N-linked Locomotion in Stokes Flow

Jair Koiller, FGV-RJ and AGIMB/Brazil

CDS 280 - Winter

February 7 2006

In the 2/3 of the talk, I show a geometrical mechanics approach for “Purcell’s animat” and its N linked generalization.

This is a warm up exercise for a more difficult problem, which I discuss (but do not solve) in the end:

Swimming as a result of the internal forces generated by the dynein molecular motors.

Outline

History: Caltech, 1970: interdisciplinary animal locomotion year

(G.I. Taylor, J. Lighthill since the 1950's)

intermission: 1980-1990, gauge theory: Shapere and Wilczek

1995 – today : internal force generators: molecular motors

bio-mimetics, robotics, nanotechnology

Part 1. Microswimming as a "gauge theory" (since Purcell, 1976)

Part 2. Discussion on 3 papers: E.Purcell, O. Pironneau, H. Stone

and our N-link version (with Gerusa Araujo)

Part 3. Some possible developments.

for more info: http://www.impa.br/~jair (a mini-course + papers)

Gallery

Howard Berg lab (Harvard) - http://www.rowland.harvard.edu/labs/bacteria/)

Charles Brokaw lab (Caltech) - http://members.cox.net/brokawc/

http://starcentral.mbl.edu/mv5d/ (gallery of friends in the microbial world)

http://www2.cnrs.fr/en/379.htm Microscopic artificial swimmer

http://www.nature.com/nature/journal/v421/n6924/suppinfo/nature01377.html (dynein power stroke)

http://www.sciencemag.org/content/vol288/issue5463/index.dtl (Special Issue of Science, 2000)

PART I: How to Model Microswimming?

It is a GAUGE theory !!

E. M. Purcell, Life at Low Reynolds Number American Journal of Physics vol. 45, pages 3-11, 1977

[*An attempt using classical optimal control:*

Pironneau, O. and Katz, D.F. Optimal swimming of flagellated microorganisms. Journal of Fluid Mechanics 66:39l-415 (1974)]

Part II . Two other papers in JFM and our own versions

1. A gauge theory for microswimming:

Shapere, A., Wilczek, Geometry of self-propulsion at low Reynolds number/Efficiencies of self-propulsion at low Reynolds number.
J. Fluid Mech. 198, 557-585/ 587-599 (1989)

JK, Richard Montgomery, Kurt Ehlers , Problems and Progress in Microswimming, J. Nonlinear Sci. 6:507-541 (1996)

2. Purcell's toy: 3- link swimmer

Becker, L.E., Koehler, S.A., Stone, H.A., On self-propulsion of micro-machines at low Reynolds number: Purcell's three-link swimmer
J. Fluid Mech. 490, pp. 15-35 (2003)

Gerusa Araujo, JK , Self-propulsion of N-hinged 'animats' at low Reynolds number, Qualit. Theor. Dynl. Systems, 1-28 (2003)

Part 3. Some possible developments

1. Not hard: Cells on optical tweezers
2. Very hard: Eukariotic flagella. Modeling the interaction with the molecular motors. Control and coordination. Systems biology.

What is Purcell's 'animat' ?

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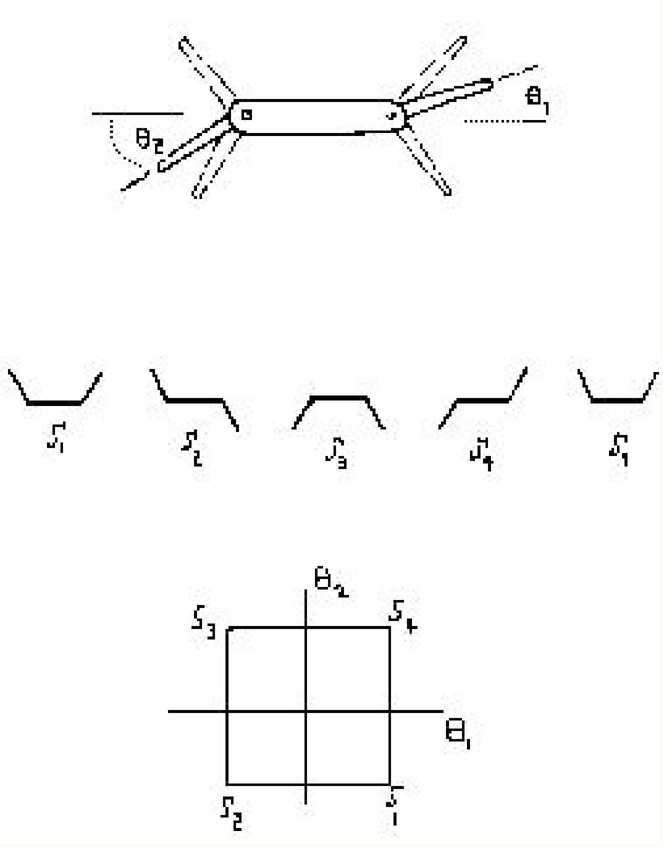

