat{X} = (x,m)$ in $\widehat{M}$, where $\widehat{M}_m := M \times \{m\}$ is the m-th cell of $\widehat{M}$

- subdivide each $\widehat{M}_m$ in subintervals, separated by points called slicers: $\{1/2\} \times \{m\}$, $\{\ell_m\} \times \{m\}$, $\{1-\ell_m\} \times \{m\}$, where $0 < \ell_m < 1/2$ for every $m \in \mathbb{Z}$ with

$$\ell_m(\alpha) = \frac{1}{\left(|m|+2^{1/\alpha}\right)^{\alpha}},\ \alpha > 0$$

- slicer map: $S : \widehat{M} \to \widehat{M}$, $\widehat{X}_{n+1} = S(\widehat{X}_n)$, $n \in \mathbb{N}$ with

$$S(x,m) = \begin{cases} (x, m-1) & \text{if } 0 \le x < \ell_m \text{ or } \frac{1}{2} < x \le 1-\ell_m, \\ (x, m+1) & \text{if } \ell_m \le x \le \frac{1}{2} \text{ or } 1-\ell_m < x \le 1. \end{cases}$$

Main result: diffusive properties

Proposition (Salari et al., 2015)

Given $\alpha \geq 0$ and a uniform initial distribution in $\widehat{M}_0$, we have

1. $\alpha = 0$: *ballistic motion with MSD* $\langle \widehat{X}_n^2 \rangle \sim n^2$
2. $0 < \alpha < 1$: *superdiffusion with MSD* $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
3. $\alpha = 1$: *normal diffusion with linear MSD* $\langle \widehat{X}_n^2 \rangle \sim n$
   non-chaotic normal diffusion with non-Gaussian density
4. $1 < \alpha < 2$: *subdiffusion with MSD* $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
   subdiffusion with ballistic peaks
5. $\alpha = 2$: *logarithmic subdiffusion with MSD* $\langle \widehat{X}_n^2 \rangle \sim \log n$
   a bit exotic
6. $\alpha > 2$: *localisation in the MSD with* $\langle \widehat{X}_n^2 \rangle \sim const.$
   non-trivial phenomenon

Higher order moments

Theorem (Salari et al., 2015)

For $\alpha \in (0, 2]$ the moments $\langle \widehat{X}_n^p \rangle$ with $p > 2$ even and uniform initial distribution in $\widehat{M}_0$ have the asymptotic behavior

$$\langle \widehat{X}_n^p \rangle \sim n^{p-\alpha}$$

while the odd moments ($p = 1, 3, ...$) vanish.

Matching to stochastic dynamics?

- one-dimensional stochastic Lévy Lorentz gas:

point particle moves ballistically between static point scatterers on a line from which it is transmitted / reflected with probability $1/2$
distance r between two scatterers is a random variable iid from the Lévy distribution

$$\lambda(r) := \beta r_0^\beta \frac{1}{r^{\beta+1}} \; , \; r \in [r_0, \infty) \; , \; \beta > 0$$

with cutoff r_0

$\rightarrow$ model exhibits only *superdiffusion*

$\rightarrow$ *all moments scale with the slicer moments* for $\alpha \in (0, 1]$ (piecewise linearly depending on parameters)

Matching to stochastic dynamics?

- Lévy walk modeled by CTRW theory:

→ *moments* calculated to $\sim t^{p+1-\beta}$ for $p > \beta$, $1 < \beta < 2$:
match to slicer *superdiffusion* with $\beta = 1 + \alpha$

→ but conceptually a totally *different process*

- correlated Gaussian stochastic processes:

modeled by a generalized Langevin equation with a power law memory kernel

→ formal analogy in the *subdiffusive* regime

→ but Gaussian distribution and a *conceptual mismatch*

II. The dissipative randomly perturbed standard map

The standard map and diffusion

- paradigmatic Hamiltonian dynamical system:

standard map

$$x_{n+1} = x_n + y_n \mod 2\pi$$
$$y_{n+1} = y_n + K \sin x_{n+1}$$

derived from kicked rot(at)or where $x_n \in \mathbb{R}$ is an angle, $y_n \in \mathbb{R}$ the angular velocity with $n \in \mathbb{N}$ and $K > 0$ the kick strength

- define **diffusion coefficient** as

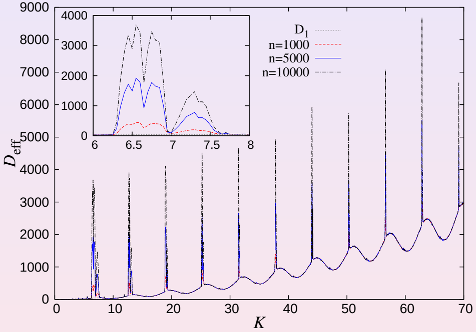
$$D(K) = \lim_{n\to\infty} \frac{1}{n} < (y_n - y_0)^2 >$$

with ensemble average over the initial density

$< \ldots >= \int dx\, dy\, \varrho(x, y) \ldots \;, x \in [0, 2\pi) \;,\; y = y_0 \in [0, 2\pi)$

