

Finite Element Modeling of Active Particles

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Abstract

In this presentation, we will discuss how to apply the Finite Element Method (FEM) to active matter problems, such as phoretic microswimmers. We use this method to solve numerically the two common phoretic microswimmers models, i.e. the self-diffusiophoretic model and the self-electrophoretic model, which are described by non-linear and coupled differential equations, e.g., Nernst-Planck Equation, Navier-Stokes Equation, and Poisson Equation, which are commonly known as electrokinetic equations. In this presentation, we will also discuss the advantages and disadvantages, when we apply FEM to solve electrokinetic equations. Furthermore, we will also discuss a scheme to reduce the non-physical error due to the discretization, namely spurious flow and spurious flux.

I. INTRODUCTION

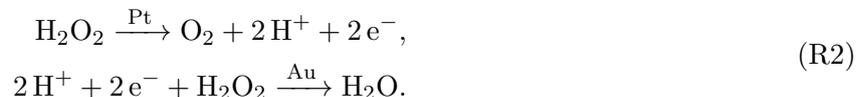
In the recent decades, active matter has attracted many scientists to study this topic. One of the interesting topics from active matter is about self-propelled colloidal particle systems (microswimmers). These systems have some potential applications for human life, such as cancer treatment [1, 2], drug delivery [3–6], and microfluidic mixing [7–10]. A particular class of active colloids, which is often connected with these applications, is artificial self-phoretic colloids [11].

Self-phoretic colloids are propelled by using self-generated fields due to the interaction between solute molecules and the colloid particle. These gradients are typically caused by chemical decomposition reactions which occur on the surface of the particle. The most common systems for understanding self-phoresis are Au-Pt bimetallic rod (Fig. 1a) and Pt-coated Janus spheres (Fig. 1b) that decompose hydrogen peroxide (H_2O_2) into water (H_2O) and oxygen (O_2) [12]. As a simple case, the decomposition of hydrogen peroxide follow the reaction:



The correct description of self-propelled motion is still under debate. Many scientists try to model the motion of Janus particles. In the previous presentations, we have already learned about one of the models to describe the motion of Janus particles, namely *self-diffusiophoresis*. In this model, the motion of a Janus particle is generated by the concentration gradient of neutral species in the solution. This concentration gradient comes from the any decomposition reaction with charge neutral product, for example reaction R1, which only occurs on the reactive side of the Janus particle, e.g. on the Pt coated side of the Janus particle in Fig. 1b.

Another model of self-phoretic motion is assuming that the decomposition mechanism of hydrogen peroxide does not occur by the simple reaction R1, but occurs partially electrochemically, e.g., in Fig. 1a, with two half reaction taking place separately on the Au and Pt:



This half reaction creates self-generated electrostatic field, which leads to a self-phoretic motion. This self-phoretic motion is called *self-electrophoresis*.

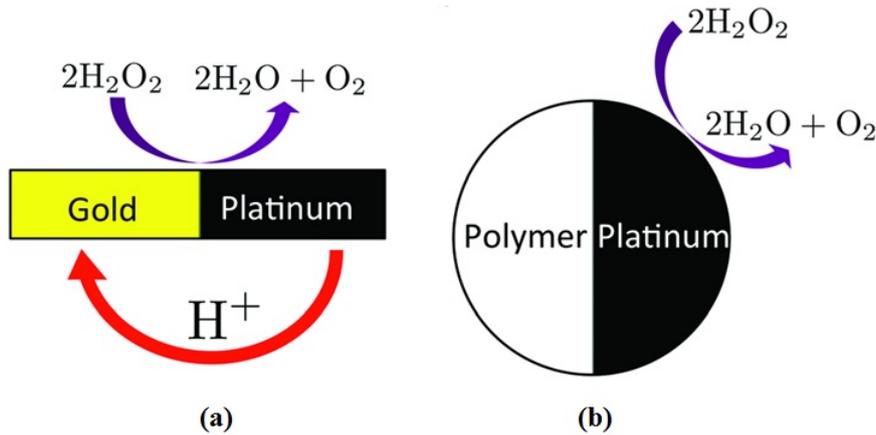


Figure 1: The examples of chemical microswimmer, which are powered by the decomposition of H_2O_2 on their surfaces: (a) Bimetallic (typically gold-platinum) rod. (b) Platinum coated-polymer (usually polystyrene) Janus sphere [12].

