Spring 2000

Numerical study of particle dynamics in a falling-ball viscometer

Peiwen Hou
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ABSTRACT

NUMERICAL STUDY OF PARTICLE DYNAMICS IN A FALLING-BALL VISCOMETER

by

Peiwen Hou

The falling-ball viscometer is a device where a spherical particle falls along the axis of a circular cylinder filled with viscous fluid. The various classical results for this device are developed under the assumption that the Reynolds number of the flow is zero, i.e., Stoke's flow. Inertial effects are not taken into account. To better understand the dynamics of the particle sedimentation process and the role of inertia in this process, we implemented a numerical simulation.

The ADI (Alternating Direction Implicit) scheme is widely used to solve the vorticity-stream function formulation of the Navier-Stokes equation in axisymmetric geometries. However, a severe timestep restriction for low Reynolds flow makes application of this method cumbersome for simulating the falling-ball viscometer. Through a study of a classical 2-D cavity problem, the cause of the instability requiring the restricted time step is identified. For this cavity problem, a modification of the usual treatment of the boundary condition for the stream function relaxes the restriction on the time step. Unfortunately, the complexity of the falling-ball viscometer simulation makes it difficult to efficiently implement this modification.

A penalty method is used here to handle the moving boundary associated with the sedimenting particles. Fluid is allowed to flow through the particle but it encounters resistance proportional to a parameter (or penalty number) that can be viewed as a porosity. For large values of the penalty number the flow converges to that for a impenetrable particle. The validity of this method is demonstrated.
The results of the numerical simulation are compared with previous work. The relationships among the sedimentation speed $U_{sed}$, the Reynolds number $Re$, the radius of cylinder $R_0$, the particle permeability $\beta$ and the dimensionless mass $\delta$ are studied. Multiparticle dynamics are easily simulated using our penalty method with virtually no additional numerical resources needed. The breaking of the time-reversal symmetry by inertia is observed and studied.
NUMERICAL STUDY OF PARTICLE DYNAMICS IN A FALLING-BALL VISCOMETER

by
Peiwen Hou

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To my parents and my wife Keke
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3.13 The variation of sedimentation velocity vs. $Re$. The sedimentation velocity decreases as the Reynolds number increase with the weight of the particle held constant.
CHAPTER 1

INTRODUCTION

The study of particle motions in a suspension has long been a subject of both theoretical and practical interest. Most of the theoretical analysis has focused on the low Reynolds number (Stokes) regime. Along these lines, Einstein's asymptotic formula for the viscosity of a dilute suspension of solid spheres is one of the most fundamental results. This result was rigorously confirmed and extended to suspensions of "fluid particles" by Keller and Rubenfeld [13] using a variational method of analysis. A second fundamental result giving the mean sedimentation speed in a dilute suspension of spheres was obtained by Batchelor [3] in 1972 using an approach that has been called "suspension renormalization".

These two fundamental results address particle dynamics in a suspension only in an indirect or averaged sense and only at zero Reynolds number. Moreover, these results (especially Batchelor's estimate of the mean sedimentation speed) are based on assumptions of how particle motions affect the statistics of the particle arrangement at the level of the suspension microstructure. It is known, however, that suspension microstructure has a significant effect on these results. For example, to obtain the next term in the asymptotic expansion of the suspension viscosity, Batchelor and Green [4] found it necessary to analyze how the interactions between pairs of particles affect particle statistics.

The importance of understanding how hydrodynamic interactions influence the statistics of the particle distribution has led to efforts to simulate numerically the motion of particles in a suspension. One significant study along these lines, performed by Caflisch et. al. [8] in 1988, considered the motion of three identical spheres sedimenting at zero Reynolds number. This work along with subsequent studies
by Golubitsky et. al. [10] revealed exceeding complex dynamics that would not likely yield to purely analytical analysis. The "Stokesian dynamics" method (Brady and Bossis [6]) is the most prominent of many numerical methods that have been developed to track many particles in an evolving suspension. However, almost all the methods have been for the case of Stokes flow. Joseph in his work on fluidized beds has pointed out the importance of inertial effects on particle dynamics. These effects arise largely due to the breaking of the time reversal symmetry of the Stokes equations.

In this thesis, we study the particle dynamics in a viscometer. The falling-ball viscometer is a device where a spherical particle falls along the axis of a circular cylinder filled with viscous fluid. As in the case of suspension dynamics mentioned above, theoretical analysis of this device has focused on the low Reynolds number regime. Stokes's equations are usually solved and the viscosity can be measured conveniently utilizing Stokes's law. Various corrections to Stokes's law were obtained due to wall effects and end effects by Lorentz and Faxen [11]. Here, we implement a numerical computation of the Navier-Stokes equations with small Reynolds number, a penalty formulation is used to simplify treatment of the moving boundary problem. Comparison with the Stokesian theory aims to gain insight into the role of inertial effects in sedimentation.
1.1 Equations of motion

We assume that the fluid motion in the falling-ball viscometer is governed by the Navier-Stokes equation,

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) + \nabla p = \mu \nabla^2 \mathbf{v} \]  
(1.1)

and continuity equation,

\[ \nabla \cdot \mathbf{v} = 0 \]  
(1.2)

for incompressible fluids where \( \mu \) is the fluid viscosity, \( \rho \) is the fluid density, \( \mathbf{v} \) is the fluid velocity and \( p \) is the pressure. For low Reynolds number flow, it is permissible to neglect the inertial terms, this reduces the Navier-Stokes equations to Stokes equations

\[ \nabla p = \mu \nabla^2 \mathbf{v}. \]  
(1.3)

Stokes's law states that the drag acting on the sphere in an infinite domain, \( D_s \), is given by

\[ D_s = 6\pi \mu a U \]  
(1.4)

where \( a \) is the radius of the sphere and \( U \) is the sedimenting speed. Since this relation is only valid in fluid media which extend to infinity in all direction, it is necessary to find corrections to Stokes's law in the viscometry problem because of the presence of the rigid walls of the finite size cylinder.

1.2 The corrections to Stokes's law

1.2.1 Cylinder wall effect

In this case, a sphere with radius \( a \) falls along the axis of an infinitely long circular cylinder of radius \( R_0 \). The total drag of the sphere \( D \), known as Faxen's correction
Thus, for Stokes flow the drag is increased by the presence of the cylinder wall.

1.2.2 Plane surface effect

We consider the motion of a sphere approaching a plane surface. Denoting the distance from the bottom of the sphere to the plane by \( h \), the full solution is developed by Brenner [7] and the drag is

\[
D = 6\pi \mu a \lambda
\]  \hspace{1cm} (1.6)

where \( \lambda = \lambda(a/h) \) is a correction to Stokes's law given by

\[
\lambda = \frac{4}{3} \sinh \alpha \sum_{n=1}^{\infty} \frac{n(n+1)}{2n-1}(2n+3) \left[ \frac{2\sinh(2n+1)\alpha + (2n+1)\sinh 2\alpha}{4\sinh^2(n+\frac{1}{2})\alpha - (2n+1)^2\sinh^2 \alpha} - 1 \right]
\]  \hspace{1cm} (1.7)

where \( \alpha = \cosh^{-1}(h/a) \).

When the sphere radius is small compared with the distance of its center from the plane, this results in

\[
\lambda = 1 + \frac{9}{8} \left( \frac{a}{h} \right) + O \left( \frac{a}{h} \right)^2
\]  \hspace{1cm} (1.8)

which agrees with Lorentz's correction exactly. Here, the drag increases due to the presence of the bottom plane as in the case of a cylindrical wall.

1.2.3 End effects

Although the separate effects of each of the boundaries alone are known, it is not correct to add these corrections to analyze the falling-ball viscometer. In this case the interactions between wall effects and end effects must be considered. More generally, free surface effects must be considered as well.
Figure 1.2 Drag curves showing that the sum (Ladenburg) of the Lorentz and Faxen correction does not give the drag on the particle in the viscometer (Tanner).

Tanner [20] did a numerical calculation solving the steady Stokes equation for the viscometry problem. Figure 1.2 shows the results. The Ladenburg drag curve shown is the sum of the Faxen drag and the Lorentz end-effect correction. Tanner’s result lies above the Faxen and Lorentz curves separately, but below the sum of the two. It is clear that end effects are negligible when end-sphere distances are greater than 1.5$R_0$, but they must be considered near the ends.

1.2.4 The inertial effect

The inertial effect must be taken into account at higher Reynolds number, typically $Re > 1$. In this case, the hydrodynamic drag force exerted on the particle is larger than Stokes’s drag $D_s$. The Stokes’s law can be expressed as

$$D_s = \frac{1}{2} \rho U^2 \pi a^2 C_D$$

where $C_D$ denotes the drag coefficient. Here $C_D = 24/Re$ in Stokes’s flow and $Re$ is defined as $2a\rho U/\mu$ and this relation is accurate when $Re < 1$ [2].

A second approximation[2] is given as

$$C_D = \frac{24}{Re} \left( 1 + \frac{3}{16} Re \right)$$

(1.10)
which is good for $Re$ slightly bigger than 1. A more accurate $C_D - Re$ relation is proposed by Concha and Almerdra [21]

$$C_D = 0.28 \left(1 + \frac{9.06}{\sqrt{Re}}\right)^2$$

which is valid for $1 < Re < 1000$. Figure 1.3 shows the comparison of these relations.

1.3 The numerical scheme: vorticity-stream function formulation

The vorticity-stream function formulation is a widely used method for solving 2-D Navier-Stokes equations. In this approach, a change of variable is made which replaces the velocity components and pressure with the vorticity $\zeta$ and the stream function $\psi$.

$$\zeta_t + u\zeta_x + v\zeta_y = \frac{1}{Re}(\zeta_{xx} + \zeta_{yy})$$

$$\psi_{xx} + \psi_{yy} = -\zeta$$

By solving transport vorticity equation (1.12) and the stream function equation (1.13) we can find the velocity field of the flow by the following relations:

$$u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}$$
where the vorticity \( \omega = (0, 0, \zeta) \) and the velocity \( \mathbf{v} = (u, v, 0) \) in a planar system.

The ADI(Alternating Direction Implicit) method is often used to solve the vorticity transport equation and stream function equation.

1.4 An brief introduction to the ADI scheme

The ADI scheme is an effective method for solving parabolic partial differential equations. A typical equation is

\[
\frac{u^{n+1} - u^n}{\Delta t} = \mu (\partial_{xx} + \partial_{yy})u^n + \frac{\mu}{2} (\partial_{xx} + \partial_{yy})u^{n+1} + \frac{f^n + f^{n+1}}{2}. \tag{1.17}
\]

Letting \( d = \Delta t \mu / 2 \), this becomes

\[
(1 - d\partial_{xx} - d\partial_{yy})u^{n+1} = (1 + d\partial_{xx} + d\partial_{yy})u^n + \Delta d(f^n + f^{n+1})/2. \tag{1.18}
\]

Assume the grid is \( M \times N \), then solving this linear system involves inverting \( MN \times MN \) matrix which is computationally very expensive. The basis of the ADI method is to approximately factor the operator \((1 - d\partial_{xx} - d\partial_{yy})\) as \((1 - d\partial_{xx})(1 - d\partial_{yy})\) to give

\[
(1 - d\partial_{xx})(1 - d\partial_{yy})u^{n+1} = (1 + d\partial_{xx})u^n + \Delta d(f^n + f^{n+1})/2. \tag{1.19}
\]
This equation can be solved in two steps by splitting the time step into two half time steps and denoting values of \( u \) at this half time step as \( u^* \), so

\[
(1 - \partial_{xx})u^* = (1 + d\partial_{yy})u^n + \Delta tf^n / 2,
\]

\[
(1 - \partial_{yy})u^{n+1} = (1 + d\partial_{xx})u^* + \Delta tf^{n+1} / 2.
\]

In this way, we solve \( M \times M \) and \( N \times N \) linear systems, (which are moreover banded) at each step with substantial reduction in computational cost in comparison with directly solving (1.19).

