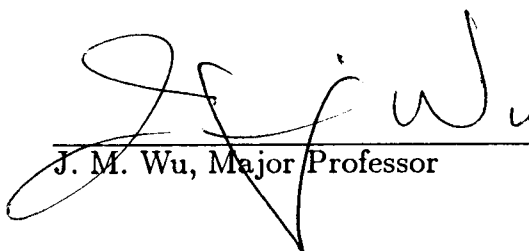


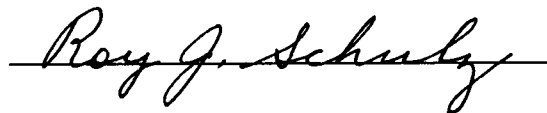
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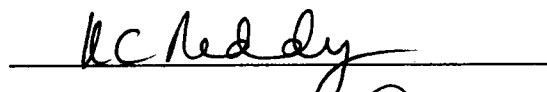
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On Vorticity-Based Numerical Methods for Incompressible Viscous Flows

A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Xiao-Hui Wu
December 1994

Dedication

To

my family and friends

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Abstract

Vorticity-based numerical methods for incompressible viscous flows are studied at a fundamental level. Important issues concerning efficient yet accurate implementation of vorticity-based methods for unsteady flows are examined from both theoretical and numerical points of view. Among them, local boundary conditions for vorticity at a solid wall and the methods of ensuring the divergence-free condition of both vorticity and velocity fields are the key subjects. The main theme is to develop the building blocks for future development of vorticity-based methods instead of a specific algorithm.

The boundary conditions of vorticity are studied based on the physical mechanism of vorticity generation from a solid wall. We observe that the dynamic condition, represented by the boundary vorticity flux, leads to a clear physical picture and robust numerical schemes.

The coupling between the boundary vorticity flux and tangential pressure gradient has been a troublesome problem in using the flux as boundary condition, since the pressure is unknown and in general has to be solved in a global way. However, it is proved that the coupling is weak for high Reynolds number flows; local decoupled approximations are therefore developed. If necessary, the coupling can be resumed by simple iteration. Numerical experiments on one-dimensional unidirectional flows and two-dimensional flow over a circular cylinder confirm our theoretical predictions, and compare favorably with exact solutions or benchmark numerical solutions, as well as fine experiments. The dynamic condition of vorticity is also extended to three-dimensional problems. Other local boundary conditions of vorticity are tested for comparison.

In vorticity-velocity formulation, the divergence-free conditions of vorticity and velocity are not automatically satisfied by numerical schemes, especially in three dimensions. In order to impose these conditions, differential and integral methods of solving the kinematic equations of velocity are studied. An efficient

method of obtaining divergence-free velocity from arbitrary vorticity distribution is established. The method also leads to an efficient scheme to project vorticity onto the divergence-free space at a minimum cost. Meanwhile, we discover the general principles of constructing true divergence-free (finite difference) schemes for solving the vorticity transport equation, i.e., a divergence-free vorticity solution is obtained without projection. The construction is thus no longer limited to central differences as in the literature; a variety of more advanced techniques are now applicable.

Three-dimensional numerical tests using the new divergence-free and projection methods are conducted for the lid-driven cavity flow at several Reynolds numbers. For high Reynolds-number unsteady flows, ensuring divergence-free condition of vorticity is crucial for obtaining physically correct results; whereas for steady-state flows it gives better accuracy. The projection method is very flexible, and is found to be valuable even for divergence-free schemes if the computation is done with relatively large roundoff error. The results are compared with other computations and experiments with good agreement.

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Chapter 1

Introduction

Numerical solutions of the incompressible Navier-Stokes (N-S) equation are playing an increasingly important role in the study of unsteady viscous fluid motion. In the last few decades (1970-1990), the N-S equation has been primarily solved in its primitive form, in terms of velocity and pressure (the $\mathbf{u}$ - p formulation). Solutions can also be obtained by solving alternative formulations derived from the original N-S equation, among which the most important one is the vorticity formulation. These vorticity-based numerical methods are the subject of this thesis.

The vorticity formulation has certain advantages over the $\mathbf{u}$ - p formulation from mathematical and physical points of view. For incompressible flows, the pressure loses its usual thermodynamic meaning and serves only as a Lagrange multiplier to secure the incompressibility. It is also a difficult term to treat numerically because it has no natural boundary conditions (BCs). Mathematically, the N-S equations can be solved without the pressure at all by projecting the N-S equation onto the divergence-free space. This projection, however, cannot be done analytically in general, but it can be conveniently represented by the vorticity equation, which is obtained by taking curl of the N-S equation. When density is constant, the pressure term is eliminated in the process, and the vorticity equation together with the kinematic equation for velocity consist of a self-contained dynamical system. This aspect is most thoroughly explored numerically by the Lagrangian vortex methods (ref. [1-5]). If density is not constant, there will be a baroclinic term left in the vorticity equation responding to vorticity generation inside the fluid. This effect, which is important for understanding geophysical flows, will not be considered here, although it poses no essential difficulties. Furthermore, the form of vorticity equation is invariant under the non-inertial transformation of

the reference frame [6], in contrast to the $\mathbf{u}$ - p formulation. The non-inertial effects enter the solution only through the initial and boundary conditions.

From physical point of view, the vorticity is a key quantity that contains insight about flows. This is determined by the nature of viscous fluid—any shear stress on a fluid element creates its rotation. Thus the vortex is the basic form of fluid motion and it is quantified by the vorticity. The situation is most dramatic when flow is turbulent. The distinct character of turbulent flows is the interaction of vortices at a vast number of scales. Therefore, one of the motivations of solving the vorticity equation is to capture the physics of flows directly, see [7–12]. On the other hand, vorticity formulation is the foundation of vortex dynamics, which has been playing a key role in the study of fluid motions. Thus it is tempting to solve the vorticity equation directly.

The above considerations do not make the vorticity formulation apparently superior to the $\mathbf{u}$ - p formulation in numerical sense. However, Gunzburger et al. [13] point out that the strength of vorticity formulation shows when the *solution phase* of the simulation process is examined. They argue strongly that the vorticity-velocity (ω - $\mathbf{u}$) formulation is “amenable to efficient solution, especially in the milieu of parallel processing architectures.” Huang and Ghia [14] note that since the vorticity is a linear function of velocity, whereas the pressure is a non-linear function of velocity, the resultant vorticity-based methods are easier to handle computationally. Besides traditional differential approaches, Wu and his co-workers adopted an integral approach [15–19]—using the generalized Biot-Savart Law to compute the velocity from known vorticity field. The integral method is naturally adaptive and can be used to construct efficient domain decomposition schemes [17]. Moreover, the vorticity formulation enables the computation to be done in a grid-free fashion as in the Lagrangian vortex method. Therefore, the flow over complicated geometries or moving boundaries becomes much easier to simulate. A major advantage of the vortex method is that by tracing the discrete vortex elements the convection of vorticity can be computed very accurately without numerical diffusion.

These numerical benefits, however, do not come free. There are sev-

eral fundamental problems to be solved. They include imposing proper numerical boundary conditions (BCs) for the vorticity on solid boundaries, and ensuring the divergence-free condition of velocity and vorticity. The first problem encountered is universal for all vorticity-based methods, whereas the latter one depends on the numerical methods as well as spatial dimensions. For example, in two dimensions, the vorticity is solenoidal since only one component perpendicular to the flow exists. Moreover, if the velocity is solved from the stream-function ψ , it is guaranteed divergence-free. It might not be divergence-free if other formulations are used. In three dimensions, all of the three problems will appear.

To be specific, we briefly analyze the problems as follows. First, we show that the problem of vorticity BC is no less difficult than that of the pressure. The vorticity BC has been said to be the “hardest problem in vortex method” [20] and still a “largely unanswered question” [5] as late as in 1993. Moreover, in his review [21], Gresho stated that “there are no BCs on the vorticity.” Therefore, it is not surprising that while a rather comprehensive analysis of the proper BCs of pressure has been given by Gresho and Sani [22] in 1987, a comparable analysis for vorticity is not available in the open literature. We shall address this tough question and show that the two are closely linked to each other.

The dispute over proper BCs for vorticity has accompanied the vorticity-based methods ever since its introduction. Unlike the adherence condition for velocity, there is no natural vorticity condition on solid walls; instead, the no-slip condition of velocity provides an integral constraint on the vorticity in the form of either the Biot-Savart law or elliptic equations that relate $\mathbf{u}$ with $\boldsymbol{\omega}$. In other words, *the vorticity condition is of global type* in contrast with the traditional local boundary conditions. Therefore, all effort of searching for rigorous vorticity BCs ended up with various integral or integro-differential conditions, e.g. [23–25]. In this sense, Gresho’s assertion is correct.

Instead of expressing the vorticity condition in integral forms, two approaches can be adopted. First, the vorticity dynamic equation and the kinematic equations can be solved in a fully coupled way, which is equivalent to imposing the integral constraints [26]. The apparent disadvantage is that six dependent variables

(three $\mathbf{u}$ components and three $\boldsymbol{\omega}$ components) have to be solved simultaneously in a fully coupled manner. Though as mentioned above, Gunzburger et al. [13] argue that the equations can be arranged to take the advantage of parallel processing. The fully coupled methods are, however, more frequently used in the computation of steady flows, e.g. [13, 27–31]. Recently, some coupled methods have been used in solving unsteady flows [32, 33]. It should be noted that Orlandi [34] designed a special scheme for two-dimensional (2-D) simulation, in which the dynamic and kinematic equations are strongly coupled and yet can be solved efficiently.

In many other unsteady flow computations, the dynamic equation and the kinematic equations are solved separately. These methods include typically the vortex methods, the integro-differential methods by Wu et al. [15, 16, 18, 19], the finite-difference vorticity-stream-function (ω - ψ) methods [35] (which are the most widely used), and more recently the $\boldsymbol{\omega}$ - $\mathbf{u}$ methods, e.g. [36–40]. These are all *decoupled approaches*. In this case, good local approximations of the vorticity BCs have to be supplied to the vorticity equation to get accurate results. Such approximations relate naturally to the physical process of *vorticity creation from solid walls*. This physical process had also been regarded as an unanswered fundamental question in the fluid mechanics [41] until a recent theoretical advance due to Wu and Wu [42]. We shall elaborate it here and adapt it into numerical methods.

It was Batchelor [43] who explained the process of vorticity generation by a model of vortex sheet creation and diffusion. The model was later used in fractional-step vortex methods, which have been the subject of intensive research after the introduction of random walk method by Chorin [44]. A similar idea was used by Wu [16] in his integro-differential type of method. In essence, a slip on a solid boundary, introduced numerically, is used to estimate the newly created vorticity through a “kinematic” manipulation. Namely, the slip is regarded equivalent to a vortex sheet and the strength of the sheet is divided by the size of vortex elements or grids to obtain the boundary vorticity. Thus, we call the resultant Dirichlet BCs as the *kinematic BCs*. The finite difference formulae of boundary vorticity [35] also belong to this category, but they are distinguished from

the vortex sheet models in that they are obtained by local Taylor series expansions of the kinematic equations. Therefore, these formulae seem to be more accurate when higher order differences are used. However, as reviewed by Gresho [21], these finite-difference BCs “often do not” work. Wu [16] tried to show that locally higher order BCs may violate the conservation of vorticity and thus give globally wrong results, while the lower order BCs could work better. Unfortunately, the example of high-order finite-difference BC he gave does not use the no-slip condition and hence is not a valid candidate for critics. However, from different points of view, we shall see indeed that formal local truncation analysis may not guarantee the finite-difference BCs to behave properly. In this respect, Hou and Wetton [45] carefully proved the convergence of a finite-difference scheme using ω - ψ (or ω - ψ in 3D, where ψ is the vector potential) with a first order Dirichlet BC of vorticity.

In his introduction to boundary layer theory [46], Lighthill presented an elegant analysis of the vorticity creation from a dynamic point of view. The essence of his argument is to apply the Navier-Stokes equations on the solid boundary and use the no-slip condition to derive a formula for the boundary vorticity flux, a Neumann BC for vorticity. For 2-D problems, Lighthill arrived at a simple balance between the vorticity flux and the tangential pressure gradient on the wall (assuming the wall is at rest). More generally, the vorticity creation is due to the balance of forces on fluid particles at solid walls, i.e. the balance of pressure force (pressure gradient), shear stress and inertial force (if the wall is accelerating). Wu et. al. [42, 47–49] studied in more detail the dynamic vorticity generation and derived general formula for the 3-D boundary vorticity flux. The resultant BCs are called the *dynamic BCs*. Compared to the kinematic model, the dynamic theory has no reference to the vortex sheet. We shall show later that the dynamic approach is more physically correct (Chapter 3).

It should be noted that Koumoutsakos, Leonard, and Pépin [50] have recently analyzed the boundary conditions for viscous vortex methods. They noted that the above mentioned vortex sheet strength can be manipulated so that either a Dirichlet or Neumann type of condition could be modeled. They further pointed out that the Neumann type of condition is better suited for vortex methods using

the Particle Strength Exchange (PSE) scheme. From a different approach, we shall show that both types of conditions can exist only in *approximate sense*, where the approximate Neumann type of condition is better. The error of these approximations, however, has never been closely analyzed.

Numerical implementation of the Neumann (dynamic) BC was initiated by Kinney and his co-workers (see [51]). They obtained the numerical BC for vorticity by a physical argument. Koumoutsakos et al. [50] arrived at virtually the same condition via a different argument. Both arguments are not rigorous, which is the key reason why the error can not be analyzed. Therefore, we shall give a more rational and rigorous analysis of the dynamic BC and propose proper numerical implementation in Chapter 3.

The divergence-free condition for velocity and vorticity are also very important both physically and mathematically. In 2-D computations, the divergence of vorticity is guaranteed zero. However, the divergence of velocity may vary for different numerical schemes. Labidi and Ta Phuoc [52, 53] found that, in some cases of their computation, a fourth-order discretization, designed to better satisfy the continuity condition, can not do the job. Following [54], a scalar potential was introduced to obtain the divergence-free velocity field at the end of each time step through an iterative process. Instead of solving the kinematic and dynamic equations separately, as in Labidi and Ta Phuoc, Orlandi [34] used a strong coupled method and avoided the problem by designing the numerical algorithm carefully. No iteration is needed to achieve solenoidal velocity in this case. Daube [55] proved that in 2-D cases such a coupled solution guarantees the velocity to be solenoidal. Similar observations in 3-D were mentioned by Guj and Stella [33].

In addition to the explicit enforcement of the divergence-free condition on the velocity, Labidi and Ta Phuoc [53] also found it to be necessary to explicitly enforce the condition on vorticity in 3-D computations. Their experience is not unique. To obtain solenoidal vorticity, Gatski et al. [39] project the vorticity field onto the divergence-free space by solving a Poisson equation for a scalar potential. On the other hand, Osswald et al. [56] as well as Guj and Stella [33] devised methods based on central difference to ensure that the divergence of vorticity vanishes

at round-off level, which can be called the divergence-free schemes. However, it is not obvious in generalizing their construction to obtain higher order schemes or better representation of the convective flux.

Although a coupled solution of the vorticity dynamic equation and the kinematic equation of velocity can avoid the problems of vorticity BC and the divergence-free conditions, they are expensive for unsteady flow problems. Since most steady problems are more or less well-addressed, we are more concerned about unsteady flows here and concentrate on the decoupled approach. Our objective is to resolve the above problems and hence establish a sound foundation for implementing the decoupled method in both theoretical and numerical aspects. Therefore, we are concentrating on the basic building blocks of efficient vorticity-based methods based on physical and mathematical analysis, rather than constructing a specific numerical algorithm. At the same time, some numerical schemes are developed to demonstrate our analysis.

The outline of the thesis is as following. The kinematic aspect of 3-D ω - u formulation is studied theoretically in Chapter 2, including both differential and integral approaches. Although some mathematical analyses exist [57–59], there are still some long standing issues which need clarification. Two questions are answered: how to solve the velocity correctly without coupling it with the vorticity equation, and how to perform the projection on vorticity correctly and efficiently without solving an extra Poisson equation. In Chapter 3, we present a rational analysis of the dynamic BC for vorticity. We show how vorticity and pressure are coupled through boundary conditions and how they can be approximately decoupled. A numerical method of implementing the dynamic BC is proposed and studied in some detail. The kinematic BCs and their connection with the dynamic one are also discussed. In Chapter 4, numerical tests of dynamic BC are performed for one-dimensional (1-D) unidirectional flows and compared with exact solutions. These flows are of pure diffusion type which might seem trivial to solve, but they exhibit fundamental difficulties of vorticity-based methods. We present a two-dimensional ω - ψ method with emphasis on the dynamic vorticity BC in Chapter 5. The impulsively started flow over a circular cylinder is solved

numerically and compared to existing benchmark solutions and experiments. In Chapter 6, we extend the implementation of dynamic BC to three-dimensions. But the main concern there is imposing the divergence-free conditions for velocity and vorticity in the ω - u approach. The divergence-free scheme for the vorticity equation is studied in a general finite-difference setting; several rules are found to be useful in constructing higher order and more sophisticated schemes. In addition the new projection method proposed in Chapter 2 is studied numerically. For demonstration, two- and three-dimensional shear driven cavity flows are solved using ω - u formulation, and the results are compared to other computations and also to experiments.

In short, in this thesis, we critically study the fundamental issues relevant to vorticity-based numerical methods; examine both physically and mathematically various existing vorticity boundary conditions; and propose and demonstrate new and efficient vorticity-based schemes with proper local boundary conditions in sample computations.

Chapter 2

The Kinematic Equations

We study the mathematical background and method of solving the kinematic equations of velocity in this chapter. The velocity $\mathbf{u}$ in general satisfies the following Cauchy-Riemann equations

$$(2.1a,b) \quad \nabla \cdot \mathbf{u} = \vartheta, \quad \nabla \times \mathbf{u} = \boldsymbol{\omega}, \quad \text{in } V,$$

$$(2.1c) \quad \mathbf{n} \cdot \mathbf{u} = u_n, \quad \text{on } \partial V.$$

Here ϑ is the dilatation, and V is a bounded domain in R^3 with boundary ∂V on which $\mathbf{n}$ is the outward normal. (we include ϑ since it adds no difficulty to the discussion that follows, and hence our results are valid for compressible flows as well.) We are interested in solving $\mathbf{u}$ from (2.1) for given ϑ and $\boldsymbol{\omega}$. The following compatibility conditions

$$(2.2a,b) \quad \int_V \vartheta dV = \oint_{\partial V} u_n dS, \quad \nabla \cdot \boldsymbol{\omega} = 0,$$

are necessary for (2.1) to have a solution. If (2.2) holds, Eq. (2.1) is well posed as proved in [57]. In the following, we assume that $\mathbf{u}$, ϑ and $\boldsymbol{\omega}$ have desired order of smoothness on $\overline{V}$, the closure of V .

Eq. (2.1) is elliptic and has to be solved at least once, depending on the numerical scheme, in each time step of unsteady computations. It is well-known that solving such elliptic problems is the most time consuming part of the whole computation, therefore, it is very important to develop efficient solution methods.

Various approaches can be used when solving Eq. (2.1) numerically. The straightforward one is to solve (2.1) directly. Several fast solvers have been proposed and studied for 2-D problems [60–63]. Note that there are two equations of two unknowns in (2.1) for 2-D problems, but four equations of three unknowns for 3-D problems. In fact, the three equations in (2.1b) are not all independent. This distinction makes the 2-D solvers of (2.1) not directly generalizable to 3-D.

For 3-D problems, Gatski et al. [39] solve the equations by a least square solution proposed by Fix and Rose [57]. Due to the compatibility condition (2.2b), Gatski et al. have to project ω onto divergence-free space by solving an additional Poisson equation. On the other hand, Huang and Ghia [14] solve (2.1) by reformulating the linear system so that an efficient multigrid technique can be developed. Their reformulation is similar to the introduction of a scalar and vector potential for $\mathbf{u}$. They also point out that the reformulated system contains a Laplacian operator and hence a better smoothing rate is obtained when performing relaxation.

Two other formulations, however, are more appreciated in the ω - $\mathbf{u}$ community, i.e. the Poisson equation for $\mathbf{u}$ (differential approach) and the generalized Biot-Savart Law (integral approach); both of them can be derived based on the vector identity

$$(2.3) \quad \Delta \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u}).$$

Obviously, the differential approach can take advantage of existing techniques for solving scalar Poisson equations, as well as ready-to-run, finely-tuned computer codes. Similarly, the integral approach can take advantage of recent development in panel methods and boundary element methods. In addition, the integral approach is attractive from theoretical point of view: it is adaptive; the far field condition is exactly built in the approach. Besides, it is a natural method to use for the Lagrangian vortex methods. However, it is fair to say that the integral method is still too expensive for large scale computations, especially in 3-D. If N is the number of grid points of vortex elements, then a direct numerical integration over the whole computational domain would cost $O(N^2)$ operations. Although the cost has been drastically cut down by a factor of 80–100 due to the development of fast multipole methods (FMM) [64–66], the integration method often cannot compete with fast Poisson solvers. On the other hand, one should note the recent development of parallel FMM [67–69], which will make large scale computations using integral method attractive in the future.

Both of the above formulations are not new subjects, yet there is still some confusion and misunderstanding to be clarified. In this chapter, we present

some new theoretical results about the formulations. These results will be the theoretical basis of our numerical schemes in Chapter 6.

The main problem of the differential approach is imposing the additional boundary conditions properly (see below). By contrast, the boundary condition (2.1c) should have been built into the integral approach; but, if not examined carefully, the result could be incorrect. These problems are analyzed in §2.1 and §2.2 below, respectively. In Section §2.3, we consider the projection of vorticity onto the divergence-free space in both approaches, which is often necessary in 3-D computations.

2.1 The Differential Approach

An effective way of solving problem (2.1) is substituting (2.1a,b) into (2.3), and then solving the Poisson equation for $\mathbf{u}$:

$$(2.4) \quad \Delta \mathbf{u} = \nabla \vartheta - \nabla \times \boldsymbol{\omega}.$$

Note that (2.4) is one order higher than (2.1), and two more component boundary conditions are needed in addition to (2.1c). These conditions have to be such that spurious solutions from raising the order of the differential equations can be excluded, so that a solution of (2.4) is also that of (2.1). This problem has been studied in [57,58]. Reference [58] contains a clear and easily understood discussion but with some minor errors. Here we make a more careful examination on the proper boundary conditions of (2.4).

We first recall the least square argument of [58] to see what additional boundary conditions we may choose from. Consider minimizing the functional

$$\mathbf{I}(\mathbf{u}) = \int_V [(\nabla \cdot \mathbf{u} - \vartheta)^2 + (\nabla \times \mathbf{u} - \boldsymbol{\omega})^2] dV.$$

Suppose that $\mathbf{I}(\mathbf{u})$ attains its minimum at $\mathbf{u}$. Let $\mathbf{w} = \mathbf{u} + \varepsilon \mathbf{v}$, where $\mathbf{v}$ is an arbitrary admissible function that satisfies $\mathbf{n} \cdot \mathbf{v} = 0$ with ε being a small parameter. Then, substitute $\mathbf{w}$ into $\mathbf{I}$, since $\mathbf{u}$ is a minimizing function, we have

$$(2.5) \quad \int_V [(\nabla \cdot \mathbf{u} - \vartheta) \nabla \cdot \mathbf{v} + (\nabla \times \mathbf{u} - \boldsymbol{\omega}) \cdot (\nabla \times \mathbf{v})] dV = 0$$

for all admissible $\mathbf{v}$. Thus, the right-hand side of the identity below must vanish

$$\begin{aligned}
 (2.6) \quad & \int_V [(\nabla \cdot \mathbf{u} - \vartheta) \nabla \cdot \mathbf{v} + (\nabla \times \mathbf{u} - \boldsymbol{\omega}) \cdot (\nabla \times \mathbf{v})] dV \\
 &= - \int_V \mathbf{v} \cdot (\Delta \mathbf{u} - \nabla \vartheta + \nabla \times \boldsymbol{\omega}) dV \\
 &\quad + \oint_{\partial V} [(\nabla \cdot \mathbf{u} - \vartheta)(\mathbf{n} \cdot \mathbf{v}) + (\nabla \times \mathbf{u} - \boldsymbol{\omega}) \cdot (\mathbf{n} \times \mathbf{v})] dS.
 \end{aligned}$$

Clearly, Eq. (2.4) follows from the requirement that the volume integral vanishes for all $\mathbf{v}$.

To assure the boundary integral be zero, we need to impose boundary conditions on $\mathbf{u}$. In [58], it was concluded that $\nabla \times \mathbf{u} - \boldsymbol{\omega} = 0$, i.e. (2.1b), should be specified at the boundary in addition to (2.1c). However, (2.1b) contains three components, which, along with (2.1c), gives one more boundary condition than necessary. Writing the last integrand in the boundary integral of (2.6) as $[(\nabla \times \mathbf{u} - \boldsymbol{\omega}) \times \mathbf{n}] \cdot \mathbf{v}$ shows that only the tangential components of (2.1b) need to be specified at ∂V .

A careful discussion is given in [36], where three alternatives were listed:

$$(2.7a) \quad \mathbf{u} = \mathbf{b}, \quad \text{on } \partial V,$$

$$(2.7b) \quad \mathbf{n} \times \mathbf{u} = \mathbf{n} \times \mathbf{b}, \quad \nabla \cdot \mathbf{u} = \vartheta, \quad \text{on } \partial V,$$

$$(2.7c) \quad \mathbf{n} \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0, \quad \mathbf{n} \cdot \mathbf{u} = u_n, \quad \text{on } \partial V,$$

The authors further remarked that (2.7a) can be used for (2.4) to avoid the coupling between the velocity components in (2.7c) at curved boundaries.

Unfortunately, both (2.7a) and (2.7b) are actually incorrect. The definition of the admissible test functions has already excluded (2.7b) from being a choice. From another point of view, the solution obtained by using (2.7b) may not satisfy the normal condition (2.1c) which, according to Gresho [21], is not violable. In contrast to (2.7b) where the class of admissible functions is enlarged, Eq. (2.7a) reduces the class by adding tangential restrictions on $\mathbf{u}$. Since (2.1) is well posed, the additional tangential boundary conditions in (2.7a) can only make the problem overdetermined. Thus, under this condition, the solution of (2.1) can exist only for a restricted class of vorticity, whereas (2.4) can be solved for a wider class of $\boldsymbol{\omega}$. It

is easy to construct ω such that (2.1) has no solution but (2.4) has a solution, and hence the solution does not satisfy (2.1). More specifically, the continuity equation (2.1a) may be violated as mentioned in [33]. On the other hand, if the vorticity distribution happens to let (2.1) and (2.7a) have a solution, then the solution must also satisfy (2.4). In the computation of fluid flow, this is guaranteed by solving (2.4) coupled with the vorticity transport equation.

Therefore, we arrive at the proper derivative formulation in differential form:

$$(2.8a) \quad \Delta \mathbf{u} = \nabla \vartheta - \nabla \times \omega, \quad \text{in } V,$$

$$(2.8b,c) \quad \mathbf{n} \cdot \mathbf{u} = u_n, \quad \mathbf{n} \times (\nabla \times \mathbf{u} - \omega) = 0, \quad \text{on } \partial V.$$

In [57], Fix and Rose proved that if the compatibility conditions (2.2a,b) hold, then the minimizing function $\mathbf{u}$ for $\mathbf{I}(\mathbf{u})$ satisfies (2.1a,b) (almost everywhere in V). Hence, the solution of (2.8) should satisfy (2.1) under the condition (2.2). (Note: Both (2.7a) and (2.7b) can fail their proof.)

We now prove a more general result concerning (2.8) via a different way that shows more detailed structure of the solution.

Lemma 2.1.1 *The problem (2.8) has at most one solution.*

Proof. Let $\mathbf{v}$ be the difference of two solutions of (2.8,) such that

$$\Delta \mathbf{v} = 0, \quad \mathbf{n} \cdot \mathbf{v} = 0, \quad \mathbf{n} \times (\nabla \times \mathbf{v}) = 0.$$

Then, owing to (2.6), we have

$$\begin{aligned} \int_V [(\nabla \cdot \mathbf{v})^2 + (\nabla \times \mathbf{v})^2] dV &= - \int_V \mathbf{v} \cdot \Delta \mathbf{v} dV \\ &\quad + \oint_{\partial V} [(\mathbf{n} \cdot \mathbf{v}) \nabla \cdot \mathbf{v} + (\nabla \times \mathbf{v}) \cdot (\mathbf{n} \times \mathbf{v})] dS. \end{aligned}$$

Note that

$$(\nabla \times \mathbf{v}) \cdot (\mathbf{n} \times \mathbf{v}) = -[\mathbf{n} \times (\nabla \times \mathbf{v})] \cdot \mathbf{v} = 0;$$

there must be $\nabla \cdot \mathbf{v} = 0$ and $\nabla \times \mathbf{v} = 0$ (almost everywhere) because the right hand side of the above integral equation vanishes. Therefore, $\mathbf{v}$ is the gradient of

some harmonic function with vanishing normal derivative on ∂V because of (2.1c). Thus $\mathbf{v} = 0$ in V , i.e. Eq. (2.8) has at most one solution. $\square$

Lemma 2.1.2 *Assume (2.2a) holds. If $\mathbf{u}$ is a solution of (2.8), then the following equations*

$$(2.9) \quad \nabla \cdot \mathbf{u} = \vartheta, \quad \nabla \times \mathbf{u} = \boldsymbol{\omega} - \nabla \psi,$$

hold (almost everywhere) in V , where ψ is defined by

$$(2.10a,b) \quad \Delta \psi = \nabla \cdot \boldsymbol{\omega}, \quad \text{in } V, \quad \text{and} \quad \mathbf{n} \times \nabla \psi = 0, \quad \text{on } \partial V.$$

Proof. Rewriting (2.8a) gives

$$(2.11) \quad \nabla(\nabla \cdot \mathbf{u} - \vartheta) - \nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0.$$

Since (2.8c) is a sufficient condition for the two terms in (2.11) to be orthogonal (in the L_2 sense), i.e.

$$\begin{aligned} & \int_V \nabla(\nabla \cdot \mathbf{u} - \vartheta) \cdot [\nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega})] dV \\ &= \oint_{\partial V} \mathbf{n} \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) \cdot \nabla(\nabla \cdot \mathbf{u} - \vartheta) dS \\ &= 0, \end{aligned}$$

it follows that

$$(2.12a,b) \quad \nabla(\nabla \cdot \mathbf{u} - \vartheta) = 0, \quad \nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0.$$

Thus $\nabla \times \mathbf{u} - \boldsymbol{\omega} = -\nabla \psi$. Taking divergence on both sides, we obtain (2.10a), and by (2.8c), Eq. (2.10b) follows. Similarly, we have $\nabla \cdot \mathbf{u} - \vartheta = \text{const}$ in V . From (2.2a), the constant must be zero. $\square$

Based on the above discussion, the following observations can be made.

Remarks:

1. If $\nabla \cdot \boldsymbol{\omega} = 0$, then $\nabla \psi = 0$ from (2.10). Thus, under the compatibility conditions (2.2a,b), if the solution of (2.8) exists, it also solves (2.1).

2. When ϑ and ω are sufficiently smooth on $\overline{V}$, the solution of (2.1) satisfies (2.8). In this case, since (2.1) is well-posed, there exists a solution for (2.1) and thus for (2.8).
3. The first remark was also proved in [58], though a wrong boundary condition was used and thus a different derivation.
4. It was argued in [13] that since (2.11) represents the Helmholtz decomposition of the null vector, and such a decomposition is unique up to an additive constant and a gradient of a scalar, Eq. (2.12) follows without any boundary conditions. This argument is only valid for an unbounded domain.
5. From (2.8c) we have

$$\frac{\partial}{\partial n}[\mathbf{n} \cdot (\nabla \times \mathbf{u} - \omega)] = 0 \quad \text{on } \partial V$$

due to the fact that $\nabla \times \mathbf{u} - \omega$ is divergence free.

Combine remarks 1 and 2, as well as the lemmas, we arrive at the main result of this section:

Theorem 2.1.1 *If (2.2a) holds, given sufficiently smooth ϑ and ω , Eq. (2.8) has a unique solution. Moreover, the solution satisfies (2.9).*

Proof. The uniqueness and the second part of the theorem has been shown in Lemmas 2.1.1 and 2.1.2. We only need to show that the solution exists.

If $\nabla \cdot \omega = 0$, then remark 2 has the answer. If $\nabla \cdot \omega \neq 0$, then (2.1) does not have a solution. But consider

$$\begin{aligned} \nabla \cdot \mathbf{u} &= \vartheta, \quad \nabla \times \mathbf{u} = \hat{\omega}, \quad \text{in } V \\ \mathbf{n} \cdot \mathbf{u} &= u_n, \quad \text{on } \partial V, \end{aligned}$$

where $\hat{\omega} = \omega - \nabla\psi$ and ψ is defined by (2.10). Since $\nabla \cdot \hat{\omega} = 0$, the above equation is again well-posed (assuming that (2.2a) is valid), and hence it has a unique solution. It is easy to verify that the solution satisfies (2.8) by using (2.3) and noting that $\nabla \times \hat{\omega} = \nabla \times \omega$. $\square$

The significance of the theorem is that $\mathbf{u}$ can be solved for *arbitrary* $\boldsymbol{\omega}$ (which may not be divergence-free) from (2.8) and the solution always has the desired divergence.

2.2 The Integral Approach

Let $G = G(\mathbf{x}, \mathbf{y})$ be the fundamental solution of the Laplace equation in the free space, hence $\Delta G = -\delta(\mathbf{x} - \mathbf{y})$, and let $\mathbf{g} = \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})$ (where $\nabla_{\mathbf{y}}$ is the gradient operator with respect to $\mathbf{y}$). By (2.3) and the identity

$$\begin{aligned} \nabla \cdot (G \nabla \mathbf{u} - \mathbf{u} \nabla G) - \nabla (G \nabla \cdot \mathbf{u}) + \nabla \times (G \nabla \times \mathbf{u}) \\ = -\nabla \cdot (\mathbf{u} \nabla G) + \nabla (\nabla G \cdot \mathbf{u}) - \nabla \cdot (\nabla G \mathbf{u}), \end{aligned}$$

from Green's second identity the generalized Biot-Savart law follows

$$(2.13) \quad \alpha \mathbf{u} = \int_V (\mathbf{g} \vartheta - \mathbf{g} \times \boldsymbol{\omega}) dV - \oint_{\partial V} [\mathbf{g}(\mathbf{n} \cdot \mathbf{u}) - \mathbf{g} \times (\mathbf{n} \times \mathbf{u})] dS.$$

Here the integration is taken with respect to $\mathbf{y}$, and $\alpha = 1$ or 0 for $\mathbf{x}$ in V or $V' = R^3 \setminus \overline{V}$ (exterior domain), respectively. If the boundary is smooth, $\alpha = 1/2$ on ∂V . Note that in (2.13) we have substituted (2.1a,b) in place of $\nabla \cdot \mathbf{u}$ and $\nabla \times \mathbf{u}$, respectively, which implies that (2.2a,b) are satisfied. However, in computations, Eq. (2.2b) may be violated because of numerical error, whose consequences will be studied in §2.3. If an exterior domain is under consideration, we need to assume ϑ and $\boldsymbol{\omega}$ vanish at infinity of order r^{-2} , and $\mathbf{u} = 0$ at infinity.

Although the generalized Biot-Savart law is derived from the differential equations, whether it is equivalent to the original equation (2.1) needs to be carefully verified. Note that (2.13) is an integral equation for $\mathbf{u}$, because the $\mathbf{n} \times \mathbf{u}$ term is unknown at ∂V . Here, we prove

Theorem 2.2.1 *A vector field $\mathbf{u}$ that satisfies (2.13) must also satisfy (2.1a,b).*

Proof. Taking divergence of (2.13) yields

$$(2.14) \quad \nabla \cdot \mathbf{u} = - \int_V \vartheta \Delta G dV + \oint_{\partial V} (\mathbf{n} \cdot \mathbf{u}) \Delta G dS, \quad (\mathbf{x} \in V).$$

Since $\Delta G = -\delta(\mathbf{x} - \mathbf{y})$, Eq. (2.1a) follows for $\mathbf{x} \in V$. The proof of (2.1b) needs a little more work. Taking curl of (2.13), for $\mathbf{x} \in V$ we obtain

$$(2.15) \quad \nabla \times \mathbf{u} = - \int_V \nabla_x \times (\mathbf{g} \times \boldsymbol{\omega}) dV + \oint_{\partial V} \nabla_x \times [\mathbf{g} \times (\mathbf{n} \times \mathbf{u})] dS,$$

where, after some manipulation,

$$(2.16) \quad - \int_V \nabla_x \times (\mathbf{g} \times \boldsymbol{\omega}) dV = \boldsymbol{\omega} + \oint_{\partial V} \mathbf{g}(\mathbf{n} \cdot \boldsymbol{\omega}) dS - \int_V \mathbf{g}(\nabla \cdot \boldsymbol{\omega}) dV,$$

$$(2.17) \quad \oint_{\partial V} \nabla_x \times [\mathbf{g} \times (\mathbf{n} \times \mathbf{u})] dS = - \oint_{\partial V} \mathbf{n} \cdot (\nabla \times \mathbf{u}) \mathbf{g} dS + \oint_{\partial V} (\mathbf{n} \times \mathbf{u}) \Delta G dS.$$

Therefore, since $\nabla \cdot \boldsymbol{\omega} = 0$ is assumed, we have

$$(2.18) \quad \nabla \times \mathbf{u} = \boldsymbol{\omega} + \oint_{\partial V} \mathbf{n} \cdot (\boldsymbol{\omega} - \nabla \times \mathbf{u}) \mathbf{g} dS \quad (\mathbf{x} \in V).$$

To prove (2.1b), then, it suffices to show that

$$(2.19) \quad \eta = \mathbf{n} \cdot (\boldsymbol{\omega} - \nabla \times \mathbf{u}) = 0 \quad (\mathbf{x} \in \partial V).$$

Let $\mathbf{x} = \mathbf{x}_0 + \rho \mathbf{n}_{x_0}$, where $\mathbf{x}_0 \in \partial V$, $\rho < 0$, so that $\mathbf{x} \in V$ and $\mathbf{x} \rightarrow \mathbf{x}_0$ as $\rho \rightarrow 0$.

Taking dot product of (2.19) with $\mathbf{n}_{x_0}$ and noting that $\mathbf{g} = -\nabla_x G$, we get

$$\mathbf{n}_{x_0} \cdot (\boldsymbol{\omega} - \nabla \times \mathbf{u}) - \frac{\partial}{\partial n_{x_0}} \oint_{\partial V} \mathbf{n} \cdot (\boldsymbol{\omega} - \nabla \times \mathbf{u}) G dS = 0.$$

Using the jump condition of double-layer potential, as $\rho \rightarrow 0$, we get the boundary integral equation

$$(2.20) \quad \frac{1}{2} \eta(\mathbf{x}) - \oint_{\partial V} \eta(\mathbf{y}) \frac{\partial}{\partial n_x} G(\mathbf{x}, \mathbf{y}) dS_y = 0.$$

Eq. (2.20) permits only trivial solution, i.e. (2.19). Therefore, Eq. (2.1c) follows from (2.18). $\square$

Remarks:

1. The above proof can be adopted for exterior problem in V' , except that instead of (2.20), we have

$$(2.21) \quad \frac{1}{2}\eta(\mathbf{x}) + \oint_{\partial V} \eta(\mathbf{y}) \frac{\partial}{\partial n_x} G(\mathbf{x}, \mathbf{y}) dS_y = 0,$$

where $\eta = \mathbf{n}' \cdot (\boldsymbol{\omega} - \nabla \times \mathbf{u})$ and $\mathbf{n}' = -\mathbf{n}$ is the outward normal of V' . Since the solution of (2.21) is unique up to a constant, it follows that $\eta = C$. However, C must be zero because both $\nabla \times \mathbf{u}$ and $\boldsymbol{\omega}$ vanish at infinity.

2. Equations (2.14) and (2.17) are valid *only* in V . Therefore, the singularities of ΔG in the surface integrals of these equations do not affect the proof.
3. The singularities in (2.14) and (2.17) are due to the discontinuous property of integrals at the boundary. One thus needs to be careful in defining differential operations at the boundary. The common way of dealing with the problem is the limit approach used in the proof.
4. Another form of the generalized Biot-Savart law, derivable from (2.13), is discussed in [70]:

$$(2.22) \quad \mathbf{u} = \int (\mathbf{g} \vartheta - \mathbf{g} \times \boldsymbol{\omega}) dV - \oint_{\partial V} [\mathbf{g}(\mathbf{n} \cdot [\mathbf{u}]) - \mathbf{g} \times (\mathbf{n} \times [\mathbf{u}])] dS,$$

where $[\mathbf{u}] = \mathbf{u}_1 - \mathbf{u}_2$ (1 and 2 indicate the inside and outside of ∂V , respectively) is the jump in $\mathbf{u}$ across the boundary. Taking curl of (2.22) gives

$$\nabla \times \mathbf{u} = \boldsymbol{\omega} + \oint_{\partial V} (\mathbf{n} \times [\mathbf{u}]) \Delta G dS.$$

Let δ be a small distance in $\mathbf{n}$ direction, then

$$(2.23) \quad \lim_{\delta \rightarrow 0} \int_{-\delta}^{\delta} \nabla \times \mathbf{u} d\mathbf{n} = \mathbf{n} \times [\mathbf{u}].$$

Note the similar singularity in (2.23) as in (2.17). If ∂V is a solid boundary, this result can be interpreted as the existence of a vortex sheet on ∂V with strength $\mathbf{n} \times [\mathbf{u}]$. When the adherence condition is satisfied, the vortex sheet no longer exists.

It remains to show how to find the correct $\mathbf{n} \times \mathbf{u}$ on ∂V such that (2.1c) is satisfied by the solution of (2.13). Substituting (2.13) into (2.1c), we obtain the boundary integral equation for $\mathbf{n} \times \mathbf{u}$ [70]:

$$(2.24) \quad \frac{1}{2}u_n = \mathbf{n} \cdot \left\{ \int_V (\mathbf{g}\vartheta - \mathbf{g} \times \boldsymbol{\omega}) dV - \oint_{\partial V} [\mathbf{g}u_n - \mathbf{g} \times (\mathbf{n} \times \mathbf{u})] dS \right\}.$$

Whether (2.24) has solutions is not easy to answer, because it seems that there is only one equation for two components of the tangential part of $\mathbf{u}$ (see [70]). To avoid this difficulty, we construct $\mathbf{n} \times \mathbf{u}$ by the method described by Lighthill [46] with some modification. In fact, by this method, we can solve $\mathbf{u}$ in V without using (2.13). In the following, we show how to solve $\mathbf{u}$ on $\bar{V}$ first, then explain how $\mathbf{n} \times \mathbf{u}$ can be obtained without actually solving $\mathbf{u}$ in the whole domain.

Denote the volume integral in (2.13) as $\mathbf{u}_v$, then $\mathbf{u}$ may be expressed as

$$(2.25) \quad \mathbf{u} = \mathbf{u}_v + \mathbf{u}_s.$$

In general, $\mathbf{u}_v$ does not satisfy (2.1c); thus, we need to find $\mathbf{u}_s$ such that $\mathbf{u}$ satisfies (2.1c). Since the solution of (2.1) is unique, by Theorem 2.2.1 there must be

$$(2.26) \quad \mathbf{u}_s = - \oint_{\partial V} [\mathbf{g}(\mathbf{n} \cdot \mathbf{u}) - \mathbf{g} \times (\mathbf{n} \times \mathbf{u})] dS.$$

It is commonly argued that $\mathbf{u}_s$ must be irrotational “since $\nabla \times \mathbf{u}_v = \boldsymbol{\omega}$ ” [46]. Then because $\nabla \cdot (\mathbf{u} - \mathbf{u}_v) = 0$, we have $\mathbf{u}_s = \nabla \phi$ and

$$(2.27a) \quad \Delta \phi = 0,$$

$$(2.27b) \quad \frac{\partial \phi}{\partial \mathbf{n}} = u_n - \mathbf{n} \cdot \mathbf{u}_v.$$

Eq. (2.27) can be solved uniquely and the desired $\mathbf{u}$ is obtained. This argument is repeated also in a recent review on vortex method [5].

Unfortunately, the above scheme works only for 2-D problems and some 3-D problems but not all. In fact, by (2.16) we have

$$\nabla \times \mathbf{u}_v = \boldsymbol{\omega} + \oint_{\partial V} (\mathbf{n} \cdot \boldsymbol{\omega}) \mathbf{g} dS,$$

and hence,

$$\nabla \times \mathbf{u}_s = - \oint_{\partial V} (\mathbf{n} \cdot \boldsymbol{\omega}) \mathbf{g} dS.$$

Clearly $\mathbf{u}_s$ is *not* irrotational if $\mathbf{n} \cdot \boldsymbol{\omega} \neq 0$ on ∂V . This happens typically for a viscous flow over rotating solid bodies.

The above method can be modified to suit general 3-D problems. Following [71], we define the extension of vorticity $\boldsymbol{\omega}' = \nabla \phi'$ in V' (similarly in V for exterior problems) where ϕ' satisfies

$$(2.28a) \quad \Delta \phi' = 0 \quad (\mathbf{x} \in V'),$$

$$(2.28b,c) \quad \frac{\partial \phi'}{\partial n} = \mathbf{n} \cdot \boldsymbol{\omega} \quad (\mathbf{x} \in \partial V), \quad \nabla \phi' \rightarrow 0 \text{ as } |\mathbf{x}| \rightarrow \infty.$$

Then, define

$$(2.29) \quad \mathbf{u} = \mathbf{u}_v + \mathbf{u}'_s + \mathbf{u}''_s,$$

where

$$(2.30) \quad \mathbf{u}'_s = - \int_{V'} \mathbf{g} \times \nabla \phi' dV = - \oint_{\partial V} \phi' (\mathbf{n} \times \mathbf{g}) dS.$$

It is easily verified that

$$\nabla \cdot \mathbf{u}'_s = 0, \quad \nabla \times \mathbf{u}'_s = \beta \nabla \phi' - \oint_{\partial V} (\mathbf{n} \cdot \boldsymbol{\omega}) \mathbf{g} dS,$$

where $\beta = 0$ or 1 for $\mathbf{x} \in V$ or $\mathbf{x} \in V'$, respectively. Thus,

$$\nabla \times \mathbf{u}''_s = \nabla \times \mathbf{u} - \nabla \times (\mathbf{u}_v - \mathbf{u}'_s) = 0,$$

and hence, $\mathbf{u}''_s = \nabla \phi''$ with

$$(2.31a) \quad \Delta \phi'' = 0 \quad (\mathbf{x} \in V),$$

$$(2.31b) \quad \frac{\partial \phi''}{\partial n} = u_n - \mathbf{n} \cdot (\mathbf{u}_v + \mathbf{u}'_s) \quad (\mathbf{x} \in \partial V),$$

which can be solved uniquely. Then the solution of (2.1) is obtained by (2.29).

Now we show how to use the above method to solve the tangential components of $\mathbf{u}$ on ∂V alone without solving $\mathbf{u}$ in V . First, we evaluate $\mathbf{u}_v$ on ∂V . Then (2.28) can be solved by recasting it into a boundary-integral equation either by representing ϕ' as a single layer potential (indirect method) or using Green's

second identity (direct method). In either case, the integral equation is of the second kind and can be solved efficiently by using iterative methods. Once ϕ' on ∂V is obtained, $\mathbf{u}'_s$ can be evaluated on ∂V by (2.30). Equation (2.31) can then be solved again by the boundary-integral equation methods and $\mathbf{u}''_s$ on ∂V is computed by a surface integral. Therefore $\mathbf{n} \times \mathbf{u}$ is obtained on ∂V by solving and evaluating quantities solely on the boundary. This procedure neither proves (2.24) has a solution nor indicates how to solve (2.24) directly. Nevertheless, after obtaining the tangential part of $\mathbf{u}$ on ∂V , Eq. (2.13) can be used to find $\mathbf{u}$ in V , though it is more convenient to use (2.29) with the potentials $\nabla\phi'$ and $\nabla\phi''$, since the discretized form of the relevant surface integrals are already available when the boundary-integral equations are solved.