II. THEORY OF SELF-PHORETIC MOTION

i. Self-Diffusiophoretic Model

To understand about self-diffusiophoretic motion, we consider a Janus microswimmer as shown in Fig. 1b with radius r . This swimmer is surrounded by the fluid, i.e. water, which contains H_2O_2 . The flux of neutral species is written as

$$\mathbf{j}_0 = c_0 \mathbf{u} - D_0 \nabla c_0 - \frac{D_0 c_0}{k_B T} \nabla \Psi^{diff}, \quad (1)$$

with \mathbf{u} the fluid velocity, k_B the Boltzmann's constant, T the temperature, D_0 the diffusivity of oxygen, c_0 the concentration of oxygen, and Ψ^{diff} the interaction potential between solute molecules, i.e. oxygen, and the swimmer's surface [11]. The first term of Eq. 1 is called *advective term*. The advective term means that the dissolved particles adopt the velocity \mathbf{u} of the fluid [13]. The second and third term of Eq. 1 are called *diffusion* and *migration term* [13]. The diffusion term means that the movement of oxygen is generated by concentration gradient, and the migration term here means that the motion of particles is caused by an interaction potential between oxygen molecules with the swimmer surface.

In this presentation, we consider that our system is in the low-Reynolds number regime. The Reynolds number (Re) is defined as $Re = \rho_f v L / \mu$, with ρ_f the mass density of the fluid, v is the maximum velocity of the swimmer relative to the fluid, L is the size of the swimmer [11]. A low Reynolds number indicates that inertial forces in the system are small compared to the viscous forces [11], and the fluid flow is laminar. Therefore, the flow of fluid is described by Stokes equation which also follows incompressible condition

$$\mu \nabla^2 \mathbf{u} = \nabla p + \mathbf{f}, \quad (2)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (3)$$

with fluid dynamic viscosity μ , hydrostatic pressure p , and force density $\mathbf{f} = c_0 \nabla \Psi^{diff}$. The incompressible condition means that a flow in which the material density is constant within a fluid parcel – an infinitesimal volume that moves with the flow velocity.

In addition, we can assume also that the system have low Péclet number. Péclet number (Pe) is defined as ratio of the rate of advection and the rate of diffusion for transport processes in hydrodynamics systems, $Pe = uL/D_0$, with u the velocity given by fluid flow field and D_0 the diffusivity of neutral species, i.e. oxygen [11]. In the low Péclet number system, for swimmers typically $Pe \leq 10^{-2} \ll 1$, the advective term in Eq. 1 can be neglected, giving

$$\mathbf{j}_0 = -D_0 \nabla c_0 - \frac{D_0 c_0}{k_B T} \nabla \Psi^{diff}. \quad (4)$$

