Computers Math. Applic. Vol. 22, No. 8, pp. 73–81, 1991
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0097-4943/91 $3.00 + 0.00
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PREDICTOR AND STEPLENGTH SELECTION IN CONTINUATION METHODS FOR THE NAVIER-STOKES EQUATIONS

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(Received March 1991)

Abstract—Continuation methods are in common use for solving the nonlinear equations resulting from discretizations of the Navier-Stokes equations. An important ingredient in these algorithms is the selection of the step size in the continuation parameter. For certain values of the Reynolds number, it is shown that the step size in the Reynolds number may be chosen independently of the particular predictor step used within the continuation algorithm. Estimates for the path derivatives are derived and used to show that the allowable step sizes are substantially greater than would be predicted by theories that apply to general nonlinear mappings.

1. INTRODUCTION

The approximation of the solution of the Navier-Stokes equations is an area of considerable interest. In practice, it is often the case that the solution is desired for some given value of the Reynolds number and that knowledge about the smoothness of the solution curve is available from experimental data. Since discretizations of the Navier-Stokes equations lead to a system of nonlinear equations, iterative methods must be employed. Methods of this type, such as Newton or quasi-Newton methods, are based on a linearization of these nonlinear equations and converge only if a "sufficiently good" initial guess is available. A popular approach for accomplishing this task is to use continuation methods. A brief description of these methods is given in Section 2 in the context of general mappings from $\mathbb{R}^{n+1} \to \mathbb{R}^n$.

The goal of this paper is to show that if a continuation method is applied to the nonlinear system of equations which result from discretizations of the Navier-Stokes equations, then more precise information can be determined concerning choices of predictor methods and step sizes in the Reynolds number. This is applicable only to portions of the solution curve where there are no singular points. The results given here apply equally well to all versions of the Navier-Stokes equations, e.g., primitive variable, streamfunction-vorticity, etc., and to any discretization method, e.g., finite difference, spectral, finite element, etc. However, only Galerkin-type methods for the primitive variable version will be considered here. In Section 3, a specific discretization of the Navier-Stokes equations is given along with certain properties that the approximating subspaces must satisfy in order to guarantee that the discretization is stable and the solution is optimally accurate. In Section 4, estimates for the path derivatives in terms of the norm of the solution of the original problem are derived. In Section 5, Newton's method is applied to the nonlinear system of equations that arise from the discretization of the Navier-Stokes equations. The main result of the paper is given in Section 6. Here it is shown that the step size that may be chosen is largely independent of the particular predictor used with the continuation algorithm. Finally, in Section 7, some numerical examples which illustrate the results of the previous sections are presented.

*Research was partially supported by the Air Force Office of Scientific Research under Grant No. AFOSR-88-0197.
**Work performed under the auspices of the U.S. Department of Energy in the Computing and Communications Division, Los Alamos National Laboratory, Los Alamos, NM 87545.

2. THE BASIC CONTINUATION METHOD

In this section, continuation methods are briefly described in the context of a general mapping $F(\mathbf{u},\lambda) : \mathbb{R}^{n+1} \to \mathbb{R}^n$, where $\mathbf{u} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$. Here, λ may be a parameter that appears naturally, such as the Reynolds number for the discrete Navier-Stokes equations, or it may be an artificially introduced parameter such as the arc length along a solution branch [1,2]. The goal is to find a $\mathbf{u}^*$ such that $F(\mathbf{u}^*,\lambda^*) = 0$ for some given value $\lambda = \lambda^*$. It is assumed that a solution $\tilde{\mathbf{u}}$ is known for some $\tilde{\lambda} < \lambda^*$, i.e., $F(\tilde{\mathbf{u}},\tilde{\lambda}) = 0$. The solution at $\lambda = \lambda^*$ is obtained by starting with the known solution at $\lambda = \tilde{\lambda}$ and then following the solution curve $\mathbf{u}(\lambda)$ for $\lambda \in [\tilde{\lambda},\lambda^*]$, where $F(\mathbf{u}(\lambda),\lambda) = 0$. This curve is determined through a predictor-corrector procedure. First, an approximation $\mathbf{u}_0$ for $\mathbf{u}(\lambda)$ is predicted for some $\lambda \in (\tilde{\lambda},\lambda^*]$; a common choice of the predictor is to follow the tangent line to the curve at the known point $(\tilde{\lambda},\mathbf{u}(\tilde{\lambda}))$. Thus,

$$\mathbf{u}_0 = \mathbf{u}(\tilde{\lambda}) + \Delta\lambda \left.\frac{d\mathbf{u}}{d\lambda}\right|_{\tilde{\lambda}}, \qquad \text{where } \Delta\lambda = \lambda - \tilde{\lambda}. \tag{2.1}$$

