

# **Search for a general fluid mechanics algorithm**

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# SEARCH FOR A GENERAL FLUID MECHANICS ALGORITHM

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## Part I - Proposed algorithm

The paper outlines the formulation of a novel algorithm which can be used for the solution of both compressible and incompressible Navier-Stokes or Euler equations. Full incompressibility can be dealt with if the algorithm is used in its semi-explicit form and its structure permits arbitrary interpolation functions to be used avoiding the Babuška-Brezzi restriction.

In a fully explicit version it introduces a rational form of balancing dissipation avoiding the use of arbitrary parameters and forms for this.



## 1. INTRODUCTION

The extensive development of the finite element procedures for the solution of compressible, high speed flow problems occurred only in the last decade. Without doubt this was due to the “rediscovery” of the Lax-Wendroff methods [1] in the context of elements as the Taylor-Galerkin process [2][3] and the introduction of the Characteristic Galerkin Method [4-6]. However while the former, Taylor-Galerkin, formulation could be used for a general form of conservation equations typical of Navier-Stokes or Euler problems with multiple variables and characteristic speeds, only the latter, Characteristic Galerkin Method, justifies the use of the particular, Galerkin, spatial discretization yielding an identical approximation only when a single variable and one characteristic speed exists. In the section 2 of this paper we recall the essentials of the *Characteristic Galerkin process and its rationale*.

While the original, Taylor-Galerkin, stabilization of the finite element discretization has been widely supplemented by the use of, empirical, artificial diffusion forms developed in the context of finite difference methods and results consequently improved, it appeared to the Author that a return to the single characteristic speed, for which the procedures were proved, could be achieved by a suitable operator splitting procedure.

The key to such a split lies in a fractional step method devised originally by Chorin [7][8] and subsequently developed by others [9-19] for incompressible flows. By adding compressibility the acoustic or compressible wave phenomena can be separated and solved by standard self adjoint formulation leaving the convection equations with the fluid velocity as a single characteristic speed [20-23].

The original Chorin method was initially devised for the purpose of implementing a time stepping process for the momentum and continuity equations in which the essential variables were the flow velocity  $\mathbf{u}$  and pressure  $p$ . The process, applicable to incompressible flows and sometimes interpreted as a projection method, starts by obtaining an approximate velocity field using the momentum equation with the pressure gradients omitted. This first step is followed by solving for the unknown pressures by inserting the velocity approximation into the continuity equation. The final stage is the correction of the velocity vector using the computed pressure terms. This led to the process sometimes being known as the velocity correction method.

The method essentially separates the pressure calculation into one involving a Laplacian form which is self adjoint and only a single characteristic velocity is involved in the first and final stages clearly achieving the desired effect. However when the transient form is used for steady state solution further benefits can arise. One of these, observed by Schneider and Rathby [11] and by Kawahara [15], is that the Babuška Brezzi stability restrictions, well known in the velocity-pressure finite element discretization,

no longer apply as the steady state equations do not have a zero diagonal term. Now a term proportional to the time increment is there inserted and this allows arbitrary and convenient interpolations to be used for  $\mathbf{u}$  and  $p$ . Here for instance any equal interpolation is possible avoiding the difficulties frequently encountered in the use of such interpolation coupled with the previously mentioned Taylor-Galerkin procedures.

The result here is in essence similar to that obtained by Hughes et al. [24], Sampaio [25] and the wider interpretation of it described by Zienkiewicz and Wu [26].

These combined merits of the use of the fractional step procedures have been realised by the author earlier [21] but so far success has been limited to applications in a non-conservative form of equations of Navier-Stokes and Euler [22] or to shallow water equations [23]. In the present paper the approach is considerably modified allowing the full form of conservation equations to be dealt with. Indeed the new approach can be simply extended to deal with the transport of additional variables such as turbulence parameters or chemical reactions.

The essential step of the new procedure is the realization that in each computational step the transport of a single scalar quantity occurs and the treatment of this is described in the next section.

## 2. THE SCALAR CONVECTION-DIFFUSION PROBLEM AND THE CHARACTERISTIC GALERKIN EXPLICIT APPROXIMATION

Before proceeding with the description of the full algorithm we shall recall the application of the characteristic Galerkin method in the explicit form to a typical convection-diffusion process with a scalar dependent variable  $\Phi$ .

