Single Particle Tracking in Anomalous Diffusion Continuous and Trapped Random Walks

Stochastic Modelling and Simulations

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Outline

1. Introduction
2. Continuous Time Random Walk (CTRW)
3. Fractional Brownian Motion (FBM)
4. Ben Arous et al.: Randomly Trapped Random Walks (RTRW)
5. Comparative Analysis Simulations
6. Conclusion

Real-World Systems: Why Traps and Waiting Times?

Examples of systems with anomalous diffusion:

- **Intracellular Transport (e.g., proteins in cells)**
  Observed: Particles move through a crowded, heterogeneous environment.
  Model: CTRW (random waiting times), RTRW (site-specific traps)
- **Diffusion in Porous Media (e.g. rocks with pores)**
  Observed: A particle moves freely in some regions but gets trapped or slowed down in others.
  Model: RTRW — random trap times depending on location
- **Glassy Systems**
  Observed: Extremely slow, irregular dynamics as particles hop between energy wells
  Model: CTRW — power-law waiting times mimic metastable states

Key phenomena captured: Subdiffusion, aging, weak ergodicity breaking, non-Markovian behavior

Motivation Context

- Single-particle tracking provides the trajectories of individual particles.
- Jean Baptiste Perrin's experiments to prove Einstein's work on Brownian motion is an example of Single-particle tracking.
- We have seen that standard Brownian motions is characterised by the following.
    - Continuous trajectories, and independent stationary Gaussian increments: $X(t) - X(s) \sim \mathcal{N}(0, \sigma^2|t-s|)$.
    - **Mean Displacement:** $\langle X(t) \rangle = 0$ *(Zero drift)*
    - **Mean Squared Displacement (MSD):** $\langle r^2(t) \rangle = 2dDt$ *(Linear in t)*
    - **Variance:** $\mathrm{Var}(X(t)) = \langle X(t)^2 \rangle - \langle X(t) \rangle^2 = 2dDt$

We characterise atypical particle movements by experiencing subdiffusion (sublinear MSD) or superdiffusion (exponential with time), or by exhibiting ergodicity breaking.

Therefore, we need to tweak our model!

Classical Diffusion v.s Anomalous Diffusion

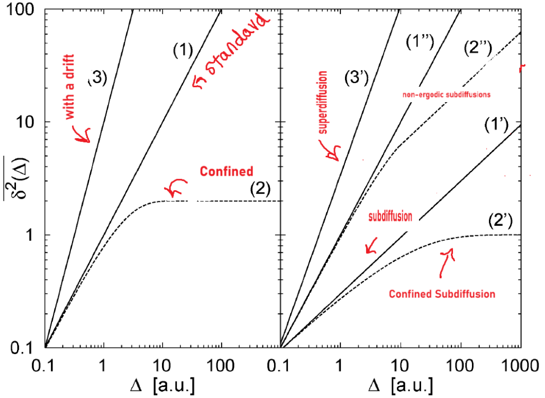


Figure: Reference [1]

Left: Classical diffusion behaviors.
(1) $\overline{\delta^2(\Delta)} \sim \Delta$.
(2) A chnage from $\overline{\delta^2(\Delta)} \sim \Delta$ to a constant.
(3) Drift diffusion: $\overline{\delta^2(\Delta)} \sim \Delta^2$.

Right: Anomalous diffusion.
(1') Subdiffusion: $\overline{\delta^2(\Delta)} \sim \Delta^\alpha$, $\alpha < 1$.
(2') Restricted subdiffusion turning over from $\overline{\delta^2(\Delta)} \sim \Delta^\alpha$ to a constant.
(1'') Non-ergodic subdiffusion: linear.
(2'') Restricted non-ergodic subdiffusion turning over from a linear to $\overline{\delta^2(\Delta)} \sim \Delta^{1-\alpha}$.
(3') Superdiffusion: $\overline{\delta^2(\Delta)} \sim \Delta^{1+\alpha}$.