Here the tangent vector $d\mathbf{u}/d\lambda$ is obtained by differentiating the defining relation $F(\mathbf{u}(\lambda),\lambda) = 0$; i.e.,

$$\frac{d\mathbf{u}}{d\lambda} = -\big(F_u(\mathbf{u}(\lambda),\lambda)\big)^{-1} F_\lambda(\mathbf{u}(\lambda),\lambda), \tag{2.2}$$

where $F_u(\mathbf{u},\cdot)$ denotes the $n \times n$ Jacobian matrix of F with respect to $\mathbf{u}$ and $F_\lambda(\cdot,\lambda)$ denotes the n-vector whose components are the partial derivatives with respect to λ of the corresponding components of F. Clearly, (2.1) is simply a forward Euler approximation to the solution of the ordinary differential equation (2.2). Of course, in order for (2.1) to be of use, F_u must be invertible for $\lambda \in [\tilde{\lambda},\lambda^*]$. If the solution is being approximated at or near a turning or bifurcation point, then special procedures must be invoked, e.g., introducing an artificial parameter or switching parameters [1,2]. Here it is assumed that the solution curve $\mathbf{u}(\lambda)$ for $\lambda \in [\tilde{\lambda},\lambda^*]$ is a section of a nonsingular branch; i.e., $F_u(\mathbf{u}(\lambda),\lambda)$ is invertible and moreover $(F_u(\mathbf{u}(\lambda),\lambda))^{-1}$ is uniformily bounded with respect to λ for $\lambda \in [\tilde{\lambda},\lambda^*]$.

After $\mathbf{u}_0$ is obtained through a predictor such as (2.1), it can be used as an initial guess for an iterative procedure such as Newton's method. Then, in principle, an arbitrarily close approximation to the exact solution $\mathbf{u}(\lambda)$ can be generated. Of course, if this corrective step is to produce a convergent sequence of approximations to $\mathbf{u}(\lambda)$, then $\mathbf{u}_0$ must be within the attraction region at λ for the chosen iterative scheme. Once the solution at $\mathbf{u}(\lambda)$ is obtained, then the procedure is repeated using this solution as the starting point.

The description of the predictor-corrector algorithm is completed by defining a method for choosing the step size $\Delta\lambda$. If the predictor (2.1) is used, then

$$\mathbf{u}(\lambda) - \mathbf{u}_0 = \frac{1}{2}\left.\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}\right|_{\tilde{\lambda}} (\Delta\lambda)^2 + \mathrm{O}(\Delta\lambda)^3.$$

If $\|\mathbf{u}(\lambda) - \mathbf{u}_0\| = \epsilon$, where ϵ is smaller than the radius of the attraction ball at λ of the corrector, then an approximation for $\Delta\lambda$ can be obtained from

$$\Delta\lambda \approx \left(\frac{2\epsilon}{\left\|\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}\right\|}\right)^{1/2} \tag{2.3}$$

for $\Delta\lambda$ sufficiently small. Here $\|\cdot\|$ represents any given norm, but usually the ℓ_2-norm is employed. In order to use the last formula, one must be able to estimate $\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}$ and ϵ. In [3] it is shown that an approximation for $\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}$ can be obtained if an additional point on the solution curve is available. Also, it is possible to obtain an estimate for ϵ using the convergence history of the corrector at previous steps; see [3] for details.

It should be noted that the procedure outlined above is not foolproof in the sense that one cannot positively guarantee that the iterative method will converge. Also, formula (2.3) and the approximation for $\frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}$ are derived using the assumption that the step size in λ is small. However, if a *general purpose* nonlinear equation solver is desired, then the above procedure is quite good.

3. A DISCRETIZATION OF THE NAVIER-STOKES EQUATIONS

The specific problem that is considered is the Navier-Stokes equations written in terms of the primitive variables. The equations are given by

$$-\frac{1}{\lambda}\Delta \mathbf{u} + \mathbf{u} \cdot \operatorname{grad} \mathbf{u} + \operatorname{grad} \mathbf{p} = \mathbf{f} \qquad \text{in } \Omega \tag{3.1}$$

$$\operatorname{div} \mathbf{u} = 0 \qquad \text{in } \Omega \tag{3.2}$$

$$\mathbf{u} = 0 \qquad \text{on } \Gamma. \tag{3.3}$$

Here Ω denotes a bounded, open, and connected subset of $\mathbb{R}^2$ or $\mathbb{R}^3$ with boundary Γ. Also $\mathbf{u}$ and p represent the unknown non-dimensionalized velocity and pressure fields, respectively; $\mathbf{f}$ is a prescribed body force per unit mass; and $\lambda = Re$ is the Reynolds number. The results derived in this paper can be extended to other problems including those involving inhomogeneous boundary conditions and other formulations of the Navier-Stokes equations.

A Galerkin formulation of (3.1)–(3.3) can be defined through the use of the bilinear forms

$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \operatorname{grad} \mathbf{u} : \operatorname{grad} \mathbf{v} \, d\Omega \tag{3.4}$$

and

$$b(\mathbf{v}, q) = -\int_\Omega q \operatorname{div} \mathbf{v} \, d\Omega, \tag{3.5}$$

the trilinear form

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \frac{1}{2}\left(\int_\Omega \mathbf{w} \cdot \operatorname{grad} \mathbf{u} \cdot \mathbf{v} \, d\Omega - \int_\Omega \mathbf{w} \cdot \operatorname{grad} \mathbf{v} \cdot \mathbf{u} \, d\Omega\right), \tag{3.6}$$

and the linear functional

$$< \mathbf{f}, \mathbf{v} > = \int_\Omega \mathbf{f} \cdot \mathbf{v} \, d\Omega.$$

