Designing Molecular Swimmers

Ramin Golestanian

Department of Physics and Astronomy
University of Sheffield

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Swimming and Length Scale

- Simplified Dynamics

$$m\frac{d^2x}{dt^2} + V\frac{dx}{dt} = F(t)$$

$F(t)$ is Periodic: *interaction with medium*

$$m \sim rL^3 \qquad\qquad V \sim hL$$

Swimming and Length Scale

- Large Scales

Inertial $$t \to -t \;\Rightarrow\; F \to F$$

? **constructive**

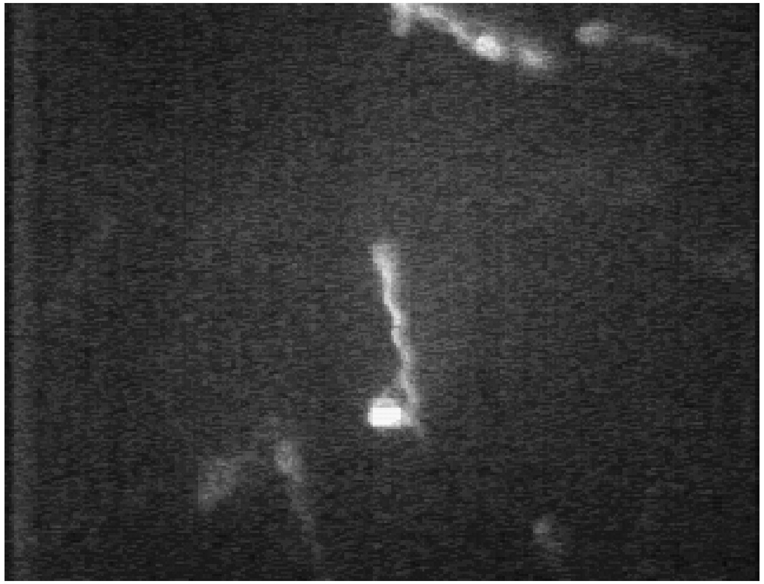
- Small Scales

Viscous $$t \to -t \;\Rightarrow\; F \to -F$$

? **destructive**

Bacterial Swimming

- *E. coli* driven by rotating flagella



L. Turner, W.S. Ryu, and H.C. Berg, *J. Bacteriol.* 182, 2793-2801 (2000)

- G.I. Taylor (1951)

  Swimming at low Reynolds number

Swimming at Low Reynolds

- Purcell Swimmer (1976)

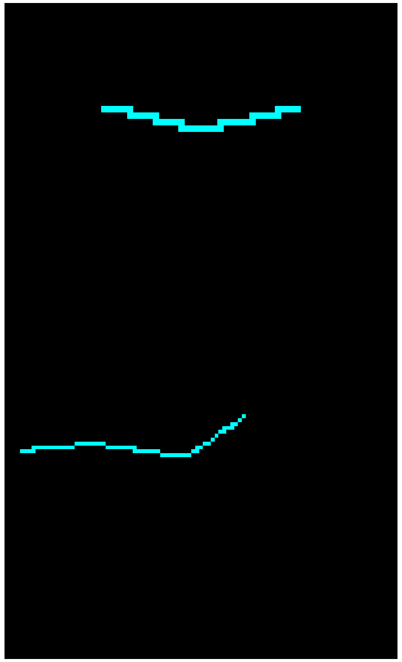
  Using the smallest number of degrees of freedom:

  - **One**, is not enough

    Scallop Theorem

  - **Two**, will just do!

  … but the passenger will get sea-sick!



