Fractional Langevin Equation with a Reflecting Barrier

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Introduction

- Diffusion is ubiquitous throughout nature
- Normal diffusion: $\langle x^2 \rangle \sim t$
- Anomalous diffusion: $\langle x^2 \rangle \neq Dt$
- Applications:
  - amorphous semiconductors
  - financial market dynamics
  - RNA motion in E coli cells
- Anomalous diffusion is not well understood in confined geometries

What is the probability density of anomalous diffusion near a reflecting wall?

Approach

To answer our big question we are using:
- Fractional Langevin equation (FLE), standard model for anomalous diffusion with long time correlations
- Reflecting Wall
- Monte Carlo Simulations

Our results show that:
- Mean-square displacement shows expected anomalous diffusion behavior,
  $$\langle x^2 \rangle \sim t^{(2-\alpha)},$$
  as in the unconfined case.
- Probability density close to the wall shows highly non-Gaussian behavior.

Model

General Langevin equation (GLE) [1]:

$$m\frac{d^2x(t)}{dt^2} = -\bar{\gamma}\int_0^t \kappa(t-t')\,\frac{dx}{dt'}dt' + \xi(t)$$

Friction Term   Random Term

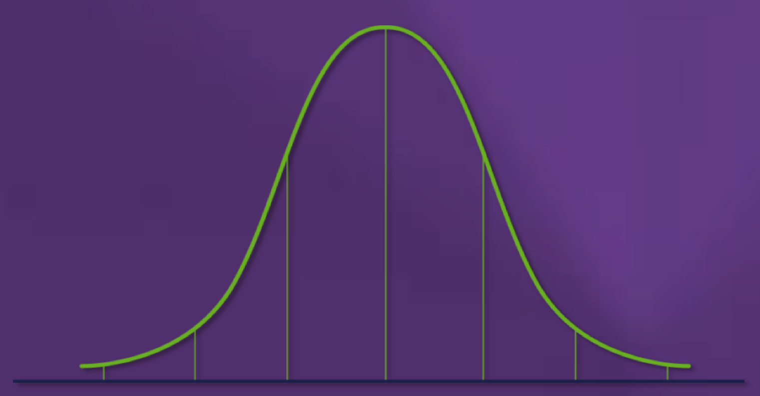
Definitions:
- x(t) - position over time
- κ - memory kernel
- λ - decay length
- α - anomalous diffusion exponent
- T - temperature

For FLE [1]:
$\xi(t) \rightarrow$ nonwhite Gaussian Noise

Gaussian mean:
$$\langle \xi(t) \rangle = 0$$

Gaussian correlation function:
$$\langle \xi(t)\xi(t') \rangle = \alpha(\alpha-1)t^{\alpha-2}$$

Equilibrium Condition:
$$\langle \xi(t)\xi(t') \rangle = k_B T \bar{\gamma}\kappa(t-t')$$



Standard Gaussian Distribution

Totally reflecting wall modeled by repulsive potential:

