A practical introduction to stochastic modeling of particles

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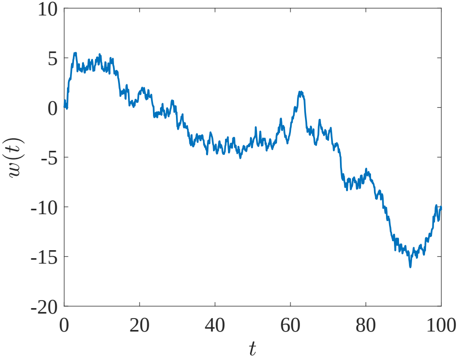
Brownian motion (or Wiener process)

Brownian motion $w(t)$ is a continuous stochastic process.



- Time-indexed random variable;
- Gaussian-distributed: $\mathbb{E}\, f(w(t)) = \int_{-\infty}^{\infty} f(\varpi)\, \frac{e^{-\varpi^2/2t}}{\sqrt{2\pi t}}\, d\varpi$;
- Mean-zero: $\mathbb{E}\, w(t) = 0$;
- Variance is $\mathbb{E}\, w^2(t) = t$ (standard BM).

Increments of Brownian motion

- Increments: $\Delta w = w(t + \Delta t) - w(t)$
- $\mathbb{E}\,\Delta w = 0$
- Variance of increment is Δt:

$$\begin{aligned}\mathbb{E}(\Delta w)^2 &= \mathbb{E}\,w^2(t+\Delta t) + \mathbb{E}\,w^2(t) - 2\,\mathbb{E}\,w(t+\Delta t)w(t)\\ &= (t+\Delta t) + (t) - 2(t)\\ &= \Delta t\end{aligned}$$

- Since

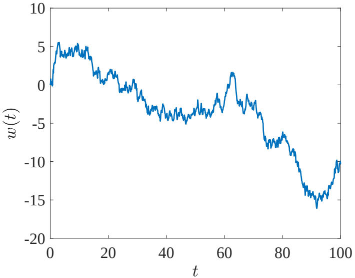
$$\Delta w/\Delta t \sim \sqrt{\mathbb{E}(\Delta w)^2}/\Delta t = 1/\sqrt{\Delta t}$$

does not have a limit as $\Delta t \to 0$, the process is continuous but rough.

Simulating Brownian motion

```
N = 1000;
dt = .1;
t = dt*(0:N);
w = zeros(1,N+1);

for i = 1:N
    w(i+1) = w(i) + sqrt(dt)*randn;
end
```



Observe: reaches distance 10 in time 100.

Stochastic differential equation (SDE)

By itself, Brownian motion is a bit limited. Much richer as part of an SDE for a stochastic process $x(t)$:

$$\dot{x} = v(x) + \Sigma(x)\,\dot{w}$$

The Brownian motion 'drives' a more complex process $x(t)$.
Probabilists call $v(x)$ the drift, and $\Sigma(x)$ the noise coupling or noise parameter or volatility (finance).

Safer to think in terms of increments:

$$\Delta x = v(x)\,\Delta t + \Sigma(x)\,\Delta w.$$

Simulating an SDE

Simulate with $v(x) = \sigma(x) = x$.

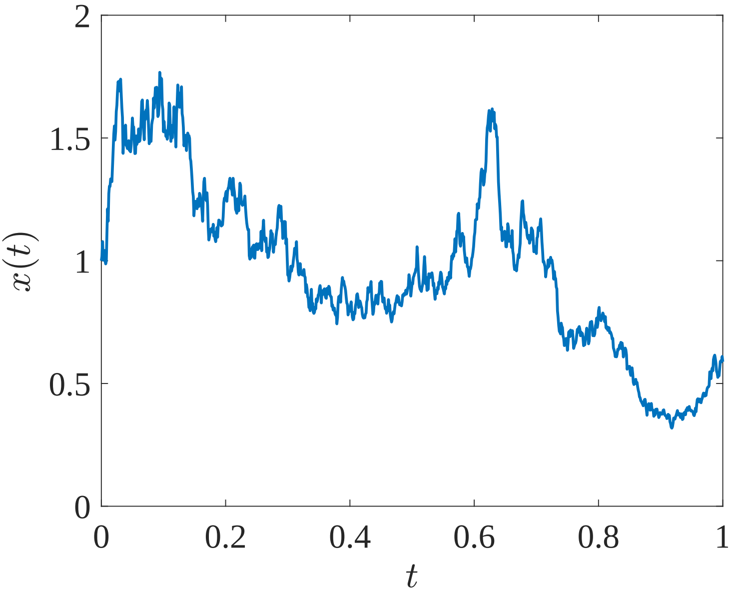
Euler–Maruyama method:

```
N = 1000; dt = .001;
t = dt*(0:N); x = zeros(1,N+1);

x(1) = 1;
v = @(x) x;
sigma = @(x) x;

for i = 1:N
    x(i+1) = x(i) + v(x(i))*dt ...
        + sigma(x(i))*sqrt(dt)*randn;
end
```