Courtesy of Daniel B. Murray

Three-Sphere Swimmer

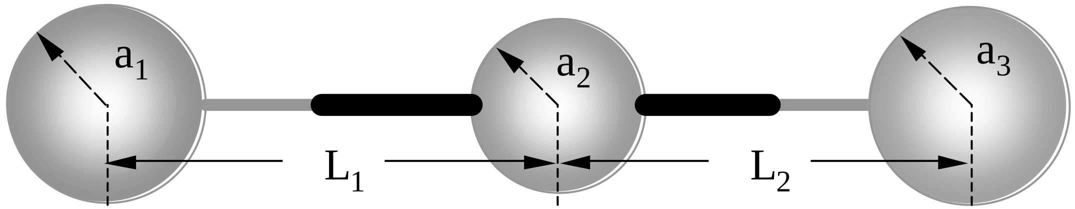
- Two Translational Degrees of Freedom

A. Najafi & R. Golestanian, PRE **69**, 062901 (2004)

Swimming Velocity

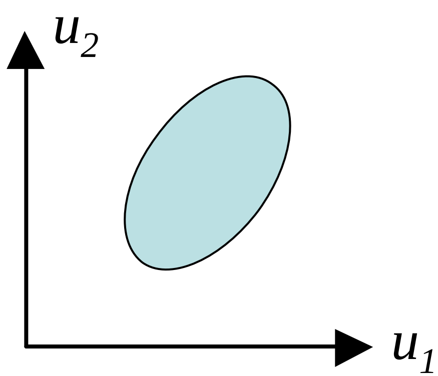
- Simple Perturbative Analysis

$$L_1 = \ell + u_1$$
$$L_2 = \ell + u_2$$



$$\overline{V} = \frac{7}{24}\frac{a}{\ell^2}\overline{(u_1\dot{u}_2 - \dot{u}_1 u_2)}$$

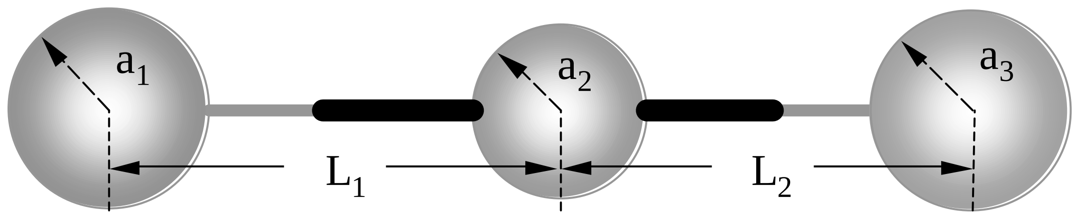
- Geometric Interpretation



Harmonic Deformations

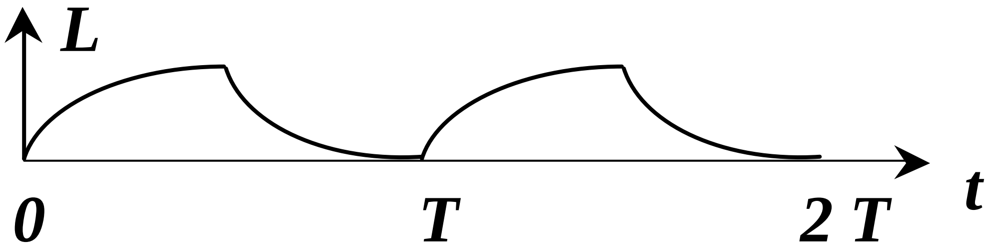
$$u_1(t) = d_1 \cos(\omega t + \varphi_1)$$

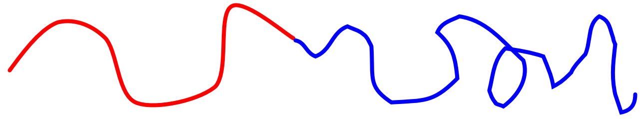
$$u_2(t) = d_2 \cos(\omega t + \varphi_2)$$



$$\overline{V} = \frac{7}{24} \frac{a}{\ell^2} \, d_1 d_2 \omega \sin(\varphi_1 - \varphi_2)$$

Exponential Relaxation





$$\overline{V} = \frac{7}{96}\frac{a}{\ell^2}\, d_1 d_2 \left(\frac{1}{\tau_1} - \frac{1}{\tau_2}\right) \mathcal{F}\left(\frac{T}{4\tau_1}, \frac{T}{4\tau_2}\right)$$

$$\mathcal{F}(x,y) = \frac{1}{\sinh x \ \sinh y}\left[\frac{\sinh(x+y)}{(x+y)} - \frac{\sinh(x-y)}{(x-y)}\right]$$