Combining the two equation recovers the factored form of the discrete equation, so the ADI method is a very efficient and accurate method for solving parabolic partial differential equations. For the classical cavity problem, we simply use the above formulation to solve the vorticity transport equation; however, in the falling-ball viscometer, we need to modify the formulation because of its complexity.

1.5 Problems and goals

1.5.1 Numerical instability

A numerical instability arises in the ADI methods for the vorticity transport equations. Although the ADI scheme is unconditional stable, the associated boundary conditions cause divergence or oscillation in the solution [19]. Bontoux et al. found a restriction [5] on the time step of the type \( \Delta t / \Delta x^2 < a \) where \( a \) goes to zero with Reynolds number. Our computation with the ADI method confirms these results. For \( \Delta x = 0.1 \) and \( Re = 0.1 \), instabilities develop for \( \Delta t \geq 10^{-3} \). For finer grids this restriction becomes intolerable. We will investigate the stability problem in Chapter 2 and give a modified scheme that overcomes this restriction for the 2-D planar cavity problem.
1.5.2 Method validation

We identify and document the strengths and weakness of the penetrable particle model analyzed in [5] and implemented here. We show the result and compare with theoretical results in Chapter 3. Issues include to what extent does the flow satisfy the no-slip boundary conditions at the particle surface, the bottom penetrations, two particle interactions, convergence of the ADI iterations and comparison of results with Stokes flow.

1.5.3 Inertial effects in sedimentation dynamics

For zero Reynolds number flow the dynamics of the single particle problem have the form

\[ \delta \ddot{X} = F(X, \dot{X}, \alpha) \]  

(1.22)

We expect that this structure might persist (in the sense of an inertial manifold) for small nonzero values of the Reynolds number. That is, we postulate approximate dynamics

\[ \delta \ddot{X} = F(X, \dot{X}, \alpha, Re) \]  

(1.23)

for sufficiently small but nonzero values of \( Re \). Assuming \( F \) depend regularly on \( Re \), we expect solutions to also exhibit regular dependence on \( Re \). Using our numerical simulations, we have performed a preliminary investigation of this dependence in the form of expansion of the solution in \( Re \) about \( Re = 0 \):

\[ X(t, Re) = X_0(t) + Re X_1(t) + Re^2 X_2(t) + \ldots \]  

(1.24)

These expansions are used to analyze two particle dynamics.
CHAPTER 2

A STABILITY STUDY OF VORTICITY-STREAM FUNCTION FORMULATION FOR NAVIER-STOKES EQUATIONS

2.1 Overview

The ADI method applied to the vorticity-stream function formulation of the Navier-Stokes equation is widely used for numerical computation in planar or axisymmetric geometries. It is well known that the ADI method is unconditionally stable for parabolic equations on periodic or unbounded domains, but one finds [5] that there is a numerical stability problem in the presence of boundaries; the time step $\Delta t$ has to be smaller than $Re\Delta x^2$ to avoid instability. This restriction can be severe for low Reynolds number flow when $Re \ll 1$. So it turns out that to solve a low Reynolds number flow ($Re \ll 1$) with the ADI method can be very time-consuming or even impossible because of the time step restriction. This situation occurs even though the solution is well approximated by solving the Stokes equations for which highly efficient methods are available.

We investigate this stability problem carefully and show that the instability in the vorticity-stream function formulation can be overcome, and the time restriction $\Delta t < Re\Delta x^2$ can be removed for low Reynolds number flow. The instability found in the literature is caused by mismatched boundary values. By implementing an extra step to get the approximate matched boundary values, we obtain a stable numerical scheme in the low Reynolds number limit.

The classical example of 2-D driven cavity problem is used for the study of stability analysis. However, for simplicity, we first analyze a reduced 1-D model and then go to the 2-D cavity problem. Results and comparisons are presented for both cases.
2.2 The vorticity-stream function formulation

The idea of the vorticity-stream function formulation for Navier-Stokes equations in planar or axisymmetric system is to take advantage of the fact that the vorticity \( \omega = (0, 0, \zeta) \) has only one component. By change of variable using the relation in (1.14) and (1.15), we solve the system of one vorticity transport equation (1.12) and one stream function equation (1.13) instead of two velocity component equations and the continuity equation for \( u, v \) and pressure \( p \). So this technique is efficient in numerical computation.

\[
\frac{\zeta_t + u \zeta_x + v \zeta_y}{R} = \frac{1}{Re} (\zeta_{xx} + \zeta_{yy})
\]

(2.1)

\[
\psi_{xx} + \psi_{yy} = -\zeta
\]

(2.2)

The specification of boundary conditions is very important since it directly affects the stability and accuracy of the solution. For the cavity problem, \( \psi \) values are constants at the wall surfaces and are usually set to zero (no permeability condition). However, there is no physical condition for vorticity at the boundaries and \( \zeta \) is determined by an expansion using no-slip conditions. The first order and second order expression [19] are the following:

First order:

\[
\zeta_w = \frac{2}{h^2} (\psi_w - \psi_{w-1}) - \frac{2u_w}{h}
\]

Second order:

\[
\zeta_w = \frac{1}{2h^2} (7\psi_w - 8\psi_{w-1} + \psi_{w-2}) - \frac{3u_w}{h}
\]

where \( \zeta_w, u_w \) are values on the walls and \( h \) is the spatial step size.

A brief description of a typical time-marching procedure [1] for solving the vorticity-stream function formulation is as follows:
1. Specify initial values for $\zeta$ and $\psi$ at time $t=0$;

2. Solve the vorticity transport equation (2.1) for $\zeta$ at each interior point at $t + \Delta t$; boundary conditions for $\zeta$ are obtained from $\psi$ at $t$.

3. Solve the stream function equation (2.2) for $\psi$ at all points;

4. Find the velocity components from $u = \psi_y$ and $v = -\psi_x$;

5. Determine boundary values of $\zeta$ using $\psi$ and $\zeta$ at interior points;

6. Return to Step 2 for the next time step.

From the above procedure, the boundary values of $\zeta$ are not treated correctly in the standard iteration procedure. As shown in Figure 2.1, the boundary values of $\zeta$ for the time step $t$ (points $\triangle$) and the time step $t + \Delta t$ (points $\circ$) are needed to update the values at interior points $\bullet$ if using ADI-type scheme to solve the vorticity transport equation; however, the boundary values of $\zeta$ at time step $t + \Delta t$ (points $\circ$) are not known yet and they are to be solved in Step 5. So the traditional scheme actually uses boundary values of $\zeta$ at time step $t$ (points $\triangle$) as values at time step $t + \Delta t$ (points $\circ$) to solve vorticity transport equation and the mismatched boundary condition causes the instability as we will see later. If the matched boundary values (points $\circ$) of $\zeta$ are used, then this scheme retains the unconditional stability as the ADI scheme does in the usual cases.
2.3 The reduced 1-D problem

In this case, the fluid flow is driven by the upper plane in an infinite long strip while the lower plane stays still. Then the problem is in 1-D domain, and we can analyze the stability more easily.

2.3.1 The governing equations

In this 1-D problem, all variables are only functions of \( y \), so the Navier-Stokes equations become

\[
\zeta_t = \frac{1}{Re} \zeta_{yy} \tag{2.3}
\]

\[
\psi_{yy} = -\zeta \tag{2.4}
\]

where \( \zeta \) is the vorticity, \( \psi \) is the stream function and \( u = \psi_y, v = 0 \). The stream function \( \psi \) is constant on the walls and is usually set to zero. The boundary values of \( \zeta \) can be approximated by the values of \( \psi \) on interior points as in previous section.
2.3.2 Discrete formulation

First we use the implicit scheme to solve (2.3) because of its simplicity. We also present similar result for the Crank-Nicholson scheme.

\[
\frac{\zeta_{m+1}^{n+1} - \zeta_{m}^{n}}{\Delta t} = \frac{1}{Re} \left( \frac{\zeta_{m+1}^{n+1} - 2\zeta_{m}^{n+1} + \zeta_{m-1}^{n+1}}{h^2} \right) \tag{2.5}
\]

\[
\frac{\psi_{m+1}^{n+1} - 2\psi_{m}^{n+1} + \psi_{m-1}^{n+1}}{h^2} = -\zeta_{m}^{n+1} \tag{2.6}
\]

where \( m = 1, 2, \ldots, N - 1 \), and the \( n \) refers to time level.

The boundary conditions are:

\[
u(0) = 0, \quad u(1) = 1
\]

\[
\psi(0) = \psi(1) = 0
\]

\[
\zeta_{0} = \frac{2\psi_{1}}{h^2}
\]

\[
\zeta_{N} = \frac{2\psi_{N-1}}{h^2} - \frac{2u_{N}}{h}
\]

Here, the boundary values of the stream function \( \psi \) are constants and are set to zero at the walls. The first order approximation of the boundary values of vorticity \( \zeta \) are used.

2.3.3 Basic analysis

We show that the discrete problem (2.5) and (2.6) is unstable with mismatched boundary condition unless \( \Delta t < 2Reh^2 \).

We use von Neumann method to study the stability problem, then

\[
\zeta_{m}^{n} = Z_{m} e^{ikm\Delta y}, \quad \psi_{m}^{n} = P_{m} e^{ikm\Delta y}.
\]
It is obvious that the implicit scheme is unconditionally stable at the interior points. But near the upper boundary, we have

\[
\frac{\zeta_{N-1}^{n+1} - \zeta_{N-1}^n}{\Delta t} = \frac{1}{Re} \left( \frac{\zeta_{N}^{n+1} - 2\zeta_{N-1}^{n+1} + \zeta_{N-2}^{n+1}}{h^2} \right)
\]  

(2.7)

\[
\frac{\psi_{N}^{n+1} - 2\psi_{N-1}^{n+1} + \psi_{N-2}^{n+1}}{h^2} = -\zeta_{N-1}^{n+1}
\]  

(2.8)

with boundary conditions

\[u_N = 1, \quad \psi_N = 0, \quad \zeta_N = -\frac{2\psi_{N-1}^{n+1} - 2u_N}{h},\]

\[\zeta_{N}^{n+1} \text{ is unknown in (2.7) and the boundary conditions are used to approximate } \zeta_{N}^{n+1} \text{ by values of } \psi_N. \text{ Because } \psi_{N}^{n+1} \text{ is unknown at this point, } \psi_{N}^{n+1} \text{ is usually adopted as the basis for the boundary value needed to approximate } \zeta_{N}^{n+1} \text{ in the usual schemes. We refer to this use of boundary values at the } n \text{th time level to approximate boundary values at the } (n + 1) \text{th time level as mismatched boundary values.}
\]

\[
\zeta_{N}^{n+1} = \frac{2\psi_{N-1}^{n+1} - 2u_N}{h^2},
\]  

(2.9)

\[\psi_N = 0 \text{ in equation (2.8) and } \psi_{N-2}^{n+1} = e^{-ik\Delta y} \psi_{N-1}^{n+1}, \text{ so (2.8) becomes}
\]

\[
0 - 2\psi_{N-1}^{n+1} + e^{-ik\Delta y} \psi_{N-1}^{n+1} = -\zeta_{N-1}^{n+1}
\]  

then we have

\[
\psi_{N-1}^{n+1} = \frac{h^2}{2 - e^{-ik\Delta y}} \zeta_{N-1}^{n+1}.
\]  

(2.10)

Substituting \(\psi_{N-1}^{n+1}\) in (2.9) by expression in (2.10) gives

\[
\zeta_{N}^{n+1} = -\frac{2}{2 - e^{-ik\Delta y}} \zeta_{N-1}^{n+1} - \frac{2u_N}{h}
\]  

(2.11)

then the discrete vorticity transport equation (2.7) becomes

\[
(Z^{n+1} - Z^n)e^{ik(N-1)\Delta y} = \frac{\Delta t}{h^2 Re} \left( -\frac{2}{2 - e^{-ik\Delta y}} Z^n e^{ik(N-1)\Delta y} + \frac{2u_N}{h} - (2 - e^{-ik\Delta y}) Z^{n+1} e^{ik(N-1)\Delta y} \right)
\]
then

\[(1 + d(2 - \alpha))Z^{n+1} = \left(1 - \frac{2d}{2 - \alpha}\right)Z^n - \frac{2du_N}{h}e^{-ik(N-1)\Delta y}\]  \hspace{1cm} (2.12)

where \(d = \Delta t/(h^2Re), \alpha = \exp(-ik\Delta y)\), so we get

\[Z^{n+1} = \lambda Z^n + C\]

where

\[
\lambda = \frac{1 - 2d/(2 - \alpha)}{1 + d(2 - \alpha)}, \quad C = -\frac{2du_Ne^{-ik(N-1)\Delta y}}{1 + d(2 - \alpha)}.
\]

The numerical scheme is stable if \(|\lambda| \leq 1\) for all obtainable values of \(d\) and \(\alpha\).

