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Immersed Particle Dynamics in Fluctuating Fluids with Memory

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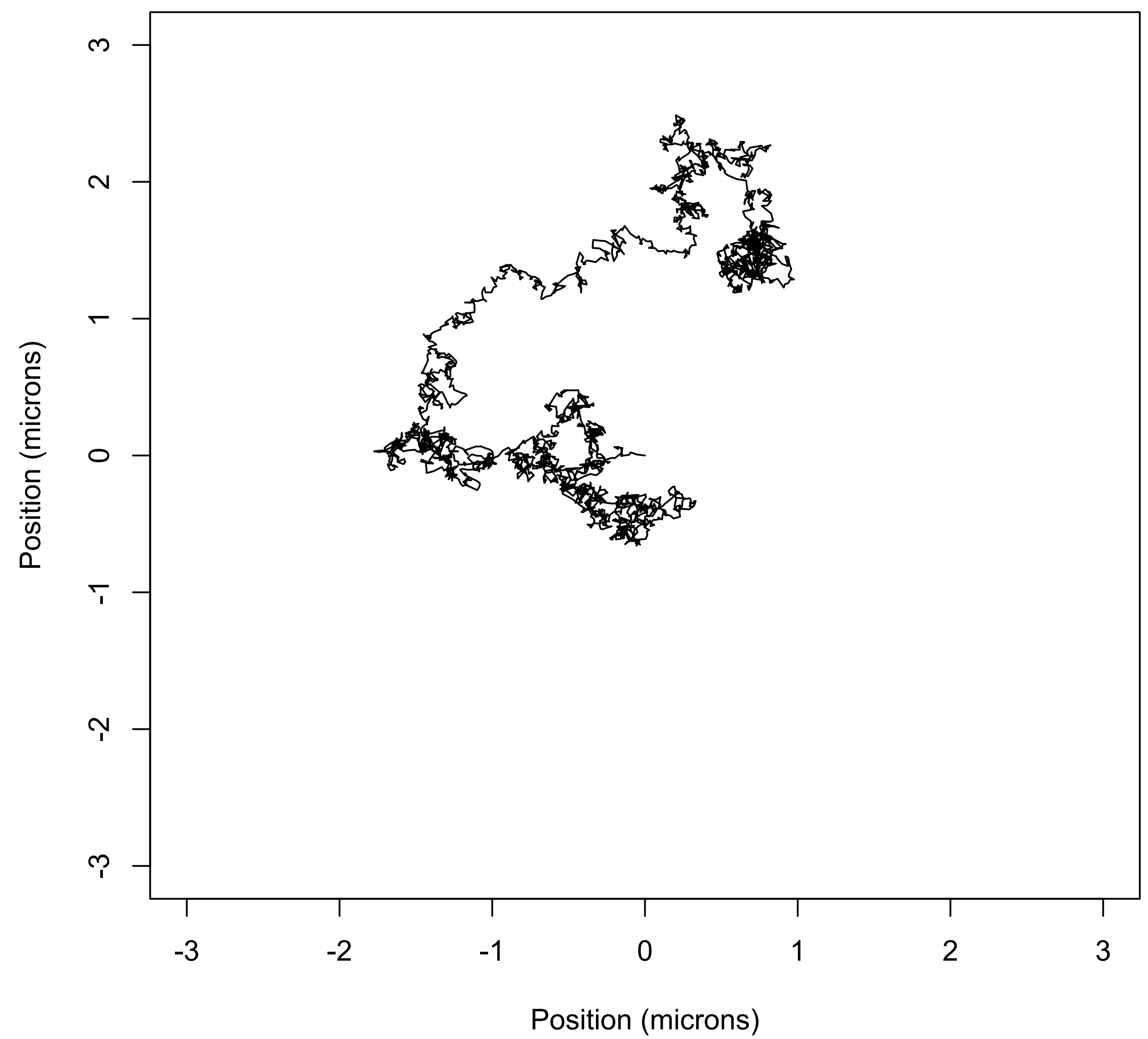
Together with Scott McKinley (University of Florida)
Inspired by Greg Forest (University of North Carolina, Chapel Hill)

Passive Microrheology

- Measure mechanical properties using material deformation and flow.
- Micro: small volume of liquid.
- Passive: no external forcing on tracers.
  - Record displacements induced by thermal fluctuations.
  - The mechanical properties are extracted via statistical analysis.
  - Used with viscous and viscoelastic liquids.

