A COMPARATIVE CFD ANALYSIS: PENALTY METHOD (PM), PRESSURE POISSON EQUATION (PPE) AND THE COUPLED FORMULATION (PPE+PM)

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Abstract. *In incompressible CFD, the development of numerical algorithms to achieve mass conservation has been extensively studied by many authors. At this context, this work has focused on a comparative analysis of three numerical approaches. They consist in addressing the inconvenient imposed by velocity divergence free restriction based on distinct mathematical formulation of the incompressible flow problem: the penalty method (PM), the pressure Poisson equation (PPE) and the coupled formulation (PPE+PM). Whereas the PM and PPE are well known and widely spread out in many fields of applied fluid flow, the PPE+PM is an innovative approach obtained by combining the PM and the PPE in the same iterative algorithm. The performance of the three formulations in terms of CPU time and mass conservation error are compared considering two benchmarks problems, lid driven cavity flow and backward facing step flow. Additionally the effect of the mesh density on the solution is observed under different penalizations of the continuity constraint. The results indicate the PPE less attractive when the CPU time consumption imposes a restriction, on the other hand, the PM is faster but the quality of the solution strongly depends of the correct choice of penalty parameter. The coupled formulation has shown being less prone to present divergent behavior, as presented by PPE in the lid driven cavity problem, leading to the best balance between low CPU time and acceptable mass conservation error.*

Keywords: *Penalty Method, Incompressible, Mass Conservation, Mesh Locking.*

1. INTRODUCTION

Nowadays one of the most important issues in numerical analysis is the computational cost involved with a problem solution. This computational cost is dependent on three main factors which are: hardware, algorithm technology and programming, (Housting and Rice, 2000). Usually, numerical simulation of viscous incompressible flow is found to be a class of problems that has been limited due to the excessively high computational cost. In this cost is included not only the parcel related to time processing but also the amount relative to numerical code development. Much has already been accomplished in CFD development but there is always room for improvement. Taking advantage of the knowledge in numerical methods, small changes in the formulation of a problem or even a different representation of some aspect of it can have a huge effect on performance. Especially in incompressible flows, the relationship between pressure and velocity is not very clear, the pressure field plays a secondary role in the solution according to Tu et al. (2008), moreover, in the pressure-velocity formulations the "*direct enforcement of zero divergence is lost*", as stated by Nordstrom et al (2007). In the words of Sheng et al. (2011): *"The pressure has long been a main source of trouble for understanding and computing solutions to the equations of incompressible flow"*. The literature is vast regarding the mass conservation problem and the diversity of ways that pressure and velocity interact to ensure conservation of mass under the incompressibility assumption (Linke, 2009 and Bolton and Thatcher, 2005). Thus, this feature permits the possibility of addressing the problem from many distinct points of view (Kwak et al., 2011). Considering the range of available methods for incompressible flow and excluding those ones associated with non-primitive variable formulations, Shen (1997) has classified the methods in three categories according to how the incompressibility constraint is treated. Under such classification, the penalty method is included in a group together with pseudo-compressibility methods, among whose are the artificial compressibility method, the pressure stabilization method, and the projection method. These methods are very similar in their formulations; the difference among them resides on the way that incompressibility constraint is relaxed. The common aspect that characterizes the Penalty Method and the Pressure Poisson Equation is the strategy adopted to achieve the mass conservation. In the first, it is enforced by introducing a penalized velocity divergence into the incompressible flow equation, acting similarly as a Lagrange multiplier. This will result in the reduction of the problem degrees of freedom, the pressure is no longer a variable. While in the PPE formulation, the pressure is present as a variable throughout a pseudo-transient schema which the pressure field evolves to achieve a solution with velocity divergence approximately null. Finally, the coupled formulation consists in aggregating both strategies to enforce mass balance, it means, via penalty parameter and via a pressure equation. Thus, the intent of this work is to compare three types of formulations that are used to obtain the solution of the Navier-Stokes equations for viscous incompressible flows: 1. Penalty method (PM), 2. Pressure Poisson equation (PPE), and 3. Coupled formulation (PM+PPE). The motivation is to show how a simple consideration into the mathematical formulation can improve the CFD performance without taking actions costly prohibitive.

