Lattice Monte Carlo simulation of anomalous diffusion and its accuracy analysis

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Outline

- Anomalous diffusion
- LMC simulation of Galilei-variant type
- Galilei-invariant type
- Modified fractional diffusion equation with two time scales

Anomalous diffusion

- Anomalous diffusion
  - observed in numerous physical, chemical and biological systems, ubiquitous
  - a nonlinear behavior for the mean square displacement as a function of time
  - “normal”

Anomalous diffusion

- Fractional Partial Differential Equation: FPDE
- Continuous Time Random Walk: CTRW
- Lattice Monte Carlo (LMC) simulation: an important and effective method when it is difficult to get analytical solutions or necessary to track the trajectory of particles

Anomalous diffusion

- Galilei–variant fractional diffusion–drift equation
- Galilei–invariant fractional diffusion–drift equation
- Modified fractional diffusion equation with two time scales

Anomalous diffusion

- LMC simulation
  - First Passage Time (FPT) distribution with double absorbing barriers
  - Montroll–Weiss equation: waiting time distribution and structure function for particle transitions
  - Accuracy analysis based on integrals or moments

Galilei-variant

$$\frac{\partial}{\partial t}P(x,t)=\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(D_\alpha\frac{\partial^2}{\partial x^2}P(x,t)+v_\alpha\frac{\partial}{\partial x}P(x,t)\right),$$

- subballistic superdiffusive behavior of the MSD observed in experiments on wild-type and mutated epithelial cells and cancer cells
- the two state model with anomalous switching between migrating and proliferating phenotypes of cancer cells
- the intracellular fluid flow in rapidly moving cells with combined diffusion and drift intermittent with brief sticking to or trapping within the actin network

Galilei-variant

- Moments

$$< x >= {}_0\partial_t^{-\alpha}\left(v_\alpha \int_{-\infty}^{+\infty} P(x,t)dx - D_\alpha \int_{-\infty}^{+\infty} (\frac{\partial}{\partial x} P(x,t))dx \right) = v_\alpha\, {}_0\partial_t^{-\alpha}(1) = \frac{v_\alpha t^\alpha}{\Gamma(1+\alpha)},$$

$$< x^2 >= 2\, {}_0\partial_t^{-\alpha}\left(v_\alpha \int_{-\infty}^{+\infty} xP(x,t)dx - D_\alpha \int_{-\infty}^{+\infty} (x\frac{\partial}{\partial x} P(x,t))dx \right) = 2\, {}_0\partial_t^{-\alpha}\left(\frac{v_\alpha^2 t^\alpha}{\Gamma(1+\alpha)} + D_\alpha \right) = \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)} + \frac{2v_\alpha^2 t^{2\alpha}}{\Gamma(1+2\alpha)},$$

$$< \Delta x^2 >=< (x-< x >)^2 >= \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)} + \left(\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma^2(1+\alpha)} \right) v_\alpha^2 t^{2\alpha},$$

- FPT distribution with double absorbing barriers

$$F_2(\ell, v_\alpha, s) = F_2^+(\ell, v_\alpha, s) + F_2^-(\ell, v_\alpha, s) = \cosh\left(\frac{v_\alpha \ell}{2D_\alpha}\right) \operatorname{sech}\left(\frac{\ell\sqrt{v_\alpha^2 + 4D_\alpha s^\alpha}}{2D_\alpha}\right)$$

Galilei-variant

- Structure function

$$\lambda(k) = \sum_{l} p(l) \exp(-ik \cdot l).$$

- Fourier transform of discrete distribution

$$P(k,t) = \mathscr{F}\left[P(l,t),k\right] = \sum_{l} P(l,t) \exp(-ik \cdot l).$$

- Montroll–Weiss equation

$$P(k,s) = \mathscr{L}\left[P(k,t),s\right] = \frac{1-\psi(s)}{s}\frac{1}{1-\lambda(k)\psi(s)},$$

Galilei–variant

- n–th differentiation

$$\frac{\partial^n P(k,s)}{\partial \lambda^n}_{|\lambda=1} = \frac{n!(\psi(s))^n(1-\psi(s))}{s(1-\lambda(k)\psi(s))^{n+1}}_{|\lambda=1} = \frac{n!(\psi(s))^n}{s(1-\psi(s))^n},$$

- with the Laplace transform of the waiting time distribution

$$\Delta_1(t) \approx \frac{D_\alpha}{v_\alpha} - \frac{\ell}{2\tanh(\ell v_\alpha / 2D_\alpha)}$$