Typical path for 500 nm beads in 2M concentration mucus.



D. Hill, CFC (UNC)

Goals

- Develop a **numerical** experiment of particles passively moving in a viscoelastic fluid.
- Why:
  - Avoid experimental noise and uncertainties;
  - Prescribe the viscoelastic model;
  - Inverse problem: recover the parameters of the viscoelastic model, statistical inference based on the fluctuations of the mean squared displacement;
  - Answer fundamental modeling questions about length and time scales of transport of memory information through the fluid and mediated by the particles;
  - Learn something new about SPDEs.
- How:
  - Fluctuating hydrodynamics. Done for a viscous fluid;
  - Do not assume a GLE for particle positions;
  - Deal with particle interactions without using a mobility matrix.

Navier-Stokes (constant temperature)

- **Conservation of linear momentum** for a volume of fluid:

$$\boxed{\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u})} = \boxed{\nabla\cdot\boldsymbol{\sigma}} + \boxed{\mathbf{f}}$$

Inertia (per volume): unsteady + convective acceleration

Contact (molecular forces): divergence of stress

Body forces (per unit volume)

- **Constitutive stress equation** (Newtonian fluid):

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{E} \quad \mathbf{E} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$$

E rate-of-strain tensor, *p* pressure, η fluid viscosity (dynamic)
pressure -> normal stresses, viscosity -> shear stresses

- **Conservation of mass**: $\nabla\cdot\mathbf{u} = 0$
Incompressibility: the density of a fluid parcel is constant

- **Conservation of angular momentum**: $\boldsymbol{\sigma}$ is symmetric

Nondimensionalization

- Pick (problem dependent) a characteristic velocity *U* and length *L.*

  Let $\mathrm{Re} = \dfrac{LU\rho}{\eta}$ be the Reynolds number. It is the ratio of the inertial to viscous forces.

- Pick *T* a characteristic time. In general, $T \neq L/U$.

  Let $\beta = \dfrac{L^2\rho}{T\mu}$ be the frequency parameter. If **f**=0, then $T=L/U$ and Re=β.

- **Stokes** equations: small Re and **f**=0:

$$0 = -\nabla p + \eta \Delta \mathbf{u} \quad \nabla \cdot \mathbf{u} = 0$$

- **Unsteady Stokes** equations: small Re:

$$\rho \partial_t \mathbf{u} = -\nabla p + \eta \Delta \mathbf{u} + \mathbf{f} \quad \nabla \cdot \mathbf{u} = 0$$

- Inviscid flow: high Re - no viscosity (nonlinear)

Fluctuating Hydrodynamics for a viscous fluid

- Model fluctuations in the thermal bath by adding fluctuations in the form of a stress (a stochastic flux). This introduces a new timescale *T≠L/U*, the timescale of fluctuations. Nondimensional numbers: $\mathrm{Re} \ll 1 \quad \beta \sim 1$

- **Fluctuating unsteady Stokes equations**:

$$\rho \partial_t \mathbf{u} = -\nabla p + \nabla \cdot \left(2\eta \mathbf{E} + \sqrt{2 k_B T \mu} \mathbf{W} \right)$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbb{E}[W_{ij}(x,t) W_{kl}(y,s)] = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \delta(t-s) \delta(x-y)$$

k_B Boltzmann constant, T temperature and $\mathbf{W} = \dot{\mathbf{B}}$ is a space-time white noise tensor.