If \(\alpha = 1\) then

\[\lambda = \frac{1 - 2d}{1 + d},\]

so \(\lambda < -1\) if \(d < 2\), which means the scheme is unstable if \(\Delta > 2Re\Delta y^2\). From the following plot, we can see that this scheme is conditionally stable for \(d < 2\), i.e., \(\Delta t < 2Re\Delta y^2\).

If we use the correct value of \(\zeta_N^{n+1}\) in (2.7) instead of the mismatched boundary value, then boundary relation (2.9) is

\[\zeta_N^{n+1} = -\frac{2\psi_{N-1}^{n+1}}{h^2} - \frac{2u_N}{h},\]  \hspace{1cm} (2.13)
Substituting $\psi^{n+1}_N$ given by expression in (2.10) we find

$$\zeta^{n+1}_{N-1} = -\frac{2}{2 - e^{-i(\Delta y)}} \zeta^{n+1}_{N-1} - \frac{2u_N}{h}. \quad (2.14)$$

Using matched boundary values of $\zeta$, the discrete vorticity transport equation (2.7) then becomes

$$\left(1 + d(2 - \alpha) + \frac{2d}{2 - \alpha}\right) Z^{n+1} = Z^n - \frac{2du_N}{h} e^{-i(\Delta y)}$$

so

$$\lambda = \frac{1}{1 + 2d/(2 - \alpha) + d(2 - \alpha)}$$

and $|\lambda| < 1$ for any $d$ and $\alpha$. So this scheme is unconditional stable if matched boundary values are used.

### 2.3.4 Modified boundary treatment

In this section we show how to find the matched boundary values. With the correct boundary values, the implicit scheme for solving the vorticity transport equation is unconditional stable.

Since the boundary values of $\zeta$ on time step $(n+1)$ are unknown in (2.7), we assume $\zeta_0^{n+1} = a, \zeta_N^{n+1} = b$, where $a, b$ can be determined later. Applying (2.5) at all interior points yields the following system of equations:

$$\begin{pmatrix} 1+2d & -d & 0 & \ldots & 0 \\ -d & 1+2d & -d & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & -d & 1+2d & -d \\ 0 & \ldots & 0 & -d & 1+2d \end{pmatrix} \begin{pmatrix} \zeta_1^{n+1} \\ \zeta_2^{n+1} \\ \vdots \\ \zeta_{N-2}^{n+1} \\ \zeta_{N-1}^{n+1} \end{pmatrix} = \begin{pmatrix} \zeta_0^n + ad \\ \zeta_1^n \\ \vdots \\ \zeta_{N-2}^n \\ \zeta_{N-1}^n + bd \end{pmatrix},$$

which can be rewritten as:

$$A\zeta^{n+1} = \zeta^n + a\zeta + b\zeta \quad (2.16)$$
where $A$ is the matrix, $\zeta = (d, 0, \ldots, 0)^T$ and $\bar{\zeta} = (0, \ldots, 0, d)^T$.

Because (2.16) is a linear system, the solution can be written as:

$$\zeta = z^* + a\bar{z} + b\bar{z}$$

(2.17)

where $z^*$, $\bar{z}$ and $\bar{z}$ are solutions of $A\zeta^{n+1} = \zeta^n$, $A\zeta^{n+1} = \zeta^n$ and $A\zeta^{n+1} = \bar{\zeta}$.

Then we can use $\zeta$ in (2.16) to force the stream function equation

$$\psi_{yy} = -z^* - a\bar{z} - b\bar{z}$$

(2.18)

and the solution can be written as

$$\psi = p^* + ap + b\bar{p}$$

where $p^*$, $p$ and $\bar{p}$ are solutions of $p^*_{yy} = -z^*$, $p_{yy} = -\bar{z}$ and $\bar{p}_{yy} = -\bar{z}$.

From the boundary condition relations, we have

$$a = -\frac{2}{h^2}\psi_1,$$

$$b = -\frac{2}{h^2}\psi_{N-1} - \frac{2u_N}{h}.$$

We then get equations for $a$ and $b$,

$$\left(1 + \frac{2}{h^2}\bar{p}_1\right) a + \frac{2}{h^2}\bar{p}_1 b = -\frac{2}{h^2}p^*_1,$$

$$\frac{2}{h^2}p_{N-1} a + \left(1 + \frac{2}{h^2}\bar{p}_{N-1}\right) b = -\frac{2}{h^2}p^*_{N-1} - \frac{2u_N}{h}.$$

Solving equations for $a$ and $b$ and substituting them back into (2.17) and (2.18), we get all solutions for $\zeta$ and $\psi$ at time step $(n+1)$.

### 2.3.5 Crank-Nicholson scheme for vorticity transport equation

If we use Crank-Nicholson scheme to solve vorticity transport equation (2.3), we have

$$\zeta^{n+1}_{N-1} - \zeta^n_{N-1} = \frac{d}{2}(\zeta^{n+1}_N - 2\zeta^{n+1}_{N-1} + \zeta^{n+1}_{N-2}) + \frac{d}{2}(\zeta^n_N - 2\zeta^n_{N-1} + \zeta^n_{N-2}).$$

(2.19)
Figure 2.4 Locus of $\lambda$ for the Crank-Nicholson scheme of vorticity transport equation.

In the usual method, the boundary values of $\zeta$ are mismatched

$$\psi_{N-1}^{n+1} = -\frac{2}{2 - e^{-iky}}c_{N-1}^n - \frac{2u_N}{h}$$

(2.20)

and thus cause instability. Analysis shows

$$\left\{1 + d\left(1 - \frac{\alpha}{2}\right)\right\}Z^{n+1} = \left\{1 - d\left(1 - \frac{\alpha}{2} + \frac{2}{2 - \alpha}\right)\right\}Z^n + C$$

where $C = -du_0e^{-iky}/h$, so

$$\lambda = \frac{1 - d(1 - \alpha/2) - 2/(2 - \alpha)}{1 + d(1 - \alpha/2)}.$$

When $\alpha = 1$, we see

$$\lambda = \frac{1 - 5d/2}{1 + d/2}$$

so $\lambda < -1$ when $d > 1$. From the Figure 2.4, we can see that this scheme is conditionally stable for $d < 1$, i.e., $\Delta t < Re\Delta y^2$. By implementing this extra step to find the correct boundary values, we get an unconditionally stable scheme as shown in previous analysis.

With the modified scheme, we take an extra step to solve the boundary values $\zeta_0^{n+1}$ and $\zeta_N^{n+1}$ at first, then (2.20) becomes

$$\psi_{N-1}^{n+1} = -\frac{2}{2 - e^{ikx}}c_{N-1}^{n+1} - \frac{2u_N}{h}$$
then the discrete vorticity transport equation becomes
\[ \left\{ 1 + d \left( 1 - \frac{\alpha}{2} + \frac{1}{2 - \alpha} \right) \right\} Z_{n+1} = \left\{ 1 - d \left( 1 - \frac{\alpha}{2} + \frac{1}{2 - \alpha} \right) \right\} Z_n + C \]
where \( C = -du_w \exp(-iky)/h \), so
\[ \lambda = \frac{1 - d(1 - \alpha/2 + 1/(2 - \alpha))}{1 + d(1 - \alpha/2 + 1/(2 - \alpha))} \]
and \(|\lambda| < 1\) for any \( d \) and \( \alpha \), so the fixed scheme is unconditionally stable.

2.3.6 Crank-Nicholson scheme for the stream function equation

If we introduce a time-dependent term \( \epsilon \psi_t \) in (2.4), then (2.4) becomes
\[ \epsilon \psi_t = \psi_{yy} + \zeta, \]
and the elliptic type equation is changed into parabolic time-dependent problem, when iteration to convergence is used and \( \epsilon \psi_t \to 0 \), we get the approximate solution of (2.4). This scheme is often useful in high dimension problems \([17]\) while the number of iterations is usually less than 32 and greater than 16 \([9]\). We will use Crank-Nicholson scheme, then the stability analysis becomes difficult to study analytically.

For simplicity, we take \( \Delta t \) and \( \Delta y \) the same as in (2.5), then the discrete form is
\[ \frac{\psi_{n+1}^{N-1} - \psi_{n-1}^N}{\Delta t/\epsilon} = \frac{1}{2} \frac{\psi_{n+1}^N - 2\psi_{n+1}^{N-1} + \psi_{n-1}^{N-1}}{\Delta y^2} + \frac{1}{2} \frac{\psi_n^N - 2\psi_{n-1}^N + \psi_{n-2}^N}{\Delta y^2} + \epsilon_{n-1}^{n+1}. \]

For the mismatched case,
\[ A = \begin{pmatrix} 1 + c - \frac{ac}{2} & -\Delta t/\epsilon \\ 0 & 1 + d - \frac{ad}{2} \end{pmatrix}, \quad B = \begin{pmatrix} 1 - c + \frac{ac}{2} & 0 \\ -\frac{2d}{h^2} & 1 - d + \frac{ad}{2} \end{pmatrix} \]
where \( c = \Delta t/(\epsilon h^2) \), \( d = \Delta t/h^2 Re \), \( \alpha = e^{-ik\Delta y} \). Solving the eigenvalue problem numerically for \( A^{-1}B \) shows that \( \max |\lambda| < 1 \) only for \( \Delta t < \epsilon a Re \Delta x^2 \), where \( a \) varies with \( Re \) and \( a \approx 1 \). Figure 2.5 shows the \( \max |\lambda| > 1 \) for \( d = 1.5, \epsilon = 1.0 \).
With matched boundary values for $\zeta$, we get

$$A \left[ \begin{array}{c} P^{n+1} \\ Z^{n+1} \end{array} \right] = B \left[ \begin{array}{c} P^n \\ Z^n \end{array} \right],$$

here

$$A = \begin{pmatrix} 1 + c - \frac{ac}{2} & -\Delta t/\varepsilon \\ \frac{d}{h^2} & 1 + d - \frac{ad}{2} \end{pmatrix}, \quad B = \begin{pmatrix} 1 - c + \frac{ac}{2} & 0 \\ -\frac{d}{h^2} & 1 - d + \frac{ad}{2} \end{pmatrix}.$$

Solving the eigenvalue problem numerically for $A^{-1}B$ shows that $\max|\lambda| < 1$ for all $\Delta t$. The Fig. 2.6 shows that $\max|\lambda| < 1$ for $d = 10, \varepsilon = 0.2$; thus, the scheme is stable in this case.

2.3.7 Remarks

From the Figure 2.6, we notice that $\lambda \to -1$ for large $d$. This means that the scheme can be oscillatory although it is stable. The numerical transient solution overshoots and oscillates about the steady state solution, as shown in Figure 2.7. These oscillations are an inherent feature of the Crank-Nicholson method when $d$ becomes big [12].
Figure 2.6 Locus of $\lambda$ for matched scheme

Figure 2.7 The oscillation behavior of Crank-Nicholson Scheme
Implicit scheme can be used to reach the steady state solution quickly and there is no oscillation for large $d$, but the transient state solution lags the exact transient solution, as shown in Figure 2.8.