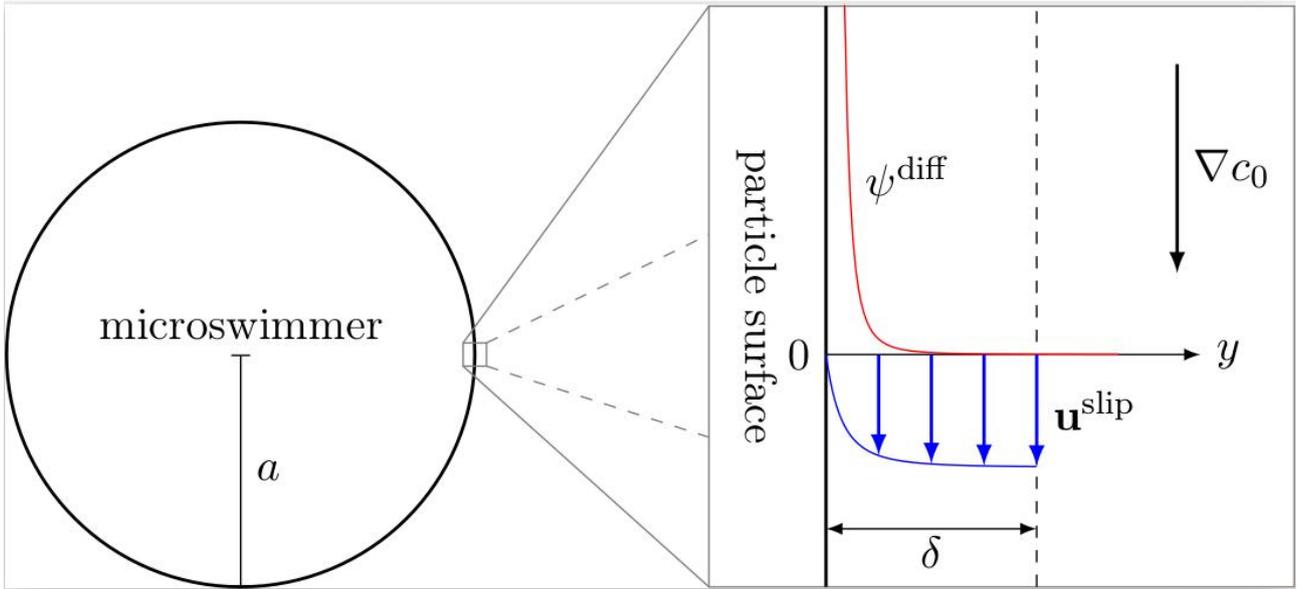


Figure 2: *The slip layer approximation scheme [14]: As the potential interaction between swimmer surface and solute particles decay so fast, then we can assume that the interaction area on microswimmer surface is very small, and the interaction is like a planar surface, and the effective force can be replaced by the slip velocity which act at a distance δ from surface.*

To get the solution for self-diffusiophoretic motion, we solve basically Eq. 2, Eq. 3, and Eq. 4 simultaneously. But, we still need to specify the boundary conditions in this system to find the exact solution. As the first boundary condition, we consider that there is no reaction in bulk [11]. Therefore, we can set

$$\nabla \cdot \mathbf{j}_0 = 0. \quad (5)$$

On the other hand, we also assume that the uniformly concentration and pressure at the point which is far away from the swimmer (we can consider it at infinity), i.e. $c_0 \rightarrow c_0^\infty = 0$ and $p_0 \rightarrow p_0^\infty$ equals atmospheric pressure [11].

To specify the boundary condition for the interaction potential Ψ^{diff} , we can consider that the potential decay so fast with the length scale $\delta \ll r$ due to the potential interaction between neutral species. Therefore, we can consider slip layer condition to self-diffusionphoretic model, which is shown by Fig. 2 and the slip velocity can be assume that acts on the surface of swimmer. The surface slip is given by

$$\mathbf{u}(\mathbf{s}) \cdot \hat{\mathbf{n}} = 0 \quad (6)$$

$$\mathbf{u}(\mathbf{s}) \cdot \hat{\mathbf{t}} = -\zeta(\mathbf{s})\hat{\mathbf{t}} \cdot \mathbf{c}_0(\mathbf{s}) \quad (7)$$

where $\hat{\mathbf{t}}$ is tangential vector to the surface, and

$$\zeta(\mathbf{s}) = \frac{1}{\mu} \int_0^\infty t \left[\exp \left(-\frac{1}{k_B T} \Psi^{diff}(\mathbf{s} + t\hat{\mathbf{n}}(\mathbf{s})) \right) - 1 \right] dt \quad (8)$$

is a parameter which describe the surface-molecules interaction [11].

To determine the velocity of swimmer, we can approach by using two kinds of frame, lab frame and co-moving frame. In lab frame, we consider that the observer does not move. In co-moving frame, we can imagine that the observer sits on the swimmer, and the fluid move. Hence, we can say that $\mathbf{u} = -\mathbf{U}$, where \mathbf{U} is the velocity of swimmer [11]. The co-moving frame is used often in the simulation of self-diffusiophoretic swimmer, because it is easier to implement the simulation setup in the co-moving than lab frame.

ii. Self-Electrophoretic Model

Fundamentally, a self-electrophoretic swimmer is quite similar to the self-diffusiophoretic swimmer, but in self-electrophoretic swimmer, the solute species are not neutral, but have charge. Therefore,

the potential interaction is now an electrostatic potential, which has to be modeled by using Poisson equation. For understanding the physical phenomena of self-electrophoretic swimmer, we consider a bimetallic Au-Pt sphere with radius r . This swimmer is suspended in a fluid, which contains three different ions. The first ion is H^+ , which are produced and consumed by the reaction on swimmer's surface. The another ions are Na^+ and Cl^- . These ions are not involved in the reaction. For simplicity, the ions will be labeled with an index $i \in \{a, +, -\}$ [11]. The index 'a' stands for 'active'. The word active means that this ion is produced or consumed by the swimmer, i.e. H^+ ions. The index (+) and (-) refer to the positive and negative salt ions in solution, i.e. Na^+ and Cl^- ions.

