

MatLab Session 3

2D Steady Advection-Diffusion-Reaction equation

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1 Introduction

This report will cover the 2D *steady state advection-diffusion-reaction* equation, seen in (1), solution with WRM using Galerkin approach for *FEM* spatial discretization with emphasis on stabilization methods proposed as exercises in laboratory session 3. The first part will briefly explain the code changes in order to implement each stabilization method: Streamline Upwind Petrov Galerkin (SUPG) and Galerkin Least Square (GLS) for both 2D bilinear and bi-quadratic 9-Noded quadrilateral elements. Following, results will be discussed.

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

2 Changes in MatLab routines

The implemented changes in MatLab routines are explained in the following subsections.

2.1 Implementation for 2D bi-quadratic quadrilateral elements

In order to enable the formulation of the problem with 9-Noded bi-quadratic quadrilateral elements the changes in the following MatLab routines were made:

2.1.1 Routine *main.m*

The proper imposition of boundary conditions for $p = 2$ was made by the following:

```

% BOUNDARY CONDITIONS
% Boundary conditions are imposed using Lagrange multipliers
nodes_y0 = [1:p*nx+1]'; % Nodes on the boundary y=0
nodes_x1 = [2*(p*nx+1):p*nx+1:(p*ny+1)*(p*nx+1)]' ; % Nodes on the boundary x=1
nodes_y1 = [p*ny*(p*nx+1)+p*nx:-1:p*ny*(p*nx+1)+1]' ; % Nodes on the boundary y=1
nodes_x0 = [(p*ny-1)*(p*nx+1)+1:-1:(p*nx+1):p*nx+2]' ; % Nodes on the boundary x=0

```

2.1.2 Routine *ShapFunc.m*

In this subroutine the definition of each shape function second order derivative, evaluated at gauss points, was made for bilinear and bi-quadratic quadrilateral elements as follows:

```

%SECOND DERIVATIVE OF SHAPE FUNCTIONS (BILINEAR ELEMENT)
N2xi = [ zeros(size(xi)), zeros(size(xi)), zeros(size(xi)), zeros(size(xi))];
N2eta = [ zeros(size(xi)), zeros(size(xi)), zeros(size(xi)), zeros(size(xi))];

```

```

%SECOND DERIVATIVE OF SHAPE FUNCTIONS (BIQUADRATIC ELEMENT)
N2xi = [eta.*(eta-1)/2 , eta.*(eta-1)/2 , eta.*(eta+1)/2,...
        eta.*(eta+1)/2 , -eta.*(eta-1) , (1-eta.^2) , ...
        -eta.*(eta+1) , (1-eta.^2) , -2*(1-eta.^2)];
N2eta = [xi.*(xi-1)/2 , xi.*(xi+1)/2 , xi.*(xi+1)/2,...
        xi.*(xi-1)/2 , (1-xi.^2) , -xi.*(xi+1) , ...
        (1-xi.^2) , -xi.*(xi-1) , -2*(1-xi.^2)];

```

2.1.3 Routine *FEM_System.m*

In this routine the definition of the transformation matrix of the second derivative from natural coordinates (ξ, η) to physical coordinates (x, y) was made. After some tenacious algebra and the consideration that for a quadrilateral element with sides aligned with physical coordinates axis the derivatives $dx/d\eta = dy/d\xi = 0$ and also $d^2x/d\xi^2 = d^2y/d\eta^2 = 0$, the transformation of the shape functions second order derivatives reduces to:

$$\left\{ \begin{array}{c} \frac{d^2N}{d\xi^2} \\ \frac{d^2N}{d\eta^2} \end{array} \right\} = \begin{bmatrix} \left(\frac{dx}{d\xi}\right)^2 & \left(\frac{dy}{d\xi}\right)^2 \\ \left(\frac{dx}{d\eta}\right)^2 & \left(\frac{dy}{d\eta}\right)^2 \end{bmatrix} \left\{ \begin{array}{c} \frac{d^2N}{dx^2} \\ \frac{d^2N}{dy^2} \end{array} \right\} \quad (2)$$

