

# **Generalized Langevin Equation**

## **Stochastic Differential Equations**

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# Agenda



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- ② Introduction to Generalized Langevin Equation
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  - Mathematical Model: Stochastic systems with memory capture anomalous diffusion
  - Model Complications and Solutions: due to memory effects
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- ③ Numerical Schemes for Solving GLE
  - Numerical Schemes: **Explicit Euler vs Splitting Schemes**
  - Comparison of Numerical Schemes: **Splitting schemes conserve first and second moments**
  - Harmonic Potential Well
- ④ Sensitivity Analysis
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Break this up a bit more: local sensitivity , global sensitivity etc
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# Scope of the Project

**What?** Generalized Langevin Dynamics is a modeling technique that can be used to model anomalous diffusive phenomena observed in viscoelastic fluids, flow and in biological systems.

**Why?** ~~Anomalous diffusion problems: Langevin model fails to capture sub-diffusive and super-diffusive behavior which the GLE succeeds in capturing.~~ But GLE is *Non-Markovian* i.e. memory kernel depends on the history of velocity. This issue is overcome by using Extended Variable GLE that considers a finite dimensional subspace for the memory kernel.

**Where?** Applications of GLE include but are not restricted to micro-rheology, biological systems, nuclear quantum effects and systems in which anomalous diffusion arise.

**How?** Study Extended Variable GLE using Prony series approximation. Accuracy of Implicit/Explicit Euler and Splitting Numerical schemes are also tested to find out the “optimal scheme”. Study the sensitivity of the solution to the changes in the parameters of the extended variable GLE.

not solutions: observables

local and global

# ~~Introduction~~ Langevin dynamics is a computational tool

**What?** **Langevin Dynamics:** Large particles in a bath of small particles, motion of large particles directly integrated while the dynamics of small particles are "averaged out".

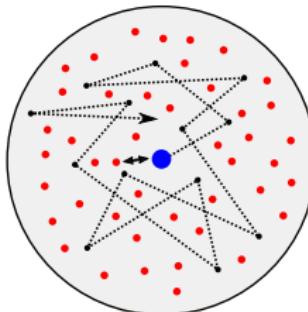
**Why?** *Molecular Dynamics* simulations involving all particles is computationally expensive. Langevin Equation model is computationally cheaper.

## Drawback

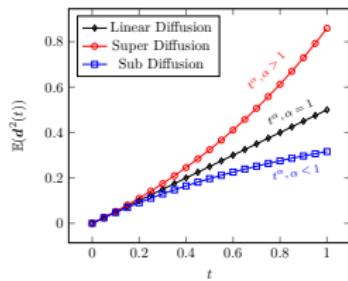
Anomalous diffusion problems arising due to *Power Law* behavior of solute-solvent systems cannot be solved.

## Solution

*Generalized Langevin Equation (GLE)*



(a) Big Particles interacting with Smaller Particles



(b) Sub-diffusive and Super-diffusive behavior of solute-solvent systems

# Mathematical Model for anomalous diffusion

The velocity term of GLE is based on *Ornstein-Uhlenbeck* process.

## GLE Equations

$$d\mathbf{X}(t) = \mathbf{V}(t)dt \quad (1)$$

$$\mathbf{M}d\mathbf{V}(t) = \underbrace{\mathbf{F}^c(\mathbf{X}(t))dt}_{\substack{\text{Conservative} \\ \text{Force due to} \\ \text{Potential}}} - \underbrace{\int_0^t \mathbf{\Gamma}(t-s)\mathbf{V}(s)dsdt}_{\substack{\text{Temporally} \\ \text{Non-Local Drag } (\mathbf{F}^d) \\ \text{Force}}} + \underbrace{\mathbf{F}^r(t)dt}_{\substack{\text{Random} \\ \text{Correlated} \\ \text{Force given by} \\ \text{FDT}}} \quad (2)$$

$$\mathbf{X}(0) = \mathbf{X}_0, \quad \mathbf{V}(0) = \mathbf{V}_0 \quad (\text{Initial Conditions}) \quad (3)$$

### Note:

$\mathbf{F}^r$  and  $\mathbf{F}^d$  are characterized by the memory kernel consistent with FDT.

# Mathematical Model

## Theorem

FDT (*Fluctuation Dissipation Theorem*) states that the equilibration to a temperature,  $T$ , requires that the two-time correlation of  $\mathbf{F}^r(t)$  and  $\mathbf{\Gamma}(t)$  be related as:

$$\langle \mathbf{F}_i^r(t+s), \mathbf{F}_j^r(t) \rangle = k_B T \mathbf{\Gamma}(s) \delta_{ij}, \quad s \geq 0 \quad (4)$$

where  $k_B$  is the Boltzmann's Constant and  $\delta_{ij}$  is the Kronecker Delta.

