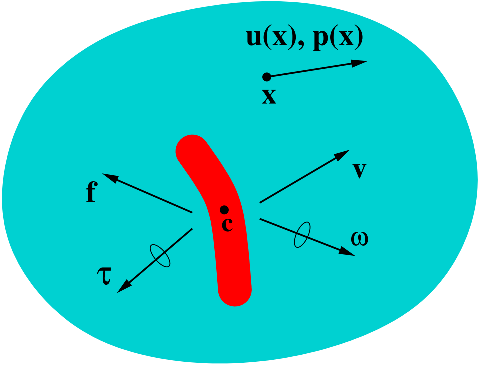
On the Stokesian hydrodynamics of rigid bodies

O. Gonzalez

University of Texas at Austin

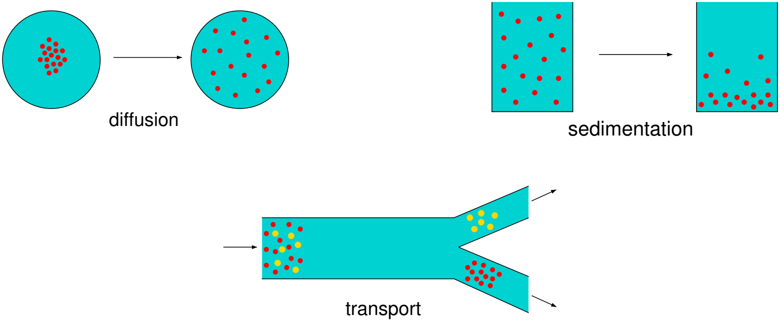
Introduction

Goal. To characterize the hydrodynamic mobility properties of a rigid body in a viscous fluid under Stokes flow conditions.



Introduction

Motivation. Hydrodynamic mobility properties of a body play a central role in models of diffusion, sedimentation and transport.



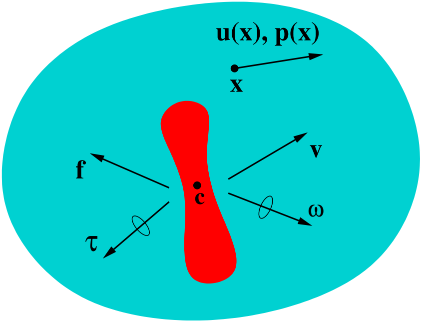
Applications. Microfluidic devices for separation and mixing of particles; magnetic microswimmers; free-soln DNA sequencing.

Outline

Background

Background

Setup. Consider slow, quasi-static motion of a body in an infinite viscous fluid.

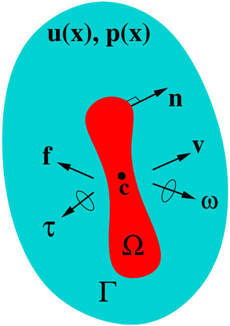


$u(x), p(x)$	velocity and pressure fields in fluid.
f, τ	external force and torque on body.
v, ω	linear and angular velocity of body.
c	reference point for velocities, loads.

Background

Fluid-body equations. Stokes system in exterior domain for fluid; balance of external and hydrodynamic loads for body.

$$\begin{aligned} \Delta u &= \nabla p && \text{in } \mathbb{R}^3 \backslash \Omega \\ \nabla \cdot u &= 0 && \text{in } \mathbb{R}^3 \backslash \Omega \\ u &= v + \omega \times (x - c) && \text{on } \Gamma = \partial\Omega \\ u, p &\to u_\infty, p_\infty && \text{as } |x| \to \infty \end{aligned}$$



$$\begin{aligned} f &+ \int_\Gamma \sigma[u,p]n \, dA &= 0 \\ \tau &+ \int_\Gamma (x-c) \times \sigma[u,p]n \, dA &= 0 \end{aligned}$$

Here $\sigma[u,p] = 2\, sym(\nabla u) - pI$ is stress field in fluid; all quantities non-dimensional.

