

MULTI-DIMENSIONAL TIME DEPENDENT CONVECTION-DIFFUSION

Extension of the Petrov-Galerkin method to the equation $\frac{\partial \phi}{\partial t} + \mathbf{V} \cdot \nabla \phi = \nabla \mathbf{D} \nabla \phi + S$ in two and three dimensions is obtained as before by adding an anisotropic diffusion and dispersion only in the direction of flow.

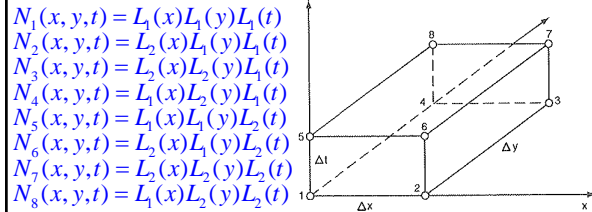
The weighting functions can be expressed in the form

$$w_i(\mathbf{x}, t) = M_i + \frac{h}{2\|\mathbf{V}\|} \left(\alpha + \frac{\beta \Delta t}{2} \frac{\partial}{\partial t} \right) \mathbf{V} \cdot \nabla M_i$$

where the functions M_i are quadratic in time and linear in space.

In two space dimensions the elements are tri-linear. The figure below shows a tri-linear space-time element together with the nodal numbering and coordinate system. Also the shape functions are given.

1



$$L_1(\zeta) = 1 - \frac{\zeta}{\Delta \zeta}, \quad L_2(\zeta) = \frac{\zeta}{\Delta \zeta}, \quad 0 < \zeta < \Delta \zeta, \quad \zeta = x, y, t$$

The functions M_i are

$$\begin{aligned} M_1(x, y, t) &= M_5(x, y, t) = L_1(x)L_1(y)T(t) \\ M_2(x, y, t) &= M_6(x, y, t) = L_2(x)L_1(y)T(t) \\ M_3(x, y, t) &= M_7(x, y, t) = L_2(x)L_2(y)T(t) \\ M_4(x, y, t) &= M_8(x, y, t) = L_1(x)L_2(y)T(t) \end{aligned} \quad T(t) = \frac{t}{\Delta t} \left(1 - \frac{t}{\Delta t} \right)$$

2

The parameters α and β are obtained from

$$\begin{aligned} \alpha &= \coth\left(\frac{\bar{\gamma}}{2}\right) - \frac{2}{\bar{\gamma}}, \quad \bar{\gamma} = \frac{\|\mathbf{V}\|\bar{h}}{D} \\ \beta &= \frac{\delta}{3} - \frac{2\alpha}{\bar{\gamma}\delta}, \quad \delta = \frac{\|\mathbf{V}\|\Delta t}{h} \end{aligned}$$

with \bar{h} defined as in the steady-state case.

When $\beta \neq 0$ the stability limit in two dimensions takes the form

$$\Delta t \leq \frac{1}{\left(\frac{|u|}{\Delta x} \right) + \left(\frac{|v|}{\Delta y} \right)}$$

In 2 and 3 dimensions the stability limit is only approximate, and it can be expressed in several different ways.

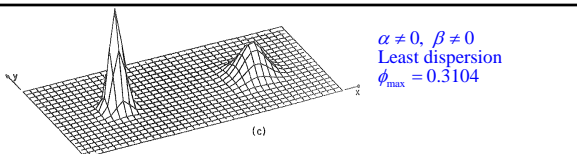
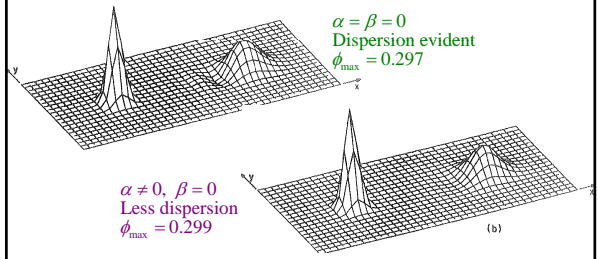
The Courant number is also approximate and given by

$$c = \left(\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} \right) \Delta t$$

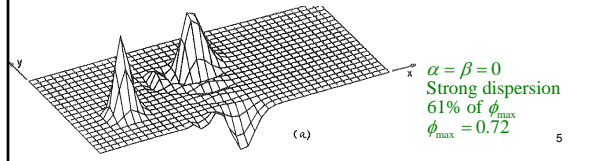
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EXAMPLES