- First proposed by Landau and Lifshitz for compressible flow. Generalized to incompressible Navier-Stokes by Bell, Donev, ... Justified using the Mori-Zwanzig formalism to ensure the correct equilibrium distribution.

Linear viscoelasticity (Maxwell fluid)

- **Viscoelastic fluid**: response of the fluid to the applied strain or stress depends on the applied force. The fluid can behave as an elastic (fast deformation) or as a liquid (slow deformation). Examples: ketchup, silly putty, corn starch.

- **Linear viscoelastic model**: Lodge equation

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\int_{-\infty}^{t} G(t-t')\mathbf{E}(t')dt' \quad G \text{ relaxation modulus}$$

$$G(t) = \int_{t}^{\infty} m(s)ds \quad m \text{ memory} \quad \eta = \int_{0}^{\infty} G(s)ds \quad \eta \text{ zero shear-rate viscosity}$$

- Rewrite (factor η and introduce causality)

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\int_{-\infty}^{\infty} K^{+}(t-t')\mathbf{E}(t')dt' \qquad K^{+}(t) = \mathbb{1}_{t\geq 0}K(t)$$

- Prony series (aka Maxwell): *K* fluid memory kernel with *N* relaxation times

$$K(t) = \frac{1}{\tau_0}\sum_{i=0}^{N-1} e^{-t/\tau_i} \quad \tau_i = \tau_0\left(\frac{N}{N-i}\right)^{p} \quad p > 1$$

Fluctuating Hydrodynamics for a viscoelastic fluid

- Let **F**(**x**,*t*) be a stationary zero mean Gaussian matrix process with

$$\mathbb{E}[F_{ij}(x,t)F_{kl}(y,s)] = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})K(|t-s|)\delta(|\mathbf{x}-\mathbf{y}|)$$

  F is a space white noise and time colored noise.

- Consider a linear **Maxwell** fluid with *N* relaxation times.

- (New) **Fluctuating Hydrodynamics Maxwell Stokes equations**

$$\rho\partial_t\mathbf{u} = -\nabla p + 2\eta\nabla\cdot(K^+ \star \mathbf{E}) + \sqrt{2k_B T\eta}\nabla\cdot\mathbf{F}$$
$$\nabla\cdot\mathbf{u} = 0$$

  * is the time convolution.

- Different than considering spacial correlation which models heterogeneous media.

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Fourier transformed system

- Motivated by
  - (Spacial) Spectral decomposition of **F**: $\mathbf{F}(\mathbf{x},t) = \frac{1}{L}\sum_{\mathbf{k}} \mathbf{F}^{\mathbf{k}}(t) e^{-i\lambda \mathbf{k}\cdot\mathbf{x}}$
  - For periodic boundary conditions, (unsteady) Stokes can be solved in Fourier space.
- Eliminate the pressure by taking the dot product with **k**.
- **Fourier transformed system**:

$$\lambda = \frac{2\pi}{L} \quad \mathbf{P} = \mathbf{I} - \frac{1}{k^2}\mathbf{k}\mathbf{k}^{\mathbf{T}} \quad k = |\mathbf{k}|$$

$$\rho \partial_t \mathbf{u}_{\mathbf{k}} = -\lambda^2 k^2 \eta K^+ \star \mathbf{u}_{\mathbf{k}} + i\lambda L \sqrt{2k_B T\eta}\mathbf{P}^{\mathbf{k}}\mathbf{F}^{\mathbf{k}}\mathbf{k}$$

$$\mathbb{E}[F^{\mathbf{k}}_{ij}(t)\overline{F^{\mathbf{l}}_{mn}}] = (\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm})\delta_{\mathbf{kl}}K(|t-s|)$$

