

A spectral element/smoothed profile method for complex-geometry flows

by

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Abstract of “A spectral element/smoothed profile method for complex-geometry flows” by Xian Luo, Ph.D., Brown University, May 2009

We combine the spectral element method with the smoothed profile method (SPM) [81] to obtain an efficient method for flows with moving boundaries in complex geometries. SPM uses a fixed non-conforming computational mesh and represents the particles by indicator functions to construct a penalty force term in the Navier-Stokes equations. The method is similar to the immersed boundary method in that they both use a force distribution to effectively impose the constraints on the fluid motion to approximate the boundary conditions. However, for spectral element discretizations, the smooth profile of SPM leads to high order accuracy.

While the original method employs a fully-explicit time-integration scheme, we develop a high-order semi-implicit splitting scheme to improve accuracy and stability. We first analyze the error of the hybrid method for several prototype flow problems. We show that the modeling error of SPM is a non-monotonic function of the time step size and the interface thickness of the smooth profile. The optimum time step size balances the thickness of the Stokes layer and that of the profile interface. Subsequently, we propose an extension of SPM to simulate *electrokinetic flows* allowing for spatially varying electrical conductivities. In addition to the Navier-Stokes equations, the Poisson-Boltzmann and electric charge continuity equations are also cast into forms based on SPM. The method is verified by benchmark problems of electroosmotic flow in straight channels and electrophoresis of charged insulating cylinders. We also present simulations on the electrophoresis of charged microtubules, and show that the simulated electrophoretic mobility and anisotropy agree with the experimental results.

In the last part we present numerical simulation results for engineering flows involving three-dimensional moving domains. In particular, the flow patterns around the vortex-induced vibrations of two tandem cylinders are successfully resolved, and results are also shown for a rotating three-bladed propeller in a duct which can

be used in waterjet propulsion. Compared to the simulation results based on an arbitrary Lagrangian Euler formulation, SPM yields satisfactory agreement, yet it is computationally much cheaper allowing for fast three-dimensional simulations on a laptop.

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This dissertation by Xian Luo is accepted in its present form
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- Xian Luo and George Em Karniadakis, *Numerical modeling of electrokinetic flows with applications to the electrophoresis of microtubules*, (in preparation 2009).
- Xian Luo, Martin R. Maxey, and George Em Karniadakis, *Smoothed profile method for particulate flows: Error analysis and simulations*, *J. Comput. Phys.*, 228, 5(2009), 1750-1769.
- Xian Luo, Martin R. Maxey, and George Em Karniadakis, *Smoothed profile method for particulate two-phase flow*, *Proceedings of ASME 2008 Fluids Engineering Division Summer Conference, 10-14 August 2008 Jacksonville*, FEDSM2008-55033.

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- Proper orthogonal decomposition (POD).
- Multiscale simulations of dense suspensions and electrokinetic flows.

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Chapter 1

Introduction

1.1 Background and motivation

Complex-geometry flows refer to the flow either around or inside complex shaped boundaries. Our primary research interest resides in the developement of fast and accurate numerical algorithms for solid-fluid two phase flows with complex geometries. Specifically, we aim to study two different but related problems: particulate flows and electrokinetic flows.

Particulate flows occur in many natural and technological situations, such as colloidal sedimentation, polymer suspensions and lubricated transport. The methods for numerical simulation of particulate flows can be broadly divided into two categories: the first one involves a Lagrangian description in which the computational mesh follows the particles or the fluid; the second one employs an Eulerian description on a fixed grid with the interactions between the solvent and the particles represented by some form of body force or appropriate interaction equations. For example, the arbitrary Lagrangian-Eulerian (ALE) method [41, 42] belongs to the first category while the distributed Lagrange multiplier (DLM) method first proposed by Glowinski et al. [27, 28] and further developed by Patankar et al. [93] falls into the second category.

The force coupling method (FCM) has been studied extensively in the past [75, 69, 66, 67], which is also a method in the second category. It represents each particle in the flow by a low-order expansion of force multipoles, which is applied as a distributed body force on the flow. It captures the far-field solution accurately and can typically resolve body forces with better than a couple of percent accuracy, though it does not fully resolve the flow field close to the particle surfaces (in the pointwise sense).

One of the most widely used methods in the second category is the immersed boundary method (IBM) of Peskin, which was originally developed for flows with immersed flexible membranes [94, 95]. The main idea of IBM is to employ a regular Eulerian mesh for the solvent over the entire domain, together with Lagrangian markers for the immersed boundary. The immersed boundary moves with the local fluid velocity, and in return exerts a “singular” force to the nearby fluid. This force is usually obtained from the elastic properties of the immersed boundary, and then distributed into the surrounding fluid using a regularized Dirac delta function. IBM was later extended to flows with rigid bodies with certain treatment, e.g. in [22, 4]. A new “formally” second-order scheme of IBM was proposed in [58], which has less numerical viscosity and might be more appropriate for high Reynolds number flows. In these references [22, 4, 58], the fluid-particle interaction force utilizes a feed-back formulation, namely the “virtual boundary method” proposed in [29]. An alternative expression for the force called “direct forcing” has been introduced to IBM by [19], which avoids introducing additional free parameters and alleviates the severe time step restrictions of the virtual boundary method. More recently, [111] proposed an improved direct forcing formulation which shows a smoother and less oscillatory boundary force for moving boundary problems.

A similar approach to IBM called “immersed interface method” (IIM) has been proposed in [61], and it was applied to Stokes flow problems in [62]. In contrast to IBM adding the forcing function into the continuous governing equations, IIM incor-

porates the jump conditions across the immersed interfaces directly into the *discrete* equations. The IIM has been shown to be second-order accurate in the maximum norm for elliptic problems. Extension to incompressible Navier-Stokes equations has been presented in [64, 60]. The entire vector or only the normal component of the singular force (from the immersed interface to the fluid) is incorporated into jump conditions for both velocity and pressure or only pressure, in [64] and [60], respectively. They both give sharp resolution of the pressure across the interface. Compared to [60], the method in [64] achieves better accuracy but it is more complicated to implement in general.

More recently, a boundaryless method called the “Smoothed Profile” method (SPM), was proposed in [81, 52, 122, 78, 79, 53, 121]; it falls into the second category as well for it uses a fixed grid. It is conceptually similar to FCM in the sense that it represents the particles by certain smooth body forces in the Navier-Stokes equations instead of treating the particles as boundary conditions to the fluid. However, it has also features of IBM in that the force distribution effectively imposes constraints on the fluid motion that approximate the boundary conditions. As with FCM and IBM, SPM solves for a single set of fluid dynamics equations in the entire domain including the particle volumes, without any internal boundary conditions. However, in contrast to FCM and IBM, a smoothly spreading interface layer is used to represent the particle boundaries to give a transition from the rigid body motion to the fluid motion. This treatment is similar to the method of PHYSALIS [101, 43], which assumes boundary layer exists next to the particle surface, where the Stokes approximation is valid; PHYSALIS uses a local analytic solution of the Stokes equations near the particle. Both PHYSALIS and SPM smear out the sharp solid-fluid interface and replace it by a smooth layer, which should be sufficiently resolved by the spatial discretization.

The key point of SPM is to update the velocity inside each particle through the integration of a “penalty” body force to ensure the rigidity of the particles. It

imposes the no-slip boundary condition implicitly without any special treatment on the solid-fluid boundaries. This feature is, of course, appealing as it corrects the near-particle behavior of FCM in an efficient manner. SPM has been verified by several test problems, and has also been applied to the sedimentation of hundreds of 2D colloidal disks in [81, 122]. The method shows great potential in fast simulations of multi-component fluids, such as charged colloids in dense suspensions [78, 79, 80]. However, this method lacks any rigorous theoretical foundation and it has only been presented as a fully-explicit scheme, hence limiting the size of time step to very small values. It has also been used in conjunction with uniform grids and simple particle shapes.

We are also interested in *electrokinetic flows*, which occur in heterogeneous fluids associated with electric field which could be either externally applied or internally induced. Two of the major effects in general electrokinetic flows are: *electroosmosis*, which is the electrically driven motion of a fluid relative to stationary charged surfaces, and *electrophoresis* which is the motion of charged particles through a solvent medium under the action of an applied electric field. These effects have many important applications in biology, forensics, environmental and energy engineering [103, 16, 117, 112, 48]. Over the century many remarkable experimental techniques have been developed to effectively image the electrokinetic systems and measure related quantities, especially in micro- and nanofluidic devices [77, 12, 55, 104, 38, 14, 113].

There have also been many successful numerical simulations on electroosmosis recently; most of them are based on solving the Poisson–Boltzmann equation to include an electrokinetic force in the Navier–Stokes equation. A numerical algorithm based on the Debye–Hückel linearization was proposed by [123] to study electrokinetic effects in pressure-driven liquid flows. A finite-volume method was developed by [92] to simulate electroosmotic injection at the intersection of two channels. Beskok et al. have developed a spectral element algorithm for solution

of mixed electroosmotic/pressure-driven flows in complex two-dimensional microgeometries [17, 18, 31]. Aluru et al. proposed meshless methods and compact methods to study steady electroosmotic flows in microfluidic devices and also investigated the validity of the Poisson–Boltzmann equation in nanochannels using molecular dynamics simulations [76, 97]. A lattice Boltzmann method was applied to study the electroosmosis in microchannels and showed chaotic advection and mixing enhancement by using heterogeneous surface potential distribution [114, 109].

However, few full numerical simulations can be found to have successfully resolved the electrophoretic flow. This is probably due to the difficulties of standard numerical methods for moving boundary problems, especially with charged complex boundaries. A finite element method, which uses a posteriori error estimation to adaptively refine the mesh, was proposed to solve for the Poisson-Boltzmann equation around charged complex surfaces such as biomolecules [3, 9]. The method has the potential to be used in combination with an effective flow solver to simulate the electrophoresis of complex particles. The smoothed profile method was extended to account for the electrohydrodynamic couplings, by integrating the modified species conservation and Navier–Stokes equations [53, 54, 121, 80]. In particular it was applied to calculate the electrophoretic mobilities of charged spheres and showed great potential for modeling colloidal dispersions. However due to the fully explicit time integration scheme used, the temporal stability and accuracy was not quite satisfactory. Also the model used a constant external electric field to calculate the electrokinetic force, which only works for particles with the same electrical conductivity as the surrounding solution, and thus is not practical for general poorly conducting materials.

1.2 Objectives

The main objective of this thesis is to develop fast and accurate numerical algorithms based on SPM for flows in complex geometries, especially when we have moving boundaries. We also want to effectively incorporate the electrokinetic effects into the hydrodynamic flow solver.

A second objective is to quantify the errors of SPM and make it more robust. Due to the absence of rigorous analysis in the original work of SPM, we aim to analyze the modeling error of the method. Also as it has only been used with fully-explicit time integration and uniform spatial discretization, possible improvement in the discretization accuracy is sought. Furthermore we will extend the numerical methodology to simulate electrokinetic flows around complex interfaces with arbitrary electrical conductivity.

A third objective is to examine if SPM can be applied to other complex flows with moving boundaries, e.g. vortex-induced vibrations and waterjet propulsion.

1.3 Outline

The thesis is organized as follows.

In Chap. 2 we present the framework of SPM in the context of high-order discretizations, and we quantify the modeling accuracy of SPM for several prototype flows. Further verification of the method is presented by simulations of flow around complex shaped particles and also for multi-particle interactions; the SPM results are critically evaluated against direct numerical simulations (DNS) and FCM solutions.

In Chap.3 we propose an efficient modeling method for electrokinetic flows, allowing for spatially varying electrical conductivities. The basic idea is to include electrokinetic forces into the flow solver in the way that the Poisson-Boltzmann equation and electric charge continuity equations are cast into forms based on SPM. We verify the modeling method by benchmark problems of electroosmotic flow in

straight channels and electrophoresis of charged cylinders. We also present the simulation results of the electrophoresis of charged microtubules, and show that the simulated electrophoretic mobility and anisotropy agree well with the experimental results.

In Chap. 4, we show simulation results for several interesting engineering applications, such as vortex induced vibrations and waterjet propulsion.

We conclude in Chap. 5 by a summary and some future work.

Chapter 2

Smoothed Profile Method for Particulate Flows

2.1 Introduction

Three dimensional particulate flow with moving complex boundaries poses great challenge for numerical simulations. In contrast to the standard numerical methods which require frequent remeshing around physical boundaries of the particles, the smoothed profile method (SPM) [81, 52, 122, 78, 79, 53, 121] is much more efficient as it avoids the direct boundary treatment and instead, a fixed non-conforming computational mesh can be used. SPM is similar in spirit to the popular immersed boundary method [94, 95] as they both use a force distribution to effectively impose the constraints associated with the flow boundary conditions. However, in combination with the spectral element method as we propose, the smooth profile of SPM leads to high-order accuracy as it does not cause Gibbs phenomena at the geometric interfaces.

We note that the original work of SPM lacks any rigorous theoretical foundation and it has only been presented as a fully-explicit scheme, hence limiting the size of time step to very small values. It has also been used in conjunction with uniform

grids and simple particle shapes. To this end, we have developed an error analysis of this method and, in particular, its semi-implicit extension that we present in the current work. In addition, we critically evaluate SPM, for first time, against direct numerical simulations (DNS) and the force coupling method (FCM) for a number of problems, including steady and unsteady particulate flows, simple and complex shaped particle evolutions. All the results we present in this section are based on *three-dimensional* simulations.

The chapter is organized in the following way. In the second section, we present the main steps of SPM in the context of high-order discretizations. Specifically, a stiffly-stable splitting scheme (up to third-order) is employed for temporal discretization and spectral element method for spatial discretization. In the third section we quantify the accuracy and analyze the modeling error of SPM for several prototype flows. We show that the modeling error has a non-monotonic dependence on the time step size Δt and interface thickness ξ . In the fourth section, a further verification of the method is presented through comparisons with other numerical methods for complex-shaped particles. The fifth section presents a SPM simulation of two interacting spheres in low Reynolds number, which is compared to both the FCM results and experimental results. We conclude in the last section.

2.2 Formulation

2.2.1 Smoothed representation of particles

SPM represents each particle by a smoothed profile (or in other words an indicator/concentration function), which equals *unity* in the particle domain, *zero* in the fluid domain, and varies smoothly between one and zero in the solid-fluid interfacial domain. In [81], several *analytical* forms of the smoothed profile for spherical

particles are presented. Among them, the following profile is mostly used:

$$\phi_i(\mathbf{x}, t) = \frac{1}{2} \left[\tanh\left(\frac{a_i - |\mathbf{x}_i - \mathbf{R}_i|}{\xi_i}\right) + 1 \right], \quad (2.1a)$$

where index i refers to the i_{th} sphere, and a_i , $\mathbf{R}_i$, ξ_i are respectively the radius, the position vector, and the interface thickness parameter for the i_{th} sphere. The indicator function ϕ_i is a function of spatial coordinates $\mathbf{x}$ and time t .

Here we extend the above formula to a more *general* form, which is effective for *any* particle shape:

$$\phi_i(\mathbf{x}, t) = \frac{1}{2} \left[\tanh\left(\frac{-d_i(\mathbf{x}, t)}{\xi_i}\right) + 1 \right], \quad (2.1b)$$

where $d_i(\mathbf{x}, t)$ is the *signed* distance to the i_{th} particle surface with positive value outside the particle and negative value inside the particle. The calculation of $d_i(\mathbf{x}, t)$ is rather straightforward if particles are in simple shapes (boxes, spheres, etc.). If, however, we deal with more complex shapes which are represented by many surface point coordinates, a closest-point searching procedure should be used to find $d_i(\mathbf{x}, t)$ and thus $\phi_i(\mathbf{x}, t)$.

For other cases where we know the *analytical* form of the particle surface functions, or where we can construct an interpolating spline function based on the surface points, we propose to use a slightly different form of the indicator function due to its convenience and efficiency:

$$\phi_i(\mathbf{x}, t) = \frac{1}{2} \left[\tanh\left(\frac{f_i(\mathbf{x}, t)}{\xi_i} \tau_i\right) + 1 \right], \quad (2.2)$$

where $f_i(\mathbf{x}, t)$ is the surface function of the i_{th} particle, which is zero on the surface, positive outside the particle, and negative inside; here τ_i is a scaling factor. We implement this form in most of the numerical simulations of flows involving spherical, ellipsoidal and biconcave particles, which are presented in the next two sections.

A smoothly spreading *concentration field* is achieved by summing up the concen-

tration functions of all the N_p non-overlapping particles:

$$\phi(\mathbf{x}, t) = \sum_{i=1}^{N_p} \phi_i(\mathbf{x}, t). \quad (2.3)$$

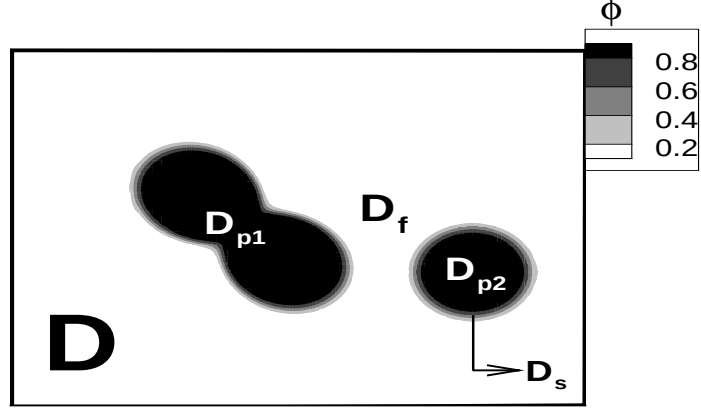


Figure 2.1: *An example of two particles:* contours of the concentration field ϕ and computational domain partitioning ($D = \sum_{i=1}^{N_p} D_{pi} + D_f + D_s$).

Fig. 2.1 shows a schematic of the smoothed profiles for an example involving two particles. The entire domain D can be subdivided into three domain types: D_{pi} is the particle domain of the i_{th} particle, where $\phi \sim 1.0$; D_f is the fluid domain, where $\phi \sim 0.0$; and D_s is the interface domain, where $0.0 < \phi < 1.0$.

Based on this concentration field, the *particle velocity field*, $\mathbf{u}_p(\mathbf{x}, t)$, is constructed from the rigid motions of the N_p particles:

$$\phi(\mathbf{x}, t) \mathbf{u}_p(\mathbf{x}, t) = \sum_{i=1}^{N_p} \{ \mathbf{V}_i(t) + \boldsymbol{\Omega}_i(t) \times [\mathbf{x} - \mathbf{R}_i(t)] \} \phi_i(\mathbf{x}, t), \quad (2.4)$$

where $\mathbf{R}_i$, $\mathbf{V}_i = \frac{d\mathbf{R}_i}{dt}$ and $\boldsymbol{\Omega}_i$ are spatial positions, translational velocity and angular velocity of the i_{th} particle, respectively. We can verify that the divergence of the

particle velocity field is identically zero, i.e.,

$$\nabla \cdot \mathbf{u}_p = \sum_{i=1}^{N_p} \{ \mathbf{V}_i(t) + \boldsymbol{\Omega}_i(t) \times [\mathbf{x} - \mathbf{R}_i(t)] \} \cdot \nabla \left(\frac{\phi_i}{\phi} \right) = 0,$$

where we have used: $\nabla \left(\frac{\phi_i}{\phi} \right) = \frac{(\nabla \phi_i) \phi - \phi_i (\nabla \phi)}{\phi^2} = \frac{\sum_{j=1}^{N_p} [(\nabla \phi_i) \phi_j - \phi_i (\nabla \phi_j)]}{\phi^2} = 0$, by the assumption of non-overlapping envelopes of different particles, i.e., $\phi_i (\nabla \phi_j) = 0$ for $\forall i \neq j$.

The *total velocity field* is then defined by a smooth combination of both the particle velocity field $\mathbf{u}_p$ and the fluid velocity field $\mathbf{u}_f$:

$$\mathbf{u}(\mathbf{x}, t) = \phi(\mathbf{x}, t) \mathbf{u}_p(\mathbf{x}, t) + (1 - \phi(\mathbf{x}, t)) \mathbf{u}_f(\mathbf{x}, t). \quad (2.5)$$

We see that inside the particle domain ($\phi = 1$), we have $\mathbf{u} = \mathbf{u}_p$, i.e., the total velocity equals the particle velocity. In the interfacial domain ($0 < \phi < 1$) the total velocity changes smoothly from the particle velocity $\mathbf{u}_p$ to the fluid velocity $\mathbf{u}_f$.

SPM imposes indirectly the no-slip constraint on the particle boundaries. This imposition can be verified by taking the curl of Eq. (2.5):

$$\nabla \times \mathbf{u} = \nabla \times [\mathbf{u}_f + \phi(\mathbf{u}_p - \mathbf{u}_f)] = (\nabla \phi) \times (\mathbf{u}_p - \mathbf{u}_f) + \phi(\nabla \times \mathbf{u}_p) + (1 - \phi)(\nabla \times \mathbf{u}_f).$$

As $\nabla \phi$ is non-zero in the interfacial domain and is perpendicular to the particle surface, the no-slip constraint can be expressed as $(\nabla \phi) \times (\mathbf{u}_p - \mathbf{u}_f) = 0$. So the imposition of the no-slip constraint comes from the assumption that the vorticity of the total flow field consists of the vorticities from both the fluid velocity and the particle velocity, i.e.,

$$\nabla \times \mathbf{u} = \phi(\nabla \times \mathbf{u}_p) + (1 - \phi)(\nabla \times \mathbf{u}_f). \quad (2.6)$$

The validity of this equation will be checked later in a numerical simulation example.

SPM also imposes the no-penetration constraint on particle surfaces. If we check the divergence of the total velocity, taking into account that the fluid solvent is incompressible and the particle velocity field is divergence-free (derived by assuming non-overlapping particle envelopes), we obtain:

$$\nabla \cdot \mathbf{u} = \nabla \cdot [\mathbf{u}_f + \phi(\mathbf{u}_p - \mathbf{u}_f)] = (\nabla \phi) \cdot (\mathbf{u}_p - \mathbf{u}_f). \quad (2.7)$$

Since $(\nabla \phi) \cdot (\mathbf{u}_p - \mathbf{u}_f) = 0$ represents the no-penetration constraint on particle surfaces, imposing the incompressibility condition of the total velocity $\nabla \cdot \mathbf{u} = 0$ ensures the no-penetration surface condition, and vice versa.

SPM solves for the total velocity, $\mathbf{u}$, in the entire domain D , including the particle domain, using the Navier-Stokes equations with an extra force density term along with the incompressibility constraint:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} + \mathbf{f}_s \quad \text{in } D \quad (2.8a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } D, \quad (2.8b)$$

where ρ is the density of the fluid, p is the pressure field, ν is the kinematic viscosity of the fluid, $\mathbf{g}$ is the gravity (and other external forces on the fluid), and $\mathbf{f}_s$ is the body force density term representing the interactions between the particles and the fluid. Here the fluid solvent is assumed to be Newtonian with constant viscosity for simplicity.

The velocity and pressure fields are solved through the following two-step semi-discrete form proposed in [81, 78]. First, SPM solves for an *intermediate* velocity and pressure fields as $\mathbf{u}^*, p^*$ from the previous step solution $\mathbf{u}^n$, by integrating the

advection and viscous stress:

$$\mathbf{u}^* = \mathbf{u}^n + \int_{t^n}^{t^{n+1}} dt [-(\mathbf{u} \cdot \nabla) \mathbf{u} - \frac{1}{\rho} \nabla p^* + \nu \nabla^2 \mathbf{u} + \mathbf{g}] \quad (2.9a)$$

$$\approx \mathbf{u}^n + \Delta t [-(\mathbf{u}^n \cdot \nabla) \mathbf{u}^n - \frac{1}{\rho} \nabla p^* + \nu \nabla^2 \mathbf{u}^n + \mathbf{g}^n] \quad \text{in } D, \quad (2.9b)$$

where Δt is the time increment $t^{n+1} - t^n$, and a forward Euler integration is used. This is solved in conjunction with the incompressibility constraint on $\mathbf{u}^*$, i.e., $\nabla \cdot \mathbf{u}^* = 0$, and hence $\frac{1}{\rho} \nabla^2 p^* = \nabla \cdot [-(\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \mathbf{g}^n]$.

Then SPM updates the total velocity and pressure fields from $\mathbf{u}^*, \mathbf{p}^*$:

$$\mathbf{u}^{n+1} = \mathbf{u}^* + \int_{t^n}^{t^{n+1}} dt [\mathbf{f}_s - \frac{1}{\rho} \nabla p_p] = \mathbf{u}^* + [\phi(\mathbf{u}_p - \mathbf{u}^*) - \frac{\Delta t}{\rho} \nabla p_p] \quad \text{in } D, \quad (2.10)$$

where p_p is the *extra pressure* field and $\mathbf{u}_p$ is calculated from Eq. (2.4). Note that the particle motions ($\mathbf{V}_i$ and $\mathbf{\Omega}_i$) could either be given or calculated from Newton's equations using the exerted forces on the particle. SPM assigns $\int_{t^n}^{t^{n+1}} \mathbf{f}_s dt = \phi(\mathbf{u}_p - \mathbf{u}^*)$ to denote the momentum change (per unit mass) due to the presence of the particle. Thus at each time step the flow is corrected by a momentum impulse to ensure that the total velocity matches that of the rigid particles within the particle volume, and hence to enforce the rigidity constraint. From the above expression we have that $\mathbf{f}_s \sim \frac{1}{\Delta t} \phi(\mathbf{u}_p - \mathbf{u}^*)$, suggesting that SPM is similar to penalty methods [25, 39], which incorporate constraints into the governing equations. Here $1/\Delta t$ serves as a penalty parameter; thus the smaller Δt is, the tighter the control of the rigidity constraint is. However, in contrast to the delta functions used in [25, 39], the smooth indicator function ϕ is used here by SPM.

The total pressure field is split into two parts as: $p = p^* + p_p$ to ensure the divergence-free of the total velocity field ($\nabla \cdot \mathbf{u} = 0$) and hence the imposition of the impermeable boundary condition on the particle boundaries. Specifically, the

following equation for p_p :

$$\frac{\Delta t}{\rho} \nabla^2 p_p = \nabla \cdot [\phi(\mathbf{u}_p - \mathbf{u}^*)] \quad \text{in } \mathbf{D}, \quad (2.11)$$

is derived by taking the divergence of Eq. (2.10) and using the divergence-free constraints $\nabla \cdot \mathbf{u}^* = 0$, $\nabla \cdot \mathbf{u}^n = 0$ and $\nabla \cdot \mathbf{u}^{n+1} = 0$.

2.2.2 Semi-discrete system: temporal integration

The original SPM [81, 78] used a fully-explicit time marching scheme for Eq. (2.9a). In the current thesis, we introduce a semi-implicit treatment, using a stiffly-stable high-order *splitting* (velocity-correction) scheme [49], in order to enhance stability and increase temporal accuracy.

In the velocity-correction splitting scheme, the fields at time level n : $\{\mathbf{u}^n, p^n, \mathbf{R}_i^n, \mathbf{O}_i^n, \phi^n, \mathbf{V}_i^n, \boldsymbol{\Omega}_i^n, \forall i = 1, \dots, N_p\}$, are advanced over a time step Δt to determine the fields $\{\mathbf{u}^{n+1}, p^{n+1}, \mathbf{R}_i^{n+1}, \mathbf{O}_i^{n+1}, \phi^{n+1}, \mathbf{V}_i^{n+1}, \boldsymbol{\Omega}_i^{n+1}, \forall i = 1, \dots, N_p\}$, through the four substeps outlined below. Note that $\mathbf{R}_i^n, \mathbf{O}_i^n$ are position vector and orientation vector of the i_{th} particle respectively, which contribute to the concentration function ϕ^n .

As a preliminary step before all substeps, we move particles from $\mathbf{R}_i^n, \mathbf{O}_i^n$ to $\mathbf{R}_i^{n+1}, \mathbf{O}_i^{n+1}$ by $\mathbf{V}_i^n, \boldsymbol{\Omega}_i^n$ using an explicit integration scheme, e.g. a high-order Adam-Bashforth method as:

$$\mathbf{R}_i^{n+1} = \mathbf{R}_i^n + \Delta t \sum_{q=0}^{J_e} a_q \mathbf{V}_i^{n-q} \quad (2.12a)$$

$$\mathbf{O}_i^{n+1} = \mathbf{O}_i^n + \Delta t \sum_{q=0}^{J_e} a_q \boldsymbol{\Omega}_i^{n-q}, \quad (2.12b)$$

where J_e is the order of the explicit time integration scheme and a_q are the coefficients in the Adam-Bashforth scheme. Then, the concentration field ϕ^{n+1} is calculated.

Velocity update due to advection

We compute the intermediate velocity field $\mathbf{u}^s$ by first integrating the non-linear (advection) term and body force term:

$$\frac{\mathbf{u}^s - \sum_{q=0}^{J_e-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q [-((\mathbf{u} \cdot \nabla) \mathbf{u})^{n-q} + \mathbf{g}^{n-q}] \quad \text{in } D, \quad (2.13)$$

where α_q, β_q are the coefficients derived from the standard stiffly-stable scheme formulation (see p. 264 in [50]). Also, $\mathbf{u}^{n-q}$ and $\mathbf{g}^{n-q}$ are the velocity and body force fields at previous time steps.

Velocity update due to pressure influence

We then update the velocity from $\mathbf{u}^s$ to $\mathbf{u}^{ss}$ to account for the pressure influence:

$$\frac{\mathbf{u}^{ss} - \mathbf{u}^s}{\Delta t} = -\nabla p^* \quad \text{in } D, \quad (2.14)$$

where the intermediate pressure field p^* is solved from:

$$\nabla^2 p^* = \nabla \cdot \left(\frac{\mathbf{u}^s}{\Delta t} \right) \quad \text{in } D. \quad (2.15)$$

This equation is derived from Eq. (2.14) by imposing the incompressibility constraint $\nabla \cdot \mathbf{u}^{ss} = 0$, following the velocity-correction splitting scheme described in [50]. The following Neumann boundary condition for p^* is used at any velocity Dirichlet boundary:

$$\frac{\partial p^*}{\partial n} = \sum_{q=0}^{J_e-1} \beta_q [-(\mathbf{u} \cdot \nabla) \mathbf{u} + \mathbf{g} - \nu \nabla \times (\nabla \times \mathbf{u})]^{n-q} \cdot \mathbf{n}, \quad (2.16)$$

assuming time-independent normal velocities at the boundary (see [50]).

Viscous effects

We obtain the intermediate velocity $\mathbf{u}^*$ based on $\mathbf{u}^{ss}$ by treating the viscous term implicitly:

$$(\nabla^2 - \frac{\gamma_0}{\nu \Delta t})\mathbf{u}^* = -\frac{\mathbf{u}^{ss}}{\nu \Delta t} \quad \text{in } D, \quad (2.17)$$

where γ_0 is the scaled coefficient of the stiffly-stable scheme with $\gamma_0 = \sum_{q=0}^{Je-1} \alpha_q$. Here the velocity $\mathbf{u}^*$ on the boundary takes the same values prescribed as boundary conditions.

Velocity update due to rigid-body motion constraint

First, the hydrodynamic force and torque on the particles exerted by the surrounding fluid are derived from the momentum conservation between the particles and the fluid. In other words, the momentum change in the particle and interfacial domain equals the time integral of the hydrodynamic force and the external force. Hence, we assign

$$\mathbf{F}_{hi}^n = \frac{1}{\Delta t} \int_D \rho \phi_i^{n+1} (\mathbf{u}^* - \mathbf{u}_p^n) d\mathbf{x} - \int_D \phi_i^{n+1} \rho \mathbf{g} d\mathbf{x} \quad (2.18a)$$

$$\mathbf{N}_{hi}^n = \frac{1}{\Delta t} \int_D \mathbf{r}_i^{n+1} \times [\rho \phi_i^{n+1} (\mathbf{u}^* - \mathbf{u}_p^n)] - \int_D \phi_i^{n+1} \mathbf{r}_i^{n+1} \times (\rho \mathbf{g}) d\mathbf{x}, \quad (2.18b)$$

where $\mathbf{r}_i^{n+1}$ is the distance vector from the rotational reference point on the i_{th} particle to any spatial point $\mathbf{x}$. Here a first order approximation is used in the force integration.

Second, the particle translational and angular velocities are updated using Newton's equations:

$$\mathbf{V}_i^{n+1} = \mathbf{V}_i^n + M_i^{-1} \cdot \Delta t \cdot \sum_{q=0}^{Je} a_q \cdot (\mathbf{F}_{hi}^{n-q} + \mathbf{F}_{ext_i}^{n-q}) \quad (2.19a)$$

$$\mathbf{\Omega}_i^{n+1} = \mathbf{\Omega}_i^n + I_i^{-1} \cdot \Delta t \cdot \sum_{q=0}^{Je} a_q \cdot (\mathbf{N}_{hi}^{n-q} + \mathbf{N}_{ext_i}^{n-q}), \quad (2.19b)$$

where M_i and I_i are the mass and the moment of inertia of the i_{th} particle, a_q are the coefficients from a Adam-Bashforth scheme. Here $\mathbf{F}_{ext_i}^{n-q}$ and $\mathbf{N}_{ext_i}^{n-q}$ are respectively the external force and torque on the i_{th} particle at previous time steps.

Third, the particle velocity field is calculated from:

$$\phi^{n+1} \mathbf{u}_p^{n+1} = \sum_{i=1}^{N_p} \phi_i^{n+1} \{ \mathbf{V}_i^{n+1} + \boldsymbol{\Omega}_i^{n+1} \times [\mathbf{x} - \mathbf{R}_i^{n+1}] \}. \quad (2.20)$$

For free motion of particles, $\mathbf{u}_p$ is coupled with the forces and torques on particles $\mathbf{F}_{hi}, \mathbf{F}_{ext_i}, \mathbf{N}_{hi}$ and $\mathbf{N}_{ext_i}$. To decouple the system, we employ Eq. (2.18), (2.19) and (2.20) using an explicit numerical scheme.

Fourth, we solve for the extra pressure field p_p due to the rigidity of the particle as:

$$\nabla^2 p_p = \gamma_0 \nabla \cdot \left(\frac{\phi^{n+1} (\mathbf{u}_p^{n+1} - \mathbf{u}^*)}{\Delta t} \right) \quad \text{in } D. \quad (2.21a)$$

The following is used as the boundary conditions for p_p at any velocity Dirichlet boundary (with time-independent normal velocities):

$$\frac{\partial p_p}{\partial n} = \frac{\gamma_0 \phi^{n+1} (\mathbf{u}_p^{n+1} - \mathbf{u}^*)}{\Delta t} \cdot \mathbf{n}. \quad (2.21b)$$

Finally, we update the total velocity field by enforcing the rigid-body motion constraint using the particle velocity field $\phi^{n+1} \mathbf{u}_p^{n+1}$:

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \gamma_0 \mathbf{u}^*}{\Delta t} = \frac{\gamma_0 \phi^{n+1} (\mathbf{u}_p^{n+1} - \mathbf{u}^*)}{\Delta t} - \nabla p_p \quad \text{in } D. \quad (2.22)$$

Eq. (2.21a) and (2.21b) are both derived from Eq. (2.22). The total pressure field is calculated by summing the intermediate pressure and the extra pressure field, i.e., $p^{n+1} = p^* + p_p$.

2.2.3 Fully-discrete system: spatial discretization

For spatial discretization of the above equations, we apply the spectral/ hp element method (see [50]). This hybrid method benefits from both finite element and spectral discretization: on one hand, for domains with complex geometry, we can increase the number of subdomains/elements (h-refinement) with the error in the numerical solution decaying algebraically. On the other hand, with fixed elemental size we can increase the interpolation order within the elements (p-refinement) to achieve an exponentially decaying error, provided the solutions are sufficiently smooth throughout the domain. Hence, the use of smoothed profiles in SPM preserves the high-order numerical accuracy of the spectral/ hp element method.

The solution domain is partitioned into non-overlapping sub-domains/elements (with characteristic size of an element to be h): $\Omega = \bigcup_{e=1}^{N_{el}} \Omega^e$. We use hexahedral or tetrahedral elements in our present numerical simulations. By constructing the standard element Ω^{st} , the local coordinates in the standard element ($\zeta \in \Omega^{st}$) can be mapped to the global coordinate in any elemental domain ($\mathbf{x} \in \Omega^e$) by an isoparametric transformation $\mathbf{x} = \chi^e(\zeta)$. Then, a polynomial expansion (with polynomial order up to P) is employed within the standard element to construct the approximate solution u^δ :

$$u^\delta(\mathbf{x}) = \sum_{e=1}^{N_{el}} \sum_{j=1}^P \hat{u}_j^e \psi_j^e(\zeta) = \sum_{i=0}^{N_{dof}} \hat{u}_i \Psi_i(\mathbf{x}), \quad (2.23)$$

where $\zeta = [\chi^e]^{-1}(\mathbf{x})$ is the local coordinate, $\psi_j^e(\zeta)$ denotes the local expansion modes, and $\Psi_i(\mathbf{x})$ are the global modes derived from the global assembly of the local modes [50].

For the expansion basis $\psi_j^e(\zeta)$, both *modal* and *nodal* basis can be used. A modal expansion is used in conjunction with Galerkin projection to solve Eq. (2.15),(2.17) and (2.21a), while a nodal expansion is used in conjunction with collocation projection of Eq. (2.13). The updating step (2.22) could be done by either collocation or Galerkin projection. The former is more efficient but the numerical solution might be

discontinuous at some element boundaries, whereas the latter guarantees C^0 continuity of the approximate solution across the elements through an appropriate choice of the boundary modes. For the modal expansion, we use a semi-orthogonal basis written in terms of the Jacobi polynomials. For the nodal basis, we employ the Lagrange-Jacobi polynomials through the Gauss-Legendre-Lobatto quadrature points.

The spectral/ hp element method allows us to accurately represent arbitrary fixed rigid boundaries of the flow domain while using SPM to represent the particles.

2.3 Prototype flows: error analysis and verification

In order to verify SPM and analyze its error, we test several prototype flow problems.

2.3.1 Planar Couette flow

We simulate the steady laminar flow of a viscous fluid between two parallel plates, one moving relatively to the other. The plates are separated by a distance h in the y -direction with the lower plate aligned with the x -axis and being stationary while the upper plate moving with constant velocity $\mathbf{V} = (V, 0, 0)$. At first, we want to see how accurately SPM captures the exact analytical solution $\mathbf{u}_{exact} = (V \cdot y/h, 0, 0)$ for $y \in [0, h]$ and $(V, 0, 0)$ for $y \in [h, 2h]$; here we specify $V = 1, h = 3$.

Specifically, using this problem, we want to analyze SPM using two different time-discretization implementations: one is the original fully-explicit scheme [81, 78], while the other is the semi-implicit scheme we proposed in the previous section. The fully-explicit SPM uses two steps in Eq. (2.9a) and (2.10), while the semi-implicit SPM uses four steps given by Eq. (2.13), (2.14), (2.17) and (2.22). The top wall ($h \leq y \leq 2h$) is treated by a ‘‘Smoothed Profile’’, with the concentration field of $\phi(\mathbf{x}, t) = \frac{1}{2}[\tanh(\frac{y-h}{\xi}) + 1]$ derived from Eq. (2.1b). The simulation domain D is

a box of $h/3 \times 2h \times h/3$, with periodic boundaries in the x- and z-directions and Dirichlet boundaries in the y-direction (i.e., $\mathbf{u}|_{y=0} = (0, 0, 0)$, $\mathbf{u}|_{y=2h} = \mathbf{V} = (1, 0, 0)$). We ignore both the gravity and the advection $(\mathbf{u} \cdot \nabla)\mathbf{u}$ in both implementations. The velocity and pressure fields are solved by a first-order temporal scheme by marching through pseudo-time to the steady state. The spectral/ hp element method is used for spatial discretization, with six non-uniform elements and a polynomial order of $P = 11$. Upon convergence to steady state, we calculate the L_2 error (L_{2er}) of the streamwise velocity u in the flow region $0 \leq y \leq h$.

We can also obtain solutions directly from the semi-discrete equations by assuming that: (1) All the field quantities are only y-dependent, i.e., $\mathbf{u}(x, y, z) = \mathbf{u}(y)$, $p(x, y, z) = p(y)$, etc.; (2) The velocity field has a nontrivial component only in the streamwise direction, i.e., $\mathbf{u}(y) = (u(y), 0, 0)$; (3) Steady state is achieved, i.e., $u^{n+1} = u^n$; (4) The pressure is uniform everywhere, i.e., $\nabla p^* = (0, 0, 0)$, $\nabla p_p = (0, 0, 0)$. Then for the *fully-explicit* implementation, from (2.9a) and (2.10), we obtain the 1D reduced system for the streamwise velocity u^n and the streamwise intermediate velocity u^* :

$$\begin{cases} (1 - \phi)\nu\Delta t \frac{\partial^2 u^n}{\partial y^2} - \phi u^n = -\phi u_p \\ u^* = u^n + \nu\Delta t \frac{\partial^2 u^n}{\partial y^2}. \end{cases} \quad (2.24)$$

Applying the same assumptions to the *semi-implicit* scheme, a *different* reduced system for u^n and u^* is derived from Eq. (2.13), (2.14), (2.17) and (2.22):

$$\begin{cases} \nu\Delta t \frac{\partial^2 u^*}{\partial y^2} - \phi u^* = -\phi u_p \\ u^n = u^* + \phi(u_p - u^*). \end{cases} \quad (2.25)$$

From the above reduced systems, for both schemes we obtain the velocity to be: $u^n = u_p$ when $\phi = 1$ (particle domain) and $u^n = u^* = ay$ when $\phi = 0$ (fluid domain), where the constant a needs to be determined by matching the velocity through the interface domain. In the limit of employing a *step function* for ϕ (i.e., $\xi = 0$), and by imposing C^0 continuity of u^n at the interface $y = h$, we find that $a = y/h$, which

means we recover the exact solution using both schemes. However, if ϕ is a smooth function with $\xi > 0$, the above two reduced systems are solved by a second-order finite difference method using a fine uniform grid (with 4001 grid points and mesh size $\Delta y = 2h/4000$).

Furthermore, in both 1D systems (2.24) and (2.25), an artificial boundary layer (scaling as $\sqrt{\nu\Delta t}$) is present. In particular, both terms $\exp(\pm y/\sqrt{\nu\Delta t})$ will be present in the velocity solution and this will lead to a non-monotonic error behavior. Our results from solving the full 3D system further verify this.

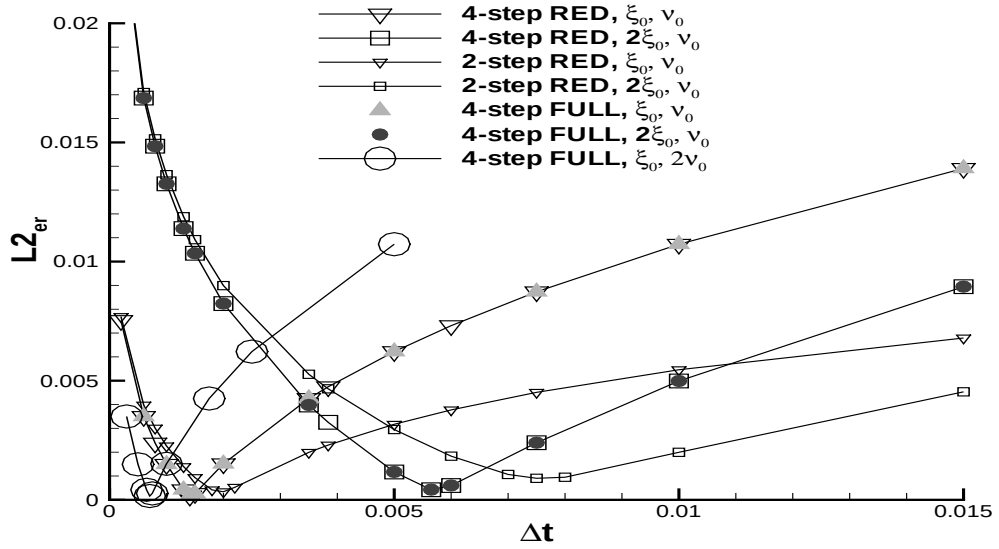


Figure 2.2: *Couette flow*: L_2 error of the streamwise velocity versus Δt for two different interface thickness ξ and two different kinematic viscosity ν . (LEGEND NOTE: ‘4-step’: 4-step semi-implicit scheme ; ‘2-step’: 2-step full-explicit scheme; ‘RED’: reduced 1D system discretized by finite difference; ‘FULL’: full 3D system discretized by spectral/ hp element; ‘ ξ_0 ’: $\xi_0 = 0.05 = 0.0167h$; ‘ ν_0 ’: $\nu_0 = 1.0$.)

Fig. 2.2 shows that the L_2 error in both implementations has a non-monotonic dependence on the time step Δt , similar in fact to the error structure of semi-Lagrangian schemes [120]. We note that the spatial discretization error is negligible since increasing the polynomial order in each element from $P = 11$ to $P = 13$ showed no change in the L_2 error. The true temporal discretization error should also vanish

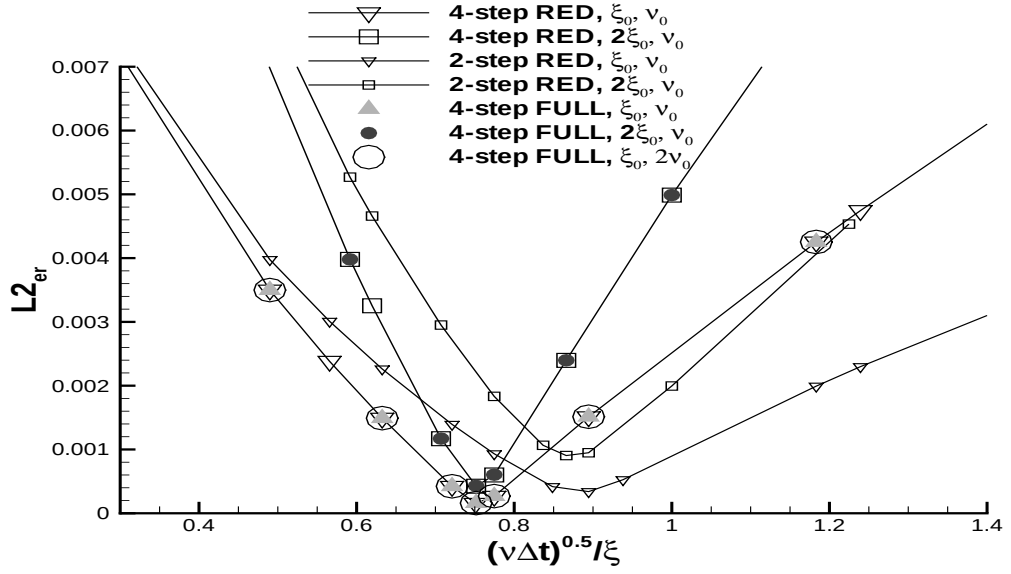


Figure 2.3: *Couette flow*: L_2 error of the streamwise velocity versus $\sqrt{\nu\Delta t}/\xi$ for the same SPM simulation results as shown in Fig. 2.2.

for the high-order splitting scheme (see [50]). The agreement of the 4-step full 3D system results with the 4-step reduced 1D system results in Fig. 2.2 indicates a negligible error of the pressure solver. So the L_2 error shown in the figures consists of the SPM modeling error from the smoothed particle representation in the Navier-Stokes equation by Eq. (2.9a) and (2.10). Simple scaling arguments of the 1D systems (2.24) and (2.25) show that the error is, in fact, a function of $\sqrt{\nu\Delta t}/\xi$, and the results from the solution of the full 3D system shown in Fig. 2.3 verify this.