Robotic implementations:

Annette Hosoi (MIT):

http://web.mit.edu/chosetec/www/robo/3link/

Remi Dreyfus et al, (ESPCI/Paris) + H.Stone (Harvard):

http://www2.cnrs.fr/en/379.htm

E. M. Purcells's paper: Life at Low Reynolds Number
American Journal of Physics vol. 45, pages 3-11, 1977.

Historical note: Purcell presented the contents of the paper in the APS annual meeting, in 1976. Since then this became a "cult paper". Purcell said he was under the influence of his ex-student
Howard Berg . Berg directs an important lab in Harvard, and was one of the first person that proposed that bacteria are powered by a rotatory motor.

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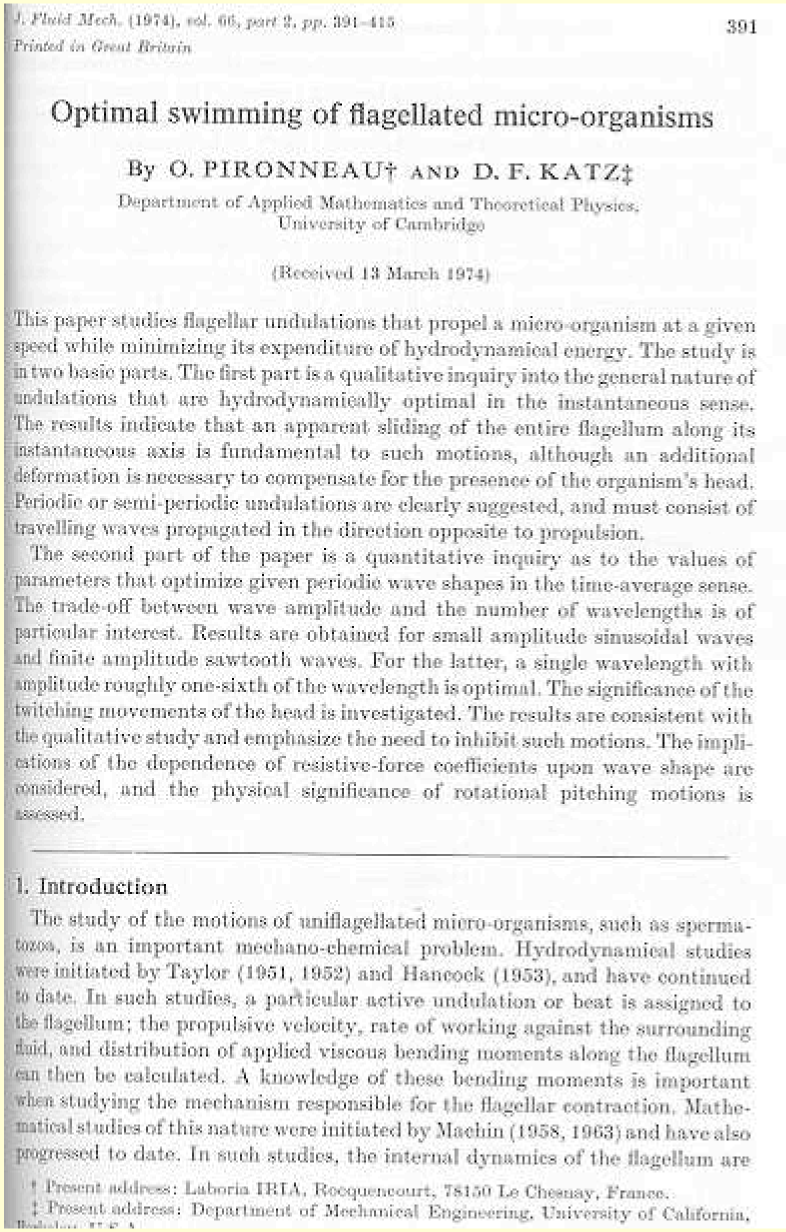