- Let $\mathbf{v}_{\mathbf{k}} = \mathrm{Re}(\mathbf{u}_{\mathbf{k}}) = \mathbf{P}\zeta\hat{\mathbf{k}} \quad \hat{\mathbf{k}} = \frac{\mathbf{k}}{k}$. Then

$$\rho\partial_t \zeta^{\mathbf{k}}_{ij} = -\lambda^2 k^2 \eta K^+ \star \zeta^{\mathbf{k}}_{ij} + L\lambda k\sqrt{2k_B T\eta}G^{\mathbf{k}}_{ij}$$

$$\mathbb{E}[G^{\mathbf{k}}_{ij}(t)G^{\mathbf{l}}_{mn}(s)] = \frac{1}{2}(\delta_{im}\delta_{jn} + \delta_{nm}\delta_{in})\delta_{\mathbf{kl}}K(|t-s|)$$

Generalized Langevin Equation for each **k**

Advection of immersed particles

- **Passive advection**: given ***X***(0)

$$\dot{\mathbf{X}}(t) = \mathbf{V}(t) = \int_\Omega \delta_a(\mathbf{x} - \mathbf{X}(t))\mathbf{u}(\mathbf{x}, t)d\mathbf{x}$$

  where δ_a is an approximate Delta function depending on the radius of the particle. Follow the evolution of a blob of liquid or distributional average.

- **Spectral representation**: $\dot{\mathbf{X}} = \frac{2}{L^2}\sum_{\mathbf{k}>0} \cos\left(\lambda\mathbf{k}\cdot\mathbf{X}\right)\mathbf{u}_\mathbf{k}\delta_{a,\mathbf{k}}$

- **Semi-Euler time stepping**: Δt time step $\quad t_n = n\Delta t$

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \frac{2}{L^2}\sum_{\mathbf{k}>0} \cos\left(\lambda\mathbf{k}\cdot\mathbf{X}_n\right)\delta_{a,\mathbf{k}}\int_{n\Delta t}^{(n+1)\Delta t} \mathbf{u}_\mathbf{k}(s)ds$$

- All we really need is $\mathbf{v}_\mathbf{k} = \mathrm{Re}(\mathbf{u}_\mathbf{k}) = \mathbf{P}\zeta\hat{\mathbf{k}}$

$$\int_{n\Delta t}^{(n+1)\Delta t} \zeta_{ij}^{\mathbf{k}}(s)ds \quad \zeta_{ij}^{\mathbf{k}} \text{ is given by a GLE}$$

Generalized Langevin equation (GLE)

- Consider the 1d simpler problem of **Brownian motion with memory**. Let *F*(*t*) be a zero mean stationary Gaussian process and $\gamma = 6\pi\eta a$ be the drag coefficient of a particle of radius a

$$m\frac{dV(t)}{dt} = -\gamma K^{+} \star V(t) + \sqrt{2k_B T\gamma}F(t)$$
$$\mathbb{E}[F(t)F(s)] = K(|t-s|)$$
$$\frac{dX}{dt} = V(t)$$

- In the previous set-up: $V = \zeta_{ij}^{\mathbf{k}} \quad m = \rho \quad \gamma = \lambda^2 k^2 \eta$

- **Facts**:
  - *V*(*t*) is Gaussian and stationary, and non Markovian. *X*(*t*) is Gaussian.
  - *V*(*t*) can be solved in Fourier space and its covariance is

$$\widehat{\rho_V(\xi)} = |\widehat{\chi}(\xi)|^2 \hat{K}(\xi) \quad \widehat{\chi}(\xi) = \frac{\sqrt{2k_B T\gamma}}{\left(mi2\pi\xi + \gamma\widehat{K_1^{+}}(\xi)\right)}$$

Covariance of the position process

- Covariance of the position process:

$$\rho_X(t,s) = \int_0^t \int_0^s \rho_V(|t'-s'|)ds'dt'.$$

- Calculus: change the order of integration

$$\rho_X(t,s) = tI_1(t) - (t-s)I_1(t-s) + sI_1(s) - [I_2(t) - I_2(t-s) + I_2(s)]$$

$$I_1(t) = \int_0^t \rho_V(u)du \quad I_2(t) = \int_0^t u\rho_V(u)du$$

- Using Fourier transforms and more calculus:

$$\boxed{\rho_X(t,s) = \frac{2}{\pi^2}\int_0^\infty \frac{\widehat{\rho_V}(\xi)}{\xi^2}\cos\left(\pi\xi(t-s)\right)\sin(\pi\xi t)\sin(\pi\xi s)d\xi}$$

- The integral exists at the origin (no singularity).