Diffusion in the standard map

analytical (Rechester, White, 1980) and numerical studies of parameter-dependent diffusion $D_{eff}(K)$:



Manos, Robnik, PRE (2014)

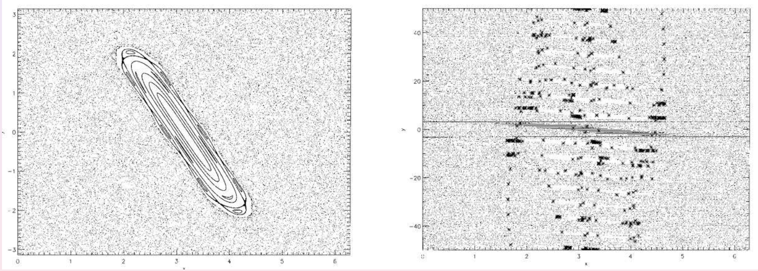
- $D(K)$ is highly irregular
- for some K there is superdiffusion with mean square displacement $< y_n^2 > \sim n^\gamma \ , \ \gamma > 1$ due to accelerator modes

The dissipative standard map

model damping in the standard map by

$$x_{n+1} = x_n + y_n \mod 2\pi$$
$$y_{n+1} = (1-\nu)y_n + f_0 \sin x_{n+1}$$

with $\nu \in [0, 1]$:



Feudel, Grebogi, Hunt, Yorke, PRE (1996)

- islands in phase space for $\nu = 0$ (left) become coexisting periodic attractors (right): 150 found for $\nu = 0.02$, $f_0 = 4$
- simple argument yields $|y_n| < y_{max}$: quick trapping

Dissipative dynamics and random perturbations

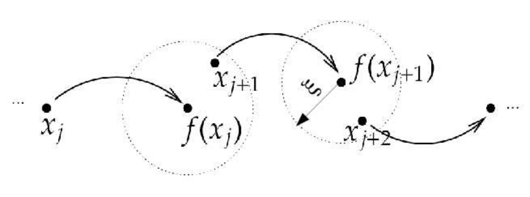
Question: What happens to dissipative deterministic dynamics $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ under random perturbations?

Consider the dissipative standard map with additive noise:

$$\begin{aligned} x_{n+1} &= x_n + y_n + \epsilon_{x,n} \mod 2\pi \\ y_{n+1} &= (1-\nu) y_n + f_0 \sin x_{n+1} + \epsilon_{y,n} \end{aligned}$$

with iid random variables $\epsilon_n = (\epsilon_{x,n}, \epsilon_{y,n})$ drawn from uniform distribution bounded by $||\epsilon_n|| < \xi$ of noise amplitude ξ

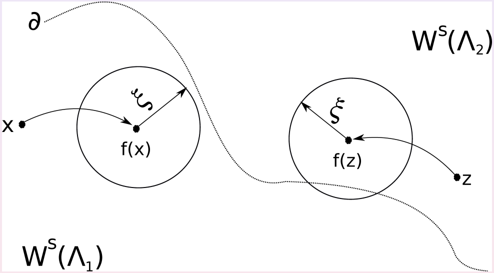
perturbed dynamics $\mathbf{F}(\mathbf{x}_j) = \mathbf{f}(\mathbf{x}_j) + \epsilon_j$:



From attractors to hopping on pseudo attractors

Consequences of the random perturbations:

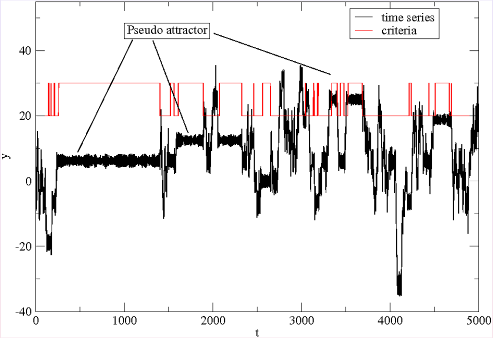
- beyond a noise threshold $\xi \geq \xi_0$ the attracting sets $W^s(\Lambda_i)$ lose their stability due to holes



- the (invariant) attractors become (quasi-invariant) pseudo attractors from which there is noise-induced escape
- the noise induces a hopping process between all coexisting pseudo attractors

Intermittency and stickiness

the resulting perturbed dissipative dynamics is intermittent:



$$f_0 = 4\ ,\ \xi = 0.06\ ,\ \nu = 0.002$$

- stickiness to pseudo attractors measured by criterion that maximal eigenvalue of the Jacobian matrix along orbit < 1