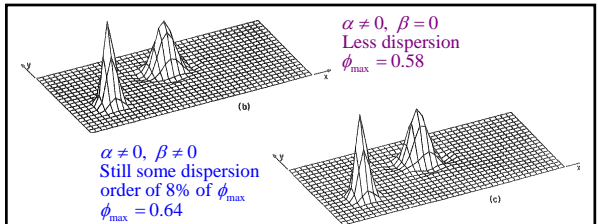
1) First consider unidirectional flow, $u = 0.25$ and $v = 0$. The initial perturbation is $\phi(x, y, 0) = \exp\left\{-\left[(x-0.25)^2 + (y-0.25)^2\right]/0.00125\right\}$. $D = 0.0003125$, $S = 0$. The domain $0 \leq x \leq 1.0$ and $0 \leq y \leq 0.5$ is discretized with a uniform mesh $\Delta x = \Delta y = 0.025$, and Δt is chosen so that $c = 0.85$ and $\gamma = 20$. Results are shown at $t = 2.04$.



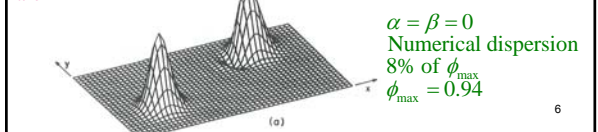
2) Purely advective transport at a 25° angle to the x-axis. $u = 0.25$, $v = 0.1166$ and the initial condition is $\phi(x, y, 0) = \exp\left\{-\left[(x-0.175)^2 + (y-0.175)^2\right]/0.00125\right\}$. $c = 0.7332$ and $\gamma = 20$ same mesh as example 1. The initial condition and the results at $t = 1.3$ are shown below.



5



These results are not all that good. In this case there are six elements to describe the initial perturbation, i. e. $L/h = 6$. If we reduce the mesh size by one half, $\Delta x = \Delta y = 0.0125$ then $L/h = 12$. The results at $t = 1.3$ are



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$\alpha \neq 0, \beta = 0$
Dispersion 4% of ϕ_{max}
 $\phi_{max} = 0.846$

$\alpha \neq 0, \beta \neq 0$
Dispersion < 1% of ϕ_{max}
 $\phi_{max} = 0.91$

REMARKS
1) The above examples illustrate how difficult it can be to simulate this type of problems and how numerical algorithms must be carefully evaluated before accepting a solution. Modifications to the algorithms may also be necessary depending on the problem.

2) The stiffness matrices of convection problems are non-symmetric which greatly increases the cost of the solutions. This can be avoided in practice by treating the convective terms explicitly. However in these methods if $\beta \neq 0$ it leads to unconditionally unstable schemes. However if $\alpha \neq 0$ and $\beta = 0$ we can still compute with $c < 1$. This argues for the use of $\alpha \neq 0$ and $\beta = 0$ in practical situations when the added accuracy is not needed.

3) A method that has been heavily used in the purely convective case is the Taylor-Galerkin method (Do-1984). In one dimension the idea is to approximate $(\partial\phi/\partial t)$ by a truncated Taylor series in time

$$\phi_t^n = \frac{\phi^{n+1} - \phi^n}{\Delta t} - \frac{\Delta t}{2} \phi_{tt}^n + \frac{\Delta t^2}{6} \phi_{ttt}^n + O(\Delta t^3)$$

where $\phi_t^n = \frac{\partial\phi}{\partial t}(x, t_n)$.

From the differential equation we have $\phi_t = -u\phi_{xx}$ which can be differentiated to get

$\phi_{tt} = u^2\phi_{xx}$ and $\phi_{ttx} = u^2\phi_{xxx}$
replacing in the Taylor expansion we have

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - u^2 \frac{\Delta t^2}{6} \phi_{xxx}^n + u\phi_x - u^2 \frac{\Delta t}{2} \phi_{xx}^n = 0$$

This can be discretized to obtain a number of different algorithms

For example, replacing the time derivative by a forward difference leads to the Euler-Taylor-Galerkin form

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - u^2 \frac{\Delta t}{6} [\phi_{xx}^{n+1} - \phi_{xx}^n] + u\phi_x - u^2 \frac{\Delta t}{2} \phi_{xx}^n = 0$$

NOTES:
i) In effect, a stabilizing diffusion has been added to the scheme.
ii) The scheme is accurate, simple and easy to implement.
iii) The solution will not approach the correct limit as it reaches steady-state.
iv) The extension to include diffusion is difficult and not as accurate

4) The Petrov-Galerkin method has the *unit Courant-Friedrich-Levy property*. That is, if $c = 1$ the perturbations travel undistorted. The convection of a Gauss form in the x-direction with $\alpha \neq 0, \beta \neq 0$ and $c = 1$ is shown below at $t = 0$ and $t = 2$. It shows no error.