Simulating an SDE (cont'd)



Higher-dimensional SDEs

Turn everything into a vector and matrix:

$$\dot{\boldsymbol{x}} = \boldsymbol{v}(\boldsymbol{x}) + \mathbb{\Sigma}(\boldsymbol{x}) \cdot \dot{\boldsymbol{w}}$$

The vector $\boldsymbol{w}(t)$ contains independent standard BMs.

Use `randn(1,N)` in Matlab.

The noise coupling matrix $\mathbb{\Sigma}$ scales and connects the BMs to $\boldsymbol{x}$.

Important: $\mathbb{\Sigma}$ is not necessarily square.

From SDEs to PDEs

What is so special about BM and SDEs? Intimate connection to PDEs.

The SDE

$$\dot{\boldsymbol{x}} = \boldsymbol{v}(\boldsymbol{x}) + \mathbb{Σ}(\boldsymbol{x}) \cdot \dot{\boldsymbol{w}}$$

has a probability density $p(\boldsymbol{x}, t)$. i.e., the probability of finding a trajectory in the small volume $\Delta_{\boldsymbol{x}} V$ centered on $\boldsymbol{x}$ at time t is

$$p(\boldsymbol{x}, t)\, \Delta_{\boldsymbol{x}} V\,.$$

The initial condition is $p(\boldsymbol{x}, 0) = \delta(\boldsymbol{x} - \boldsymbol{x}_0)$, where $\boldsymbol{x}(0) = \boldsymbol{x}_0$.

From SDEs to PDEs (cont'd)

The striking fact is that, given the SDE

$$\dot{\boldsymbol{x}} = \boldsymbol{v}(\boldsymbol{x}) + \mathbb{\Sigma}(\boldsymbol{x}) \cdot \dot{\boldsymbol{w}}\,,$$

then its probability density satisfies the Fokker–Planck equation

$$\boxed{\partial_t p = -\nabla \cdot (\boldsymbol{v}\, p) + \nabla\nabla : (\mathbb{D}\, p)}$$

with initial condition $p(\boldsymbol{x}, 0) = \delta(\boldsymbol{x} - \boldsymbol{x}_0)$, and diffusion matrix

$$\boxed{\mathbb{D} = \tfrac{1}{2}\, \mathbb{\Sigma} \cdot \mathbb{\Sigma}^\top.}$$

This is an exact correspondence, which means we can use the SDE to solve the PDE, or vice-versa.

(In fact mathematicians go back and forth when proving theorems.)

Itô vs Stratonovich and all that

I have swept under the rug a big issue, regarding the interpretation of the stochastic product. Earlier we defined the increment:

$$\Delta \boldsymbol{x} = \boldsymbol{v}(\boldsymbol{x}(t))\,\Delta t + \mathbb{\Sigma}(\boldsymbol{x}(t)) \cdot \Delta \boldsymbol{w} \qquad \text{(Itô).}$$

where on the right $\Sigma(\boldsymbol{x})$ is evaluated at t. In ODEs this doesn't matter.