MSD and Ergodicity in Single Particle Tracking

Mean Squared Displacement (MSD)

- **Ensemble MSD:**

$$\langle r^2(t)\rangle = \int r^2 P(r,t)\, d^3 r$$

- **Time-averaged MSD:**

$$\overline{\delta^2(\Delta;T)} = \frac{1}{T-\Delta}\int_0^{T-\Delta} [r(t+\Delta) - r(t)]^2 dt$$

Ergodicity: A process is ergodic if:

$$\lim_{T\to\infty} \overline{\delta^2(\Delta;T)} = \langle r^2(\Delta)\rangle$$

Observation:

- Brownian motion and FBM are ergodic.
- CTRW (with heavy-tailed waiting times) exhibits **weak ergodicity breaking**.

Biological Observations of Subdiffusion

Anomalous diffusion:

$$\langle r^2(t) \rangle \sim t^\alpha \quad \text{with} \quad 0 < \alpha < 1$$

Typical exponents from experiments:

- **mRNA in E. coli:** $\alpha \approx 0.7$–0.8
- **DNA loci:** $\alpha \approx 0.4$
- **Telomeres:** $\alpha \approx 0.3$–0.5
- **Viruses/lipid granules:** $\alpha \approx 0.5$–0.9

Conclusion: Classical models (Brownian motion) are insufficient — we need new stochastic models.

Continuous Time Random Walks

Definition:

- A random walk with *random waiting times* between jumps, so the position at time t:
  $X(t) = \sum_{i=1}^{N(t)} \xi_i$ where $N(t) = \max\{n : \sum_{i=1}^{n} \tau_i \leq t\}$
- Described by two PDFs:
  - $\xi_i \sim \psi(x)$: Jump length distribution
  - $\tau_i \sim \phi(t)$: Waiting time distribution

Anomalous behavior emerges when:

- $\phi(t) \sim t^{-(1+\alpha)}$ with $0 < \alpha < 1$ Leads to subdiffusion: $\langle r^2(t) \rangle \sim t^{\alpha}$.
- Waiting time survival probability: $\Psi(t) = \int_t^{\infty} \phi(t') dt'$ leading to trapping.
- Ergodicity breaking: $\overline{\delta^2(\Delta, T)} \neq \langle r^2(t) \rangle$

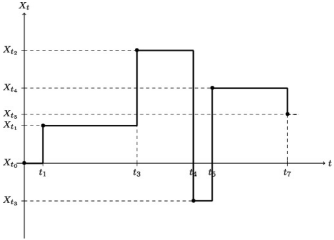
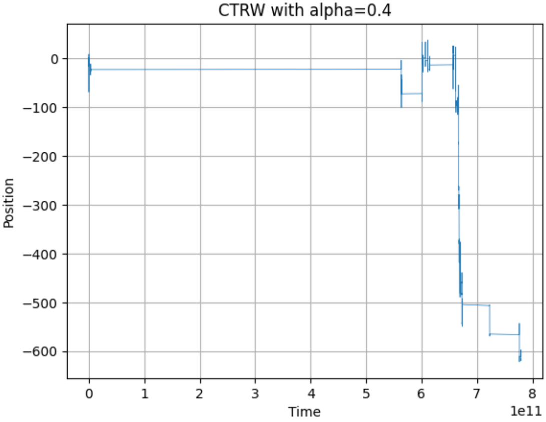
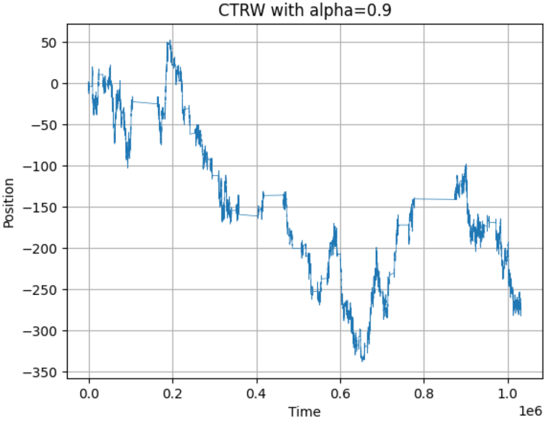


Figure: Reference [3]

Simulation



CTRW with alpha=0.4
Position
Time
1e11
0
−100
−200
−300
−400
−500
−600
0
1
2
3
4
5
6
7
8



CTRW with alpha=0.9
Position
Time
1e6
50
0
−50
−100
−150
−200
−250
−300
−350
0.0
0.2
0.4
0.6
0.8
1.0