Background

Basic BVP. Given $(u_\infty, p_\infty, f, \tau)$ determine (u, p, v, ω).

$$\begin{aligned} \Delta u &= \nabla p && \text{in } \mathbb{R}^3 \backslash \Omega \\ \nabla \cdot u &= 0 && \text{in } \mathbb{R}^3 \backslash \Omega \\ u &= v + \omega \times (x - c) && \text{on } \Gamma = \partial\Omega \\ u, p &\to u_\infty, p_\infty && \text{as } |x| \to \infty \end{aligned}$$

$$\begin{aligned} f &+ \int_\Gamma \sigma[u,p] n \, dA &&= 0 \\ \tau &+ \int_\Gamma (x - c) \times \sigma[u,p] n \, dA &&= 0 \end{aligned}$$

Assume Γ is closed, bounded, non-self-intersecting and class $C^{1,\alpha}$; well-developed analysis/numerics based on potential theory.

Background

Stokes matrices. When conditions at infinity are zero, there is an invertible linear map between $(v, \omega) \in \mathbb{R}^6$ and $(f, \tau) \in \mathbb{R}^6$.

$$\begin{aligned} \Delta u &= \nabla p && \text{in } \mathbb{R}^3 \backslash \Omega \\ \nabla \cdot u &= 0 && \text{in } \mathbb{R}^3 \backslash \Omega \\ u &= v + \omega \times (x - c) && \text{on } \Gamma = \partial\Omega \\ u, p &\to 0, 0 && \text{as } |x| \to \infty \end{aligned}$$

$$\begin{aligned} f &+ \int_\Gamma \sigma[u, p] n \, dA &&= 0 \\ \tau &+ \int_\Gamma (x - c) \times \sigma[u, p] n \, dA &&= 0 \end{aligned}$$

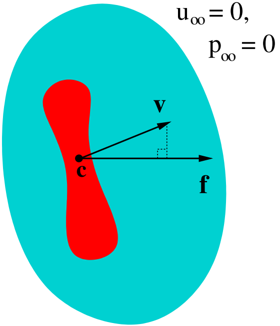
$$(v, \omega) = M(f, \tau), \qquad M = \begin{bmatrix} M_1 & M_3 \\ M_2 & M_4 \end{bmatrix}, \qquad M = M^T > 0$$

$$(f, \tau) = L(v, \omega), \qquad L = \begin{bmatrix} L_1 & L_3 \\ L_2 & L_4 \end{bmatrix}, \qquad L = L^T > 0$$

Mobility coefficient

Mobility coefficient

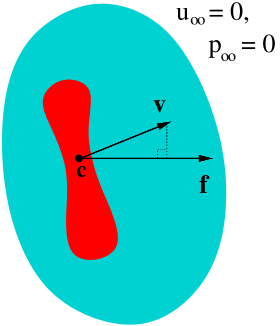
Definition. Consider body subject to a unit force in fluid at rest at infinity; consider velocity along force, average over orientations.



Mobility coefficient

Definition. Consider body subject to a unit force in fluid at rest at infinity; consider velocity along force, average over orientations.

v, f	velocity, force at c
$v_f = v \cdot f$	component along f
$\mathcal{M} = \underset{f \in S^2}{avg}\, v_f$	average over $\lvert f \rvert = 1$

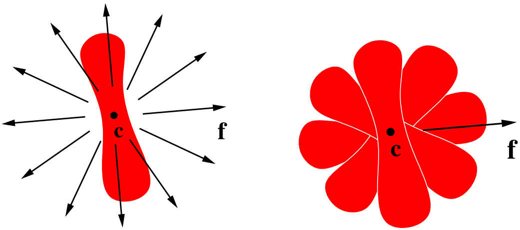


$\mathcal{M}$ is called the mobility coefficient; it is the average velocity imparted to the body along an imposed unit force.

Mobility coefficient

Interpretation. $\mathcal{M}$ is average velocity along a unit force when either force or body orientation are fixed, and other is randomized.

$$\mathcal{M} = \underset{f \in S^2}{avg}\ v_f$$



$\mathcal{M}$ naturally arises in transport problems; proportional to diffusion, sedimentation coefficients.