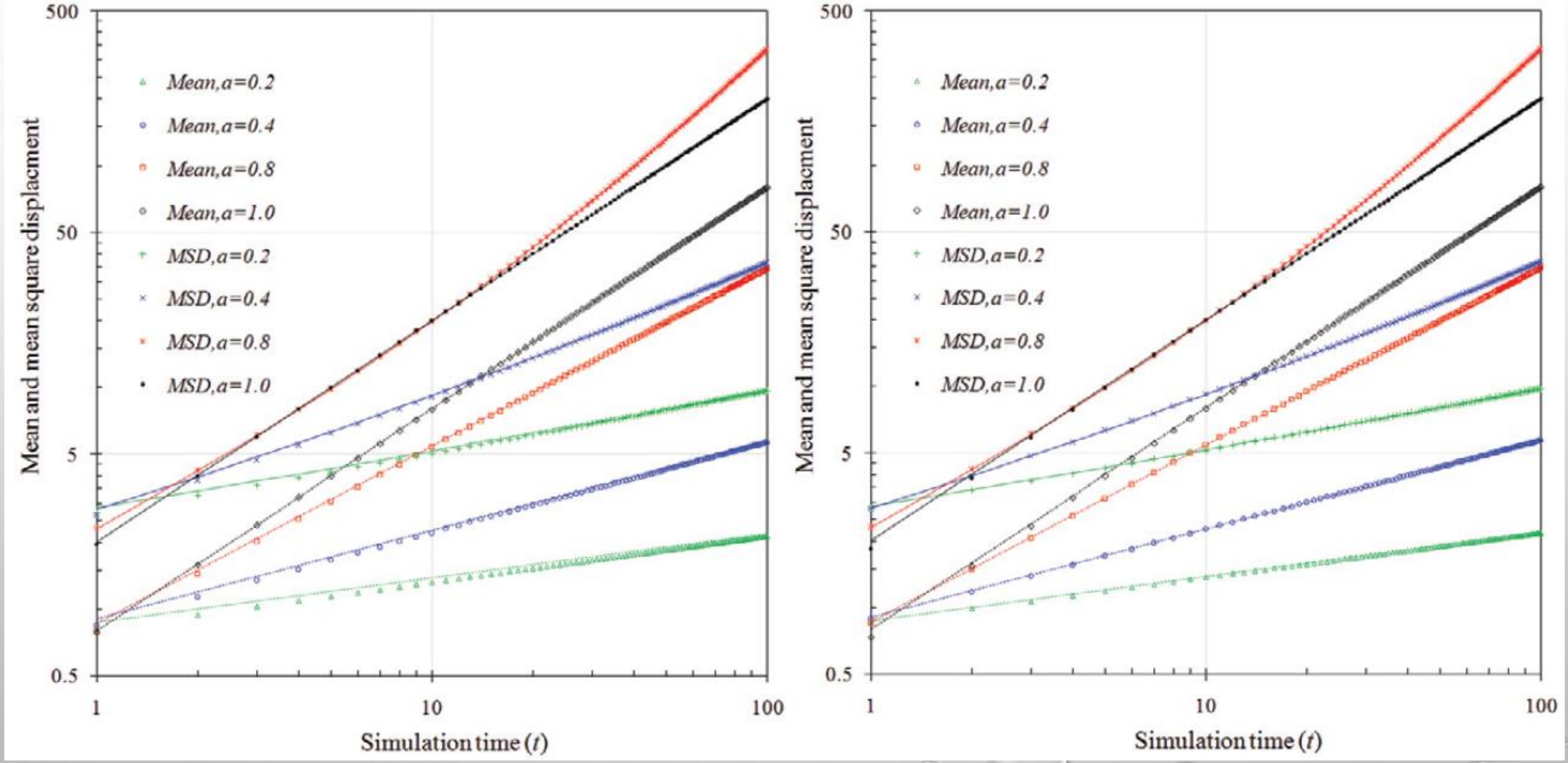
$$\Delta_2(t) = \overline{l_t^2} - \langle x^2 \rangle \approx \left(2D_\alpha - \frac{\ell v_\alpha}{\tanh(\ell v_\alpha / 2D_\alpha)}\right)\frac{t^\alpha}{\Gamma(1+\alpha)}$$

$$\Delta l_t^2 = \overline{l_t^2} - \overline{l_t}^2 \approx \left(\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma^2(1+\alpha)}\right)v_\alpha^2 t^{2\alpha} + \left(\frac{2}{\Gamma(1+\alpha)}\right)D_\alpha t^\alpha$$