The implementation of this transformation becomes:

```

%SECOND DERIVATIVE
N2xi_ig = N2xi(ig,:);
N2eta_ig = N2eta(ig,:);
%TRANSFORMATION MATRIX
J2 = [(Nxi_ig*(Xe(:,1)))^2 (Nxi_ig*(Xe(:,2)))^2
       (Neta_ig*(Xe(:,1)))^2 (Neta_ig*(Xe(:,2)))^2];
res2 = J2\[N2xi_ig;N2eta_ig];
%SECOND DERIVATIVES IN PHYSICAL COORDINATES
Nxx = res2(1,:);
Nyy = res2(2,:);

```

2.2 Implementation of SUPG

For the SUPG stabilization method, the stabilization term in the case of advection-diffusion-reaction becomes:

$$\sum_e \int_{\Omega^e} P(w) \tau R(u) d\Omega = \sum_e (\tau \mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u) - (\tau \mathbf{a} \cdot \nabla w, \nabla \cdot (\nu \nabla u)) + (\tau \mathbf{a} \cdot \nabla w, \sigma u) \quad (3)$$

The source term contribution becomes:

$$\sum_e (\tau \mathbf{a} \cdot \nabla w, s) \quad (4)$$

Thus, the code implementation becomes:

```

% SUPG
Ke = Ke + (nu*(Nx'*Nx+Ny'*Ny) + N_ig'*(ax*Nx+ay*Ny) + N_ig'*(sig*N_ig)+ ...
          tau*(ax*Nx+ay*Ny)'*((ax*Nx+ay*Ny) - nu*(Nxx+Nyy) + sig*N_ig))*dvolu;
aux = N_ig*Ke;
f_ig = SourceTerm(aux);
fe = fe + (N_ig + tau*(ax*Nx+ay*Ny))*f_ig*dvolu;

```

2.3 Implementation of GLS

For the SUPG stabilization method, the stabilization parameter in the case of advection-diffusion-reaction becomes:

$$\begin{aligned} \sum_e \int_{\Omega^e} P(w) \tau R(u) d\Omega = & \sum_e (\tau \mathbf{a} \cdot \nabla w, \mathbf{a} \cdot \nabla u) - (\tau \mathbf{a} \cdot \nabla w, \nabla \cdot (\nu \nabla u)) + (\tau \mathbf{a} \cdot \nabla w, \sigma u) + \\ & -(\tau \nabla \cdot (\nu \nabla w), \mathbf{a} \cdot \nabla u) + (\tau \nabla \cdot (\nu \nabla w), \nabla \cdot (\nu \nabla u)) - (\tau \nabla \cdot (\nu \nabla w), \sigma u) + \\ & + (\tau \sigma w, \mathbf{a} \cdot \nabla u) - (\tau \sigma w, \nabla \cdot (\nu \nabla u)) + (\tau \sigma w, \sigma u) \end{aligned} \quad (5)$$

The source term contribution becomes:

$$\sum_e (\tau \mathbf{a} \cdot \nabla w, s) - (\tau \nabla \cdot (\nu \nabla w), s) + (\tau \sigma w, s) \quad (6)$$

Finally the code implementation gets the following form:

```

% GLS
Ke = Ke + (nu*(Nx'*Nx+Ny'*Ny) + N_ig'*(ax*Nx+ay*Ny) + N_ig'*sig*N_ig+ ...
          tau*(ax*Nx+ay*Ny)'*((ax*Nx+ay*Ny) - nu*(Nxx+Nyy) + sig*N_ig)+...
          -tau*nu*(Nxx+Nyy)'*((ax*Nx+ay*Ny) - nu*(Nxx+Nyy) + sig*N_ig)+...
          tau*sig*N_ig'*((ax*Nx+ay*Ny) - nu*(Nxx+Nyy) + sig*N_ig))*dvolu;
aux = N_ig*Ke;
f_ig = SourceTerm(aux);
fe = fe + (N_ig + tau*(ax*Nx+ay*Ny) - tau*nu*(Nxx+Nyy) + tau*sig*N_ig)*f_ig*dvolu;

```

3 Results

In this section, three exercises problems will be solved and the stabilization methods will be compared. Those three are particular cases of the skew to mesh (30°) advection velocity \mathbf{a} in a square domain ([0,1]x[0,1]).

