

Generalized Langevin Equation

Stochastic Differential Equations

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① Scope of the Project

② Introduction

③ Generalized Langevin Equation

Scope of the Project

What? Generalized Langevin Dynamics is a modeling technique that can be used to model anomalous diffusive phenomena observed in viscoelastic fluid 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.

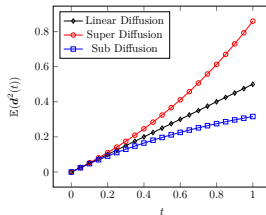


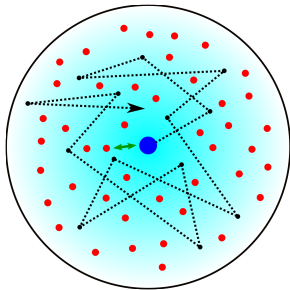
Figure: Anomalous Diffusion: Linear, Sub and Super Diffusive nature

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

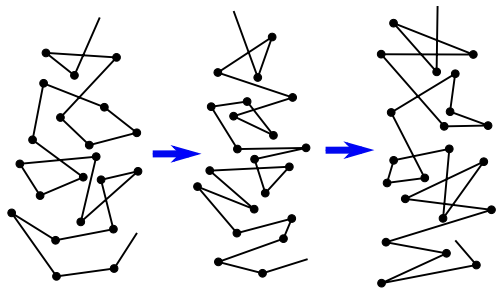
How? The theory behind extended variable GLD is studied. Accuracy of Implicit/Explicit Euler and Splitting Numerical schemes are also tested to find out the optimal scheme. Study the sensitivity of the solution to the changes in the parameters of the extended variable Prony series.

Introduction

Langevin Dynamics is a modeling technique in which the motion of a set of massive bodies in the presence of a bath of smaller solvent particles is directly integrated, while the dynamics of the solvent are "averaged out".



(a) Big particle interacting with the smaller particles.



(b) Evolution of a molecule over time due to interaction with smaller particles.

Generalized Langevin Equation

Mathematical Model

GLE equations are based on *Ornstein-Uhlenbeck* equations

GLE Equations

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

$$M d\mathbf{V}(t) = \mathbf{F}^c(\mathbf{X}(t))dt - \int_0^t \Gamma(t-s)\mathbf{V}(s)dsdt + \mathbf{F}^r(t)dt \quad (2)$$

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

Temporally Non-Local Drag Force (\mathbf{F}^d)

$$\mathbf{F}^d(t) = - \int_0^t \Gamma(t-s)\mathbf{V}(s)dsdt \quad (4)$$

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Mathematical Model

$\mathbf{F}^c : \mathcal{R}^{dN_p} \rightarrow \mathcal{R}^{dN_p}$	Conservative Force
$\mathbf{F}^r : \mathcal{R}^{dN_p} \rightarrow \mathcal{R}^{dN_p}$	Random Correlated Force
M	Diagonal Mass Matrix
Γ	Memory Kernel

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

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 $\Gamma(t)$ be related as:

$$\langle \mathbf{F}_i^r(t+s), \mathbf{F}_j^r(t) \rangle = k_B T \Gamma(s) \delta_{ij}, \quad s \geq 0 \quad (5)$$

k_B	Boltzmann's Constant
δ_{ij}	Kronecker Delta

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Model Complications

Discrete Problem:

Solve for $\mathbf{X}(t)$ and $\mathbf{V}(t)$ at N_t uniformly spaced discrete points in time.

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

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

- ② Integration scheme to conserve moments of velocity.

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Extended Variable GLE