$$F_{wall} = F_0 e^{-\frac{x}{\lambda}}$$

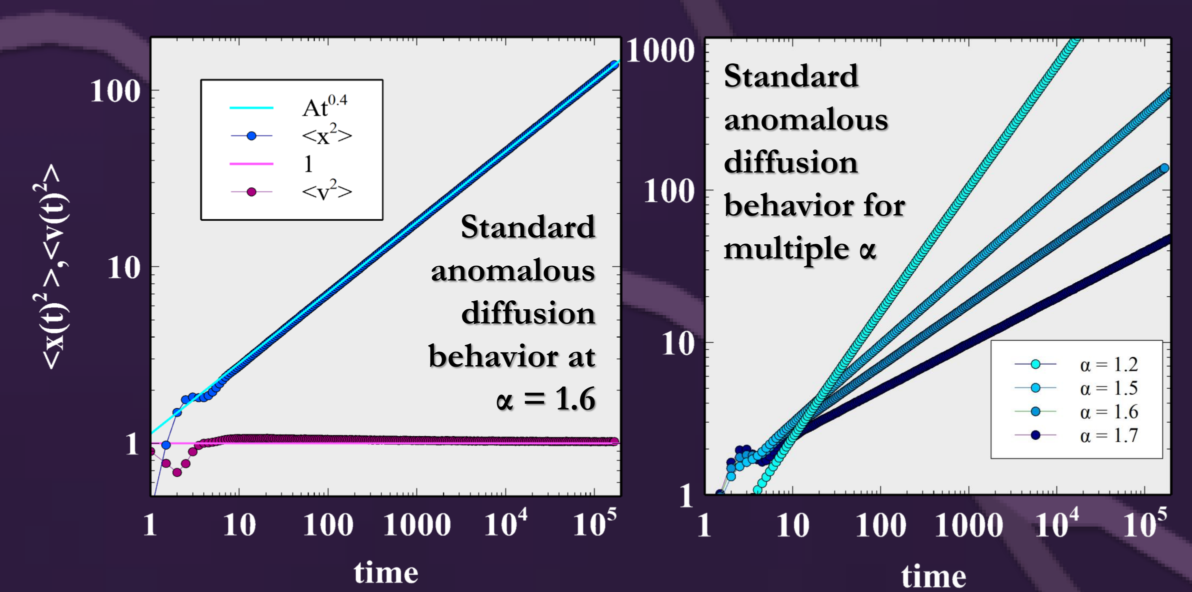
Numerical Methods

- Discretized time and gaussian noise
- Solved Caputo fractional derivative with L1 method variation [2]
- To reduce computation time, approximated friction term using Taylor series expansion

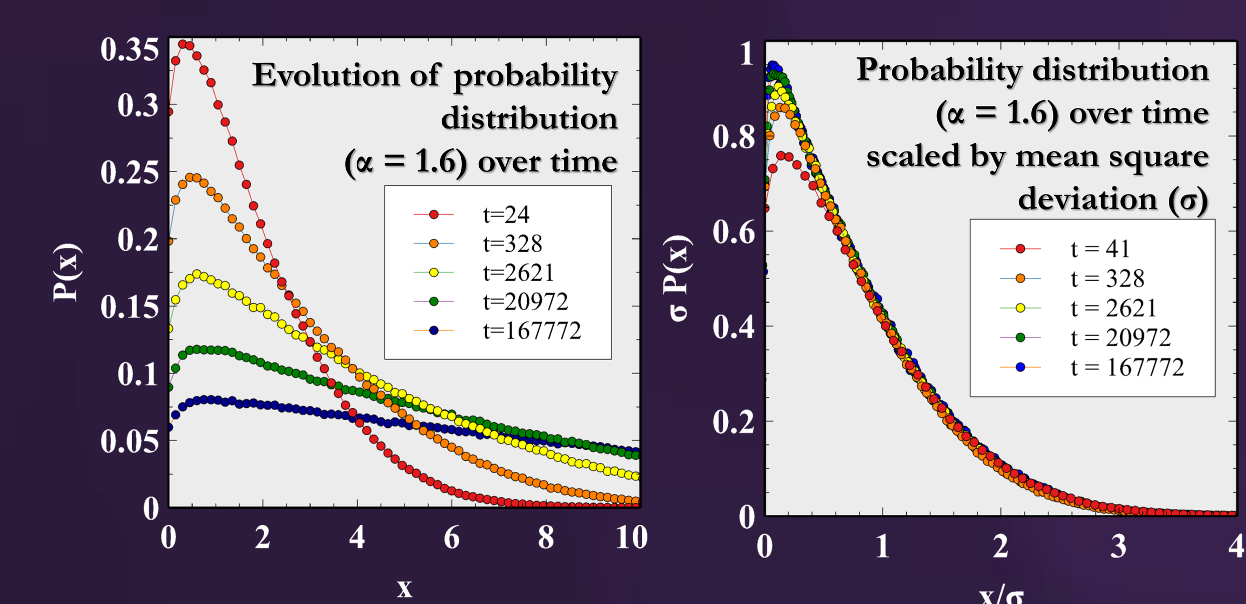
Simulation Parameters

- α = 1.2, 1.3, 1.4, 1.5, 1.6, 1.7
- Timestep size = 0.01
- Timesteps ⩽ 2^25
- Number of walkers ⩽ 10^6
- $\gamma = k_B T = m = 1$
- $F_0 = \lambda = 5$