Time-Averaged MSD

Definition: Time-averaged mean squared displacement (TAMSD)

$$\overline{\delta^2(\Delta; T)} = \frac{1}{T-\Delta} \int_0^{T-\Delta} [x(t+\Delta) - x(t)]^2 \, dt$$

Ensemble average:

$$\left\langle \overline{\delta^2(\Delta; T)} \right\rangle = \frac{1}{T-\Delta} \int_0^{T-\Delta} \left\langle [x(t+\Delta) - x(t)]^2 \right\rangle dt$$

Relation to Number of Jumps

In processes with discrete jumps:

$$\left\langle [x(t+\Delta) - x(t)]^2 \right\rangle = \langle \delta x^2 \rangle \cdot n(t, t+\Delta)$$

where:

- $\langle \delta x^2 \rangle$ = variance of single jump
- $n(t, t+\Delta)$ = average number of jumps in interval $[t, t+\Delta]$

Brownian Motion

- Constant jump rate: $n(t, t+\Delta) = \Delta/\langle\tau\rangle$
- TAMSD becomes:

$$\left\langle \overline{\delta^2(\Delta; T)} \right\rangle = \frac{\langle \delta x^2 \rangle}{\langle \tau \rangle} \Delta = 2K_1 \Delta$$

- Consistent with ensemble MSD: **ergodic behavior**

CTRW Subdiffusion

- Waiting times: $\psi(\tau) \sim \tau^{-1-\alpha}$, with $0 < \alpha < 1$
- Number of jumps up to t: $n(0, t) \sim t^{\alpha}$
- Then:

$$n(t, t+\Delta) \approx \alpha t^{\alpha-1}\Delta$$

- TAMSD scales as:

$$\left\langle \overline{\delta^2(\Delta; T)} \right\rangle \sim \frac{\Delta}{T^{1-\alpha}}$$

Aging and Ergodicity Breaking

- TAMSD has **linear** dependence on Δ, like Brownian motion
- But effective diffusion constant decays:

$$K_{\text{eff}}(T) \sim T^{\alpha-1}$$

- Process becomes **slower with time**: aging
- **Weak ergodicity breaking**:

$$\left\langle \overline{\delta^2} \right\rangle \neq \langle x^2(t) \rangle$$

CTRW vs. Brownian Motion: Visual Comparison

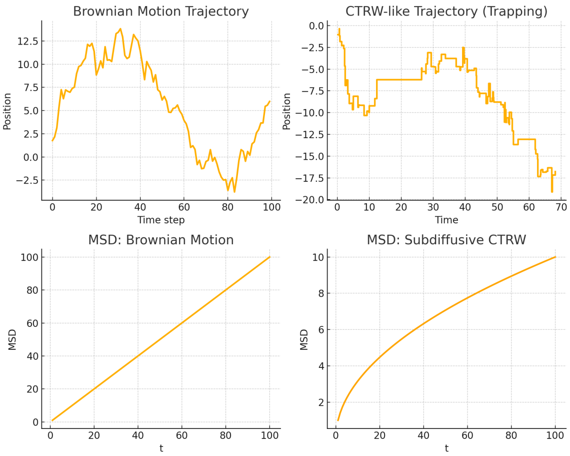


Figure: Up: BM (regular step intervals) V.S CTRW (random waiting jumps)
Down: $\mathrm{MSD}(t) \sim t$ V.S. $\mathrm{MSD}(t) \sim t^{\alpha}$, $\alpha < 1$

Fractional Brownian Motion (FBM)

Introduced by B. Mandelbrot and J. Van Ness (1968) as a generalization of Brownian motion to account for long-range dependence.

Definition: FBM $B_H(t)$ is a Gaussian process with:

$$\mathbb{E}[B_H(t)] = 0, \quad \mathbb{E}[B_H(t)B_H(s)] = \frac{1}{2}\left(t^{2H} + s^{2H} - |t-s|^{2H}\right)$$

where $H \in (0,1)$ is the Hurst exponent.