Here $A : B$ denotes the scalar product of the tensors A and B. A weak formulation of (3.1)–(3.3) is the following: seek $\mathbf{u} \in \mathbf{V}$ and $p \in P$ such that

$$\frac{1}{\lambda} a(\mathbf{u}, \mathbf{v}) + \mathbf{c}(\mathbf{u}, \mathbf{u}, \mathbf{v}) + \mathbf{b}(\mathbf{v}, \mathbf{p}) + \mathbf{b}(\mathbf{u}, \mathbf{q}) = < \mathbf{f}, \mathbf{v} > \qquad \forall \, \mathbf{v} \in \mathbf{V}, \mathbf{q} \in \mathbf{P}. \tag{3.7}$$

Here $\mathbf{V} = \mathbf{H}_0^1(\Omega)$ and $P = L_0^2(\Omega)$, where

$$\mathbf{H}_0^1(\Omega) = \left\{ \mathbf{v} \mid v_i \in L^2(\Omega), \ \frac{\partial v_i}{\partial x_j} \in L^2(\Omega) \text{ for } i, j = 1, \ldots, n, \text{ and } \mathbf{v} = 0 \text{ on } \Gamma \right\}$$

and

$$L_0^2(\Omega) = \left\{ q \in L^2(\Omega) \mid \int_\Omega q \, d\Omega = 0 \right\}.$$

The number of space dimensions is $n = 2$ or $n = 3$. It is easily verified that sufficiently smooth solutions of (3.7) are also solutions of (3.1)–(3.3). For example, see [4] for details.

Equation (3.7) also represents a discretization of the Navier-Stokes if one chooses $\mathbf{V} = \mathbf{V^h}$ and $P = P^h$, where $\mathbf{V^h}$ and P^h are finite dimensional subspaces of $\mathbf{H}_0^1(\Omega)$ and $L_0^2(\Omega)$, respectively. It is assumed that these subspaces satisfy all the conditions which insure that the discretization is a stable one and that the discrete solution is optimally accurate. This includes all continuity, coercivity, and stability conditions; again, see [4] for details.

The norm which will be used for both $\mathbf{H}_0^1(\Omega)$ and any discrete subspace $\mathbf{V^h} \subset \mathbf{H}_0^1(\Omega)$ is given by

$$\|\mathbf{v}\| = \left(\int_\Omega |\operatorname{grad} \mathbf{v}|^2 \, d\Omega\right)^{1/2}.$$

Some specific properties of the forms (3.4)–(3.6) that will be needed are

$$a(\mathbf{v},\mathbf{v}) = \|\mathbf{v}\|^2 \qquad \forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega)\,, \tag{3.8}$$

$$a(\mathbf{u},\mathbf{v}) = a(\mathbf{v},\mathbf{u}) \qquad \forall\, \mathbf{u},\mathbf{v} \in \mathbf{H}_0^1(\Omega)\,, \tag{3.9}$$

$$|c(\mathbf{u},\mathbf{v},\mathbf{w})| \le \gamma \|\mathbf{u}\|\,\|\mathbf{v}\|\,\|\mathbf{w}\| \qquad \forall\, \mathbf{u},\mathbf{v},\mathbf{w} \in \mathbf{H}_0^1(\Omega)\,, \tag{3.10}$$

and

$$c(\mathbf{u},\mathbf{v},\mathbf{w}) = -c(\mathbf{u},\mathbf{w},\mathbf{v}) \qquad \forall\, \mathbf{u},\mathbf{v},\mathbf{w} \in \mathbf{H}_0^1(\Omega)\,, \tag{3.11}$$

where γ depends only on Ω and n; see [4,5] for the proofs of these properties.

4. ESTIMATES FOR THE PATH DERIVATIVES

Equations that determine the derivatives of $\mathbf{u}$ and p with respect to $\lambda = Re$ can be derived from (3.7). If $\mathbf{u}^{(\mathbf{k})} = \frac{\mathbf{d}^{\mathbf{k}}\mathbf{u}}{\mathbf{d}\lambda^{\mathbf{k}}}$ and $p^k = \frac{d^k p}{d\lambda^k}$, then by formally differentiating (3.7) one obtains

$$\begin{aligned}\frac{1}{\lambda}\, a(\mathbf{u}^{(\mathbf{k})},\mathbf{v}) + c(\mathbf{u}^{(\mathbf{k})},\mathbf{u},\mathbf{v}) + \mathbf{c}(\mathbf{u},\mathbf{u}^{(\mathbf{k})},\mathbf{v}) + \mathbf{b}(\mathbf{v},\mathbf{p}^{\mathbf{k}}) + \mathbf{b}(\mathbf{u}^{(\mathbf{k})},\mathbf{q}) \\ = \mathcal{G}_k(\mathbf{u}^{(\mathbf{k-1})},\ldots,\mathbf{u}^{(1)},\mathbf{u};\mathbf{v};\lambda) \qquad \forall\, \mathbf{v} \in \mathbf{V},\ \mathbf{q} \in \mathbf{P} \text{ and } \mathbf{k} = 1,2,\ldots\,.\end{aligned} \tag{4.1}$$