Fig. 2.3 also indicates that the optimum time step size $(\Delta t)_o$ depends only on $\sqrt{\nu}/\xi$, i.e., for the 2-step fully-explicit scheme $\sqrt{\nu(\Delta t)_o}/\xi \sim 0.88$, while for the 4-step semi-implicit scheme $\sqrt{\nu(\Delta t)_o}/\xi \sim 0.75$. A physical explanation of this error behavior can be put forward by considering the following two aspects. On the one hand, recall that SPM essentially adds a penalty term $\mathbf{f}_s \sim \phi(\mathbf{u}_p - \mathbf{u}^*)/\Delta t$ in the Navier-Stokes equations. Hence, smaller Δt would have a tighter control of the flow and thus achieve better accuracy. But on the other hand, physically SPM simulates the particle by impulsively applying a momentum change to the particle

domain at each time step, which in turn creates an impulse on the flow as in the Stokes' first problem. The thickness of the diffusive layer (within which the impulsive momentum change has an effect) is thus scaled as $\delta = 2.76\sqrt{\nu\Delta t}$ [57]. So a smaller Δt will produce a thinner Stokes layer thickness δ ; in particular, if Δt is so small that δ cannot be spatially resolved by the smoothed profile used, it will lead to an increase in error. Let us introduce the “effective” smooth interface thickness l_e , which is expected to be scaled as 2ξ . The optimum time step size $(\Delta t)_o$, which produces the smallest error, comes from the balance of the Stokes layer scale δ and the effective interface thickness l_e . The numerical results in Fig. 2.3 verify this by showing that $l_e = 2.07\xi$ for the 4-step semi-implicit implementation. But for the 2-step fully-explicit scheme, a larger $l_e = 2.42\xi$ is indicated. By treating the viscous term implicitly in the 4-step scheme, we have a stricter control of the viscous layer throughout the interface domain, thus the intermediate velocity $\mathbf{u}^*$ is more sharply defined and hence the effective smooth interface thickness l_e is thinner.

Furthermore, we check the spectral convergence of the L_2 error of the streamwise velocity for increasing polynomial order P in figure 2.4. Since the modeling error dominates over the spatial discretization error if we use a large P , we present the discretization error by the difference in the L_2 error between arbitrary P and $P = 13$, i.e. $\log_{10}(L2_{er} - L2_{er,P=13})$. The figure indicates that spectral convergence in the spatial discretization is achieved.

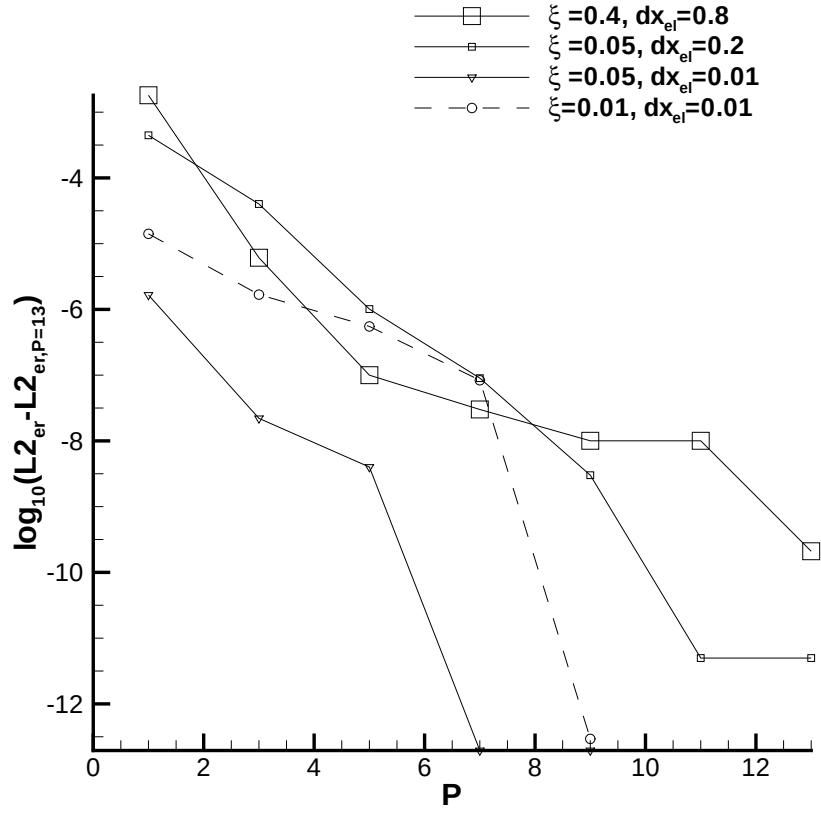


Figure 2.4: *Couette flow*: difference in L_2 error of the streamwise velocity $\log_{10}(L2_{er} - L2_{er,P=13})$ versus polynomial order P for different interface thickness ξ and element size dx_{el} near the interface.

2.3.2 Periodic array of spheres

Next we apply SPM to another benchmark problem describing the sedimentation of spheres (of radius a) arranged in a periodic cubic lattice (of length L). The particle concentration c is defined by the ratio of the particle volume (Ω_p) over the domain volume (Ω): $c = \Omega_p/\Omega = \frac{4\pi a^3}{3}/L^3$. For low c , Hasimoto [34] has derived a relationship between the external force ($\mathbf{F}$) on each sphere and the sedimentation velocity ($\mathbf{V}_{exact}$) as follows:

$$\mathbf{V}_{exact} = (1 - 1.7601c^{\frac{1}{3}} + c - 1.5593c^2 + O(c^{\frac{8}{3}})) \frac{\mathbf{F}}{6\pi a \rho \nu}, \quad (2.26)$$

where $\frac{\mathbf{F}}{6\pi a \rho \nu}$ is the Stokes velocity of a particle settling in a unbounded fluid under the external force $\mathbf{F}$.

The simulation here adopts a configuration of $L = 12$ and $a = 2$. Hence $c = 0.0194$, and Eq. (2.26) can be used to compare with the settling velocity results from the numerical simulations. In order to maintain the system in equilibrium, a uniform pressure gradient is applied to balance the net force exerted on the spheres: $\nabla p \cdot \Omega = -\mathbf{F}$. The net volume flux is zero in this frame of reference. Alternatively, if we change the reference frame to move with the particle (with velocity $\mathbf{V}$), the particles can be viewed as a fixed bed flushed by fluid driven by a pressure gradient. The superficial velocity is defined by the net displacement or volume flux of flow throughout the domain D :

$$\mathbf{V}_s = \frac{1}{\Omega} \int_D \mathbf{u} d\mathbf{x}, \quad (2.27)$$

where $\mathbf{u}$ is the flow velocity at any spatial point $\mathbf{x}$. As this reference frame is moving with velocity $\mathbf{V}$, from the zero net volume flux under the original fixed frame, we have $\Omega \mathbf{V}_s + \Omega \mathbf{V} = 0$, thus $\mathbf{V}_s = -\mathbf{V}$, i.e., the superficial velocity in the second reference frame equals the negative settling velocity in the first reference frame. This, in fact, is the result of Galilean invariance, which we have verified also numerically.

In addition to the settling velocity, we want to examine the accuracy of SPM in

the *pointwise* sense with comparisons against *well-resolved* Direct Numerical Simulations (DNS) using the spectral/*hp* element code [56], and also against the Force Coupling Method (FCM) with spectral/*hp* element discretizations as presented in [75, 67]. For the SPM simulation, flows in both reference frames are resolved with an identical grid of 1728 uniform hexahedral elements and $P = 7$ polynomial order. Also, the same uniform pressure gradient $\nabla p = (-5.88 \times 10^{-4}, 0, 0)$ is applied in both reference frames. Within the first reference frame, an external force $\mathbf{F} = -\nabla p \cdot \Omega$ is applied on each sphere, and the sedimentation velocity $\mathbf{V}$ is calculated. In the second reference frame, the particle velocity is zero, and the superficial velocity $\mathbf{V}_s$ is calculated.

Both DNS and FCM simulations are performed to resolve the flow in the second reference frame. DNS simulation applies a pressure gradient of $\nabla p' = \nabla p \cdot \Omega / \Omega_f$ to ensure the same value of the drag force, and hence the same flow problem as in SPM and FCM simulations is solved. A non-uniform mesh of 11,232 tetrahedral elements and $P = 7$ polynomial order is used. FCM simulation uses a penalty method to calculate the external force in order to fix the particle in position as proposed in [68]. The same pressure gradient ∇p and the same mesh as in the SPM simulation is used for FCM.

Fig. 2.5 shows the streamwise velocity profiles along the cross-flow direction (y-axis) using DNS, FCM and SPM, all in the second reference frame. The agreement of SPM and DNS is very good everywhere; SPM has a similar error to FCM in the far-field, but SPM resolves the near-field velocity much better. This is due to the rigid-body constraint imposition of SPM, which is not present in the FCM implementation. Also the errors of the superficial velocity for FCM and SPM simulations are very similar; both are around 0.05%.

The error plots in Fig. 2.6 confirm the conclusions of the last subsection, namely that the SPM modeling error is a function of $\nu \Delta t$ and ξ , and the optimum time step size $(\Delta t)_o$ is determined by the balance of the Stokes layer $\delta = 2.76\sqrt{\nu \Delta t}$ and the

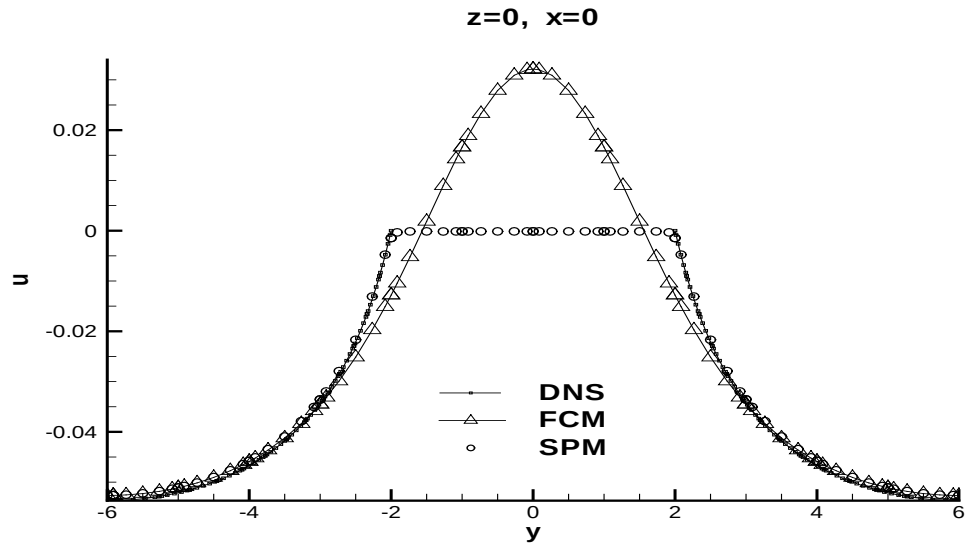


Figure 2.5: *Periodic array of spheres*: streamwise velocity u along the center line y -axis, using DNS, FCM and SPM (with $\nu = 0.34, \xi = 0.1 = 0.05a, \Delta t = 0.015$).

effective smooth interface thickness l_e . We find from the above data that $l_e \sim 2.07\xi$ for sufficiently small ξ ($\xi = 0.025a$), which is the same as the result we obtained for the Couette problem! (We note that l_e is slightly smaller ($l_e \sim 1.97\xi$) if we employ a larger value of ξ , e.g. $0.05a$.) Fig. 2.6 also verifies that the relative difference between the absolute values of the superficial velocity $\mathbf{V}_s$ and the settling velocity $\mathbf{V}$ is negligible.

2.3.3 Rotating sphere at low Reynolds number

Next we investigate the accuracy of SPM in simulating the steady flow induced by a sphere rotating with constant angular velocity in a viscous incompressible fluid which is at rest at large distances from the sphere. This problem in an open domain has been treated analytically by Bickley [5], who obtained a second-order approximation for the fluid velocity and pressure, which is quite accurate when the Reynolds number

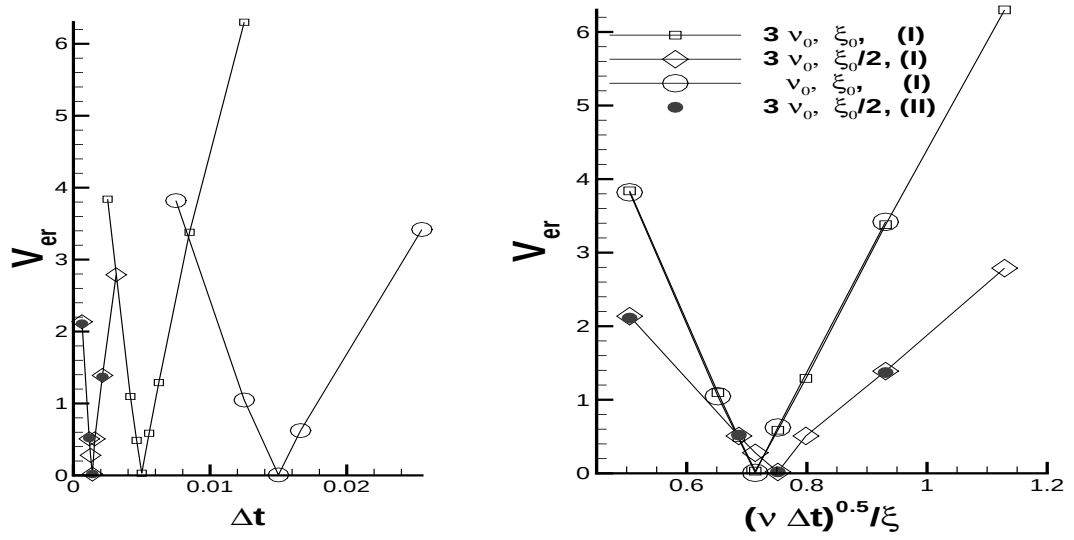


Figure 2.6: *SPM* for a periodic array of spheres: percentage error in settling velocity ($V_{er} = \frac{|\mathbf{V} - \mathbf{V}_{exact}|}{V_{exact}} \cdot 100$) versus time step Δt (left) and versus $\sqrt{\nu\Delta t}/\xi$ (right), for two values of viscosity ν and for two values of the interface thickness ξ . (LEGEND NOTE: ' ν_0 ': $\nu_0 = 0.34$; ' ξ_0 ': $\xi_0 = 0.1 = 0.05a$; '(I)': simulation done in the first reference frame to calculate $\mathbf{V}$; '(II)': simulation done in the second reference frame with fixed spheres, $-\mathbf{V}_s$ calculated to substitute $\mathbf{V}$.)

is small. We use this open-domain solution as a reference to validate our numerical simulation results for a finite domain, at Reynolds number less than or equal to 8.0.

The computational domain is $[-\pi, \pi] \times [-\pi, \pi] \times [-\pi, \pi]$, with a sphere of radius $a = 0.261$ centered at the origin and spinning with an angular velocity of $\omega = (0, 0, \omega_z)$. We use this configuration of $L/2a = 2\pi/2a = 12.036$ with periodic treatment on domain boundaries in all three directions to simulate the unbounded flow domain. By the definition of the rotation Reynolds number $Re_w = \omega_z a^2 / \nu$, we set $\omega_z = 10.01$ and simply change the fluid kinematic viscosity ν to obtain different values of Reynolds number, from 0.25 to 8.

The required external torque T_{ext} on the sphere to achieve a Reynolds number Re_w is estimated from the asymptotic approximation obtained by Takagi [108]:

$$2T_{ext}/\rho a^5 \omega_z^2 = 16\pi(1 + f(Re_w))/Re_w,$$

This is a correction to Lamb's result $M = 16\pi/Re_w$ for Stokes flow [59], and has been confirmed by numerical simulations of Dennis [15] for $Re \leq 10$. Numerical results of the hydrodynamic torque obtained from Eq. (2.18b) are compared to this given external torque.

For the SPM simulations we used 4096 nonuniform hexahedral elements and a polynomial order of $P = 5$. The following indicator function, utilizing the form of (2.2), was applied:

$$\phi(\mathbf{x}, t) = \frac{1}{2} \left[\tanh\left(\frac{f(\mathbf{x}, t)}{\xi} \tau\right) + 1 \right], \quad \text{with} \quad f = 1 - |\mathbf{x}|^2/a^2, \quad \tau = a/2. \quad (2.28)$$

Compared to the original spherical envelope (2.1), this envelope is slightly different and thus the effective smooth interface thickness l_e is slightly different from 2.07ξ obtained for (2.1). Let us define the effective interface thickness l_e to be twice the distance from the particle surface to the spatial point whose concentration function is $\phi_e = (\tanh(\frac{-2.07/2\xi}{\xi}) + 1)/2 = 0.112$. For the original envelopes (2.1), with $\xi =$

$0.05a = 0.013$, $l_e = 2.07\xi = 0.0269$; with the new envelope (2.28), using the same ξ , we have $l_e = 2 \times 0.0127 = 0.0254$. The time step size is thus chosen according to the expected optimum time step derived from $2.76\sqrt{\nu(\Delta t)_o} = l_e$. DNS results were obtained using 6600 hexahedral elements with polynomial order $P = 7$. The FCM results from [11], which were obtained by a Fourier pseudo-spectral method with 64^3 grid points for the same domain, are also included for comparison.

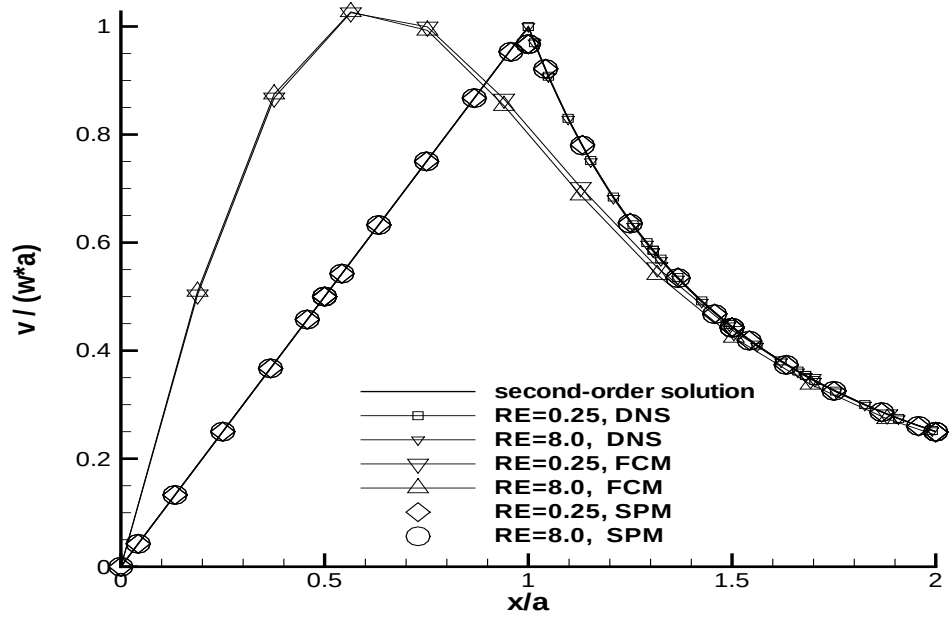


Figure 2.7: *Rotating sphere*: Non-dimensional *azimuthal* velocity v versus radial distance along the x -axis. Comparison between the second-order approximation solution and results from DNS, FCM and SPM (with $\xi = 0.05a$) for two different Reynolds numbers.

We see from Fig. 2.7 that SPM captures the primary azimuthal velocity quite well, with a maximum pointwise error of about 3.2% near the sphere surface (with $\xi = 0.05a$). This error goes up to about 4.9% if we use a thicker smooth interface, $\xi = 0.077a$. The radial velocity is more challenging to resolve, for it comes from the secondary flow at finite Reynolds numbers and its magnitude is much smaller

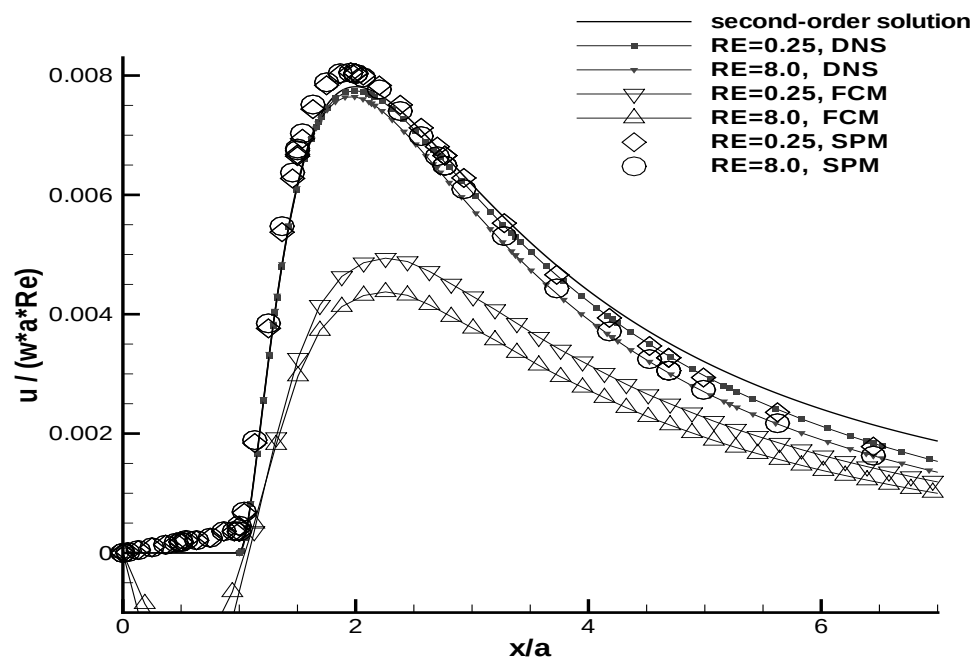


Figure 2.8: *Rotating sphere*: Non-dimensional *radial* velocity u versus radial distance the along x -axis. Comparison between the second-order approximation solution and results from DNS, FCM and SPM (with $\xi = 0.05a$) for two different Reynolds numbers.

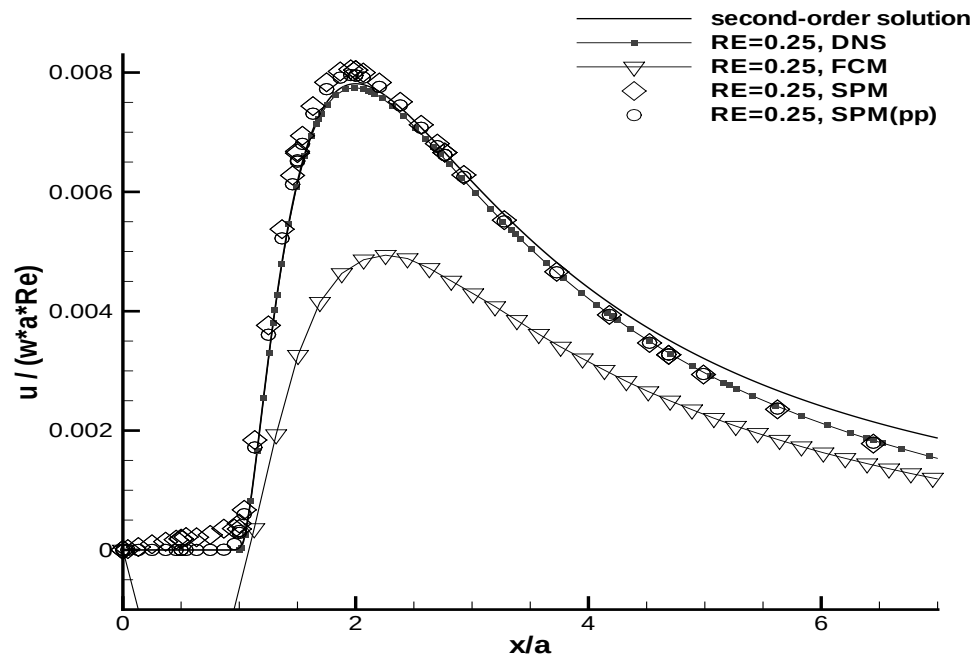


Figure 2.9: *Rotating sphere at Reynolds number 0.25*: Non-dimensional *radial* velocity u versus radial distance along the x -axis. Comparison between the second-order approximation solution and results from DNS, FCM, SPM (with $\xi = 0.05a$). (LEG-
END NOTE: ‘SPM(pp)’: SPM with p_p modification step as in Eq. (2.29).)

than the dominant azimuthal velocity. Fig. 2.8 shows that there is some effect due to the periodic boundary conditions as manifested by the difference between the SPM results and the second-order approximate solution [5]. The relative difference in the azimuthal velocity is around 0.00063 on the domain boundaries. Thus, we employ DNS results for a more fair comparison, and the agreement with SPM is good everywhere. We also see that SPM is resolving the radial velocity much better than FCM near the particle surface ($x/a < 1.3$), and it resolves the far-field velocity as well as FCM. By reducing the SPM interface thickness parameter from $\xi = 0.077a$ to $\xi = 0.05a$, the peak pointwise error in the radial velocity reduces from about 8.5% to 3.6% for Reynolds number 0.25.

With the above SPM setup, we now check the indirect imposition of the *no-slip constraint* on the sphere boundary by validating Eq. (2.6) on the equator plane $z = 0$. The right hand side (RHS) is calculated using ϕ from (2.28), $\mathbf{u}(r \leq a) = \omega \times \mathbf{x}$ and $\mathbf{u}(r > a) = (\omega \times \mathbf{x})a^3/|x|^3$ which is the exact Stokes solution for an open domain. The left hand side (LHS) is computed by taking the numerical gradient of the total velocity. We obtain the relative error between RHS and LHS (in L2-sense) to be around 1.1%. By noting that this error mainly comes from the periodic boundary treatment instead of a open domain, and this problem features in sharp transition of the vorticity across the interface, the above test serves as a sufficient verification of the imposition of no-slip boundary constraint in SPM.

Fig. 2.8 also shows a non-zero radial velocity inside the particle, which is of the same order of magnitude as the peak error in the radial velocity. This particle-penetrating phenomenon arises from the final updating step Eq. (2.22), where ∇p_p has a non-zero value even inside the particle. In order to suppress this erroneous velocity we modify (2.22) to:

$$\gamma_0 \frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{dt} = \gamma_0 \frac{\phi(\mathbf{u}_p^{n+1} - \mathbf{u}^*)}{dt} - (1 - \phi)\nabla p_p. \quad (2.29)$$

We see from Fig. 2.9 that the result is satisfying, as this modification ensures the

non-penetrating constraint is satisfied strictly inside the particle as well and this has as a result a further reduction in the error of the radial velocity outside the particle. However, this modification introduces some compressibility inside and on the particle boundary (i.e., $\phi \neq 0$), see Eq. (2.21a) and (2.29). Indeed, the numerical results show that the divergence of the total velocity $\nabla \cdot \mathbf{u}^{n+1}$ is slightly larger than the divergence of the intermediate velocity $\nabla \cdot \mathbf{u}^*$ inside the particle, however, both are of comparable magnitude.

2.3.4 Stokes oscillating plate

Next we study an *unsteady* problem in order to evaluate the temporal discretization error and how it compares to the modeling error inherent in SPM. To this end, we consider the problem of an infinite plate oscillating in an unbounded fluid. The simulation domain is $[0, 1] \times [0, 6] \times [0, 1]$, where $y \in [0, 3]$ is the solid plate modeled by SPM and the fluid flow is in the interval $y \in [3, 6]$. The plate moves with an oscillating velocity $\mathbf{V} = (\sin(\omega t), \mathbf{0}, \mathbf{0})$. The exact solution given in [89] is

$$\mathbf{u}_{ex} = (e^{-Y/\sqrt{2}} \sin(T - Y/\sqrt{2}), 0, 0),$$

where $Y = \frac{y-3}{(\nu/\omega)^{1/2}}$ and $T = \omega t$ for our case. We treat the boundary at $y = 6$ as a Dirichlet boundary using the exact solution; periodicity is imposed along both the x- and z-directions.

We calculate the L_2 error of the streamwise velocity in the domain ($y \in [0, 3]$) at each time step and then calculate the mean error after convergence (to a constant-amplitude *sine* function in time). Here we specify the fluid kinematic viscosity as $\nu = 1$ and the oscillating frequency parameter to be $\omega = 1$. SPM simulations are performed on a mesh of 6 non-uniform hexahedral elements with $P = 7$ polynomial order. Different order ($J_e = 1, 2$ or 3) in time integration for solving the intermediate velocity $\mathbf{u}^*$ is employed.

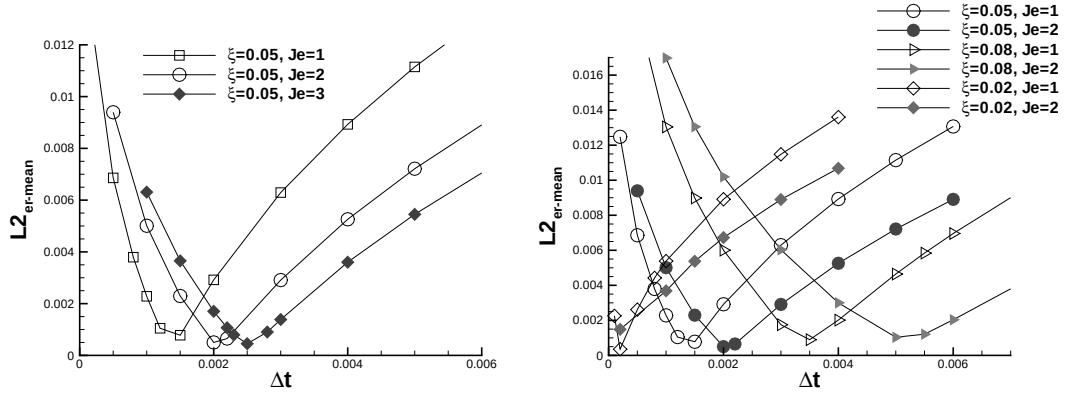


Figure 2.10: *Oscillating plate*: Mean L_2 error ($L2_{er-mean}$) versus time step size Δt for different order J_e (left) and different interface thickness parameter ξ (right).

From Fig. 2.10, we see that indeed higher time-integration order J_e leads to smaller errors beyond the optimum time step size where the temporal discretization error dominates over the SPM modeling error. This behavior, in fact, confirms that the temporal error has two contributions: (1) the SPM modeling error, which is a function of $\nu\Delta t$ and ξ , and (2) the discretization error from the time-integration scheme we use for the intermediate velocity field solving Eq. (2.13), (2.15), (2.14) and (2.17); the second error scales as $(\nu\Delta t)^{J_e}$ for unsteady problems (see details in [49]). With regards to the effect of the profile thickness ξ , our results suggest that larger thickness ξ and higher order J_e would lead to larger optimum time step $(\Delta t)_o$, which is clearly advantageous in production simulations.

2.4 Flow past complex-shaped particles

So far we have modeled particles with simple shapes but in this section we employ the new general envelopes (Eq. (2.2)) to model flow past complex-shaped particles. SPM is advantageous in that it does not require complex meshes around the particle surfaces, as the computational domain is the entire domain including particle domains. The way it represents the complex-shaped particles is rather straightforward. As

long as we know the surface function of the particles or we have the coordinates of a sufficient number of points on the particle surfaces, we can obtain the concentration field ϕ representing the particles, and then solve the governing equations for the flow. In the following we examine the accuracy of SPM for ellipsoidal and biconcave particles.

2.4.1 Stokes flow past an ellipsoid

We first study ellipsoidal particles, specifically spheroids. Similar to what we employed for the rotating sphere, here too we use an indicator function utilizing Eq. (2.2) with

$$f = 1 - (x^2/a^2 + y^2/b^2 + z^2/c^2), \quad \text{and} \quad \tau = \sqrt[3]{abc}/2,$$

where a, b, c are the semi-axes of the ellipsoid centered at the origin.

With this concentration function we apply SPM to the problem of Stokes flow past a spheroid (aligned with the flow) between two infinite parallel walls. The simulation domain is $[80, 80] \times [-3.3333, 10] \times [-20, 20]$ with $y = -3.3333$ and $y = 10$ to be the walls. Periodicity is imposed in both x- and z- directions. A spheroid with semi-axes of $a = 2, b = 1$ and $c = 1$ is centered at the origin with its long axis aligned with x-axis. A uniform pressure gradient of $\nabla p = (0.06075, 0, 0)$ is applied to drive the flow. Thus, the flow far from the ellipsoid can be modeled as a fully developed Poiseuille flow driven by this pressure gradient, and correspondingly the centerline velocity is $U_{cl} = 1.35$. Based on these values, we obtain from table 7-5.1 in [33] the “exact” drag force $(F_x)_{ex} = 29.1765$ for a fixed ellipsoid immersed in an infinite Poiseuille flow. We use this force value as the “exact” drag force to compare against our SPM results on a finite computational domain.

In the SPM simulation we use 4560 rectilinear elements with polynomial order $P = 3$, with finer resolution around the spheroid (see Fig. 2.11). We choose the

interface thickness to be $\xi = 0.1b$.

For comparison, we have also performed both DNS and FCM simulations. In FCM we employed the same mesh as in the SPM simulation (i.e., 4560 elements with $P = 3$), and we computed the hydrodynamic force and torque using a penalty method as in [68]. DNS simulation employs 7168 hexahedral elements with polynomial order $P = 4$. The meshes, displaying the elements only, are shown in Fig. 2.11.

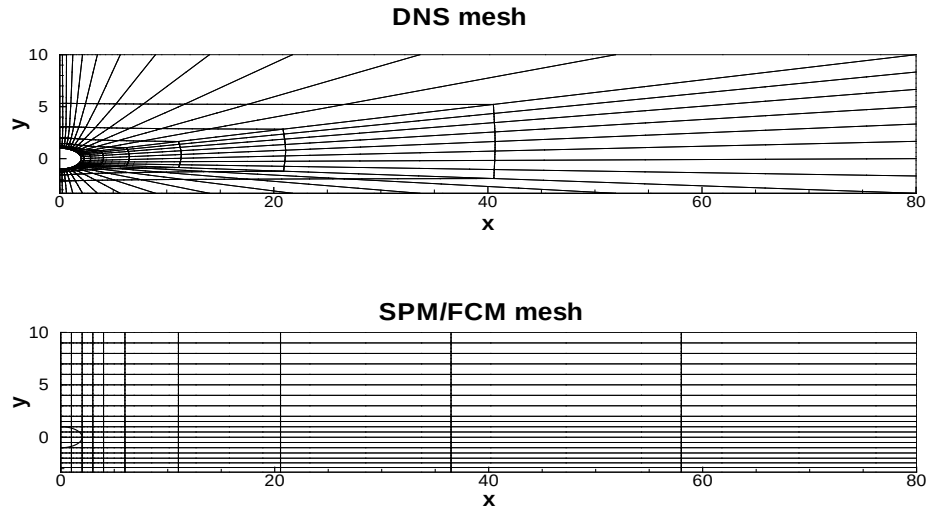


Figure 2.11: *Flow past an ellipsoid*: slices ($z=0$ plane) of meshes used in the simulations of DNS (top), SPM and FCM (bottom). Due to the symmetry in the streamwise (x -) direction, only half of the domain is shown.

We have summarized the results of our simulations in Tab. 3.1. It shows that for this value of ξ , the optimum time step size is around 0.005, which, in fact, is the value expected from the balance of the Stokes layer thickness δ and the effective interface thickness l_e , i.e., $\delta = 2.76\sqrt{\nu(\Delta t)_o} = l_e$ (obtained from the Couette problem). For $\xi = 0.1b$, we obtain the effective interface thickness in x , y and z direction as $(l_e)_x = 2 \times 0.1529$, $(l_e)_y = (l_e)_z = 2 \times 0.07645$. Let us define the total effective interface thickness as the geometric mean of all three directions to obtain

$l_e = \sqrt[3]{(l_e)_x(l_e)_y(l_e)_z} = 2 \times 0.09632$, and hence $(\Delta t)_o = (\frac{l_e}{2.76})^2/\nu = 0.00524$, which agrees with the SPM simulation results. Tab. 3.1 also shows that the boundary treatment at the inlet and outlet has certain effects in the numerical results.

Table 2.1: *Flow past an ellipsoid*: hydrodynamic force in streamwise direction F_x and torque in z-direction T_z . Two different boundary conditions are applied at $x = \pm 80.0$: ‘periodic’ means periodic at both the inlet $x = -80.0$ and the outlet $x = 80.0$; ‘inflow’ means inflow type at the inlet and Neumann type at the outlet.

	F_x	difference from exact	T_z	difference from DNS
exact ([33])	29.1765			
DNS (periodic)	28.89703	0.958%	4.29880	
FCM (periodic)	29.43436	0.884%	4.38510	2.01%
SPM (periodic, $\Delta t=0.003$)	29.90128	2.484%	4.61497	7.35%
SPM (periodic, $\Delta t=0.005$)	28.98194	0.667%	4.28673	0.28%
SPM (periodic, $\Delta t=0.01$)	27.55520	5.557%	3.81726	11.20%
DNS (inflow)	29.61001	1.486%	4.32863	
FCM (inflow)	29.62734	1.545%	4.42328	2.187%
SPM (inflow, $\Delta t=0.005$)	29.170	0.022%	4.31411	0.335%

Next, we compare the SPM results against DNS and FCM results for the same conditions (with periodic boundary treatment) in the pointwise sense, e.g., we compare velocity profiles at different locations, in Fig. 2.12, 2.13 and 2.14. The results indicate that if we choose the time step wisely and the interface thickness reasonably, SPM resolves the near velocity fields better than FCM while in far-field it is comparable to FCM.

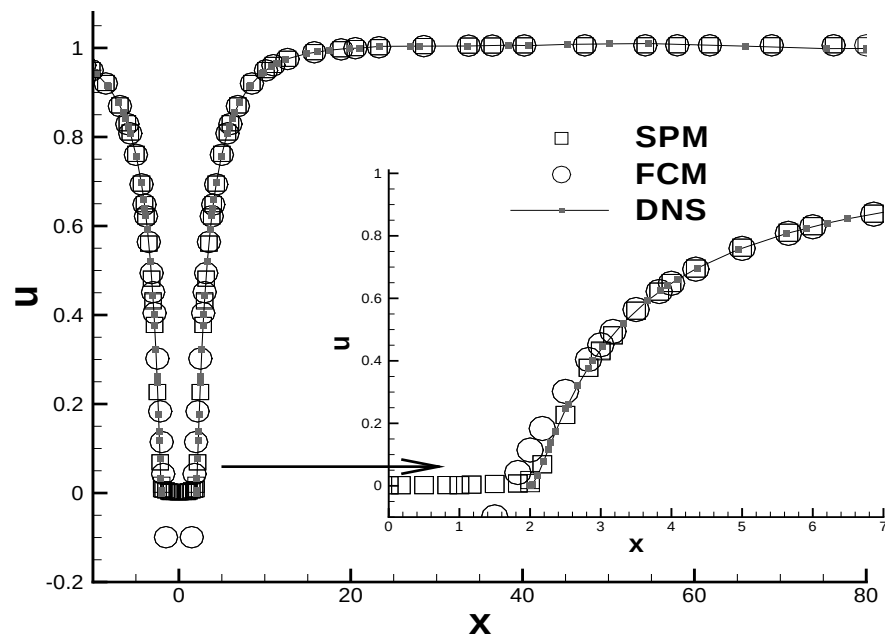


Figure 2.12: *Flow past an ellipsoid*: Comparison between SPM, FCM and DNS of streamwise velocity (u) versus streamwise distance (x) along the long axis of the ellipsoid (x -axis). In the bottom right a close-up around the spheroid surface is shown.

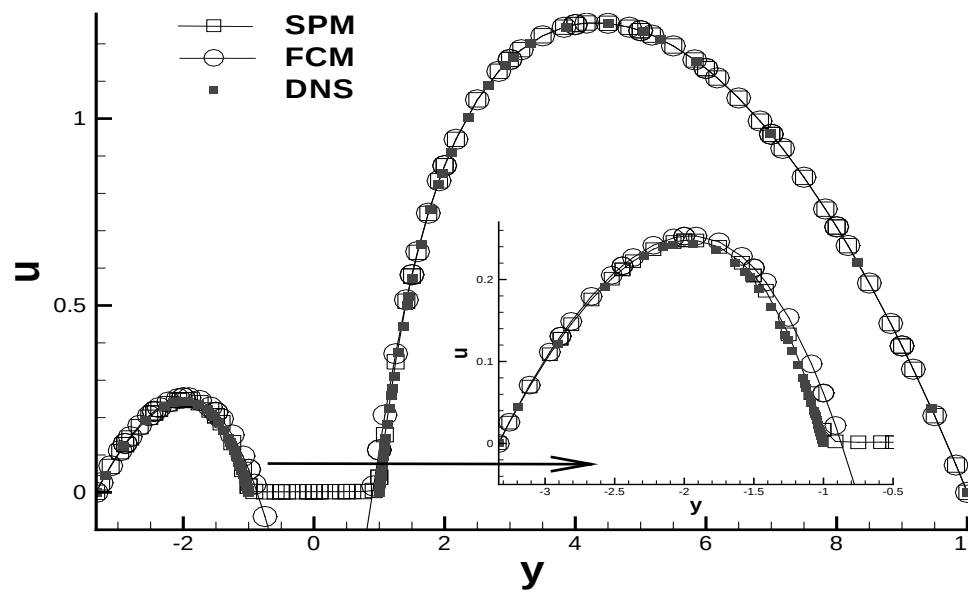


Figure 2.13: *Flow past an ellipsoid*: Comparison between SPM, FCM and DNS of streamwise velocity (u) versus inter-wall distance (y) along the short axis of the ellipsoid (y -axis). In the bottom right a close-up around the spheroid surface is shown.

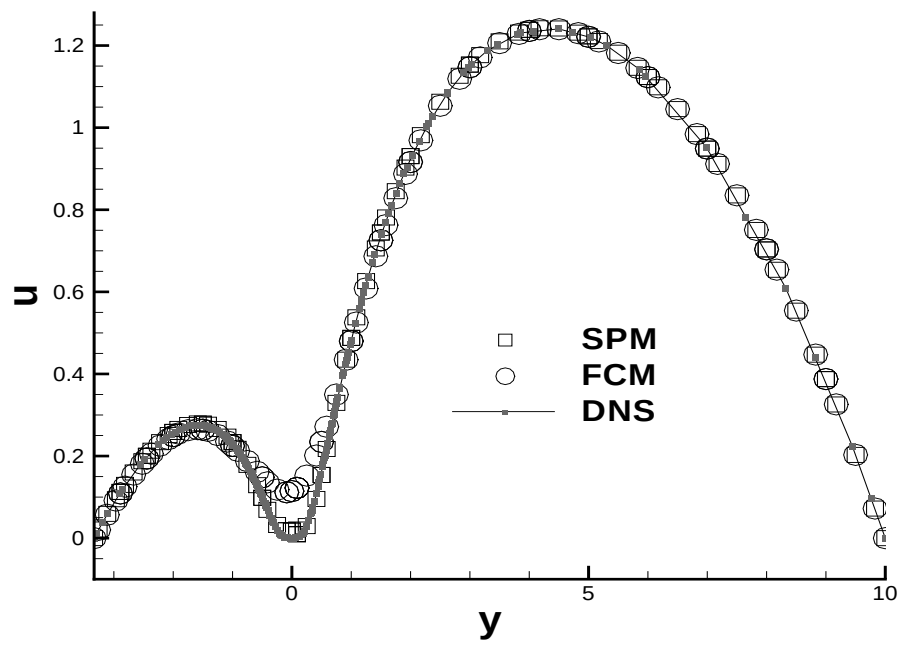


Figure 2.14: *Flow past an ellipsoid:* Comparison between SPM, FCM and DNS of streamwise velocity (u) versus inter-wall distance (y) along the tangential line ($z = 0, x = -2$)

2.4.2 Flow past a biconcave particle

Biconcave shaped particles resemble red blood cells, so we are interested to assess the accuracy of SPM for flow past a single particle tilted with respect to the flow direction. The concentration function for biconcave is derived from (2.2) using the surface function f given in [71]:

$$f(\mathbf{x}, t) = |\mathbf{x}| - (a - b) \sin^q \theta + b, \quad \text{and} \quad \tau = 1$$

where a, b are the semi-axes of the biconcave, θ is the orientation angle as $\theta = \arccos(x_I/|\mathbf{x}|)$, and x_I is the projection of $\mathbf{x}$ onto the symmetry axis of the biconcave. We simulate the steady Stokes flow past a tilted biconcave particle between two walls. The simulation domain is $[-6, 6] \times [-4, 4] \times [-6, 6]$, with a particle of $a = 2.22, b = 0.62$ centered at the origin and tilted in the z -direction by an angle of $-\pi/4$. Two walls are located at $y = \pm 4$, and periodicity is imposed along the x - and z -directions. A pressure gradient $\nabla p = (0.05, 0, 0)$ is prescribed to drive the flow. As the biconcave is tilted, both drag force F_x and lift force F_y are expected.

The SPM simulation uses 7200 nonuniform hexahedral elements with fourth-order polynomials, while DNS uses 50941 tetrahedral elements and a polynomial order of $P = 8$; the meshes (elements only) are shown in Fig. 2.15. Compared to the DNS mesh, the rectilinear mesh for SPM is much simpler and more manageable.

Typical results for velocity profiles at different locations are shown in Fig. 2.16, 2.17 and 2.18. We could not obtain FCM results for this complex shape so we compare against the DNS results with spectral element method. The agreement is very good and comparable to the simple shaped particle simulations we considered in previous sections.

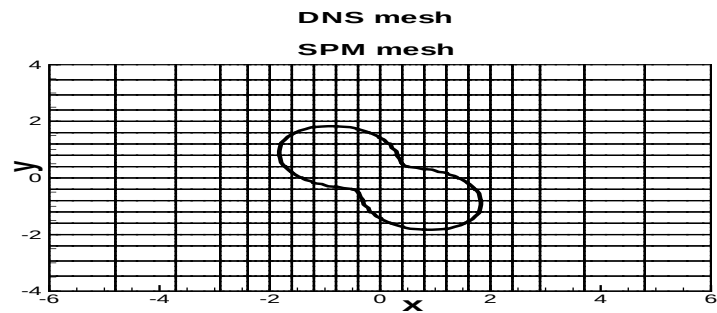


Figure 2.15: *Flow past a biconcave particle*: slices ($z=0$ plane) of meshes used in the simulations of DNS (top) and SPM (bottom), for the same computational domain.