Remarks:

1. In the above integral method, only $\mathbf{u}_v$ needs to be evaluated by a volume integral. Both volume and surface integrals can be computed efficiently by the fast multipole method [64–66]. Moreover, an efficient scheme based on a fast multipole method is used to solve the boundary-integral equations of potential problems with arbitrary geometry [64, 72]. These advances make the above scheme ready to be implemented.
2. As mentioned above, Eq. (2.24) is a scalar equation for two components of $\mathbf{u}$. When $\mathbf{n} \cdot \boldsymbol{\omega} = 0$, as discussed in [70, 73], the two components are dependent, thus the unknowns are reduced by one. This can also be seen from the above procedure where we note that only one scalar function ϕ needs to be solved. On the other hand, when $\mathbf{n} \cdot \boldsymbol{\omega} \neq 0$, solving two scalar functions ϕ' and ϕ'' is necessary.
3. The problem of $\mathbf{n} \cdot \boldsymbol{\omega} \neq 0$ can also be treated by adding a vortex sheet on ∂V as originated in [74]. For a detailed discussion see [59]. This method should relate to the method given above, though we shall not discuss it here.

Finally, when $\mathbf{n} \cdot \boldsymbol{\omega} = 0$, using Green's identity and (2.27)

$$\phi = \oint_{\partial V} \frac{\partial \phi}{\partial n} G dS - \oint_{\partial V} \phi \frac{\partial G}{\partial n} dS.$$

Thus,

$$(2.32) \quad \nabla \phi = - \oint_{\partial V} \frac{\partial \phi}{\partial n} \mathbf{g} dS + \oint_{\partial V} \mathbf{g} \times (\mathbf{n} \times \nabla \phi) dS,$$

where the relation between double layers and vortex layers is used (see [43, 59, 70]).

Since $\mathbf{u}_s = \nabla \phi$, Eq. (2.31) can be rewritten as

$$\mathbf{u}_s = - \oint_{\partial V} [(\mathbf{n} \cdot \mathbf{u}_s) \mathbf{g} - \mathbf{g} \times (\mathbf{n} \times \mathbf{u}_s)] dS.$$

Therefore, comparing this with (2.26), we obtain an interesting property of $\mathbf{u}_v$

$$(2.33) \quad \oint_{\partial V} [(\mathbf{n} \cdot \mathbf{u}_v) \mathbf{g} - \mathbf{g} \times (\mathbf{n} \times \mathbf{u}_v)] dS = 0.$$

2.3 The Projection of Vorticity

It has been mentioned (§2.1) that in computations the divergence of $\boldsymbol{\omega}$ may not be zero because of numerical approximation. In this case, Eq. (2.1) does not have a solution. However, (2.8) has a unique solution, the only difference being that $\nabla \times \mathbf{u}$ equals $\hat{\boldsymbol{\omega}} = \boldsymbol{\omega} - \nabla \psi$ (rather than $\boldsymbol{\omega}$) which is nothing but a projection of $\boldsymbol{\omega}$ onto the divergence-free space because $\nabla \cdot \hat{\boldsymbol{\omega}} = 0$. The projection has important application in the numerical methods [39], hence it deserves some detailed discussion.

First, for free space, the projection is uniquely defined. In fact, we have

$$\Delta \psi = \nabla \cdot \boldsymbol{\omega},$$

and hence

$$\psi = - \int G \nabla \cdot \boldsymbol{\omega} dV.$$

This gives

$$(2.34) \quad \hat{\boldsymbol{\omega}} = \boldsymbol{\omega} - \int \mathbf{g} (\nabla \cdot \boldsymbol{\omega}) dV.$$

Furthermore, the projection is orthogonal [75] in the sense

$$\int \hat{\boldsymbol{\omega}} \cdot \nabla \psi dV = 0.$$

Interestingly, this projection is ensured in the integral formulation. Consider $\mathbf{u} = \mathbf{u}_v$ in free space. By using (2.16) it is easy to show that $\nabla \times \mathbf{u} = \hat{\boldsymbol{\omega}}$. Therefore when $\mathbf{u}_v$ is computed from the integral, the divergence-free part of $\boldsymbol{\omega}$ is “picked up” automatically and the projected vorticity can be obtained by differentiating the velocity. This is in fact part of the 3-D vortex method of [75].

When the domain is bounded, the projection is not uniquely defined unless some boundary conditions are specified. In [39], the Neumann condition

$$(2.35) \quad \frac{\partial \psi}{\partial n} = 0 \quad (\mathbf{x} \in \partial V)$$

was used (without explanation). We can see that when $\nabla \cdot \boldsymbol{\omega} = 0$, the projection has no effect, as expected. On the other hand,

$$(2.36) \quad \psi = \text{const} \quad (\mathbf{x} \in \partial V)$$

is another reasonable choice. However, the projections defined by (2.35) and (2.36) are different. For the former there is $\mathbf{n} \cdot \hat{\boldsymbol{\omega}} = \mathbf{n} \cdot \boldsymbol{\omega}$, whereas for the latter, $\mathbf{n} \times \hat{\boldsymbol{\omega}} = \mathbf{n} \times \boldsymbol{\omega}$. Moreover, since

$$\int_V \hat{\boldsymbol{\omega}} \cdot \nabla \psi dV = \oint_{\partial V} \psi (\mathbf{n} \cdot \hat{\boldsymbol{\omega}}) dS,$$

the projection defined by (2.35) is orthogonal if $\mathbf{n} \cdot \hat{\boldsymbol{\omega}} = \mathbf{n} \cdot \boldsymbol{\omega} = 0$; but the one defined by (2.36) is *always* orthogonal.

Since the projections are determined by the boundary conditions of which the number could be infinity, it is necessary to find the optimum one. Because in practice the problem is due to the numerical discretization of continuous equations, we should choose the projection that preserves the numerical accuracy as well as the physical content of the solution. Naturally, if the projected vorticity is closer to the unprojected one, then we have a better reason to believe that less useful information is lost during the projection.

Mathematically, we can formulate the problem as minimizing the L_2 norm of the difference between $\boldsymbol{\omega}$ and $\hat{\boldsymbol{\omega}}$, namely

$$I(\psi) = \int_V (\boldsymbol{\omega} - \hat{\boldsymbol{\omega}})^2 dV = \int_V (\nabla \psi)^2 dV,$$

by imposing a proper boundary condition on ψ . Let ψ be the minimizing function, and $\psi + \epsilon\psi'$ be a variation of ψ . Clearly ψ' must be a harmonic function in V , and hence satisfies

$$(2.37) \quad \oint_{\partial V} \frac{\partial \psi'}{\partial n} dS = 0.$$

By a standard minimization argument, it is straightforward to show that

$$(2.38) \quad \int_V \nabla \psi \cdot \nabla \psi' dV = \oint_{\partial V} \psi \frac{\partial \psi'}{\partial n} dS = 0$$

must be valid for all ψ' . Next, we show that ψ should be constant on ∂V .

Obviously, if $\psi = \text{const}$ on ∂V , Eq. (2.38) holds for all ψ' , then ψ is a minimizing function. Conversely, if $\psi \neq \text{const}$, it is possible to construct ψ' such that (2.38) is violated. We present a proof for 2-D cases: Assume ψ is not constant but a function of the arc length s of ∂V , then there exists an interval $[-s_0, s_0]$ on which $\psi(s)$ does not change sign and increases (or decreases) monotonically. Let

$$\frac{\partial \psi'}{\partial n} = \begin{cases} s(|s| - s_0)^2 & \text{if } s \in [-s_0, s_0], \\ 0 & \text{otherwise,} \end{cases}$$

which is a smooth function of s . Thus (2.37) is valid and the corresponding harmonic function ψ' exists; however,

$$\oint_{\partial V} \psi \frac{\partial \psi'}{\partial n} ds = \int_{-s_0}^{s_0} \psi \frac{\partial \psi'}{\partial n} ds \neq 0.$$

For 3-D problems, similar constructions of ψ' can be done.

If we compare Theorem 2.1.1 with the above discussion, the meaning of the theorem becomes apparent—the solution $\mathbf{u}$ of (2.8) corresponds automatically to the optimum projection of $\boldsymbol{\omega}$, and its curl is nothing but the projection. Numerically, it means that instead of performing any projection by solving one more scalar function ψ (as in [39]), we may solve $\mathbf{u}$ directly from (2.8) and then taking curl of $\mathbf{u}$ to obtain the projected vorticity.

Now consider the integral formulation. We are interested in whether the similar projection property can be reserved as for the free space and (2.8).

Formally, we can still use (2.29) to compute $\mathbf{u}$, where $\mathbf{u}_v$, ϕ' and ϕ'' are defined by (2.13), (2.28), and (2.31), respectively. Suppose $\hat{\omega} = \nabla \times \mathbf{u}$, then

$$(2.39) \quad \hat{\omega} = \omega - \int_V \mathbf{g}(\nabla \cdot \omega) dV.$$

Note that

$$\nabla \times \int_V \mathbf{g}(\nabla \cdot \omega) dV = 0,$$

hence (2.39) can be rewritten in the form of (2.33) and defines yet another projection. Note that the corresponding boundary condition for the potential is different from both (2.35) and (2.36), thus this projection is not optimum.

This observation naturally leads to a further question: does the integral approach inherently correspond to the non-optimum projection? For a closer look, we follow a derivation similar to that of (2.32) and get

$$\nabla \psi = \int_V \mathbf{g}(\nabla \cdot \omega) dV - \oint_{\partial V} \frac{\partial \psi}{\partial n} \mathbf{g} dS + \oint_{\partial V} \mathbf{g} \times (\mathbf{n} \times \nabla \psi) dS.$$

Therefore, we have

$$(2.40) \quad \hat{\omega} = \omega - \int_V \mathbf{g}(\nabla \cdot \omega) dV + \oint_{\partial V} \mathbf{n} \cdot (\omega - \hat{\omega}) \mathbf{g} dS + \oint_{\partial V} \mathbf{g} \times (\mathbf{n} \times (\omega - \hat{\omega})) dS,$$

which contains the three projections defined by (2.35), (2.36) and (2.39). As shown by (2.40), the common part of the three projections is the volume potential (integral); the differences are the surface potentials that are determined by the boundary conditions. If in the construction of ϕ' we use $\hat{\omega}$, the projected vorticity, instead of ω in (2.28b), then we get (2.40) instead of (2.39). Therefore, the optimum projection can be included in the integral formulation if correct projection boundary condition is used to determine $\hat{\omega}$. Unfortunately, this argument indicates that the optimum projection has to be obtained by solving it explicitly.

Chapter 3

Vorticity Generation and Boundary Conditions

The boundary condition for vorticity at a solid surface is encountered in various vorticity-based formulations and numerical methods, and is considered to be one of the most difficult problems in this area. In the past two decades, great efforts have been made toward solving the problem. For recent reviews see Gresho [21, 76]. As mentioned in Chapter 1, the difficulty lies in the fact that there is no natural boundary condition for vorticity; instead, only integral constraints can be rigorously derived [23–25].

The counterpart of mathematical derivation is the physical understanding of vorticity creation from solid surfaces. The two are closely related. This relation becomes more important when we solve the dynamic equation for vorticity with local BCs and the kinematic equation of velocity separately. In practice, the physical interpretation of vorticity creation often leads directly to the numerical modeling. These local models are convenient for computations, but their accuracy are often hard to estimate because of the introduction of free parameters and the ambiguity of some physical arguments. Therefore, in this study, we pay special attention to the mathematical derivation that leads to the approximate BCs.

After briefly discussing the physical process of vorticity creation, we present the general theory relevant to the dynamic vorticity BC, especially the coupling between ω and p . Then we study the approximate decoupling of ω and p and estimate its accuracy.

3.1 Vorticity Generation from Solid Walls

The question of how vorticity is generated from solid walls has puzzled fluid dynamists for a long time. While there is no doubt that the solid wall is the most important source of vorticity for an incompressible flow, the details of

generation process have not been clear. The understanding of the process is often gained through qualitative physical argument about certain idealized flow models, but there is a lack of quantitative description for general problems. The boundary vorticity and the boundary vorticity flux are usually used to quantify the process. They lead to two different descriptions of vorticity creation.

3.1.1 Kinematic Description

The well known description of the development of vorticity in the interior of flows was given by Batchelor [43]. There are three stages: first, vorticity is created on the solid boundary; then, it is diffused into the interior of the flow; in the third stage, the vorticity is convected downstream. Notably in this description, the vorticity creation and its diffusion are considered separately as a sequence of events. For a continuous vorticity creation and diffusion, the sequence occurs in every infinitesimal time interval. It is, however, impossible to infer exactly how much vorticity is created on the boundary for each sequence (which is equivalent to specifying the Dirichlet condition for vorticity) in general. Therefore, an idealized flow model is introduced so that quantitative information about boundary vorticity can be obtained.

Consider the fluid response to the motion of a solid body which is at rest at $t < 0$ and suddenly given a finite velocity at $t = 0$. The infinite acceleration of the solid body may be caused by an inertial impulse. The fluid motion has to be irrotational at $t = 0$, then the normal condition of velocity (no-penetration condition) determines the potential flow completely. Thus, the tangential velocity of the fluid is generally different from that of the solid, i.e. the no-slip condition is violated at $t = 0$. Batchelor then points out that “the discontinuity in tangential velocity at the boundary” is equivalent to a vortex sheet. Moreover, “the line integral of ω along the normal to the boundary at any point is equal in magnitude to the local jump in tangential velocity and is thus finite.” On the other hand we may consider vorticity to be infinitely large along the boundary with a δ -function like distribution along the normal direction. Right after $t = 0$, the vortex sheet

disappears because of diffusion and the vorticity becomes finite on the boundary. Diffusion also takes vorticity into the interior of the flow. Since the strength of the vortex sheet can be determined exactly at each point of the solid surface, the boundary vorticity is thus known exactly in an integral sense.

The equivalence of the jump in tangential velocity to vortex sheet needs careful justification. There are two important concepts need to be clarified. First, a vortex sheet is a sheet of concentrated vorticity *inside the fluid*, whose strength equals the jump of tangential velocity *of fluid* on the two sides of the sheet. Second, the jump of tangential velocity can be regarded as a form of concentrated vorticity *only* when the flow is considered as the limit of a viscous flow as the viscosity approaches zero [42]. The distinction between purely inviscid flows and the limit of viscous flows was first clearly addressed by Lagerstrom [77]. Wu et al. [78] show that the two concepts are of crucial importance for correct interpretation of the vorticity generation from solid walls, especially from moving walls. Moreover Wu [79] indicates that the second concept leads to an important constraint on the movement of fluid-fluid interface.

Thus, in Batchelor's argument, the no-slip condition has to be "turned on" at $t = 0^+$, so that the tangential velocity jump *from fluid to solid* becomes a vortex sheet with a strength equal that jump. From another point of view, the artificial turn-on of the no-slip condition can be avoided by insisting that it is satisfied in the whole process from $t < 0$ to $t > 0$, and a discontinuity in tangential velocity of the fluid is created at $t = 0$ due to the impulsive movement of the solid body. Wrong conclusions can be drawn from careless use of the concept of vortex sheet. For example, the following argument is given in [59, 70]. Starting from the generalized Biot-Savart Law (2.22), a boundary integral equation of $\mathbf{n} \times [\mathbf{u}]$ which depends only on the normal velocity condition at the solid boundary can be derived (ref. §2.2). It is shown that that $\mathbf{n} \times [\mathbf{u}]$ can be solved uniquely from the integral equation and hence the tangential velocity condition, i.e. the no-slip condition, is not needed. Since $\mathbf{n} \times [\mathbf{u}]$ is interpreted as the vortex sheet strength, it is concluded that the vorticity generation is determined by normal condition alone. However, we note that $\mathbf{n} \times [\mathbf{u}]$ is the jump of tangential velocity from fluid

to solid rather than inside the fluid.

The no-slip condition and viscous effect are closely connected. Without viscosity the no-slip condition is meaningless. In [80], it is argued that since the jump in velocity is an instantaneous response to the inertial force acted by the solid body, diffusion has no effect at that moment, thus "viscosity plays no role in the generation of vorticity" and hence "the generation of vorticity at the boundary ... is an inviscid process." Therefore, the no-slip condition has no effect on the flow and "the no-slip boundary condition can in no way provide a mechanism for the generation of vorticity and indeed plays no role in its generation." This conclusion, however, is erroneous as pointed out by Wu and Wu [42]. They show that if the flow is regarded as truly inviscid, there is no no-slip condition, and the jump in tangential velocity from fluid to solid does not create any rotation of fluid particles (or more precisely the principal axes of the strain rate tensor, see [42]); instead, the fluid particles slide on the solid surface. Therefore, there is no vortex sheet created. The remedy to this situation is to consider the inviscid flow to be the limit of a viscous flow as the viscosity approaches zero, thus the no-slip condition is effective, and the jump from fluid to solid can be translated as a jump inside the fluid which creates singular vorticity.

Batchelor's model is difficult to apply to vorticity generation process in general. After the impulsive start, the vorticity keeps being created continuously in time except for very special cases like the Rayleigh flow. Morino [59] suggested modeling the continuous motion of the solid body by a piecewise continuous motion which consists of a sequence of impulsive accelerations. Then the Batchelor's model can be used for each impulsive segment. A more widely adopted approach is the operator splitting in vortex methods: the convection (inertial) and diffusion (viscous) processes are treated successively. After the inviscid convection, there exists a slip on the solid body. The slip is converted to a vortex sheet by turning on the viscosity and no-slip condition. This is in essence the same as Batchelor's model except that in the small time intervals, the initial inviscid flow may be rotational instead of potential. In both cases, the vortex sheet strength is determined by solving the kinematic equations of velocity. Thus the vorticity generation is de-

terminated solely by the kinematics. However, the kinematic description should be distinguished from the real physical process. Indeed, the impulsively started flow is physically unrealistic, and the operator splitting is nothing but a mathematical treatment.

While the operator splitting provides a way to calculate the amount of vorticity generated on the boundary in a singular form at the artificial singular moments in each time step, vorticity continues to be generated after those moments. The reason is that a free diffusion of the vortex sheet does not satisfy the global constraint on vorticity imposed by the no-slip condition. In fact, new vorticity needs to be created in addition to that in the vortex sheet such that the resultant vorticity distribution satisfies the global constraint (see §3.3.1 below). In this case, the generation of vorticity is strongly coupled with the diffusion and they cannot be separated. Thus the amount of vorticity created at each point of the boundary is again undetermined. Since the viscous diffusion can not be further divided into an inviscid-viscous sequence, the kinematic description of vorticity creation can not proceed any further and hence is incomplete.

Another difficulty of computing vortex sheet diffusion was observed by Gresho [21]. The singular vorticity makes the vorticity diffusion difficult to tackle numerically, whereas it is easy to handle in u - p formulations because it is just a finite jump of velocity. However, this difficulty can be avoided by using the integral formulation presented in §3.2.2, and it can be alleviated by carefully approximating the singular vorticity on grid points as in finite difference or similar methods shown in §4.1.3.

3.1.2 Dynamic Description

Lighthill [46] took a different approach to explain the vorticity generation from solid walls. He emphasized the dynamical aspects of the process. Consider a 2D flow over a piece of plane solid surface. Let x and y be the tangential and

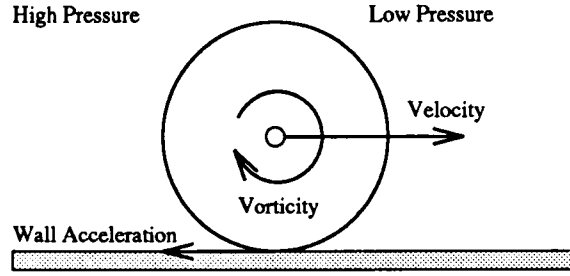


Figure 3.1: Vorticity creation due to force balance on a solid boundary.

normal directions. Applying the N-S equation at $y = 0$, the solid surface, we have

$$(3.1a) \quad -\nu \frac{\partial \omega}{\partial y} = \frac{Du}{Dt} + \frac{1}{\rho} \frac{\partial p}{\partial x},$$

$$(3.1b) \quad \nu \frac{\partial \omega}{\partial x} = \frac{Dv}{Dt} + \frac{1}{\rho} \frac{\partial p}{\partial y}.$$

Note that the acceleration of fluid particles Du/Dt and Dv/Dt should equal that of the solid boundary due to adherence condition. Eq. (3.1) represents exactly the force balance of a fluid particle on the solid body (Fig. 3.1). Denote $\sigma = -\nu \partial \omega / \partial y$ and $\delta = \partial p / \partial y$; they are called the boundary vorticity and compressing flux analogous to heat flux [42]. Since σ can be regarded as source of vorticity per unit area per unit time, Lighthill called it the vorticity source strength and considered the solid boundary as a distributed source of vorticity. From (3.1a), Lighthill also observed that the tangential vorticity is created in the direction of the surface isobars.

Wu and Wu [42] indicated that σ is responsible for both the generation of boundary vorticity and sending ω into the flow field. Therefore, there is no need to separate the production and diffusion of vorticity as they occur simultaneously in general, except that at the beginning of an impulsively started flow, the generation at the singular moment is too fast for diffusion to take place. Wu and Wu also derived the general formula of σ and δ for 3-D flows, from which they were able to identify various physical mechanisms of vorticity generation due to 3-D effects. In contrast, these details can not be studied within the kinematic frame work because no local expressions for the boundary vorticity are available. Therefore,

the dynamic description of vorticity generation, deduced directly from the N-S equation, is more natural than the kinematic one.

Unfortunately, even with exact local equation (3.1a), the rate of vorticity creation is still undetermined due to the unknown tangential pressure gradient $\partial p/\partial x$. To obtain $\partial p/\partial x$, however, one needs to know the vorticity as shown by (3.1b). Therefore, the vorticity and pressure are coupled through viscosity and the no-slip condition. This coupling is in fact another form of the coupling between vorticity and the velocity. To obtain more quantitative information about the rate of vorticity generation, Lighthill side-stepped this difficulty by returning to the vortex sheet argument as described in the last subsection, and he made no connection between the creation of vortex sheet with (3.1a). However, Wu and Wu [42] show that (3.1a) is very useful for understanding the dynamics of the vortex sheet generation. They pointed out that the impulsively started flow must come from an impulsive pressure gradient, and the impulsively started wall motion must cause impulsive inertial force, then by (3.1a) a singular boundary vorticity flux is needed to balance the sum of the impulsive pressure gradient and the inertial force. This singular σ is responsible for the creation of the initial vortex sheet. Note that the no-slip condition is imposed through out the whole argument.

Like the kinematic description, the dynamic description can also benefit from operator splitting, but from a different point of view—the approximate decoupling between vorticity and pressure. This topic will be studied in detail in the next section. The significance of the dynamic description is its ability to treat the singular as well as regular vorticity creation in a consistent and unified way. In some simple situations, where the tangential pressure gradient is known, Eq. (3.1a) gives the exact Neumann BC for vorticity; while it is still impossible to obtain a local Dirichlet BC for vorticity from the kinematic description alone. This shows the advantage of having an exact local equation for the vorticity flux, from which the vorticity and pressure solution can be formulated in an integral form, convenient for studying the approximate decoupling of ω and p .

3.2 Vorticity-Pressure Coupling

In this section, we present the general theory of ω - p coupling due to Wu et al. [81], including the integral formulation of the solution structure of vorticity and pressure. Then, based on these general results, we examine the strength of ω - p coupling and the method to decouple the two approximately.

Consider an incompressible flow of unit density past a solid body. Let the flow domain be V with boundary ∂V moving with velocity $\mathbf{b}$. For neatness denote

$$(3.2) \quad \mathcal{L}(\mathbf{u}) = \mathbf{a} - \nu \nabla^2 \mathbf{u} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u}$$

where $\mathbf{a} = D\mathbf{u}/Dt$ is acceleration, such that the Navier-Stokes and continuity equations read

$$(3.3a) \quad \mathcal{L}(\mathbf{u}) + \nabla p = 0$$

$$(3.3b) \quad \nabla \cdot \mathbf{u} = 0.$$

The initial and boundary conditions are

$$(3.3c) \quad \mathbf{u} = \mathbf{u}_0 \quad \text{at } t = 0 \quad \text{in } V,$$

$$(3.3d,e) \quad \mathbf{n} \times \mathbf{u} = \mathbf{n} \times \mathbf{b}, \quad \text{and} \quad \mathbf{n} \cdot \mathbf{u} = \mathbf{n} \cdot \mathbf{b}, \quad \text{on } \partial V.$$

Hereafter $\mathbf{n}$ is the unit normal vector on the boundary ∂V , pointing out of the fluid. The boundary ∂V may consist of a solid surface B and an infinite boundary ∂V_∞ . In the latter case we can still imagine an “adherence” there, since (3.3d,e) apply as well, with $\mathbf{b}$ being assumed as a uniform vector, say $\mathbf{U}(t)$. Then, instead of solving problem (3.3) in terms of primary variables, the vorticity-based methods seek the solution of

$$(3.4a,b) \quad \mathcal{N}(\mathbf{u}, \boldsymbol{\omega}) = \nabla \times \mathcal{L}(\mathbf{u}) = 0, \quad \boldsymbol{\omega} = \nabla \times \mathbf{u},$$

under constraints (3.3b~e). An immediate problem is that due to raising the order of differential equation, Eq. (3.4) may have solutions that do not satisfy (3.3a). In

general, these spurious solutions are removed by imposing *compatibility* conditions. On the other hand, as long as the problem (3.4) with (3.3b~e) is well-posed and its solution $\mathbf{u}$ is obtained, then, there must be

$$\mathcal{L}(\mathbf{u}) + \nabla\phi = 0$$

for some ϕ , which can only be identified as the pressure p . Then, there is no need for solving p simultaneously. Eqs. (3.3b), (3.4b) and (3.3e) consist of the kinematic equations for $\mathbf{u}$ which can be solved easily by the methods presented in Chapter 2. However, difficulty arises in implementing (3.3d) directly in terms of ω . This motivated us to appeal to the dynamic boundary conditions.

3.2.1 Dynamic Neumann Conditions for the (ω, p) Field

It is easy to understand that the velocity adherence implies *acceleration adherence*:

$$(3.5a,b) \quad \mathbf{n} \times \mathbf{a}_B = \mathbf{n} \times \mathbf{a}_b \quad \text{and} \quad \mathbf{n} \cdot \mathbf{a}_B = \mathbf{n} \cdot \mathbf{a}_b, \quad t \geq 0,$$

where $\mathbf{a}_b$ is the wall acceleration, and where and below the subscript B implies the value of fluid quantities on solid surface B . To recover (3.3d,e), one simply adds an initial velocity adherence [25,49]

$$(3.6a,b) \quad \mathbf{n} \times \mathbf{u}_B = \mathbf{n} \times \mathbf{b} \quad \text{and} \quad \mathbf{n} \cdot \mathbf{u}_B = \mathbf{n} \cdot \mathbf{b}, \quad t = 0.$$

Note that, as shown by Wu and Wu [42], in vorticity-based formulations the no-slip condition should be and can be imposed at $t = 0$, even if there is an (idealized) impulsive start from a potential flow along with a singular vortex sheet on B , since only the no-slip condition can determine the sheet strength (see also §3.1.1 and §3.2.2 below). But in the $(\mathbf{u}, p)$ formulation there is no such need, and it is acceptable to impose no-slip only for $t > 0$ as Gresho [21,76] stressed.

Now, the local dynamic boundary conditions of the Neumann type for ω and p follow from applying (3.3a) to the wall and using (3.5a,b). It is then immediately clear that once these dynamic boundary conditions are used in solving

the vorticity field, the (ω, p) coupling becomes inevitable. Thus, theoretically, one has to solve the (ω, p) equations simultaneously. Symbolically, these equations and respective dynamic boundary conditions are

$$(3.7a,b) \quad \nabla \times \mathcal{L}(\mathbf{u}) = 0, \quad \mathbf{n} \times \mathcal{L}(\mathbf{u})_B = -\mathbf{n} \times \nabla p_B,$$

$$(3.8a,b) \quad \nabla^2 p = -\nabla \cdot \mathcal{L}(\mathbf{u}), \quad \mathbf{n} \cdot \nabla p_B = -\mathbf{n} \cdot \mathcal{L}(\mathbf{u})_B.$$

We shall see below that like (3.8b), Eq. (3.7b) can be cast to an explicit formula for *boundary vorticity flux* $\sigma = \nu (\partial\omega/\partial n)_B$. Equations (3.5a) and (3.5b) are necessary in fixing $(\partial\omega/\partial n)_B$ and $(\partial p/\partial n)_B$, respectively.

Our first concern is whether the solution to this set of equations is also a solution of the original equation (3.3). We have

Theorem 3.2.1 *Assume $\mathbf{u}$ satisfies (3.7a) and (3.8a). Then it is the solution of (3.3a), if either (3.7b) or (3.8b) holds.*

Proof. From (3.7a) we have $\mathcal{L}(\mathbf{u}) + \nabla\phi = 0$ for some ϕ . Substitute this into (3.8a), we get

$$(3.9) \quad \nabla \cdot \nabla(p - \phi) = \nabla^2\phi' = 0$$

for $\phi' = p - \phi$. But (3.7b) implies $\mathbf{n} \times \nabla\phi' = 0$ or $\phi' = \text{const.}$ on B , thus $\nabla\phi' = 0$ in V . Alternatively, (3.8b) implies $\partial\phi'/\partial n = 0$ on B and the same result follows. In both cases (3.3a) holds. $\square$

Therefore, by introducing acceleration adherence (3.5a,b), the boundary conditions and compatibility conditions are merged into one. In this case, (3.7b) and (3.8b) represent the mathematically natural boundary conditions for ω and p , respectively. They are also physically natural: as shown by Wu and Wu [42] (see also §3.1.2 and §3.2.2 below), they precisely reflect the physics of (ω, p) creation from the wall.

The above theorem can be restated as

Corollary 3.2.1 *Let $\mathbf{u}$ be a solution of problem (3.7a, b) (or (3.8a, b)). Then it is also a solution of (3.3a), if and only if it satisfies (3.8a) (or (3.7a)) simultaneously.*

Proof. The “only if” part is trivial. To prove the “if” part, for example, from (3.7a,b) we obtain $\mathcal{L}(\mathbf{u}) = -\nabla\phi$ with $\mathbf{n} \times \nabla(\phi - p) = 0$; but by (3.8a) we must have $\nabla^2(\phi - p) = 0$. The rest of the proof is obvious. $\square$

As mentioned before, once the velocity field of an incompressible flow has been solved by whatever method, ∇p can be inferred from the Navier-Stokes equation (3.3a). One can also solve the second-order pressure equation (3.8a,b). However, Corollary 3.2.1 shows that this approach needs to satisfy the vorticity equation as a prerequisite. Similarly, solving the vorticity equation (3.7a,b) also requires the second-order pressure equation.

Problems (3.7a,b) and (3.8a,b), along with initial condition (3.3c) plus a given initial vorticity distribution ω_0 in V at $t = 0$, constitute a well-posed initial-boundary value problem for the coupled (ω, p) field. The pressure part of this problem has been extensively studied by Gresho and Sani; [22] so we shall mainly concentrate on the vorticity part of the problem. However, the (ω, p) coupling on B , and hence an interior (ω, p) coupling over the whole flow domain V , should not be ignored or oversimplified. The effect of this coupling will be analyzed theoretically in §3.2.2, and numerical aspects of handling this coupling will be presented in §3.3.

We now recover the detailed form of equations and boundary conditions. For incompressible flow the (ω, p) equations (3.7a) and (3.8a) read

$$(3.10) \quad \frac{\partial \omega}{\partial t} + \nabla \times \mathbf{L} - \nu \nabla^2 \omega = 0, \quad \mathbf{L} \equiv \omega \times \mathbf{u},$$

$$(3.11) \quad \nabla^2 p_0 = -\nabla \cdot \mathbf{L}, \quad p_0 \equiv p + \frac{1}{2}|\mathbf{u}|^2.$$

The general formula for the boundary vorticity flux σ on a solid wall, as well as that for the normal pressure gradient, have been given by Wu [47], Wu et al. [48] and Wu and Wu [42]. The incompressible version reads

$$(3.12) \quad \sigma \equiv \nu \left(\frac{\partial \omega}{\partial n} \right)_B = \mathbf{n} \times \mathbf{a}_b + (\mathbf{n} \times \nabla) \cdot (p_B \mathbf{I} + \nu \omega'_B \times \mathbf{nn}),$$

$$(3.13) \quad \delta \equiv - \left(\frac{\partial p}{\partial n} \right)_B = \mathbf{n} \cdot \mathbf{a}_b + (\mathbf{n} \times \nabla) \cdot \nu \omega_B,$$

where $\mathbf{I}$ is the unit tensor, and $\boldsymbol{\omega}'_B = \boldsymbol{\omega}_B - 2\boldsymbol{\Omega}(t)$ is the relative vorticity with $\boldsymbol{\Omega}$ being the angular velocity of the wall. The two-dimensional form of these formulas is well known (see Eq. (3.1)), and in three-dimensions there is an extra term $(\mathbf{n} \times \nabla) \cdot (\nu \boldsymbol{\omega}'_B \times \mathbf{n})$ in $\boldsymbol{\sigma}$, indicating its dependence on $\boldsymbol{\omega}_B$ or skin-friction $\boldsymbol{\tau}_B = \nu \mathbf{n} \times \boldsymbol{\omega}'_B$ and the surface curvature [42, 47, 48]. The physical aspects of $\boldsymbol{\sigma}$ have been discussed by Wu and Wu [42] in depth, where it is also shown that this flux, first introduced by Lighthill [46], is the uniquely correct measure of vorticity source strength on a solid wall.

3.2.2 The Solution Structure of Vorticity

We now examine the detailed structure of formal $(\boldsymbol{\omega}, p)$ solutions by the standard Green's function method. This study provides a foundation to the later design of numerical (both integral and local) schemes.

We first concentrate on the vorticity part, and assume temporarily that the p_B distribution is known. Let $\mathbf{r} = \mathbf{x} - \boldsymbol{\xi}$, $r = |\mathbf{r}|$, and

$$(3.14) \quad G^*(\mathbf{x}, \boldsymbol{\xi}; t, \tau) = \frac{H(t - \tau)}{[4\pi\nu(t - \tau)]^{d/2}} \exp \left[-\frac{r^2}{4\nu(t - \tau)} \right]$$

be the fundamental solution of the heat equation in free space, with H being the step function and d the spatial dimensionality. From Green's second identity it follows that

$$(3.15) \quad \begin{aligned} \boldsymbol{\omega}(\mathbf{x}, t) = & \int_V G_0^* \boldsymbol{\omega}_0 dV + \int_0^t d\tau \oint_B \left(G^* \boldsymbol{\sigma} - \nu \boldsymbol{\omega}_B \frac{\partial G^*}{\partial n} \right) dS \\ & - \int_0^t d\tau \oint_B G^* \mathbf{n} \times \mathbf{L}_B dS + \int_0^t d\tau \int_V \nabla G^* \times \mathbf{L} dV. \end{aligned}$$

Here the subscript 0 implies values at $\tau = 0$, and $\boldsymbol{\sigma}$ is given by (3.12). The first volume integral represents the effect of initial $\boldsymbol{\omega}$ distribution, and the last two, the nonlinear convection effect. The $\partial G^* / \partial n$ term can be eliminated if the Green's function with zero normal derivative can be found. For simple boundaries such as flat plate or circular cylinder, this can be achieved by using the image method.

Note that great care is necessary in determining the effect of a moving boundary. Although velocity adherence implies acceleration adherence, in the Eulerian description the local and convection accelerations of fluid particles on B , $(\partial \mathbf{u}/\partial t)_B$ and $(\mathbf{u} \cdot \nabla \mathbf{u})_B$, are not equal to those of the solid surface, $\partial \mathbf{b}/\partial t$ and $\mathbf{b} \cdot \nabla \mathbf{b} = \boldsymbol{\Omega} \times \mathbf{b}$, respectively. Rather, it can be shown that [78]

$$\left(\frac{\partial \mathbf{u}}{\partial t}\right)_B = \frac{\partial \mathbf{b}}{\partial t} - (\mathbf{n} \cdot \mathbf{b})(\boldsymbol{\omega}'_B \times \mathbf{n}), \quad (\mathbf{u} \cdot \nabla \mathbf{u})_B = \boldsymbol{\Omega} \times \mathbf{b} + (\mathbf{n} \cdot \mathbf{b})(\boldsymbol{\omega}'_B \times \mathbf{n}).$$

Moreover, a normal motion of B will generally lead to the time dependence of the normal vector $\mathbf{n}$ and the flow domain V . All these make flow problems with moving walls (for instance, an oscillating flap) much more complicated than those with stationary walls. For an analysis of the effect of a moving boundary on the time-averaged vorticity flux see Wu et al. [78]. For simplicity, we assume $\mathbf{n} \cdot \mathbf{b} = 0$ in the rest of the thesis. Thus,

$$\mathbf{n} \times \mathbf{L}_B = -\mathbf{b}\mathbf{n} \cdot \boldsymbol{\omega}_B = -2\mathbf{b}\mathbf{n} \cdot \boldsymbol{\Omega}.$$

As shown by Wu and Wu [42], if in an idealized model the flow is started by either an *impulsive* pressure gradient and/or an *impulsive* body motion, the boundary vorticity flux $\boldsymbol{\sigma}$ must contain a δ -function at $t = 0$ and creates an infinitely thin vortex sheet with strength γ_0 :

$$(3.16) \quad \boldsymbol{\sigma} = \mathbf{n} \times (\mathbf{b}_0 - \mathbf{u}_0)\delta(t) = \gamma_0\delta(t), \quad 0^- \leq t \leq 0^+,$$

where $\mathbf{u}_0$ denotes a suddenly gained flow velocity above the wall at $t = 0$ due to the impulsive pressure gradient. In (3.15), this singular behavior of $\boldsymbol{\sigma}$ can be easily separated from its regular part:

$$(3.17) \quad \oint_0^t d\tau \oint_B G^* \boldsymbol{\sigma} dS = \oint_B G_0^* \gamma_0 dS + \int_{0^+}^t d\tau \oint_B G^* \boldsymbol{\sigma} dS.$$

Note that the initial velocity no-slip condition has been implied through (3.17), and without such a condition the initial vortex sheet strength γ_0 would be uncertain and has to be prescribed in advance.

To illustrate the implication of (3.15), we apply it to a unidirectional flow $u(y, t)$ over a flat plate at $y = 0$. Assume the fluid and wall are at rest for $t < 0$. Take $d = 1$ and $r = y - \eta$ in (3.14) and eliminate $\partial G^*/\partial n$ in (3.15) by the method of images. Then we readily obtain

(3.18a)

$$\omega(y, t) = \frac{\gamma_0}{\sqrt{\pi\nu t}} \exp\left(-\frac{y^2}{4\nu t}\right) + \int_{0^+}^t \frac{\sigma(\tau)}{\sqrt{\pi\nu(t-\tau)}} \exp\left[-\frac{y^2}{4\nu(t-\tau)}\right] d\tau,$$

where $\gamma_0 = b_0 - u_0$ and

(3.18b)
$$\sigma(t) = \frac{db}{dt} + P(t),$$

with $P(t) \equiv \partial p/\partial x$ that can only be a function of t . In particular, the boundary vorticity is

(3.19)
$$\omega_B(t) = \frac{\gamma_0}{\sqrt{\pi\nu t}} + \frac{1}{\sqrt{\pi\nu}} \int_{0^+}^t \frac{\sigma(\tau)}{\sqrt{t-\tau}} d\tau.$$

For example, the solution of Stokes' first problem (the Rayleigh problem) simply follows from letting $\sigma = 0$ for $t \geq 0^+$ in (3.18a) and (3.19), yielding the boundary vorticity

(3.20)
$$\omega_B = \frac{\gamma_0}{\sqrt{\pi\nu t}}.$$

Or, if $P(t) = 0$, $u_0 = 0$, and $b = b_0 \cos t$, Eq. (3.19) yields

(3.21)
$$\omega_B = \frac{b_0}{\sqrt{\pi\nu t}} + b_0 \sqrt{\frac{2}{\nu}} [S(\sqrt{t}) \cos t - C(\sqrt{t}) \sin t],$$

where $S(x)$ and $C(x)$ are Fresnel's functions. This is the solution of the generalized Stokes' second problem including the transient effect, which has been thoroughly studied by Panton [82]. As $t \rightarrow \infty$, Eq. (3.21) gives the classical result $\omega_B(t) = (b_0/\sqrt{\nu}) \cos(t + \pi/4)$. In Chapter 4 we shall give numerical results of these two typical problems as the first test of numerical algorithms, but the flat plate is replaced by a circular cylinder.

The special case with $b = 0$ and $P = \text{const.}$ in (3.18) was used by Gresho [21] to explain the singular behavior of ω_B and σ at $t = 0$. He concludes that the vortex sheet "is a primary evil when using vorticity based methods". But this evil disappears in the integral formulation.

Note that in the above example, there is no way to infer the boundary condition in advance from kinematic relations only (either theoretically or numerically), since the effect of p is "unknown" in the kinematics. This statement is also valid for general *gradually* started flows due to a sudden appearance of a *finite* pressure gradient. This is another indication that vorticity creation can only be fully understood dynamically.

Return to (3.15), and further confine attention to the case with $\mathbf{b} = 0$ and hence $\mathbf{n} \cdot \omega_B = 0$. By (3.12) we have

$$G^* \sigma = (\mathbf{n} \times \nabla) \cdot [G^*(p_B \mathbf{I} + \nu \omega_B \times \mathbf{nn})] - (\mathbf{n} \times \nabla G^*) \cdot (p_B \mathbf{I} + \nu \omega_B \times \mathbf{nn}).$$

Here, owing to a consequence of the generalized Stokes theorem

$$(3.22) \quad \oint (\mathbf{n} \times \nabla) \circ \mathcal{F} dS = 0$$

for any tensor $\mathcal{F}$ and meaningful operation $\circ$, the first term has no contribution to the surface integral of $G^* \sigma$; while the second term is

$$-(\mathbf{n} \times \nabla G^*) \cdot (p_B \mathbf{I} + \nu \omega_B \times \mathbf{nn}) = \nabla G^* \times \mathbf{n} p + \mathbf{n} \nabla G^* \cdot \nu \omega_B.$$

Therefore, since

$$(3.23a) \quad \mathbf{n} p_B + \mathbf{n} \times \nu \omega_B = \mathbf{t}_B$$

is the wall stress, it follows from (3.15) and (3.17) that, for stationary B ,

$$(3.23b) \quad \begin{aligned} \omega(\mathbf{x}, t) = & \oint_B G_0^* \gamma_0 dS + \int_V G_0^* \omega_0 dV + \int_{0^+}^t d\tau \oint_B \nabla G^* \times \mathbf{t}_B dS \\ & + \int_0^t d\tau \int_V \nabla G^* \times \mathbf{L} dV. \end{aligned}$$

We make three remarks on (3.23). First, although in deriving (3.23b) we only used the free-space Green's function (3.14), the $G^* \partial \omega / \partial n$ term is remarkably absent in the surface integral. Thus, along with the corresponding pressure equation (3.26) below, we arrive at an innovative integral formulation of a *Dirichlet problem with free-space Green's function*. However, this problem is not for ω alone; rather, it is for the coupled (ω, p) . Second, since by (3.14) ∇G^* is along the direction of $\mathbf{r} = \mathbf{x} - \boldsymbol{\xi}$, we see that the boundary stress $\mathbf{t}_B$ at a point $\boldsymbol{\xi}_B \in B$ affects the vorticity field at a point $\mathbf{x} \in V$ only by its components *perpendicular* to $\mathbf{r}$, through diffusion. Third, applying (3.23b) to B implies a dynamic integral constraint to the boundary vorticity ω_B , or a global and implicit Dirichlet condition for ω in V . Unlike the boundary vorticity flux σ , however, there exists no local equation for ω_B . This is factually a mathematical manifestation of the underlying physics [42]: it is the boundary vorticity flux rather than boundary vorticity that reflects the vorticity source directly, and the boundary vorticity itself arises through a time-accumulated effect of the flux (see (3.19)).

We use the integral formulation here mainly for clarifying the structure of the solution and the effect of boundary conditions. In numerical computations integral methods are usually more time-consuming than finite-difference methods. But, owing to the desire to remove the less-accurate random-walk approach from Chorin's vortex methods, some authors have recently turned to deterministic diffusion algorithms, which are mostly of integral type since then a smooth connection between the Lagrangian convection substep and the Eulerian diffusion substep can be achieved (in contrast, to connect a Lagrangian convection and a finite-difference diffusion one has to use the vortex-in-cell technique at the expense of artificial viscosity). For example, the PSE method (Degond and Mas-Gallic [83]; Pépin [68] and references cited therein) uses an approximate estimation of σ as the Neumann condition; and, to avoid the appearance of ω_B , it starts from Green's first identity instead of (3.15), bringing about some error due to the inevitable appearance of a volume integral of a Taylor expansion (Cottet [84]; Leonard 1991, private communication). On the other hand, Lu and Ross [85] use an integral equation for ω_B to construct the Dirichlet condition, and introduce an approximate image Green's

function (with respect to a flat plate) to remove the vorticity flux σ . Now, despite the large consumption of computational resources inherent in these integral methods, we see that (3.15) and (3.23) provide a foundation to deterministic diffusion methods.

3.2.3 Boundary Pressure

So far we have assumed that p_B is known in (3.12) or (3.23). We now turn to the pressure problem (3.11) and (3.13), which in turn depends on ω_B . This can also be seen clearly from the solution structure for p . Let

$$(3.24) \quad G(\mathbf{x}, \boldsymbol{\xi}) = \begin{cases} -\ln r/2\pi, & \text{if } d = 2 \\ 1/4\pi r, & \text{if } d = 3 \end{cases}$$

be the fundamental solution of the Laplace equation in free space. Similar to (3.15), from Green's second identity it readily follows that

$$(3.25) \quad p_0(\mathbf{x}) = - \oint_B \left(G\delta + p_0 \frac{\partial G}{\partial n} \right) dS + \oint_B G \mathbf{n} \cdot \mathbf{L}_B dS - \int_V \nabla G \cdot \mathbf{L} dV,$$

where δ is given by (3.13). Hence, substituting (3.13) into (3.25) and using (3.22), for a stationary wall we find that the counterpart of (3.23) is

$$(3.26) \quad p_0(\mathbf{x}) = - \oint_B \nabla G \cdot \mathbf{t}_B dS - \int_V \nabla G \cdot \mathbf{L} dV,$$

where $\mathbf{t}_B$ is defined by (3.23a). It follows from (3.26) that the component of $\mathbf{t}_B$ parallel to $\mathbf{r} = \mathbf{x} - \boldsymbol{\xi}$ at $\boldsymbol{\xi}_B \in B$ has an effect on p_0 at $\mathbf{x}$. Again, Eq. (3.26) contains a boundary integral equation for p_B (note that $p_0 = p$ on stationary B).

In principle, p_B or its tangential gradient can be solved simultaneously with vorticity. However, such a global coupling is computationally undesirable, especially for vortex methods; for otherwise the methods would lose some of their main advantages, i.e. getting rid of p and working in the rotational flow region only. In many $(\omega, \mathbf{u})$ -based methods, ω is solved coupled with $\mathbf{u}$ through the no-slip condition. This certainly avoids solving p , but it only switches the coupling from dynamics to kinematics. Therefore, it is important to study the methods of decoupling ω and p .

3.3 Decoupled Approximations and Vorticity Boundary Conditions

Any decoupling of ω and p has to be approximate. The operator splitting scheme provides a natural way to carry out the approximation, since the vorticity and pressure are fully decoupled in the vorticity convection equation. The slip generated on the solid boundary by the convection represents the inertial effect on vorticity creation. Intuitively, we expect that most of the vorticity are created due to the inertial force at high Reynolds numbers. Boundary layer flows are typical cases of vorticity generation being solely determined by the convection of flows outside the thin layer near the wall; therefore, decoupling of ω and p is achieved rather completely in these flows.