J. Fluid Mech. (1974), *vol.* 66, *part* 2, *pp.* 391–415 391
Printed in Great Britain

Optimal swimming of flagellated micro-organisms

By O. PIRONNEAU† AND D. F. KATZ‡

Department of Applied Mathematics and Theoretical Physics,
University of Cambridge

(Received 13 March 1974)

This paper studies flagellar undulations that propel a micro-organism at a given speed while minimizing its expenditure of hydrodynamical energy. The study is in two basic parts. The first part is a qualitative inquiry into the general nature of undulations that are hydrodynamically optimal in the instantaneous sense. The results indicate that an apparent sliding of the entire flagellum along its instantaneous axis is fundamental to such motions, although an additional deformation is necessary to compensate for the presence of the organism's head. Periodic or semi-periodic undulations are clearly suggested, and must consist of travelling waves propagated in the direction opposite to propulsion.

The second part of the paper is a quantitative inquiry as to the values of parameters that optimize given periodic wave shapes in the time-average sense. The trade-off between wave amplitude and the number of wavelengths is of particular interest. Results are obtained for small amplitude sinusoidal waves and finite amplitude sawtooth waves. For the latter, a single wavelength with amplitude roughly one-sixth of the wavelength is optimal. The significance of the twitching movements of the head is investigated. The results are consistent with the qualitative study and emphasize the need to inhibit such motions. The implications of the dependence of resistive-force coefficients upon wave shape are considered, and the physical significance of rotational pitching motions is assessed.

1. Introduction

The study of the motions of uniflagellated micro-organisms, such as spermatozoa, is an important mechano-chemical problem. Hydrodynamical studies were initiated by Taylor (1951, 1952) and Hancock (1953), and have continued to date. In such studies, a particular active undulation or beat is assigned to the flagellum; the propulsive velocity, rate of working against the surrounding fluid, and distribution of applied viscous bending moments along the flagellum can then be calculated. A knowledge of these bending moments is important when studying the mechanism responsible for the flagellar contraction. Mathematical studies of this nature were initiated by Machin (1958, 1963) and have also progressed to date. In such studies, the internal dynamics of the flagellum are

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‡ Present address: Department of Mechanical Engineering, University of California,

This paper is an extended version of their article in Caltech's proceedings of the animal locomotion year (1973).

modelled via consideration of the equilibrium between the applied viscous bending moment and an internally induced bending moment. This internal moment, which is decomposed into passive and active effects, physically characterizes the contraction mechanism. The result of such a study is the determination of the flagellar undulations. Thus, studies of the contraction mechanism can be coupled with hydrodynamic determinations of swimming trajectories, e.g. Brokaw (1972).

In this paper, we present a third approach. We start with the fact that an organism is swimming forward at a certain rate, and we inquire as to the most economical way of doing so. The object of this approach is to determine the flagellar undulations responsible for the 'optimal' propulsion. Thus our study is intimately connected with the two previous types of investigations. It would seem reasonable to stipulate that an economical way of swimming is one in which the hydrodynamical energy expenditure by the organism is kept to a minimum. Indeed, this is a problem with which nature was originally faced when designing flagella. Thus our results reflect upon the facility of the evolutionary process, as well as presenting criteria upon which to evaluate the hydrodynamic efficiency of swimming organisms. Of course, when more is understood about the internal mechanics and dynamics of flagella, it may be possible to include specific internal considerations as well. Ideally we might ask, "Given that an organism swims from A to B in a given time, how can the total energy expenditure during this interval be minimized?" This is an optimal control problem of non-standard type,[†] for which no general theory has been developed. We shall therefore solve an alternative, though closely related problem in which the instantaneous rate of working is minimized at each time.