5) Many other methods have been proposed, amongst them:
The Method of Moments (P-B), Variational approaches (Id), Euler-Lagrange (Var-Finn), Hermite cubics (Allen), etc.

6. The method has been extended to the non-linear Burgers equation. Results show that in the presence of very sharp fronts small oscillations develop just ahead and behind the front.

EXAMPLE

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0.01 \frac{\partial^2 u}{\partial x^2} \quad 0 < x < 2, \quad u(0,t) = u(2,t) = 0,$$

$$u(x,0) = \begin{cases} \cos[2\pi(x-0.25)], & 0 \leq x \leq 0.5 \\ 0, & \text{otherwise} \end{cases}, \quad \Delta x = \Delta t = 0.025$$

VISCOUS INCOMPRESSIBLE FLOW

The Navier-Stokes equations (in two-dimensions for simplicity) are normally written either in terms of velocity or in terms of stresses.

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$\rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) + \rho B_x$$

$$\rho \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial y} \right) + \rho B_y$$

or $\rho \frac{Du_i}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho B_i, \quad \sigma_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$

$$\frac{\partial u_i}{\partial x_i} = 0$$

Example

Flow over a backward facing step

The boundary segments are

$$\Gamma_1 = \{y=0, L_1 \leq x \leq L_2\} \cup \{x=L_1, 0 \leq y \leq H/2\} \cup \{y=H/2, 0 \leq x \leq L_2\} \cup \{x=0, H/2 \leq y \leq H\} \cup \{y=H, 0 \leq x \leq L_2\}$$

$$\Gamma_2 = \{x=L_2, 0 \leq y \leq H\}$$

$$\Gamma_3 = \emptyset$$

Remarks:

1) Notice that the boundary segments Γ_1, Γ_2 , and Γ_3 need not be the same for both velocity components. For example, symmetry boundary conditions occur often and are applied as a combination of a Dirichlet condition normal to the symmetry plane and a Neumann condition along the symmetry plane.

2) Boundary conditions of mixed type are rarely encountered in fluid flow.

3) Boundary conditions at free surfaces will be discussed later.

4) In general no boundary conditions are needed for the pressure. However, a reference value must be provided. This is usually done fixing the pressure at one point in the domain.

5) In some calculations cyclic conditions are imposed along otherwise open boundaries. This can be done in various ways depending on the problem and will be discussed later.

The weak form is stated as follows: Find functions u^* and v^* in $H^1(\Omega)$ that satisfy the Dirichlet boundary conditions in Γ_1 , and a function p^* in $\mathcal{L}^2(\Omega)$ such that

$$\int_{\Omega} \left\{ U \rho \left(\frac{\partial u^*}{\partial t} + u^* \frac{\partial u^*}{\partial x} + v^* \frac{\partial u^*}{\partial y} \right) - \frac{\partial U}{\partial x} p^* + \mu \left(\frac{\partial U}{\partial x} \frac{\partial u^*}{\partial x} + \frac{\partial U}{\partial y} \frac{\partial u^*}{\partial y} \right) - \rho B_x \right\} d\Omega$$

$$+ \int_{\Gamma} \left[-p^* + \mu \frac{\partial u^*}{\partial x} \right] n_x + \mu \frac{\partial u^*}{\partial y} n_y \, d\Gamma = 0$$

$$\int_{\Omega} \left\{ V \rho \left(\frac{\partial v^*}{\partial t} + u^* \frac{\partial v^*}{\partial x} + v^* \frac{\partial v^*}{\partial y} \right) - \frac{\partial V}{\partial y} p^* + \mu \left(\frac{\partial V}{\partial x} \frac{\partial v^*}{\partial x} + \frac{\partial V}{\partial y} \frac{\partial v^*}{\partial y} \right) - \rho B_y \right\} d\Omega$$

$$+ \int_{\Gamma} \left[\mu \frac{\partial v^*}{\partial y} n_x + \left(-p^* + \mu \frac{\partial v^*}{\partial y} \right) n_y \right] d\Gamma = 0$$

and $\int_{\Omega} Q \left(\frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial x} \right) d\Omega = 0$

for all pairs of weighting functions U and V in $H_0^1(\Omega)$ and all functions Q in a space S that will be defined below.