The linear functionals $\mathcal{G}_k(\cdots;\mathbf{v};\cdot)$, $k = 1,2,\ldots$, are defined by

$$\begin{aligned}\mathcal{G}_k(\mathbf{u}^{(\mathbf{k-1})},\ldots,\mathbf{u}^{(1)},\mathbf{u};\mathbf{v};\lambda) = &\sum_{j=0}^{k-1} \frac{\alpha_{kj}}{(-\lambda)^{k+1-j}}\, a(\mathbf{u}^{(\mathbf{j})},\mathbf{v}) \\ &- \sum_{j=1}^{k-1} \beta_{kj}\, c(\mathbf{u}^{(\mathbf{j})},\mathbf{u}^{(\mathbf{k-j})},\mathbf{v}) \qquad \forall\, \mathbf{v} \in \mathbf{H}_0^1(\Omega)\,,\end{aligned} \tag{4.2}$$

where $\mathbf{u}^{(0)} = \mathbf{u}$; the positive constants α_{kj} and β_{kj} do not depend on λ. For example,

$$\mathcal{G}_1(\mathbf{u};\mathbf{v};\lambda) = \frac{1}{\lambda^2}\, a(\mathbf{u},\mathbf{v})\,, \tag{4.3}$$

$$\mathcal{G}_2(\mathbf{u}^{(1)},\mathbf{u};\mathbf{v};\lambda) = \frac{2}{\lambda^2}\, a(\mathbf{u}^{(1)},\mathbf{v}) - \frac{2}{\lambda^3}\, \mathbf{a}(\mathbf{u},\mathbf{v}) - 2\mathbf{c}(\mathbf{u}^{(1)},\mathbf{u}^{(1)},\mathbf{v})\,, \tag{4.4}$$

$$\begin{aligned}\mathcal{G}_3(\mathbf{u}^{(2)},\mathbf{u}^{(1)},\mathbf{u};\mathbf{v};\lambda) = &\frac{3}{\lambda^2}\, a(\mathbf{u}^{(2)},\mathbf{v}) - \frac{6}{\lambda^3}\, \mathbf{a}(\mathbf{u}^{(1)},\mathbf{v}) + \frac{6}{\lambda^4}\, \mathbf{a}(\mathbf{u},\mathbf{v}) \\ &- 3c(\mathbf{u}^{(2)},\mathbf{u}^{(1)},\mathbf{v}) - 3\mathbf{c}(\mathbf{u}^{(1)},\mathbf{u}^{(2)},\mathbf{v})\,,\end{aligned} \tag{4.5}$$

and

$$\begin{aligned}\mathcal{G}_4(\mathbf{u}^{(3)},\mathbf{u}^{(2)},\mathbf{u}^{(1)},\mathbf{u};\mathbf{v};\lambda) = &\frac{4}{\lambda^2}\, a(\mathbf{u}^{(3)},\mathbf{v}) - \frac{12}{\lambda^3}\, \mathbf{a}(\mathbf{u}^{(2)},\mathbf{v}) \\ &+ \frac{24}{\lambda^4}\, a(\mathbf{u}^{(1)},\mathbf{v}) - \frac{24}{\lambda^5}\, \mathbf{a}(\mathbf{u},\mathbf{v}) - 4\mathbf{c}(\mathbf{u}^{(3)},\mathbf{u}^{(1)},\mathbf{v}) \\ &- 6c(\mathbf{u}^{(2)},\mathbf{u}^{(2)},\mathbf{v}) - 4\mathbf{c}(\mathbf{u}^{(1)},\mathbf{u}^{(3)},\mathbf{v})\,.\end{aligned} \tag{4.6}$$

Note that (4.1) is a linear system for the path derivatives $\mathbf{u}^{(\mathbf{k})}$, p^k, and only the right-hand side depends on k; i.e., the linear operator on $\mathbf{u}^{(\mathbf{k})}$ and p^k appearing in the left-hand side of (4.1) does not depend on k.

Using the choice $\mathbf{v} = \mathbf{u}^{(\mathbf{k})}$, $q = -p^k$ in (4.1) and applying (3.8)–(3.11), one obtains

$$\frac{\sigma}{\lambda}\|\mathbf{u}^{(\mathbf{k})}\| \le \sum_{\mathbf{j}=0}^{\mathbf{k-1}} \frac{\alpha_{\mathbf{kj}}}{\lambda^{\mathbf{k+1-j}}}\|\mathbf{u}^{(\mathbf{j})}\| + \gamma \sum_{\mathbf{j}=1}^{\mathbf{k-1}} \beta_{\mathbf{kj}}\|\mathbf{u}^{(\mathbf{j})}\|\,\|\mathbf{u}^{(\mathbf{k-j})}\|\,, \tag{4.7}$$

where

$$\sigma = 1 - \gamma\|\mathbf{u}\|\lambda\,. \tag{4.8}$$

It is well known that $\sigma > 0$ implies that the solution of (3.7) is uniquely determined; see [4,5]. Furthermore, $\sigma > 0$ implies that the point $(\lambda, \mathbf{u}(\lambda), \mathbf{p}(\lambda))$ is on a nonsingular branch, or equivalently, (4.1) is uniquely solvable. Thus, under the assumptions made here, there exists a $\hat{\sigma}$ such that $\sigma \geq \hat{\sigma} > 0$. Whenever $\sigma > 0$, it follows from (4.7)–(4.8) that