## Note:

- $\mathbf{F}^d(t)$  depends on the velocity history unlike in *Langevin Equation* where it depends on the velocity at that instant.
- The random forces are not just delta correlated but are correlated by the memory kernel. Memory Kernel choice and approximation important based on the problem to be studied.

# Model Complications and Solutions

## Complications

- ① Storage of subset of the time history of  $\mathbf{V}(t)$ .
- ② Sequence of  $\mathbf{F}^r(t)$  given by FDT.
- ③ Numerical SDE solution should converge in distribution.

## Solution

- ① Using extended variable Prony Series for Memory Kernel.

$$\Gamma(t) \approx \sum_{k=1}^{N_k} \frac{c_k}{\tau_k} \exp\left[-\frac{t}{\tau_k}\right], \quad t \geq 0 \quad (5)$$

where  $N_k$  is the number of terms used in approximating the memory kernel.

- ② Using a suitable integration scheme for the numerical method.

# Model Complications and Solutions

## Why use extended variable Prony Series?

- Approximation of memory kernel to map **Non-Markovian GLE** to **Markovian** system of  $N_k$  variables.
- Typically used for modelling *Power Law* based decay/growth as observed in sub/super diffusive systems.

## Importance of choice of integration scheme?

- Conservation of moments of variables of interest such as displacement and velocity (usual variables of interest for MD simulations)
- Convergence of **GLE** to Langevin equation in the limit of small  $\tau_k$  as observed in theory.



# Extended Variable GLE

## Main Extended Variable GLE Equations

$$m_i dV_i(t) = F_i^C(\mathbf{X}(t))dt + \sum_{k=1}^{N_k} S_{i,k} dt \quad (6)$$

$$dX_i(t) = V_i(t)dt \quad (7)$$

$$dS_{i,k}(t) = -\frac{1}{\tau_k} S_{i,k}(t)dt - \frac{c_k}{\tau_k} V_i(t)dt + \frac{1}{\tau_k} \sqrt{2k_B T c_k} dW_{i,k}(t) \quad (8)$$

## Auxiliary Extended Variable GLE Equations

$$S_{i,k}(t) = Z_{i,k}(t) + F_{i,k}(t) \quad (9)$$

$$dZ_{i,k}(t) = -\frac{1}{\tau_k} Z_{i,k}(t)dt - \frac{c_k}{\tau_k} V_i(t)dt \quad Z_{i,k}(t) = - \int_0^t \frac{c_k}{\tau_k} \exp \left[ -\frac{(t-s)}{\tau_k} \right] V_i(s) ds \quad (10)$$

$$dF_{i,k}(t) = -\frac{1}{\tau_k} F_{i,k}(t)dt + \frac{1}{\tau_k} \sqrt{2k_B T c_k} dW_{i,k}(t) \quad \langle F_{i,k}(t+s), F_{i,k}(t) \rangle = k_B T \frac{c_k}{\tau_k} \exp \left[ -\frac{s}{\tau_k} \right] \quad (11)$$

$$F_i^r(t) = \sum_{k=1}^{N_k} F_{i,k}(t) \quad (12)$$

# Numerical Schemes

## Numerical Schemes:

- Explicit Euler Scheme.
- Splitting Scheme.

### Which numerical scheme to choose for solving the problem?

Therefore Scheme that is able to conserve the first and second moments of quantities of interest i.e.  $\mathbf{V}(t)$  and  $\mathbf{X}(t)$  are essential for validating simulations.

**Reason:** General observables/physical quantities that are measured to understand the behavior of a system. For example, Mean Square Displacement (MSD) in microrheology. simulations.

E.g.,

Sp.

and velocity autocorrelation functions (VACF)

## Implementation Details:

- Uniform time-step size,  $\Delta t$ , where  $N_t \Delta t = T_{\text{tot}}$  ( $T_{\text{tot}}$  represents the total time of the simulation and  $N_t$  represents the # of time-steps.)
- All  $N_p$  particles are seeded with the same constant  $\mathbf{X}(0)$  and  $\mathbf{V}(0)$  (**Note:** We could also seed the initial conditions based on the p.d.f if known.)
- The composite variable  $S_{i,k}(t)$  is assumed to be zero initially.