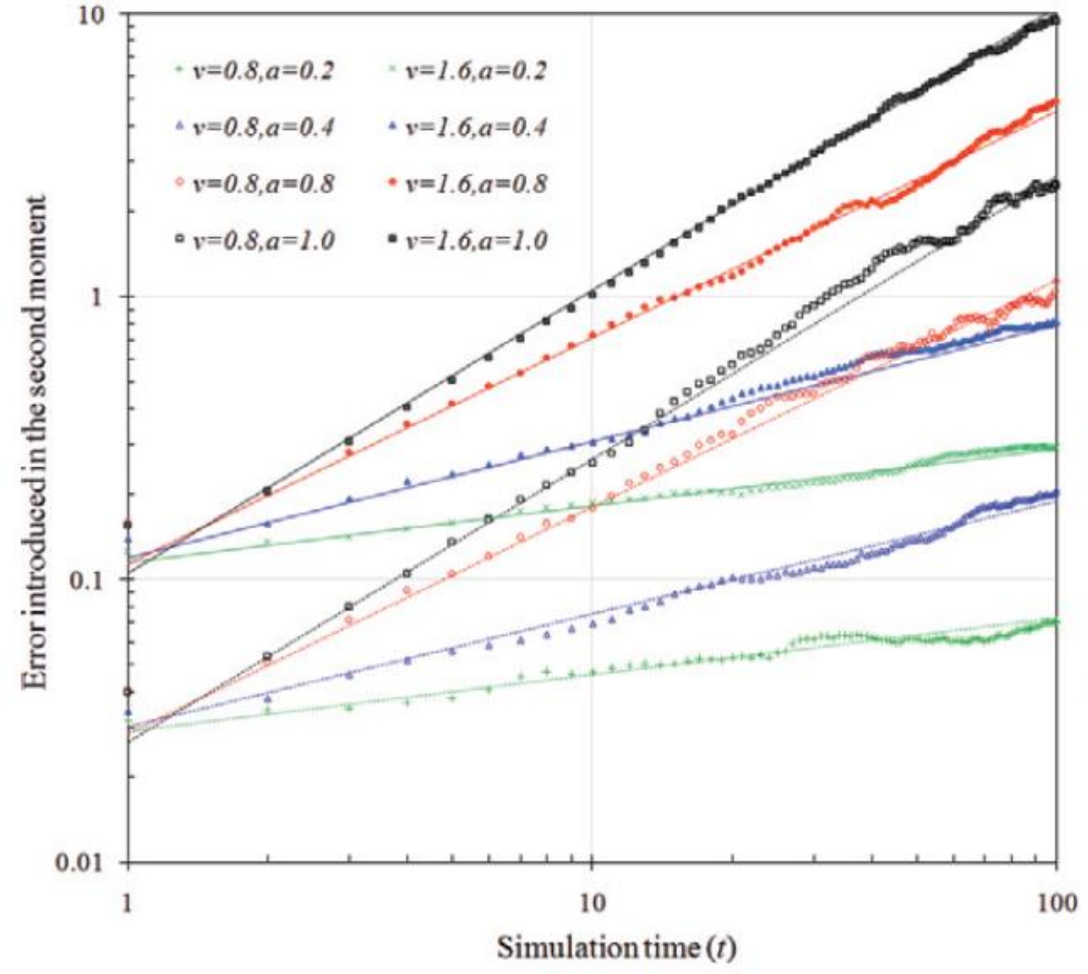
Galilei-variant

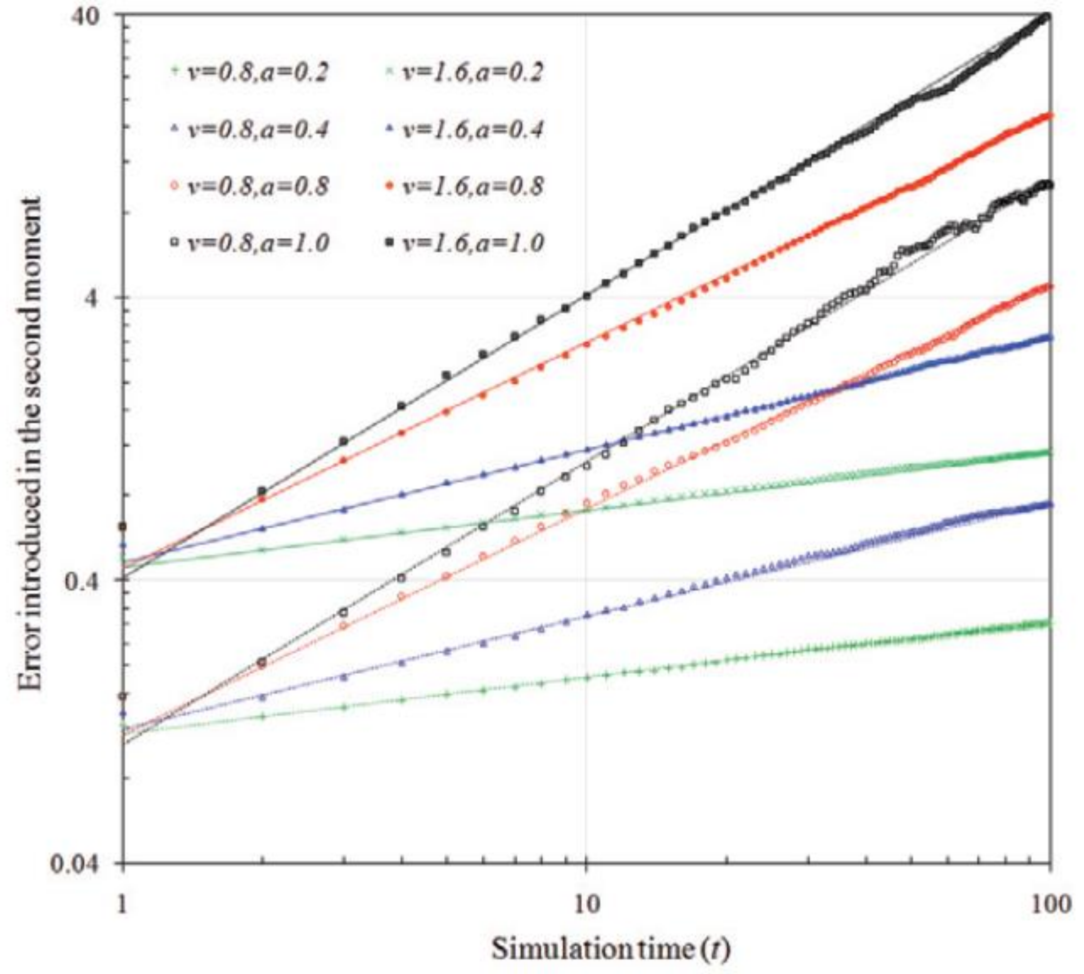
- The error introduced in the second moment of the distribution is due to the fluctuations in the time duration of each jump and the lattice step
- The absolute error in the 2nd moment can be controlled within a specified tolerance

Galilei-variant



Galilei–variant





Galilei-invariant

$$\frac{\partial}{\partial t}P(x,t)=\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(D_\alpha\frac{\partial^2}{\partial x^2}P(x,t)\right)+v_\alpha\frac{\partial}{\partial x}P(x,t).$$

- FPT distribution with one absorbing barrier

$$F_1(\ell,v_\alpha,s)=\exp\left(\frac{\ell v_\alpha s^{\alpha-1}}{2D_\alpha}-\ell\sqrt{\frac{v_\alpha^2 s^{2\alpha-2}}{4D_\alpha^2}+\frac{s^\alpha}{D_\alpha}}\right).$$

- However, for $0<\alpha<1$, it is not completely monotonic and hence not a valid pdf.
- Still some work to do ...

Modified fractional diffusion equation with two time scales