3.3.1 Operator Splitting

The operator splitting (or fractional-step) methods can partially but greatly reduce the (ω, p) coupling. In these methods, one solves the Euler and Stokes equations

$$(3.27a) \quad \frac{\partial \mathbf{u}_1}{\partial t} + \mathbf{u}_1 \cdot \nabla \mathbf{u}_1 + \nabla p_1 = 0,$$

$$(3.27b) \quad \frac{\partial \mathbf{u}_2}{\partial t} + \nabla p_2 = \nu \nabla^2 \mathbf{u}_2$$

successively for each time step. In this process, $\mathbf{u}_1$ solved from (3.27a) is used as the initial condition for (3.27b). Here the scalars p_1 and p_2 are needed to guarantee the solenoidal condition (3.3b); they are only implicitly related through the relation between $\mathbf{u}_1$ and $\mathbf{u}_2$. Symbolically, the solution of the N-S equation (3.3a) can be written as

$$(3.28) \quad \mathbf{u}(\Delta t) = S(\Delta t)\mathbf{u}^0 = H(\Delta t)E(\Delta t)\mathbf{u}^0,$$

where $\mathbf{u}^0$ is the initial velocity for a time step, and $S(t)$, $H(t)$, and $E(t)$ are the solution operators for the N-S, Stokes, and Euler equations, respectively. Eq. (3.28) is rigorously valid as $\Delta t \rightarrow 0$. The scheme is proved to be $O(\nu\Delta t)$ accurate in time for unbounded flow by Beale and Majda [86], and $O(\Delta t)$ accurate for flow bounded

by solid boundaries by Ying [87] and Beale and Greengard [88]. Higher-order schemes can be designed; e.g. Strang splitting scheme:

$$\mathbf{u}(\Delta t) = S(\Delta t)\mathbf{u}^0 = H(\Delta t/2)E(\Delta t)H(\Delta t/2)\mathbf{u}^0,$$

which is $O(\nu\Delta t^2)$ and $O(\Delta t^2)$ accurate for unbounded and bounded flows, respectively. Here we only discuss (3.28); the results are also valid for the Strang splitting.

It should be mentioned that while $\mathbf{u}_2$ (solved from (3.27b) with $\mathbf{u}_1$ as the initial condition) is a valid approximation of the original Navier-Stokes equation, it remains unclear whether the same is true for p_2 . In fact, Eq. (3.27b) shows that p_2 satisfies the Laplace equation, whose solution may be qualitatively different from that of (3.11).

Corresponding to (3.27a,b), we have

$$(3.29a) \quad \frac{\partial \boldsymbol{\omega}_1}{\partial t} + \nabla \times \mathbf{L}_1 = 0, \quad \mathbf{L}_1 = \boldsymbol{\omega}_1 \times \mathbf{u}_1,$$

$$(3.29b) \quad \frac{\partial \boldsymbol{\omega}_2}{\partial t} = \nu \nabla^2 \boldsymbol{\omega}_2,$$

as the vorticity convection and diffusion equations. Note that $\boldsymbol{\omega}_1$ and p_1 are fully *decoupled* in (3.29a) since only (3.3e) is required on B . In other words, Eq. (3.29a) can be solved without regard to p , and in this substep there is no need of the vorticity BC at all. Here Lagrangian vortex methods exhibit most of their strength. On the other hand, the coupling between $\boldsymbol{\omega}_2$ and p_2 persists in (3.29b) due to the no-slip condition, which causes the problem of vorticity BCs. Thus, as Gresho [89] observed, the Stokes part is most difficult to deal with. Now the coupling is revealed by the reduced version of (3.23) and (3.26), i.e.

$$(3.30) \quad \boldsymbol{\omega}_2(\mathbf{x}, t) = \oint_B G_0^* \boldsymbol{\gamma}_0 dS + \int_V G_0^* \boldsymbol{\omega}_{20} dV + \int_{0^+}^t d\tau \oint_B \nabla G^* \times \mathbf{t}_{2B} dS,$$

$$(3.31) \quad \frac{1}{2} p_{2B} + \oint_B \nabla G \cdot (\mathbf{n} p_{2B} + \mathbf{n} \times \nu \boldsymbol{\omega}_{2B}) dS = 0.$$

Two benefits can be seen from (3.30) and (3.31). First, the equations are linearly coupled, which makes it easier to solve. Second, the velocity does not appear in the coupling, hence it can be solved separately after $\boldsymbol{\omega}$ is obtained.

We also note that the first two integrals of (3.30) are the diffusion of vortex sheet γ_0 and initial vorticity ω_0 in free space; the third integral corrects the results of the first two integrals so that the global constraint on vorticity is satisfied. From the derivation of (3.23b), it is clear that the third integral contains additional vorticity generation. Thus, the vorticity diffusion is coupled with generation (ref. §3.1.1).

3.3.2 Local Vorticity BCs and (ω, p) Decoupling

In the original Chorin-Marsden product formula [90], the solution operator is approximated by

$$S(\Delta t) = H(\Delta t)\Phi(\Delta t)E(\Delta t),$$

where $\Phi(t)$ is called the “vorticity creation operator”. The effect of this operator is to *model* vorticity creation from a solid wall and hence provides local vorticity BCs for $H(t)$. Note that $\Phi(t)$ includes only the inertial effect on vorticity creation of $E(t)$. Usually, the modeling does not use the information of pressure directly, and so ω is decoupled from p . This, in fact, is also true for some implementation of the local kinematic vorticity BCs in conventional finite-difference methods.

The modeling of the vorticity creation can only be approximate, and has been very often based on intuition. After the substep of inviscid convection (i.e. solving (3.29a)), a slip velocity $\mathbf{u}_s = \mathbf{u}_b - \mathbf{b}$ always appears on the solid boundary B . Thus, like (3.17), there must be a singular vortex sheet with strength

$$\gamma = -\mathbf{n} \times \mathbf{u}_s$$

This vortex sheet is then used to either estimate the variation in boundary vorticity (i.e., a Dirichlet condition):

$$(3.32) \quad \Delta\omega_B \simeq \frac{\gamma}{h}$$

with h being a chosen small normal distance, [19] or to determine the circulation of the discrete vortices newly created from B [91]. One common choice is to set

$h = \sqrt{\pi\nu\Delta t}$, implying that (3.20) is used to approximate ω_B everywhere, and some dynamics is thereby introduced. We see that this choice is essentially a local unidirectional-flow approximation.

Another way of utilizing γ is the dynamic approach that has been applied in some ω -based methods in 2D computations [50, 51, 68, 92]. The following Neumann condition is adopted (the argument leading to this will be given below):

$$(3.33) \quad \sigma \simeq \frac{\gamma}{\Delta t}.$$

Equations (3.32) and (3.33) are both decoupled from the pressure and hence they are *not exact*. It should be stressed that the reverse reasoning that (3.32) and (3.33) imply no explicit coupling between ω and p is incorrect.

Both (3.32) and (3.33) are often criticized as being inaccurate. However, because of the singularity and the “unusual” way of computing the BCs, the error estimate is not so straightforward. As we discussed above, the vorticity creation and diffusion are not really separable because of the (ω, p) coupling; therefore, it is better to look at how accurate the final solution, obtained from solving (3.29b) and (3.32) or (3.33), will be. When no exact solution or benchmark numerical solution is available, the judgment is difficult to make. However, we may infer, at least, how well the decoupled methods approximate the global (ω, p) coupling by checking the velocity no-slip condition (since it is the reason for all the trouble). But this check cannot be easily done analytically (see Hou and Wetton [45]) and numerical experiments are needed in many cases.

To gain some insight into the above decoupled approaches, we need to clarify the hidden assumptions of the approximate BCs, especially (3.33). The common argument that leads to (3.33) has been clearly summarized by Gresho [21]. A more rational analysis is as follows.

For the sake of simplicity, we consider a two-dimensional flow over a solid surface $y = 0$, with x and y being the tangential and normal directions of the surface, respectively. The flow occurs at $y > 0$. For the tangential velocity u , at

the surface we have

$$(3.34) \quad \frac{\partial u}{\partial t} + P = -\nu \frac{\partial \omega}{\partial y} = \sigma,$$

where $P \equiv \partial p_{2B}/\partial x$. Assume initially there is a slip velocity $u_s = u_b - b$ (where b is the tangential velocity of the solid wall) at $y = 0$ for $t = 0$. Since for $t > 0$, the no-slip condition is resumed, there must be a singular boundary vorticity flux to balance the infinite deceleration of the fluid. It is important to keep in mind that P is always finite because there is no pressure impulse. Integrating (3.34) from 0 to Δt yields

$$(3.35) \quad u(\Delta t) - u_b = \Delta t(\bar{\sigma} - \bar{P})$$

where

$$\bar{\sigma} = -\frac{1}{\Delta t} \int_0^{\Delta t} \nu \frac{\partial \omega}{\partial y} dt \quad \text{and} \quad \bar{P} = \frac{1}{\Delta t} \int_0^{\Delta t} P dt.$$

are the time averaged values of σ and P . Since the diffusion substep should make the no-slip condition satisfied for $t > 0$, hence $u(\Delta t) = b$ and we have

$$(3.36) \quad \bar{\sigma} = -\frac{u_s}{\Delta t} + \bar{P}.$$

Here, $\bar{P}$ is unknown, and by dropping it we return to the decoupled approximate expression (3.33) for the averaged vorticity flux. Since u_s represents the initial singularity, $\bar{P}$ should give the “regular part” of σ . This implies that as $\Delta t \rightarrow 0$ there is

$$(3.37) \quad \int_0^{\Delta t} \sigma dt = -u_s,$$

from which we may get $\bar{\sigma} = -u_s/\Delta t$ too. It shows that the decoupling is exact when $\Delta t \rightarrow 0$. For any finite Δt , dropping $\bar{P}$ introduces an error of order $O(\Delta t)$. We note that Koumoutsakos et al. obtained (3.37) via a different approach. First, they obtain an integral equality (for two-dimensional problems), which in our notation reads

$$\int_0^{\Delta t} \oint \sigma ds = - \oint u_s ds,$$

where the closed line integral is along the surface of a solid body. Then follows their key step: Eq. (3.37) is sufficient for the integral equality to be satisfied. Note that adding a tangential gradient of a single valued scalar function on the right-hand side of (3.37) would also ensure the above equality. Compare to (3.34) or (3.35), the scalar function can be identified as the pressure. Therefore, the use of (3.34) avoids such ambiguity and clearly reveals the coupling with pressure.

To further evaluate the accuracy of this decoupled approximation, it suffices to compare $\bar{P}$ with $u_s/\Delta t$. Assume that $\mathbf{u}_0$ satisfies the no-slip condition, so that after the inviscid convection substep there should be $u_s = O(\Delta t)$. Thus, $u_s/\Delta t = O(1)$. On the other hand, by (3.31) we may estimate $p_{2B} = O(\nu\omega_B)$. For high Reynolds-number flows $\omega_B = O(\nu^{-\frac{1}{2}})$, hence

$$(3.38) \quad \bar{P} \sim \nu \frac{\partial \omega_B}{\partial x} \sim \nu^{\frac{1}{2}}.$$

Therefore, if $\nu \ll 1$ (i.e. $Re \gg 1$), the error due to dropping $\bar{P}$ is of order $\nu^{\frac{1}{2}}$, which is much smaller than $u_s/\Delta t$. In (3.38) we have assumed ω_B varies smoothly along the body surface such that $\partial \omega_B / \partial x = O(\omega_B)$. This is not the case for complicated separating flows, since near separation the tangential gradient of ω_B may be much larger. By the triple-deck theory (ref. [93]) the streamwise length scale near separation is $\nu^{\frac{3}{8}}$. Thus, $\partial \omega_B / \partial x \sim \nu^{-\frac{7}{8}}$ and $\bar{P} \sim \nu^{\frac{1}{8}} \gg \nu^{\frac{1}{2}}$. In this case dropping $\bar{P}$ might be numerically unsatisfactory, although it is still asymptotically small as $Re \rightarrow \infty$.

Similarly, for three-dimensional flows, the extra term in $\boldsymbol{\sigma}$, i.e. $(\mathbf{n} \times \nabla) \cdot (\nu \boldsymbol{\omega}_B \times \mathbf{n})$, is also small in general. This term involves the possible sharp curvature of the body surface and the critical-point behavior of skin-friction lines; see Wu and Wu [42] for detailed analysis.

Overall, we conclude that (3.33) is a good approximation when the Reynolds number of the flow is high and no separation from a smooth surface occurs. In any case, due to ignoring the effect of $\bar{P}$, there will be a residual slip on the boundary even after diffusion.

If the assumption of local unidirectional flow is valid (e.g. Δt is small and the surface is smooth, etc.), and h is taken to be proportional to $\sqrt{\nu \Delta t}$, then (3.32)

may give results close to those given by (3.33). However, carrying the accuracy analysis of (3.32) further is difficult in general, solely because of the lack of a local equation for ω_B . Moreover, the arbitrariness of h is an undesirable feature for both theoretical analysis and numerical computation. The error will again show up in the form of slip. In the next chapter, we present an analysis of (3.32) type of vorticity BC for the simple Rayleigh flow.

We end this subsection with the following comments. First, the above analysis seems to support our doubt about p_2 being the pressure solution of the Navier-Stokes equation. In fact, at a high Reynolds number p_2 is only a small part of the pressure, associated with diffusion. In contrast, p_1 , the driving force for convection, is dominant. Indeed, from (3.27a) we have $p_{1B} = O(1)$. In the above fractional-step scheme, the effect of this pressure is already reflected by the $O(\Delta t)$ order $\mathbf{u}_s$ after the convection.

Second, there is a general trend of the coupling strength between ω and p . By strength we mean how well the decoupled solutions approximates the coupled one. The weaker the coupling, the better the approximation. Therefore, under the setting of fractional-step methods, we can conveniently quantify the definition of the coupling strength by the ratio between p_2 and p_1 , which leads naturally to the Reynolds-number dependence. The above analysis shows that the coupling is stronger when Re is smaller. The strongest coupling happens if $Re \ll 1$: in a two-dimensional steady Stokes flow the relation between p and ω is simply that of the real and imaginary part of an analytical function. On the other hand, for the attached boundary layer approximation with $Re \gg 1$, the coupling disappears since p is given. But, when separation occurs the coupling becomes stronger. Note that the decoupled approximation discussed here is different from the parabolic boundary layer approximation: when separation occurs, the former only becomes less accurate but the latter breaks down due to the Goldstain singularity.

Third, the slip due to decoupled approximation does not accumulate during time marching. Obviously, any slip left by a diffusion substep will be carried over to the initial condition for the diffusion substep in the next time step. Thus, if at the end of a time step, the vorticity is under- or over-created, it will some-

how be automatically corrected at the next time step. This self-adjusting feature is common to the above decoupled approximations. However, the ability of self-adjustment varies among different schemes, as will be shown by the numerical examples in the next chapter.

Finally, although the strength of the coupling between ω and p is most naturally revealed via operator splitting, the decoupled approximation can also be constructed using non-splitting methods. As far as the local vorticity BC is concerned, the most useful feature of operator splitting is that for high Re flow, the vorticity generation due to inertial motion of fluid, the dominating portion, is obtained easily. While operator splitting has some other advantages, it is limited to at most second order accurate in time. When higher order methods are desired, decoupled approximations similar to that described above can be used with non-splitting schemes. This is studied in details in Chapters 5 and 6.

Chapter 4

Unidirectional Flows

Unidirectional flows of this chapter contain only one velocity component tangent to the solid boundaries. These flows are pure diffusion problems and hence the simplest ones to solve; yet, they contain an essential difficulty of general vorticity-based methods—the singular vorticity distribution due to impulsively started wall motion or pressure impulse. However, the coupling between vorticity and pressure is absent in these flows, which simplifies the comparison of different vorticity BCs. Pressure gradient can still exist along the tangential direction of solid walls, but it has to be a given constant. We shall see that the presence of a finite pressure gradient makes the kinematic BCs difficult to apply while it adds no difficulty for the dynamic BC.

4.1 The Rayleigh Flow

Consider a stationary infinitely long flat plate at $y = 0$ with fluid above it. The fluid is at rest for $t < 0$, but suddenly starts to flow with a constant speed $U = 1$ in x direction parallel to the plate. The flow is described by

$$(4.1a) \quad \frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} \quad (t > 0)$$

with initial

$$(4.1b) \quad u(y, 0) = 0 \quad (y > 0)$$

and boundary conditions

$$(4.1c,d) \quad u(0, t) = 0 \quad (\text{for all } t), \quad u(\infty, t) = 1 \quad (t \geq 0).$$

Our objective is to solve the vorticity equation, that is

$$(4.2) \quad \frac{\partial \omega}{\partial t} = \nu \frac{\partial^2 \omega}{\partial y^2} \quad (t > 0),$$

where $\omega = -\partial u / \partial y$, instead of (4.1a). The initial condition for (4.2) is $\omega(y, 0) = 0$ or $-\delta(y)$ depending on whether no-slip condition is imposed; the far field BC is $\omega(\infty, t) = 0$. It remains to determine the BC at $y = 0$. The exact solutions of the problem are

$$(4.3) \quad u(y, t) = \operatorname{erf}\left(\frac{y}{2\sqrt{\nu t}}\right) \quad \text{and} \quad \omega = -\frac{1}{\sqrt{\pi\nu t}} e^{-y^2/4\nu t}.$$

4.1.1 The Finite Difference Scheme

Let h be the size of a uniform grid in y direction, and Δt be the time step. We use the Crank-Nicolson scheme

$$(4.4) \quad \frac{\omega^{n+1} - \omega^n}{\Delta t} = \frac{\nu}{2} \left(\frac{\omega_{j+1}^{n+1} - 2\omega_j^{n+1} + \omega_{j-1}^{n+1}}{h^2} + \frac{\omega_{j+1}^n - 2\omega_j^n + \omega_{j-1}^n}{h^2} \right),$$

with j and n for the indices of grid point and time step. By Taylor expansion, the scheme is formally second order in time and space. It is also unconditionally stable for regular problems. These conclusions, however, have to be carefully studied in the present problem because of the singularity in ω as $t \rightarrow 0$ and possible inexact vorticity BCs.

4.1.2 Numerical Boundary Conditions for Vorticity

The local numerical BCs are closely related to the solution of velocity on the solid surface. For the present problem, the velocity can be obtained by integrating ω along y , but here we introduce the stream-function ψ to simulate more general 2-D situations. Thus, we solve

$$(4.5a,b,c) \quad \frac{\partial^2 \psi}{\partial y^2} = -\omega, \quad \psi(0, t) = 0, \quad \frac{\partial \psi}{\partial y}(\infty, t) = 1.$$

The exact solution is

$$(4.6) \quad \psi(y, t) = y \operatorname{erf}\left(\frac{y}{2\sqrt{\nu t}}\right) + 2\sqrt{\frac{\nu t}{\pi}} (e^{-y^2/4\nu t} - 1);$$

it can be used to set the far field condition at the boundary of truncated domain of computation. Eq. (4.5a) can be discretized by central difference:

$$(4.7) \quad \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{h^2} = -\omega_j.$$

Under (4.5b,c), the resultant tridiagonal matrix can be inverted exactly. If we use central difference scheme

$$(4.8) \quad u_j = \frac{\psi_{j+1} - \psi_{j-1}}{2h} \quad (j > 0)$$

to compute velocity, the result can be proved to be exactly the same as integrating ω by trapezoidal rule. For slip velocity u_s , which equals u_0 because the solid boundary is a rest, a variety of schemes can be used; among them only

$$(4.9) \quad u_s = \frac{\psi_1 - \psi_0}{h} + \frac{h}{2}\omega_0$$

is equivalent to the trapezoidal integration. It can be obtained by applying (4.7) and (4.8) at $j = 0$ and canceling ψ_{-1} . Formula (4.9) is second order accurate by Taylor expansion. Another second order formula for u_s is the forward difference

$$(4.10) \quad u_s = \frac{-3\psi_0 + 4\psi_1 - \psi_2}{2h}.$$

Third order formulas are also available:

$$(4.11) \quad u_s = \frac{-11\psi_0 + 18\psi_1 - 9\psi_2 + 2\psi_3}{6h},$$

$$(4.12) \quad u_s = u_{\frac{1}{2}} + \frac{h}{2}\omega_0 + \frac{h^2}{8} \left(\frac{\partial \omega}{\partial y} \right)_0 = u_{\frac{1}{2}} + \frac{h}{8}(3\omega_0 + \omega_1),$$

where $(\partial \omega / \partial y)_0$ is approximated as $(\omega_1 - \omega_0)/h$. In computations, if (4.11) and (4.12) are used together with (4.7), their accuracy is limited by ψ 's accuracy. The error of u , which is solved from (4.7) and (4.8), and the u_s for given exact ω are shown in Fig. 4.1. Note that y_∞ is the upper boundary of the computational domain.

It can be seen that (4.7) and (4.8) give second order velocity solution provided that the viscous layer is well-resolved. Further tests show that $h \leq 2\sqrt{\nu t}$ seems to be appropriate, which corresponds to more than 40 grid points in Fig. 4.1. This can be explained by the exact solution (4.3), which shows that $\eta = y/2\sqrt{\nu t}$ is the similarity variable. Thus the spacial accuracy is determined by how well η is resolved. We also note that the convergence rates of u_s are higher than expected (when the flow is well-resolved): extremely high-order for (4.9) and third-order for

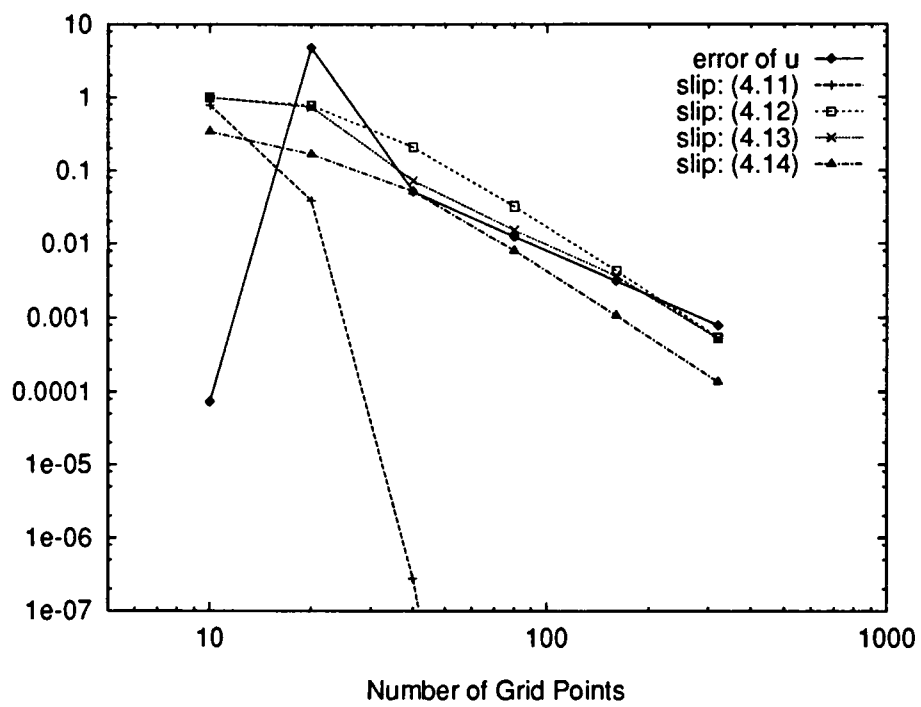


Figure 4.1: Max norm error of velocity and slip, computed from exact vorticity distribution at $t = 0.01$. Upper boundary at $y_\infty = 0.2$ and $\nu = 0.001$.

(4.10) and (4.12). However, scheme (4.11) behaves less consistently. It seems that these results are attributed to the special distribution of vorticity of the present problem.

When u_s is obtained, according to (3.32) and (3.33), the Dirichlet and Neumann condition of ω at $y = 0$ are

$$(4.13) \quad \omega_B^{n+1} = \omega_B^n - u_s^n/h',$$

$$(4.14) \quad \bar{\sigma} = -u_s^n/\Delta t,$$

where h' is an arbitrarily small normal distance from the wall. Since there is no pressure gradient, condition (4.14) is exact. Two other Dirichlet BCs can be obtained from (4.9) and (4.12):

$$(4.15) \quad \omega_B = -2(\psi_1 - \psi_0)/h^2,$$

$$(4.16) \quad \omega_B = -8u_{1/2}/3h - \omega_1/3,$$

in which $u_s = 0$ has been used. Many other formulas like (4.15) and (4.16) have been derived [35,94] but will not be considered here, because they do not yield any new information. In both formulas, ω and ψ *should be evaluated at the same time level*, say $n+1$ for the implicit scheme (4.4). This implies that ω^{n+1} and ψ^{n+1} have to be solved in a coupled manner. Then (4.15) and (4.16) are *not truly local*. One way to avoid the coupled solution is to use the iterative scheme described in [94], the other way is to localize them by using ψ^n to predict ω_B^{n+1} as in [95]. The price is reduced accuracy in time.

The Neumann condition is second order accurate in time if we assume

$$(4.17) \quad \bar{\sigma} = \frac{1}{2}(\sigma^n + \sigma^{n+1}) = -\frac{\nu}{2} \left(\frac{\partial \omega^n}{\partial y} + \frac{\partial \omega^{n+1}}{\partial y} \right).$$

Its spatial accuracy should be determined by that of u_s^n . The accuracy of (4.13) is not clear because of the arbitrariness in h' . But substituting (4.9) and (4.12) for u_s into (4.13) yields nothing but the localized forms of (4.15) and (4.16) with $h' = h/2$ and $h' = 3h/8$, respectively. Thus the localized kinematic BCs can be written in a single form as (4.13); the differences are just choices of h' and the methods of computing u_s , but they should have similar accuracy in time.

The kinematic BCs also relate to the dynamic one. Apply (4.4) at $j = 0$ and use central difference

$$(4.18) \quad \frac{\partial \omega}{\partial y} = -\frac{\sigma}{\nu} = \frac{\omega_1 - \omega_{-1}}{2h} + O(h^2)$$

to implement the Neumann condition, we get at $j = 0$

$$(4.19) \quad (1 + 2\lambda)\omega_B^{n+1} - 2\lambda\omega_1^{n+1} = (1 - 2\lambda)\omega_B^n + 2\lambda\omega_1^n - 2\frac{u_s}{h},$$

where $\lambda = \nu\Delta t/2h^2$. It follows from (4.19) that $\omega_B^{n+1} - \omega_B^n = -2u_s/h$ as $\Delta t \rightarrow 0$. Note that no assumption has been made about how u_s is solved in this derivation, thus $h' = h/2$ seems to be a valid choice independent of u_s . In fact, Anderson [25] proved that $-2u_s/h$ is the vorticity “induced” by a vortex sheet with strength u_s via a different argument when considering fractional step method for Prandtl boundary layer equations.

It is easy to see that the solutions using local kinematic BCs cannot satisfy the no-slip condition exactly for any finite Δt for general unsteady problems. If on the contrary that no-slip condition is satisfied, then there will be no change in the boundary vorticity, which is generally not true. To obtain $u_s = 0$ results, either coupled solution or iteration needs to be used to get ω and ψ at the same time level. In contrast, if $u_s = 0$ in the dynamic BC (4.14), one get the exact vorticity BC $\partial\omega/\partial y = 0$ ($t > 0$) for the present problem; no iteration is needed.

4.1.3 Numerical Tests

In the following, we study the performance of local kinematic and dynamic BCs of vorticity derived above through numerical experiments. These tests are very simple, so they have been overlooked in the literature, yet they exhibit some basic and interesting properties of the local numerical BCs of vorticity, which are often covered up in computations of more complicated problems. In all tests $\nu = 0.001$, and $y_\infty = 0.2$ are used. The exact solutions are used to impose boundary conditions at y_∞ . The kinematic BCs are treated in the unified form of (4.13) with $h' = h/2$; different schemes are obtained by choosing different formulas for u_s . The dynamic and kinematic BCs are shorthand as DBC and KBC below.

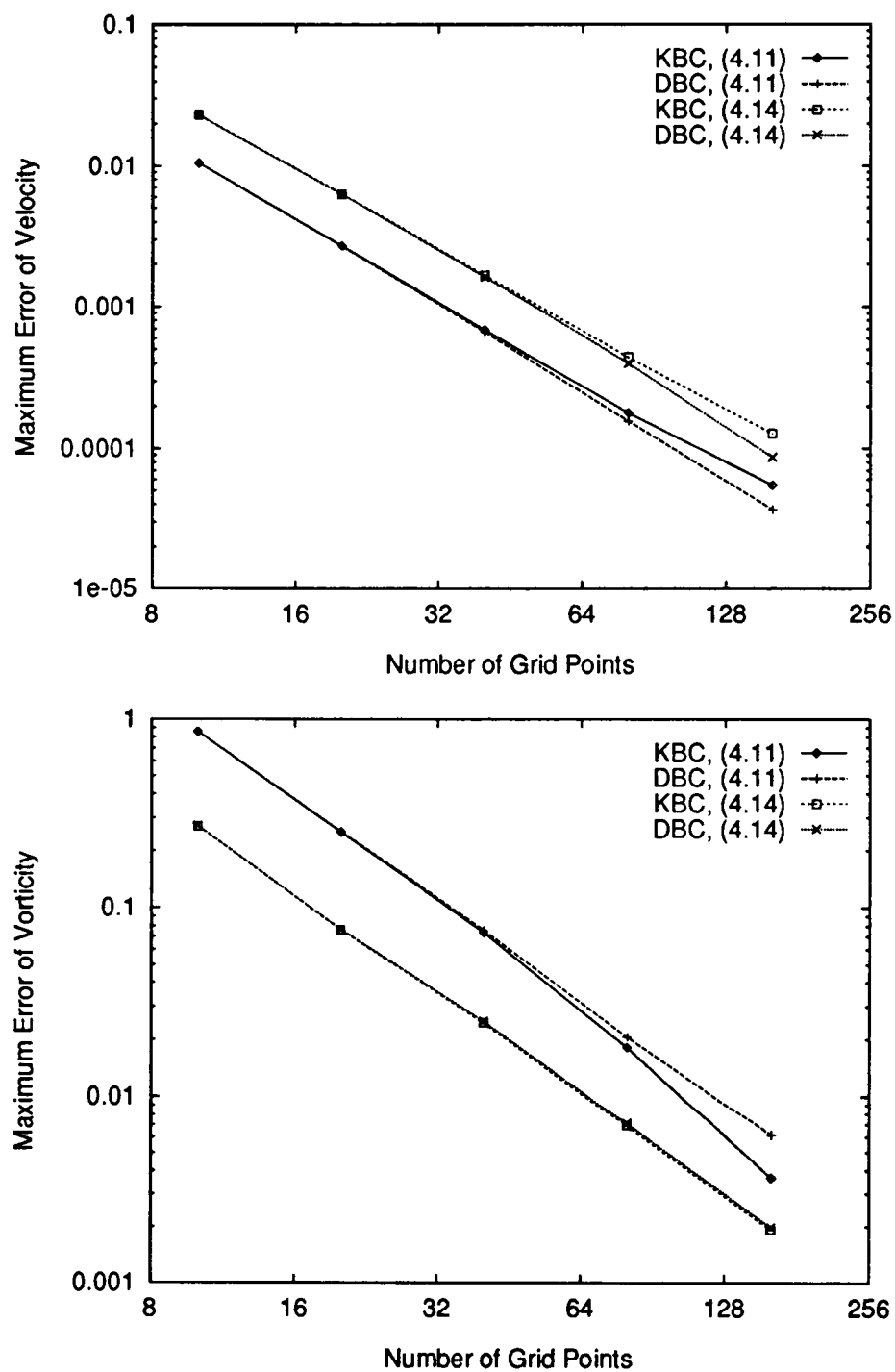


Figure 4.2: Spatial convergence of velocity and vorticity solutions using different BCs and methods of computing u_s .

First, we test the spatial accuracy of the schemes, i.e. whether the schemes converge to second order as predicted by the Taylor expansion. In the results of numerical tests shown by Fig. 4.2, $\Delta t = 0.0001$, and solutions of u and ω are computed at $t = 0.5$ with different numbers of grid points. It is clear that the convergence rates of the schemes are influenced by both the boundary condition and formula of u_s . From the results, we also observe that more accurate ω solutions correspond to less accurate u solutions. This observation is in contradiction with Gresho's comment [21] that an fairly accurate vorticity solution should lead to very accurate velocity solution. It may be anticipated that schemes used to compute velocity should be more accurate than those used to compute vorticity. For the DBC u converges with second order accuracy or close to it, while ω converges slower than u . As grid number increases, the convergence of both u and ω slows down due to error in time. For the KBC the trends are less predictable; the convergence seems to be sensitive to the evaluation of u_s . One important distinction between KBCs and DBC can be seen from the convergence of u_s as t increases, as discussed above and shown in Fig. 4.3 (where N is the number of grid points).

We need to mention that formula (4.10) for u_s was also tested. When KBC is used, the results oscillate and diverge as t increases. The smaller the h , the faster the blow up. On the contrary, when the DBC is used, the oscillation converge as t increases; the rate is faster as h becomes smaller. In any case, the results are not satisfactory. The reason of the oscillation is caused solely by the large error in u_s . However, the DBC has a stronger ability than KBC to adjust the solution onto the right track; therefore, it is more robust.

The tests of accuracy of the schemes in time further reveal the robustness of DBC. In the tests, we need to keep h small and Δt relatively large so that the spatial error is negligible compared to timewise error. In this case, the tests for KBCs become hard to manage because the computation keeps diverging in an oscillatory fashion until Δt is sufficiently small.

It is easy to understand the difficulty in the above localized KBCs. For both local KBCs and DBC, the amount of vorticity created is solely determined by the magnitude and sign of the residual slip u_s . If the correct amount of vor-

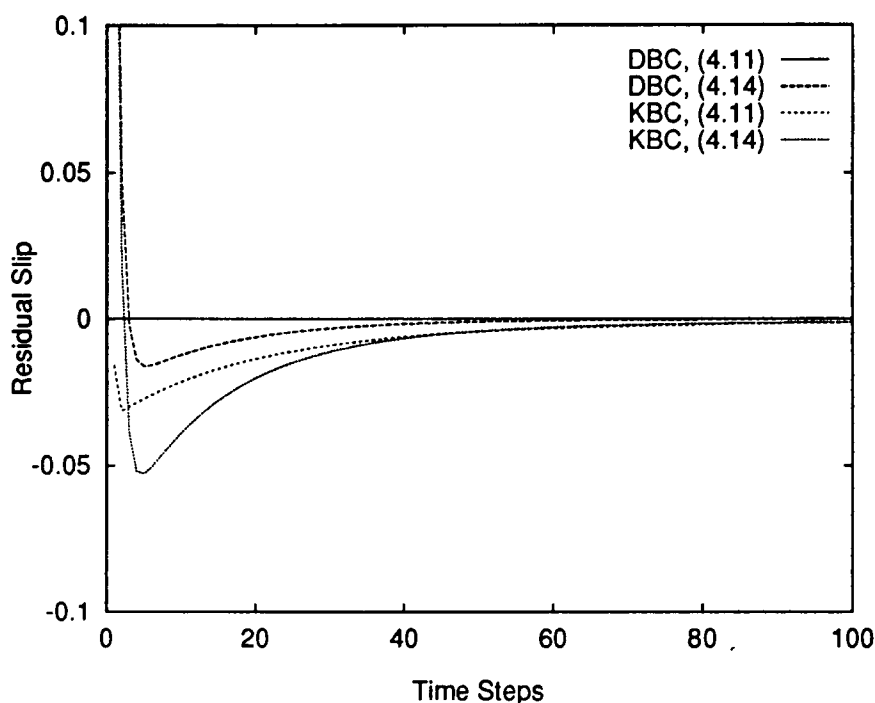


Figure 4.3: Variation of residual slip u_s with time step. $N = 81$, $\Delta t = 0.0001$.

ticity is generated from the boundary and diffused into the flow, then after the process u_s should be zero. However, if vorticity is under-created, the residual slip may reduce but will not be zero; this slip will continue to create more vorticity in the next time step. On the other hand, if vorticity is over-created, then the slip may be over-reduced to the opposite sign; in the next time step, vorticity with opposite sign is created and partly cancels the over-created vorticity. This is the basic self-adjusting feature of the local vorticity BCs, which, for obvious reasons, are also called “vorticity BCs of creation type” [45]. If the adjustment goes right, the computation will converge to the right solution and u_s . An example of convergence has been shown in Fig. 4.3 for Δt relatively small. On the other hand, the oscillation may diverge if the over-creation of vorticity is too severe. Since the localized KBCs are Δt independent and accurate only in the limit of $\Delta t \rightarrow 0$, thus, large error will be introduced when Δt is large. It is found that for KBCs there is a critical Δt , proportional to h^2/ν , beyond which the Crank-Nicolson scheme becomes unstable. This constraint on time step is similar to that for conditionally

stable explicit schemes. The unconditionally stable feature of the Crank-Nicolson scheme is thus lost. In contrast, the DBC can adjust itself when Δt increases to predict vorticity creation with tolerable error, hence the Crank-Nicolson scheme remains stable.

The result of test of convergence in time using KBC is obtained for limited range of Δt as in Fig. 4.4. The convergence rate of ω is rather irregular due to the sharp turn in the result at $\Delta t = 0.00125$. By reducing h , the error at $\Delta t = 6.25 \times 10^{-4}$ can be reduced; however, it is still larger than that at $\Delta t = 0.00125$. Since velocity is solved from vorticity, its convergence rate in time should perceptibly follow that of vorticity. However, this is not the case—the solution converges regularly with about first-order accuracy.

In the test using DBC, we can reduce both Δt and h simultaneously (because the scheme is stable) to avoid the interference between time and spatial errors. First-order convergence in both ω and u is shown in Fig. 4.4. When (4.12) is used instead of (4.9), same results are obtained.

Although the above results are obtained for only a special problem and a particular finite difference method, they are far more general. For impulsively started flow over general solid bodies, the initial development is similar locally to the Rayleigh problem. Therefore, we may expect the same problem of degeneration of accuracy in time would present. In fact, Anderson and Reider [96] meet the problem in their computation of impulsively started flow over circular cylinder. Their fourth order Runge-Kutta explicit time integration becomes exactly first order. To preserve the time accuracy, they modified the initial vorticity so that the no-slip condition is satisfied. Their construction is to perform one step Euler integration with a step size ε and then consider the vorticity in the limit as $\varepsilon \rightarrow 0$. For the present problem, Anderson and Reider's method leads to $\omega_j^0 = 0$ for $j > 0$ and $\omega_B^0 = -2u_s^0/h$ (instead of $\omega_B^0 = 0$), which can also be seen from (4.19).

Performing the same tests as above using the DBC and the modified initial vorticity, we obtain second-order convergence in ω and u as shown in Fig. 4.4. Again, the use of (4.12) gives about the same result except that the velocity is less accurate, while vorticity is more accurate. By comparison of the results in

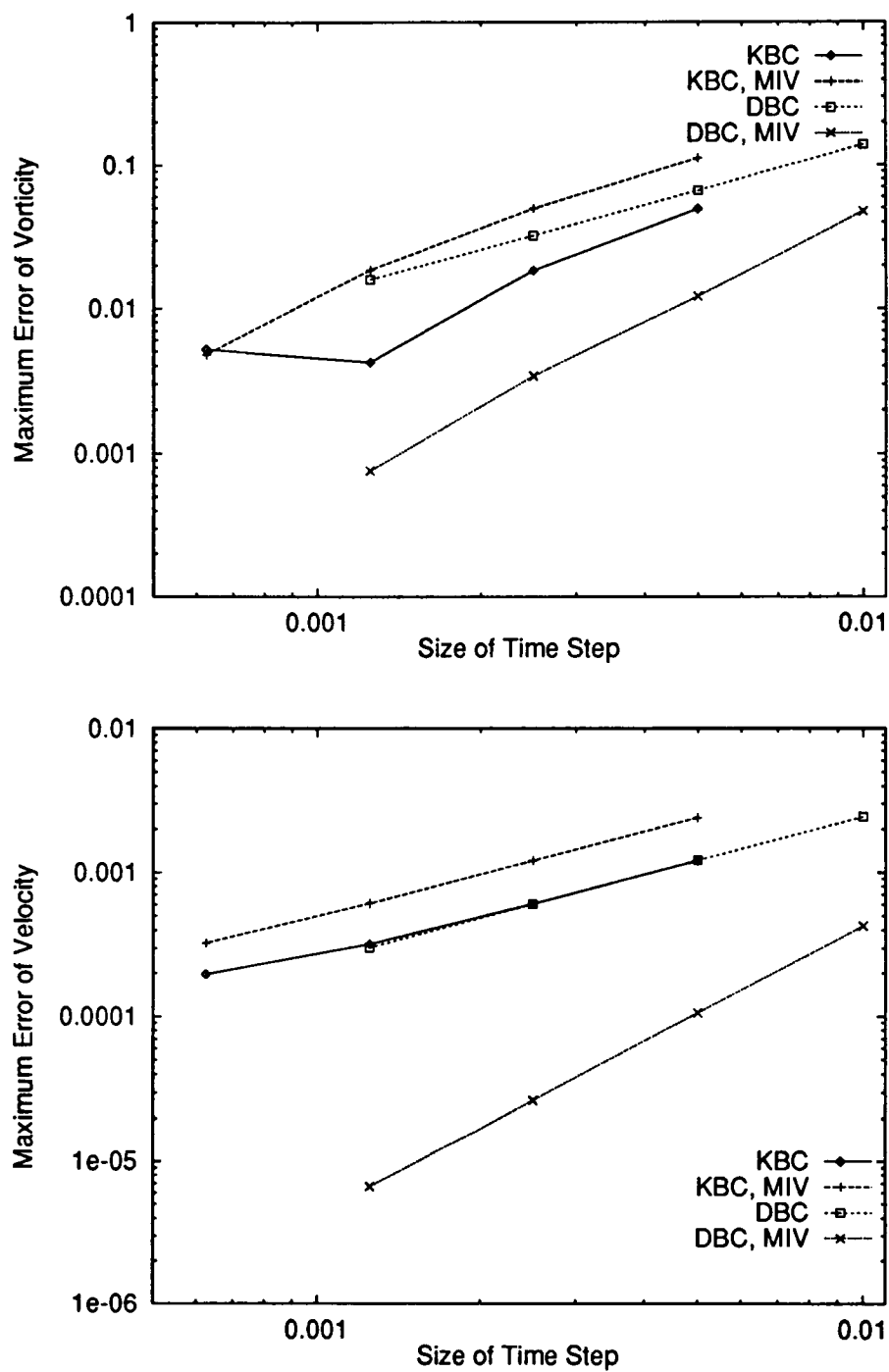


Figure 4.4: Convergence of ω and u in time with and without modified initial vorticity (MIV).

Fig. 4.4, we find great improvement not only in the convergence rate but also the accuracy for the same Δt (and h) with modified initial vorticity. It should be noted that the modification is nothing but replacing an infinite jump in the vorticity by a finite jump. The key is to ensure the no-slip condition initially at *discrete level*. Another interesting observation is that, with modified ω^0 , the magnitude of oscillation discussed above could be larger than that without the modification. However, when the oscillation converges, the result with modified ω^0 is more accurate.

The author [97] proposed a method by smoothing the initial vorticity similar to the above modification. Furthermore, we may start at a smooth solution at t_0 . For the present problem we can use the exact solution; for general problems, we may need to use the integral formulation in Chapter 3 to construct the solution. As observed by Anderson and Reider [96], as $t_0 \rightarrow 0$, the accuracy in time returns to first order. Therefore, they conclude that the above modification of ω^0 is better. We believe the reason is that as t_0 approaches zero, the solution approaches to singular and is worse resolved on a fixed grid. Therefore, we can start at a small $t_0 \neq 0$ but large enough for a relatively smooth representation of the initial data; actually, $t_0 = h^2/\nu$ seems to be good enough as observed in our tests. When the computation starts from a smooth initial condition of vorticity, then the magnitude and number of oscillation can be greatly reduced. In case of the scheme being sensitive to oscillations, this approach may be desirable.

Neither modification of initial vorticity nor smooth start can save the result using local KBCs from diverging when $\Delta t/h^2$ exceeds a critical value. The test using the KBC is repeated with modified ω^0 , see Fig. 4.4. The modification does not improve the convergence rate nor the accuracy. Other tests were performed with the KBC including start the computation from a smoothed exact solution at $t = 0.5$, the constraint on the time step and $O(\Delta t)$ convergence were again observed.

A set of numerical tests was also performed using the modified initial vorticity and the exact Neumann condition $(\partial\omega/\partial y)_B = 0$ (for $t > 0$). The results are essentially the same as the one using DBC (4.14). Note that in this case the

no-slip condition is not imposed except at $t = 0$, rather it is the acceleration no-slip being imposed for $t > 0$. This ensures the solution to maintain velocity no-slip for $t > 0$. The DBC is different from the exact condition in that the velocity no-slip is imposed in *each* time step. This set of tests shows how well the modified initial vorticity distribution works, because any error in the initial distribution will *not* be corrected later by the exact BC, which basically says that no vorticity is created after $t = 0$.

In summary, the DBC we tested has two main advantages over the KBCs: preserving the stability and accuracy of the Crank-Nicolson scheme (if the initial vorticity satisfies the no-slip condition). It is not fair though to say that DBC is generally better than the KBCs, the result will depend on the numerical scheme used; for implicit time integration schemes, our tests and discussion indicate that the DBC is likely to give better results. Moreover, the interpolation methods for u_s are very important: the spatial accuracy and the speed of convergence will be determined by the accuracy of u_s . Not all formulas with the same order of accuracy can be equivalently used. As shown by the tests, the forward difference type of formulas are not good choices for the present computation. It seems that only when ω_B is used, reasonably accurate u_s can be obtained especially if the flow is under-resolved.

Finally, it is interesting to note that there are other methods for discretizing the Neumann condition for ω , such as forward difference like (4.10) for $\partial\psi/\partial y$, which is also second order. In this case, it is (4.9) inappropriate to use but (4.10) works fine. It is anticipated that there exists certain matching rules between the formula for u_s and $\partial\omega/\partial y$, however, we shall insist on the central difference type of discretization of viscous terms because they are more accurate than one-sided differences. This is important particularly in the near wall region.

4.2 Unidirectional Flows around a Circular Cylinder

In this section, more examples of pure diffusion problem of vorticity are studied; they include (1) the impulsively started rotating circular cylinder, i.e. a

generalized Stokes' first problem with known exact solution; (2) circular cylinder performing rotatory oscillation, with impulsive start, i.e. a generalized Stokes' second problem including transient period, whose exact solution is known only for steady state ($t \rightarrow \infty$). The flows are rotationally symmetric, so the nonlinear convection and the coupling with tangential pressure gradient are both absent. We first use finite difference method to solve the problems, then devote subsection 4.2.2 to the application of integral formulations presented in Chapter 3.

4.2.1 Finite Difference Results

In the polar coordinate system (r, θ) , after the transformation $z = \log r$, the vorticity equation for the present case reads

$$(4.20) \quad r^2 \frac{\partial \omega}{\partial t} = \frac{1}{Re} \frac{\partial^2 \omega}{\partial z^2},$$

with $\omega = 0$ as $r \rightarrow \infty$. Introducing stream-function ψ , we have

$$(4.21a) \quad \frac{\partial^2 \psi}{\partial z^2} = -r^2 \omega, \quad -\frac{\partial \psi}{\partial z} = ru,$$

where u is the velocity along the θ -direction. The boundary conditions are

$$(4.21b) \quad \psi(0, t) = 0, \quad -\frac{\partial \psi}{\partial z}(0, t) = b(t), \quad \frac{\partial \psi}{\partial z}(0, z) = 0 \quad (\text{as } z \rightarrow \infty).$$

As above, Eq. (4.20) is discretized by using the Crank-Nicolson scheme and all spatial derivatives are discretized via central difference. The local BCs for vorticity (4.13)–(4.16) can be modified easily for the present problem. It should be noted that for varying tangential velocity of the solid body, instead of $-u_s^n$ in (4.14), we need to use $b^{n+1} - u_0^n$ to assure the no-slip condition at the $(n+1)$ th step and the second order accuracy in time. This substitution already includes the effect of tangential acceleration of the boundary. Three BCs are used. The first two are based on (4.13) with $h' = \Delta z/2$ and $h' = \sqrt{\pi \nu \Delta t}$. The third one is the dynamic one. We denote them as BC1, BC2 and BC3, respectively.