However, in an SDE we can choose to evaluate the noise matrix at a different time, for instance at the midpoint of the interval:

$$\Delta \boldsymbol{x} = \boldsymbol{v}(\boldsymbol{x}(t))\,\Delta t + \mathbb{\Sigma}\big(\boldsymbol{x}(t + \tfrac{1}{2}\Delta t)\big) \cdot \Delta \boldsymbol{w} \qquad \text{(Stratonovich).}$$

There are other interpretations as well (i.e., anti-Itô, at endpoint).

Itô vs Stratonovich (cont'd)

However, a Stratonovich equation can be solved as Itô equation with an additional drift

$$\left[\tfrac{1}{2}\ \mathrm{Tr}(\mathbb{\Sigma}^\top \cdot \nabla \mathbb{\Sigma})\right]_i = \tfrac{1}{2} \sum_{j,k} \Sigma_{jk} \frac{\partial \Sigma_{ik}}{\partial x_j} \qquad \text{(Stratonovich correction).}$$

The choice of interpretation (which is a choice of drift) is a modeling issue.

It must be dictated by some physical consideration, often the desire for a specific type of equilibrium.

Additive vs multiplicative noise

$$\dot{\boldsymbol{x}} = \boldsymbol{v}(\boldsymbol{x}) + \mathbb{\Sigma}(\boldsymbol{x}) \cdot \dot{\boldsymbol{w}}\,,$$

In the literature one often reads

> *If $\mathbb{\Sigma}$ is constant then the noise is additive.*
> *Otherwise it is multiplicative.*

This is not quite correct. A more accurate statement is

> *If $\mathrm{Tr}(\mathbb{\Sigma}^\top \cdot \nabla\mathbb{\Sigma}) = 0$ then the noise is additive.*
> *Otherwise it is multiplicative.*

This distinction will matter to us soon. For additive noise little care is required when integrating.

Langevin equation

The noisy motion of a small particle in a fluid at rest is given by the Langevin equation:

$$\dot{\boldsymbol{x}} = \boldsymbol{u}$$
$$m\,\dot{\boldsymbol{u}} = -\mathbb{K}\cdot\boldsymbol{u} + \mathbb{S}\cdot\dot{\boldsymbol{w}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\boldsymbol{x}\\ \boldsymbol{\pi}\end{pmatrix} = \begin{pmatrix} m^{-1}\,\boldsymbol{\pi} \\ -\mathbb{K}\cdot m^{-1}\,\boldsymbol{\pi}\end{pmatrix} + \begin{pmatrix}\mathbb{O}\\ \mathbb{S}\end{pmatrix}\cdot\dot{\boldsymbol{w}}$$

Compare to earlier standard SDE form:

$$\dot{\boldsymbol{X}} = \boldsymbol{V} + \mathbb{\Sigma}\cdot\dot{\boldsymbol{w}}$$

$\boldsymbol{X} = \begin{pmatrix}\boldsymbol{x}\\ \boldsymbol{\pi}\end{pmatrix}$ is a vector of 6 variables. $\mathbb{\Sigma}$ is a 6×3 matrix (not square).

Additive or multiplicative?

$$\mathbb{\Sigma} = \begin{pmatrix} \mathbb{0} \\ \mathbb{S}(\boldsymbol{x}) \end{pmatrix}$$

A priori, the noise in our Langevin equation 'looks' multiplicative. However,

$$\begin{aligned} [\mathrm{Tr}(\mathbb{\Sigma}^\top \cdot \nabla \mathbb{\Sigma})]_i &= \sum_{j=1}^{6} \sum_{k=1}^{3} \Sigma_{jk} \frac{\partial \Sigma_{ik}}{\partial X_j} \\ &= \sum_{j=1}^{3} \sum_{k=1}^{3} S_{jk} \frac{\partial \Sigma_{ik}}{\partial \pi_j} \\ &= 0 \end{aligned}$$

since $\mathbb{S}(\boldsymbol{x})$ does not depend on the momentum variables.

Additive! No Itô or Stratonovich shady business.