Throughout the analytical development of the problem we shall use resistive-force theory to describe the propulsive hydrodynamics. That is, we regard the local tangential and normal forces per unit length acting on the flagellum as proportional to the local tangential and normal velocities of the axis of the flagellum, the coefficients of proportionality being the resistance coefficients C_L and C_N, respectively. In the qualitative studies of this paper in §§3 and 4, we assume that C_N and C_L are constant. Later, in the quantitative studies of §§5, 6 and 7, we consider the dependence of C_N and C_L upon the flagellar wave shape. We shall make use of a complementary resistive-force approximation when considering the influence of the head of an organism. The head contributes a drag force $\mathbf{D}_H$ and moment $\mathbf{M}_H$ to the net viscous reactions acting upon the organism. We assume that $\mathbf{D}_H$ and $\mathbf{M}_H$ depend only upon the movements of the head itself, and that the head is sufficiently symmetrical that its translational and rotational motions are not coupled.[‡] Thence we can introduce resistive-force and moment coefficients for the head; throughout this paper we consider an effectively spherical head of radius a. Thus

$$\mathbf{D}_H = C_H \mathbf{v}_H, \quad \mathbf{M}_H = T_H \boldsymbol{\omega}_H, \tag{1.1), (1.2}$$

[†] The problem is non-standard in the sense of optimal control theory in that the boundaries are not stationary.

[‡] This assumption is implicit in the resistive-force treatment of the flagellum.

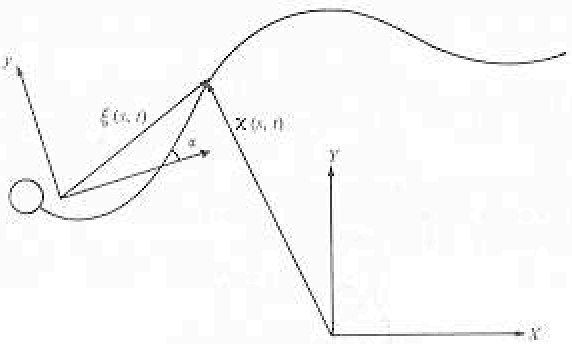


FIGURE 1. $\boldsymbol{\chi}(s,t)$ is the position vector as measured in the fixed X, Y frame of reference. $\boldsymbol{\xi}(s,t)$ is the position vector as measured in the x, y frame moving with the organism.

where $\mathbf{v}_H$ and $\boldsymbol{\omega}_H$ are respectively the absolute linear and angular velocities of the head, and $C_H = 6\pi\mu a$ and $T_H = 8\pi\mu a^3$, the values for an isolated sphere, μ being the viscosity. Despite our analytical use of resistive-force theory, we shall, however, pose the general hydrodynamical problem first, since the applicability of the methods of optimal control theory does not require use of this approximation.

2. Statement of the problem

Our micro-organism is comprised of a deformable flagellum attached to a rigid head. We consider a slender cylindrical flagellum of radius r_0 and length L such that $r_0 \ll L$, and assume that it does not stretch or twist about its local axis. Since all points on a particular cross-section then move with approximately the same velocity, we can describe the motion of the flagellum by the position vector $\boldsymbol{\chi}(s,t)$, with $s \in [0,L]$ and $t \in [0,T]$, to a point M on the axis, where $\boldsymbol{\chi}$ is measured in a co-ordinate system fixed in space (see figure 1). The absolute velocity $\mathbf{v}(s,t)$ of M is given by

$$\mathbf{v}(s,t) = \partial\boldsymbol{\chi}/\partial t = v_l \mathbf{l} + \mathbf{v}_n \mathbf{n}, \tag{2.1}$$

where $\mathbf{l}(s,t)$ and $\mathbf{n}(s,t)$ are respectively the unit forward tangent and normal to the flagellum and, for algebraic clarity, we have considered only two-dimensional flagellar undulations. Thus,