Figures 4.5 shows the results of the Stokes' first problem with $\Delta z = 0.0067$ and $\Delta t = 0.02$. For BC3, the initial vorticity is modified as in the last subsection.

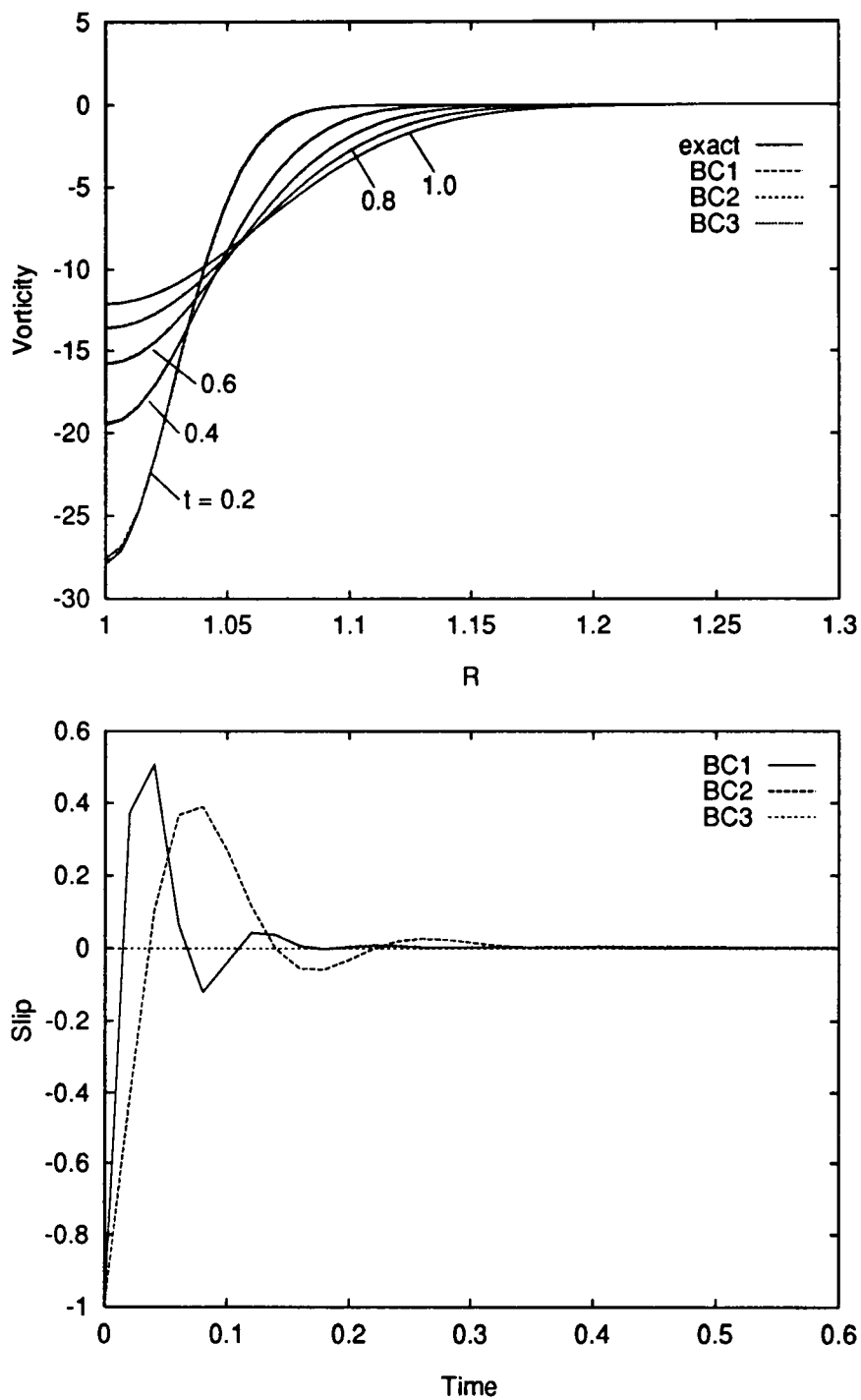


Figure 4.5: Generalized Stokes' first problem. Top: Solutions of vorticity at $t = 0.4, 0.8, 1.2, 1.6, 2.0$. bottom: Variation of residual slip with time.

The Stokes' second problem is solved with the three different BCs. The comparison is shown in Fig. 4.6. Essentially, no new difficulties occur except that the slip using the first two BCs are larger in this unsteady moving boundary problem than in steady one.

4.2.2 Integral Method and Smoothed Heat Kernel

For the above generalized Stokes' first and second problems, the basic integral formula is the purely diffusive version of (3.15):

$$(4.22) \quad \omega(t) = 2 \oint_B G_0^* \gamma_0 dS + \int_V \hat{G}_0^* \omega_0 dV + 2 \int_0^t d\tau \oint_B G^* \sigma dS,$$

where $\hat{G}_0^*$ is G^* plus its image with respect to the cylinder and can be obtained by the same method as Coulombic kernel. Here the flux σ is exactly known: for the first problem $\sigma = 0$ for $t > 0$; and for the second, $\sigma = \partial b / \partial t = \sin t$ (we assume $b = \cos t$ so that there is an impulsive start). Thus our task was merely to improve the accuracy of numerical integration, which was carried out by the repeated use of (4.22) in each time step Δt . After the first Δt the volume integral in (4.22) is no longer zero, which becomes the most time-consuming part. Therefore, six-point Gaussian quadrature formula was used for surface integrals, while the volume integral was first done by simple summation.

To perform the integration, a grid with equal size in the θ -direction was used. For the radial direction, we set $z = \log r$ and divide the z interval equally so that the resulting grid is more clustered near the boundary to help to resolve the large vorticity gradient there. Due to symmetry, the main factor influencing the accuracy is Δz , the grid size in the z direction. In all test cases presented in this subsection, $\Delta t = 0.02$ was used. The solution for the Stokes' first problem is shown in Fig. 4.7 with $Re = 1000$ and $\Delta z = 0.00084$. Note that the error near the boundary is rather significant, which is mainly due to the inaccurate volume integral.

Two methods can be used to improve the accuracy. One is a higher-order volume integration method, such as Gaussian quadrature, and the other is a

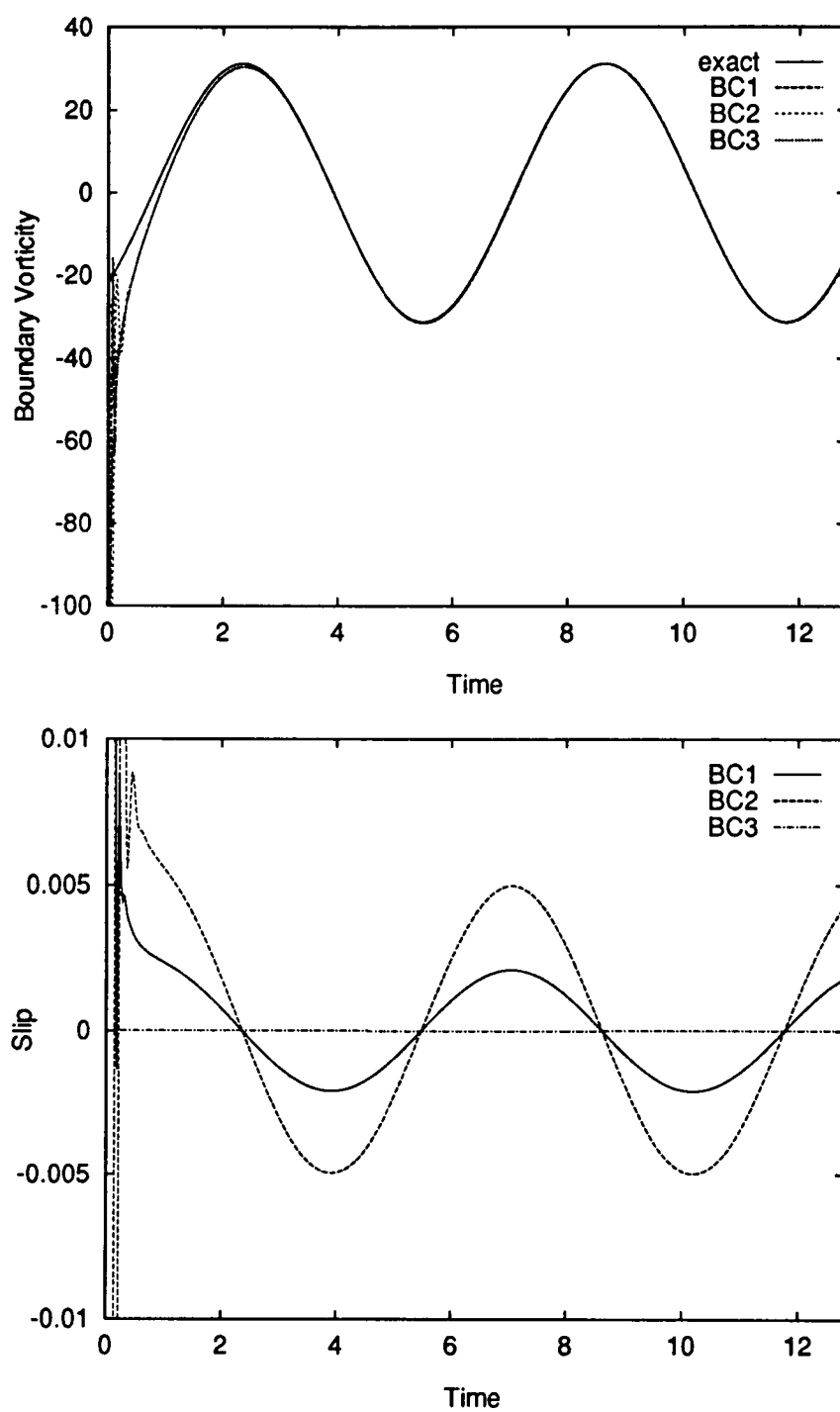


Figure 4.6: Generalized Stokes' second problem. Top: Solutions of boundary vorticity; bottom: Variation of residual slip with time.

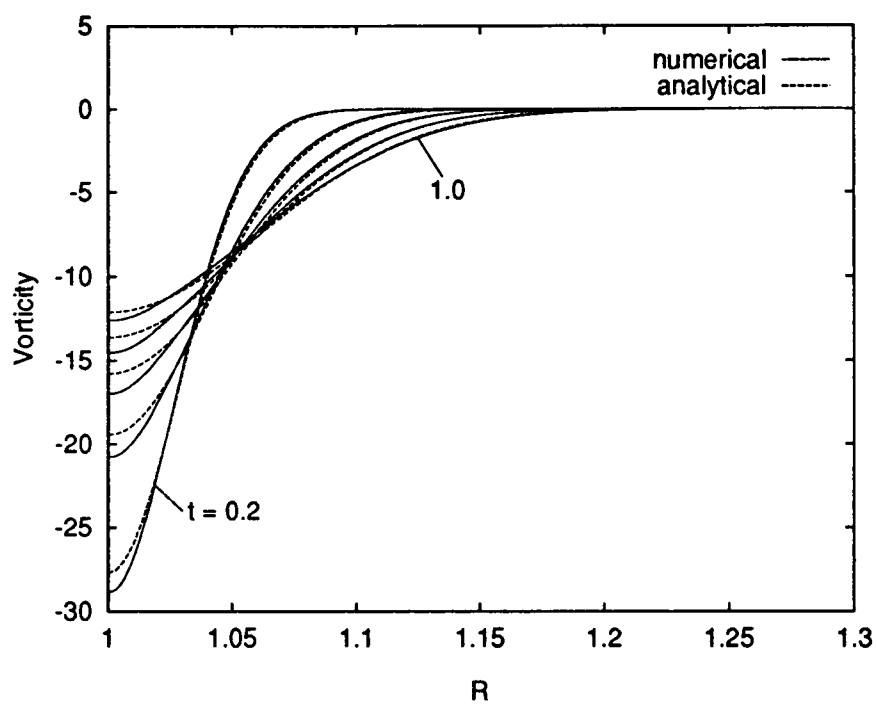


Figure 4.7: Generalized Stokes' first problem computed using non-smoothed kernel. Solution at $t = 0.2, 0.4, 0.6, 0.8$, and 1.0 .

smoothed kernel method. We chose the latter because it is simple to implement. More importantly, it is generally applicable to the deterministic diffusion part of a vortex method. Thus, we replace G^* by a smoothed kernel G_δ^* , even though in computations G^* did not show any singularity. The technique is borrowed from that for the Coulombic kernel G , defined by (3.24), which has been successfully applied in vortex methods. The smoothing function is of the form

$$(4.23) \quad \psi(\delta) = \frac{1}{\pi\delta^2} e^{-r^2/\delta^2}.$$

The following results are due to J. Z. Wu and H. Y. Ma (private communication). After some straightforward algebra involving special functions, the convolution of $\psi(\delta)$ with G^* gives

$$(4.24) \quad G_\delta^{*(2)} = \frac{1}{\pi(a^2 + \delta^2)} \exp\left(-\frac{r^2}{a^2 + \delta^2}\right), \quad a^2 \equiv 4\nu t,$$

where the index (2) implies that this is a second-order kernel. Beale and Majda [98] showed that proper linear combinations of functions like (4.23) can be used to construct higher-order smoothed Coulombic kernels, and their results can well be applied to heat kernel. For instance, the sixth-order smoothing function found by Beale and Majda is

$$\psi_\delta = \frac{1}{\pi\delta^2} \left(\frac{8}{3} e^{-r^2/\delta^2} - e^{-r^2/2\delta^2} + \frac{1}{12} e^{-r^2/4\delta^2} \right),$$

for which we obtain

$$(4.25)$$

$$(4.26) \quad G_\delta^{*(6)} = \frac{8}{3\pi(a^2 + \delta^2)} \exp\left(-\frac{r^2}{a^2 + \delta^2}\right) - \frac{2}{\pi(a^2 + 2\delta^2)} \exp\left(-\frac{r^2}{a^2 + 2\delta^2}\right) + \frac{1}{3\pi(a^2 + 4\delta^2)} \exp\left(-\frac{r^2}{a^2 + 4\delta^2}\right).$$

The result of $G_\delta^{*(6)}$ with $\Delta z = 0.0034$ and $\delta = 2.5\Delta z$ is shown in Fig. 4.8, where the agreement is excellent.

Both non-smoothed and smoothed kernels were used to compute Stokes' second problem with $Re = 1000$. Figure 4.9 shows the time variation of boundary

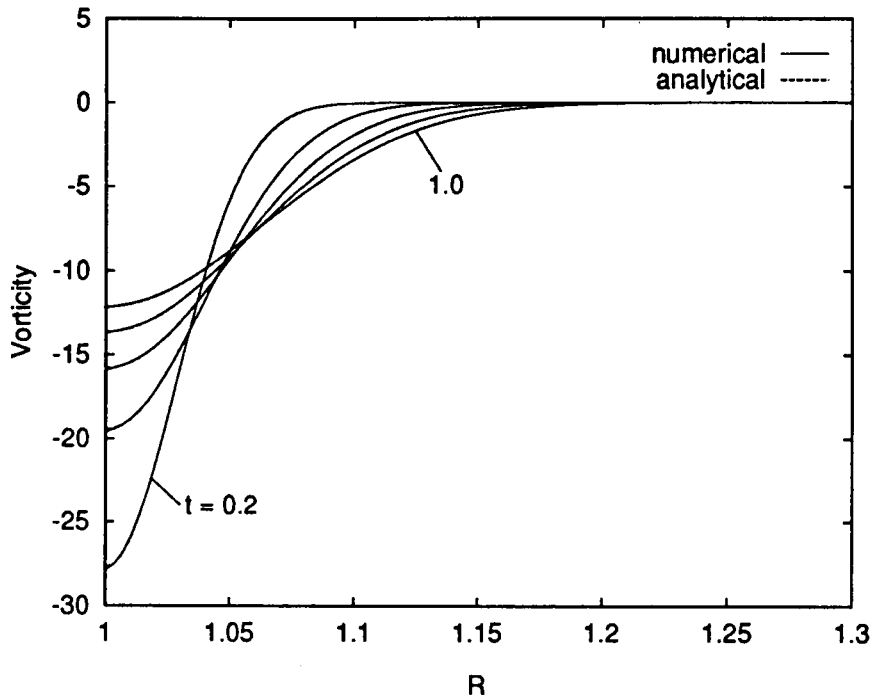


Figure 4.8: Generalized Stokes' first problem computed using 6th order smoothed kernel.

vorticity, using $G_\delta^{*(6)}$ with $\delta = 2.0\Delta z$ and the non-smoothed kernel. The grid sizes are the same as above for the two kernels respectively. The short dashed line is the analytical steady-state solution ($t \rightarrow \infty$) and the solid line is the solution using the smoothed kernel which contains the transient part. The agreement in the smoothed kernel case is again very good. But using direct summation of the non-smoothed kernel made the scheme blow up after the first period of oscillation (see the dashed line). Although the reason is not totally clear at the moment, we observe that with the smoothed kernel the scheme is not only more accurate but also more stable.

It is evident that if we set $\delta^2 = 4\nu\delta t$, the smoothed heat kernels have a simple interpretation: the diffusion process is numerically moved forward by a δt (which has no direct relation with the computation time step Δt). In particular,

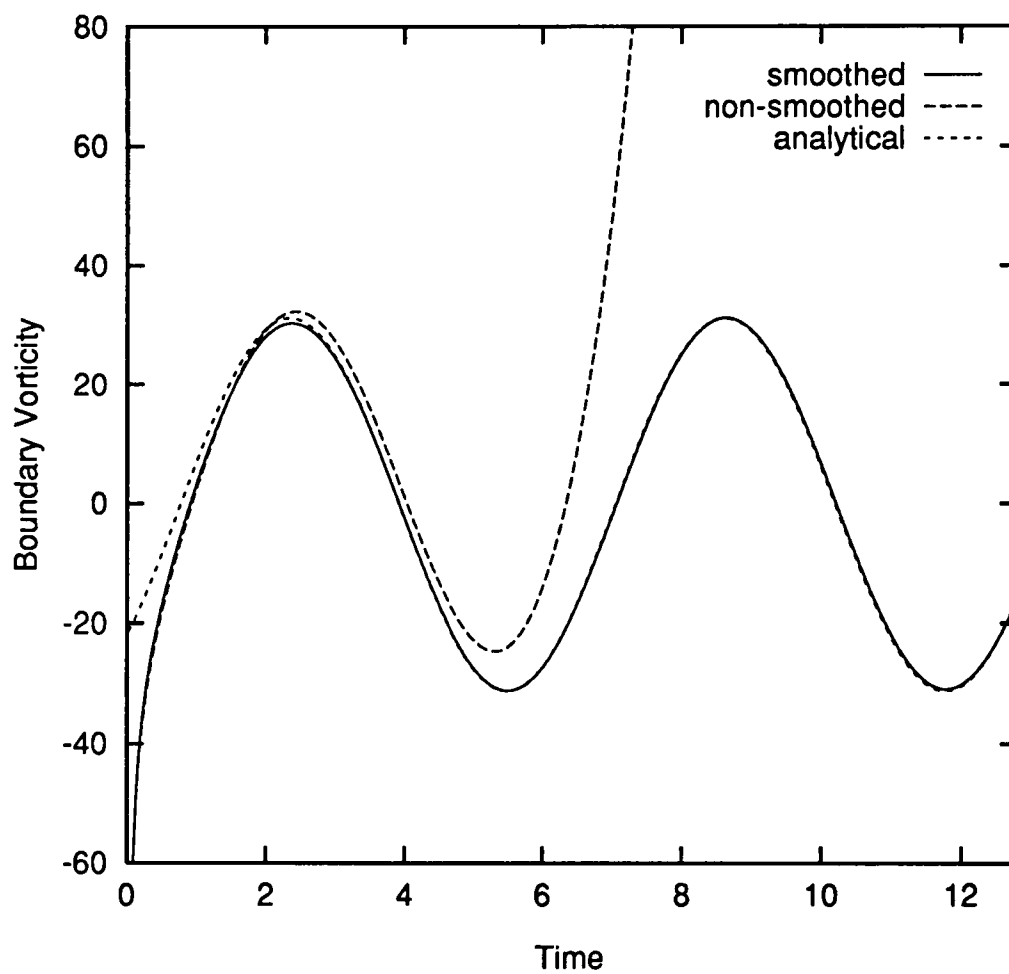


Figure 4.9: Boundary vorticity variation with time for the generalized Stokes' second problem. Comparison between smoothed and non-smoothed kernels.

(4.24) simply becomes

$$G_{\delta}^{*(2)} = \frac{1}{4\pi\nu(t+\delta t)} \exp\left[-\frac{r^2}{4\nu(t+\delta t)}\right],$$

thus at $t = 0$,

$$G_{\delta 0}^{*(2)} = \frac{1}{4\pi\nu\delta t} \exp\left(-\frac{r^2}{4\nu\delta t}\right),$$

which is regular even for $r = 0$. This implies that the singular initial condition of vorticity is smoothed out. The application of this idea to finite-difference schemes was tested numerically for the above problems by Wu [97].

Finally, a fast summation algorithm for heat kernels, of great value in integral methods, has been developed by Greengard and Strain [99,100]. Based on the same principle, Koumoutsakos et al. [50] successfully developed and applied a fast deterministic diffusion scheme for the vortex method.

4.3 Effect of Pressure Gradient

In this section, we examine the effect of pressure gradient on the application of local vorticity boundary conditions. Because the pressure is eliminated from the vorticity equation, the effect of pressure gradient must be accounted for through the initial or boundary conditions. Since the dynamic BC is derived by applying momentum equation on the solid wall, the pressure effect is automatically included as shown by the vorticity flux formulas of Chapter 3. However, the kinematic BCs do not contain any information of the pressure gradient and hence the pressure effect can only enter the solution through initial condition or boundary conditions *of velocity*.

To be more specific, consider an impulsively started flow over a solid body. At the beginning, the pressure impulse establishes an initial velocity field spontaneously, thus its effect is represented by the initial condition. After the start, pressure gradient will continue to affect the flow field. To see how pressure effect enters the solution based on vorticity, it suffices to consider the Rayleigh

flow with a constant pressure gradient term below

$$(4.27) \quad \frac{\partial u}{\partial t} = -P + \frac{\partial^2 u}{\partial y^2}.$$

Applying (4.27) at $y = 0$, it is easy to obtain the correct dynamic BC. On the other hand, since the kinematic BC is determined solely by u_s , the effect of P has to be found from the BCs for velocity. The no-slip condition provides no information about the pressure, but the far field BC does. Let $y \rightarrow \infty$ in (4.27), since the vorticity is zero, so is its derivative. Then the viscous term can be dropped, which gives

$$u(\infty, t) = u(\infty, 0) - Pt,$$

thus the pressure effect is included by the far field boundary condition of velocity. In this special case, the vorticity equation can be solved without reference to velocity if the no-slip condition is assumed at the beginning and the exact dynamic BC is used. For more general problems, the pressure gradient on solid boundaries is not known, and it has to be solved together with the velocity or vorticity.

Now, we demonstrate an interesting situation where the kinematic BCs are useless for obtaining correct solutions based on vorticity. Consider a plane Poiseuille flow caused by a constant *finite* pressure gradient along the plane channel. The flow will reach steady state due to the balance of pressure and viscous forces. Note that the flow develops gradually instead of instantaneously as it does under a pressure impulse. The equation to solve is the same as (4.27), but now the far field velocity condition is replaced by a no-slip condition at the upper solid wall. The solution can be obtained easily by solving the vorticity equation with exact dynamic BC. The interesting part is that there is no way to compute the flow using kinematic BCs, either local or global; because the only driving force of the flow, the pressure gradient, is absent from both the initial and boundary conditions. There are more examples like this; however, the point is that the dynamic BC contains more information about the flow, especially the pressure, than the kinematic one. This makes it convenient for modeling the vorticity generation from solid walls, which is consistent with the physical arguments presented in Chapter 3.

Chapter 5

Numerical Experiments of Vorticity-Pressure Decoupling

In this chapter, we examine the ω - p decoupling numerically by solving the impulsively started flow over a circular cylinder. The decoupling methods based on both operator-splitting and non-splitting approaches are studied. Although we shall implement both by using finite difference method, the former approach can be considered as resembling vortex methods. Thus, the conclusion drawn from the numerical experiment below should be equally applicable to vortex methods. Since vorticity and pressure are coupled through the no-slip condition at solid surfaces, the decoupling schemes are indeed numerical treatments of vorticity boundary conditions. It should be noted that talking about the coupling of vorticity with pressure is not very meaningful when kinematic BCs are under consideration. However, the ω - p coupling still exists, although it appears as a global one between vorticity and velocity.

While the operator-splitting is a natural way to decouple the vorticity and pressure, the non-splitting approach is important to study because it is more widely used and not limited to second order accuracy in time, like the splitting methods. For non-splitting methods, the construction of the decoupling varies with numerical schemes used to solve the vorticity equation. However, the derivations of the decoupling schemes are basically the same. Therefore, we shall study only one example here. The kinematic BCs will also be studied for comparison. In addition, an iteration scheme is derived for use with the dynamic BC to efficiently recover the ω - p coupling when necessary.

5.1 The ω - ψ Formulation

Consider a circular cylinder with radius R in a cross flow with free stream speed U . Define the Reynolds number as $Re = 2UR/\nu$. Using U and R to non-

dimensionalize the vorticity and stream-function equations yields

$$(5.1a) \quad \frac{\partial \omega}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\partial \psi}{\partial \theta} \omega \right) - \frac{\partial}{\partial \theta} \left(\frac{\partial \psi}{\partial r} \omega \right) = \frac{2}{Re} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial^2 \omega}{\partial r^2} \right) + \frac{1}{r^2} \frac{\partial^2 \omega}{\partial \theta^2} \right],$$

$$(5.1b) \quad \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = -\omega.$$

The initial condition is potential flow around the cylinder

$$(5.1c) \quad \psi(r, \theta) = -r \sin \theta \left(1 - \frac{1}{r^2} \right),$$

and the boundary conditions are

$$(5.1d,e) \quad \psi(1, \theta) = 0, \quad \frac{\partial \psi}{\partial r}(1, \theta) = 0.$$

For convenience, we shall use ν for $2/Re$ below as the dimensionless viscosity.

Introducing coordinate transformation in r direction

$$(5.2) \quad z = \log(r + a),$$

where $-1 < a < 0$ is a constant (strain parameter). Then Eq. (5.1a,b) can be recast as

$$(5.3) \quad A \frac{\partial \omega}{\partial t} + \frac{\partial}{\partial z} \left(\frac{\partial \psi}{\partial \theta} \omega \right) - \frac{\partial}{\partial \theta} \left(\frac{\partial \psi}{\partial z} \omega \right) = \nu \left(C \frac{\partial^2 \omega}{\partial z^2} + B \frac{\partial \omega}{\partial z} + \frac{1}{C} \frac{\partial^2 \omega}{\partial \theta^2} \right),$$

$$(5.4) \quad C \frac{\partial^2 \psi}{\partial z^2} + B \frac{\partial \psi}{\partial z} + \frac{1}{C} \frac{\partial^2 \psi}{\partial \theta^2} = -A\omega,$$

where

$$(5.5) \quad A = e^z(e^z - a), \quad B = ae^{-z}, \quad C = 1 - ae^{-z}.$$

The effect of the transformation is to make the grid points more clustered near the cylinder surface, for fixed grid size Δz , we have

$$\Delta r = (r + a)\Delta z$$

approximately.

5.2 The Poisson Solver

Since the local vorticity BCs are used, Eqs. (5.3) and (5.4) can be solved separately. In this section, we describe the method to solve ψ from Poisson equation (5.4). It is crucial to have a fast Poisson solver to make the computation efficient and affordable. Here, we take the advantage of periodicity of the problem. The stream-function and vorticity can be expanded as finite Fourier series

$$\psi(z, \theta) = \sum_{k=-N/2}^{N/2-1} \hat{\psi}_k(z) e^{ik\theta}, \quad \omega(z, \theta) = \sum_{k=-N/2}^{N/2-1} \hat{\omega}_k(z) e^{ik\theta},$$

from which we get

$$(5.6) \quad C \frac{d^2 \hat{\psi}_k}{dz^2} + B \frac{d\hat{\psi}_k}{dz} - \frac{1}{C} k^2 \hat{\psi}_k = -A \hat{\omega}_k.$$

Therefore, we may use FFT (Fast Fourier Transform) to transform ω to $\hat{\omega}$, then solve (5.6) for $\hat{\psi}$ using standard finite difference method (here we use second-order central difference), and finally, ψ is obtained from an inverse FFT of $\hat{\psi}$. Note that this method is spectrally accurate in the θ direction if ω is given exactly. A true second-order scheme can be obtained by changing k^2 in (5.6) to $(2 - 2 \cos k\Delta\theta)/\Delta\theta^2$ [96]. Nevertheless, since our solution of ω is second order in both z and θ directions, the resulting ψ will be second order.

5.3 Solving the Vorticity Transport Equation

In this section, we discuss methods to solve (5.1a) via operator splitting and non-splitting approaches. We consider the splitting approach first, where convection and diffusion of vorticity are computed successively. Then, we obtain a non-splitting scheme by adding viscous diffusion to the convection scheme used in the splitting approach and give the derivation of ω - p decoupling.

5.3.1 Upwind Schemes for Convection

The main problem of discretizing the convection terms when Re is high is to avoid excessive numerical diffusion while keeping the numerical scheme stable.

For incompressible flow, central differences can be used to get stable schemes with no second-order numerical diffusion, but they produce numerical oscillations. For this reason, we choose to use upwind schemes instead of centered ones. To avoid the second-order diffusion of the upwind scheme on a three-point stencil, we need to use larger stencils and higher order methods. These methods can be obtained systematically from the ENO (Essentially Non-Oscillatory) schemes, which has been proven to be very effective for compressible flow computations. However, due to the dynamic selection of stencils, the ENO schemes are time consuming. On the other hand, the QUICK (Quadratic Upwind Interpolation for Convective Kinematics) scheme [101], which has been popular in computing incompressible flows, suffices for our purpose.

The QUICK scheme can be explained simply as follows. Consider solving the 1-D linear convection equation

$$\frac{\partial u}{\partial t} + \frac{\partial(au)}{\partial x} = 0,$$

on a set of grid points x_i . Denote the flux au by f , integration gives

$$\frac{\partial \bar{u}}{\partial t} = \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} \quad \text{with} \quad \bar{u} = \int_{x_{i-1/2}}^{x_{i+1/2}} u dx / \Delta x.$$

The task is to find $f_{i+1/2}$, the flux at cell interface. Since the values of f are known on x_i , we may form a unique quadratic polynomial $\hat{f}(x)$ using values on stencil $\{x_{i-1}, x_i, x_{i+1}\}$ or on $\{x_i, x_{i+1}, x_{i+2}\}$. Then $f(x_{i+1/2})$ is approximated by the numerical flux $\hat{f}(x_{i+1/2})$. The choice of which stencil to use is determined by the local velocity of convection: if $a_{i+1/2} > 0$ then the former is used, otherwise the latter is used. Therefore, upwinding is achieved through stencil selection. The final scheme can be written as

$$(5.7) \quad f_{i+1/2} = \begin{cases} \frac{1}{2}(f_i + f_{i+1}) - \frac{1}{8}(f_{i-1} - 2f_i + f_{i+1}) & \text{if } a_{i+1/2} > 0, \\ \frac{1}{2}(f_i + f_{i+1}) - \frac{1}{8}(f_i - 2f_{i+1} + f_{i+2}) & \text{otherwise.} \end{cases}$$

In finite volume formulation, Eq. (5.7) leads to third order results. However, in our application, $\bar{u}_i$ is replaced by u_i and the resulting scheme is second-order according to Taylor series expansion.

The QUICK scheme is tested against the linear convection equation with $a = 1$ on interval $[-1, 1]$ with periodic boundary condition, and

$$u(x, 0) = \begin{cases} -x \sin(\frac{3\pi}{2}x^2), & -1 \leq x \leq -\frac{1}{3}, \\ |\sin(2\pi x)|, & -\frac{1}{3} < x < \frac{1}{3}, \\ 2x - 1 - \sin(3\pi x)/6, & \frac{1}{3} \leq x \leq 1, \end{cases}$$

as the initial condition. A second-order TVD (Total Variation Diminishing) Runge-Kutta scheme [102] is used for time integration. In Fig. 5.1, the result at $t = 8.5$ is compared with that of second- and third-order ENO schemes (with a third-order TVD R-K scheme) [102]. Except for a little numerical oscillation, QUICK scheme compares well with the third-order ENO scheme, and its numerical diffusion is much smaller than the second-order ENO. It should be noted that the ENO schemes use longer stencils (seven-point for second order; nine-point for third order) than the five-point one of QUICK, and take much longer CPU time. On the other hand, the ENO schemes are stable for strong non-linear equations, like the Burgers equation; whereas QUICK is unstable when strong discontinuity occurs. However, such discontinuities are unlikely to happen in incompressible flows. In two or more dimensions, we use (5.7) in each direction. The QUICK scheme will be used in both splitting and non-splitting methods.

5.3.2 Diffusion and Vorticity Boundary Conditions

In a splitting approach, the vorticity diffusion equation

$$(5.8) \quad A \frac{\partial \omega}{\partial t} = \nu \left(C \frac{\partial^2 \omega}{\partial z^2} + B \frac{\partial \omega}{\partial z} + \frac{1}{C} \frac{\partial^2 \omega}{\partial \theta^2} \right)$$

needs to be solved after the inviscid convection substep. Integrating (5.8) gives

$$(5.9) \quad A(\omega^{n+1} - \omega^{n+1/2}) = \nu \Delta t \left(C \frac{\partial^2 \bar{\omega}}{\partial z^2} + B \frac{\partial \bar{\omega}}{\partial z} + \frac{1}{C} \frac{\partial^2 \bar{\omega}}{\partial \theta^2} \right),$$

where $\bar{\omega}$ is the time average of ω and superscript $(n + 1/2)$ denotes values after the convection. The Crank-Nicolson scheme follows from the approximation

$$(5.10) \quad \bar{\omega} = \frac{1}{2}(\omega^{n+1} + \omega^{n+1/2}),$$

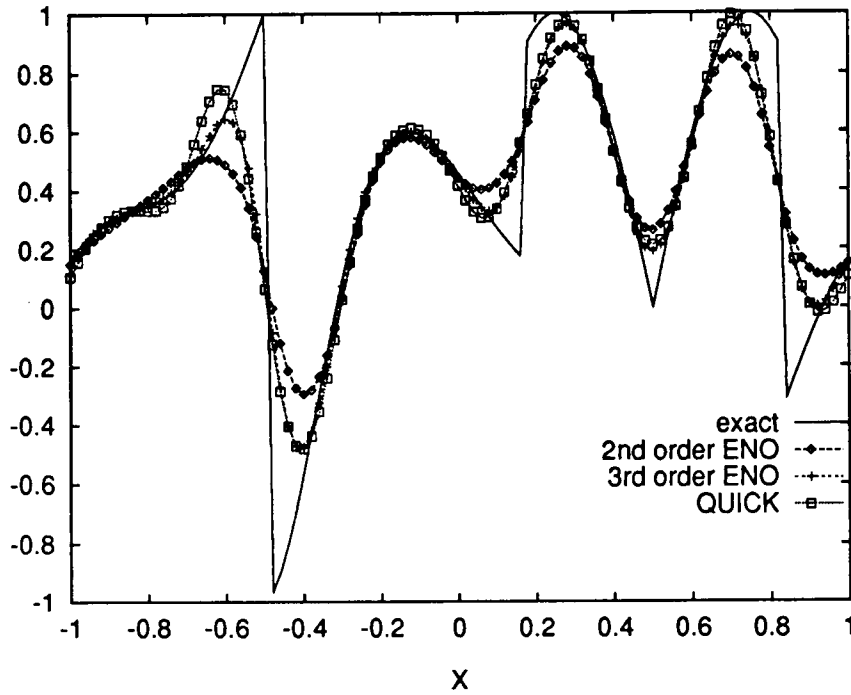


Figure 5.1: Comparison of QUICK and ENO schemes. $t = 8.5$, $\Delta x = 0.02$, $\Delta t = 0.01$.

and is second order accurate in time. Eq. (5.9) is then discretized by using central difference, which leads to second order accuracy in space. The resulting linear system of equations of ω^{n+1} can be efficiently solved by approximate factorization.

We still need to specify the boundary condition of ω to close the system of equations. The kinematic BCs described in Chapter 4 can be applied in the same manner, however, the dynamic BC needs more consideration here because of the presence of the unknown pressure gradient term in the tangential momentum equation at the cylinder surface, which is

$$(5.11) \quad \frac{\partial u}{\partial t} = -e^z \frac{\partial p}{\partial \theta} + \nu \frac{\partial \omega}{\partial z} = -P - \sigma.$$

Note that $u = -\partial\psi/\partial z$ is the transformed tangential velocity in θ direction. By the same procedure in Chapter 3, there is

$$(5.12) \quad \bar{\sigma} = (u^{n+1/2} - u^{n+1})/\Delta t - \bar{P}.$$

Since no-slip condition is applied at t_{n+1} , then

$$(5.13) \quad \bar{\sigma} = (u^{n+1/2} - b^{n+1})/\Delta t - \bar{P},$$

where b is the *transformed* tangential velocity of the boundary. Dropping unknown term $\bar{P}$ in (5.13), we get the approximate dynamic BC for ω , which is decoupled from P . According to Chapter 3, the error, represented by a residual slip u_s^{n+1} , should be small if the Reynolds number is sufficiently high.

The numerical BC (5.13) can be incorporated into (5.9) directly. In fact, the central difference of the viscous term in (5.9) at the boundary is

$$\nu \Delta t \left[\frac{2C}{\Delta z^2} (\bar{\omega}_{i,j+1} - \bar{\omega}_{i,j}) + \frac{1}{C \Delta \theta^2} (\bar{\omega}_{i+1,j+1} - 2\bar{\omega}_{i+1,j} + \bar{\omega}_{i-1,j}) \right] + \Delta t \left(\frac{2C}{\Delta z^2} - B \right) \bar{\sigma},$$

where subscripts i and j denotes the nodal index in θ and z directions, respectively.

As in Chapter 4, the modified initial vorticity can be obtained by letting $\Delta t \rightarrow 0$ in the Crank-Nicolson scheme, which yields

$$(5.14) \quad \omega_{i,B}^{n+1/2, mod} = \omega_{i,B}^{n+1/2} + \left(\frac{2}{\Delta z} - a \right) u_{s,i}^{n+1/2} / (1 + a)^2$$

on the cylinder surface. It should be noted that (5.14) remains the same if the full vorticity equation (5.3) is under the consideration. Eq. (5.14) can be used at the impulsive start and at the beginning of each diffusion substep or whenever there is a slip on the solid boundary. When used before the diffusion substep, the no-slip condition is resumed, and (5.13) becomes

$$\bar{\sigma} = (b^{n+1/2} - b^{n+1})/\Delta t - \bar{P}.$$

If there is no tangential acceleration of the boundary, so that the first term vanishes, the equation reduces to $\bar{\sigma} = \bar{P}$. Now, dropping $\bar{P}$ implies $\bar{\sigma} = 0$. This is an alternative treatment of the dynamic condition. We note that (5.14) does not enhance the accuracy of solutions when used in this way. The reason is that once the no-slip condition is established after $t = 0$, the inviscid convection substep produces a $u_s^{n+1/2}$ of order $O(\Delta t)$, which tends to zero as $\Delta t \rightarrow 0$; therefore $u_s^{n+1/2}$, artificially created, does not represent a true singular problem. In addition, the

accuracy in $\bar{\sigma}$ is not improved by the alternative treatment. Nevertheless, the modification of initial vorticity is still useful at the true impulsive start at $t = 0$. It can also be used at the end of each time step to take into account the vorticity contained in the residual slip.

With the convection and diffusion schemes of vorticity presented in the last and present subsections, we can now construct either first- and second-order splitting schemes. For the second-order splitting there is

$$\begin{aligned} \mathbf{u}^n &= (H(\Delta t/2)E(\Delta t)H(\Delta t/2))^n \mathbf{u}^0 \\ &= H(\Delta t/2)(E(\Delta t/2)H(\Delta t/2))^{n-1}E(\Delta t)H(\Delta t/2)\mathbf{u}^0, \end{aligned}$$

thus the method will not cost much more than the first-order one, because the increase of computation occurs only when intermediate results are needed for output.

5.3.3 Recover Global Coupling by Iteration

Iteration can be used with local vorticity BCs to obtain results that satisfy the no-slip condition at the end of each substep of diffusion. For the local kinematic BC

$$(5.15) \quad \omega_B^{n+1} = \omega_B^{n+1/2} + u_s^{n+1/2}/h',$$

the following iteration is obvious:

$$(5.16) \quad \omega_B^{n+1,m+1} = \omega_B^{n+1,m} + u_s^{n+1,m}/h',$$

where $\omega_B^{n+1,0}$ is given by (5.15). When u_s^{n+1} becomes zero, the iteration converges. To accelerate the convergence, a relaxation parameter α can be introduced and there is

$$(5.16') \quad \omega_B^{n+1,m+1} = \omega_B^{n+1,m} + \alpha u_s^{n+1,m}/h'.$$

This scheme is basically the same as the one given in [94]. The disadvantage of this scheme is again due to the fact that (5.15) is Δt independent. As discussed

in Chapter 4, when Δt is large (which is typical in an implicit scheme), the initial guess of $\omega_B^{n+1,0}$ may be too far-off from the actual value and leads to divergent iteration. Therefore, the speed of convergence of (5.16) or (5.16') depends on Δt . For (5.16') this means that the relaxation parameter has to be tuned according to Δt to get optimum convergence. These problems, however, are relieved by using the dynamic BC which depends on Δt .

The iteration scheme using dynamic BC can be derived as follows. First the initial guess $\bar{\sigma}^0$ is given by (5.13) with $\bar{P}$ dropped, i.e.,

$$(5.17) \quad \bar{\sigma}^0 = \frac{u^{n+1/2} - b^{n+1}}{\Delta t}.$$

For fully decoupled implementation, Eq. (5.17) is the boundary condition to use. On the other hand, there is $u^{n+1,0} \neq b^{n+1}$ in general due to the assumption $\bar{P}^0 = 0$. Since (5.12) should be satisfied for $\bar{\sigma}^0$ and $u^{n+1,0}$, $\bar{P}^0$ has to be updated to $\bar{P}^1$. Subtracting (5.17) from (5.12) gives

$$(5.18) \quad \bar{P}^1 = -\frac{u^{n+1,0} - b^{n+1,0}}{\Delta t} = -\frac{u_s^{n+1,0}}{\Delta t},$$

a first-order approximation of $\bar{P}$. Substitute (5.18) into (5.13), we get updated vorticity flux

$$\bar{\sigma}^1 = \bar{\sigma}^0 + u_s^{n+1,0}/\Delta t,$$

and hence in general,

$$(5.19) \quad \bar{\sigma}^{m+1} = \bar{\sigma}^m + u_s^{n+1,m}/\Delta t.$$

One may notice the similarity between (5.19) and (5.16); in fact, both of them have the same physical interpretation, namely when vorticity is less (more) than required so that there is a slip in the direction of (opposite) the flow, there should be an increase (decrease) in vorticity production. However, the similarity does not imply that (5.16) and (5.19) behaves similarly in computations. As mentioned above, the convergence of (5.19) is less dependent on Δt . Moreover, we find from computations that there is no need to introduce relaxation parameters at all,

the convergence is always fast, which can be achieved in just two or three iterations at sufficiently high Re (above 1000). In contrast, the relaxation parameter has to be finely tuned to achieve such a speed of convergence when using (5.16').

Both of (5.16') and (5.19) can be used in a non-splitting methods. Furthermore, for the operator splitting methods, the iterations only requires the value of slip on the boundary; therefore, integral methods like the generalized Biot-Savart Law can be used to make the iterations very efficient. However, this may not be the case for certain non-splitting schemes, i.e., the whole velocity field has to be solved for every iteration. For the present computations, we have to solve the whole velocity field because integral method is not used. However, our Poisson solver is fast enough to make the iteration schemes perform at satisfactory speed.

5.3.4 The Non-splitting Methods

There are many non-splitting methods that can be used for solving the present problems. We only give an example of such methods, an explicit scheme using second-order TVD Runge-Kutta time integration:

$$(5.20a) \quad \omega^* = \omega^n - \Delta t F(\omega^n, \psi^n),$$

$$(5.20b) \quad \omega^{n+1} = \frac{1}{2}\omega^n + \frac{1}{2}[\omega^* - \Delta t F(\omega^*, \psi^*)],$$

where superscript $*$ denotes intermediate values, and F includes the QUICK discretization for the convection terms and central difference for the viscous terms. Equation (5.20) can be used to update the interior vorticity ω^{n+1} if ω^n is given, the boundary vorticity ω_B^{n+1} needs to be computed by imposing boundary conditions. Either kinematic or dynamic BC can be used. The latter is the main concern here.

The kinematic BC can be imposed in a straightforward manner for the present schemes. Note that the solution of ψ^{n+1} does not require knowing ω_B^{n+1} . Thus, once the interior ω^{n+1} is found, ψ^{n+1} can be solved, then we can interpolate ω_B^{n+1} by using those formulas given in §4.1.2. Note that the kinematic BC is now truly local and there is no loss of time accuracy, in contrast to its implementation in implicit schemes. On the other hand, it is not always possible to compute ω_B^{n+1}

in this way, particularly when higher order difference scheme is used to solve ψ^{n+1} , which may require the knowledge of ω_B^{n+1} in advance. In this case, ω_B^{n+1} should be solved together with ψ^{n+1} ; it is not too bad because the coupling between ω and ψ is now greatly reduced. There are ways to avoid the coupling by using one-sided difference instead of central difference for (5.4) at the boundary [96]. However, from our experience (see also below), one-sided difference at the boundary could be significantly less accurate than the centered one, because of the large normal gradient of vorticity usually existing at the boundary. Nevertheless, the kinematic BC is more natural and easier to use in explicit schemes than in implicit ones.

In the present situation, the dynamic BC is a little bit more complicated to impose than the kinematic one. In explicit schemes, the dynamic BC is no longer advantageous in the sense of preserving the stability of numerical methods. However, the dynamic BC enables us to evaluate the boundary vorticity for the next time step before solving the stream-function. Thus, there is no coupling between ω_B and ψ at all. This could be an advantage when higher order schemes are used. Of course, we have to pay the price that there will be a residual slip on the boundary. One can use the iteration method described in §5.3.3 to reduce the residual slip to below the discretization level. But here we are more interested in solving the problem from a different angle: Since ω and ψ solved from the second order Runge-Kutta scheme are at best $O(\Delta t^2)$, therefore, it would be reasonable to accept a residual slip of order $O(\Delta t^2)$.