Noisy Deformations

$$\overline{V} = \frac{7}{24}\frac{a}{\ell^2}\frac{1}{T}\int \frac{d\omega}{2\pi}\, i\omega\overline{[u_2(\omega)u_1(-\omega) - u_1(\omega)u_2(-\omega)]}$$

$$u_i(t) = \sum_n d_{in}\cos(\omega_n t + \varphi_{in})$$

$$\overline{V} = \frac{7}{24}\frac{a}{\ell^2}\sum_n \overline{d_{1n}d_{2n}\omega_n \sin(\varphi_{1n} - \varphi_{2n})}$$

Load-Velocity Response

- Force-Velocity Relation

$$\overline{V}(F) = \frac{7}{24}\frac{a}{\ell^2}\overline{(u_1\dot{u}_2 - \dot{u}_1 u_2)} + \frac{F}{18\pi\eta a}$$

- Stall Force

$$F_s = -18\pi\eta a\overline{V}(0)$$

Mechanical Efficiency

- Power Consumption

$$\overline{\mathcal{P}} = 2\pi\eta a \left[\overline{\dot{u}_1^2} + \overline{\dot{u}_2^2} + \overline{(\dot{u}_1 + \dot{u}_2)^2}\right]$$

- Lighthill's Efficiency $\eta_{\mathrm{L}} = \dfrac{18\pi\eta a \overline{V}^2}{\overline{\mathcal{P}}}$

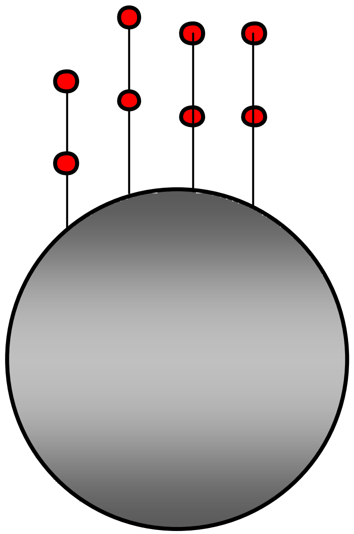
$$\eta_{\mathrm{L}} = \frac{49}{64}\frac{a^2}{\ell^4}\,\frac{\overline{(u_1\dot{u}_2 - \dot{u}_1 u_2)}^2}{\overline{\dot{u}_1^2} + \overline{\dot{u}_2^2} + \overline{(\dot{u}_1 + \dot{u}_2)^2}}$$

