

LEAST SQUARES FINITE ELEMENT METHOD IN VELOCITY-PRESSURE-VORTICITY FORMULATION THE APPLICATION OF LARGE EDDY SIMULATION METHODOLOGY

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Abstract. *In this work, simulations of incompressible fluid flows have been done by a Least-Squares Finite Element Method (LSFEM) using velocity-pressure-vorticity formulation, here called $u-p-\omega$ formulation. This formulation is used because the resulting equations are partial differential equations of first order, which is convenient for implementation by LSFEM. The main purposes of this work are the numerical computation fluid flows by LSFEM through the application of large eddy simulation (LES) methodology. The Navier-Stokes equations in $u-p-\omega$ formulation are filtered and the eddy viscosity of Smagorinsky is used for modeling the sub-grid-scale variables. The backward facing-step flow has been solved to study the influence of the constant of Smagorinsky on the velocity profile for different Reynolds numbers. The results are presented and compared with available results from the literature.*

Keywords: Navier-Stokes equations, large eddy simulation, least-squares finite element, fluid flows.

1 INTRODUCTION

The finite element method (FEM) is one of the most used techniques for numerical solution of partial differential equations in engineering and applied sciences. The mathematical foundation of the finite element method can be based on the weight residual method (WRM), Finlayson, (1972), which originate different formulations according to the weight functions used. The main versions of the FEM are the Bubnov-Galerkin, Petrov-Galerkin, Collocation, Sub-domain and Least-Squares formulations. Another classification underlining the variational principle considers three major groups: the Rayleigh-Ritz method, The Galerkin Method and the Least-squares method. For convection dominated problems the Galerkin-based methods present often spurious oscillation of the solutions (Jiang, 1998). In recent works, Romão et al. (2003) and Romão (2004) applied different versions of the finite element method for convection-diffusion problems. Several authors have investigated the LSFEM for solution of incompressible and compressible fluid flows. Jiang (1998) presented a list of such works. Winterscheidt & Surana (1994) have applied p-versions of least-squares finite element method for fluid flows. The least squares have also been used for stabilization of the Galerkin finite element method. Jansen (1999) presented a LSFEM for computing turbulent flows in unstructured-grids. Some previous works have been presented: Pereira et al. (2004), Pereira and Campos_Silva (2005), Pereira et al. (2006a, b). Pereira (2005) has presented the u - p - ω formulation employed in this work. In that work some questions were not satisfactory answered. One of them was the influence of the constant of Smagorinsky in the LES methodology with the present formulation. In Pereira et al. (2006a, b) was tried to continue that investigation, but no high Reynolds number flow was still simulated for the present geometry. This work is a continuation of the previous works. Although, turbulence is a 3D phenomenon, in this work, only 2D simulations have been considered to understand the behavior of the LSFEM in the proposed formulations and due to the computational capacity available.

Jiang (1998) enumerated several features of the LSFEM, among them: universality, efficiency, robustness, optimality, concurrent simulation of multiple physics and general-purpose coding. Jiang also claimed that no upwind technique is necessary for numerical calculation of convection dominated problems, because the resulting matrix systems of equations from the LSFEM application are always symmetrical and positive-definite.

In this work, the backward-facing step flow has been solved with quadratic quadrilateral elements for investigation of different values of the constant of Smagorinsky. The results are compared with results from other authors. Beyond of this introduction, the paper covers some aspects of formulation of the proposed model, presents some results, discussions, conclusions and references.

2- NOMENCLATURE

k = turbulent kinetic energy

L = length of reference

p = pressure

$P = \frac{P - P_o}{\rho u_0^2}$ = dimensionless pressure

Re = Reynolds number

t = Time

u = component of dimensional velocity in the x_i - axis direction

u_i = component of velocity in the x_i - axis direction

u_0 = reference velocity

$U = u/u_o$ - dimensionless component of velocity in the X -axis direction

U_i = dimensionless component of velocity in the X_i -axis direction

v = component of dimensional velocity in the y -axis direction

$X = x/L$ = dimensionless X coordinate

x_i = i^{th} - axis in Cartesian coordinates

$X_i = x_i/L$ = i^{th} dimensionless coordinate

$Y = y/L$ = dimensionless Y coordinate

Greek Symbols

α = index that indicates local node number inside an element

δ_{ij} = Krönecker delta

θ = time discretization parameter

μ = dynamic viscosity

μ_t = dynamic eddy viscosity

ρ = density

ϕ = any scalar variable

ψ = stream function

ω_j = vorticity around the j-axis

$\varepsilon_{ijk} = 1$; if $ijk = 123, 231, 312$

$\varepsilon_{ijk} = -1$; if $ijk = 132, 213, 321$

$\varepsilon_{ijk} = 0$ for any two equal indices

Superscripts

n = variable evaluated at time t

$n+1$ = variable evaluated at time $t + \Delta t$

Subscripts

i = direction of the axis in the system of coordinates or component

j = direction of the axis in the system of coordinates or component

k = direction of the axis in the system of coordinates or component

3 – FORMULATION

3.1 - Governing Equations

The Navier-Stokes equations for incompressible transient fluid flows in vector notation can be written as follow:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p + \mu \nabla^2 \mathbf{u} = \mathbf{f} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

where ρ is the fluid density, \mathbf{u} is the velocity vector with components u_i , p is the pressure, μ is the dynamic viscosity and \mathbf{f} is the body forces vector with components f_i .