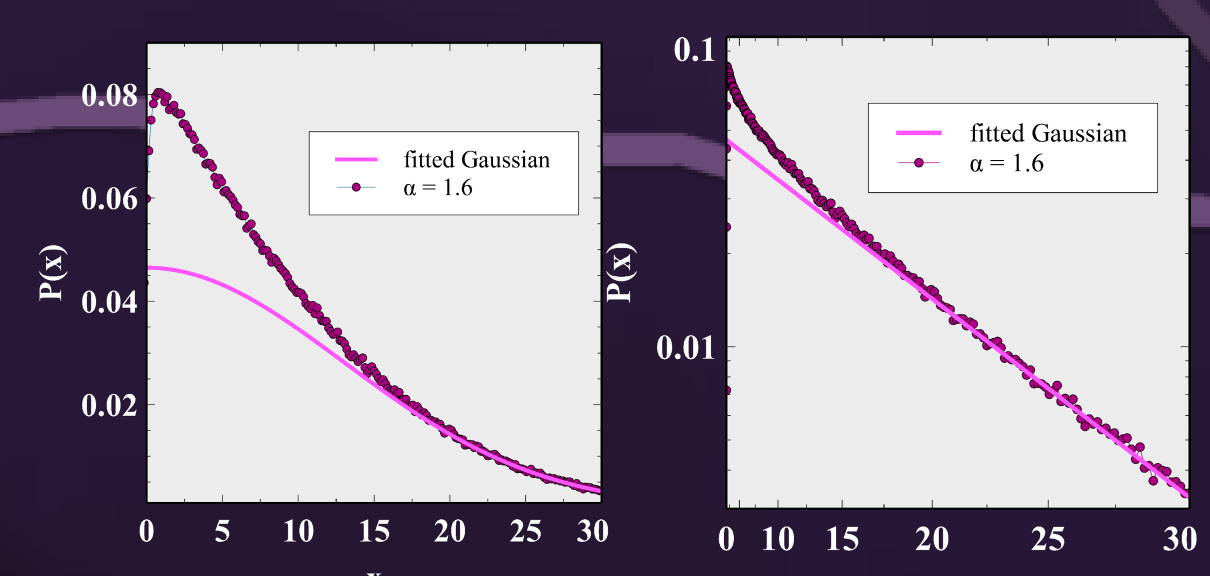
Results



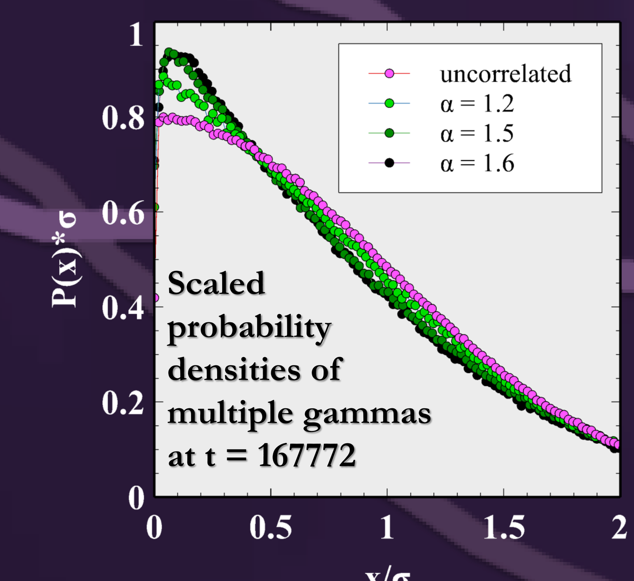
Long time behavior of mean square displacement and mean square velocity follows standard anomalous diffusion: $\langle x^2 \rangle \sim t^{2-\alpha}$ $\langle v^2 \rangle \sim 1$