Key Features:

- Stationary increments: $x(t+\Delta) - x(t) \sim \mathcal{N}(0, \Delta^{2H})$
- **Hurst exponent:** $H = \alpha/2$, controls correlation.
- **MSD:** $\langle x^2(t) \rangle \sim t^{2H}$
- **Correlated increments:**
  - $H > 0.5$: persistent (superdiffusion)
  - $H < 0.5$: anti-persistent (subdiffusion)
  - $H = 0.5$: classical Brownian motion

FBM and Fractional Gaussian Noise

FBM solves the Langevin equation:

$$\frac{dx(t)}{dt} = \xi_\alpha(t), \quad x(t) = \int_0^t \xi_\alpha(t')dt'$$

where $\xi_\alpha(t)$ is **fractional Gaussian noise (fGn)**:

$$\langle \xi_\alpha(t_1)\xi_\alpha(t_2) \rangle = \alpha K_\alpha^*(\alpha - 1)|t_1 - t_2|^{\alpha-2}$$

Interpretation:

- **Anti-correlation:** for $\alpha < 1$, noise reverses direction — "trapping" effect
- Unlike CTRW, FBM has **no jumps** and is **ergodic**.
- Diffusion is **smooth and continuous** but not Markovian.
- Unlike BM, noise is not white: system has **long-term memory**.

BM, CTRW, and FBM

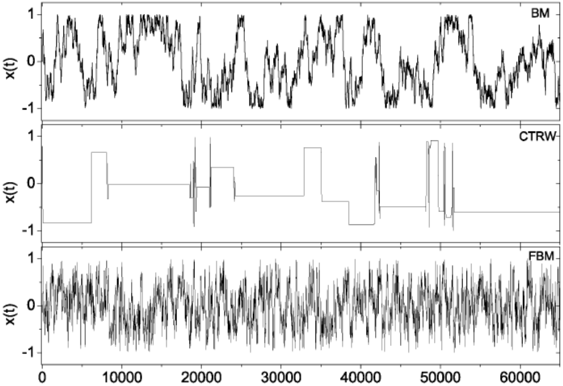


Figure: Brownian motion (top), CTRW (middle), and FBM (bottom).Reference [1]

FBM: Time-Averaged MSD Ergodicity

Time-Averaged MSD ($\overline{\delta^2(\Delta, T)}$) For FBM:

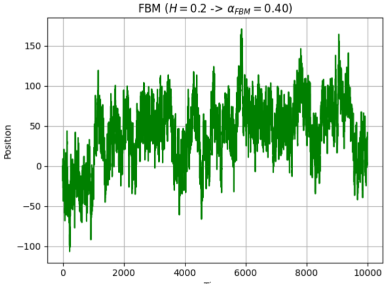
$$\langle\overline{\delta^2(\Delta, T)}\rangle = \sigma^2\Delta^{2H} = \sigma^2\Delta^{\alpha}$$

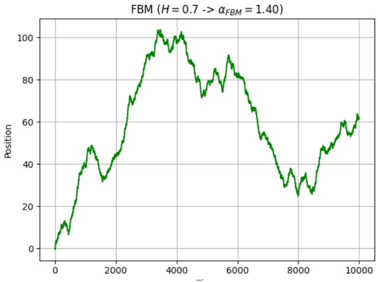
The time-averaged MSD directly reflects the anomalous exponent.
Ergodicity
FBM is an ergodic process.

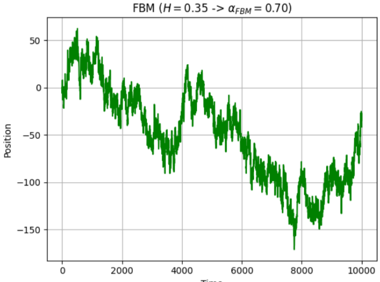
$$\overline{\delta^2(\Delta, T)} \xrightarrow{T\to\infty} \langle B_H(\Delta)^2\rangle$$

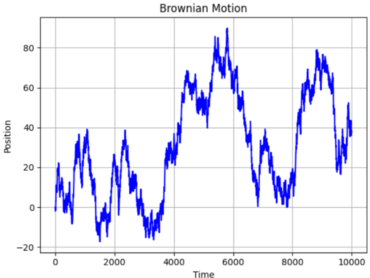
However, convergence can be algebraically slow, especially for $H \neq 1/2$. Scatter in TA-MSD for finite T is much smaller than for CTRW.