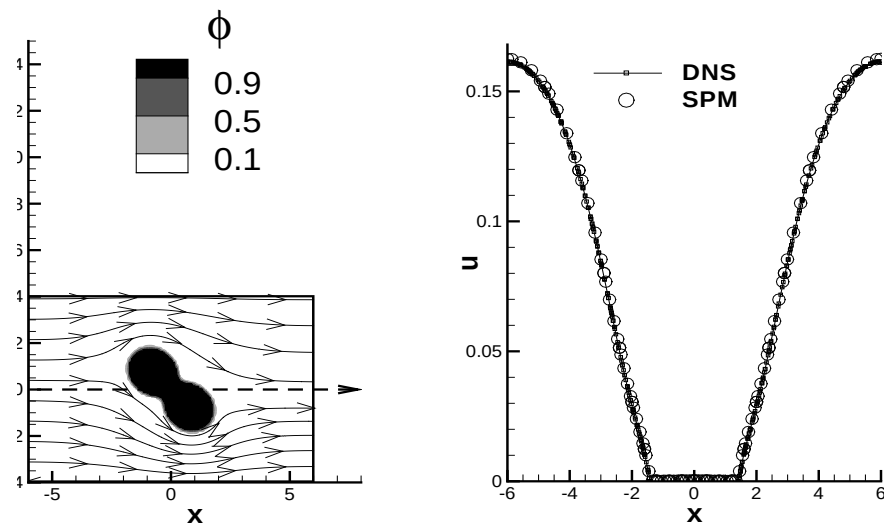


Figure 2.16: *Flow past a biconcave particle*: Left: 2-D streamlines and concentration function contour in $z=0$ plane by SPM; Right: comparison between SPM and DNS: streamwise velocity (u) versus streamwise distance (x) along the center line: $z=0, y=0$.

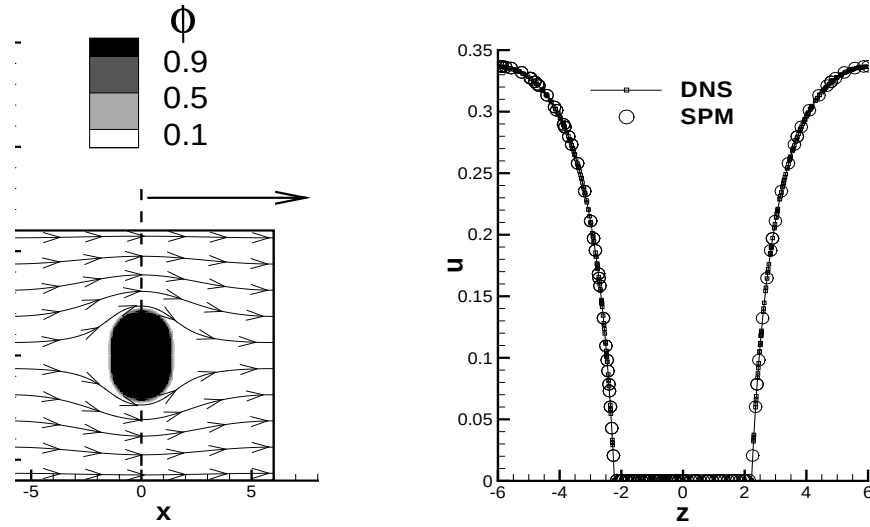


Figure 2.17: *Flow past a biconcave particle*: Left: 2D streamlines and concentration function contours at the $y=0$ plane by SPM. Right: comparison between SPM and DNS: streamwise velocity (u) versus depth distance (z) along the center line: $y = 0, x = 0$.

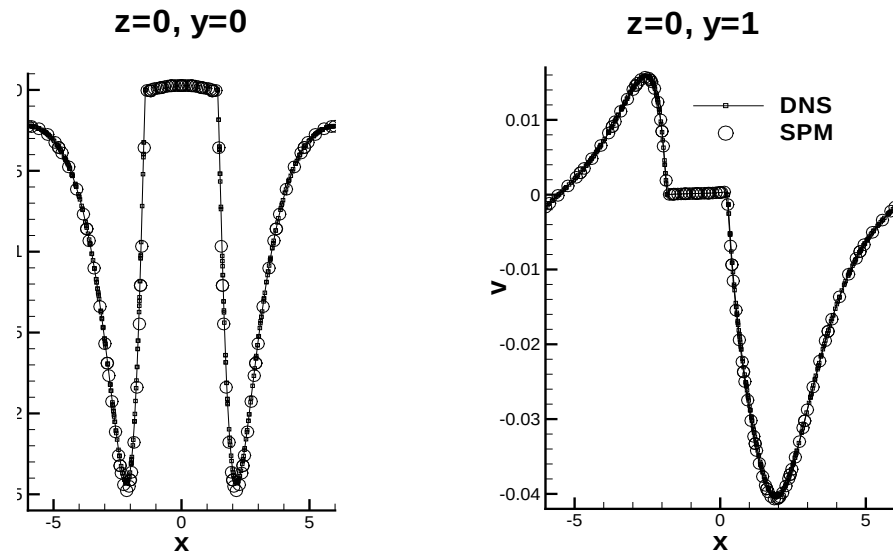


Figure 2.18: *Flow past a biconcave particle*: Inter-wall velocity (v) versus streamwise distance (x). Left: along the center line $z = 0, y = 0$. Right: along the line $z = 0, y = 1$.

2.5 Two interacting spheres

We employ SPM to study the pairwise interaction between two spheres rising in a vertical channel at low Reynolds number. We check if the SPM simulation can reproduce the drafting-kissing-tumbling (DKT) scenario observed in the experiments [47, 23]. The numerical results are compared with both the experimental and FCM results presented in [70].

The experimental setup was a vertical channel of $[0, 150] \times [-5, 5] \times [-50, 50]$ (all in *mm*s). The channel was filled with a mixture of glycerol and water with density $\rho_f = 1.094g/cm^3$. Two spheres with radius $a = 1mm$ and density $\rho_p = 1.081g/cm^3$ were introduced into the channel through small holes in the bottom, as in the third set of experiment in Table 1 of [70]. Hence, the particles were rising under the combination of the gravity and buoyant force $\mathbf{F} = (\rho_p - \rho_f)(4\pi a^3/3)\mathbf{g}$. Based on the Stokes settling velocity, the Reynolds number was about 13.5.

The simulation domain for SPM is $[0, 40] \times [-5, 5] \times [-10, 10]$ (all in *mm*s), with periodic boundaries in x- and z-direction, and two walls at $y = \pm 5$. The two spheres are initially placed at $(18.65, -1.03, 1.13)$ and $(27.2, 0.1, 0.655)$, and they are driven by the force $\mathbf{F}$. To discretize the domain, 6400 hexahedral elements with fifth-order polynomials are used. We choose $\xi = 0.1a$ for the concentration function of Eq. (2.1a), and the optimum time step $(\Delta t)_o$ from $\delta = l_e$ is used in the time integration.

The particle trajectories from the SPM simulation are shown in Fig. 2.19, with comparison against the experimental and FCM results in [70]. Fig. 2.19 indicates that SPM reproduces the DKT process and yields satisfactory agreement with the experimental and FCM data, despite the fact that we could not obtain exactly the same initial conditions as in the experiment or FCM simulation and also the simulation domain is somewhat different.

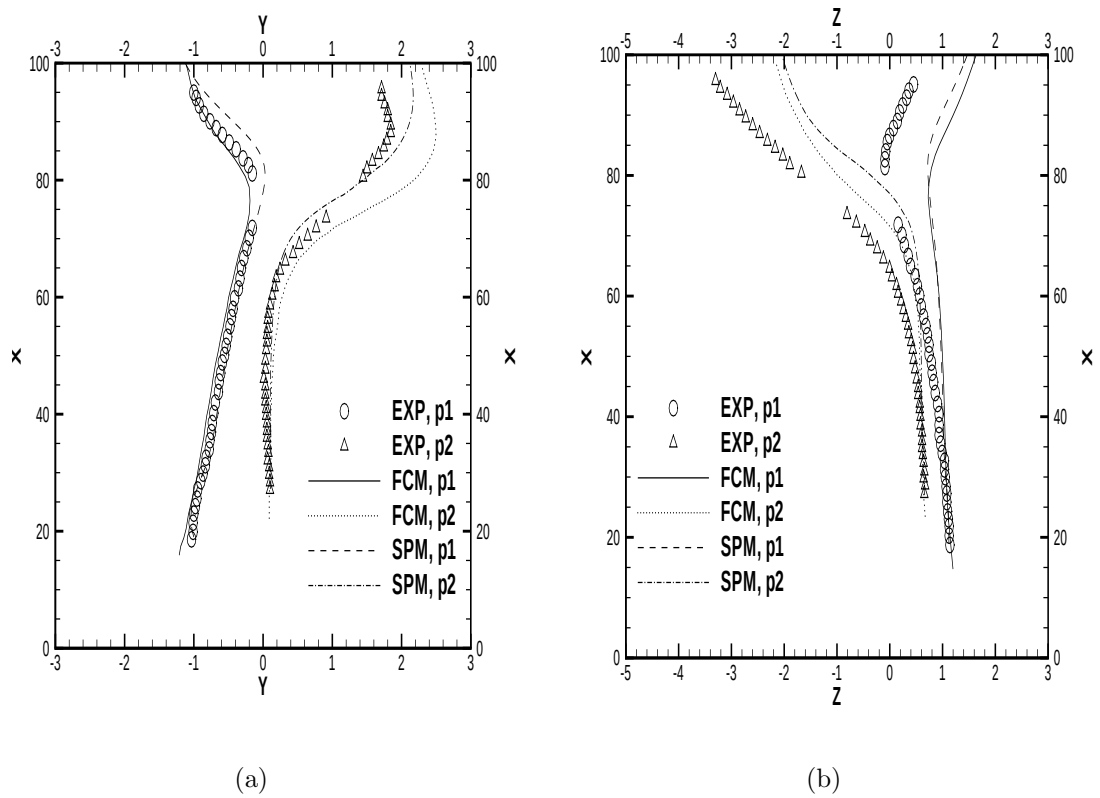


Figure 2.19: *Two interacting spheres*: trajectories of the two particles (center positions) projected into the Z-plane (a) and Y-plane (b), with ‘p1’ referring to the first particle and ‘p2’ to the second.

2.6 Concluding remarks

In this chapter, we have reviewed and analyzed a new computational method for particulate flows, the Smoothed Profile method (SPM). We extended the original fully-explicit time-integration scheme to a semi-implicit high-order splitting scheme and implemented it with a spectral/*hp* element discretization in space. We showed that the modeling error of SPM has a *non-monotonic* dependence on time step size, with the optimum time step $(\Delta t)_o$ obtained from a balance between the effective interface thickness and the Stokes layer thickness. Also, the minimum error (corresponding to $\Delta t = (\Delta t)_o$) decreases with decreasing interface thickness, and SPM recovers the exact solution if a limiting interface thickness is used, i.e. $\xi = 0$ and ϕ equals a step function.

Furthermore, extended the application of the method to flows past complex-shaped particles. Comparisons with the force coupling method (FCM) and direct numerical simulations (DNS) for several problems show that SPM is resolving accurately the near-field flows as well as the far-field flows.

Besides its accuracy, SPM is also a fast method for modeling particulate flows. Our numerical results show that compared to DNS, SPM is generally much less expensive, since SPM avoids complicated discretizations around the particles, and hence it can reduce computational complexity significantly, especially for complex-shaped particles. Moreover, SPM is advantageous for simulating flows involving moving particles, whereas ALE-based methods require frequent re-meshing. When compared to another fast method FCM, SPM is about 50% more expensive if the same computational meshes are used, as SPM needs to solve the extra equations (Eq. (2.21a) and (2.22)). Also, SPM requires slightly higher spatial resolution than FCM, since it adopts a sharper interface representation (tanh function) instead of the Gaussian envelope used by FCM. Typically, taking the grid spacing Δx around the particle surface to scale as the interface thickness parameter ξ , i.e. $\Delta x \sim \xi$, would resolve the interface sufficiently. This extra work of SPM is a trade-off for

better near-field resolution (thus advantageous for dense concentration particulate flow) and also for greater flexibility in modeling complex-shaped particles than FCM.

Chapter 3

Smoothed Profile Method for Electrokinetic Flows

3.1 Introduction

Electrokinetic flows have important applications in diverse fields such as biomedical, forensics, environmental and energy engineering [103, 16]. The electrokinetic phenomena is a family of interesting effects that occur in heterogeneous fluids associated with electric field. Due to various combinations of the driving force and moving phase, electrokinetic phenomena can be divided into the following categories [72, 96]:

- *Electroosmosis*, or *electroosmotic flow (EOF)*, as electrically driven motion of a fluid relative to the stationary charged surfaces which bound it;
- *Electrophoresis*, or *electrophoretic flow (EPF)*, as motion of charged particles through a solvent medium under the action of an applied electric field;
- *Diffusiphoresis*, as motion of particles under influence of a chemical potential gradient;

- *Capillary osmosis*, as motion of liquid in porous body under influence of the chemical potential gradient;
- *Sedimentation potential*, as electric field generated by sedimenting colloid particles;
- *Streaming potential/current*, as either electric potential or current generated by fluid moving through porous body, or relative to flat surface;
- *Colloid vibration current*, as electric current generated by particles moving in fluid under influence of ultrasound;
- *Electric sonic amplitude*, as ultrasound generated by colloidal particles in oscillating electric field.

There are many books published with detailed descriptions of electrokinetic phenomena in colloid and interface science [45, 100]. For a historical review of electrokinetic theory, we refer the reader to [7]. In the rest of this section, we present a brief review of historical developments and recent research on EOF and EPF as they are the two major effects in general electrokinetic flows.

EOF was first reported by Reuss (1809), who demonstrated that water could percolate through porous clay diaphragms due to an applied electric field. A porous medium such as clay provides a complex network of microchannels for the motion of the liquid. The mechanism is the same as in typical capillary electrophoresis, with a single long narrow cylindrical fused silica capillary [26]. The solid fused silica substrate (like many other materials such as most minerals, glass, and certain polymeric materials) acquires a surface charge when brought into contact with a polar medium, due to ionization or ion adsorption or ion dissolution. The resulting surface charge attracts the counterions (ions of opposite charge) and repels the co-ions (ions of the same charge) in the electrolyte, creating a layer of highly concentrated ions next to it which screens the surface charge. This is known as the *electrical double layer (EDL)*

or Debye layer. When an external electric field is applied, the ions in the diffuse layer acquire momentum which is transmitted to adjacent layers of fluid through the effect of viscosity, thus causes the fluid to flow. One of the most useful applications of EOF is microfluidic pumping and flow control using electric fields [48, 116], avoiding the use of mechanical pumps or valves with moving components. There are many remarkable experimental works which developed effective imaging techniques and revealed interesting electroosmotically driven flows in various microscale geometries and with different coating materials [77, 12, 55, 104, 38]. There have been many successful numerical simulations on EOF over recent decades. Most of them are based on solving the Poisson–Boltzmann and Navier–Stokes equations with boundary conditions specified directly on immersed interfaces, please see section 1.1 for a detailed review.

In contrast, electrophoresis, or, in some older literature, cataphoresis, is the motion of charged particles relative to the stationary fluid. EPF can be thought as the mirror image of EOF; its presence is also due to EDL, which results from the interaction of the particle charges and the surrounding ionized solution. The electrophoretic motion is determined by a balance between the electric force due to the net particle charge under the EDL screening and the opposing hydrodynamic force. Therefore, electrophoretic velocity is proportional to the external electric field and the net charge of the particle, and inversely proportional to the fluid viscosity. According to Reed and Morrison [98], electrophoretic motion does not disturb the surrounding fluid to a great extent, and thus the steady electrophoresis can be modeled by using a simple mobility concept, i.e. $\mathbf{V}_{EP} = \mu_{EP} \mathbf{E}_{ext}$. By taking advantage of the differences in the electrophoretic mobilities of different particles, separation and detection of macromolecules such as DNA, RNA, and microtubules is possible and useful in many fields like modern biology and forensics [117, 112]. The experimental techniques to measure the particle velocity in suspensions has been quite well developed over recent decades, such as microelectrophoresis and electrophoretic

light scattering [14]. Especially fluorescence microscopy can be used to image the electrophoretic motion of individual particles such as microtubules and virus particles, which are confined in microfabricated slit-like fluidic channels [113, 63]. The measured electrophoretic mobility data are useful for estimating zeta-potential of dispersions based on established electrophoretic theories.

Theories and analytical approximations on μ_{EP} for various particle shapes have been developed through the last century. The first complete analytical solution of the electrophoretic mobility for a sphere or a cylinder in a inertia-free flow was obtained by Henry [37], which accounts for the retardation effects. Henry’s formula takes as input arbitrary electrical conductivity of the particles and the electrostatic potential distribution due to EDL. Further simplified formulations for the mobility has been derived by invoking the Debye-Huckel linearization under the assumption of small zeta-potentials [100, 84, 86]. More recently, O’Brien and White [82] developed perturbation methods and derived linearized equations to numerically compute the mobility, which allows for small deformation of EDL and thus includes the relaxation effect. In contrast to the well-developed theories and analytical approximations, few full numerical simulations have been successful in resolving the electrophoretic flow. This is probably due to the difficulties of standard numerical methods with moving charged boundaries which are often in complex shapes. A boundaryless method called smoothed profile method [53, 121, 80] was extended to solve for the electrohydrodynamic couplings by integrating the modified species conservation and Navier–Stokes equations. It was applied to simulate the EPF of charged spheres and showed great potential for modeling colloidal dispersions. However, due to the fully explicit time integration scheme used, the temporal stability and accuracy was not quite satisfying. Also a constant external electric field is used to calculate the electrokinetic force, which only works for particles with same electrical conductivity as the surrounding solution, and thus is not generally applicable.

In this chapter we propose an efficient modeling method for electrohydrodynamic flows, allowing for spatially varying electrical conductivities. The basic idea is to include electrokinetic forces into the flow solver which we developed in Chap. 2. In the second section, we present fundamental theories and governing equations for electrokinetic flows. In the third section, we introduce our numerical methodology where the Poisson-Boltzmann equation and electric charge continuity equation are cast into forms based on SPM. In the fourth section we verify the modeling method by benchmark problems of electroosmotic flow in straight channels and electrophoresis of charged cylinders. We present in the last section the simulation results of the electrophoresis of charged microtubules, and show that the simulated electrophoretic mobility and anisotropy agree with the experimental results of [113].

3.2 Fundamentals

3.2.1 Electrical double layer (EDL)

Most substrates acquire charge when brought into contact with ionized solution; an EDL is formed to effectively screen the surface charge and thus generates all kinds of interesting and useful electrokinetic flows. The earliest model to describe EDL is the Helmholtz model, which treated EDL mathematically as a simple capacitor, where a single layer of ions is adsorbed at the surface. Gouy and Chapman made significant improvements by introducing a diffuse model of EDL, in which the electric potential decreases exponentially away from the surface to the fluid bulk [30, 8]. As this Gouy-Chapman model fails for highly charged EDLs, Stern improved the model by introducing an additional internal layer where some of the counter-ions specifically adsorb to the surface; this is now referred to as Stern layer [106]. This Gouy-Chapman-Stern model is now the most commonly used model to describe EDL structure. The Stern layer has a typical thickness of one hydrated ionic radius [96], and it is immobilized under strong electrostatic force to the charged surface, as

demonstrated by molecular dynamics studies [73]. The outer part of the screening layer which can move under the influence of tangential stress is referred to as the *diffuse layer*. In equilibrium state, the ion density in the diffuse layer obeys the Boltzmann distribution [30, 8]. This is consistent with the derivations based on statistical-mechanics theories [21].

An illustration of the electric potential and ion distribution throughout EDL of a negatively charged surface is shown in Figure 3.1. Here the surface potential ψ_o refers to the electric potential difference between the charged surface and the fluid bulk; while zeta-potential ζ is the potential on the shear plane which separates mobile fluid from stagnant fluid attached to the surface. For most practical cases, we can employ the zeta-potential as the boundary condition of electrokinetic flows rather than the wall potential ψ_o , because the Stern layer is very thin and it is immobilized. The characteristic thickness of EDL is Debye length λ_d , which refers to the distance from the charged surface where the electrokinetic potential energy equals the thermal energy. In aqueous solution λ_d is usually on the order of nanometers and it decreases with increasing ion concentration. It is very common in literature to use the reciprocal Debye length or the so called Debye-Hückel parameter (κ):

$$\kappa = \frac{1}{\lambda_d} = \sqrt{\frac{\sum_i e^2 z_i^2 n_{i,\infty}}{\epsilon \epsilon_0 k_B T}}, \quad (3.1)$$

where the subscript i indicates the i th ion species, e is the elementary charge, z_i is the ion algebraic valence, k_B is the Boltzmann constant, T is the absolute temperature, ϵ_0 is the permittivity of vacuum, ϵ is the dielectric constant of the solvent and $n_{i,\infty}$ is the ionic concentration (number density with SI unit m^{-3}) in the bulk solution.

The local electric potential ψ in the aqueous solution is related to the charge density through the Poisson equation of electrostatics:

$$\nabla^2 \psi = -\frac{\rho_e}{\epsilon \epsilon_0} = -\frac{1}{\epsilon \epsilon_0} \sum_i e z_i n_i, \quad (3.2)$$

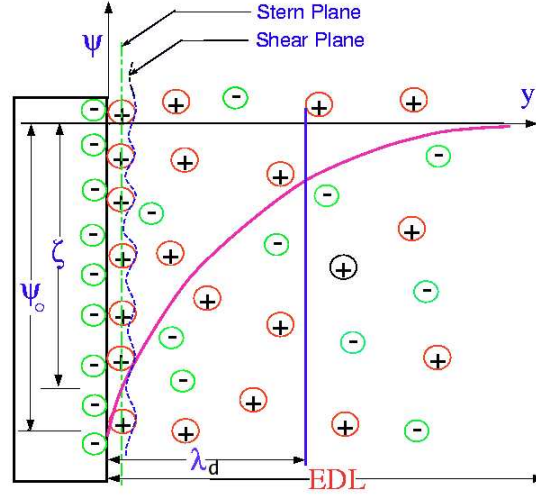


Figure 3.1: Schematic diagram of the electric double layer (EDL) next to a negatively charged solid surface. The red curve is the electric potential ψ along the distance measured from the wall y . Here ψ_0 is the surface electric potential, ζ is the zeta potential and λ_d is the Debye length respectively. [After Karniadakis et al., 2005 [48]. With permission.]

where the dielectric constant ϵ_0 is assumed to be uniform. Here ρ_e is the net electric charge density (with SI unit Cm^{-3}), and n_i is the local ionic concentration (number density) for the i th ion species. It is governed by the species conservation equation including transport and reaction [65]:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \mathbf{j}_i + \lambda_i n_i = R_i, \quad (3.3)$$

where λ_i is a radioactive decay constant and R_i the chemical reaction rate of the i th species. $\mathbf{j}_i$ denotes the number flux of the i th species (with SI unit $m^{-2}s^{-1}$), and follows the Nernst-Planck equation [65, 96]:

$$\mathbf{j}_i = -\frac{ez_i D_i}{kT} n_i \nabla \psi - D_i (\nabla n_i + n_i \nabla \ln \gamma_i) + n_i \mathbf{u}, \quad (3.4)$$

where the first term on the right refers to electrochemical migration, the second term is aqueous diffusion, and the last term is advective transport. Here γ_i is the activity

coefficient and D_i is the diffusivity (with SI unit m^2s^{-1}). Note that diffusivity is directly related to the electrical conductivity of the solution as:

$$\sigma = \sum_i \frac{e^2 z_i^2 D_i}{kT} n_i \quad (Sm^{-1}). \quad (3.5)$$

For electrolyte solutions with no radiation or chemical reactions, equations (3.3) and (3.4) can be further simplified as:

$$\frac{\partial n_i}{\partial t} + \mathbf{u} \cdot \nabla n_i = D_i \nabla^2 n_i + \frac{e z_i D_i}{kT} \nabla \cdot (n_i \nabla \psi), \quad (3.6)$$

which is fully coupled with equation (3.2) and poses great challenges for numerical solving. When the electric potential is continuously derivable and the ionic convection is negligible, equation (3.6) has a simple solution as being the Boltzmann distribution:

$$n_i = n_{i,\infty} \exp\left(-\frac{e z_i \psi}{kT}\right), \quad (3.7)$$

where we recall that $n_{i,\infty}$ is the ionic concentration in the bulk solution far away from EDL. Substituting equation (3.7) into equation (3.2) yields the famous Poisson-Boltzmann equation [40]:

$$\nabla^2 \psi = -\frac{1}{\epsilon \epsilon_0} \sum_i e z_i n_{i,\infty} \exp\left(-\frac{e z_i \psi}{kT}\right), \quad (3.8)$$

which decouples the electric potential from ionic concentration and thus enables fast numerical simulations. The boundary conditions for equation (3.8) can be derived from either the zeta-potential ζ or the surface charge density σ_e . The former leads to a Dirichlet-type boundary condition and the latter to a Neumann-type [96] as

follows:

$$\psi = \zeta \quad \text{or,} \quad (3.9a)$$

$$\nabla\psi \cdot \mathbf{n} = -\frac{\sigma_e}{\epsilon\epsilon_0} \quad \text{at} \quad \Gamma_p, \quad (3.9b)$$

where Γ_p refers to the interface of the immersed particles and the surrounding medium, and $\mathbf{n}$ is the unit normal vector of the interface. Here we use as boundary condition the zeta-potential instead of the surface potential, as it is the diffuse layer which obeys the Poisson-Boltzmann statistics, and the Stern layer is usually very thin. We also need the boundary conditions for far field in bulk solution where we have electroneutrality $\sum_i e z_i n_{i,\infty} = 0$ and the potential is constant; we usually set the constant to zero:

$$\psi = 0 \quad \text{at} \quad \infty. \quad (3.9c)$$

We note that exact analytical solution for equation (3.8) is not *generally* obtainable as the equation is nonlinear. For small zeta potential ($|z_i \zeta| \leq \frac{kT}{e} \sim 25mV$ for all species i), it is possible to linearize equation (3.8) by expanding the right-hand side via a Taylor series and discarding quadratic and higher order terms. This results in the Debye–Hückel approximation as :

$$\nabla^2 \psi = \kappa^2 \psi. \quad (3.10)$$

This linearized equation reveals simple analytical solution of the potential ψ and concentration n_i for simple EDL geometries. For example, for a charged plane with zeta-potential ζ introduced in an electrolyte where the Debye–Hückel approximation is valid, it is easily derived that $\psi = \zeta \exp(-\kappa x)$, with x to be the distance to the plate. The Debye length κ^{-1} is thus seen to be the $1/e$ decay distance for the electric potential, or in other words, the thickness of the diffuse layer which effectively shields

the surface charge.

3.2.2 Externally applied electric field

Once an external electric field $\mathbf{E}_{ext}$ is applied, the ions in the diffuse layer and the charged surface will acquire motion under electric forces. According to Henry [37], the electrophoresis mobility would be much different, depending on whether or not the particles have the same electrical conductivity as the medium fluid. In the analysis of Debye and Hückel [13, 44] and many other analytical or numerical computations, it was assumed that the applied electric potential gradient is constant everywhere and not disturbed by the presence of the particles. But this is only true if the electrical conductivity of the particles are the same as the medium, which rarely happen in reality. Most particles (such as colloids, microtubules) would be more like insulators when the electrical conductivity is compared to that of the surrounding electrolyte solution. Although many papers report findings of the surface conductivities of particles such as microtubules to be hundreds of times the conductivity of the medium, this phenomenon is only due to the highly concentrated counter-ions and co-ions in EDL near the charged surfaces. So in this subsection we discuss the theories and equations for the applied electric field.

Following the assumption made by Henry [37] that the applied field may be taken as simply superimposed on the electric field due to EDL, we consider separately when EDL effect is absent, how the applied uniform electric field is reconstructed near surfaces of insulators or with electrical conductivity different from the ionized solution.

The applied field $\mathbf{E}_{ext}$ is related to the electrostatic potential ψ_{ext} as:

$$\mathbf{E}_{ext} = -\nabla\psi_{ext}. \quad (3.11)$$

The current continuity or the charge conservation equation states that:

$$\nabla \cdot \mathbf{i} = -\nabla \cdot (\sigma \nabla \psi_{ext}) = -\frac{d\rho_{ext}}{dt}, \quad (3.12)$$

where $\mathbf{i}$ is the current density, σ is the electrical conductivity and ρ_{ext} is the charge density due to the conductivity difference. The relation used $\mathbf{i} = \sigma \mathbf{E}_{ext}$ is an expression of Ohm's law, with the assumptions of no charge convection and no ordinary diffusion [96], which is generally satisfied in the cases we are studying in this subsection.

If we assume the charge distribution (due to the conductivity difference) is instantaneously derivable or in quasi-equilibrium state, the last term in equation (3.12) vanishes, and we derive the following equation:

$$\nabla \cdot (\sigma \nabla \psi_{ext}) = 0, \quad (3.13)$$

where σ could either be the conductivity of the fluid medium σ_f or the one of the immersed particles or boundaries σ_p . Alternatively we can write $\sigma = \sigma_f H(d) + \sigma_p (1 - H(d))$, where d is the distance to the interface and H is the Heaviside step function which is one in fluid medium and zero in particles. If both σ_f and σ_p are constants, equation (3.13) reduces to two Laplace equations:

$$\nabla^2 \psi_{ext,f} = 0 \quad \text{in} \quad \Omega_f \quad (3.14a)$$

$$\nabla^2 \psi_{ext,p} = 0 \quad \text{in} \quad \Omega_p \quad (3.14b)$$

where Ω_f, Ω_p are domains of fluid medium and particles respectively. The boundary conditions for the applied potentials are:

$$\nabla \psi_{ext,f} = -\mathbf{E}_\infty \quad \text{at} \quad \infty \quad (3.15a)$$

$$\psi_{ext,f} = \psi_{ext,p}, \quad \text{at} \quad \Gamma_p \quad (3.15b)$$

$$\mathbf{s} \cdot (\nabla \psi_{ext,f}) = \mathbf{s} \cdot (\nabla \psi_{ext,p}) \quad \text{at} \quad \Gamma_p \quad (3.15c)$$

$$\mathbf{n} \cdot (\sigma_f \nabla \psi_{ext,f}) = \mathbf{n} \cdot (\sigma_p \nabla \psi_{ext,p}) \quad \text{at} \quad \Gamma_p \quad (3.15d)$$

where Γ_p refers to the interface with conductivity jumps, $\mathbf{E}_\infty$ is the external field strength in far field, and $\mathbf{s}, \mathbf{n}$ are the unit tangential and normal vectors of the surfaces Γ_p respectively. Henry [37] provided exact solutions of ψ_{ext} for a sphere and an infinitely long cylinder with arbitrary σ_p , and utilized them to calculate the electrophoretic mobilities.

We note that for insulating boundaries ($\sigma_p = 0$), the condition (3.15d) becomes $\partial \psi_{ext,f} / \partial n = 0$, which combined with (3.15a) can be used to solve equation (3.14a) alone in the fluid domain, either theoretically or numerically. However for nontrivial values of σ_p , equations (3.14a) and (3.14b) need to be solved in both domains, which challenges the numerical solvers, as general direct methods only simulate the fluid domain. We are in need of a numerical methodology which effectively solves equation (3.13) or its approximate form in the entire domain. We also note that although the potential ψ_{ext} is continuous across the interface Γ_p , the field $\mathbf{E}_{ext}$ is discontinuous and has finite jumps across the interface. Moreover, the resulting charge distribution $\rho_{ext} = -\epsilon \epsilon_0 \nabla^2 \psi_{ext}$ includes a Dirac delta function, and its radial integral reveals a surface charge whose density varies along the interface. This non-smooth nature of the exact solution brings big challenges to numerical solvers.

3.2.3 Electrohydrodynamic coupling

Providing the equations and solutions for both the electric potential due to EDL and the applied electric field, we can couple the electrokinetic effects with the hydrodynamic effects by adding an electrokinetic force to the local fluid. Assuming the fluid medium to be incompressible and Newtonian with constant viscosity, the

incompressible Navier–Stokes equations are used to model the bulk fluid motion:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} + \mathbf{f}_{EK} \quad \text{in} \quad \Omega_f \quad (3.16)$$

where ρ is the fluid density, $\mathbf{u}$ is the velocity field which is assumed to be divergence free $\nabla \cdot \mathbf{u} = 0$, p is the pressure, ν is the kinematic viscosity of the fluid, $\mathbf{g}$ is the gravity (and other external forces on the fluid), and $\mathbf{f}_{EK}$ is the electrokinetic body force.

According to Stratton [107], the electrokinetic force density is in the form of :

$$\mathbf{f}_{EK} = \rho_e \mathbf{E} - \frac{1}{2} (\mathbf{E} \cdot \mathbf{E}) \epsilon_o \nabla \epsilon + \frac{\epsilon_o}{2} \nabla \left(\rho \frac{\partial \epsilon}{\partial \rho} \mathbf{E} \cdot \mathbf{E} \right), \quad (3.17)$$

where ρ_e is the net charge density and $\mathbf{E}$ is the external electric field. The last two terms refer to the forces arising from permittivity variations which are important for liquid/gas interfaces and in ionized gas flows [107]. For simplicity, we assume a constant electric permittivity ϵ throughout the fluid medium, and hence only the first term on right hand side is considered: $\mathbf{f}_{EK} = \rho_e \mathbf{E}$.

Here we interpret ρ_e as the net charge density in the electrolyte solution due to EDL (3.2), and $\mathbf{E}$ as the applied electric field $\mathbf{E}_{ext}$ (3.11). Therefore, we can rewrite the incompressible Navier–Stokes equations (3.16) as:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} - \rho_e \nabla \psi_{ext} \quad \text{in} \quad \Omega_f \quad (3.18a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega_f, \quad (3.18b)$$

with no-slip boundary condition specified on the immersed boundaries:

$$\mathbf{u} = 0 \quad \text{at} \quad \Gamma_p. \quad (3.19)$$

The whole set of simplified governing equations for electrokinetic flows are:

1. Poisson–Boltzmann equation (3.8) and (3.2) for EDL, with boundary conditions (3.9);
2. The current continuity equations (3.14) and (3.11) for applied electric field, with boundary conditions (3.15);
3. The incompressible Navier–Stokes equations (3.18) for fluid motion, with boundary conditions (3.19).

Here we summarize the main assumptions and approximations used in these equations as follows:

- The ionic convection is negligible and electric potential is continuously derivable in EDL, so that Poisson–Boltzmann equation (3.8) is valid.
- The ions are point charges.
- The applied electric field can be simply superimposed on the field due to EDL.
- The fluid solution is assumed to be Newtonian and viscosity is constant. The fluid viscosity is independent of the ion concentration and local electric field strength in EDL, which is only true for dilute solutions.
- The permittivity of the solution is constant and not affected by the local electric field strength.
- The charge on the immersed particles or boundaries is uniform and shall not change by the applied field or the motion.

3.3 Numerical methodology

In this section, we present a numerical methodology for modeling electrokinetic flows by solving the Poisson–Boltzmann equation, the current continuity equation and the incompressible Navier–Stokes equations respectively. We present a new modeling

method based on the smoothed profile method, which avoids applying the exact boundary conditions on the particle/solution interfaces and hence avoids using complex conforming computational meshes.

3.3.1 Solving the Poisson–Boltzmann (PB) equation for EDL

Direct boundary treatment

We follow the spectral element algorithm developed by Beskok et al. [17, 18, 31], in solving the Poisson–Boltzmann equation with direct boundary treatment at particle/solution interfaces; it successfully resolves electroosmotic/pressure-driven flows in complex two-dimensional geometries. Here we briefly review the algorithm and extend it to study three-dimensional EDLs by solving the Poisson–Boltzmann equation.

We rewrite the Poisson–Boltzmann equation (3.8) and (3.2) for a non-dimensional potential ψ_d for a binary electrolyte solution (i.e. $z_i = \pm 1$):

$$\nabla^2 \psi_d = \beta \sinh(\psi_d) \quad \text{in} \quad \Lambda_f \quad (3.20a)$$

$$\rho_e = \left(-\frac{\epsilon \epsilon_0 \zeta_e}{h^2} \right) \beta \sinh(\psi_d), \quad (3.20b)$$

where Λ_f is the dimensionless domain of fluid medium, h is the characteristic length used to normalize the length scale, $\zeta_e = k_B T / ez$ (corresponding to 25.69 mV at 25°C) is used to scale the electric potential as $\psi_d = \psi / \zeta_e$. We also introduce the parameter $\beta = (\kappa h)^2$.

A semi-discrete system is obtained from equation (3.20) by using a Newton iteration strategy to treat the exponential nonlinearity, i.e.,

$$[\nabla^2 - \beta \cosh(\psi^n)] \psi^{n+1} = \beta \sinh(\psi^n) - \beta \cosh(\psi^n) \psi^n \quad \text{in} \quad \Lambda_f, \quad (3.21a)$$

$$\rho_e^{n+1} = \left(-\frac{\epsilon \epsilon_0 \zeta_e}{h^2} \right) \beta \sinh(\psi^{n+1}), \quad (3.21b)$$

where index $n, n+1$ refer to the iteration number. The resulting equation is a variable coefficient Helmholtz equation, which can be solved by either a direct method (Cholesky decomposition) or a conjugate gradient iterative method. The weak variational form of equation (3.21) is solved via a Galerkin projection in the context of spectral element discretization (see Sec. 2.2.3). The boundary condition $(\psi)^{n+1} = \zeta$ is imposed at the particle/solution interface Γ_p ; this is what we call the *direct boundary treatment* or *direct boundary method*.

SPM boundary treatment

The direct boundary treatment for solving the Poisson–Boltzmann equation is readily applicable to electrostatic problems such as electroosmotic flows, where the charged surfaces are fixed. However, for other electrokinetic problems, e.g. electrophoretic flows with moving boundaries, the required remeshing is difficult and challenging. To this end, we apply the smoothed profile method to the Poisson–Boltzmann equation, aiming for an efficient modeling method for problems with moving EDLs induced by charged surfaces or bodies in an electrolyte solution. The direct implementation of the boundary conditions on the charged surfaces are removed, thus a simple computational mesh can be used.

The first attempt is to modify the Poisson–Boltzmann equation with a smoothed profile as:

$$[\nabla \cdot (c_0 \nabla - \beta \cosh(\psi^n) + \frac{1}{\Delta\tau})](\psi^*)^{n+1} = \frac{\psi^n}{\Delta\tau} + c_1 \beta \sinh(\psi^n) - \beta \cosh(\psi^n) \psi^n, \quad (3.22a)$$

$$\psi^{n+1} = (\psi^*)^{n+1} + \phi \cdot [\psi_p^{n+1} - (\psi^*)^{n+1}], \quad (3.22b)$$

in the entire domain Λ including inside the particles. Here ψ_p is the prescribed particle potential field obtained from the individual zeta-potential on each particle, as $\phi\psi_p = \sum_{i=0}^{N_p} \phi_i \cdot (\zeta_p)_i$. The assumptions made here are that the zeta potentials are known and the electric potential is constant inside the particles, i.e. the particles

are surface charged. Also, c_0, c_1 are coefficients to suppress potential variation inside the particles, which are chosen to be 1 or $1 - \phi$.

Due to the limitation of the assumptions made by SPM model of Eq. (3.22), we modify the nondimensionalized Poisson-Boltzmann equation (3.20) by specifying the charges on the immersed particles and extending to the entire computational domain Λ :

$$\nabla^2 \psi_d = [(1 - \phi)\beta \sinh(\psi_d) - \rho_{ep}] \quad \text{in } \Lambda \quad (3.23a)$$

$$\rho_{edl} = \left(\frac{\epsilon \epsilon_0 \zeta_e}{h^2} \right) [-(1 - \phi)\beta \sinh(\psi_d) + \rho_{ep}], \quad (3.23b)$$

where ϕ is a smooth function termed as indicator function in Sec. 2.2.1. Here ρ_{ep} is the dimensionless charge density on the particles and $-(1 - \phi)\beta \sinh \psi = \rho_{ef}$ refers to the dimensionless charge density in electrolyte solutions with $1 - \phi$ adopted to suppress inside the particle. Thus, the total dimensionless charge density is $\rho_{edl,d} = \rho_{ef} + \rho_{ep}$; it is related to the total charge density ρ_{edl} through $\rho_{edl} = \left(\frac{\epsilon \epsilon_0 \zeta_e}{h^2} \right) \rho_{edl,d}$.

We can adopt different forms of dimensionless ρ_{ep} due to different charge patterns:

$$\rho_{ep} = \gamma_v \phi \quad (3.24a)$$

$$= \gamma_s \nabla \phi \quad (3.24b)$$

$$= \gamma'_s \phi (1 - \phi) \quad (3.24c)$$

Here γ_v and γ_s are prescribed dimensionless volume or surface charge density, scaled by the total dimensionless volume $V_p = \int_{\Lambda} \phi d\mathbf{x}_d$ or total surface area $S_p = \int_{\Lambda} \nabla \phi d\mathbf{x}_d$ of the immersed particle, respectively. By recovering the dimensional equations, it is easy to show that $\gamma_s = \frac{h}{\epsilon \epsilon_0 \zeta_e} e \delta_p$, where $e \delta_p$ is the surface charge density with SI unit C/m^2 .

It is easy to show from Gauss's theorem that for symmetric shapes such as spheres and infinite circular cylinders, either the uniform surface charge or the uniform vol-

ume charge will result in exactly the same electric field and potential outside the particles. So to switch between the volume charge and surface charge patterns, we keep the total charge of the particle to be the same to obtain comparable results, i.e. $Q_p = \gamma_v V_p = \gamma_s S_p$. As $\nabla\phi$ is not always analytically available for all particle shapes, and errors are introduced by the numerical differentiation, here we propose another way to introduce the surface charges as in Eq. (3.24c). We see that $\phi(1 - \phi)$ has the expected peak at the surface, and γ'_s need to be scaled correspondingly to have the prescribed total charge. That is, to switch between all three charge patterns, we keep the total charge of particles the same:

$$Q_{p,d} = \gamma_v V_p = \gamma_s S_p = \int_{\Lambda} \gamma'_s \phi(1 - \phi) d\mathbf{x}_d, \quad (3.25)$$

where $Q_{p,d}$ is the dimensionless total charge scaled from the total charge Q_p through $Q_{p,d} = Q_p / (\epsilon\epsilon_0\zeta_e h)$. For simplicity, only uniform volume charged or surface charged particles are considered, i.e. all γ in Eq. (3.24) are constant. However, we could also adopt a varying γ to simulate inhomogeneous charged particles.

For the smooth profile/indicator function ϕ , we use the following expression:

$$\phi = \frac{\tanh(-d/\xi_p) + 1}{2}, \quad (3.26)$$

$$\text{where} \quad \xi_p = \xi \quad (3.27a)$$

$$\text{or} \quad = \xi \exp(-\frac{c|d|}{\xi}). \quad (3.27b)$$

Note that here d is the *signed* distance to the particle surface (negative inside and positive outside the particle), ξ is a constant named the interface thickness parameter, and ξ_p is the local interface thickness which can be either a constant (3.27a) or a variable (3.27b). Also, c is a constant which is 2 if not specifically

indicated. We see that for variable thickness (3.27b), $\xi_p = \xi$ at particle surface ($d = 0$) and ξ_p decreases exponentially away from the surface.

The semi-discrete scheme utilizing the Newton iteration strategy is thus:

$$[\nabla^2 - (1 - \phi)\beta \cosh(\psi^n)](\psi)^{n+1} = (1 - \phi)\beta \sinh(\psi^n) - (1 - \phi)\beta \cosh(\psi^n)\psi^n + \rho_{ep} \quad \text{in } \Lambda, \quad (3.28)$$

where index n is the iteration number. This equation is also a variable coefficient Helmholtz equation, just as equation (3.21) with direct boundary treatment, but the simulation domain is different. The numerical solution is obtained by solving the weak varitional form of equation (3.28) using the spectral element method (see Sec. 2.2.3). As equation (3.28) is for the entire domain Ω including the particle domain, there is no boundary condition imposed at particle/solution interface Γ_p ; this is what we call the *SPM boundary treatment* or *SPM-PB solver*.

3.3.2 Solving the current continuity equation for applied electric field

Here we solve the electric charge continuity equation for the applied electric potential and field, which is distorted around interfaces with conductivity differences. Due to the physical discontinuity in the exact solution of E_{ext} from equation (3.13), the spectral method with truncated expansions of polynomials suffers from the Gibbs phenomenon. Therefore we propose a smooth approximation of the equation (3.13) as follows:

$$\nabla \cdot (\sigma \nabla \psi_{ext}) = \nabla \cdot ([\phi \sigma_p + (1 - \phi) \sigma_f] \nabla \psi_{ext}) = 0 \quad \text{in } \Omega, \quad (3.29)$$

where σ_p , σ_f are the electrical conductivity of the particles and surrounding fluid medium respectively and the equation is solved in the entire domain Ω . We use

a smooth function ϕ to approximate the conductivity jumps across the interfaces between particles and surrounding solution as $\sigma = \phi\sigma_p + (1 - \phi)\sigma_f$. Note that if ϕ and hence σ is a step function across the particle surfaces, Equation (3.29) breaks down to two Laplace equations (3.14) for potential in and out the particle, where the boundary conditions need to be matched on the particle surfaces (3.15). With the utilization of smooth ϕ , the boundary conditions on the particle surfaces are avoided and we impose only the far field condition, which normally would be $\nabla\psi_{ext} = \mathbf{E}_\infty$. This condition serves as a Neumann condition to be imposed on the boundaries of the computational domain. Alternatively, if our simulation domain includes the electrodes, we have boundary conditions from the known electrode potential: $\psi_{ext} = \zeta_{ext}$, which is a Dirichlet type boundary condition.

We apply the spectral element method to discretize equation (3.29) and to solve its weak variational form. An iterative (conjugate gradient) method is used to update the solution until the residual is reduced beyond a certain level (typically 10^{-12}). As the applied electric field and the resulting charge density have jump discontinuities in the exact solution, we use Galerkin projections to solve the following equations:

$$\mathbf{E}_{ext} = -\nabla\psi_{ext}. \quad (3.30a)$$

$$\rho_{ext} = -\epsilon\epsilon_0\nabla^2\psi_{ext} \quad (3.30b)$$

A better approach would be to adopt a discontinuous Galerkin formulation, but this requires change in the expansion bases of the spectral element solver.

3.3.3 Solving the Navier–Stokes equation for electrohydrodynamic coupling

Finally, the incompressible Navier–Stokes equation is modified to include the elec-

trokinetic force in the entire domain:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} + \mathbf{f}_s + \mathbf{f}_{ek} \quad \text{in} \quad \Omega, \quad (3.31a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega, \quad (3.31b)$$

where $\mathbf{f}_s$ is the penalty force representing the rigid particles (see section 2.2), and $\mathbf{f}_{ek}$ is the electrokinetic force density, which differs from $\mathbf{f}_{EK}$ in equation (3.16). $\mathbf{f}_{ek}$ includes the force both on the electrolyte solution and on the charged particles, and can be written in the form of:

$$\mathbf{f}_{ek} = \rho_{edl} \mathbf{E}_{ext} + \rho_{ext} \mathbf{E}_{edl} \quad (3.32a)$$

$$\text{or} \quad = \rho_{edl} \mathbf{E}_{ext}, \quad (3.32b)$$

where the second expression (3.32b) is a possible simplification when the second term is zero or negligible, e.g. in the electroosmosis in straight channels with an external electric field parallel to the walls. We recall that ρ_{edl} is the charge density in EDL which includes the particle charges (3.23b), $\mathbf{E}_{edl} = -\nabla \psi$ is the corresponding electric field due to EDL, and $\mathbf{E}_{ext}, \rho_{ext}$ are the external applied field and corresponding charge distribution respectively. Note that here we do not explicitly include the forces $\rho_{edl} \mathbf{E}_{edl}$ and $\rho_{ext} \mathbf{E}_{ext}$, as their effects are already included in the Poisson–Boltzmann equation and the current density equation. More specifically if we consider the static charges and corresponding electric field in an equilibrium EDL, the electric force $\rho_{edl} \mathbf{E}_{edl}$ on any ion is balanced by the force due to the concentration gradient and thus all the ions and fluid mass are stationary $u \equiv 0$; similar argument can be made if we consider only the applied field around stationary interfaces.

