Comments on the Fractional Step Method

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One of the more subtle, but profound advances in the understanding of fractional step methods for the incompressible Navier-Stokes equations has been the realization that these methods should be analyzed from a discrete point of view [1][2]. Even though a fractional step method is fundamentally a method for advancing the solution in time, the analysis of such methods can not be divorced from the spatial discretization of the various spatial operators. This important point clears up two of the most vexing questions accompanying traditional fractional step methods. Namely, what form should the boundary conditions on the intermediate velocity and presure take, and how can the time accuracy of fractional step methods be improved. Since this very fundamental point has been misunderstood, and misrepresented in recent literature, it is reviewed below. In particular, a reply to the comments of Abdallah [3] is presented.

The fully discretized incompressible Navier-Stokes equations take the form

$$\begin{pmatrix} A & G \\ D & 0 \end{pmatrix} \begin{pmatrix} v^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix} + \begin{pmatrix} bc \\ bc \end{pmatrix} \tag{1}$$

Where G is the discrete gradient operator, D is the discrete divergence operator, and A contains contributions from the time derivative, and convection and diffusion operators if they are computed implicitly. The vector r contains forcing terms plus any explicit convection and diffusion. Inhomogeneous boundary conditions appear in the vector bc. Note that the operators A, G, and D also incorporate boundary condition information. The vectors v^{n+1} and p^{n+1} represent the unknown velocities and pressures respectively.

The block matrix form of the evolution equation (1) can formally be factored as follows,

$$\begin{pmatrix} A & 0 \\ D & -DA^{-1}G \end{pmatrix} \begin{pmatrix} I & A^{-1}G \\ 0 & I \end{pmatrix} \begin{pmatrix} v^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix} + \begin{pmatrix} bc \\ bc \end{pmatrix} \tag{2}$$

which reduces still further to the following set of operations,

$$Av^* = r + bc \tag{3a}$$

$$DA^{-1}Gp^{n+1} = Dv^* - bc \tag{3b}$$

$$v^{n+1} = v^* - A^{-1}Gp^{n+1} \tag{3c}$$

This is sometimes referred to as the Uzawa method [4]. The variable v^* is known in the literature as the intermediate velocity. Note that the Uzawa method is extremely expensive computationally since the matrix A must effectively be inverted for every iteration of the discrete Poisson equation (3b). Traditional fractional step methods approximate equation (3), and significantly reduce the computational complexity, by assuming that $A^{-1} = \Delta t I$.

At this point a number of important statements can be made. First, boundary conditions on the intermediate velocity are not required. The intermediate velocity is simply a mathematical construction, used to go from equation (2) to equation (3). It is only defined at points where the velocity is unknown. This seems trivial from the previous analysis but has in the past been the topic of widespread debate. The confusion results from the traditional approach of posing equation (3) with continuous (undiscretized) spatial operators. Second, the accuracy of the traditional fractional step method is first order in time no matter how the actual diffusive and convective terms are approximated. The first order accuracy results from the approximation for A^{-1}.

With this background, it is now possible to address the comments of Abdallah [3] in some detail. It was demonstrated by Perot [2] that the traditional fractional step method is equivalent to the approximation $A^{-1} = \Delta t I$. This approximation and its resulting error, were not "assumed" in Ref. [2], nor were they "considered acceptable", or "rationalized". In fact higher order approximations for A^{-1} were both proposed and demonstrated to be effective. The work of Dukowicz & Dvinsky [1] presents an alternative (possibly preferable) route to higher order accuracy.

In addition, the work of Perot [2] does not suggest the boundary condition $\partial p/\partial n = 0$. Though in a brief aside it does mention that this boundary condition, when applied to the traditional (continuous) fractional step method, will give a system identical to equation (3) once it is spatially discretized. In fact, the conclusion found in Perot [2] is that "boundary conditions on v^* and p^{n+1} are not required" (See also Zang, Street & Koseff [5]). The fact that boundary conditions on the pressure are not required (when the pressure variables are located interior to the domain, such as at cell centers) is not a result of the fractional step approximation ($A^{-1} = \Delta t I$), but is also true of the original discrete system, equation (1).

Abdallah [3] suggests that Eq. (3b) "can be easily solved for the pressure if A^{-1} and G commute". Unfortunately, A^{-1} (or its approximation) and G do not in general commute. G is typically not even square, so it could not possibly commute (even with the identity matrix). Therefore, it is most emphatically *not* possible to create a variable $\phi = A^{-1} p^{n+1}$ and eliminate the matrix A^{-1} as is suggested in the latter part of Ref. [3]. Contrary to the assertion that "Perot's approximations (2) and (3) satisfy and require (commutivity)", Perot [2] actually asserts the very opposite (section 6), and goes on to state that in general it is not even possible to define a matrix Q such that $A^{-1}G = GQ$, which is the more general concept of commutivity that should be used when presenting this (erroneous) argument.

It is well known that fractional step methods exhibit a layer of reduced accuracy near

boundaries [6]. The conclusion has always been that this layer is a result of the boundary conditions on v^* and p^{n+1} (hence Abdallah's interest in Perot's pressure boundary conditions, or more accurately, the lack of one). However, the analysis of Perot [2] suggests that the problem is really due to a lack of generalized commutivity of the discrete operators ($A^{-1}G \neq GQ$). Not surprisingly the lack of commutivity in these operators happens to be at the boundaries (the only exception to this rule known to the author is periodic boundaries). This does not mean that the classic approach of creating "higher order boundary conditions" can not lead to improved accuracy by somehow canceling the effects of the lack of commutivity. But this classic approach does seems a rather complicated (and very difficult to analyze) solution to the problem. A much more straightforward solution, proposed in Perot [2], is to simply use better approximations for A^{-1}, and perform the fractional step splitting *after* the system has been fully discretized so that no boundary conditions on the intermediate variables are required.

The errors found in Ref [3] stem from a single basic misconception, one that readers would be wise to avoid in their own work. Discrete systems (the things we actually solve numerically) do not retain all the properties of their continuous counterparts. One should be very careful when analyzing numerical systems based solely on an understanding of the continuous physical operators. For example, while the continuous operators in this problem (the gradient, and typically the Laplacian) *do* commute, their discrete counterparts may not. While the continuous version of Eq. (3) (the version found in almost all references to the fractional step method) requires boundary conditions on both the pressure and the intermediate velocity, the discrete version requires neither.

The concept of analyzing the discrete system rather than its continuous counterpart applies in time as well as space. The computed pressure can only really be understood in a discrete context. Previous calculations have shown that the numerical pressure is always first order accurate in time (no matter what method is used to advance the solution), and that this first order accuracy does not influence the temporal order of accuracy of the velocity field. To understand this phenomenon, note that the discrete system of equations is equivalent to the continuous equations integrated over the time interval n to $n+1$. The pressure variable that is computed (usually some combination of p^{n+1} and p^n) is therefore actually the average pressure over the interval. By the mean value theorem this average pressure equals the real pressure at some point in the interval, but in general this point is unknown. The best that can be said is that the average pressure equals the pressure at time $n+1/2$ to order $\Delta t/2$, and hence is first order accurate. This first order accuracy does not effect the velocity, because the average pressure (not the pressure at time $n+1/2$) is the quantity required by the discrete system for the update of the velocity.

The fractional step method is a powerful tool for the efficient solution of the incompressible Navier-Stokes equations. However, the simplicity of the fractional step method can be deceptive. In the context of the analysis of such methods it is extremely important to consider the fully discrete system of equations and not be mislead by the properties of its continuous counterpart.

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