ON THE PERFORMANCE OF COUPLED AND SEGREGATED METHODS FOR SOLVING TWO-DIMENSIONAL INCOMPRESSIBLE FLOWS EMPLOYING UNSTRUCTURED GRIDS

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Abstract. *In this work, a detailed comparison of the performance of different solution techniques to solve the momentum and mass conservation equations for bidimensional incompressible flows is realized. This kind of comparison is common in the literature, but, in this case, it was done using unstructured grids in the framework of the Element-based Finite Volume Method. Unstructured grids, as very well known, requires the use of co-located arrangements of variables in order to avoid excessive complexity of the code. The interpolation function of the FIELDS method was used to overcome the checkerboard pressure problem, which arises from the co-located arrangement. Coupled solution, as well as the solution involving pressure-velocity coupling methods where used and compared. When compared to the other methods, the coupled solution has shown a great numerical stability and reduced computational effort most of the time.*

Keywords: *unstructured grids, segregated solution, coupled solution, element based finite volume method.*

1. INTRODUCTION

Real engineering and technological problems, such as 3D, viscous and advective-dominated flows involving complex physical phenomena like compressibility, shock waves and turbulence, started to be solved only after the second half of XX century through the development of numerical techniques for solving partial differential equations. Particularly, for the Navier-Stokes set of equations, two numerical strategies are well known and mostly applied for its solution: the segregated and the fully-coupled methods. Segregated methods remained as the best alternative for more than three decades, since there was no computational facilities for using routinely coupled solvers.

Basically, segregated methods propose the solution of each conservation equations independently, obtaining the solution for one specific variable. As the iterative process goes on, all variables must gradually satisfy all conservation equations. For compressible flows this type of methods works pretty well since each variable has a clear evolutive equation. That is, the velocities are calculated by the momentum equations, the density by the mass conservation equation and the pressure by the equation of state. For incompressible flows, however, the equation of state is no longer suitable for the pressure calculation, since it does not depend on density anymore. Additionally, pressure does not show up in mass conservation equation. It gives rise to the pressure-velocity coupling problem the segregated methods have to deal with. Some of the most known methods of this type are the SIMPLE (Patankar and Spalding, 1972), SIMPLEC (Doormaal and Raithby, 1984), SIMPLER (Patankar, 1981) and PRIME (Maliska, 1981), which will be considered in this work.

On the other hand, if one decides to solve all conservation equations simultaneously in one system of algebraic equations, necessarily, all variables must fully satisfy all conservation equations at the same time. Thus, there is no need of a pressure-velocity coupling method. In this case, iterations are still needed only to take into account for the non-linearities. Macarthur and Patankar (1989) compared different techniques to handle the non-linearities and concluded the successive substitution (Picard method), despite its simplicity, is almost as efficient as the Newton and Broyden methods. Another problem that shows up is how to handle the zeros in the main diagonal of the system of equations due to the absence of pressure in continuity equation. A common way to overcome this problem is the employment of a proper interpolation function that considers the neighboring pressure effect on the velocities (Schneider and Raw, 1987; Rhie and Chow, 1983). This technique is of special interest since it introduces pressure into the continuity equation and, at the same time, helps to avoid the checkerboard problem (Patankar, 1980).

The segregated methods give rise to smaller systems of equations when compared to the fully-coupled methods. Thus, specially for finer grids, it requires less computational memory and, for this reason, it has always been preferred. The computational capabilities available nowadays, however, allow fully-coupled algorithms to be run without compromising computational performance. The discussion about the performance of both type of methods is not sufficiently addressed in the literature, specially when unstructured co-located grids are employed. Thus, since it is an open subject for debate, this work aims to perform a systematic comparison between these two types of methods in order to contribute for filling up this gap and to deep the understanding of their behavior.

2. NUMERICAL TECHNIQUES

Firstly proposed by Baliga (1978) and later improved by Schneider and Raw (1987), in the element based finite volume method (EbFVM) the control volumes (CV) are constructed around every grid nodes (element vertices) by the union of all sub-control volumes (SCV) that share a same element vertex, as depicted in Figure 1. All sub-control volumes are built based only on the information contained in the element they belong to. Also, the fluxes in the integration points (j), required by the conservation equations, can be evaluated based on the same element information. This allows an element by element approach that, together with the element shape functions, is the key for handling unstructured grids.
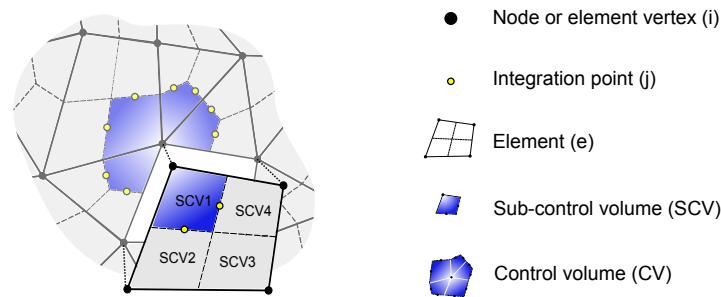

Figure 1: Control volume construction and geometric entities.