Solutions of equation 3.31 are obtained by solving its dimensionless form:

$$\frac{\partial \mathbf{u}_d}{\partial t} + (\mathbf{u}_d \cdot \nabla) \mathbf{u}_d = -\nabla p_d + \frac{1}{Re_0} \nabla^2 \mathbf{u}_d + \mathbf{g}_d + \mathbf{f}_{s,d} + \mathbf{f}_{ek,d} \quad \text{in} \quad \Lambda, \quad (3.33a)$$

$$\nabla \cdot \mathbf{u}_d = 0 \quad \text{in} \quad \Lambda, \quad (3.33b)$$

where $\mathbf{u}_d$ is the dimensionless velocity scaled by the characteristic velocity u_0 , p_d is the dimensionless pressure scaled by the dynamic pressure ρu_0^2 , the length is scaled by the characteristic length h , and Re_0 is the Reynolds number $Re_0 = u_0 h / \nu$. All the body forces $\mathbf{g}_d$, $\mathbf{f}_{s,d}$ and $\mathbf{f}_{ek,d}$ are nondimensionalized by $\rho u_0^2 / h$. Equation (3.33) is solved by using a stiffly-stable high-order splitting scheme for temporal discretization and spectral element method for spatial discretization; we refer the readers to section 2.2 for details.

3.4 Numerical verification

In this section, we validate the modeling method with SPM boundary treatment for several benchmark problems of electrokinetic flows induced by charged particles in ionized solutions under an applied electric field. The numerical results of electric potential and charge density are compared with analytical solutions and also numerical results with direct boundary treatment.

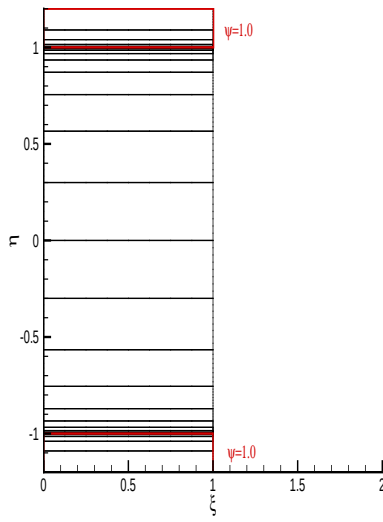
3.4.1 Accuracy of SPM–PB solver

EDL near charged plates

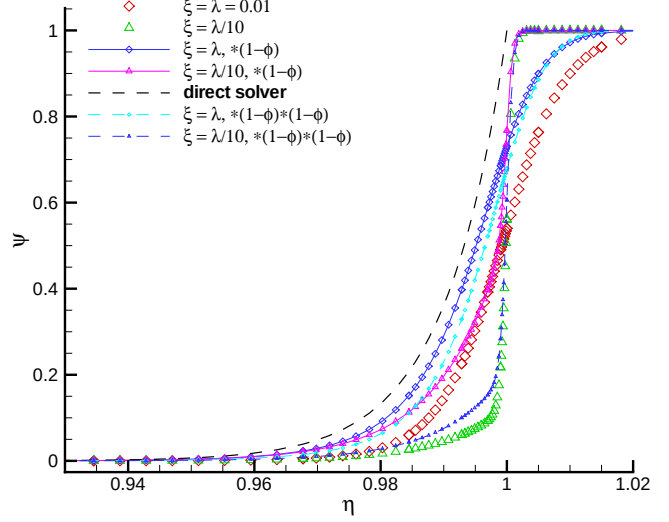
The formation of EDL near a charged plate in contact with an ionized solution is fundamental in the electroosmosis in two-dimensional channels. We simulate the problem to verify the two different modeling methods with modified Poisson–Boltzmann equations: one with specification of the zeta-potentials (3.22), and the other with prescribed charge density on the particles (3.23).

We consider two charged parallel plates, which are separated by a distance of $2h$ in y -direction, and infinite length is assumed for the other two dimensions. The geometry and computational mesh is shown in figure 3.2(a), with two “smoothed particles” representing the two walls located at $1.0 \leq |\eta| \leq 1.2$; all length scales are non-dimensionalized by h . We use 32 hexahedral elements with a finer grid near

the plates, and the polynomial order is chosen from $P = 6$ to $P = 14$ to check the convergence.



(a)



(b)

Figure 3.2: *EDL in a channel with two zeta potential patterned walls*: geometry of the problem (a), and dimensionless electric potential ψ along the interwall distance η (b). The numerical solutions of the SPM method with zeta-potential boundaries (3.22) is compared with the direct boundary solver (3.21). ξ refers to the SPM interface thickness, $\lambda = 0.01$ is the Debye length, $*(1 - \phi)$ stands for $c_1 = 1 - \phi$ and $*(1 - \phi) * (1 - \phi)$ stands for $c_0 = 1 - \phi, c_1 = 1 - \phi$.

Figure 3.2(b) presents the numerical solution of the dimensionless electric potential using SPM with zeta-potential boundaries (3.22), which is compared with the results of the direct boundary method (3.21). It is shown that reducing the interface thickness parameter ξ would improve the potential results inside and on the particle, but it leads to larger error in the fluid domain near the wall, e.g. $\eta = 0.98 \sim 1$. We see that by introducing $c_1 = 1 - \phi$ in (3.22), better accuracy is achieved, but still it fails to resolve very accurately the exact potential variation near the interface. This might be a result of the artificial correction of the potential inside the particles.

We proceed to the SPM–PB solver with *prescribed particle charge density* (3.23) and aim to gain better computational results. The same mesh is used as for the zeta–potential PB solver. We specify the surface charge density $e\sigma_e$ (with SI unit of C/m^2) by using its dimensionless form $I = \frac{e\sigma_e}{\epsilon\epsilon_0} kT\lambda_d$, which is related to our dimensionless parameter in (3.24) through $I = \gamma_s/\kappa h$. In order to examine the numerical accuracy based on the charge specification, we determine the analytical zeta–potential from the Grahame equation [46]:

$$I = 2\sinh\left(\frac{\zeta_{exact}}{2}\right), \quad (3.34)$$

where ζ_{exact} is the exact dimensionless zeta–potential scaled by kT/e , which we use as the “exact” solution. The assumption made in this equation is that the Debye length is very small compared to the particle dimensions $\kappa h = h/\lambda_d \gg 1$.

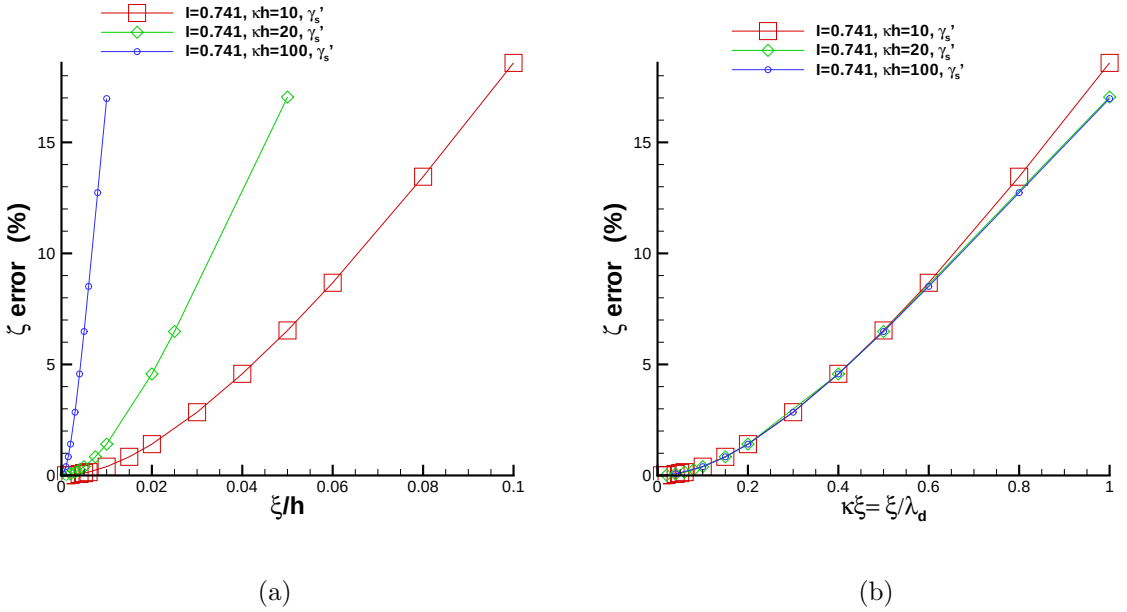


Figure 3.3: *EDL in a channel with two charged walls*: percentage error in zeta–potential with prescribed particle charge density (I) and Debye length ($\kappa h = h/\lambda_d$), showing the error dependence on the SPM interface thickness parameter (ξ/h) (a) and on the ratio of ξ/λ_d .

Figure 3.3 presents the percentage errors in the zeta–potential $\frac{|\zeta - \zeta_{exact}|}{\zeta_{exact}} \cdot 100$. We

argue that the error is mainly due to the modeling error of the smooth approximation used in (3.23), since the discretization error (spatial) is shown to be negligible by increasing the polynomial order beyond $P = 9$. The left plot shows that for a fixed Debye length, the error decreases with smaller interface thickness parameter ξ . It also shows that for a particular interface thickness used, the error goes up if we increase κh and reduce the Debye length. In order to examine the error dependence on the ratio of interface thickness to Debye length $\kappa\xi$, we replot the same data in 3.3(b). The agreement in all the results for different Debye length indicates that the error is only dependent on the ratio of $\kappa\xi$. It verifies that a better resolution of the double layer would be achieved if we use a smaller ratio $\kappa\xi$. In order to have a sufficiently good representation of the double layer with a characteristic thickness κ^{-1} , we need to use a relatively smaller SPM interface thickness. Recall that the effective interface thickness is scaled as $l_e = 2.07\xi$ (see section 2.3), so for adequate resolution, we suggest that $2.07\xi < \lambda_d$, i.e. $\kappa\xi < 0.483$. This is verified by our numerical results, which shows that the error is less than 6.5% if $\kappa\xi < 0.5$.

In order to examine the numerical results in a pointwise sense, we include for comparison the exact solution of the dimensionless potential by [18]:

$$\psi_{exact,d} = 4\zeta_{exact} \tanh^{-1}[\tanh(1/4) \exp(-\kappa h(1 - |\eta|))], \quad (3.35)$$

where ζ_{exact} is obtained from (3.34). Note that the derivation of (3.35) assumes that the potential is zero at the channel center, i.e. $\psi_d(\eta = 0) = 0$. In order to have a fair comparison with the analytical results of (3.34) and (3.35), we use small Debye length in our numerical simulations $\lambda_d/h \leq 0.1$. We plot the potential profiles across the channel in figure 3.4, where the potential is scaled by ζ_{exact} . It shows that SPM successfully resolves the potential variation in EDL with the parameters used.

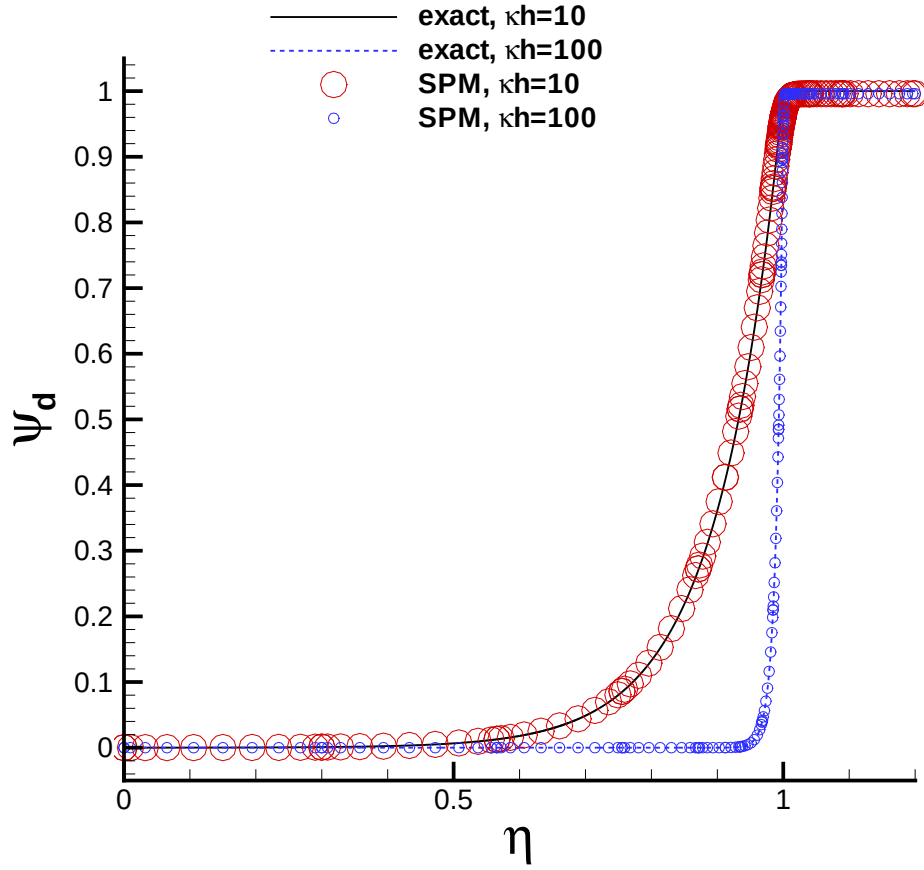


Figure 3.4: *EDL in a channel with two charged walls*: profile of the dimensionless electric potential ψ_d versus interwall distance η compared to the exact solutions. Parameters used are $I = 0.741$, $\xi/\lambda_d = 0.1$ and $\kappa h = 10$ or 100 . Only half of the domain is shown due to symmetry.

EDL around a charged sphere

We consider a charged spherical particle immersed in an electrolyte solution; a spherical shell of diffuse layer with high concentrations of counterions will be induced. Based on the Debye–Hückel approximation for low zeta-potentials, the linearized Poisson–Boltzmann equation (3.10) has a simple analytical solution in spherical coordinates [96]:

$$\psi_{DH,sph} = \frac{A}{r} \exp(-\kappa r) = \frac{A}{r} \exp\left(\frac{-r}{\lambda_d}\right),$$

where r is the distance to the sphere center and A is a constant of integration. The boundary condition on the sphere surface is $\psi = \zeta_{exact}$ at $r = a$, where we use the zeta-potential instead of the surface potential, as the Stern layer is very thin. Hence, the Debye–Hückel solution of the potential outside the particle ($r \geq a$) is as follows:

$$\psi_{DH,sph} = \zeta_{exact} \frac{a}{r} \exp(-\kappa(r - a)). \quad (3.36)$$

We solve equation (3.28) by spectral element discretization, given an uniform surface charge density γ_s, γ'_s or volume charge density γ_v in (3.24). The computational domain is $[-12, 12] \times [-12, 12] \times [-12, 12]$. A sphere with radius $a = 1$ is placed at the origin. A total number of 4096 nonuniform hexahedral elements with polynomial order $P = 6$ is employed for spatial discretization. Periodicity is imposed in all directions at the domain boundary.

Figure 3.5 shows the contours at $z = 0$ plane for the dimensionless electric potential ψ_d and charge density $\rho_{edl,d}$ in EDL around a positively surface charged sphere with $\gamma_s = 2.03, \kappa a = 1, \xi/a = 0.05$. The double layer structure is clearly illustrated with one layer of charge on particle surface and another layer of concentrated ions in the solution. We also see that, as expected, the electric potential is uniform *in* and *on* the sphere, and it decays very fast away from the surface.

To rigorously examine the potential distribution, we look at the potential profiles extracted at $z = 0$ plane and compare to the Debye–Hückel solution (3.36). Figure

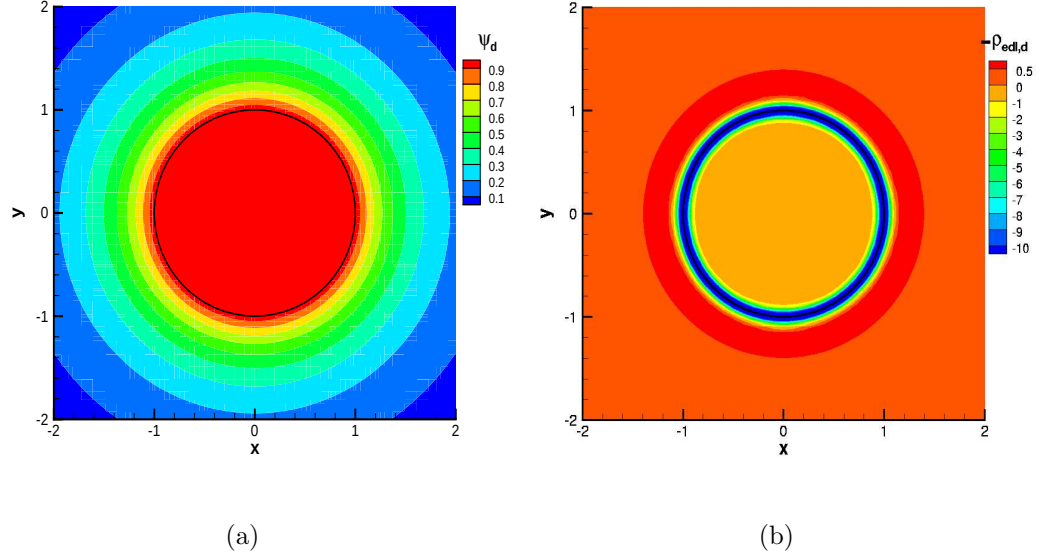


Figure 3.5: *EDL around a sphere*: contours of the dimensionless electric potential ψ_d (a) and dimensionless charge density $-\rho_{edl,d}$ (b), with $\gamma_s = 2.03$, $\kappa a = 1$, $\xi/a = 0.05$. The black curve shows the exact surface of the sphere.

3.6 shows good agreement between the SPM results with surface charge and the analytical approximation, except when close to the particle surface $r = a$, the sharp interfacial transition is smoothed out by SPM implementation. We also provide for comparison the SPM results using a volume charge pattern (3.24a) with prescribed total charge. The agreement with the Debye–Hückel approximation is even better for the potential outside the particle, although it loses the uniformity inside the particle. Next we explain how we obtain ζ_{exact} , provided the charge density on the sphere.

Ohshima et al. [85, 88] derived a second-order approximate solution of the surface charge density/surface potential relationship for a spherical particle, which was found to be very accurate for $\zeta \leq 1$, $\kappa a \geq 1$. We use this analytic expression as the exact solution of zeta-potential to examine the numerical accuracy of SPM–PB solver. Provided dimensionless surface charge density I and scaled radius $A = \kappa a$ as in equation [24] and table [I] in [88], the exact dimensionless potential y_s and thus

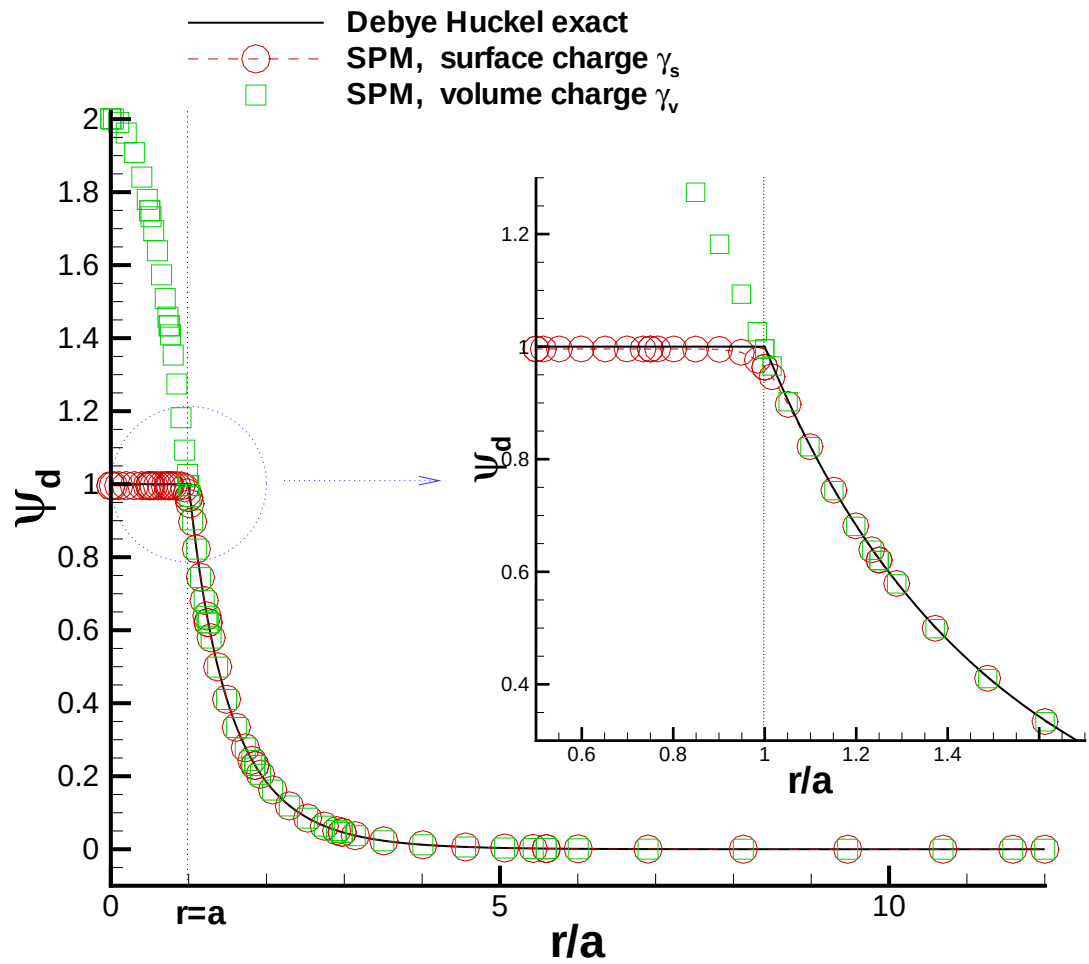


Figure 3.6: *EDL around a sphere*: profile of the dimensionless electric potential ψ_d along centerline $z = 0, y = 0$ with $\gamma_s = 2.03, \kappa a = 1, \xi/a = 0.05$. Only half of the domain is shown due to symmetry, and the right plot is a close-up around the sphere surface $r = a$.

the exact zeta-potential ζ_{exact} is obtained. Based on this ζ_{exact} , we calculate the relative error of the numerical zeta-potential, which is the potential interpolated on the sphere. Percentage errors in the zeta-potential ($\frac{|\zeta - \zeta_{exact}|}{\zeta_{exact}} \cdot 100$) are plotted in figure 3.7, for different physical and numerical parameters.

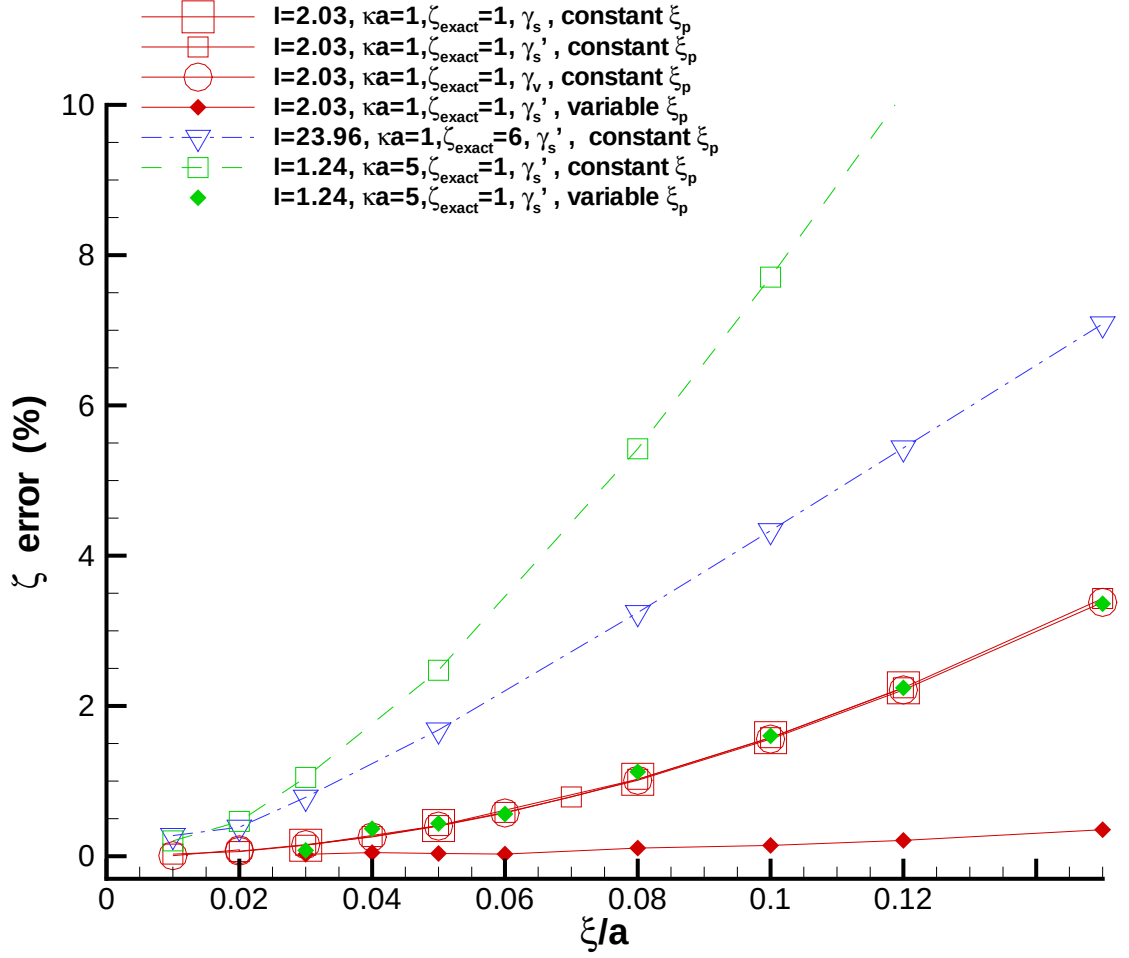


Figure 3.7: *EDL around a sphere*: percentage error in zeta-potential versus SPM interface thickness parameter (ξ/a), with various reduced radius (κa), particle charge density (I) and variable interface thickness (ξ_p in (3.27)).

In figure 3.7, the dimensionless surface charge density I is adopted from [85, 88], which is related to our surface charge density parameter through $I = \gamma_s / \kappa h$. We

use I as the reference indicating the prescribed total charge. The particular charge pattern applied in our simulations is one of the following: equation (3.24a) with γ_v , equation (3.24b) with γ_s and equation (3.24c) with γ'_s . The first three sets of data (with $I = 2.03, \kappa a = 1$ in red hollow symbols) in figure 3.7 show equivalence of all three implementations of particle charge patterns (3.24). For this I and κa , the error is less than 1.5% if $\xi/a < 0.1$, and it further decreases with decreasing ξ . Blue symbols in the figure show that for higher charge density $I = 23.96$ which corresponds to $\zeta_{exact} = 6$, the error increases to about 4.3% for $\xi/a = 0.1$. This increase might come from the fact that Ohshima's approximation was derived under small ζ conditions.

For smaller Debye length $\kappa a = 5, \lambda_d = 0.2a$ (green hollow symbols in figure 3.7) the error increases to about 7.7% for $\xi/a = 0.1$. This is due to the comparable scale of smooth interface thickness ξ to the Debye length λ_d . We argue that in order to resolve the potential variation in the diffuse layer, the effective interface thickness ($l_e = 2.07\xi$ for constant ξ_p in section 2.3) needs to be smaller than the effective thickness of the diffuse layer, i.e. $l_e < \lambda_d$ and thus $\xi < 0.48\lambda_d$. With this condition satisfied, we see that the error is bounded by 7%.

Furthermore, the filled small symbols in figure 3.7 show big improvement of accuracy when a variable interface thickness (equation (3.27b) with $c = 2$) is used instead of the usual constant thickness ((3.27a)). It is specially useful for problems with larger κa , as the error decreases to the error scale of smaller κa .

EDL around an infinitely long charged circular cylinder

We consider a charged circular cylinder immersed in an electrolyte solution. As our ultimate goal is to have comparable results with microtubules, we adopt a configuration based on the geometries of microtubules as in [113]. First, as the spanwise dimension of a real microtubule is about a hundred times the cross-section dimension, we start with infinitely long (two-dimensional) cylinders (however, our SPM

simulations are still 3D). Second, as real microtubules are hollow structures, we need to investigate how the hollowness would affect the EDL and thus the electrophoresis mobility. Hence, we begin with simulations for solid cylinders and then proceed to hollow cylinders and microtubules.

The radius of the cylinder is adopted as $a = 11.0 \text{ nm}$ to match the average outer radius of the microtubule structures [113]. We choose the scaling factor for length to be $h = 1 \text{ nm}$ and thus all the length scales in the rest of this section are dimensionless. The simulation domain is chosen to be $[-176, 176] \times [-176, 176] \times [0, 10]$, with a cylinder of radius $a = 11$ placed at origin and its axis aligned with the z-axis. Note that a small spanwise dimension is used to study the 2D problem by a single layer of elements with periodicity imposed in the z-direction.

The modified Poisson–Boltzmann equations (3.22) or (3.28) are solved by the spectral element method, given the zeta-potential or the charge on the cylinder (γ_s, γ'_s or γ_v in (3.24)). For spatial discretization we use 1156 nonuniform hexahedral elements with polynomial order $P = 5$ or $P = 7$. We see in figure 3.8 that with the SPM zeta-potential solver (3.22), a smaller interface thickness ξ would lead to better accuracy, but still it fails to resolve the potential both inside and outside the particle at the same time. Next, we verify the SPM–PB solver with *charge specifications* as in (3.22).

From the analytical approximation of Ohshima [87] for the surface charge density/surface potential relationship for a cylinder, we can obtain the exact zeta-potential ζ_{exact} , given the charge on the cylinder. The numerical errors of zeta-potentials are calculated and listed in table 3.1 for a given dimensionless surface charge density $I = 1.47$ with $\kappa a = 1$. The results show that the error of the zeta-potential is less than 1% for all the interface thickness included, i.e. $\xi/a \leq 0.1$. The Debye–Hückel approximate solution for a cylinder with low zeta-potential is used as

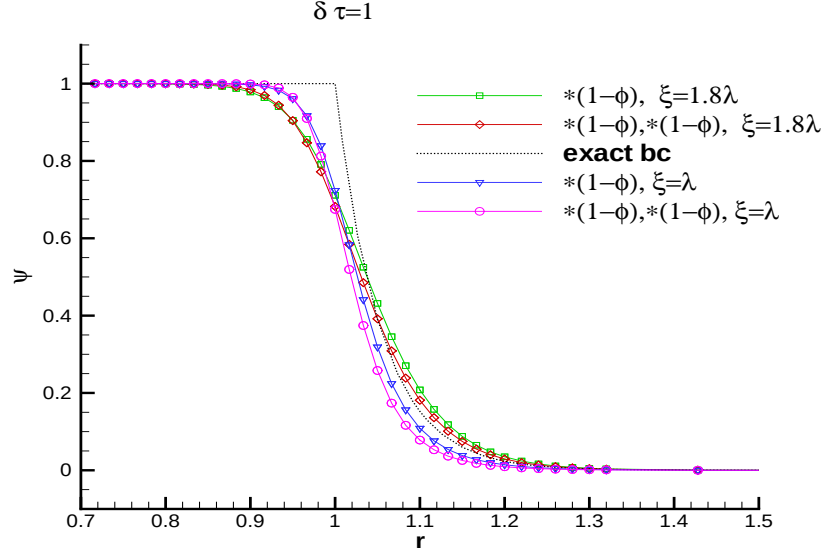


Figure 3.8: *Zeta potential patterned cylinder in a periodic box*: comparison of direct boundary solver with exact BC (3.21) and SPM zeta-potential solver (3.22), dimensionless electric potential ψ along the radial distance r , with various interface thickness ξ . In the legend, $*(1 - \phi)$ refers to $c_1 = 1 - \phi$ and $*(1 - \phi) * (1 - \phi)$ to $c_0 = 1 - \phi, c_1 = 1 - \phi$ in equation (3.22).

Table 3.1: *Electric potential of an infinitely long cylinder*: dimensionless potential at the surface and the center of the cylinder with $I = 1.47, \kappa a = 1, \zeta_{exact} = 1$

ξ/a	ζ	ψ_{center}	error= $\frac{ \zeta - \zeta_{exact} }{\zeta_{exact}}$
0.01	0.999218	0.999890	0.0782 %
0.02	0.999675	0.999680	0.0325 %
0.03	0.999298	0.999299	0.0702 %
0.05	0.998151	0.998151	0.1849 %
0.1	0.993016	0.993016	0.6984 %

a reference to compare with the numerical results:

$$\psi_{DH,cyl} = \zeta_{exact} \frac{K_0(\kappa r)}{K_0(\kappa a)}, \quad (3.37)$$

where K_0 is the zero order modified Bessel function of the second kind. Figure 3.9 shows profiles of the dimensionless potential ψ_d along the radial distance to the cylinder center r . Here we prescribe the total charge and Debye length as $I = 2.06, \kappa a = 11$ and investigate the effects of different particle charge patterns and smooth indicator functions. We see first that the three sets of blue symbols agree very well outside the cylinder and they verify the equivalence of three different implementations of particle charge distribution (3.24). Figure 3.9 also shows significant improvement by decreasing the interface thickness parameter ξ , or by using a variable thickness ξ_p (3.27b).

Percentage errors in zeta-potential ($\frac{|\zeta - \zeta_{exact}|}{\zeta_{exact}} \cdot 100$) for various computational parameters are plotted in figure 3.10 and 3.11. We see that for the blue and black symbols in figure 3.10 which corresponds to $I = 1.47, \kappa a = 1$ and thus $\zeta_{exact} = 1$, the numerical error in ζ is less than 1% for all the values of the interface thickness $\xi/a \leq 0.1$. Also, the volume charge distribution model γ_v produces comparable error as the surface charge model γ'_s , with a relative difference of 0.5% for $\xi/a = 0.1$. The purple symbols show that the error increases when a higher charge density is imposed as $I = 2.06, \kappa a = 1$ and correspondingly $\zeta_{exact} = 6.08$. However, we are able to reduce the error by using a variable interface thickness ξ_p as in (3.27b); the resulting error is less than 1.5% as long as $\xi/a \leq 0.1$. Similarly, we have greater numerical error when a smaller Debye length is presented $\kappa a = 11$, as the cyan symbols shown in figure 3.10. For such a small Debye length $\lambda_d/a = 0.09$, we need to use a sharper interface representation, either by reducing ξ or by using a variable ξ_p . In order to resolve the diffuse layer with a thickness scaled as λ_d , the effective smooth interface thickness needs to be bounded by the Debye length as $l_e = 2.07\xi < \lambda_d$. Our numerical results (cyan squares) verify this statement by showing the error to be less

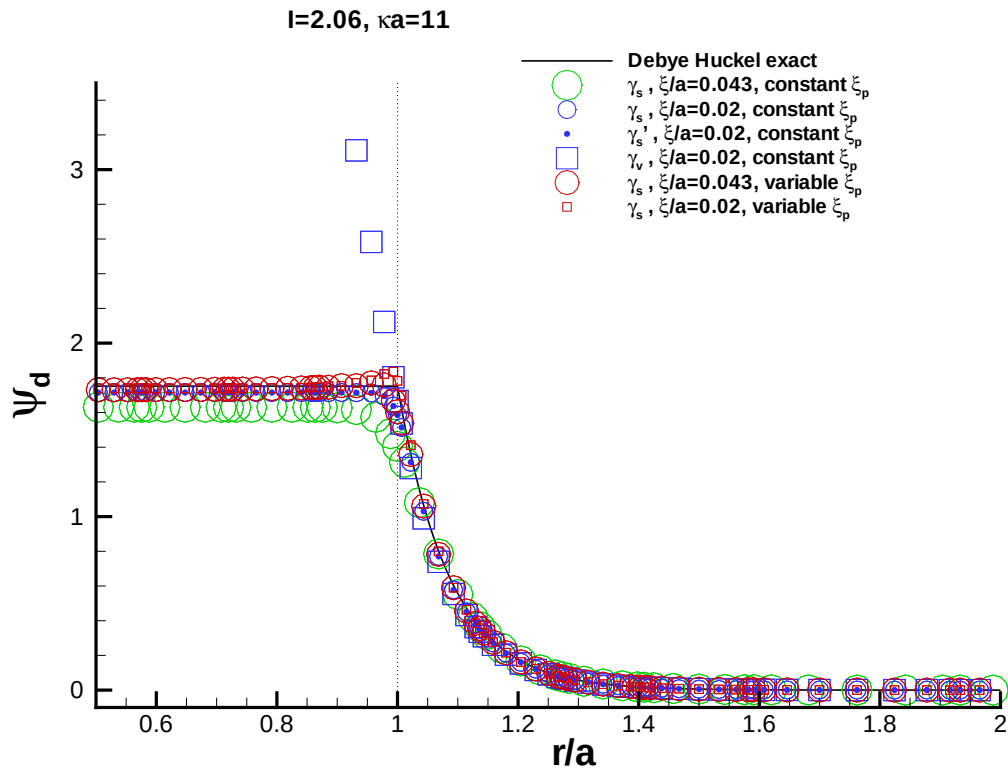


Figure 3.9: *SPM simulations for EDL around an infinite cylinder*: non-dimensional electric potential ψ_d versus radial distance r , compared to the Debye–Hückel approximation. The black dotted line indicates the cylinder surface.

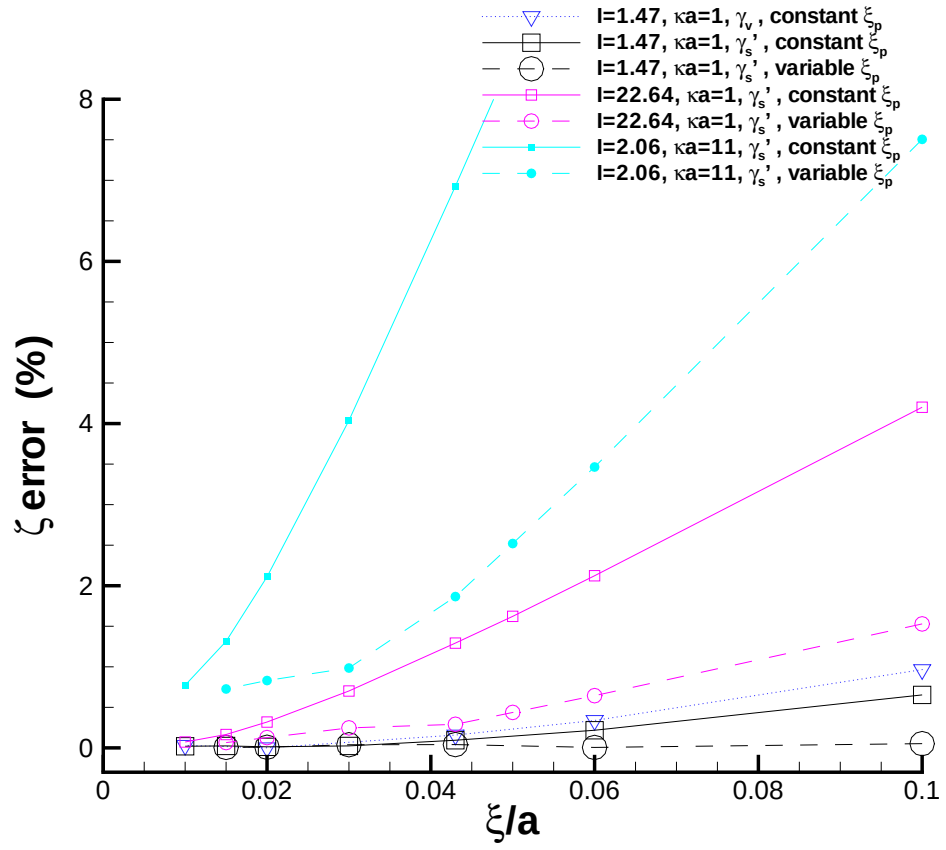


Figure 3.10: *SPM simulations for EDL around a infinite cylinder*: percentage error in dimensionless zeta-potential ζ_d versus SPM interface thickness parameter (ξ/a), for various dimensionless particle charge density (I), reduced radius (κa), and charge distribution (γ).

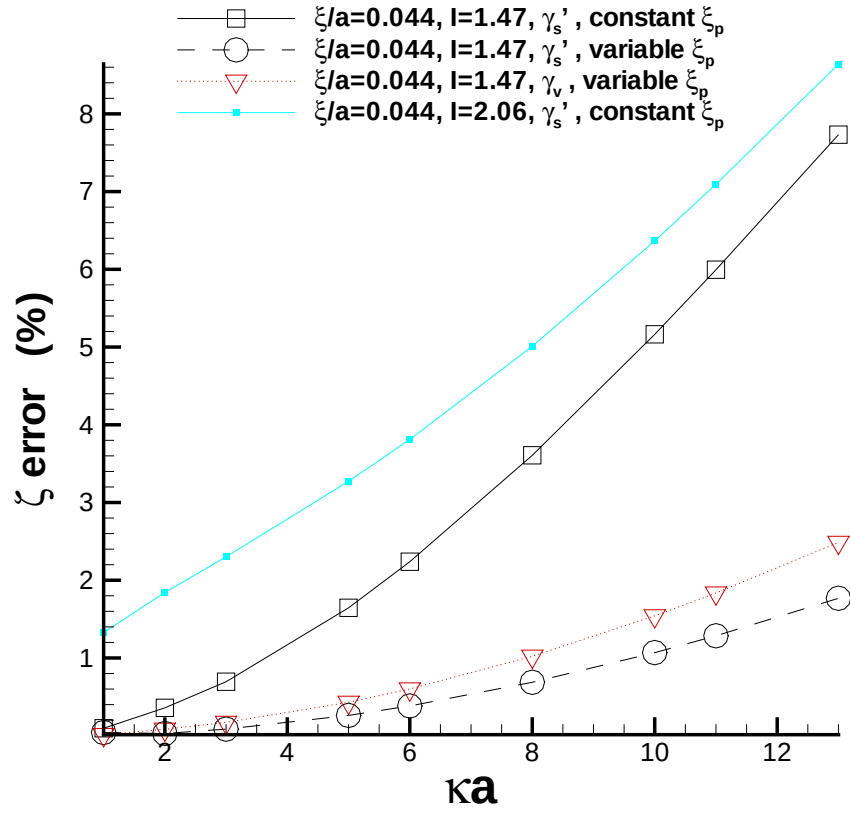


Figure 3.11: *SPM simulations for EDL around an infinite cylinder*: percentage error in dimensionless zeta-potential ζ_d versus reduced radius (κa), for various dimensionless particle charge density (I), reduced radius (κa), and charge distribution (γ).

than 7% if the above condition is satisfied; we note that this critical error is similar to the one obtained in the spherical EDL simulations in the proceeding subsection. Furthermore, we are able to control the error to be within 2.5% if we use a variable interface thickness ξ_p with $\xi/a \leq 0.05$.

Figure 3.11 demonstrates the error dependence on the reduced radius κa . It shows that for a fixed interface thickness ξ , the error grows with increasing κa and hence decreasing Debye length λ_d . The square symbols again confirm that the error is bounded by $\leq 7\%$, if we resolve the diffuse layer adequately by $l_e = 2.07\xi < \lambda_d$. The last two sets of data show big improvement in accuracy by using variable ξ_p , which is due to the resulting smaller effective interface thickness. They also indicate that no significant difference is caused by using different charge patterns, as either surface charge or volume charge.

3.4.2 Accuracy of SPM current continuity solver

We investigate the accuracy of the SPM solver of current continuity equations (3.29) by solving for the applied external electric field which is distorted around poorly conducting particles in an electrolyte solution with high electrical conductivity. We examine the numerical accuracy by comparing it with analytical solutions for simple particle shapes, e.g. spheres and cylinders.

Applied field around a sphere

We solve equation (3.29), (3.30a) and (3.30b) by spectral element discretization, with a smooth indicator function for spheres (3.26). The computational configuration is the same as the problem of EDL around a sphere, i.e. with a cubic domain of 24^3 and a sphere of radius $a = 1$ at the center. Also, we use the same spatial discretization with 4096 nonuniform hexahedral elements and polynomial order $P = 6$. However in contrast, Neumann BCs are applied at all the domain boundaries, i.e. $\frac{\partial \psi_{ext}}{n} = \nabla \psi_{ext} \cdot \mathbf{n} = -\mathbf{E}_\infty \cdot \mathbf{n}$. Here we assume that the domain is large enough compared to the sphere dimension, so that far field condition $\mathbf{E}_{ext} = \mathbf{E}_\infty$ can be applied as boundary condition.

The exact solution for the applied electric potential around a sphere with conductivity jumps ($\sigma_f \neq \sigma_p$) in an open domain is as follows [37]:

$$\begin{aligned}\psi_{ext,out} &= -\mathbf{E}_\infty \left(1 + \frac{\sigma_f - \sigma_p}{2\sigma_f + \sigma_p} \cdot \frac{a^3}{(x^2 + y^2 + z^2)^{3/2}} \right) x, \\ \psi_{ext,in} &= -\mathbf{E}_\infty \left(1 + \frac{\sigma_f - \sigma_p}{2\sigma_f + \sigma_p} \right) x,\end{aligned}\tag{3.38}$$

respectively for the outer and inner fields, respectively. The exact electric field $\mathbf{E}_{ext,out}$ and $\mathbf{E}_{ext,in}$ is derived correspondingly. We use this exact solution to verify our modeling method by comparing with the numerical results. We prescribe the conductivity ratio σ_p/σ_f to be 0.1 or 0.001, and the far field condition is given as $\mathbf{E}_\infty = (4000 \text{ V/m}, 0, 0)$.

Figure 3.12 illustrates how the applied field E_{ext} is distorted around a sphere with small conductivity of $\sigma_p/\sigma_f = 0.1$. The charge density contours demonstrate the charge accumulation near the interface with a conductivity jump. We note that instead of the Dirac delta distribution of the charge as in the exact solution, SPM results in a smooth diffusion of the surface charge into the particles.

