Langevin simulations of protoplasmic streaming in non-Euclidean geometry

Shuta Noro(1), Masahiko Okumura, Satoshi Hongo, Shinichiro Nagahiro, Toshiyuki Ikai, Madoka Nakayama and Hiroshi Koibuchi(2)
National Institute of Technology (KOSEN), Sendai College, Natori, Japan
E-mail: (1)noro@sendai-nct.ac.jp, (2)koi-hiro@sendai-nct.ac.jp

Abstract. The protoplasmic streaming in plant cells enables the transportation of biological materials. This circular flow was experimentally observed with laser Doppler velocimetry, and it was reported that there are two peaks in the velocity distribution. Recently, we reported that these peaks are numerically reproduced by the stochastic or Langevin Navier-Stokes (N-S) simulation technique. However, interactions between fluid and the biological materials have not yet been implemented. In this report, we show that this complex interaction can be simulated in the N-S equation with the Finsler geometry (FG) modeling technique by including an internal directional degree of freedom $\sigma (\in S^1$: circle) corresponding to the small biological materials. We find that the interaction effectively makes the viscosity coefficient small when the variable $\sigma$ is uniformly aligned.

1. Introduction

Flows in cells of living organisms such as animals and plants are considered to be multiphase flows. This multiphase flow is complex because the fluid, called protoplasm, includes several biological materials, and details regarding the interaction of the fluid with the biological materials are unknown. This flow in the cells is called protoplasmic streaming.

Kamiya et al. observed a velocity distribution of streaming in rhizoid, leaf and internode cells of Nitella flexilis [1]. This streaming inside the cells enables the transportation of biological materials. Kawakubo et al. reported that the motion of chlorophyll in Chara cells is induced by myosin molecules interacting with the actin filaments [2]. Several studies have focused on the molecular motors, and at present, the transportation in the flow system inside cells is understood to be caused by the myosin-actin mechanism [3].

R. Mustacich et al. experimentally observed the velocity of the protoplasmic streaming of living algae cells using laser Doppler velocimetry (LDV) [4]. They reported that there are two peaks in the velocity distribution. Meent et al. found that the flow is not parallel but rotating in a cylindrical cell of Characean algae [5]. Recently, we reported that these peaks are numerically reproduced by the stochastic Navier-Stokes (N-S) simulation technique without the rotation of streaming and concluded that the origin of the peaks is the stochastic nature of the fluid particles [6].

However, in the simulation of Ref. [6], the interaction of fluids with biological materials is neglected. Here, in this report, we show that this complex interaction can be simulated by using the N-S equation based on the Finsler geometry (FG) modeling technique. In this FG modeling,
we include an internal directional degree of freedom $\sigma (\in S^1$: circle) corresponding to the small biological materials.

In this study, 2-dimensional (2D) Couette flow (Fig. 1(a)) representing the surface of a cylindrical cell is solved by using a hybrid technique combining the N-S simulation with Brownian random force and a Monte Carlo (MC) simulation. In the N-S simulation, the flow field is obtained by solving the N-S equation with a random force, and in the MC simulation, the internal degrees of freedom $\sigma$ are updated for the Finsler metric. We show that the viscosity coefficient effectively becomes small (large) when the variable $\sigma$ is randomly (uniformly) aligned. This result implies that the complex interaction between fluids and biological materials, which are assumed to be solid, is implemented in the model constructed on the basis of the FG modeling technique.

![Figure 1](image_url)

**Figure 1.** (a) Computational domain, and (b) internal variable $\sigma_{ij}$ at the lattice site $(i,j)$, where the site and its nearest neighbor sites are denoted by the numbers 0, 1, 2, 3, and 4.

2. Computational method

2.1. Governing equation

The 2D incompressible N-S equations, which we solve in this paper, are written in the form of the vorticity equation with Brownian random force such that

$$\frac{\partial \omega}{\partial t} = - (\vec{V} \cdot \nabla) \omega + \nu \Delta \omega + (\nabla \times \vec{\eta}(t))_z,$$

where $\vec{V} = (V_x, V_y)$ is the fluid velocity obtained from the stream function $\psi$ and $\omega$ is the vorticity, $\omega = (\nabla \times \vec{V})_z$. The parameter $\nu$ is the kinematic viscosity coefficient; $\nu \simeq 1 \times 10^{-6}$ m$^2$/s in the case of water at room temperature. $\vec{\eta}(t)$ is a Gaussian white noise or a Gaussian random force corresponding to the Brownian motion of fluid particles or a lump of fluid particles. The components of $\vec{\eta}(t)$ are assumed to satisfy

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D \delta_{ij} \delta^{mm} \delta(t-t'),$$

where $\langle \cdot \rangle$ denotes the expectation. $D$ is the strength of the random force, and the suffix $i$ denotes the fluid position. No confusion is expected between the symbols of the kinematic viscosity $\nu$ and the superscript of the Gaussian random force $\eta^i(t)$.

In the discrete form of the Laplace operator for $\Delta \omega$ and $\Delta \psi$ in Eq. (1), the Finsler metric

$$g_{ab} = \begin{pmatrix} 1/v_{i,x}^2 & 0 \\ 0 & 1/v_{i,y}^2 \end{pmatrix}$$

(3)
is used (detailed information will be reported elsewhere). Here, \( v_x \) and \( v_y \) are the Finsler lengths along the \( x \) and \( y \) directions at \((x, y)\). The discrete expressions at the site \((i, j)\) on a regular square lattice are

\[
v_{i,x} = |\sigma_{i,x}| + v_0, \quad v_{i,y} = |\sigma_{i,y}| + v_0,
\]

where \( \sigma_{i,x(y)} \) is the \( x \) (or \( y \)) component of the internal degrees of freedom \( \sigma_i \) at the site \( i \) (Fig. 1(b)). \( v_0 \) is a cutoff, which effectively plays a role in the anisotropic strength for the variable \( \sigma \).