The Equation (1) is a second order partial differential equation and this is not the most appropriated form for solution by LSFEM. The LSFEM generally is applied for first order differential equations. However, second order partial differential can be transformed in first order system by using auxiliary variables. This is another advantage of the least-squares method: the direct calculation of secondary variables that have physical interpretation such as heat and mass fluxes, stresses and vorticity. According to Brodkey (1967), using vectorial identities: $\mathbf{u} \cdot \nabla \mathbf{u} = \nabla(\mathbf{u} \cdot \mathbf{u})/2 - \mathbf{u} \times \nabla \times \mathbf{u}$ and $\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u})$, the Navier-Stokes can be rewritten, now, in tensorial notation as

$$\rho \left(\frac{\partial u_i}{\partial t} - \varepsilon_{ijk} u_j \omega_k \right) + \frac{\partial (p + u_i^2 / 2)}{\partial x_i} + \varepsilon_{ijk} \mu \frac{\partial \omega_k}{\partial x_j} = f_i; \quad (3)$$

$$\frac{\partial u_i}{\partial x_i} = 0; \quad (4)$$

$$\omega_i = \varepsilon_{ijk} \frac{\partial u_k}{\partial x_j} . \quad (5)$$

For application of the large-eddy simulation methodology, the equations must be filtered for separation of the large scales from the sub-grid scales. So, the large scales are simulated by solution of the equations for the filtered variables after modeling the sub-grid scales terms that come from the filter process. Large-eddy simulation has been studied by a several researchers. Some few references are Moin & Kim (1982), Germano et al. (1991), Silveira-Neto (2002, 2003), Tejada-Martinez (2002). Chidambaram (1998) presented different filter functions for LES. The filtered Equations (3)–(5) are of the form

$$\begin{aligned} \rho \left(\frac{\partial \bar{u}_i}{\partial t} - \varepsilon_{ijk} \bar{u}_j \bar{\omega}_k + \frac{1}{2} \frac{\partial \bar{u}_i^2}{\partial x_i} \right) + \frac{\partial [\bar{p} + \rho(\bar{u}_i^2 - \bar{u}_i^2) / 2]}{\partial x_i} + \\ + \varepsilon_{ijk} \mu \frac{\partial \bar{\omega}_k}{\partial x_j} - \varepsilon_{ijk} \rho (\overline{u_j \omega_k} - \bar{u}_j \bar{\omega}_k) = \bar{f}_i \end{aligned} \quad (6)$$

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 ; \quad (7)$$

$$\bar{\omega}_i = \varepsilon_{ijk} \frac{\partial \bar{u}_k}{\partial x_j} . \quad (8)$$

The differences between Eq. (3) and Eq. (6) are the additional term to the pressure and in the fourth term of left hand side of Eq. (6) that originated from the convection term of the Navier-Stokes equations. These terms correspond to the turbulent kinetic energy and the vorticity of the sub-grid scales respectively. The purpose of this work is the modeling of the fourth term, by analogy with the modeling of the sub-grid scale stresses in the conventional formulation of the Navier-Stokes equations. So, it is defined the sub-grid scale effects and the turbulent pressure as

$$\overline{u_j \omega_k} - \bar{u}_j \bar{\omega}_k = -\mu_t \frac{\partial \bar{\omega}_k}{\partial x_j} ; \quad p_t = \bar{p} + \rho(\bar{u}_i^2 - \bar{u}_i^2) / 2 . \quad (9)$$

Now, after modeling of the sub-grid scale effects, the dimensionless form of the Eqs. (6)-(8) is as follow, Pereira (2005):

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial X_j} + \frac{\partial P_t}{\partial X_i} + \varepsilon_{ijk} \left(\frac{1}{\text{Re}} + \nu_t \right) \frac{\partial \Omega_k}{\partial X_j} = S_i ; \quad (10)$$

$$\frac{\partial U_i}{\partial X_i} = 0 ; \quad (11)$$

$$\Omega_i = \varepsilon_{ijk} \frac{\partial U_k}{\partial X_j} . \quad (12)$$

The dimensionless variables in Eqs. (10)-(12) are defined in function of the characteristic parameters of length L and velocity u_0 as

$$X_i = \frac{x_i}{L} ; \quad U_i = \frac{\bar{u}_i}{u_0} ; \quad P_t = \frac{p_t - p_0}{\rho u_0^2} ; \quad t = \frac{t^*}{L/u_0} ; \quad \nu_t = \frac{\nu_t^*}{u_0 L} = \left(C_s \frac{\Delta}{L} \right)^2 (2 \bar{S}_{kl} \bar{S}_{kl})^{1/2} ; \quad \Omega_i = \frac{\bar{\omega}_i L}{u_0} ; \quad \text{Re} = \frac{\rho u_0 L}{\mu} .$$