The motion of ions in fluid will create a flux of each ion species, which is defined as

$$\mathbf{j}_i = c_i \mathbf{u} - D_i \nabla c_i - \frac{D_i z_i e c_i}{k_B T} \nabla \Phi^{el}, \quad (9)$$

with \mathbf{u} the fluid velocity, D_i the diffusivity of ion, c_i the concentration of ion, z_i valency of ion and Φ^{el} the electrostatic potential, which can be described by Poisson equation

$$\nabla^2 \Phi^{el} = -\frac{\rho_e}{\epsilon}, \quad (10)$$

with charge density

$$\rho_e = e \sum_i z_i c_i, \quad (11)$$

and the solvent permittivity ϵ , which we assume constant. Similarly with self-diffusiophoretic model, the first term of Eq. 9 is called *advective term*. The second and third term of Eq. 9 are called *diffusion* and *migration term* [13]. The diffusion term here means that the movement of ions is generated by the concentration gradient, and the migration term here means that the motion of ions is caused by the electrostatic interaction. In analogy with self-diffusiophoretic model, if we consider that our system have low Péclet number, then the advective term of Eq. 9 can be neglected. As a result, Eq. 9 can be written as

$$\mathbf{j}_i = -D_i \nabla c_i - \frac{D_i z_i e c_i}{k_B T} \nabla \Phi^{el}. \quad (12)$$

The motion of fluid in the self-electrophoretic model is also described by the Stokes equation (Eq. 2 and Eq. 3). But in this model, we use now electrostatic interaction to describe the force density. Therefore, the force density \mathbf{f} can be written as

$$\mathbf{f} = - \sum_i z_i e c_i \nabla \Phi^{el}. \quad (13)$$

To get the solution of self-electrophoretic problem, we solve fundamentally Eq. 9 (Nernst-Planck equation), Eq. 10, Eq. 2, and Eq. 3 (Stokes equation) simultaneously. The combination of these equations is known as *electrokinetic equations*. Nevertheless, we need also the boundary conditions to determine the exact solution for our system. As the first boundary condition, we assume that solute molecules are produced or consumed only on the swimmer surface [11]. Because of this, we can set in bulk condition that

$$\nabla \cdot \mathbf{j}_i = 0. \quad (14)$$

In addition, we also assume that the charge density in the bulk is

$$\rho_e^\infty = e \sum_i z_i c_i^\infty = 0, \quad (15)$$

the concentration and pressure are uniform at the point, which is far away from the swimmer, i.e. $\Phi^{el} \rightarrow 0$ and $p_i \rightarrow p_i^\infty$ equals atmospheric pressure [11].

Additionally, the production or consumption rate of salt is zero. However, the existence of these salt ions leads to electrostatic screening, the strength of which is characterized by the Debye length κ^{-1} , where the inverse Debye length κ is given by

$$\kappa = \sqrt{\frac{e^2 \sum_i z_i^2 c_i}{\epsilon k_B T}}. \quad (16)$$

In contrast to self-diffusiophoretic model, we do not consider any slip layer approximation, since the low concentration of salt ions and long range interaction. To specify the boundary condition for Poisson equation, we can apply at the surface (s) a von Neumann boundary condition

$$\hat{\mathbf{n}} \cdot \nabla \Phi^{el}(s) = -\frac{\sigma}{\epsilon}, \quad (17)$$

which can be used to a swimmer with vanishing dielectric constant and surface charge density σ [11].

To determine the velocity of swimmer, we can, similarly to self-diffusiophoretic model, approach by using two kinds of frame, lab frame and co-moving frame. As well as self-diffusiophoretic model, it is also easier in this model to implement the simulation setup in the co-moving than lab frame. Therefore, this frame is used often in self-electrophoretic swimmer simulation.

III. FINITE ELEMENT METHOD IN SELF-PHORETIC PROBLEM

i. Finite Element Method

The Finite Element Method (FEM) is a numerical method for solving the ordinary differential equation (ODE) and the partial differential equation (PDE). By using this method, we can also solve the set of nonlinear, coupled partial differential equations. In this section, we will discuss how to implement the FEM to electrokinetic equations.

The first step to use this method is reformulating the differential equation into the weak formulation [15]. To illustrate this procedure, first we will develop the weak form for the Poisson equation Eq. 10. Multiplying both sides of Eq. 10 by test function Ψ and integrating over the whole domain Ω leads to:

$$\int_{\Omega} \Psi \nabla^2 \Phi^{el} dV = - \int_{\Omega} \Psi \frac{\rho_e}{\epsilon} dV \quad (18)$$

Integration by parts gives the weak form of the Poisson equation:

$$\int_{\Omega} \nabla \Psi \nabla \Phi^{el} dV = - \int_{\Omega} \Psi \frac{\rho_e}{\epsilon} dV + \int_{\partial\Omega} \Psi \nabla \Phi^{el} d\mathbf{A}. \quad (19)$$

The reason why we use weak form in FEM, because this form can assure us the smoothness of our solution. Even our system has the discontinuity, the integral form of weak formula still can treat this discontinuity [16].