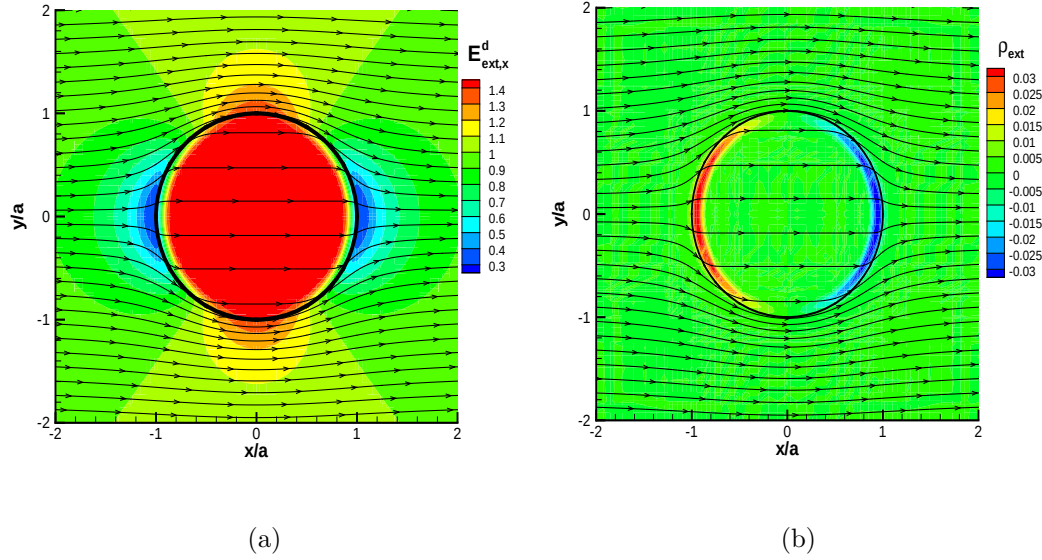


Figure 3.12: *SPM simulations for applied field around a sphere*: contours of the primary component of the dimensionless applied external electric field $E^d_{ext,x} = E_{ext,x}/E_{\infty,x}$ (a), and the corresponding charge density ρ_{ext} (b) in a plane cutting through the sphere center $z = 0$. The electric field lines are shown with arrows, and the sphere surface is indicated with wide black line.

The profiles of the applied electric potential and electric field near the sphere surface are examined and compared against the above analytical solution in figures 3.13 and 3.14. Figure 3.13 shows excellent agreement between the SPM potential results ψ_{ext} and the exact solution outside the sphere. However, in order to resolve the sharp transition on the interface and hence to resolve the field inside, we have to use a very thin SPM interface representation. Using a variable ξ_p with $\xi/a = 0.05$, the L_∞ error is around 2.1% for the case $\sigma_p/\sigma_f = 0.1$. The L_∞ error goes up to

about 4.0% for a smaller ratio $\sigma_p/\sigma_f = 0.001$, which comes from the fact that the equation (3.29) is more ill-conditioned.

For the applied electric field $\mathbf{E}_{ext}$, figure 3.14 shows features which are similar to the potential results. Smaller interface thickness improves the accuracy inside, but it also introduces oscillations near the interface, which comes from insufficient spatial resolution of the SPM interface. The big blue circles in figure 3.14 refer to the result of $\mathbf{E}_{ext}$ before the Galerkin projection, i.e. the gradient (3.30a) is calculated element-wise in the nodal space by using Lagrange interpolation polynomials. Comparison between the two sets of blue symbols shows that the Galerkin projection of the solution effectively removes the discontinuity at elemental boundaries and reduces the magnitude of the oscillation.

Applied field around a cylinder

We further examine the accuracy of the SPM current continuity solver (3.29) for the applied electric field around an infinitely long circular cylinder. Same as the simulation setup for cylindrical EDL problems, a cylinder of radius $a = 11$ is aligned with z-axis, and a computational domain of $[-176, 176] \times [-176, 176] \times [0, 10]$ is used. The same spatial discretization is used, i.e. with 1156 nonuniform rectilinear (hexahedral) elements and polynomial order $P = 7$. Also, periodicity is imposed in the spanwise z-direction, but here, we apply Neumann BCs for the other boundaries of the domain, i.e. $\frac{\partial \psi_{ext}}{\partial \mathbf{n}} = -\mathbf{E}_\infty \cdot \mathbf{n}$. The external electric field is uniform in the far field, i.e. $\mathbf{E}_\infty = (4000, 0, 0) \text{ V/m}$.

For comparison, we provide the exact solutions of the applied field and potential as follows:

$$\psi_{ext,out} = -\mathbf{E}_\infty \left(1 + \frac{\sigma_f - \sigma_p}{\sigma_f + \sigma_p} \cdot \frac{a^2}{(x^2 + y^2 + z^2)} \right) x, \quad (3.39a)$$

$$\psi_{ext,in} = -\mathbf{E}_\infty \left(1 + \frac{\sigma_f - \sigma_p}{\sigma_f + \sigma_p} \right) x. \quad (3.39b)$$

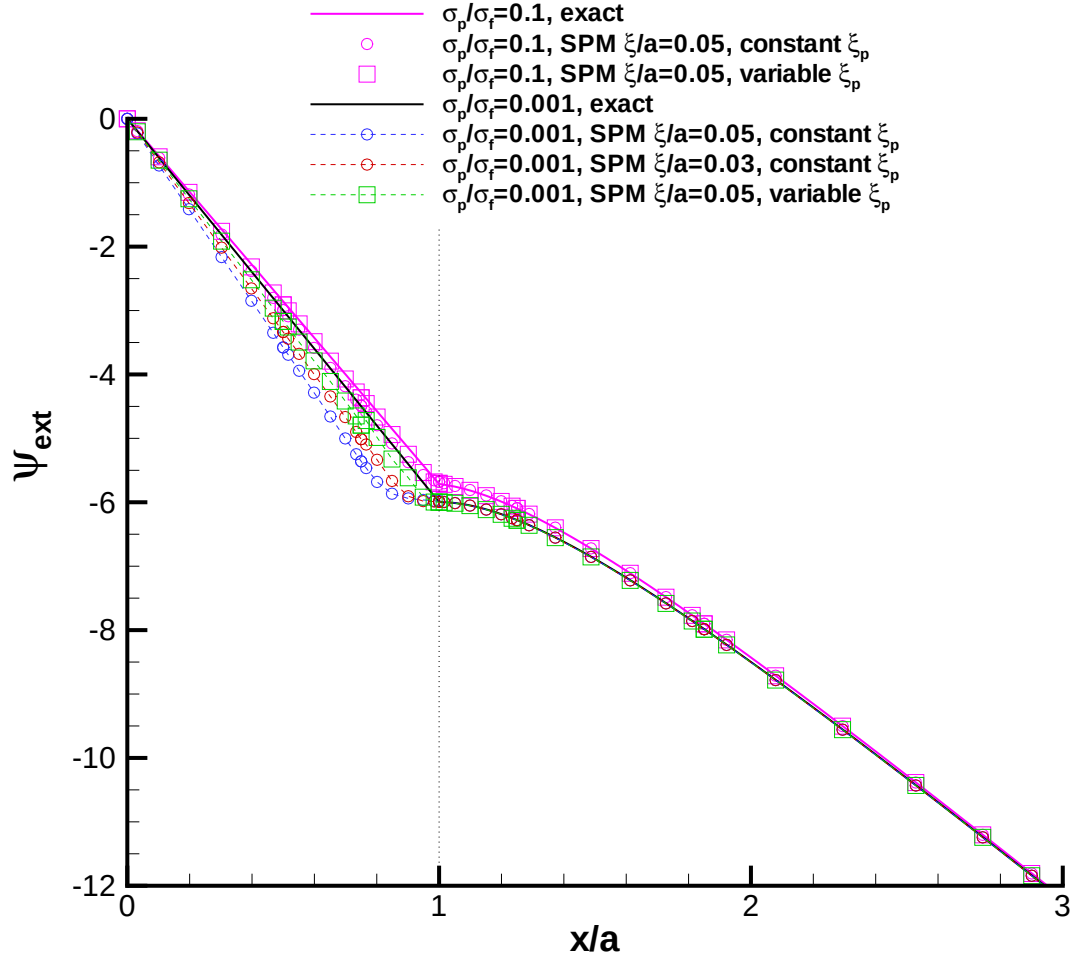


Figure 3.13: *SPM simulations for applied field around a sphere*: the applied external electric potential ψ_{ext} along the primary axis x , for two different ratios of σ_p/σ_f . The sphere surface is indicated by the black dotted line.

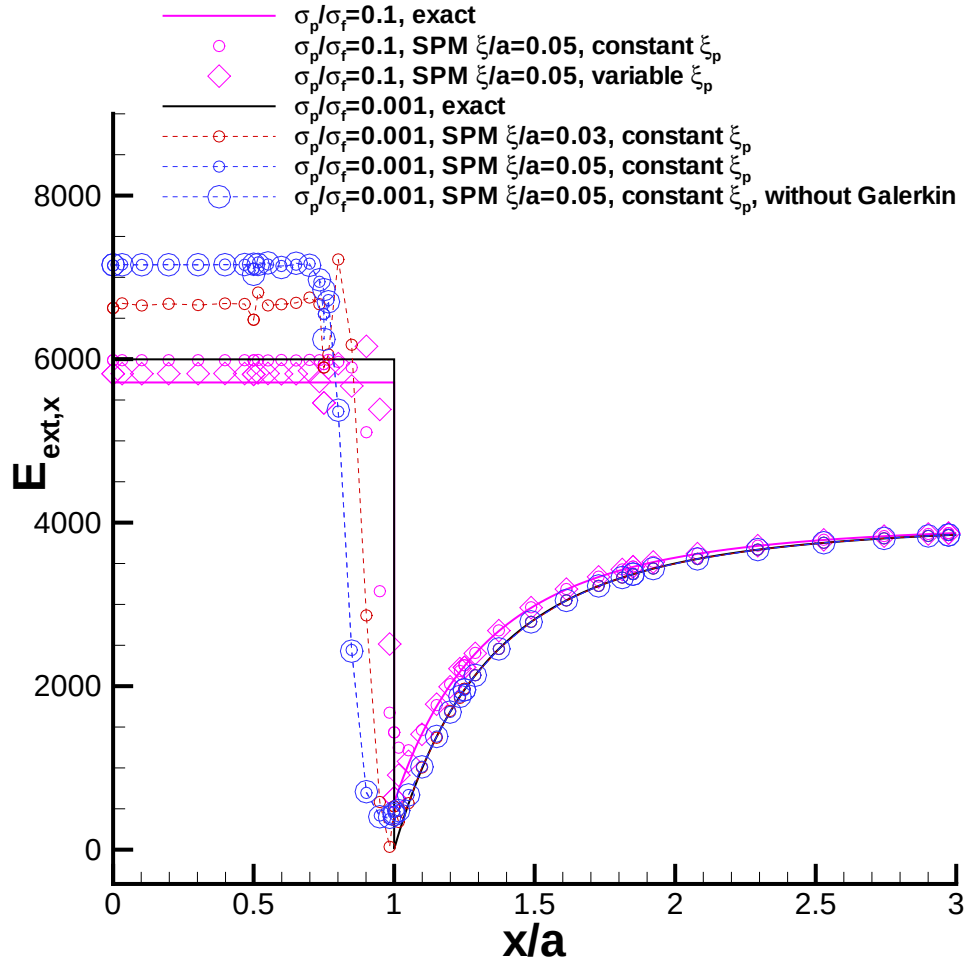


Figure 3.14: *SPM simulations for applied field around a sphere*: the dimensionless applied electric field $E_{ext,x}^d = E_{ext,x}/E_{\infty,x}$ along the primary axis x , for two different ratios of σ_p/σ_f . The sphere surface is indicated by the black dotted line.

The exact electric field $\mathbf{E}_{ext,out}$ and $\mathbf{E}_{ext,in}$ is obtained correspondingly. These exact solutions can be applied at the domain boundaries as Dirichlet BCs; the resulting numerical solution are compared with the Neumann BC implementation to check the finite-domain effect.

We also want to include for comparison the SPM results using a limiting step function $\phi = H(\xi = 0)$ in equation (3.29), against the general SPM solution using a smooth $\phi(\xi \neq 0)$. So a curvilinear mesh conforming to the particle surface is employed for spectral element discretization, to avoid the Gibbs phenomenon due to the polynomial expansion in each spectral element. A total of 580 hexahedral elements with polynomial degree $P = 9$ are used for both cases: $\xi = 0$ and $\xi \neq 0$. The elemental mesh is shown in figure 3.15(b), with a comparison against the rectilinear mesh used for general smooth ϕ as in figure 3.15(a). We see that the results for the applied field by using these two different meshes are very similar.

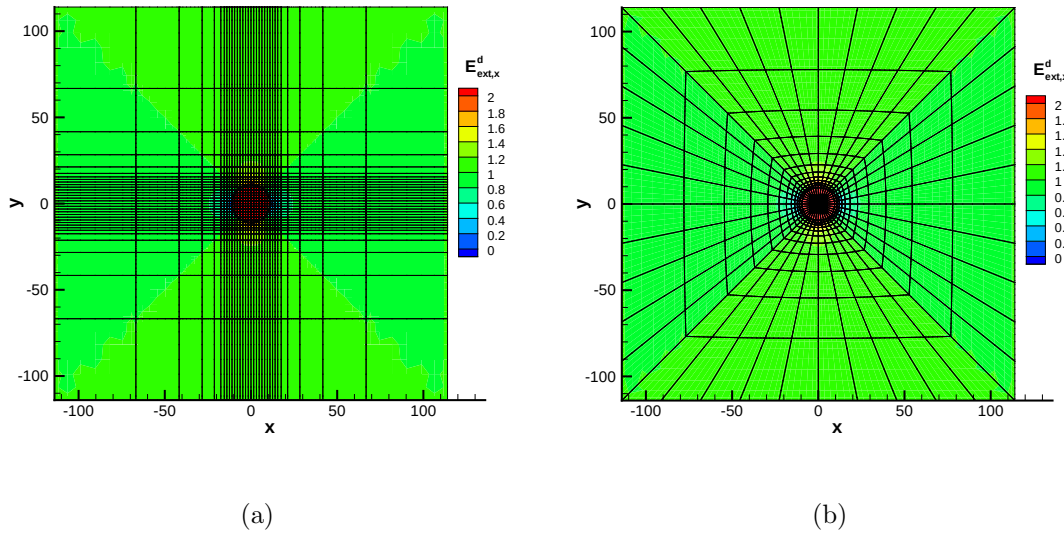


Figure 3.15: *SPM simulations for applied field around an infinitely long cylinder*: the elemental meshes and contours of the external electric field $E_{ext,x}^d = E_{ext,x}/E_{\infty,x}$, with a conductivity ratios of $\sigma_p/\sigma_f = 0.001$. The left plot refers to the rectilinear mesh and the right to the curvilinear mesh; the thick black curves indicate the cylinder surface.

Next we present near-field profiles of the applied electric potential in figure 3.16. The filled symbols in the figure show excellent agreement between the SPM results with $\xi = 0$ and the exact solution for all the conductivity ratios σ_p/σ_f included. However, note that due to the body-conforming mesh required, this model is not generally applicable, especially for moving complex boundaries. The hollow circles corresponding to $\xi \leq 0$ show that the error grows with decreasing ratio σ_p/σ_f ; worse accuracy inside the particle is presented while the outer field is resolved very accurately. For the small ratio of $\sigma_p/\sigma_f = 0.001$, a small smooth interface thickness is required to resolve the interfacial field, e.g. $\xi/a = 0.01$ would control the error under $L_\infty < 3\%$. Comparison of the blue hollow squares and circles indicates that the relative difference between the two BC types is small ($L_\infty < 1\%$), and hence the finite-domain effect is negligible. Also, we note that the difference between using either rectilinear or curvilinear mesh is small, as shown by the red hollow symbols with identical $\sigma_p/\sigma_f = 0.1, \xi/a = 0.043$. This indicates that the results are mesh independent, and it suggests the use of simple rectilinear mesh regardless of the shape of the particles.

Figure 3.17 presents variations of the numerical solutions of the applied electric field near the cylinder surface, with a small conductivity ratio $\sigma_p/\sigma_f = 0.001$. SPM results with various interface thickness ξ_p are compared against the exact solution and numerical solution with limiting $\xi = 0$. The agreement is very good for the outer field, but is worse inside the particle. By using a thin SPM interface of variable ξ_p with $\xi/a = 0.043$ and $c = 5$ in (3.27), the electric field at the center of the cylinder has a small error $< 2\%$, although some oscillations are present near the surface which is due to the resolution issue. It is again verified by the red symbols that the two different meshes result in only small differences in the numerical solution.

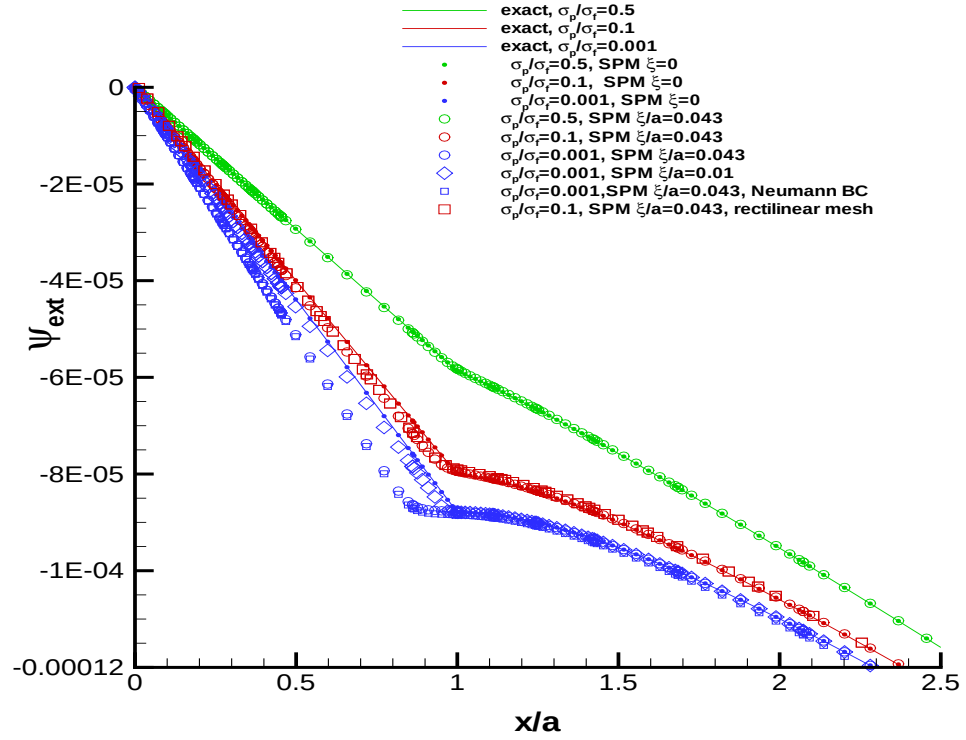


Figure 3.16: *SPM simulations for applied field around an infinitely long cylinder:* external electric potential ψ_{ext} versus the primary axis x , with different conductivity ratios σ_p/σ_f . The black dotted line refers to the cylinder surface. A curvilinear mesh with Dirichlet BC is used if not indicated.

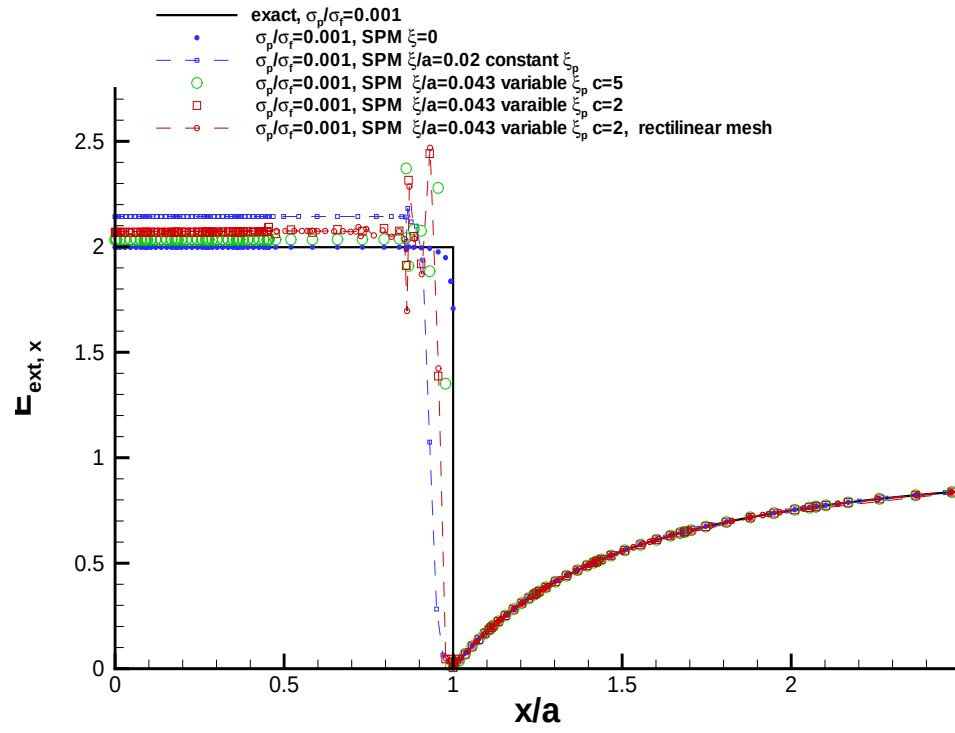


Figure 3.17: *SPM simulations for applied field around an infinitely long cylinder: the dimensionless external electric field $E_{\text{ext},x}^d = E_{\text{ext},x}/E_{\infty,x}$ along the primary axis x , with various SPM interface representations.*

3.4.3 Accuracy of SPM electrohydrodynamic solver

In this section, we simulate the electrokinetic flows around simple particle shapes to investigate the accuracy of our SPM electrohydrodynamic solver (3.31).

Electroosmosis in a microchannel

We first consider the problem of EOF in a two-dimensional microchannel under the influence of an applied electric field which is uniform and parallel to the channel walls. Since there is no distortion of the applied field due to the simple geometry, the electrokinetic force consists of only one term (3.32b) and thus the error from the current density solver is not included in the numerical results. The same geometry and computational mesh are used as for the planar EDL problem, see figure 3.2(a). Here we specify the non-dimensionalization factor $h = 0.5 \times 10^{-6} \text{ m}$ for a channel of one micron wide. The other physical parameters are: the fluid density $\rho = 999.9 \text{ kg/m}^3$, the dielectric constant $\epsilon\epsilon_o = 6.95 \times 10^{-10} \text{ C}^2/Jm$, the dynamic viscosity $\nu = 0.889 \times 10^{-3} \text{ Pa} \cdot s$, the temperature $T = 25^\circ\text{C}$, and the external electric field $\mathbf{E}_\infty = (4000 \text{ V/m}, 0, 0)$.

The analytical solution of the electroosmotic velocity is provided by [18] for zero pressure gradient and given the Stokes assumption:

$$u_{exact}^d(\eta) = 1 - \frac{\psi_{exact,d}}{\zeta_{exact}}, \quad (3.40)$$

where $\zeta_{exact}, \psi_{exact,d}$ can be obtained from equations (3.34) and (3.35) from the prescribed dimensionless charge density on the channel walls. Here, the velocity is scaled by the Helmholtz–Smoluchowski electroosmotic velocity $u_{HS} = -\zeta_{exact} \frac{\epsilon\epsilon_o E_\infty}{\mu}$, which is the velocity at the center of the channel assuming $\kappa h \gg 1$ and $\psi_{center} = 0$. We use this “exact” solution to verify our numerical results.

Figure 3.18 shows typical velocity profiles across the channel. Note that we use the numerical solution of the electric potential and charge density in EDL with

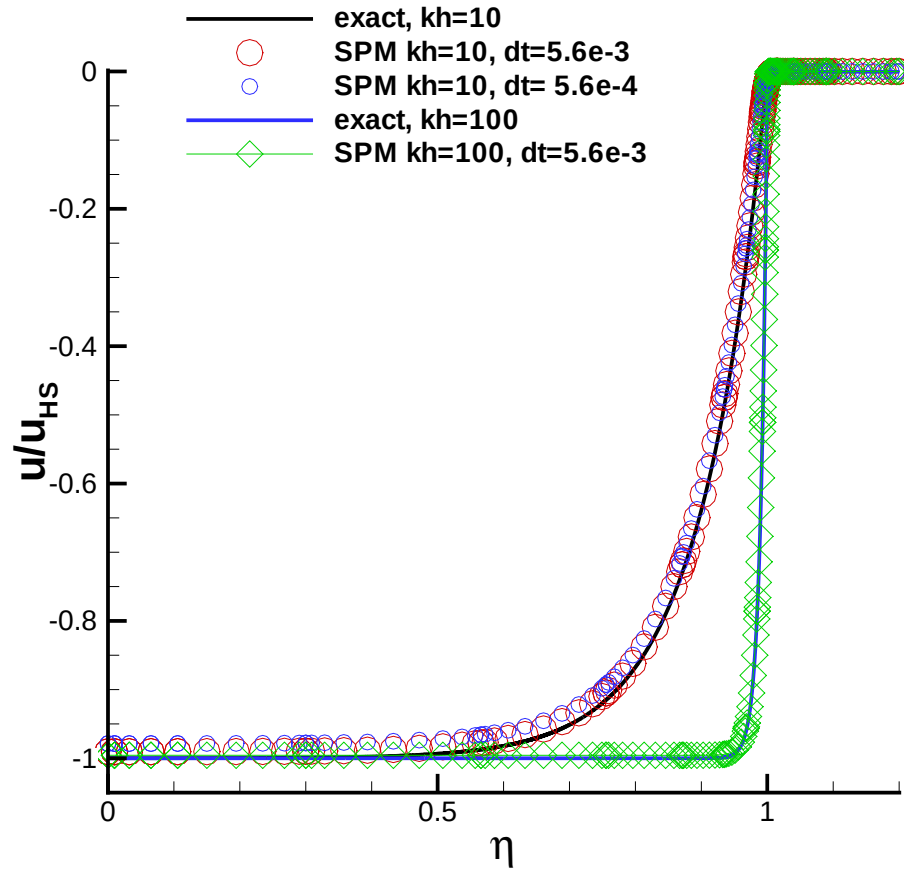


Figure 3.18: *Electroosmosis in a microchannel*: dimensionless streamwise velocity u/u_{HS} versus interwall distance η compared to the exact solution (3.40), with different reciprocal Debye length $\kappa h = h/\lambda_d$ and computational time step dt .

specified charge density $I = 0.741$ and thickness ratio $\kappa\xi = 0.1$ as in figure 3.4. We see that SPM successfully resolves the electroosmotic motion and shows that the velocity profile is more uniform for a smaller Debye length, i.e. larger κh . The figure also indicates that the numerical accuracy depends on the time step size used to iterate to a steady state.

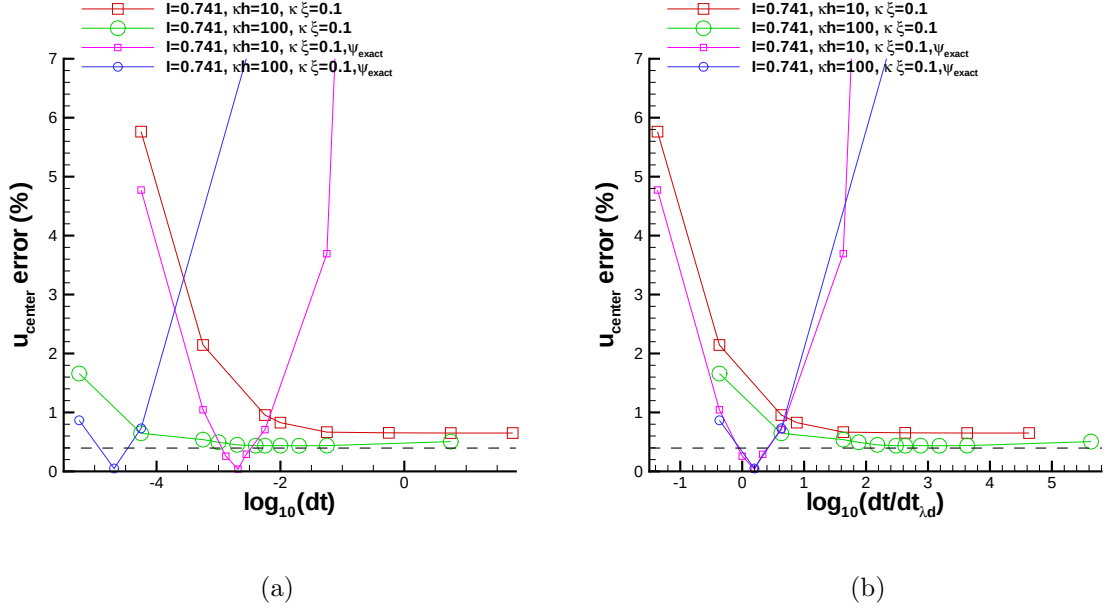


Figure 3.19: *Electroosmosis in a microchannel*: percentage error in centerline velocity versus time step size dt (a) and versus time step ratio dt/dt_{λ_d} (b), with specified particle charge density (I), reciprocal Debye length ($\kappa h = h/\lambda_d$) and thickness ratio $\kappa\xi$. Dashed line indicates the error in the zeta-potential from the SPM-PB solver.

In order to examine more closely this error dependence, we plot in figure 3.19 the percentage error of the center velocity $u(\eta = 0)$ compared to the Helmholtz–Smoluchowski results u_{HS} , i.e. $\frac{|u(\eta=0) - u_{\text{HS}}|}{u_{\text{HS}}} \cdot 100$. Again, we interpret the error as the modeling error of SPM, provided that both the temporal and spatial discretization errors are negligible. Note that this modeling error consists of three parts, i.e. the first one is due to the representation of rigid bodies by a penalty force in NS equation (3.31), which we have already quantified in section 2.3; the second one comes from the SPM-PB solver (3.23), which depends on $\kappa\xi$ as we showed in section 3.4.1; the

last is attributed to the modeling error from the electrokinetic force constitution, which uses a smooth approximation of the EDL charges both on the particle and in the solution (3.23b).

Figure 3.19 shows by the big symbols the error of velocity when we use the numerical solutions of EDL potential and charge from the SPM–PB solver (3.23). The error is very small ($< 1\%$) for the small Debye length $\lambda_d/h = 0.01$ for all time steps included, as shown by the big circles. Particularly, we note that the minimum error (around 0.43%) is consistent with the zeta-potential error from the SPM–PB solver, as shown by the dashed line, which is about 0.4% for both cases with different Debye lengths but the same thickness ratio. For a bigger Debye length $\lambda_d/h = 0.1$ as presented by the big squares, the error goes up, which may be partially due to the worse accuracy of the “exact” solutions for the zeta-potential and Helmholtz–Smoluchowski velocity, with the assumption of infinitesimally small Debye length. Furthermore, we note that in contrast to the non-monotonic error behavior of the pure hydrodynamic solver in section 2.3, the modeling error of the electrokinetic solver is more like a monotonic function, which reaches a plateau beyond certain time step size.

In order to decouple the error of the SPM–NS solver from the SPM–PB solver, we show in figure 3.19 by the small symbols the velocity results when the exact solution of EDL potential (3.35) is used to calculate the charge density (3.23b) and thus the electrokinetic force. We see that the error dependence is non-monotonic, just as the error behavior from the hydrodynamic solver. However, the optimum time step is much bigger than the one from our previous analysis in section 2.3. An explanation can be put forth by a similar argument as in section 2.3. Smaller time step would have a tighter penalty control and tend to achieve better accuracy. However meanwhile, a smaller time step also leads to a thinner Stokes diffusive layer $\delta = 2.76\sqrt{\nu dt}$ which is induced by the momentum impulse when imposing the rigidity constraint. If this thin Stokes layer fails to be resolved by the SPM

interface $l_e = 2.07\xi$, it will result in a larger error. Similarly, this Stokes layer need to be thicker than the electric diffuse layer which has a characteristic length of λ_d , i.e. $\delta > \lambda_d$. So we conclude that the optimum time step is from the balance of the Stokes diffusive thickness δ and the larger of the two: effective SPM interface thickness $l_e = 2.07\xi$ and Debye length λ_d . Our numerical results confirm this statement by figure 3.19(b), where dt_{λ_d} is the optimum time step expected from $\delta = \lambda_d$ (provided here $l_e < \lambda_d$). In fact, we can define an “effective” thickness of the electric diffuse layer λ_e by matching the numerical optimum time step to the relationship $\delta = \lambda_e$; our numerical data suggest that $\lambda_e = 1.25\lambda_d$ for this particular problem. We note that at such a distance away from the channel wall, the dimensionless potential drops to a value of $\psi_{exact}/\zeta_{exact} = 0.25$ according to equation (3.35).

Furthermore, in figure 3.19 by comparing the results between the the one using the numerical solutions of the SPM–PB solver and the one with the exact potential solution, we find that beyond certain time step size, the coupled electrokinetic solver leads to a cancellation in the errors from SPM–PB and SPM–NS solutions, and thus results in a plateau.

Electrophoretic mobility of a charged infinite cylinder in a transverse or a parallel electric field

Provided the numerical solutions of the electric potential and field for both the EDL and the applied electric field in the presence of a particle, we arrive at a point to validate the SPM electrohydrodynamic solver (3.31) by studying the electrophoretic mobility. The problem of the electrophoresis flow around a charged infinite cylinder is studied, under either a transverse or a parallel electric field.

We use the same computational configuration as in the EDL and the applied field simulations for a cylinder with $a = 11$. The domain $[-176, 176] \times [-176, 176] \times [0, 10]$ is discretized using 1156 nonuniform hexahedral elements and polynomial order $P = 7$. Also, periodicity is imposed in the spanwise z -direction.

We present comparisons with Henry’s exact solution [37] for the electrophoretic velocity ($V_{p,Henry}$) of an cylinder in a transverse field, which was derived from cylindrical Stokes equation with Oseen’s correction. The analytical expressions take as input an arbitrary conductivity ratio σ_p/σ_f and the electric potential solution due to EDL. Here we obtain the “exact” zeta-potential ζ_{exact} from the potential-charge relationship expression in [87], and use the Debye-Hückel approximation (3.37) for the “exact” potential field. It is assumed that the zeta-potential is small and thus linearization of the Poisson-Boltzmann equation is possible. The “exact” solution for the mobility with a parallel orientation is given by Smoluchowski’s formula: $V_{p\parallel} = u_{HS} = E_\infty \epsilon \epsilon_o \zeta \eta$, where small Debye length is assumed $\kappa a \gg 1$. These analytical results are also used as the Dirichlet BC on the boundaries of the computational domain to alleviate the finite-domain effect.

We prescribe the dimensionless charge on the cylinder ($I = 2.06$) with a reduced radius $\kappa a = 11$ and the undistorted external electric field $\mathbf{E}_\infty = (4000V/m, 0, 0)$. For the small ratio of $\sigma_p/\sigma_f = 0.001$, Henry’s solution indicates that $V_{p\perp} = 1.028e - 4$ for a cylinder perpendicularly oriented with the applied field and $V_{p\parallel} = 1.250e - 4$ for the parallel orientation; hence the anisotropy is $V_{p\perp}/V_{p\parallel} = 0.822$. However, if an

identical conductivity is present $\sigma_p/\sigma_f = 1$ and thus the external field is uniform, the transverse mobility and hence the anisotropy drops significantly, i.e. $V_{p\perp} = 6.249e-5$ and $V_{p\perp}/V_{p\parallel} = 0.5$. Note that this anisotropy is exactly the same as that of an infinite cylinder in pure hydrodynamic flow.

Figure 3.20 presents profiles of the streamwise velocity scaled by the Smoluchowski velocity u_{HS} for a cylinder with a perpendicular orientation. All SPM results are using an indicator function of variable ξ_p with $\xi/a = 0.43, c = 2$ in (3.27b). The figure shows that SPM successfully resolves the electrophoretic flow features; it verifies that the mobility decreases with increasing conductivity ratio σ_p/σ_f . An alternative mesh for a smaller domain is used to check the finite-domain effect, i.e. $[-114, 114] \times [-114, 114] \times [0, 10]$ with 1024 elements and 7th polynomial order. A comparison between the circle symbols for the two different simulation domains indicates that the finite-domain effect is small. It is also shown by the two sets of red symbols that including both terms in the electrokinetic force (3.32a) has a better representation of the flow than using a single term (3.32b).

Furthermore, figure 3.20 shows that the volume charge implementation γ_v results in an overshoot of the particle velocity, while the surface charge pattern γ'_s always leads to an undershoot. Since these two charge patterns have been verified to equivalently resolve the cylindrical EDL potential, the difference in the mobility comes from the inadequate resolution of the applied field near the interfaces, which results in an underestimation of the driving electric force for the surface charge.

We also include for comparison in figure 3.20 the numerical results for a pure hydrodynamic motion of a cylinder in a periodic box. The external nonelectric force applied on the cylinder is set to be the same value as the electric force based on the total charge on the cylinder, i.e. $F_x = Q_p E_\infty = 1.015 \times 10^{-13}$ N. A negative uniform pressure gradient is applied on the fluid to ensure the zero net flux out of the domain. The velocity shown is scaled by the particle velocity $V_p = 1.53 \times 10^{-3}$, which is an order of magnitude larger than the typical electrophoretic velocity scale u_{HS} . The

figure also shows that the electrophoretic motion has a much shorter disturbance length in the surrounding fluid, when compared to the pure hydrodynamic motion. This is due to the opposite electric force on the surrounding fluid via the counter-ions, which is termed as the *retardation effect*.

In figure 3.21, the percentage error of the electrophoretic velocity ($\frac{|V_p - V_{p, Henry}|}{V_{p, Henry}} \cdot 100$) is plotted versus the time step size used in the NS solver (3.31). It is again verified by the first two sets of data that including both force components (3.32a) leads to better accuracy. The figure also indicates that increasing the size of the simulation domain leads to a smaller error, as shown by the circle symbols. We note that using the applied field solution $\mathbf{E}_{ext}$ without Galerkin projection causes greater error in the particle velocity for large time steps, which is due to the erroneous discontinuity of $\mathbf{E}_{ext}$ at elemental boundaries near the interfaces.

Furthermore, comparison between the green symbols in figure 3.21 indicates that by increasing the conductivity ratio to $\sigma_p/\sigma_f = 1$ and thus excluding the error from the current density solver, the error is reduced for most time steps, but it is still of a comparable scale. This suggests that the error comes mainly from the PB solver and the NS solver; we recall that the error in the zeta-potential is around 2% for the parameters used. For a larger Debye length $\kappa a = 1$, the error is below 2% for all the time steps involved, as shown by the big squares. This is due to the better accuracy in the PB solution, since the error in the zeta-potential is as small as 0.3%. We also note that the error tends to form a plateau when time step size goes beyond certain value, which is very similar to the error behavior in the electroosmotic flow problem. This again verifies that the coupling of the PB solution with NS solution leads to a cancellation in the modeling error and thus tends to favor larger time steps.

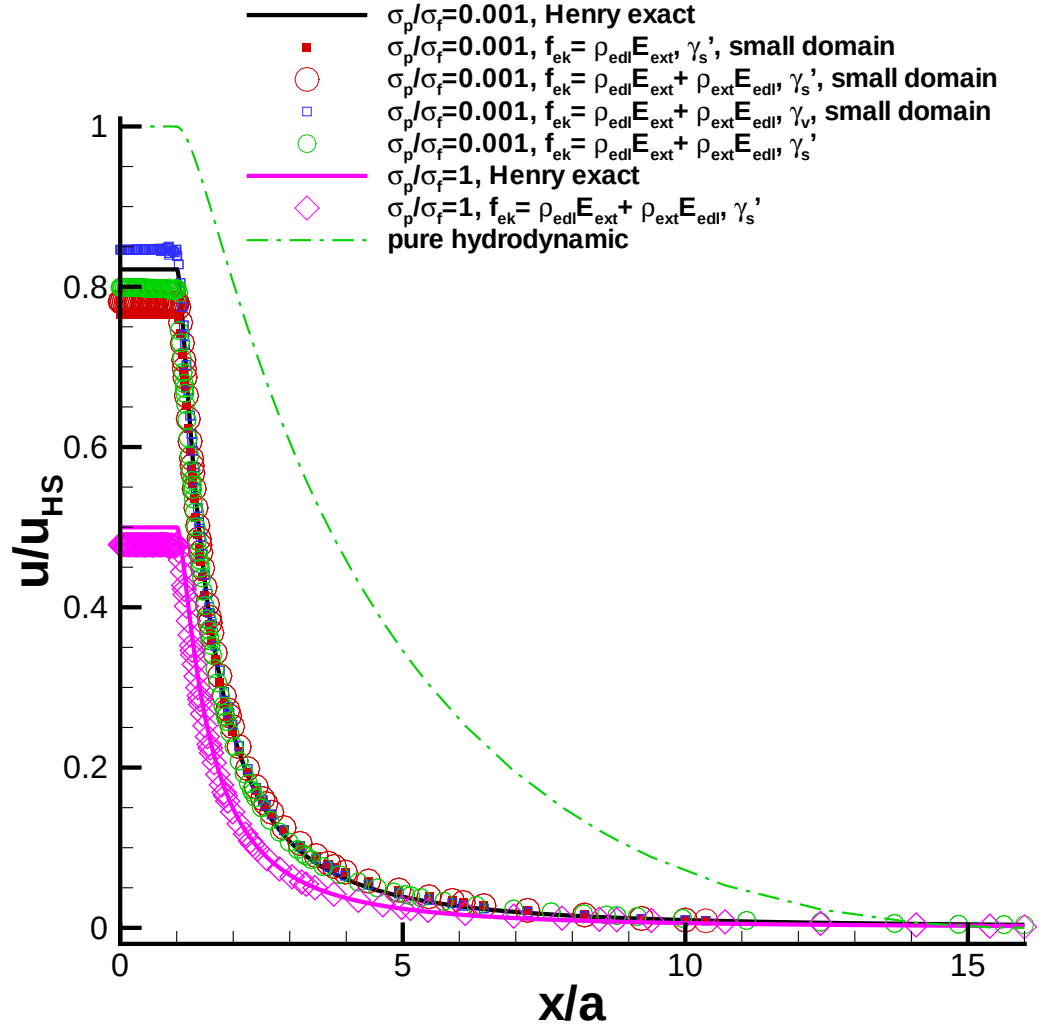


Figure 3.20: *Electrophoresis of an infinite cylinder in a transverse electric field: dimensionless streamwise velocity along streamwise distance, compared to Henry's solution [37], with two different conductivity ratios σ_p/σ_f .*

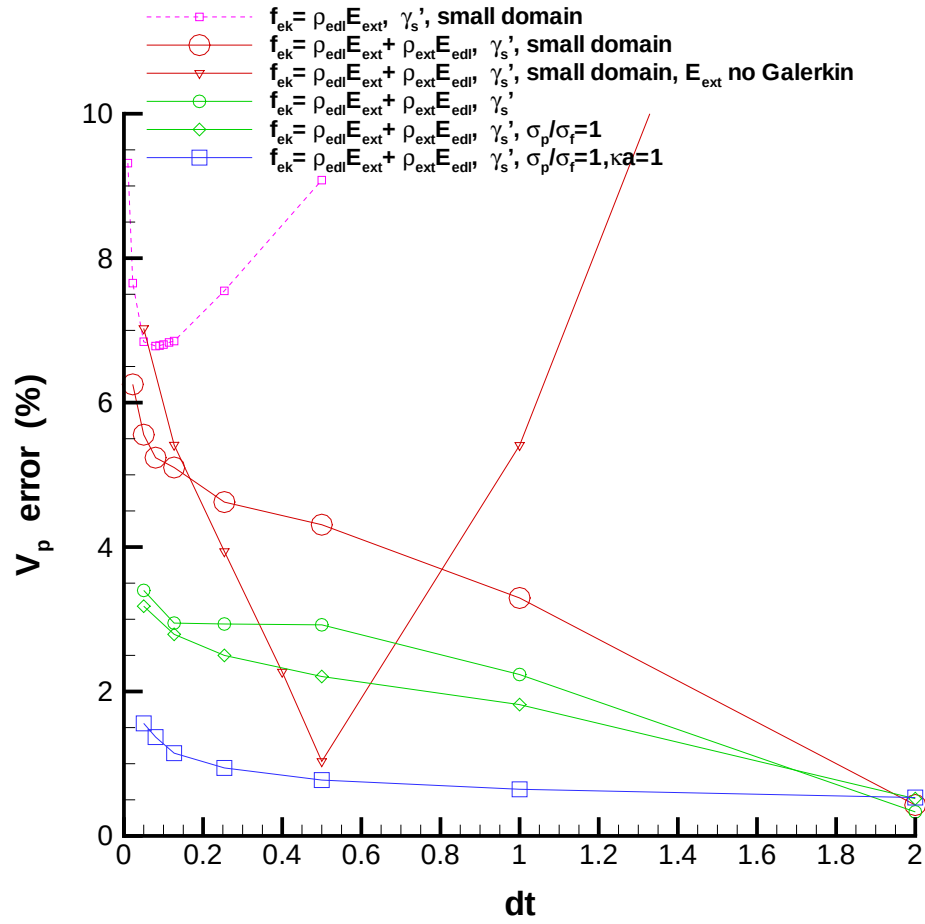


Figure 3.21: *Electrophoresis of an infinite cylinder in a transverse electric field*: percentage error in electrophoretic velocity versus time step, with a variable ξ_p and $\xi/a = 0.43$. If not indicated, $\sigma_p/\sigma_f = 0.001$ and $\kappa a = 11$.

3.5 Simulations

3.5.1 Electrophoretic flows of microtubules

Microtubules have very complex structures. According to the results by an axial projection of the electron-density map [113, 102], a single microtubule can be modeled as 13 protofilaments around a thin cylindrical shell, with an inner radius of $a_i = 8.4 \text{ nm}$ and an outer radius of $a_o = 9.5 \text{ nm}$. Each protofilament is a half-ellipsoid with radius $a_a = 2.3 \text{ nm}$ and $a_b = 3.0 \text{ nm}$. Due to this complexity in geometry, numerical simulations of the electrokinetic flow around microtubules with standard computational methods are challenging. Our SPM electrohydrodynamic solver is a good candidate for such a problem as it removes the difficulty on applying the boundary conditions for complex shapes.

We simulate the electrophoretic flow of an individual microtubule and aim to gain qualitative agreement with the experimental results in [113]. In order to examine how the surface roughness of microtubules affects the EDL, the applied field and thus the electrophoretic motion, we include for comparison the simulation results for a circular cylinder with a similar “effective” radius.

EDL of microtubules

According to [113], the Debye length is around $\lambda_d = 0.7 \text{ nm}$ and the surface charge density is about $e\delta_p = -36.7 \times 10^{-3} \text{ C/m}^2$, corresponding to the dimensionless charge density $I = 1.39$. Thus, we set the corresponding charge density coefficient in equation (3.24) to be $\gamma_s = 1.992$, and γ_v, γ'_s calculated correspondingly with fixed total charge. Note that although it is normally assumed that the microtubules are uniformly surface charged, the real charge distribution is uncertain. Therefore, we will use and examine both uniform surface charge and uniform volume charge patterns in our SPM–PB solver (3.23).

The simulation domain is $[-176, 176] \times [-176, 176] \times [0, 10]$, with periodicity

imposed in all directions. Note that the scaling factor for length is $h = 1 \text{ nm}$ and thus all the length scales in the section are dimensionless. We use 1156 nonuniform hexahedral elements with polynomial order $P = 7$ for spatial discretization with spectral element method. This identical mesh is used to simulate the EDL problem for a microtubule or a cylinder which is aligned with the z-axis. Different shapes are represented by different smooth indicator functions with analytical expressions of the distance to the surface. The interface thickness parameter is set to $\xi/a = 0.02$ for a good representation of the shapes by SPM. For comparisons with a microtubule, the cylinder adopts the same inner radius $a_i = 8.4$ and an outer radius of $a = 11.0$, which is chosen to match the average outer radius of the microtubule $a = a_o + a_b/2$.

