Dynamics of Motile Microbes

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Outline

- Microbial motility and adhesion
- Finite size Lyapunov exponent (FSLE) for Levy processes
- Numerical modeling of transport in a pore with sticky boundaries
- Theoretical evaluation of MFPT in a pore
- Challenges and topics for future research
Microbial Motility

- Motile microbes are equipped with swimming devices consisting of a set of rotary motors and thin helical filaments (flagella).

- Flagella coalesce and the motor rotate to either self-propel the microbe or to change its direction.
Microbial Motility

- Self-propelled Movement of flagella imparts a run and tumble behavior.
- motion of microbes are random in nature.
- Mean square displacement grows faster than $t$ indicating a super-diffusion process.

(courtesy: Howard Berg, Harvard Univ)
Microbial Motility

Super-diffusion (Levy motion) and Classical diffusion (Brownian motion)

Microbial motion and Levy motion
Microbial Adhesion

- Adhesion is guided by flagellar movement and chemical & biological considerations.
- Detachment process results in elution curves with long and heavy tail.
- Power-law scaling of waiting times explains the observed characteristics.
Microbes in Porous Media

- Swimming characteristics of microbes exhibit anomalous dispersion characteristic even in a homogeneous medium.
- Using classical ADE to model microbial transport invariably leads to the usage of fitting parameters.
The Finite Size Lyapunov Exponent

- The FSLE describes the exponential divergence of two trajectories starting a specified distance apart.
- If $r$ is the initial separation between two trajectories, and $T_a(r)$ is the mean time it takes the separation to grow by a factor $a > 1$, then
  \[
  \lambda_a(r) = \frac{1}{T_a(r)} \ln a.
  \]
- The FSLE is obtained experimentally by generating trajectories and then employing particle tracking methods.
FSLE for $\alpha$-stable Levy Processes

- $\Delta x_i^1$ and $\Delta x_i^2$, are described by the same $\alpha$-stable distribution.
- Observe the system from a reference frame attached to Particle 1. The only mobile entity now is Particle 2.
- $(\Delta x_i^1 - \Delta x_i^2)$ is an $\alpha$-stable distribution with a modified $\sigma$.
- Passage plane are treated as absorbing barriers to find $T_\alpha(r)$.
FSLE for $\alpha$-stable Levy Processes

\[ T_\alpha(r) = \frac{2^{2+\alpha}}{\pi^{1+\alpha} D} a^\alpha (r)^\alpha \sum_{m=0}^{\infty} \frac{(-1)^m \sin\left[(2m+1)\left(1 + \frac{1}{a}\right) \frac{\pi}{2}\right]}{(2m+1)^{1+\alpha}} \]

\[ \lambda_\alpha(r) = \frac{\pi^{1+\alpha} D \ln(a)}{2^{2+\alpha} a^\alpha P(a, \alpha)} (r)^{-\alpha} \quad \text{where} \quad P(a, \alpha) = \sum_{m=0}^{\infty} \frac{(-1)^m \sin\left[(2m+1)\left(1 + \frac{1}{a}\right) \frac{\pi}{2}\right]}{(2m+1)^{1+\alpha}} \]

- The power-law relation between FSLE and $r$, when plotted on a log-log scale, will yield $\alpha$ as the slope.
- The scaling factor $\sigma$ can be estimated from the constant of proportionality [Parashar and Cushman, *Physical Rev E*, 2007].
Numerical modeling of a pore with sticky boundaries

- A three-dimensional pore with boundaries in z-direction located at $\pm \infty$.
- Microbial transport is modeled as a Levy motion and the boundary conditions are sticky, prompting us to model the local sorption time as absolute values of an $\alpha$-stable distribution.
Numerical modeling of a pore with sticky boundaries

- We take Lagrangian perspective (solving SDE) as Eulerian statement for sticky boundary conditions could not be formulated.
- Particles attach to the boundaries upon collision and are released back after a waiting period described by an absolute $\alpha$-stable distribution.
- Numerical model track microbes as they are transported (diffusion + advection) towards the passage plane.
- First passage time (FPT) density is computed and analyzed for various statistical properties.
Numerical modeling of a pore with sticky boundaries
Numerical modeling of a pore with sticky boundaries

- A large number of variables affecting the evolution of the plume justifies the need of a sensitivity study.
- Variables can be clubbed together to form meaningful non-dimensional parameters.
- Non-dimensionalisation is accomplished by employing the fractional Eulerian equation and by evaluating the expected value of waiting time on the sticky boundaries.
Non-Dimensionalization

FADE to nd-FADE in 2d:

\[
\frac{\partial C}{\partial t} = D \frac{\partial^{\alpha_f} C}{\partial x^{\alpha_f}} + D \frac{\partial^{\alpha_f} C}{\partial y^{\alpha_f}} - \nu \frac{\partial C}{\partial x}
\]

\[
\frac{\partial C_0}{\partial T} = \frac{1}{P} \frac{\partial^{\alpha_f} C_0}{\partial X^{\alpha_f}} + \frac{1}{R} \frac{\partial^{\alpha_f} C_0}{\partial Y^{\alpha_f}} - \frac{\partial C_0}{\partial X}
\]

where \( P = \frac{\nu L^{\alpha_f-1}}{D} = \frac{L^{\alpha_f}}{(DL/\nu)} \) and \( R = \frac{b^{\alpha_f}}{(DL/\nu)} \)