After we reformulate the Poisson equation into weak form, we can approximate the solution. We use linear expansion as an solution ansatz for electrostatic potential $\Phi(\mathbf{r})$ and charge density $\rho(\mathbf{r})$

$$\Phi^{el}(\mathbf{r}) = \sum_k \Phi_k b_k(\mathbf{r}), \quad \rho_e(\mathbf{r}) = \sum_k \rho_k b_k(\mathbf{r}), \quad (20)$$

where b_k is basis (ansatz) function [15].

For determining the test function, we have theoretically infinitely convergence choices. In this presentation, one of the common approximation for test function is introduced, namely *Galerkin approximation*. In the Galerkin approximation, the test function Φ is expanded into the same set of basis function, i.e. $\Phi \sim \sum_i \Phi_i b_i$. After we have already chosen Galerkin approximation for determining the test function, then the Eq. 19 leads to

$$\sum_k \Phi_k \int_{\Omega} \nabla b_i(\mathbf{r}) \nabla b_k(\mathbf{r}) dV = \sum_k \frac{\rho_k}{\epsilon} \int_{\Omega} b_i(\mathbf{r}) b_k(\mathbf{r}) dV + \sum_k Q(b_i, b_k), \quad (21)$$

where $\sum_k Q(b_i, b_k)$ belongs to the integral over $\partial\Omega$ in the weak form and represent the boundary conditions matrix. For all components of i , we can represent Eq. 21 with matrix representation:

$$\sum_k K_{ik} \Phi_k = f_i(\rho) + Q_i. \quad (22)$$

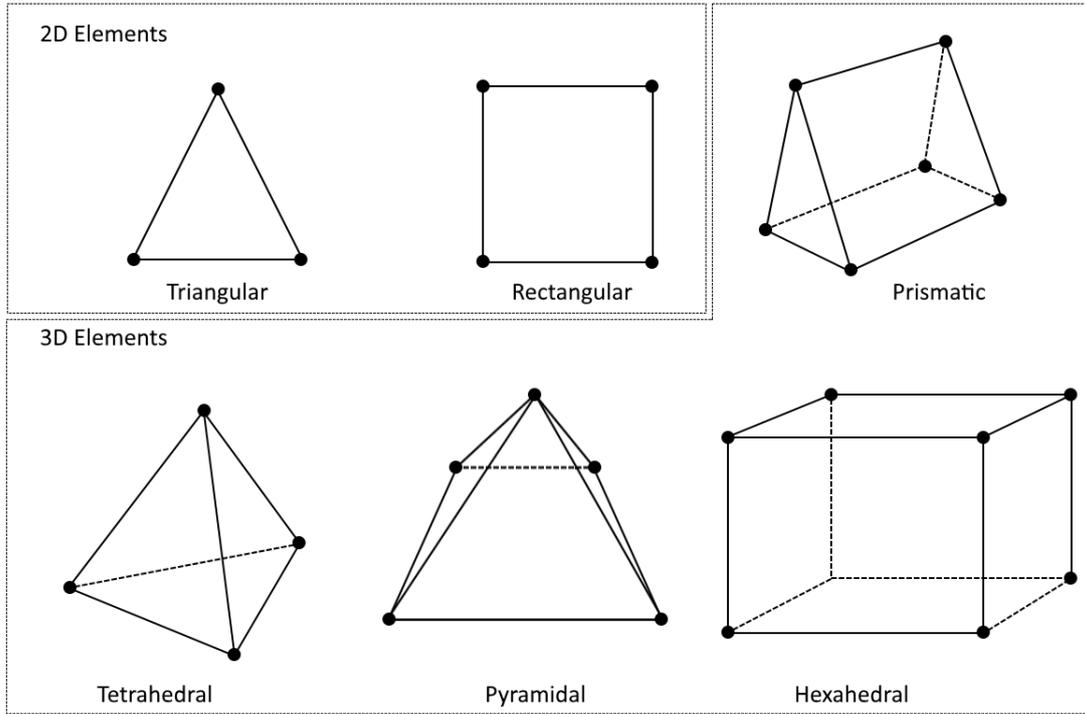


Figure 3: Some shapes, which can be used for creating mesh 2D and 3D in Finite Element Method (FEM) [17]