The previous stability analysis is based on a first order approximation for boundary values of $\zeta$, if second order approximation is used, then the stability analysis is similar. The relation (2.10) becomes

$$\zeta_{N+1}^{n+1} = -\frac{8 - \alpha}{4 - 2\alpha} \zeta_{N-1}^{n+1} - \frac{2u_N}{h}$$

and for implicit scheme, mismatched case, we can find that

$$\lambda = \frac{1 - d(8 - \alpha)/(4 - 2\alpha)}{1 + d(2 - \alpha)}$$

If $\alpha = 1$ then

$$\lambda = \frac{1 - 7d/2}{1 + d}$$

so $\lambda = -1$ when $d = 4/5$, the scheme is unstable for $\Delta t < (4/5)h^2Re$.

If the boundary values are matched, similarly we get

$$\lambda = \frac{1}{1 + d(8 - \alpha)/(4 - 2\alpha) + d(2 - \alpha)}$$

and $|\lambda| < 1$ for any $d$ and $\alpha$, so the scheme is unconditionally stable.
The stability analysis for the Crank-Nicholson scheme is much similar to the implicit scheme.

To find the correct boundary values with second order approximation, we need to change the equations for $a$ and $b$ in section 2.3.4 by

$$a = -\frac{1}{h^2}(-7\psi_0 + 8\psi_1 - \psi_2) - \frac{3u_0}{h}$$

$$b = -\frac{1}{h^2}(-7\psi_N + 8\psi_{N-1} - \psi_{N-2}) - \frac{3u_N}{h}$$

The steady state solution of (2.3) and (2.4) can be found by solving

$$\zeta_{yy} = 0, \quad \psi_{yy} = -\zeta$$

with boundary conditions

$$\psi(0) = \psi(1) = 0, \quad u(0) = 0, u(1) = 1$$

where $u = \psi_y$. The solutions are

$$\zeta(y) = -6y + 2, \quad \psi(y) = y^3 - y^2, \quad u(y) = 3y^2 - 2y.$$

### 2.4 Analysis for the 2-D cavity problem

The 2-D cavity problem illustrated in Figure 2.9 is a classical example to test the numerical method for solving the incompressible Navier-Stokes equations. The upper lid is moving with velocity $U$ and the other wall surfaces remain still with viscous fluid in the enclosed region.

We will study the Stokes problem first and show that the instability can be fixed by introducing an extra step to get the exact boundary values of $\zeta$. For low Reynolds number Navier-Stokes problem, we can approximate the matched boundary values of $\zeta$ by solving Stokes problem and using them to solve N-S equations.
Figure 2.9 The classical cavity problem.

2.4.1 Stability analysis of 2-D Stokes problem

The Stokes equations in 2-D domain are

\[ \zeta_t = \frac{1}{Re} (\zeta_{xx} + \zeta_{yy}) \]  
\[ (2.21) \]

\[ \psi_{xx} + \psi_{yy} = -\zeta \]  
\[ (2.22) \]

Assume we solve (2.21) by implicit scheme and solve (2.22) directly, then the discrete forms are

\[ \frac{\zeta_{i,j}^{n+1} - \zeta_{i,j}^{n}}{\Delta t} = \frac{1}{Re} \left\{ \frac{\zeta_{i+1,j}^{n+1} - 2\zeta_{i,j}^{n+1} + \zeta_{i-1,j}^{n+1}}{\Delta x^2} + \frac{\zeta_{i,j+1}^{n+1} - 2\zeta_{i,j}^{n+1} + \zeta_{i,j-1}^{n+1}}{\Delta y^2} \right\} \]  
\[ (2.23) \]

\[ \frac{\psi_{i+1,j}^{n+1} - 2\psi_{i,j}^{n+1} + \psi_{i-1,j}^{n+1}}{\Delta x^2} + \frac{\psi_{i,j+1}^{n+1} - 2\psi_{i,j}^{n+1} + \psi_{i,j-1}^{n+1}}{\Delta y^2} = -\zeta_{i,j}^{n+1} \]  
\[ (2.24) \]

We use first order expression to approximate the boundary values of \( \zeta \)

\[ \zeta_{w} = -\frac{2}{h^2} \psi_{w-1}^{n} - \frac{2u_{w}}{h} \]

where \( \Delta x = \Delta y = h \) for simplicity, \( \zeta_{w} \) and \( u_{w} \) are values on the wall.

Using the von Neumann method, we take a general Fourier component of \( \zeta_{i,j}^{n} \) and \( \psi_{i,j}^{n} \) as follows:

\[ \zeta_{i,j}^{n} = Z^n e^{i(m(\theta_2 i \Delta x + \theta_2 j \Delta y))} \]
where $I_m = \sqrt{-1}$, $\theta_x$ and $\theta_y$ are wave numbers.

On the grid point $(N - 1, j)$ we have

\[
\zeta_{N,j} = -\frac{2}{h^2} \psi_{N-1,j} - \frac{2u_{N,j}}{h}
\] (2.25)

Also from (2.24),

\[
0 - 2\psi_{N-1,j}^{n+1} + \psi_{N-2,j}^{n+1} + \frac{1}{h^2} (2\cos(\theta_y \Delta y) - 2) \psi_{N-1,j}^{n+1} = -\zeta_{N-1,j}^{n+1}
\]

and $\psi_{N-2,j}^{n+1} = e^{-i\theta_x \Delta x} \psi_{N-1,j}^{n+1}$, so

\[
\{(2 - e^{-i\theta_x \Delta x}) + (2 - 2\cos(\theta_y \Delta y))\} \psi_{N-1,j}^{n+1} = h^2 \zeta_{N-1,j}^{n+1}.
\]

Denoting $e^{-i\theta_x \Delta x} = \alpha, \theta_y \Delta y = 2\beta$, then

\[
\psi_{N-1,j}^{n+1} = \frac{h^2}{2 - \alpha + 4\sin^2 \beta} \zeta_{N-1,j}^{n+1}.
\]

Substituting $\psi_{N-1,j}$ into (2.25) and $u_N = 0$ we get

\[
\zeta_{N,j} = -\frac{2}{2 - \alpha + 4\sin^2 \beta} \zeta_{N-1,j}.
\]

The mismatched boundary values of $\zeta$ are used in the standard scheme, where the values of $\psi_{w-1}$ at time step $(n)$ are used to approximate the values of $\zeta_w$ at time step $(n + 1)$ in (2.25), then we get

\[
\zeta_{N,j}^{n+1} = -\frac{2}{2 - \alpha + 4\sin^2 \beta} \zeta_{N-1,j}^{n}.
\]
Putting this into (2.23) we get

$$\zeta_{N-1,j}^{n+1} - \zeta_{N-1,j}^n = d \left( \zeta_{N,j}^{n+1} - 2\zeta_{N-1,j}^{n+1} + \alpha \zeta_{N-1,j}^{n+1} \right) + 4d \sin^2 \beta \zeta_{N-1,j}^{n+1},$$

where \( d = \Delta t / (h^2 Re) \), so

$$Z^{n+1} = \lambda Z^n$$

where

$$\lambda = \frac{1 - 2d/(2 - \alpha + 4\sin^2 \beta)}{1 + 4d \sin^2 \beta + d(2 - \alpha)}.$$

If \( \beta = 0, \alpha = 1 \), then

$$\lambda = \frac{1 - 2d}{1 + d}$$

\( \lambda < -1 \) when \( d > 2 \), the scheme is unstable.

If we use the matched boundary values of \( \zeta \) in (2.25), then

$$\zeta_{N,j}^{n+1} = -\frac{2}{2 - \alpha + 4\sin^2 \beta} \zeta_{N-1,j}^{n+1}$$

is used in (2.23), so

$$\lambda = \frac{1}{1 + 4d \sin^2 \beta + d(2 - \alpha) + 2d/(2 - \alpha + 4\sin^2 \beta)}.$$

Thus, \(|\lambda| < 1\) for all \( \alpha, \beta \) and \( d \), so the scheme with matched boundary values is unconditional stable.

### 2.4.2 The matched boundary value scheme

It is clear that if matched boundary values of \( \zeta \) are used in solving the vorticity transport equation, then the scheme is unconditional stable. In the 2-D case, it is more difficult to find the matched boundary values than in the 1-D case. Assume the grid is of \((N) \times (N)\) then there are \(4N - 4\) unknown boundary values of \( \zeta \) at time step \((n+1)\). Denoting them by \( \alpha_i, i = 1, 2, \ldots, 4(N - 1) \) as shown in Figure 2.11, we will solve these \( \alpha \)'s first, then use these correct boundary values to solve (2.23).
Equation (2.23) can be written as:

\[ M \zeta^{n+1} = \zeta^n + d \sum_{i}^{4N-4} e^{(i)} \alpha_i \]

where

\[
M_{(N-1)^2 \times (N-1)^2} = \begin{pmatrix}
D & E & 0 & \ldots & 0 \\
E & D & E & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & E & D & E \\
0 & \ldots & 0 & E & D \\
\end{pmatrix},
\]

\[
D_{(N-1) \times (N-1)} = \begin{pmatrix}
1+4d & -d & 0 & \ldots & 0 \\
-d & 1+4d & -d & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & -d & 1+4d & -d \\
0 & \ldots & 0 & -d & 1+4d \\
\end{pmatrix},
\]

\[ E_{(N-1) \times (N-1)} = d I_{(N-1) \times (N-1)} \]

and \( e^{(i)} = (0, \ldots, 0, 1, 0, \ldots, 0, 0)^T \).

We can write the solution as

\[ \zeta = z^* + \sum_{i}^{4N-4} z^{(i)} \]

where \( z^*, z^{(i)} \) correspond to the solutions of \( M\zeta^{n+1} = \zeta^n, M\zeta^{n+1} = de^{(i)} \).
Then we can use \( \zeta \) to solve stream function equation

\[
\psi_{xx} + \psi_{yy} = -z^* - \sum_{i}^{4N-4} z^{(i)}
\]

and the solution can be written as

\[
\psi = p^* + \sum_{i}^{4N-4} p^{(i)}
\]

where \( p^*, p^{(i)} \) correspond to the solutions of \( \Delta \psi = -z^*, \Delta \psi = -z^{(i)} \).

From the boundary conditions, we get equations for \( \alpha_i \):

\[
\alpha_i = -\frac{2}{h^2} (p_{w-1}^* + \sum_{k=1}^{4N-4} \alpha_k p_{w-1}^{(k)}) - \frac{2u_w}{h}
\]

where \( i = 1, \ldots, 4N - 4 \). Solving these equations for \( \alpha \)'s then we get the matched boundary values for \( \zeta \) at current time. From the previous stability analysis, using these matched boundary values for \( \zeta \) in (2.23) will give a stable scheme.

As we can see, we need to solve the system \( Mx = e^{(i)} \) once before the time-march, and solve the transport equation with \( \zeta^{n+1} = 0 \) at the boundary and corresponding stream function equation one more time and solve a \( (4N - 4) \times (4N - 4) \) system for \( \alpha \)'s (the matched boundary values of \( \zeta \)) during each iteration. These are the tradeoffs to retain the stability of vorticity-stream function formulation. Notice that the matrix \( M \) is sparse and symmetric, so we may use a fast iteration method such as CJG (Conjugate Gradient method) to solve the linear system instead of using ADI method or solving directly it.