# Numerical Schemes

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## Explicit Euler Scheme

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**Input:**  $\mathbf{X}(0), \mathbf{V}(0), \mathbf{S}(0)$

**Output:**  $\mathbf{X}(t), \mathbf{V}(t)$

```
1: for  $n = 0$  to  $N_t$  do
2:    $V_i^{n+1} = V_i^n + \frac{\Delta t}{m_i} F_i^c(\mathbf{X}^n) + \frac{\Delta t}{m_i} \sum_{k=1}^{N_k} S_{i,k}^n$            ▷ Advance  $\mathbf{V}(t)$  by a full step
3:    $X_i^{n+1} = X_i^n + \Delta t V_i^n$                                      ▷ Advance  $\mathbf{X}(t)$  by a full step
4:    $S_{i,k}^{n+1} = \left(1 - \frac{\Delta t}{\tau_k}\right) S_{i,k}^n - \frac{c_k \Delta t}{\tau_k} V_i^n + \frac{1}{\tau_k} \sqrt{2k_B T c_k} \Delta W_{i,k}$  ▷ Advance  $\mathbf{S}(t)$  by a full step
5: end for
```

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## Splitting Scheme

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**Input:**  $\mathbf{X}(0), \mathbf{V}(0), \mathbf{S}(0)$

**Output:**  $\mathbf{X}(t), \mathbf{V}(t)$

```
1: for  $n = 0$  to  $N_t$  do
2:    $V_i^{n+1/2} = V_i^n + \frac{\Delta t}{2m_i} F_i^c(\mathbf{X}^n) + \frac{\Delta t}{2m_i} \sum_{k=1}^{N_k} S_{i,k}^n$            ▷ Advance  $\mathbf{V}(t)$  by a half step
3:    $X_i^{n+1} = X_i^n + \Delta t V_i^{n+1/2}$                                      ▷ Advance  $\mathbf{X}(t)$  by a full step
4:    $S_{i,k}^{n+1} = \theta_k S_{i,k}^n - (1 - \theta_k) c_k V_i^{n+1/2} + \alpha_k \sqrt{2k_B T c_k} \Delta W_{i,k}$  ▷ Advance  $\mathbf{S}(t)$  by a full step
5:    $V_i^{n+1} = V_i^{n+1/2} + \frac{\Delta t}{2m_i} F_i^c(\mathbf{X}^{n+1}) + \frac{\Delta t}{2m_i} \sum_{k=1}^{N_k} S_{i,k}^{n+1}$           ▷ Advance  $\mathbf{V}(t)$  by a half step
6: end for
```

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## Comparison of Numerical Schemes

### Case Study:

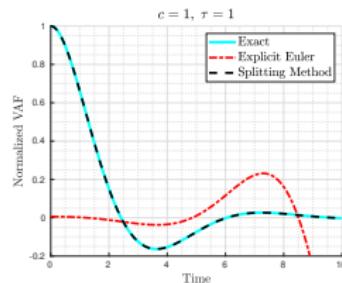
- One dimensional problem,  $d = 1$
- Single mode in the Prony series approximation,  $N_k = 1$
- Zero conservative force acting on the particles,  $\mathbf{F}^c(\mathbf{X}(t)) = 0$

The case study is simulated using both numerical schemes, *Explicit Euler* and *Splitting Method*, for three different  $\tau$  and  $c$  values in the Prony Series approximation (Table 1)

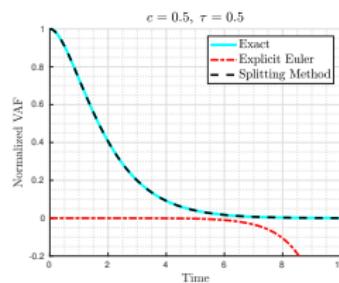
Type of System	$c$	$\tau$
Under-damped	1	1
Critically-damped	0.5	0.5
Over-damped	0.25	0.25

Table:  $c$  and  $\tau$  values used for the case study

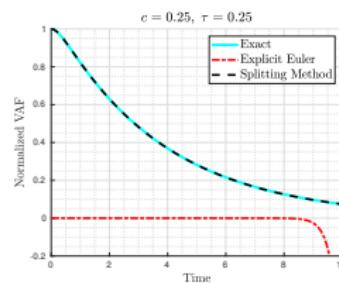
# Comparison of Numerical Schemes - Results



(a) Under-damped



(b) Critically-damped



(c) Over-damped

**Figure:** Comparison of different numerical schemes w.r.t. Normalized VAF  
how many extended variables? how many samples are these based on? for what step sizes?

Normalized VAF (*Velocity Autocorrelation Function*)

$$\frac{\langle \mathbf{V}(t), \mathbf{V}(0) \rangle}{\langle \mathbf{V}(0), \mathbf{V}(0) \rangle} = \begin{cases} \exp\left[-\frac{t}{2\tau}\right] \left(\cos(\Omega t) + \frac{1}{2\tau\Omega} \sin(\Omega t)\right) & \text{for } \Omega \neq 0 \\ \exp\left[-\frac{t}{2\tau}\right] \left(1 + \frac{t}{2\tau}\right) & \text{for } \Omega = 0 \end{cases} \quad (13)$$

$$\Omega = \sqrt{c/\tau - 1/4\tau^2}$$

**Note:** VAF is for one mode Prony series approx. without any conservative force terms.

# Comparison of Numerical Schemes - Results

**Observation:** Explicit Euler scheme produces wrong results for the Normalized VAF as when compared to the Splitting scheme (*Reason: Independent updates for  $X(t)$  and  $V(t)$  when using Explicit Euler scheme.*)

**Solution:** Using the Splitting scheme as the preferred integration scheme for all proceeding cases.

numerical experiments (and SA).