The use of element shape functions by the EbFVM is a feature inherited from the finite element method. These shape functions transform an irregular element in the global coordinate system into a regular element, with fixed dimensions, in the transformed coordinate system. In practice, they allow the interpolation of any quantity stored at the element vertices in any position inside the element. In general, quantities are needed to be interpolated only at the integration points of the faces and at the centroids of the sub-control volumes, where the local coordinates are known and, therefore, the shape functions can be calculated. For example, supposing Φ_i is a scalar stored at the vertices (i) of a given element, the value ϕ_j evaluated at the integration point (j) of an element face is given by,

$$\phi_j = \sum_{i=1}^{N_{EV}} N_{ij}\Phi_i \tag{1}$$

where Nv is the number of element vertices. The sub-index i of N_{ij} refers to the shape function associated with the vertex i of the element and it is evaluated at the local coordinates of the integration point j.

The gradient of a scalar can also be obtained from the spatial derivatives of the shape functions, as shown in equation 2. As it can be seen, all derivatives can be evaluated at any point inside the element based only on the values stored at its vertices, which is indispensible for the dicretization processes.

$$\vec{\nabla}\phi_j = \sum_{i=1}^{N_{EV}} \left[\frac{\partial N_{ij}}{\partial x} \quad \frac{\partial N_{ij}}{\partial y} \right]^T \Phi_i \tag{2}$$

Beyond being the main tools for obtaining the algebraic representation of the differential equations, as will be seen ahead, the Equations 1 and 2 allow some geometric calculations, such as the volumes Ω of the control volumes and the area

vectors $\vec{S}$ defined on faces. These calculations are shown by Schneider and Raw (1987).

2.1 Velocity interpolation function

It is well known (Maliska, 2004) that, when low Reynolds numbers are involved, the 2º order interpolation schemes, such as the central differencing scheme (CDS), are suitable since diffusion dominates the flow and, therefore, the downstream values, as well as the upstream ones, affect the property value at the integration point. When the Reynolds number begins to rise, the advection terms come into play causing the 2º order schemes to show oscilations (and instabilities) near sharp gradient regions, due to their non-dissipative nature. In these cases (high Reynolds) 1º order schemes, such as the upwind differencing scheme (UDS), are more suitable since they are stable and do not introduce oscilations in the solution, although they do present the "false difusion" problem.

The above discussion leads to the idea of a hybrid method that gradually switches from 1º to 2º order as the Reynolds number starts to decrease. In another words, an interpolation scheme that suitably balances the advection and diffusion effects. However, as discussed by Raw (1985), in the case of momentum equations the inclusion of the pressure gradient effects are of utmost importance for also avoiding the "false diffusion" problem. The interpolation function of the FIELDS method, developed by Schneider and Raw (1987), naturally takes these effects into account by using the differential form of the momentum equations, evaluated at the integration point, to its deduction. For the x-component of the velocity vector, u, for example, one may start by the following equation,

$$\rho|\vec{V}_j| \left.\frac{\partial u}{\partial s}\right|_j = -\left.\frac{\partial p}{\partial x}\right|_j + \mu\nabla^2 u\big|_j \tag{3}$$

where ρ is the fluid density, μ is the fluid viscosity and s is the stream line direction at the integration point. When properly discretized, Equation 3 will give the value of u_j as a function of U and P (x-component of the velocity vector and pressure, respectively) stored at the element vetices, i, that contains the integration point, j. Performing the discretization, the following expression is obtained,

$$u_j = \sum_{i=1}^{N_{EV}} \left(\frac{\gamma_{ij}}{\psi_j} U_i - \frac{1}{\psi_j} \frac{\partial N_{ij}}{\partial x} P_i \right) \tag{4}$$

The Equation 4 gives an expression of u_j as a function of U_i and P_i weighted by the shape function derivatives and the coefficients ψ_j and γ_{ij}. These coefficients take advection and diffusion effects into account and their expressions and deduction can be seen in Honório (2013).

3. MATHEMATICAL MODEL AND NUMERICAL FORMULATION

In this work, as already mentioned, different solution strategies were employed for the solution of two-dimensional incompressible flows. Also considering single-phase flow, no heat transfer or chemical reactions, newtonian fluid and constant viscosity, the mathematical model is comprised only by the continuity equation (5) and the momentum conservation equations (6) as the following,

$$\vec{\nabla}.\vec{V} = 0 \tag{5}$$

$$\frac{\partial}{\partial t}\left(\rho\vec{V}\right) + \vec{\nabla}.\left(\rho\vec{V}\vec{V}^T\right) = -\vec{\nabla}.\overline{\overline{P}} + \vec{\nabla}.\left(\mu\vec{\nabla}\vec{V}^T\right) \tag{6}$$

where $\overline{\overline{P}} = p\overline{\overline{I}}$. For cartesian components, Equation (6) results in both x and y momentum equations.