### 2.4.3 2-D Navier-Stokes problem

For the 2-D Navier-Stokes problem, it is more complicated because of the nonlinear terms. Because the velocity components \( u \) and \( v \) for the current time step are unknown when solving vorticity transport equation, we can not find the exact matched boundary values of \( \zeta \) by the previous technique. However, for low Reynolds
number flow, these nonlinear terms are perturbations compared to the linear terms \( \Delta \zeta / Re \). Thus, we can solve the matched boundary values of the Stokes problem, and use these to approximate the boundary values of \( \zeta \) for current time step. Since the analytical stability analysis is very difficult for the Navier-Stokes equation, we only present the numerical comparison of the modified scheme and the standard scheme.

In this test case, the width and height of the cavity are both 1, the computation domain is on 20 \( \times \) 20 grid points. The Reynolds number of the flow is \( Re = 0.1 \), the driving force on the top lid has velocity \( u(x) = -16x^2(1 - x)^2 \) in order to avoid the singularities around the corner. For the standard scheme, the largest time step can be taken is \( \Delta t = Re \Delta x^2 = 2.5 \times 10^{-4} \) where the modified scheme is unconditional stable. There is no restriction on \( \Delta t \), but a large diffusion number \( d = \Delta t/(Re \Delta x^2) \) will cause transient solution to oscillate speciously. In this example, we take \( \Delta t = 2.5 \times 10^{-3} \); hence \( d = 10 \). The steady state solutions of vorticity agree up to 4 digit accuracy.
Figure 2.13 The steady state solution of the vorticity $\zeta$ in the cavity problem

Figure 2.14 The steady state solution of the stream function $\psi$ in the cavity problem
CHAPTER 3

THE NUMERICAL STUDY OF THE VISCOMETER PROBLEM

3.1 Overview

In this chapter, we present a numerical simulation of the falling-ball viscometer problem. The aim of this simulation is to capture the unsteady nature of and the inertial effects in this problem. The vorticity-stream function scheme is used to formulate the Navier-Stokes equations, and the ADI (Alternating Direction Implicit) method [1] is used to solve the vorticity transport equation and stream function equation. Because the fluid domain is changing with time due to the falling particle, we use a penalty region method to handle the moving boundary.

We will show the comparison of our numerical results to theoretical and experimental results in Stokes flow. The numerical stability problem and validation of this method is discussed. We also present a basic numerical study of the two-particle dynamics for small but nonzero Reynolds number flow.

3.1.1 The vorticity-stream function formulation in cylindrical coordinates

In the viscometer problem, the particle falls along the axis of the cylinder, so the flow is axisymmetric and cylindrical coordinate system is used. Introducing stream function $\psi$ and vorticity $\omega$. The velocity $v = (u, 0, w)$ and vorticity $\omega = (0, \zeta, 0)$ components in cylindrical coordinates $(r, z)$ can be expressed as

$$u = \frac{1}{r} \frac{\partial \psi}{\partial z}, \quad w = -\frac{1}{r} \frac{\partial \psi}{\partial r}, \quad \zeta = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial r},$$

combining the three relations gives the stream function equation:

$$\frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \psi}{\partial r} \right) + \frac{1}{r} \frac{\partial^2 \psi}{\partial z^2} = \zeta.$$

(3.1)
Taking curl of Navier-Stokes equation gives the vorticity transport equation:

\[
\frac{\partial \omega}{\partial t} - \nabla \times (v \times \omega) + \nu \nabla \times (\nabla \times \omega) = 0,
\]

in cylindrical coordinate system, this can be written as:

\[
\frac{\partial \zeta}{\partial t} + rw \frac{\partial}{\partial z} \left( \frac{\zeta}{r} \right) + ru \frac{\partial}{\partial r} \left( \frac{\zeta}{r} \right) = \nu \left[ \frac{\partial^2 \zeta}{\partial z^2} + \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r \zeta) \right) \right]
\]

(3.2)

Solving the coupled equations (3.1) and (3.2) with corresponding boundary conditions will get the flow field of the system.

### 3.1.2 The equations of falling ball viscometry

The equations of motion for the falling ball viscometer with one or more particles consists of Navier-Stokes equations which govern the fluid motion and ordinary differential equations which describe the motion of the particle under the forces exerted by gravity and the surrounding fluid,

\[
\rho \left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) + \nabla p = \mu \nabla^2 v \quad \text{in } D - \sum B_i
\]

\[
\nabla \cdot v = 0 \quad \text{in } D - \sum B_i
\]

\[
v = 0 \quad \text{on } \partial D
\]

\[
v = V_i \quad \text{on } \partial B_i
\]

\[
m_i \dot{V}_i = F_i + \int_{\partial B_i} \sigma \cdot n \, ds
\]

\[
\dot{X}_i = V_i
\]

where $D$ is the fluid domain, $B_i$ denotes the particles, $m_i$ are the particle mass, $\sigma$ is the stress tensor, $F_i$ is the external force acting on the particle which is usually gravity force excluding the buoyancy force, $X_i$ is the position of the particle and $V_i$ is the particle velocity. This formulation models multiple particles interacting with the fluid.
3.1.3 The boundary condition and penalty method

The moving particles cause the boundary of the fluid domain to change in time, the direct approach to the boundary condition is difficult. For this reason, a penalty method is used to give an approximate solution. By introducing a penalty term containing $\alpha$, the domain of the fluid equation is changed into a fixed one. The approximate system is then

$$\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) + \nabla p = \mu \nabla^2 \mathbf{v} + \alpha \sum_{i} \chi_{i} (\mathbf{V}_{i} - \mathbf{v}) \quad \text{in } D$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } D$$

$$m_{i} \dot{\mathbf{V}}_{i} = F_{i} - \alpha \sum_{i} \int_{B_{i}} (\mathbf{V}_{i} - \mathbf{v}) \, dx$$

$$\dot{\mathbf{X}}_{i} = \mathbf{V}_{i}$$

where $\chi_{i}$ is the characteristic function for each particles,

$$\chi = \begin{cases} 
1 & |\mathbf{x} - \mathbf{X}_{i}| < a \\
0 & \text{otherwise}
\end{cases}$$

$$\mathbf{V}_{i} = \begin{pmatrix} 0 \\ 0 \\ U_{i} \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} u \\ 0 \\ w \end{pmatrix}$$

Physically, the penalty method models the particles as a porous media. This system has a fixed domain; thus it provides an easier approach for numerical computation. As $\alpha \to \infty$, this converges exactly to the original system [14]. While we have introduced the porosity as a parameter for numerical purposes, our simulation naturally allows us to study sedimentation of porous particles.

3.1.4 The nondimensional form and the characteristic parameters

Before we start numerical computation, the system needs to be nondimensionalized. Let $L'$ be the characteristic length which we take to be the radius of the particle $a$, 

\begin{align*}
L' &= a + \dfrac{1}{\sqrt[3]{1 - \frac{\rho_{p}}{\rho}}} \\
U' &= \left( 1 + \dfrac{\rho_{p}}{\rho} \right) \dfrac{V_{m}}{L'} \\
\rho' &= \dfrac{\rho_{p}}{\rho_{m}} \\
T' &= T_{m} \left( 1 + \dfrac{\rho_{p}}{\rho} \right) \left( 1 + \dfrac{\rho_{p}}{\rho_{m}} \right) \\
\mu' &= \mu_{m} \\
\gamma' &= \gamma_{m} \\
\beta' &= \beta_{m} \\
\lambda' &= \lambda_{m}
\end{align*}
and let $U^*$ be the characteristic velocity. The characteristic time is then $\tau = L^*/U^*$. One choice for $U^*$ is the Stoke's velocity

$$U_{st} = \frac{F}{6\pi \mu a}$$

where $F = \tilde{m}g$ is the gravity force excluding the buoyancy force on the particle. We apply this choice to the dynamic sedimentation process. Another choice is to use the steady sedimentation velocity of the particle as the characteristic velocity. This choice is often used in some previous work where the position of the particle is fixed.

The Darcy-Brinkman law states:

$$\frac{\mu}{k} v_p + \nabla p = \mu \nabla^2 v_p.$$ 

Here the fluid velocity $v_p$ is the velocity field inside the porous sphere and $k$ is defined by the dimensionless permeability $\beta$ of sphere as:

$$\beta = a/\sqrt{k}$$

where $a$ is the radius of the particle. So, the penalty number $\alpha$ is a dimensional term related to $\beta$ by $\alpha = \mu \beta^2 / a^2$. Hence, the penalty term in our equations is consistent with the Darcy-Brinkman model of porous media [21].

Because the sedimentation velocity of particle is changing during the sedimentation process, we can not use the sedimentation velocity as the characteristic velocity. Thus, the Stokes's velocity is used to scale the velocity. We take $v = U^*v', V = U^*V', t = \tau t', x = ax', \alpha = \mu \beta^2 / a^2$. Dropping the primes (')
and considering the one particle case, we have

\[
\frac{\rho U_{st}^2}{a} \left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) + \nabla p = \mu \frac{U_{st}}{a^2} \nabla^2 v + \mu \frac{\beta^2 U_{st}}{a^2} \chi (V - v) \quad \text{in } D,
\]

\[
\nabla \cdot v = 0 \quad \text{in } D,
\]

\[
m \frac{U_{st}^2}{a} \dot{V} = \ddot{m} g - \alpha U_{st} a^3 \int_B (V - v) \, dx,
\]

\[
\dot{X} = V.
\]

The nondimensional form of the system is then

\[
\left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) + \nabla p = \frac{1}{Re} \nabla^2 v + \frac{\beta^2}{Re} \chi (V - v) \quad \text{in } D, \tag{3.3}
\]

\[
\nabla \cdot v = 0 \quad \text{in } D, \tag{3.4}
\]

\[
\delta \dot{V} = k - \frac{\beta^2}{6\pi} \int_B (V - v) \, dx, \tag{3.5}
\]

\[
\dot{X} = V, \tag{3.6}
\]

where

\[
Re = \frac{a U_{st} \rho}{\mu}, \quad \delta = \frac{m U_{st}^2}{\ddot{m} g} = \frac{2 \rho_p}{\rho_f} Re, \quad \beta = a \sqrt{\frac{\alpha}{\mu}}
\]

and \( k \) is the unit vector in the \( z \) direction.

If we want to study the steady state when the particle is settling at some static position, then we can use the particle velocity as the scaling velocity. In this case, the steady state of the equations are

\[
\frac{\rho U_{st}^2}{a} (v \cdot \nabla v) + \nabla p = \mu \frac{U}{a^2} \nabla^2 v + \mu \frac{\beta^2 U}{a^2} \chi (k - v) \quad \text{in } D
\]

\[
\nabla \cdot v = 0 \quad \text{in } D
\]

\[
0 = \ddot{m} g - \alpha U a^3 \int_B (k - v) \, dx.
\]
The nondimensional form of the system in this case is

\[
\left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) + \nabla p = \frac{1}{Re} \nabla^2 v + \frac{\beta^2}{Re} \chi(k - v) \quad \text{in } D \tag{3.7}
\]

\[
\nabla \cdot v = 0 \quad \text{in } D \tag{3.8}
\]

\[
F = \frac{\beta^2}{6\pi} \int_B (k - v) \, dx \tag{3.9}
\]

where

\[
\text{Re} = \frac{a \rho U}{\mu}, \quad F = \frac{\tilde{m}g}{6\pi \mu a U}, \quad \beta = a \sqrt{\frac{\alpha}{\mu}}.
\]

