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Discrete Compatibility in Finite Difference Methods for Viscous Incompressible Fluid Flow

HUAXIONG HUANG*,[1] AND BRIAN R. WETTON†,[2]

*Department of Mathematics & Statistics, Simon Fraser University, Burnaby, Canada British Columbia, V5A 1S6;
†Department of Mathematics, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z2

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Thom's vorticity condition for solving the incompressible Navier–Stokes equations is generally known as a first-order method since the local truncation error for the value of boundary vorticity is first-order accurate. In the present paper, it is shown that convergence in the boundary vorticity is actually second order for steady problems and for time-dependent problems when $t > 0$. The result is proved by looking carefully at error expansions for the discretization which have been previously used to show second-order convergence of interior vorticity. Numerical convergence studies confirm the results. At $t = 0$ the computed boundary vorticity is first-order accurate as predicted by the local truncation error. Using simple model problems for insight we predict that the size of the second-order error term in the boundary condition blows up like $C/\sqrt{t}$ as $t \to 0$. This is confirmed by careful numerical experiments. A similar phenomenon is observed for boundary vorticity computed using a primitive method based on the staggered marker-and-cell grid. © 1996 Academic Press, Inc.

1. INTRODUCTION

We consider finite-difference (FD) methods for two-dimensional (2D) viscous incompressible flow based on the vorticity-streamfunction ($\omega - \psi$) formulation. Typically, values of boundary vorticity are related to the interior streamfunction values by matching Taylor series, although other approaches have been taken [1, 13, 24]. The simplest of these so-called $\omega - \psi$ boundary conditions was proposed by Thom [23] in 1933. It is generally known as a first-order method [18, 4] since the local truncation error for the boundary vorticity expression is first order. However, results for the Stokes equation [7] indicated that stream function solution converges in the order of $h^{3/2}$, faster than first order (h), if standard second-order approximations are used in the interior. Hou and Wetton [11] proved second-order convergence of the vorticity values in the interior for the Navier–Stokes equations. However, they reported a first-order convergence of the vorticity values at the boundary. Recently, this result was improved in [15] to show second-order convergence of solutions including boundary vorticity for the steady Stokes equations using Thom's boundary condition. In the present paper, a discrete error for boundary voriticity is estimated to be of order h^2 for steady state Navier–Stokes equations and for time dependent problems for $t > 0$. The uniform second-order convergence of the vorticity values here and in [15] is established by more carefully examining the asymptotic error results from [11]. The fundamental idea here is very simple: that Thom's voriticity boundary condition is generated from a second-order approximation of the more fundamental no-slip condition. We prove that Thom's boundary approximation is a second-order method even at the boundary, contrary to popular belief. We demonstrate this result numerically in smooth domains and in the ubiquitous driven cavity, where the smoothness assumptions of the asymptotic error analysis are violated at the corners. Here, second-order convergence of boundary vorticity is observed in regions bounded away from the corners.

For time-dependent problems, the situation is more complicated. The asymptotic error results are valid assuming numerous compatibility conditions are satisfied at $t = 0$. Formally, the results are still valid for $t > 0$ even if the compatibility conditions are violated. The result is second-order convergence even in boundary vorticity for $t > 0$. This was observed numerically in [25]. However, at $t = 0$ the boundary vorticity converges with first order, as predicted by the straightforward Taylor series analysis. It is clear that if the computed boundary vorticity error is bounded asymptotically by $K(t)h^2$ then $\lim_{t\to 0^+} K(t) = \infty$. In fact, we show using model examples and numerical experiments that $K(t) \sim C/\sqrt{t}$. Through the model problems we also observe the error behaviour for stronger incompatibilities. It is interesting to note that for FD methods there can be incompatibilities in the error expansion terms leading to singular behaviour in the error at $t = 0$ even if the continuous problem satisfies all compatibility conditions.

Thom's boundary condition is actually used infrequently

[1] Email: hhuang@cs.sfu.ca. Supported by an NSERC Canada postdoctoral fellowship.

[2] Email: wetton@math.ubc.ca. Supported by an NSERC Canada grant.

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in practice and almost always hidden in pure streamfunction methods such as [20, 10], where the confusion over its accuracy is not apparent. More often, "higher order" boundary conditions are used (see [18, pp. 185–187] for a list). However, our results show that using these more complicated boundary conditions is not necessary to attain second-order convergence, even in boundary vorticity. We also show in Section 5 of this paper that the use of higher order boundary conditions does not in general improve the singular behaviour in convergence of derived quantities (like vorticity) at the boundary near $t = 0$ in time-dependent computations.

We observe a similar phenomenon for primitive variable incompressible flow calculations. When a staggered grid MAC approximation is used for the velocity and pressure values, linear interpolation or "reflection" conditions must be used to approximate the Dirichlet velocity data. The use of these conditions results in an apparently inconsistent approximation of the diffusion terms at the boundary [6], although it can be proven that the pressure and velocity converge at second order for time-independent flow and for $t > 0$ for time-dependent flow using the same techniques as above [12]; other authors have explained this phenomenon by borrowing FEM results [27]. Here also, second-order convergence in boundary vorticity is seen, although it appears to be calculated only to first order. At $t = 0$ the second-order error terms for boundary vorticity and for pressure blow up like $C/\sqrt{t}$ as above.