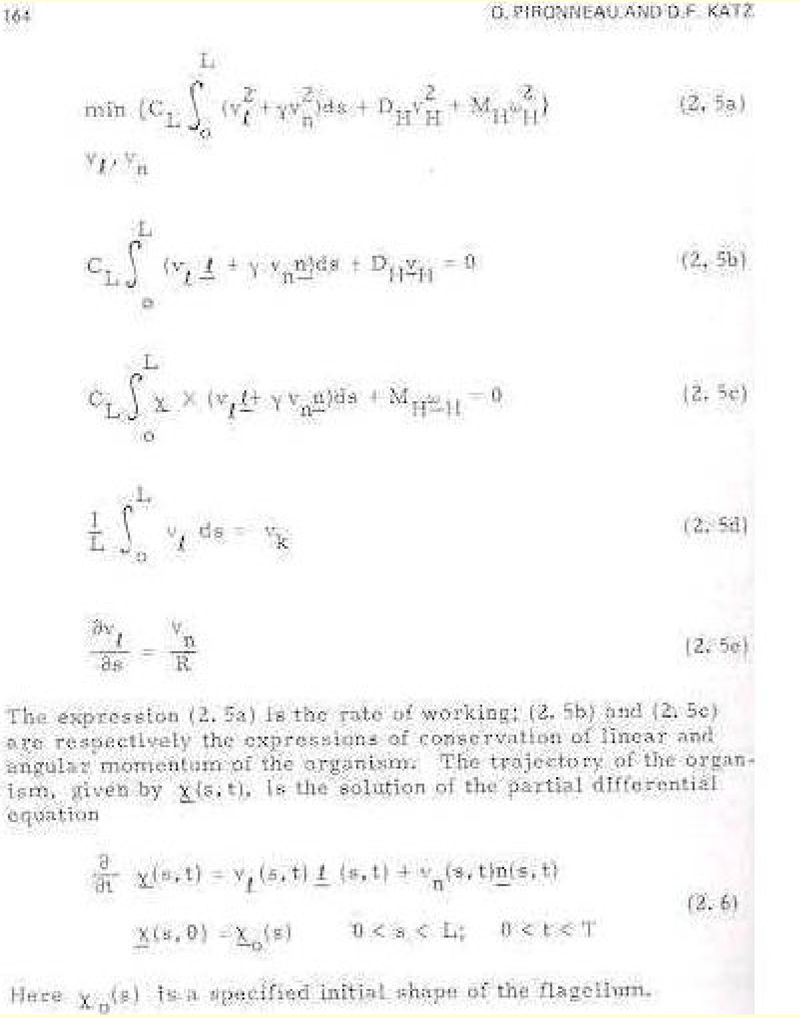
$$\mathbf{l} = \frac{\partial\boldsymbol{\chi}/\partial s}{\|\partial\boldsymbol{\chi}/\partial s\|}, \quad \mathbf{n} = R\,\partial\mathbf{l}/\partial s, \tag{2.2), (2.3}$$

where $R(s,t)$ is the local radius of curvature. The inextensibility condition for the flagellum implies that

$$\partial\,|\boldsymbol{\chi}(s+\delta s,t)-\boldsymbol{\chi}(s,t)|^2/\partial t = 0 \quad \text{for all} \quad s \in [0,L], \quad t \in [0,T]. \tag{2.4}$$

Equation (2.4) yields the relation

$$\partial v_l/\partial s = v_n/R. \tag{2.5}$$



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$$\min_{v_\ell,\, v_n} \left(C_L \int_0^L (v_\ell^2 + \gamma v_n^2)\,ds + D_H v_H^2 + M_H \omega_H^2\right) \tag{2, 5a}$$

$$C_L \int_0^L (v_\ell \underline{\ell} + \gamma v_n \underline{n})\,ds + D_H \underline{v}_H = 0 \tag{2, 5b}$$

$$C_L \int_0^L \underline{\chi} \times (v_\ell \underline{\ell} + \gamma v_n \underline{n})\,ds + M_H \underline{\omega}_H = 0 \tag{2, 5c}$$

