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| Report no. | 3   |
| Topic      | 2D steady and unsteady Transport Equation |

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# 1 2D steady transport equation

## 1.1 Developing discrete form of the Galerkin/Least-Square (GLS) for steady convection-diffusion-reaction equation

The steady convection-diffusion-reaction equation is given by:

$$\mathbf{a} \cdot \nabla u - \nabla \cdot (\nu \nabla u) + \sigma u = s \quad (1)$$

which is alternatively written as:

$$\mathcal{R}(u) = \mathcal{L}(u) - s = 0 \quad (2)$$

The Galerkin weak form of equation (1) is written as:

$$(w, \mathbf{a} \cdot \nabla u)_{\Omega} + (\nabla w, \nu \nabla u)_{\Omega} + (w, \sigma u)_{\Omega} = (w, s)_{\Omega} + (w, h)_{\Gamma_N} \quad (3)$$

The general form of a consistent stabilization technique is:

$$(w, \mathbf{a} \cdot \nabla u)_{\Omega} + (\nabla w, \nu \nabla u)_{\Omega} + (w, \sigma u)_{\Omega} + \sum_e \int_{\Omega_e} \mathcal{P}(w) \tau \mathcal{R}(u) \, d\Omega = (w, s)_{\Omega} + (w, h)_{\Gamma_N} \quad (4)$$

For Galerkin/Least Square (GLS), the operator  $\mathcal{P}$  applied to the test function  $w$  is defined as:

$$\mathcal{P}(w) = \mathcal{L}(w) = \mathbf{a} \cdot \nabla w - \nabla \cdot (\nu \nabla w) + \sigma w \quad (5)$$

Therefore, the weak form for the GLS method is written as:

$$\begin{aligned} & (w, \mathbf{a} \cdot \nabla u)_{\Omega} + (\nabla w, \nu \nabla u)_{\Omega} + (w, \sigma u)_{\Omega} \\ & + \sum_e \int_{\Omega_e} [\mathbf{a} \cdot \nabla w - \nabla \cdot (\nu \nabla w) + \sigma w] \tau [\mathbf{a} \cdot \nabla u - \nabla \cdot (\nu \nabla u) + \sigma u] \, d\Omega \\ & = (w, s)_{\Omega} + (w, h)_{\Gamma_N} + \sum_e \int_{\Omega_e} [\mathbf{a} \cdot \nabla w - \nabla \cdot (\nu \nabla w) + \sigma w] \tau s \, d\Omega \end{aligned} \quad (6)$$

and the corresponding part of the Matlab code is:

```
1 % GLS
2 Ke = Ke + (N_ig'*(ax*Nx+ay*Ny) + nu*(Nx'*Nx+Ny'*Ny) + N_ig'*sigma*N_ig + ...
3         tau*((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig))*...
4         ((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig))*dvolu;
5 aux = N_ig*Xe;
6 f_ig = SourceTerm(aux);
7 fe = fe + (N_ig + tau*((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig))*...
8         (f_ig*dvolu);
```

## 1.2 2D steady convection-diffusion

### 1.2.1 Downwind homogeneous natural boundary conditions

Considering a homogeneous convection-diffusion problem on a square domain  $[0, 1] \times [0, 1]$  shown in Figure 1. Discontinuous Dirichlet boundary conditions are imposed on the inlet boundary. On the outlet boundary (drawn in green), homogeneous (zero) Neumann boundary (natural) condition is applied. The convection velocity is of magnitude  $\|a\| = 1$  and is skew to the mesh with an angle  $30^\circ$ , and the diffusion coefficient is  $\nu = 10^{-4}$ . The mesh is composed of 10 bilinear quadrilateral elements in each direction. The solutions obtained using different spatial discretization techniques are shown in Figure 2. It is noticed that Galerkin formulation doesn't satisfactorily resolve the discontinuity and produces spurious oscillations (nearly pure convection). The artificial diffusion method introduces too much crosswind diffusion. The SUPG and GLS produce much better results, where less crosswind diffusion is added and the oscillations of the Galerkin formulation are reduced.

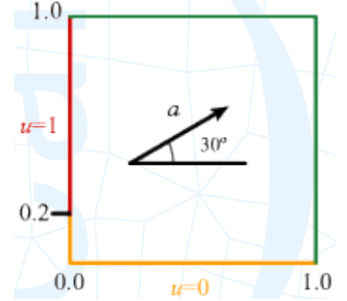


Figure 1: Problem setup

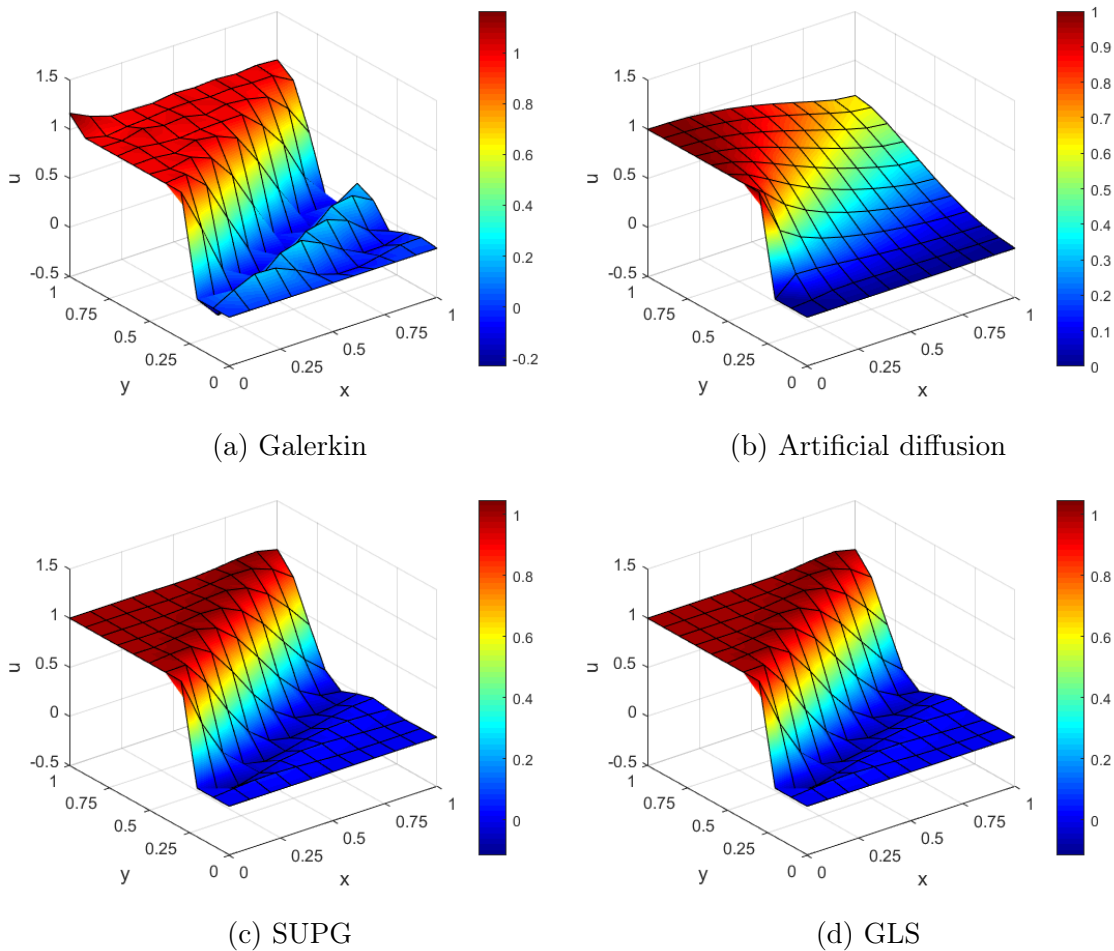


Figure 2: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-diffusion problem with downwind natural conditions, using bi-linear quadrilateral elements. (Peclet number = 500)

Keeping all the parameters the same but changing the order of elements from  $p = 1$  to  $p = 2$ , i.e. using bi-quadratic quadrilaterals, the solutions obtained are shown in Figure 3. Better representation of the discontinuity is obtained. However, the Galerkin and artificial diffusion methods still don't provide acceptable results. The results prove that the modifications made to the code, to account for quadratic elements, are correct. The details of the modifications and additions to the code are shown in appendix A.1.

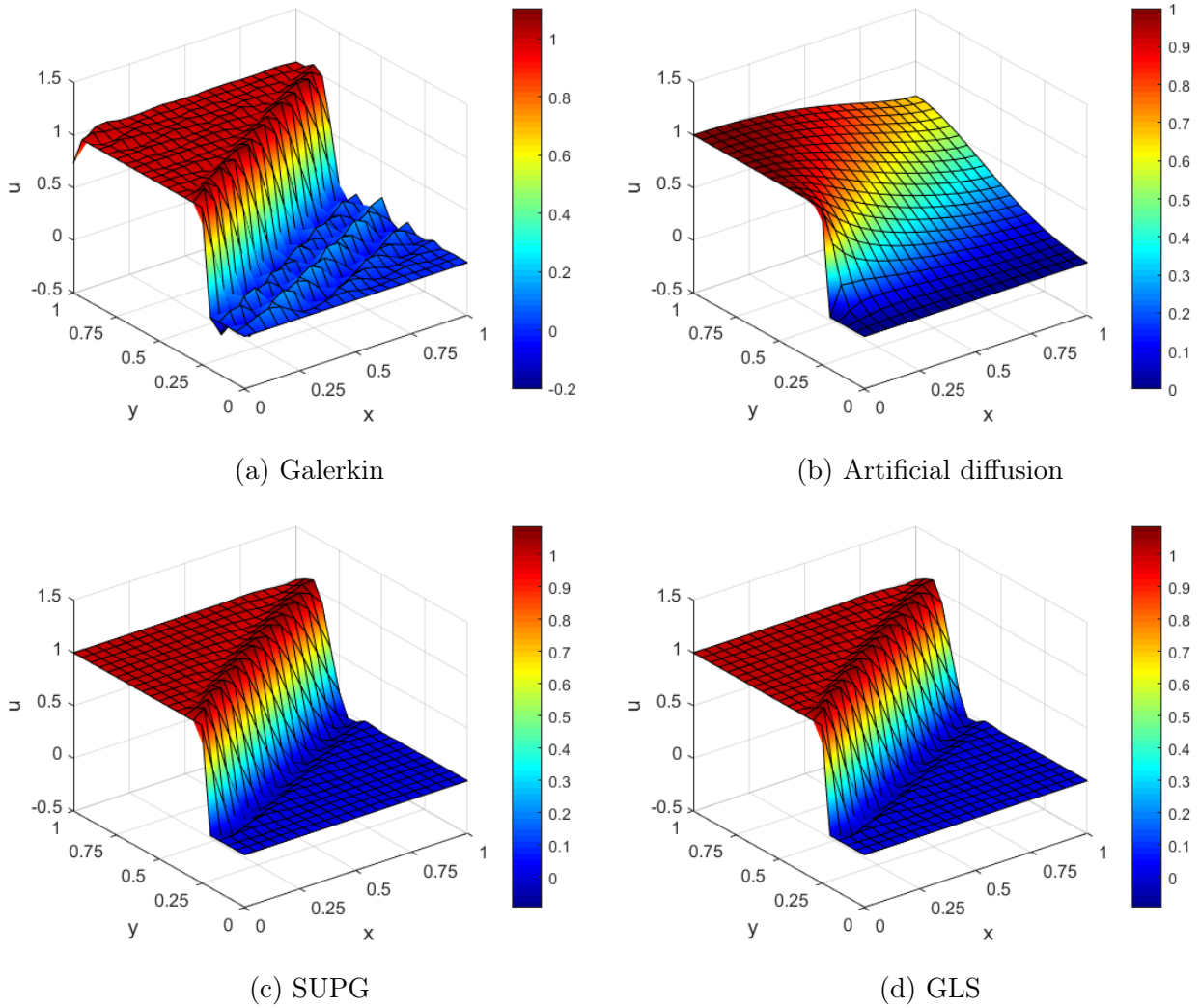


Figure 3: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-diffusion problem with downwind natural conditions, using bi-quadratic quadrilateral elements. (Peclet number = 500)

### 1.2.2 Downwind homogeneous essential boundary conditions

Next, the problem is solved with homogeneous essential boundary conditions (zero Dirichlet) on the outlet boundary. The solution now involves a thin boundary layer at the outlet as seen in Figure 4. However, the boundary layer is not well captured because of the coarse mesh employed. It is observed that the Galerkin formulation yields completely unstable solution. Again, the artificial diffusion method introduces excessive numerical diffusion. Better results are obtained using SUPG and GLS.

The modifications to the code, to account for zero Dirichlet boundary conditions on the outlet boundary, are shown in appendix A.1.1 (lines 43 to 46 and 80 to 87).