Simulation


FBM ($H = 0.2$ -> $\alpha_{FBM} = 0.40$)
Position
150
100
50
0
−50
−100
0
2000
4000
6000
8000
10000


FBM ($H = 0.7$ -> $\alpha_{FBM} = 1.40$)
Position
100
80
60
40
20
0
0
2000
4000
6000
8000
10000


FBM ($H = 0.35$ -> $\alpha_{FBM} = 0.70$)
Position
50
0
−50
−100
−150
0
2000
4000
6000
8000
10000


Brownian Motion
Position
80
60
40
20
0
−20
0
2000
4000
6000
8000
10000
Time

RTRW: Generalizing Trapping Models

Motivation CTRW is a specific instance of trapping. RTRW provides a much wider class.

The Model

- Consider a graph $G = (V, E)$.
- **Trapping Landscape:** A collection $\pi = (\pi_x)_{x \in V}$ of probability measures on $(0, \infty)$.
- π_x is the distribution of random trapping/sojourn duration at vertex x.
- Particle stays at x for a duration sampled from π_x, then moves to a random neighbor. New duration sampled if x is revisited.
- **Random Trapping Landscape:** The collection $(\pi_x)_{x \in V}$ is itself an i.i.d. sample from a distribution P on the space of probability measures. This introduces an extra layer of randomness.

RTRW: Scaling Limits on $\mathbb{Z}$

The paper focuses on RTRW on $G = \mathbb{Z}$. **Classification Theorem (Thm 2.8)** If $X_t^\epsilon = \epsilon X_{\rho(\epsilon)^{-1}t}$ converges to a non-trivial limit U_t as $\epsilon \to 0$:

1. If $\rho(\epsilon) = \epsilon^2 L(\epsilon)$ (L slowly varying), then U_t is a scaled Brownian Motion.
2. If $\rho(\epsilon) = \epsilon^\alpha L(\epsilon)$ with $\alpha > 2$, then U_t is an **FK-SSBM mixture**.

- **Fractional Kinetics (FK) Process:** $Z_t^\alpha = B_{\psi_t^\alpha}$, where B is BM and ψ_t^α is the inverse of an α-stable subordinator.

RTRW: Example - Transparent Traps

Model Setup

At site x, trap of "depth" τ_x (i.i.d., $P(\tau_0 > u) \sim u^{-\alpha_0}$). Particle is trapped for time τ_x with probability $\tau_x^{-\beta}$, otherwise stays for unit time (trap is "transparent"). The trapping measure is $\pi_x = (1 - \tau_x^{-\beta})\delta_1 + \tau_x^{-\beta}\delta_{\tau_x}$. (Paper uses δ_0 for simplicity in some calculations for unit time).

Rich Phase Diagram (Theorem 3.2)

Depending on $\alpha_0 + \beta$:

- If $\alpha_0 + \beta > 1$: Converges to Brownian Motion.
- If $\alpha_0 + \beta < 1$ and $\alpha_0 > \beta$: Converges to FIN diffusion.
- If $\alpha_0 + \beta < 1$ and $\alpha_0 < \beta$: Converges to FK process.
- If $\alpha_0 + \beta < 1$ and $\alpha_0 = \beta$: Converges to a new SSBM (Poissonian SSBM).

Comparing Trajectories MSDs

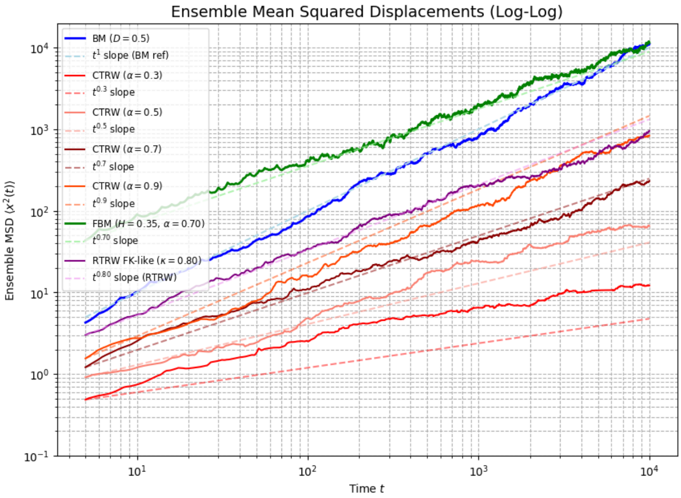


Figure: Comparison of simulated trajectories.