Remarks:

1) The mathematical theory is complex and beyond our scope, we will be satisfied with stating the results. There are several very good text books that the interested reader can consult.

2) This is called a "Mixed Variational Formulation" because the pressure is found in a space different than the velocities. The pressure is sought in a subset of $\mathcal{L}^2(\Omega)$ that we refer to as " $\mathcal{L}^2(\Omega)$ modulo constants" and is denoted by $S = \mathcal{L}^2(\Omega)/\mathcal{R}$. Because the pressure is only determined up to an arbitrary constant, therefore, two functions that differ by a real constant number are the same function in this space.

3) Mathematically results can only be proved for the continuity equation coupled to the linear Stokes equations

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$\rho \frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \rho B_x$$

$$\rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \rho B_y$$

The existence and uniqueness of solutions requires that the subspaces containing the solution be compatible. This requires the existence of a constant $\beta > 0$ such that

$$\sup_{\substack{V \in H^1(\Omega) \\ V \neq 0}} \frac{\int_{\Omega} q \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) d\Omega}{\|V\|_1} \leq \beta \|q\|_0$$

for all $q \in S$.

This guarantees that the velocity and pressure spaces are consistent and is known as the "LBB" condition (after Ladyzhenskaya, Babuska and Brezzi)

Clearly the analytical spaces automatically satisfy this condition. However the discretized spaces often violate it, and the elements cannot be used or must be modified to satisfy the condition.

CONSTANT DENSITY FLOWS

Let us assume that $B_x = 0$ and $B_y = 0$, and that ρ and μ are constant. Write the momentum equations in non-dimensional form

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \frac{1}{\text{Re}} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)$$

Re is the Reynolds number defined as $\text{Re} = \frac{\bar{U} \rho_0 L}{\mu}$, where \bar{U} is a characteristic velocity, ρ_0 is the reference density, L is the characteristic length and μ is the dynamic viscosity.

The reference pressure is $p_0 = \rho_0 \bar{U}^2$ and the time scale is $\tau = L/\bar{U}$.

MIXED FORMULATION

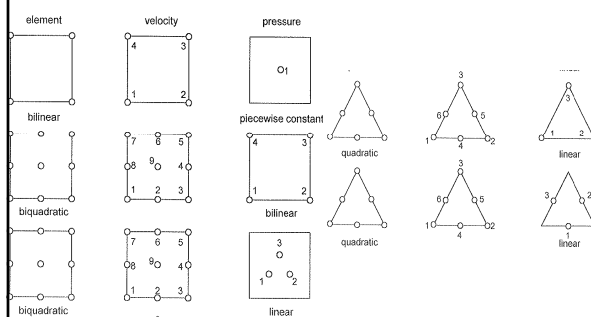
The velocity and pressure are approximated using shape functions

$$u(x, y, t) = \sum_j N_j(x, y) u_j(t)$$

$$v(x, y, t) = \sum_j N_j(x, y) v_j(t)$$

$$p(x, y, t) = \sum_k M_k(x, y) p_k(t)$$

To satisfy the LBB condition the shape functions for the pressure must be polynomials one order less than for the velocities. The combinations of mixed shape functions most often used are



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The first, third and fifth combination involve a discontinuous pressure field. These are usually more accurate than using a continuous pressure field. We will use only the first combination.

The Galerkin formulation using n-node shape functions for the velocity, and m-node elements for pressure result in element equations that are $(2n+m) \times (2n+m)$ of the form

$$\mathbf{M}\dot{\mathbf{d}} + \mathbf{K}\mathbf{d} = \mathbf{F}$$

where $\mathbf{d}^T = [u_1, u_2, \dots, u_n, v_1, v_2, \dots, v_n, p_1, p_2, \dots, p_m]$

The Mass Matrix \mathbf{M} is defined as $\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}$

where \mathbf{A} is the $n \times n$ matrix $[a_{ij}] = \left[\int_{\Omega} N_i N_j d\Omega \right]$

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To avoid having to combine the time stepping with a non-linear iteration, as well as having to invert a stiffness matrix at each time step, the convective terms are treated explicitly evaluating them at The current known time step.