The governing equations can here be written always in a conservation form as

$$\frac{\partial \Phi}{\partial t} + \frac{\partial F_i}{\partial x_i} + \frac{\partial G_i}{\partial x_i} + Q = 0 \quad (1)$$

with  $x_i$  being  $i$ -th the coordinate ( $i = 1, 2, 3$ ),

$$F_j = u_j \Phi \quad (2a)$$

the convected flux,

$$G_i = -k \frac{\partial \Phi}{\partial x_i} \quad (2b)$$

the diffusion flux,

$$Q = Q(\mathbf{x}) \quad (2c)$$

the source term, and

$$\mathbf{u} = \mathbf{u}(\mathbf{x}) \quad (2d)$$

is the velocity field which is assumed to be known.

The full equation can thus be alternatively written as

$$\frac{\partial \Phi}{\partial t} = -u_j \frac{\partial \Phi}{\partial x_j} + \frac{\partial}{\partial x_i} \left( k \frac{\partial \Phi}{\partial x_i} \right) - Q - \Phi \frac{\partial u_j}{\partial x_j} \quad (3)$$

in which only the first term on the R.H.S. is not self-adjoint. As that term corresponds precisely to an advection wave moving with a velocity  $u_i$ , a change of co-ordinates to the characteristic ones given by

$$dx'_i = dx_i - u_i dt \quad (4)$$

makes the offending term vanish leaving a fully self-adjoint system.

For such a self-adjoint system it is known that the standard Galerkin approximation in space is optimal but the inconvenience of a moving co-ordinate system is introduced. To avoid this difficulty a local approximation has been used [3-5]. This is fully described in [6] and results in an explicit form written in fixed co-ordinates (noting that the last term of Eq.3 simply adds to the source) as

$$\begin{aligned} \Delta \Phi &= \Phi^{n+1} - \Phi^n \\ &= \Delta t \left[ -\frac{\partial F_i}{\partial x_i} + \frac{\partial}{\partial x_i} \left( k \frac{\partial \Phi}{\partial x_i} \right) - Q \right]_n \\ &\quad + \frac{\Delta t^2}{2} \left[ u_i \frac{\partial}{\partial x_i} \left( u_j \frac{\partial \Phi}{\partial x_j} + \Phi \frac{\partial u_j}{\partial x_j} + Q \right) \right]_n \\ &= \Delta t \left[ -\frac{\partial F_i}{\partial x_i} + \frac{\partial}{\partial x_i} \left( k \frac{\partial \Phi}{\partial x_i} \right) - Q \right]_n \\ &\quad + \frac{\Delta t^2}{2} \left[ u_i \frac{\partial}{\partial x_i} \left( \frac{\partial}{\partial x_j} (u_j \Phi) - Q \right) \right]_n \end{aligned} \quad (5)$$

An identical expression can be here derived by using a higher order time approximation for a single scalar variable of the Lax-Wendroff type. However, as Eq.(5) is derived from a self-adjoint form spatial discretization by the Galerkin method is optimally used. We can write thus the approximation

$$\Phi = \mathbf{N} \bar{\Phi} \quad (6)$$

and use the weighting  $\mathbf{N}^T$  in the integrated residual expression. Thus we obtain

$$\mathbf{M}(\bar{\Phi}^{n+1} - \bar{\Phi}^n) = -\Delta t[(\mathbf{C}\bar{\Phi}^n + \mathbf{K}\bar{\Phi}^n + \mathbf{f}^n) - \Delta t(\mathbf{K}_u\bar{\Phi}^n + \mathbf{f}_s^n)] \quad (7)$$

where

$$\begin{aligned} \mathbf{M} &= \int_{\Omega} \mathbf{N}^T \mathbf{N} d\Omega & \mathbf{C} &= \int_{\Omega} \mathbf{N} u_i \frac{\partial \mathbf{N}^T}{\partial x_i} d\Omega \\ \mathbf{K} &= \int_{\Omega} \frac{\partial \mathbf{N}^T}{\partial x_i} k \frac{\partial \mathbf{N}}{\partial x_i} d\Omega & \mathbf{f} &= \int_{\Omega} \mathbf{N}^T Q d\Omega + b.t. \end{aligned} \quad (8.a)$$

and  $\mathbf{K}_u$  and  $\mathbf{f}_s^n$  come from the new term introduced by the discretization along the characteristics. After integration by parts, the expression of  $\mathbf{K}_u$  and  $\mathbf{f}_s$  is

$$\begin{aligned} \mathbf{K}_u &= -\frac{1}{2} \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) \frac{\partial}{\partial x_j} (u_j \mathbf{N}) d\Omega \\ \mathbf{f}_s &= -\frac{1}{2} \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) Q d\Omega + b.t. \end{aligned} \quad (8.b)$$

The approximation is valid for any scalar convected quantity even if that is the velocity  $\mathbf{u}$  itself, as is the case with the momentum conservation equations. For this reason we have elaborated the full details of the spatial approximation as the matrices will be repeatedly used.