The eddy viscosity is calculated according to the Smagorinsky model in the form

$$v_t^* = (C_s \Delta)^2 (2\bar{s}_{kl}\bar{s}_{kl})^{1/2}; \bar{s}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (13)$$

where C_s is the constant of Smagorinsky and Δ is the filter width defined as: $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$ for 3D or $\Delta = (\Delta x \Delta y)^{1/2}$ for 2D geometry.

The first order system (10)-(12) for 2D problems, after discretizing the transient term can be written in a compact form as

$$L\Phi^{n+1} = f^n; \quad (14)$$

where $\Phi = [U, V, P, \Omega]^T$ is the vector of unknown variables, $f = [S_u, S_v, 0, 0]^T$ is the vector of independent terms and now L is a matrix differential operator defined as

$$L = \begin{pmatrix} \frac{1}{\Delta\tau} + \theta \left(U \frac{\partial(\cdot)}{\partial X} + V \frac{\partial(\cdot)}{\partial Y} \right) & 0 & \frac{\partial(\cdot)}{\partial X} & v_e \frac{\partial(\cdot)}{\partial Y} \\ 0 & \frac{1}{\Delta\tau} + \theta \left(U \frac{\partial(\cdot)}{\partial x} + V \frac{\partial(\cdot)}{\partial y} \right) & \frac{\partial(\cdot)}{\partial Y} & -v_e \frac{\partial(\cdot)}{\partial X} \\ \frac{\partial(\cdot)}{\partial X} & \frac{\partial(\cdot)}{\partial Y} & 0 & 0 \\ -\frac{\partial(\cdot)}{\partial Y} & \frac{\partial(\cdot)}{\partial X} & 0 & 1 \end{pmatrix} \quad (15)$$

The source terms S_u and S_v are:

$$S_u = f_x + \frac{U^n}{\Delta t} - (1 - \theta) \left(U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} + \frac{\partial P}{\partial X} + \mu_e \frac{\partial \Omega}{\partial Y} \right)^n; \quad (16)$$

$$S_v = f_y + \frac{V^n}{\Delta t} - (1 - \theta) \left(U \frac{\partial V}{\partial X} + V \frac{\partial V}{\partial Y} + \frac{\partial P}{\partial Y} - \mu_e \frac{\partial \Omega}{\partial X} \right)^n. \quad (17)$$

and $0 \leq \theta \leq 1$ is a parameter of time discretization.

The variable Φ in finite element methods, for equal order interpolation of all degrees of freedom, can be interpolated inside an element in the form:

$$\Phi^e(X, Y, t) = \sum_{j=1}^{Ne} N_j(X, Y) \begin{Bmatrix} U \\ V \\ P \\ \Omega \end{Bmatrix}_j (t); \quad (18)$$

where N_j is the interpolation function associated to the node j of the element and Ne is the number of nodes. It has been pointed out that the LSFEM is not restricted by LBB (Ladyzhenskaya-Babuska-Brezzi) condition like the Galerkin-based method, Jiang (1998), Winterscheidt & Surana (1994).

3.2 - Least-Squares Finite Element Method

Substituting Eq. (18) in Eq. (14) a residual vector can be defined inside an element as

$$R = LN\Phi^{n+1} - f^n. \quad (19)$$

The application of LSFEM consists in the minimization of a functional defined as the integral of the squared residuals. If inside an element ones define a functional as $J_e(\Phi^{n+1}) = \int_{A_e} R^T \bullet R dA$, the functional, in the whole domain divided in $Nelem$ elements, can be calculated as follow

$$J(\Phi^{n+1}) = \sum_{e=1}^{Nelem} \int_{A_e} R^T \bullet R dA. \quad (20)$$

The minimization of the functional requires that $\delta J(\Phi^{n+1}) = 0$, which results in the following matrix system:

$$K\Phi = F \quad (21)$$

Now, in Eq. (21), Φ is the global vector of nodal values. The global matrix K is assembled from the element matrices,

$$K_e = \int_{A_e} \langle LN_1, LN_2, \dots, LN_{Ne} \rangle^T \langle LN_1, LN_2, \dots, LN_{Ne} \rangle dA \quad (22)$$

where A_e is the area of the finite element, T denotes the transpose and the global vector F is assembled with the contribution of the element vectors

$$F_e = \int_{A_e} \langle LN_1, LN_2, \dots, LN_{Ne} \rangle^T f dA ; \quad (23)$$