$$\frac{\partial}{\partial t}P(x,t) = \left(K_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} + K_\beta \frac{\partial^{1-\beta}}{\partial t^{1-\beta}} \right) \frac{\partial^2}{\partial x^2} P(x,t),$$

for decelerating subdiffusion processes

- Finite solution

$$P(x,t) = \sum_{n=1}^{\infty} \left\{ A_n \sin\left(\frac{n\pi(x+\ell)}{2\ell}\right) \sum_{k=0}^{\infty} \frac{(\lambda_n K_\beta t^\beta)^k}{k!} H_{1,2}^{1,1}\left(-\lambda_n K_\alpha t^\alpha \left| \begin{matrix} (-k,1) & \\ (0,1) & (-\beta k, \alpha) \end{matrix} \right. \right) \right\}$$

$$= \sum_{n=1}^{\infty} \left\{ A_n \sin\left(\frac{n\pi(x+\ell)}{2\ell}\right) \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{n^2\pi^2 K_\beta t^\beta}{4\ell^2} \right)^k H_{1,2}^{1,1}\left(\frac{n^2\pi^2 K_\alpha t^\alpha}{4\ell^2} \left| \begin{matrix} (-k,1) & \\ (0,1) & (-\beta k, \alpha) \end{matrix} \right. \right) \right\}$$

$$A_n = \frac{1}{\ell} \sin\left(\frac{n\pi}{2}\right), \quad n = 1, 2, \ldots.$$