It is of interest to remark that the explicit form of the equation (7) is conditionally stable. For one-dimensional problems, the stability condition is given by (neglecting the effect of sources)

$$\Delta t \leq \Delta t_{crit} = \frac{h}{|u|} \left( \sqrt{\frac{1}{P^2} + \frac{1}{3}} - \frac{1}{P} \right) \quad (9)$$

for linear elements. In above the Peclet number  $P$  is defined as

$$P = \frac{|u|h}{2k} \quad (10)$$

In 2D problems the critical time step size may be computed as [27]

$$\Delta t_{crit} = \frac{\Delta t_{\sigma} \Delta t_{\nu}}{\Delta t_{\sigma} + \Delta t_{\nu}}$$

where  $\Delta t_{\sigma}$  is given by (9) and  $\Delta t_{\nu} = h^2/2k$  is the diffusive limit for the critical one-dimensional time step size.



Further, with  $\Delta t = \Delta t_{crit}$  the steady state solution results in an (almost) identical diffusion change to that obtained by using the optimal stream line upwinding procedures [6]. Thus if steady state solution are the main objective of the computation such a value of  $\Delta t$  should be used in connection with the  $K_u$  term.

### 3. THE GENERAL FRACTIONAL STEP ALGORITHM FOR THE NAVIER-STOKES EQUATIONS

#### 3.1 The equations of flow

The full conservation form of the Navier-Stokes equations for compressible flow is traditionally written as

$$\frac{\partial \mathbf{V}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q} = 0 \quad (11)$$

with

$$\mathbf{V}^T = [\rho, \rho u_1, \rho u_2, \rho u_3, \rho E] \quad (12a)$$

being the independent variable vector

$$\mathbf{F}_i^T = [\rho u_i, \rho u_1 u_i + \delta_{1i} p, \rho u_2 u_i + \delta_{2i} p, \rho u_3 u_i + \delta_{3i} p, u_i(\rho E + p)] \quad (12b)$$

defining the convective flux vector and

$$\mathbf{G}_i^T = [0, \tau_{1i}, -\tau_{2i}, -\tau_{3i}, -k \frac{\partial T}{\partial x_i} - \tau_{ij} u_j] \quad (12c)$$

defining the diffusion flows. Finally

$$\mathbf{Q}^T = [0, g_1, g_2, g_3, 0] \quad (12d)$$

gives the source terms.

In above the stress components  $\tau_{ij}$  are related to velocity gradients by

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (13)$$

$\rho$  is the density,  $u_i$  are the velocity components,  $p$  is the pressure,  $E$  the internal energy and  $T$  the absolute temperature.

The equations are completed by the universal gas law

$$p = \rho RT \quad (14)$$

where  $R$  is the gas constant.

The sound velocity is defined assuming constant entropy as

$$c^2 = \frac{\partial p}{\partial \rho} = \frac{\gamma p}{\rho} \quad (15)$$

Further we can write conveniently

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p} \frac{\partial p}{\partial t} = \frac{1}{c^2} \frac{\partial p}{\partial t} \quad (16)$$

though this expression assumes again constant entropy and is therefore only an approximation. We shall, in what follows use Eq. 16 but later will discuss the possibility of correcting any errors involved by an amendment of the algorithm.

While in gas flow all the equations are fully coupled, for incompressible flow in which  $c = \infty$  the energy equations can be solved independently after the velocity field has been established. Nevertheless a single algorithm for the solution of both problems is possible as we shall now show.

### 3.2 The general algorithm

For convenience we shall rewrite the Eq.(11) in a more direct form, omitting initially the energy equation. These equations can be solved completely in a time increment  $\Delta t$  as the only coupling which exists is through the speed of sound  $c$  for which we shall simply use the value at time  $t_n$  due to the explicit nature of the time stepping algorithm.