# Harmonic Potential Well

## Harmonic Potential Well GLE

$$d\mathbf{V}(t) = \underbrace{-\omega_0^2 \mathbf{X}(t)}_{\text{Conservative Force}} dt - \underbrace{\int_0^t \frac{\gamma_\lambda}{\Gamma_0(1-\lambda)} (t-s)^{-\lambda} \mathbf{V}(s) ds dt + \mathbf{M}^{-1} \mathbf{F}^r(t) dt}_{\substack{\text{Power Law decay} \\ \text{memory kernel} \\ \text{function}}} \quad (14)$$

## Question?

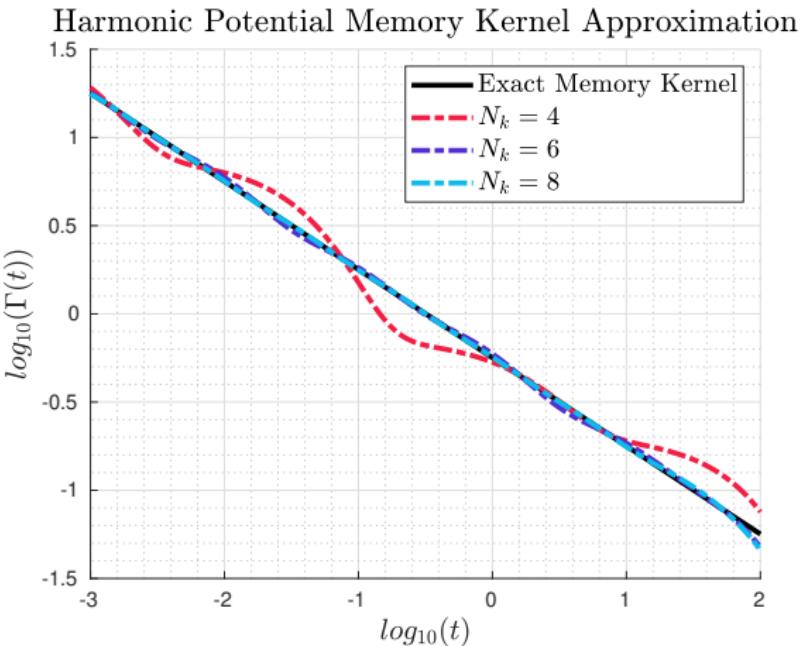
Approximation of the memory kernel in Equation (14) using Prony series

## Answer:

*log-spaced values for  $\tau_k$  from  $\Delta t/10$  to  $10N_t\Delta t$  and then linearly fitting  $c_k$  using least squares regression i.e.*

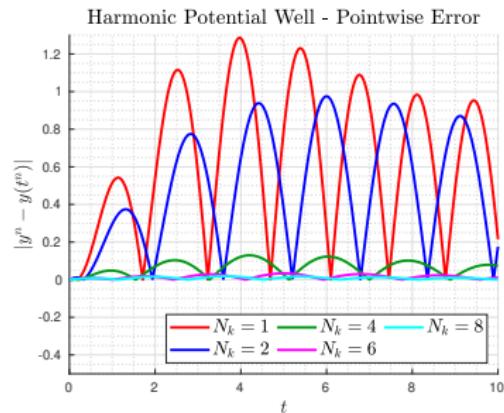
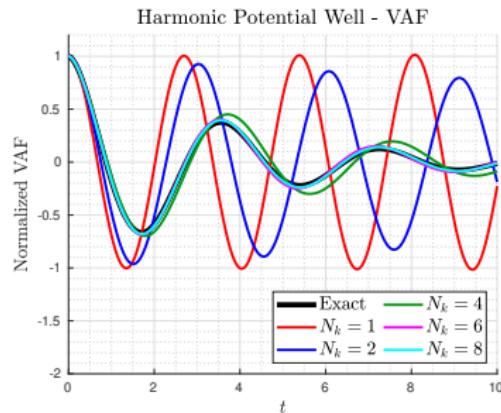
$$\min_{\mathbf{x}} \|\mathbf{A} \cdot \mathbf{x} - \mathbf{b}\|^2, \quad \mathbf{x} = \{c_k\} \quad \forall k = 1, \dots, N_k$$