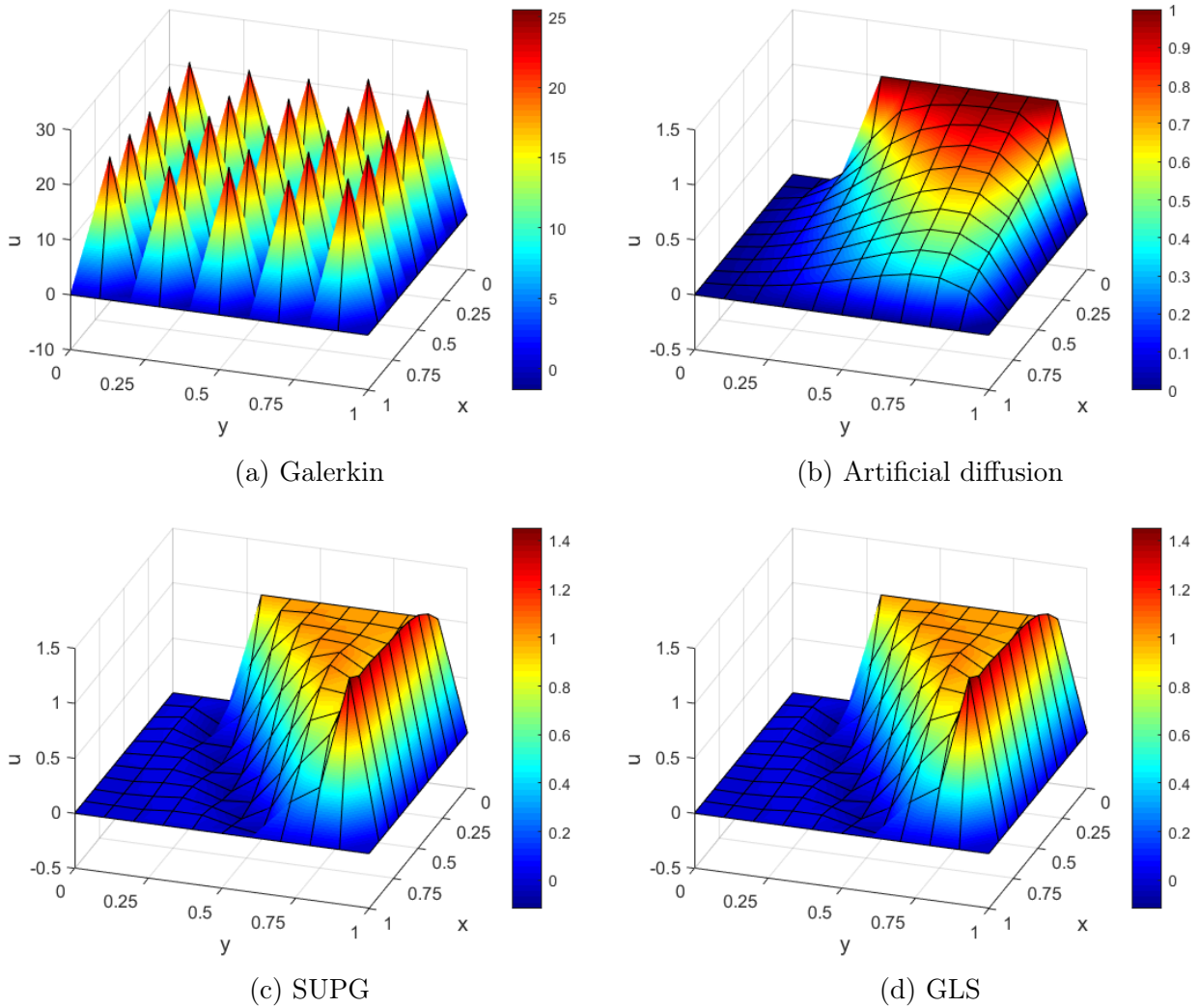


Figure 4: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-diffusion problem with downwind essential boundary conditions, using bi-linear quadrilateral elements. (Peclet number = 500)

The solution for the problem with zero Dirichlet condition on the outlet boundary using bi-quadratic quadrilaterals is shown in Figure 5. Similar conclusions as in the case of bi-linear elements are obtained. However, it is clearly seen the more accurate representation of the boundary layer at the outlet in the stable solutions.

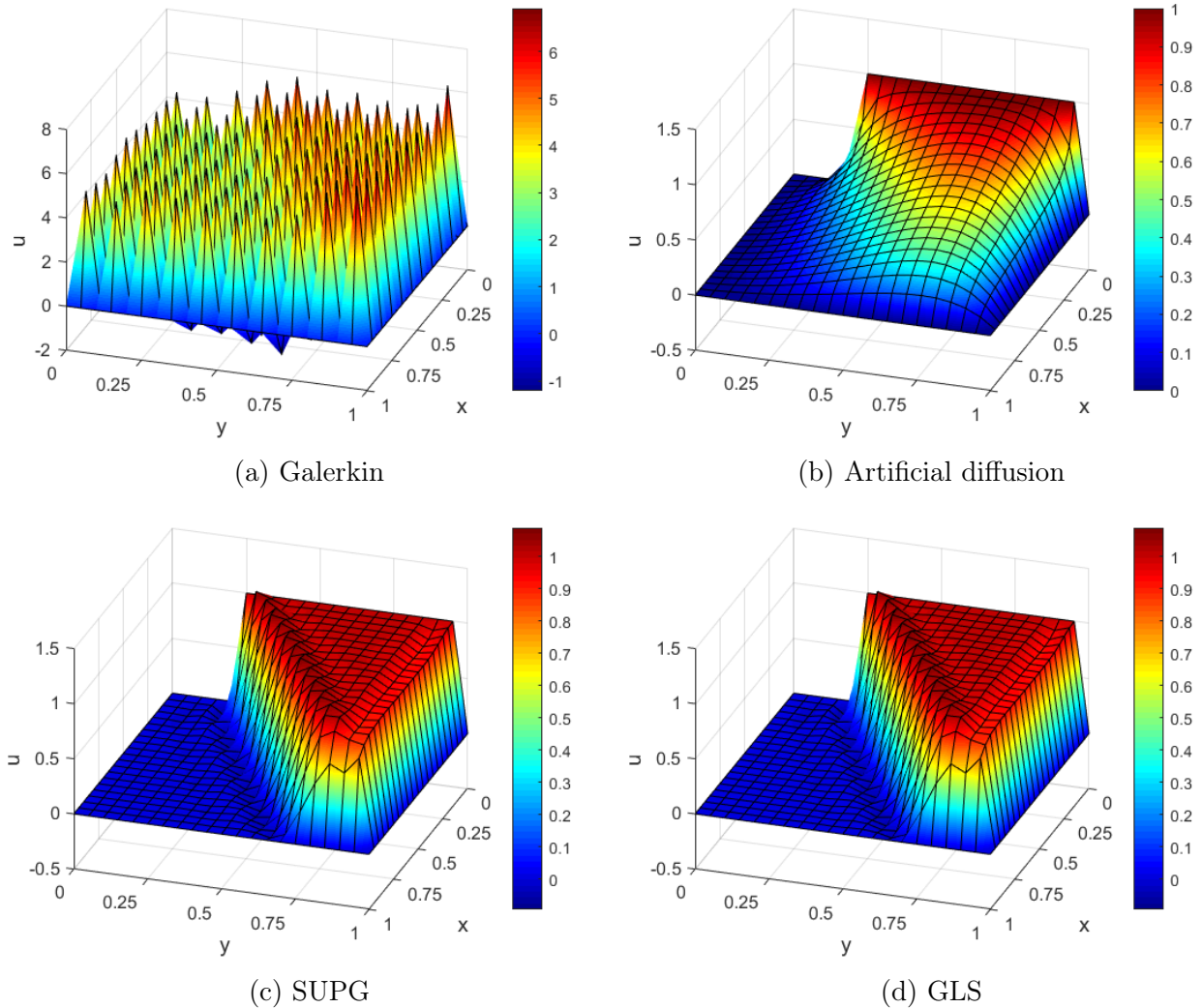


Figure 5: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-diffusion problem with downwind essential boundary conditions, using bi-quadratic quadrilateral elements. (Peclet number = 500)

## 1.3 2D steady convection-diffusion-reaction

### 1.3.1 Convection-reaction-dominated case

Setting the following parameters:  $\|a\| = 1/2$ ,  $\nu = 10^{-4}$ ,  $\sigma = 1$ ,  $s = 0$ , downwind essential boundary conditions, bi-linear quadrilateral elements. The solution is shown in Figure 6. It is seen that the Galerkin formulation yields unstable solution because the Peclet number is 250 (more than 1) as the problem is convection dominated. It is also noted that the stabilized methods yields satisfactory solutions.

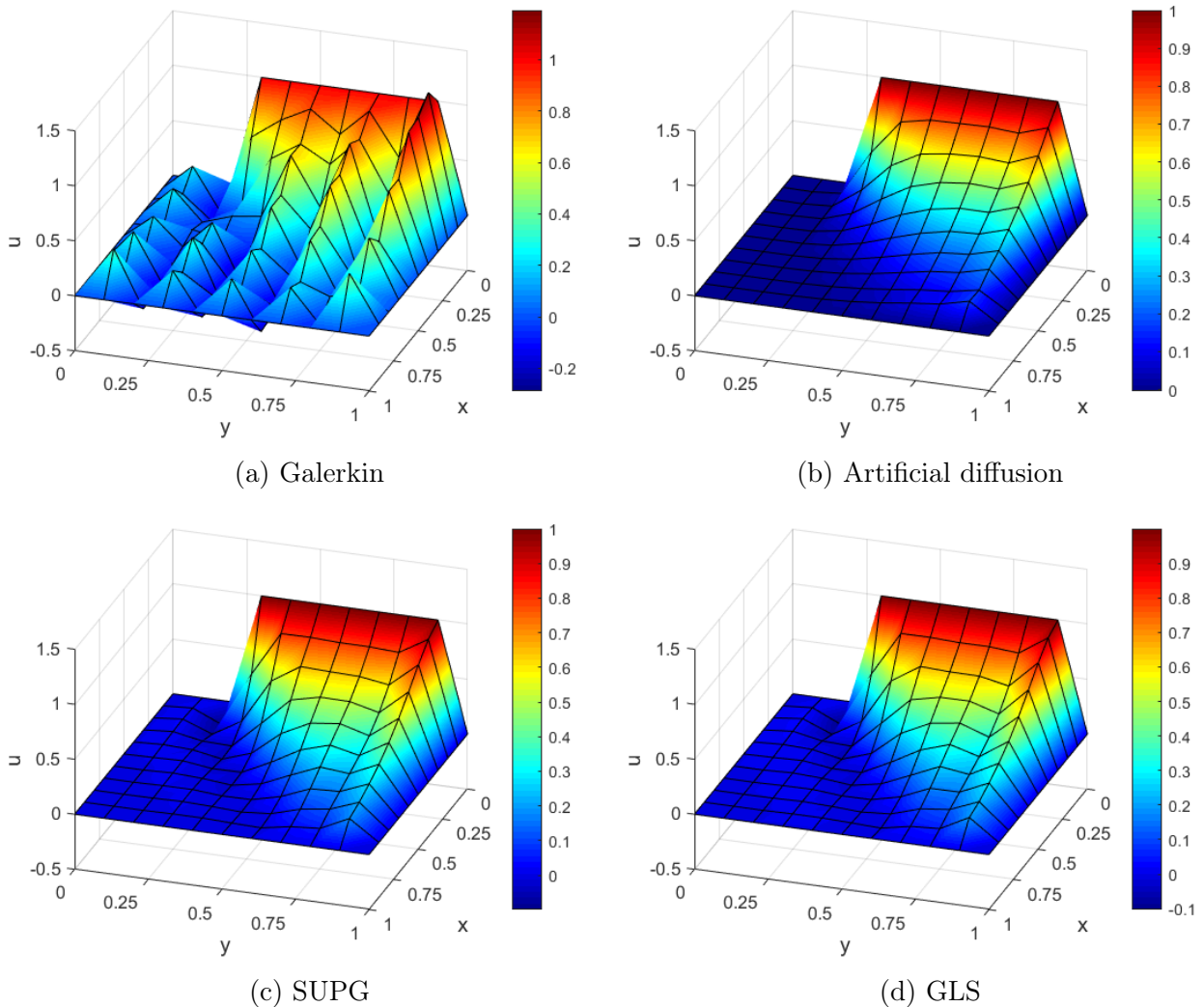
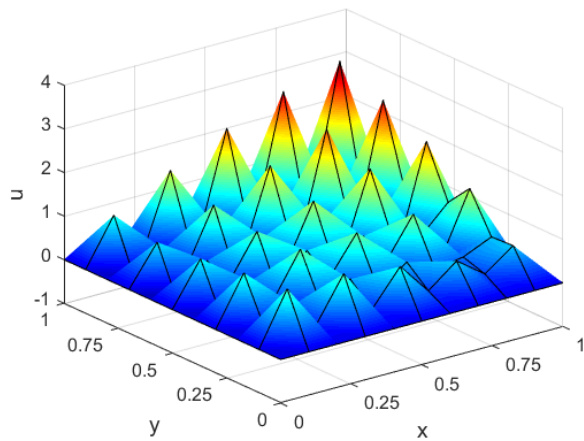


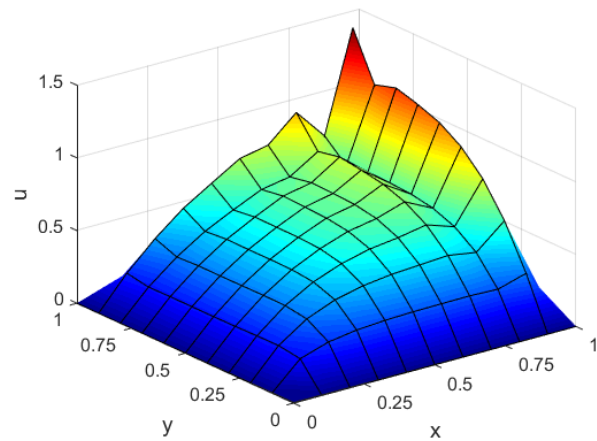
Figure 6: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-reaction dominated problem with downwind essential boundary conditions and no source term, using bi-linear quadrilateral elements. (Peclet number = 250)



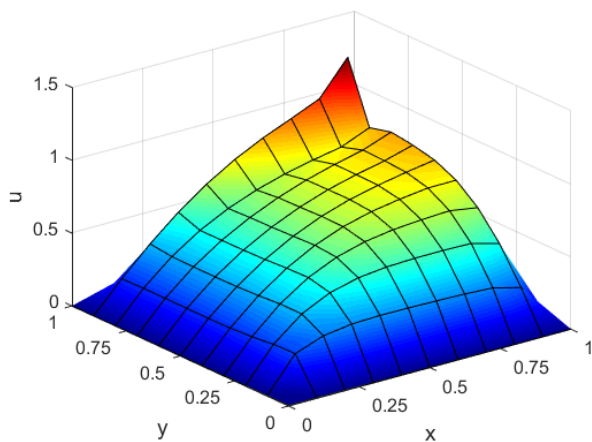
To duplicate the results obtained in the book at page 77 (Fig. 2.21), the following parameters are used:  $\|a\| = 1/2$ ,  $\nu = 10^{-4}$ ,  $\sigma = 1$ ,  $s = 1$  homogeneous essential boundary conditions everywhere, bi-linear quadrilateral elements. The variation here is that the source term is not zero and that all boundaries are homogeneous Dirichlet. The solution is shown in Figure 7. Again, the Galerkin formulation gives unstable solution (Peclet = 250 > 1). The SUPG and GLS formulations gives better solutions that the Artificial diffusion formulation.