in which

$$LN_j = \begin{pmatrix} \frac{N_j}{\Delta\tau} + \theta \left(U \frac{\partial N_j}{\partial X} + V \frac{\partial N_j}{\partial Y} \right) & 0 & \frac{\partial N_j}{\partial X} & \mu_e \frac{\partial N_j}{\partial Y} \\ 0 & \frac{N_j}{\Delta\tau} + \theta \left(U \frac{\partial N_j}{\partial x} + V \frac{\partial N_j}{\partial y} \right) & \frac{\partial N_j}{\partial Y} & -\mu_e \frac{\partial N_j}{\partial X} \\ \frac{\partial N_j}{\partial X} & \frac{\partial N_j}{\partial Y} & 0 & 0 \\ -\frac{\partial N_j}{\partial Y} & \frac{\partial N_j}{\partial X} & 0 & N_j \end{pmatrix} \quad (24)$$

3.3 - Backward-Facing Step Flow

In this section some results for backward-facing step flow are presented for Reynolds number in the range of 100 to 1000 and values of the constant of Smagorinsky of 0.1, 0.17 and 0.21. The geometry of the problem and dimensions of the channel are shown in Figure 1. The Figure 2 illustrates a mesh utilized composed by 1840 finite elements and 7541 nodes. The ratio of expansion in this case is of 1:2. At the entrance of the channel was imposed a parabolic velocity profile of the form: $u = 3u_0/2 \left[2(y-h)/r_w - (y-h)^2/r_w^2 \right]$, where h is the step height, r_w is the half spacing of the small channel and in this case $r_w = h/2$. At all other walls was imposed zero velocities and at exit of the channel was imposed null pressure. For the vorticity was not necessary to impose any boundary condition, Jiang (1998).

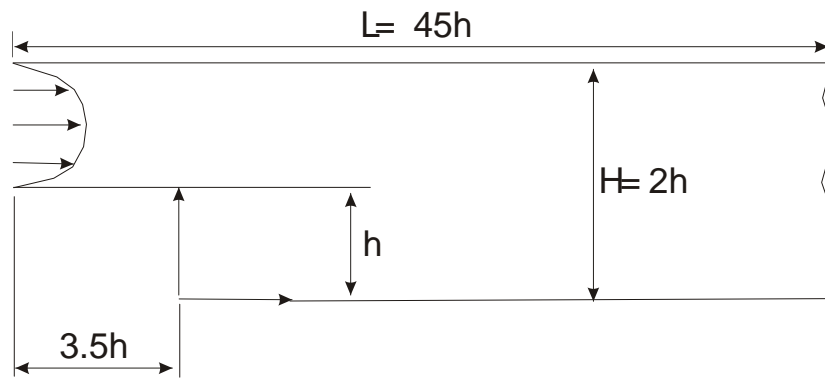


Figura 1. Non symmetric channel with a step.

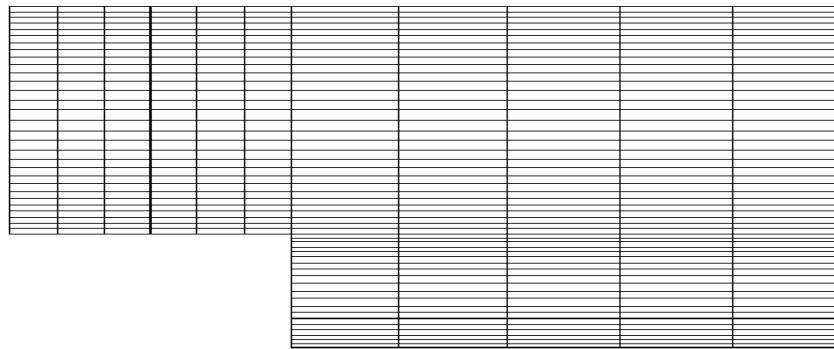


Figura 2. Mesh with 1840 finite elements and 7841 nodes.

The Reynolds numbers has been based on the step height, h . The computational code has been validated by Pereira (2005). Here, the main objective has been to analyze the influence of constant of Smagorinsky, in the simulation of the backward-facing step flow. The results presented below are for Reynolds numbers of 700 and 1000. Others low Reynolds numbers have been considered, in previous works, however, for lacking of spacing was not possible to present all results. The intent of this work is simulating high Reynolds number flows; however, until the present moment due to the computational resource available it was not possible to attain such objective. Figures 3 and 4 show velocity profiles at some positions along the channel, for different values of the constant of Smagorinsky. Differences between the velocities profiles appear only at some intermediate position along the channel. Figures 5 to 7 and 8 to 10 show the streamlines for Re equal to 700 and 1000 respectively for constant of Smagorinsky $C_s = 0.1, 0.17$ and 0.21 . The behavior of the flow has been simulated satisfactorily. The non-dimensional reattachment lengths are approximately, 10 and 15 times step height for $Re = 700$ and 1000 respectively. The reattachment length result from Barber & Fonty (2003) for a similar flow and a Reynolds number are of 300 is about 7 times step height. Barber & Fonty presented results until Re of 600. For the Reynolds number of 400 and 600 respectively, the reattachment length of 10 and 16 times step height were showed by Barber & Fonty. For this low Reynolds numbers, the use of the Smagorinsky constant seems to create an effect of a more high Reynolds number. Until now, only one case of $Re = 2000$ has been simulated with $C_s = 0.1$. The stream functions are presented in Figure 11. This last result, however, presents a strange behavior and shall be investigated in future works. The profiles of velocity of this case, not included by lacking of space, seem to have been qualitatively and correctly simulated.