# Harmonic Potential Well - Parameter Fitting



**Figure:** A Prony series fit of the *power law* memory kernel in eq. (14) for  $\gamma\lambda = 1$ ,  $\lambda = 0.5$  for different  $N_k$

## Harmonic Potential Well - Normalized VAF & Pointwise Error



(a) Normalized VAF at different times for different no. of modes used in Prony series approximation

(b) Pointwise error in VAF at different times for different no. of modes used in Prony series approximation

**Figure:** Approximation of the Harmonic Potential Well problem for  $\gamma_\lambda = 1$ ,  $\lambda = 0.5$  and  $\omega_0 = 1.4$  using Prony series approximation

# Harmonic Potential Well - Normalized VAF & Pointwise Error

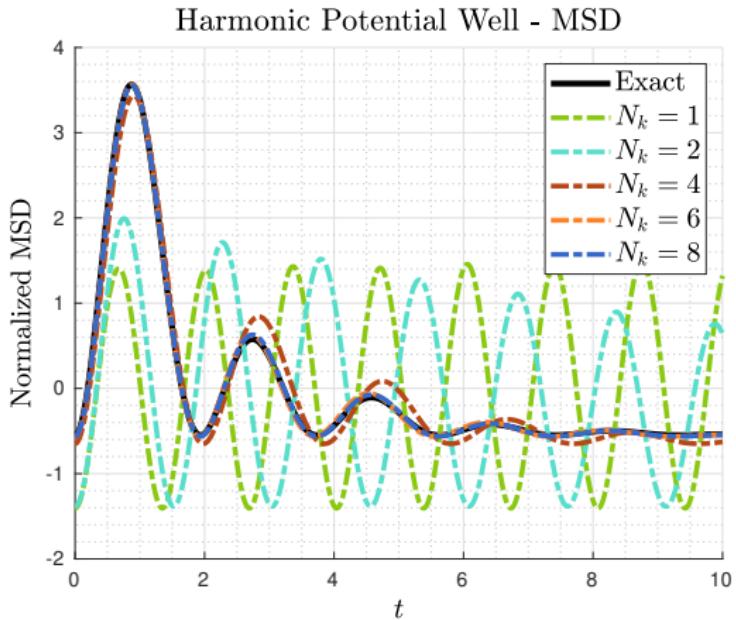
## Normalized VAF - Exact Solution

$$\underbrace{C_V(t)}_{\text{Normalized VACF}} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} (\omega_0 t)^{2k} \mathcal{E}_{2-\lambda, 1+\lambda k}^{(k)} (-\gamma_\lambda t^{2-\lambda})$$

where  $\mathcal{E}_{\alpha, \beta}^{(k)}(y)$  represents the  $k^{\text{th}}$  derivative of the *Generalized Mittag-Leffler function* given by:

$$\mathcal{E}_{\alpha, \beta}^{(k)}(y) = \sum_{j=0}^{\infty} \frac{(j+k)! y^j}{j! \Gamma_0(\alpha(j+k)+\beta)}$$

# Harmonic Potential Well - Normalized MSD



**Figure:** Normalized MSD at different times for different no. of modes used in Prony series approximation. ( $\gamma_\lambda = 1$ ,  $\lambda = 0.5$  and  $\omega_0 = 1.4$ )

# Harmonic Potential Well - Normalized MSD

## Normalized MSD - Exact Solution

$$\underbrace{\left\langle [\mathbf{X}(t + \tau) - \mathbf{X}(t)]^2 \right\rangle}_{\text{Normalized MSD}} = \frac{2k_B T}{m} I(\tau) - 2x_0 v_0 \omega_0^2 [G(t + \tau) - G(t)] [I(t + \tau) - I(t)] \\ + \left( v_0^2 - \frac{k_B T}{m} \right) [G(t + \tau) - G(t)]^2 \\ + \omega_0^2 \left( x_0^2 \omega_0^2 - \frac{k_B T}{m} \right) [I(t + \tau) - I(t)]^2$$

$$I(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \omega_0^{2k} t^{2(k+1)} \mathcal{E}_{2-\lambda, 3+\lambda k}^{(k)} (-\gamma_\lambda t^{2-\lambda}) \quad (\text{Kernel integral})$$

$$G(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \omega_0^{2k} t^{2k+1} \mathcal{E}_{2-\lambda, 2+\lambda k}^k (-\gamma_\lambda t^{2-\lambda}) \quad (\text{Relaxation function})$$

where  $v_0, x_0$  represent the velocity and position of the particles at time  $t = 0$ .

# Sensitivity Analysis

## Inference:

- Devised an integration scheme that is able to conserve first and second moments of  $V(t)$  and  $X(t)$  (Observables for understanding the behavior of physical systems.)
- Adequately able to approximate exact memory kernel using finite no. of modes of Prony series.