This phenomenon is different from some other cases reported in the literature where better convergence is observed than expected at first glance. It is not the same phenomenon as described by Gustafsson [8] for the approximation of exiting characteristic data for hyperbolic problems. It is similar in appearance but cannot properly be called supra-convergence [2] since that phenomenon is due to an incorrect interpretation of truncation error. In our case, we expect second-order convergence because the true boundary conditions of the problem are satisfied to second order accuracy. We consider the loss of convergence order at $t = 0$ to be due to a lack of *discrete compatibility*. Although we consider incompressible fluid flow as our main example, our work explains similar phenomena in other problems.

In the next section we show a model of the behaviour we wish to investigate. This allows us to show the asymptotic error result explicitly for a simple case. In Section 3 we consider the $\omega - \psi$ formulation of viscous incompressible flow using Thom's "first-order" boundary condition. We show that it gives second-order vorticity values even at the boundary (for $t > 0$) and examine the behaviour near $t = 0$ numerically. In Section 4 we consider a primitive variable method based on the MAC grid. In Section 5 we consider model problems showing the growth rate of the second-order error constant as $t \to 0^+$ in various situations.

2. THE PHENOMENON AND ANALYSIS

We demonstrate the type of phenomenon considered in this paper first in simple one-dimensional problems below. We apply the insight here to discretizations of incompressible flow in later sections.

2.1. Steady State (Elliptic) Problems

We present the phenomenon we study through a simple model problem. The problem is to compute the solution $u(x)$ for $x \in [0, 1]$ to

$$u'' - u = e^x, \tag{1}$$

satisfying boundary conditions $u'(0) = 0$ and $u'(1) = 0$. The exact solution is

$$u(x) = c_1 e^x + c_2 e^{-x} + \frac{x}{2} e^x,$$

where

$$c_1 = \frac{1/2 + e^2}{e^2 - 1}; \quad c_2 = c_1 + \frac{1}{2}.$$

We were careful to choose this problem so that no derivatives of u vanished at the boundary to "fool" our numerical tests of convergence rates.

We consider a standard centered difference approximation of this problem on a regular grid with spacing h. Capital letters will denote numerical approximations $U_i \approx u(ih)$ for $i = 0, 1, ..., N$, where $N = 1/h$. Standard second-order finite difference operators for derivatives of order k are denoted by D_k, i.e., $D_2 U_i = (U_{i+1} - 2U_i + U_{i-1})/h^2$. Equation (1) is approximated by

$$D_2 U_i - U_i = e^{ih} \tag{2}$$

for $i = 0, 1, ..., N$. The boundary conditions are also approximated to second order

$$D_1 U_0 = 0, \quad D_1 U_N = 0. \tag{3}$$

These boundary conditions can be used to eliminate the artificial values U_{-1} and U_{N+1} in Eqs. (2) for $i = 0$ and $i = N$, leading to the expressions

$$D_2 U_0 = 2(U_1 - U_0)/h^2, \quad D_2 U_N = 2(U_{N-1} - U_N)/h^2. \tag{4}$$

The system (2) with modifications (4) near the boundaries is easily solved. Since we have approximated the equations and boundary conditions to second order, we expect sec-

TABLE I

Normalized Second-Order Errors in U for the Model Elliptic Problem

$N = 1/h$	$\|U - u\|/h^2$
8	0.2983
16	0.2990
32	0.2992
64	0.2993

ond-order convergence unless we are confused by the terms (4) which are only first-order accurate as written, i.e.,

$$2(u(h) - u(0))/h^2 = u_{xx}(0) + \frac{h}{3}u_{xxx}(0) + \cdots \tag{5}$$

when $u_x(0) = 0$.

However, our original logic is correct; second-order approximations of the boundary conditions and equations lead to second-order accurate solutions. There are a number of ways to show this. One technique, involving asymptotic error expansions, is shown in the subsection below. Here, we prove that, in fact, the discrete solutions U^h tend asymptotically to $u + h^2u^{(2)} + O(h^4)$, where $u^{(2)}(x)$ is a smooth function. This implies that

$$\lim_{h\to 0} \|U^h - u\|/h^2 = K, \tag{6}$$

where $K = \|u^{(2)}\|$ is a constant independent of h. We use maximum norms throughout the paper. We demonstrate this asymptotic second order convergence with discrete solutions to the model problem described above in Table I.

While this is not so surprising, the following fact is: the expressions (4) also give asymptotic second order accurate values for u_{xx}. This is certainly not intuitive since the exact solution has a first-order error in this expression as shown by (5). We demonstrate the second-order convergence numerically for our model problem in Table II. Second-order convergence is also seen for D_2U in the interior of the domain. This phenomenon is due to a matching of error terms at the boundary as shown by the asymptotic error analysis below. We call this effect discrete compatibility.

TABLE II

Normalized Second-Order Errors in D_2U_0 for the Model Elliptic Problem

$N = 1/h$	$\|D_2U_0 - u_{xx}(0)\|/h^2$
8	0.3324e − 1
16	0.3328e − 1
32	0.3329e − 1
64	0.3329e − 1

2.1.1. *Asymptotic Error Analysis*

In this section we show the asymptotic result discussed above. We determine $u^{(2)}$ so that $\tilde{u} = u + h^2u^{(2)}$ satisfies the discrete equations (2) and boundary conditions (3) to fourth-order accuracy. We plug $\tilde{u}$ into the discrete equations, expand in Taylor series, and equate terms with the same powers of h. At order zero, we recover the original equation for u (i.e., the scheme is consistent). At order 2 (h^2) we get

$$u^{(2)\prime\prime} - u^{(2)} = -\tfrac{1}{12}u^{\prime\prime\prime\prime} \tag{7}$$

from (2) and

$$u^{(2)\prime}(0) = -\tfrac{1}{6}u^{\prime\prime\prime}(0) \tag{8}$$

and a similar term at $x = 1$ from (3), where the terms on the right-hand sides of the two equations above come from the second-order errors in D_2 and D_1, respectively. The requirements for $u^{(2)}$ above are a solvable problem with smooth solution. Because there are only even powers of h in the trunction error, $\tilde{u}$ now satisfies (2), (3) to fourth-order accuracy.