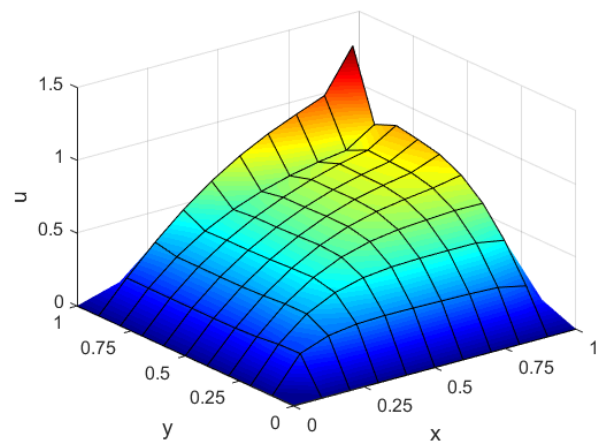
(a) Galerkin



(b) Artificial diffusion



(c) SUPG



(d) GLS

Figure 7: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady convection-reaction dominated problem with homogeneous essential boundary conditions everywhere and a source term  $s = 1$ , using bi-linear quadrilateral elements. (Peclet number = 250)

### 1.3.2 Reaction-dominated case

Setting the following parameters:  $\|a\| = 10^{-3}$ ,  $\nu = 10^{-4}$ ,  $\sigma = 1$ ,  $s = 0$ , downwind essential boundary conditions, bi-linear quadrilateral elements. The solution is shown in Figure 8. It is seen that all formulations yields very similar solutions. In this case, the Peclet number is 0.5 which is less than the stability limit ( $Pe=1$ ), therefore the Galerkin formulation is able to yield stable solution.

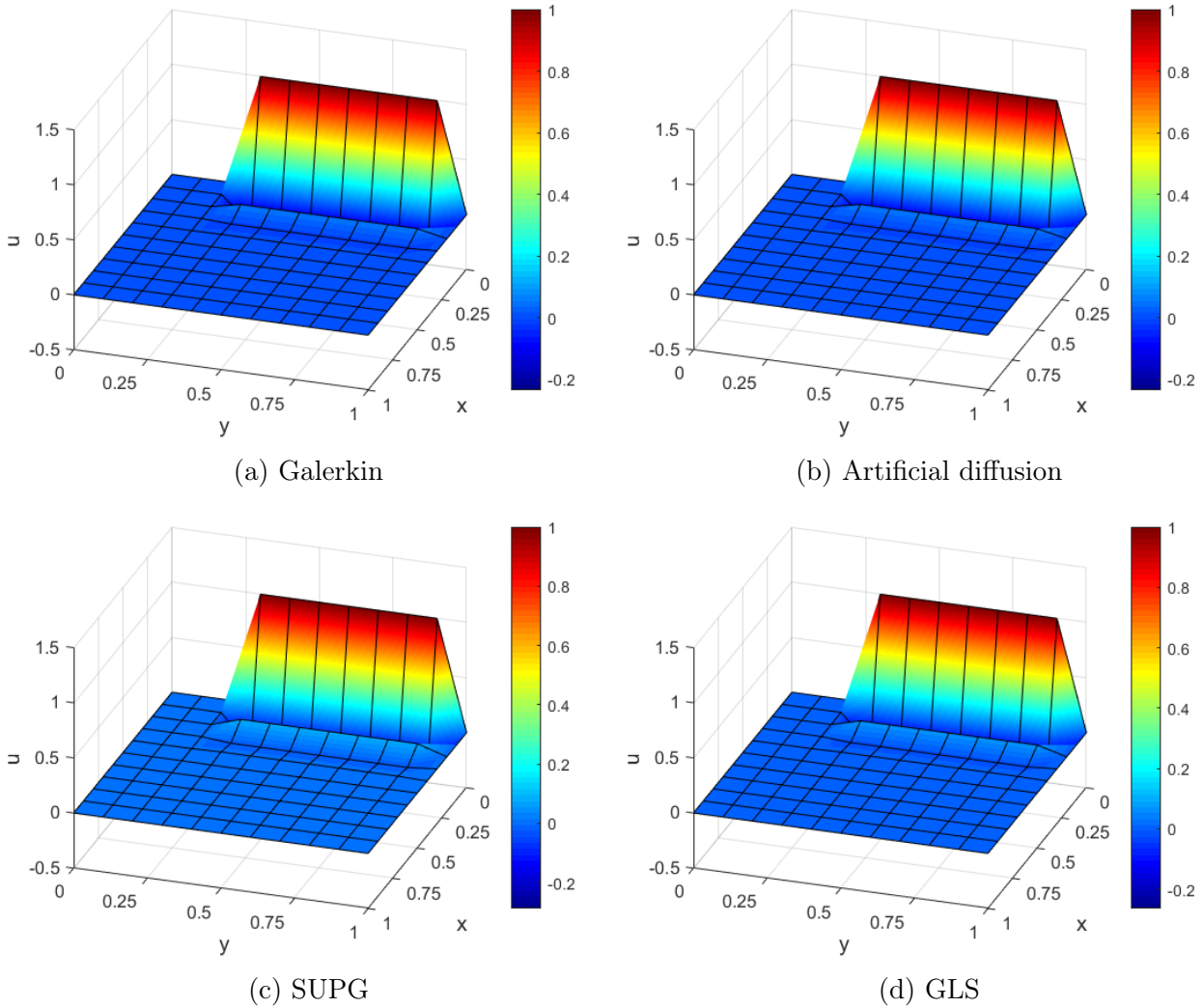
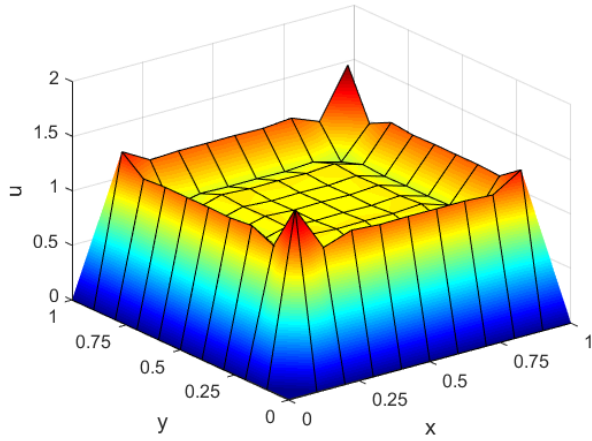
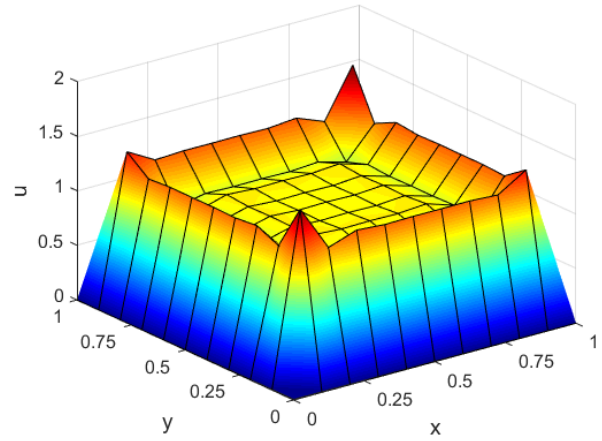


Figure 8: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady reaction dominated problem with downwind essential boundary conditions and no source term, using bi-linear quadrilateral elements. (Peclet number = 0.5)

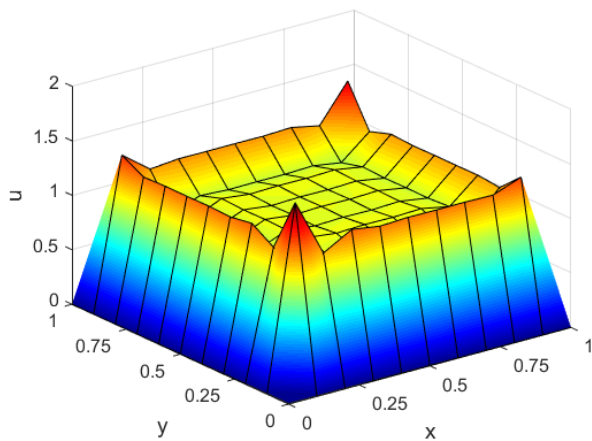
To duplicate the results obtained in the book at page 77 (Fig. 2.22), the following parameters are used:  $\|a\| = 10^{-3}$ ,  $\nu = 10^{-4}$ ,  $\sigma = 1$ ,  $s = 1$ , homogeneous essential boundary conditions everywhere, bi-linear quadrilateral elements. The variation here is that the source term is not zero and that all boundaries are homogeneous Dirichlet. The solution is shown in Figure 9.



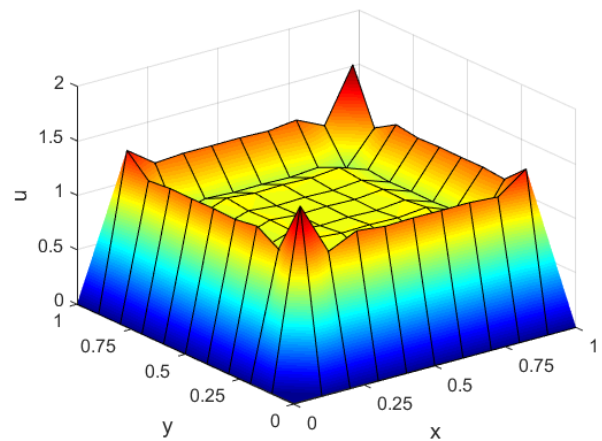
(a) Galerkin



(b) Artificial diffusion



(c) SUPG



(d) GLS

Figure 9: Galerkin, artificial diffusion, SUPG and GLS solution for the 2D steady reaction dominated problem with homogeneous essential boundary conditions everywhere and a source term  $s = 1$ , using bi-linear quadrilateral elements. (Peclet number = 0.5)

## 2 2D unsteady transport equation

In this section, the 2D unsteady pure convection equation is considered

$$u_t + \mathbf{a} \cdot \nabla u = s \quad (7)$$

### 2.1 Lax-Wendroff method + Galerkin formulation

The time discretization is given by:

$$\frac{\Delta u}{\Delta t} = -\mathbf{a} \cdot \nabla u^n + \frac{\Delta t}{2} (\mathbf{a} \cdot \nabla)^2 u^n + s^n + \frac{\Delta t}{2} (s_t^n - \mathbf{a} \cdot \nabla s^n) \quad (8)$$

The Galerkin weak form is:

$$\left(w, \frac{\Delta u}{\Delta t}\right)_\Omega = -\left(w, \mathbf{a} \cdot \nabla u^n\right)_\Omega + \frac{\Delta t}{2} \left(w, (\mathbf{a} \cdot \nabla)^2 u^n\right)_\Omega + \left(w, s^n\right)_\Omega + \frac{\Delta t}{2} \left(w, s_t^n\right)_\Omega - \frac{\Delta t}{2} \left(w, \mathbf{a} \cdot \nabla s^n\right)_\Omega \quad (9)$$

Integration by parts for the first two terms and the last term on the RHS yields:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega &= \left(\mathbf{a} \cdot \nabla w, u^n\right)_\Omega - \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n\right)_\Omega + \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, s^n\right)_\Omega \\ &\quad - \left((\mathbf{a} \cdot \mathbf{n})w, u^n\right)_\Gamma + \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n\right)_\Gamma - \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, s^n\right)_\Gamma \\ &\quad + \left(w, s^n\right)_\Omega + \frac{\Delta t}{2} \left(w, s_t^n\right)_\Omega \end{aligned} \quad (10)$$

Given that the boundary  $\Gamma = \Gamma^{in} \cup \Gamma^{out}$ , and recalling that for hyperbolic problems the boundary conditions are applied only to inflow boundaries. Furthermore, the inflow boundary could be a Neumann part and a Dirchlet part, i.e.  $\Gamma^{in} = \Gamma_N^{in} \cup \Gamma_D^{in}$ . Since  $w = 0$  on the Dirchlet boundary, therefore the weak form is written as:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega &= \left(\mathbf{a} \cdot \nabla w, u^n\right)_\Omega - \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n\right)_\Omega + \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, s^n\right)_\Omega \\ &\quad - \left((\mathbf{a} \cdot \mathbf{n})w, u^n\right)_{\Gamma^{out}} + \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n\right)_{\Gamma^{out}} - \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, s^n\right)_{\Gamma^{out}} \\ &\quad - \left((\mathbf{a} \cdot \mathbf{n})w, u^n\right)_{\Gamma_N^{in}} + \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n\right)_{\Gamma_N^{in}} - \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, s^n\right)_{\Gamma_N^{in}} \\ &\quad + \left(w, s^n\right)_\Omega + \frac{\Delta t}{2} \left(w, s_t^n\right)_\Omega \end{aligned} \quad (11)$$

For a problem with homogeneous Dirchlet boundary condition at the inlet, and assuming a source term that is not time-dependent, i.e.  $s_t = 0$ , therefore the weak form is simplified to:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega &= \left(\mathbf{a} \cdot \nabla w, u^n\right)_\Omega - \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n\right)_\Omega + \frac{\Delta t}{2} \left(\mathbf{a} \cdot \nabla w, s\right)_\Omega \\ &\quad - \left((\mathbf{a} \cdot \mathbf{n})w, u^n\right)_{\Gamma^{out}} + \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n\right)_{\Gamma^{out}} - \frac{\Delta t}{2} \left((\mathbf{a} \cdot \mathbf{n})w, s\right)_{\Gamma^{out}} + \left(w, s\right)_\Omega \end{aligned} \quad (12)$$

Using the following definitions:

$$\begin{aligned}
\mathbf{M}\mathbf{U} &= (w, u)_{\Omega}, \\
\mathbf{C}\mathbf{U} &= (\mathbf{a} \cdot \nabla w, u)_{\Omega}, \\
\mathbf{K}\mathbf{U} &= (\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u)_{\Omega}, \\
\mathbf{v}_1 &= (w, s)_{\Omega}, \\
\mathbf{v}_2 &= (\mathbf{a} \cdot \nabla w, s)_{\Omega}, \\
\mathbf{M}_o\mathbf{U} &= ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma^{out}}, \\
\mathbf{C}_o\mathbf{U} &= ((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n)_{\Gamma^{out}}, \\
\mathbf{v}_o &= ((\mathbf{a} \cdot \mathbf{n})w, s)_{\Omega}
\end{aligned} \tag{13}$$