Mobility coefficient

Characterization. The mobility coefficient $\mathcal{M}$ can be expressed in terms of the Stokes matrix M.

$$(v, \omega) = M(f, \tau), \quad \tau = 0 \qquad \Longrightarrow \qquad v = M_1 f$$

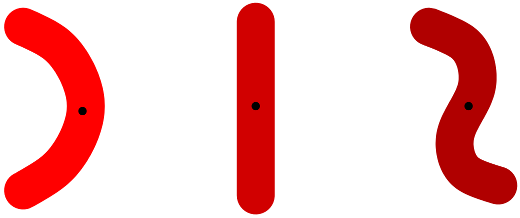
$$v_f = v \cdot f = f \cdot M_1 f$$

$$\mathcal{M} = \underset{f \in S^2}{avg}\, v_f = \frac{1}{3}\, tr(M_1)$$

Can compute using boundary-element techniques; but there are various natural questions for analysis.

Mobility coefficient

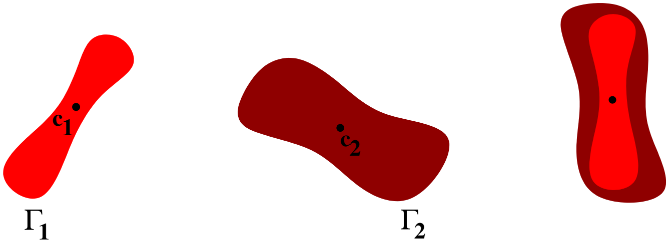
Questions. How does $\mathcal{M}$ vary among bodies of different shape? Are there simple criteria for ordering shapes by $\mathcal{M}$?



Mobility coefficient

Inclusion monotonicity theorem. [Hill & Power; and others]. Let Γ_1 and Γ_2 be body surfaces, with reference points c_1 and c_2. If Γ_1 can be enclosed by Γ_2, with c_1 and c_2 superimposed, then

$$\mathcal{M}_1 \geq \mathcal{M}_2.$$



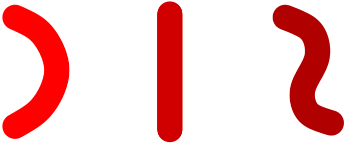
Mobility coefficient

Remarks.

- Inclusion theorem implies

$$\text{“smaller body”} \quad \Longrightarrow \quad \text{“higher mobility”}.$$

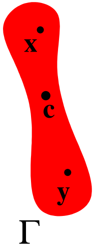
- Result provides little insight for filament-type bodies



Mobility coefficient

Inverse chord theorem. Let Γ be a body surface with reference point c at its centroid. Then

$$2\min_{\mathbf{x},\mathbf{y}\in\Gamma}\frac{1}{|\mathbf{x}-\mathbf{y}|} \;\le\; 6\pi\mathcal{M} \;\le\; \operatorname*{avg}_{\mathbf{x},\mathbf{y}\in\Gamma}\frac{1}{|\mathbf{x}-\mathbf{y}|}.$$



Mobility coefficient

Remarks.

- Theorem implies geometric inequality for arbitrary surfaces

$$2 \min_{x,y\in\Gamma} \frac{1}{|x-y|} \quad \leq \quad \operatorname*{avg}_{x,y\in\Gamma} \frac{1}{|x-y|}.$$

- Theorem implies existence of a characteristic chord length $|x_* - y_*|$ such that

$$6\pi\mathcal{M} = \frac{1}{|x_* - y_*|}.$$

Mobility coefficient

Remarks.

- Lower bound in theorem suggests the heuristic

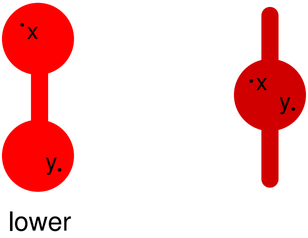
$$\text{“higher } \min_{x,y\in\Gamma} \frac{1}{|x-y|}\text{”} \quad \Longrightarrow \quad \text{“higher mobility”}.$$

Mobility coefficient

Remarks.