### 3.1.5 The vorticity-stream function formulation for the falling ball viscometer problem

To make use of the vorticity-stream function method, the characteristic function \( \chi \) has to be smoothed to mollify the singularity that arises in vorticity transport equation. Here,

\[
\chi(x - X) = \begin{cases} 
1 & |x - X| < a - \varepsilon \\
\frac{1}{2} - \frac{1}{2} \sin \frac{\pi |x - X|}{2\varepsilon} & a - \varepsilon < |x - X| < a + \varepsilon \\
0 & |x - X| > a + \varepsilon
\end{cases}
\]

where \( \varepsilon \ll a \), so we have the following formulation:

\[
\frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial r} - \frac{u \zeta}{r} + w \frac{\partial \zeta}{\partial z} = \frac{1}{Re} \left[ \frac{\partial^2 \zeta}{\partial r^2} + \frac{1}{r} \frac{\partial \zeta}{\partial r} - \frac{\zeta}{r^2} + \frac{\partial^2 \zeta}{\partial z^2} \right] - \frac{\beta^2}{Re} \left[ u \frac{\partial \chi}{\partial z} + (U - w) \frac{\partial \chi}{\partial r} \right] - \frac{\beta^2}{Re} \chi(x - X), \tag{3.10}
\]

\[
\frac{1}{r} \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r^2} \frac{\partial \psi}{\partial r} + \frac{1}{r} \frac{\partial^2 \psi}{\partial z^2} = \zeta, \tag{3.11}
\]

\[
\delta \dot{U} = 1 - \frac{\beta^2}{6\pi} \int_D (U - w) \chi(x - X) \, dx, \tag{3.12}
\]

\[
\dot{Z} = U. \tag{3.13}
\]
3.1.6 The numerical scheme—ADI method

The ADI (Alternating Direction Implicit) method is a stable and efficient method that is extensively used to solve parabolic type partial differential equations. We use the ADI scheme to solve the stream function equation by adding a time-dependent term $\psi_t$ which becomes very small after a few iterations. Thus, we get an approximate solution of the original equation. The discrete form of equations are the following:

\[
\frac{\psi_{i,j}^{n+1} - \psi_{i,j}^n}{\Delta t/2} = \frac{\psi_{i+1,j}^{n+1} - 2\psi_{i+1,j}^n + \psi_{i-1,j}^n}{r \Delta r^2} \\
- \frac{\psi_{i+1,j}^n - \psi_{i-1,j}^n}{r^2 \Delta r} + \frac{\psi_{i,j+1}^{n+1} - 2\psi_{i,j+1}^n + \psi_{i,j-1}^n}{r \Delta z^2} - \zeta_{i,j},
\]

\[
\frac{\psi_{i,j}^{n+1} - \psi_{i,j}^n}{\Delta t/2} = \frac{\psi_{i+1,j}^{n+1} - 2\psi_{i,j}^{n+1} + \psi_{i-1,j}^{n+1}}{r \Delta r^2} \\
- \frac{\psi_{i+1,j}^n - \psi_{i-1,j}^n}{r^2 \Delta r} + \frac{\psi_{i,j+1}^{n+1} - 2\psi_{i,j+1}^{n+1} + \psi_{i,j-1}^{n+1}}{r \Delta z^2} - \zeta_{i,j}.
\]

The vorticity transport equation is also solved using the ADI scheme, but here we need some modifications because of the penalty term that introduces stiffness into the system and must be handled correctly.

The vorticity transport equation can be rewritten as

\[
\zeta_t + u\zeta_r + v\zeta_z = \mu(\zeta_{rr} + \zeta_{zz}) - \alpha f - \gamma \zeta
\]

where $\mu$ denotes $1/Re$, $\alpha f$ denotes $\frac{\beta^2}{Re} (u \chi_z + (U - w) \chi_r)$ and $\gamma \zeta$ denotes $\frac{\beta^2}{Re} \zeta \chi$.

The averaged form of the discrete equation is

\[
\frac{\zeta^{n+1} - \zeta^n}{\Delta t} + \frac{u\zeta_r^{n+1} + v\zeta_z^{n+1}}{2} \left( \frac{u\zeta_r^n + v\zeta_z^n}{2} \right) = \frac{\mu}{2} (\partial_{rr} + \partial_{zz})\zeta^{n+1} + \frac{\mu}{2} (\partial_{rr} + \partial_{zz})\zeta^n \\
- \frac{\alpha}{2} (f^n + f^{n+1}) - \frac{\alpha}{2} (\zeta^n + \zeta^{n+1}).
\]

Denoting $D_r = \mu \partial_{rr} - \mu_r$, $D_z = \mu \partial_{zz} - v \partial_z$, $d = \Delta t/2$ and $e = \alpha \Delta t/2$ we have

\[
(1 - dD_r - dD_z + e)\zeta^{n+1} = (1 + dD_r + dD_z - e)\zeta^n - e(f^n + f^{n+1})
\]
this can be rewritten as
\[
(1 + e) \left( 1 - \frac{d}{1 + e} D_r - \frac{d}{1 + e} D_z \right) \zeta^{n+1} = (1 - e) \left( 1 + \frac{d}{1 - e} D_r - \frac{d}{1 - e} D_z \right) \zeta^{n+1} - e(f^n + f^{n+1})
\]
and factor as
\[
(1 + e) \left( 1 - \frac{d}{1 + e} D_z \right) \zeta^* = \left( 1 + \frac{d}{1 - e} D_r \right) \zeta^n - e f^n
\]
\[
\left( 1 - \frac{d}{1 + e} D_r \right) \zeta^{n+1} = (1 - e) \left( 1 + \frac{d}{1 - e} D_z \right) \zeta^* - e f^{n+1}.
\]
This leads to the following discrete form of the vorticity transport equation for the falling-ball viscometer problem with one particle. It is easily extended to multi-particle sedimentation problems with very little additional arithmetic needed in the simulation.
\[
\frac{\tilde{\zeta}_{i,j} - \zeta^n_{i,j}}{\Delta t/2} + w_{i,j} \frac{\zeta^n_{i,j+1} - \zeta^n_{i,j-1}}{2\Delta z} + u_{i,j} \frac{\tilde{\zeta}_{i+1,j} - \tilde{\zeta}_{i-1,j}}{2\Delta r} - \frac{u_{i,j}\tilde{\zeta}}{r}
\]
\[
= \frac{1}{\text{Re}} \left[ \frac{\zeta^n_{i,j+1} - 2\zeta^n_{i,j} + \zeta^n_{i,j-1}}{\Delta z^2} + \frac{\tilde{\zeta}_{i+1,j} - 2\tilde{\zeta}_{i,j} + \tilde{\zeta}_{i-1,j}}{\Delta r^2} + \frac{\tilde{\zeta}_{i+1,j} - \tilde{\zeta}_{i-1,j}}{r2\Delta r} \right]
\]
\[
- \frac{\tilde{\zeta}_{i,j}}{r^2} - \frac{\beta^2}{\text{Re}} \left[ u_{i,j} \left( \frac{\partial X}{\partial z} \right)_{i,j} + (U - w_{i,j}) \left( \frac{\partial X}{\partial r} \right)_{i,j} \right] - \frac{\beta^2}{\text{Re}} \tilde{\zeta}_{i,j} X_{i,j}
\]
\[
\frac{\zeta^{n+1}_{i,j} - \tilde{\zeta}_{i,j}}{\Delta t/2} + w_{i,j} \frac{\zeta^{n+1}_{i,j+1} - \zeta^{n+1}_{i,j-1}}{2\Delta z} + u_{i,j} \frac{\tilde{\zeta}_{i+1,j} - \tilde{\zeta}_{i-1,j}}{2\Delta r} - \frac{u_{i,j}\tilde{\zeta}}{r}
\]
\[
= \frac{1}{\text{Re}} \left[ \frac{\zeta^{n+1}_{i,j+1} - 2\zeta^{n+1}_{i,j} + \zeta^{n+1}_{i,j-1}}{\Delta z^2} + \frac{\tilde{\zeta}_{i+1,j} - 2\tilde{\zeta}_{i,j} + \tilde{\zeta}_{i-1,j}}{\Delta r^2} + \frac{\tilde{\zeta}_{i+1,j} - \tilde{\zeta}_{i-1,j}}{r2\Delta r} \right]
\]
\[
- \frac{\tilde{\zeta}_{i,j}}{r^2} - \frac{\beta^2}{\text{Re}} \left[ u_{i,j} \left( \frac{\partial X}{\partial z} \right)_{i,j} + (U - w_{i,j}) \left( \frac{\partial X}{\partial r} \right)_{i,j} \right] - \frac{\beta^2}{\text{Re}} \zeta^{n+1}_{i,j} X_{i,j}
\]
3.1.7 The boundary conditions

The computational domain is bounded by rigid walls and the axis of the cylinder. The boundary conditions of the stream function are $\psi = 0$ on all rigid walls and on the axis. The values of vorticity on the rigid walls can be approximated by the values of the stream function from inner points using Taylor’s expansion. Also $\zeta = 0$ on the axis by symmetry.

On the top and bottom, we have

$$\psi_{b-1} = \psi_b - \Delta z \frac{\partial \psi_b}{\partial z} + \frac{\Delta z^2}{2} \frac{\partial^2 \psi_b}{\partial z^2},$$

$$\frac{\partial \psi}{\partial r} = ru, \quad \psi_b = 0$$
on the boundary, so

$$\psi_{b-1} = \frac{\Delta z^2}{2} \frac{\partial u}{\partial z}, \quad \text{and} \quad \zeta_b = \frac{2\psi_{b-1}}{r\Delta z^2}$$

On the side of the cylinder,

$$\psi_m = 0, \psi_{m-1} = \psi_m - \Delta r \frac{\partial \psi_m}{\partial r} + \frac{\Delta r^2}{2} \frac{\partial^2 \psi_m}{\partial r^2}$$

since $\frac{\partial \psi}{\partial r} = -rw$, then

$$\psi_{m-1} = \psi_m + \Delta r rw + \frac{\Delta r^2}{2}(-w + r\zeta).$$

Hence,

$$\zeta_m = \frac{2}{r\Delta r^2}(\psi_{m-1} - \Delta rrw) + \frac{w}{r}.$$  

On the axis of the cylinder, because the flow is axisymmetric, we have the following Taylor’s expansion for $\psi$:

$$\psi(r) = \psi(0) + \frac{r^2}{2} \psi''(0) + \frac{r^4}{24} \psi'''(0) + \ldots$$

and

$$\psi'(r) = r\psi''(0) + \frac{r^3}{6} \psi'''(0) + \ldots$$
where
\[ w(r) = -\frac{\psi'(r)}{r} = \psi''(0) + \frac{1}{6} r^2 \psi'''(0) + \ldots \]

Let
\[ \psi(r) = A + Br^2 + cr^4; \]
\[ \psi(0) = A = \psi_0 = 0, \]
\[ \psi(\Delta r) = A + B\Delta r^2 + C\Delta r^4 = \psi_1, \]
\[ \psi(2\Delta r) = A + 4B\Delta r^2 + 16C\Delta r^4 = \psi_2, \]

so
\[ w(0) = -\frac{16\psi_1 - \psi_2}{6\Delta r^2}. \]

3.2 Results and Discussion

3.2.1 Comparison with Faxen's line

Faxen's line gives the relationship between the hydrodynamic drag and Stokes' drag for a solid particle falling in an infinitely long cylinder.

\[ D = D_s \left( 1 + 2.1048 \left( \frac{a}{R} \right) \right) \]

Nondimensionalizing this result with \( D = \tilde{m}g, D_s = 6\pi \mu a U' \) and \( U' = UU_{st}, F = 6\pi \mu a U_{st} \) we have

\[ 1 = U \left\{ 1 + 2.1048 \left( \frac{a}{R} \right) \right\}. \]

This formula holds for low Reynolds number flow.

If the Reynolds number increases and the inertial effect is not ignored, then the drag and velocity relationship is described as

\[ D = (\pi a^2)(U^2)C_D/2 \]
where $C_D$ denotes the drag coefficient. The value of $C_D$ is $24/Re$ for Stokes’s flow. In this case, the above expression recovers Stokes’ law $D_s = 6\pi \mu a U$. For a larger Reynolds number, the following expression

$$C_D = 0.28 \left( 1 + \frac{9.06}{\sqrt{Re}} \right)^2$$

holds for $1 < Re < 1000$. In this case, the drag law is modified as

$$D_s = 6\pi \mu a U C_D / (24/Re)$$

so

$$U = \frac{24}{C_D Re (1 + 2.1048(a/R))}$$

for a particle falling in an infinitely long cylinder.