Therefore, the weak form given by (12) is written in discrete form as:

$$\frac{1}{\Delta t} \mathbf{M} \Delta \mathbf{U} = \mathbf{C} \mathbf{U}^n - \frac{\Delta t}{2} \mathbf{K} \mathbf{U}^n + \frac{\Delta t}{2} \mathbf{v}_2 - \mathbf{M}_o \mathbf{U}^n + \frac{\Delta t}{2} \mathbf{C}_o \mathbf{U}^n - \frac{\Delta t}{2} \mathbf{v}_2 + \mathbf{v}_1 \tag{14}$$

and is further simplified to:

$$\mathbf{M} \Delta \mathbf{U} = \Delta t \left[ \mathbf{C} - \frac{\Delta t}{2} \mathbf{K} - \mathbf{M}_o + \frac{\Delta t}{2} \mathbf{C}_o \right] \mathbf{U}^n + \Delta t \left[ \mathbf{v}_1 + \frac{\Delta t}{2} (\mathbf{v}_2 - \mathbf{v}_2) \right] \tag{15}$$

and written in the following format, for the ease of implementation in Matlab:

$$\mathbf{A} \Delta \mathbf{U} = \mathbf{B} \mathbf{U}^n + \mathbf{f}$$

and the corresponding part of the Matlab code is:

```

1 % COMPUTATION OF MATRICES FOR THE TRANSIENT ANALYSIS
2 if meth == 1
3     A = M;
4     B = dt*(C - (dt/2)*K - Mo + (dt/2)*Co);
5     f = dt*(v1 + (dt/2)*(v2-v0));

```

If lumped mass matrix is used, the corresponding part of the Matlab code is:

```

1 elseif meth == 2
2     Md = diag(M*ones(numnp, 1));
3     Mod = diag(Mo*ones(numnp, 1));
4     A = Md;
5     B = dt*(C - (dt/2)*K - Mod + (dt/2)*Co);
6     f = dt*(v1 + (dt/2)*(v2-v0));

```

## 2.2 Crank-Nicholson method + Galerkin formulation

The time discretization is given by:

$$\frac{\Delta u}{\Delta t} + \frac{1}{2}(\mathbf{a} \cdot \nabla) \Delta u = \frac{1}{2}s^{n+1} + \frac{1}{2}s^n - \mathbf{a} \cdot \nabla u^n \quad (16)$$

The Galerkin weak form is:

$$\left(w, \frac{\Delta u}{\Delta t}\right)_\Omega + \frac{1}{2}(w, (\mathbf{a} \cdot \nabla) \Delta u)_\Omega = \frac{1}{2}(w, s^{n+1})_\Omega + \frac{1}{2}(w, s^n)_\Omega - (w, \mathbf{a} \cdot \nabla u^n)_\Omega \quad (17)$$

Integration by parts for the second term on the LHS and the last term on the RHS yields:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega - \frac{1}{2}(\mathbf{a} \cdot \nabla w, \Delta u)_\Omega + \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, \Delta u)_\Gamma \\ = \frac{1}{2}(w, s^{n+1})_\Omega + \frac{1}{2}(w, s^n)_\Omega + (\mathbf{a} \cdot \nabla w, u^n)_\Omega - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_\Gamma \end{aligned} \quad (18)$$

Given that the boundary  $\Gamma = \Gamma^{in} \cup \Gamma^{out}$ , and recalling that for hyperbolic problems the boundary conditions are applied only to inflow boundaries. Furthermore, the inflow boundary could be a Neumann part and a Dirchlet part, i.e.  $\Gamma^{in} = \Gamma_N^{in} \cup \Gamma_D^{in}$ . Since  $w = 0$  on the Dirchlet boundary, therefore the weak form is written as:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega - \frac{1}{2}(\mathbf{a} \cdot \nabla w, \Delta u)_\Omega + \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, \Delta u)_{\Gamma^{out}} + \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, \Delta u)_{\Gamma_N^{in}} \\ = \frac{1}{2}(w, s^{n+1})_\Omega + \frac{1}{2}(w, s^n)_\Omega + (\mathbf{a} \cdot \nabla w, u^n)_\Omega - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma^{out}} - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma_N^{in}} \end{aligned} \quad (19)$$

Moving the fourth term on the LHS to the RHS yields:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega - \frac{1}{2}(\mathbf{a} \cdot \nabla w, \Delta u)_\Omega + \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, \Delta u)_{\Gamma^{out}} \\ = \frac{1}{2}(w, s^{n+1})_\Omega + \frac{1}{2}(w, s^n)_\Omega + (\mathbf{a} \cdot \nabla w, u^n)_\Omega - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma^{out}} \\ - \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, u^{n+1})_{\Gamma_N^{in}} - \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma_N^{in}} \end{aligned} \quad (20)$$

For a problem with homogeneous Dirchlet boundary condition at the inlet, and assuming a source term that is not time-dependent, i.e.  $s^{n+1} = s^n = s$ , therefore the weak form is simplified to:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega - \frac{1}{2}(\mathbf{a} \cdot \nabla w, \Delta u)_\Omega + \frac{1}{2}((\mathbf{a} \cdot \mathbf{n})w, \Delta u)_{\Gamma^{out}} \\ = \frac{1}{2}(w, s)_\Omega + \frac{1}{2}(w, s)_\Omega + (\mathbf{a} \cdot \nabla w, u^n)_\Omega - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma^{out}} \end{aligned} \quad (21)$$

Using the previous definitions given by (13), the weak form given by (21) is written in discrete form as:

$$\frac{1}{\Delta t} \mathbf{M} \Delta \mathbf{U} - \frac{1}{2} \mathbf{C} \Delta \mathbf{U} + \frac{1}{2} \mathbf{M}_o \Delta \mathbf{U} = \mathbf{v}_1 + \mathbf{C} \mathbf{U}^n - \mathbf{M}_o \mathbf{U}^n \quad (22)$$

further simplification yields:

$$\left[ \mathbf{M} - \frac{\Delta t}{2} \mathbf{C} + \frac{\Delta t}{2} \mathbf{M}_o \right] \Delta \mathbf{U} = \left[ \Delta t \mathbf{C} - \Delta t \mathbf{M}_o \right] \mathbf{U}^n + \Delta t \mathbf{v}_1 \quad (23)$$

and for ease of implementation in Matlab, it is written as:

$$\mathbf{A} \Delta \mathbf{U} = \mathbf{B} \mathbf{U}^n + \mathbf{f}$$

The corresponding part of the Matlab code is:

```

1 elseif meth == 4
2     A = M - (dt/2)*C + (dt/2)*Mo;
3     B = dt*C - dt*Mo;
4     f = dt*v1;

```

If lumped mass matrix is used, the corresponding part of the Matlab code is:

```

1 elseif meth == 5
2     Md = diag(M*ones(numnp,1));
3     Mod = diag(Mo*ones(numnp,1));
4     A = Md - (dt/2)*C + (dt/2)*Mod;
5     B = dt*C - dt*Mod;
6     f = dt*v1;

```

### 2.3 Third-order Taylor-Galerkin (TG3) + Galerkin formulation

Assuming that the source term is not time dependent, therefore the time discretization using third-order Taylor-Galerkin method is given by:

$$\left[ 1 - \frac{\Delta t^2}{6} (\mathbf{a} \cdot \nabla)^2 \right] \frac{\Delta u}{\Delta t} = -(\mathbf{a} \cdot \nabla) u^n + \frac{\Delta t}{2} (\mathbf{a} \cdot \nabla)^2 u^n + s - \frac{\Delta t}{2} \mathbf{a} \cdot \nabla s \quad (24)$$

The Galerkin weak form is given by:

$$\left( w, \frac{\Delta u}{\Delta t} \right)_\Omega - \frac{\Delta t^2}{6} \left( w, (\mathbf{a} \cdot \nabla)^2 \frac{\Delta u}{\Delta t} \right)_\Omega = - \left( w, \mathbf{a} \cdot \nabla u^n \right)_\Omega + \frac{\Delta t}{2} \left( w, (\mathbf{a} \cdot \nabla)^2 u^n \right)_\Omega + \left( w, s \right)_\Omega - \frac{\Delta t}{2} \left( w, \mathbf{a} \cdot \nabla s \right)_\Omega \quad (25)$$

Integration by parts yields:

$$\begin{aligned} & \left( w, \frac{\Delta u}{\Delta t} \right)_\Omega + \frac{\Delta t^2}{6} \left( \mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla \frac{\Delta u}{\Delta t} \right)_\Omega - \frac{\Delta t^2}{6} \left( (\mathbf{a} \cdot \mathbf{n}) w, \mathbf{a} \cdot \nabla \frac{\Delta u}{\Delta t} \right)_\Gamma \\ & = \left( \mathbf{a} \cdot \nabla w, u^n \right)_\Omega - \left( (\mathbf{a} \cdot \mathbf{n}) w, u^n \right)_\Gamma - \frac{\Delta t}{2} \left( \mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n \right)_\Omega + \frac{\Delta t}{2} \left( (\mathbf{a} \cdot \mathbf{n}) w, \mathbf{a} \cdot \nabla u^n \right)_\Gamma \\ & + \left( w, s \right)_\Omega + \frac{\Delta t}{2} \left( \mathbf{a} \cdot \nabla w, s \right)_\Omega - \frac{\Delta t}{2} \left( (\mathbf{a} \cdot \mathbf{n}) w, s \right)_\Gamma \end{aligned} \quad (26)$$

For a problem with homogeneous Dirichlet boundary condition at the inlet, the weak form is written as:

$$\begin{aligned}
& \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega + \frac{\Delta t^2}{6} (\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla \frac{\Delta u}{\Delta t})_\Omega - \frac{\Delta t^2}{6} ((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla \frac{\Delta u}{\Delta t})_{\Gamma_{out}} \\
& = (\mathbf{a} \cdot \nabla w, u^n)_\Omega - ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma_{out}} - \frac{\Delta t}{2} (\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n)_\Omega + \frac{\Delta t}{2} ((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n)_{\Gamma_{out}} \\
& + (w, s)_\Omega + \frac{\Delta t}{2} (\mathbf{a} \cdot \nabla w, s)_\Omega - \frac{\Delta t}{2} ((\mathbf{a} \cdot \mathbf{n})w, s)_{\Gamma_{out}}
\end{aligned} \tag{27}$$

Using the previous definitions given by (13), the weak form given by (27) is written in discrete form as:

$$\frac{1}{\Delta t} \mathbf{M} \Delta \mathbf{U} + \frac{\Delta t}{6} \mathbf{K} \Delta \mathbf{U} - \frac{\Delta t}{6} \mathbf{C}_o \Delta \mathbf{U} = \mathbf{C} \mathbf{U}^n - \mathbf{M}_o \mathbf{U}^n - \frac{\Delta t}{2} \mathbf{K} \mathbf{U}^n + \frac{\Delta t}{2} \mathbf{C}_o \mathbf{U}^n + \mathbf{v}_1 + \frac{\Delta t}{2} \mathbf{v}_2 - \frac{\Delta t}{2} \mathbf{v}_o \tag{28}$$

further simplification yields:

$$\left[ \mathbf{M} + \frac{\Delta t^2}{6} (\mathbf{K} - \mathbf{C}_o) \right] \Delta \mathbf{U} = \Delta t \left[ \mathbf{C} - \frac{\Delta t}{2} \mathbf{K} - \mathbf{M}_o + \frac{\Delta t}{2} \mathbf{C}_o \right] \mathbf{U}^n + \Delta t \left[ \frac{\Delta t}{2} (\mathbf{v}_2 - \mathbf{v}_o) + \mathbf{v}_1 \right] \tag{29}$$

and for ease of implementation in Matlab, it is written as:

$$\mathbf{A} \Delta \mathbf{U} = \mathbf{B} \mathbf{U}^n + \mathbf{f}$$

The corresponding part of the Matlab code is:

```

1 elseif meth == 3
2     A = M + (dt^2/6) * (K - Co);
3     B = dt * (C - (dt/2) * K - Mo + (dt/2) * Co);
4     f = dt * ((dt/2) * (v2 - vo) + v1);

```

## 2.4 Two-step third-order Taylor-Galerkin (TG3-2S) + Galerkin formulation

The time discretization of two-step third-order Taylor-Galerkin method is given by:

$$\tilde{u}^n = u^n + \frac{1}{3} \Delta t u_t^n + \alpha \Delta t^2 u_{tt}^n, \tag{30a}$$

$$u^{n+1} = u^n + \Delta t u_t^n + \frac{1}{2} \Delta t^2 \tilde{u}_{tt}^n \tag{30b}$$

It is important to recall that:

$$u_t^n = s^n - \mathbf{a} \cdot \nabla u^n \tag{31}$$

$$u_{tt}^n = s_t^n - \mathbf{a} \cdot \nabla u_t^n = s_t^n - \mathbf{a} \cdot \nabla s^n + (\mathbf{a} \cdot \nabla)^2 u^n \tag{32}$$

and similarly:

$$\tilde{u}_{tt}^n = s_t^n - \mathbf{a} \cdot \nabla s^n + (\mathbf{a} \cdot \nabla)^2 \tilde{u}^n \tag{33}$$



Substituting (31) and (32) into (30a), and (31) and (33) into (30b) yields:

$$\tilde{u}^n = u^n + \frac{1}{3}\Delta t s^n - \frac{1}{3}\Delta t \mathbf{a} \cdot \nabla u^n + \alpha \Delta t^2 s_t^n - \alpha \Delta t^2 \mathbf{a} \cdot \nabla s^n + \alpha \Delta t^2 (\mathbf{a} \cdot \nabla)^2 u^n \quad (34a)$$

$$u^{n+1} = u^n + \Delta t s^n - \Delta t \mathbf{a} \cdot \nabla u^n + \frac{1}{2}\Delta t^2 s_t^n - \frac{1}{2}\Delta t^2 \mathbf{a} \cdot \nabla s^n + \frac{1}{2}\Delta t^2 (\mathbf{a} \cdot \nabla)^2 \tilde{u}^n \quad (34b)$$

Assuming that the source term is not time dependent, then the Galerkin weak form is given by:

$$(w, \tilde{u}^n)_\Omega = (w, u^n)_\Omega + \frac{1}{3}\Delta t (w, s^n)_\Omega - \frac{1}{3}\Delta t (w, \mathbf{a} \cdot \nabla u^n)_\Omega - \alpha \Delta t^2 (w, \mathbf{a} \cdot \nabla s^n)_\Omega + \alpha \Delta t^2 (w, (\mathbf{a} \cdot \nabla)^2 u^n)_\Omega \quad (35a)$$

$$(w, u^{n+1})_\Omega = (w, u^n)_\Omega + \Delta t (w, s^n)_\Omega - \Delta t (w, \mathbf{a} \cdot \nabla u^n)_\Omega - \frac{1}{2}\Delta t^2 (w, \mathbf{a} \cdot \nabla s^n)_\Omega + \frac{1}{2}\Delta t^2 (w, (\mathbf{a} \cdot \nabla)^2 \tilde{u}^n)_\Omega \quad (35b)$$