## Question?

Why

Need for performing sensitivity analysis

## Answer:

- Extended variable GLE fitted by matching MSD or VAF obtained from experimental data ~~to~~ Prony series parameters  $c_k, \tau_k, N_l$  sensitive to experimental data i.e. to errors in measurement or lack of data.
- *Ergodicity breaking:* Time averaged statistics such as MSD do not converge to ensemble averages.  
IE a large "spread" is observed

Further, how can one decide on  $N_k$

# ~~Sensitivity Analysis~~

What tools are available for local sensitivity analysis?

## Sensitivity Analysis

Let  $\mathcal{S}(t, \theta; f)$  denote the sensitivity of the stochastic process  $\mathbf{X}_t(\theta)$  where  $\theta$  is a parameter that affects the stochastic process and  $f$  is the given observable. We are interested in calculating:

$$\mathcal{S}(t, \theta; f) = \frac{\partial \mathbb{E}[f(\mathbf{X}_t(\theta))]}{\partial \theta}$$

## Methods of Calculation:

- *Finite Difference Stencils*: Approximating derivative by a finite difference stencil and obtain the required moments by Monte Carlo.
- *Likelihood Ratio*: Expressing sensitivity as an expectation of  $f$  under a change of measure.
- *Malliavin Calculus*: Extension of calculus of variations to stochastic processes.

# ~~Methods for calculating sensitivity~~

## Finite Difference Stencil

$$\mathcal{S}_\varepsilon(t, \theta; f) = \frac{\mathbb{E}[f(\mathbf{X}_t(\theta + \varepsilon))] - \mathbb{E}[f(\mathbf{X}_t(\theta))]}{\varepsilon}$$

## Likelihood Estimator

$$\begin{aligned}\mathcal{S}_{LR}(t, \theta; f) &= \frac{\mathbb{E}[f(\mathbf{X}_t(\theta))]}{\partial \theta} = \int f(x_t) [\partial_\theta \log g(\theta, x_t)] g(\theta, x_t) dx_t \\ &= \mathbb{E}[f(\mathbf{X}_t(\theta)) \partial_\theta \log g(\theta, \mathbf{X}_t)]\end{aligned}$$

where  $g$  represents the change in measure by a p.d.f.  **$g$  is unknown  $\Rightarrow$  difficulty in calculating sensitivity using likelihood estimator**

and not possible for c\_k, tau\_k appearing in drift + diffusion as there is no appropriate change of measure on path space

## Malliavin Calculus

$$\mathcal{S}_M(t, \theta; f) = \mathbb{E} \left[ f(\mathbf{X}_T) h \left( \{\mathbf{X}_s\}_{0 \leq s \leq T} \right) \right]$$

where  $h(\cdot)$  represents the Malliavin weights.  **$h(\cdot)$  is computationally expensive to calculate.**

$h$  is not unique. Is it possible to find  $h$ ?

## Sensitivity Estimators using Finite Difference Stencils

To find a reduced variance sampling strategy for calculating sensitivity (since that is the method we are left with) ...

**Objective:** To calculate the sensitivity of the stochastic process efficiently using finite difference stencils ~~X~~ right sampling strategy to reduce variance.

**Methodology:** Let  $\hat{\phi}(\theta)$  represent the expected value of the observable  $f(\mathbf{X}_t(\theta))$ . Then we can write,

$$\hat{\phi}(\theta) = M^{-1} \sum_{i=1}^M f(X_{i,t}(\theta)) \Rightarrow S_\varepsilon(t, \theta; \hat{\phi}) \approx \Delta_c(M, \varepsilon) = \frac{\hat{\phi}(\theta + \varepsilon) - \hat{\phi}(\theta - \varepsilon)}{2\varepsilon}$$

where each random variable is sampled independently of each other.

$$\begin{aligned} \Rightarrow \text{Var}[\Delta_c] &= \varepsilon^{-2} \text{Var} [\hat{\phi}(\theta + \varepsilon) - \hat{\phi}(\theta - \varepsilon)] \\ &= \varepsilon^{-2} M^{-1} \text{Var} \left[ \underbrace{f(\mathbf{X}_t(\theta + \varepsilon))}_{R_1} - \underbrace{f(\mathbf{X}_t(\theta - \varepsilon))}_{R_2} \right] \end{aligned}$$

where the variance can be rewritten as

$$\text{Var}[\Delta_c] = \varepsilon^{-2} M^{-1} (\text{Var}[R_1] + \text{Var}[R_2] - 2\text{Cov}[R_1, R_2])$$

