Modeling of Single Flagellum
Bacterial Motion

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Purpose

- Simulate motion in a low Reynolds number environments
- Applications: micromachines, nanotech
- Most applications in medicine
Bacteria Model

- Particles connected by springs of varying elasticities

- Torque and counter torques applied by a motor at the junction

Optimization Recap

- Stokes Equations:
  \[ \Delta u = \nabla P - f \]
  \[ \nabla u = 0 \]

- Regularized Stokeslet:
  \[ U_s(x; x_0, f) = \frac{(r^2 + 2\delta^2)}{8\pi(r^2 + \delta^2)^{3/2}} f_0 + \frac{[f_0 \cdot (x - x_0)]}{8\pi(r^2 + \delta^2)^{3/2}} (x - x_0) \]

- Regularized rotlet:
  \[ U_r(x; x_0, L_0) = \frac{(2r^2 + 5\delta^2)}{16\pi(r^2 + \delta^2)^{3/2}} L_0 \times (x - x_0) \]
Optimization Recap (Cont)

- **Constraints:**
  \[
  \dot{x}_k = \sum_{i=0}^{3} U_r(x_k; x_n, L_i) + \sum_{j=1}^{N_s} U_s(x_k; x_j, f_j)
  \]

- **Functional:**
  \[
  J(\alpha) = \frac{1}{2} \left( \frac{||\bar{x}(T; \alpha) - \bar{x}(0; \alpha)||_{L_2}}{T} \right)^2
  \]

- Use adjoint optimization and gradient over elasticity distribution

Model #1

- Bacteria head and flagellum
- Freely moving
- Measure distance traveled
Model #1 Simulation

Velocity Field Plots
CMU Experiments

![Image of CMU Experiments setup]

CMU Results

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Dimensions of the helical tail of the scaled-up prototype</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Design I</td>
</tr>
<tr>
<td>Filament thickness, w</td>
<td>0.43</td>
</tr>
<tr>
<td>Amplitude, A</td>
<td>0.8</td>
</tr>
<tr>
<td>Wavelength, λ</td>
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</tr>
<tr>
<td>Length, L</td>
<td>20</td>
</tr>
</tbody>
</table>

![Graph showing Frequency vs Force]
Differences in Assumptions

- Completely rigid flagellum
- Long, thin cylindrical flagellum
- No non-slip boundary condition

Model #2

- Remove bacteria head
- Replace hook with different envelope
- Apply forces to fix position of junction
- Sum applied forces to find force generated
Model #2 Simulation

Matching Data

- Many factors to take into account
  - Dimensionalizing values
    \[ \text{Force} = f_0 \frac{\mu [L]^2}{[T]} \]
  - Length of tail
    - Number of rotations
Actual Data Comparison

- For Design II:
  - $\mu=0.3395 \text{ kg/(m*s)}$, $D=0.63 \text{ mm}$, $L=10$, $\lambda = 5 \text{ Hz}$
  - Experimental Force: 1.7 mN

- From Simulation:
  - $D = 0.02 \text{ m}$, $L=4$, $\tau = 104.5$
  - Calculated Force: 0.15621 mN

- Off by a factor of 10.8829

Problems with Model #2
Model #3

- Fix two points near junction instead of one
- Not working quite yet

Force Calculations

- Apply $f_0 = <f_{0x}, f_{0y}, f_{0z}>$ and $f_1 = <0, f_{1y}, f_{1z}>$
- Want $v_0 = <0,0,0>$ and $v_1 = <v_{1x},0,0>$
**Force Matrix**

\[ A = \frac{1}{8\pi} \begin{bmatrix}
\frac{2}{\delta} & 0 & 0 & x_{01x}^* \cdot x_{01y} \cdot \frac{2}{r^2 + \delta^2} \\
0 & \frac{2}{\delta} & 0 & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} \\
0 & 0 & \frac{2}{\delta} & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} \\
x_{01x}^* \cdot x_{01y} \cdot \frac{2}{r^2 + \delta^2} & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} & \frac{2}{\delta} & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} \\
x_{01x}^* \cdot x_{01y} \cdot \frac{2}{r^2 + \delta^2} & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} & \frac{2}{\delta} & x_{01y}^2 \cdot \left(\frac{r^2 + 2\delta^2}{r^2 + \delta^2}\right)^{\frac{3}{2}} \\
\end{bmatrix} \]

**Model #3 Simulation**

![Model #3 Simulation Graph]
Future Work

- Get Model #3 working properly
- Theoretically solve perfectly rigid flagellum problem using force matrix
- Try to incorporate wall effects

References


- Lobaton, Edgar and Alexandre Bayen. “Modeling and Optimization Analysis of Single Flagellum Bacterial Motion”. 