Integration by parts, and applying homogeneous Dirichlet boundary condition at the inlet yields:

$$\begin{aligned} (w, \tilde{u}^n)_\Omega &= (w, u^n)_\Omega + \frac{1}{3}\Delta t (w, s^n)_\Omega + \frac{1}{3}\Delta t (\mathbf{a} \cdot \nabla w, u^n)_\Omega + \alpha \Delta t^2 (\mathbf{a} \cdot \nabla w, s^n)_\Omega \\ &\quad - \alpha \Delta t^2 (\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u^n)_\Omega - \frac{1}{3}\Delta t ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma_{out}} \\ &\quad - \alpha \Delta t^2 ((\mathbf{a} \cdot \mathbf{n})w, s^n)_{\Gamma_{out}} + \alpha \Delta t^2 ((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla u^n)_{\Gamma_{out}} \end{aligned} \quad (36a)$$

$$\begin{aligned} (w, u^{n+1})_\Omega &= (w, u^n)_\Omega + \Delta t (w, s^n)_\Omega + \Delta t (\mathbf{a} \cdot \nabla w, u^n)_\Omega + \frac{1}{2}\Delta t^2 (\mathbf{a} \cdot \nabla w, s^n)_\Omega \\ &\quad - \frac{1}{2}\Delta t^2 (\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla \tilde{u}^n)_\Omega - \Delta t ((\mathbf{a} \cdot \mathbf{n})w, u^n)_{\Gamma_{out}} \\ &\quad - \frac{1}{2}\Delta t^2 ((\mathbf{a} \cdot \mathbf{n})w, s^n)_{\Gamma_{out}} + \frac{1}{2}\Delta t^2 ((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla \tilde{u}^n)_{\Gamma_{out}} \end{aligned} \quad (36b)$$

Using the previous definitions given by (13), the weak form given by (36) is written in discrete form as:

$$\mathbf{M}\tilde{\mathbf{U}}^n = \mathbf{M}\mathbf{U}^n + \frac{1}{3}\Delta t \mathbf{v}_1 + \frac{1}{3}\Delta t \mathbf{C}\mathbf{U}^n + \alpha \Delta t^2 \mathbf{v}_2 - \alpha \Delta t^2 \mathbf{K}\mathbf{U}^n - \frac{1}{3}\Delta t \mathbf{M}_o \mathbf{U}^n - \alpha \Delta t^2 \mathbf{v}_o + \alpha \Delta t^2 \mathbf{C}_o \mathbf{U}^n, \quad (37a)$$

$$\mathbf{M}\mathbf{U}^{n+1} = \mathbf{M}\mathbf{U}^n + \Delta t \mathbf{v}_1 + \Delta t \mathbf{C}\mathbf{U}^n + \frac{1}{2}\Delta t^2 \mathbf{v}_2 - \frac{1}{2}\Delta t^2 \mathbf{K}\tilde{\mathbf{U}}^n - \Delta t \mathbf{M}_o \mathbf{U}^n - \frac{1}{2}\Delta t^2 \mathbf{v}_o + \frac{1}{2}\Delta t^2 \mathbf{C}_o \tilde{\mathbf{U}}^n \quad (37b)$$

further simplification yields:

$$\mathbf{M}(\tilde{\mathbf{U}}^n - \mathbf{U}^n) = \left[ \frac{\Delta t}{3}(\mathbf{C} - \mathbf{M}_o) - \alpha \Delta t^2(\mathbf{K} - \mathbf{C}_o) \right] \mathbf{U}^n + \left[ \frac{\Delta t}{3}\mathbf{v}_1 + \alpha \Delta t^2(\mathbf{v}_2 - \mathbf{v}_o) \right], \quad (38a)$$

$$\mathbf{M}(\mathbf{U}^{n+1} - \mathbf{U}^n) = \left[ \Delta t(\mathbf{C} - \mathbf{M}_o) \right] \mathbf{U}^n - \left[ \alpha \Delta t^2(\mathbf{K} - \mathbf{C}_o) \right] \tilde{\mathbf{U}}^n + \left[ \Delta t \mathbf{v}_1 + \frac{\Delta t^2}{2}(\mathbf{v}_2 - \mathbf{v}_o) \right] \quad (38b)$$

and for ease of implementation in Matlab, it is written as:

$$\mathbf{A}_1(\tilde{\mathbf{U}}^n - \mathbf{U}^n) = \mathbf{B}_1 \mathbf{U}^n + \mathbf{f}_1, \quad (39a)$$

$$\mathbf{A}_2(\mathbf{U}^{n+1} - \mathbf{U}^n) = \mathbf{B}_2 \mathbf{U}^n + \mathbf{C}_2 \tilde{\mathbf{U}}^n + \mathbf{f}_2 \quad (39b)$$

The corresponding part of the Matlab code is:

```

1 elseif meth == 7
2     alpha = 1/9;
3     A1 = M;
4     B1 = -(dt/3)*C' - alpha*dt^2*(K - Co);
5 %     B1 = (dt/3)*(C-Mo) - alpha*dt^2*(K - Co);
6     f1 = (dt/3)*v1 + alpha*dt^2*(v2 - v0);
7     A2 = M;
8     B2 = -dt*C';
9 %     B2 = dt*(C-Mo);
10    C2 = - (dt^2/2)*(K-Co);
11    f2 = dt*v1 - (dt^2/2)*(v2 - v0);

```

In the original code, the third term in the RHS of equation (35) wasn't integrated by parts. Both variations are valid and they give exactly the same results.

## 2.5 Fourth-order Taylor-Galerkin (TG4) + Galerkin formulation

The time discretization of fourth-order Taylor-Galerkin method is given by:

$$\frac{\Delta u}{\Delta t} = \frac{1}{2}(u_t^{n+1} + u_t^n) - \frac{\Delta t}{12}(u_{tt}^{n+1} - u_{tt}^n) \quad (40)$$

Substituting (31) and (32) into (40) yields:

$$\frac{\Delta u}{\Delta t} = \frac{1}{2}(s^{n+1} - \mathbf{a} \cdot \nabla u^{n+1} + s^n - \mathbf{a} \cdot \nabla u^n) - \frac{\Delta t}{12}(s_t^{n+1} - \mathbf{a} \cdot \nabla s^{n+1} + (\mathbf{a} \cdot \nabla)^2 u^{n+1} - s_t^n + \mathbf{a} \cdot \nabla s^n - (\mathbf{a} \cdot \nabla)^2 u^n) \quad (41)$$

Assuming that the source term is not time dependent, i.e.  $s_t = 0$  and  $s^{n+1} = s^n$ , simplifies the equation into:

$$\frac{\Delta u}{\Delta t} = s - \frac{1}{2}\mathbf{a} \cdot \nabla u^{n+1} - \frac{1}{2}\mathbf{a} \cdot \nabla u^n - \frac{\Delta t}{12}(\mathbf{a} \cdot \nabla)^2 \Delta u \quad (42)$$

Re-writing the third term on the RHS yields:

$$\frac{\Delta u}{\Delta t} = s - \frac{1}{2}\mathbf{a} \cdot \nabla u^{n+1} + \frac{1}{2}\mathbf{a} \cdot \nabla u^n - \mathbf{a} \cdot \nabla u^n - \frac{\Delta t}{12}(\mathbf{a} \cdot \nabla)^2 \Delta u \quad (43)$$

Gathering the 2nd and third term on the RHS yields:

$$\frac{\Delta u}{\Delta t} = s - \frac{1}{2}\mathbf{a} \cdot \nabla \Delta u - \mathbf{a} \cdot \nabla u^n - \frac{\Delta t}{12}(\mathbf{a} \cdot \nabla)^2 \Delta u \quad (44)$$

Re-arranging:

$$\frac{\Delta u}{\Delta t} + \frac{1}{2}\mathbf{a} \cdot \nabla \Delta u + \frac{\Delta t}{12}(\mathbf{a} \cdot \nabla)^2 \Delta u = s - \mathbf{a} \cdot \nabla u^n \quad (45)$$

The Galerkin weak form is given by:

$$(w, \frac{\Delta u}{\Delta t})_{\Omega} + \frac{1}{2}(w, \mathbf{a} \cdot \nabla \Delta u)_{\Omega} + \frac{\Delta t}{12}(w, (\mathbf{a} \cdot \nabla)^2 \Delta u)_{\Omega} = (w, s)_{\Omega} - (w, \mathbf{a} \cdot \nabla u^n)_{\Omega} \quad (46)$$

Integration by parts for the third term on the LHS, and considering only Dirichlet boundary conditions at the inlet boundary yields:

$$\begin{aligned} \left(w, \frac{\Delta u}{\Delta t}\right)_\Omega + \frac{1}{2} \left(w, \mathbf{a} \cdot \nabla \Delta u\right)_\Omega - \frac{\Delta t}{12} \left(\mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla \Delta u\right)_\Omega + \frac{\Delta t}{12} \left((\mathbf{a} \cdot \mathbf{n})w, \mathbf{a} \cdot \nabla \Delta u\right)_{\Gamma_{out}} \\ = \left(w, s\right)_\Omega - \left(w, \mathbf{a} \cdot \nabla u^n\right)_\Omega \end{aligned} \quad (47)$$

Using the previous definitions given by (13), the weak form given by (47) is written in discrete form as:

$$\frac{1}{\Delta t} \mathbf{M} \Delta \mathbf{U} + \frac{1}{2} \mathbf{C} \Delta \mathbf{U} - \frac{\Delta t}{12} \mathbf{K} \Delta \mathbf{U} + \frac{\Delta t}{12} \mathbf{C}_o \Delta \mathbf{U} = \mathbf{v}_1 - \mathbf{C} \mathbf{U}^n \quad (48)$$

further simplification yields:

$$\left[ \mathbf{M} + \frac{\Delta t}{2} \mathbf{C} - \frac{\Delta t^2}{12} (\mathbf{K} - \mathbf{C}_o) \right] \Delta \mathbf{U} = -\Delta t \mathbf{C} \mathbf{U}^n + \Delta t \mathbf{v}_1 \quad (49)$$

and for ease of implementation in Matlab, it is written as:

$$\mathbf{A} \Delta \mathbf{U} = \mathbf{B} \mathbf{U}^n + \mathbf{f}$$

The corresponding part of the Matlab code is:

```
1 elseif meth == 8
2     A = M + (dt/2)*C' - (dt^2/12)*(K - Co);
3     B = -dt*C';
4     f = dt*v1;
```

## 2.6 Two-step fourth-order Taylor-Galerkin (TG4-2S) + Galerkin formulation

By changing the value of  $\alpha$  in (30) to  $1/12$ , the two-step fourth-order Taylor-Galerkin time discretization is obtained.

```
1 elseif meth == 9
2 alpha = 1/12;
3     A1 = M;
4     B1 = -(dt/3)*C' - alpha*dt^2*(K - Co);
5 %     B1 = (dt/3)*(C-Mo) - alpha*dt^2*(K - Co);
6     f1 = (dt/3)*v1 + alpha*dt^2*(v2 - vo);
7     A2 = M;
8     B2 = -dt*C';
9 %     B2 = dt*(C-Mo);
10    C2 = - (dt^2/2)*(K-Co);
11    f2 = dt*v1 - (dt^2/2)*(v2 - vo);
```

## 2.7 Numerical results of the rotating cone problem

The rotating cone problem presented in [1] is solved on a uniform mesh of  $30 \times 30$  linear quadrilateral elements over the unit square  $[-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$ . The numerical solution, using the different methods presented earlier, is obtained after a complete revolution of the cone, i.e.  $t_{end} = 2\pi$ . For the explicit methods, 200 time steps ( $\Delta t = 2\pi/200$ ) are used, while for the implicit Crank-Nicholson method, three increasing values of the time step are employed ( $\Delta t = 2\pi/120, 2\pi/60$  and  $2\pi/30$ ).

To compare the accuracy of the explicit methods (Lax-Wendroff/Lumped mass LW-FD, Lax-Wendroff/Consistent mass TG2, TG3, TG3-2S, TG4, TG4-2S), the maximum and minimum values of the computed solution are recorded in Table 1. Similarly, for the implicit Crank-Nicholson method, the maximum and minimum values of the computed solution are recorded in Table 1 using different values of time step.

It is noticed in Figure 10 that the TG2 and TG3 methods are more accurate than the LW-FD method. However, TG2 and TG3 uses consistent mass matrices which makes them computationally more expensive than LW-FD that has a diagonal mass matrix. The results using TG3-2S and the fourth-order methods TG4 and TG4-2S are shown in Figure 11. The high accuracy of the solutions is clearly apparent.

For the implicit Crank-Nicholson method which is unconditionally stable, the solutions obtained, using different values of the time step, are shown in Figure 3d. Higher values of  $\Delta t$  are used to check the behaviour of the method beyond the stability limit of the explicit methods. It is noticed that the method is not dissipative. However, the accuracy of the method decreases by increasing  $\Delta t$  which can be interpreted from the higher non-physical oscillations.

| Method | $\Delta t$ | $u_{max}$ | $u_{min}$ | Figure             |
|--------|------------|-----------|-----------|--------------------|
| LW-FD  | $2\pi/200$ | 0.818575  | -0.177432 | Figure 10 (Top)    |
| TG2    | $2\pi/200$ | 0.983041  | -0.018619 | Figure 10 (Middle) |
| TG3    | $2\pi/200$ | 0.983465  | -0.014839 | Figure 10 (Bottom) |
| TG3-2S | $2\pi/200$ | 0.982845  | -0.014939 | Figure 11 (Top)    |
| TG4    | $2\pi/200$ | 0.992350  | -0.017285 | Figure 11 (Middle) |
| TG4-2S | $2\pi/200$ | 0.982536  | -0.014973 | Figure 11 (Bottom) |
| CN     | $2\pi/120$ | 0.996931  | -0.045350 | Figure 12 (Top)    |
| CN     | $2\pi/60$  | 0.969116  | -0.109591 | Figure 12 (Middle) |
| CN     | $2\pi/30$  | 0.889308  | -0.269427 | Figure 12 (Bottom) |

Table 1: The maximum and minimum values of the computed solution after one complete revolution using different methods.