2.2. Hamiltonian for the internal variable

The internal variable \( \sigma \) is updated by the MC technique with the Hamiltonian corresponding to the term \( \nu \Delta \omega \) in Eq. (1). The discrete expressions for the total Hamiltonian \( S \) for \( \sigma \) are obtained by including several terms such that

\[
S = \lambda S_0 + \nu S_\nu + S_E, \quad S_0 = \frac{1}{2} \sum_{ij} \left[ 1 - 3(\sigma_i \cdot \sigma_j)^2 \right], \quad S_\nu = \sum_{ij} \nu_{ij} (\omega_j - \omega_i)^2, \quad S_E = -E \sum_{ij} (\sigma_i \cdot \vec{e})^2, \quad \vec{E} = E\vec{e}.
\]

The first term \( S_0 \) is the Lebwohl-Lasher potential for \( \sigma \) [7], the second term is the term corresponding to \( \nu \Delta \omega \) in Eq. (1), and the final term represents the energy for the external field \( \vec{E} \). In the Hamiltonian, \( \sum_{ij} \) denotes the sum over bond \( ij \) connecting two neighboring vertices \( i \) and \( j \). The coefficient \( \nu \) is the kinematic viscosity coefficient. The symbol \( \nu_{ij} \) in \( S_\nu \) is given by

\[
\nu_{ij} = \frac{1}{4} \left( \frac{v_{i,x}}{v_{i,y}} + \frac{v_{j,x}}{v_{j,y}} \right), \quad \nu_{ij} = \nu_{ji}.
\]

The partition function is defined by

\[
Z = \sum_\sigma \exp (-S),
\]

where \( \sum_\sigma \) denotes the sum over all possible configurations.

2.3. Hybrid simulation technique

The simulation procedure is as follows: The first step is to update the variable \( \sigma \) by the canonical (or Metropolis) MC technique using the Hamiltonian \( S \) in Eq. (5). This variable is randomly updated to new \( \sigma'(\in S^1) \) with the probability \( \text{Min}[1, \exp(-\delta S)] \). This first step is performed for sufficiently many MC sweeps (MCSs). The next step is to solve the N-S equation in Eq. (1) by the iteration technique. These two steps are repeated. The initial configurations of \( \sigma \) are randomly generated. The total number of MCSs for \( \sigma \) is fixed to \( 10^5 \) in every step.

2.4. Boundary conditions and input parameters

The computational domain is shown in Fig. 1(a). The \( x- \) and \( y\)-axis denote the wall-parallel and wall-normal directions. This computational domain covers the following region: 0.5 mm in \( x \) and 0.5 mm in \( y \). The total number of grid points is 100 and 100 in the \( x \) and \( y \) directions, respectively. On the upper and lower boundaries, the fluids are driven by constant velocity \( V_B = 0.5 \text{ mm/s} \). The periodic boundary condition is given in the parallel direction. The discrete time step is \( \Delta t = 8 \times 10^{-7} \text{ s} \), and the strength of the Brownian force is fixed at \( D = 400 \) in the simulation unit (see Ref. [6]).
3. Results and discussion

Figure 2(a) shows the distribution or normalized histogram $h(V_x)$ of the absolute velocity $|V_x|$. The height of $h(V_x)$ is normalized such that the maximum height is equal to 1; the horizontal axis is also normalized. In Figs. 2(a),(b), the symbol (○), denoted by Regular, represents the results in Ref. [6], where the Finsler metric is not used and the variable $\sigma$ is not included. The symbol (△), denoted by FG(iso), represents the results of the FG model for the isotropic case, where the direction of $\sigma$ is random. The symbol (▽), denoted by FG(aniso), represents the results of the FG model for the anisotropic case, where the direction of $\sigma$ is aligned with some spontaneous direction.

We find that the result of FG(iso) is almost the same as the Regular data. This outcome is reasonable because the isotropic case in the FG model should have no influence on any physical quantities. We also find that the peak position of FG(aniso) moves to the right of the Regular data. This observation implies that the viscosity is effectively reduced by the interaction of fluids with biological materials [6]. Indeed, it is numerically confirmed in Ref. [6] that the peak position moves to the right (left) along the $|V_x|$ axis if $D$ is decreased (increased). Moreover, if the kinematic viscosity $\nu_e$ is decreased, then $D$ is expected to decrease because the macroscopic relaxation time is nontrivially dependent on $\nu_e$ [6].

Figure 2(b) shows the velocity $V_x$ vs. $y$. Both of the plotted $V_x$ results are found to be linear, and this linear behavior indicates that the nontrivial behavior of $h(V_x)$, which has two different peaks, is not always reflected in the dependence of $V_x$ on $y$.

![Image](image_url)

Figure 2. (a) The distribution $h(V_x)$ vs. $|V_x|$, and (b) $V_x$ vs. $y$.

The simulation unit of the N-S equation is not always the same as that of the MC simulations; detailed information, including the discretization of the Laplace operator, will be reported elsewhere.

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