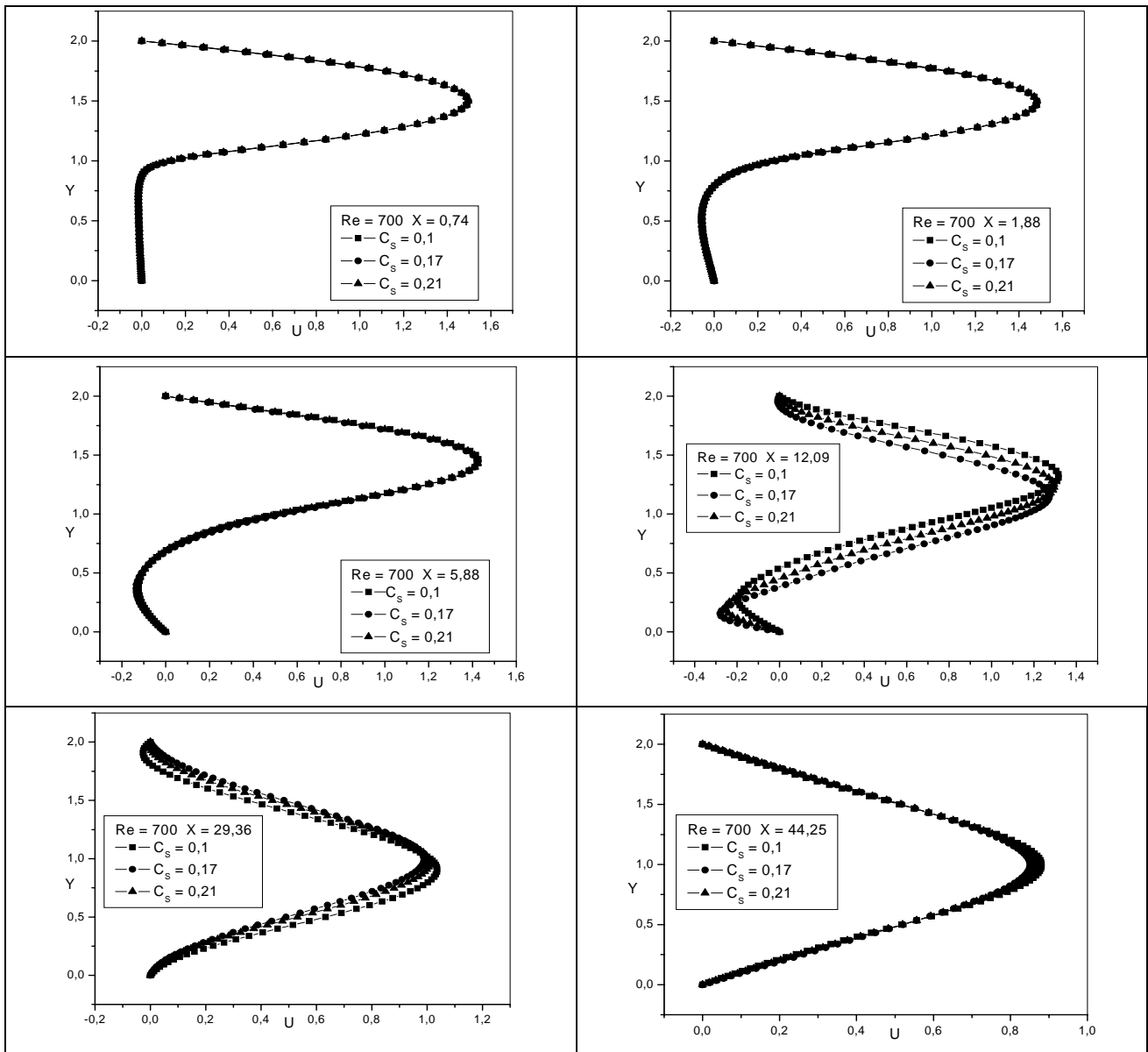


Figure 3. Profiles of velocity at some stations along the channel, for $Re = 700$.