- \( P \) is analogous to the Peclet number of classical ADE.
- \( R \) can be interpreted as the ratio between width of the pore and transverse diffusive length. A smaller value of \( R \) means that the boundaries constricts the evolution of the plume in transverse direction.
When sticky boundary effects are included,

\[
N_s = \frac{2^{1+\alpha_f/2} \Gamma \left( \frac{1}{2} + \frac{\alpha_f}{4} \right) \Gamma (-1/2)}{\alpha_f \sqrt{\pi} \Gamma (-\alpha_f/4)} \left( \frac{2b}{\sigma_f} \right)^{\alpha_f/2}
\]

\[
N_H = \frac{(L/(v\Delta t))}{N_s}
\]

Multiplying \( N_H \) by expected value of the waiting time distribution, a non-dimensional parameter can be formulated to measure the ratio of time spent on the wall vs time spent in the fluid phase,

\[
S = \frac{N_H \left[ 2\Gamma(1-1/\alpha_w) \right]}{\pi \sigma_w} \frac{(L/v)}{L/v}
\]

\[
C_0(X,Y;T) = f(\alpha_f, \alpha_w, P, R, S)
\]
Analysis of Results w.r.t to non-dimensionalised Parameters

- First Passage time (FPT) densities are computed and its sensitivity w.r.t non-dimensionalised parameters are examined.
- MFPT gives a measure of the retardation of the centroid of the plume.
- Higher order moments (\(>\alpha\)) are nonexistent for processes driven by Levy motion. However, \(T_W\) (width of central 80% of FPT density) still gives vital insight into the spread.
- Comparison of MFPT and \(T_p\) (time to peak) helps in analyzing the relative length of rising and falling limbs (skewness).
Analysis of Results w.r.t to non-dimensionalised Parameters

- Solution of SDE are used to develop plots (MFPT, $T_p$, and $T_W$) incorporating permutations of wide ranges of $P$, $R$, $S$, $\alpha_f$, and $\alpha_w$ values.

Plots for a given $\alpha_f$ and $\alpha_w$ values. $P$ (1 to 20) is plotted on x-axis. The three lines in each plot correspond to $S$ values of 0.1 (blue), 0.03 (green), and 0.001 (red).
Analysis of Results w.r.t to non-dimensionalised Parameters

- P, R, and S influence the value of MFPT in a highly coupled way. The stability parameters have only a mild influence on MFPT.
- For all possible combinations of P, R, S, \( \alpha_f \), and \( \alpha_w \), \( T_p \) is smaller than MFPT.
- An increasing P lengthens the falling limb as it influences the growth of MFPT more than the growth of \( T_p \). The difference in these two growth rates are non-linear for smaller values of P, and gradually becomes linear as P increases.
- For non-negligible sorption (higher S), \( T_W \) first decreases and then increases with increasing P. For a P value of somewhere between 1 to 10, the lowering effect of P on \( T_W \) is completely offset by the other factors which serve to increase \( T_W \).
- Different regimes of flow can be identified (marked by high or low value of a non-dimensional parameter), where P, R, or S may or may not effect the statistical quantities in a significant way [Parashar and Cushman, *Journal of Computational Physics*, 2008].
Theoretical Evaluation of MFPT in a Pore

A point source in the central pore: $G(y, n)$
Theoretical Evaluation of MFPT in a Pore

\[ G^i(y,n;m) = \int_0^{2b} G(y,n;\chi,\delta^i(\chi,m))d\chi \]

\[ = \int_0^{2b} \delta^i \sum_{k=1}^{\infty} \sin \left[ \frac{k\pi}{2b} (\chi) \right] \sin \left[ \frac{k\pi}{2b} (y) \right] \exp \left[ -D \left( \frac{k\pi}{2b} \right)^\alpha n\Delta t \right] d\chi \]

\[ \delta^i(\chi,m) = f_\alpha(\chi) \times R^{i-1} \quad R^{i-1}(m) = \Delta \int_0^{2b} \sum_{l=i-1}^{m} G^{i-1}(y,m;l) \] dy

\[ G^i(y,n) = \sum_{m=i}^{n} G^i(y,n;m) \quad \rightarrow \quad G(y,n) = \sum_{i=1}^{\infty} G^i(y,n) \]
Theoretical Evaluation of MFPT in a Pore
Theoretical Evaluation of MFPT in a Pore

\[ MTD = \sum_{n=1}^{N} \int_{y=0}^{2b} G(y, n) v(y) dy \]

\[ \mathcal{R} = N_{hit} \frac{2\Gamma(1 - 1/\alpha_w)\sigma_w}{\pi} \]

\[ MFPT = \frac{v_{av} (\mathcal{R} + N\Delta t)}{MTD} \]

[Parashar et al., *Physical Rev E*, 2008]
Challenges and Topics for Future Research

- Study the implication of microbial transport on engineering techniques such as bio-stimulation or bio-augmentation.
- Conduct laboratory experiments to quantify anomalous characteristics of microbial motion.
- Find the necessary and sufficient conditions (FSLE?) for identification of a Levy process.
- Examine if and when a state of equilibrium is reached for Levy motion in a pore with sticky boundaries.
- Develop upscaling methods for cases with sticky boundaries.
- Explore the spatial-temporal density function for a selectively coupled CTRW with dual-region waiting time density function.