## Sensitivity Estimators using Finite Difference Stencils

*Statistical Error* is given by  $\epsilon_M = \frac{C_\alpha \sigma}{\sqrt{M}}$  where  $\sigma = \sqrt{\text{Var}[\Delta_c]}$  and  $C_\alpha$  is a constant based on the confidence level of the solution

### Coupled vs. Decoupled Noise:

- If  $R_1$  and  $R_2$  are not correlated, then  $\text{Var}[\Delta_c] = \mathcal{O}(\varepsilon^{-2} M^{-1})$
- If  $R_1$  and  $R_2$  are positively correlated, then  $\text{Var}[\Delta_c] = \mathcal{O}(M^{-1})$

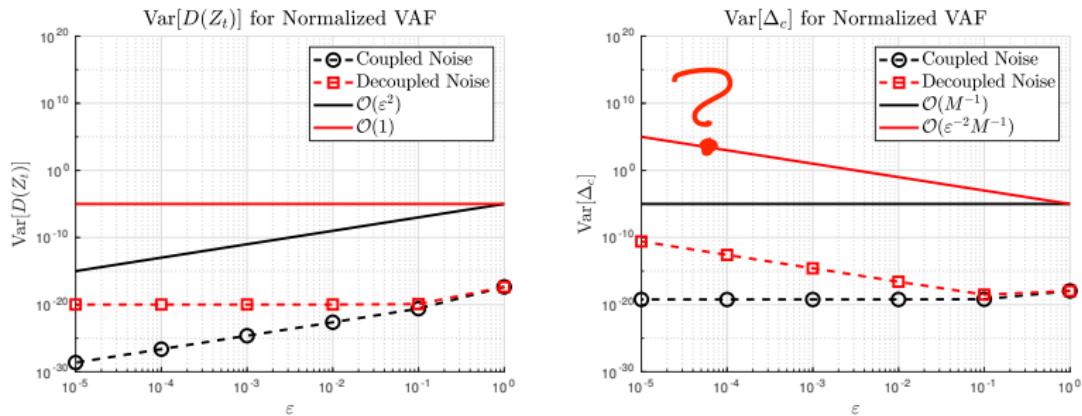
### Observation:

Let  $\varepsilon = 0.1$ . In order to reduce the error by a factor of 10.

- *Coupled Noise*:  $M = 10^4$  samples
- *Decoupled Noise*:  $M = 10^2$  samples

Hence the statistical error becomes independent of the perturbation parameter on using a common random path coupling i.e.  $R_1$  and  $R_2$  use the same Wiener process  $dW$ .

# Sensitivity Analysis - Results

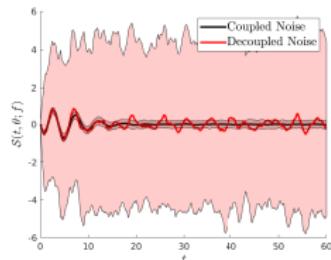


**(a)**  $\text{Var}[D(Z_t)]$  for Normalized VAF where  
 $D(Z_t) = (\hat{f}(\theta + \varepsilon) - \hat{f}(\theta - \varepsilon))$

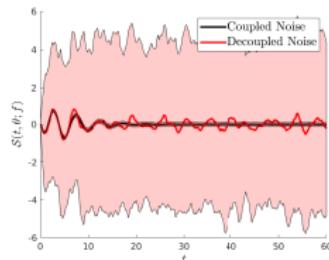
**(b)**  $\text{Var}[\Delta_c]$  for Normalized VAF where  
 $\Delta_c = (\hat{\phi}(\theta + \varepsilon) - \hat{\phi}(\theta - \varepsilon)) / 2\varepsilon$

**Figure:** Order of variance reduction when using *Coupled* vs. *Decoupled* noise term on perturbing  $c_1$ . ( $M = 200, \delta t = 0.1, N_p = 1000$ )

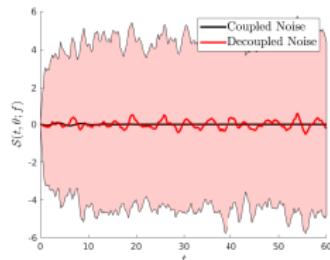
# Sensitivity Analysis - Results



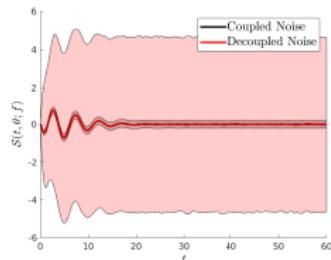
(a)  $S_\varepsilon(t, c_1; \text{VAF})$ ,  $M = 10^2$



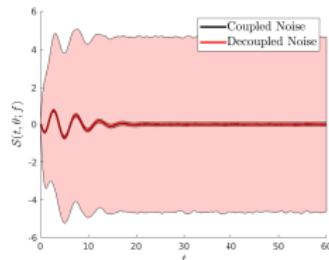
(b)  $S_\varepsilon(t, c_3; \text{VAF})$ ,  $M = 10^2$