Equilibrium

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\boldsymbol{x}\\ \boldsymbol{\pi}\end{pmatrix} = \begin{pmatrix} m^{-1}\,\boldsymbol{\pi} \\ -\mathbb{K}\cdot m^{-1}\,\boldsymbol{\pi}\end{pmatrix} + \begin{pmatrix}\mathbb{O}\\ \mathbb{S}\end{pmatrix}\cdot\dot{\boldsymbol{w}}$$

Recall the corresponding Fokker–Planck equation for $p(\boldsymbol{x},\boldsymbol{\pi},t)$:

$$\partial_t p = -\nabla_{\boldsymbol{x}}\cdot(m^{-1}\,\boldsymbol{\pi}\,p) + \nabla_{\boldsymbol{\pi}}\cdot(\mathbb{K}\cdot m^{-1}\,\boldsymbol{\pi}\,p) + \nabla_{\boldsymbol{\pi}}\nabla_{\boldsymbol{\pi}} : (\mathbb{E}\,p)$$

where $\mathbb{E} = \frac{1}{2}\mathbb{S}\cdot\mathbb{S}^\top$ is a (6×6) momentum diffusion tensor.

The FP equation has a Gaussian equilibrium:

$$p \sim \exp(-\tfrac{1}{2}\,\boldsymbol{\pi}\cdot\mathbb{A}^{-1}\cdot\boldsymbol{\pi})$$

where the covariance matrix $\mathbb{A}$ satisfies the lovely matrix equation:

$$\mathbb{K}\cdot\mathbb{A} + \mathbb{A}\cdot\mathbb{K}^\top = 2m\mathbb{E}$$

Equilibrium (cont'd)

$$p \sim \exp(-\tfrac{1}{2}\,\boldsymbol{\pi}\cdot\mathbb{A}^{-1}\cdot\boldsymbol{\pi})$$

$$\mathbb{K}\cdot\mathbb{A} + \mathbb{A}\cdot\mathbb{K}^{\top} = 2m\mathbb{E}$$

This is a Sylvester equation or a continuous time Lyapunov equation (control theory). Just like a regular linear equation where the 'vector' is a matrix $\mathbb{A}$. Easy! Existence and uniqueness an interesting equation (noise has to collaborate with dissipation).

Thermodynamic equilibrium puts a heavy constraint: $\mathbb{A} = mk_{\mathrm{B}}T\,\mathbb{1}$:

$$p \sim \exp(-\tfrac{1}{2}\,|\boldsymbol{\pi}|^2/(mk_{\mathrm{B}}T))$$

Maxwell–Boltzmann distribution.

Fluctuation-dissipation theorem

$$\mathbb{K} \cdot \mathbb{A} + \mathbb{A} \cdot \mathbb{K}^\top = 2m\mathbb{E}$$

Insert

$$\mathbb{A} = m k_{\mathrm{B}} T \, \mathbb{1}$$

to find

$$k_{\mathrm{B}} T \, (\mathbb{K} + \mathbb{K}^\top) = 2\mathbb{E}$$

Usually the resistance matrix $\mathbb{K}$ is symmetric:

$$\boxed{k_{\mathrm{B}} T \, \mathbb{K} = \mathbb{E}}$$

This is the fluctuation-dissipation theorem (in momentum form). It tells us how to choose the noise matrix $\mathbb{E}$ to guarantee the correct physics.
Depends on particle shape!

Greg Voth: use larger particles to measure $\mathbb{K}$!

Overdamping

$$\dot{\boldsymbol{x}} = \boldsymbol{u}$$
$$m\,\dot{\boldsymbol{u}} = -\mathbb{K}\cdot\boldsymbol{u} + \mathbb{S}\cdot\dot{\boldsymbol{w}}$$

In practice, evolving the Langevin equation is tricky, especially when the damping is strong. We waste a lot of time doing very small steps.

Overdamped limit: neglect inertia, assume drag and noise are always balanced:

$$0 = -\mathbb{K}\cdot\boldsymbol{u} + \mathbb{S}\cdot\dot{\boldsymbol{w}}$$

Solve for $\boldsymbol{u}$:

$$\boldsymbol{u} = \mathbb{K}^{-1}\cdot\mathbb{S}\cdot\dot{\boldsymbol{w}}$$

Insert back in $\dot{\boldsymbol{x}}$:

$$\dot{\boldsymbol{x}} = \mathbb{K}^{-1}\cdot\mathbb{S}\cdot\dot{\boldsymbol{w}}.$$

Easy! But wrong, in general. (Ok for spheres in uniform env.)