The following simulation keeps the particle at a particular position (by setting $X = 0$) and obtains the steady state solution. In this case a particle with radius $a = 1$ falls along the axis of a cylinder with height $L = 20$ and radius $R = 10$; the Reynolds number is $Re = 1.0$; the particle is fixed at $z = 10$—the center of the cylinder. The particle is emulated by a porous particle with a layer having thickness $\varepsilon$ and the porosity number $\beta$. We estimate the settling speed for the particle with $\varepsilon = 0$ by linear interpolation approximated from the results with different layer thickness $\varepsilon$’s. Stiffness associated with small $\varepsilon$ precludes direct computations for $\varepsilon = 0$. Figure 3.1 shows the settling speed with $\beta = 15.8$. Here the falling speed from Faxen’s correction is $1/(1+2.1048 \times 0.1) \approx 0.826$ and the result from simulation is 0.92. With the porosity property $\beta$ increased to 50, the approximate falling speed as shown in Figure 3.2 is about 0.84 which is very close to Faxen’s correction. Particles with porosity greater than approximately 50 can be regarded as nonporous particles [21]. Our simulations agree with Faxen’s correction when the results are extrapolated to the limits $\varepsilon \to 0$ and $\beta \to \infty$ and $Re = 1.0$. 
Figure 3.1 Sedimenting speed vs. different layer thickness ($\varepsilon$) for $Re = 1.0$, $\beta = 15.8$. Linear extrapolation from the cases $\varepsilon = 0.15, 0.20, 0.25$ and $0.30$ gives a sedimentation velocity of $0.92$.

Figure 3.2 Sedimenting speed vs different layer thickness ($\varepsilon$) for $Re = 1.0$, $\beta = 50$. Linear extrapolation from the cases $\varepsilon = 0.15, 0.20, 0.25$ and $0.30$ gives a sedimentation velocity of $0.84$ in good agreement with Faxen’s correction.
3.2.2 Comparison with Lorentz’s correction

Lorentz’s correction gives the modification of Stoke’s law for a solid particle approaching an infinite plane. Similarly, we can get the dimensionless form for our simulation as follows

\[ U = \frac{24}{C_D Re (1 + (9a/8H))} \]

where \( H = L - z \) is the distance from the particle to the bottom. Figure 3.3 shows that our simulation result agree well with the Lorentz’s correction near the end of the bottom. In this case, the particle with radius \( a = 1 \) falls along a cylinder with radius \( R = 10 \), height \( L = 20 \), here \( Re = 1.0 \).

3.2.3 Mesh refinement and comparison between dynamic and static simulations

The second test case is to compare the numerical results with refined timestep and refined spatial grid to show the convergence and consistency of the method. Here, simulation results with height \( L = 10 \), radius \( R = 5 \) with spatial step \( dx = 0.1, 0.05 \) and 0.025 are shown in the Figure 3.4 (porosity number \( \beta = 10, Re = 1.0 \)).
Result for dynamic sedimentation simulation can also be compared with steady state solution for particles fixed at particular positions. Table 3.1 shows the comparison of a dynamics simulation vs. results from stationary particles in a thin cylinder \((R = 2.5, L = 20), Re = 1.0, \beta = 15.8\). The dynamic trajectories start falling from \(z = 7\) and reach a quasi-steady state between \(z = 11\) to \(z = 16\). When the particle approaches the bottom, the difference increases because the end effect decelerate the particle and the sedimentation is not quasi-steady.

**Table 3.1** The comparison of dynamic and steady state sedimentation velocity

<table>
<thead>
<tr>
<th>(h/d)</th>
<th>(z)</th>
<th>velocity (dynamic)</th>
<th>velocity (stationary)</th>
<th>difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.0</td>
<td>11.0</td>
<td>0.2888</td>
<td>0.2890</td>
<td>0.07</td>
</tr>
<tr>
<td>3.0</td>
<td>13.0</td>
<td>0.2888</td>
<td>0.2890</td>
<td>0.07</td>
</tr>
<tr>
<td>2.0</td>
<td>15.0</td>
<td>0.2888</td>
<td>0.2890</td>
<td>0.07</td>
</tr>
<tr>
<td>1.5</td>
<td>16.0</td>
<td>0.2887</td>
<td>0.2890</td>
<td>0.10</td>
</tr>
<tr>
<td>1.0</td>
<td>17.0</td>
<td>0.2884</td>
<td>0.2886</td>
<td>0.07</td>
</tr>
<tr>
<td>0.5</td>
<td>18.0</td>
<td>0.2786</td>
<td>0.2770</td>
<td>0.58</td>
</tr>
<tr>
<td>0.3</td>
<td>18.4</td>
<td>0.2548</td>
<td>0.2488</td>
<td>2.40</td>
</tr>
<tr>
<td>0.2</td>
<td>18.6</td>
<td>0.2233</td>
<td>0.2169</td>
<td>2.90</td>
</tr>
</tbody>
</table>
3.2.4 Single particle sedimentation with different starting positions

In this numerical computation, a sphere with radius $a = 1$ falls along the axis of a circular cylinder with height $L = 20$ and radius $R = 10$, the sphere starts falling from different positions $L = 3, 5, 8, 10, 12, 15$ and down to the bottom ($L = 20$), the picture of sedimenting speed vs. sphere position with $Re = 1.0$ is presented in Figure 3.3.

In above simulations, particles are accelerated from rest initially by gravity. The particles far from the bottom reach a position dependent quasi-steady sedimentation velocity towards the middle of the cylinder. When these particles are close to the bottom, we see the numerical results agree with Lorentz’s correction very well and this is expected because Tanner’s numerical results show that the correction of a sphere approaching an infinite plane dominates other boundary effects when the sphere is very close to the bottom.

3.2.5 Multi-particle dynamics

Another capability of our simulation code is to simulate multiple particle dynamics. Simulating more than one particle involves almost no additional computational cost. The following are numerical results of two particle sedimentation processes. In these simulations, two identical particles with same radius $a = 1.0$ and porosity $\beta = 15.8$ fall along the axis of a cylinder with radius $R_0 = 10$ and length $L = 20$. The starting positions of the two particles are $z = 4$ and $z = 8$. We performed the computation for different Reynolds number $Re = 0.2, 0.3, 0.4$ and used the results to get an approximate relation of settling velocity vs. position as follows:

$$U(X, Re) = a(X) + Re b(X) + \frac{Re^2}{2} c(X).$$  \hspace{1cm} (3.14)
Then we use the approximation to predict the velocities at different positions for small Reynolds number $Re = 0.1$ and $Re = 0.5$. The comparison of prediction with simulation results are also presented.

In Figure 3.5 we see the velocity of the trailing particle as a function of its position for $Re = 0.2, 0.3$ and 0.4. All three experiments produce similar particle trajectories. Initially, the sedimentation velocity is larger for the smaller Reynolds numbers. This result is consistent with the energy dissipation analysis presented in sections 3.2.7 and 3.2.8. At a point between $x = 8$ and $x = 10$, this results is
Figure 3.7 Prediction and simulation result for the top particle with $Re = 0.1, 0.5$, sedimentation velocity vs. position. Trajectories from direct simulation and extrapolation from $Re = 0.2, 0.3, 0.4$ match well.

reversed and the sedimentation velocity is smaller for the smaller Reynolds numbers. A possible explanation for the result is the inertial diminution of the range of the end effect.

In Figure 3.6, we see the separation or gap between the two particles as a function of time. Initially, the gap increases with this effect most pronounced for the lower Reynolds numbers. This effect appears due to the resistance of the trailing particle to being pulled away from the top of the container. As the particles fall at some point, the gap begins shrink. Thus, the Lorentz correction appears to be diminished by inertia. This occurs due to the trailing particle drafting in the wake of the first particle. As the wake is an inertial effect, it is expected that the gap closes most rapidly for the higher Reynolds numbers.

We note that the lower Reynolds number simulations are more symmetric than the higher Reynolds number simulation. For Stokes flow, the falling trajectory is symmetric due to the time-reversal symmetry.
Figure 3.8 Prediction and simulation result for the lower particle with $Re = 0.1, 0.5$, sedimentation velocity vs. position. Trajectories from direct simulation and extrapolation from $Re = 0.2, 0.3, 0.4$ match well.

Figure 3.9 Two particle settling speeds vs. time with $Re = 1.0$. 
Figure 3.10 The velocity component w profile for two particle dynamics.

Figure 3.11 Streamlines for two particle sedimentation.
3.2.6 Discussion of simulation parameters

There are four parameters in the system. We focus on the $Re$ and how it affects the flow. The drag coefficient $C_D$ given in (3.2.1) characterizes the deviation from Stokes’s law for $1 < Re < 1000$. When $Re$ increase, the particle experience more hydrodynamic resistance. Since in low Reynolds number flow $\hat{U}$ is small, the hydrodynamic force fluid acting on the particle $(\beta^2/6\pi) \int \chi(x - X)(V - v) \, dx$ would be approximately equal to the scaled gravity force $F = 1$ in our example, so the sedimenting speed would decrease as shown in figure 3.13.

The parameter $\beta$ depicts the porosity of the particle and $\beta \to \infty$ is the limiting case when the particle becomes a rigid one. The Figure 3.12 shows that the particle is more susceptible to having fluid flow through it with smaller $\beta$ and becomes more like a rigid particle for larger $\beta$. As $\beta$ is increased the flow inside the particle is more consistent with the rigid body motion of a solid sphere.

The parameter $\epsilon$ is the layer thickness which we used to mollify the singularity in vorticity transport equation that arises at the interface between the particle and the fluid. From the numerical experiment, we can derive the settling speed for $\epsilon \to 0$ by linear interpolation. The parameter $\delta$ in section 3.1.4 indicates the relaxation
time for the particle to reach its quasi-steady velocity (when the magnitude of the hydrodynamic force acting on the particle converges to that of the gravity).

### 3.2.7 The inertial effect on sedimentation speed

Because of the inertial term effect, the hydrodynamic drag exerted on the particle is larger than Stokes's drag. This result is verified in the next subsection. So for a fixed weight particle, when Reynolds number increases, the dimensionless velocity decreases. This result can be verified as follows.

Assume $w$ denotes the weight of the particle, $w = f(v, Re)$ where $f$ is a function depends on two independent variables: the steady sedimentation velocity $v$ and the Reynolds number $Re$. Likewise, the steady state sedimentation velocity can be found in terms of $w$ and $Re$, $v = g(w, Re)$. The rate of energy dissipation $\dot{E} = w \cdot g(w, Re) = v \cdot f(v, Re)$.

Since $w = f(v, Re) = f(g(w, Re), Re)$, we have

$$1 = \frac{\partial f}{\partial v} \frac{\partial g}{\partial w}, \quad 0 = \frac{\partial f}{\partial v} \frac{\partial g}{\partial Re} + \frac{\partial f}{\partial Re}$$

so

$$\frac{\partial g}{\partial Re} = -\frac{\frac{\partial f}{\partial Re}}{\frac{\partial f}{\partial v}}$$

Since the sedimentation velocity is monotonically related to weight, so $\frac{\partial f}{\partial v} \geq 0$. Also, $\frac{\partial f}{\partial Re} \geq 0$ because the rate of energy dissipation increase with $Re$ according to the minimization principle of section 3.2.8 (with $v$ fixed). Thus we have

$$\frac{\partial g}{\partial Re} = -\frac{\frac{\partial f}{\partial Re}}{\frac{\partial f}{\partial v}} \leq 0$$

that is the sedimentation velocity decreases with increasing Reynolds number provided the hydrodynamic drag is fixed.
Figure 3.13 The variation of sedimentation velocity vs. $Re$. The sedimentation velocity decreases as the Reynolds number increase with the weight of the particle held constant.