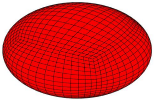
- Upper bound in theorem suggests the heuristic

$$\text{“lower } \underset{x,y\in\Gamma}{avg} \frac{1}{|x-y|}\text{”} \quad \Longrightarrow \quad \text{“lower mobility”}.$$

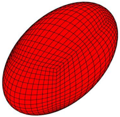


Mobility coefficient

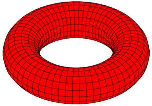
Example bounds. $2\, min_{x,y\in\Gamma} \frac{1}{|x-y|} \ \leq \ 6\pi\mathcal{M} \ \leq \ avg_{x,y\in\Gamma} \frac{1}{|x-y|}.$



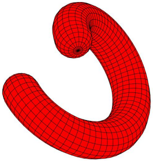
$1.000 \leq 1.209 \leq 1.220$



$1.000 \leq 1.521 \leq 1.533$



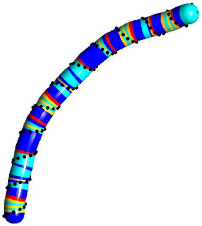
$0.750 \leq 0.966 \leq 0.992$



$0.712 \leq 0.892 \leq 0.921$

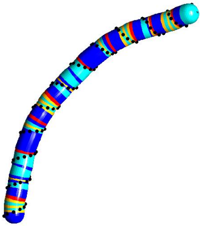
Mobility coefficient

Example application. Mobility coefficient $\mathcal{M}$ can be used to estimate structural features of molecular bodies.



Mobility coefficient

Example application. Mobility coefficient $\mathcal{M}$ can be used to estimate structural features of molecular bodies.



If DNA is modeled as a filament, what would be its effective radius in solution?

Can estimate radius by fitting computed values of $\mathcal{M}$ to experimental data.

Mobility coefficient

Geometric models. For comparison, consider two different models for a DNA sequence S; each has uniform radius r.

Straight model:

axial length determined by number of basepairs in S.

Mobility coefficient

Geometric models. For comparison, consider two different models for a DNA sequence S; each has uniform radius r.

Straight model:

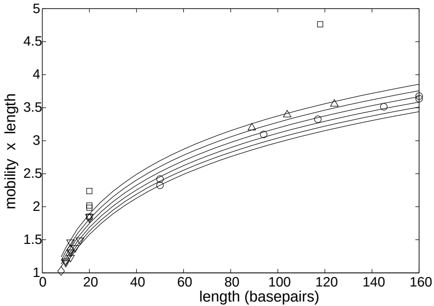
axial length determined by number of basepairs in S.

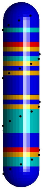
Curved model:

axial length, curvature determined by sequence composition of S.

Mobility coefficient

Results for straight model.





Curves: numerics with $r = 10, 11, \ldots, 15$Å from top to bottom.

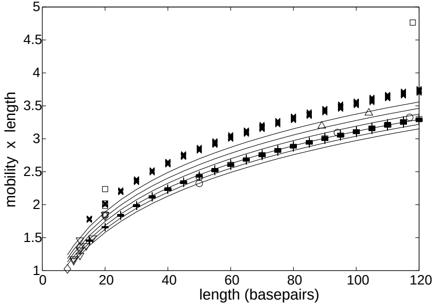
Open circles, triangles: data from sedimentation, diffusion.

Open squares: data from electrophoresis.

Estimate of hydrated radius: $r = 10 - 15$Å.

Mobility coefficient

Results for curved model.



Curves: numerics on straight model as before.

Open symbols: experimental data as before.

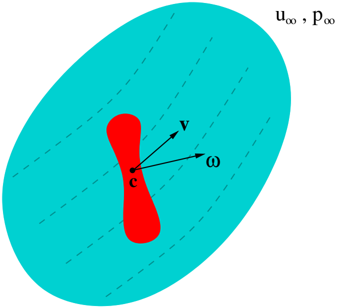
Crosses, pluses: numerics on curved model w/$r = 10$, $r = 15$Å.

Revised estimate of hydrated radius: $r = 12 - 17$Å.

Transport velocity

Transport velocity

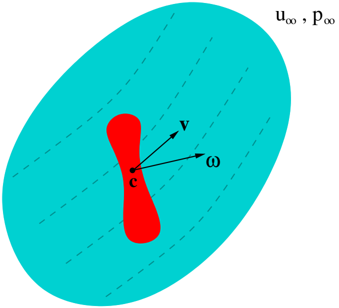
Definition. Consider body in an ambient fluid flow; let flow freely carry body with no external forces acting.