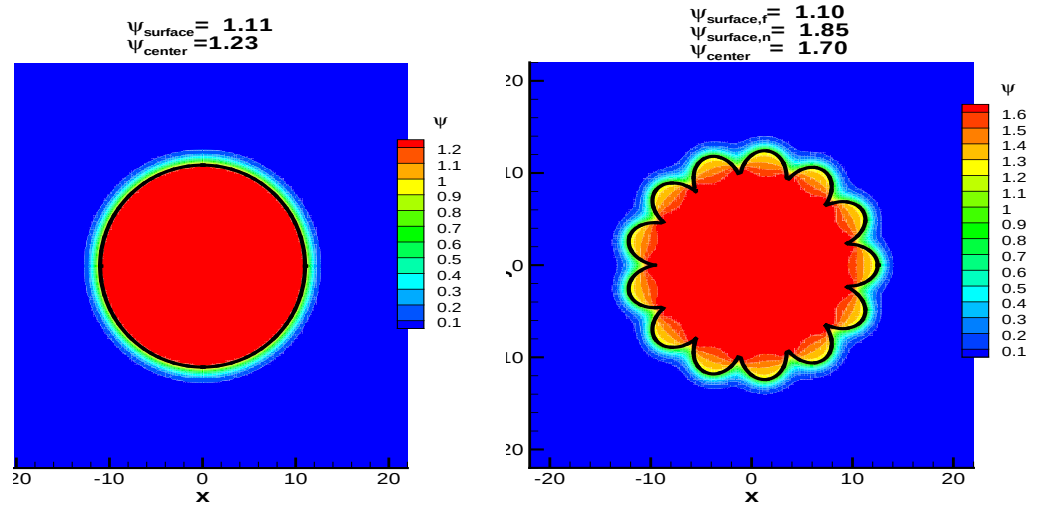


Figure 3.22: *SPM simulations for EDL around a surface charged solid cylinder and a “solid” microtubule: contours of dimensionless electric potential due to electrical double layer, with identical surface charge density. The black curves are showing the particles’ boundaries.*

To study the effect of hollowness in EDL potential variation, we begin with solid cylinders and “solid” microtubules and compare with the hollow structures. In figure 3.22, 3.23 and 3.24 we plot the dimensionless electric potential contours in EDL

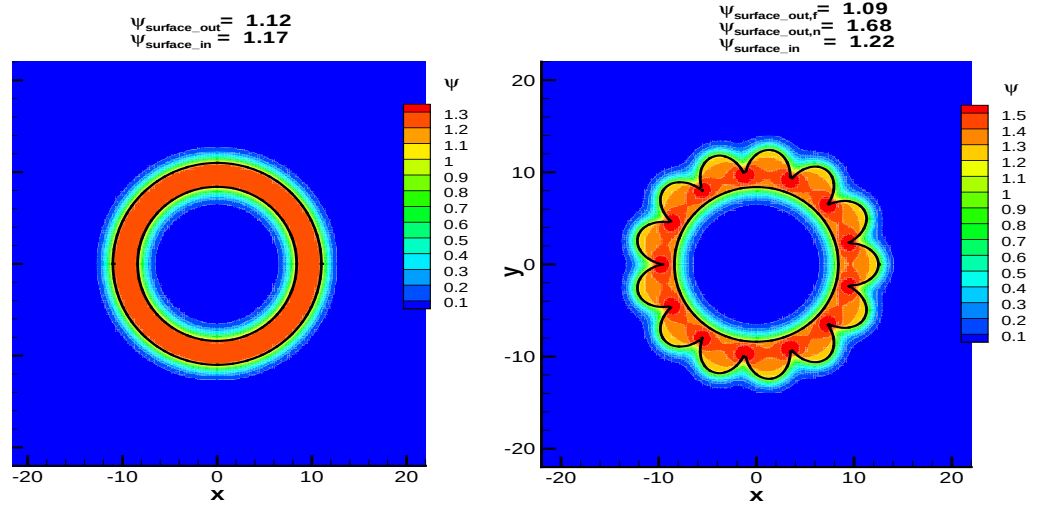


Figure 3.23: *SPM simulations for EDL around for a surface charged hollow cylinder and a hollow microtubule: contours of dimensionless electric potential due to electrical double layer, with the same surface charge density as above.*

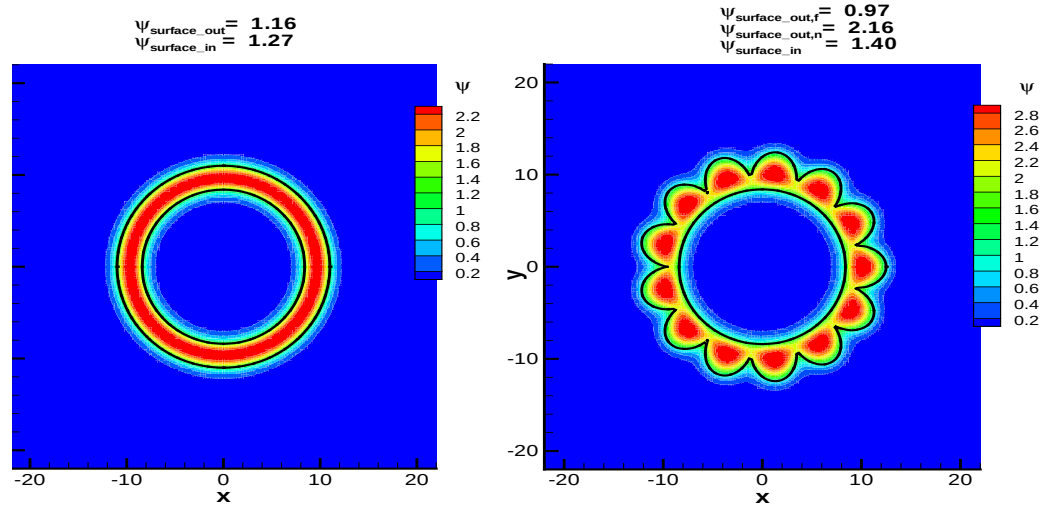


Figure 3.24: *SPM simulations for EDL around a volume charged hollow cylinder and a hollow microtubule: contours of dimensionless electric potential due to electrical double layer, with the same total charge as above.*

around a microtubule with comparisons to a cylinder. We also present the value of the potential for typical spatial points. Here, $\psi_{surface}$ refers to surface points, ψ_{center} to the center, $\psi_{surface_out}$ to the outer surface of cylinder (11, 0, 0), $\psi_{surface_out,f}$ to the furthest outer surface point on microtubule (12.5, 0, 0), $\psi_{surface_out,n}$ to the nearest outer surface point on microtubule (−9.5, 0, 0), and $\psi_{surface_in}$ to the inner surface (8.4, 0, 0). Figure 3.22 and 3.23 show that with surface charges, in contrast to the uniformity of the potential present in a cylindrical particle, the potential on the surface and inside a microtubule has big variations. This is due to the irregularity and asymmetry of the microtubule geometry. Although the surface charge density of a microtubule is assumed to be constant, the charge on the surface near the protofilaments joints is higher than the rest of the surface; the relative difference in the potential between two typical surface points is as high as $\frac{\psi_{surface,out,n} - \psi_{surface,out,f}}{\psi_{surface,out,f}} = 54\%$. It is indicated by figure 3.23 that the hollowness does not influence much the potential distribution outside the cylinder or the microtubule, with a difference less than 10% in the surface potential when compared to the solid structures.

Figure 3.24 indicates that for a hollow cylinder, the charge patterns of either surface or volume distribution have little impact on the electric potential on the surface and outside the particle; the difference in ψ is around 3.6% for the same outer surface point (11, 0, 0), and about 8.5% for the inner surface point (8.4, 0, 0). However, for a microtubule, the resulting differences from the different charge patterns are as large as about 28.6% for the outer surface point (−9.5, 0, 0) and 14.8% for the inner surface. This comes from the asymmetric geometry of the microtubules with undulated outer surfaces. Compared to the findings of [113] which reported the average surface potential to be $32.6mV = 1.27\zeta_e$, the results from our SPM–PB model show qualitative agreements. Note that we use a more accurate model which resolves the potential variations on the surface.

Applied electric field around microtubules

We apply the SPM–current continuity solver (3.29) to solve for the applied external electric field around poorly conducting microtubules in an electrolyte solution. Comparisons are made against the numerical results for an infinitely long hollow circular cylinder with the same conductivity and effective radius. Same simulation domain and spatial discretization are used as for the EDL problem around a microtubule.

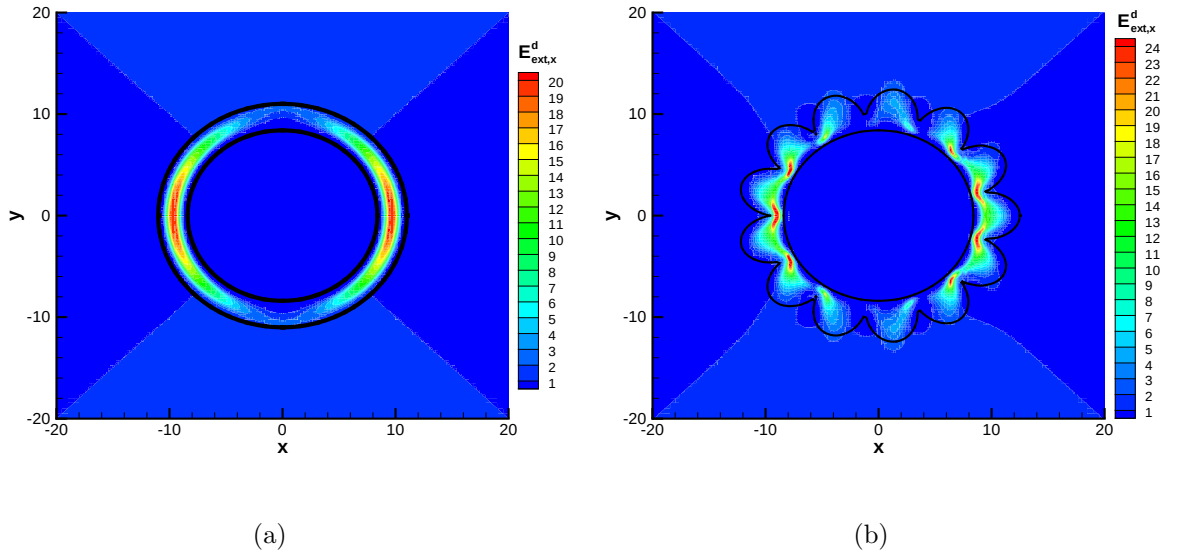


Figure 3.25: *Applied electric field distorted by poorly conductive hollow structures:* comparison of the primary component of the dimensionless applied field $E^d_{ext,x} = E_{ext,x}/E_{\infty,x}$ between a cylinder (a) and a microtubule (b) of infinite spanwise length, with an external electric field of $\mathbf{E}_\infty = (4000, 0, 0)V/m$ and a ratio of $\sigma_p/\sigma_f = 0.001$.

Figure 3.25 shows that the electric field inside a hollow cylinder is much stronger than that inside a solid structure, which is $E^d_{ext,x} = E_{ext,x}/E_\infty = 2$ by the analytical solution (3.39b). A microtubule has a similar magnitude in the electric field as a hollow cylinder, but the field is distorted to a much greater extent due to the undulated surface geometry, as shown in figure 3.25(b). In particular we note that the resulting field for a microtubule loses its symmetry in x–direction as expected from the asymmetric geometry; this suggests that the problem is orientational dependent.

In figure 3.26, we examine the charge density variations due to the accumulation of charges on the interfaces with conductivity jumps. It is shown that the surface charges have been smeared into the particles by our SPM representation. Also, the complex geometry of the microtubule leads to a more complicated distribution of the charges, which needs to be sufficiently resolved by the spatial discretization.

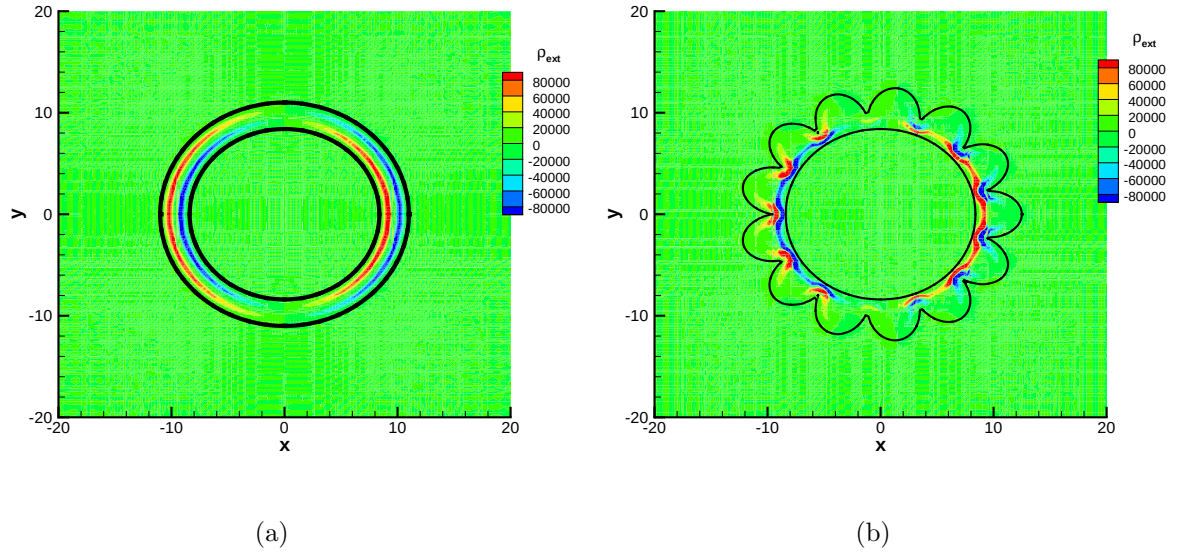


Figure 3.26: *Charge distribution due to the distorted applied electric field around poorly conductive hollow structures: comparison between a cylinder (a) and a microtubule (b) of infinite spanwise length, with an external electric field of $\mathbf{E}_{\infty} = (4000, 0, 0)V/m$ and a ratio of $\sigma_p/\sigma_f = 0.001$.*

Electrophoretic flows of microtubules

We apply the electrohydrodynamic solver (3.31) to study the electrophoretic motion of cylinders and microtubules, which are oriented either parallel or perpendicular to the external applied field. Typical numerical results of the electrophoretic velocity and anisotropy for various particles are listed in table 3.1. Comparisons are made against the exact solution for an infinite solid cylinder by [37]. The same reference surface charge density $I = 1.39$ is used for all the particles listed, so the hollow particles have more total charge due to the extra charge on the inner surface. In all the simulations, we use volume charge pattern to alleviate the effects of the numerical error in the applied field near the undulated surfaces; γ_v is calculated correspondingly from the particular total charge according to equation (3.25). Also, the ratio of the electrical conductivity is prescribed as $\sigma_p/\sigma_f = 0.001$.

Table 3.2: *Electrophoretic velocity and anisotropy*: different particles with same surface charge density. $V_{p\parallel}$ refers to particle velocity with parallel orientation with respect to the applied field, and $V_{p\perp}$ refers to perpendicular orientation.

	$V_{p\parallel}$	$V_{p\perp}$	<i>anisotropy</i>
exact , solid cyl, infinite	1.038e-4	8.936e-5	0.861
solid cyl, infinite	9.860e-5	8.391e-5	0.851
hollow cyl, infinite	1.009e-4	8.109e-5	0.804
microtubule, infinite	1.135e-4	8.964e-5	0.790
microtubule, finite L/a=4	8.132e-5	5.961e-5	0.731
microtubule, finite L/a=8	8.784e-5	6.790e-5	0.773

It is shown by table 3.2 that the electrophoretic velocity of an infinite cylinder with transverse or parallel external field is resolved qualitatively, with errors of 5.0% and 6.1% respectively. A hollow cylinder has a larger parallel mobility than a solid cylinder, which might come from the higher charge and hence larger electric force on the cylinder. In contrast, the transverse mobility of a hollow cylinder is smaller than the solid one, which may result from the oppositely charged fluid confined inside the cylinder. We also see that the mobilities of a microtubule are significantly larger than the ones for a hollow cylinder, which is again due to the higher net charge and hence

larger electric driving force on the microtubule. The anisotropy $V_{p\perp}/V_{p\parallel} = 0.790$ of a microtubule is in agreement with the value 0.83 reported in experiments of [113]. Furthermore, the table indicates that by reducing the length of the microtubule to a small value $L/a = 4$, the mobility and also the anisotropy drops significantly. Note that a different computational domain is used for finite microtubules, i.e. $[-88, 88] \times [-88, 88] \times [-165, 165]$ with a number of 10816 nonuniform rectilinear elements.

We plot in figure 3.27 the contours of the primary electrophoretic velocity (i.e., the component which is parallel to the applied field $\mathbf{E}_\infty$) in a cross-section of an infinitely long microtubule. We see that with a parallel orientation, the microtubule moves in the direction of the applied field, while the fluid inside has an opposite flow direction which is similar to standard electroosmosis in stationary channels. Also, the disturbance introduced into the fluid outside the microtubule is limited within a very short distance away from the outer surface. In contrast, for the perpendicular configuration as shown in 3.27(b), the inner fluid moves with the microtubule and the disturbance distance outside is significantly larger. Figure 3.27(b) shows that a nonuniform velocity exist inside near the joints of the protofilaments, which could be problematic, as we expect that the inner fluid is fully confined and thus should move strictly together with the microtubule. This might come from the high charge density in the solution near the protofilaments joints and the resulting large electric force that affects the local fluid momentum.

Figure 3.28 and 3.29 show the electrophoretic motion of a microtubule with a short spanwise length $L/a = 4$. It is indicated that compared to the infinite microtubules, such a limited spanwise dimension leads to a significant decrease in the mobilities. However, the finite structures disturb the surrounding fluid to a greater extent, e.g. an inverse flow is present outside the microtubule as shown in figure 3.28(a). Also for the perpendicular orientation in figure 3.28(b), the non-uniformity of the inner fluid velocity is alleviated; this is due to the fact that the fluid inside is not fully confined anymore because of the open-ends. Figure 3.29 further confirms

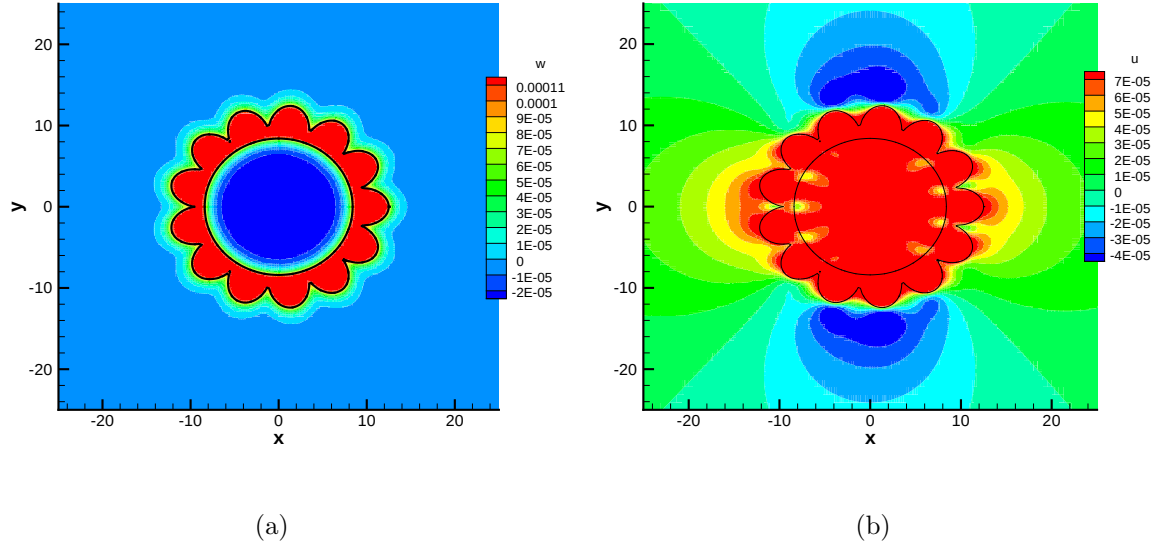


Figure 3.27: *Electrophoresis of an infinitely long microtubule with either axial or perpendicular orientations:* velocity contour in the cross-section $z = 0$, with an external electric field of $\mathbf{E}_\infty = (0, 0, 4000) \text{ V/m}$ (a) and $\mathbf{E}_\infty = (4000, 0, 0) \text{ V/m}$ (b).

these statements by showing a different angle of view, i.e. there exists large variations of the velocity near the free ends, and the outer fluid is influenced greatly by the finite dimension effects.

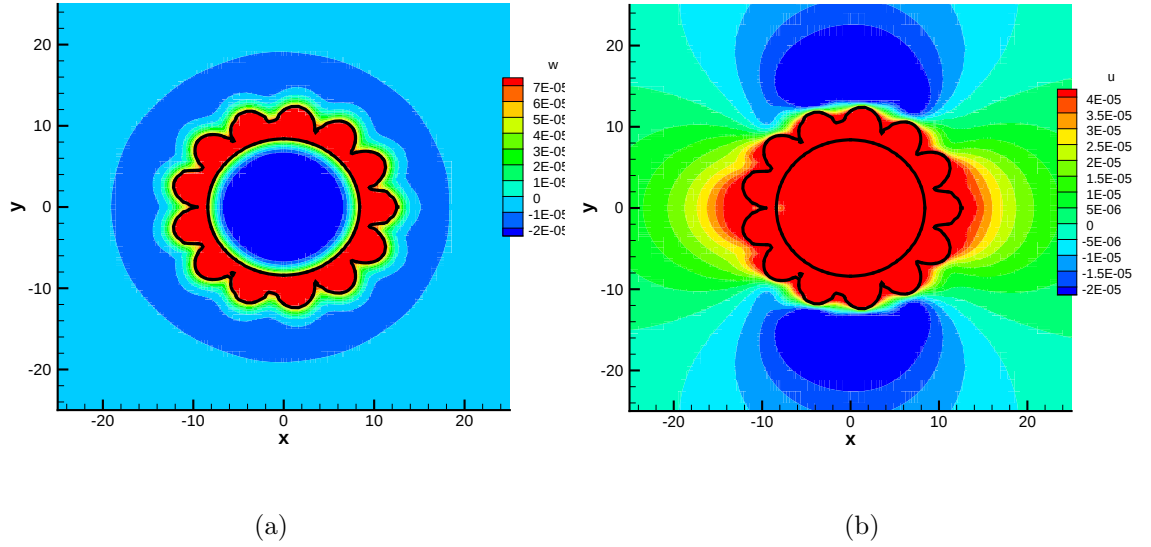


Figure 3.28: *Electrophoresis of a microtubule of length $L/a = 4$ with either axial or perpendicular orientations: velocity contour in the cross-section $z = 0$, with an external electric field of $\mathbf{E}_\infty = (0, 0, 4000)V/m$ (a) and $\mathbf{E}_\infty = (4000, 0, 0)V/m$ (b).*

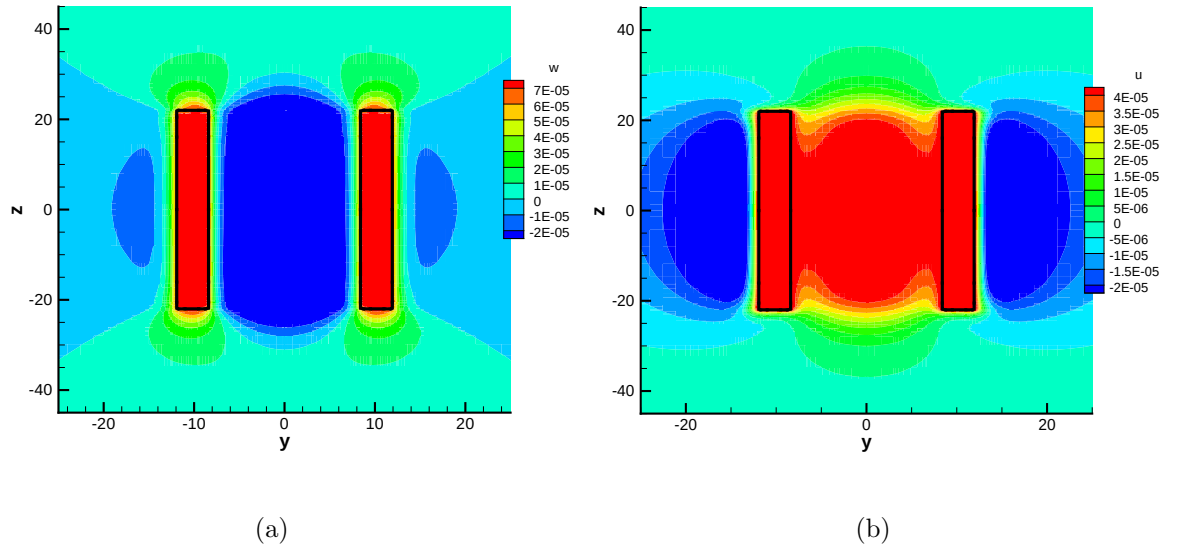


Figure 3.29: *Electrophoresis of a microtubule of length $L/a = 4$ with either axial or perpendicular orientations: velocity contour in the axial plane $x = 0$, with an external electric field of $\mathbf{E}_\infty = (0, 0, 4000)V/m$ (a) and $\mathbf{E}_\infty = (4000, 0, 0)V/m$ (b).*

3.5.2 Micromixers with heterogeneously charged channel walls

Heterogeneously charged surfaces can be used to control the flow direction or to change the interface wetting property, which have many important applications in microfluidics, such as micromixing enhancement [83, 6, 115] and microchip switch [105, 20]. In this section, we present preliminary simulation results for electrokinetic flows inside a heterogeneously charged microchannel. We investigate how the heterogeneous surface charge would influence the electric potential distribution, the corresponding flow pattern, and thus introduce effective mixing.

Figure 3.30(a) shows the geometry of the problem with a heterogeneously charged microchannel. Each wall is charged with uniform charge density, but with positive charges on one half and negative charges on the other half. The channel is periodic in both x-direction and z-direction. The external electric field is uniform and parallel to the channel wall, i.e. $\mathbf{E}_{ext} = (4000, 0, 0)V/m$. We prescribe the channel width as $2h = 6 \mu m$, the Debye length $\kappa h = 0.1$, dimensionless charge $I = 0.206$, and all other physical parameters are the same as in the problem of EOF in a straight channel. We use 480 rectilinear elements and 7th polynomial order to discretize the computational domain of $[-3, 3] \times [-3.6, 3.6] \times [-3, 3]$.

Figure 3.30(a) shows that the electric potential has sharp variations near the joint point of the two oppositely charged electrodes. For comparison, we also include the numerical results of the direct boundary method for PB equation (3.20), where the zeta-potential are prescribed on the channel walls. The potential profiles in figure 3.30(b) indicate that compared to the DNS results with constant zeta-potentials, the SPM solutions with prescribed uniform surface charges results in larger potential variation in x-direction, which may suggest better mixing efficiency.

Figure 3.31 shows typical streamlines and also pressure contours in a 2D plane $z = 0$. We see that four vortices are induced and they are strongly interacting with each other. Large variation in the pressure are created across the channel, due to the change in the local flow directions. This flow pattern would result in efficient mixing

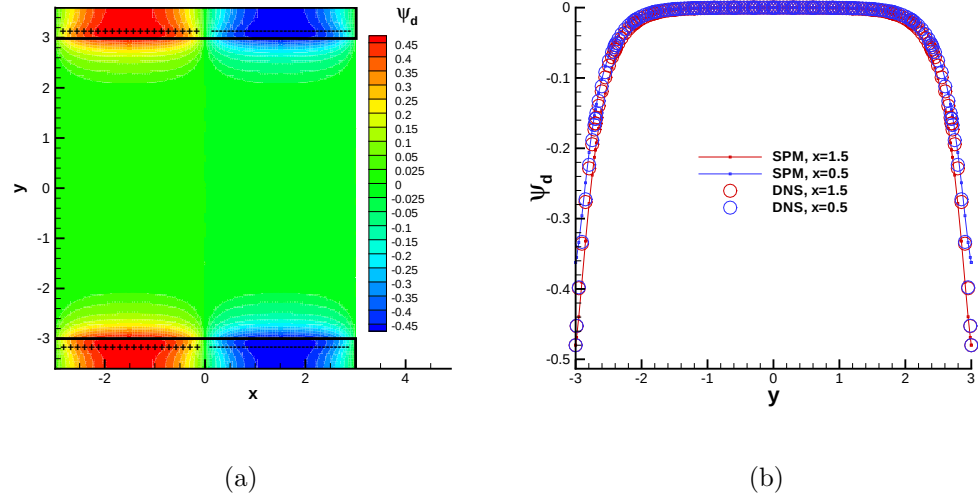


Figure 3.30: *EDL in a heterogeneously charged microchannel*: the dimensionless electric potential ψ_d , 2D contour (a) and profiles across the channel compared to DNS results (b).

if a multi-component complex fluid is utilized. We note that there are nontrivial pressure variations inside the plates which could be erroneous, but the resulting velocity is much smaller (100 times) in magnitude than the maximum velocity in the channel. Furthermore, the figure indicates certain circulation immediately near the walls (e.g. $x \sim 3, y \sim 3$). This is a result of the SPM modeling using a fixed charge density. In the region very near the joints of the two electrodes, the ions in the solvent are under the influences of both electrodes, so the net charge density is much lower than elsewhere away from the joints region but with the same interwall distance. Since the electric force is very small there, certain circulation zones are induced. But we note that the magnitude of the velocity there is very small compared to the major circulation velocities.

Figure 3.31(b) shows that a larger external electric field $E_\infty = 8000$ results in greater variation in the pressure. Also in figure 3.32, the velocity field is shown to increase almost linearly with the external field, which is due to the small Reynolds number involved ($Re \sim 10^{-8}$).

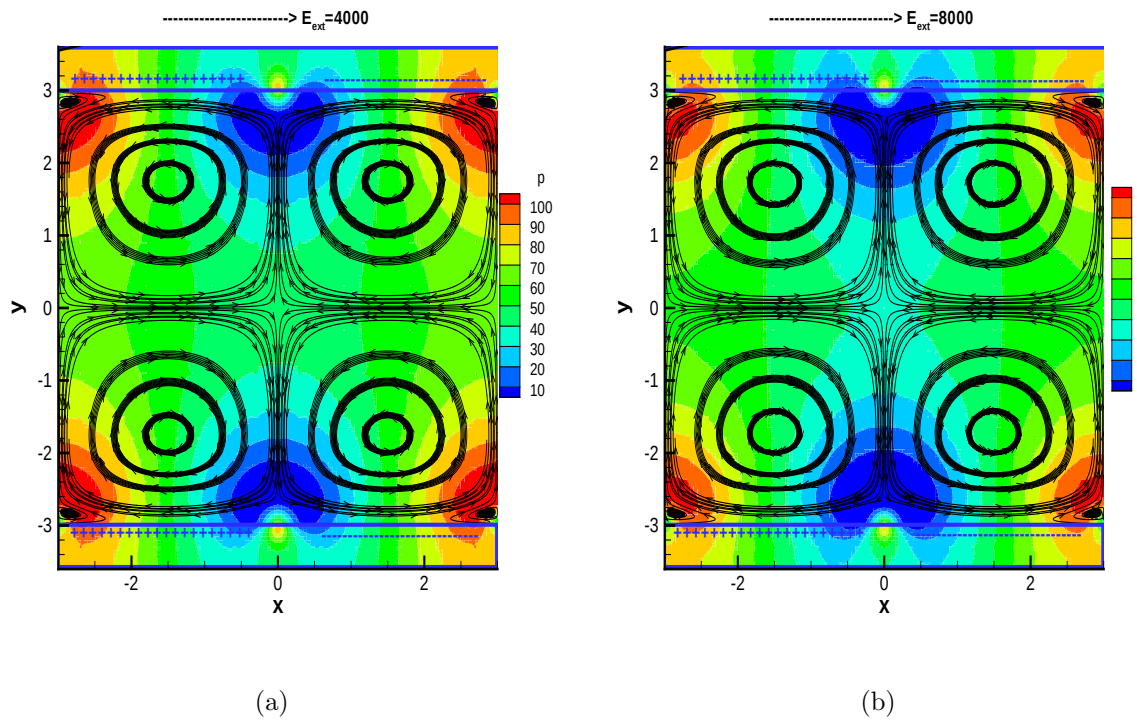


Figure 3.31: A heterogeneously charged microchannel with a uniform external electric field: streamlines and pressure contour shown in a 2D plane $z = 0$, with two different external field strength $E_{\infty,x} = 4000$ (a) and $E_{\infty,x} = 8000$ (b).

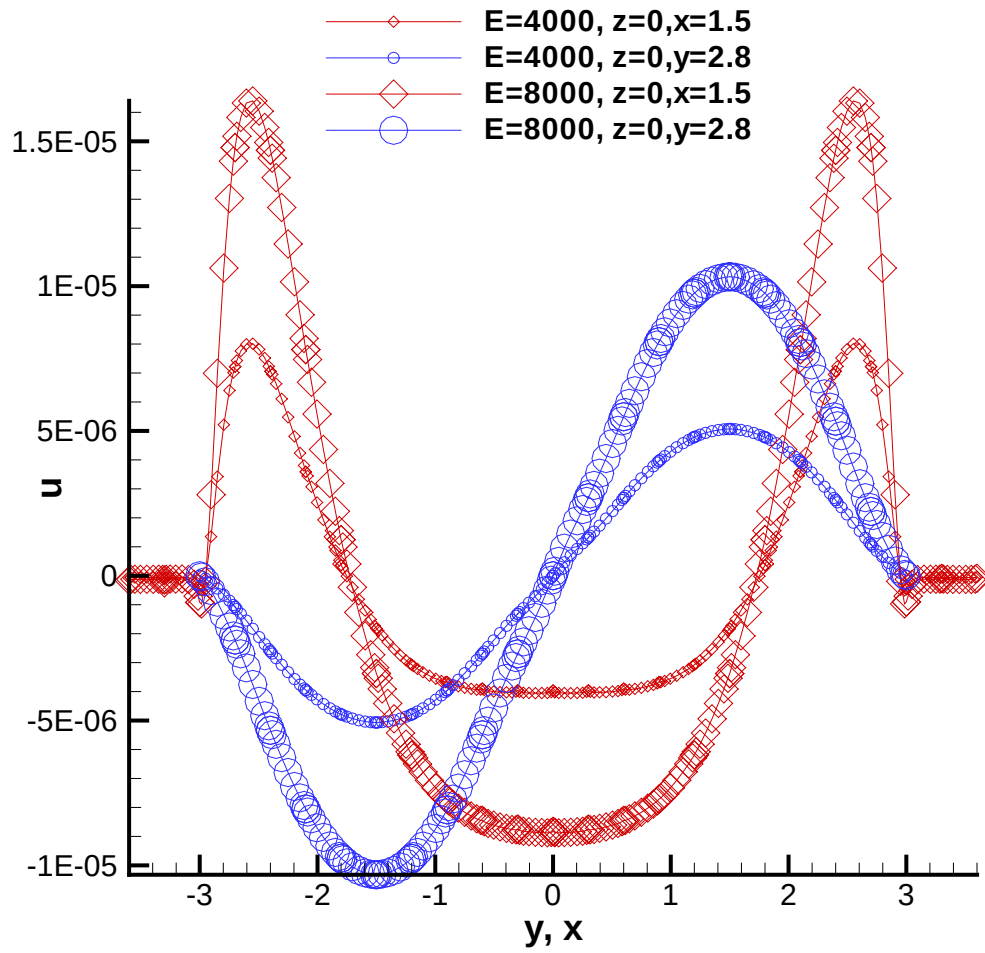


Figure 3.32: A heterogeneously charged microchannel with a uniform external electric field: comparison of velocity profiles, with two different external field strength $E_{\infty,x} = 4000$ and $E_{\infty,x} = 8000$.

3.6 Concluding remarks

In this chapter, we have developed a modeling method for electrokinetic flows where particles with arbitrary electrical conductivity are present. We modified the Poisson–Boltzmann (PB) and electric charge continuity equations based on a *smoothed profile* technique, to account for the entire domain including the particles. These equations were solved numerically in conjunction with the modified incompressible Navier–Stokes equations, to include the electrokinetic forces.

We verified the method by benchmark problems of electroosmotic flows in straight channels and the electrophoresis of charged cylinders. The modeling error of the coupled electrokinetic solver was quantified, and it showed a significant difference from the error behavior of the pure hydrodynamic solver. By excluding the error from the PB solution, we showed that the modeling error is nonmonotonic; the optimum time step comes from a balance between the thickness of the Stokes diffusive layer and the one of the electrical diffuse layer, i.e. $\delta = 2.76\sqrt{\nu dt} \sim \lambda_d$.

As the direct boundary conditions at particle/solution interfaces are removed, the proposed method is advantageous for simulating electrokinetic flows with moving complex-shaped particles which are charged. Simulation results for the electrophoresis of charged microtubules were presented and the simulated electrophoretic mobility and anisotropy agreed with the experimental results. We also showed the capability of the method to study the enhanced mixing inside a heterogeneously charged channel.

We note that further improvement can be made to the proposed modeling method. Since one limitation comes from the current continuity solver, a better approach can be used to solve for the “discontinuous” electric field, such as a discontinuous Galerkin formulation or a spectral filtering method. Another limitation is due to the assumptions made in deriving the PB and current continuity equations. It is assumed that the charge distribution is instantaneously derivable or in equilibrium state, i.e. ionic advection is negligible. A more accurate model would be using the

Nernst–Planck equation (3.4) for ionic transport instead of the hypothesized Boltzmann distribution. A possible way to effectively solve the Poisson–Nernst–Planck equations (3.2) and (3.6) would be to rewrite them to account for the entire domain by using a smooth approximation of the diffusivity D_i . However, since the transport processes of all the species are influenced by each other, the governing equations are coupled together, and thus pose a great challenge to numerical modeling.

Chapter 4

Engineering Applications

4.1 Introduction

Engineering flows, e.g. turbomachinery, are characterized by complex geometries, probably moving domains and complex flow physics. The flow past a cylinder represents a simplified problem of a complex engineering flow. There have been several efforts via direct numerical simulations to study the two- and three-dimensional wake structure behind a circular cylinder with a low to moderate Reynolds number [35, 51, 110, 36], and the recent developments in large-scale computations enables fast and reliable simulation results for this problem. From our stand point, we pose the following question: is an immersed-boundary type method, as SPM, capable of resolving the complicated flow structures at moderately high Reynolds number flows? We note that there are very few reported results on simulations of flows with $Re > 200$ using a boundary-less method where the exact boundary conditions are avoided. This is due to the inaccuracy in resolving the near field motion by using approximate boundary treatments instead of the exact conditions. To this end, we want to examine the accuracy of SPM in simulating moderate Reynolds number flows, for both two- and three-dimensional wake patterns, and to cover both stationary and moving boundary problems.

In addition, we are interested in the applicability of SPM to important engineering flow problems, such as waterjet propulsion systems [1, 91]. Standard numerical methods are greatly challenged for such problems as propellers in free-space and impellers in ducts. In contrast, SPM has potentially a great advantage in simulating such problems with 3D complex moving domains, as it avoids the direct boundary conditions imposed at the interfaces.

4.2 Moderate Reynolds number flow past a circular cylinder

Although in previous work SPM has been applied only to zero and low Reynolds number flow problems ($Re < 20$), extensions to moderate and high Reynolds number flows are feasible. For higher Reynolds number flow, both the Stokes layer thickness ($\delta \sim 2.76\sqrt{\nu\Delta t}$) and the boundary layer thickness ($\delta_{bl} \sim x/\sqrt{Re}$) become thinner. For best modeling accuracy, we need to choose a time step close to the optimum size $(\Delta t)_o$ which balances the effective interface thickness ($l_e = 2.07\xi$) and the Stokes layer thickness (δ), i.e., $l_e = \delta$ as stated in section 2.3. In addition, we need to make sure that the smooth interface adequately resolves the boundary layer (i.e., $l_e < \delta_{bl}$), which is *usually* automatically satisfied in our simulations if the optimum time step $(\Delta t)_o$ is used and it is below the CFL limit.

Next, we examine the accuracy of SPM for moderate Reynolds number flow problems by simulating both two-dimensional and three-dimensional circular cylinder flows.

4.2.1 Two-dimensional flow

We apply SPM to simulate two-dimensional cylinder flow at Reynolds number up to 1000. Comparisons are made against the DNS results using the same simulation domain and boundary conditions. The domain is $[-15, 25] \times [-9, 9] \times [0, 1]$ with

a circular cylinder of radius $r = 0.5$ fixed at origin. Periodicity is imposed in z -direction with a single layer of elements used, so the flow is in fact two-dimensional. We impose Dirichlet boundary condition (BC) at the inlet $x = -15$ by prescribing a uniform velocity $\mathbf{u}_{in} = (1.0, 0.0, 0.0)$; the outlet at $x = 25$ is given as a Neumann type BC with $\partial/\partial n = 0$. Periodicity is also imposed in the y -direction. In SPM simulation, we employ 888 hexahedral elements with polynomial order up to 7. In contrast, DNS simulation uses a two-dimensional mesh with 412 triangle elements and up to 13th polynomial order. Figure 4.1 shows a comparison between the two meshes.

Table 4.1: *Two-dimensional flow past a cylinder with $Re=100\sim 1000$* : the Strouhal number St , drag force F_x , lift force F_y , mean drag coefficient C_D , and percentage errors compared to Henderson's results [35].

	St	error %	$F_{x,max}$	$F_{x,min}$	$F_{y,max}$	C_D	error %
<i>Henderson [35] (Re=100)</i>	0.1662					1.350	
DNS (Re=100)	0.1700	2.29	0.697	0.687	0.172	1.384	2.52
SPM (Re=100, $\xi=0.009$)	0.1698	2.17	0.706	0.695	0.176	1.401	3.77
SPM (Re=100, $\xi=0.005$)	0.1692	1.81	0.700	0.690	0.174	1.390	2.93
<i>Henderson [35] (Re=200)</i>	0.1967					1.341	
DNS (Re=200)	0.2004	1.90	0.665	0.712	0.354	1.377	2.65
SPM (Re=200, $\xi=0.009$)	0.1985	0.90	0.674	0.721	0.373	1.395	4.00
<i>Henderson [35] (Re=500)</i>	0.2251					1.445	
DNS (Re=500)	0.2279	1.23	0.796	0.656	0.594	1.452	2.02
SPM (Re=500, $\xi=0.005$)	0.2255	0.16	0.821	0.674	0.611	1.495	3.47
<i>Henderson [35] (Re=1000)</i>	0.2370					1.509	
DNS (Re=1000)	0.2406	1.53	0.895	0.648	0.749	1.544	2.28
SPM (Re=1000, $\xi=0.005$)	0.2417	1.98	0.914	0.665	0.761	1.580	4.67

After convergence to the steady state, we calculate typical average quantities, such as the Strouhal number St and the mean drag coefficient C_D . We compare our numerical results with the following data-fit expressions of Henderson [35], which were found to be very accurate for Reynolds number up to 1000.

$$C_D = 1.4114 - 0.2668Re^{0.1648}\exp(-3.375e^{-3}Re) + 2.5818/Re^{0.4369}, \quad (4.1a)$$

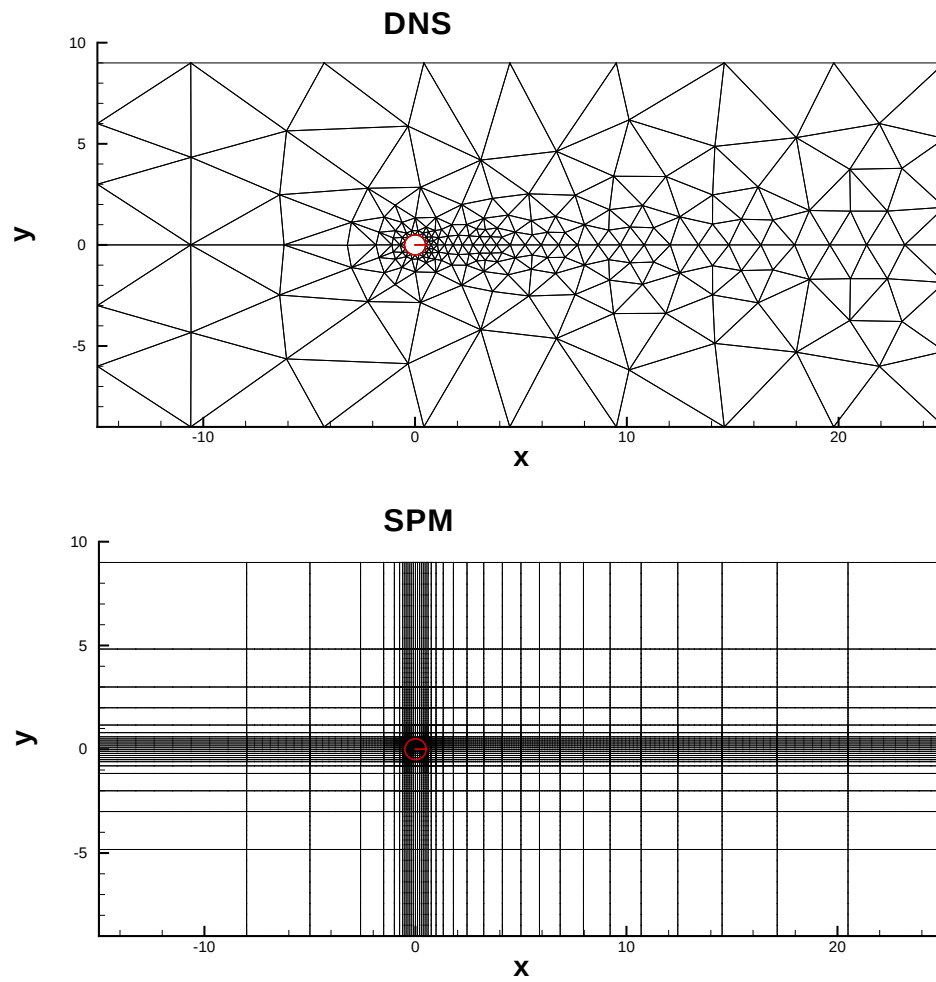


Figure 4.1: *Two-dimensional flow past a cylinder*: elemental mesh shown for both DNS and SPM simulations.

$$S_t = 0.2417 - 0.8328Re^{-0.4808} \exp(-0.001859Re). \quad (4.1b)$$

In table 4.1 we list the computed quantities from SPM simulations, with comparisons to both DNS results. The errors are calculated by using the expressions (4.1). Note that for $Re = 1000$, we use a larger computational domain as $[-10, 40] \times [-9, 9]$ for both DNS and SPM simulations, as the smaller domain leads to a numerical instability due to the shorter outflow region. DNS employs 2382 triangle elements and polynomial order $P = 9$, while SPM uses 912 hexahedral elements and $P = 7$.

Table 4.1 shows that SPM obtains very accurate Strouhal number, when compared to Henderson's results. The relative difference is within 2.2% for all the Reynolds number included. The error in the drag coefficient is relatively larger, but it is indicated that a smaller SPM interface thickness ξ would improve the results. Furthermore, when compared to DNS results, SPM reveals good agreement, with differences smaller than 0.5% in Strouhal number and 2.5% in drag coefficient. This stands for a more fair comparison, considering the effects from the finite domain and the boundary conditions imposed.

We also compare SPM simulation results with the experimental results of Hammache et al. [32] and obtain a good agreement. The relative error in the Strouhal number is about 1.9% and 0.9%, for $Re = 100$ and 150 respectively.