$$\|\mathbf{u}^{(\mathbf{k})}\| \leq \frac{\mathbf{k}! r_{\mathbf{k}}(\sigma)}{\lambda^{\mathbf{k}} \sigma^{2\mathbf{k}-1}} \|\mathbf{u}\| \qquad \text{for } k = 1, 2, \ldots, \tag{4.9}$$

where $r_k(\sigma)$ denotes a monic polynomial of degree $2k-2$. For example,

$$r_1(\sigma) = 1\,, \quad r_2(\sigma) = \sigma^2 + 1\,, \quad r_3(\sigma) = \sigma^4 + 2\sigma^2 - \sigma + 2$$

and

$$r_4(\sigma) = \sigma^6 + 3\sigma^4 - 3\sigma^3 + 7\sigma^2 - 5\sigma + 5\,.$$

Since $0 < \hat{\sigma} \leq \sigma \leq 1$, (4.9) implies that

$$\|\mathbf{u}^{(\mathbf{k})}\| \leq \frac{\mathbf{C_k}}{\lambda^{\mathbf{k}} \hat{\sigma}^{2\mathbf{k}-1}} \|\mathbf{u}\|;$$

i.e., for $\lambda >> 1$ one has that $\|\mathbf{u}^{(\mathbf{k})}\| = \mathbf{O}(\lambda^{-\mathbf{k}})$.

For large ranges in λ, the computations indicate that

$$\frac{d}{d\lambda} \|\mathbf{u}\| \geq 0\,. \tag{4.10}$$

For sufficiently small λ, (4.10) can be shown rigorously to be true. From (3.8)–(3.9),

$$\frac{d}{d\lambda} \|\mathbf{u}\|^2 = \frac{\mathbf{d}}{\mathbf{d}\lambda} \mathbf{a}(\mathbf{u}, \mathbf{u}) = 2\mathbf{a}(\mathbf{u}, \mathbf{u}^{(1)})\,. \tag{4.11}$$

Setting $k = 1$, $\mathbf{v} = \mathbf{u}$, and $q = 0$ in (4.1), one obtains

$$a(\mathbf{u}, \mathbf{u}^{(1)}) = \frac{1}{\lambda} \mathbf{a}(\mathbf{u}, \mathbf{u}) - \lambda \mathbf{c}(\mathbf{u}, \mathbf{u}^{(1)}, \mathbf{u})\,, \tag{4.12}$$

where (3.11) and the fact that $b(\mathbf{u}, \mathbf{q}) = 0$ for all $q \in P$ have been invoked. One then combines (4.11)–(4.12) and uses (3.8) and (3.10) to produce the estimate

$$\begin{aligned} \frac{d}{d\lambda} \|\mathbf{u}\| &\geq \frac{1}{\lambda} \|\mathbf{u}\| - \lambda\gamma \|\mathbf{u}\| \, \|\mathbf{u}^{(1)}\| \\ &\geq \frac{1}{\lambda} \|\mathbf{u}\| \left(1 - \frac{\gamma\lambda}{\sigma} \|\mathbf{u}\|\right)\,, \end{aligned}$$

where (4.9) with $k = 1$ has been used as well. The substitution of (4.8) into this expression yields

$$\frac{d}{d\lambda} \|\mathbf{u}\| \geq \frac{1}{\lambda} \|\mathbf{u}\| \left(\frac{1 - 2\gamma\lambda\|\mathbf{u}\|}{1 - \gamma\lambda\|\mathbf{u}\|}\right)\,.$$

It is well known [4–6] that the estimate $\|\mathbf{u}\| \leq \lambda \|\mathbf{f}\|_{-1}$ holds, where $\|\cdot\|_{-1}$ denotes the norm on the dual space of $\mathbf{H}_0^1(\Omega)$. Thus, for λ sufficiently small, (4.10) follows. In addition, from (4.8), one easily finds that

$$\frac{d\sigma}{d\lambda} = -\gamma \|\mathbf{u}\| - \gamma\lambda \frac{\mathbf{d}}{\mathbf{d}\lambda} \|\mathbf{u}\|\,, \tag{4.13}$$

so that $d\sigma/d\lambda \leq 0$ whenever $d\|\mathbf{u}\|/\mathbf{d}\lambda \geq 0$.

It should be noted that all the results of this section hold for both the continuous and discrete problem, i.e., $\mathbf{u}$ may denote either the solution of (3.7) when $\mathbf{V} = \mathbf{H}_0^1(\Omega)$ or when $\mathbf{V} = \mathbf{V^h}$, some finite dimensional subspace of $\mathbf{H}_0^1(\Omega)$.