Transport velocity

Definition. Consider body in an ambient fluid flow; let flow freely carry body with no external forces acting.

u_∞, p_∞	ambient flow fields
v, ω	body velocities



(v, ω) are called transport velocities; they are imparted to the body as it is carried by the fluid.

Transport velocity

BVP formulation. Given (u_∞, p_∞) we can determine (v, ω) and disturbed flow (u, p) via the following

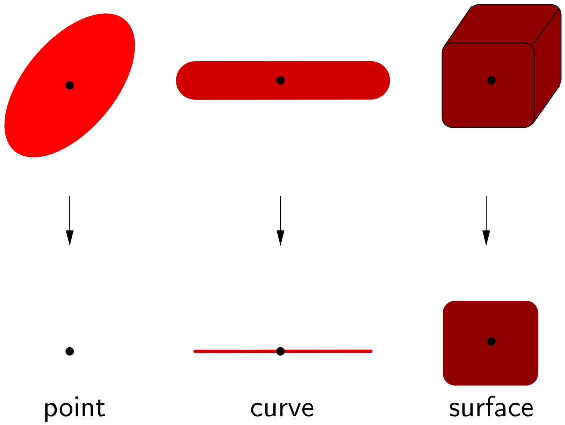
$$
\begin{array}{rcll}
\Delta u & = & \nabla p & \text{in } \mathbb{R}^3 \backslash \Omega \\
\nabla \cdot u & = & 0 & \text{in } \mathbb{R}^3 \backslash \Omega \\
u & = & v + \omega \times (x - c) & \text{on } \Gamma = \partial \Omega \\
u, p & \to & u_\infty, p_\infty & \text{as } |x| \to \infty
\end{array}
$$

$$
\begin{array}{ll}
\int_\Gamma \sigma[u, p] n \, dA & = 0 \\
\int_\Gamma (x - c) \times \sigma[u, p] n \, dA & = 0
\end{array}
$$

Can characterize (v, ω) in terms of Stokes matrix M and loads (f_∞, τ_∞) associated with ambient flow.

Transport velocity

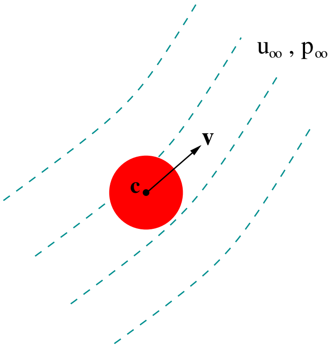
Questions. How do transport velocities depend on body shape? What happens in limiting cases as body volume tends to zero?



Transport velocity

Sphere limit theorem. Consider a sphere of radius r and center c. Then

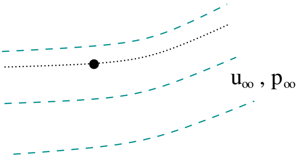
$$\lim_{r \downarrow 0} v = u_\infty(c).$$



Transport velocity

Remarks.

- Theorem implies limiting sphere would follow streamlines.



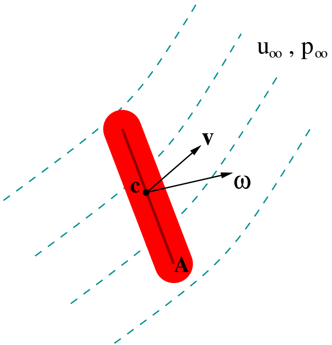
- Theorem extends to zero-radius limit of more general shapes.

Transport velocity

Cylinder limit theorem. Consider a cylinder with axis A and radius r, with capped ends, and reference point c at its centroid. Then

$$\ell_A \cdot \lim_{r \downarrow 0} v = \int_A u_\infty \, ds$$

$$I_A \cdot \lim_{r \downarrow 0} \omega = \int_A (x - c) \times u_\infty \, ds$$

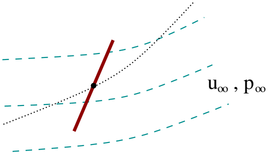


where ℓ_A and I_A are the length and second-moment matrix for the line segment A.

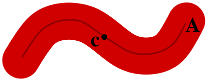
Transport velocity

Remarks.

- Theorem implies limiting cylinder may not follow streamlines.



- Theorem extends to zero-radius limit of general tubular shapes.



Thank You