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Abstract

In this paper we present an application of matrix exponentiation via Krylov subspace projection, to the solution of fluid dynamics problems. The main idea is to approximate the operation $exp(A)v$ by means of a projection-like process onto a Krylov subspace. This results in a computation of an exponential matrix vector product similar to the one above but of a much smaller size. Time integration schemes can then be devised to exploit this basic computational kernel. The motivation of this approach is to provide time-integration schemes that are essentially of an explicit nature but which have good stability properties.

1 Introduction

This paper presents some results of the application of a new integration technique to the Navier-Stokes equations. The originality of the new method is that it attempts to exploit the local exponential behavior of the solution with respect to time. Roughly speaking, evaluating the solution of a nonlinear system of equation $w' = F(w)$ at time $t + \Delta t$ involves the computation of a vector of the form $exp(\Delta t A)w(t)$, where $w(t)$ is the approximation at the current time and A is the linearization of the nonlinear mapping F at $w(t)$. This type of approximation is exact for linear problems. Although it may seem difficult to exploit this local bahavior in practice because it involves the computation of the exponential of a matrix times a vector, we will show that using a Krylov subspace approach, a number of efficient integration schemes can be derived based on it. Moreover the scheme is of an explicit nature in that the only operations that it requires with the Jacobian A are matrix by vector products.

Many of the integration schemes for solving time dependent problems do exploit, implicitly, the local behavior mentioned above. In particular, explicit schemes make use of polynomial approximations to the exponential whereas implicit schemes employ rational approximations. It is well known that the stability properties of implicit schemes resulting from these approximations make their use more attractive than an explicit scheme. The price paid for this stability is the necessity to solve one or more large linear systems at each time step. On the other hand explicit schemes suffer from their requirement of using small time steps. The Krylov subspace approach presented in this paper avoids the solution of large linear systems of equations necessitated by the use of implicit time integration schemes while retaining the stability properties of these schemes. The elimination of the necessity of solving large systems of equations makes the use of higher order polynomials and their concomitant higher order accuracy very attractive from the practical point of view. The immediate object of this work is to demonstrate the feasibility of using these methods to obtain steady state solutions of the Navier-Stokes equations.

Krylov subspace methods form the basis of powerful linear system solvers such as the conjugate gradient and generalized minimum residual method. In section two of this paper we indicate how Krylov subspaces can also be used to approximate the product of a matrix exponential times a given vector. The basic idea has been suggested in several previous articles, see for example [3, 1, 9]. In the same section we also briefly discuss how the approximation can be used to solve time dependent nonlinear partial differential equations.

Section 3 deals with the application of the method to the problem of incompressible viscous flow. The Navier-Stokes equations in primitive variables form are solved using a pseudo compressibility approach. In this work the spacial derivatives are approximated by second order centered differences on a staggered mesh. The resulting nonlinear differential equations are then manipulated into a form suitable for the application of the Krylov exponential method.

2 The Krylov subspace approach

In this section we address the problem of computing an approximation to a vector $w = e^{-A}v$ by using polynomial approximation, i.e., we seek an approximation of the form:

$$e^{-A}v \approx p_{m-1}(A)v, \tag{1}$$

where p_{m-1} is a polynomial of degree $m-1$. A systematic way in which such an approximation can be found is to start by observing that the vector $w = e^{-A}v$ is an element of the Krylov subspace

$$K_m \equiv span\{v, Av, \ldots, A^{m-1}v\}.$$

One would like to get an element of this subspace that approximates $e^{-A}v$, ideally in some least squares sense. To facilitate working with vectors in K_m, it is convenient to generate an orthonormal basis $V_m = [v_1, v_2, v_3, \ldots, v_m]$. Starting with the vector $v_1 = v/\|v\|_2$ we will generate the basis V_m with the well-known Arnoldi algorithm, described below.

Algorithm: Arnoldi

1. Initialize:

Compute $v_1 := v/\|v\|_2$.

2. Iterate: Do $j = 1, 2, \ldots, m$

1. Compute $w := Av_j$.

2. Compute a set of j coefficients h_{ij} so that

$$w := w - \sum_{i=1}^{j} h_{ij}v_i$$

is orthogonal to all previous v_i's.