The discretization procedure for obtaining the algebraic equations starts by a time integration followed by a volume integration of Equations (5) and (6). The total implicit formulation (Maliska, 2004) were employed to evaluate the time

integrals. The divergence theorem is applied to transform the control volume integrals into surface integrals. The surface integrals are taken by parts at each face of the controle volumes. The integrands of the surface integrals are assumed to be constant over each face, so they can be evaluated at the center of the faces (integration points). This procedure leads to the following discretized representation of Equations 5 and 6 for a control volume centered at a node p (or element vertex),

$$\sum_{j=1}^{N_{FP}} \left(S_j^x u_j + S_j^y v_j \right) = 0 \tag{7}$$

$$\frac{M_p U_p}{\Delta t} + \sum_{j=1}^{N_{FP}} \dot{m}_j u_j = \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(\mu \beta_{ij} U_i - S_j^x N_{ij} P_i \right) \right\} + \frac{M_p^o U_p^o}{\Delta t} \tag{8}$$

$$\frac{M_p V_p}{\Delta t} + \sum_{j=1}^{N_{FP}} \dot{m}_j v_j = \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(\mu \beta_{ij} V_i - S_j^y N_{ij} P_i \right) \right\} + \frac{M_p^o V_p^o}{\Delta t} \tag{9}$$

where N_{FP} is the number of faces surrounding the control volume p, M_p is the control volume mass, $\dot{m}_j$ is the mass flux crossing the face j and the superscript ^{o} denotes the evaluation of a property at the previous time step (Δt). The x and y components of the area vector are being represented by S_j^x and S_j^y. The diffusive term of the momentum equations (last term of the right-hand side of Equation 6) were evaluated using Equation 2, which originated the diffusive operator β_{ij}, given by,

$$\beta_{ij} = \frac{\partial N_{ij}}{\partial x} S_j^x + \frac{\partial N_{ij}}{\partial y} S_j^y \tag{10}$$

Equations 8 and 9 also show that the shape functions N_{ij} were used to represent the pressure value at an integration point j as a function of its nodal values P_i. What is left now is to adequately represent u_j and v_j, which is done by the velocity interpolation function of the FIELDS method, discussed in the last section. Then, by substitution of the Equation 4 for u_j and a similar one for v_j into the Equations 7, 8 and 9 and conveniently grouping the terms, the dicretized forms of the governing equations are finally obtained,

$$\sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(A_{ij}^{pp} P_i + A_{ij}^{pu} U_i + A_{ij}^{pv} V_i \right) \right\} = 0 \tag{11}$$

$$\frac{M_p U_p}{\Delta t} + \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(A_{ij}^{uu} U_i + A_{ij}^{up} P_i \right) \right\} = \frac{M_p^o U_p^o}{\Delta t} \tag{12}$$

$$\frac{M_p V_p}{\Delta t} + \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(A_{ij}^{vv} V_i + A_{ij}^{vp} P_i \right) \right\} = \frac{M_p^o V_p^o}{\Delta t} \tag{13}$$

More details on the deduction of the above equations can be found in (Honório, 2013).

3.1 Solution Strategies

As stressed out by Maliska (2004), solving Equations 11 to 13 by a segregated method means to find a pressure field (P) that when introduced into the momentum equations (12 and 13) results in a velocity field (U and V) that satisfies not just the momentum equations, but also the continuity equation (11). In fact, this will happen only when the pressure field

($P - V$ coupling) and the coefficients (non-linearities) of the momentum equations are correct. There are a number of strategies for achieving that and each one of them deals with these two points in different manners.

The PRIME method, for example, solves the Equation 11 implicitly for pressure (using guessed U and V). This pressure field is then introduced into the momentum equations, which are solved in a explicit manner to obtain a new velocity field. This new velocity field satisfy only partially the momentum equations and it will satisfy the continuity equation only when the iterative process is converged. In this method, the only mechanism that "guides" the velocity field to satisfy the continuity equation is the pressure field introduced into the momentum equation, since it is obtained from the mass conservation equation. For this reason, although there is just one linear system being solved at each iteration step, it is expected a slow convergence rate.