After we reform the weak function for Poisson equation, we do basically the same way to reform the rest electrokinetic equations to the weak formulation [15]. After that, we can represent all of three electrokinetic equations in a matrix:

$$\begin{pmatrix} \mathbf{K}_1(\Phi, \mathbf{u}) & 0 & 0 \\ 0 & \mathbf{K}_2 & 0 \\ 0 & 0 & \mathbf{K}_3 \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \Phi \\ \mathbf{u} \end{pmatrix} - \begin{pmatrix} 0 \\ \mathbf{f}_2(\mathbf{c}) \\ \mathbf{f}_3(\Phi, \mathbf{c}) \end{pmatrix} - \begin{pmatrix} \mathbf{Q}_1 \\ \mathbf{Q}_2 \\ \mathbf{Q}_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad (23)$$

where \mathbf{K}_1 represents the Nernst-Planck equation, \mathbf{K}_2 and \mathbf{f}_2 represent the Poisson equation, and \mathbf{K}_3 and \mathbf{f}_3 represent the Stokes equation. Eq. 23 can be solved now by using a Newton solver:

$$\mathbf{DF} \begin{pmatrix} \mathbf{c}_n \\ \Phi_n \\ \mathbf{u}_n \end{pmatrix} \begin{pmatrix} \mathbf{c}_{n+1} - \mathbf{c}_n \\ \Phi_{n+1} - \Phi_n \\ \mathbf{u}_{n+1} - \mathbf{u}_n \end{pmatrix} = -\mathbf{F} \begin{pmatrix} \mathbf{c}_n \\ \Phi_n \\ \mathbf{u}_n \end{pmatrix}, \quad (24)$$

where

$$\mathbf{F} \begin{pmatrix} \mathbf{c}_n \\ \Phi_n \\ \mathbf{u}_n \end{pmatrix} = \begin{pmatrix} \mathbf{K}_1(\Phi, \mathbf{u}) & 0 & 0 \\ 0 & \mathbf{K}_2 & 0 \\ 0 & 0 & \mathbf{K}_3 \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \Phi \\ \mathbf{u} \end{pmatrix} - \begin{pmatrix} 0 \\ \mathbf{f}_2(\mathbf{c}) \\ \mathbf{f}_3(\Phi, \mathbf{c}) \end{pmatrix} - \begin{pmatrix} \mathbf{Q}_1 \\ \mathbf{Q}_2 \\ \mathbf{Q}_3 \end{pmatrix}, \quad (25)$$

and \mathbf{DF} is the total derivative of \mathbf{F} [15]. Hence, Eq. 23 is a standard form to solve electrokinetic equations using FEM.

After we understand the standard equation for finite element simulation, the important steps to do the simulation using FEM are dividing the simulation domain into smaller subdomains by creating mesh and setting the boundary conditions. In FEM, there are many ways to determine the shape of mesh. The shape of mesh could be intervals in one dimension or triangles or quadrilaterals in two dimensions or tetrahedrons, cuboids, etc in three dimensions, which are shown by Fig. 3 [17]. In addition, we can also apply the mixing of mesh shape during the numerical calculation using FEM, for example mixing between triangles and quadrilaterals, which is shown by Fig. 4.

The accuracy of our numerical calculation in FEM depends not only on the number of mesh, but also on the choice of our polynomial basis ansatz. Therefore, we have possibility to save our simulation time and computer memory due to the reducing of mesh number. The right choice of mesh and polynomial degree will produce the accurate result of our simulation.