As before, we derive the numerical dynamic condition for vorticity by applying the numerical scheme of the original N-S equation corresponding to the vorticity-based scheme to the solid boundary. Here we present a general derivation which is applicable to 3-D computations. Corresponding to (5.20a,b), we have

$$\begin{aligned} \mathbf{u}^* &= \mathbf{u}^n - \Delta t(\mathbf{u}^n \cdot \nabla \mathbf{u}^n + \nabla p^* - \nu \Delta \mathbf{u}^n), \\ \mathbf{u}^{n+1} &= \frac{1}{2}\mathbf{u}^n - \frac{1}{2}[\mathbf{u}^* - \Delta t(\mathbf{u}^* \cdot \nabla \mathbf{u}^* + \nabla p^{n+1} - \nu \Delta \mathbf{u}^*)]. \end{aligned}$$

It should be noted that p is treated implicitly in the above two equations as required by the fact that when $\mathbf{u}$ is obtained from ψ (which is solved from ω), the divergence

free conditions

$$\nabla \cdot \mathbf{u}^* = 0 \quad \text{and} \quad \nabla \cdot \mathbf{u}^{n+1} = 0$$

are satisfied. Apply the tangential part of these two equations on the cylinder surface, and denote $\mathbf{u}_{||} = \mathbf{n} \times \mathbf{u}$, $P_{||} = \mathbf{n} \times \nabla p$, and $\boldsymbol{\sigma}_{||} = \nu \mathbf{n} \times (\nabla \times \boldsymbol{\omega})$ (note that $\boldsymbol{\sigma}_{||}$ is not equal to $\mathbf{n} \times \boldsymbol{\sigma}$ in general, though it reduces to $\boldsymbol{\sigma}$ in 2-D), we have

$$(5.21a) \quad \mathbf{u}_{||}^* = \mathbf{u}_{||}^n - \Delta t (\mathbf{n} \times (\mathbf{u}^n \cdot \nabla \mathbf{u}^n) + P_{||}^* + \boldsymbol{\sigma}_{||}^n),$$

$$(5.21b)$$

$$\mathbf{u}_{||}^{n+1} = \frac{1}{2} \mathbf{u}_{||}^n - \frac{1}{2} [\mathbf{u}_{||}^* - \Delta t (\mathbf{n} \times (\mathbf{u}^* \cdot \nabla \mathbf{u}^*) + P_{||}^{n+1} + \boldsymbol{\sigma}_{||}^*)].$$

Assume that the no-slip condition holds initially, i.e. $\mathbf{u}^n = \mathbf{b}^n$, and $\boldsymbol{\sigma}_{||}^n$ is known, then we can use (5.20a) on the boundary to compute ω_B . The result, however, will not satisfy the no-slip condition $\mathbf{u}^* = \mathbf{b}^*$. This is obvious if the boundary is stationary. There is

$$\mathbf{u}_{||}^* = -\Delta t (P_{||}^* + \boldsymbol{\sigma}_{||}^n) = O(\Delta t^2),$$

since $P_{||}^n = -\boldsymbol{\sigma}_{||}^n$ by our assumption that no-slip condition is satisfied, and $P_{||}^* = P_{||}^n + O(\Delta t)$. Therefore, it is generally impossible to ensure the no-slip condition unless $\boldsymbol{\sigma}$ is implicitly treated, i.e. we may assume

$$\mathbf{b}_{||}^* = \mathbf{u}_{||}^n - \Delta t (\mathbf{n} \times (\mathbf{u}^n \cdot \nabla \mathbf{u}^n) + P_{||}^* + \boldsymbol{\sigma}_{||}^n),$$

where $\mathbf{b}_{||}^* = \mathbf{n} \times \mathbf{b}^*$. Subtract this equation from (5.21a), we get

$$(5.22a) \quad \boldsymbol{\sigma}_{||}^* = \boldsymbol{\sigma}_{||}^n + (\mathbf{u}_{||}^* - \mathbf{b}_{||}^*)/\Delta t = \boldsymbol{\sigma}_{||}^n + \mathbf{u}_{||}^*/\Delta t.$$

Equation (5.22a) gives the method to update $\boldsymbol{\sigma}_{||}^*$, which is needed for computing ω_B^{n+1} (see (5.21b)). After updating $\boldsymbol{\sigma}^*$, we impose the no-slip condition $\mathbf{u}^* = \mathbf{b}^*$. Following the procedure of deriving (5.22a), we can get

$$(5.22b) \quad \boldsymbol{\sigma}_{||}^{n+1} = \boldsymbol{\sigma}_{||}^* + (2\mathbf{u}_{||}^{n+1} - \mathbf{u}_{||}^*)/\Delta t,$$

It is obvious from (5.22b) that $\mathbf{u}_{||}^{n+1} = O(\Delta t^2)$. In the computation, we modify the vorticity according to (5.14) at the end of each time step, and then set $\mathbf{u}_s^{n+1} = 0$.

5.3.5 Far Field Condition

Since the computational domain has to be truncated to a finite region, we need to specify boundary conditions at the boundary of truncation r_∞ . In the computations below, we impose Dirichlet condition on ψ by using the exact potential flow solution at r_∞ , which has to be sufficiently far away from the solid body. For the vorticity equation, we assume the viscous diffusion is negligible at r_∞ and vorticity is convected out of the computational domain. The disadvantage of this method is that r_∞ has to be much larger than the necessary radius that encompass the region in which vorticity is not zero. Thus, more grid points in r direction need be used to get sufficiently small grid size near the cylinder surface to resolve the normal gradient of vorticity. The strain parameter introduced in the coordinate transformation helps to make the grid clustered near the boundary; but if it is too large, the accuracy of the scheme will be degraded. Nevertheless, this approach is the simplest and fits the objectives of present study.

A more accurate treatment was used by Anderson and Reider [96] They used a domain decomposition method so that the far field condition is treated exactly while the computational domain is just large enough to contain almost all the vorticity with a negligible portion left outside. This provides tremendous saving for high Re flow when vorticity is concentrated. Their method, however, utilized the harmonic analysis peculiar to circular geometry and hence is not general. The more general approach is the integral approach proposed by J.C. Wu et al. [18] in 1970s. In this approach, one computes the velocity induced by vorticity from the Biot-Savart Law as well as the contribution of the surface potential which takes care of the normal velocity condition (see Chapter 2). The far field condition is thus treated exactly and the computational domain needs only to include main portion of the vorticity like AR's method. Unfortunately, the fast integration methods [65] are beyond the capability of the author's computing facility.

5.4 Result and Discussion

The numerical schemes described in previous sections were applied to impulsively started flow over a circular cylinder. We are mainly interested in the high Re flows, e.g. $Re = 9500$, which is interesting because of its fine vortex structures. The results are compared to the benchmark solutions obtained by Anderson and Reider [96] (abbreviated as AR below) who used a fourth order scheme in both space and time, as well as the widely quoted experiment by Bouard and Coutureau [103].

5.4.1 Results of Operator Splitting and Strength of (ω, p) Coupling

The first-order splitting scheme, most commonly used in the context of vortex method, is used to compute the impulsively started flow with $Re = 9500$. At this Reynolds number, the flow exhibits a rich vortex structure which makes the computation difficult in general. In the following results, the far field boundary is taken to be $r_\infty = 5$ unless otherwise stated; a 512×301 grid was used, except for Figs. 5.2 and 5.3 below where the grid was 256×301 . The computation was done in double precision on a Sun SPARC10 workstation. With the 256×301 grid, it took about 5 CPU seconds for one time step without iteration.

Figure 5.2 shows the computed flow field using the first-order splitting and no iteration, compared with experiment [103] and the computation by Ta Phuoc Loc and Bouard [104]. The results were obtained with $a = -0.5$, so the grid sizes are $\Delta\theta = 0.0245$ and $\Delta z = 0.0073$, and we have $\Delta r = 0.0037$ adjacent to the wall which will be denoted by Δr_B . The time step is $\Delta t = 0.005$. The agreement is good. It needs to be stressed that such comparison is only of qualitative value. Later, we shall compare the results of ω_B , and the drag coefficient C_D , which gives more quantitative information about our scheme. In Fig. 5.3, the velocity at the symmetry plane behind the cylinder is compared with the experiment. The solid lines are for the numerical results and the symbols for experiment data. We note that the wake length of our computation is always smaller than that of the experiment [103] as well as Ta Phuoc Loc and Bouard's results (Fig. 5.2). On the

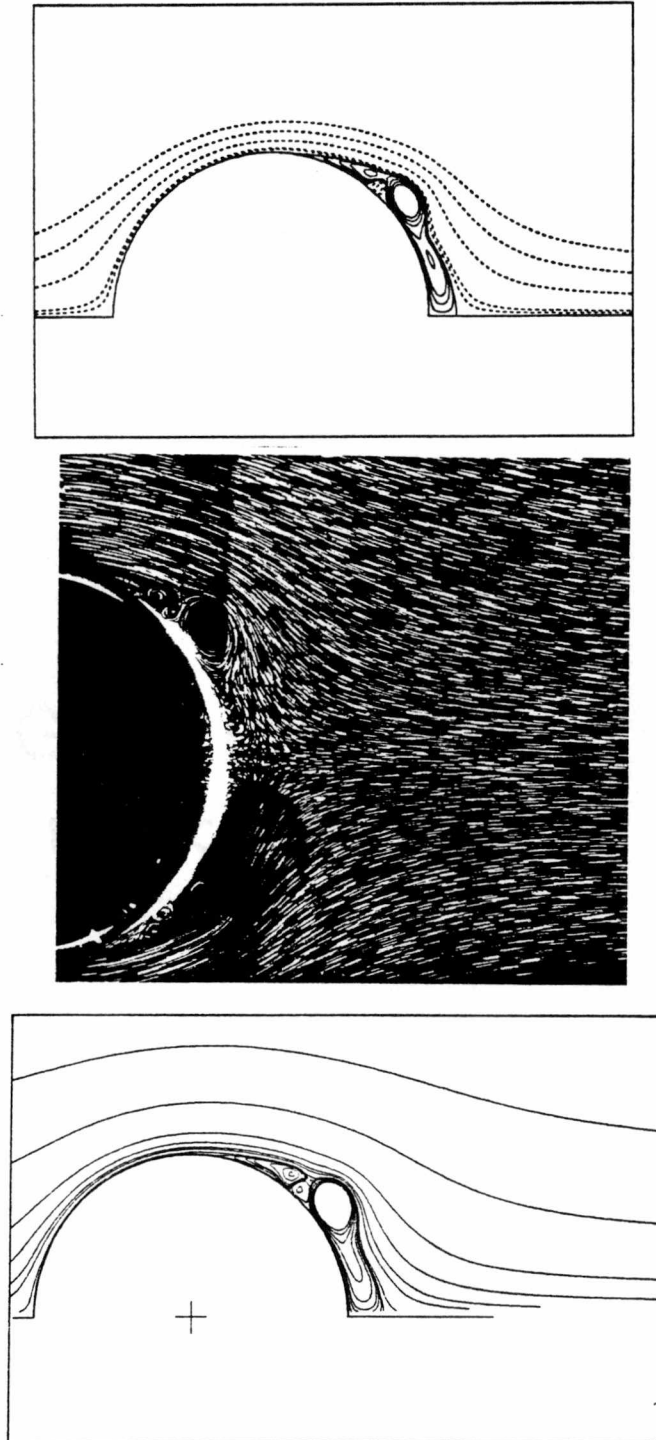


Figure 5.2: Flow structures for $Re = 9500$. Top: result of the first-order splitting scheme (256×301 grid, $a = -0.5$, $r_\infty = 5$, $\Delta t = 0.005$); middle: flow visualization; bottom: numerical simulation of Ta Phuoc Loc and Bouard [104].

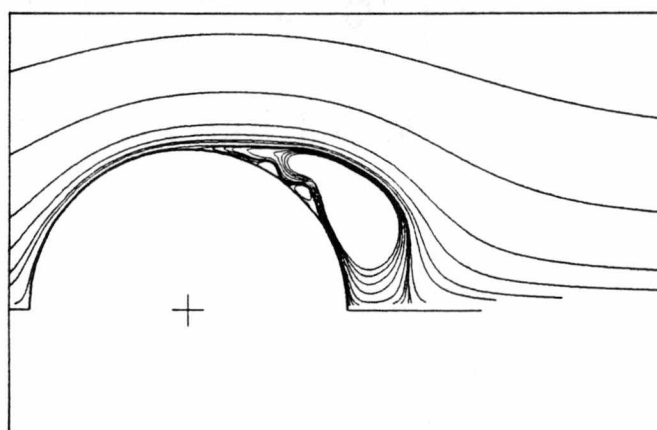
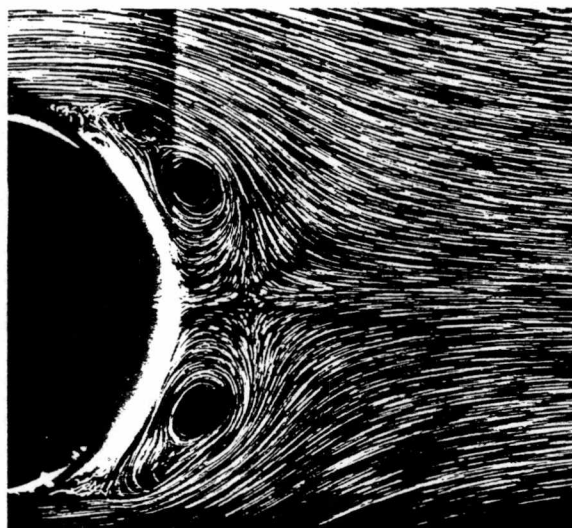
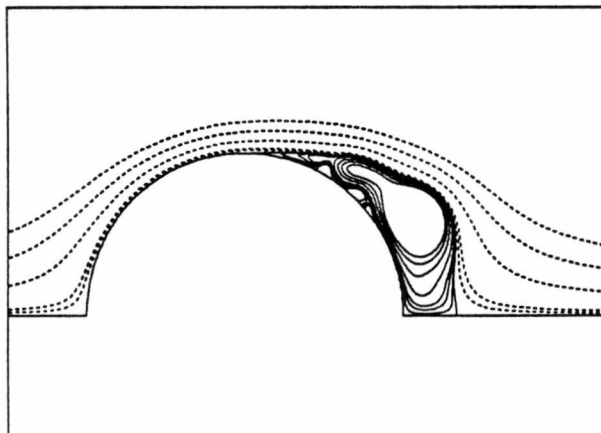
$t = 2.8$ 

Figure 5.2 (continued).

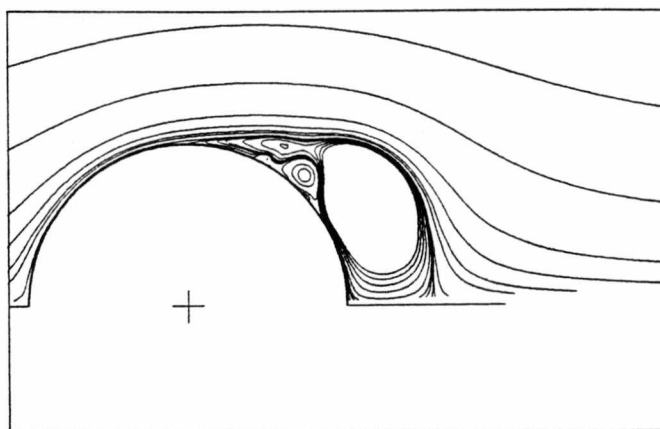
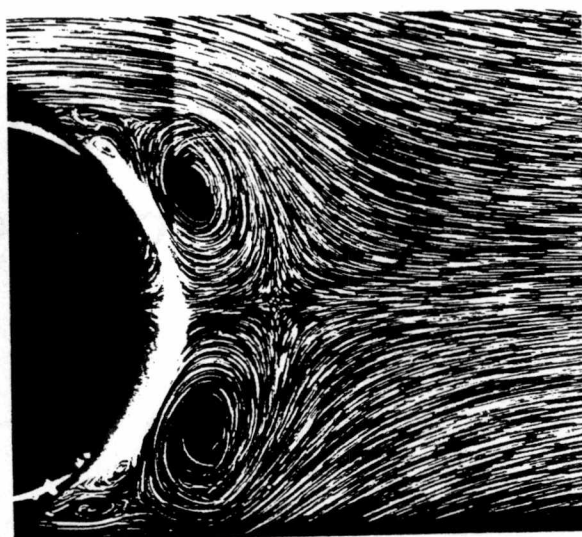
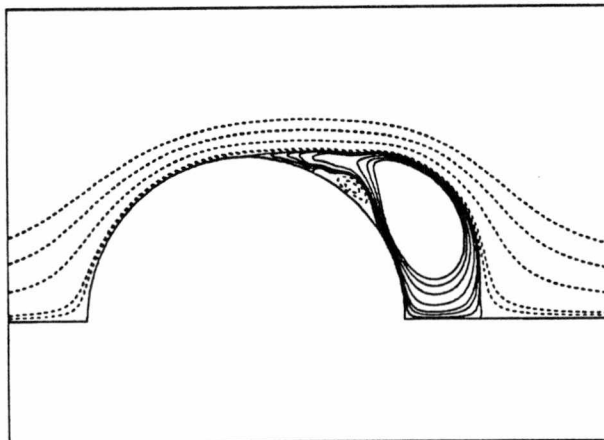
$t = 3.2$ 

Figure 5.2 (continued).

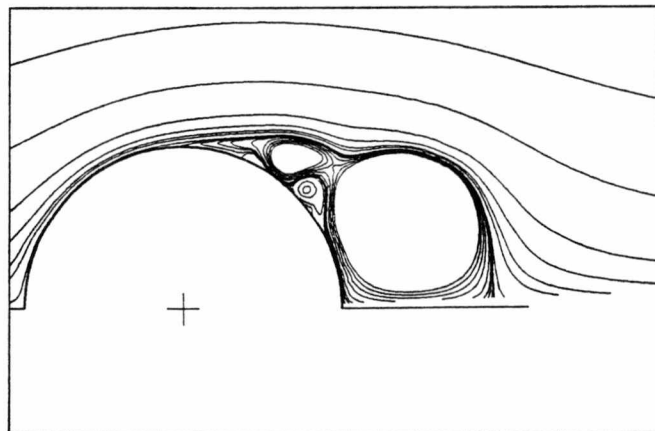
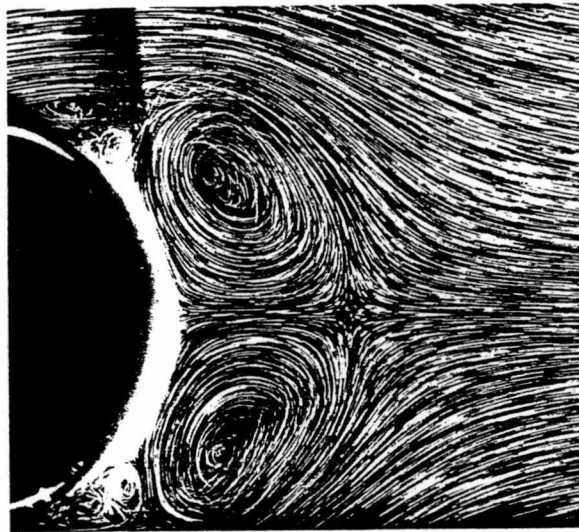
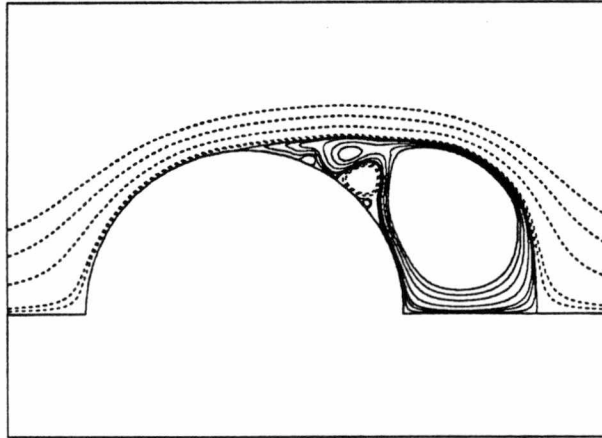
$t = 4.0$ 

Figure 5.2 (concluded).

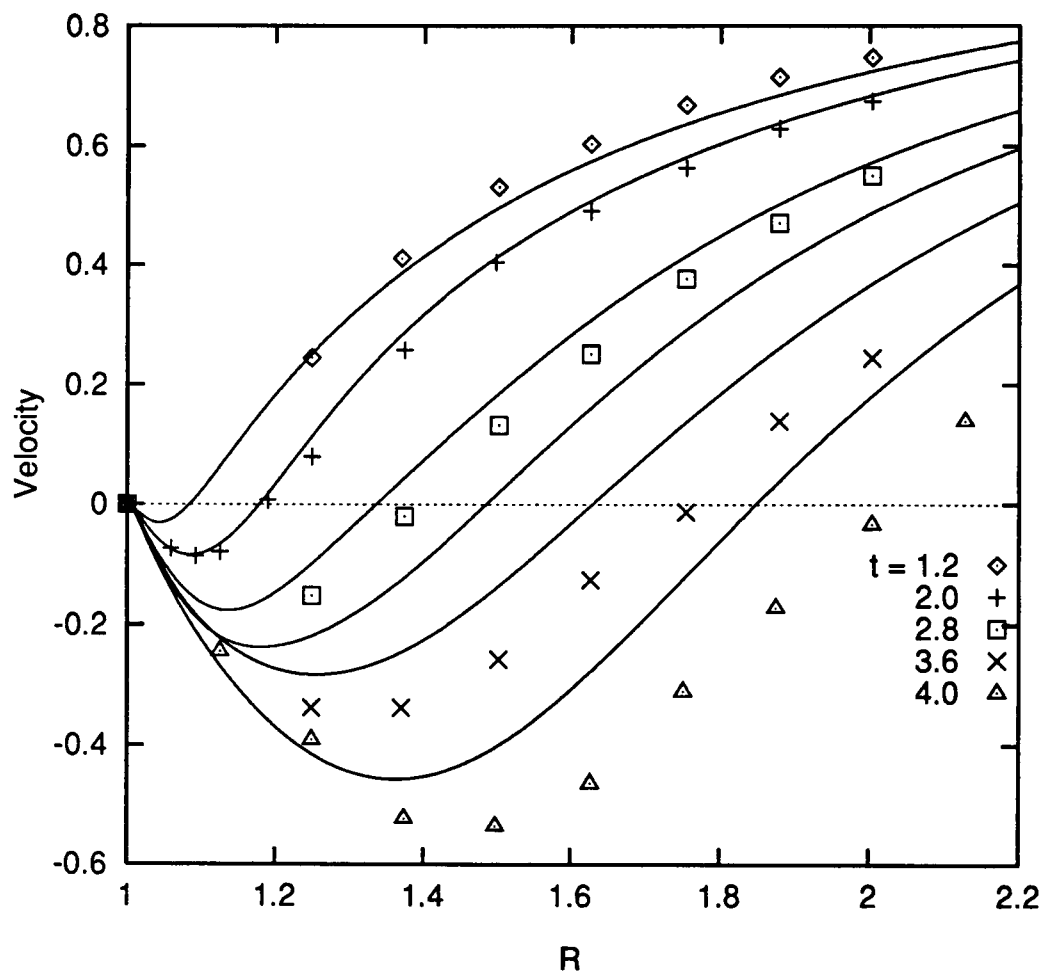


Figure 5.3: Comparison of the wake velocity on the symmetry plane between numerical and experimental results. See figure 5.2 for parameters. Solid lines are for the numerical results and symbols for experimental data (read from [104]).

other hand, however, our result agrees well with AR's fourth-order computation (see Fig. 5.11 below). We believe that besides the grid-size and r_∞ effect to be discussed below, the different treatment of the initial condition is an important source of the discrepancy with the solutions of Ta Phuoc Loc and Bouard. In both the present and AR's computations, a potential flow (with modification in the latter case) was used to model the "impulsive" start, while an initial Stokes flow with a sudden change in the Reynolds number was used by Ta Phuoc Loc and Bouard [104].

The comparison in Fig. 5.2 seems to suggest that the flow is well resolved. Indeed, a comparison of the ω_B by using the above grid with AR's fourth-order solution (obtained on a uniform grid with $\Delta\theta = 0.00307$, $\Delta r = 0.00195$, and $\Delta t = 0.00033$) showed that the attached and smooth separating flows are well resolved with our much larger $\Delta\theta$. However, for resolving the more complicated separating flow, smaller $\Delta\theta$ is necessary. Thus we reduced $\Delta\theta$ to 0.0123 by increasing the grid number in θ -direction n_θ to 512 (Δt was reduced to 0.0025). The results of ω_B with and without iteration are shown in Fig. 5.4. The agreement is good except for the extreme values.

The time variation of the maximum and averaged slip (under L_2 norm) is shown in Fig. 5.5. To the authors' knowledge, in the literature only Cottet [84] mentioned that in his computation the averaged slip is about 2%. It is interesting to note that, after keeping at a constant level (with maximum slip 0.0125%) for some time, the slip rises up. The time of slip rising is about the time when the first secondary vortex starts to form. Due to these small vortices, rather than the primary large vortex, the boundary vorticity no longer varies smoothly along the surface; large gradient occurs. This can also be seen clearly in Fig. 5.4. Comparing Fig. 5.4 with Fig. 5.5 shows that when $t = 2$, there are high peaks in ω_B distribution (in fact, the maximum boundary vorticity occurs at about this time), so that not only ω_B but also its gradient is large. Correspondingly, the slip is larger, about the maximum point in the curve. This observation is in qualitative agreement with our previous discussion on the accuracy of decoupled schemes (§3.3).

There are two ways to further improve the accuracy in ω_B . First, when

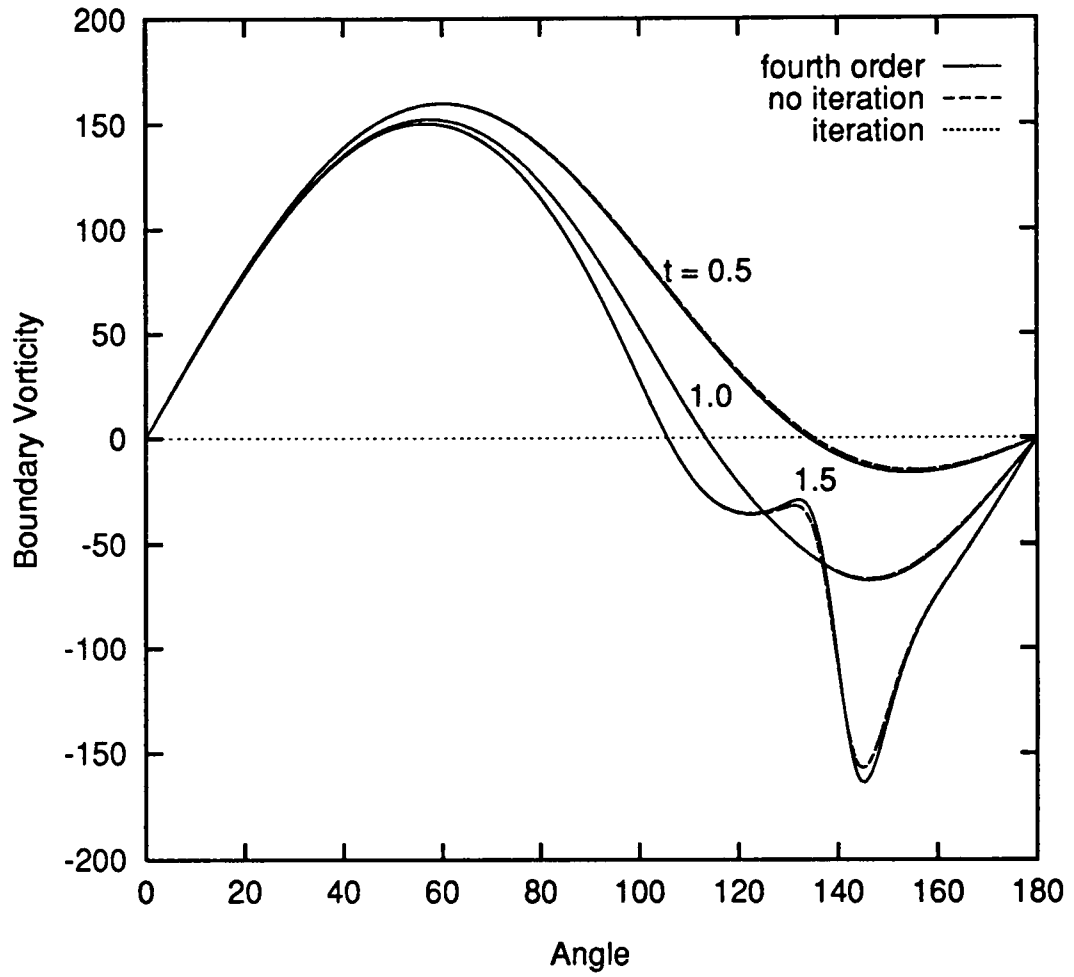


Figure 5.4: Comparison of the boundary vorticity on a 512×301 grid ($a = -0.5$, $r_\infty = 5$, $\Delta t = 0.0025$) and the fourth-order result of AR.

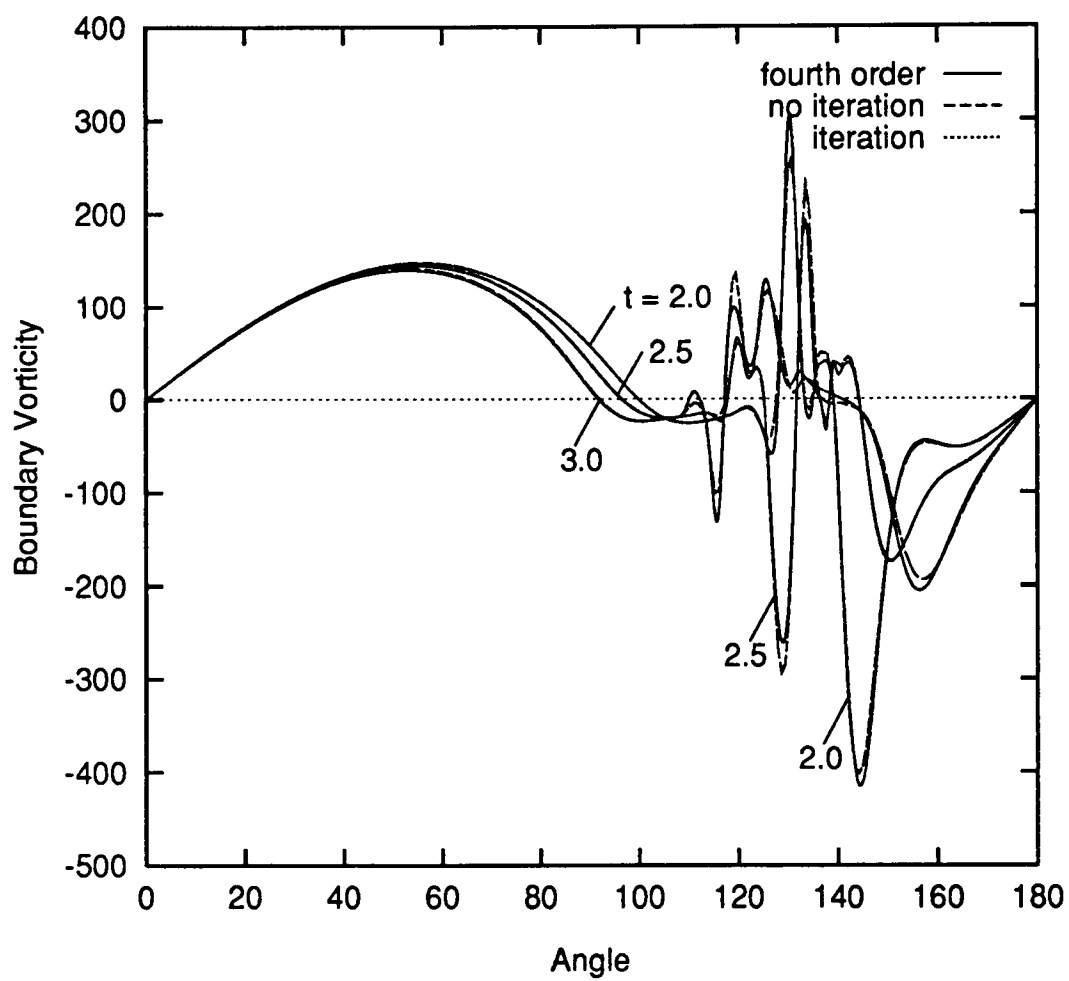


Figure 5.4 (continued).

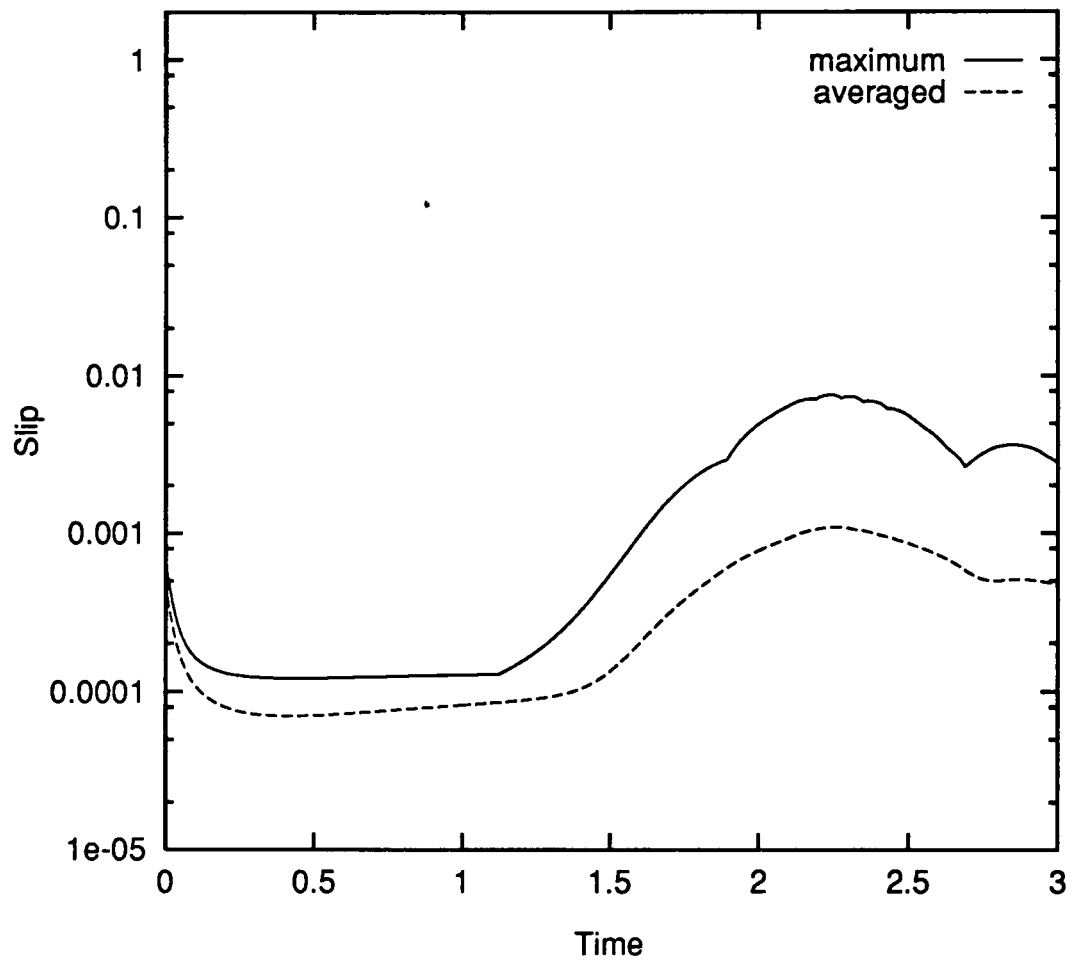


Figure 5.5: The time variation of the maximum and averaged slip velocity. See figure 5.4 for parameters.

there is a high peak in ω_B , the normal gradient near the wall is likely to be very high. Thus reducing Δr near the wall will give better resolution. The other way is to use the iteration method so that the slip can be further reduced and the global coupling is better satisfied. We need to point out, however, that *the slip does not directly relate to the accuracy of ω_B* , although vorticity is created by the no-slip condition (recall that ω_B is the space-time integrated effect of σ , see §3.2.2).

We implemented the iterative scheme and let the averaged slip reduce to below 10^{-6} , which is below the discretization error. Only two or three iterations were needed for convergence. The fast convergence of the iterative scheme is mainly because of the weak coupling as discussed in §3.3.2. The result (Fig. 5.4) is almost identical to the non-iterative one. This indicates that for the present high Reynolds number flow the (ω, p) coupling is so weak that the decoupled approximation is good enough, at least in the range of the present second-order accuracy. On the other hand, the second-order method of computing slip might degrade the effectiveness of the iteration. Note that the slip is most influenced by the vorticity distribution near the wall; when large gradients present in that region, the slip could be difficult to compute accurately even by the second-order method. To make the iteration more beneficial, therefore, higher-order methods might be needed for computing the slip. Examples of these methods, but in different contexts, include that by Ta Phuoc Loc and Bouard [104] who used a compact fourth-order scheme to compute the stream-function and velocity, and by AR [96] who tested a hybrid-scheme with higher-order computation of both u_s and ω_B .

Now, we reduce Δr close to the wall by choosing the strain parameter $a = -0.9$ ($\Delta r_B = 0.00124$) and use two different Δt s, i.e. 0.001 and 0.01. The results for ω_B (without iteration) are shown in Fig. 5.6. Compare to Fig. 5.4, the improvement in the peak values of ω_B is obvious. The influence of Δt is also shown in the figure, which turns out to be small. It seems that the time accuracy is not crucial in the present early-stage computation.

Figure 5.7 shows a comparison of the slip variation with different time steps (no iteration). It clearly indicates that the residual slip after the diffusion substep is proportional to Δt . Recall that the first estimate of $\bar{P}$ is just the

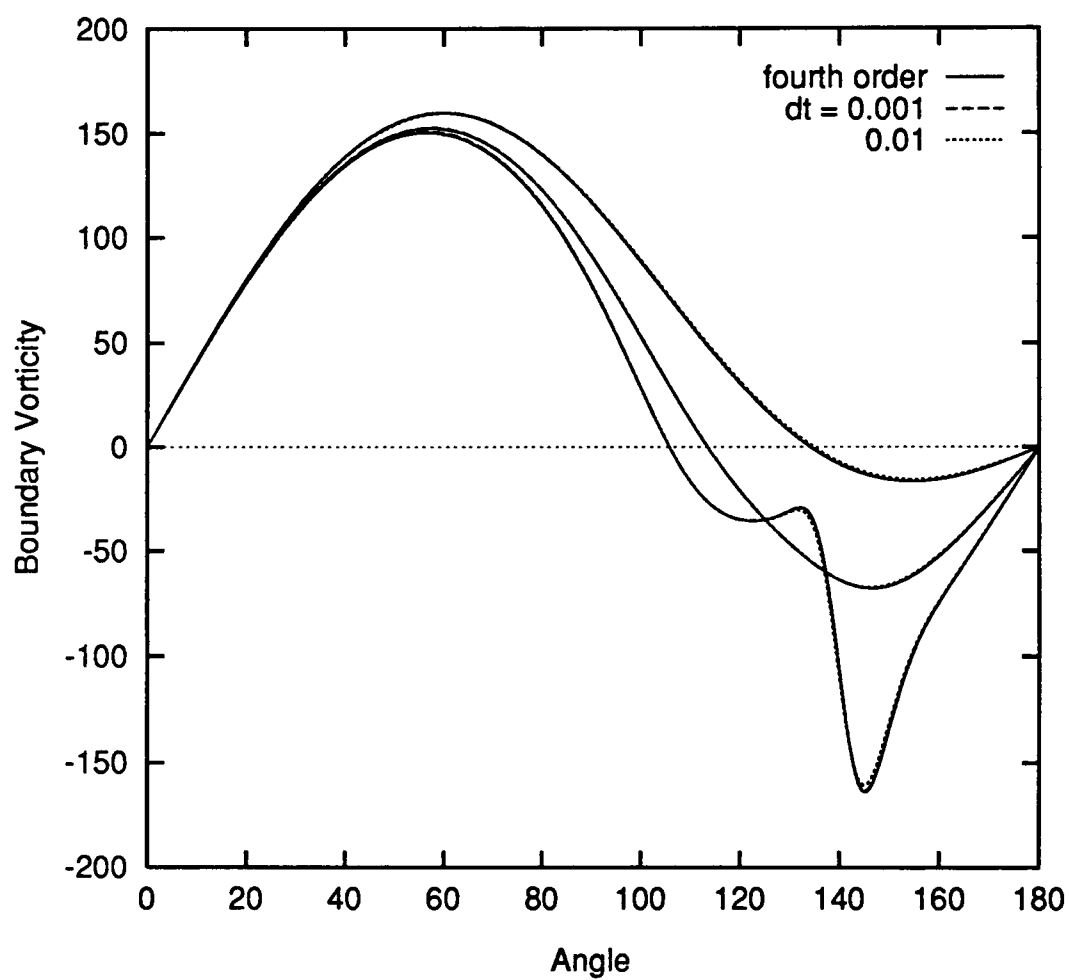


Figure 5.6: As figure Fig. 5.4; $a = -0.9$ and $\Delta t = 0.001, 0.01$.

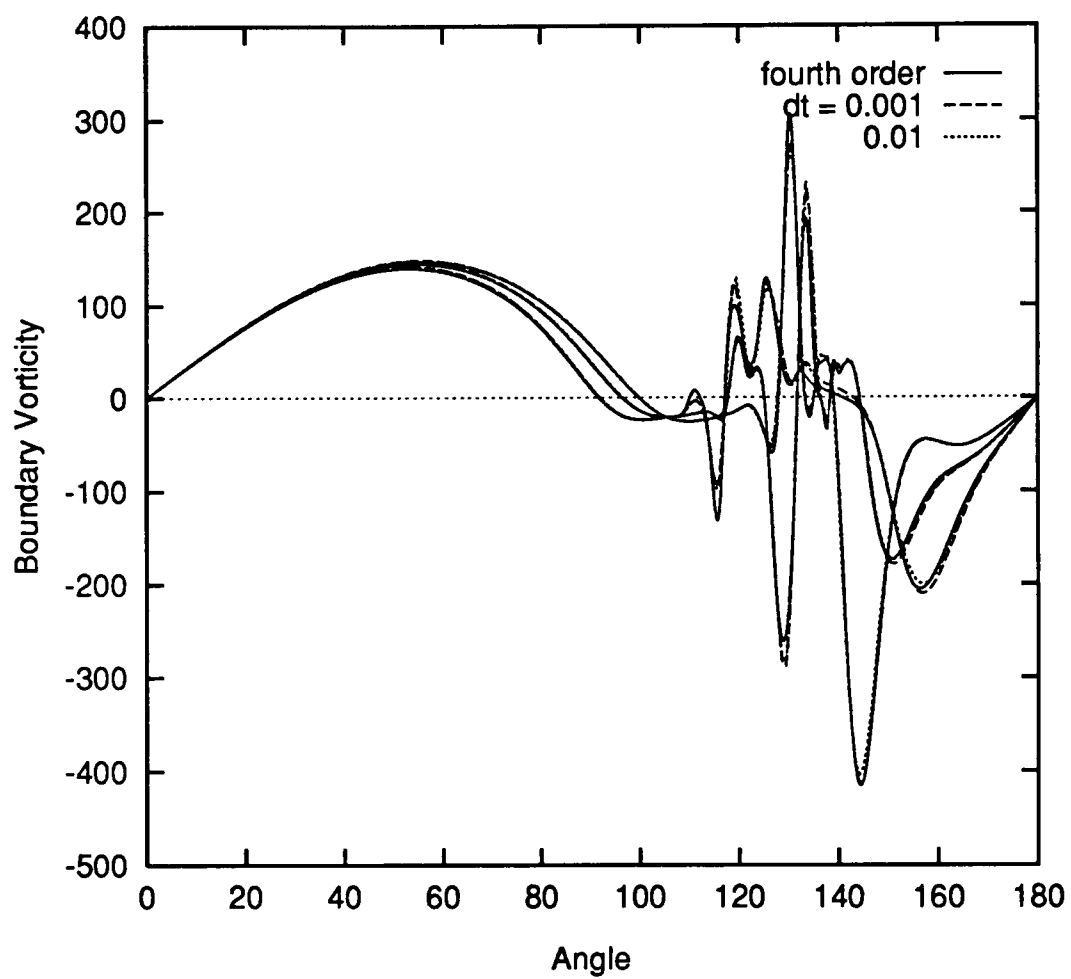


Figure 5.6 (continued).

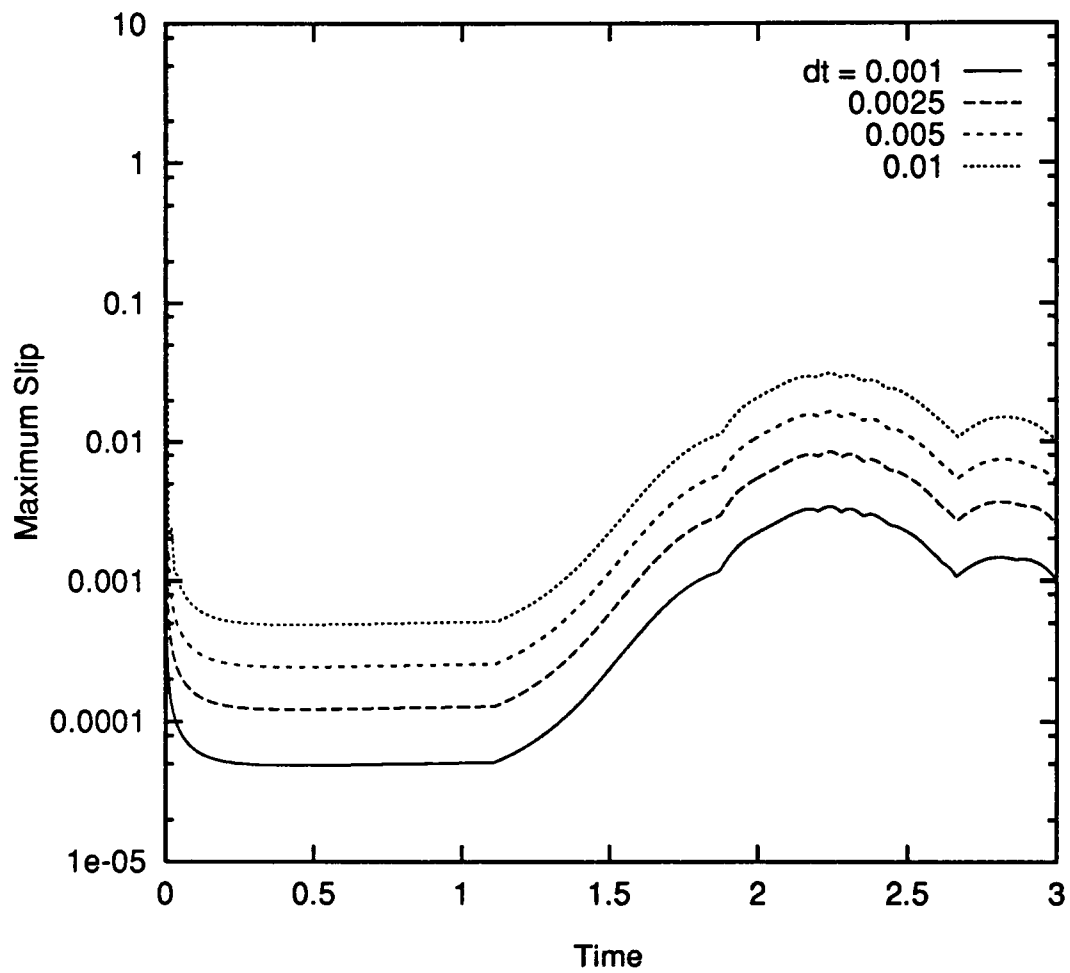


Figure 5.7: Effect of Δt on the maximum slip. See figure 5.6 for the parameters of the grid.

ratio of this residual slip to Δt (Eq. (5.18)), therefore, $\bar{P}$, and whence the error introduced by dropping $\bar{P}$, is *independent* of Δt , which is physically correct. This error should depend mainly on the Reynolds number as discussed in §3.3. Similar Δt -independence holds for the performance of the iterative method. Compare the maximum slip in Fig. 5.5 with the one obtained with $\Delta t = 0.0025$ in Fig. 5.7, we see very similar slip variation. In fact, our numerical experiments showed that the magnitude of slip has little dependence on the grid sizes.