2. MATHEMATICAL FORMULATION

This section presents the governing equations, the two-dimensional mathematical model, mass conservation and momentum equations for a laminar incompressible flow which are given by Eq. (1) and Eq. (2):

$$\vec{\nabla}\cdot\left(\rho\,\vec{V}\right)=0 \tag{1}$$

$$\rho\left(\frac{\partial\vec{V}}{\partial t}+\vec{V}\cdot\vec{\nabla}\vec{V}\right)=\rho\vec{g}-\vec{\nabla}P+\vec{\nabla}\cdot\left[\,\mu(\vec{\nabla}\vec{V})+\mu(\vec{\nabla}\vec{V})^{\mathrm{T}}\right] \tag{2}$$

Although the approach presented herein covers steady-state problems, the transient term is preserved in the Eq. (2) to derive the PPE formulation. In the PM, the transient term is removed and the formulation is derived directly from the momentum equation with the penalty term introduction.

Table 1 gives the definition of symbols and mathematical nomenclature used along this work.

Table 1. Nomenclature.

Symbol	Nomenclature	Symbol	Nomenclature
A	Area	Re	Reynolds number
E	Mass conservation error	s	Step size
$\vec{g}$	Gravity acceleration vector	$(\ )^T$	Transpose tensor
h	Inlet size	u, v	Velocity component, x and y coordinates
H	Outlet size	$\vec{V}$	Velocity vector
L	Square cavity length	x, y	Cartesian coordinate system
P	Pressure	X1	Reattachment length
Δt	Pseudo time interval	$\vec{\vec{\delta}}$	Unitary tensor
λ	Penalty parameter	$\vec{\nabla}(\ )$	Gradient operator
μ	Dynamic viscosity of fluid	$\vec{\nabla}\cdot(\ )$	Divergence operator
ρ	Density of fluid	∇^2	Laplacian operator
Subscript		**Subscript**	
D	Domain	m	Average
i	inlet	calc	Calculated
o	outlet	ref	Benchmark reference
Superscript			
n	Time level		

2.1. Penalty Method (PM)

In 1968, Temam (1968) presented a theoretical analysis to demonstrate the convergence of velocity and pressure solutions concerning to the Navier-Stokes solution in finite differences. In that study, the existence of an approximation associating the pressure multiplied by a negative constant with velocity divergence for incompressible flow was verified. Later the constant received the name: penalty parameter. According to Kardestuncer et al. (1988) the popularity of penalty finite element method grew in the seventies. The first to use the penalty method in conjunction with finite method was Babuska (1988), but applications in incompressible viscous flow took place with Zienkiewicz (1975). The penalty method applicability has been extensively spread out in a lot of applied CFD fields during the last years. Examples include: rotating machinery analysis by Pelletier et al. (1991), forming processes by Reddy and Reddy (1992), the Non-Newtonian fluid flow by Huang et al. (1999), analysis of fluid-structure interaction by Kerh et al. (1998), wind engineering by Choi and Yu (1999), multiphase flow with solid interaction by Vincent et al. (2007).

Considering the alternatives to deal with the incompressibility constraint, the simplest approach is the penalty method. The method consists in replacing the pressure by the relation given by Eq. (3):

$$P = -\lambda \nabla . \vec{V} \tag{3}$$

For the case when the penalty parameter is assumed as constant, the momentum equation derived for the penalty method results in Eq. (4):

$$\rho \left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \vec{\nabla} \vec{V} \right) = \rho \vec{g} \;\; + \lambda . \vec{\nabla} \cdot \left[\; (\vec{\nabla} \cdot \vec{V}) \; \vec{\vec{\delta}} \right] + \vec{\nabla} \cdot \left[\; \mu (\vec{\nabla} \vec{V}) + \mu (\vec{\nabla} \vec{V})^{\mathrm{T}} \right] \tag{4}$$

Theoretically, as the penalty parameter tends to infinity the solution of Eq. (4) must attend better the constraint. But in fact, the need for a relatively high value to the penalty parameter to satisfy the mass balance properly results in the "meshing locking" problem (Heinrich and Pepper, 1999). As indicated in Shahbazi (2005) this method requires the proper choice of a penalty parameter that is dependent on the mesh and interpolation order. The penalty parameter should be relatively small, to prevent degradation of the iterative procedure performance and at the same time, large enough to prevent the solution to became unstable.