3. Compute $h_{j+1,j} := \|w\|_2$ and $v_{j+1} := w/h_{j+1,j}$.

The above algorithm produces an orthonormal basis $V_m = [v_1, v_2, \ldots, v_m]$, of the Krylov subspace K_m. If we denote the $m \times m$ upper Hessenberg matrix consisting of the coefficients h_{ij} computed from the algorithm by H_m we have the relation

$$AV_m = V_m H_m + h_{m+1,m}v_{m+1}e_m^T. \tag{2}$$

Because of the orthogonality of the matrix V_m we have the relation $H_m = V_m^T A V_m$ and as a result H_m represents the projection of the linear transformation A to the subspace K_m, with respect to the basis V_m. The vector $x_{opt} = V_m V_m^T e^{-A}v$ is the projection of $e^{-A}v$ on K_m,

i.e., it is the closest approximation to $exp(-A)v$ from K_m. Defining $\beta \equiv \|v\|_2$, it follows immediately that,

$$V_m V_m^T e^{-A} v = \beta V_m V_m^T e^{-A} v_1 = V_m V_m^T e^{-A} V_m e_1.$$

The optimal fit is therefore $x_{opt} \equiv V_m y_{opt}$ in which $y_{opt} \equiv \beta V_m^T e^{-A} V_m e_1$. Unfortunately, y_{opt} is not practically computable, since it involves e^{-A}. The alternative which will be used throughout is to approximate $V_m^T e^{-A} V_m$ by e^{-H_m}, leading to the approximation, $y_{opt} \approx \beta e^{-H_m} e_1$ and, .

$$e^{-A} v \approx \beta V_m e^{-H_m} e_1. \tag{3}$$

We are now left with the problem of computing efficiently the vector $e^{-H_m} e_1$ which is similar to the problem we started with but typically of much smaller size. We will not discuss the aspect of this computation here. The reader is referred to [4, 3] for one approach based on rational approximation to the exponential. More standard techniques such as those based on spectral decomposition may also be used[2] although these are typically more expensive. More generally, one can approximate $w = \phi(A)v$ for any function which is analytic around the eigenvalues of A in the same manner.

The theory of the above approximation has been examined in Gallopoulos and Saad [3] and [9]. Applications to the solution of systems of Ordinary Differential Equations have been discussed by several authors [1, 5, 7, 8]

We now give a brief overview on the ways in which the above approximation can be exploited to solve systems of Ordinary Differential Equations. We start with the simplest such equation, namely the homogeneous linear system

$$w' = -Aw$$

which can be solved by using a time integration scheme of the form

$$w(t + \Delta t) = e^{-\Delta t A} w(t).$$

We can exploit the previous approximation to evaluate the above expression at any given time t. Note that the accuracy of the above scheme is basically dictated by that of the approximation (3) and that if the solution is desired at a certain time then in theory one may be able to compute it in one single time-step provided m is sufficiently large to make the approximation accurate enough.

To solve more realistic time dependent equations we must start by looking at the slightly more general case:

$$w' = -Aw + r \tag{4}$$

in which we assume for now that r does not depend on time. The exact solution to the above equation is known to be

$$w(t) = A^{-1} r + e^{-tA}(w_0 - A^{-1} r) \tag{5}$$

which can be rewritten as

$$w(t) = w_0 + t\phi(tA)(r - Aw_0). \tag{6}$$

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where we define
$$\phi(z) = \frac{1 - e^{-z}}{z}. \tag{7}$$

Therefore, similarly to the homogeneous case consider above we can devise an integration scheme based on the following formula

$$w(t + \Delta t) = w(t) + \Delta t \phi(\Delta t A)(r - Aw(t)). \tag{8}$$

The use of the above formula, as opposed to the more standard equation (5) avoids the solution of linear systems. The evaluation of $\phi(H_m)e_1$ has been discussed in detail [9].

The simplest way to generalize the above formula to nonlinear equations of the form

$$w' + L(w) = 0 \tag{9}$$

is to rewrite it in a given interval $[t, t + \Delta t]$ as

$$w' = -Aw + (Aw - L(w)) \equiv -Aw + r(w(t))$$

in which A is the differential of L with respect to w at $w(t)$, and then to replace the variable term $Aw - L(w)$ by some constant r_c in the interval $[t, t + \Delta t]$. The original equation (9) is therefore replaced by an equation of the form (4) which is advanced from t to $t + \Delta t$ by a formula of the form (8). Many variations to this basic scheme are possible.