5. NEWTON'S METHOD AND AN ESTIMATE FOR ITS ATTRACTION BALL

There are a variety of iterative methods in use for solving discrete versions of the Navier-Stokes equations. At least in the context of two-dimensional problems, one popular choice is Newton's method. For the discrete Navier-Stokes problem of finding $\mathbf{u}^h \in \mathbf{V}^h$ and $p^h \in P^h$ satisfying

$$\frac{1}{\lambda} a(\mathbf{u}^h, \mathbf{v}) + \mathbf{c}(\mathbf{u}^h, \mathbf{u}^h, \mathbf{v}) + \mathbf{b}(\mathbf{v}, p^h) + \mathbf{b}(\mathbf{u}^h, q) = <\mathbf{f}, \mathbf{v}> \qquad \forall\, \mathbf{v} \in \mathbf{V}^h, q \in P^h, \tag{5.1}$$

Newton's method is defined as follows. Given an initial guess $\mathbf{u}_0 \in \mathbf{V}^h$ for the velocity, then the sequence of Newton iterates $\{\mathbf{u_m} \in \mathbf{V}^h,\ \mathbf{p_m} \in \mathbf{P}^h\}$, $m = 1, 2, \ldots$, is determined by solving the sequence of problems

$$\begin{aligned} \frac{1}{\lambda} a(\mathbf{u_m}, \mathbf{v}) + c(\mathbf{u_m}, \mathbf{u_{m-1}}, \mathbf{v}) + \mathbf{c}(\mathbf{u_{m-1}}, \mathbf{u_m}, \mathbf{v}) + \mathbf{b}(\mathbf{v}, p_m) + \mathbf{b}(\mathbf{u_m}, q) \\ = <\mathbf{f}, \mathbf{v}> + c(\mathbf{u_{m-1}}, \mathbf{u_{m-1}}, \mathbf{v}) \qquad \forall\, \mathbf{v} \in \mathbf{V}^h, q \in P^h \text{ and } \mathbf{m} = 1, 2, \ldots. \end{aligned} \tag{5.2}$$

Note that no initial guess for the pressure is necessary.

It is known [4,5,7] that if $(\lambda, \mathbf{u}(\lambda))$ is a point on a nonsingular branch, and if $\mathbf{u}_0$ is sufficiently close to the exact solution $\mathbf{u}^h$ of the discrete Navier-Stokes equation (5.1), then the sequence $\{\mathbf{u_m}, p_\mathbf{m}\}$ is locally and quadratically convergent to $\{\mathbf{u}^h, p^h\}$. In particular, for the case $\sigma > 0$, it can be shown [5,7] that the Newton iteration converges quadratically whenever $\mathbf{u}_0 \in \mathbf{V}^h$ satisfies $\|\mathbf{u}_0 - \mathbf{u}^h\| \leq \epsilon$, where

$$\epsilon = \frac{\sigma}{2(1-\sigma)} \|\mathbf{u}\|. \tag{5.3}$$

Note that by using (4.13), one obtains

$$\frac{d\epsilon}{d\lambda} = -\frac{1}{2\gamma\lambda^2} - \frac{1}{2}\frac{d}{d\lambda}\|\mathbf{u}\|,$$

so that $\frac{d\epsilon}{d\lambda} \leq 0$ if $\frac{d\|\mathbf{u}\|}{d\lambda} \geq 0$. Thus, whenever (4.10) holds, the attraction ball for Newton's method decreases as the Reynolds number increases.

6. CONTINUATION METHODS FOR THE DISCRETE NAVIER-STOKES EQUATIONS

For "small" values of the Reynolds number λ, the attraction ball is relatively large and it is easy to find an initial guess $\mathbf{u}_0$ such that the Newton iteration converges. For example, one may define $\mathbf{u}_0$ to be the solution of a linear Stokes problem. For larger values of λ one needs a better starting guess; one method for generating such a guess is to use continuation methods.

First, assume that a solution $\mathbf{u}(\tilde{\lambda}) \in \mathbf{V}^h$, $p(\tilde{\lambda}) \in P^h$ at a particular value $\tilde{\lambda}$ of the Reynolds number has been determined. Then using the predictor (2.1), one can generate an initial guess $\mathbf{u}_0$ for the Newton iteration at $\lambda > \tilde{\lambda}$ from

$$\mathbf{u}_0 = \mathbf{u}(\tilde{\lambda}) + \mathbf{u}^{(1)}(\tilde{\lambda})\Delta\lambda, \tag{6.1}$$

where $\Delta\lambda = \lambda - \tilde{\lambda}$ and $\mathbf{u}^{(1)} = \frac{\mathbf{du}}{\mathbf{d}\lambda} \in \mathbf{V}^h$ is the solution of (4.1) with $k = 1$ and $\lambda = \tilde{\lambda}$. Standard mean value theorems [8] for multivariate mappings yield

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| = \|\mathbf{u}(\lambda) - \mathbf{u}(\tilde{\lambda}) - \mathbf{u}^{(1)}(\tilde{\lambda})\Delta\lambda\| \leq \sup_{\tilde{\lambda} \leq \xi \leq \lambda} \frac{1}{2} \left\| \frac{\mathbf{d}^2\mathbf{u}}{\mathbf{d}\lambda^2}(\xi) \right\| (\Delta\lambda)^2.$$