2.2. Pressure Poisson Equation Formulation (PPE)

The pressure Poisson equation is the most common strategy found in incompressible flow problems, some examples include the works of Liu (2009), Hirsh (2007) and Aubry et al. (2008). The application of PPE to computational fluid dynamics can be obtained considering two forms, classified as consistent and inconsistent by Gresho and Sani (1999). The first form, used in finite element by Rice and Spike (1985) and in finite volume method by Patankar (1980), consists of taking the momentum conservation equation in the discrete form to be rearranged with the discrete mass conservation equation, while the order of pressure and velocity field interpolation are different. In the formulation contained herein, the discretization used in the momentum conservation equation and pressure Poisson equation are realized independently with equal order of interpolation for pressure and velocity field and the divergence operator is applied to the conservative form of the momentum conservation equation, then the resulting expression is given by Eq. (5):

$$\nabla^2 P + \vec{\nabla} \cdot \left\{ - \rho \vec{g} - \vec{\nabla} \cdot \left[\mu \, (\vec{\nabla} \vec{V}) + \mu \, (\vec{\nabla} \vec{V})^{\mathrm{T}} \right] + \vec{\nabla} (\vec{V} \vec{V}) \right\} = - \frac{\partial \, [\, \vec{\nabla} \cdot (\vec{V}) \,]}{\partial t} \tag{5}$$

Although the right hand side of Eq. (5) is null in the exact solution, the temporal term has been maintained because the iterative procedure considers the final solution as a result of a pseudo-transient. During this procedure the algorithm must seek for a velocity field that satisfies the mass balance. Thus the discretization of the right hand side of Eq. (5) is performed with Euler scheme, resulting in Eq. (6):

$$\nabla^2 P^{n+1} + \vec{\nabla} \cdot \left\{ - \rho \vec{g} - \vec{\nabla} \cdot \left[\mu \, (\vec{\nabla} \vec{V}) + \mu \, (\vec{\nabla} \vec{V})^{\mathrm{T}} \right] + \vec{\nabla} (\vec{V} \vec{V}) \right\}^n = \frac{\left[\vec{\nabla} \cdot \vec{V} \right]^n - \left[\vec{\nabla} \cdot \vec{V} \right]^{n+1}}{\Delta t} \tag{6}$$

The velocity field results at the n-iteration do not satisfy the mass balance, resulting that Eq. (7) is:

$$\left(\vec{\nabla} \cdot \vec{V} \right)^n \neq 0 \tag{7}$$

But the goal here is to build an algorithm that attempts to find a velocity field conserving mass. Therefore the results of the next iteration will try to reach a condition equivalent to the expression, given by Eq. (8):

$$\left(\vec{\nabla} \cdot \vec{V} \right)^{n+1} = 0 \tag{8}$$

Equation (6) can be interpreted as presented in Williams and Baker (1996), "the pressure assumes the dual role of both a Lagrangian multiplier instantaneously enforcing an isochoric constraint on the flow field (conservation of mass) and of a dynamical state variable acting as a part of the mechanical force balance law for the flow (conservation of linear momentum)".