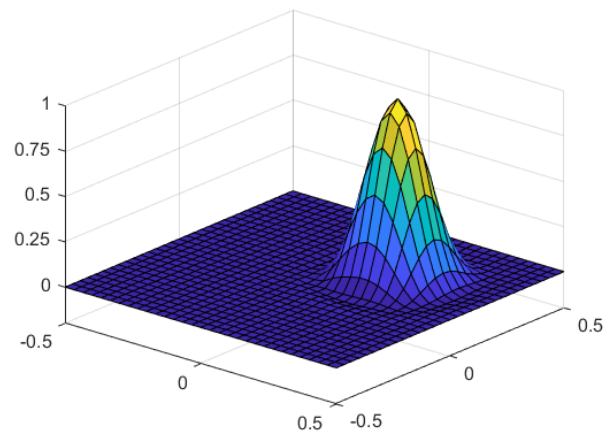
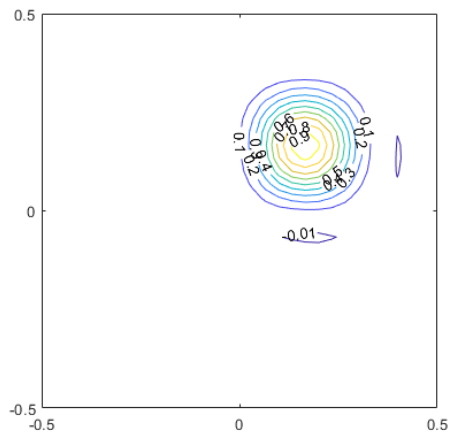
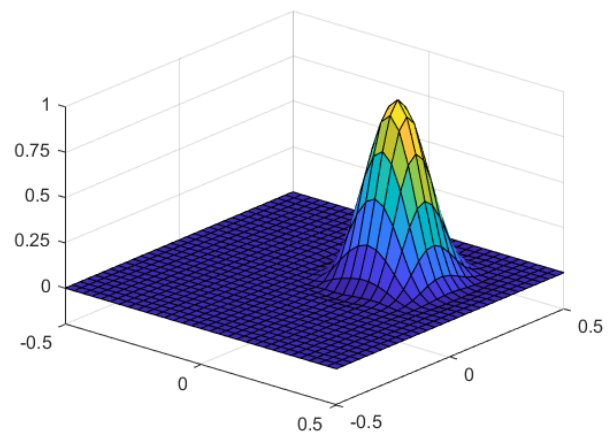
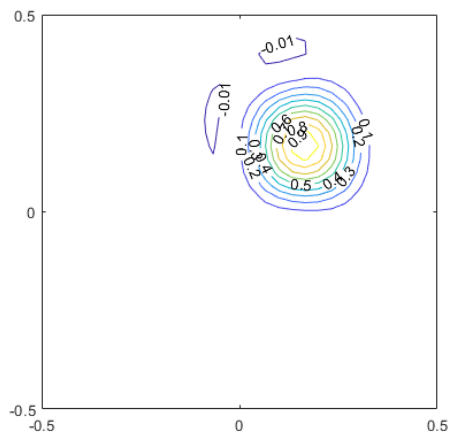
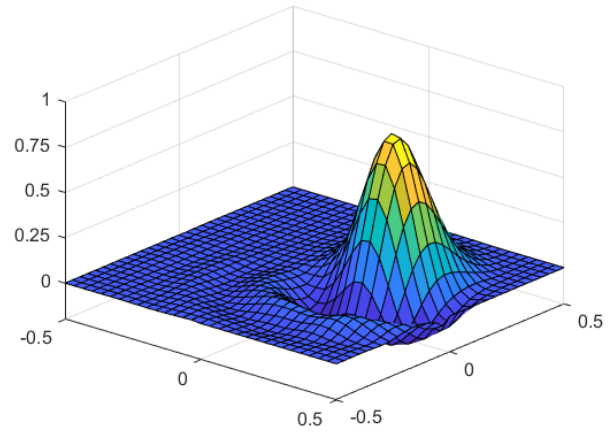
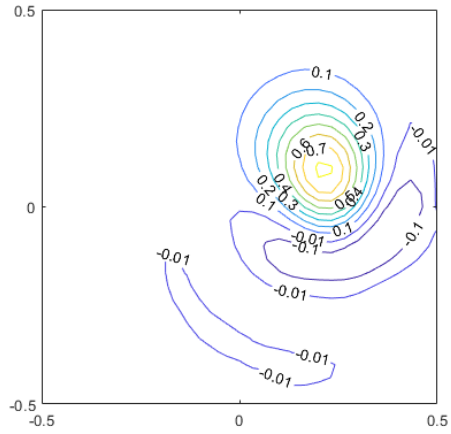


Figure 10: Convection of a cosine hill in a pure rotation velocity field: comparison of the numerical solutions after a complete revolution calculated with  $\Delta t = 2\pi/200$  by means of (Top): Lax-Wendroff/Lumped mass matrix ( $u_{max} = 0.818575, u_{min} = -0.177432$ ); (Middle): Lax-Wendroff/Consistent mass matrix ( $u_{max} = 0.983041, u_{min} = -0.018619$ ); and (Bottom): TG3 ( $u_{max} = 0.983465, u_{min} = -0.014839$ ).

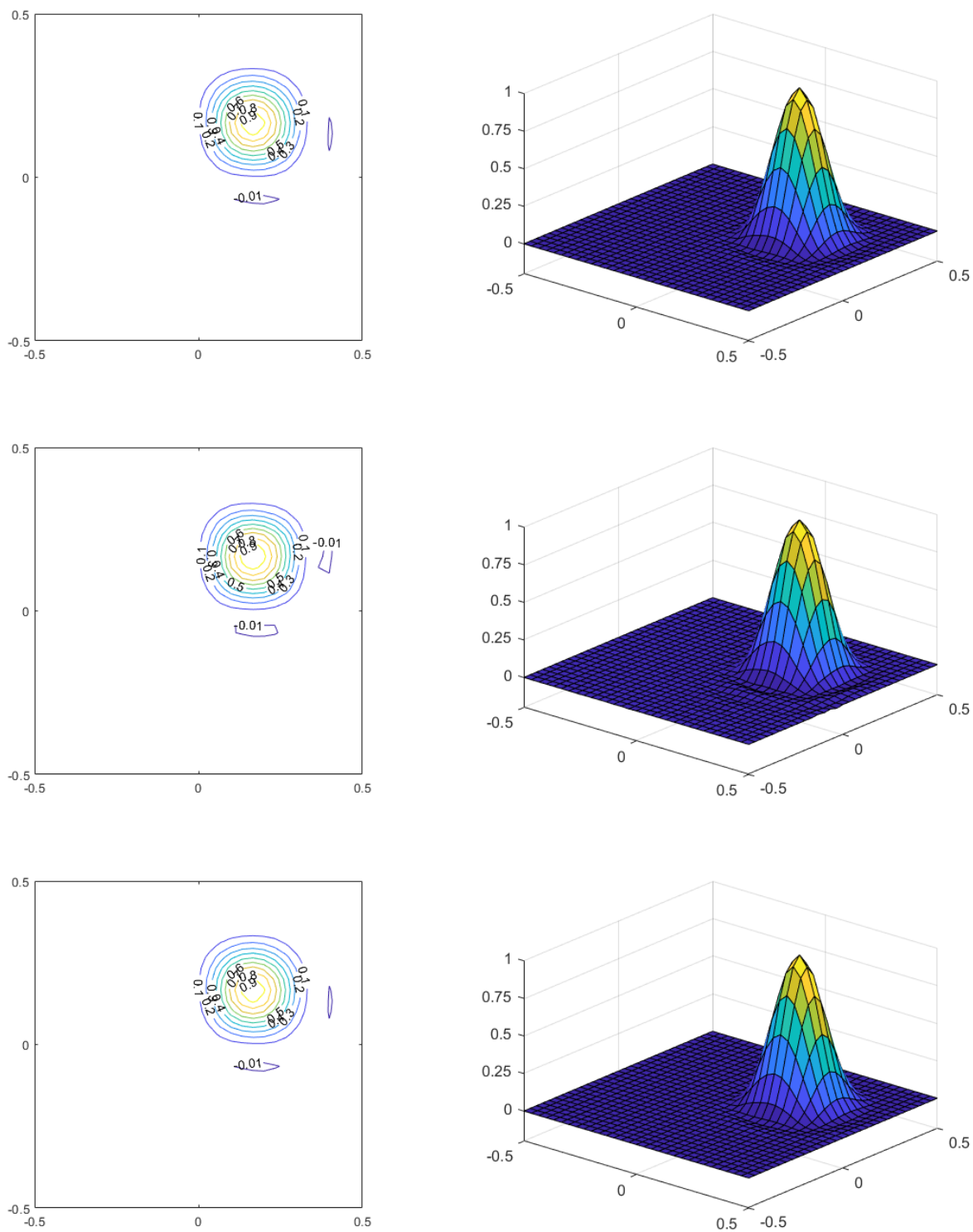


Figure 11: Convection of a cosine hill in a pure rotation velocity field: comparison of the numerical solutions after a complete revolution calculated with  $\Delta t = 2\pi/200$  by means of (Top): TG3-2S ( $u_{max} = 0.982845$ ,  $u_{min} = -0.014939$ ); (Middle): TG4 ( $u_{max} = 0.992350$ ,  $u_{min} = -0.017285$ ); and (Bottom): TG4-2S ( $u_{max} = 0.982536$ ,  $u_{min} = -0.0124973$ ).

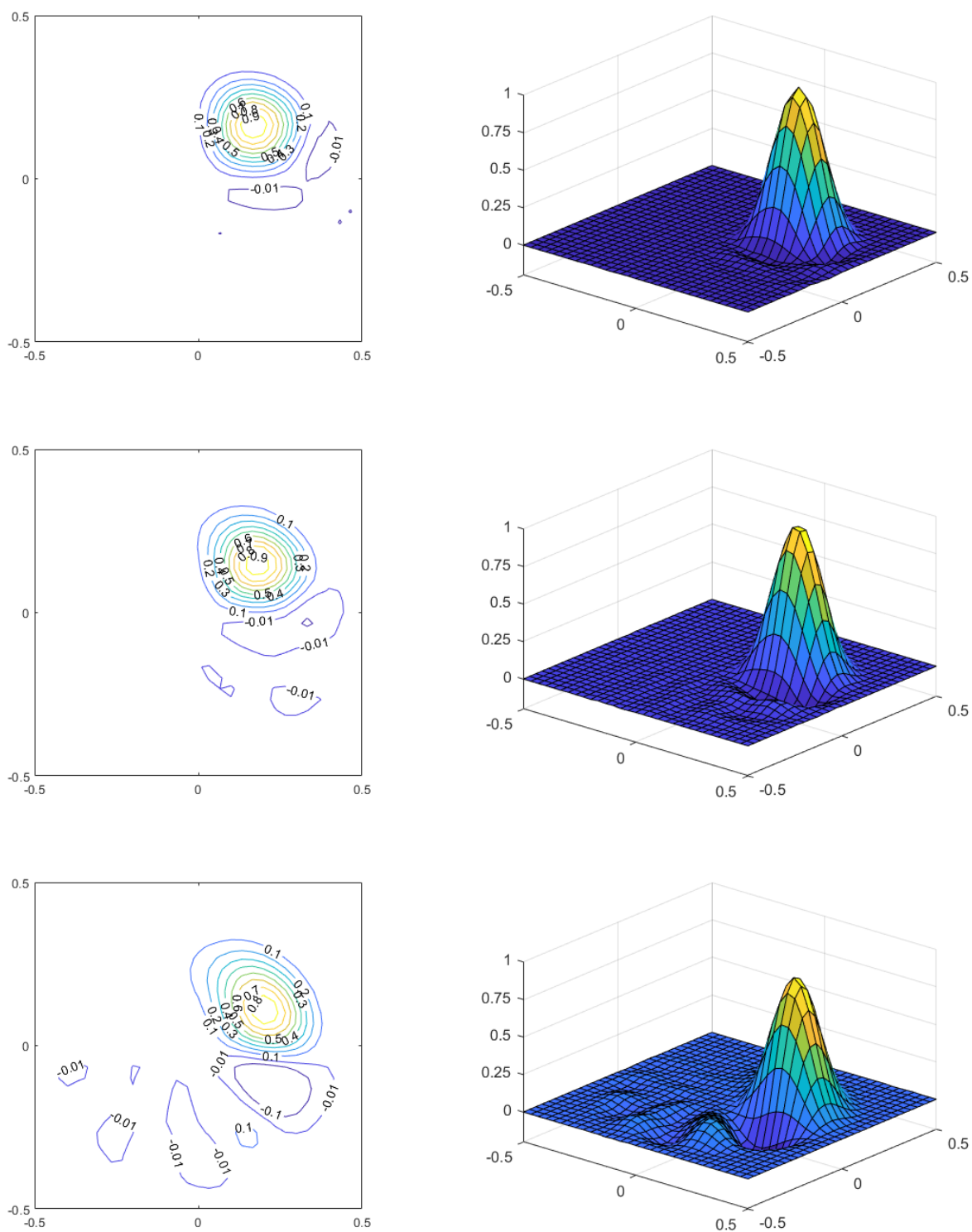


Figure 12: Convection of a cosine hill in a pure rotation velocity field using the Crank-Nicholson/Galerkin method: comparison of the numerical solutions after a complete revolution calculated with (Top):  $\Delta t = 2\pi/120$ ,  $u_{max} = 0.996931$ ,  $u_{min} = -0.045350$ ; (Middle):  $\Delta t = 2\pi/60$ ,  $u_{max} = 0.969116$ ,  $u_{min} = -0.109591$ ; and (Bottom):  $\Delta t = 2\pi/30$ ,  $u_{max} = 0.889308$ ,  $u_{min} = -0.269427$ .