We rewrite the first term of (4) as it was derived,

$$D_2\tilde{u}_0 = \frac{\tilde{u}_{-1} - 2\tilde{u}_0 + \tilde{u}_1}{h^2} + \frac{\tilde{u}_1 - \tilde{u}_{-1}}{h^2},$$

where $\tilde{u}_1$ is the smooth extension of $\tilde{u}$ through the boundary. The first term on the right-hand side matches the interior discretization and leads to a fourth-order accurate expression in the discrete equations; the second term is $O(h^3)$ from (8). Therefore the truncation error of $\tilde{u}$ in the discrete equations is $O(h^4)$ in the interior and $O(h^3)$ at the boundary. In this paper we will concern ourselves with questions about the accuracy rather than stability of various numerical methods. All schemes considered here have been proven to be stable. Standard stability estimates for this problem [19] show that $\|U - \tilde{u}\| \leq Kh^3$, which from the form of $\tilde{u}$ proves (6).

If we include a further term in the asymptotic series (i.e., $\tilde{u} = u + h^2u^{(2)} + h^4u^{(4)}$, where $u^{(4)}$ satisfies equations and boundary conditions from h^4 terms) then we can show that

$$\|U - \tilde{u}\| \leq Ch^5. \tag{9}$$

Following the argument above we can show that

$$D_2\tilde{u}_0 = u''(0) + h^2 u^{(2)''}(0) + \frac{h^2}{12} u''''(0) + O(h^4).$$

Combining this result and (9) we see that

$$D_2 U_0 = u''(0) + h^2 u^{(2)''}(0) + \frac{h^2}{12} u''''(0) + O(h^3), \qquad (10)$$

or D_2U_0 converges asymptotically with second order as observed above. The essential idea here is that asymptotic error terms match errors near the boundary, giving a higher order convergence rate than expected. This is the phenomenon we call discrete compatibility.

2.1.2. *Discussion of Asymptotic Error Techniques*

The idea of asymptotic error expansions for discrete equations was first considered by Strang [21]. In that first work and other applications, i.e., [5, 16], the use of the expansions was to handle the stability of nonlinear terms. In this paper and other works [11, 12] the error expansions can be used to explain some confusing issues of how the errors from boundary terms enter the solutions. In some sense, there are not the ideal tools to use since they require solutions to be smooth, which is often not the case. In the process above, we use the smoothness of the solutions essentially to overcome some weaknesses in the stability arguments. However, error expansions do provide insight into some confusing numerical issues such as that described above and the predictions are often valid in situations where the smoothness assumptions break down as seen in the next section and Section 3.1.2.

2.2. Time-Dependent (Parabolic) Problems

We now turn to a time-dependent model problem. Behaviour similar to that described above is obtained for time continuous or method of lines FD spatial discretizations. As above we consider a specific simple model, to find $u(x, t)$ for $t \geq 0$, $x \in [0, 1]$, that satisfies

$$u_t = \nu u_{xx}$$

with initial data $u(x, 0) = \sin(\pi x)/\pi$ and Neumann boundary conditions

$$u_x(0, t) = \sin t + 1, \quad u_x(1, t) = -1.$$

In the computations described below we take $\nu = 0.01$.

We consider spatial approximations on a regular grid as above, continuous in time, i.e., $U_i(t) \approx u(ih, t)$ for $i = 0, 1, ..., N$. As above we use second-order centered approximation of the boundary conditions to modify the stencils near the boundaries. Here,

TABLE III

Normalized Second-Order Errors in D_2U_0 at $t = \frac{1}{4}$ for the Model Parabolic Problem

$N = 1/h$	$\lvert D_2^h U_0^h - D_2^{2h} U_0^{2h} \rvert / h^2$
32	1265
64	1229
128	1228
256	1228
512	1229

$$\begin{aligned} D_2U_0 &= 2(U_1 - U_0 - h(\sin t + 1))/h^2, \\ D_2U_N &= 2(U_{N-1} - U_N - h)/h^2. \end{aligned} \qquad (11)$$

In this time-dependent computation and others described below, we use explicit fourth-order Runge–Kutta time-stepping with very small time steps; the results reported essentially have no temporal errors. As above, we observe asymptotic second-order convergence in U. This follows a similar asymptotic analysis as above and is discussed in the next section for this problem. For $t > 0$ this behaviour is also seen for D_2U_0. To examine the asymptotic error we consider

$$\lim_{h \to 0} \tfrac{1}{3} \lvert D_2^h U_0^h - D_2^{2h} U_0^{2h} \rvert / h^2,$$

i.e., we compare numerical solutions at double grid spacing. The asymptotic results show that this also should tend to the asymptotic second-order error constant K (for $t > 0$). This is clearly shown in Table III.