Ergodicity Fluctuations of TA-MSD

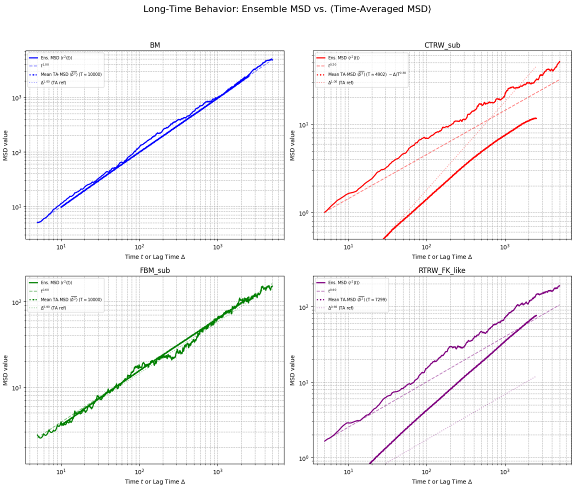


Figure: Comparison of simulated Ergodicities.

Comparative Summary: MSD, Ergodicity, Mechanisms

Property	CTRW (Subdiff.)	FBM (Subdiff.)	RTRW (e.g., Transparent Traps)
Anomaly Origin	Heavy-tailed $\psi(\tau)$	Correlated noise $\xi_H(t)$	Random landscape (π_x), $P(\pi)$
$\langle r^2(t)\rangle$	$\sim t^\alpha$	$\sim t^{2H}$	Regime-dependent (BM, t^γ, etc.)
$\langle\overline{\delta^2(\Delta, T)}\rangle$ (unconf.)	$\sim \Delta/T^{1-\alpha}$	$\sim \Delta^{2H}$	Regime-dependent
$\langle\overline{\delta^2(\Delta, T)}\rangle$ (conf.)	$\sim (\Delta/T)^{1-\alpha}$	Saturates	Regime-dependent
Ergodicity	Weakly Broken	Ergodic	Often broken / complex
Typical PDF $P(x,t)$	Non-Gaussian (Lévy)	Gaussian	Varied
Memory Type	Renewal (trapping)	Long-range correlations	Quenched disorder + dynamic

Table: Distinguishing features of the diffusion models.

Summary Key Takeaways

- **Brownian Motion:** Well-defined, ergodic, linear MSD. Serves as a baseline.
- **CTRW:** Characterized by waiting time distributions. Subdiffusive CTRWs show:
  - Discrepancy between ensemble and time-averaged MSD.
  - Weak ergodicity breaking significant trajectory-to-trajectory variations.
- **FBM:** Characterized by correlated increments. Subdiffusive FBMs show:
  - TA-MSD directly reflects anomalous exponent.
  - Ergodic, less scatter for long trajectories.
- **RTRW (Ben Arous et al.):** Provides a unifying and generalized framework for trapping phenomena.
  - Introduces random trapping landscapes.
  - Predicts rich scaling limits including FK, FIN, and novel SSBMs.
  - Offers deeper insight into how microscopic trap structure affects macroscopic diffusion.
- Choice of model depends on the underlying physical mechanisms (trapping vs. viscoelastic memory).
- Careful analysis of time-averaged quantities and their fluctuations is crucial for interpreting experimental SPT data.

References

S. Burov, J.-H. Jeon, R. Metzler, E. Barkai. (2011). Single particle tracking in systems showing anomalous diffusion: the role of weak ergodicity breaking. *Phys. Chem. Chem. Phys.*, 13, 1800-1812.

G. Ben Arous, M. Cabezas, J. Černý, R. Royfman. (2015). Randomly Trapped Random Walks. *The Annals of Probability*, 43(5), 2405-2457.

Hasan A. Fallahgoul and Sergio M. Focardi and Frank J. Fabozzi. (2017). Fractional Calculus and Fractional Processes with Applications to Financial Economics. *Academic Press*, 978-0-12-804248-9,

Thank You!

Questions?