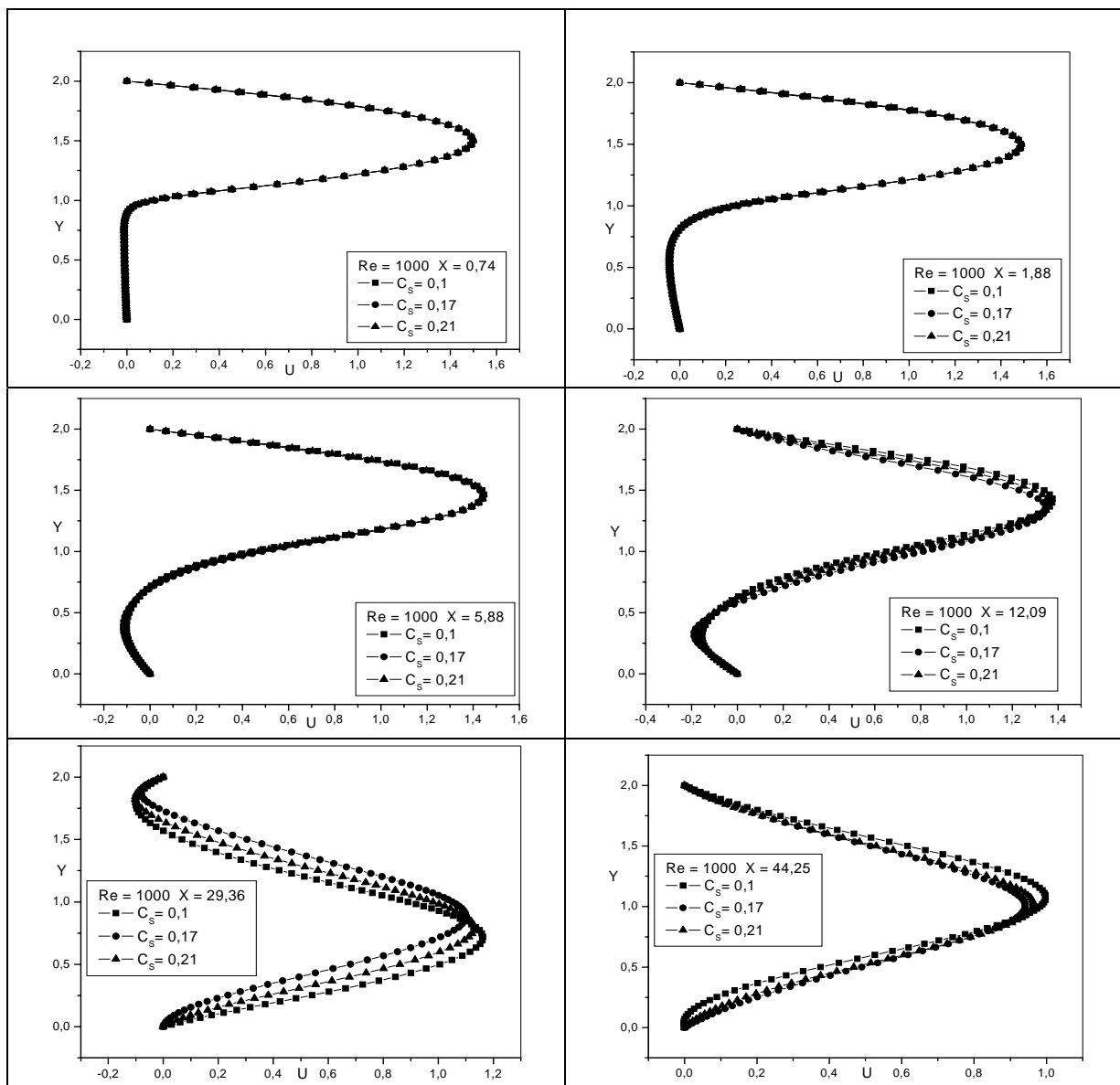


Figure 4. Profiles of velocity at some stations along the channel, for $Re = 1000$.

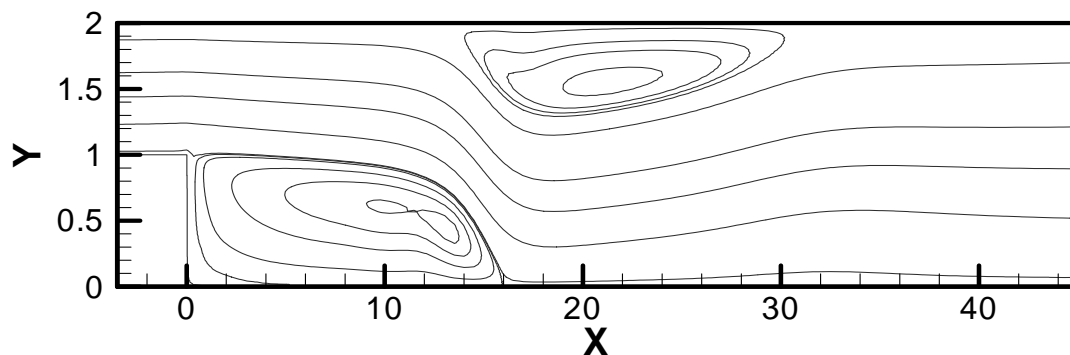


Figure 5. Streamlines for $Re = 700$ and $C_s = 0.1$.