Functional form of probability distribution of position x fulfills the scaling equation: $P(x) = \frac{1}{\sigma} Y\left(\frac{x}{\sigma}\right)$

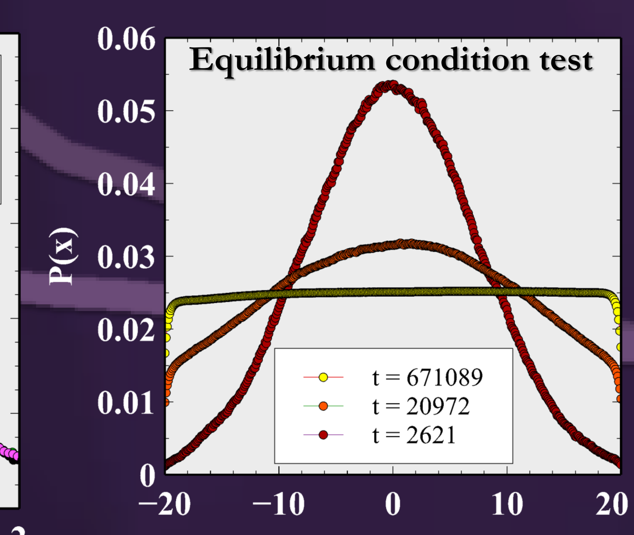


Probability density of position x (t = 167772, α = 1.6):
- Close to wall, highly non-gaussian behavior
- Far from wall, gaussian behavior



Scaled probability densities of multiple gammas at t = 167772

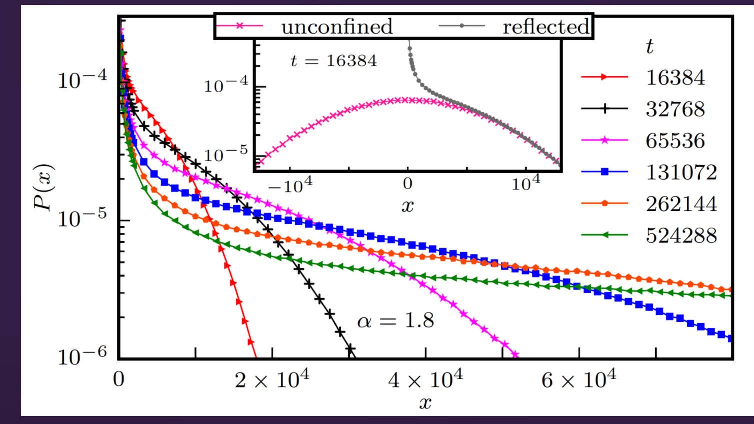
Deviations from Gaussian behavior (uncorrelated case) increases with increasing α



Probability distribution of position x on interval with a wall on either side to show the simulation does reach equilibrium in the infinite case

Discussion

- Average position and velocity show anomalous diffusion behaves as expected
- Average behaves as expected
- Probability densities show strong deviations from uncorrelated case
  - As alpha increased, deviation increased
- When we compare this to fractional Brownian motion (FBM) with a reflecting wall [3]:
  - Both lead to non-Gaussian behavior near the wall
  - For FBM, there's a power law divergence at the wall
  - For FLE, there's a cusp at the wall



References

[1] R. Kubo, Reports on Progress in Physics 29, 255 (1966).
[2] YN Zhang, ZZ Sun, HL Liao, Finite difference methods for the time fractional diffusion equation on non-uniform meshs, J Comput Phys 263 (2014)
[3] A.H.O. Wada and T. Vojta, Physics Review E 97, 0201012 (2018)

Special Thanks

This work is supported in part by the NSF under Grant No. DMR-1506152 and DMR-1828489.