Rhodobacter Spheroides

- Flagella are filaments used for motion
- When the filament spin, it is helical and the cell runs
- When the filament stops, it coils up and the cell stops. The coiling tends to reorient the cell body.

http://www.rowland.harvard.edu/labs/bacteria/
Modeling
Modeling of Bacteria

- Due to scale of the system we use the Stokes Equations for modeling

\[
0 = -\nabla P + \Delta u + f \\
0 = \nabla \cdot u.
\]

- We consider an elastic model since the dynamics of the system are of interest.

- The Method of Regularized Stokeslets is used for modeling the system, which gives analytic solutions for the velocity.
Optimization
Energy Functional

- NO analytic expression for the forward velocity. Instead we look at the average distance traveled.

- Assume that the position can be modeled by
  
  \[ x(t) = v_1 t \hat{e}_1 + a \cos(wt) \hat{e}_2 + a \sin(wt) \hat{e}_3 \]

- The square of the average velocity gives
  
  \[ \left( \frac{||x(T)||}{T} \right)^2 = v_1^2 + \left( \frac{a}{T} \right)^2 \]

- Hence, we consider the energy functional
  
  \[ J(\alpha) = \frac{1}{2} \sum_{i=1}^{N_x} ||x_i(T) - x_i(0)||^2 \]

Optimization Problem

- Maximize:
  
  \[ J(\alpha) = \frac{1}{2} \sum_{i=1}^{N_x} ||x_i(T) - x_i(0)||^2 \]

- With Constraints:
  
  \[ \dot{x}_k = \sum_{i \in R} U_r(x_k; x_i, L_i) + \sum_{j=1}^{N_x} U_s(x_k; x_j, f_j) \]
  
  \[ b_{lower} \leq \alpha_k \leq b_{upper} \]

- From Adjoint Method:
  
  \[ \frac{\partial J}{\partial \alpha_j}(\alpha) = \int_0^T \sum_{k=1}^{N_x} G^F_{k,j}(S(t))y_k(t) \, dt \]
  
  \[ \dot{y}_k(t) = -\sum_{k=1}^{N_x} F^F_{k,k}(S(t))y_k \]
  
  \[ y_k(T) = x_i(T) - x_i(0), \]
Optimization Problem (cont…)

- Issues:
  - Minimize the effect from transition to steady state
  - Functional is depend on Initial Conditions (IC)

- Solution:
  - Use final condition from previous iteration as IC for new iteration
  - This allows for quicker transition and randomizes IC so we do not get stuck at local minimum (i.e. we change the energy functional)
  - However, not well behaved for regular optimization

Preliminary Results

- Little Transition time to steady state
- Distribution appears to be periodic over with a decreasing amplitude over the flagellum
References

J.P. Armitage et al. 'Transformations in Flagellar Structure of Rhodobacter sphaeroides and Possible Relationship to Changes in Swimming Speed'

H. Flores et al. 'A Study of Bacterial Flagellar Bundling.'

Applications

Fluid dynamics study of the motion
Comparing Optimal Values to Real Values
Design of Propulsion Mechanism for Nanobots