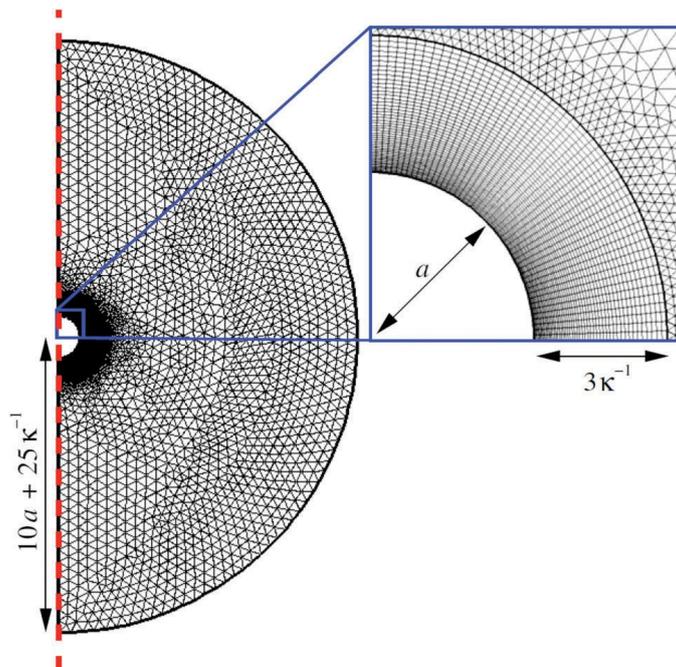


Figure 4: An example of meshing for active matter system: The domain from simulation system in [12]. The simulation domain is divided into two region of mesh, i.e. triangular and quadrilateral elements are used. In a range of $3\kappa^{-1}$ around the colloid the domain consists of quadrilaterals, which grow in size geometrically, which is shown by blue box. Outside this range the shape of mesh are triangular and is allowed to grow out linearly to best fit the domain boundary and reduce the total number of elements.

ii. Example of Result

If we solve the self-phoretic motion problem using FEM, our outputs are the distribution of velocity, concentration and electric or diffusion potential as a function of position. An example for the output of finite element simulation is shown by Fig. 5.

In Fig. 5, there are the normalized concentration field and normalized fluid flow field from two model swimmer, self-diffusiophoresis and self-electrophoresis. Fig. 5a and Fig. 5c show simulation results for half-coated swimmers and Fig. 5b and Fig. 5d show swimmers with delta-distribution-like production profiles. According to the result from [11], we learn that the speed of swimmer can be improved by changing the distribution reactive surface of swimmer.

IV. ADVANTAGES AND DISADVANTAGES FEM

i. Disadvantages

As a numerical method, applying FEM to solve differential equation system has some disadvantages. The first disadvantage of FEM is this method is quite complex method, since we reform the differential equation into the weak form, and also do integration for our basis ansatz function. Furthermore, using this method will produce numerical error due to discretization, which in self-phoretic problem is known as spurious flow and spurious flux. The explanation about one scheme for reducing this numerical error will be discussed in more detail in the section V.

ii. Advantages

Nevertheless, by using FEM have so many advantages. First of all, we can solve the non-linear and coupled differential equation system. Secondly, this method is also good for solving the systems, which have discontinuity. It is possible to do it, because the integral form in weak differential equation formula can solve the discontinuity, whereas by using the strong form, the discontinuity point in our system leads to produce the divergence at that point. Then, we have possibility to solve the system with large

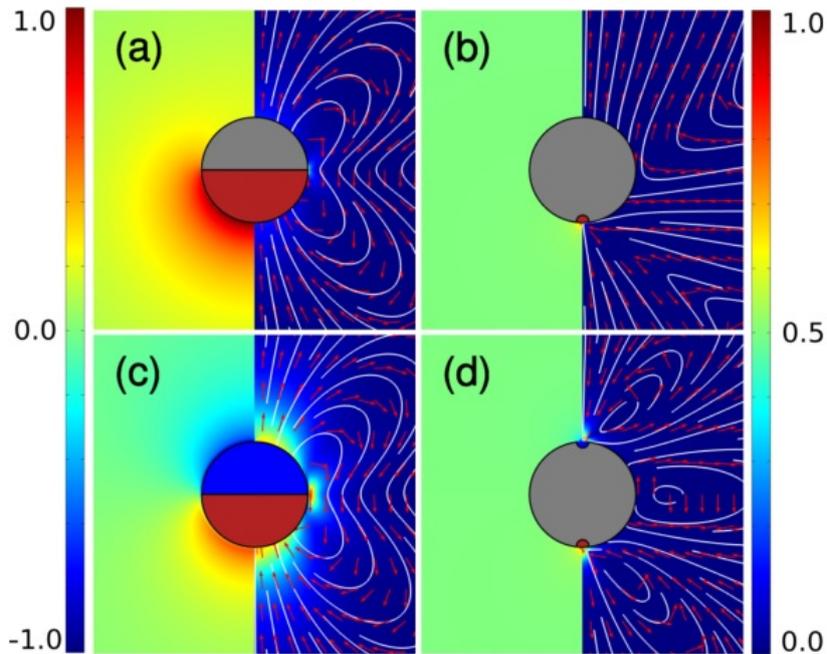


Figure 5: Normalized concentration field (left) and normalized fluid flow field (right) in the lab frame for self-diffusiophoretic swimmers ((a) and (b)) and self-electrophoretic swimmers ((c) and (d)). Figures ((a) and (c)) show simulation results for half-coated swimmers and ((b) and (d)) show swimmers with delta-distribution-like production profiles. The white lines depict stream lines, the red arrows represent the normalized of flow field [11].

domain. By using this method, we have also many choice for design the mesh, including the density and shape of the mesh. This point is important in self-phoretic swimmer, because the interesting physical phenomena in swimmer usually happen in a small environment around the swimmer. Furthermore, we can also create mix meshing when we use FEM. For example, creating quadrilateral mesh around the surface and triangle mesh for far region from the surface (see Fig. 4). Using quadrilateral mesh for the area near the surface is more useful than triangle, because this shape is better to handle the curve shape of the swimmer surface, such that we will have more smooth solution, especially for perpendicular direction to the surface.