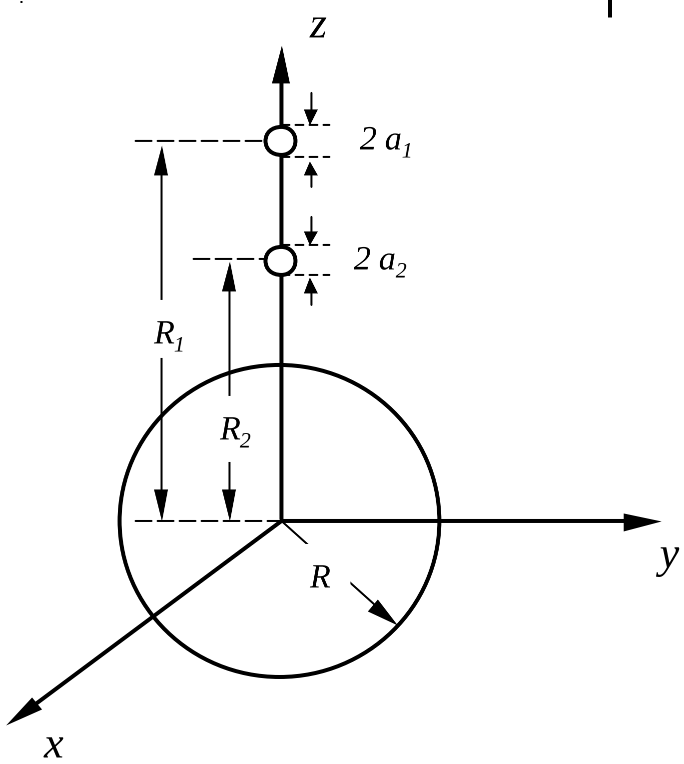
Swimmer with Cargo

- Small deformations

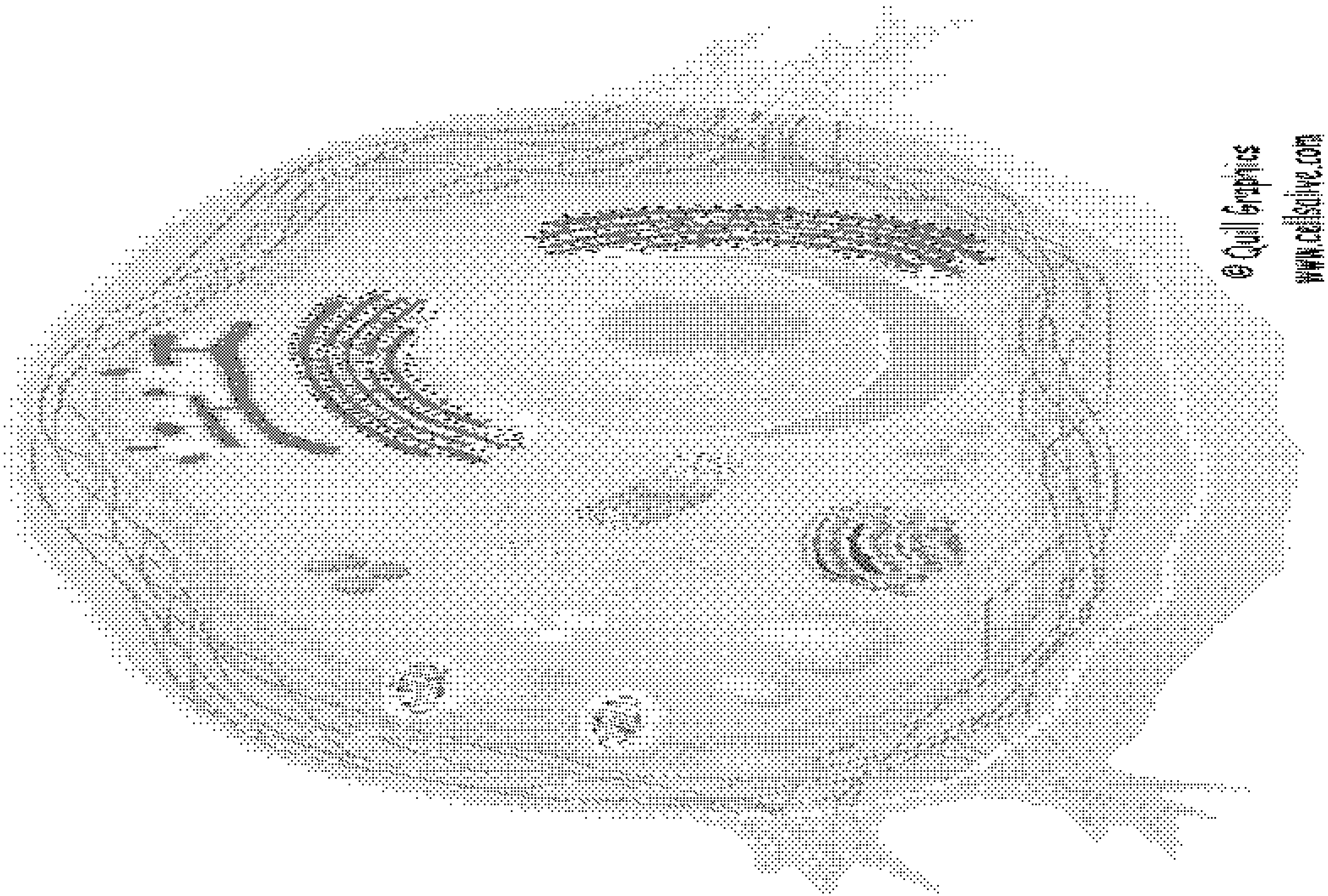
$$\overline{V} = \frac{9}{4}\left(\frac{a_1 a_2}{R^3}\right)\frac{\ell_2^2\,(3\ell_1 + 2\ell_2)}{\ell_1^2\,(\ell_1 + 2\ell_2)}\,\overline{(\dot{u}_1 u_2 - \dot{u}_2 u_1)}\Big|$$