At $t = 0$ the formula for D_2U_0 in (11) involves the initial data $u(x, 0)$ and is *first-order accurate*. At $t = 0$ there are no second-order error terms present to correct for this error. To reconcile this with the observation of second-order convergence for $t > 0$ above, we must have $\lim_{t \to 0} K(t) = \infty$. We observe the rate of growth in $K(t)$ in Table IV. We see that $\lim_{t \to 0} K(t) = \infty$ as predicted. It becomes

TABLE IV

Estimated $K(t)$ for the Model Parabolic Problem, Ratios of Successive K's, the Number N_r of Grid Points Needed to Resolve $K(t)$ to 1% Accuracy

t	$3K(t)$	N_r	$K(t/2)/K(t)$
$\frac{1}{4}$	1229	128	1.20
$\frac{1}{8}$	1471	256	1.28
$\frac{1}{16}$	1876	512	1.37
$\frac{1}{32}$	2508	1024	1.37
$\frac{1}{64}$	3445	1024	1.39
$\frac{1}{128}$	4791	2048	1.41
$\frac{1}{256}$	6732	2048	1.41
$\frac{1}{512}$	9469	4096	

harder to resolve $K(t)$ for t small, but convergence is still asymptotically second order. It is also observed that if t is halved, K increases by a factor of $1.41 \approx \sqrt{2}$. This is consistent with the formula $K(t) \sim C/\sqrt{t}$. We show formally why this is true in the next section.

2.2.1. *Asymptotic Error Analysis and Small Time Behaviour*

As before, we consider an asymptotic error expansion for the discrete solution $\tilde{u} = u + h^2 u^{(2)}$. Here, $u^{(2)}$ obeys the equation

$$u_t^{(2)} = \nu u_{xx}^{(2)} - \frac{\nu}{12} u_{xxxx}$$

and boundary condition

$$u_x^{(2)}(0, t) = -\tfrac{1}{6} u_{xxx}(0, t) \tag{12}$$

with a similar condition at $x = 1$. At time 0 we make no error so $u^{(2)}(x, 0) \equiv 0$. This is a problem that has a solution near $t = 0$ in the sense of distributions only (discussed below) but with smooth solution for $t > 0$. We can consider higher order terms in the expansion and derive (10) as above, also valid for $t > 0$. Let us now consider the difficulty at $t = 0$. The second-order error expression for $D_2 U_0$ involves $u_{xx}^{(2)}(0, t)$ and $u_{xxxx}(0, t)$. However, the values for $u_x^{(2)}(0, 0)$ from initial and boundary data do not match at $(0, 0)$. From the initial data $u_x^{(2)}(0, 0)$ is 0 but from (12) it is $-1/(6\nu)$ (obtained by differentiating the interior equation to get $u_{xxx}(0, 0) = (1/\nu) u_{xt}(0, 0)$ and evaluating the right-hand side by differentiating the boundary data in time). This is called an incompatibility in the initial data.

To give the idea for the behaviour of the solution in this situation, we consider a similar effect in the unbounded case $u(x, t)$ with $x \in (-\infty, \infty)$ (this can be related to the present case by extending the solution in a suitable manner through the boundary). We consider initial data $u(x, 0) = u_0(x)$ that is smooth, except for a jump in the derivative at $x = 0$. The solution is

$$\begin{aligned} u(x, t) = G * u_0 &:= \int G(\xi, t) u_0(x - \xi)\, d\xi \\ &= \int G(x - \xi, t) u_0(\xi)\, d\xi, \end{aligned} \tag{13}$$

where

$$G(x, t) = \sqrt{1/4\nu\pi t}\, e^{-x^2/(4\nu t)} \tag{14}$$

is the Green's function for the heat equation.

For $x > 0$ we can take a derivative of the first integral expression to get

$$u_x(x, t) = \int G(\xi, t) u_0'(x - \xi)\, d\xi$$

which behaves boundedly as $t \to 0$ for $x > 0$ and right limiting values at $x = 0$. For the next derivative, we switch this to the form of the second integral expression in (13) and take the derivative of G:

$$u_{xx}(x, t) = -\frac{1}{2\nu} \int \frac{x - \xi}{t} G(x - \xi, t) u_0'(\xi)\, d\xi.$$

We change variables $\tau = (x - \xi)^2/t$ to get

$$u_{xx}(x, t) = \frac{1}{4\nu} \sqrt{1/\nu t} \int_0^\infty e^{-\tau/(4\nu)} u_0'(x + \sqrt{t\tau})\, d\tau,$$

plus another similar integral for negative τ. Except for the $1/\sqrt{t}$ term above, the remaining integral remains bounded as $t \to 0$ for $x > 0$ and right limiting values. What we have shown here is just that a discontinuity in the first derivative of the initial data acts as a δ-function source for the second derivative.

We now examine the other term ($u_{xxxx}(0, t)$) in the second-order error for $D_2 U_0$. This term will also give trouble at $t = 0$ since there is a mismatch in $u_{xxx}(0, 0)$. From the initial data, u_{xxx} is $-\pi^2$. As above we also calculate $u_{xxx}(0, 0) = 1/\nu$, using the boundary data. This incompatibility in u_{xxx} at $(0, 0)$ leads to growth like $C/\sqrt{t}$ in $u_{xxxx}(0, t)$ as $t \to 0$, using the same arguments as above. Thus both parts of the error in $D_2 U_0$ have this behaviour. The term u_{xxxx} also appears as a singular source term in the equation for $u^{(2)}$ but this effect is of lower order as $t \to 0$.

The incompatibility in u_{xxx} comes from the continuous problem. However, in Section 5 we show that the continuous problem can be compatible at all orders but incompatibilities can occur in the equations for the asymptotic error expansion equations. We note that additional terms in the error expansion will grow faster as $t \to 0$; i.e., the fourth-order error terms in $D_2 U_0$ will grow like $t^{-3/2}$. This is what makes the computations above so hard to resolve for small t.