The stiffness matrix \mathbf{K} will contain only the linear part of the spatial operator, that is the pressure and viscous terms and the continuity constraint.

$$\mathbf{K} = \begin{bmatrix} \mathbf{B} & \mathbf{0} & \mathbf{C}_x \\ \mathbf{0} & \mathbf{B} & \mathbf{C}_y \\ -\mathbf{C}_x^T & -\mathbf{C}_y^T & \mathbf{0} \end{bmatrix}$$

The matrices \mathbf{B} , \mathbf{C}_x and \mathbf{C}_y are

$$\mathbf{B} = [b_{ij}] = \left[\int_{\Omega} \frac{1}{\text{Re}} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega \right]$$

$$\mathbf{C}_x = [(c_x)_{ik}] = \left[-\int_{\Omega} \frac{\partial N_i}{\partial x} M_k d\Omega \right] \quad \mathbf{C}_y = [(c_y)_{ik}] = \left[-\int_{\Omega} \frac{\partial N_i}{\partial y} M_k d\Omega \right]$$

The non-linear terms are computed explicitly and placed in \mathbf{F} that Takes the form

$$\mathbf{F} = \begin{bmatrix} \mathbf{F}_x \\ \mathbf{F}_y \\ \mathbf{0} \end{bmatrix}$$

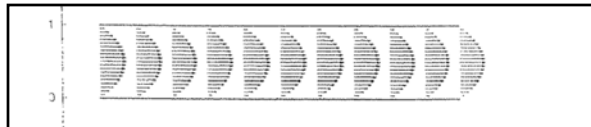
$$\mathbf{F}_x = [(f_x)_i] = \left[-\int_{\Omega} N_i \left\{ \left(\sum_j N_j u_j \right) \left(\sum_k \frac{\partial N_k}{\partial x} u_k \right) + \left(\sum_j N_j v_j \right) \left(\sum_k \frac{\partial N_k}{\partial y} u_k \right) \right\} d\Omega \right]$$

$$\mathbf{F}_y = [(f_y)_i] = \left[-\int_{\Omega} N_i \left\{ \left(\sum_j N_j u_j \right) \left(\sum_k \frac{\partial N_k}{\partial x} v_k \right) + \left(\sum_j N_j v_j \right) \left(\sum_k \frac{\partial N_k}{\partial y} v_k \right) \right\} d\Omega \right]$$

The boundary line integrals are almost always zero, except in some cases involving open boundaries. They will be discussed in the context of stratified flows.

EXAMPLE

Poiseuille flow between parallel plates. The figure shows a region of height H and length $5H$ non-dimensionalized using $L=H$. 22



The exact solution is $u(x, y) = 4u_m y(1 - y)$, $v(x, y) = 0$, $\frac{\partial p}{\partial x} = \frac{8u_m}{\text{Re}}$ where u_m is the maximum velocity at the center of the channel

The Figure shows the finite element solution obtained for $\text{Re} = 100$ using bilinear elements for velocity, piecewise constant pressure and a uniform mesh of size $\Delta x = 0.1, \Delta y = 0.05$.

The initial condition is zero velocities and pressure throughout.

The boundary conditions are developed flow at the entry $x = 0$, no slip, $u = v = 0$ along solid walls and along the outflow boundary

$$-p + \mu \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0.$$

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The steady state solution was calculated using a time dependent formulation. We can also do it through a direct non-linear iteration. The present approach is preferable though because if there are bifurcations in the mode of circulation direct iterative solutions often follow branches that are not physically stable, this does not happen with time dependent solutions.

Treating the convective terms explicitly introduces the stability limitation $c \leq 1$. If the time evolution of the flow is to be captured accurately this does not constitute a restriction, since we should not calculate with $c > 1$.

An unconditionally stable algorithm possibly combined with a Newton-Raphson iteration can be used if only the final steady-state is of interest and larger time steps are desired. Also, recall that for highly convective flows the Re number may have to be increased gradually.

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At high Re numbers the use of a stabilizing method such as Petrov Galerkin is necessary. For non-linear problems the algorithms become complex, and the understanding of how the different pieces interact is limited. For example, experience shows that in problems involving body forces the consistent P-G weighting of the body forces leads to unstable schemes.

The results of extensive calculations show that in practice in many situations we should apply the P-G weights only to the convective terms and use only the parameter α . In general for problems of forced flow such as the backward facing step, first order accuracy in time suffices. For problems involving the free transport of perturbations second order accuracy in time is a must.