Algorithm to generate sample paths

- Given $\hat{\rho}_V$ and *N* the length of the path.
- Build the covariance matrix **R**: $R_{ij} = \rho_X(i\Delta t, j\Delta s)$
  Integrals are evaluated numerically using adaptive Gauss-Kronrod quadrature (Matlab)
- Let **C** be the Cholesky (lower triangular) decomposition of **R**.
- Let **Y** be a vector of length *N* of unitary normal random variables.
- Let **X**=**CY**. Then **X** has the correct covariance structure (Asmussen and Glynn).
- Error:
  - Statistically exact (drawn from of the exact distribution);
  - Deterministic: approximation of the integral.

Summary

- Particle advection:

$$\dot{\mathbf{X}}(t) = \mathbf{V}(t) = \int_{\Omega} \delta_a(\mathbf{x} - \mathbf{X}(t))\mathbf{u}(\mathbf{x}, t) d\mathbf{x}$$

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \frac{2}{L^2} \sum_{\mathbf{k}>0} \cos\left(\lambda \mathbf{k} \cdot \mathbf{X}_n\right) \delta_{a,\mathbf{k}} \int_{n\Delta t}^{(n+1)\Delta t} \mathbf{u}_{\mathbf{k}}(s) ds$$

- Fluctuating Viscoelastic Hydrodynamics fluid: Fourier space

$$\rho \partial_t \zeta_{ij}^{\mathbf{k}} = -\lambda^2 k^2 \eta K^+ \star \zeta_{ij}^{\mathbf{k}} + L\lambda k \sqrt{2k_B T \eta} G_{ij}^{\mathbf{k}}$$

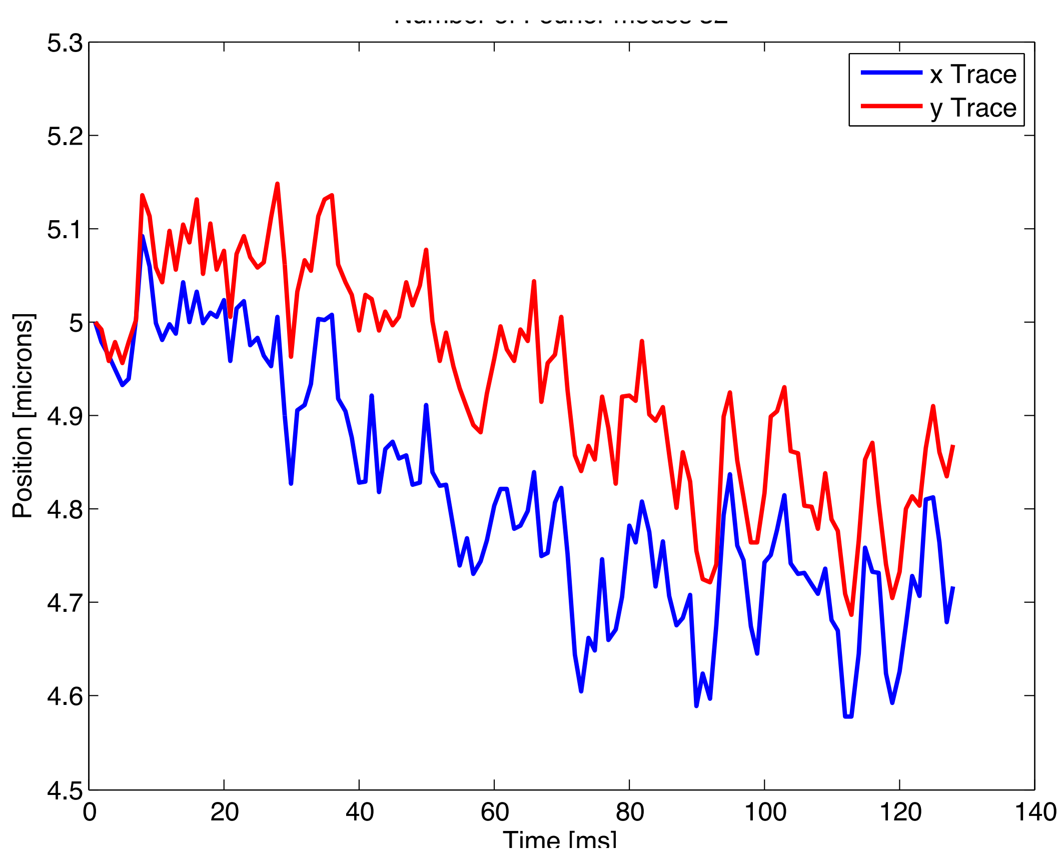
$$\mathbb{E}[G_{ij}^{\mathbf{k}}(t) G_{mn}^{\mathbf{l}}(s)] = \frac{1}{2}(\delta_{im}\delta_{jn} + \delta_{nm}\delta_{in})\delta_{\mathbf{kl}} K(|t-s|)$$