2.3. Summary of the Phenomenon and Analysis

We intend this paper as a practical guide to understanding some aspects of the way the errors from boundary conditions enter the discrete solutions. Some analysis is presented above for 1D model elliptic and parabolic computations to give the flavour of the arguments. The results show that the error introduced into the discrete solution at the boundary occurs at the order at which the underlying boundary condition is approximated. Even derived quantities can converge with the overall accuracy for $t > 0$ (however, this is not true for higher order wide schemes where numerical boundary layers are present). If the derived quantities are not compatible at $t = 0$ (i.e., their accuracy is less than predicted for $t > 0$) then the error constant for these quantities behaves like C/t^p as $t \to 0$ for some $p > 0$. We consider model cases which have different values of p in Section 5. We note that for hyperbolic problems data incompatibilities are not smoothed out and can be observed in computations for $t > 0$ [17].

In the next two sections, we will extend these results to incompressible fluid flow problems in higher dimensions. Some of the extensions are rigorous, but others pose tough analytical questions. We verify all predictions with careful numerical tests.

3. VORTICITY-STREAMFUNCTION ($\omega - \psi$) METHODS

We consider now the type of phenomenon discussed above in the context of finite difference methods for incompressible flow. We limit the discussion to 2D flow for simplicity, although our results also apply to 3D flows as well. First, we consider $\omega - \psi$ methods and then primitive variable methods in the next section. The equations for incompressible flow in vorticity form are

$$\omega_t + \mathbf{u} \cdot \nabla\omega = \nu\,\Delta\omega, \tag{15}$$

where $\mathbf{u} = (u, v)$ is the velocity vector, $\omega = v_x - u_y$ is the vorticity, and ν is the kinematic viscosity. Using the incompressibility condition $\nabla \cdot \mathbf{u} = 0$, we can introduce a stream function ψ that satisfies

$$\psi_x = -v; \quad \psi_y = u: \quad \Delta\psi = -\omega. \tag{16}$$

We consider a single boundary at $y = 0$ at which we specify no-flow $\psi = 0$ and given slip $\psi_y(x, 0) = u_s(x)$ velocity.

We approximate values on a regular grid with spacing h in both directions (we still consider continuous time approximations), i.e., $\Psi_{i,j}(t) \approx \psi(ih, jh, t)$ and Ω approximates ω values similarly. We use standard second-order centered differences in space to approximate the equations. Details can be found in, e.g., [11]. At the boundary we use Thom's [23] first-order $\omega - \psi$ boundary condition

$$\Omega_{i,0} = -\frac{2(\Psi_{i,1} - hu_s(ih))}{h^2}. \tag{17}$$

This boundary condition is first-order accurate as written. However, it can be derived from the formal relationship

$$\frac{\Psi_{i,1} - \Psi_{i,-1}}{2h} = u_s(ih)$$

which is a second-order accurate approximation of the slip condition. As in the model problems in Section 2, this leads to second-order convergence of the solution, including the boundary vorticity, for both steady state and time-dependent (for $t > 0$) computations. The corresponding error expansion analysis is presented in [11], although the fact that this led to second-order accurate boundary vorticity values was not recognized at that time. The details of the matching of the discrete error terms at the boundary are shown in [15] for the steady Stokes case.

Below, we show computational evidence for second-order convergence of boundary vorticity, first in a smooth steady case, then in a steady case that violates the smoothness assumptions of the analysis, and finally in a time-dependent case. Numerical resolution of the behaviour near $t = 0$ shows blowup of $C/\sqrt{t}$ in the second-order error coefficient for boundary vorticity computed using (17).

3.1. Steady State Computations

We do two steady state numerical computations below. The first is in a periodic channel, where the solution is smooth and our asymptotic error analysis above is justified rigorously. The second is the ubiquitous driven cavity, where higher derivatives do not exist in the domain corners and so the asymptotic analysis is only formal. Still, second-order convergence in boundary vorticity is seen computationally away from the corners.

3.1.1. *Periodic Channel* (*Smooth*) *Computation*

We compute flow in the square domain $[0, 1] \times [0, 1]$, periodic in the horizontal x direction with walls at the top and bottom of the domain. The wall $y = 0$ is fixed (no-flow and no-slip) and the upper wall $y = 1$ has slip velocity $u_s(x) = \cos(\cos(2\pi x))$. This slip velocity is 1-periodic and has components at all wavenumbers. Calculations based on the $\omega - \psi$ formulation were performed with $\omega = 0.01$ (leading to a Reynolds number Re = 100). The moderate Reynolds number and the simple geometry here and in other computations allow us to resolve the subtle numerical effects completely.

Interior values of the streamfunctions and the vorticity converge with second order. The computational results shown in Table V show that boundary vorticity also converges with second order (recall the numbers shown in the table should tend to a constant as $h \to 0$ if the scheme converges asymptotically with second order) as predicted by our theory.

3.1.2. *Driven Cavity* (*Nonsmooth*) *Computation*

In this section we describe steady state computations in the smoothed driven cavity problem (see, e.g., [18, p. 199]) with slip velocity on the upper surface of $u_s(x) = x^2(1 - x)^2$. Viscosity is chosen to give Re = 100. Even

TABLE V

Normalized Second-Order Errors in Computed Boundary Vorticity Ω_b for the Periodic Channel Calculation

$N = 1/h$	$\|\Omega_b^h - \Omega_b^{2h}\|/(3h^2)$
80	4.30e3
120	4.91e3
160	5.10e3
200	5.17e3

TABLE VII

Normalized Second-Order Errors in Computed Boundary Vorticity Ω_b for the Time-Dependent Calculation at $t = \frac{1}{8}$

$N = 1/h$	$\|\Omega_b^h - \Omega_b^{2h}\|/(3h^2)$
32	128
64	174
128	184
256	186

though this data is smoothed to avoid the worst singularities in the upper corners, the solution still has singularities in higher derivatives of the solution in the corners and so the asymptotic results above do not apply directly in this case. However, formally the analysis still applies away from the corners and we still observe second-order convergence in boundary vorticity. We consider the boundary vorticity Ω_{b*}, excluding portions of the boundary of distance less than $\frac{1}{10}$ from the corner. Second-order convergence of Ω_{b*} is shown in Table VI.