We thus write the first of equations (13), i.e. the mass flow continuity as

$$\frac{\partial \rho}{\partial t} = \frac{1}{c^2} \frac{\partial p}{\partial t} = -\frac{\partial U_i}{\partial x_i} \quad (17)$$

in which we use the Eq.(16). Further, for each of the momentum conservation equations we write similarly

$$\frac{\partial U_i}{\partial t} = -\frac{\partial F_i^j}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} - g_i \quad (18)$$

In above we define

$$U_i = \rho u_i$$

and

$$F_i^j = u_j(\rho u_i) = u_j U_i \quad (19)$$

Since

$$\frac{\partial F_i^j}{\partial x_j} = \frac{\partial u_j}{\partial x_j} U_i + u_j \frac{\partial U_i}{\partial x_j} \quad (20)$$

we can discretize in time Eq.(8) using the Characteristic Galerkin process. Except for the pressure term this equation is similar to the convection-diffusion problem of Eq.(3). We shall have

$$\begin{aligned} U_i^{n+1} - U_i^n &= \Delta t \left[ -\frac{\partial F_i^j}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - g_i + \frac{\Delta t}{2} u_k \frac{\partial}{\partial x_k} \left( \frac{\partial F_i^j}{\partial x_j} + g_i \right) \right]_n \\ &\quad - (1 - \theta_2) \Delta t \left[ \frac{\partial p}{\partial x_i} - \frac{\Delta t}{2} u_k \frac{\partial}{\partial x_k} \frac{\partial p}{\partial x_i} \right]_n - \theta_2 \Delta t \left[ \frac{\partial p}{\partial x_i} \right]_{n+1} \end{aligned} \quad (21)$$

Observe that the pressure term has been evaluated at  $t_n + \theta_2 \Delta t$ .

Before proceeding further it is convenient to introduce an auxiliary variable  $\tilde{U}_i$  such that

$$\Delta \tilde{U}_i = \tilde{U}_i^{n+1} - U_i^n = \Delta t \left[ -\frac{\partial F_i^j}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - g_i + \frac{\Delta t}{2} u_k \frac{\partial}{\partial x_k} \left( \frac{\partial F_i^j}{\partial x_j} + g_i \right) \right]_n \quad (22)$$

and therefore

$$\begin{aligned} \Delta U_i &= U_i^{n+1} - U_i^n = \Delta \tilde{U}_i - \Delta t (1 - \theta_2) \left[ \frac{\partial p}{\partial x_i} - \frac{\Delta t}{2} u_k \frac{\partial}{\partial x_k} \frac{\partial p}{\partial x_i} \right] \\ &\quad - \theta_2 \Delta t \left[ \frac{\partial p}{\partial x_i} \right]_{n+1} = \Delta \tilde{U}_i - \Delta t \left[ \frac{\partial p^n}{\partial x_i} + \theta_2 \frac{\partial \Delta p}{\partial x_i} \right] + (1 - \theta_2) \frac{\Delta t^2}{2} u_k \frac{\partial}{\partial x_k} \frac{\partial p^n}{\partial x_i} \end{aligned} \quad (23)$$

where  $\Delta p = p^{n+1} - p^n$  and the last term as before represents the ‘‘source’’ correction. From Eq.(17) we have omitting third order terms

$$\begin{aligned} \Delta \rho &= \left( \frac{1}{c^2} \right)_n \Delta p = -\Delta t \frac{\partial U_i^{n+\theta_1}}{\partial x_i} \\ &= -\Delta t \left[ \frac{\partial U_i^n}{\partial x_i} + \theta_1 \frac{\partial \Delta \tilde{U}_i}{\partial x_i} - \Delta t \theta_1 \left( \frac{\partial^2 p^n}{\partial x_i \partial x_i} + \theta_2 \frac{\partial^2 \Delta p}{\partial x_i \partial x_i} \right) \right]_n \end{aligned} \quad (24)$$

It is clear that the equations can be solved after spatial discretization in the following order

