Generalized Langevin Equation

Stochastic Differential Equations

Sankarasubramanian Ragunathan

389851

RWTH Aachen

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: sub-diffusion and super-diffusion can be captured only with GLE as Langevin model fails. Move from GLE model to Extended Variable GLE to capture the diffusion phenomenon

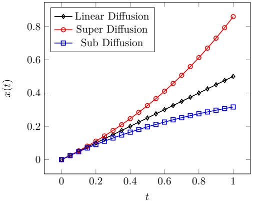

Figure: Anomalous Diffusion: Linear,Sub and Super Diffusive nature

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".

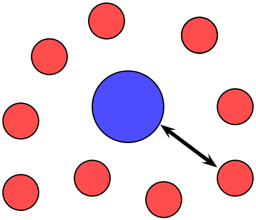

Figure: Big particle (Blue) being bombarded by smaller solvent particles (Red)

Generalized Langevin Equation

- GLE equations are based on *Ornstein-Uhlenbeck* equations
- Need to model memory kernel using extended variable methods like Prony series

GLE Equations

$$d\boldsymbol{q} = \boldsymbol{M}^{-1}\boldsymbol{p}dt \qquad d\boldsymbol{p} = -\nabla U(\boldsymbol{q})dt - \int_0^t \boldsymbol{\Gamma}(t-s)\boldsymbol{p}(s)ds dt + d\boldsymbol{B} \tag{1}$$

Initial Conditions

$$\boldsymbol{q}(0) = \boldsymbol{q}_0 \qquad \boldsymbol{p}(0) = \boldsymbol{p}_0 \tag{2}$$

Drag Force ($\boldsymbol{F}_d$) and Random Force $\boldsymbol{R}(t)$

$$\boldsymbol{F}_d = -\int_0^t \boldsymbol{\Gamma}(t-s)\boldsymbol{p}(s)ds dt \qquad d\boldsymbol{B} = \boldsymbol{R}(t)dt \tag{3}$$

$\boldsymbol{\Gamma}(t) = (\gamma_{ij}(t))$ is a $N_c \times N_c$ matrix-valued function of t which we refer to as the `memory kernel`.