$$\frac{1}{L} \int_0^L v_\ell \, ds = v_k \tag{2, 5d}$$

$$\frac{\partial v_\ell}{\partial s} = \frac{v_n}{R} \tag{2, 5e}$$

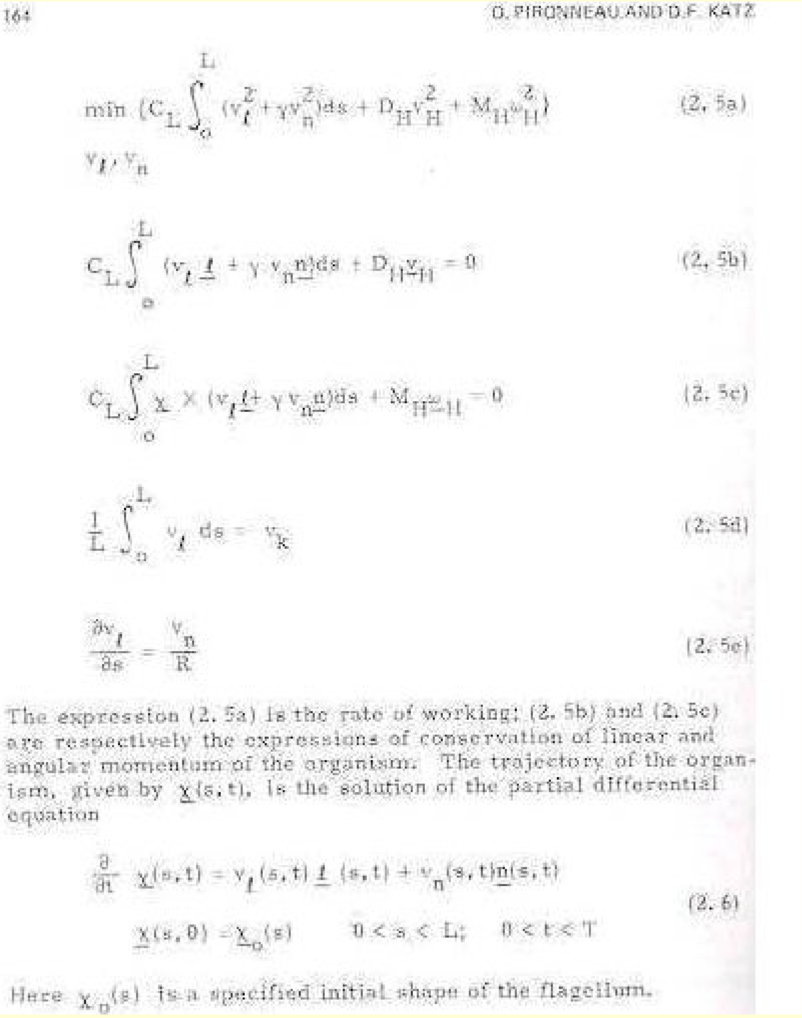
The expression (2, 5a) is the rate of working; (2, 5b) and (2, 5c) are respectively the expressions of conservation of linear and angular momentum of the organism. The trajectory of the organism, given by $\underline{\chi}(s,t)$, is the solution of the partial differential equation

$$\begin{aligned} \frac{\partial}{\partial t}\, \underline{\chi}(s,t) &= v_\ell(s,t)\,\underline{\ell}(s,t) + v_n(s,t)\,\underline{n}(s,t) \\ \underline{\chi}(s,0) &= \underline{\chi}_0(s) \qquad 0 < s < L; \quad 0 < t < T \end{aligned} \tag{2, 6}$$

Here $\chi_0(s)$ is a specified initial shape of the flagellum.

EXERCISE:

What is the problem of using the traditional optimal control approach ?



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$$\min_{v_\ell,\, v_n} \left(C_L \int_o^L (v_\ell^2 + \gamma v_n^2)\,ds + D_H v_H^2 + M_H \omega_H^2\right) \tag{2, 5a}$$