In order to further confirm the estimate (3.38), a group of tests were performed with fixed Δt to check the dependence of the residual slip, and hence $\bar{P}$, on Re . We define the reduction factor of the slip by

$$f_R = u_s^{n+1} / u_s^{n+\frac{1}{2}},$$

where $u_s^{n+\frac{1}{2}}$ and u_s^{n+1} are the slip after the convection and diffusion substeps, respectively. Evidently f_R also represents the ratio between p_1 and p_2 , or the inverse of the strength of (ω, p) coupling. To determine the variation of f_R with Re , we define the index of f_R as

$$I_R = \frac{\ln(f_{R2}/f_{R1})}{\ln(Re_2/Re_1)}.$$

According to (3.38), I_R should be about 0.5. To compute I_R , we need to compare two flows with different Re . This is done carefully by choosing Re_1 and Re_2 close enough (10% difference) so that the flows do not differ qualitatively. We use the averaged slip for calculating f_R and I_R because it reflects the global character of the flow. Table 5.1 clearly confirms the predicted value 0.5 especially as Re becomes higher. It also presents the L_2 -norm relative error in $\omega_B(E)$ of the decoupled scheme compared to the fully coupled one using iteration. The index of this error I_E is similarly defined as I_R and also has a similar trend. Another indication of the strength of (ω, p) coupling is the number of iterations required to achieve convergence in u_s . As expected, more iterations were needed for lower Re in our tests. A test with $Re = 9500$ shows that (3.38) is valid for smoothly separated flow, which corresponds to the “flat” part of the averaged slip in Fig. 5.5. As the flow becomes more complicated and the slip rises, the estimate becomes invalid

Table 5.1: Variation of decoupling error with Re

Re	f_R	I_R	E	I_E
10	1.552	0.359	5.093e-3	-0.398
100	4.226	0.475	1.992e-3	-0.423
1000	12.94	0.497	7.104e-4	-0.459
10000	37.49	0.508	2.659e-4	-0.466

Note: Results are obtained with $\Delta t = 0.01$ at $t = 1$.

Table 5.2: L_2 -norm of relative error in boundary vorticity due to decoupling for $Re = 9500$ flows

Time	0.5	1.0	1.5	2.0	2.5	3.0
Error	6.200e-5	6.171e-5	1.773e-4	1.607e-3	1.985e-3	1.577e-3

Note: See legend of Fig. 5.4 for parameter of the computation.

and the error of decoupling is larger. In Table 5.2 we show the error in boundary vorticity at different time. More importantly, we found that both f_R and hence the error in ω_B due to decoupling seem to be *independent* of grid size when the flow is well resolved. This would imply that the present fractional-step decoupled scheme is not suitable for pursuing very-high-resolution computations. On the other hand, for fixed-precision simulations in practice, the method could be very useful as long as the decoupling error is smaller than the discretization error. For example, the largest decoupling error in Table 5.2 would be well acceptable if the required precision is 1%. Amazingly, even at $Re = 10$, about the lowest Reynolds number of most practical interest, the decoupling error might be considered as still sufficiently small. It is not feasible to give a criterion for whether a decoupled scheme can be used in general, but one can always find it out by comparing the decoupled result to fully coupled one using the efficient iteration scheme described above.

A similar test on the influence of time step on residual slip was performed

for the second-order splitting method. The result shows that the slip is again proportional to Δt although lower than that of the first-order splitting for same Δt .

Therefore, we summarize that the present decoupled scheme with dynamic condition is capable of capturing the fine vortex structures of high Re flow, while it can also be used for flow with Re as low as 10. The accuracy of short time simulation depends solely on the grid size, especially in the near-wall and separation regions.

In the present computation, the boundary vorticity flux σ is directly affected by the accuracy of computing the slip, and hence so is the pressure solution as it is computed by integrating the flux. Therefore, again, higher-order methods of computing the slip is desirable.

Our results also clearly indicates the importance of choosing r_∞ . For $r_\infty = 5$, although reducing Δr_B leads to better ω_B (Fig. 5.6), it does not improve p_B significantly or might be even worse for separating flow. But with the same Δr_B , using $r_\infty = 20$ leads to a much better result, see Fig. 5.8. It is interesting to note that the difference in σ due to different r_∞ is much less significant than that in p_B , especially when Δr_B keeps the same (Fig. 5.9). Figure 5.10 shows the C_D variation. For the attached flow where friction drag is dominant, smaller Δr_B makes the result more accurate due to improving ω_B . When complicated flow separation occurs and large vortex structure forms behind the cylinder, the pressure drag is dominant and r_∞ becomes an important factor in determining the accuracy of C_D . Note that the result in Fig. 5.10 was not expected to converge because the number of grid points was kept the same although Δr_B are different. This explains the apparent difference between our result and that of AR.

In Fig. 5.11, we compare the wake velocity on the symmetry plane behind the cylinder with the fourth order solution. The Δr_B effect is not as significant as that in other figures. Note that the relatively large error of the result computed with $\Delta\theta = 0.0245$ shows that the flow is too under-resolved. The r_∞ effect is clearly seen again at $t = 3$. From this figure, and the above observation, we conclude that, if only the simplest treatment of the far field condition like ours is

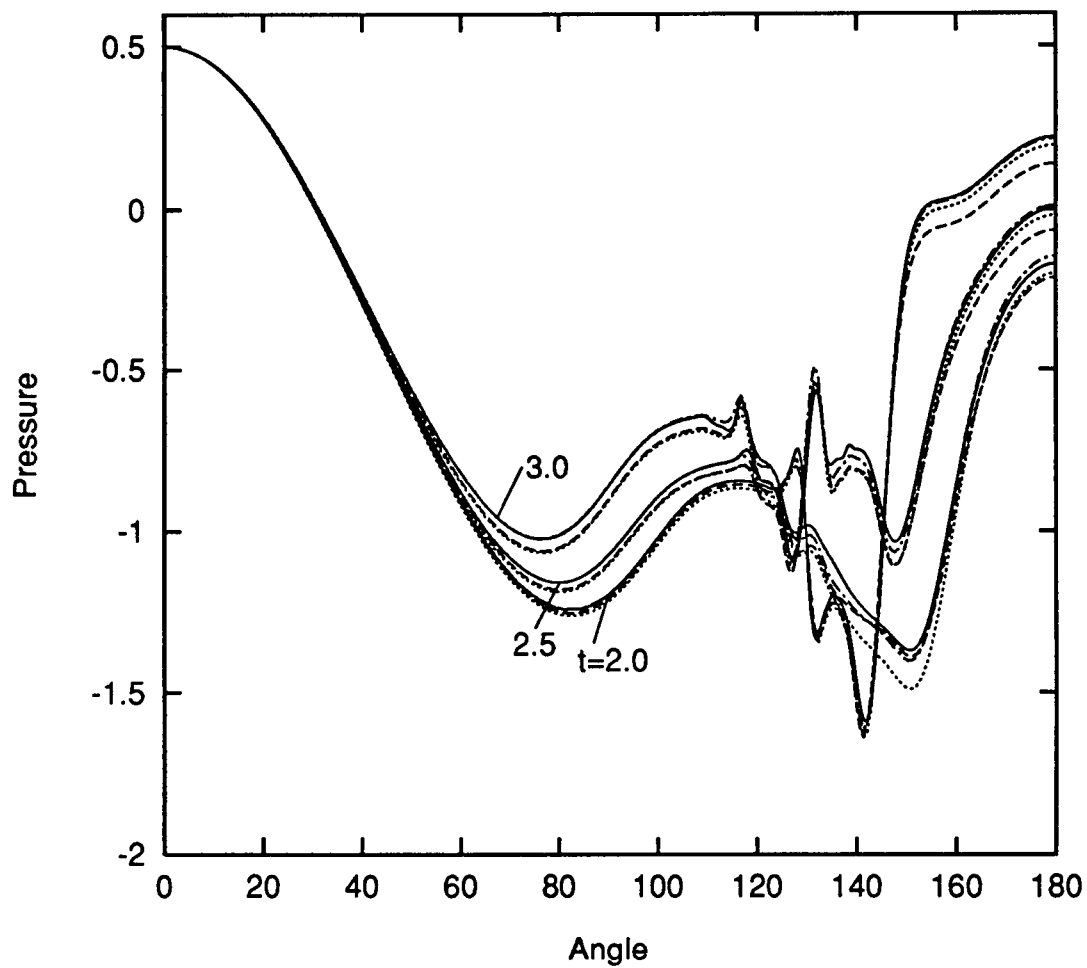


Figure 5.8: Pressure solution with different Δr_B and r_∞ compared to the fourth-order result. — AR's fourth-order solution; --- $\Delta r_B = 0.0037$, $r_\infty = 5$; $\Delta r_B = 0.002$, $r_\infty = 5$; - - - $\Delta r_B = 0.002$, $r_\infty = 20$.

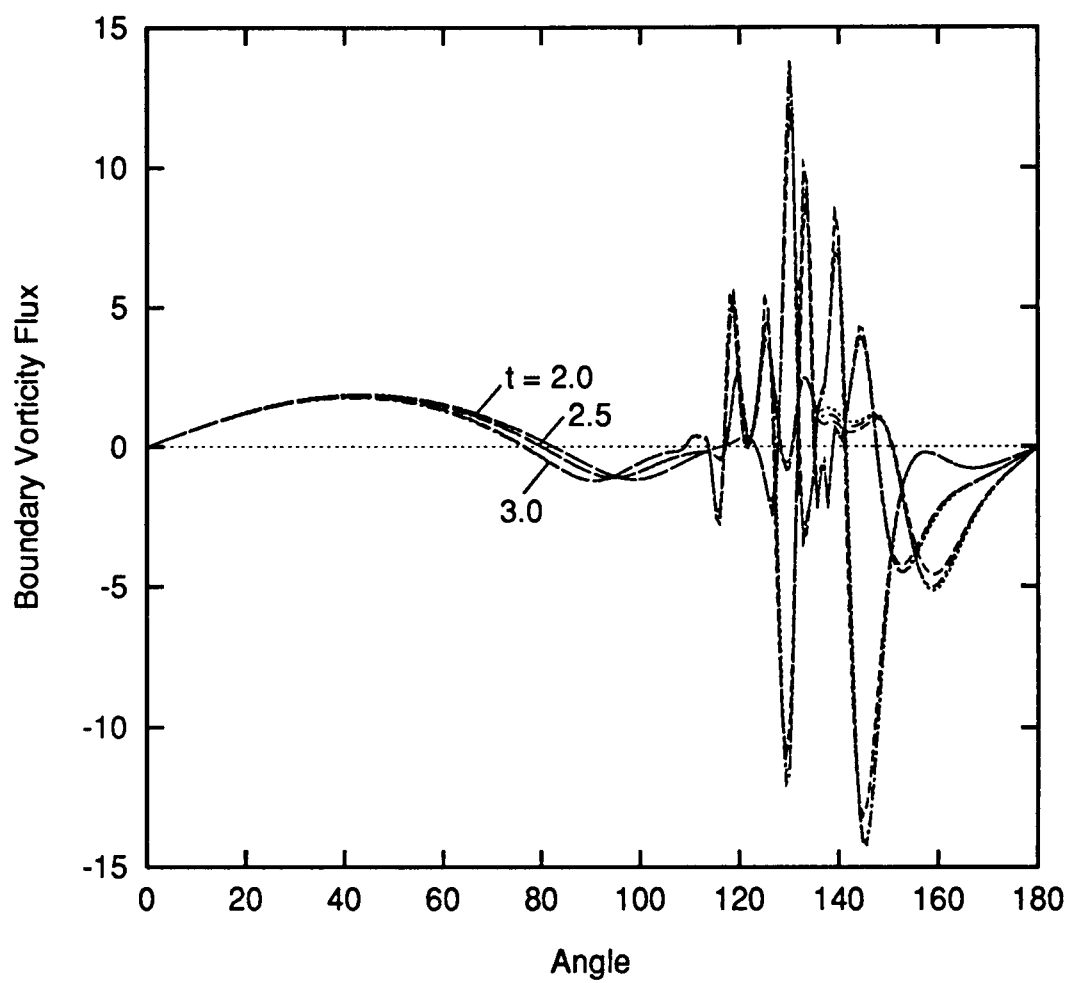


Figure 5.9: Solution of boundary vorticity flux with different Δr_B and r_∞ . For notation of curves see figure 5.8.

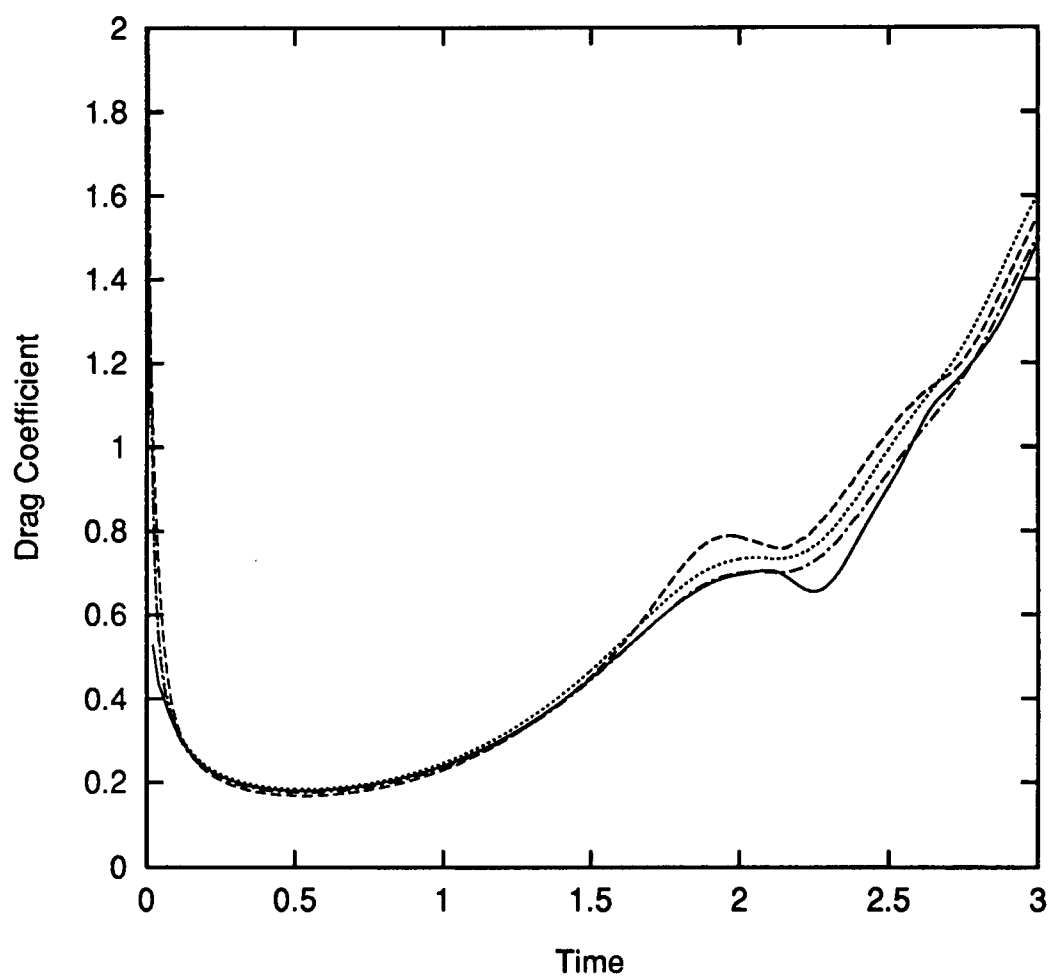


Figure 5.10: Drag coefficient with different Δr_B and r_∞ compared to AR's fourth-order result; $Re = 9500$. For notation of curves see figure 5.8.

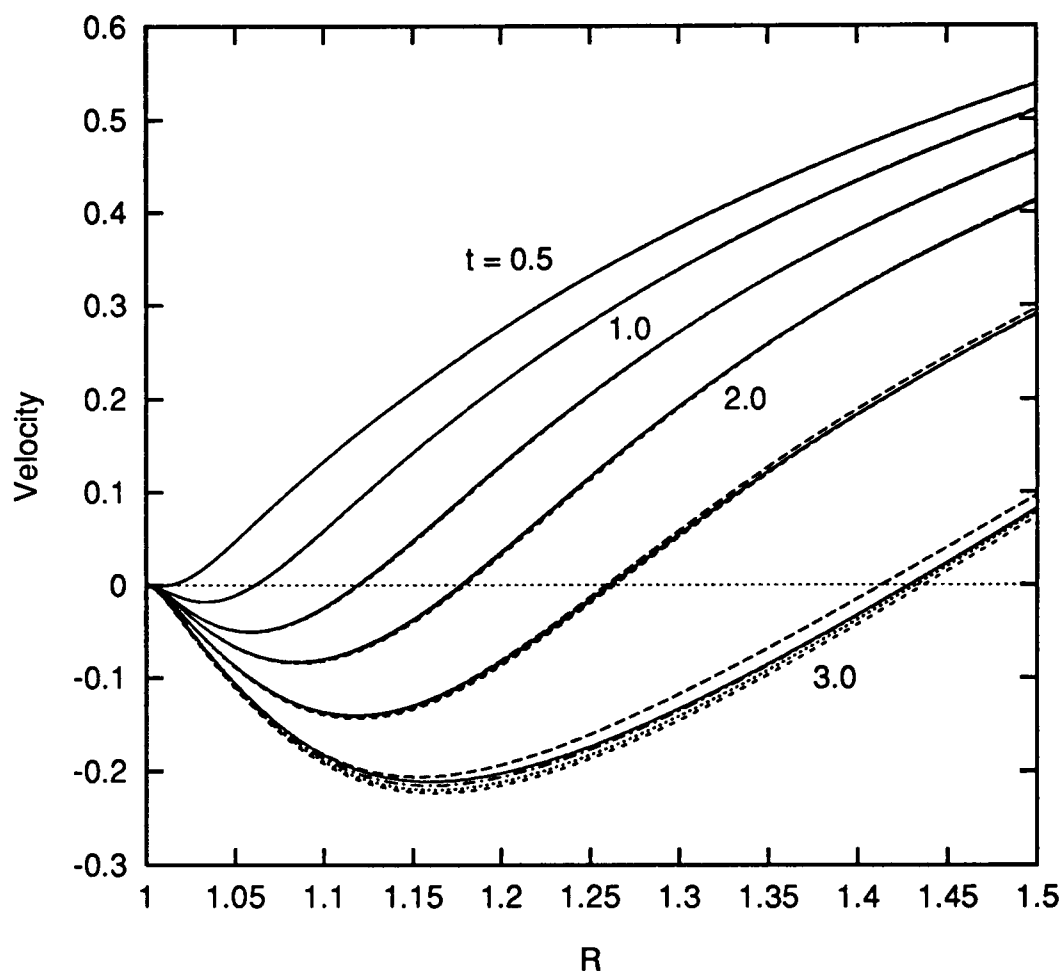


Figure 5.11: Wake velocity on the symmetry plane obtained with different grid sizes compared to the fourth-order result. — AR's fourth-order solution; --- $\Delta r_B = 0.0037$, $\Delta\theta = 0.0245$, $r_\infty = 5$; - - - $\Delta r_B = 0.0037$, $\Delta\theta = 0.0123$, $r_\infty = 5$; $\Delta r_B = 0.002$, $\Delta\theta = 0.0123$, $r_\infty = 5$; - · - · - $\Delta r_B = 0.002$, $\Delta\theta = 0.0123$, $r_\infty = 20$.

to be used, choosing r_∞ far enough from the cylinder is important even for the early stage computation of a high Reynolds number flow.

5.4.2 More Results and Comparisons

In this subsection, we present more numerical results, including those obtained from the second-order splitting scheme and the non-splitting schemes with dynamic and kinematic vorticity BCs. We shall compare the accuracy of different schemes and observe the effect of modifying the vorticity distribution according to (5.14), and we are also interested in the variation of residual slip with Δt for the second-order splitting scheme and the non-splitting one with dynamic BC.

To compare the accuracy among different schemes, we compute $Re = 1000$ flow with three different grids (see Table 5.3 below), where $r_\infty = 10.0$ and $a = -0.715$. The choice of a is made to give Δr_B close to that of AR, when the same number of grid in r direction is used. Therefore, our grid has about the same resolution as theirs near the boundary, but worse away from it because of grid stretching. The results of boundary vorticity at $t = 1.5$ are compared with AR's fourth order solution on a 512×128 grid. For comparison, the error obtained by AR using fourth-order, second-order, and hybrid schemes are listed in Table 5.4. It should be noted that AR computed the error by comparing to the fourth order result on a 1024×256 grid. However, as seen from Table 5.4, our comparison is still valid. Except for the first scheme in Table 5.3, all other schemes use (5.14) to modified the vorticity distribution when there is a slip on the boundary (except before the diffusion substep of the splitting scheme). From the table, it is seen that all schemes have about the same accuracy and using (5.14) does not necessarily increase the accuracy of the results. Moreover, the two non-splitting schemes have almost identical results. All results in Table 5.3 are more accurate than the second-order and hybrid schemes of [105], which is quite interesting. We need to be careful, though, to extrapolate this observation to finer grids because the convergence of the schemes in Table 5.4 seem to be faster than ours. It is reasonable to believe

Table 5.3: Relative error of boundary vorticity for $Re = 1000$ flows compared to AR's fourth-order results

		Schemes				
grid size	Δt	A	B	C	D	E
L_2 norm						
64×33	0.02	0.0500	0.0487	0.0457	0.0533	0.0533
128×64	0.01	0.0132	0.0185	0.0101	0.0104	0.0104
256×128	0.005	0.0045	0.0051	0.0031	0.0034	0.0034
Max norm						
64×33	0.02	0.0664	0.0607	0.0589	0.0640	0.0640
128×64	0.01	0.0235	0.0198	0.0158	0.0169	0.0168
256×128	0.005	0.0069	0.0076	0.0047	0.0045	0.0045

Note: Schemes are (A) first-order splitting (without modified initial vorticity), (B) first-order splitting, (C) second-order splitting, (D) non-splitting scheme with dynamic BC, and (E) non-splitting scheme with dynamic BC.

Table 5.4: L_2 norm of relative error of boundary vorticity for $Re = 1000$ flows¹

grid size	fourth order	second order	hybrid
128×33	0.116	0.237	0.145
256×64	0.0093	0.071	0.025
512×128	0.00039	0.019	0.006

1. Source: C. R. Anderson and M. B. Reider. A high order explicit method for the computation of flow about a circular cylinder, to appear in *J. Comput. Phys.*

that the error listed above also reflects the error of vorticity in the interior of the domain. Table 5.3 also indicates that the non-splitting methods converge to second order in max norm.

As seen in the last subsection that when dynamic BC is used, the residual slip contains information of the flow development. By examining slip variation with Δt , we may also have an estimate of the time accuracy of the scheme, which is difficult to obtain here by using traditional tests (such as those in Chapter 4) here. In Fig. 5.12, the residual slips computed from the operator-splitting schemes with different time steps and grid sizes (see Table 5.3) are shown. The slip curves of both splitting schemes look almost identical except that the second-order splitting gives smaller slips for the same Δt . However, in both cases, the slips converge only in first order. Therefore, second-order splitting scheme we tested should actually be only first order accurate in time. This is not surprising if we consider the fact that the procedure applied to solve the second diffusion substep ($H(\Delta t/2)$ after $E(\Delta t)$) is exactly the same as in first-order splitting, thus the error are of the same type. It is anticipated that to gain higher order accuracy, the local dynamic BC should be used with iteration to retain the ω - p coupling.

For the non-splitting scheme with dynamic BC, the slip curves are presented in Fig. 5.13. The distinct feature here is the second order convergence of slip with respect to Δt , as expected by previous analysis, and that the slips are much smaller than those of the splitting schemes. Therefore, the error due to slip is negligible and hence no iteration would be needed. This also explains why the result of using dynamic BC is so close to that using kinematic BC, which satisfies the no-slip condition exactly in the sense that there are no other error in the boundary velocity except truncation. Another notable feature of the curves are the small wiggles on the curves for larger Δt . This is indeed the effect of grid size, especially Δr near the wall, rather than the time step. In this computation, the ratio of grid size to Δt was fixed, so larger Δt corresponds to larger Δr . The wiggles disappear when Δr is sufficiently small.

In both Figs. 5.12 and 5.13, the trend of the curves are rather independent of the grid size and time step. However, the trend for splitting and non-splitting

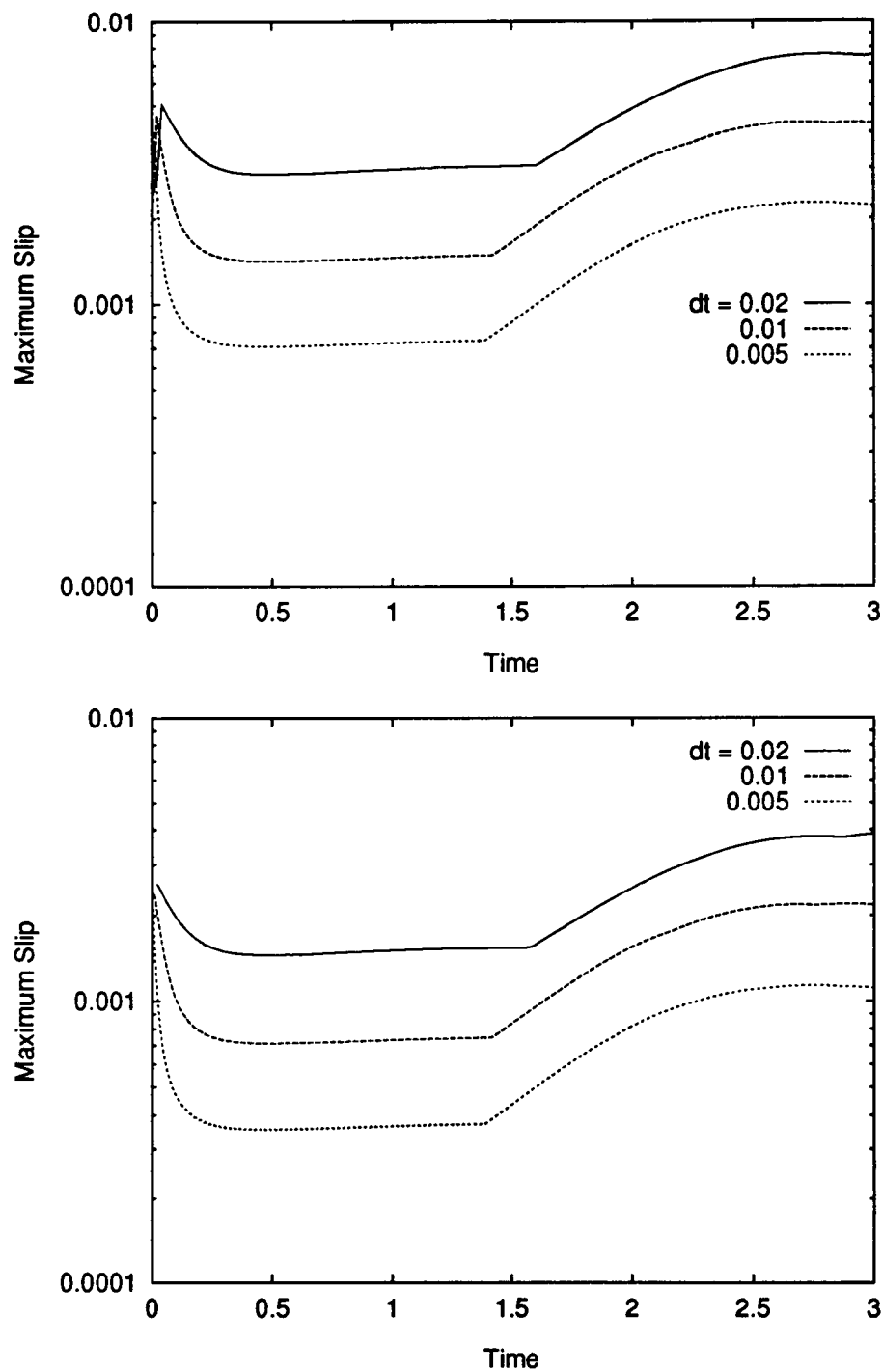


Figure 5.12: Residual slip computed using the operator-splitting schemes for $Re = 1000$ flows. Top: first-order splitting; bottom: second-order splitting.

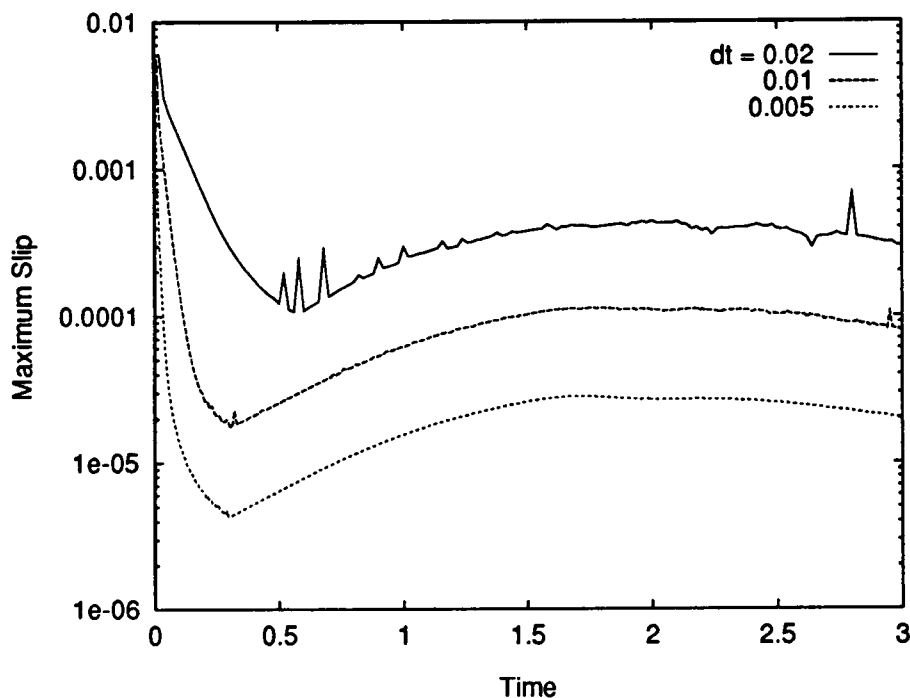


Figure 5.13: Residual slip computed using the non-splitting scheme for $Re = 1000$ flows.

schemes are different. This can be attributed to the different responses of the schemes to the physical development of the flow field. For the splitting schemes, like the case of $Re = 9500$, the rise of slip occurs at the time when the secondary vortex starts to form, as can be seen clearly from Fig. 5.14. We note that for $\Delta t = 0.02$, the rise is a little bit late, which is due to the larger Δt and the coarser grid that cannot well resolve the secondary vortex at the time it is forming. The slip of the non-splitting scheme is insensitive to the formation of the secondary vortex; however, the abrupt turn of the curve at about $t = 0.3$ is a clear response to the formation of the primary separation, as shown in Fig. 5.15.

When dynamic BC is used, the drag coefficient can be conveniently computed from ω_B and σ . But if the kinematic BC is used, it is very crucial to obtain accurate values of σ from the solution of vorticity. The obvious way is to use one-sided finite differences at the boundary. However, since the vorticity is likely to have large normal gradients, we find that the one-sided differences are not always

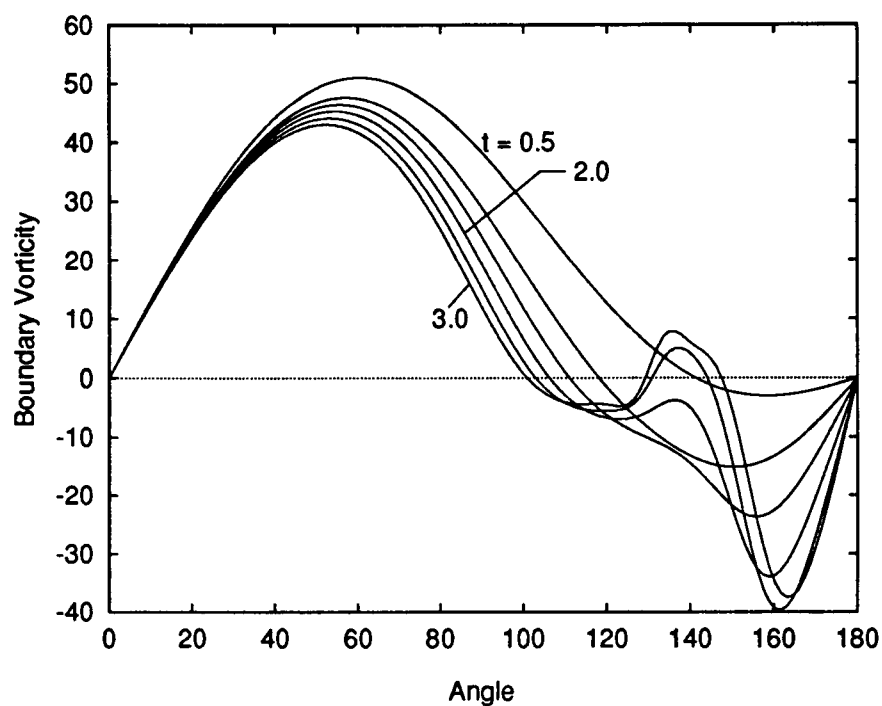


Figure 5.14: Boundary vorticity for $Re = 1000$ flows at different time.

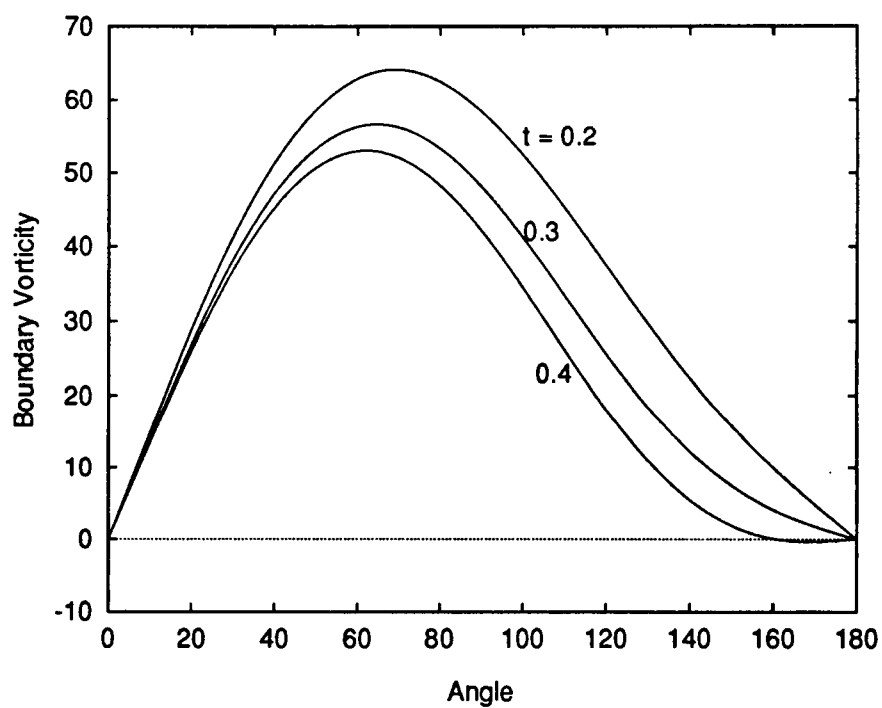


Figure 5.15: Boundary vorticity for $Re = 1000$ flows before and after the primary separation.

satisfactory, especially when the flow is not very well resolved. To obtain resolution, we approximate the normal gradient by central difference at the solid surface, and incorporate this approximation into the dynamic process of the variation of the boundary vorticity. More specifically, we assume that ω_B is obtained from the dynamic scheme (5.20), where the diffusion term and the normal gradient of ω are approximated by central differences instead of the kinematic one as it really is. Then, using the known value of ω_B we solve for σ . This approach is compared with the second- and third-order one-sided differences in Fig. 5.16. The dynamic approach with central difference is obviously superior to the one-sided differences. Not only is it more accurate, but also it converges faster to the fully resolved solution of [105]. We note that this method gives almost identical drag coefficients as those computed from the non-splitting scheme with dynamic BC. The figure also shows that higher order does not mean more accuracy. In fact, the third-order finite difference gives the worst and even non-physical results.

The second-order splitting and non-splitting schemes are also used to compute $Re = 9500$ flows. Since the results are not significantly more accurate than those already presented, they are not included here. The observation made in this subsection are valid for higher Re flows, except that the flow is more complicated because of more secondary vortices, so the slip due to using the dynamic BC varies in a more complicated fashion.

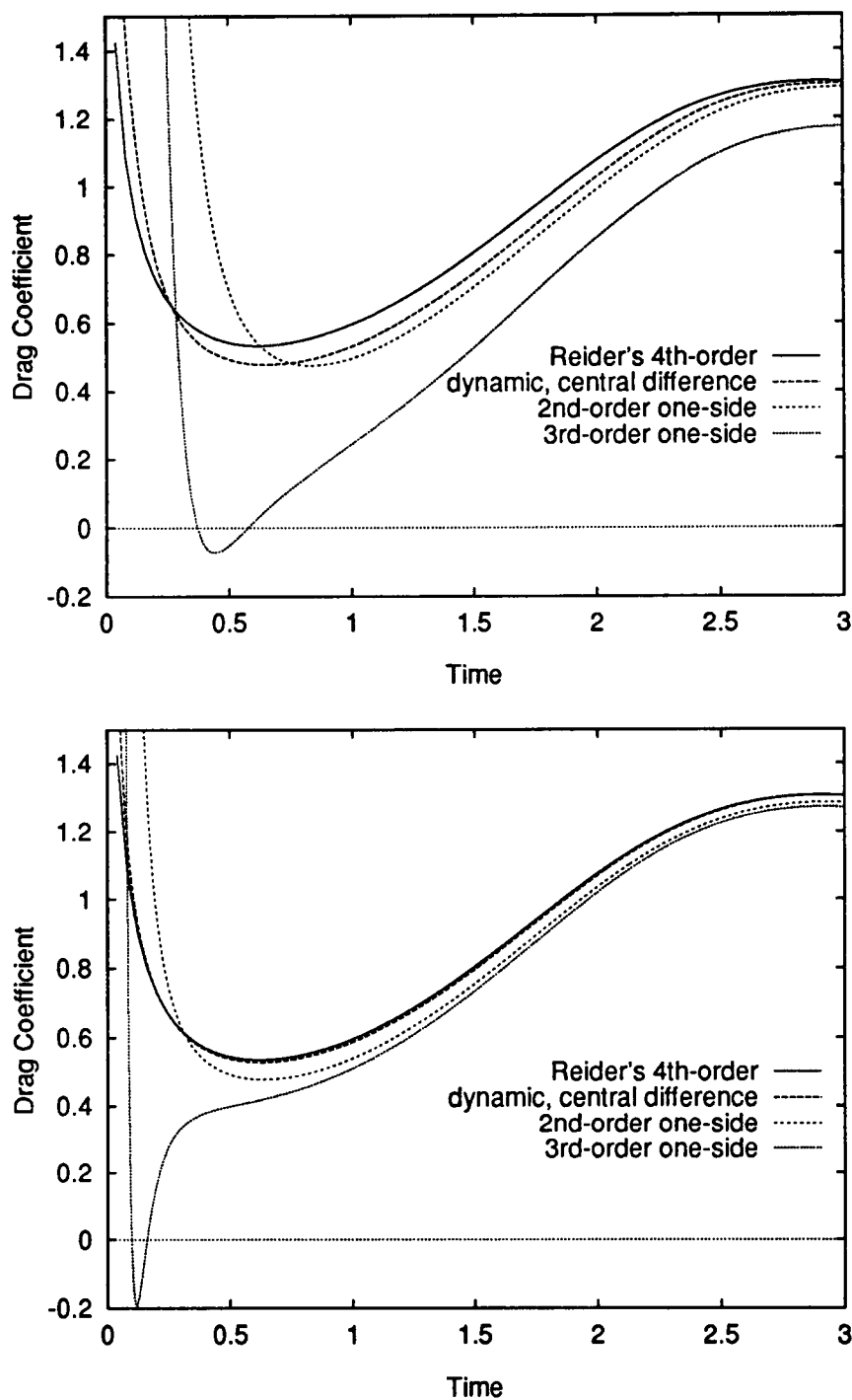


Figure 5.16: Drag coefficients for $Re = 1000$ flows computed with $r_\infty = 40.0$ and $a = -0.75$. Top: results of 128×64 grid; bottom: results of 256×128 grid.

Chapter 6

Vorticity-Velocity Formulation

As discussed in the introduction, the ω - ψ method, although convenient for solving 2-D problems, are not easy to be extended to 3-D due to the difficulties in specifying boundary conditions for the vector potential. This chapter is devoted to developing the building blocks of ω - $\mathbf{u}$ method for solving 2-D and 3-D problems. In 2-D cases, compared to ω - ψ formulation, the ω - $\mathbf{u}$ method may seem to cost more computation because two components of $\mathbf{u}$ need to be solved from a vector elliptic type of equation instead of only one scalar function ψ . However, we shall demonstrate that this is not the case if we utilize the theoretical results proved in Chapter 2. Except the method of solving of $\mathbf{u}$, other methods and techniques presented for the ω - ψ method in the last chapter are applicable here.

Two additional problems arise from the ω - $\mathbf{u}$ approach—we need to ensure divergence-free conditions for $\mathbf{u}$ and ω . The first is required by incompressibility; the second, which is automatically satisfied in 2-D, is a result of $\omega = \nabla \times \mathbf{u}$. Note that the two conditions are not interrelated. The divergence-free condition of ω has many consequences of key importance to vortex dynamics; if this condition is not satisfied accurately, then the numerical results could be non-physical. These two conditions cause many numerical problems in the ω - $\mathbf{u}$ methods as mentioned in Chapter 1.

Special discretizations of the vorticity equation and the boundary conditions have been constructed in such a way that the vorticity satisfies the *discrete* divergence-free condition to the round-off level, if the initial vorticity does [33,56]. We call these methods *fully divergence-free*. If only the vorticity equation, but not the boundary conditions, is carefully discretized, the method will be called *divergence-free*, which refers only to the treatment of the interior of the domain. Although constructed differently, the schemes in [56] and [33] are essentially the

same because both of them are based on the second-order central difference. In this chapter, we present a unified and general approach of constructing fully divergence-free schemes, which is independent of any particular difference method.

On the other hand, the fully divergence-free scheme may not be the best choice, or may be even impossible to construct due to various numerical considerations. The projection type of approach, like that of [39], is much more flexible in this regard, because there are no constraints on the discretization of vorticity equations and the boundary conditions. However, the method given in [39] requires solving an additional Poisson equation which makes the projection inefficient. In addition, the projection is not unique; one should project the vorticity solution with minimum loss of physical information. Here, based on the mathematical study of Chapter 2, we develop a new and very efficient method of solving $\mathbf{u}$ from ω ; its by-product is an optimum projection which can be performed at almost no cost.

Another objective of this chapter is to extend the implementation of dynamic vorticity BCs to 3-D; we shall only consider the non-splitting method. The extension is straightforward, except that in 3-D we need to take care of the normal vorticity condition which is absent in 2-D.

For the purpose of demonstration and comparison, the 2-D and 3-D lid-driven cavity flows are solved. In 3-D, both divergence-free and projection methods are used. The geometry of the selected problem is simple while the flows exhibit interesting vortical structures especially at relatively high Reynolds number. Both steady and unsteady problems are computed and compared with existing numerical solutions and experiments. We shall concentrate on discussing the 3-D methods here, the 2-D methods are just simplifications.

6.1 The ω - $\mathbf{u}$ Formulation

Consider a lid-driven flow inside a rectangular cavity (Fig. 6.1). We are interested in solving

$$(6.1a) \quad \frac{\partial \omega}{\partial t} + \nabla \cdot (\mathbf{u}\omega - \omega\mathbf{u}) = \nu \Delta \omega, \quad \text{in } V,$$

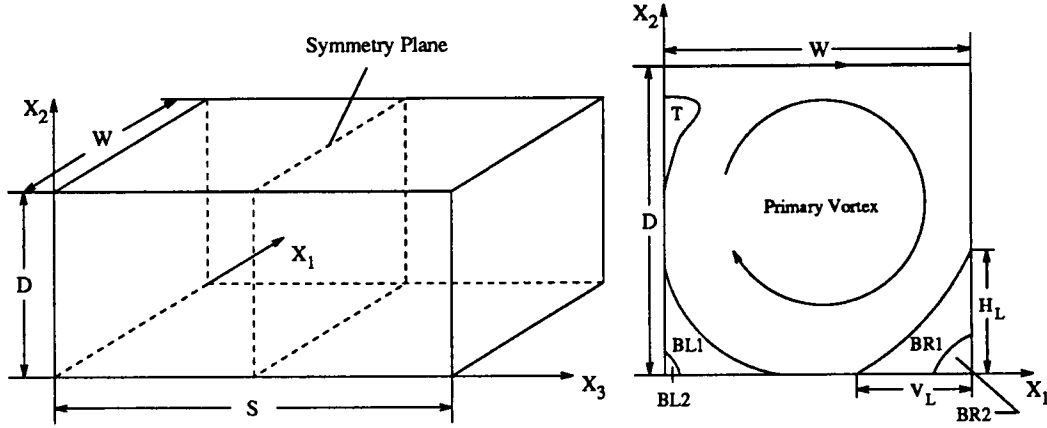


Figure 6.1: The lid-driven cavity flow. Left: Three-dimensional configuration. Right: Vortex structures of two-dimensional flow, follow [106].

where V is the interior of the cavity, and the kinematic equations

$$(6.1b,c) \quad \nabla \cdot \mathbf{u} = 0, \quad \nabla \times \mathbf{u} = \boldsymbol{\omega}, \quad \text{in } V,$$

with boundary conditions

$$(6.1d,e) \quad \mathbf{n} \cdot \mathbf{u} = \mathbf{n} \cdot \mathbf{b} \quad \text{and} \quad \mathbf{n} \times \mathbf{u} = \mathbf{n} \times \mathbf{b} \quad \text{on } \partial V.$$

The compatibility conditions

$$(6.1f,g) \quad \int_{\partial V} \mathbf{n} \cdot \mathbf{u} dS = 0 \quad \text{and} \quad \nabla \cdot \boldsymbol{\omega} = 0$$

should also be satisfied. For the present problem, Eq. (6.1f) is guaranteed by (6.1d) because $\mathbf{n} \cdot \mathbf{b} = 0$; while securing Eq. (6.1g) is one of the main subject of this chapter.

Theoretically, if the whole set of equations and boundary conditions in (6.1) are solved together, then both (6.1b) and (6.1g) are satisfied. However, as mentioned in the introduction, such a coupled method is not efficient for unsteady flows. Therefore, we consider solving (6.1a) and (6.1b,c) separately. Note that the normal velocity condition (6.1d) should be used with the kinematic equations, while the no-slip condition (6.1e) is the constraint on the vorticity equation.

As discussed in Chapter 2, there are several methods of solving the kinematic equations (6.1b,c) with boundary condition (6.1d). Among them, we prefer to use the alternative formulation

$$(6.2a) \quad \Delta \mathbf{u} = -\nabla \times \boldsymbol{\omega}, \quad \text{in } V,$$

$$(6.2b,c) \quad \mathbf{n} \cdot \mathbf{u} = 0, \quad \mathbf{n} \times (\nabla \times \mathbf{u}) = \mathbf{n} \times \boldsymbol{\omega}, \quad \text{on } \partial V.$$

because of several advantages. From Theorem 2.1.1 and §2.3, we first know that when $\mathbf{u}$ is solved from (6.2), it is automatically divergence-free. Second, the curl of $\mathbf{u}$ is nothing but the orthogonal and optimum projection of $\boldsymbol{\omega}$ onto the divergence-free space. Therefore, in the computation, the projection can be performed by taking numerical differentiation of velocity at little cost *after* $\mathbf{u}$ is solved. Furthermore, because (6.1b) is ensured, we need only to solve *two* components of $\mathbf{u}$ from two scalar Poisson equations instead of three; the third component can be integrated directly from (6.1b). Therefore, our method is about 30% faster than other methods solving three Poisson equations. In 2-D, only one Poisson equation needs to be solved, thus the amount of computation is the same as the ω - ψ approach. In fact, the two 2-D formulations can be made identical algebraically by discretizing (6.2) on a staggered grid (Fig. 6.3). Compared to the present approach, the direct solution of (6.1b,c) needs (6.1g) to hold in the first place, for otherwise there is no solution. Thus, either $\boldsymbol{\omega}$ has to be solved from a fully divergence-free scheme or it has to be projected onto the divergence-free space first. The projection, however, can only be done by solving an extra Poisson equation. Later we shall see that, in some cases, the projection may be desirable even when a fully divergence-free scheme is used.