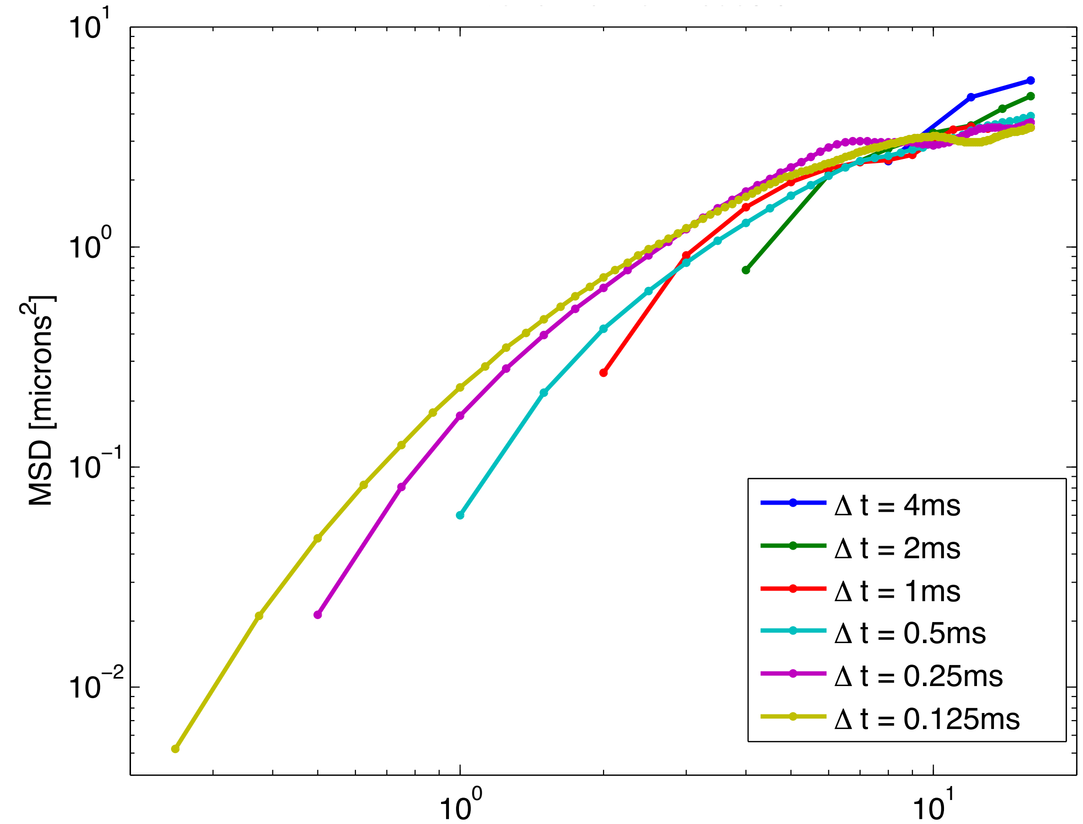
$$\mathbf{v}_{\mathbf{k}} = \mathrm{Re}(\mathbf{u}_{\mathbf{k}}) = \mathbf{P}\boldsymbol{\zeta}\hat{\mathbf{k}}$$