### 3.2.8 Energy transport and conversion

In the scaled equations (3.3) the kinetic energy in the fluid is given by

$$\frac{1}{2} Re \int_D |\mathbf{v}|^2 \, dx,$$

and the kinetic energy of the particle is given by

$$\frac{1}{2} (6\pi \delta)|\mathbf{V}|^2.$$

In this subsection, we derive equations governing the conversion of the gravitational potential energy associated with the particle into kinetic energy and the conversion of kinetic energy into heat through viscous friction. Taking the inner product of (3.3) with $\mathbf{v}$ and integrating over the entire fluid domain $D$ gives (after some manipulation)

$$\frac{d}{dt} \frac{1}{2} Re \int_D |\mathbf{v}|^2 \, dx = - 2 \int_D e : e \, dx + \beta^2 \int_D \chi (\mathbf{V} \cdot \mathbf{v} - |\mathbf{v}|^2) \, dx \quad (3.15)$$

Taking the inner product of (3.5) with $\mathbf{V}$ gives

$$\frac{d}{dt} \frac{1}{2} (6\pi \delta)|\mathbf{V}|^2 = 6\pi \mathbf{V} \cdot \mathbf{k} + \beta^2 \int_D \chi (\mathbf{V} \cdot \mathbf{v} - |\mathbf{V}|^2) \, dx. \quad (3.16)$$
Adding (3.15) and (3.16) together gives an equation for the rate of change of the total kinetic energy

\[
\frac{d}{dt} \left[ \frac{1}{2} Re \int_D |\mathbf{v}|^2 \, dx + \frac{1}{2} (6\pi \delta)|\mathbf{V}|^2 \right] = 6\pi \mathbf{V} \cdot \mathbf{k} - 2 \int_D e : e \, dx - \beta^2 \int_D \chi |\mathbf{V} - \mathbf{v}|^2 \, dx.
\]

(3.17)

The three terms on the right hand side of (3.17) have clear physical interpretations: The first represents the power due to the conversion to gravitational potential energy to kinetic energy of the falling particle. The second is the usual expression in an incompressible fluid for the conversion of kinetic energy in the particle to heat through viscous friction. The third term represents an additional conversion of heat through viscous friction as the fluid squeezes through the porous media. This last term is a macroscopic theory for viscous energy dissipation in the microstructure of the porous media. In steady state, the energy converted from gravitational potential energy to kinetic energy balances the viscous dissipation of energy:

\[
6\pi \mathbf{V} \cdot \mathbf{k} = 2 \int_D e : e + \beta^2 \int_D \chi |\mathbf{V} - \mathbf{v}|^2 \, dx.
\]

(3.18)

If we take \( \mathbf{V} \) to be given and minimize the rate of energy dissipation (the right hand side of (3.18)) over incompressible flows \( \mathbf{v} \) satisfying the no-slip condition on \( \partial \Omega \), we find that \( \mathbf{v} \) satisfies (3.4) with \( Re = 0 \). That is, we obtain a generalization of the well-known result of Helmholtz that the rate of energy dissipation is minimized by the Stokes flow. Interestingly, if we fix the drag on the particle as a constraint rather than the velocity, the rate of energy dissipation is minimized by a Stokes flow but the particle velocity vanishes.

3.2.9 The stability problem

The mismatched boundary condition causes the instability which we resolved for the 2-D planar cavity example. However it turns out to be very difficult to resolve in the
viscometer simulation problem. The main reason is our treatment of the penalty term appear to be incompatible with the remedy for instability we see in the 2-D cavity problem. Hence, we are compelled to use very small time steps in our numerical simulations.
We implemented a numerical simulation for the dynamics of an axisymmetric flow in a falling-ball viscometer using a penalty method to overcome the moving boundary problem caused by the falling particles. By introducing a penalty number, the particle becomes a porous one and permeable to the fluid. When the penalty number goes to infinity, the flow converges to that for a rigid particle. This theoretical result was validated numerically. The method, however, is naturally increasing stiff as the porosity is increased. The extension to multiple particle simulation is natural and does not require significant additional computational resources.

By the penalty method, we are able to simulate the dynamics of fluid flow instead of using steady state approximations used in earlier work. For low Reynolds number flow, the full dynamical process does converge to quasi-steady approximation; nonetheless, significant dependence of the particle trajectories is found even for Reynolds number less than one.

We observed that the inclusion of inertia for a fixed drag decreases the sedimentation speed. A minimization principle tells us Stokes flow minimizes the energy dissipation in the flow for a particle with a fixed velocity. If a particle is falling in fluid with constant drag, then the velocity of the particle will decrease with the inclusion of inertia because the drag required to maintain the velocity increases.

The ADI scheme is an efficient method to solve high dimension parabolic partial differential equations. But it is also well known that this method becomes unstable for low Reynolds number flow in the presence of no-slip boundary condition unless a very stringent time step restriction is observed. We studied a simplified 1-D problem and uncovered the cause of the instability. We developed a modified scheme that is
unconditionally stable. We extended this technique to standard 2-D cavity problem and found a way to recover the unconditional stability for low Reynolds number flow. However, in the falling-ball viscometer simulation problem, the complexity that the penalty term makes the instability problem difficult to overcome, and it is impractical to modify the scheme. So, there is still a severe time step restriction for small Reynolds number: $\Delta t \sim Re \Delta x^2$.

Numerical simulation of two particle sedimentation reveals detailed feature of the particle interaction with each other and with the walls of the device. Our computations reveal the potential for using this simulation to probe the effects of inertia in sedimentation.
Consider the flow generated by a falling sphere in a bounded cylinder, it’s axisymmetric, so the velocity and vorticity field are:

\[ \mathbf{v} = (u, 0, w), \quad \mathbf{\omega} = (0, \zeta, 0) \]

where the velocity field can be retrieved from stream function,

\[ u = \frac{1}{r} \frac{\partial \psi}{\partial z}, \quad w = -\frac{1}{r} \frac{\partial \psi}{\partial r} \]

the vorticity \( \zeta \) is then:

\[ \mathbf{\omega} = \nabla \times \mathbf{v} = \begin{vmatrix} \frac{1}{r} \frac{\partial}{\partial r} & i_\phi & \frac{1}{r} \frac{\partial}{\partial z} \\ \frac{\partial}{\partial r} & 0 & \frac{\partial}{\partial z} \\ u & 0 & w \end{vmatrix} = \left[ \frac{\partial}{\partial z} \left( \frac{1}{r} \frac{\partial \psi}{\partial z} \right) + \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \psi}{\partial r} \right) \right] i_\phi \]

So, the stream function equation is:

\[
\frac{1}{r} \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r^2} \frac{\partial \psi}{\partial r} + \frac{1}{r} \frac{\partial^2 \psi}{\partial z^2} = \zeta \tag{A.1}
\]

and the incompressibility is satisfied:

\[
\nabla \cdot \mathbf{u} = \frac{1}{r} \frac{\partial}{\partial r} (ru) + \frac{\partial w}{\partial z} = 0 \tag{A.2}
\]

The standard vorticity transport equation is

\[
\frac{\partial \mathbf{\omega}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{\omega}) + \nu \nabla \times (\nabla \times \mathbf{\omega}) = 0
\]
On the left side,

\[ \mathbf{v} \times \omega = \begin{vmatrix} i_r & i_\phi & i_z \\ u & 0 & w \\ 0 & \zeta & 0 \end{vmatrix} = (-w\zeta, 0, u\zeta) \]

and

\[ \nabla \times (\mathbf{v} \times \omega) = \begin{vmatrix} \frac{1}{r}i_r & i_\phi & \frac{1}{r}i_z \\ \frac{\partial}{\partial r} & 0 & \frac{\partial}{\partial z} \\ -w\zeta & 0 & u\zeta \end{vmatrix} = \frac{\partial}{\partial z}(-w\zeta) - \frac{\partial}{\partial r}(u\zeta) \]

so

\[ -\nabla \times (\mathbf{v} \times \omega) = \frac{\partial}{\partial z} \left( rw\frac{\zeta}{r} \right) + \frac{\partial}{\partial r} \left( ru\frac{\zeta}{r} \right) = rw \frac{\partial}{\partial z} \left( \frac{\zeta}{r} \right) + ru \frac{\partial}{\partial r} \left( \frac{\zeta}{r} \right) \]

where

\[ \frac{\zeta}{r} \frac{\partial}{\partial z} (rw) + \frac{\zeta}{r} \frac{\partial}{\partial r} (ru) = 0 \]

from equation (A.2), and

\[ \nabla \times \omega = \begin{vmatrix} \frac{1}{r}i_r & i_\phi & \frac{1}{r}i_z \\ \frac{\partial}{\partial r} & 0 & \frac{\partial}{\partial z} \\ 0 & r\zeta & 0 \end{vmatrix} = \left( -\frac{\partial \zeta}{\partial z}, 0, \frac{1}{r} \frac{\partial}{\partial r} (r\zeta) \right) \]

so

\[ \nabla \times (\nabla \times \omega) = \begin{vmatrix} \frac{1}{r}i_r & i_\phi & \frac{1}{r}i_z \\ \frac{\partial}{\partial r} & 0 & \frac{\partial}{\partial z} \\ -\frac{\partial \zeta}{\partial z} & 0 & \frac{1}{r} \frac{\partial}{\partial r} (r\zeta) \end{vmatrix} = -\frac{\partial^2 \zeta}{\partial z^2} - \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r\zeta) \right) \]
Thus the vorticity transport equation is then:

$$\frac{\partial \zeta}{\partial t} + r w \frac{\partial}{\partial z} \left( \frac{\zeta}{r} \right) + ru \frac{\partial}{\partial r} \left( \frac{\zeta}{r} \right) = \nu \left[ \frac{\partial^2 \zeta}{\partial z^2} + \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r \zeta) \right) \right] \quad (A.3)$$

The Navier-Stokes equation is:

$$\rho (v_t + v \cdot \nabla v) + \nabla p = \mu \Delta v + \alpha (V - v)x (x - X) \quad (A.4)$$

where $V = (0, 0, U), v = (u, 0, w)$, denoting $f = \alpha (V - v)x$, then

$$\nabla \times f = \alpha \begin{vmatrix} \frac{1}{r} \hat{r} & \hat{\phi} & \frac{1}{r} \hat{z} \\ \frac{\partial}{\partial r} & 0 & \frac{\partial}{\partial z} \\ -u \chi & 0 & (U - w) \chi \end{vmatrix} = \frac{\partial}{\partial z} (-u \chi) - \frac{\partial}{\partial r} ((U - w) \chi)$$

so

$$\nabla \times f = -\alpha \zeta \chi - \alpha (u \chi_x + (U - w) \chi_r)$$
APPENDIX B

THE CONJUGATE GRADIENT METHOD

Conjugate gradient method is an efficient method for solving linear equations

$$Ax = b$$

provided that A is a symmetric matrix, otherwise, preconditioning on matrix A should performed first. The idea of the method is using a sequence of $\xi_i$ to minimize $A\xi_i - b$. When $\xi_i$ converges to $\xi^*$, then we get the approximate solution $x = \xi^*$.

The procedure is as follows:

Given $\xi^0 = (x_1, x_2, \ldots, x_n)$ and $d^0 = -r^0$ where $r^k = A\xi^k - b$, start the iteration until $\xi^k$ converge:

$$\alpha_k = -\frac{r^k \cdot d^k}{d^k \cdot Ad^k}$$

$$\xi^{k+1} = \xi^k + \alpha_k d^k$$

$$r^{k+1} = A\xi^{k+1} - b$$

$$\beta_k = \frac{r^{k+1} \cdot Ad^k}{d^k \cdot d^k}$$

$$d^{k+1} = -r^{k+1} + \beta_k d^k$$

Here the new search direction $d^{k+1}$ is conjugate with respect to the old direction $d^k$ because $d^{k+1} \cdot Ad^k = 0$. 

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REFERENCES