Next, we examine the numerical accuracy in a pointwise manner. We present the velocity profiles averaged over several Strouhal periods at different locations in figure 4.2, 4.3 and 4.4. Excellent agreement between SPM and DNS results are indicated, except for the discrepancy in streamwise velocity near the outlet. This is due to the outflow boundary condition and different spatial resolution in the outflow region.

Furthermore the velocity profiles at Reynolds number $Re = 500$ are shown in figure 4.5. Again SPM shows very good agreement with the DNS results in the near field. But there exists considerable difference in the velocity results near the outflow region, which is a result of the erroneous outflow boundary condition we impose. To alleviate this boundary effect, a larger domain is required for more accurate solutions.

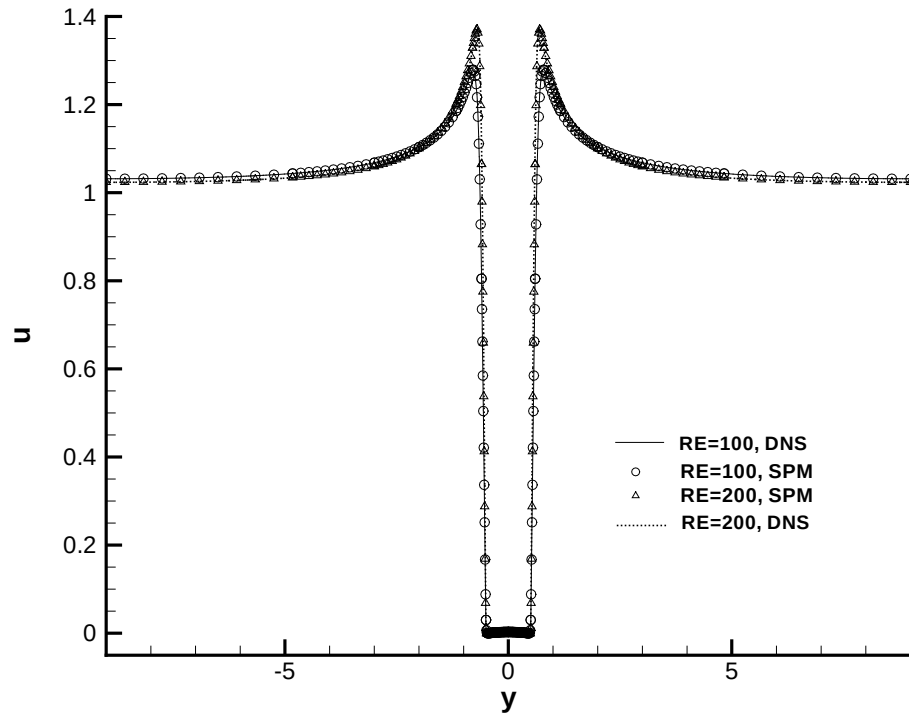


Figure 4.2: *Two-dimensional flow past a cylinder at Reynolds number 100 and 200: comparison of SPM and DNS simulation results of streamwise velocity (u) versus the cross-section distance (y) at $x = 0$.*

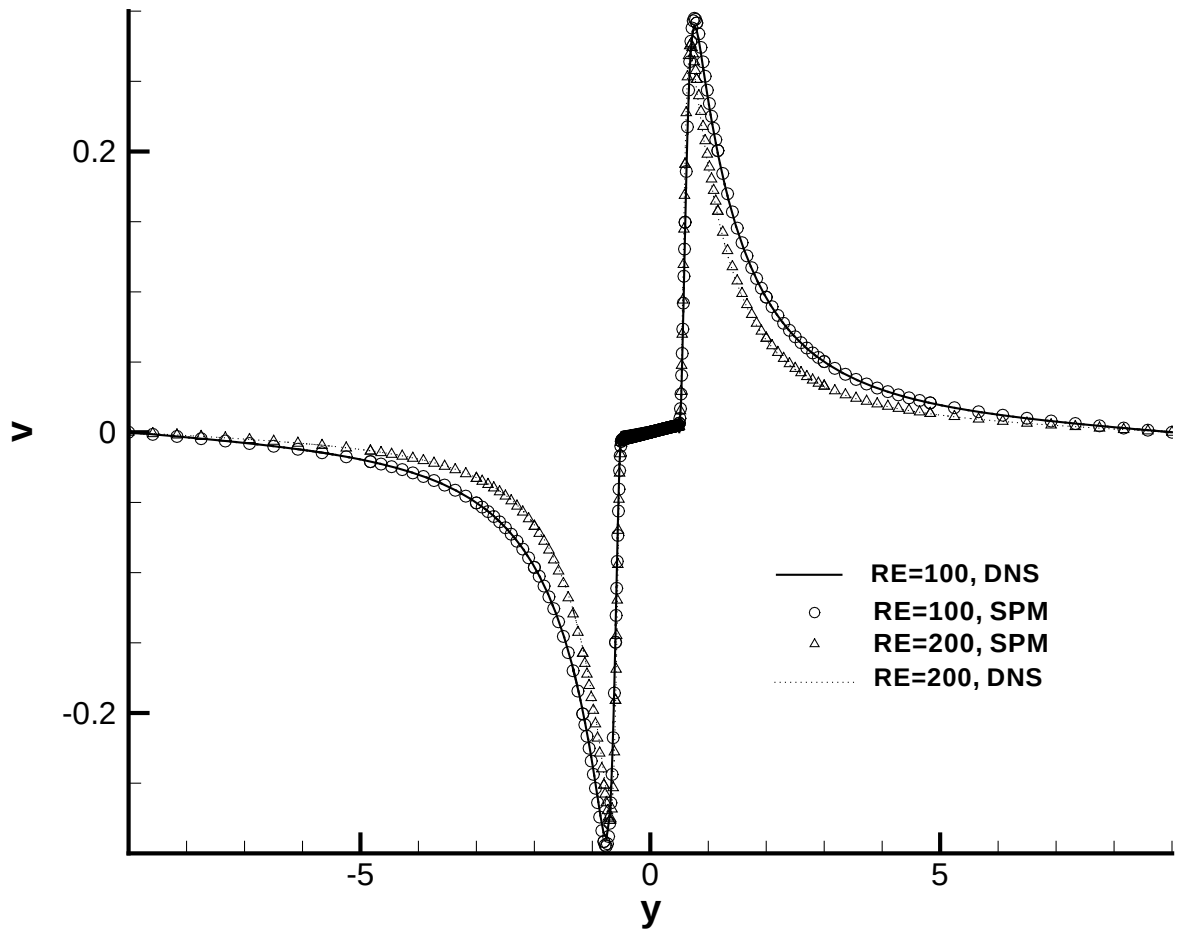


Figure 4.3: *Two-dimensional flow past a cylinder at Reynolds number 100 and 200: crossflow velocity (v) versus the cross-section distance (y) at $x = 0$.*

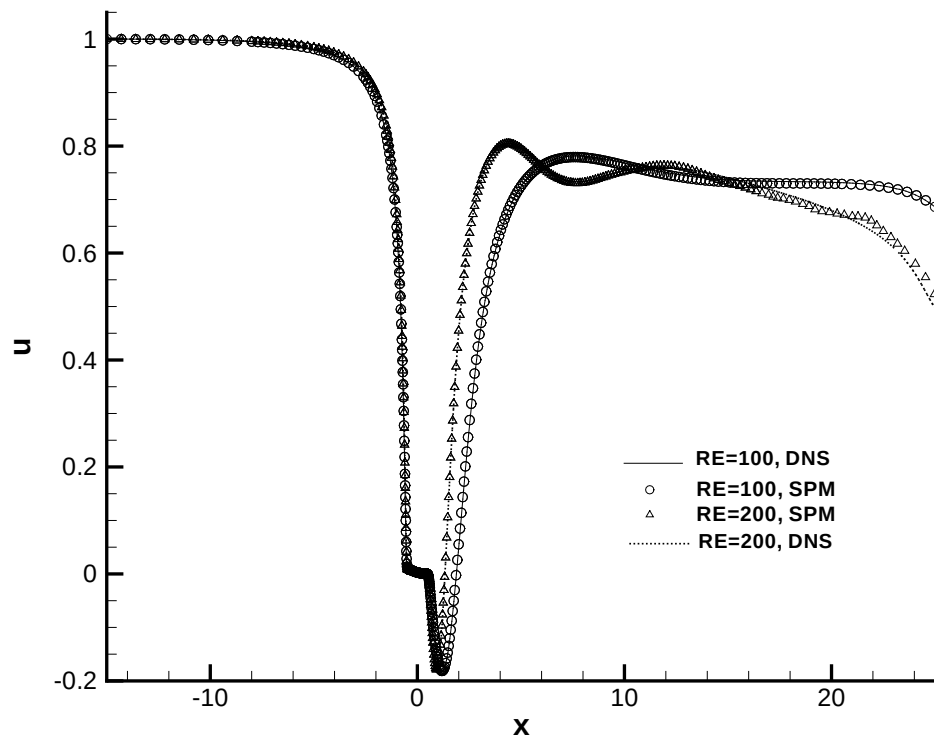


Figure 4.4: *Two-dimensional flow past a cylinder at Reynolds number 100 and 200: streamwise velocity (u) versus the downstream distance (x) at $y = 0$.*

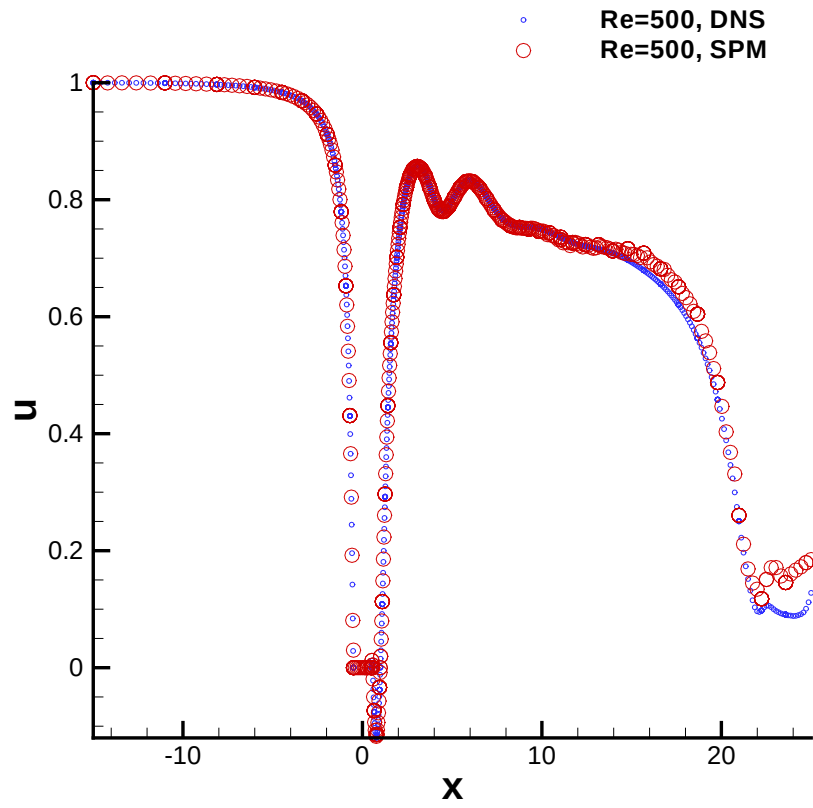


Figure 4.5: *Two-dimensional flow past a cylinder at Reynolds number 500: stream-wise velocity (u) versus the downstream distance (x) at $y = 0$.*

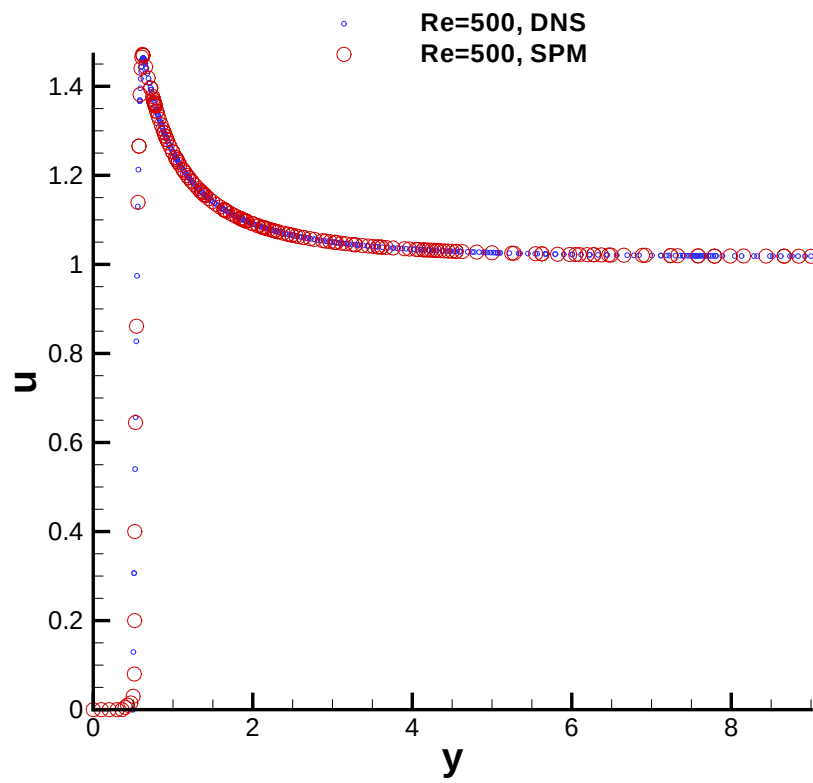


Figure 4.6: *Two-dimensional flow past a cylinder at Reynolds number 500*: stream-wise velocity (u) versus the cross-section distance (y) at $x = 0$. Only half of the domain is shown due to symmetry.

4.2.2 Three-dimensional flow

Three-dimensional instabilities in the wake of a circular cylinder have been observed both in experiments and in numerical simulations. At a Reynolds number of around 190, the two-dimensional periodic vortex shedding undergoes a transition to three-dimensionality, which was observed by [99] through irregularities in the wake velocity fluctuations. Williamson demonstrated by experiments [118, 119] that the wake transition regime involves two modes of three-dimensional instability, modes 'A' and 'B', dominant over different Reynolds number ranges. These two modes are quite distinct in spanwise lengthscale and in symmetry, and they are found to scale on different physical features of the flow.

When the wake first becomes three-dimensional, at $Re \sim 190$ [119, 36], mode A vortex shedding appears. This is characterized by regular streamwise vortices appearing in the wake, with a spanwise wavelength of approximately $\lambda \sim 4D$. In the transition region of $Re = 230 \sim 260$, mode B starts to appear, consisting of a more irregular array of streamwise vortices with a shorter spanwise wavelength (about $\lambda \sim D$). In this range both modes coexist, and at larger $Re > 260$, mode B structures contain more energy. At each of these transitions, there occurs a discontinuity in the Strouhal–Reynolds number curve.

There have been many direct numerical simulations to study the *three-dimensionalities* in the wake of a cylinder [51, 110, 36]. Here, we investigate if SPM is capable of resolving the complicated three-dimensional wake structures, despite the fact that it discards the exact boundary conditions and results in great computational efficiency for complex moving domain problems.

The computational domain is $[-15, 25] \times [-9, 9]$ in constant- z planes; we investigate the effect of using different spanwise dimensions following the numerical procedures of [36]. We study the critical Reynolds number of $Re = 265$ corresponding to the bifurcation to mode B instabilities. SPM employs a spatial discretization of 3552 hexahedral elements for $L_z = 3.288$ and 1776 elements for $L_z = 0.822$;

the polynomial order is set to 5. To subject the flow to three-dimensionalities in our SPM simulation, we introduce an initial disturbance in spanwise direction by starting from a two-dimensional higher Reynolds number flow ($Re=500$) and using a small spanwise perturbation force for the first few hundreds of time steps. We check the evolution of the instability by examining the velocity and pressure histories of several near wake points.

For comparison, we include the simulation results for the same domain using $2\frac{1}{2}D$ DNS, i.e. spectral element discretization with a two-dimensional mesh in constant- z plane and a Fourier spectral method for spanwise direction. DNS simulation uses 2084 quadrature elements with $P = 4$ for each Fourier plane; in spanwise direction it uses 64 Fourier modes for $L_z = 3.288$ and 32 modes for $L_z = 0.822$. The elemental meshes for both DNS and SPM simulations are demonstrated in figure 4.7.

First, we consider perturbations to the wake near the short-wavelength instability threshold, where the spanwise dimension of the simulation domain is set to be the same as the critical mode B wavelength, $L_z = \lambda'_2 = 0.822D$ for $Re = 265$ [36]. Figures 4.8 and 4.9 show spatial pattern formation in the streamwise and crossflow velocity field. They indicate that the 3D instability results in only a slight distortion of the two-dimensional flow, and the amplitude of this distortion decays rapidly with distance downstream. The converged flow is time-periodic and the spatial pattern is stationary. This flow pattern shows qualitative similarities with experimental observations of mode B instability, but this “pure” state is not realistic because the wake is absolutely unstable to mode A for this Reynolds number. In our simulations, it is due to the restricted size of the domain that mode A does not appear. We also note that the simulation results from SPM and DNS show very similar flow patterns for the same spanwise length.

Next, we simulate the three-dimensional flow system with spanwise dimension four times the critical mode B wavelength, $L_z = 4\lambda'_2 = 3.288D$. Figures 4.10 and 4.11 indicate that Mode B appears in the near wake, i.e. there exists a small-scale

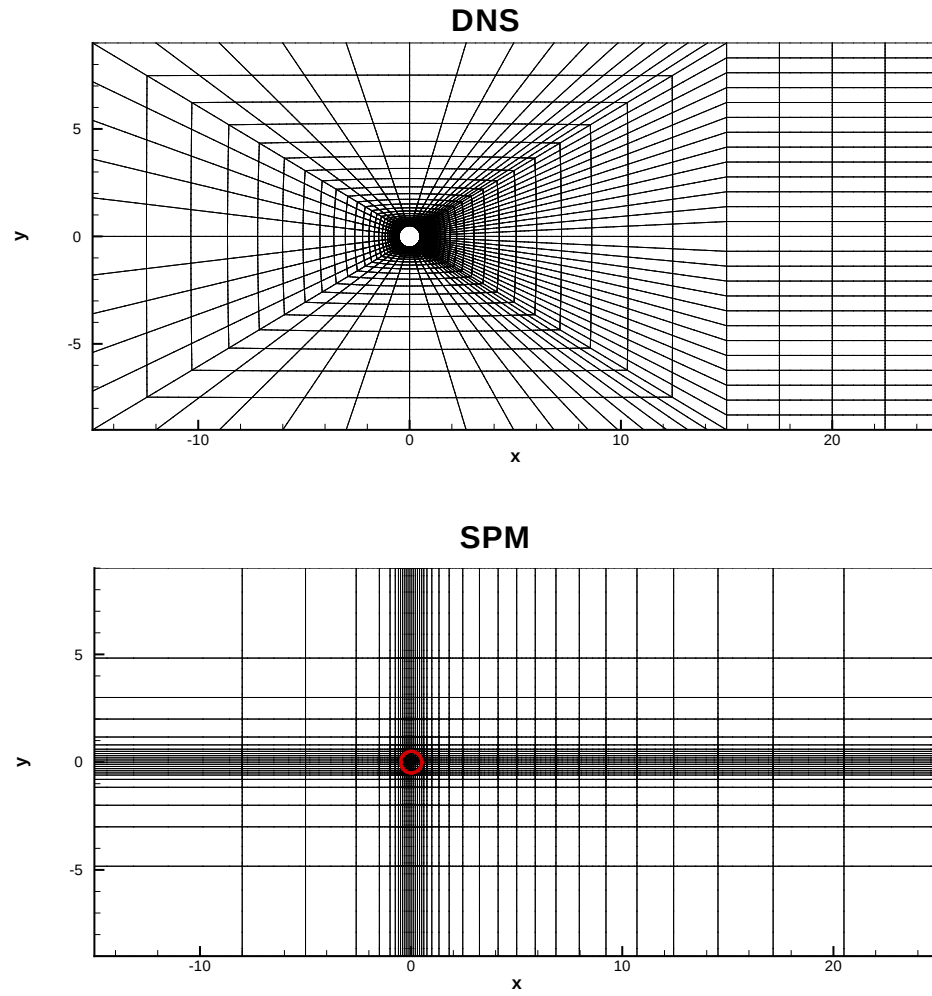


Figure 4.7: *Three-dimensional flow past a cylinder*: elemental mesh for both DNS and SPM simulations. Red circle indicates the cylinder surface in SPM ($\phi = 0.5$).

pattern superimposed over the larger-scale mode A pattern. The asymptotic state is a mixture of both instability modes with the amplitude of mode B decaying quickly with downstream distance. These two figures are shown at the same spanwise scale as in figures 4.8 and 4.9 to emphasize the relationship between the long- and short-wavelength instabilities.

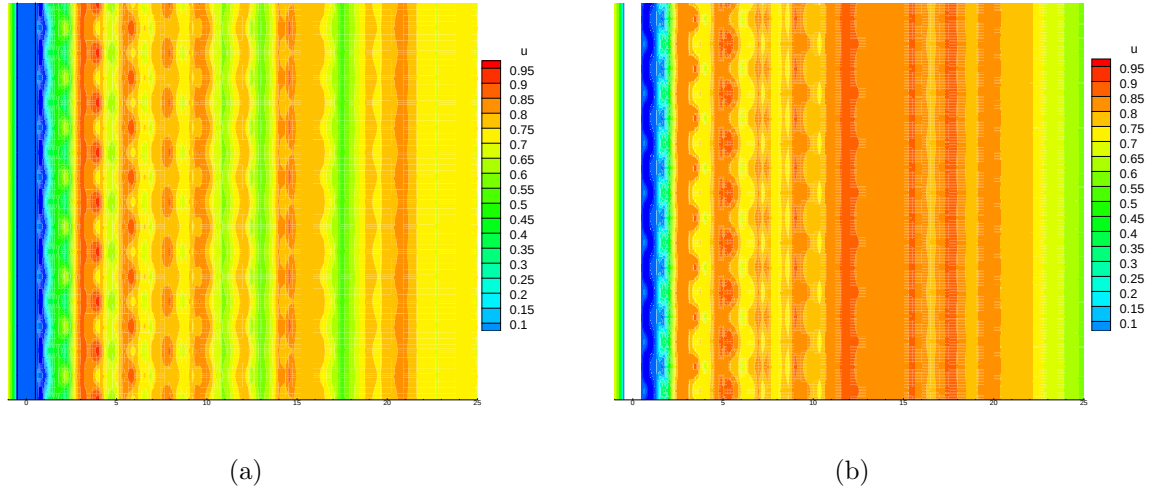


Figure 4.8: *Three-dimensional flow past a cylinder at Reynolds number 265 and spanwise domain length $L_z = \lambda'_2$: contours of streamwise velocity u in the plane $y = 0$, SPM results (a) versus DNS results (b). The cylinder surface ($\phi = 0.5$ in SPM) is indicated by vertical black lines. The image plane is $x=(-1,25)$ and $z=(0,6.576)$. The asymptotic state reveals a *mode B*.*

Since the three-dimensional flow structures calculated by SPM and DNS reveal great similarity, we further examine the numerical accuracy by the averaged quantities of 3D vortex shedding. Table 4.2 presents the simulated results of the Strouhal number St , the mean drag coefficient C_D and the lift force amplitude $|F_y| = F_{y,max} - F_{y,min}$ for the aforementioned three dimensional flow patterns. Compared to Henderson's full 3D DNS results with $L_z = 16\lambda'_2$ [36], both the SPM and DNS overestimate the mean drag force, which is mainly due to the effects of limited

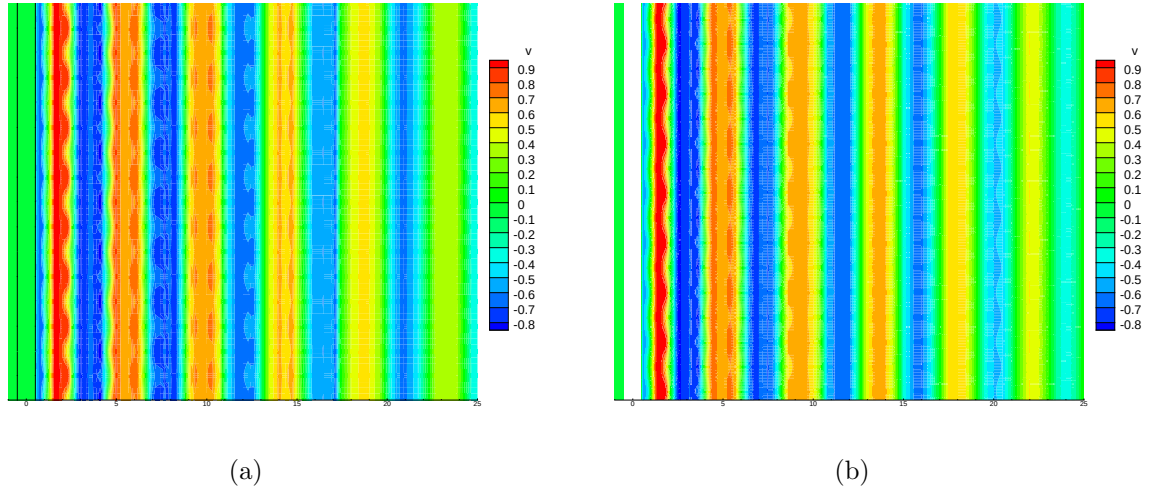


Figure 4.9: *Three-dimensional flow past a cylinder at Reynolds number 265 and spanwise domain length $L_z = \lambda'_2$: contours of crossflow velocity v in the plane $y = 0$, SPM results (a) versus DNS results (b). The cylinder surface ($\phi = 0.5$ in SPM) is indicated by vertical black lines. The image plane is $x=(-1,25)$ and $z=(0,6.576)$. The asymptotic state reveals a *mode B instability*.*

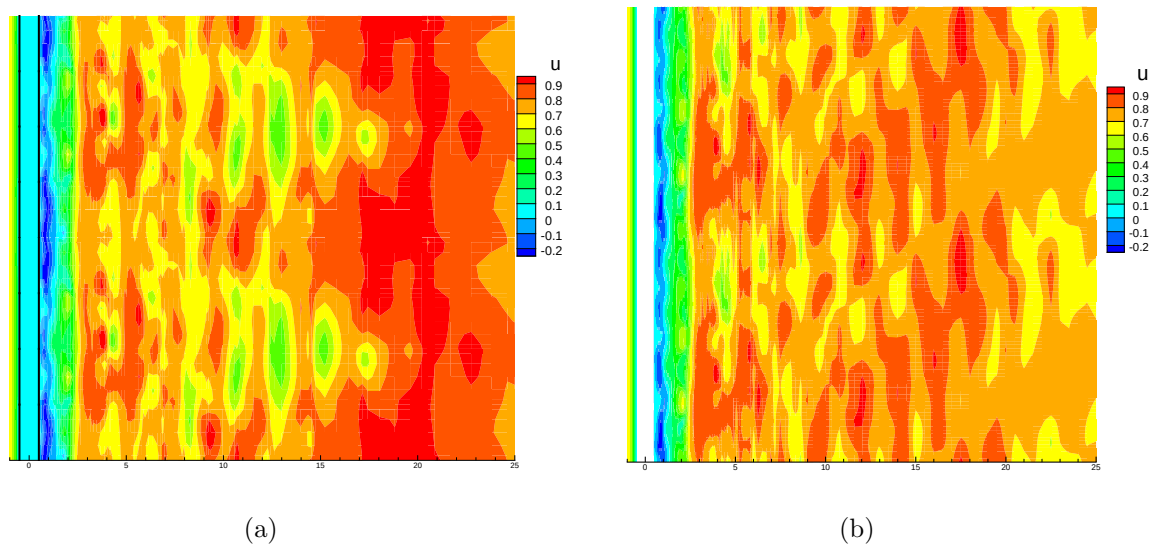


Figure 4.10: *Three-dimensional flow past a cylinder at Reynolds number 265 and spanwise domain length $L_z = 4\lambda'_2$: contours of streamwise velocity u in the plane $y = 0$, SPM results (a) versus DNS results (b). The cylinder surface in SPM ($\phi = 0.5$) is indicated by vertical black lines. The image plane is $x=(-1,25)$ and $z=(0,6.576)$. The asymptotic state corresponds to a *mixture of both mode A and mode B*.*

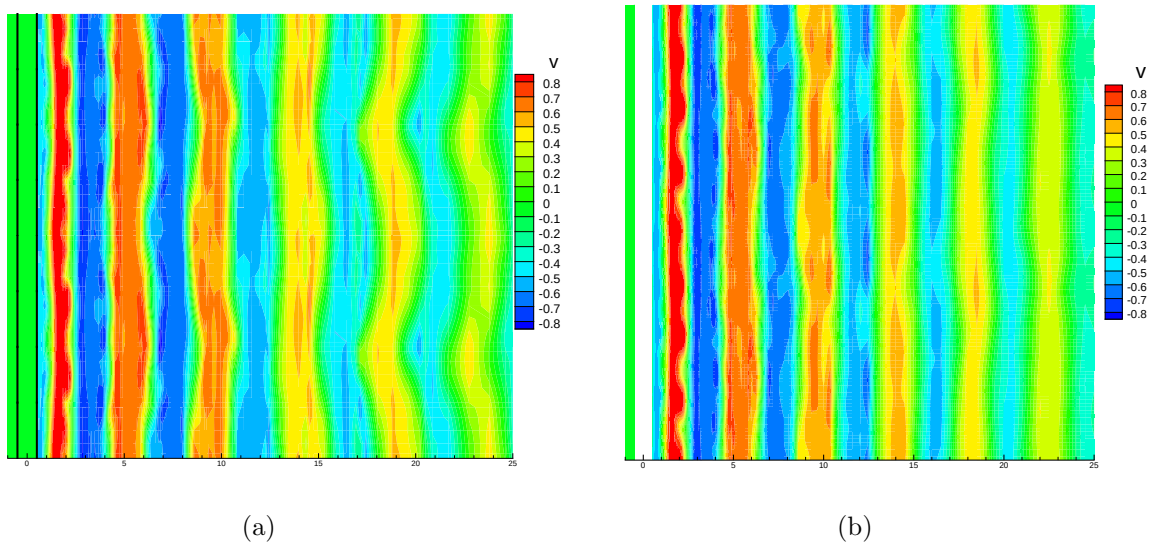


Figure 4.11: *Three-dimensional flow past a cylinder at Reynolds number 265 and spanwise domain length $L_z = 4\lambda'_2$: contours of crossflow velocity v in the plane $y = 0$, SPM results (a) versus DNS results (b). The cylinder surface in SPM ($\phi = 0.5$) is indicated by vertical black lines. The image plane is $x=(-1,25)$ and $z=(0,6.576)$. The asymptotic state corresponds to a *mixture of both mode A and mode B*.*

Table 4.2: *Three-dimensional flow past a cylinder at Reynolds number 265*: Strouhal number St , mean drag coefficient C_D and lift force amplitude $|F_y| = F_{y,max} - F_{y,min}$, with percentage differences indicating comparisons between SPM and DNS results, e.g. $\frac{|St_{SPM} - St_{DNS}|}{St_{DNS}} \cdot 100$.

	St	C_D	$ F_y $	St diff%	C_D diff%	$ F_y $ diff%
[36] ($Re=265$, $L_z = 16\lambda'_2$)	0.205	1.21				
DNS ($Re=265$, $L_z = \lambda'_2$)	0.209	1.378	0.805			
SPM ($Re=265$, $L_z = \lambda'_2$)	0.205	1.427	0.818	2.33	3.52	1.61
DNS ($Re=265$, $L_z = 4\lambda'_2$)	0.208	1.328	0.672			
SPM ($Re=265$, $L_z = 4\lambda'_2$)	0.204	1.369	0.679	1.93	3.05	1.11

domain sizes; Henderson showed that large L_z results in chaotic behavior characterized by irregular large-scale structures in the wake. However, the table shows good agreement (with a maximum difference of 3.5%) between the SPM and DNS results if the same computational domain is used.

4.3 Vortex induced vibrations

A cylinder in cross flow exhibits oscillations with large amplitude if the natural frequency of cylinder vibration is close to the vortex-shedding frequency of the stationary cylinder. The cylinder then sheds vortices at the natural frequency, which is called *lock-in*. The locked-in region plotted in an amplitude-versus-frequency bifurcation diagram is similar to the Arnold tongues or resonance horns. The interaction of two cylinders occurs in diverse applications, including piles of offshore risers, heat exchangers and suspension bridges. It is shown both experimentally and numerically [74, 90] that Arnold tongues also exist in two-cylinder systems, but the shape may be sensitive to the phase angle between the two cylinders and it may suggest the existence of holes in the Arnold tongues.

SPM is advantageous in simulating VIV flows, as a simple stationary computation mesh can be used. We apply SPM to study the fundamental problem concerning the sensitive region in the Arnold tongues, by simulating coupled oscillators which are subject to resonant excitation. In particular, we present comparisons with the numerical results from an arbitrary Lagrangian Eulerian (ALE) formulation associated with a hybrid moving mesh [90]. Specifically, we consider two cylinders of diameter $D = 1$ in tandem arrangement with a center-to-center spacing $2.5D$. The two cylinders oscillate in transverse direction with the same amplitude (A) and frequency (f_e), i.e. $Y_p(t) = A \cos(2\pi f_e t + \pi/2)$. The Reynolds number is $Re = 160$ based on the free-stream velocity $u_\infty = 1$ and the diameter D .

The computational domain we use for SPM simulations is $[-15, 25] \times [-9, 9] \times [0, 1]$, with periodicity imposed in the z -direction to study the two-dimensional problem. A total of 1440 hexahedral elements with $P = 5$ are used for spectral element discretizations. The two cylinders are represented in SPM by an indicator function (2.1), with $\xi = 0.0085$. We note that the ALE results are obtained by using a two-dimensional moving mesh with 1748 triangle elements and $P = 6$ for a slightly larger domain. The elemental meshes for the two different methods are shown in figure 4.12

for comparison.

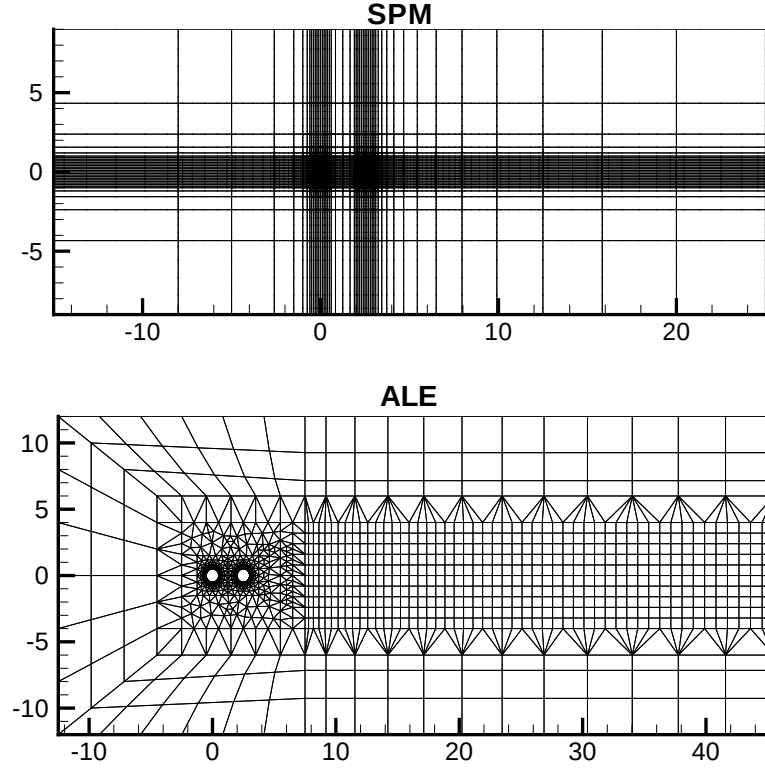


Figure 4.12: *Two-dimensional flow past two oscillating cylinders*: elemental mesh shown for both ALE and SPM simulations, with the red circles representing the cylinders surfaces in SPM ($\phi = 0.5$).

We prescribe the oscillation amplitude $A/D = 0.35$ and examine different excitation frequencies f_e . For each run, we check the flow development by the time history of velocity components for a few downstream points. After convergence to a steady state, we plot the phase portrait based on the two velocity components (u, v) of each history point. We note that the shedding frequency for two stationary cylinders with the same separation is $f_0 = 0.128$, so we investigate the excitation frequency in the region of $f_e = 0.12 \sim 0.22$.

Figures 4.13, 4.14 and 4.15 show the phase portraits of several history points

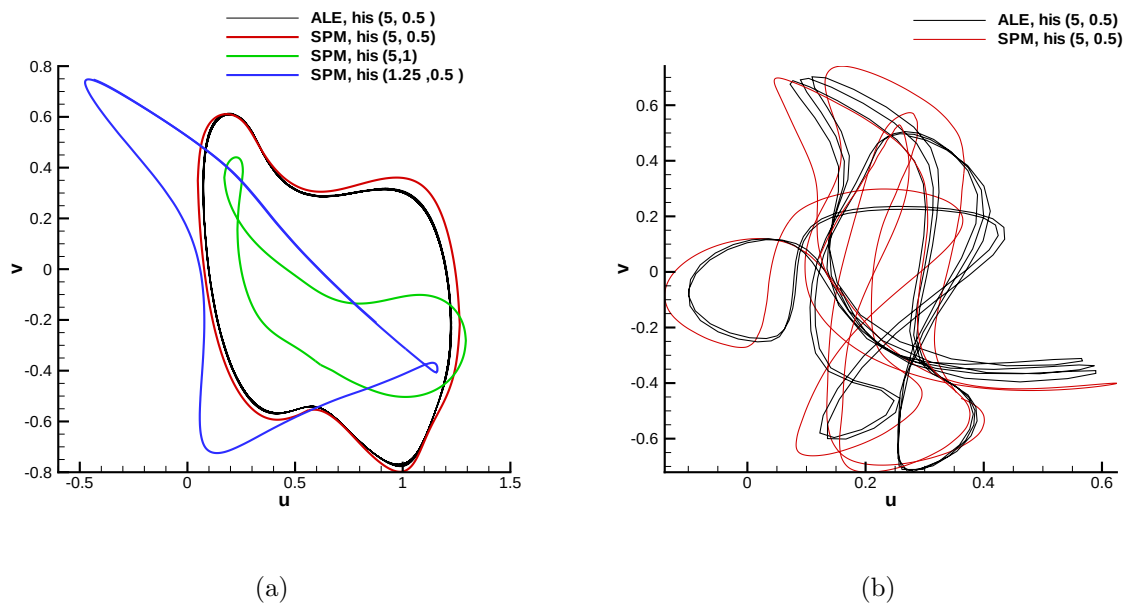


Figure 4.13: *Two-dimensional flow past two oscillating cylinders*: phase portrait of the crossflow velocity v versus the streamwise velocity u for points in the near wake. (a) refers to excitation frequency $f_e = 0.1253$, *locked-in*; (b) refers to $f_e = 0.1567$, *quasiperiodic*.

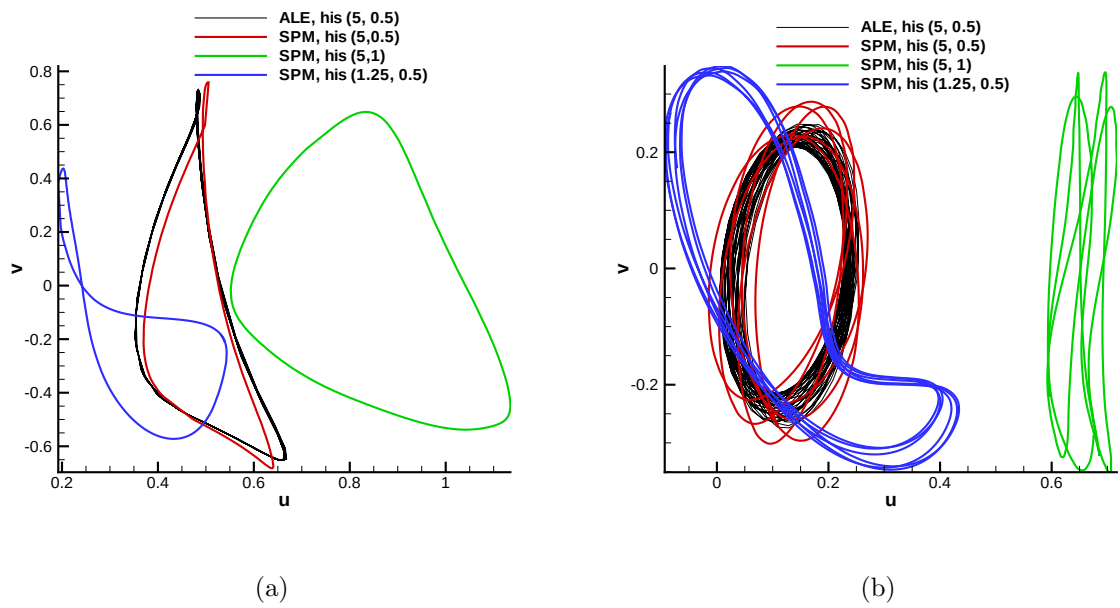


Figure 4.14: *Two-dimensional flow past two oscillating cylinders*: phase portrait of the crossflow velocity v versus the streamwise velocity u for points in the near wake. (a) refers to excitation frequency $f_e = 0.1723$, *locked-in*; (b) refers to $f_e = 0.1880$, *transitional*.

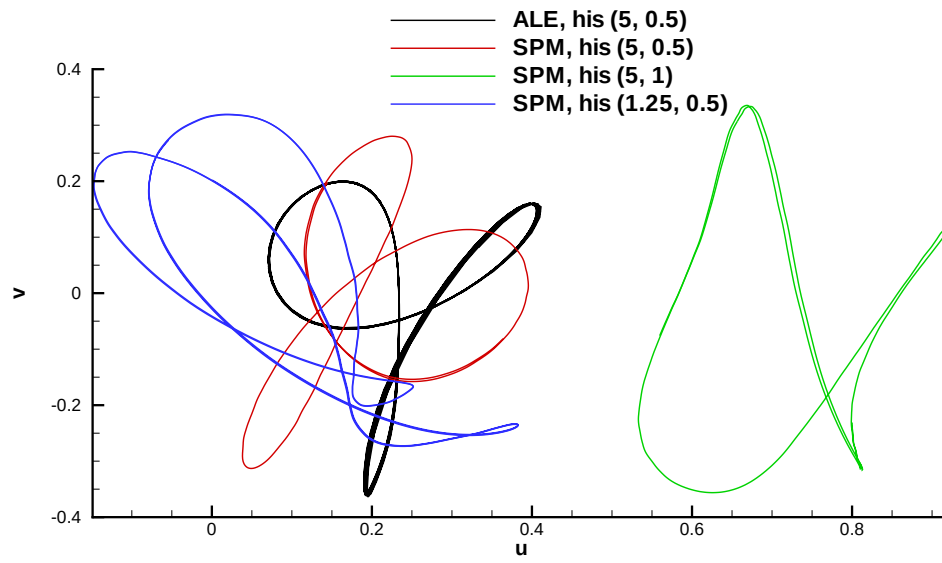


Figure 4.15: *Two-dimensional flow past two oscillating cylinders*: phase portrait of the crossflow velocity v versus the streamwise velocity u for points in the near wake of the downstream, with excitation frequency $f_e = 0.2200$, *period doubling*.

for several typical f_e . We see that $f_e = 0.1253$ (figure 4.13(a)) and $f_e = 0.1723$ (figure 4.14(a)) lead to locked-in states, since the wake spectrum peaks at f_e and its integer multiples (superharmonics). In contrast, $f_e = 0.1567$ (figure 4.13(b)) results in quasiperiodic shedding, with frequency peaks $f_e, f_e/2$. An even larger excitation frequency $f_e = 0.188$ (figure 4.14(b)) corresponds to a transitional state; there exists small peaks other than the dominant $f_e, 2f_e$ which cause modulations of the wake. More interestingly, further increase of f_e to 0.220 results in period doubling, with prominent peaks at $f_e/2$ and its integer multiples.

In summary, by increasing the excitation frequency, the wake changes from locked-in states to quasiperiodic shedding, then it returns to a locked-in state, and subsequently it switches to period doubling. Most importantly, these phase portraits indicate qualitative agreements between SPM and ALE results for the same near wake point. We note that the small discrepancy mainly comes from the different simulation domains.

To closely examine the flow patterns corresponding to the aforementioned distinguished states, we plot instantaneous streamwise velocity contours from SPM simulations in figures 4.16, 4.17 and 4.18. It is shown that for the locked-in frequencies $f_e = 0.1253$ and $f_e = 0.1723$, the wake features with well organized structures, while $f_e = 0.1567$ leads to a very unorganized wake corresponding to a quasiperiodic shedding. In contrast, $f_e = 0.1880$ results in an organized wake near the cylinders, but the structure collapses further downstream. This transitional wake pattern is consistent with the power spectra results, i.e. the prominent peak at f_e corresponds to organized structures in the near wake, while the smaller peaks at lower frequencies represents disturbances in the downstream flow. Furthermore, for $f_e = 0.2200$ which leads to period doubling, we see that the wake downstream is organized as in locked-in states, but the wake is wider and coarser. This is due to the merging of neighboring vortices which also results in spectrum peaks at frequencies of $f_e/2$ and its integer multiples. These findings are consistent with the ALE simulation results

[90], and also with the experimental results of [74] which reported that “modulated or locked-in response can exist intermittently”.