2.3. Coupled formulation (PM+PPE)

The coupled formulation presented herein may be obtained as a combination of the above mentioned formulations. It must be pointed out that the degrees of freedom for these two configurations are in terms of pressure and velocity field, differently from PM in which the degrees of freedom are composed necessarily by velocity components. The present formulation does not employ reduced integration; pressure and velocity fields are integrated with the same order of interpolation. Equation (9) is obtained introducing the Laplacian pressure term into the Eq. (5) from PM.

$$\rho\left(\frac{\partial\vec{V}}{\partial t}+\vec{V}\cdot\vec{\nabla}\vec{V}\right)=\rho\vec{g}-\vec{\nabla}P+\lambda.\vec{\nabla}\cdot\left[(\vec{\nabla}\cdot\vec{V})\,\vec{\vec{\delta}}\right]+\vec{\nabla}\cdot\left[\mu(\vec{\nabla}\vec{V})+\mu(\vec{\nabla}\vec{V})^{\mathrm{T}}\right] \tag{9}$$

Equation (10) is obtained from PPE formulation introducing the penalty term, which results in:

$$\nabla^2P^{n+1}+\vec{\nabla}\cdot\left\{-\rho\vec{g}-\vec{\nabla}\cdot\left[\mu\,(\vec{\nabla}\vec{V})+\mu\,(\vec{\nabla}\vec{V})^{\mathrm{T}}-\lambda\,(\vec{\nabla}\cdot\vec{V})\,\vec{\vec{\delta}}\right]+\vec{\nabla}(\vec{V}\vec{V})\right\}^n=\frac{\left[\vec{\nabla}\cdot\vec{V}\right]^n}{\Delta t} \tag{10}$$

The Neumann boundary condition for pressure is considered in the two formulations employing the Pressure Poison Equation. It is necessary to specify a value to the pressure at one point in the boundary to determine an unique solution.

2.4. Error assessment

The mass conservation error assessment is based on calculating the integral of the absolute value of the velocity divergence over the area of the domain (AD), according to Eq. (11):

$$\mathrm{E_D}=\frac{1}{U_mA_D^2}\int_D\left|\vec{\nabla}\cdot(\vec{V})\right|dx\,\mathrm{dy} \tag{11}$$

Differently from the other benchmark problem considered here the backward-facing step flow is an open boundary problem, this requires the definition of an error criteria based on the balance between the inlet and the outlet of problem. Thus, the integral of the velocity at the inlet and the integral of velocity at the outlet of the domain have been evaluated and the error representing this difference is given by Eq. (12):

$$E_{io}=\frac{\left|\int u.dy\right|_i-\left|\int u.dy\right|_o}{\left|\int u.dy\right|_i}.100\% \tag{12}$$

It must be verified that smaller is the value of E_D, better is the mass conservation achieved, while for the E_{io} error, the ideal result should give zero, meaning that the mass flux entering in the domain is equal to mass flux leaving the domain. Additionally, to verify the quality of the solution the reattachment length of the primary recirculation zone in the backward-facing step has been evaluated according to Eq. (13):

$$E=\frac{\mathrm{X_1^{calc}}-\mathrm{X_1^{ref}}}{X_1^{ref}}.100\% \tag{13}$$

3. NUMERICAL RESULTS

The numerical solution of the governing partial differential equations and associated boundary conditions that are presented here has been obtained through the computational program PDEase2D (1996). This program utilizes the Galerkin finite element technique to transform the original partial differential equations system into the algebraic equations system. The code also performs the domain discretization using an adaptive unstructured mesh, comprised of second order triangular elements with six nodes per element.

3.1. Lid-driven cavity flow

The lid driven cavity flow has been used as a model problem for testing and evaluating numerical techniques. The fluid motion generated in this cavity is an example of closed streamline problem that is of theoretical importance because it belongs to the broader field of steady, separated flows. For this problem the numerical simulations were carried out to Reynolds number of 100, 400 and 1000. Figure (1) presents the square cavity with dimension L, in which the top wall moves with constant velocity from left to right. The coordinate system origin is at the left bottom corner of the cavity. The germane dimensionless parameter for lid-driven cavity flow problems is the Reynolds number, defined as: $Re = L.U.\rho/\mu$.