6.2 Solving Velocity from the Kinematic Equations

At the first sight, it might seem to be straightforward to discretize (6.2) and solve the resulting linear system of equations. But indeed an arbitrary discretization of (6.2) might *not* behave as predicted by the theory. This is a rather particular and fundamental problem for ω - $\mathbf{u}$ methods. As a simple example, we

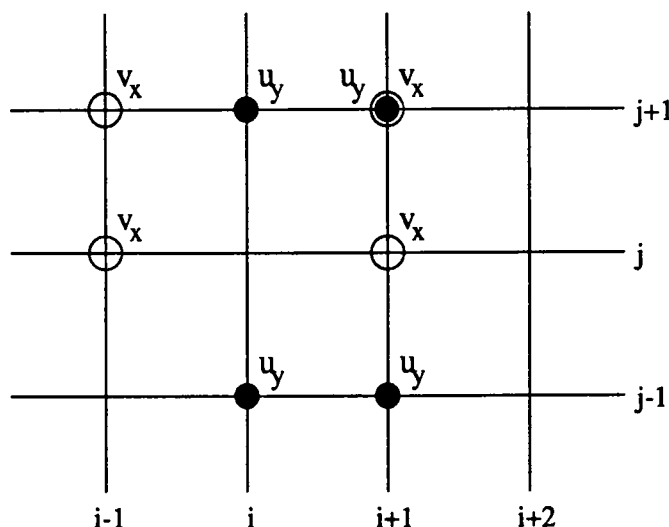


Figure 6.2: Grid point used by $(v_x)_{ij}$ (circles) and $(u_y)_{ij}$ (black dots).

know that the curl of the gradient of a scalar function should be *identically zero*. Assume that the gradient of a 2-D function ϕ is computed using forward difference as

$$\nabla^h \phi_{ij} = (u_{ij}, v_{ij}) = \left(\frac{\phi_{i+1,j} - \phi_{i,j}}{h}, \frac{\phi_{i,j+1} - \phi_{i,j}}{h} \right),$$

on a uniform grid with size h in both i and j directions. Now, we use central difference to compute the curl of $\nabla^h \phi$ as

$$\nabla^h \times \nabla^h \phi_{ij} = (v_x - u_y)_{ij} = \frac{v_{i+1,j} - v_{i-1,j}}{2h} - \frac{u_{i,j+1} - u_{i,j-1}}{2h}.$$

It is easy to check that the right-hand side is not identically zero. As shown in Fig. 6.2, $(v_x)_{ij}$ and $(u_y)_{ij}$ are computed by using different sets of ϕ values and hence they cannot cancel each other, unlike the continuous problem.

This type of problem happens to other vector identities as well, for example, $\nabla \cdot (\nabla \times \mathbf{u}) = 0$. The key of these identities is that the mixed partial derivatives are equal, that is $\phi_{yx} = \phi_{xy}$. However, this important property is not preserved by the definition of above discrete partial differential operations, which are “order dependent.” The resolution is simple—*define the discrete differential operators uniquely*. In the above case, insisting on either central or forward difference gives

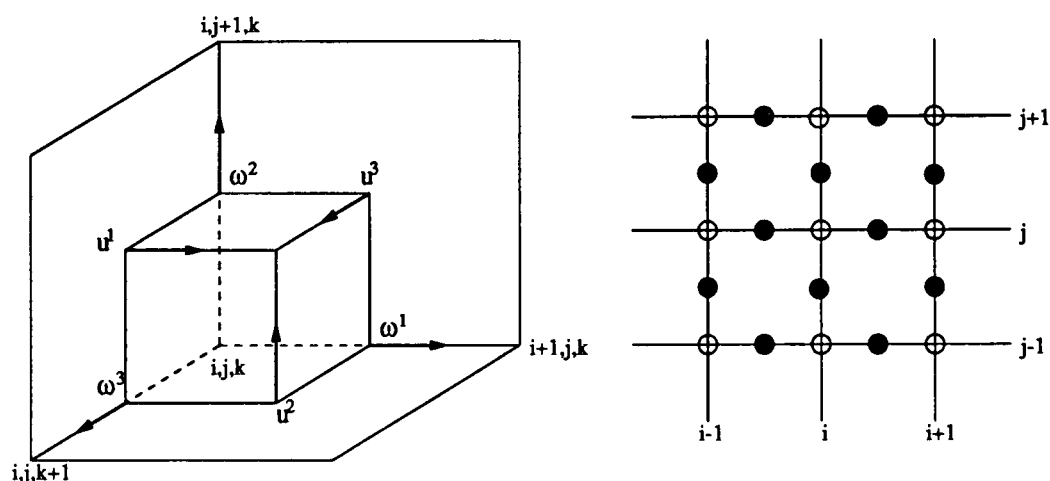


Figure 6.3: The staggered grid for ω - u method. Left: The 3-D grid. Right: The 2-D grid; u^1 , u^2 , and ω^3 are defined on the black, gray, and white dots, respectively.

desired result, namely, the vector identity $\nabla \times \nabla \phi$ is satisfied *identically*. Note that the term “identically” or “exactly” means “within round-off error” for numerical problems. Another necessary condition, which is implicit in the above example, is ϕ being uniquely defined at each spatial points. This condition is not as trivial as it sounds. In many situations, the discrete differential operator uses values that are not on the grids but have to be interpolated from the grid values. A typical example is the calculation of numerical flux in conservative type of schemes for the N-S equation. Then, it is crucial to make sure that the interpolation gives unique values at the same spatial location. As shown in the next section, these two general principles lead directly to the unified method of constructing divergence-free schemes.

The staggered grid, which depicted in Fig. 6.3, is used to discretize (6.2). This grid has proved to be valuable for preserving mass conservation [33, 56]. We have three more advantages here. First, it is easy to impose boundary condition (6.2c) on the staggered grid. Second, the tangential components of ω_B are not used in solving u , which makes it easy to impose the kinematic BCs for vorticity. Furthermore, it is convenient to perform the numerical projection on the staggered grid.

In the following, i , j , and k denote the grid indices along x_1 , x_2 , and x_3 directions; the numeric superscripts denote the direction of a vector components. Thus, according to Fig. 6.3, the velocity components are defined as $u_{i,j+1/2,k+1/2}^1$, $u_{i+1/2,j,k+1/2}^2$, and $u_{i+1/2,j+1/2,k}^3$; the vorticity components are $\omega_{i+1/2,j,k}^1$, $\omega_{i,j+1/2,k}^2$, and $\omega_{i,j,k+1/2}^3$, respectively. Define the discrete gradient operator as

$$(6.3) \quad \nabla^h = (D_1, D_2, D_3) = \left(\frac{\delta_1}{\Delta x_1}, \frac{\delta_2}{\Delta x_2}, \frac{\delta_3}{\Delta x_3} \right),$$

where δ_i and Δx_i ($i = 1, 2, 3$) are the central difference operator and grid sizes in the i th direction, hence $D_1 f_{i,j,k} = (f_{i+1/2,j,k} - f_{i-1/2,j,k})/\Delta x_1$, etc. We shall also use the notation $(D_1 f)_{i,j,k} = D_1 f_{i,j,k}$ to group several operations together. Thus, the velocity and vorticity are related as

$$\begin{aligned} \omega_{i+1/2,j,k}^1 &= (D_2 u^3 - D_3 u^2)_{i+1/2,j,k}, \\ \omega_{i,j+1/2,k}^2 &= (D_3 u^1 - D_1 u^3)_{i,j+1/2,k}, \\ \omega_{i,j,k+1/2}^3 &= (D_1 u^2 - D_2 u^1)_{i,j,k+1/2}, \end{aligned}$$

which is in fact our projection scheme. It is easy to verify that the projected vorticity is divergence-free inside the domain, i.e.

$$(D_1 \omega^1 + D_2 \omega^2 + D_3 \omega^3)_{i,j,k} = 0.$$

The divergence of vorticity on the boundary is determined by the boundary conditions.

Using the above definition, the discretization of (6.2a) in x_1 direction is

$$(6.4a) \quad (D^2 u^1 = D_3 \omega^2 - D_2 \omega^3)_{i,j+1/2,k+1/2},$$

where $D^2 = (D_1^2 + D_2^2 + D_3^2) = \Delta^h$ is the discrete Laplacian operator. At the boundary we have

$$(6.4b) \quad u_{i,j+1/2,k+1/2}^1 = 0, \quad i = 1 \text{ and } N_1;$$

$$(6.4c) \quad D_2 u_{i,j,k+1/2}^1 = -\omega_{i,j,k+1/2}^3, \quad j = 1 \text{ and } N_2;$$

$$(6.4d) \quad D_3 u_{i,j+1/2,k}^1 = \omega_{i,j+1/2,k}^2, \quad k = 1 \text{ and } N_3.$$

Here, N_i ($i = 1, 2, 3$) is the number of grid points in i th direction. By (6.4d) there is

$$\begin{aligned} D_3^2 u_{i,j+1/2,k+1/2}^1 &= \frac{1}{\Delta x_3} (D_3 u_{i,j+1/2,k+1}^1 - D_3 u_{i,j+1/2,k}^1) \\ &= \frac{1}{\Delta x_3} (D_3 u_{i,j+1/2,k+1}^1 - \omega_{i,j+1/2,k}^2) \quad (k = 1 \text{ and } N_3). \end{aligned}$$

Note that $\omega_{i,j+1/2,k}^2$, the tangential vorticity components on the boundary, cancels the corresponding term in $D_3 \omega_{i,j+1/2,k}^2$ on the right-hand-side of (6.4), and thereby does not appear in the linear system of equations. Similarly, neither does the boundary value of ω^3 . Thus, Eq. (6.4) leads to a closed linear system of equations for interior values of u^1 without using tangential components of ω_B . Similar discretization can be done for u^2 and u^3 .

In the above discretization, we have assumed that the grid is uniformly spaced. On such a grid, Eq. (6.4) can be solved efficiently by using FFT. For non-uniform grids, other solution techniques, such as multigrid methods, can be used. The numerical tests show that the solution of $\mathbf{u}$ is indeed divergence-free in the sense that

$$(6.5) \quad \vartheta_{i+1/2,j+1/2,k+1/2} = (D_1 u^1 + D_2 u^2 + D_3 u^3)_{i+1/2,j+1/2,k+1/2} = 0$$

is identically satisfied. Therefore, we need only to solve two components of $\mathbf{u}$, say u^1 and u^2 , and compute u^3 from (6.5). To avoid the accumulation of round-off error at one end of the integration, we can alternate the direction of integration between time steps or substeps in a multistep time integration method.

To put the scheme on solid ground, we still need to prove that the above implementation does ensure (6.5). Although we have proved $\nabla \cdot \mathbf{u} = 0$ in Chapter 2, however, the proof does not relate directly to the above discretization. We first present another proof for the continuous problem whose discrete analog provides a general way of proving (6.5) immediately. Taking divergence of (6.2a) yields

$$(6.6) \quad \Delta \vartheta = 0.$$

If we can show that (6.6) has a homogeneous boundary condition

$$(6.7) \quad \frac{\partial \vartheta}{\partial n} = 0 \quad \text{on } \partial V,$$

then $\vartheta = \text{const}$ in V , and due to the compatibility condition (6.1f), there is $\nabla \cdot \mathbf{u} = 0$ in V . But (6.7) follows from (6.2c) and

$$\begin{aligned} \mathbf{n} \cdot \nabla(\nabla \cdot \mathbf{u}) &= \mathbf{n} \cdot (\nabla \times (\nabla \times \mathbf{u}) + \Delta \mathbf{u}) \\ &= \mathbf{n} \cdot (\nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega})) \\ &= -\nabla \cdot (\mathbf{n} \times (\nabla \times \mathbf{u} - \boldsymbol{\omega})) \\ &= 0, \end{aligned}$$

where we have used the fact that $\nabla \times \mathbf{n} = 0$ on ∂V , and the vector identity

$$\mathbf{a} \cdot (\nabla \times \mathbf{b}) = -\nabla \cdot (\mathbf{a} \times \mathbf{b}) + \mathbf{b} \cdot (\nabla \times \mathbf{a}).$$

Roughly speaking, if we can show that the discrete analog of (6.6) and (6.7) holds, then the same conclusion can be drawn for the discrete problem. Such an approach is rather independent of the grid although we only use uniform Cartesian grid here. For higher order methods, the same principle can be used. By (6.4) and the corresponding equations of u^2 and u^3 , it is straightforward to verify

$$(6.8) \quad D^2 \vartheta_{i+1/2, j+1/2, k+1/2} = 0$$

for $i = 2, \dots, N_1 - 2$; $j = 2, \dots, N_2 - 2$; $k = 2, \dots, N_3 - 2$. For the rest of grid points in the neighborhood of the cavity walls, edges, and corners, special derivation need to be made. At the first glance, if we can derive (6.8) on these near-boundary points and show that the discrete version of (6.7)

$$(6.9a) \quad D_1 \vartheta_{i, j+1/2, k+1/2} = 0 \quad \text{for } i = 1 \text{ and } N_1 - 1$$

$$(6.9b) \quad D_2 \vartheta_{i+1/2, j, k+1/2} = 0 \quad \text{for } j = 1 \text{ and } N_2 - 1$$

$$(6.9c) \quad D_3 \vartheta_{i+1/2, j+1/2, k} = 0 \quad \text{for } k = 1 \text{ and } N_3 - 1$$

is valid on the boundary, then it is easy to show that the linear system of equations for ϑ has at most nontrivial constant solution. But the constant has to be zero because the summation of ϑ over the all domain, i.e., the net mass flux out of the boundary, is zero.

Unfortunately, it is impossible to derive (6.8) and (6.9) separately. But note that in actual solving ϑ , Eq. (6.9) is used to cancel the unknown boundary terms in (6.8), resulting in an equation of ϑ at grid points next to the boundary. Thus, it is indeed the combination of (6.8) and (6.9) that is important. Therefore, we only need to derive the equation for ϑ at next-to-boundary points, and show that it is the same as the above combination. As an example, we prove the equivalence at the lower edge of the cavity with $i = 1$, $j = 1$, and $k \neq 1$ and $N_3 - 1$. For other edges, corners and surfaces, the derivations are similar. First the combination of (6.8) and (6.9) for $i = 1$ and $j = 1$ is

$$(6.10) \quad \frac{D_1}{\Delta x_1} \vartheta_{i+1,j+1/2,k+1/2} + \frac{D_2}{\Delta x_2} \vartheta_{i+1/2,j+1,k+1/2} + D_3^2 \vartheta_{i+1/2,j+1/2,k+1/2} = 0.$$

Now, we derive (6.10) from (6.4) and corresponding equations of u^2 and u^3 . Apply (6.4a) to $i = 1$ and $j = 1$, and use (6.4b), we can get

$$(D_1^2 + D_3^2) u_{i+1,j+1/2,k+1/2}^1 + \frac{D_2}{\Delta x_2} u_{i+1,j+1,k+1/2}^1 = D_3 \omega_{i+1,j+1/2,k+1/2}^2 - \frac{\omega_{i+1,j+1,k+1/2}^3}{\Delta x_2}$$

by straightforward algebra. Dividing the equation by Δx_1 , since $u_{i,j+1/2,k+1/2}^1 = 0$, we obtain

$$(6.11a) \quad \frac{D_1}{\Delta x_1} D_1 u_{i+1,j+1/2,k+1/2}^1 + \frac{D_2}{\Delta x_2} D_1 u_{i+1/2,j+1,k+1/2}^1 + D_3^2 D_1 u_{i+1/2,j+1/2,k+1/2}^1 = \frac{D_3}{\Delta x_1} \omega_{i+1,j+1/2,k+1/2}^2 - \frac{\omega_{i+1,j+1,k+1/2}^3}{\Delta x_1 \Delta x_2}.$$

Similarly, it can be shown for u^2 that

$$(6.11b) \quad \frac{D_1}{\Delta x_1} D_2 u_{i+1,j+1/2,k+1/2}^2 + \frac{D_2}{\Delta x_2} D_2 u_{i+1/2,j+1,k+1/2}^2 + D_3^2 D_2 u_{i+1/2,j+1/2,k+1/2}^2 = -\frac{D_3}{\Delta x_2} \omega_{i+1/2,j+1,k+1/2}^1 + \frac{\omega_{i+1,j+1,k+1/2}^3}{\Delta x_1 \Delta x_2}.$$

For u^3 there is

$$\frac{D_1}{\Delta x_1} u_{i+1,j+1/2,k}^3 + \frac{D_2}{\Delta x_2} u_{i+1/2,j+1,k}^3 + D_3^2 u_{i+1/2,j+1/2,k}^3 = \frac{\omega_{i+1/2,j+1,k}^1}{\Delta x_2} - \frac{\omega_{i+1,j+1/2,k}^2}{\Delta x_1}.$$

Subtracting this equation from the one with i replaced by $(i + 1)$ yields

$$(6.11c) \quad \frac{D_1}{\Delta x_1} D_3 u_{i+1,j+1/2,k+1/2}^3 + \frac{D_2}{\Delta x_2} D_3 u_{i+1/2,j+1,k+1/2}^3 + D_3^2 D_3 u_{i+1/2,j+1/2,k+1/2}^3 = \frac{D_3}{\Delta x_2} \omega_{i+1/2,j+1,k+1/2}^1 - \frac{D_3}{\Delta x_1} \omega_{i+1,j+1/2,k+1/2}^2.$$

Now, it is clear that the summation of (6.11a–c) is (6.10).

We stressed again that not every discretization of (6.2) can preserve the desired properties of the continuous problem; it is always desirable to check the numerical methods. The above procedure is a simple but general way to do so.

6.3 Solution of the Vorticity Transport Equations

In this section, we study the construction of divergence-free schemes for vorticity, and a proper way of imposing 3-D vorticity BCs. Denote $\vartheta_\omega = \nabla \cdot \omega$, then taking divergence of (6.1a) yields

$$(6.13) \quad \frac{\partial}{\partial t} \vartheta_\omega = \nu \Delta \vartheta_\omega.$$

In the derivation, the skew-symmetric property of $\nabla \cdot (\mathbf{u}\omega - \omega\mathbf{u})$ is used. From (6.13), if $\vartheta_\omega = 0$ initially and on the boundary, then it will be zero in the whole domain for later time. Another form of the vorticity equation is writing the viscous term as $-\nu \nabla \times (\nabla \times \omega)$, then (6.13) becomes $\partial \vartheta_\omega / \partial t = 0$; thus, a zero initial condition for ϑ_ω is sufficient to ensure $\vartheta_\omega = 0$. The second form of viscous term leads to a stronger result, however, neither of the formulations ensures that the same is true for the discrete version of (6.1a).

6.3.1 Divergence-Free Scheme in the Interior of Domain

Consider the following semi-discretized vorticity transport equation

$$(6.14) \quad \frac{\partial \omega}{\partial t} + \nabla^h \cdot (\mathbf{u}\omega - \omega\mathbf{u}) = \nu \Delta^h \omega.$$

Since the components of vorticity are defined at different locations, Eq. (6.14) should be applied correspondingly. By (6.3), we note that (6.14) is a conservative scheme. In our computation, the second-order Runge-Kutta method is used for time integration (see Chapter 5).

To get divergence-free schemes, we need

$$(6.15) \quad \nabla^h \cdot [\nabla^h \cdot (\mathbf{u}\omega - \omega\mathbf{u})]$$

to vanish identically, then the discrete divergence of (6.14) resembles (6.13); otherwise (6.15) will act like a source term in the diffusion equation of ϑ_ω to produce error continuously in time. To see more details, we write out (6.14) as follows:

$$\begin{aligned} \left[\frac{\partial}{\partial t} \omega^1 + D_2(F^{21} - F^{12}) + D_3(F^{31} - F^{13}) = \nu D^2 \omega^1 \right]_{i+1/2, j, k}, \\ \left[\frac{\partial}{\partial t} \omega^2 + D_1(F^{12} - F^{21}) + D_3(F^{32} - F^{23}) = \nu D^2 \omega^2 \right]_{i, j+1/2, k}, \\ \left[\frac{\partial}{\partial t} \omega^3 + D_1(F^{13} - F^{31}) + D_2(F^{23} - F^{32}) = \nu D^2 \omega^3 \right]_{i, j, k+1/2}, \end{aligned}$$

where $F^{12} = u^1 \omega^2$ and $F^{21} = u^2 \omega^1$, and similarly for F^{13} , F^{23} , F^{31} , and F^{32} . From these equations, the equation for ϑ_ω can be derived as

$$(6.16) \quad \left[\frac{\partial}{\partial t} \vartheta_\omega + D_1 D_2 (F^{21} - F^{12}) + D_2 D_1 (F^{12} - F^{21}) + \dots = \nu D^2 \vartheta_\omega \right]_{i, j, k},$$

in which we have omitted terms similar to the second and third terms on the left-hand side. Thus, a divergence-free scheme requires the two terms with F^{12} and the two with F^{21} to cancel, which might seem to be trivial from (6.16). However, one should keep in mind that F^{21} represents the convection effect in the second term but vortex stretching effect in the third. In both cases the value of $F_{i+1/2, j+1/2, k}^{21}$ (with different signs) is used. Since neither u^2 nor ω^1 is defined at $\{i + 1/2, j + 1/2, k\}$, interpolation is necessary. Then how to do it so that $F_{i+1/2, j+1/2, k}^{21}$ is *uniquely defined*, and hence the desired cancellation in (6.16) could happen? An obvious answer is to *calculate $F_{i+1/2, j+1/2, k}^{21}$ only once, and use the result in both convection and stretching terms.*

Thus, we just need to consider the construction of $F_{i+1/2, j+1/2, k}^{21}$ as a convection term. First we interpolate $u_{i+1/2, j, k}^2$ from $u_{i+1/2, j, k+1/2}^2$. Any method can be used, but in most of the computation done below,

$$(6.17) \quad u_{i+1/2, j, k}^2 = 0.5(u_{i+1/2, j, k+1/2}^2 + u_{i+1/2, j, k-1/2}^2)$$

is used. Then $F_{i+1/2, j, k}^{21} = (u^2 \omega^1)_{i+1/2, j, k}$ can be computed. Next, we may interpolate $F_{i+1/2, j+1/2, k}^{21}$ (values at the cell interfaces) from $F_{i+1/2, j, k}^{21}$ by using QUICK, ENO, or any other suitable methods. Calculation of other flux values is done in the same way. If centered interpolation is used, the algorithm will be the same as

those in [33, 56]. However, our method is not limited by central difference. Moreover, it should be noted that defining F^{21} (and similar terms) uniquely is *sufficient* for the cancellation but not necessary. There could be other ways to achieve the cancellation. However, they will be more complicated and may not resemble the actual continuous equations. At present, we cannot conceive any reason to do so.

6.3.2 3-D Kinematic Boundary Conditions

The above divergence-free scheme eliminates the source of ϑ_ω in the interior of domain. To ensure no error to be produced from the boundary, the boundary condition of vorticity has to be carefully imposed. We first examine imposing the kinematic BCs, then the dynamic BC.

The kinematic BC is nothing but $\omega = \nabla \times \mathbf{u}$. It follows that $\vartheta_\omega = 0$ on the boundary, and hence the divergence-free condition is ensured theoretically. Again, this argument does not guarantee numerical methods having the same property. In component form, the boundary conditions at the bottom of the cavity are

$$\omega^1 = \frac{\partial u^3}{\partial x^2}, \quad \omega^2 = 0, \quad \omega^3 = -\frac{\partial u^1}{\partial x_2}.$$

For ω^1 and ω^3 , local Taylor expansion can be used to get the interpolation methods. We have for $j = 1$

$$\begin{aligned} u_{i+1/2, j+1/2, k}^3 &= u_{i+1/2, j, k}^3 + \frac{\Delta x_2}{2} \omega_{i+1/2, j, k}^1 + \frac{\Delta x_2^2}{8} \left(\frac{\partial^2 u^3}{\partial x_2^2} \right)_{i+1/2, j, k} + O(\Delta x_2^3), \\ u_{i, j+1/2, k+1/2}^1 &= u_{i, j+1/2, k}^1 - \frac{\Delta x_2}{2} \omega_{i, j+1/2, k}^3 + \frac{\Delta x_2^2}{8} \left(\frac{\partial^2 u^1}{\partial x_2^2} \right)_{i, j+1/2, k} + O(\Delta x_2^3). \end{aligned}$$

If the second- and higher-order terms are ignored, apply the no-slip condition $u_{i+1/2, j, k}^3 = u_{i, j+1/2, k}^1 = 0$, we can get first order formulas for ω^1 and ω^3 at the boundary. Second-order formulas can be obtained by combining the above two expansions with those of $u_{i+1/2, j+3/2, k}^3$ and $u_{i, j+3/2, k+1/2}^1$. All these formulas can be written in the form of

$$(6.18) \quad \omega_{i+1/2, j, k}^1 = I_2(u^3)/\Delta x_2 \quad \text{and} \quad \omega_{i, j, k+1/2}^3 = -I_2(u^1)/\Delta x_2,$$

where $I_2(f)$ denotes a linear interpolation of function f in x_2 direction. Note that in case of dynamic BC, ω^1 and ω^3 are known, we can use the Taylor expansions method to get the boundary velocity and hence the residual slip.

While it is straightforward to apply the tangential kinematic BCs of vorticity, the normal vorticity condition needs to be treated more carefully. In the following, we show how to impose the condition for ω^2 in a way consistent with (6.18) to get fully divergence-free schemes.

First it is easy to show that, if $D_1\omega^1 + D_2\omega^2 + D_3\omega^3 = 0$ for all $\{i, j, k\}$, where $i = 2$ to $N_1 - 1$, $j = 2$ to $N_2 - 1$, and $k = 2$ to $N_3 - 1$, then

$$(6.19) \quad D_1 D^2 \omega^1 + D_2 D^2 \omega^2 + D_3 D^2 \omega^3 = 0,$$

is valid at $\{i, j, k\}$, where $i = 3$ to $N_1 - 2$, $j = 3$ to $N_2 - 2$, and $k = 3$ to $N_3 - 2$; this means that the viscous term does not contribute error to ϑ_ω at interior points (except the grid points closest to but not on the boundary). Further it can be shown by some algebra that, to ensure (6.19) to hold at grid points with $j = 2$, it is necessary for $(D_1\omega^1 + D_2\omega^2 + D_3\omega^3)_{i,j,k}$ to vanish identically for $j = 1$. This means

$$D_2\omega_{i,j,k}^2 = -D_1\omega_{i,j,k}^1 - D_3\omega_{i,j,k}^3, \quad (\text{for } j = 1).$$

Suppose the same interpolation operator is used for *both* tangential velocity components u^1 and u^3 , then by (6.18) we get

$$\begin{aligned} (6.20) \quad D_2\omega_{i,j,k}^2 &= -(\omega_{i+1/2,j,k}^1 - \omega_{i-1/2,j,k}^1)/\Delta x_1 - (\omega_{i,j,k+1/2}^3 - \omega_{i,j,k-1/2}^3)/\Delta x_3 \\ &= (-I_2(D_1 u^3) + I_2(D_3 u^1))/\Delta x_2 \\ &= I_2(\omega^2)/\Delta x_2. \end{aligned}$$

Furthermore, it can be shown that Eq. (6.20) implies $\omega_{i,1,k}^2 = 0$, i.e. the original condition for the normal vorticity. In the computation, Eq. (6.20) is used to update $\omega_{i,1\frac{1}{2},k}^2$. We note that $D_2\omega^2$ is the discrete normal derivative of ω^2 at the boundary.

Equation (6.20) can be seen as the definition of D^2 operator at the boundary. We may also consider it as a consistent extrapolation scheme for artificial

vorticity values outside the boundary, i.e.

$$\omega_{i,j-1/2,k}^2 = \omega_{2,j+1/2,k}^2 - I_2(\omega^2).$$

Again, the kinematic BCs at other boundaries can be derived similarly. We anticipate that the analysis given above is applicable for more general problems with different geometry and moving boundaries.

6.3.3 3-D Dynamic Boundary Conditions

Due to the use of explicit time integration scheme and the present second order method of solving $\mathbf{u}$, the kinematic BCs are easy to apply. If an implicit scheme is used, or the solution of $\mathbf{u}$ requires knowing boundary vorticity in advance, then the application of kinematic BCs will be much more complicated. As discussed in the last Chapter, the Dynamic BC would be easier to use in this case. For the present non-splitting scheme, the method discussed in §5.3.4 can be directly applied here. However, we note that (5.22) only gives two componentwise boundary conditions for $\boldsymbol{\omega}$. One more condition is needed.

The general vorticity flux formula has been given by Wu and Wu [42] (see also (3.12)). In fact, applying the N-S equation to a solid wall gives

$$(6.21) \quad -\nu \mathbf{n} \times (\nabla \times \boldsymbol{\omega}) = \mathbf{n} \times \mathbf{a}_b + \mathbf{n} \times \nabla p.$$

The left-hand side of (3.12) is obtained by recasting the left-hand side of (6.21) and using the no-slip condition. Since in our implementation, there is a residual slip on the boundary (which has important utility), we shall not use (3.12). Instead, we have

$$(6.22) \quad \begin{aligned} -\mathbf{n} \times (\nabla \times \boldsymbol{\omega}) &= \mathbf{n} \cdot (\nabla \boldsymbol{\omega}) - (\nabla \boldsymbol{\omega}) \cdot \mathbf{n} \\ &= \frac{\partial \boldsymbol{\omega}}{\partial n} - \nabla(\omega_n) - \nabla \mathbf{n} \cdot \boldsymbol{\omega}. \end{aligned}$$

The first term on the right-hand side of the second equality is the vorticity flux; the third term reflects the 3-D geometric effect which does not introduce any difficulty in our explicit scheme; however, the second term causes some trouble.

From (6.22) we can obtain the fluxes of the tangential components of ω , provided that ω_n is known on the boundary. Although ω_n can be computed from the boundary velocity, due to the sharp edges and corner of the cavity geometry, the $\nabla\omega_n$ term in (6.22) requires values of ω_n outside the boundary. We found that it is very hard if not impossible to manage the extrapolation of ω_n to meet the divergence-free requirement, unless $\nabla\omega_n$ is obtained in an implicit manner. For smooth and closed solid geometry, this problem disappears. For the cavity flow computation, we simplify the above implementation by setting $\omega_n = 0$ on the solid boundaries. This of course conflicts with the presence of residual slip, therefore, error in ϑ_ω is produced, and the resulting scheme is not fully divergence-free. The error can be relatively large at the beginning of an impulsively started flow because of large slip. Once the slip is reduced as the flow becomes smooth, the error also reduces. Moreover, the error can be filtered out by projection. Even if no projection is used, these error will be gradually reduced by diffusion and tends to zero in the steady state because the slip tends to zero. In the 3-D numerical tests below, we shall show that the error due to non-divergence-free discretization is much larger than that introduced here and does not vanish even in the steady state.

For implicit schemes, the dynamic BC needs to be calculated before the solution of whole vorticity field. Therefore, it is impossible to calculate ω_n in advance because the boundary velocity is not available. In this case, we may use $\vartheta_\omega = 0$ instead of ω_n condition on the boundary. This method introduces coupling of vorticity components on the boundary. On the other hand, we may impose $\omega_n = 0$ by sacrificing the divergence-free condition of ω temporally and recover it later by projection.

6.4 Two-Dimensional Result

The 2-D lid-driven flow in a square cavity is solved using the ω - u method given above. The Reynolds number of the problem is defined by $Re = UW/\nu$, where W is the width of the cavity. At $Re = 3200$, the flow reaches steady state

as $t \rightarrow \infty$. In the present computations, the residual slip because of using the dynamic BC is very small (10^{-11}) when reaching the steady state. Thus there is no difference between the solutions of using dynamic and kinematic BCs. In the computation, only one velocity component is solved from ω , the other one is obtained by integration. All results are obtained on uniform grids.

In Figs. 6.4 and 6.5, the contours of the stream-function and vorticity obtained on a 129×129 grid are shown, and are compared with the result of Ghia et al. [106] which has been widely used as a reference. Note that the stream-function is used here only to show the flow field, it is not used in the computation. The QUICK scheme is used for the convection of vorticity. Both first- and second-order vorticity BCs are used. The contour values are chosen to be the same as in [106]. At $t = 400$, our results are close to the steady-state results. From Fig. 6.4, the primary vortex and the down-stream secondary vortex of our solution is a bit weaker than that of [106], especially the result using first-order BC; but the upstream secondary vortex is stronger. A more quantitative comparison of the sizes of the secondary vortices are given in Table 6.1, where all results are computed on 129×129 grid. Here BL (bottom left), BR (bottom right) and T (top) indicate the positions of the secondary vortices in the cavity, and 1 and 2 denote the level of secondary separation; H_L and V_L are the normalized horizontal and vertical length of the vortices (see Fig. 6.1). Clearly, the present solution are in good agreement with existing results.

We also performed the computation on a 65×65 grid to see how well can the flow be resolved. The results of velocity profiles are given in Fig. 6.6. Clearly, the second-order BC leads to better results. The sizes of vortices are given in Table 6.2. Both small eddies BL2 and BR2 are captured by using the second-order BC, while BL2 is not resolved when using only the first-order BC.

It should be noted that Hayase et al. [107] were able to resolve the $Re = 10^4$ flow using a QUICK scheme for primitive variables on a 80×80 grid; the result compares well with that of Ghia et al. [106] obtained on a 257×257 grid. This would imply that for the present computation, a 65×65 grid should be sufficient to resolve the $Re = 3200$ flow if QUICK scheme is used. However, the present scheme

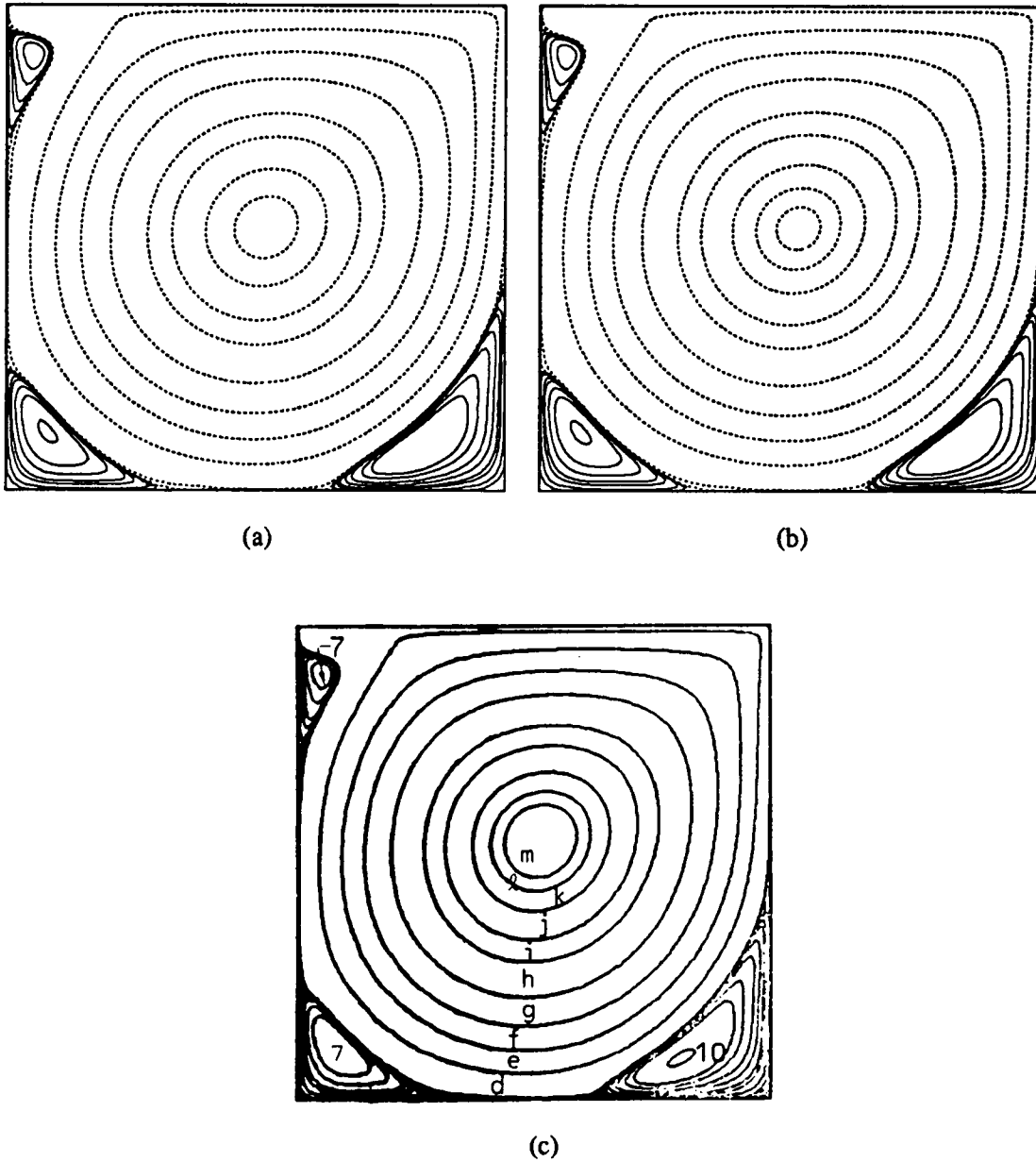


Figure 6.4: Stream-function contour of $Re = 3200$ 2-D flow (on 129×129 grid). (a) Present solution with first-order BC. (b) Present solution with second-order BC. (c) Steady-state solution of Ghia et al. [106].

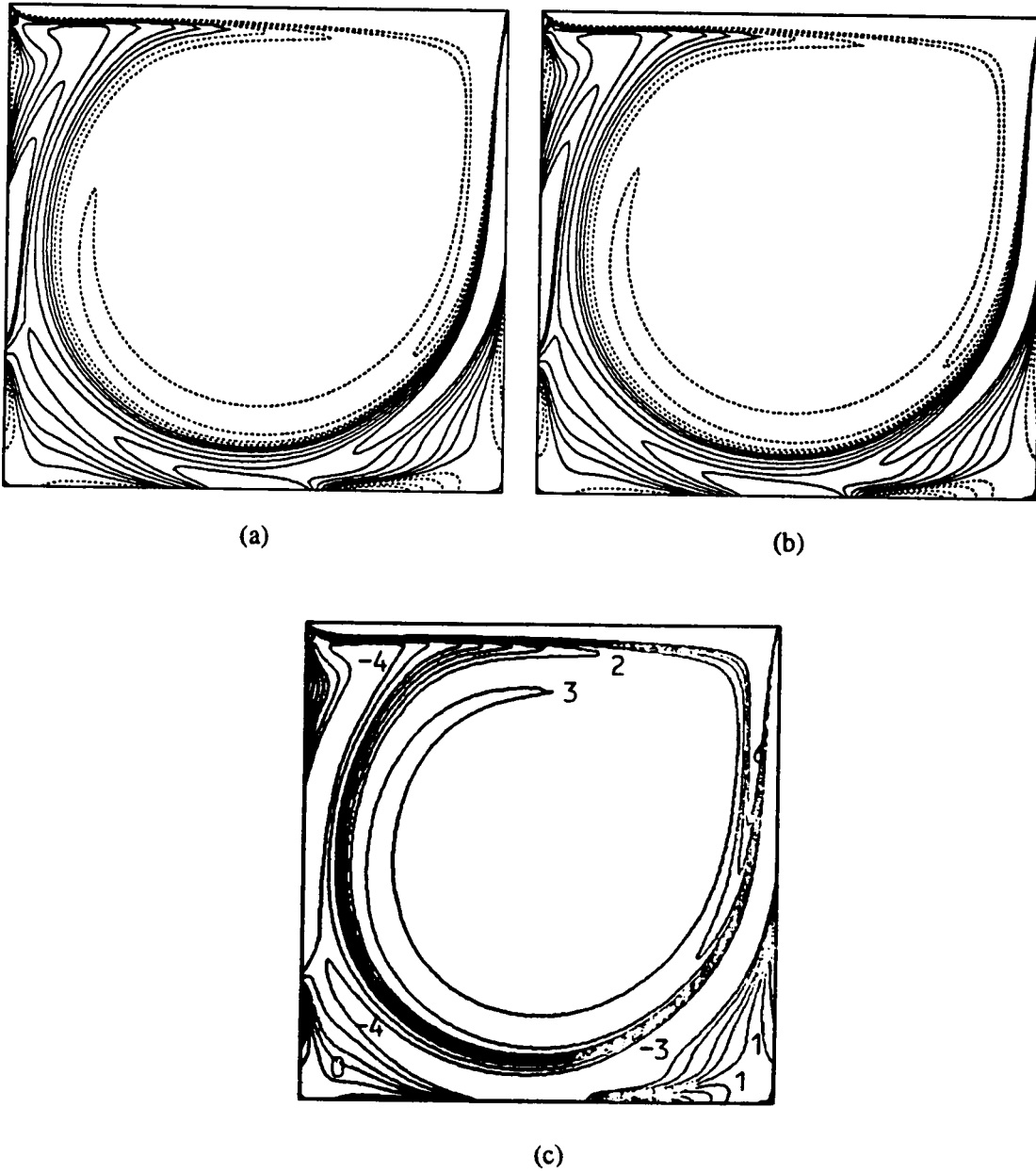


Figure 6.5: Vorticity contour of $Re = 3200$ 2-D flow (on 129×129 grid). (a) Present solution with first-order BC. (b) Present solution with second-order BC. (c) Steady-state solution of Ghia et al. [106].

Table 6.1: Sizes of secondary vortices for $Re = 3200$ flows

Eddy	Length	1st-order BC	2nd-order BC	Ghia et al. ¹	Perng and Street ²
BL1	H_L	0.3043	0.3071	0.2844	0.3047
	V_L	0.2445	0.2460	0.2305	0.2461
BR1	H_L	0.3485	0.3462	0.3406	0.3516
	V_L	0.4148	0.4145	0.4102	0.4180
T	V_L	0.2191	0.2200	0.2057	0.2187
BL2	H_L	0.0126	0.0156	0.0078	—
	V_L	0.0122	0.0150	0.0078	—
BR2	H_L	0.0262	0.0267	0.0254	—
	V_L	0.0246	0.0251	0.0234	—

1. Source: U. Ghia, K. N. Ghia, and C. T. Shin. High- Re solution for incompressible flow using Navier-Stokes equations and a multigrid method. *J. Comput. Phys.*, vol 48, pp 387–411, 1982.

2. Source: C.-Y. Perng and R. L. Street. Three-dimensional unsteady flow simulations: Alternative strategies for a volume-averaged calculation. *Int. j. numer. methods fluids*, vol 9, pp 341–362, 1989.

Table 6.2: Sizes of secondary vortices for $Re = 3200$ flows using a 65×65 uniform grid

Number	Length	1st-order BC	2nd-order BC
BL1	H_L	0.2946	0.3069
	V_L	0.2347	0.2409
BR1	H_L	0.3591	0.3482
	V_L	0.4525	0.4544
T	V_L	0.2122	0.2188
BL2	H_L	—	0.0039
	V_L	—	0.0039
BR2	H_L	0.0234	0.0244
	V_L	0.0211	0.0219

Note: Short line means the vortex is not resolved.

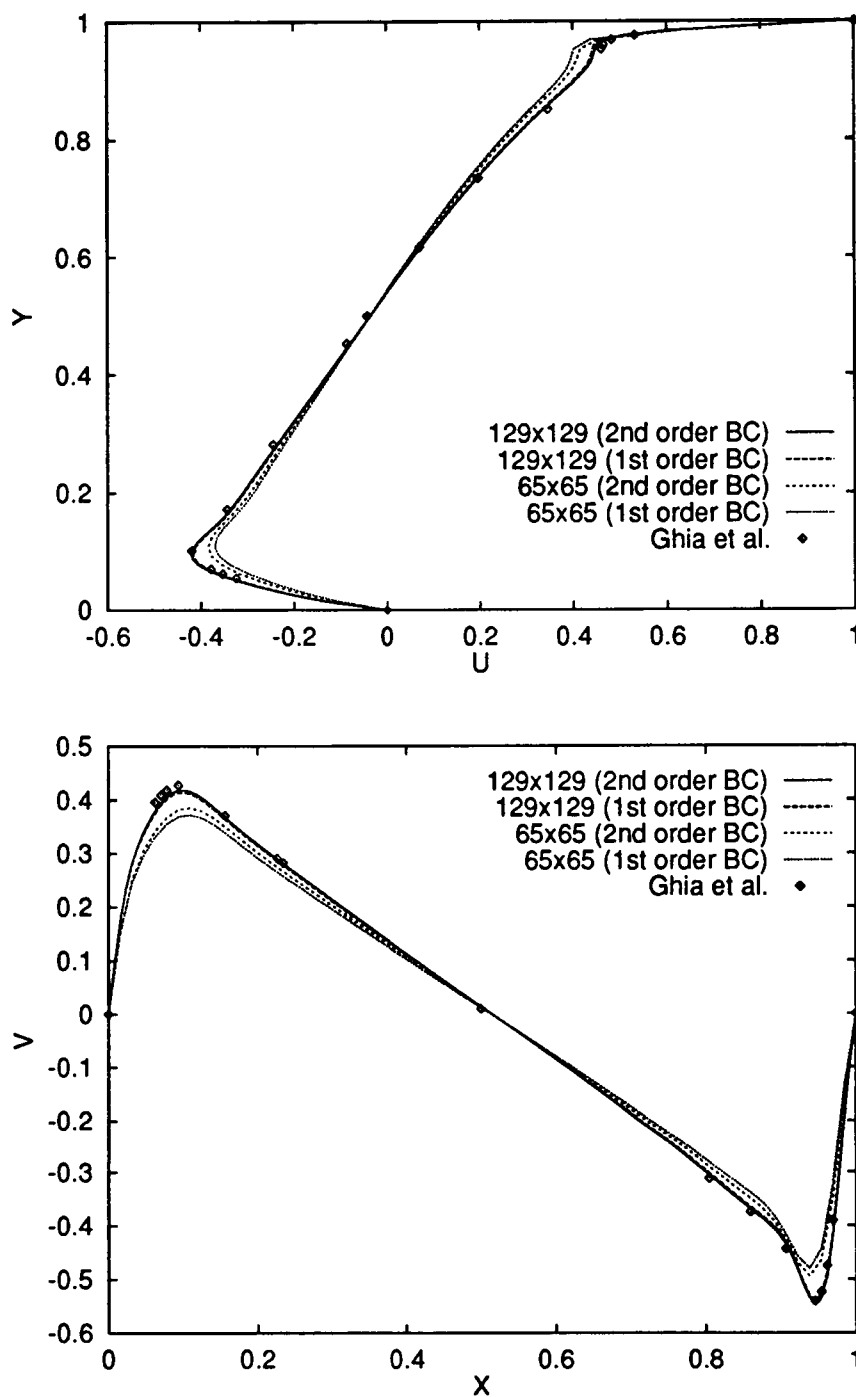


Figure 6.6: Velocity profiles for $Re = 3200$ 2-D flows. Top: u^1 profile on the vertical centerline; bottom: u^2 profile on the horizontal centerline.

fails in this respect. We note that the linear interpolation in (6.17) is in fact a smoothing process. To avoid it, we can use quadratic interpolation instead of the linear averaging. A test was performed and marginal improvement was found in the primary vortex. A centered scheme was also used for the convection, and the result is almost identical with that of QUICK. Therefore, we anticipate that more severe smoothing may occur due to the solution of velocity from vorticity. On the other hand, as shown later in 3-D computations, the QUICK and centered schemes do not always leads to the same results.