Convergence is second order if a region near the corners, however small, is excluded, although the convergence becomes harder to resolve. Second-order convergence of the boundary vorticity including the corner is not obtained, although the streamfunction values do converge with second order up to the corner. A careful analysis involving the corner singularity structure would explain these results more fully.

3.2. Time-Dependent Computation

We consider time-dependent flow in the periodic channel geometry, beginning with streamfunction values

$$\psi(x, y) = (3y^2 - 2y^3) + 16y^2(1 - y)^2 \sin(2\pi x)/(2\pi). \quad (18)$$

The first term of (18) is unit Poiseuille flow and the second term is a perturbation. We take viscosity $\nu = 0.1$ leading to Re ≈ 17. This represents a very viscous flow, where the perturbation will die out. It is again an "easy" computation which will allow us to resolve the asymptotic numerical behaviour. We use 4RK time-stepping to make the temporal error negligible as before. From our analysis (formal because there are incompatibilities at $t = 0$ discussed below) we expect second-order convergence in the boundary vorticity for $t > 0$. This is observed in Table VII. At $t = 0$, however, the boundary voriticity converges only with first-order accuracy as predicted by the straightforward Taylor series analysis. We have the same situation as in the introductory model of Section 2 and can argue formally that a mismatch of order h to h^2 at $t = 0$ in a second-order (nonlocal here) parabolic problem will lead to a $C/\sqrt{t}$ behaviour in the second-order error coefficient as $t \to 0$. The analysis of the effect of incompatibilities at $t = 0$ in the Navier–Stokes equations presented in [9] supports this reasoning. We show $K(t)$, the second-order constant associated with boundary vorticity (i.e., $K(\frac{1}{8}) \approx 186$ Table VII), for $t \to 0$ in Table VIII. We resolve $K(t)$ only to 10% since it is hard to resolve this further for this 2D computation. The results are consistent with the hypothesis $K(t) \sim C/\sqrt{t}$ (recall this is consistent if the last column in Table VIII tends to $\sqrt{2} \approx 1.41$).

4. PRIMITIVE VARIABLE METHODS

We now consider a method based on the primitive variable formulation of the Navier–Stokes equations in the periodic channel. The equations are

TABLE VI

Normalized Second-Order Errors in Computed Boundary Vorticity Ω_b Excluding Corners for the Driven Cavity Calculation

$N = 1/h$	$\|\Omega_{b*}^h - \Omega_{b*}^{2h}\|/(3h^2)$
80	1.81e2
120	1.61e2
160	1.55e2
200	1.53e2

TABLE VIII

Estimated $K(t)$ for Boundary Vorticity from the $\omega - \psi$ Computation, Ratios of Successive K's, the Number N_r of Grid Lines in Each Direction Needed to Resolve $K(t)$ to 10% Accuracy

t	$K(t)$	N_r	$K(t/2)/K(t)$
$\frac{1}{32}$	252	128	1.25
$\frac{1}{64}$	315	256	1.31
$\frac{1}{128}$	413	512	1.36
$\frac{1}{256}$	562	512	1.44
$\frac{1}{512}$	810	512	

$$\mathbf{u}_t = -\mathbf{u}\cdot\nabla\mathbf{u} + \nu\,\Delta\mathbf{u} - \nabla p \tag{19}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{20}$$

where p is the pressure. Initial data $\mathbf{u}_0 = (u_0, v_0)$ are given that are derived from the streamfunction initial data (18). Viscosity is taken as 0.1 as above.

We consider a discretization based on the staggered MAC grid, where

$$\mathbf{U}_{i,j}(t) = (U_{i,j}(t), V_{i,j}(t)) \quad \text{and} \quad P_{i,j}(t) \tag{21}$$

approximate

$$u((i+\tfrac{1}{2})h, (j-\tfrac{1}{2})h, t), \quad v(ih, jh, t), \quad p(ih, (j-\tfrac{1}{2})h, t). \tag{22}$$

Since the U (slip velocity) points are not on the boundary, the no-slip condition must be approximated. We use the so-called reflection conditions at the lower boundary

$$U_{i,0} = -U_{i,1} \tag{23}$$

with a similar expression at the upper boundary. These relationships are derived from an approximation of the no-slip condition by linear interpolation (second-order accurate). A short, centered difference approximation of the vorticity is

$$\Omega_{i,j} = \frac{V_{i+1,j} - V_{i,j}}{h} - \frac{U_{i,j+1} - U_{i,j}}{h}.$$

Note that $\Omega_{i,j} = \omega((i+\frac{1}{2})h, jh)$ to second order. However, the use of (23) in the expression for the boundary vorticity

$$\omega(x,0) = u_y(x,0) \approx \Omega_{i,0} = 2U_{i,1}/h$$

is formally only first-order accurate. The same results as in the examples considered above apply here. For steady state computations and for time-dependent computations for $t > 0$ second-order convergence in computed boundary vorticity is seen. The error expansion analysis is presented in [12], although this fact was not realized in this work. At $t = 0$ the boundary vorticity is only first-order accurate and in the transition from second-order accuracy at $t \to 0$ the second-order constant in the error for the computed boundary vorticity behaves like $C/\sqrt{t}$. This is shown in