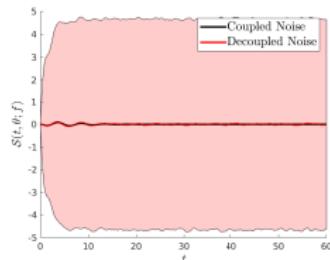
(c)  $S_\varepsilon(t, c_6; \text{VAF})$ ,  $M = 10^2$



(d)  $S_\varepsilon(t, c_1; \text{VAF})$ ,  $M = 10^4$



(e)  $S_\varepsilon(t, c_3; \text{VAF})$ ,  $M = 10^4$



(f)  $S_\varepsilon(t, c_6; \text{VAF})$ ,  $M = 10^4$

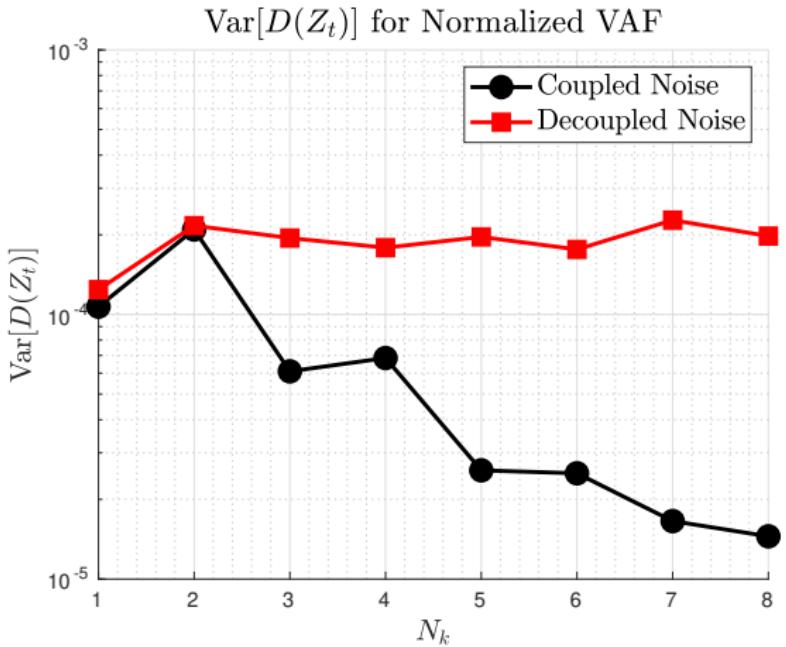
*Local*

**Figure:** Sensitivity of solution due to perturbation of  $c$  ( $\varepsilon = 0.01, \omega_0 = \frac{8}{9}, k_B T = 10^{-5}$ )

These plots of the Sensitivity Indices are nice. Could you calculate a ranking? That would be an interesting bar chart to add. That is,  $r_i = \text{SI\_parameter}_i / \sum_j \text{SI\_parameter}_j$

# ~~Sensitivity Analysis~~ Results

A global sensitivity analysis result.



**Figure:**  $\text{Var}[D(Z_t)]$  where the difference in solution,  $D(Z_t)$ , is between the nominal model with  $N_k = n$  and the perturbed model with  $N_k = n + 1$  where  $n = 1, \dots, 8$  ( $\omega_0 = 8/9, k_B T = 10^{-5}, t = 100$ ) •

# Conclusion

## Extended Variable GLE:

- Non-Markovian GLE problem converted to Markovian extended variable GLE problem using Prony series approximation.
- Explicit Euler scheme does not conserve 1<sup>st</sup> and 2<sup>nd</sup> moments of  $\alpha(t)$  and  $v(t)$  unlike Splitting scheme.
- Number of modes used in Prony series approximation affects the memory kernel fit.

## Sensitivity Analysis:

- Significant reduction in variance of the calculated sensitivity on using a common coupled random path for the diffusion term of GLE.
- Order of variance reduction for  $D(Z_t)$  was observed to be  $\mathcal{O}(\varepsilon^2)$  for coupled noise and  $\mathcal{O}(1)$  for decoupled noise.
- Order of variance reduction for  $\Delta_c$  was observed to be  $\mathcal{O}(M^{-1})$  for coupled noise and  $\mathcal{O}(\varepsilon^{-2}M^{-2})$  for decoupled noise.

I would add one more slide: Outlook. In it, put some ideas you have for things that you would investigate if you have more time. Think of it as a 30 second pitch for what value you could add if someone offered you money to continue working on the project. In particular, Raul has HIWI money so it is good to keep your options open!

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