3.1 Problem I : Convection - Diffusion case

For this problem the velocity norm is $\|\mathbf{a}\| = 1$, $\nu = 10^{-4}$, $\sigma = 0$ and $s = 0$. Discontinuous Dirichlet B.C. are imposed at inlet ($u = 1 \forall y \in \Gamma_{in} | y > 0.2$ and $u = 0$ elsewhere in Γ_{in}). Homogeneous Neumann (Natural) boundary conditions and Homogeneous Dirichlet (essential) at outlet boundary are tested. Figure (1), shows the results for the case with homogeneous Neumann B.C prescribed at outlet and a 20x20 bilinear elements mesh.

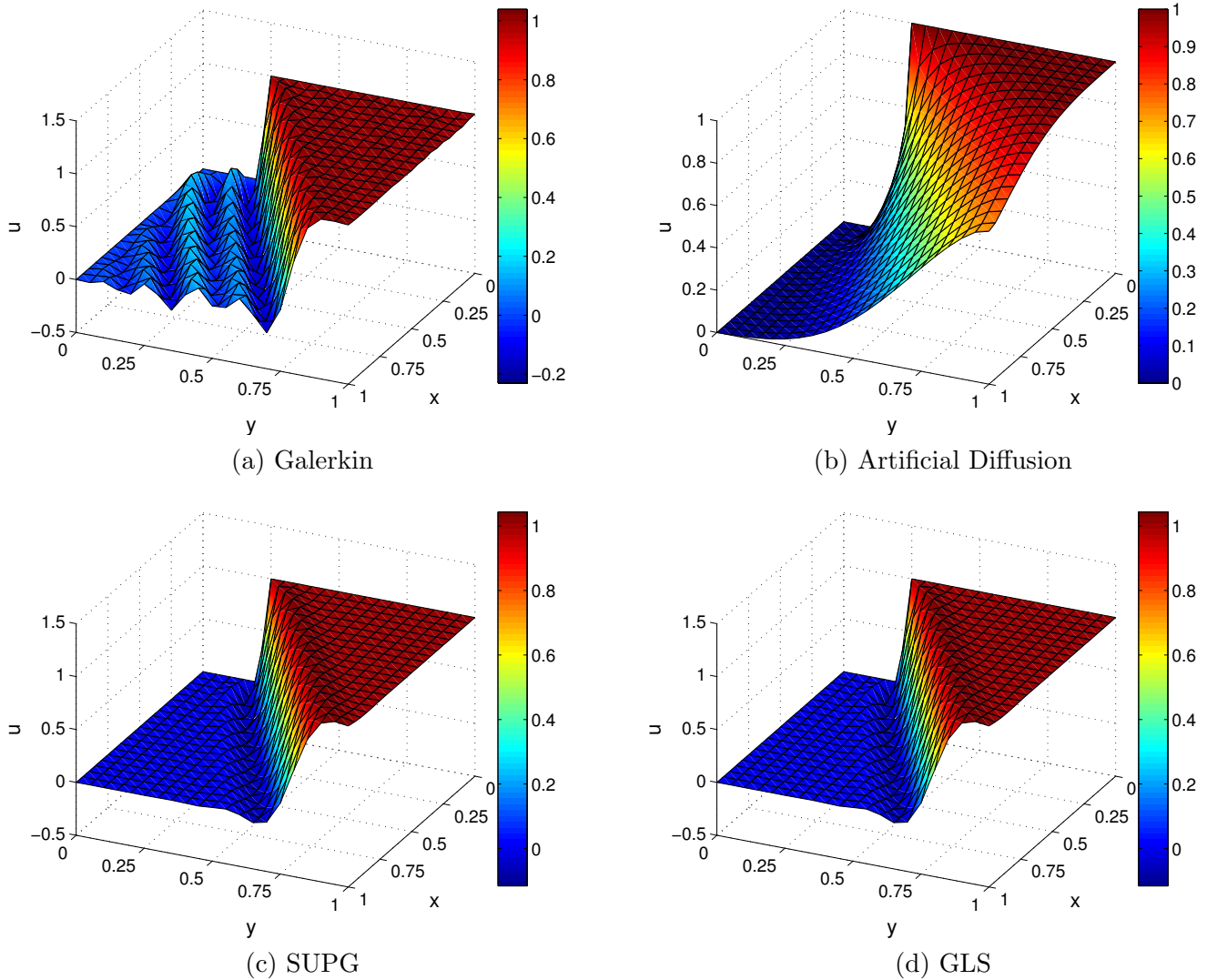


Figure 1: Convection-Diffusion case: Homogeneous Neumann (Natural) boundary conditions at outlet boundary

In this case its clear the over diffusive response of the Artificial Diffusion in cross-wind direction, Figure (1) (b), stabilization method when compared with SUPG and GLS. Further, SUPG and GLS presents, Figure (1) (c) and (d), almost same behavior reducing oscillations in the Galerkin solution.

Figure (2), show the results for the case with homogeneous Neumann B.C prescribed at outlet and a 20x20 bilinear elements mesh. This case is characterized by a thin boundary-layer at outlet

Again, in this case its clear the over diffusive response of the Artificial Diffusion, Figure (2) (b), stabilization method when compared with SUPG and GLS. Further, SUPG and GLS presents, Figure (2) (c) and (d), almost same behavior reducing oscillations in the Galerkin solution, which in this case are completely spurious.