TABLE IX

Estimated $K(t)$ for Boundary Voriticity from the Primitive Variable Computation, Ratios of Successive K's, the Number N_r of Grid Lines in Each Direction Needed to Resolve $K(t)$ to 10% Accuracy

t	$K(t)$	N_r	$K(t/2)/K(t)$
$\frac{1}{64}$	25.19	64	1.36
$\frac{1}{128}$	34.38	64	1.37
$\frac{1}{256}$	46.95	128	1.38
$\frac{1}{512}$	64.92	256	1.42
$\frac{1}{1024}$	92.23	256	

Table IX. Simple models similar to those in Section 2 can be used to predict this behaviour. The results are obtained using simple centered difference codes like those described in [12] modified to use the more accurate 4RK time-stepping.

Using the ideas in [26] it can be shown that the computed pressure at $t = 0$ is only first-order accurate due to the discrete incompatibility of the reflection condition but formally second order for $t > 0$. In Table X we observe that the second-order error constants for P also behave like $C/\sqrt{t}$ as $t \to 0$.

5. MORE MODEL PROBLEMS

We presented a simple 1D model of discrete compatibility in Section 2 and then showed how this same phenomenon occurred in 2D incompressible flow calculations in Sections 3 and 4. Now, we return to 1D model problems to investigate this idea in more detail.

5.1. Stronger Incompatibilities

We return again to the model parabolic problem of Section 2.2 with the same boundary data $u_x(0, t) = \sin t + 1$, $u_x(1, t) = -1$, but with different initial data, $u_0(x) = \sin(\pi x)/\pi + x$. Here $u_0'(0) = 2$ but the boundary data predict $u_x(0, 0) = 1$. This is a strong data incompatibility (like a tangential impulsive start for incompressible fluid

TABLE X

Estimated Second-Order Error Constant $K(t)$ for Pressure from the Primitive Variable Computation and Ratios of Successive K's

t	$K(t)$	$K(t/2)/K(t)$
$\frac{1}{64}$	28.2	1.38
$\frac{1}{128}$	38.9	1.40
$\frac{1}{256}$	52.1	1.34
$\frac{1}{512}$	72.1	1.38
$\frac{1}{1024}$	96.3	

TABLE XI

Estimated Second-Order Error Constant $K(t)$ for the Approximation of the Second Derivative on the Boundary for the 1D Parabolic Model Problem with Strong Data Discontinuity and the Ratios of Successive K's

t	$K(t)$	$K(t/2)/K(t)$
$\frac{1}{4}$	1225	2.43
$\frac{1}{8}$	2973	2.57
$\frac{1}{16}$	7647	2.70
$\frac{1}{32}$	20,390	2.76
$\frac{1}{64}$	56,280	2.81
$\frac{1}{128}$	158,200	

flow). Approximations of the second derivative at the boundary will still be second-order accurate for $t > 0$. The second-order error constant has terms proportional to $u_{xxxx}(0, t)$ and $u_{xx}^{(2)}(0, t)$. Following the reasoning of Section 2.2.1 we see that $u_{xx}(0,t)$ behaves like $C/\sqrt{t}$. Taking two more derivatives of the Greens function we obtain $u_{xxxx}(0, t) \sim C/t^{3/2}$. Careful examination shows that the second term $u_{xx}^{(2)}$ also has this behaviour. We observe this in Table XI. Note that $2^{3/2} \approx 2.83$.

In this case, convergence even in values U_0 at the boundary is affected. Computations show that these values converge with second order for $t > 0$, but that the second-order error coefficients blow up like $C/\sqrt{t}$ for this example as shown in Table XII.

5.2. Purely Discrete Incompatibility

We have examined the effect of incompatibilities in the continuous problem and in the error terms on the error constants of computed differences at the boundary. In the example below, we see that the original problem can be compatible to all orders, but incompatibilities can still be introduced in the discrete scheme. We consider the parabolic problem of Section 2.2 with modified boundary data

TABLE XII

Estimated Second-Order Error Constant $K(t)$ for the Approximation of the Solution on the Boundary (U_0) for the 1D Parabolic Model Problem with Strong Data Discontinuity and the Ratios of Successive K's

t	$K(t)$	$K(t/2)/K(t)$
$\frac{1}{4}$	2.22	2.04
$\frac{1}{8}$	4.54	1.63
$\frac{1}{16}$	7.44	1.52
$\frac{1}{32}$	11.3	1.46
$\frac{1}{64}$	16.5	1.44
$\frac{1}{128}$	23.7	