If $\hat{\sigma} \leq \sigma(\xi) < 1$ for $\xi \in [\tilde{\lambda}, \lambda]$, then from (4.9) with $k = 2$,

$$\left\| \frac{\mathbf{d}^2\mathbf{u}}{\mathbf{d}\lambda^2}(\xi) \right\| \leq \frac{4}{\tilde{\lambda}^2\hat{\sigma}^3} \|\mathbf{u}(\xi)\|,$$

so that

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \frac{2}{\tilde{\lambda}^2\hat{\sigma}^3} \sup_{\tilde{\lambda}\leq\xi\leq\lambda} \|\mathbf{u}(\xi)\| (\Delta\lambda)^2 .$$

If, in addition, (4.10) holds, then

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \frac{2}{\tilde{\lambda}^2\hat{\sigma}^3} \|\mathbf{u}(\lambda)\| (\Delta\lambda)^2 . \tag{6.2}$$

Of course, $\mathbf{u}_0$ should be chosen so that it belongs to the attraction ball at λ for Newton's method; by (5.3) this will be assured if

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \frac{\hat{\sigma}}{2} \|\mathbf{u}(\lambda)\| \tag{6.3}$$

for $\hat{\sigma} \leq \sigma(\lambda) < 1$. One then combines (6.2) and (6.3) to obtain that $\mathbf{u}_0$ will be in the attraction ball at λ whenever

$$\Delta\lambda < \tilde{\lambda}\frac{\hat{\sigma}^2}{2} , \tag{6.4}$$

i.e., the maximum allowable step size is at least as large as $\tilde{\lambda}\hat{\sigma}^2/2$. Note that unlike (2.3), the condition (6.4) has been derived without assuming that $\Delta\lambda << 1$. The important thing to note about (6.4) is that for $\tilde{\lambda} >> 1$, a large step size in the Reynolds number can be taken when using the predictor (6.1). However, as the target Reynolds number increases, $\hat{\sigma}$ must be chosen smaller so that exact proportionality to λ cannot be expected for larger values of λ. For example, $\hat{\sigma} \to 0$ as one nears a bifurcation point, and then a small step size in the Reynolds number is necessary to keep the predicted value (6.1) within the attraction ball for Newton's method.

A natural question to ask is whether or not the allowable step size may be appreciably increased by using higher order predictors. For example, one may use the second order Taylor predictor

$$\mathbf{u}_0 = \mathbf{u}(\tilde{\lambda}) + \mathbf{u}^{(1)}(\tilde{\lambda})\,\Delta\lambda + \frac{1}{2}\mathbf{u}^{(2)}(\tilde{\lambda})\,(\Delta\lambda)^2 , \tag{6.5}$$

where $\mathbf{u}^{(2)} = \frac{\mathrm{d}^2\mathbf{u}}{\mathrm{d}\lambda^2}$ is the solution of (4.1) with $k = 2$ and $\lambda = \tilde{\lambda}$. One also may ask if the allowable step size is seriously affected if a lower order predictor such as

$$\mathbf{u}_0 = \mathbf{u}(\tilde{\lambda}) \tag{6.6}$$

is used. Of course, (6.6) simply states that the Newton iteration at λ is started with the solution $\mathbf{u}(\tilde{\lambda})$ at a lower value of the Reynolds number. This "simple-minded" predictor is actually the one in prevalent use in engineering calculations for the Navier-Stokes equations.

The answer to both of the above questions is that insofar as the dependence of the allowable step size on the Reynolds number, it does not matter which of the three predictors (6.1), (6.5), or (6.6) is used. For example, for (6.6) one has that

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \sup_{\tilde{\lambda}\leq\xi\leq\lambda} \left\| \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\lambda}(\xi) \right\| \Delta\lambda .$$

If $\hat{\sigma} \leq \sigma(\xi) < 1$ for $\xi \in [\tilde{\lambda}, \lambda]$, then from (4.9) with $k = 1$,

$$\left\| \frac{d\mathbf{u}}{\mathrm{d}\lambda}(\xi) \right\| \leq \frac{1}{\tilde{\lambda}\hat{\sigma}} \|\mathbf{u}(\xi)\| ,$$

so that

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \frac{1}{\tilde{\lambda}\hat{\sigma}} \sup_{\tilde{\lambda}\leq\xi\leq\lambda} \|\mathbf{u}(\xi)\| \Delta\lambda ,$$

or, whenever (4.10) holds,

$$\|\mathbf{u}(\lambda) - \mathbf{u}_0\| \leq \frac{1}{\tilde{\lambda}\hat{\sigma}} \|\mathbf{u}(\lambda)\| \Delta\lambda .$$

The relation (6.4) is again obtained by combining this expression with (6.3). Similarly, it can be shown that if one uses the predictor (6.5), then again $\Delta\lambda$ can be chosen proportional to $\tilde{\lambda}\hat{\sigma}^2$.

Of course, what we have shown is that for the three predictors considered, the maximum allowable step size in λ exceeds $\tilde{\lambda}\hat{\sigma}^2/2$; this does not, in itself, preclude having one predictor which allows a larger step size than another. However, we note that it is probable that the inequalities we have used are sharp in the sense that for some problem they hold with near equality and thus for this case the maximum allowable step size for all three predictors will indeed be the same and equal to $\tilde{\lambda}\hat{\sigma}^2/2$. Furthermore, from a practical point of view, it is unlikely that one could obtain any better information concerning the maximum allowable step size, so that the fact that we have demonstrated that this step size exceeds the same (large) quantity in all three cases provides useful information.