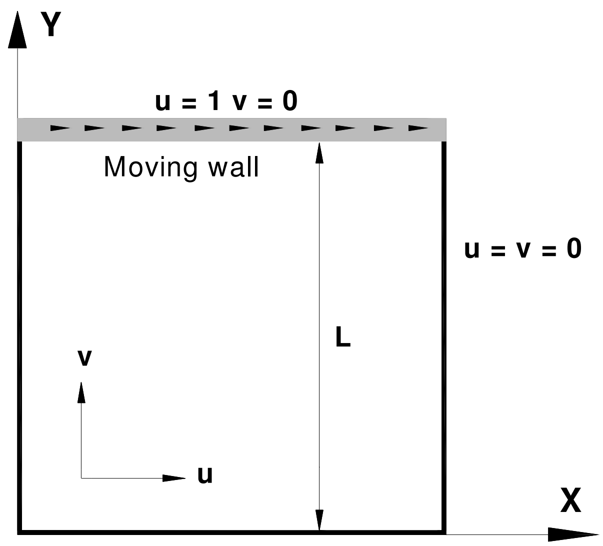


Figure 1. Square cavity schematic representation.

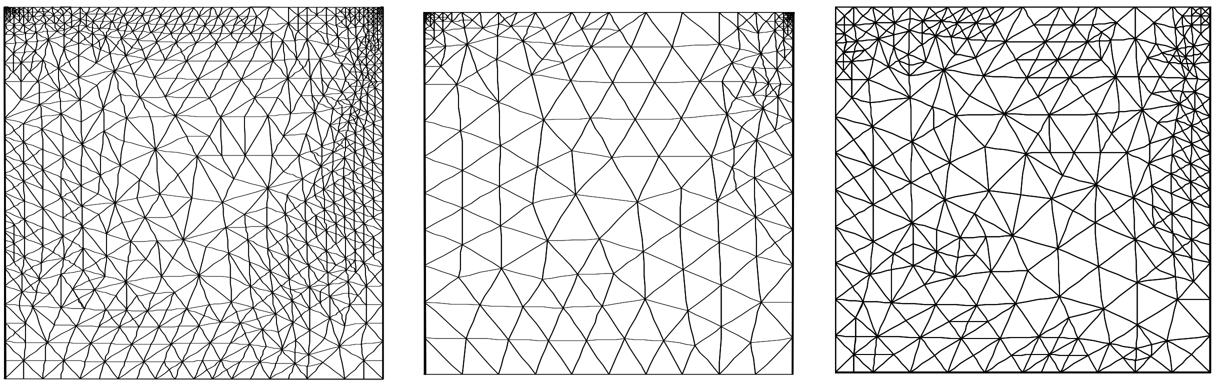
The penalty term that is common for PPE+PM and PM formulations is equal to 10^3 and the pseudo time interval (or "pressure weight") that is common parameter for PPE+PM and PPE formulations is equal to 0.1.

Table (2) presents the values of the mass conservation and the CPU time normalized by CPU time of the PM simulation for each Reynolds number. The table shows the differences of each formulation over the computational performance for different Reynolds numbers.

Table 2. Results for lid-driven cavity flow problem.

Re	Formulation	$1/\Delta t$	λ	E_D	Relative CPU time
100	PPE	10	-	5.5×10^{-4}	37
	PPE+PM	10	10^3	2.4×10^{-5}	7
	PM	-	10^3	4.3×10^{-5}	1
400	PPE	10	-	9.2×10^{-4}	65
	PPE+PM	10	10^3	7.7×10^{-6}	12
	PM	-	10^3	8.3×10^{-5}	1
1000	PPE	10	-	9.0×10^{-4}	74
	PPE+PM	10	10^3	8.4×10^{-6}	11
	PM	-	10^3	8.3×10^{-5}	1