Eq.(22) giving  $\Delta\tilde{U}_i$

Eq.(23) giving  $\Delta p$

Eq.(24) giving  $\Delta U_i$  thus establishing the values at  $t_{n+1}$

In all of the equations given below the standard Galerkin procedure can be used with a discretization

$$U_i = \mathbf{N}\bar{U}_i, \quad \Delta U_i = \mathbf{N}\Delta\bar{U}_i, \quad \Delta\tilde{U}_i = \mathbf{N}\Delta\tilde{\bar{U}}_i \quad (25)$$

and

$$p = \mathbf{N}_p\bar{p}$$

This gives from Eq.(22) the solution for  $\tilde{\bar{U}}_i$  as

$$\text{Step 1} \quad \boxed{\Delta\tilde{\bar{U}} = -\mathbf{M}^{-1}\Delta t[(\mathbf{C}\bar{U} + \mathbf{K}\bar{U} - \mathbf{f}) - \Delta t(\mathbf{K}_u\bar{U} + \mathbf{f}_s)]^n} \quad (26)$$

where all the discretization matrices *are the same* as those defined by Eq.8.

Discretization of eq.24 gives similarity

$$\text{Step 2} \quad \boxed{(\tilde{\mathbf{M}} + \Delta t^2\theta_1\theta_2\mathbf{H})\Delta\bar{p} = \Delta t[\mathbf{Q}(\bar{U}^n + \theta_1\Delta\tilde{\bar{U}}) - \Delta t\theta_1\mathbf{H}\bar{p} - \mathbf{f}_p]^n} \quad (27)$$

which can be solved for  $\Delta\bar{p}$ .

The new matrices arising here are

$$\begin{aligned} \mathbf{H} &= \int_{\Omega} \left( \frac{\partial \mathbf{N}_p^T}{\partial x_i} \right) \frac{\partial \mathbf{N}_p}{\partial x_i} d\Omega \\ \tilde{\mathbf{M}} &= \int_{\Omega} \mathbf{N}_p^T \left( \frac{1}{c^2} \right)_n \mathbf{N}_p d\Omega \\ \mathbf{Q} &= \int_{\Omega} \frac{\partial \mathbf{N}_p^T}{\partial x_i} \mathbf{N} d\Omega \end{aligned} \quad (28)$$

The question of establishing the boundary conditions for the pressure is discussed in detail in Appendix A.

The final stage of the computation of the mass flow vector  $\mathbf{U}_i^{n+1}$  is completed by discretization of Eq.(23) and we have now simply

$$\text{Step 3} \quad \boxed{\Delta\bar{U} = \Delta\tilde{\bar{U}} - \mathbf{M}^{-1}\Delta t[\mathbf{Q}^T(\bar{p}^n + \theta_2\Delta\bar{p}) + \frac{\Delta t}{2}\mathbf{P}\bar{p}^n]} \quad (29)$$

where

$$\mathbf{P} = (1 - \theta_2) \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}_p^T) \frac{\partial \mathbf{N}_p}{\partial x_i} d\Omega$$

At the completion of this stage the values of  $\bar{U}_i^{n+1}$  and  $\bar{p}^{n+1}$  are fully determined but the computation of the energy  $\rho E^{n+1}$  is needed so that new values of  $c^{n+1}$ , the speed of sound, can be determined.

The last of Eq.(11) i.e., the energy conservation equation can be written as

$$\frac{\partial(\rho E)}{\partial t} = -\frac{\partial}{\partial x_j} (u_j \rho E) + \frac{\partial}{\partial x_i} (k \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_j} (u_j p) \quad (30)$$

Once again the equation is identical in form to that of the scalar problem of Eq.(3) if we observe that  $p$ ,  $U_i$  etc. have been determined. Now the last term can be evaluated at time  $(n + \theta_3)$  for improved accuracy but in what follows we shall take  $\theta_3 = 0$  for simplicity.

Using the Characteristic Galerkin approximation of Eq.(5) and discretizing as

$$\rho E = \mathbf{N}_E \bar{\mathbf{E}}_v \quad (31a)$$

we have

$$\text{Step 4} \quad \boxed{\Delta \bar{\mathbf{E}}_v = -\Delta t [\mathbf{C} \bar{\mathbf{E}}_v^n + \mathbf{K} \mathbf{T}^n + \mathbf{f}_e^n - \Delta t (\mathbf{K}_u \bar{\mathbf{E}}_v^n + \mathbf{f}_{es}^n)]} \quad (31b)$$

where  $\bar{\mathbf{E}}_v$  contains the nodal values of  $\rho E$  and again the matrices are identical to those previously obtained (assuming that  $\rho E$  and  $T$  can be suitably scaled in the conduction term).