Continuous time random walk theory

match simulation results to **CTRW theory** (Montroll, Weiss, Scher, 1973): define stochastic process by master equation with *waiting time distribution* $w(t)$ and *jump distribution* $\lambda(x)$

$$\varrho(x,t) = \int_{-\infty}^{\infty} dx' \lambda(x-x') \int_0^t dt' \; w(t-t') \; \varrho(x',t') + \\ + (1 - \int_0^t dt' w(t'))\delta(x)$$

structure: jump + no jump for points starting at $(x,t)=(0,0)$
$\hat{\text{F}}$ourier-$\tilde{\text{L}}$aplace transform yields **Montroll-Weiss eqn (1965)**

$$\boxed{\hat{\tilde{\varrho}}(k,s) = \frac{1-\tilde{w}(s)}{s} \frac{1}{1-\hat{\lambda}(k)\tilde{w}(s)}}$$

with mean square displacement $\tilde{\langle x^2(s) \rangle} = -\left.\frac{\partial^2 \hat{\tilde{\varrho}}(k,s)}{\partial k^2}\right|_{k=0}$

Predictions of CTRW theory

according to CTRW theory solving the MW eqn. for

1. a power law waiting time distribution $w(t) \sim t^{-(\gamma+1)}$

   with jump distribution $\lambda(x) = \delta(|x| - const.)$

2. yields a mean square discplacement of $< x^2(t) > \sim t^\gamma$

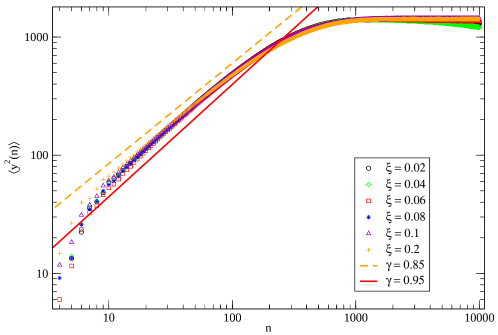
   and

3. a stretched exponential position pdf, approximately given by $P_n(y) \sim \exp\left(-cx^{2/(2-\gamma)}\right)$

crucial fit parameter: γ; check these three predictions in numerical experiments

CTRW theory and mean square displacement

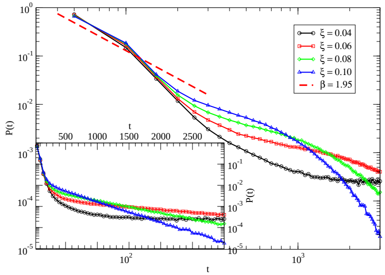
$< y^2(n) >$ for different noise amplitudes ξ at $\nu = 0.002$:



- transient subdiffusion $< y^2(n) > \sim n^\gamma$ up to $n < 1000$
- only small variation of $0.85 < \gamma < 0.95$ for different ξ; for $\xi = 0.06$ we have $\gamma \simeq 0.95$

CTRW theory and escape time distribution

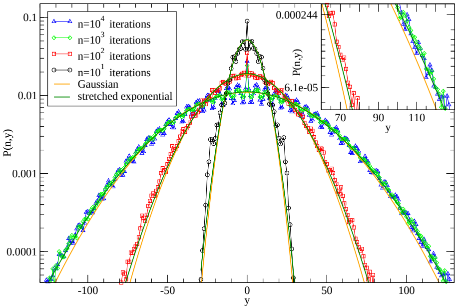
probability distributions $P(t)$ of escape times t from pseudo attractors; dissipation $\nu = 0.002$ with different noise strength ξ:



- transition from power law (stickiness) to exponential
- transition takes longer when $\xi \to 0$
- the dashed red line represents the CTRW theory prediction of $P(t) \sim t^{-1.95}$ corresponding to $< y^2(n) > \sim n^{0.95}$

CTRW theory and position pdf

$P_n(y)$ for position y at different time steps n:



$\xi = 0.06$, $\nu = 0.002$

- 'Gaussian-like' diffusive spreading up to $n < 1000$
- localization trivially due to boundedness of pseudo attractors
- CTRW theory pdf (green lines) for $\gamma = 0.95$ corrects mismatch in tails

III. A random dynamical system

Constructing a random dynamical system

to be published

Diffusion in a simple random dynamical system

to be published

Main results

to be published

Summary

- **central theme:** interplay between *dynamical systems, diffusion and stochastic modeling*

- **main results:**
  1. dynamical systems can feature *novel types of (anomalous) diffusion*
  2. naive matching to stochastic models can be misleading and difficult

- **outlook:** perhaps dynamical systems theory can inspire stochastic theory to invent new stochastic processes? *and* take your data *seriously*!!!

Acknowledgement and references

work performed with all authors on the following references:

- slicer: L.Salari, L.Rondoni, C.Giberti, RK, Chaos **25**, 073113 (2015)
- standard map: C.S.Rodrigues A.V.Chechkin, A.P.S. de Moura, C.Grebogi, RK, Europhys.Lett. **108**, 40002 (2014)
- random dynamical system: Y.Sato, RK, to be published