The first evidence revealed by these results is the higher CPU time required by the PPE formulation compared with the PM and the PPE+PM formulations. Although, the PPE+PM formulation has presented less efficiency in terms of CPU time than the PM formulation, a better mass conservation is attained. Another observation that is noted, the higher is the Reynolds number the higher is the CPU time necessary to PPE formulation, while in the PPE+PM formulation the CPU time keeps practically unchanged. The resulting meshes established from the adaptive procedure were based on the evolution of the iterative process using the same error criteria for all variables in the three formulations. For Re=1000, the PPE formulation used 3481 nodes with a mass conservation error equal to 9.0×10^{-4}, the PPE+PM formulation used 1123 nodes with a mass conservation error equal to 8.4×10^{-6} and the PM formulation used 1244 nodes with a mass conservation error equal to 8.3×10^{-5}. It must be noted that the PPE+PM formulation, for the same numerical error criteria, has required the lowest amount of nodes and has furnished the best result in terms of mass conservation. Particularly for this problem the main difficulty to achieve mass conservation is verified in the regions around the top corners of the cavity. This characteristic is evidenced during the evolution of the mesh in the adaptive procedure and this effect for each formulation is shown in Figs. (2a), (2b) and (2c).



(a) PPE formulation (b) PPE+PM formulation (c) PM formulation

Figure 2. Typical patterns of mesh for lid driven cavity flow at Re =1000.

Traditionally, the PPE type formulations are characterized by its large requirements in CPU consumption as verified by the present work and corroborated by the work of Sheu and Chiu (2007) while the PM type formulation suffer from mesh locking problem.

3.2. Backward-facing step flow

The second example considered here is a backward facing step flow. Differently from the previous problem, this one presents an inlet and an outlet face in which is possible to evaluate another important aspects, global mass conservation error beyond the local error. For the purpose of the present work the simulations were carried out at Re = 100.

Figure (3) shows schematically the region of flow separation and the flow pattern. The boundary conditions used for this problem are: the top and bottom walls were taken as zero velocity; Poiseuille flow was prescribed at the inlet (with size, h); the outlet plane was treated using natural boundary conditions for both u and v velocity components; for the pressure, it was assumed constant pressure at the outlet and natural boundary condition at inlet for both components. The definition of the Reynolds number for this problem is given by Re =2.ρ.h.U_m /μ..

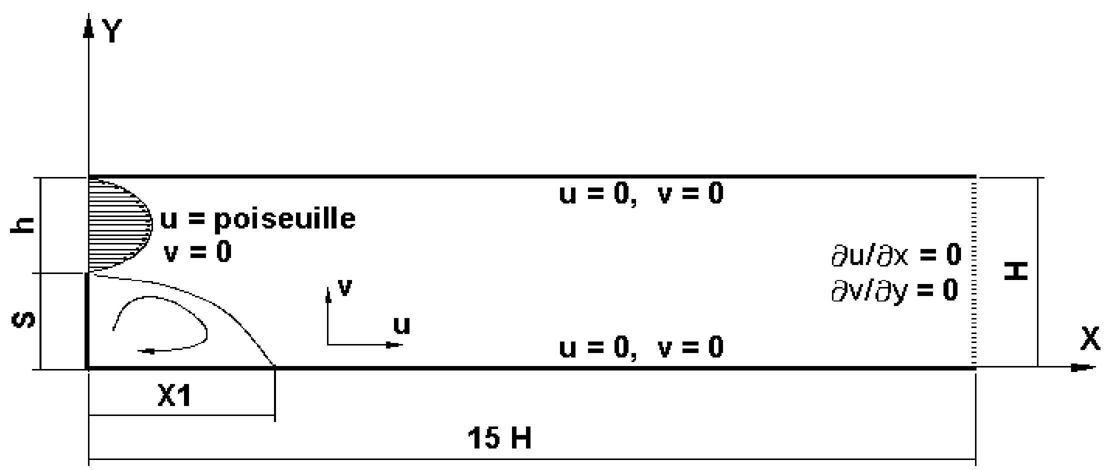


Figure 3. Backward facing step flow geometry and boundary conditions.

For this problem, the preliminary analysis performed on the three formulations has shown that the PPE formulation presented poor convergence characteristics. This behavior could be associated to the instabilities introduced by pressure due to improper combination of interpolation function for velocity and pressure as mentioned in Tezduyar et al. (1990). Based on this fact the results contained in this section includes only the PPE+PM and the PM formulations.