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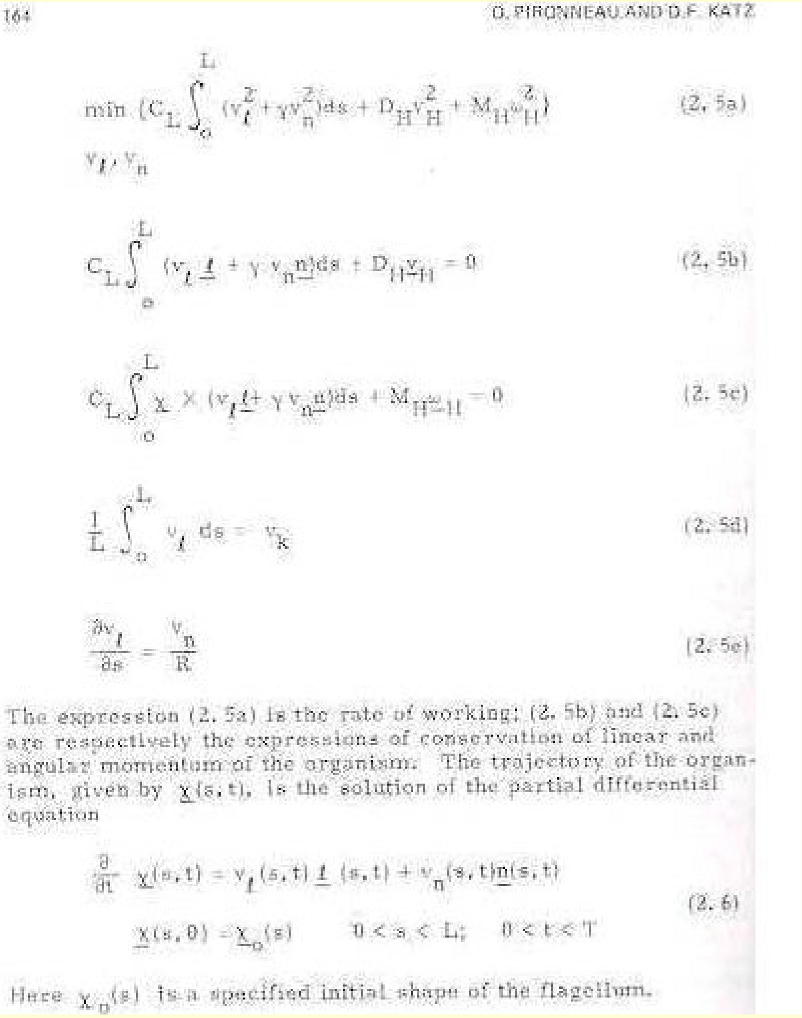
NO TIME!!!!!!



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$$\min_{v_\ell, v_n} \left(C_L \int_0^L (v_\ell^2 + \gamma v_n^2)\,ds + D_H v_H^2 + M_H \omega_H^2\right) \qquad (2.5a)$$

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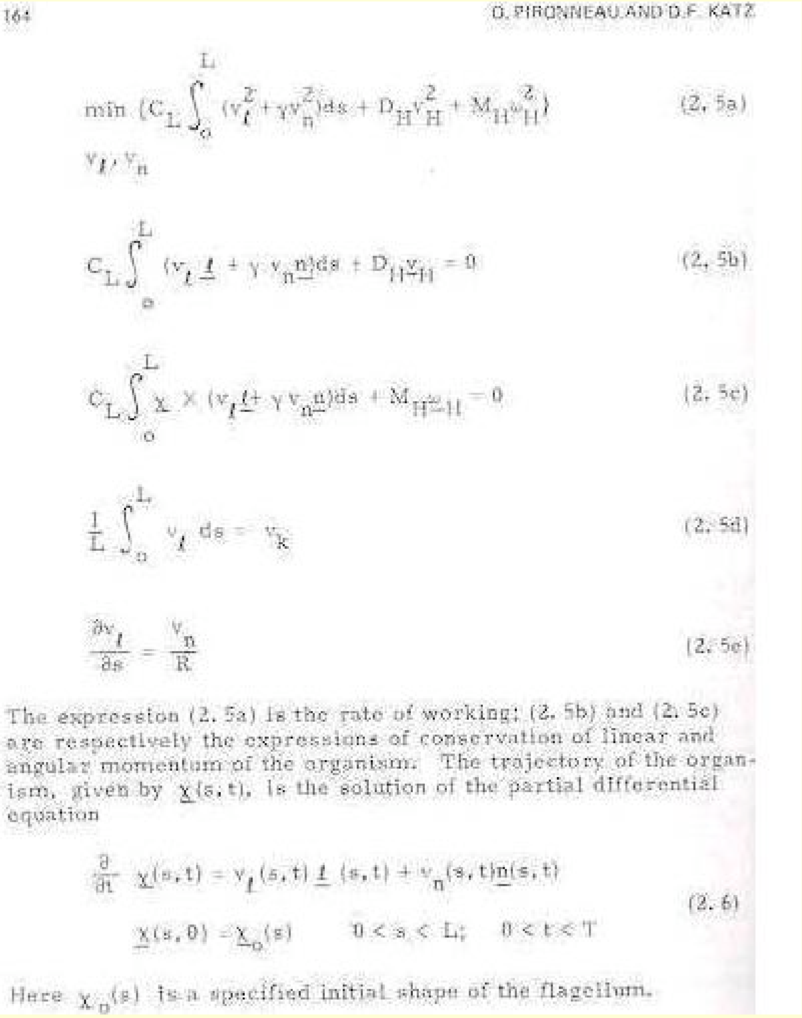
NO TIME!!!!!!