More generally, one can devise time marching procedures by attempting to exploit the expression for the exact solution of (9) at time $t + \Delta t$, which is given by

$$w(t + \Delta t) = w(t) + \int_0^{\Delta t} e^{-(\Delta t - \tau)J} \left[r(w(t + \tau)) - Aw(t) \right] d\tau \tag{10}$$

One can develop numerous schemes by applying quadrature formulas to the above equation, in the same spirit that prevails in the development of Runge Kutta methods. An important aspect of these is that the integrand involves the matrix exponential function.

An important detail concerning the practical use of the above idea is that of estimating the error a posteriori. This is important because it allows us to determine whether or not the computation that has been performed using (3) is accurate enough. Such an estimator has been presented in [9]. In case the accuracy obtained is insufficient, one can easily backtrack by reducing the time step Δt. An important point here is that, according to the formula (3) the Krylov subspace need not be recomputed. We only need to redo the computation of $exp(-\Delta t H_m)e_1$ involving the small matrix. In addition it is known that roughly the error behaves like $C \times (\Delta t)^m$ where C is a constant. This allows to determine an almost optimal Δt after the first attempt. In practice it is extremely rare that more than one backtracking step is performed which makes the process of adjusting time steps very economical.

3   Application to Fluid Dynamics

This section examines the use of the matrix exponential approach to solve computational fluid dynamics problems. In particular, the case of incompressible flow is addressed and

methods for steady state problems are presented. We begin with an introduction to the incompressible Navier-Stokes equations. The equations in nondimensional form are:

$$V_\tau - \frac{1}{Re}\Delta V + \nabla P = -(V \cdot \nabla)V \tag{11}$$

$$\nabla \cdot V = 0 \tag{12}$$

In two dimensions, the velocity vector is made up of the x and y components of the velocity

$$V = \begin{pmatrix} u \\ v \end{pmatrix}$$

and P is the pressure. The gradient operator is ∇, $\nabla\cdot$ is the divergence operator and Δ represents the Laplacian $\partial^2/\partial x^2 + \partial^2/\partial y^2$. The dissipation is scaled by Re, the Reynolds number.

3.1 Steady State Case

The artificial or pseudo compressibility method is the starting point in the application of exponential propagation by Krylov subspaces. The method involves adding a time derivative of pressure to the continuity equation and then solving the perturbed system. The equations to be solved are:

$$V_\tau - \frac{1}{Re}\Delta V + (V \cdot \nabla)V = -\nabla P \tag{13}$$

$$P_\tau + \beta\nabla \cdot V = 0 \tag{14}$$

where β is the compressibility parameter. For a mor detailed discussion of pseudo compressibility methods, the reader is refered to the early paper by Chorin [10] and the more recent work of Kwak and Chang [11, 12]. The usual method of solution of the above system is as follows:

- knowing V_n and P_n integrate equation (13) for V_{n+1}

- $P_{n+1} = P_n - \Delta\tau\beta\nabla \cdot V_{n+1}$

Time integration of equation (13) can be achieved by either implicit or explicit methods.

3.2 Use of Matrix Exponentials

After discretization in space, the perturbed Navier-Stokes equations can be written as,

$$W_t + f(W) = b. \tag{15}$$

In this system the vector W contains the unknown velocities and pressure at the nodes. The vector b contains the known boundary values, which are constant, and the function f which is nonlinear in W is defined by,

$$f(W) = \begin{pmatrix} -\frac{1}{Re}\Delta V + \nabla P + (V \cdot \nabla)V \\ \beta\nabla \cdot V \end{pmatrix} \tag{16}$$

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The system (15) represents a nonlinear system of ordinary differential equations.

In order to apply the methods of the previous section the nonlinear equations are linearized around the current value of W, $W(t)$.

$$W_t + f(W(t)) + J(W - W(t)) + [f(W) - f(W(t)) - J(W - W(t))] = b \qquad (17)$$

After some manipulation we obtain the equation,

$$W_t + JW = b - f(W) + JW = r(W) \qquad (18)$$

where J is the Jacobian of f evaluated at $W(t)$ or $J = \partial f / \partial W$.

The solution of equation (18) can be written in terms of matrix exponentials.

$$W(t + \Delta t) = W(t) + \int_0^{\Delta t} e^{-(\Delta t - \tau)J} [r(W(t + \tau)) - JW(t)] d\tau \qquad (19)$$

Application of this formula to advance the solution of equation (15) in time requires the approximation of the integral by a quadrature formula. This is complicated by the fact that the integrand is not an explicit function of τ. However, the principle of approximately integrating equations similar to (19) using numerical quadrature has been at the basis of methods of Runge Kutta type.