- Optimal Design



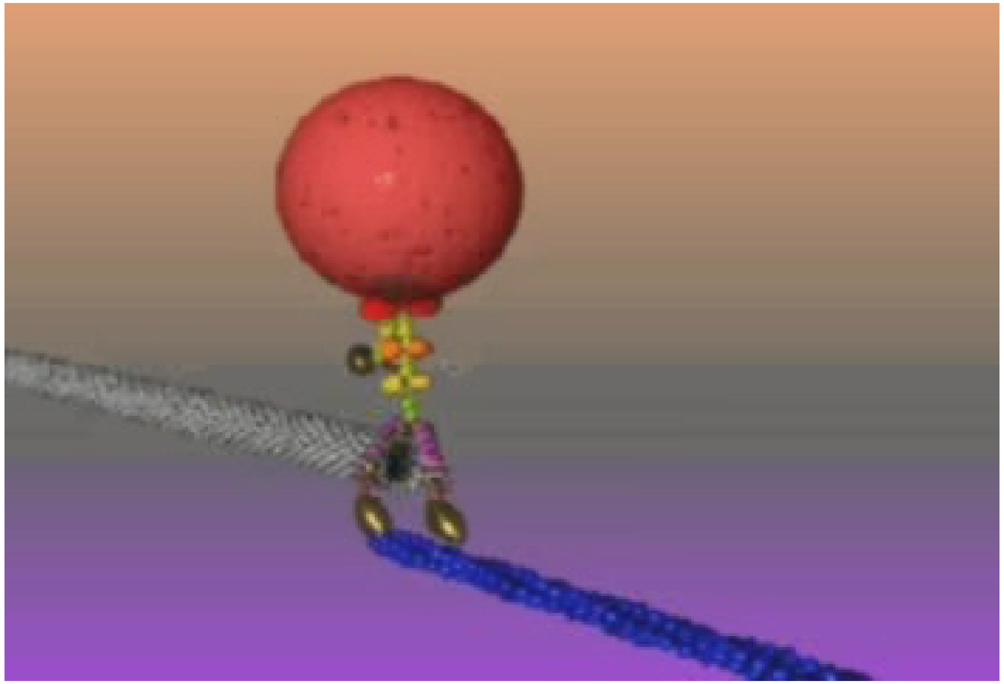


Transport System in the Cell



Molecular Motors

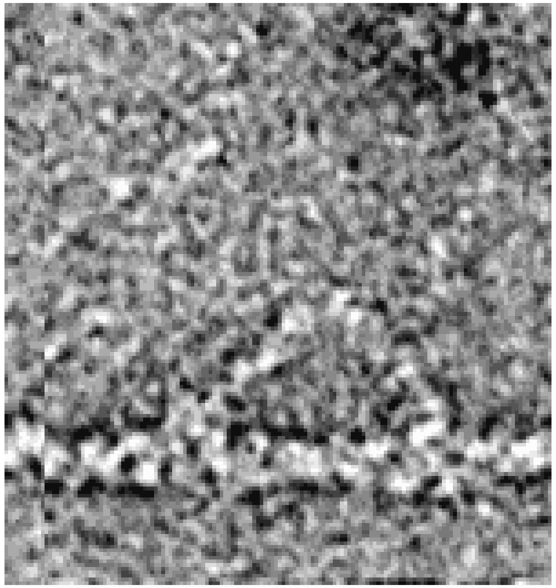
- Motion of myosin-V molecules on actin



Courtesy of Dr. George Langford

Molecular Motors

- Myosin-V: ``Electron Video Microscopy''