Overdamping (cont'd)

$$\dot{\boldsymbol{x}} = \mathbb{M} \cdot \mathbb{S} \cdot \dot{\boldsymbol{w}}, \qquad \mathbb{M} = \mathbb{K}^{-1} \quad \text{(mobility)}.$$

Note here our noise matrix is $\Sigma(\boldsymbol{x}) = \mathbb{M} \cdot \mathbb{S}$.

The Stratonovich correction is nonzero in this case! (Unlike the underdamped case.)

Summary of how we went wrong:

- We begin with the underdamped Langevin equation, with additive noise.
- We reduce to an overdamped equation, with multiplicative noise.
- Do we get to 'choose' Itô or Stratonovich or anti-Itô?
- No! Should be a unique overdamped limit. Much more subtle and requires several pages of math.

Overdamping (cont'd)

In the end get an 'added drift' in the overdamped equation:

$$\dot{\boldsymbol{x}} = \nabla \cdot \mathbb{D} + \mathbb{\Sigma} \cdot \dot{\boldsymbol{w}}, \qquad \mathbb{\Sigma} = \mathbb{M} \cdot \mathbb{S}.$$

with the spatial diffusivity

$$\mathbb{D} = \tfrac{1}{2}\,\mathbb{\Sigma} \cdot \mathbb{\Sigma}^\top = \mathbb{M} \cdot (\tfrac{1}{2}\mathbb{S} \cdot \mathbb{S}^\top) \cdot \mathbb{M} = \mathbb{M} \cdot \mathbb{E} \cdot \mathbb{M}$$

Using the FD theorem $\mathbb{E} = k_\mathrm{B}T\,\mathbb{K}$ and $\mathbb{M} \cdot \mathbb{K} = \mathbb{1}$,

$$\boxed{\mathbb{D} = k_\mathrm{B}T\,\mathbb{M}}$$

For a spherical particle, $\mathbb{M} = (6\pi\mu a)^{-1}\,\mathbb{1}$, so

$$\boxed{D = \frac{k_\mathrm{B}T}{6\pi\mu a}.}$$

This is the Stokes–Einstein equation.

The added drift

The added drift $\nabla \cdot \mathbb{D}$:

$$\boxed{\dot{\boldsymbol{x}} = \nabla \cdot \mathbb{D} + \mathbb{\Sigma} \cdot \dot{\boldsymbol{w}}}$$

plays an important role. FP equation for $p(\boldsymbol{x}, t)$:

$$\begin{aligned} \partial_t p &= -\nabla \cdot (\nabla \cdot \mathbb{D}\, p - \nabla \cdot (\mathbb{D}\, p)) \\ &= -\nabla \cdot (\mathbb{D} \cdot \nabla p) \end{aligned}$$

The added drift ensures that $p \equiv$ const. is an equilibrium (in the absence of other forcing).

Without the added drift, multiplicative noise causes spurious accumulation of particles.

Note: *not* the same as anti-Itô, as is sometimes claimed in the literature. That is only true in 1D.

Rotation

I've cheated a bit: used a particle of arbitrary shape, but we did not keep track of its orientation.

The 'full' Langevin system is

$$\begin{aligned}
\dot{\boldsymbol{x}} &= \boldsymbol{u} \\
\dot{\boldsymbol{\phi}} &= \mathbb{L} \cdot \boldsymbol{\omega} \\
\dot{\boldsymbol{\pi}} &= -\mathbb{K}_{\boldsymbol{xx}} \cdot \boldsymbol{u} - \mathbb{K}_{\boldsymbol{x\phi}} \cdot \boldsymbol{\omega} + \overline{\boldsymbol{f}} + \widetilde{\boldsymbol{f}} \\
\dot{\boldsymbol{\ell}} &= -\mathbb{K}_{\boldsymbol{\phi x}} \cdot \boldsymbol{u} - \mathbb{K}_{\boldsymbol{\phi\phi}} \cdot \boldsymbol{\omega} + \bar{\boldsymbol{\tau}} + \widetilde{\boldsymbol{\tau}}
\end{aligned}$$

$\boldsymbol{\phi}$ is a vector of 3 numbers that represent a rotation (i.e., Euler angles, quaternions, ...)