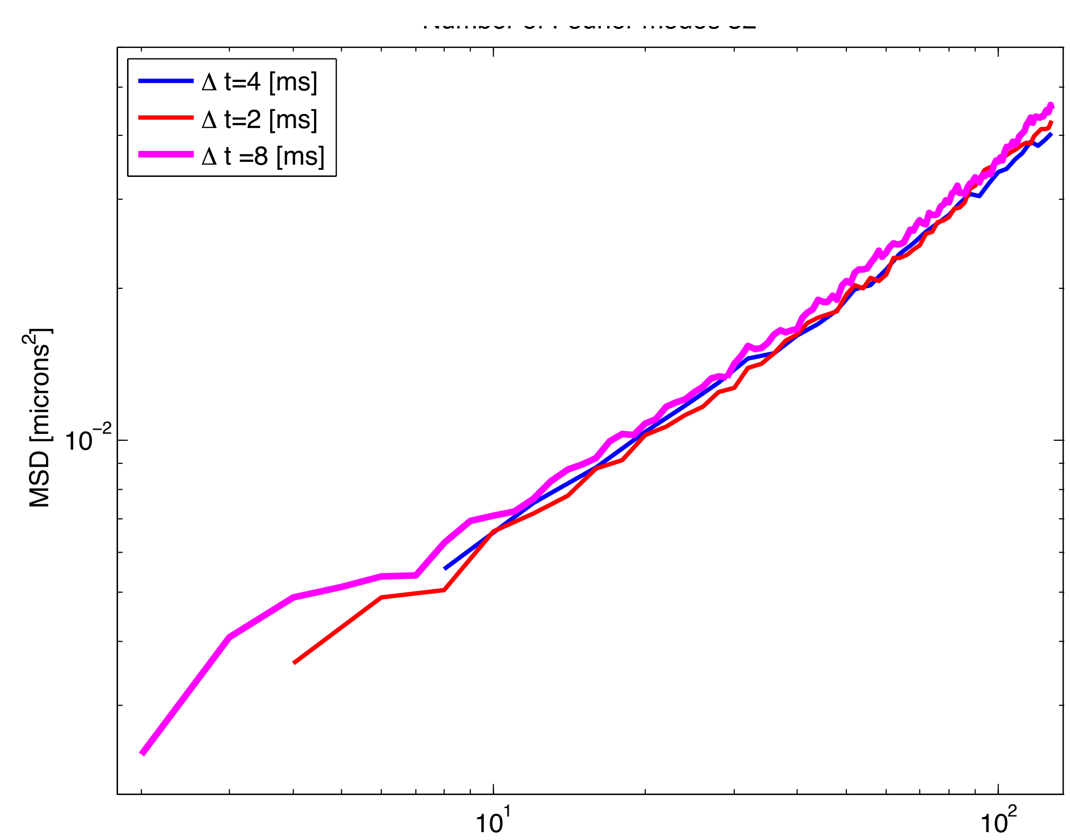
- For each **k**, the integral of the GLE is simulated using the Cholesky decomposition of the covariance matrix of the underlying Gaussian process.

- Realizations of particle paths up to a final time are generated in one step. Not a forward marching scheme.

Sample paths







Five memory kernels

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