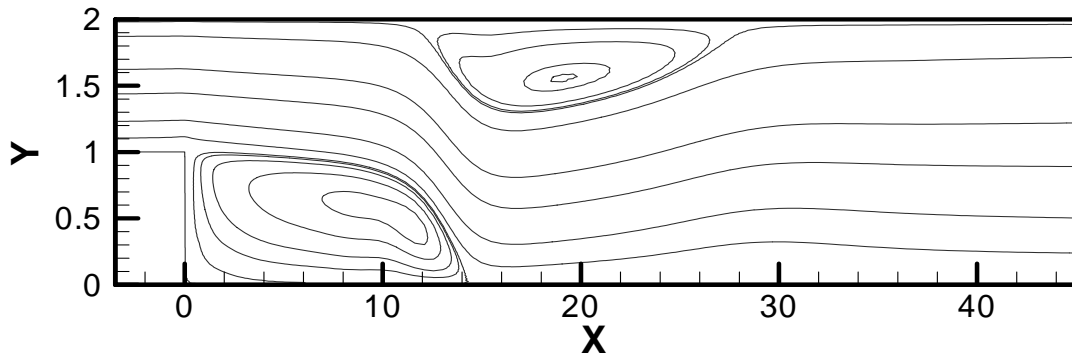


Figure 6. Streamlines for $Re = 700$ and $Cs = 0.17$

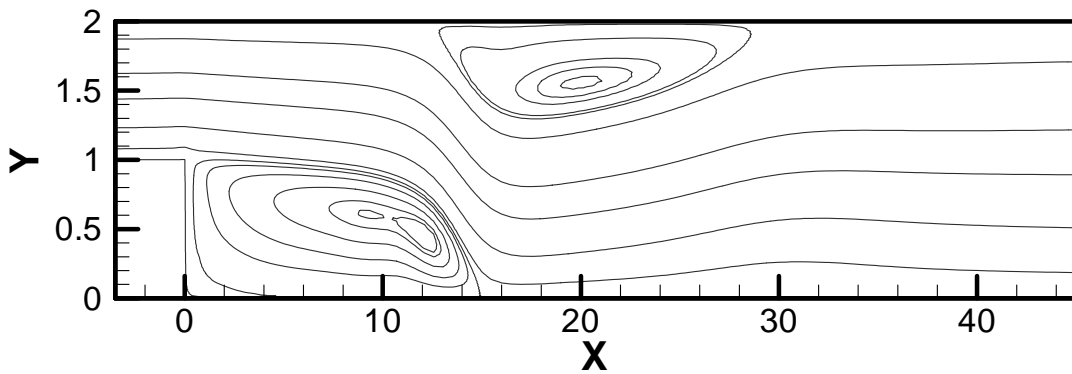


Figure 7. Streamlines for $Re = 700$ and $Cs = 0.21$

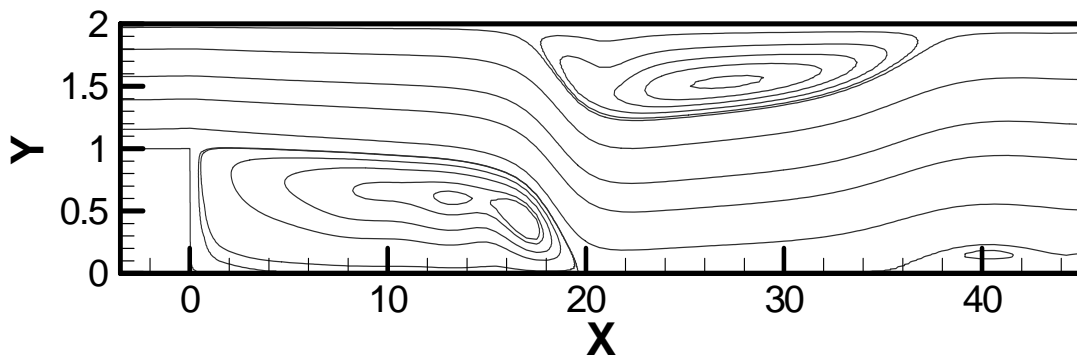


Figure 8. Streamlines for $Re = 1000$ and $Cs = 0.1$.