3.3 Solution of the Driven Cavity Problem

The problem of viscous flow in a lid driven cavity was used as a test case for solutions of the Navier-Stokes equations via equation (19). This problem has the attractive feature of no inflow or outflow boundaries. The boundary conditions for this case are simply the specification of the velocities on the boundaries. Since the problem is discretized on a staggered mesh, no pressure boundary condition is required.

The integral in equation (19) was evaluated in two ways. The evaluation of r at $W(t)$ yields, after evaluation of the integral, the first of two formula for evaluating $W(t + \Delta t)$.

$$W(t + \Delta t) = W(t) + \Delta t(I - e^{-\Delta t J})(\Delta t J)^{-1}(b - f(W(t))) \qquad (20)$$

We call this formula the left point rule because the value of the term in brackets in equation (19) is assumed to have a constant value in the entire interval from t to $t + \Delta t$. This value is the value of the term at the left of the interval. The midpoint rule is arrived at by similar means. Evaluating the term in brackets at the midpoint of the interval results in the following formula for $W(t + \Delta t)$.

$$W(t + \Delta t) = W(t) + \Delta t e^{-\frac{\Delta t}{2}J} \left[r(W(t + \frac{\Delta t}{2})) - JW(t) \right] \qquad (21)$$

The left point rule is used to predict the value of $r(W(t + \frac{\Delta t}{2}))$ and then the mid point formula is used to correct the solution.

Both the left point method alone and the predictor-corrector method composed of the left point and mid point rules were validated on the driven cavity problem. An equally

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spaced staggered grid was used for space discretization. The methods of the previous section were used to evaluate the matrix exponential terms which appear in the two formulas. The matrix exponential methods shown above required only the evaluation of a matrix vector product. In this particular case finite differences were used to approximate the Jacobian matrix vector product.

$$Jv = \frac{f(W(t) + \epsilon v) - f(W(t))}{\epsilon} \tag{22}$$

This technique makes the explicit computation of the matrix J and its storage unnecessary.