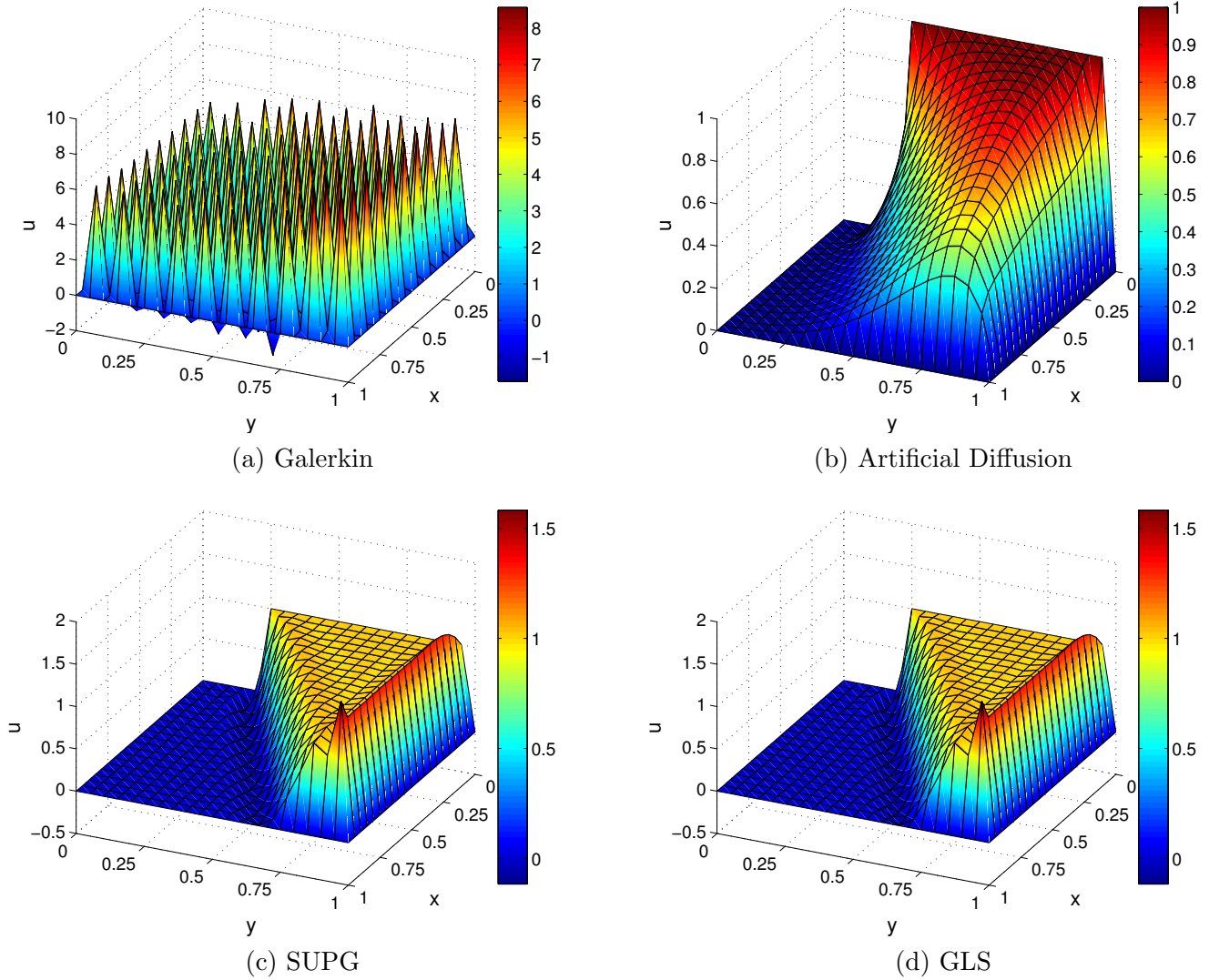
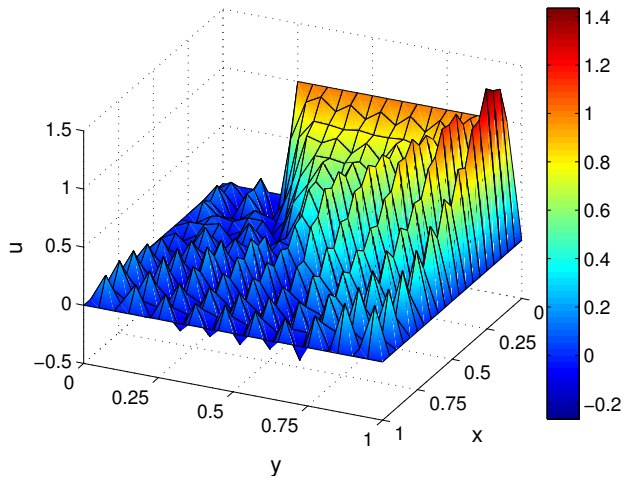


Figure 2: Convection-Diffusion case: Homogeneous Dirichlet (essential) boundary conditions at outlet boundary

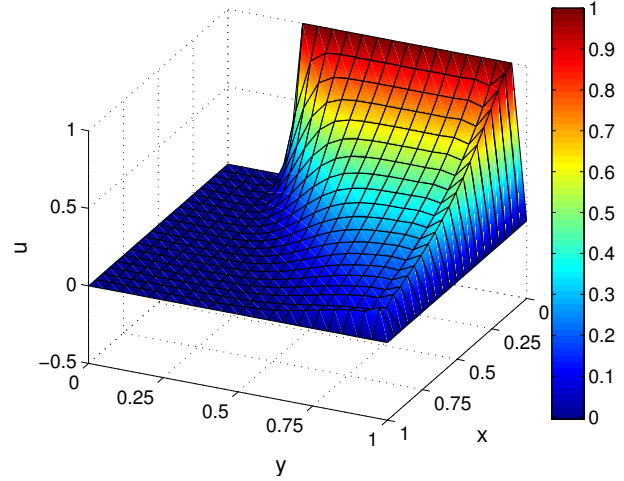
3.2 Problem II : Convection - Reaction dominated case