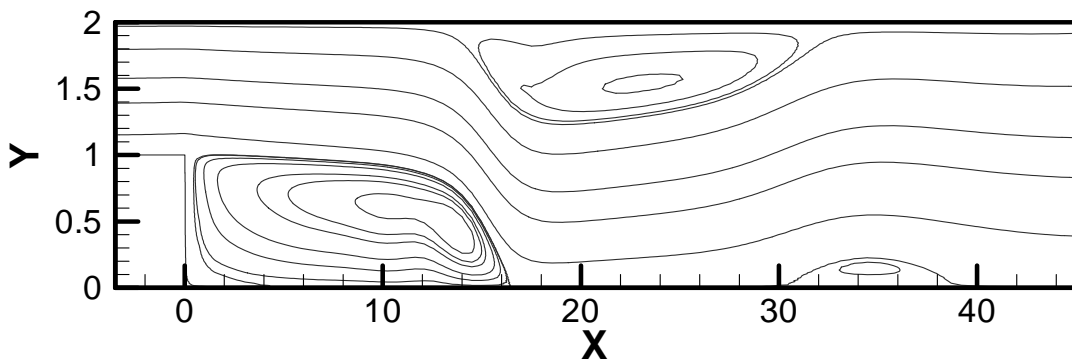


Figure 9. Streamlines for $Re = 1000$ and $Cs = 0.17$.

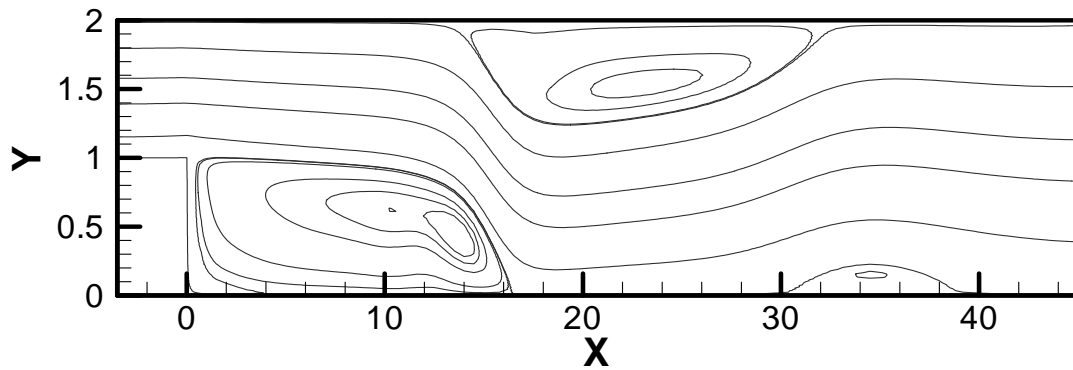


Figure 10. Streamlines for $Re = 1000$ and $Cs = 0.21$.

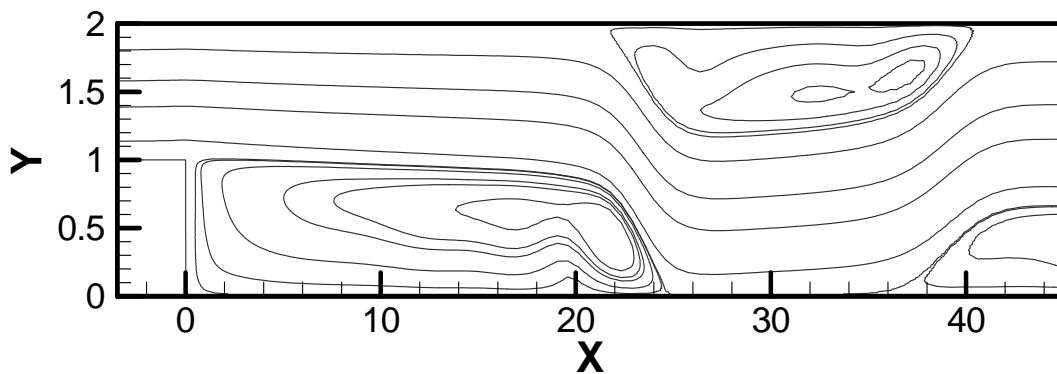


Figure 11. Streamlines for $Re = 2000$ and $Cs = 0.1$.

A comparison of Figures 5, 8 and 11 shows a crescent reattachment length with the increase of Reynolds number. However, was not possible to compare the results in this range of Reynolds with another results form the literature. The simulations have to be continued to investigate this behavior. Simulations by other numerical techniques present short reattachment length for high Reynolds number. Even this result is not true, it serves to indicate that the present numerical modeling has to be better investigated and calibrated for this kind of problem. More simulations are need in this case.

4 – CONCLUSIONS

A least-squares finite element method with eddy viscosity model of Smagorinsky has been applied in this work for simulation of Navier-Stokes equations, in $u-p-\omega$ formulation. The results were obtained for several low Reynolds numbers and $Cs = 0.1$; 0.17 and 0.21 . Since, the interest is to simulate high Reynolds flows, more investigation is still necessary for improvement of the model. Since turbulence is a three-dimensional phenomenon, cases of 3D geometry shall be treated in future works. In this work, was applied the frontal method, with storage in hard disk and only steady flows have been simulated in personal computers. Unsteady flows need to be also investigated in more details. For 3D and high Reynolds numbers flows the challenge still goes on for the present numerical method in this kind of problem. The solution method has to be changed to a method like conjugate gradient method for symmetrical matrices considering the sparsity of matrices for simulation of very large problems. So the solutions shall be faster than the solution by frontal method.

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