6.5 Three-Dimensional Result

In this section, we present the results of the 3-D lid-driven cavity flow. Both $Re = 1000$ and 3200 flows are solved using the ω - u method with dynamic or kinematic vorticity BCs. For $Re = 1000$, steady-state solution exists; whereas for $Re = 3200$, the flow is unsteady and has rather complicated 3-D vortical structures. To reduce the computation, we impose spanwise symmetry condition at the symmetry plane (see Fig. 6.1) so that only half-cavity flow is solved. Such an approach is justifiable for $Re = 3200$ flow, although there are moving Taylor-Görtler-like (TGL) vortices in the spanwise direction. Perng and Street [108] pointed out that the end walls provides only symmetric perturbations to the vortices; their numerical simulation of full cavity flow also proved this point of view.

The flow in a cavity with depth to width ration 1:1 and the span to width ratio 3:1 was investigated experimentally by Koseff and Street [109]. Later, numerical simulation at $Re = 3200$ was performed by Freitas et al. [110] using primitive variables, and by Tromeur-Dervout and Ta Phouc [111], Huang et al. [112], Huang and Ghia [14] ($Re = 3300$) using ω - u method. Unfortunately, the accuracy of these simulations has not been carefully verified. But for flows in a cubic cavity ($1 \times 1 \times 1$) at $Re = 400$ and 1000 , accurate steady-state solutions were obtained by Ku et al. [113] using pseudospectral method. The problem was also solved recently by Guj and Stella [33] using ω - u method. Their results are in good agreement. Therefore, we shall use the pseudospectral solutions of Ku et al. for

checking the accuracy of our method. Then, a more interesting flow at $Re = 3200$ is simulated by using different schemes. All results below (for the cubic cavity) are obtained on a $65 \times 65 \times 33$ grid with single precision.

The projection type of method has been successfully used in several applications [114], however, it is never truly justified from theoretical or numerical point of view. Therefore, one of the main objective of the following numerical tests is to see how well the projection method works comparing to fully divergence-free schemes. The comparison is done for both steady and unsteady flows. Another problem we shall investigate is the effect of different discretizations of the vortex stretching term, which is absent in 2-D computations. Moreover, it is interesting to observe the effect of error in ϑ_ω on the solution.

Several schemes can be constructed by combining different discretizations of the convection and stretching terms, the vorticity BCs, and the projection. Thus, it is convenient to use short-handed names for the schemes. The following convention is used: a scheme labeled as A-B means that the interpolation methods A and B are used for the convection and stretching terms (notice the order), respectively. Moreover, we shall use Q for QUICK and C for centered schemes. If the projection is used, then the label becomes A-B-P. From the previous discussion, we know that the Q-C scheme is not divergence-free; the Q-Q and C-C schemes are divergence-free but may not be fully divergence-free if error is introduced from the boundary.

For the $Re = 1000$ flow, we first compare the results of using dynamic and kinematic BCs. The difference in $\mathbf{u}$ and ω solutions are listed in Table 6.3. The solutions are very close, in particular, the velocity solutions can be regarded as identical. Thus, as in the 2-D case, we shall not distinguish the two methods below. It should be mentioned that the above result of dynamic BC is obtained without projection, so that we can observe the variation of ϑ_ω , the divergence of vorticity. We find that ϑ_ω varies as expected. At the beginning of the computation (one and two time steps after the lid starts to move), a large ϑ_ω is created close to the boundary, whose averaged value is about 1.04, which would be unacceptable. But then ϑ_ω decreases because of diffusion and quick reduction of the slip. After 100

Table 6.3: Difference in the results of using dynamic and kinematic BCs for $Re = 1000$ flows

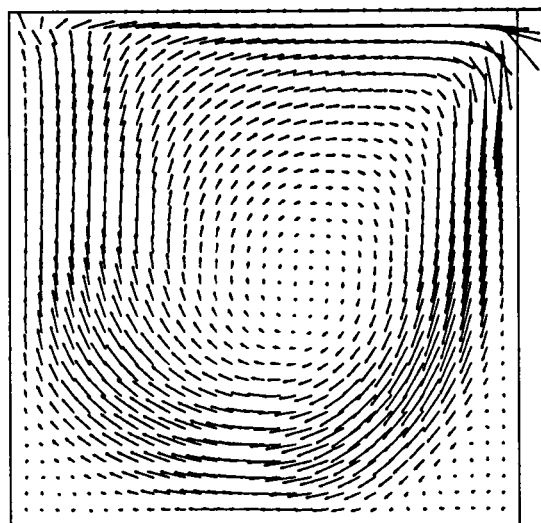
	Δu^1	Δu^2	Δu^3	$\Delta \omega^1$	$\Delta \omega^2$	$\Delta \omega^3$
Max norm	5.96e-7	8.05e-7	1.46e-6	3.15e-4	2.53e-4	7.25e-5
L_2 norm	1.05e-7	9.83e-8	1.64e-7	1.43e-5	7.37e-6	3.46e-6

time steps, the averaged value is about 1.2×10^{-3} . In this case, further reduction of ϑ_ω slows down (see below).

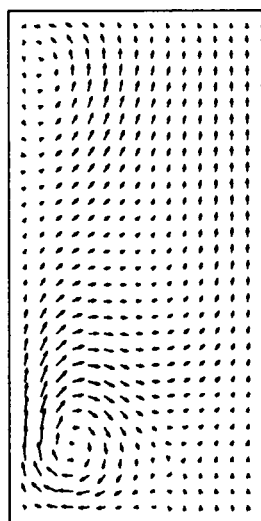
In the present single-precision computation, we find that the accumulation of round-off error of ϑ_ω is rather severe. When steady-state solution is reached at about $t = 40$, the fully divergence-free Q-Q scheme gives ϑ_ω an averaged value of 5.83×10^{-4} and maximum value of 1.18×10^{-2} . In case of using dynamic BC, the accumulation of round-off error prevents continuous reduction of ϑ_ω ; in steady-state, the slip is reduced to 3.5×10^{-6} but averaged and maximum ϑ_ω equal 3.06×10^{-4} and 5.66×10^{-3} , respectively. A test using double precision was conducted and we found that ϑ_ω did not exceed 10^{-11} for the Q-Q scheme; thus the accumulation of round-off error has no effect on the solution.

The flow field in the cavity are projected onto x_1 - x_2 , x_2 - x_3 and x_1 - x_3 mid-planes and plotted in Fig. 6.7. They are in good agreement with Guj and Stella's results [33]. In the next two figures, the profile of u^1 on the vertical centerline and the profile of u^2 on the horizontal centerline of the symmetry plane are compared with the pseudospectral results of Ku et al [113].

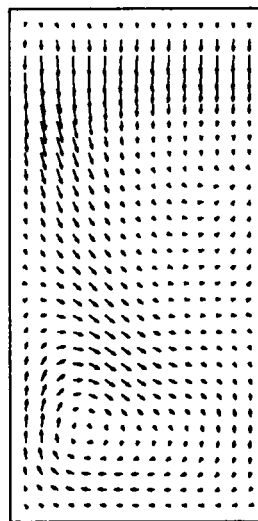
Figure 6.8 shows the results using first order vorticity BC. It can be seen that all the solutions are in good agreement, except that the two schemes without projection are slightly less accurate, which is evidently due to larger error in ϑ_ω . The figure implies that even a small residual ϑ_ω (below 10^{-3} for the Q-Q scheme) might not be good enough. On the other hand, the averaged value of ϑ_ω at steady state due to the Q-C scheme is very large, about 0.87; but interestingly, the flow field seems not severely affected by the error. We may explain this situation by



(a)



(b)



(c)

Figure 6.7: Velocity vector plots for $Re = 1000$ flow projected on: (a) x_1 - x_2 mid-plane; (b) x_2 - x_3 mid-plane; (c) x_1 - x_3 mid-plane.

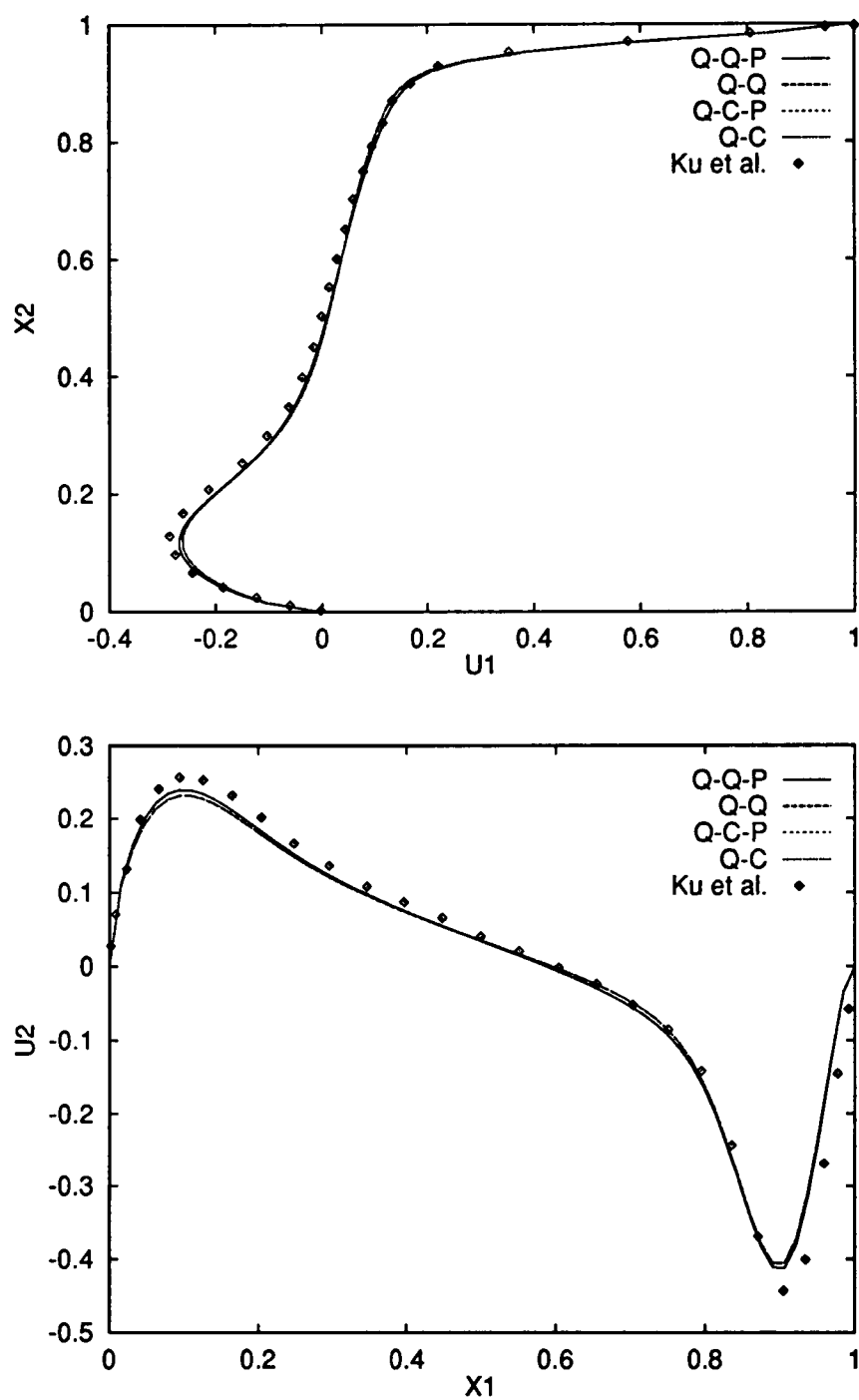


Figure 6.8: Velocity profiles on centerlines of the symmetry plane using first-order vorticity BC. Top: u^1 profile; bottom: u^2 profile.

Table 6.4: L_2 norm of difference in velocity solved from different schemes

	Q-Q vs. Q-Q-P	Q-Q-P vs. Q-C-P	Q-C-P vs. Q-C	Q-C vs. Q-Q
u^1	3.32e-3	1.39e-4	3.56e-3	9.32e-4
u^2	3.30e-3	1.46e-4	3.62e-3	9.31e-4
u^3	2.60e-3	9.06e-6	7.98e-4	6.77e-4

noting that the divergence of vorticity corresponds to the second-order derivative of velocity, hence a small error in velocity field can be greatly amplified. In other words, a large ϑ_ω does not necessarily mean a large error in $\mathbf{u}$. In Table 6.4, we present the differences among velocity fields solved from those schemes in Fig. 6.8. The table also shows that although the residual ϑ_ω of the Q-Q scheme is much smaller than that of the Q-C scheme, the difference between the velocity solutions of the Q-Q and Q-Q-P schemes is about the same as that between the Q-C and Q-C-P schemes. Furthermore, the table indicates that the discretization of the stretching term does not have a strong influence on the present steady-state result, at least less than that due to ϑ_ω .

The second-order vorticity BC is also used with different schemes to solve the problem. In one scheme, labeled as Q-Q-PI (I for inconsistent), we intentionally use the second-order BC in a way violating the consistency requirement given in §6.3.2, so that in each time step a rather large error of ϑ_ω is introduced on the boundary. Then, projection is used to filter the error out. Figure 6.9 compares the results of using first- (Q-Q-P1) and second-order BCs (Q-Q-P2 and Q-Q-PI). Clearly, the second-order BC leads to better accuracy. But more interestingly, the Q-Q-PI scheme seems to give most accurate result, particularly the solution of u^2 . Moreover, by comparing the $\mathbf{u}$ solutions of Q-Q-P, Q-C-P, and C-C-P, we find that the difference between Q-Q-P (or Q-C-P) and C-C-P (10^{-3}) is much larger than that between Q-Q-P and Q-C-P (10^{-4}). Therefore, the discretization of the convection term has stronger effect on the results than the discretization of the stretching term. In all cases, the projection works very well.

At $Re = 3200$, the flow is unsteady and quite complicated. First the

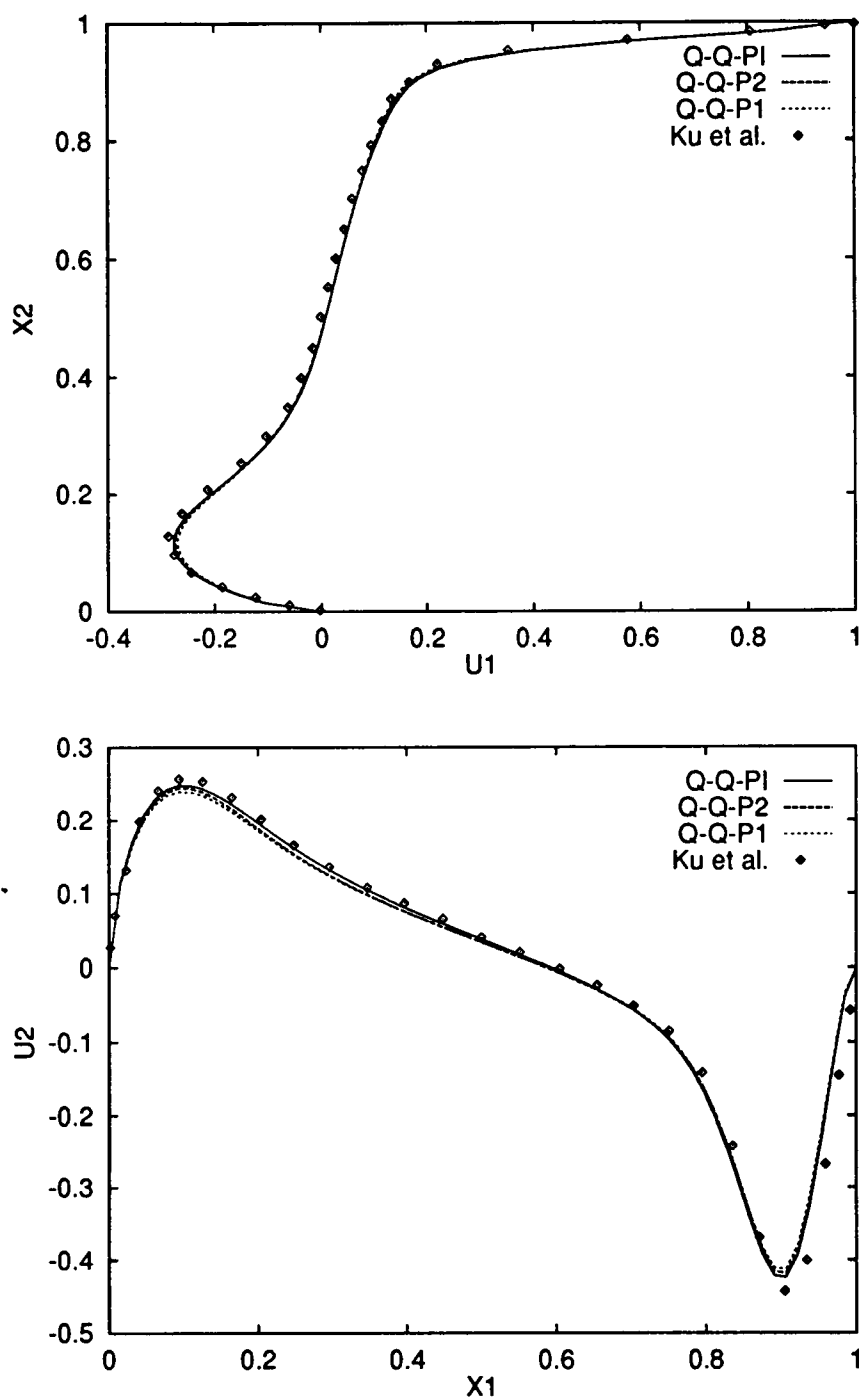


Figure 6.9: Velocity profiles on centerlines of the symmetry plane ($Re = 1000$).

Top: u^1 profile; bottom: u^2 profile.

primary vortex as well as the upstream and downstream secondary vortices (see Fig. 6.1) develop. Then, the TGL vortices and corner vortex (see Fig. 6.11 below) start to form close to the downstream sidewall. The flow remains unsteady because of the meandering of the TGL vortices and variation in the size of the downstream secondary vortex. It was found experimentally that the TGL vortices are very time dependent, thus a time accurate numerical method is required to capture the flow features correctly. Unfortunately, we cannot assess the time accuracy of our methods, because no accurate time dependent experimental or numerical data are available. Since the corner vortex, which is due to the adjustment of shear and pressure forces acting on the recirculating fluid to the no-slip condition, has a strong influence on the TGL vortices, we may also expect strong effect of vorticity BCs and near-wall grid resolution on the numerical results.

According to [115], the flow reaches fully developed state about 6 minutes after the start-up. In terms of our non-dimensional time it is about $t = 51.2$. The projected velocity field on the symmetry plane at this time is shown in Fig. 6.10. Results of different schemes with the first-order vorticity BC are compared. Clearly, the result of the Q-C scheme is significantly different from others. The same can be seen from the comparison in Fig. 6.11, where u is projected onto $x_1 = 0.766$ plane (i.e. $i = 50$). The difference is caused by the large error in ϑ_ω (whose average is about 3.1) for the Q-C scheme. For the Q-Q scheme, the error accumulated from round-off seems to be independent of Re . The residual ϑ_ω at $t = 51.2$ is about the same as the $Re = 1000$ case. However, the speed of accumulation is slower. In contrast, for the Q-C scheme, the residual ϑ_ω increases with Re , because the diffusion of ϑ_ω out of the boundary is weaker. It is plausible to conclude that for high Re flows, the non-divergence-free scheme without projection is not appropriate. On the other hand, the simplified method of imposing the dynamic BC is again justified. In fact, the result of Q-Q scheme in Fig. 6.10 is obtained by using this approach. The maximum residual slip at $t = 51.2$ is 2.3×10^{-5} and the averaged ϑ_ω is 4.7×10^{-4} .

In addition to the above observation, we note that there are some notable differences among the results of Q-C-P, C-C-P, and Q-Q, especially in Fig. 6.11.

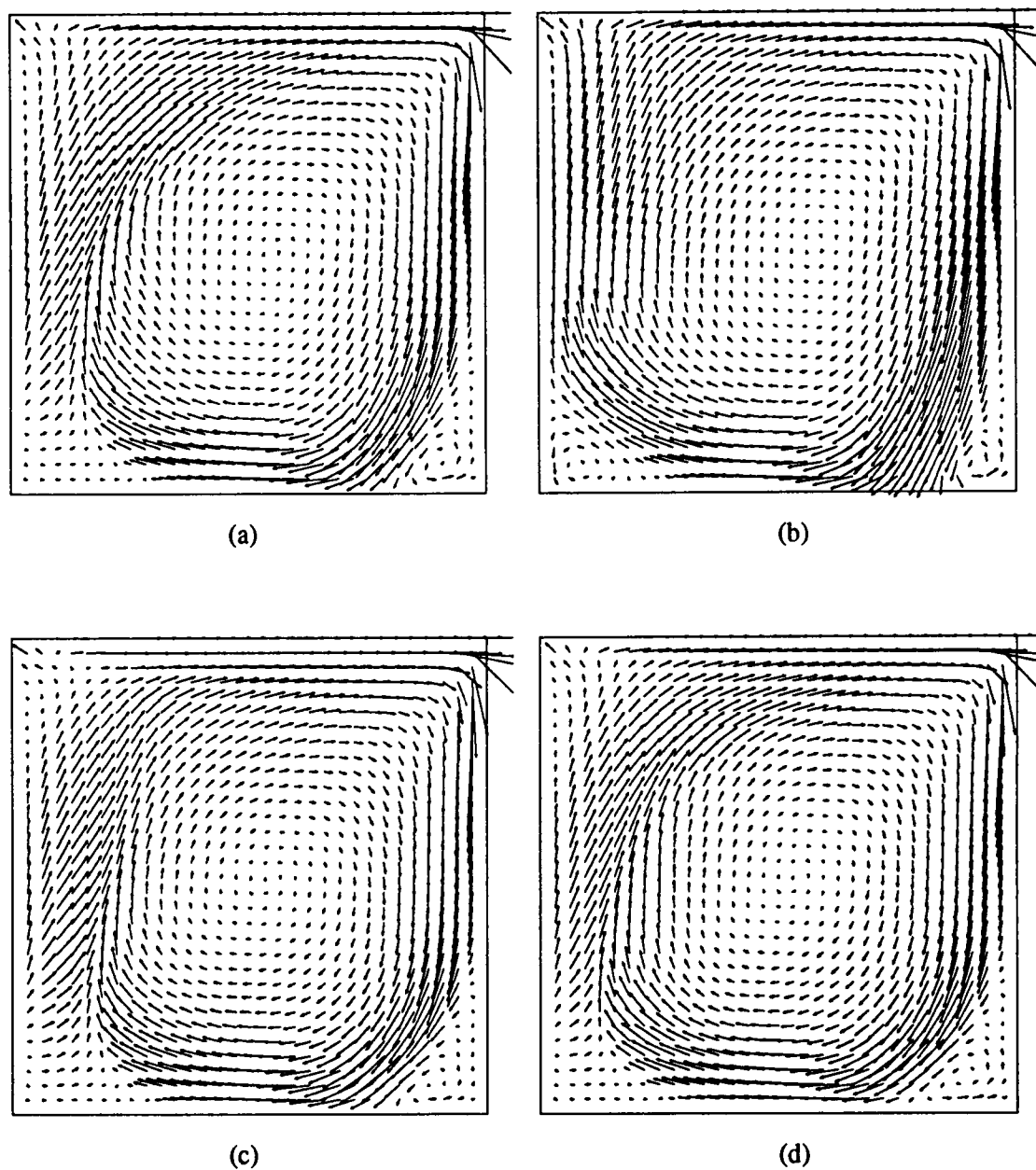


Figure 6.10: Velocity field for $Re = 3200$ flow, projected in the symmetry plane.
(a) Q-Q; (b) Q-C; (c) C-C-P; (d) Q-C-P.

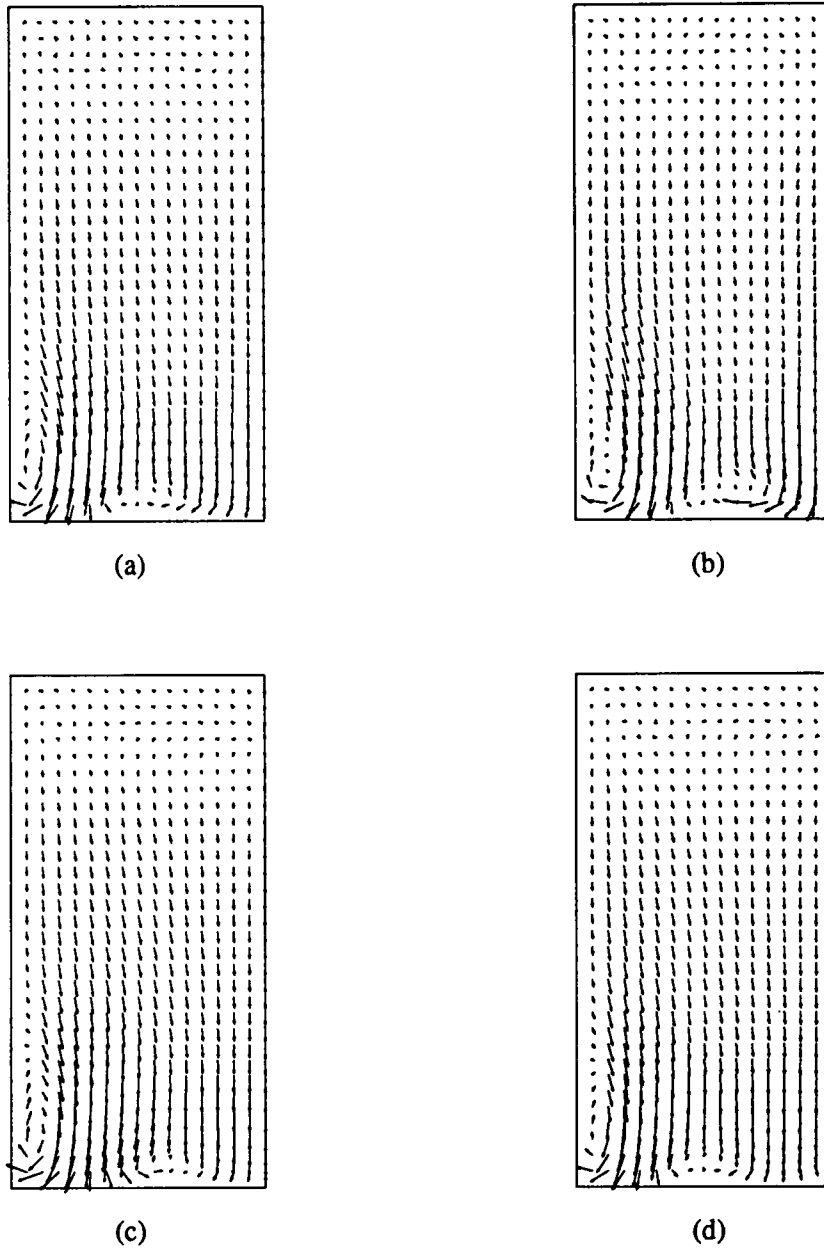


Figure 6.11: Velocity field for $Re = 3200$, projected in $x_1 = 0.766$ plane. (a) Q-Q; (b) Q-C; (c) C-C-P; (d) Q-C-P.

The only difference in these schemes is the discretization. Without a benchmark solution, we cannot judge which discretization is better here. The next figure, Fig. 6.12, show the results of Q-Q-P and C-C-P schemes with second-order vorticity BC. Comparing Figs. 6.12 with Figs. 6.10 and 6.11, it may be concluded that the solution is more sensitive to the boundary condition than to the discretization of the vorticity equation.

Because our grid is rather coarse, especially at the boundary, the solution we obtained here are only of qualitative value. Quantitative discussion of the time variation of the flow, particularly those features associated with the TGL vortices, would not be informative. In Fig. 6.13, the time averaged velocity profiles at the symmetry plane is compared with the experimental measurements [115]. The Q-Q-P scheme with first- and second-order BCs is used. Our time averages are obtained over the period of 7–10, 10–13, and 11–13 minutes after the start-up. The experimental data are averages over a 5-minute time period for the fully developed flow. The agreement is good considering the coarse grid. Perng and Street [108] used a non-uniform grid with grid size equals to 0.005 (ours is 0.0156) near the boundaries and get excellent agreement by using a time average over the period of 7–10 minutes. However, it should be noted that the time average is affected by the time period used, at least in our computation (see Fig. 6.13). At last, we show the velocity field computed using the Q-Q scheme with first-order BC at 7, 10, and 13 minutes after the start-up (Fig. 6.14). The figure shows possible structures of the TGL vortices. The motion of these vortices is complicated. Figs. 6.14a and 6.14b are very similar to those reported in [108], though for different time. Nevertheless, the current simulation seems to be able to capture the fine vortex structures. To get time accurate results of the above problem is a challenging but valuable task. However, we shall leave it for future study.

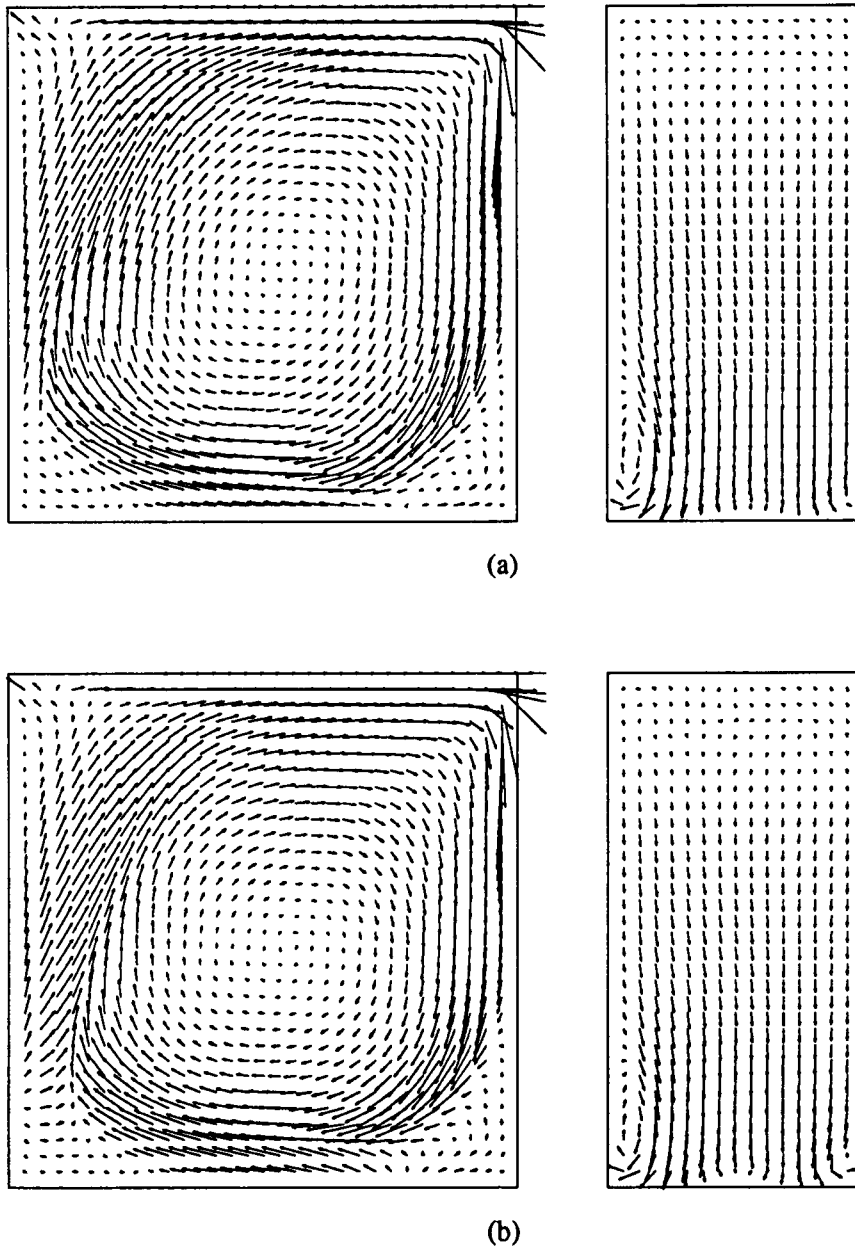


Figure 6.12: Velocity field for $Re = 3200$ using second order vorticity BC, projected in the symmetry plane (left) and $x_1 = 0.766$ plane (right). (a) Q-Q-P; (b) C-C-P.

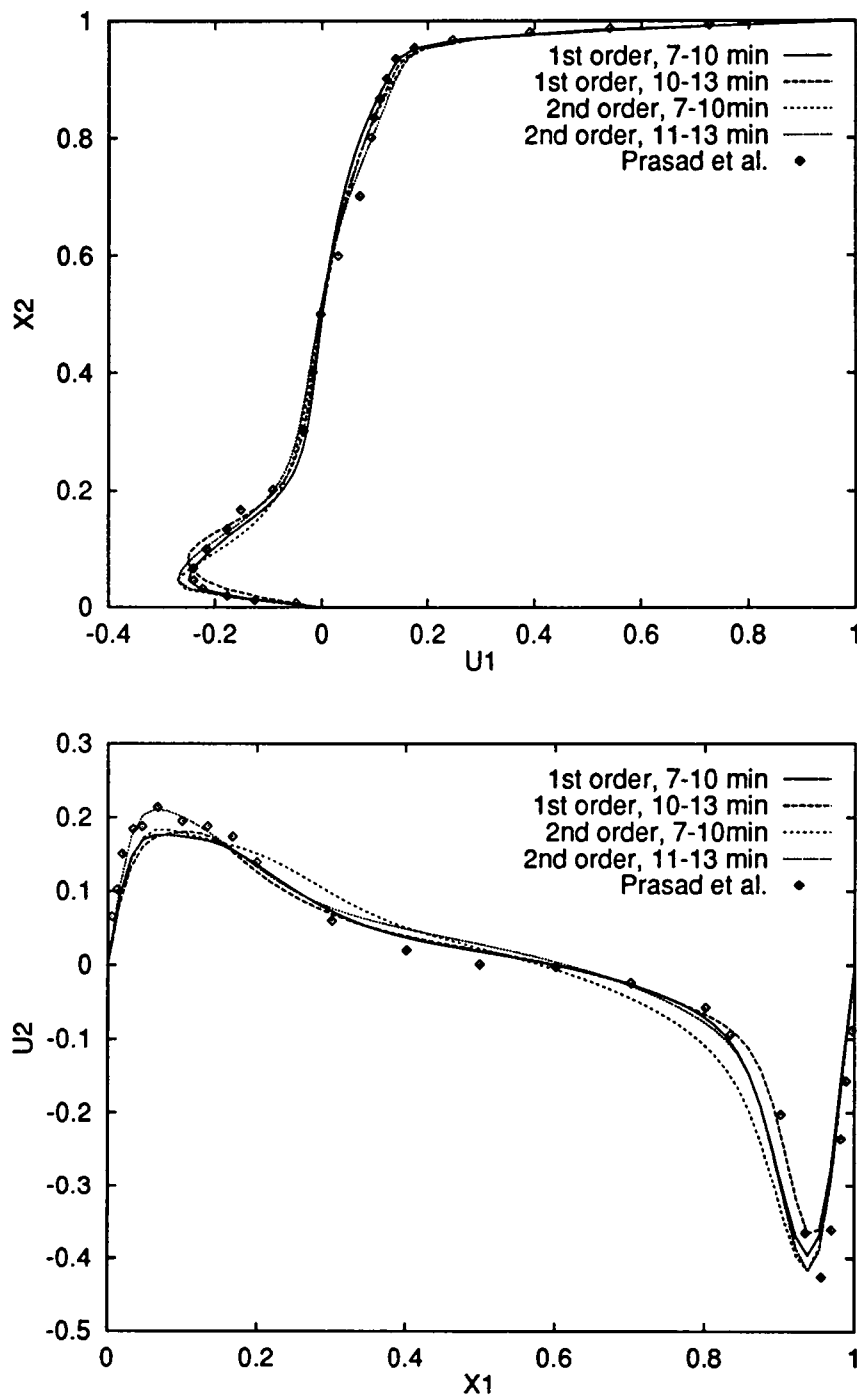


Figure 6.13: Time averaged velocity profile at the symmetry plane ($Re = 3200$).

Top: u^1 profile; bottom: u^2 profile.

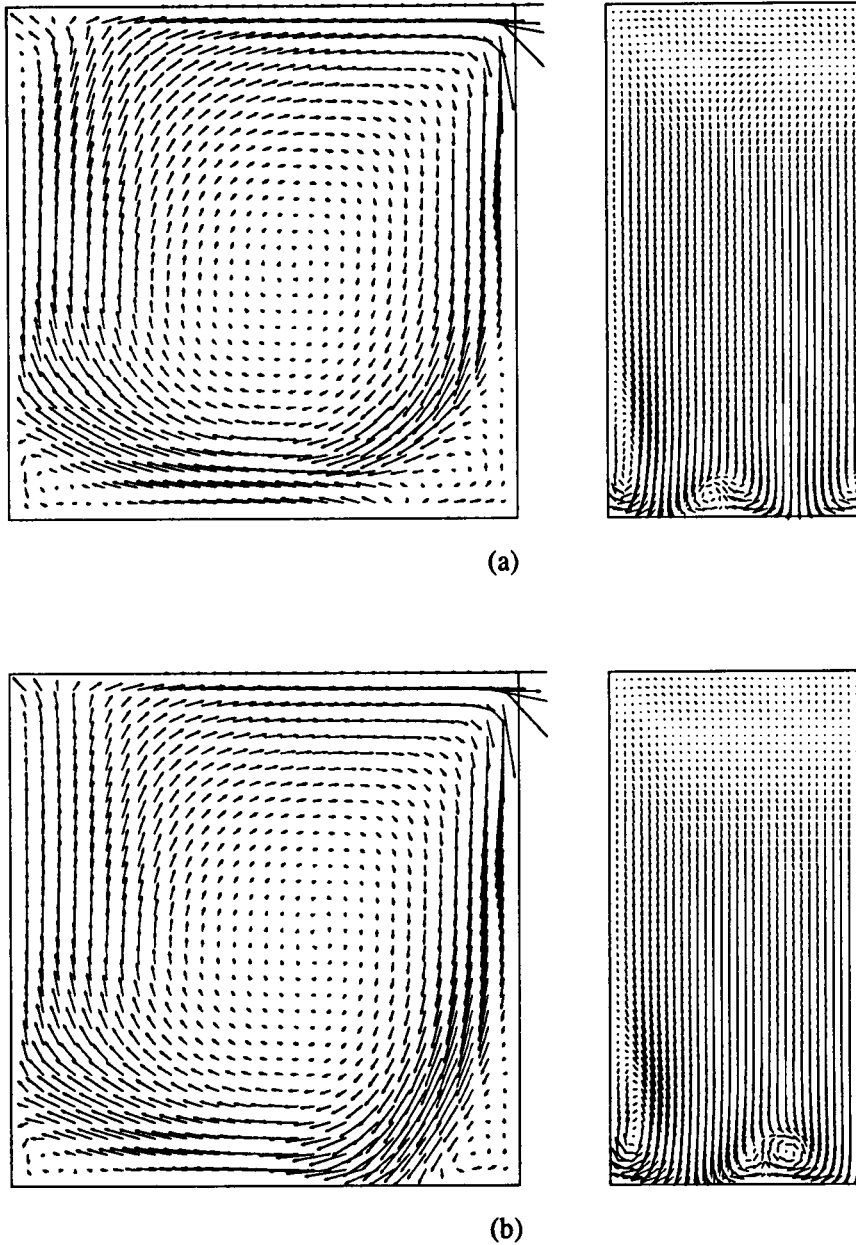
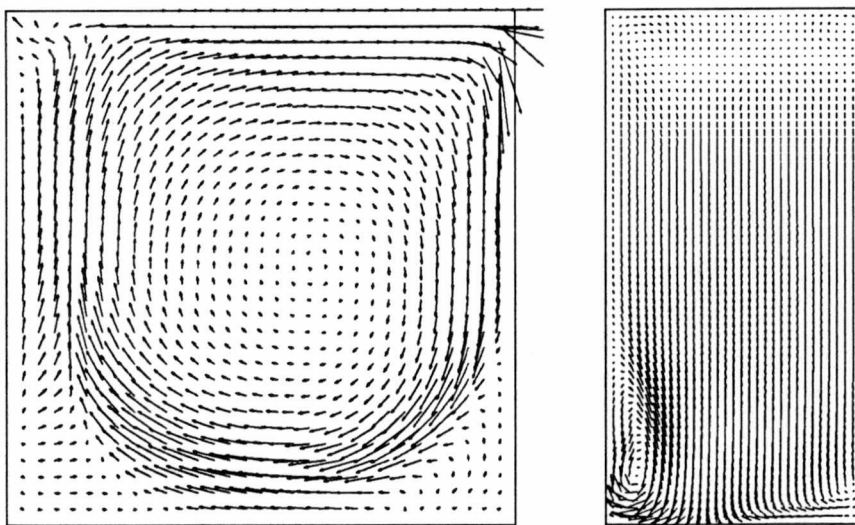


Figure 6.14: Projected velocity field at symmetry plane (left) and $x_1 = 0.766$ plane (right) for $Re = 3200$ flow. (a) $t = 7$ min. (b) $t = 10$ min. (c) $t = 13$ min.



(c)

Figure 6.14 (continued).

Chapter 7

Summary and Conclusions

Vorticity-based numerical methods are important alternatives to the conventional velocity-pressure methods for simulating viscous flows. In many cases, more physical insight can be gained by dealing with vorticity directly. This is especially true for vortex dominating flows. We have concentrated on incompressible flows, and emphasized on unsteady problems because incompressible steady-state problems are more or less settled. Several crucial issues surrounding the vorticity-based numerical methods under the above conditions were critically studied. We found that for unsteady problems, the preferred numerical method is to solve the dynamic equation for vorticity and the kinematic equation for velocity in a decoupled manner. Relevant physical, mathematical, and numerical issues, which are of key importance to successful decoupled methods, have been carefully examined. A general frame work of building the decoupled methods is established and demonstrated with sample computations. Moreover, during the study, we indeed gained better physical insight to the incompressible fluid dynamics, in particular about the generation of vorticity from solid boundaries, and applied the insight to modeling numerical vorticity boundary conditions. Important results and conclusions of this research are summarized below:

1. For the first time, a systematic and rigorous study of the dynamic boundary condition for vorticity, namely the boundary vorticity flux, was conducted. Based on the physics of vorticity creation from solid walls and with the help of mathematical analysis, we showed that the vorticity creation is inherently a dynamical process and is *coupled* with pressure through the viscous effect and no-slip condition. The strength of this coupling was then studied. By both analysis and numerical tests of flow over a circular cylinder, we proved that the strength of the coupling decreases as Reynolds number increases; for

smooth flows, it is proportional to $Re^{-1/2}$. This is the *foundation of decoupling* vorticity from pressure in the operator-splitting schemes, which are most often adopted in Lagrangian vortex methods. Our computation for cylinder flow at $Re = 9500$ on a relatively coarse grid agrees well with the fourth-order results of Anderson and Reider's [96] and experiments [104]. Moreover, we found that the decoupling between vorticity and pressure could be a valid approximation even at $Re = 10$. Thus, it is not surprising why some known ad hoc implementations of the dynamic BC work well for a wide range of Re . We conclude that for most practical flows, the above approximate decoupling is accurate enough. For very high resolution computations, the approximation is inappropriate because the decoupling gives at best first order accuracy in time. However, the vorticity-pressure coupling can be efficiently recovered by our iteration method based on the dynamic BC.

2. The residual slip on solid boundaries due to the approximate decoupling, which has been ignored in the literature, played a key role in the above study. This important quantity not only reflects the accuracy of the numerical methods, but also responds to the physical development of the flow. Our computation shows that the slip is higher when the flow has more complicated vortex structures, such as secondary vortices.
3. The kinematic boundary conditions for vorticity are *inherently global* and more difficult to localize than the dynamic BC. The localized kinematic BCs are found to convey a simple unified form; thus they can be viewed as whole. We found that the localized kinematic BCs severely degrade the stability of implicit time integration schemes, whereas the dynamic BC preserves the stability. This difference can be explained based on physical understanding and numerical evidence. In short, the localized kinematic BCs contain less physical information about vorticity creation than the dynamic BC. Thus, the dynamic BC is a more favorable choice especially for implicit methods. For some explicit time integration schemes, however, the kinematic BCs could be simpler and more convenient to implement. An accurate method of computing the

drag coefficient when using the kinematic BCs is developed. Again, we used a dynamic approach to evaluate the boundary vorticity flux instead of usual finite-difference schemes.

4. A method of decoupling vorticity from pressure for non-splitting schemes was studied. For Eulerian type of numerical methods, the non-splitting approach may be more desirable because it is not limited by second-order accuracy in time, unlike the splitting schemes. The mechanism of decoupling here is different from that in the operator-splitting methods; it is achieved in a time lagged fashion. For our example scheme, the resultant slip is proportional to $O(\Delta t^2)$ and much smaller than that due to the previous decoupling. The non-splitting method seems more suitable for high resolution computations.
5. The problem of solving kinematic equations of velocity was studied from both mathematical and numerical points of view. Mathematically, we clarified the correct boundary conditions to use for solving the vector Poisson equation of velocity derived from the original equations. We also proved that the velocity solution thus obtained satisfies the continuity equation even for arbitrarily given vorticity field. Moreover, an orthogonal projection of the vorticity onto the divergence-free space can be obtained by taking the curl of the velocity solution. These theoretical results lead directly to a new efficient finite-difference scheme for solving the velocity as well as projecting the vorticity. This method enables us to solve velocity 50% and 30% faster for 2-D and 3-D problems respectively than other vorticity-velocity methods. The projection of vorticity can then be done at almost no cost. Compared to solving an extra Poisson equation, as done by common projection schemes, the saving of computation cost is rather significant.
6. The integral formulation of solving the velocity kinematic equations, i.e., the generalized Biot-Savart Law, was studied. We proved that the integral formulation does indeed solve the original kinematic equations. We clarified some misunderstanding towards the use of the generalized Biot-Savart Law, and showed a correct and efficient implementation of the integral formulation. The

projection of vorticity was considered with the integral approach.

7. When developing the three-dimensional vorticity-velocity methods, it is common that the numerical scheme does not have the desired properties of their continuous counterparts. One important problem is to ensure that numerically the divergence of vorticity be zero. Although, some special schemes have been constructed in the literature, there lacks a general guideline for developing more sophisticated schemes. This situation is greatly improved by our finding of two simple and general principles, which ensures the discrete equations to resemble the corresponding continuous problems. Based on these principles, we were able to develop the above method for solving velocity, and divergence-free schemes for the vorticity equation. We gave a proper way of imposing three-dimensional kinematic BCs to ensure no error of vorticity divergence would be introduced from the boundary. Moreover, the implementation of dynamic BC was extended to three-dimensions.
8. Numerical tests were performed for 2-D and 3-D lid-driven cavity flows. Our 2-D results and 3-D results for $Re = 1000$ flow are in good agreement of existing accurate numerical results. However, we were more interested in comparing different schemes of our own, to identify the influence of different discretization and boundary conditions on the results. For steady-state problems (2-D and 3-D), a higher order vorticity BC does provide better accuracy. By comparing the results of the projection and fully divergence-free schemes, we justified that the projection is a powerful tool to remove non-physical error in the vorticity, and helps to retain the accuracy of the solutions. The projection method is highly recommend for extensive use, because it allows much more flexible discretization of the vorticity equation and treatment of boundary conditions. Furthermore, large error in the divergence of vorticity is found to damage the accuracy of numerical solutions, particularly for high Re unsteady cavity flows. For $Re = 1000$ steady 3-D flow, all schemes tested gave consistent results. However, the situation changed drastically for the long time simulation of the $Re = 3200$, unsteady, 3-D flow. Many factors can contribute to the discrepancy

among different schemes. We have not investigated these factors in detail and shall leave this interesting problem for the future.

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Vita

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