The Muscle Group, Leeds 2000

M L. Walker, S A. Burgess, J R. Sellers, F Wang, J.A. Hammer, J Trinick, & P J. Knight, Nature **405**, 804-807 (2000)

Molecular Motors

- Principal Characteristics
  - Nano-scale machines
  - Highly accurate despite Brownian agitation
  - Converting *chemical* energy directly to useful *mechanical* work

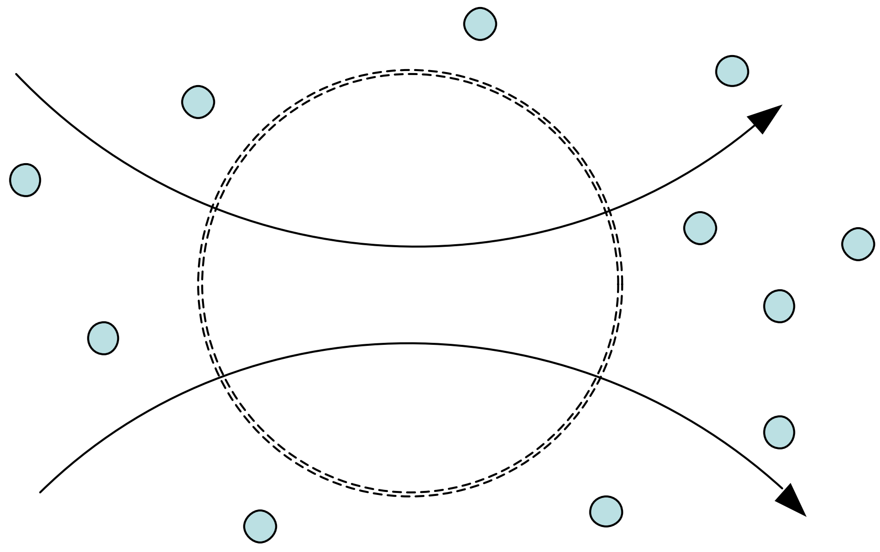
Can we design such a machine?

Phoretic Locomotion

- Osmio-phoresis

Motion of lipid vesicles under a gradient of sugar molecules

? Nardi, Sackmann & Bruinsma, PRL **82**, 5168 (1999)