Converged solutions for both the methods were obtained on meshes with 32 points in each of the coordinate directions. The Reynolds numbers for both tests was 400 and the compressibility parameter β and time step were 2.5 and 0.01 respectively. The initial conditions were velocity and pressure set to zero inside the cavity. A plot of the vorticity of the converged solution is shown in figure 2. Both methods gave identical solutions. Only the results of the mid point formula are shown. Figure 1 contains three plots of convergence history for the first 2000 iterations of the method. The three plots represent the behavior of the logrithm of the norm of the vector $b - f(W)$. The information is separated into the parts of the vector corresponding to the steady state u momentum, v momentum and continuity equations. The continuity equation data is a direct measure of the divergence of the velocity field. All the plots show convergence of the algorithm.
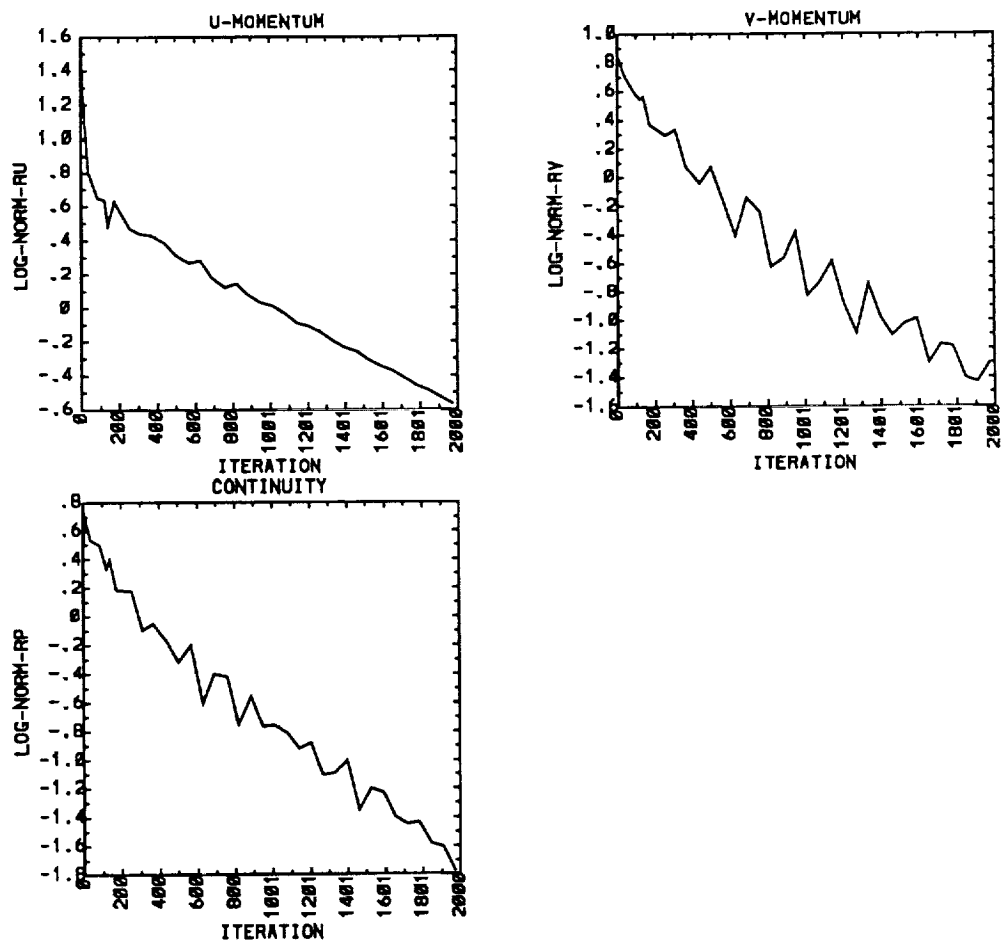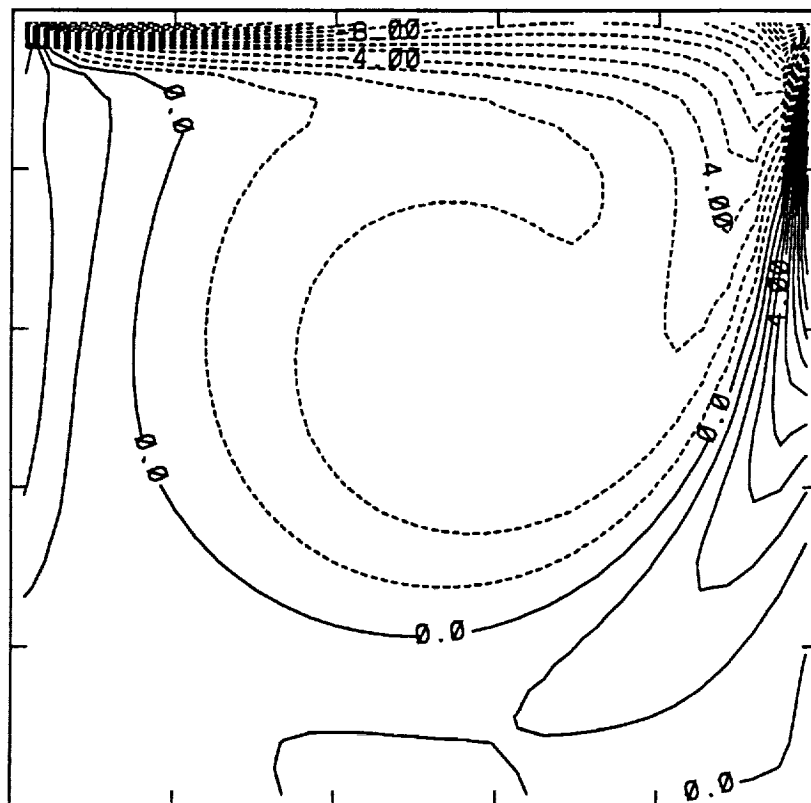
Figure 1: Convergence History

Figure 2: Vorticity

4 Conclusion

The results shown in this paper, although preliminary, show the feasibility of using matrix exponential methods based on Krylov subspaces, for solving fluid dynamics problems. The schemes that we used for handling the integral are based on the simplest quadrature rules possible. Yet the results obtained show good accuracy and the corresponding schemes are fairly efficient. It has been encouraging to see that the method seems very insensitive to the choice of the time step suggesting robust stability properties. A full study of the exact stability behavior remains to be done. We note that a number of related schemes presented in [3] for linear problems and using a different method for handling the integral, have been examined from this point of view and were shown to be either stable or A_0 stable.

It is hoped that more sophisticated integration schemes will lead to efficient procedures similar to Runge Kutta schemes but based on exploiting the matrix exponential.

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