The need to generate “areas” in shape space was not taken in consideration.



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NO TIME!!!!!!

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So this approach was not OK.

What is in order?

WHAT IS IN ORDER?

Answer: Geometric Mechanics!!!

- **A principal bundle structure with located (Q) and unlocated (S) shapes, and group G = SE(3)**
- **A metric on Q and a "fat" connection in the bundle (G , Q , S)**

H _ V

Optimization: subriemannian metric ; prescribed holonomy

References:

Shapere/Wilczek (1989, J.Fluid Mechanics)
JK,R.Montgomery, K.Ehlers (1996,J. Nonlinear Sci. 6:507-541)

JFM paper on Purcell’s swimmer by H.Stone’s group

_ Modeling is based on [we think correct, by complicated, approach]

“torque difference or *strain forcing* that the mechanism …
applies to the surrounding fuid, and represents the external
torque applied to link S1 minus that on link S2.

… This strain forcing of the motion may be thought of as resulting from a rubber band stretched across the active joint, or alternatively as twice the torque exerted by one side on the other via a motor, for example.”

_ The authors justify rigorously the use of the zero order Purcell approximations for Stokes equations solutions.

_ They compute the curvature of the connection at the straight configuration (but they do not use our jargon).

_ They analyze and explain some of the motions.

(they are sometimes not intuitive!)

Gerusa Araujo, JK , Self-propulsion of N-hinged 'animats' at low Reynolds number, Qualit. Theor. Dynl. Systems, 1-28 (2003)

_ Modeling is based directly on the fundamental insight for self propulsion at low Reynolds number (masterfully summarized by J. Lighthill in his 1975 John von Neumann lecture):

"The organism's motile activity, in fact, is able to specify the instantaneous rate of deformation of its external surface only *to within an arbitrary rigid body movement*. That movement, comprising a translation and a rotation, is uniquely determined by the requirement that the forces between the body and the fluid form a system of forces with zero [force] resultant and zero moment".

_ The " linear algebra of Aristotelian physics" is systematically explored.

Further developments (in order, quite doable)

_ Curvature of the connection, at any point of shape space.

_ Get, via genetic algorithms, intuition for better locomotion strategies.
Hook with optimization codes.

_ Cells on optical tweezers (motion subject to external forces)

Part 3. The next wave: Modeling the action of dynein molecular motors

_ Find a simple, but reasonable, model for the sliding of microtubules - perhaps based on Lighthill's "doublets"

_ Show that this internal force generation becomes equivalent to Peskin's immersed boundary method as Reynolds tends to zero.

http://www.siam.org/meetings/an99/peskin.htm

_ Combine with (calcium) control vs. hydrodynamical effects

_ Tie with Systems Biology

http://www.cds.caltech.edu/~doyle/shortcourse.htm

Many research groups on each piece (google them)

A crash course on Eukariotic flagella

http://www.cytochemistry.net/Cell-biology/cilia.htm

Charles Brokaw (Caltech)
http://www.cco.caltech.edu/~brokawc/Demo1/BeadExpt.html

Michael Holwill
http://www.foresight.org/Conferences/MNT6/Papers/Taylor/

Peter Satir

http://www.wadsworth.org/albcon97/abstract/guevara.htm

Information about Molecular Motors

Feynman http://www.zyvex.com/nanotech/feynman.html

Three sites to start from...

http://www.bmb.leeds.ac.uk/illingworth/motors/

http://mitacs-gw.phys.ualberta.ca/mmpd/tutorials/cell/motor_proteins.php?

http://www.foresight.org/Conferences/MNT11/

Thanks to …

Control and Dynamical Systems Alliance !!

http://www.cds.caltech.edu/~murray/projects/ed02-fipse/

INFORMATION SECTION COMING SOON!