For this problem the velocity norm is $\| \mathbf{a} \| = 0.5$, $\nu = 10^{-4}$ and $\sigma = 1$. Discontinuous Dirichlet B.C. are imposed at inlet ($u = 1 \forall y \in \Gamma_{in} | y > 0.2$ and $u = 0$ elsewhere in Γ_{in}). Homogeneous Dirichlet (essential) boundary condition at outlet boundary is prescribed. Figure (3), show the results for a 20x20 bilinear elements mesh.

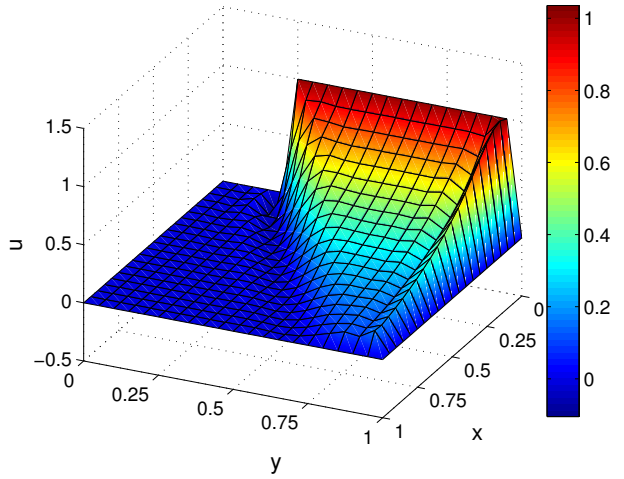
In this case the Artificial Diffusion adds more in cross-wind diffusion as previously, however the effect is not so noticeable as reaction is present. Further, SUPG and GLS presents, Figure (1) (c) and (d), almost same behavior reducing oscillations in the Galerkin solution.