The sequence of the simulation were performed with $\lambda = 10^3$, $\lambda = 10^5$, and $\lambda = 10^7$, varying the mesh density. The main intent of these simulations is to verify the characteristics of the solution furnished by each formulation under different the mesh densities. As a secondary purpose, the mesh independence on the solution is presented.

Table (3) presents the error calculated by Eqs. (9) and (10), respectively indicating the local mass conservation and the global mass balance. To state precisely that the incompressibility constraint is being suitably satisfied, the velocity field must satisfy both error criteria simultaneously. The Tab. (3) groups the results accordingly with the mesh size; course for a mesh density smaller than 700 nodes, medium for a mesh density varying from 800 nodes thru 2000 nodes and fine for a mesh greater than 3000 nodes. It must be noted that each value found in the Tab. (3) is an average on the respective range in consideration.

Table 3. Mesh size and associated mass conservation error.

		E_{IO} (Averaged)			Log (E_D) (Averaged)		
Formulation	Mesh	$\lambda = 10^3$	$\lambda = 10^5$	$\lambda = 10^7$	$\lambda = 10^3$	$\lambda = 10^5$	$\lambda = 10^7$
PM	Course	43.3 %	0.8 %	0	1.2	-0.6	-0.8
	Medium	43.2 %	0.9 %	Diverged	1.2	≈0	Diverged
	Fine	42.5 %	Diverged	Diverged	1.3	Diverged	Diverged
PPE+PM	Course	0.2 %	0	0	-0.9	-2.2	-2.6
	Medium	0.1 %	0	1.6 %	-1.4	-2.3	0.1
	Fine	0.1 %	0	0	-1.4	-3.0	-4.3

Focusing the attention on the results given by PM formulation it is possible to note clearly a trend related with the mesh size and the penalty parameter magnitude. In terms of mass conservation, the increase in the penalty parameter for a courser mesh yields in a benefic action on the solution. Contrarily to the expectation as the mesh becomes fine the solution diverges, consequently compromising the performance. While for the results of PPE+PM formulation a completely different comportment is observed. The quality of the results in terms of mass conservation comes together with the increase in the mesh density and with the choice of an optimum penalty parameter. The curves given by the Figs. (4) and (5) account for the error in the reattachment length, estimated as a percentage from the benchmark results (Armaly et al., 1983).

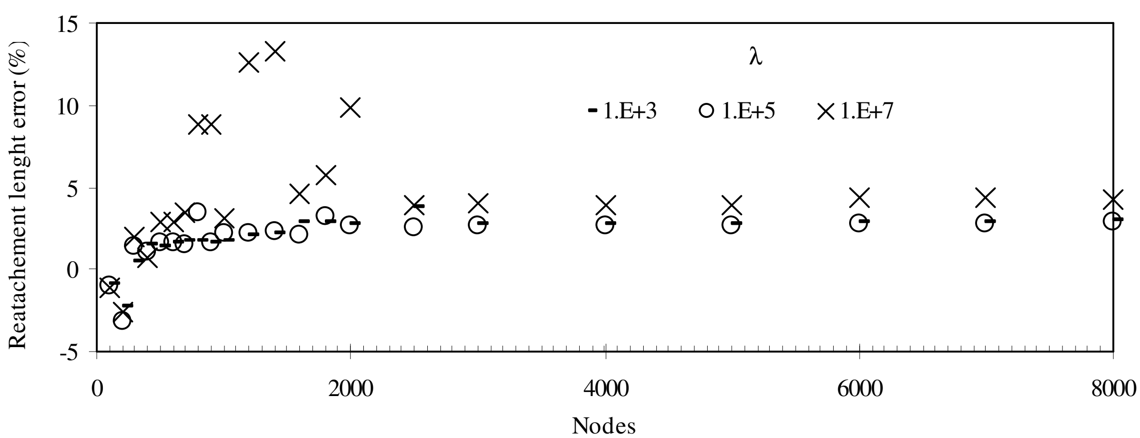


Figure 4. Reattachment length versus mesh size, PPE+PM formulation.