7. NUMERICAL EXAMPLES AND CONCLUDING REMARKS

It has been shown that whenever the Navier-Stokes equations possess a unique solution and when one is not in the neighborhood of singular points, then the step size used in predicting an initial guess for Newton's method may be chosen independently of the choice of predictor algorithm. Thus, it is not unreasonable to employ a "simple-minded" predictor such as initializing Newton's method with the solution at a lower value of the Reynolds number at least for smooth portions of the solution curve.

These results, as well as some others of this paper, are confirmed by computational experience; e.g., it is observed that indeed large step sizes in the Reynolds number are allowable even when one uses the predictor (6.6). We illustrate this fact with some numerical results for the driven cavity problem. The domain is the unit square, which is subdivided into quadrilaterals that are then divided into two triangles by drawing a diagonal. The choice of finite element spaces is Taylor-Hood; i.e, continuous piecewise quadratic functions over the triangles for $\mathbf{V}^h$ and continuous piecewise linear functions over the triangles for P^h. In all computations a uniform 9×9 grid was used.

Table 1 gives the value of $||\mathbf{u}^{(k)}||$ for the driven cavity problem, where $\mathbf{u}^{(k)} = \frac{d^k\mathbf{u}}{d\lambda^k}$ and λ denotes the Reynolds number. From this table one notes that for $\lambda = 100$, the values of $||\mathbf{u}^{(k)}||$ are $O(\lambda^{-k})$ as predicted; however, for $\lambda = 1000$, the values are considerably larger than λ^{-k}. This is due to the fact that σ is becoming smaller and the estimate (4.9) has the term σ^{1-2k} appearing in it. However, even at $\lambda = 1000$, one sees that $||\mathbf{u}^{(k)}||$ decreases with k.

Table 1. Norms of the velocity Taylor basis functions for the driven cavity problem.

RE	$\|\|\mathbf{u}\|\|$	$\|\|\mathbf{u}^{(1)}\|\|$	$\|\|\mathbf{u}^{(2)}\|\|$	$\|\|\mathbf{u}^{(3)}\|\|$	$\|\|\mathbf{u}^{(4)}\|\|$
100	3.51	1.03×10^{-2}	1.12×10^{-4}	2.22×10^{-6}	7.07×10^{-8}
500	4.27	4.22×10^{-3}	1.62×10^{-5}	1.56×10^{-7}	1.75×10^{-8}
1000	4.84	3.10×10^{-2}	1.77×10^{-5}	1.84×10^{-7}	1.39×10^{-8}

Next, the maximum allowable step size is computed to the nearest 100 for the three different predictors given by (6.1), (6.5), and (6.6). Newton's method is used for the corrector in all cases. These results are given in Table 2. Clearly, the maximum allowable step size is independent of which predictor is employed. The entries in the table are determined as follows. For each choice of the predictor and each initial value of the Reynolds number, the Reynolds number is increased by increments of 100 until nonconvergence is achieved. For example, at a Reynolds number of 10, the predictor (6.6) produced an initial guess which was in the attraction region for Newton's method at Reynolds number 110, 210, 310, 410, and 510 but not for Reynolds number 610. The allowable step size is, in almost all cases, very large.

Any step size is acceptable if it is in the range of convergence of the corrector. However, if one wishes to get to some fixed Reynolds number as efficiently as possible, then the number of Newton iterations per step must be taken into account. One must then determine if it is more efficient to take several smaller steps or one large step. Table 3 addresses this issue.

Table 2. Maximum possible step size using three different predictors.

RE	Maximum step size		
	Predictor (6.6)	Predictor (6.1)	Predictor (6.5)
10	500	500	400
50	500	500	500
100	700	700	700
500	300	300	300
1000	200	200	200
1500	700	700	700

Table 3 gives the number of Newton steps taken for the maximum possible step size as well as the total number of Newton steps taken if several smaller steps of equal size were taken to reach the same Reynolds number. The tolerance for the convergence criterion was set to the discretization error. The results are reported for the predictor given by (6.6); comparable results were obtained for the other two predictors. Seemingly, it is more efficient to take one large step in the Reynolds number than to take several smaller steps.

Table 3. Comparison of the number of Newton iterations needed to reach a fixed Reynolds number.

RE	Total number of Newton iterations						
	1 step	2 steps	3 steps	4 steps	5 steps	6 steps	7 steps
$10 \rightarrow 500$	7	8	12	16	19	18	21
$100 \rightarrow 800$	7	10	12	15	17	19	24
$500 \rightarrow 800$	5	8	9	12	15		

It should be emphasized that in the neighborhood of singular points, i.e., bifurcation points and turning points, small step sizes in the Reynolds number are necessary in order to keep the predicted value within the attraction ball for Newton's method. Moreover, it is difficult, if not impossible, to pass through such points using algorithms which involve continuation in the Reynolds number. In order to lessen these difficulties, it is recommended that near such points one switch to some other continuation parameter such as the arc length along the solution curve or some judiciously chosen component of the solution. See [1,2] for details.

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