# A Developed codes

## A.1 Developed codes for 2D steady transport equation

### A.1.1 Modified main.m

The modifications were made to account for linear and quadratic elements, and also to account for zero Dirchlet boundary conditions at the outlet boundary.

```
1 % This program solves a convection-diffusion problem
2 % in a square domain [0,1]x[0,1]
3
4 clear; close all; clc
5
6 disp(' ')
7 disp('This program solves a convection-diffusion equation on [0,1]x[0,1]')
8 disp(' ')
9 disp('No source term is considered');
10
11 % PDE coefficients
12 disp('Convection velocity is');
13 a_magnitude = 10^-3;
14 velo = [cos(pi/6), sin(pi/6)];
15 disp(velo);
16 a = norm(velo);
17 nu = cinput('Diffusion coefficient', 0.0001);
18 sigma = cinput('Reaction coefficient sigma', 1);
19 disp(' ')
20
21 dom = [0,1,0,1];
22
23 example.dom = dom;
24 example.velo = velo;
25 example.a = a;
26 example.nu = nu;
27 example.sigma = sigma;
28
29 % Element type
30 elem = 1; p = 1;
31 referenceElement = SetReferenceElement(elem,p);
32
33 nx = cinput('Number of elements in each direction (multiple of 5)= ', 10);
34 ny = nx;
35 [X,T] = CreateMesh(dom,nx,ny,referenceElement);
36 PlotMesh(T,X,'b-');
37
38 h = 1/nx;
39 Pe = a*h/(2*nu);
40 disp(' ')
41 disp(strcat('Peclet number: ', num2str(Pe)))
42
43 disp(' ')
44 disp('The following BCs at the outlet can be used:');
45 disp('      [1] Homogeneous natural condition ');
46 disp('      [2] zero Dirchlet condition');
```



```

47 disp ('      [3] zero Dirichlet condition everywhere (for this a source ...
      term s=1 is used)');
48 iOutletBC = cinput('Choose a BC at the outlet: ', 3);
49
50 disp(' ')
51 disp ('The following methods can be used:');
52 disp ('      [0] Galerkin');
53 disp ('      [1] Artificial diffusion');
54 disp ('      [2] SUPG');
55 disp ('      [3] GLS');
56 method = input ('Choose a method for solving the problem: ');
57 example.method = method;
58
59 % SYSTEM RESULTING OF DISCRETIZING THE WEAK FORM
60 [K, f] = FEM_system(X, T, referenceElement, example);
61
62 % BOUNDARY CONDITIONS
63 % Boundary conditions are imposed using Lagrange multipliers
64 nodes_x0 = find(abs(X(:,1)) < 10e-6);
65 nodes_x0 = nodes_x0(2:end-1);
66 nodes_x1 = find(abs(X(:,1)-1) < 10e-6);
67 nodes_x1 = nodes_x1(2:end);
68 nodes_y0 = find(abs(X(:,2)) < 10e-6);
69 nodes_y1 = find(abs(X(:,2)-1) < 10e-6);
70 nodes_y1 = nodes_y1(1:end-1);
71
72 if iOutletBC == 1
73     % nodes on which solution is u=1
74     nodesDir1 = nodes_x0( X(nodes_x0,2) > 0.2 );
75     % nodes on which solution is u=0
76     nodesDir0 = [nodes_x0( X(nodes_x0,2) ≤ 0.2 ); nodes_y0];
77     % Boundary condition matrix
78     C = [nodesDir1, ones(length(nodesDir1),1);
79         nodesDir0, zeros(length(nodesDir0),1)];
80 elseif iOutletBC == 2
81     % nodes on which solution is u=1
82     nodesDir1 = nodes_x0( X(nodes_x0,2) > 0.2 );
83     % nodes on which solution is u=0
84     nodesDir0 = [nodes_x0( X(nodes_x0,2) ≤ 0.2 ); nodes_y0; nodes_x1; ...
85                 nodes_y1];
86     % Boundary condition matrix
87     C = [nodesDir1, ones(length(nodesDir1),1);
88         nodesDir0, zeros(length(nodesDir0),1)];
89 elseif iOutletBC == 3
90     % nodes on which solution is u=0
91     nodesDir0 = [nodes_x0; nodes_y0; nodes_x1; nodes_y1];
92     % Boundary condition matrix
93     C = [nodesDir0, zeros(length(nodesDir0),1)];
94 end
95 nDir = size(C,1);
96 neq = size(f,1);
97 A = zeros(nDir, neq);
98 A(:,C(:,1)) = eye(nDir);
99 b = C(:,2);
100
101 % SOLUTION OF THE LINEAR SYSTEM
102 % Entire matrix
103 Ktot = [K A'; A zeros(nDir, nDir)];

```

```

103 ftot = [f;b];
104
105 sol = Ktot\ftot;
106 Temp = sol(1:neq);
107 multip = sol(neq+1:end);
108
109 % POSTPROCESS
110 figure(2), clf
111 xx = reshape(X(:,1), p*ny+1, p*nx+1)';
112 yy = reshape(X(:,2), p*ny+1, p*nx+1)';
113 sol = reshape(Temp, p*ny+1, p*nx+1)';
114 surface(xx,yy,sol,'FaceColor','interp');
115 set(gca, 'xTick',0:0.25:1, 'yTick',0:0.25:1, 'FontSize',12)
116 xlabel('x','FontSize',14);
117 ylabel('y','FontSize',14);
118 zlabel('u','FontSize',14);
119 zlim([-0.5 1.5])
120 % zlim([0 2])
121 colormap jet
122 grid on; view(3)

```

### A.1.2 Modified ShapeFunc.m

The modifications were made to account for linear and quadratic elements. The second derivatives of the shape functions are added since they are needed in GLS formulation.

```

1 function [N,Nxi,Neta,N2xi,N2eta,N2xieta] = ShapeFunc(elem,p,z)
2 % [N,Nxi,Neta] = ShapeFunc(elem,z)
3 % N, Nxi, Neta: matrices storing the values of the shape functions on the ...
   Gauss points
4 %
   of the reference element
5 %
   Each row concerns to a Gauss point
6 % z: coordinates of Gauss points in the reference element
7 % elem: type of element (0: quadrilatera, 1: triangles)
8 % p: interpolation degree
9
10 xi = z(:,1); eta = z(:,2); ngauss = length(z);
11 if elem == 0
12     if p == 1
13         N = [(1-xi).*(1-eta)/4, (1+xi).*(1-eta)/4, (1+xi).*(1+eta)/4, ...
              (1-xi).*(1+eta)/4];
14         Nxi = [(eta-1)/4, (1-eta)/4, (1+eta)/4, -(1+eta)/4];
15         Neta = [(xi-1)/4, -(1+xi)/4, (1+xi)/4, (1-xi)/4];
16         N2xi = zeros(ngauss,4);
17         N2eta = zeros(ngauss,4);
18         N2xieta = 1/4*[ones(size(xi)), -ones(size(xi)), ones(size(xi)), ...
                       -ones(size(xi))];
19     elseif p == 2
20         N = [xi.*(xi-1).*eta.*(eta-1)/4, xi.*(xi+1).*eta.*(eta-1)/4, ...
              xi.*(xi+1).*eta.*(eta+1)/4, xi.*(xi-1).*eta.*(eta+1)/4, ...
              (1-xi.^2).*eta.*(eta-1)/2, xi.*(xi+1).*(1-eta.^2)/2, ...
              (1-xi.^2).*eta.*(eta+1)/2, xi.*(xi-1).*(1-eta.^2)/2, ...
              (1-xi.^2).*(1-eta.^2)];
21         Nxi = [(xi-1/2).*eta.*(eta-1)/2, (xi+1/2).*eta.*(eta-1)/2, ...
                 (xi+1/2).*eta.*(eta+1)/2, (xi-1/2).*eta.*(eta+1)/2, ...

```

```

27         -xi.*eta.*(eta-1),          (xi+1/2).*(1-eta.^2),      ...
28         -xi.*eta.*(eta+1),          (xi-1/2).*(1-eta.^2),      ...
29         -2*xi.*(1-eta.^2)];
30     Neta = [xi.*(xi-1).*(eta-1/2)/2,  xi.*(xi+1).*(eta-1/2)/2, ...
31            xi.*(xi+1).*(eta+1/2)/2,  xi.*(xi-1).*(eta+1/2)/2, ...
32            (1-xi.^2).*(eta-1/2),      xi.*(xi+1).*(-eta),      ...
33            (1-xi.^2).*(eta+1/2),      xi.*(xi-1).*(-eta),      ...
34            (1-xi.^2).*(-2*eta)];
35     N2xi = [ eta.*(eta - 1)/2,      eta.*(eta - 1)/2, ...
36            eta.*(eta + 1)/2,      eta.*(eta + 1)/2, ...
37            -eta.*(eta - 1),      1 - eta.^2,      ...
38            -eta.*(eta + 1),      1 - eta.^2,      ...
39            2*eta.^2 - 2];
40     N2eta = [ xi.*(xi - 1)/2, xi.*(xi + 1)/2, ...
41            xi.*(xi + 1)/2, xi.*(xi - 1)/2, ...
42            1 - xi.^2, -xi.*(xi + 1),      ...
43            1 - xi.^2, -xi.*(xi - 1),      ...
44            2*xi.^2 - 2];
45     N2xieta = [ (eta.*(xi - 1/2))/2 + ((eta - 1).*(xi - 1/2))/2, ...
46                (eta.*(xi + 1/2))/2 + ((eta - 1).*(xi + 1/2))/2, ...
47                (eta.*(xi + 1/2))/2 + ((eta + 1).*(xi + 1/2))/2, ...
48                (eta.*(xi - 1/2))/2 + ((eta + 1).*(xi - 1/2))/2, ...
49                - eta.*xi - xi.*(eta - 1), -2*eta.*(xi + 1/2), ...
50                - eta.*xi - xi.*(eta + 1), -2*eta.*(xi - 1/2), ...
51                4*eta.*xi];
52     else
53         error('not available interpolation degree')
54     end
55 elseif elem == 1
56     if p == 1
57         N = [1-xi-eta, xi, eta];
58         Nxi = [-ones(size(xi)), ones(size(xi)), zeros(size(xi))];
59         Neta = [-ones(size(xi)), zeros(size(xi)), ones(size(xi))];
60         N2xi = zeros(ngauss,3);
61         N2eta = zeros(ngauss,3);
62         N2xieta = zeros(ngauss,3);
63     elseif p == 2
64         N = [2*(xi+eta).^2-3*(xi+eta)+1, 2*xi.^2-xi, ...
65            2*eta.^2-eta, -4*xi.^2 - 4*xi.*eta+4*xi, ...
66            4*xi.*eta, -4*eta.^2-4*xi.*eta + 4*eta];
67         Nxi = [4*eta + 4*xi - 3, 4*xi - 1, zeros(size(xi)), ...
68            4 - 8*xi - 4*eta, 4*eta, -4*eta];
69         Neta = [ 4*eta + 4*xi - 3, zeros(size(xi)), 4*eta - 1, ...
70            -4*xi, 4*xi, 4 - 4*xi - 8*eta];
71         N2xi = [ 4*ones(size(xi)), 4*ones(size(xi)), zeros(size(xi)), ...
72            -8*ones(size(xi)), zeros(size(xi)), zeros(size(xi))];
73         N2eta = [ 4*ones(size(xi)), zeros(size(xi)), 4*ones(size(xi)), ...
74            zeros(size(xi)), zeros(size(xi)), -8*ones(size(xi))];
75         N2xieta = [ 4*ones(size(xi)), zeros(size(xi)), zeros(size(xi)), ...
76            -4*ones(size(xi)), 4*ones(size(xi)), -4*ones(size(xi))];
77     else
78         error('not available interpolation degree')
79     end
80 else
81     error('not available element')
82 end

```

### A.1.3 Modified FEMsystem.m

The GLS method is added to the code where the stabilization parameter  $\tau$  is computed in (lines 66 to 74) and the elemental matrices are computed in (lines 159 to 166). Another main addition to this function is the mapping of the second order derivatives from the reference element to the physical one which is added in (lines 104 to 139). The details of mapping of second order derivatives are shown in appendix B.

```
1 function [K,f] = FEM_system(X,T,referenceElement,example)
2 % [K,f] = FEM_system(X,T,referenceElement,example)
3 % Matrix K and r.h.s vector f obtained after discretizing a 2D ...
   convection-diffusion equation
4 %
5 % X:          nodal coordinates
6 % T:          connectivities (elements)
7 % referenceElement: reference element properties (quadrature, shape ...
   functions...)
8 % example: example properties
9
10 velo = example.velo;
11 a = example.a;
12 nu = example.nu;
13 sigma = example.sigma;
14 method = example.method;
15 ax = velo(1);
16 ay = velo(2);
17 Te = T(1,:); Xe = X(Te,:);
18 hx = max(Xe(:,1)) - min(Xe(:,1));
19 hy = max(Xe(:,2)) - min(Xe(:,2));
20 h = (hx+hy)/2;
21
22 nen = referenceElement.nen;
23 ngaus = referenceElement.ngaus;
24 wgp = referenceElement.GaussWeights;
25 N = referenceElement.N;
26 Nxi = referenceElement.Nxi;
27 Neta = referenceElement.Neta;
28 N2xi = referenceElement.N2xi;
29 N2eta = referenceElement.N2eta;
30 N2xieta = referenceElement.N2xieta;
31
32 % Number of elements and number of nodes in the mesh
33 nElem = size(T,1);
34 nPt = size(X,1);
35
36 K = zeros(nPt,nPt);
37 f = zeros(nPt,1);
38
39 if method == 0
40     % Galerkin
41     tau = 0;
42 elseif method == 1
43     % Artificial Diffusion
44     Pe_x = ax*h/(2*nu);
45     Pe_y = ay*h/(2*nu);
46     alpha_x = coth(Pe_x)-1/Pe_x;
```

```

47     alpha_y = coth(Pe_y)-1/Pe_y;
48     tau = h*(ax*alpha_x + ay*alpha_y)/2;
49     nubar_p = tau*a*a;
50     disp(strcat('Recommended value for the artificial diffusion = ...
    ',num2str(nubar_p)));
51     nubar = cinput('Artificial diffusion to be used', nubar_p);
52     if isempty(nubar)
53         nubar = nubar_p;
54     end
55     nu = nu + nubar;
56     tau=0;
57 elseif method == 2
58     % SUPG
59     Pe = a*h/(2*nu);
60     tau_p = h*(1 + 9/Pe^2)^(-1/2)/(2*a);
61     disp(strcat('Recommended stabilization parameter = ',num2str(tau_p)));
62     tau = cinput('Stabilization parameter',tau_p);
63     if isempty(tau)
64         tau = tau_p;
65     end
66 elseif method == 3
67     % GLS
68     Pe = a*h/(2*nu);
69     tau_p = h*(1 + 9/Pe^2)^(-1/2)/(2*a);
70     disp(strcat('Recommended stabilization parameter = ',num2str(tau_p)));
71     tau = cinput('Stabilization parameter',tau_p);
72     if isempty(tau)
73         tau = tau_p;
74     end
75 else
76     error ('Unavailable method')
77 end
78
79 % Loop on elements
80 for ielem = 1:nElem
81     % Te: global number of the nodes in the current element
82     Te = T(ielem,:);
83     % Xe: coordinates of the nodes in the current element
84     Xe = X(Te,:);
85     % Element matrices
86     [Ke, fe] = ...
        EleMat (Xe, nen, ngaus, wgp, N, Nxi, Neta, N2xi, N2eta, N2xieta, method, tau, velo, nu, sigma);
87     % Assemble the element matrices
88     K(Te, Te) = K(Te, Te) + Ke;
89     f(Te) = f(Te) + fe;
90 end
91
92
93
94 function [Ke, fe] = ...
    EleMat (Xe, nen, ngaus, wgp, N, Nxi, Neta, N2xi, N2eta, N2xieta, method, tau, velo, nu, sigma)
95 %
96 ax = velo(1);
97 ay = velo(2);
98
99 Ke = zeros (nen, nen);
100 fe = zeros (nen, 1);
101