In the Fig. (4) it is possible to the note the independence of the solution occurs for a mesh greater than 3000 nodes. After this, the solution presents a constant difference (around 3%) from the benchmark results, for low and moderate penalty parameter values, respectively $\lambda=10^3$ and $\lambda=10^5$. For high penalty parameter value, $\lambda=10^7$, the corresponding curve presents a visible difference compared to the previous ones. Although the difference is small it indicates the effect of mesh locking in the solution. In the Fig. (5) the missing points are due to the results which the solution has diverged. For low penalty parameter, there is no problems related to convergence, but the results are corrupted due to high mass conservation error. The behavior of the solution for moderate and high penalty parameters is substantially deteriorated in consequence of mesh locking.

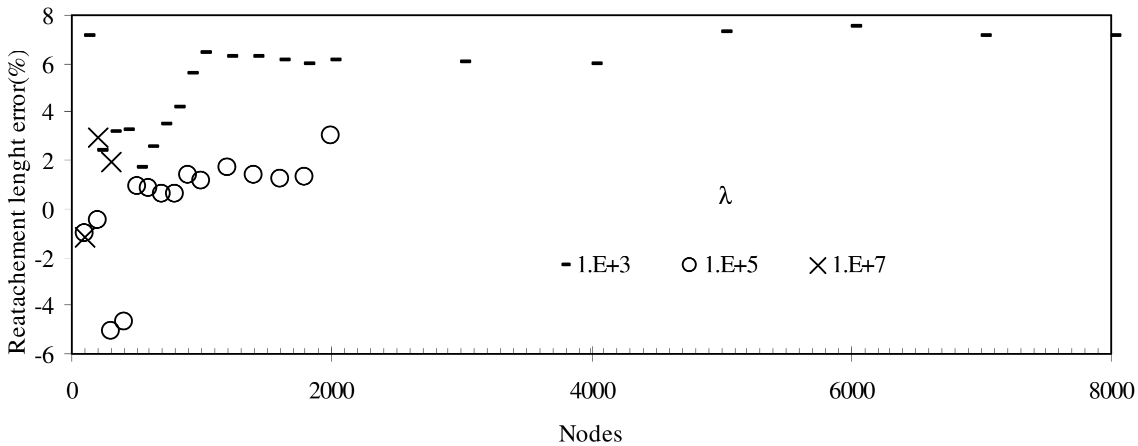


Figure 5. Reattachment length versus mesh size, PM formulation.

One important aspect to be highlighted is related to the poor efficiency that has presented the PM formulation in the backward facing step flow. In this kind of problem configuration, with inlet/outlet it is necessary a higher penalty parameter to satisfy the mass balance than the required on lid driven cavity flow.

4. CONCLUSIONS AND REMARKS

The coupled formulation considering the penalty method and the pressure Poisson equation has been presented and its results are compared to the penalty method and the pressure Poisson equation formulations applied independently. The results of the comparison traced for the three formulations may be understood and interpreted within a limited scope, hence some considerations must be taken into account:

1) Reduced integration was not employed into the PM formulation. It is well known that reduced integration precludes mesh-locking appearance and improves penalty method performance.
2) The word length used in the calculation was 15 bit. It is another mitigation to justify the poor penalty method performance. The numerical solution employed in methods based on penalties handle very large or very small quantities during the iterative procedure. Such characteristic causes a magnification of the truncation error and divergence of the solution as the iterative procedure evolutes. A common practice to reduce this behavior is to use 64-bit world length.
3) All the settings in the numerical solver (such as normalized error to the variables, iterations limits, etc) were kept the same to allow the comparison of the three formulations. This could be a reasoning to explain the problems of convergence presented by PPE formulation in the backward facing step flow.

The coupled formulation has shown to reduce the trend to mesh-locking, presented in the penalty method, at same time the pressure is calculated without post-processing with a lower time consumption than the required by pressure Poisson equation. Even without using the reduced integration, the coupled formulation can reasonable accommodate high penalty parameter values, keeping the mesh-lock problem under control.

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