Again the forcing vectors can be appropriately defined as

$$\begin{aligned} \mathbf{f}_e &= \int_{\Omega} \mathbf{N}_E^T \frac{\partial}{\partial x_j} (u_j p) d\Omega \\ \mathbf{f}_{es} &= -\frac{1}{2} \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) \frac{\partial}{\partial x_j} (u_j p) d\Omega \end{aligned} \quad (32)$$

It is of interested to observe that the process of Step 4 can be extended in an identical manner to equations describing the transport of such quantities as turbulence parameters, chemical concentrations etc. once the first essential steps 1-3 have been completed.

#### 4. SEMI-IMPLICIT AND EXPLICIT FORMS OF THE ALGORITHM

The algorithm described can be used in a semi-implicit form and indeed only in this form can incompressible problems in which  $c = \infty$  and  $\tilde{M} = 0$  be solved. Taking

$$\begin{aligned} 1 &\geq \theta_1 \geq \frac{1}{2} \\ 1 &\geq \theta_2 \geq \frac{1}{2} \end{aligned} \quad (33)$$

the algorithm is conditionally stable. The permissible time step is governed by the critical step of the explicit relation solved in Step I of the algorithm. This is the standard convection-diffusion problem discussed in section 2 and the same stability limits apply reaching for an inviscid fluid a value close to

$$\Delta t_{crit} = \frac{h}{|\mathbf{u}|} \quad (34)$$

For slightly compressible or incompressible problems in which  $\tilde{M}$  is small or zero the semi-implicit form is efficient and it should be noted that the matrix  $\mathbf{H}$  of Eq.(27) does not vary during the computation process and can be partially inverted.

In other semi-implicit forms when compressibility exists the question of the correctness of the approximation of Eq.(16) remains still unanswered and has to be further investigated. Here of course an iterative correction can be used.

However it is possible to revert to a fully explicit form by putting  $\theta_2 = 0$ . Now of course the critical step will be reduced to the order of

$$\frac{h}{c} \quad (35)$$

and this is indeed the same limit as that encountered in other explicit forms of Euler or Navier-Stokes computational schemes currently effectively used.

The four Eqs.(26), (27), (29) and (31) can be solved simultaneously if the correction step in the R.H.S of Eq.(27) is omitted. This of course is an additional approximation and is not necessary but is here introduced to mimic artificial diffusions previously extensively used with standard Galerkin form.

Further the use of the approximation of Eq.(16) is now no longer necessary as the density increment is directly obtained if we note that

$$\tilde{M}\Delta\bar{p} \equiv M\Delta\bar{p} \quad (36)$$

With above simplifications we can return to the original equations (11) and using the Galerkin approximation on these we can write directly

$$\Delta \bar{\mathbf{V}} = -\mathbf{M}^{-1} \Delta t \left[ \int_{\Omega} \mathbf{N}^T \left( \frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} \right) d\Omega + \frac{1}{2} \Delta t \int_{\Omega} \mathbf{N}^T \mathbf{D} d\Omega \right]_n \quad (37)$$

omitting the source terms for clarity. The added diffusion terms  $\mathbf{D}$  are defined below and have to be integrated by parts in the usual manner.

$$\mathbf{D} = \left\{ \begin{array}{l} 2 \frac{\partial^2}{\partial x_i \partial x_i} p \\ u_i \frac{\partial}{\partial x_i} \left[ \frac{\partial}{\partial x_j} (u_j \rho u_1) + \frac{\partial p}{\partial x_1} \right] \\ u_i \frac{\partial}{\partial x_i} \left[ \frac{\partial}{\partial x_j} (u_j \rho u_2) + \frac{\partial p}{\partial x_2} \right] \\ u_i \frac{\partial}{\partial x_i} \left[ \frac{\partial}{\partial x_j} (u_j \rho u_3) + \frac{\partial p}{\partial x_3} \right] \\ u_i \frac{\partial}{\partial x_i} \left[ \frac{\partial}{\partial x_j} (u_j \rho E + u_j p) \right] \end{array} \right\} \quad (38)$$

The “diffusions” added are simple and largely streamline oriented (for divergence-free velocities) thus not masking the true effects of viscosity as happens in some schemes. The importance of the various terms will be discussed in Part II of this paper where detailed comparisons with other explicit schemes are made.

If steady state results only are sought it would appear that  $\Delta t$  in the definition of the matrix  $\mathbf{D}$  should be set at its optimal value of  $\Delta t_{crit} \approx \frac{h}{|\mathbf{u}|}$ .