TABLE XIII

Estimated Second-Order Error Constants $K(t)$ for the Approximation of the Second Derivative at the Boundary for the Pure Discrete Incompatibility Case

t	$K(t)$	$K(t/2)/K(t)$
$\frac{1}{32}$	1701	1.37
$\frac{1}{64}$	2332	1.40
$\frac{1}{128}$	3253	1.41
$\frac{1}{256}$	4584	

$$u_x(0, t) = t; \quad u_x(1, t) = 1/2\nu$$

and initial data

$$u_0(x) = x^3/6\nu.$$

At (0, 0) the compatibility conditions of all orders are satisfied: $u_x(0, 0) = 0$ from both initial and boundary data, $(d/dt)u_x(0, 0) = \nu u_{xxx}(0, 0) = 1$; and so on. However, the compatibility conditions for $u^{(2)}$ (the second-order error expansion term) are violated. Referring to Section 2.2.1 we see that $u_0^{(2)}(x) \equiv 0$, so $u_x^{(2)}(0, 0) = 0$ from the boundary data. However, $u^{(2)}$ has boundary data

$$u_x^{(2)}(0, t) = -\tfrac{1}{6}u_{xxx}(0, t)$$

which predicts $u_x^{(2)}(0, 0) = -1/(6\nu)$. This is a strong incompatibility in $u^{(2)}$. Since the second-order error in D_2U_0 has a term proportional to $u_{xx}^{(2)}$ we expect to see $C/\sqrt{t}$ blow up in the error constant and we do observe it computationally, as shown in Table XIII. This shows that data incompatibilities can be introduced by finite difference schemes; it is not just a matter of checking the compatibility of the continuous problem.

5.3. Higher Order Boundary Extrapolation

We could also use a higher order formula to approximate the derivative condition at $x = 0$. For instance, we could use the third-order approximation

$$\frac{-2U_{-1} - 3U_0 + 6U_1 - U_2}{6h} = g$$

to $u_x(0) = g$. After eliminating U_{-1} this leads to the expression

$$D_2U_0 = \frac{-7U_0 + 8U_1 - U_2 - 6hg}{2h^2}. \tag{24}$$

This is a second-order approximation to $u_{xx}(0)$, even by

TABLE XIV

Estimated Second-Order Error Constants $K(t)$ for the Approximation of the Second Derivative at the Boundary for the Original Model with Weak Incompatibility Using Third-Order Extrapolation

t	$K(t)$	$K(t/2)/K(t)$
$\frac{1}{32}$	875	1.37
$\frac{1}{64}$	1206	1.39
$\frac{1}{128}$	1680	1.40
$\frac{1}{256}$	2351	

formal Taylor series analysis. It corresponds to the Wilkes $\omega - \psi$ boundary condition (see, e.g., [18, p. 186]).

At $t = 0$ the calculated values from (24) will be second order, as well as for $t > 0$. If the continuous problem has a weak incompatibility, then the second-order error coefficients for this expression will still behave like $C/\sqrt{t}$ as $t \to 0$ since the error term for this expression will have a term proportional to u_{xxxx}. We return to the original model problem of Section 2.2 using the third-order extrapolation above and observed this behaviour in Table XIV.

However, if we use the higher order scheme, where the underlying continuous problem is compatible, we can delay the singular behaviour of the error to higher order error terms. For instance, if we use the third-order scheme for the problem from the section above, the problem for $u^{(2)}$ will have $u_x^{(2)}(0, t) \equiv 0$ (since our scheme implements the boundary condition to third-order accuracy, we make no error at second order). Now, the problem for $u^{(2)}$ is compatible and so $u_{xx}^{(2)}$ is bounded as $t \to 0$. The discrete incompatibility will occur in the third-order error term $h^3 u^{(3)}$. Therefore, we would expect the second-order error in (24) to remain bounded as $t \to 0$ in this case. This is seen in Table XV, where we modify the initial data of Section 5.2 to $u_0(x) = x^3/(6\nu) + 100x^4$. The term $100x^4$ does not effect compatibility (only odd derivative terms do for the Neumann problem), but it gives a large constant second-order error term to help us resolve this against the singular third-order error term.

TABLE XV

Estimated Second-Order Error Constants $K(t)$ for the Approximation of the Second Derivative at the Boundary for the Pure Discrete Incompatibility Case

t	$K(t)$
$\frac{1}{32}$	516
$\frac{1}{64}$	530
$\frac{1}{128}$	532
$\frac{1}{256}$	524

In general, it is not possible to guarantee that initial data for the continuous problem is compatible, especially for incompressible flow where the conditions are nonlinear and nonlocal [9]. Therefore, using higher order boundary conditions to avoid discrete incompatibilities is not really an issue since in general there will always be incompatibilities from the continuous problem. Rather, we presented the above material just to gain insight into the behaviour of incompatibilities on the discrete scheme. Of course, using higher order boundary conditions may be useful in reducing the size of errors after the incompatibility has been smoothed out [25].

6. DISCUSSION

We have presented the idea of discrete compatibility in finite difference methods for elliptic and parabolic problems. Convergence in the discrete solution is observed at an order equal to the minimum of the accuracy of the interior equations and the boundary conditions as expected. For steady state problems and time dependent problems for $t > 0$, convergence of derived quantities at the boundary is seen at this same order, even when local truncation error analysis predicts lower order convergence. We show this rigorously for smooth steady problems and formally for time-dependent problems. For the computational PDE practitioner, these ideas should explain some confusing issues around the nature of approximation at the boundary. Through formal analysis and computational studies, we resolve the transition between the lower order convergence rate at $t = 0$ and the rate for $t > 0$. For incompressible flow computations, we show that these ideas can fully explain the approximation of vorticity at the boundary using Thom's vorticity boundary condition or reflection boundary conditions for the slip velocity in a MAC grid primitive variable computation.

We have restricted our analysis here to the case of semi-discrete schemes (continuous in time) and have used very accurate time stepping techniques to approximate this idealized situation in our numerical studies. For more realistic time-stepping methods we expect to observe the same kind of transition from a lower (at $t = 0$) to a higher order ($t > 0$) accurate approximation at the boundary. This is observed in [25], for example. However, we believe the exact behaviour depends on the discrete smoothing properties of the combined spatial and temporal discretization (see [22] for a discussion of these ideas without the effects from the boundary). This will be the subject of further investigation.

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