```

```

102 % Loop on Gauss points
103 for ig = 1:ngaus
104     N_ig = N(ig, :);
105     Nxi_ig = Nxi(ig, :);
106     Neta_ig = Neta(ig, :);
107     N2xi_ig = N2xi(ig, :);
108     N2eta_ig = N2eta(ig, :);
109     N2xieta_ig = N2xieta(ig, :);
110
111     dxdx_i = Nxi_ig*(Xe(:,1));
112     dydx_i = Nxi_ig*(Xe(:,2));
113     dxde_i = Neta_ig*(Xe(:,1));
114     dyde_i = Neta_ig*(Xe(:,2));
115     d2xdx_i2 = N2xi_ig*(Xe(:,1));
116     d2xde_i2 = N2eta_ig*(Xe(:,1));
117     d2ydx_i2 = N2xi_ig*(Xe(:,2));
118     d2yde_i2 = N2eta_ig*(Xe(:,2));
119     d2xdxieta = N2xieta_ig*(Xe(:,1));
120     d2ydxieta = N2xieta_ig*(Xe(:,2));
121
122     % mapping of 1st order derivatives
123     Jacob = [dxdx_i dydx_i;
124             dxde_i dyde_i];
125     dvolu = wgp(ig)*det(Jacob);
126     res = Jacob\[Nxi_ig;Neta_ig];
127     Nx = res(1, :);
128     Ny = res(2, :);
129     % mapping of 2nd order derivatives
130     mappingMatrix = [dxdx_i^2      dydx_i^2      2*dxdx_i*dydx_i;
131                    dxde_i^2      dyde_i^2      2*dxde_i*dyde_i;
132                    dxdx_i*dxde_i  dydx_i*dyde_i  ...
133                    dxdx_i*dyde_i+dxde_i*dydx_i];
134     referenceVector = [N2xi_ig - Nx*d2xdx_i2 - Ny*d2ydx_i2 ;
135                      N2eta_ig - Nx*d2xde_i2 - Ny*d2yde_i2;
136                      N2xieta_ig - Nx*d2xdxieta - Ny*d2ydxieta];
137     physicalVector = mappingMatrix\referenceVector;
138     N2x = physicalVector(1, :);
139     N2y = physicalVector(2, :);
140     Nxy = physicalVector(3, :);
141     if method == 0
142         % Galerkin
143         Ke = Ke + (nu*(Nx'*Nx+Ny'*Ny) + N_ig'*(ax*Nx+ay*Ny) + ...
144                 N_ig'*sigma*N_ig)*dvolu;
145         aux = N_ig*Xe;
146         f_ig = SourceTerm(aux);
147         fe = fe + N_ig'*(f_ig*dvolu);
148     elseif method == 1
149         % Artificial diffusion
150         Ke = Ke + (nu*(Nx'*Nx+Ny'*Ny) + N_ig'*(ax*Nx+ay*Ny) + ...
151                 N_ig'*sigma*N_ig)*dvolu;
152         aux = N_ig*Xe;
153         f_ig = SourceTerm(aux);
154         fe = fe + N_ig'*(f_ig*dvolu);
155     elseif method == 2
156         % SUPG
157         Ke = Ke + ( nu*(Nx'*Nx+Ny'*Ny) + N_ig'*(ax*Nx+ay*Ny) + ...
158                 N_ig'*sigma*N_ig + ...
159                 tau*(ax*Nx+ay*Ny)'*( ( ax*Nx+ay*Ny) - nu*(N2x+N2y) + ...

```

```

        sigma*N_ig) )*dvolu;
156     aux = N_ig*Xe;
157     f_ig = SourceTerm(aux);
158     fe = fe + (N_ig + tau*(ax*Nx+ay*Ny))'*(f_ig*dvolu);
159 elseif method == 3
160     % GLS
161     Ke = Ke + (N_ig'*(ax*Nx+ay*Ny) + nu*(Nx'*Nx+Ny'*Ny) + ...
        N_ig'*sigma*N_ig + ...
162         tau*((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig)'*...
163         ((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig))*dvolu;
164     aux = N_ig*Xe;
165     f_ig = SourceTerm(aux);
166     fe = fe + (N_ig + tau*((ax*Nx+ay*Ny) - nu*(N2x+N2y) + sigma*N_ig ...
        ))'*(f_ig*dvolu);
167     end
168 end

```

## A.2 Developed codes for 2D unsteady transport equation

Two higher-order methods are added to the code, which are TG4 and TG4-2S.

```
1 elseif meth == 8 % TG4
2     A = M +(dt/2)*C' - (dt^2/12)*(K - Co);
3     B = -dt*C';
4     f = dt*v1;
5 elseif meth == 9 % TG4-2S
6     alpha = 1/12;
7     A1 = M;
8     B1 = -(dt/3)*C'- alpha*dt^2*(K - Co);
9 %     B1 = (dt/3)*(C-Mo)- alpha*dt^2*(K - Co);
10    f1 = (dt/3)*v1 + alpha*dt^2*(v2 - vo);
11    A2 = M;
12    B2 = -dt*C';
13 %    B2 = dt*(C-Mo);
14    C2 = - (dt^2/2)*(K-Co);
15    f2 = dt*v1 - (dt^2/2)*(v2 - vo);
```



## B Mapping of second order derivatives from the reference element to the physical one

For 2D elements, the first order derivatives of the shape functions in the reference element can be written using chain-rule as:

$$\begin{aligned}\frac{\partial \mathbf{N}}{\partial \xi} &= \frac{\partial \mathbf{N}}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial y}{\partial \xi}, \\ \frac{\partial \mathbf{N}}{\partial \eta} &= \frac{\partial \mathbf{N}}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial y}{\partial \eta}.\end{aligned}\tag{B.1}$$

To derive an expression for a second derivative, consider for instance:

$$\begin{aligned}\frac{\partial^2 \mathbf{N}}{\partial \xi^2} &= \frac{\partial}{\partial \xi} \left( \frac{\partial \mathbf{N}}{\partial \xi} \right) \\ &= \frac{\partial}{\partial \xi} \left( \frac{\partial \mathbf{N}}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial y}{\partial \xi} \right) \\ &= \frac{\partial}{\partial \xi} \left( \frac{\partial \mathbf{N}}{\partial x} \right) \frac{\partial x}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} + \frac{\partial}{\partial \xi} \left( \frac{\partial \mathbf{N}}{\partial y} \right) \frac{\partial y}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2} \\ &= \left[ \frac{\partial}{\partial x} \left( \frac{\partial \mathbf{N}}{\partial x} \right) \frac{\partial x}{\partial \xi} + \frac{\partial}{\partial y} \left( \frac{\partial \mathbf{N}}{\partial x} \right) \frac{\partial y}{\partial \xi} \right] \frac{\partial x}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} + \left[ \frac{\partial}{\partial x} \left( \frac{\partial \mathbf{N}}{\partial y} \right) \frac{\partial x}{\partial \xi} + \frac{\partial}{\partial y} \left( \frac{\partial \mathbf{N}}{\partial y} \right) \frac{\partial y}{\partial \xi} \right] \frac{\partial y}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2} \\ &= \frac{\partial^2 \mathbf{N}}{\partial x^2} \left( \frac{\partial x}{\partial \xi} \right)^2 + \frac{\partial^2 \mathbf{N}}{\partial y \partial x} \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \xi} + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} + \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} + \frac{\partial^2 \mathbf{N}}{\partial y^2} \left( \frac{\partial y}{\partial \xi} \right)^2 + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2} \\ &= \frac{\partial^2 \mathbf{N}}{\partial x^2} \left( \frac{\partial x}{\partial \xi} \right)^2 + \frac{\partial^2 \mathbf{N}}{\partial y^2} \left( \frac{\partial y}{\partial \xi} \right)^2 + \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \left( 2 \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} \right) + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2}\end{aligned}\tag{B.2}$$

Similarly the other second order derivatives are derived, which yields:

$$\frac{\partial^2 \mathbf{N}}{\partial \eta^2} = \frac{\partial^2 \mathbf{N}}{\partial x^2} \left( \frac{\partial x}{\partial \eta} \right)^2 + \frac{\partial^2 \mathbf{N}}{\partial y^2} \left( \frac{\partial y}{\partial \eta} \right)^2 + \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \left( 2 \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \eta} \right) + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \eta^2} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \eta^2}\tag{B.3}$$

$$\frac{\partial^2 \mathbf{N}}{\partial \xi \partial \eta} = \frac{\partial^2 \mathbf{N}}{\partial x^2} \left( \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} \right) + \frac{\partial^2 \mathbf{N}}{\partial y^2} \left( \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} \right) + \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \left( \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \right) + \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi \partial \eta} + \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi \partial \eta}\tag{B.4}$$

By combining the three equations (B.2), (B.3) and (B.4) into a matrix form, it yields:

$$\begin{bmatrix} \left( \frac{\partial x}{\partial \xi} \right)^2 & \left( \frac{\partial x}{\partial \xi} \right)^2 & 2 \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} \\ \left( \frac{\partial x}{\partial \eta} \right)^2 & \left( \frac{\partial x}{\partial \eta} \right)^2 & 2 \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \eta} \\ \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} & \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \end{bmatrix} \begin{Bmatrix} \frac{\partial^2 \mathbf{N}}{\partial x^2} \\ \frac{\partial^2 \mathbf{N}}{\partial y^2} \\ \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \end{Bmatrix} = \begin{Bmatrix} \frac{\partial^2 \mathbf{N}}{\partial \xi^2} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2} \\ \frac{\partial^2 \mathbf{N}}{\partial \eta^2} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \eta^2} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \eta^2} \\ \frac{\partial^2 \mathbf{N}}{\partial \xi \partial \eta} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi \partial \eta} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi \partial \eta} \end{Bmatrix}\tag{B.5}$$

Therefore, the second order derivatives in the physical element are obtained using the following mapping:

$$\begin{Bmatrix} \frac{\partial^2 \mathbf{N}}{\partial x^2} \\ \frac{\partial^2 \mathbf{N}}{\partial y^2} \\ \frac{\partial^2 \mathbf{N}}{\partial x \partial y} \end{Bmatrix} = \begin{bmatrix} \left(\frac{\partial x}{\partial \xi}\right)^2 & \left(\frac{\partial x}{\partial \xi}\right)^2 & 2\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} \\ \left(\frac{\partial x}{\partial \eta}\right)^2 & \left(\frac{\partial x}{\partial \eta}\right)^2 & 2\frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \eta} \\ \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} & \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \end{bmatrix}^{-1} \begin{Bmatrix} \frac{\partial^2 \mathbf{N}}{\partial \xi^2} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi^2} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi^2} \\ \frac{\partial^2 \mathbf{N}}{\partial \eta^2} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \eta^2} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \eta^2} \\ \frac{\partial^2 \mathbf{N}}{\partial \xi \partial \eta} - \frac{\partial \mathbf{N}}{\partial x} \frac{\partial^2 x}{\partial \xi \partial \eta} - \frac{\partial \mathbf{N}}{\partial y} \frac{\partial^2 y}{\partial \xi \partial \eta} \end{Bmatrix} \quad (\text{B.6})$$

Recalling the isoparametric mapping between the reference element and a physical element  $e$ :

$$\begin{aligned} x^{(e)}(\xi, \eta) &= \sum_i x_i^{(e)} N_i(\xi, \eta), \\ y^{(e)}(\xi, \eta) &= \sum_i y_i^{(e)} N_i(\xi, \eta) \end{aligned} \quad (\text{B.7})$$

Then, the first and second order derivatives of  $x^{(e)}(\xi, \eta)$  and  $y^{(e)}(\xi, \eta)$  w.r.t  $\xi$  and  $\eta$  are given by:

$$\begin{aligned} \frac{\partial x^{(e)}(\xi, \eta)}{\partial \xi} &= \sum_i x_i^{(e)} \frac{\partial N_i(\xi, \eta)}{\partial \xi}, \\ \frac{\partial y^{(e)}(\xi, \eta)}{\partial \xi} &= \sum_i y_i^{(e)} \frac{\partial N_i(\xi, \eta)}{\partial \xi}, \\ \frac{\partial x^{(e)}(\xi, \eta)}{\partial \eta} &= \sum_i x_i^{(e)} \frac{\partial N_i(\xi, \eta)}{\partial \eta}, \\ \frac{\partial y^{(e)}(\xi, \eta)}{\partial \eta} &= \sum_i y_i^{(e)} \frac{\partial N_i(\xi, \eta)}{\partial \eta} \end{aligned} \quad (\text{B.8})$$

and

$$\begin{aligned} \frac{\partial^2 x^{(e)}(\xi, \eta)}{\partial \xi^2} &= \sum_i x_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \xi^2}, \\ \frac{\partial^2 y^{(e)}(\xi, \eta)}{\partial \xi^2} &= \sum_i y_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \xi^2}, \\ \frac{\partial^2 x^{(e)}(\xi, \eta)}{\partial \eta^2} &= \sum_i x_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \eta^2}, \\ \frac{\partial^2 y^{(e)}(\xi, \eta)}{\partial \eta^2} &= \sum_i y_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \eta^2}, \\ \frac{\partial^2 x^{(e)}(\xi, \eta)}{\partial \xi \partial \eta} &= \sum_i x_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \xi \partial \eta}, \\ \frac{\partial^2 y^{(e)}(\xi, \eta)}{\partial \xi \partial \eta} &= \sum_i y_i^{(e)} \frac{\partial^2 N_i(\xi, \eta)}{\partial \xi \partial \eta} \end{aligned} \quad (\text{B.9})$$

## References

- [1] Donea, J., Huerta, A. (2004). *Finite Element Methods for Flow Problems*. Chichester: Wiley, pp.135.