However the oversimplified scheme of Eq.(38) loses some accuracy and even when steady state is reached will give slightly different results than those obtained using the full sequential updating. The additional cost involved in computing the sequence  $\Delta \bar{\mathbf{U}} \rightarrow \Delta \mathbf{p} \rightarrow \Delta \bar{\mathbf{U}} \rightarrow \Delta \bar{\mathbf{E}}_v$  will have to be balanced against the accuracy increase.

It is of interest to note here in passing that the full sequential scheme introduces a so called “fourth order” diffusion proportional to  $\Delta t \mathbf{Q}^T \mathbf{M}^{-1} \mathbf{Q} \bar{\mathbf{p}}$  in addition to the second order diffusion proportional to  $\Delta t \mathbf{H} \bar{\mathbf{p}}$  into the computation. We shall indicate how this arises in the next section.

## 5. WHY THE BB RESTRICTIONS ARE CIRCUMVENTED

### Steady state results

We examine here the structure of equations reached in steady conditions. For simplicity we shall consider here only the Stokes form of governing equations in which the convective terms disappear. Further we shall take the fluid as incompressible and thus uncouple the energy equations. Now the three steps of Eqs.(26), (27) and (29) are written as

$$\Delta \tilde{\bar{\mathbf{U}}} = -\Delta t \mathbf{M}^{-1} [\mathbf{K} \bar{\mathbf{U}}^n - \mathbf{f}] \quad (39a)$$

$$\Delta \bar{\mathbf{p}} = \frac{1}{\Delta t \theta_1 \theta_2} \mathbf{H}^{-1} [\mathbf{Q}(\bar{\mathbf{U}}^n + \theta_1 \Delta \tilde{\bar{\mathbf{U}}}) - \Delta t \theta_1 \mathbf{H} \bar{\mathbf{p}}^n - \mathbf{f}_p] \quad (39b)$$

$$\Delta \bar{\mathbf{U}} = \Delta \tilde{\bar{\mathbf{U}}} - \Delta t \mathbf{M}^{-1} \mathbf{Q}^T (\bar{\mathbf{p}}_n + \theta_2 \Delta \bar{\mathbf{p}}) \quad (39c)$$

In steady state  $\Delta \bar{\mathbf{p}} = \Delta \bar{\mathbf{U}} = 0$  and eliminating  $\Delta \tilde{\bar{\mathbf{U}}}$  we can write (dropping now the superscript  $n$ )

$$\mathbf{K} \bar{\mathbf{U}} + \mathbf{Q}^T \bar{\mathbf{p}} = \mathbf{f} \quad (40)$$

from Eq.(39a) and (c) and

$$\mathbf{Q} \bar{\mathbf{U}} + \theta_1 \Delta t \mathbf{Q} \mathbf{M}^{-1} \mathbf{Q}^T \bar{\mathbf{p}} - \Delta t \theta_1 \mathbf{H} \bar{\mathbf{p}} - \mathbf{f}_p = 0 \quad (41)$$

from Eqs.(39b) and (c).

We finally have a system which can be written in a form

$$\begin{bmatrix} \mathbf{K} & \mathbf{Q}^T \\ -\mathbf{Q} & \Delta t \theta_1 [\mathbf{H} - \mathbf{Q} \mathbf{M}^{-1} \mathbf{Q}^T] \end{bmatrix} \begin{Bmatrix} \bar{\mathbf{U}} \\ \bar{\mathbf{p}} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{Bmatrix} \quad (42)$$

where  $\mathbf{f}_1$  and  $\mathbf{f}_2$  arise from the forcing terms.

This system has a non-zero diagonal which is proportional to  $\Delta t$  and which, as already mentioned, is very similar to the forms suggested by other reasoning [27,24].

Further it will be immediately observed that if the additional simplification introduced in Eq.(38) is made to avoid the sequential operations, the term  $\Delta t \mathbf{Q} \mathbf{M}^{-1} \mathbf{Q}^T$  disappears. This term is however very useful adding a “smoothing” by spreading the effect of jumps etc. to a wider pattern of elements.

It can be easily verified that if the pressure gradient term is retained in Eq.(22) (which would seem to give a better approximation) the diagonal term of Eq.(42) is identically zero and the BB conditions are still necessary.