V. REDUCING SPURIOUS FLOW AND SPURIOUS FLUX

i. The Origin of Spurious Flow and Spurious Flux

Unfortunately, discretization in our system will produce non-physical numerical errors. These errors are called by *spurious flux* and *spurious flow*. The simple explanation to describe these errors is at the equilibrium condition, we expect that our swimmer has the condition, that the flux of species (\mathbf{j}) and the fluid velocity (\mathbf{u}) equals zero. But at the end of the day, there is a non zero flux and velocity in our numerical calculation. These number give a hint on the numerical error in the system. Hence, we have to do some improvement in our numerical strategy to minimize the number of spurious flow and spurious flux in our simulation result.

ii. The Methods to Reduce Spurious Flow and Spurious Flux

In order to reduce the number of spurious flux and spurious flow, we can conservatively increase the number of mesh or grid resolution. Although we have to pay more computational cost, when we increase the number of mesh. Another way to decrease the number of spurious flux and spurious flow is by increasing the order of polynomial basis ansatz. However, the higher order of basis ansatz will decrease the number of zero elements in finite element matrix [18]. As a result, we have to also pay more computational cost, whether we increase the order of polynomial basis ansatz, even though this

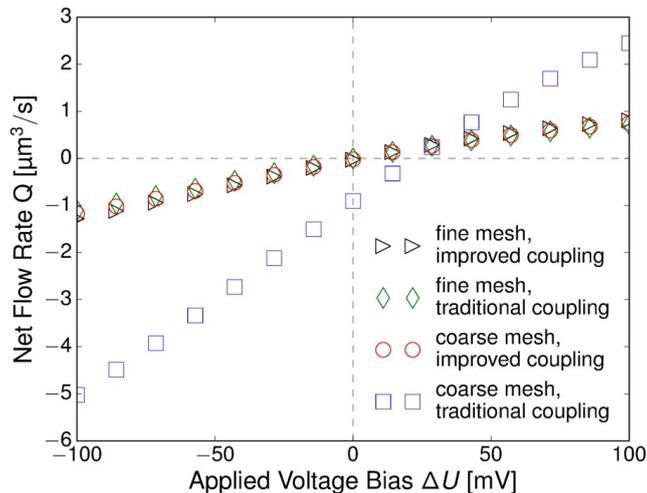


Figure 6: An example of simulations using the improved fluid coupling (Eq. 26) and the coarse mesh in nanopore system with applying a bias voltage, which is taken from [15].

way is sometimes more cheaper than we increasing the number of mesh [15].

Another way to minimize the spurious flux and spurious flow in electrokinetic equations without increasing the number of mesh and the order of polynomial basis ansatz is by reformulating the hydrodynamic driving force \mathbf{f} in Eq. 13 with modifying the gradient field without change the resulting velocity of \mathbf{u} . One way to reformulate this force is by extending the hydrodynamic force, which can be written as

$$\mathbf{f} = - \sum_i (k_B T \nabla c_i + z_i e c_i \nabla \Phi^{el}). \quad (26)$$

In contrast to common hydrodynamic force (Eq. 13), the advantage of this choice is that the force density acting on the fluid vanishes in equilibrium, and as a result there is no build up pressure to counter this force. Applying this extended hydrodynamic force (Eq. 26) can reduce also the number spurious flux and spurious flow for a system nanopore, which is illustrated by Fig. 6 [15].

VI. CONCLUSION

The Finite Element Method (FEM) is a numerical method which can be used for solving non-linear and coupled equations. Hence, we can apply this method for solving numerically the equations, which describe self-diffusiophoretic motion and self-electrophoretic motion. Indeed, by using this method we still have numerical error, like another numerical methods. Nevertheless, we have so many advantages by applying this method for simulation of self-phoretic motion. For example, this method can handle the discontinuity region due to the integral form in weak formula. Finally, FEM is a good method for solving active matter problems, i.e. self-diffusiophoretic motion and self-electrophoretic motion, because we have many advantages if we use this method.

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