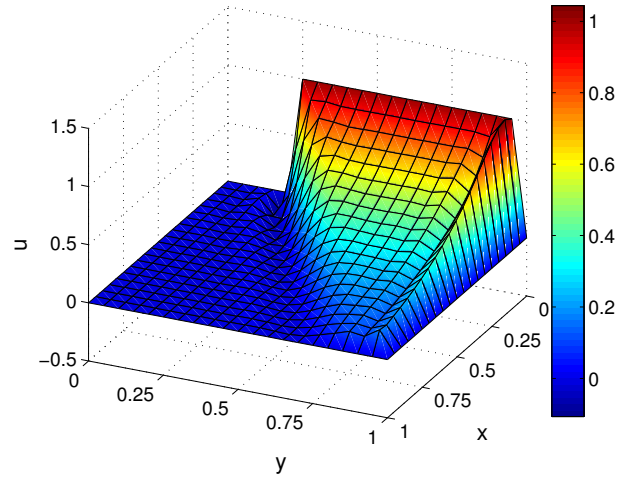
(a) Galerkin



(b) Artificial Diffusion



(c) SUPG



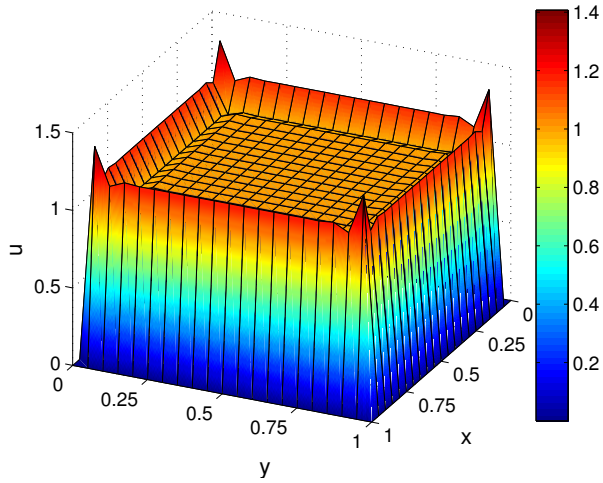
(d) GLS

Figure 3: Convection-Reaction dominated case

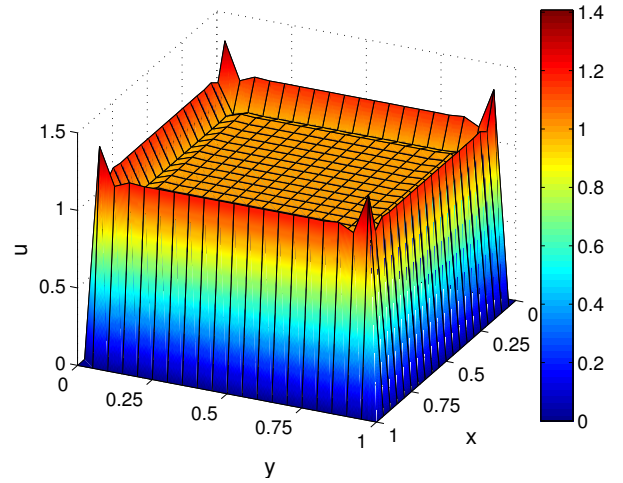
3.3 Problem III: Reaction dominated case

For this problem the velocity norm is $\| \mathbf{a} \| = 10^{-3}$, $\nu = 10^{-4}$, $\sigma = 1$ and $s = 1$ (uniform source term). Homogeneous Dirichlet boundary condition at both inlet and outlet boundaries are prescribed. Figure (4), show the results for a 20x20 bilinear elements mesh.

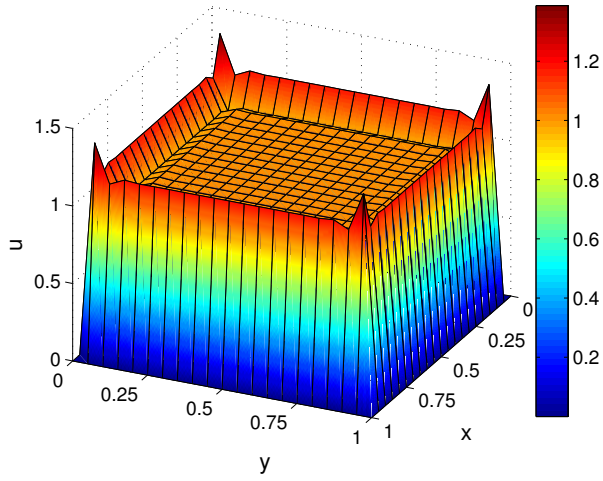
In this case all methods have similar behavior as a low convective situation is present and stabilization has lower effects due to higher Pe number.



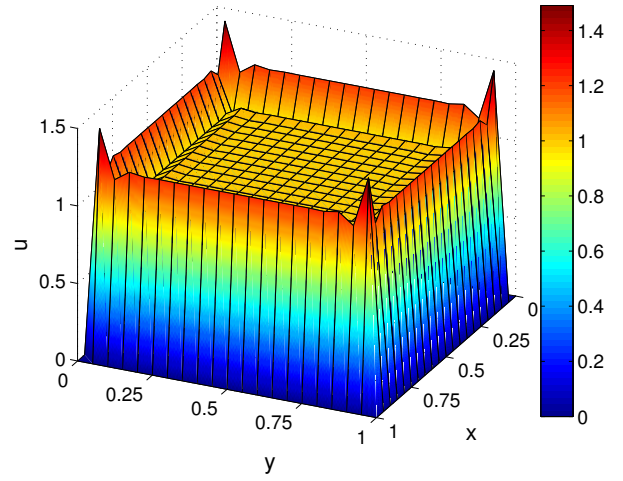
(a) Galerkin



(b) Artificial Diffusion



(c) SUPG



(d) GLS

Figure 4: Reaction dominated case