## 5. SUMMARY

The algorithm here introduced follows similar lines of reasoning as were used in previous attempts to derive the “universal” algorithm. Details however are different and in particular the introduction of the “Characteristic Galerkin” diffusion is more direct and different. In further parts of this paper numerical tests will be made and accuracy tested in various applications.

Application of the identical procedure to shallow water equation is obvious and indeed very similar to that given in ref [23].



## APPENDIX A

We shall consider in this appendix the boundary conditions to be imposed for equation (24). Observe first that Eq.(23) may be written as

$$\Delta U_i = \Delta \tilde{U}_i - \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \quad (1A)$$

where

$$\begin{aligned} p^{n+\theta_2}(\mathbf{x}) &= (1 - \theta_2)p^n(\tilde{\mathbf{x}}) + \theta_2 p^{n+1}(\mathbf{x}) \\ &= (1 - \theta_2)\left[p^n(\mathbf{x}) - \frac{\Delta t}{2} u_i \frac{\partial}{\partial x_i} p^n(\mathbf{x})\right] + \theta_2 p^{n+1}(\mathbf{x}) \end{aligned} \quad (2A)$$

The pressure boundary conditions we use are the continuity of the normal component of the momentum equation at the boundary. It may be readily checked that this is equivalent to the verification of the normal component of Eq.(1A) at the boundary, that is

$$n_i \Delta U_i = n_i \Delta \tilde{U}_i - \Delta t n_i \frac{\partial p^{n+\theta_2}}{\partial x_i} \quad (3A)$$

Multiplying Eq.(24) by a pressure test function  $N_p$  and integrating by parts we obtain, using Eq.(3A)

$$\begin{aligned} \int_{\Omega} \frac{1}{c^2} \mathbf{N}_p^T \Delta p d\Omega &= -\Delta t \left[ - \int_{\Omega} \frac{\partial \mathbf{N}_p^T}{\partial x_i} U_i^n d\Omega + \int_{\partial\Omega} \mathbf{N}_p^T n_i U_i^n d\Gamma \right. \\ &\left. + \theta_1 \int_{\partial\Omega} \mathbf{N}_p^T n_i \Delta U_i d\Gamma - \theta_1 \int_{\Omega} \frac{\partial \mathbf{N}_p^T}{\partial x_i} \Delta \tilde{U}_i^n d\Omega + \Delta t \theta_1 \int_{\Omega} \frac{\partial \mathbf{N}_p^T}{\partial x_i} \frac{\partial p^{n+\theta_2}}{\partial x_i} d\Gamma \right] \end{aligned} \quad (4A)$$

from where it follows that the term  $\mathbf{f}_p$  in Eq.(27) is given by

$$\mathbf{f}_p = - \int_{\partial\Omega} \mathbf{N}_p^T n_i U_i^n - \theta_2 \int_{\partial\Omega} \mathbf{N}_p^T n_i \Delta U_i d\Gamma \quad (5A)$$

This expression involves  $\Delta U_i$ , which is unknown at the moment of solving the pressure equation. However, the second term in the RHS of Eq.(5A) may be neglected. This approximation is exact if  $\mathbf{U}$  is prescribed on the whole boundary  $\partial\Omega$ . On the other hand, and in order to avoid the need to compute the boundary integral, in Eq.(4A) we may rewrite

$$-\int_{\Omega} \frac{\partial \mathbf{N}_p^T}{\partial x_i} U_i^n d\Omega + \int_{\partial\Omega} \mathbf{N}_p^T n_i U_i^n d\Gamma = \int_{\Omega} \mathbf{N}_p^T \frac{\partial U_i^n}{\partial x_i} d\Omega \quad (6A)$$

Instead of Eq.(27) we shall have

$$(\tilde{\mathbf{M}} + \Delta t^2 \theta_1 \theta_2 \mathbf{H}) \Delta \bar{\mathbf{p}} = \Delta t [\tilde{\mathbf{Q}} \bar{\mathbf{U}}^n + \theta_1 \mathbf{Q} \Delta \bar{\bar{\mathbf{U}}} - \Delta t \theta_1 \mathbf{H} \bar{\mathbf{p}}]^n \quad (7A)$$

where

$$\tilde{\mathbf{Q}} = - \int_{\Omega} \mathbf{N}_p^T \frac{\partial \mathbf{N}}{\partial x_i} d\Omega$$

Observe that no term  $\mathbf{f}_p$  appears in Eq.(7A).

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