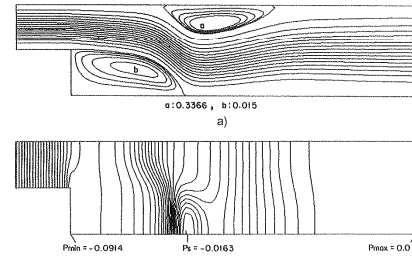
When the Newton-Raphson iteration is used, the convective term in the tangent matrix for the x-momentum equation takes the form

$$u^k \frac{\partial \Delta u}{\partial x} + \frac{\partial u^k}{\partial x} \Delta u + v^k \frac{\partial \Delta u}{\partial y} + \frac{\partial u^k}{\partial y} \Delta v$$

and similarly in the y-direction. Here a straight forward application of the P-G weights is not correct and eventually leads to lack of convergence. Corrections have been proposed by Harari-Hughes and Idelsohn.

Steady-state flow over a backward facing step at Re=900. Irregular mesh of 3,000 bilinear elements with piecewise constant pressure (mixed formulation). Backward implicit time stepping combined with Newton-Raphson and Petrov-Galerkin.

The figure shows the steady-state streamlines when $L_1 = 3H$, $L_2 = 19H$, and the step height is $H/2$



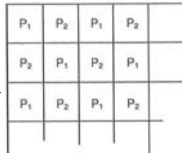
REMARKS:

- 1) The backward facing step together with the flow in a driven cavity are the most commonly used benchmark problems and there is a very large amount of data available for comparison.
- 2) In this elements the pressure is piecewise constant. In some cases, if the data is not smooth, the pressure oscillate from element to element. This is called a "CHECKERBOARD MODE" and appears because the solution space admits functions that are not constant, but for which the divergence vanishes.

This means that there exists a piecewise constant function $p^*(x, y) \neq Const.$ such that

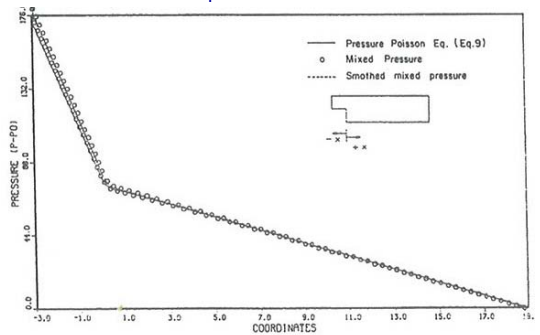
$$\int_{\Omega} p^* \left[\sum_j \frac{\partial N_j}{\partial x} u_j + \sum_j \frac{\partial N_j}{\partial y} v_j \right] d\Omega = 0.$$

It is not hard to show that for the bilinear velocity-piecewise constant pressure element mixed formulation on a square mesh, a checkerboard field as shown in the figure satisfies the equation.



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An example where the checkerboard mode is excited is shown below for the backward facing step at Re=100. The pressure along the top wall together with a smoothed pressure are shown. Methods to smooth the pressure are discussed below and later.



- 3) The appearance of the checkerboard mode does nothing to the accuracy of the velocity solution and the pressure can be readily smoothed using a least squares fit with bilinear elements.

Let $P(x, y) = \sum_j N_j P_j$ denote the bilinear interpolant of the pressure field where P_j are the values of the pressure at the nodes, and $p(x, y) = \sum_k M_k p_k$ denote the piecewise constant, calculated pressure. So that $M_k = \begin{cases} 1 & \text{in element } k \\ 0 & \text{in all other elements} \end{cases}$

Construct the functional $J = \int (P - p)^2 d\Omega$ and minimize it with respect to the values P_j . The Euler equations are

$$\frac{\partial J}{\partial P_i} = 2 \int_{\Omega} N_i \left[\sum_j N_j P_j - \sum_k M_k p_k \right] d\Omega = 0$$

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This results in a system of equations $\mathbf{AP} = \mathbf{B}$ where \mathbf{A} is the

usual mass matrix $\mathbf{A} = [a_{ij}] = \left[\int_{\Omega} N_i N_j d\Omega \right]$ and \mathbf{B} is

$$\mathbf{B} = [b_i] = \left[\int_{\Omega} N_i \left(\sum_k M_k p_k \right) \right]$$

In rectangular meshes, the use of mass lumping gives the weighted average of the values of the pressure over adjacent elements. The above form is more accurate and extends to isoparametric elements.

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