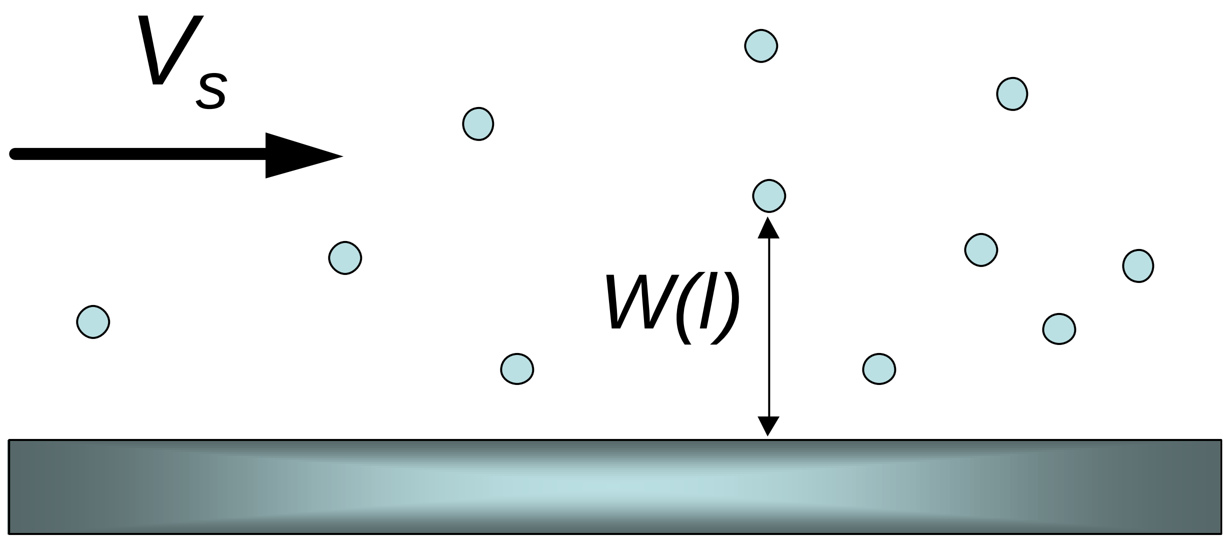


Phoretic Locomotion

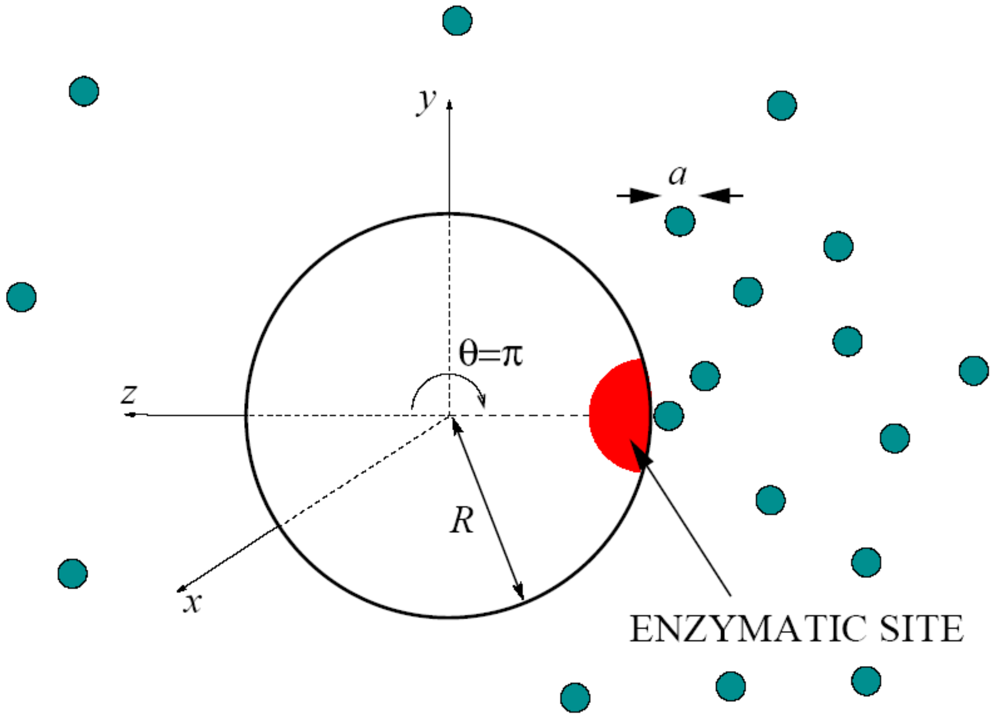
- Diffusio-phoresis

? Derjaguin, Dukhin, Korotkova, Kolloidn. Zh. **23**, 53 (1961)

? Anderson & Prieve, Sep. Purif. Methods **13**, 67 (1984)



Reaction-Driven Propulsion



R. Golestanian, T.B. Liverpool & A. Ajdari, PRL **94,** 220801 (2005)

Propulsion Velocity

$$v_0 = \frac{\ell}{\tau_{\mathrm{f}}} \qquad \ell = a \left(\frac{3\,\lambda^2}{4\,R^2} \right)$$