Modified fractional diffusion equation with two time scales

- Semi-infinite solution

$$P(x,t) = \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{K_\beta}{K_\alpha} t^{\beta-\alpha}\right)^k \left\{ \frac{1}{2\left(K_\alpha t^\alpha\right)^{\frac{1}{2}}} H_{2,2}^{1,1}\left(\frac{|x-\ell|}{\left(K_\alpha t^\alpha\right)^{\frac{1}{2}}} \middle| \begin{matrix} \left(\frac{1}{2}-k, \frac{1}{2}\right) & \left(1-(\alpha-\beta)k-\frac{\alpha}{2}, \frac{\alpha}{2}\right) \\ (0,1) & \left(\frac{1}{2}, \frac{1}{2}\right) \end{matrix} \right) \right.$$

$$\left. - \frac{1}{2\left(K_\alpha t^\alpha\right)^{\frac{1}{2}}} H_{2,2}^{1,1}\left(\frac{(x+\ell)}{\left(K_\alpha t^\alpha\right)^{\frac{1}{2}}} \middle| \begin{matrix} \left(\frac{1}{2}-k, \frac{1}{2}\right) & \left(1-(\alpha-\beta)k-\frac{\alpha}{2}, \frac{\alpha}{2}\right) \\ (0,1) & \left(\frac{1}{2}, \frac{1}{2}\right) \end{matrix} \right) \right\}.$$

Modified fractional diffusion equation with two time scales

- **FPT distribution with two absorbing barriers**

$$F_2(\ell,s)=\frac{2}{\exp(\lambda\ell)+\exp(-\lambda\ell)}=\mathrm{sech}\left(\ell\left(\frac{s}{s^{1-\alpha}K_\alpha+s^{1-\beta}K_\beta}\right)^{\frac{1}{2}}\right)$$

$$f_2(\ell,t)=-\sum_{n=1}^{\infty}\left\{\frac{4}{n\pi}\sin\left(\frac{n\pi}{2}\right)\sum_{k=0}^{\infty}\frac{(\lambda_n K_\beta)^k}{k!}t^{\beta k-1}H_{2,3}^{1,2}\left(-\lambda_n K_\alpha t^\alpha\left|\begin{matrix}(-\beta k,\alpha) & (-k,1) & \\ (0,1) & (-\beta k,\alpha) & (1-\beta k,\alpha)\end{matrix}\right.\right)\right\}$$

$$=-\sum_{n=1}^{\infty}\left\{\frac{4}{n\pi}\sin\left(\frac{n\pi}{2}\right)\sum_{k=0}^{\infty}\frac{(\lambda_n K_\beta)^k}{k!}t^{\beta k-1}H_{1,2}^{1,1}\left(-\lambda_n K_\alpha t^\alpha\left|\begin{matrix}(-k,1) & \\ (0,1) & (1-\beta k,\alpha)\end{matrix}\right.\right)\right\}$$

$$=-\sum_{n=1}^{\infty}\left\{\frac{4}{n\pi}\sin\left(\frac{n\pi}{2}\right)\sum_{k=0}^{\infty}\frac{1}{k!}\left(-\frac{n^2\pi^2K_\beta}{4\ell^2}\right)^k t^{\beta k-1}H_{1,2}^{1,1}\left(\frac{n^2\pi^2K_\alpha t^\alpha}{4\ell^2}\left|\begin{matrix}(-k,1) & \\ (0,1) & (1-\beta k,\alpha)\end{matrix}\right.\right)\right\}$$

Modified fractional diffusion equation with two time scales

- However, no LMC simulation algorithms yet …

Future work

- Analytical solutions, FPT distributions, LMC simulation algorithms …
- Accuracy analysis and parallelization
- Theorem of the existence of equivalent separable CRTW model for anomalous diffusions (to reveal the microscopic physical or mathematical mechanism …)

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Questions?