The matrix $\mathbb{L}$ 'translates' between the rotation vector and the representation. (More in a bit.)

The grand resistance matrix

Greg Voth already introduced the grand resistance/mobility matrices:

$$\begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{\omega} \end{pmatrix} = \widehat{\mathbb{M}} \cdot \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{\tau} \end{pmatrix}, \qquad \widehat{\mathbb{M}} := \begin{pmatrix} \mathbb{M}_{\boldsymbol{xx}} & \mathbb{M}_{\boldsymbol{x\phi}} \\ \mathbb{M}_{\boldsymbol{\phi x}} & \mathbb{M}_{\boldsymbol{\phi\phi}} \end{pmatrix}$$

$$\widehat{\mathbb{K}} = \widehat{\mathbb{M}}^{-1} = \begin{pmatrix} \mathbb{K}_{\boldsymbol{xx}} & \mathbb{K}_{\boldsymbol{x\phi}} \\ \mathbb{K}_{\boldsymbol{\phi x}} & \mathbb{K}_{\boldsymbol{\phi\phi}} \end{pmatrix}$$

Must be rotated from body frame (fixed matrix) to lab frame:

$$\widehat{\mathbb{K}} = \begin{pmatrix} \mathbb{Q} & \mathbb{0} \\ \mathbb{0} & \mathbb{Q} \end{pmatrix} \cdot \widehat{\mathbb{K}}^{(0)} \cdot \begin{pmatrix} \mathbb{Q}^{\top} & \mathbb{0} \\ \mathbb{0} & \mathbb{Q}^{\top} \end{pmatrix}$$

Representation for rotation matrices

$$\dot{\boldsymbol{\phi}} = \mathbb{L} \cdot \boldsymbol{\omega}, \qquad \boldsymbol{\phi} = (\phi_1, \phi_2, \phi_3)$$

How to compute $\mathbb{L}$: for a given parametrization of rotation $\mathbb{Q}(\boldsymbol{\phi})$,

$$(\,\mathbb{L}^{-1}\,)_{k\mu} = \tfrac{1}{2}\epsilon_{ijk} Q_{ip}\,\frac{\partial Q_{jp}}{\partial \phi_\mu}.$$

That's it! Now we can do this with Euler angles $\boldsymbol{\phi} = (\psi, \theta, \phi)$, or quaternions $\boldsymbol{\phi} = (q_1, q_2, q_3)$, etc. Each has its advantages.

This also tells us how to define $\nabla_{\boldsymbol{\phi}}$:

$$\nabla_{\boldsymbol{\phi}} = \mathbb{L}^{\top} \cdot \frac{\partial}{\partial \boldsymbol{\phi}}\,.$$

Overdamped limit again

Stokes–Einstein, now including angles:

$$\widehat{\mathbb{D}} = k_{\mathrm{B}}T\,\widehat{\mathbb{M}}$$

$\widehat{\mathbb{D}}$ is a 6×6 diffusion matrix! It tells us how positions and angles diffuse.

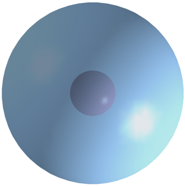
But don't forget the drift correction!

$$[\hat{\nabla} \cdot \widehat{\mathbb{D}}]_{\boldsymbol{x}} = \nabla_{\boldsymbol{x}} \cdot \mathbb{D}_{\boldsymbol{x}\boldsymbol{x}} + \nabla_{\boldsymbol{\phi}} \cdot \mathbb{D}_{\boldsymbol{\phi}\boldsymbol{x}} = \boldsymbol{\epsilon} : \mathbb{D}_{\boldsymbol{\phi}\boldsymbol{x}}$$

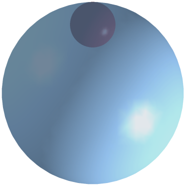
This correction is nonzero when the center of mass does not coincide with the center of mobility.