- Diffusio-phoresis

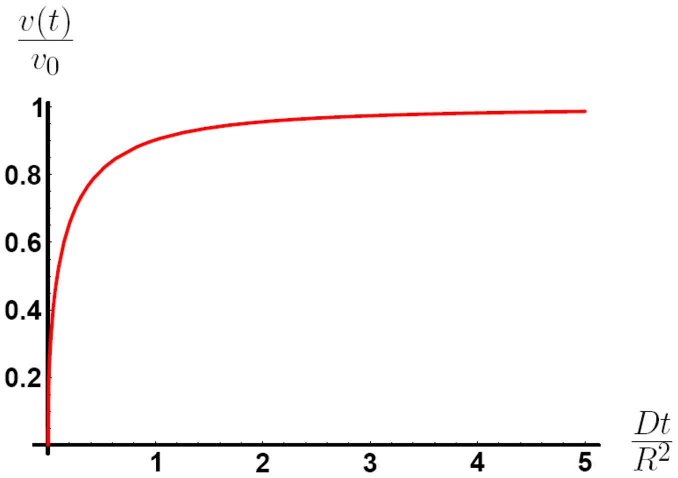
$$\lambda_D^2 = \int_0^\infty dl\; l \left[1 - \mathrm{e}^{-W(l)/k_{\mathrm{B}}T} \right]$$

- Osmio-phoresis

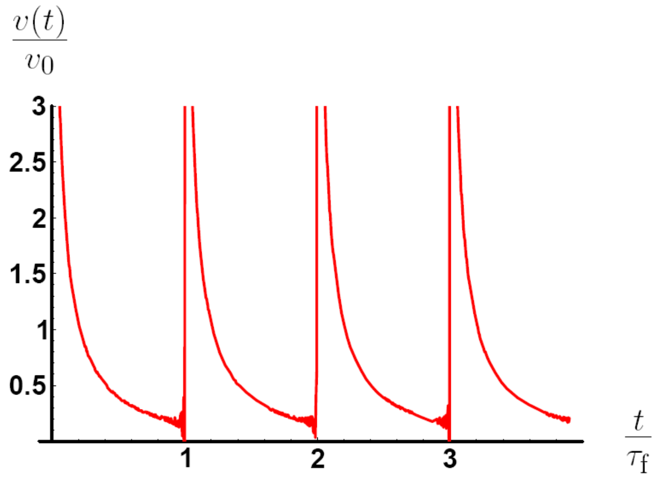
$$\lambda_O^2 = R^2 \left[\frac{\eta L_p/R}{2+20\;\eta L_p/R} \right]$$

Time Response

- Relaxation:



- Periodic particle release:



- Fluctuations: $\frac{(\Delta v)^2}{v_0^2} \sim D\tau_f / R^2$

Reaction Kinetics

- Michaelis-Menten Rule

$$\mathcal{S} + \mathcal{E} \xrightarrow{k_1} \mathcal{S}\mathcal{E} \xrightarrow{k_2} \mathcal{P}_2\mathcal{E} + \mathcal{P}_1 \xrightarrow{k_3} \mathcal{P}_1 + \mathcal{P}_2 + \mathcal{E}$$

$$\frac{1}{\tau_{\mathrm{f}}} = \left(\frac{k_2 k_3}{k_2 + k_3}\right) \frac{C_{\mathcal{S}}(\mathcal{E})}{K_M + C_{\mathcal{S}}(\mathcal{E})}$$

Michaelis constant: $K_M \equiv \frac{1}{k_1} \left(\frac{k_2 k_3}{k_2 + k_3}\right)$

Brownian Agitation

- Rotational Diffusion Time

$$\tau_R = 8\pi\eta R^3/(k_\mathrm{B}T)$$

Directional persistence increases with size

Optimal Design

- Vesicle/bead of radius: $R = 2\ \mu\mathrm{m}$
- Acetylcholinesterase: $1/\tau_{\mathrm{f}} \simeq 25000\ \mathrm{s}^{-1}$
- Propulsion velocity: $v_0 \sim 0.5\,\mu\mathrm{m/s}$
- Rotational diffusion time: 50 s

? *Directional Locomotion*

Conclusion

- **Model A:**

  ? externally controlled

- **Model B:**

  ? reaction-driven