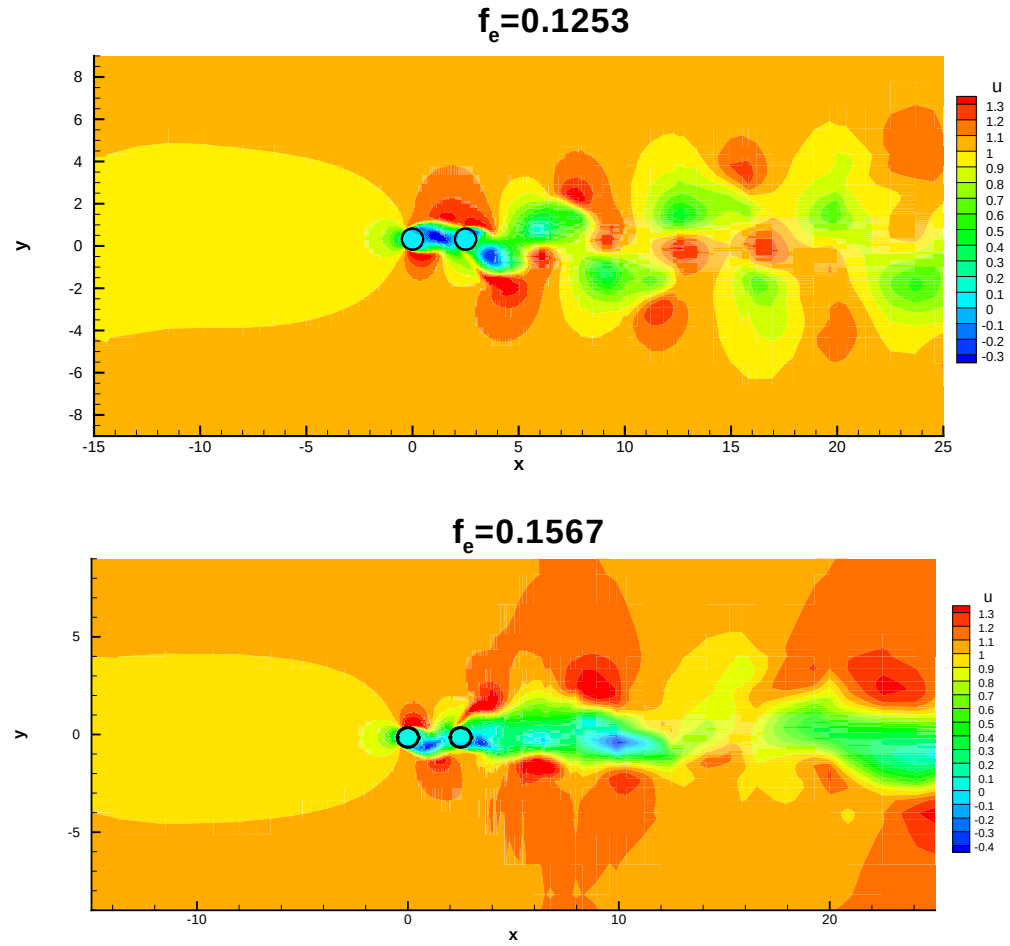


Figure 4.16: *Two-dimensional flow past two oscillating cylinders: contours of the streamwise velocity u in plane $z = 0.5$. (a) refers to excitation frequency $f_e = 0.1253$, locked-in; (b) refers to $f_e = 0.1567$, quasiperiodic.*

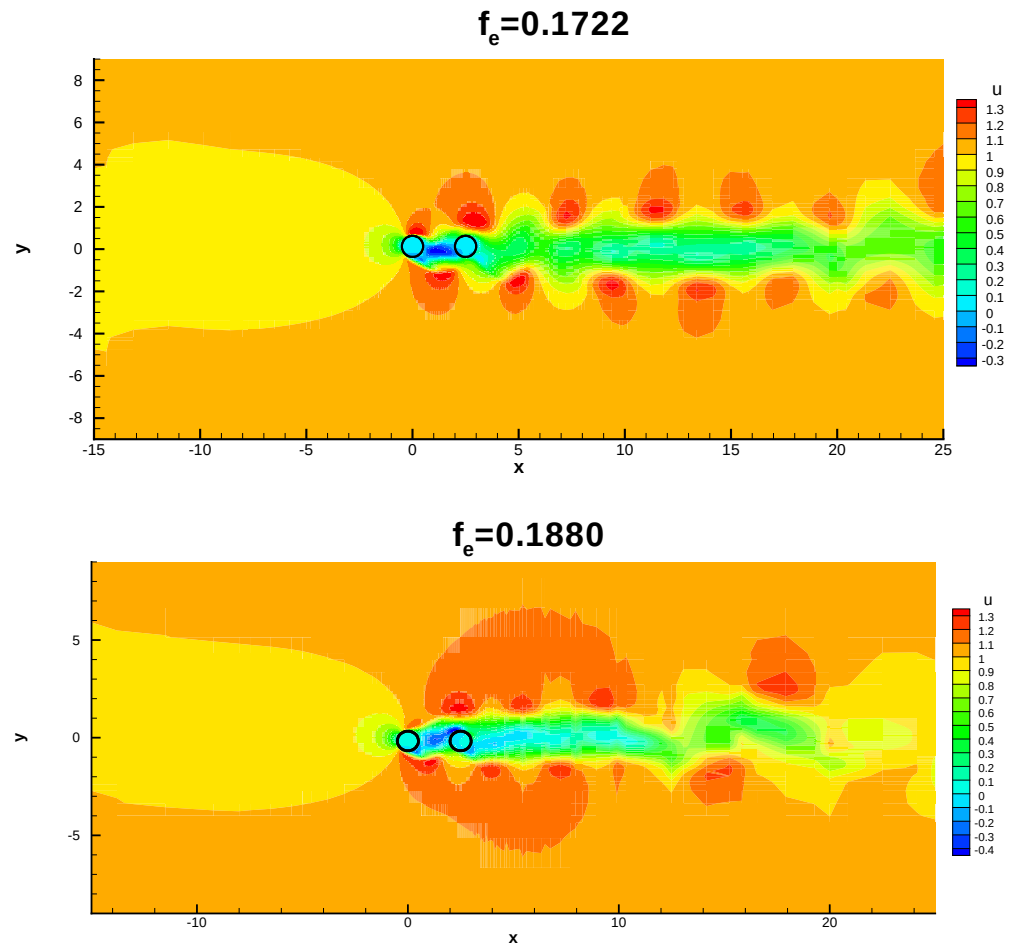


Figure 4.17: *Two-dimensional flow past two oscillating cylinders: contours of the streamwise velocity u in plane $z = 0.5$. (a) refers to excitation frequency $f_e = 0.1723$, locked-in; (b) refers to $f_e = 0.1880$, transitional.*

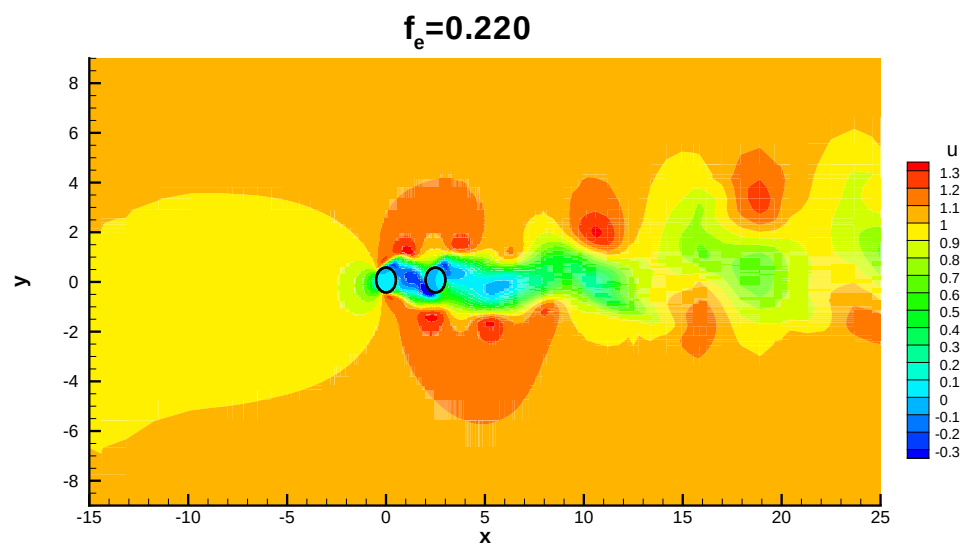


Figure 4.18: *Two-dimensional flow past two oscillating cylinders: contours of the streamwise velocity u in plane $z = 0.5$, with excitation frequency $f_e = 0.2200$, period doubling.*

4.4 Waterjet propulsion

Modern waterjet propulsion systems are very competitive with high-performance propellers, and are used for high speed marine vessels as well as military amphibian vehicles operating at low speeds with good maneuverability and reduced vibrations. The use of waterjets in commercial applications has grown recently with current designs having diameters of about 3 meters and delivering power of 25 MW per installation. Further optimization of their design using computational fluid dynamics tools will lead to more efficient designs that are smaller and alleviate cavitation problems. However, standard numerical methods are greatly challenged for such problems as propellers in free-space and impellers in ducts, which are key components of a waterjet propulsion system. In contrast, SPM avoids the direct boundary conditions imposed on the interfaces and thus it has great advantages in simulating such problems with 3D complex moving domains. In this section, we present fast 3D flow simulations of a typical waterjet propulsion system.

We consider a rotating three-bladed propeller, where each blade is modeled as an ellipsoid of axis $a = 4, b = 2, c = 1$. The propeller is placed at the center of a circular duct with a radius of $R = 10$ and a length of $L = 30$.

4.4.1 Verification for flows past a fixed propeller

First we verify the accuracy of our SPM simulation results by comparisons with the DNS results for a stationary propeller. DNS simulation adopts 100357 tetrahedral elements and a 7th polynomial order, in order to resolve the irregular geometry of the blades, especially near the joint region. In contrast, SPM uses a much simpler mesh, i.e. 10584 hexahedral elements and polynomial order of 3rd or 5th. The SPM indicator function is constructed using equation (2.1b), with d as the shortest distance to the ellipsoidal surfaces and the interface thickness as $\xi = 0.1$.

The SPM simulation applies a pressure gradient in the axial direction to drive

the flow, i.e. $\partial p / \partial z = 0.1$ everywhere in the entire domain Ω . Periodicity is imposed in the z -direction. In order to study the same problem by specifying the same total force, DNS simulation uses a different pressure gradient $\frac{\partial p'}{\partial z} = \frac{\partial p}{\partial z} \frac{\Omega}{\Omega - \Omega_p}$. Here, Ω_p is the volume of the propeller which we calculate numerically by integrating the indicator function ϕ , i.e. $\Omega_p = \int_{\Omega} \phi d\mathbf{x}$.

To examine the effects of the orientation angle of the blades θ , i.e. the angle between the blade primary plane and the central cross-section plane of the duct $z = 0$, we simulate a stationary propeller in the pressure driven flow, with both flat ($\theta = 0$) and tilted ($\theta = \pi/4$) orientations. We demonstrate in figure 4.19 the computational domain and the geometry of the propellers.

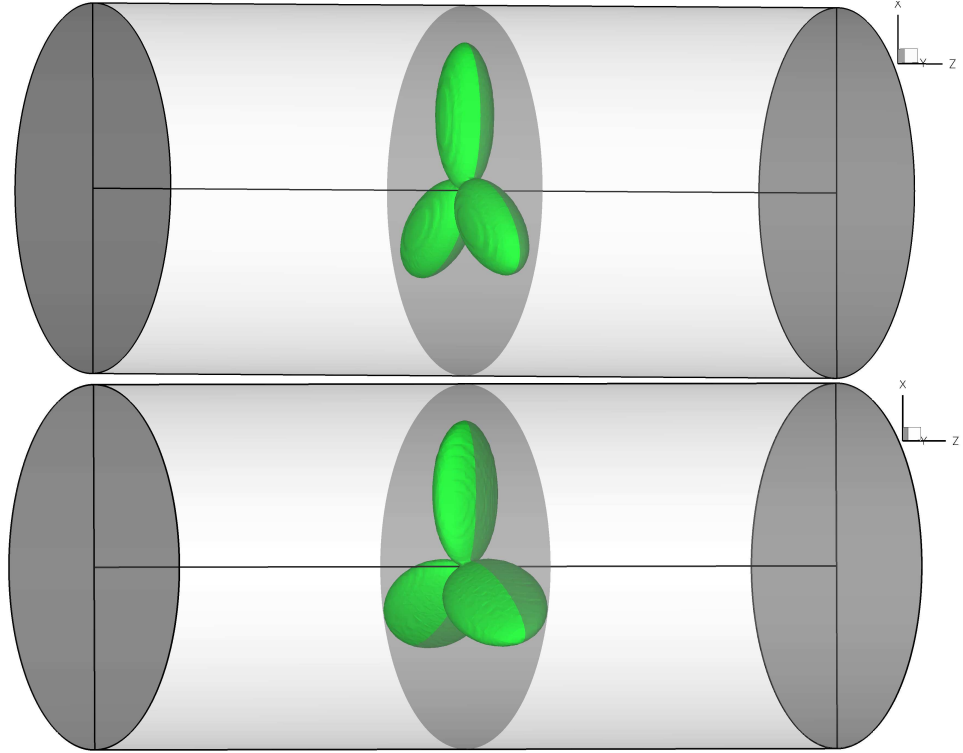


Figure 4.19: *Propeller in a circular duct*: geometries of the problem with a flat propeller (a) and a tilted propeller (b).

Figures 4.20 and 4.21 present comparisons between the results of SPM and DNS

simulations, for a flat propeller with $\partial p / \partial z = 0.1$. We see excellent agreements in the velocity and pressure field between the two methods, although the complicated mesh around the propeller surface has been avoided in SPM simulations.

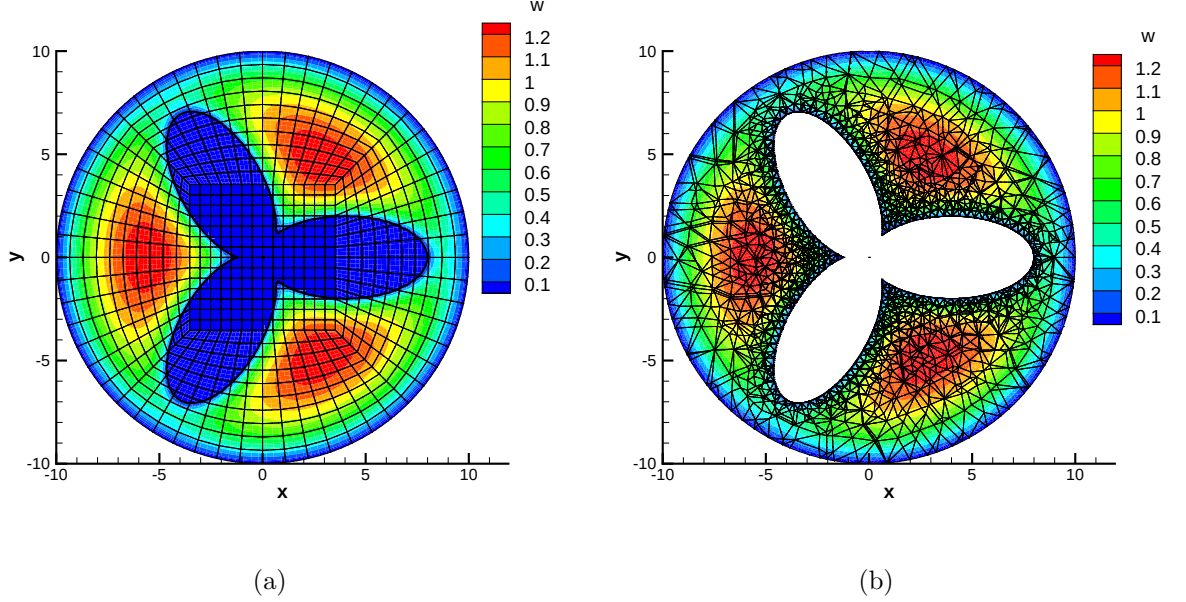


Figure 4.20: *Pressure driven flow past a stationary propeller*: streamwise velocity contour in the plane $z = 0$ with comparison between SPM (a) and DNS (b). The thin black lines indicate the elemental mesh, and the thick black curves represent the propeller surface.

Also, we examine the velocity profiles at different positions to check the pointwise accuracy, as shown in figure 4.22. It is indicated that SPM resolves the flow as well as DNS, except in the proximity of the joints between the blades. This difference could be due to the errors made in constructing the DNS mesh in the complicated intersection region, while SPM adopts a smooth representation of the surfaces.

We further examine the accuracy of SPM by comparing the simulated hydrodynamic forces with DNS simulations, as presented in table 4.3. It is shown that the relative differences are small, i.e. around 2% for all the pressure gradients involved. We also note that a tilted propeller has a smaller drag force than a flat one, which is due to the smaller cross-section area of the blades at $z = \text{constant}$.

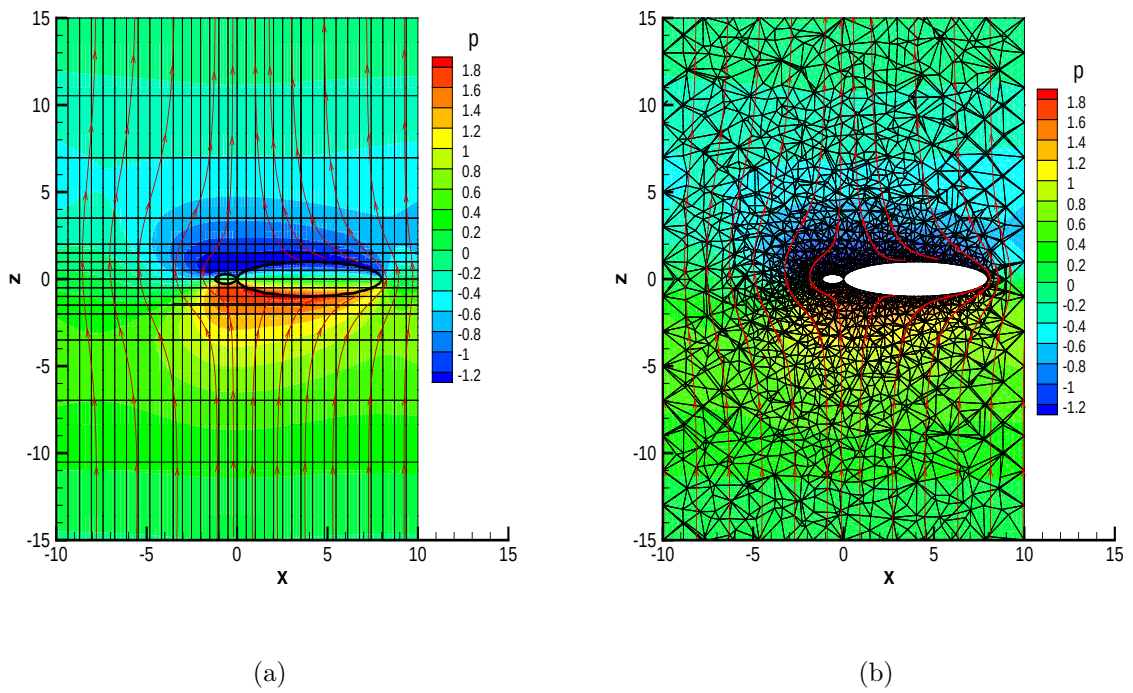


Figure 4.21: *Pressure driven flow past a stationary propeller*: pressure contour and streamlines in the plane $y = 0$ with comparison between SPM (a) and DNS (b). The thin black lines indicate the elemental mesh, and the thick black curves represent the propeller surface.

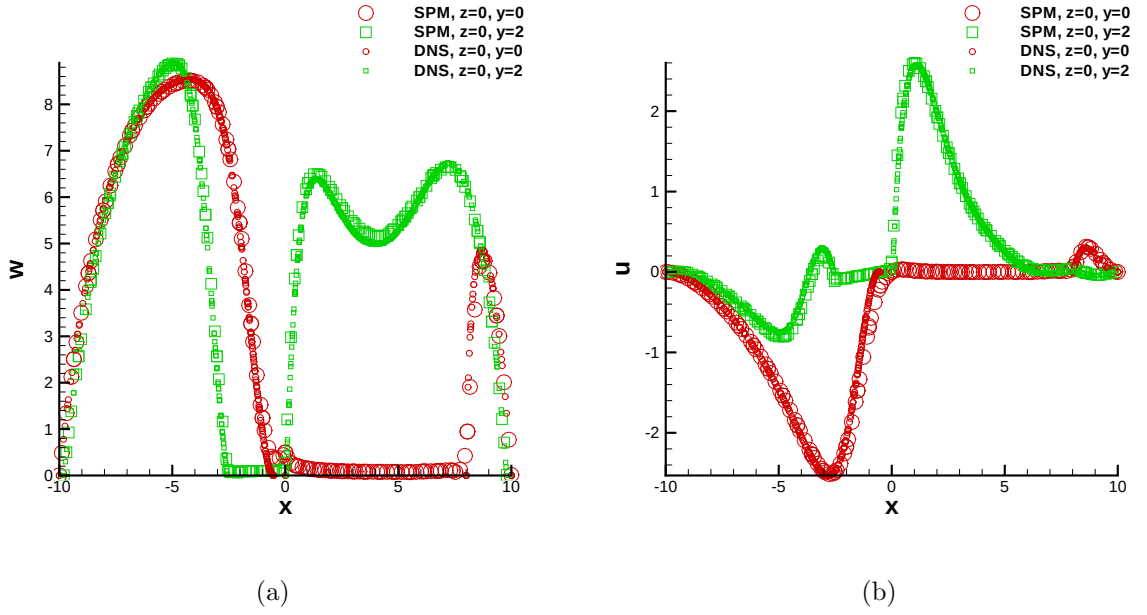


Figure 4.22: *Pressure driven flow past a tilted propeller*: velocity profiles along $z = 0, y = 0$ and $z = 0, y = 2$, with comparisons between SPM and DNS. (a) shows the streamwise velocity w and (b) shows the x-direction velocity component u .

4.4.2 Simulations of a rotating propeller

In this subsection we apply SPM to simulating flows around a rotating propeller. For this challenging problem with complex moving domains, SPM is advantageous since the same simple mesh can be used as for simple stationary geometries. This results in great computational efficiency; we note that SPM is more than 100 times faster than the often-employed Arbitrary Lagrangian Eulerian (ALE) formulations for such a problem.

In order to examine the effect of the rotational speed on the flow pattern, we plot the velocity results for two different angular velocities ω in the z -direction, as in figure 4.23. The Reynolds number is 200 and 800 respectively for $\omega = \pi$ and $\omega = 4\pi$ (rad/s), based on the rotational speed and the chord length of the blades. A constant pressure gradient of $\frac{\partial p}{\partial z} = 0.1$ is imposed on the flow. Here (u', v') refers to the velocity relative to the propeller, i.e. with a subtraction of the rotational

Table 4.3: *Pressure driven flow past a stationary propeller*: hydrodynamic forces with comparison between SPM and DNS.

	DNS Fz	SPM Fz	difference %
$\partial p/\partial z=0.1$	343.56	349.09	1.61
$\partial p/\partial z=1$	3872.16	3953.97	2.11
$\partial p/\partial z=4$	17395.50	17861.80	1.87
tilted, $\partial p/\partial z=1$	3614.81	3687.18	1.96
tilted v.s. flat, diff%	-6.65	-6.75	

speed ω as $u' = u + \omega y$ and $v' = v + \omega x$. We note that compared to the flow past a stationary propeller with the same pressure gradient as shown in figure 4.20, a rotating propeller results in a strong asymmetry of the flow between the two blades; maximum streamwise velocities are located very close to the front edge of each blade. The figure also indicates that a larger angular velocity of the propeller leads to a stronger flow in the streamwise direction, which suggests a propulsion effect on the fluid.

We also check the effects of a larger pressure gradient, or equivalently a stronger inflow. Figure 4.24 presents the simulation results using $\frac{\partial p}{\partial z} = 1.0$ and a angular velocity of $\omega = \pi$. Different blade angles are examined, i.e. a flat propeller $\theta = 0$ or a tilted one $\theta = \pi/4$. For this larger pressure gradient, we obtain a stronger and more uniform streamwise flow, as compared to the results with the smaller gradient shown in figure 4.23(a). But the increase in velocity with increasing pressure gradient is not as linear as in Stokes flows. Figure 4.24(b) indicates that a tilted geometry creates a more complex flow pattern; the streamwise flow velocity near the rear surface of the blades is as large as the one around the front surface. This is because the leading edge of a tilted blade cuts through the fluid first, and by rotation it repels the fluid away in the same direction as its angular velocity, and then the fluid leaves the blade at its trailing edge. Also, the typical magnitude of the streamwise velocity is larger than that of a flat propeller, which is what we desire in a waterjet propeller design.

Furthermore, we present the simulation results for a rotating tilted propeller with zero pressure gradient applied on the fluid. Note that the flow would be static

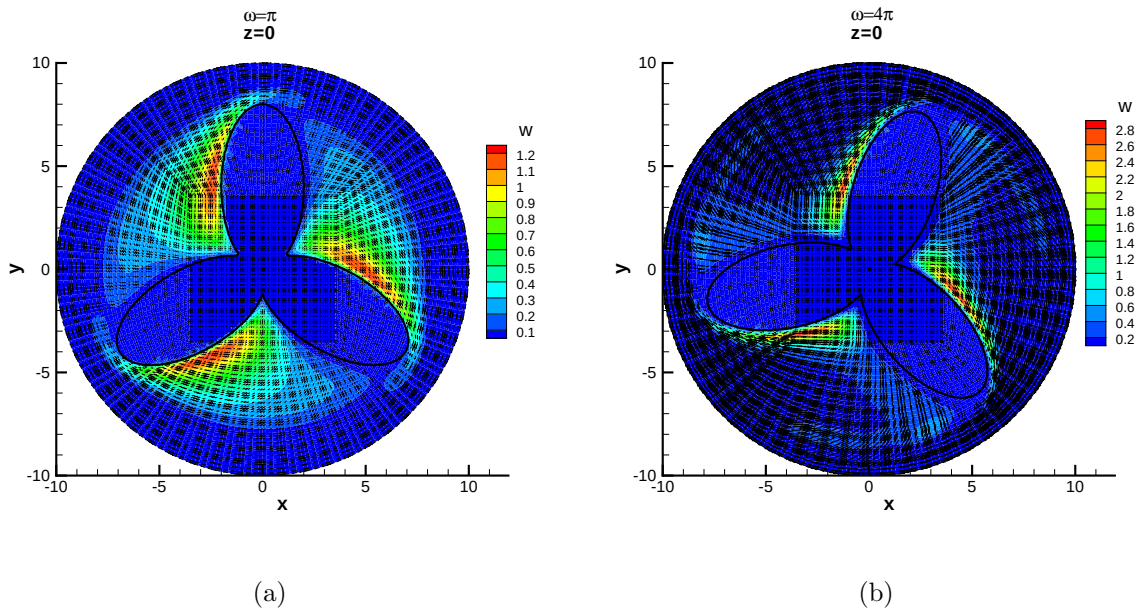


Figure 4.23: *Rotating flat propellers*: instance contours of z -direction velocity w and two-dimensional vectors of the relative velocity (u', v') in the plane $z = 0$, with a pressure gradient of $\frac{\partial p}{\partial z} = 0.1$. (a) refers to an angular velocity of $\omega = \pi \text{ rad/s}$ and (b) refers to $\omega = 4\pi \text{ rad/s}$.

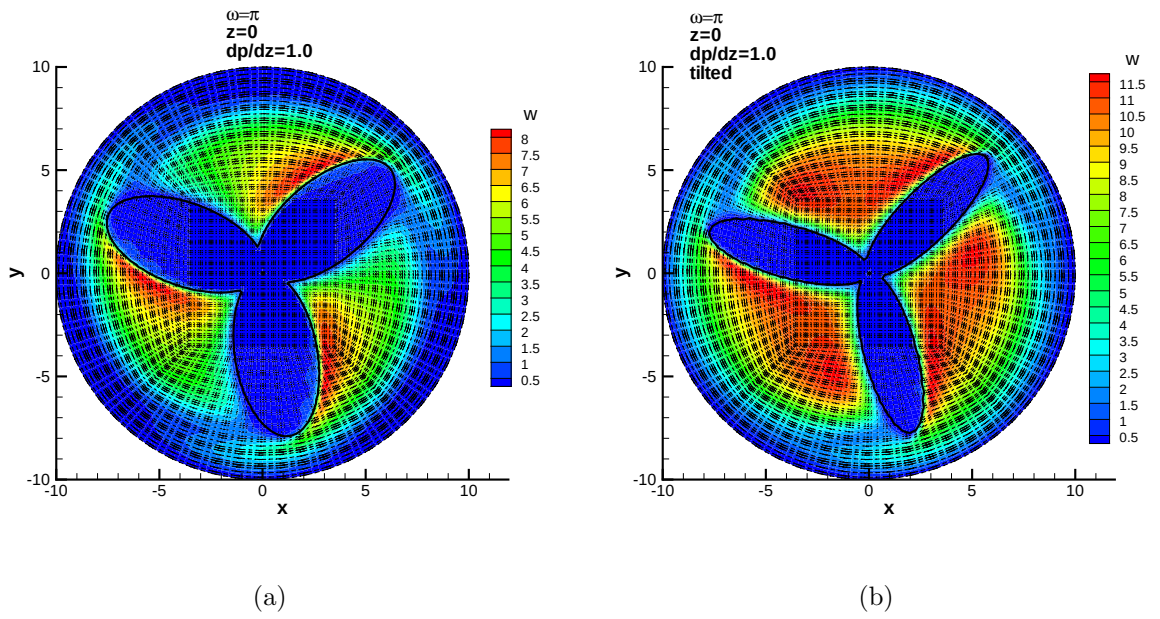


Figure 4.24: *Rotating propellers*: instantaneous contours of z-direction velocity w and two-dimensional vectors of the relative velocity (u', v') in the plane $z = 0$, with a pressure gradient of $\frac{\partial p}{\partial z} = 1.0$ and angular velocity of $\omega = \pi \text{ rad/s}$. (a) refers to a flat propeller and (b) refers to a tilted one.

without the motion of the propeller, and the effects of different rotating speeds are examined in figure 4.25. We see that the larger angular velocity $\omega = 4\pi$ results in a stronger streamwise motion of the fluid, with a maximum velocity about six times bigger than the one with $\omega = \pi$. It also leads to a greater variation in the velocity of the fluid between any two blades. This is shown more clearly by 3D streamwise velocity iso-contours in figures 4.26 and 4.27, for rotational speeds of $\omega = \pi$ and $\omega = 4\pi$. We see that by using $\omega = 4\pi$ the fluid is strongly repelled by the propeller towards z-direction, which leads to a great propulsion performance (in negative z-direction). Also, the instantaneous streamwise vorticity iso-contours are shown in figures 4.28 and 4.29.

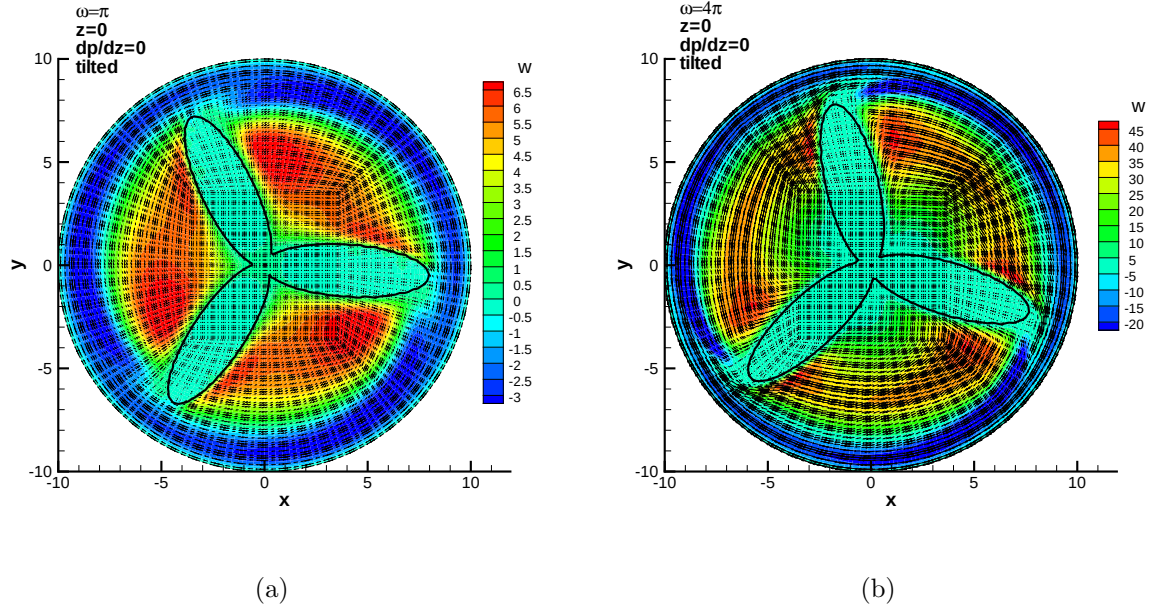


Figure 4.25: *Rotating tilted propellers*: instantaneous contours of z-direction velocity w and two-dimensional vectors of the relative velocity (u', v') in the plane $z = 0$, with zero pressure gradient $\frac{\partial p}{\partial z} = 0$. (a) refers to an angular velocity of $\omega = \pi$ rad/s and (b) refers to $\omega = 4\pi$ rad/s.

In order to examine the thrust and torque performance, we list the calculated

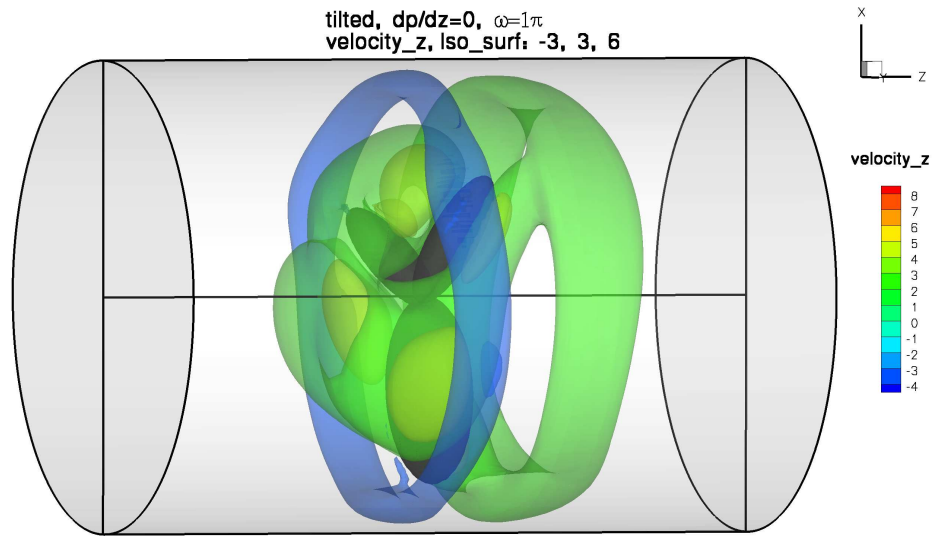


Figure 4.26: *Rotating tilted propellers*: instantaneous iso-surfaces of z-direction velocity w , with zero pressure gradient $\frac{\partial p}{\partial z} = 0$ and angular velocity $\omega = \pi \text{ rad/s}$. The propeller surfaces are indicated by deep gray contours.

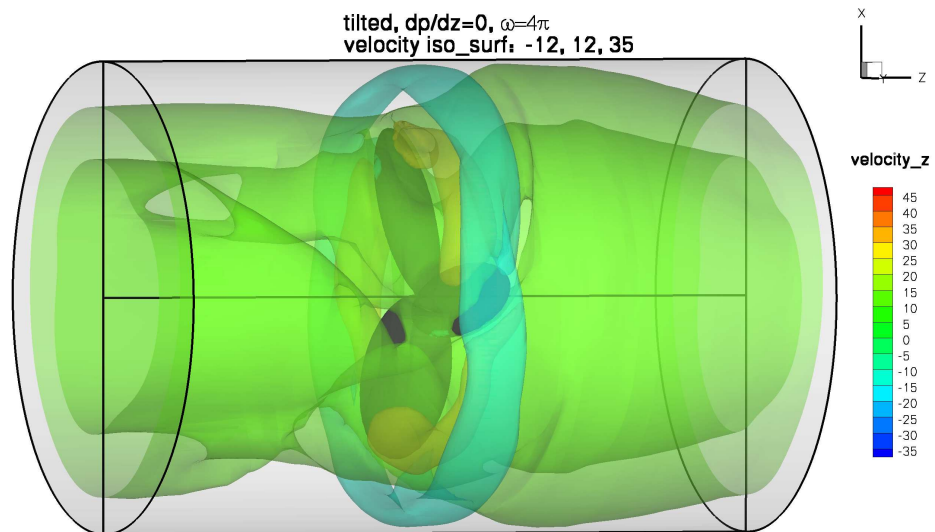


Figure 4.27: *Rotating tilted propellers*: instantaneous iso-surfaces of z-direction velocity w , with zero pressure gradient $\frac{\partial p}{\partial z} = 0$ and angular velocity $\omega = 4\pi \text{ rad/s}$.

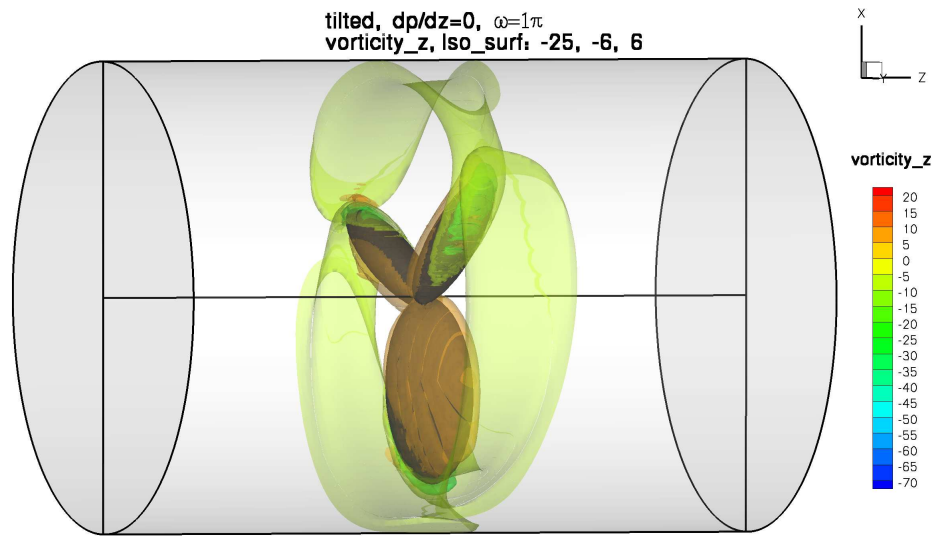


Figure 4.28: *Rotating tilted propellers*: instantaneous iso-surfaces of z-direction vorticity w_z , with zero pressure gradient $\frac{\partial p}{\partial z} = 0$ and angular velocity $\omega = \pi \text{ rad/s}$.

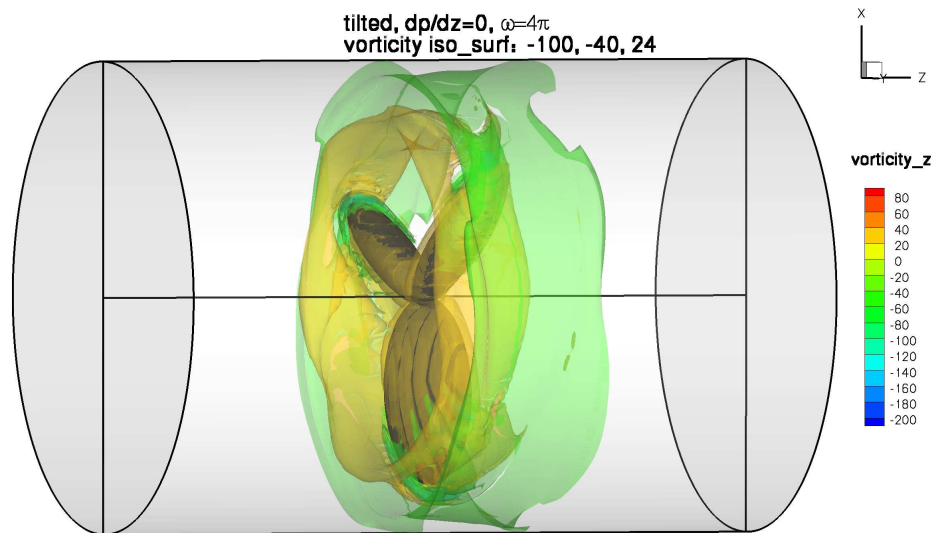


Figure 4.29: *Rotating tilted propellers*: instantaneous iso-surfaces of z-direction vorticity w_z , with zero pressure gradient $\frac{\partial p}{\partial z} = 0$ and angular velocity $\omega = 4\pi \text{ rad/s}$.

mean hydrodynamic forces and torques on the propeller, as in table 4.4. The relative differences in the forces and the torques between a tilted propeller and a flat one are presented. For propellers with the same $\omega = \pi$ and $\frac{\partial p}{\partial z} = 1.0$ but different blade angle θ , we see that a tilted propeller results in a significant drop in the drag force (-22.8%). This drop is much larger than the one for two stationary propellers (-6.75% as in table 4.3), which is because the rotational motion of the propeller further aids the fluid to get through. To see this effect more clearly, we check the forces on rotating propellers in static fluid ($\frac{\partial p}{\partial z}=0$). A flat propeller results in a zero drag force in z-direction, corresponding to no propulsion on the fluid and thus only rotational motion in constant-z plane. In contrast, a tilted propeller bears a significant negative drag force, which means that it exerts a large propulsion force on the fluid to make it move in the z-direction; this is consistent with the velocity contours in figure 4.25. We also note with a four times larger rotational speed $\omega = 4\pi$, the hydrodynamic force increases with a factor of about 16, i.e. the thrust is proportional to ω^2 . Figure 4.30 shows the time evolution of the forces on the propellers with different rotational speeds. Large oscillations in the force are present for $\omega = 4\pi$, as the Reynolds number is about $Re = 800$ based on the rotational velocity at blade tip. Furthermore, if we enlarge the blades by using $a = 4, b = 4, c = 1$ instead of $a = 4, b = 2, c = 1$, a greater propulsion is achieved, since the thrust of the propeller increases by a factor of almost four as shown in table 4.4.

Table 4.4: *Rotating propellers*: average hydrodynamic forces and torques with comparisons between different propeller angles.

	flat, Fz	Tz	tilted, Fz	Tz	Fz diff%	Tz diff%
$\omega = \pi, \frac{\partial p}{\partial z}=0.1$	554.1	-33313				
$\omega = 4\pi, \frac{\partial p}{\partial z}=0.1$	2430.8	-406211				
$\omega = \pi, \frac{\partial p}{\partial z}=1.0$	5170.6	-32871	3989.1	-35606	-22.8	+8.3
$\omega = 4\pi, \frac{\partial p}{\partial z}=1.0$	6771.2	-402685				
$\omega = \pi, \frac{\partial p}{\partial z}=0$	0	-33300	-982.5	-42380	∞	+27.3
$\omega = 4\pi, \frac{\partial p}{\partial z}=0$			-15110.7	-726046		
$\omega = \pi, \frac{\partial p}{\partial z}=0, b=4$			-2550.4	-59200		

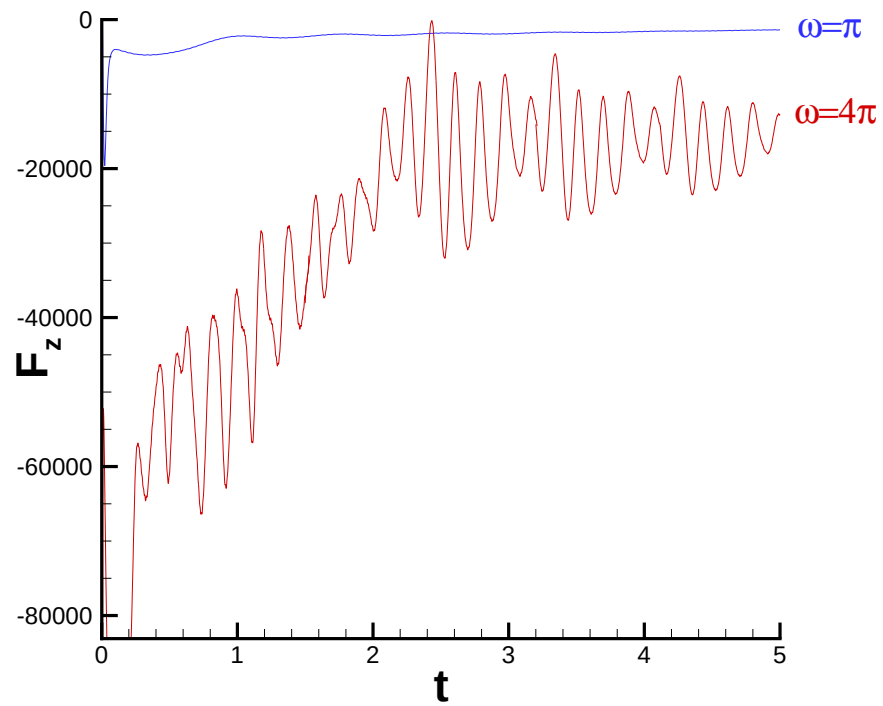


Figure 4.30: *Rotating propellers*: time evolution of the hydrodynamic forces on the propellers with different rotational speeds $\omega = \pi \text{ rad/s}$ and $\omega = 4\pi \text{ rad/s}$.

4.5 Concluding remarks

In this chapter, we focused on examining the applicability of SPM to interesting engineering flow problems. We first showed that SPM can resolve accurately two-dimensional cylinder flows at moderate Reynolds numbers up to 1000. Our numerical results also revealed its capability in capturing the three-dimensional instabilities in the wake of a cylinder. Furthermore, SPM was shown to be able to simulate vortex induced vibrations; it showed good agreement with the results of ALE two-dimensional simulations.

Subsequently, we presented fast 3D SPM simulations of a typical waterjet propulsion system with a rotating three-bladed propeller in a circular duct. Verification was achieved by comparisons against DNS results for pressure driven flows past a stationary propeller. We found the method to be stable for various rotational speeds. Propulsion performance was examined by using various rotational speed of the propeller, different blade angles and shapes. This analysis can be utilized in the optimization of a waterjet propulsion design.

Chapter 5

Summary and Future Work

In this thesis, we have analyzed and improved the smoothed profile method (SPM) for particulate flows. We extended the original fully-explicit time-integration scheme to a semi-implicit high-order splitting scheme and implemented it with a spectral/ hp element discretization in space. We showed that the modeling error of SPM has a *non-monotonic* dependence on time step size, with the optimum time step $(\Delta t)_o$ resulted from a balance between the effective interface thickness and the Stokes layer thickness. We also extended the application of the method to flows past complex-shaped particles and flows with multi-particle interactions. Comparisons with the force coupling method (FCM) and direct numerical simulations (DNS) showed that SPM is resolving accurately the near-field flows as well as the far-field flows.

Subsequently, we proposed an extension of SPM to simulate electrokinetic flows allowing for spatially varying electrical conductivities. In addition to the Navier–Stokes equations, the Poisson–Boltzmann and electric charge continuity equations were also cast into forms based on SPM. We verified the method for prototype problems of electroosmotic flows and electrophoresis of cylinders, where the modeling error is quantified. We also presented simulations on the electrophoresis of charged microtubules, and showed that the simulated electrophoretic mobility and anisotropy agree with the experimental results.

Furthermore, since SPM avoids complicated discretizations around the particles, it can lead to significant reduction in computational cost when compared to direct numerical simulations, especially for complex-shaped particles. Moreover, SPM is advantageous for simulating flows involving moving particles, whereas ALE-based methods require frequent re-meshing. To demonstrate this advantage, we applied the method to simulate several engineering flow problems which involve three-dimensional moving complex domains. Our numerical results showed that SPM successfully resolved the complex flow patterns in vortex-induced vibrations of two tandem cylinders. We also presented simulation results for a rotating three-bladed propeller, which can be used for the design of waterjet propulsion systems. Compared to the simulation results based on an arbitrary Lagrangian Euler (ALE) formulation, SPM yields satisfactory agreement with a much lower computational cost.

The following improvements in the development and implementation of SPM are recommended for future work.

- Parallel implementation. The structured mesh allows for great optimization of parallel performance.
- Extensions to modeling compressible flows. There is no limitation of the method to compressible flows, but SPM needs to be properly reformulated.
- Applications to turbomachinery such as water turbines and compressors, where both stationary and moving complex geometries are present, e.g. the intake duct, rotor, stator, and discharge nozzle.
- Developing a Poisson–Nernst–Planck model based on the smoothed profile technique, for a more general modeling method to simulate electrokinetic flows.
- Multiscale modeling of colloidal suspensions, where construction of proper models is required to represent the solid contact force and the Brownian motion. Results from using a contact force model which includes also the friction

between particles in [24] are encouraging. Another extension is to include representations of the Brownian motion of particles due to thermal fluctuations. This can be done by modifying the fluid equations via random stress terms [10, 2].

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