'Wobbly particle.'

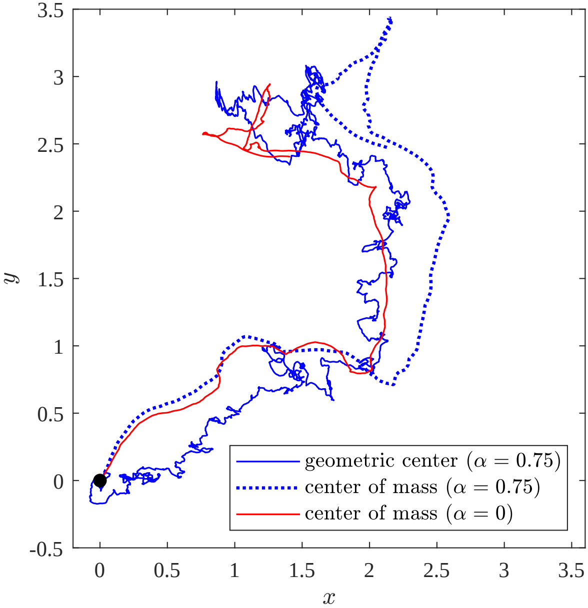
A wobbly sphere



$\alpha = 0$

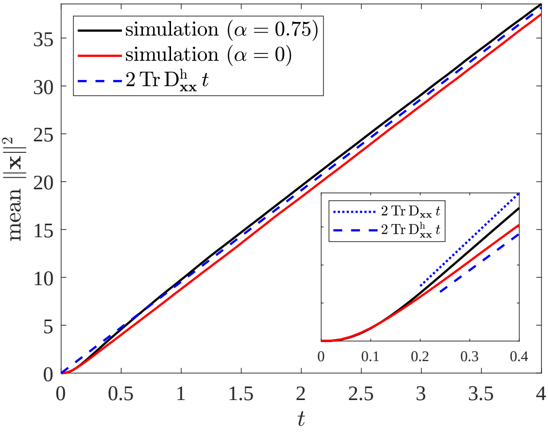


$\alpha = 0.75$



A wobbly sphere: dispersion

Inset: wobbly spheres appear to disperse faster, because of the added drift.



But at long times they're the same! [Thiffeault & Guo, preprint (2025)]

Position of center of mass is irrelevant, at least for thermal particles.

Hands-on activity

Winding around a point! Use Matlab, Python, or whatever.

- Simulate 2D Brownian motion in the plane: $\dot{\boldsymbol{x}} = \sqrt{2D}\,\dot{\boldsymbol{w}}$.
- 1. For a large ensemble of particles, what is the distribution of winding angle around the origin: $\theta(t) = \arctan(y(t)/x(t))$?
- Hint: it should be close to a Cauchy–Lorentz distribution. This is the famous Spitzer's Law (1958).
- 2. Now prevent the radius from growing too large by limiting the motion to $|r| < a$. (Rejection sampling.) What is the distribution?
- 3. Then add a vortex: $\boldsymbol{v} = (\Omega/r)\,\hat{\boldsymbol{\theta}}$. What is the distribution then?
- 4. Consider doing this for other types of vortices; perhaps compare to heavy particles.

Some references

- Textbooks on stochastic dynamics:
  [Øksendal (2003); Gardiner (2009); Pavliotis (2014); van Kampen (2007); Risken (1996)]
- Resistance matrices and low-Re hydro:
  [Happel & Brenner (1983); Kim & Karrila (1991); Brenner (1965, 1967)]
- Overdamped limit and noise-induced drift: [Kupferman *et al.* (2004); Lau & Lubensky (2007); Farago & Grønbech-Jensen (2014); Farago & Grønbech-Jensen (2014); Herzog *et al.* (2016); Farago (2017); Thiffeault & Guo (2022); Hottovy *et al.* (2012, 2014); Volpe & Wehr (2016)]
- Integrating quaternions: [Rucker (2018)]
- Active particle dynamics:
  [Cates & Tailleur (2013); Thiffeault & Guo (2022); Sevilla (2016); Sandoval (2013)]

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