The SIMPLE-like methods (SIMPLE, SIMPLEC and SIMPLER), on the other hand, ensures that the velocity field satisfies the continuity equation at the end of every iteration cycle. In these methods, the momentum equations (12 and 13) are solved implicitly with a guessed pressure field to obtain a velocity field. This velocity field, which satisfy momentum equations, must then be corrected in order to satisfy the continuity equation. So, at one iteration cycle, the velocity field satisfies the momentum equations and then the continuity equation, but not both at the same time, except when the iterative process is converged. The equations for correcting the velocities are based on the definition of a pressure correction field, defined as $P' = P - P^*$, where P^* is the pressure field of the previous iteration step. An equation for obtaining the pressure correction field can be obtained through the continuity equation (7) using correction equations, obtained with the aid of the FIELDS interpolation functions, to evaluate the integration point velocities (u_j and v_j). This leads to,

$$\sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} A_{ij}^{p'p'} P_i' \right\} = \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left[A_{ij}^{p'u} U_i^* + A_{ij}^{p'u} V_i^* - A_{ij}^{p'p} P_i^* \right] \right\} \tag{14}$$

which is also solved implicitly. Once the pressure correction field is obtained, the velocities stored at the element vertices are also corrected to ensure the mass conservation in each control volume. The equation used to correct the U velocity, for example, is

$$U_p = U_p^* - d_p^u \sum_{j=1}^{N_{FP}} \left\{ \sum_{i=1}^{N_{EV}} \left(A_{ij}^{up} P_i' \right) \right\} \tag{15}$$

where $d_p^u = 1/A_p^u$ for SIMPLE and SIMPLER methods, and $d_p^u = 1/\left(A_p^u + \sum_{nb} A_{nb}^u \right)$ for the SIMPLEC method. A similar equation is also used to correct the V velocity. The velocity correction equations are the way the SIMPLE-like methods treats the non-linearities of the momentum equations, which is not done by the PRIME method. The complete deduction of Equations 14 and 15, as well as their coefficients, can be found in Honório (2013).

Once the linear systems of Equations 12 and 13 are solved, the pressure correction field is obtained from Equation 14 and the velocities at the element nodes are corrected, a new pressure field must be calculated to be used in the next iteration step. With this purpose, the SIMPLER method solves another linear system, originated from equation 11, while the SIMPLE and SIMPLEC methods explicitly calculates a new pressure field using the pressure correction field definition,

$$P = P^* + \alpha P' \tag{16}$$

where α is a sub-relaxation factor. As suggested by I. Demirdzic and Peric (1987), in this work, α was set to $1/\left(1 + E \right)$, where E is proportional to the time step, as explained by Doormaal and Raithby (1984)). It is important to stress that the SIMPLER, SIMPLE, SIMPLEC and PRIME methods solve, respectively, four, three, three and one linear system at each iteration cycle. Each linear system has dimensions $N_{CV} \times N_{CV}$, being N_{CV} the number of control volumes of the grid.

The other strategy considered in this work was the coupled solution technique. In this method, the three Equations 11, 12 and 13 are solved altogether in just one system of equations of dimensions $3N_{CV} \times 3N_{CV}$, which has the structure

presented in Equation 17. Because all the variables are solved implicitly, the velocity field obtained fully satisfy the continuity and the momentum equations so it is tightly coupled with the pressure field. However, the velocities used to calculate the coefficients are wrong due to the non-linearities issue. Therefore, the system of equations 17 has to be solved iteratively until the convergence criteria is reached.

$$
\begin{matrix}
Continuity & \longrightarrow \\
Momentum - x & \longrightarrow \\
Momentum - y & \longrightarrow
\end{matrix}
\begin{bmatrix}
A^{pp} & A^{pu} & A^{pv} \\
A^{up} & A^{uu} & 0 \\
A^{vp} & 0 & A^{vv}
\end{bmatrix}
\begin{bmatrix}
P \\
U \\
V
\end{bmatrix}
=
\begin{bmatrix}
0 \\
B^u \\
B^v
\end{bmatrix}
\tag{17}
$$

4. RESULTS AND DISCUSSION

Once the algorithms implemented were validated, tests were carried in order to assess the performance of both fully-coupled and segregated techniques. The efficiency of a method can be understood as directly proportional to stability and robustness, and inversely proportional to the computational effort (CPU time consumed). For all methods, stability and CPU time are dependent of the time step chosen (or the E parameter) since it acts as a relaxation parameter to reach the steady state solution. Besides, the methods studied deal with different numbers of system of equations, with different sizes. So it is expected the increasing of CPU time to be different for each method as the grid is refined, that is, methods' performances may be grid dependent. One of the problems considered in order to test these different scenarios was the well known lid driven cavity problem for $Re = 100$. As it can be seen in Figure 2a, the fully-coupled and the SIMPLE methods showed a good stability compared to the other methods since they converge for a wider range of the E parameter. As the grid is refined, Figure 2b showed a great performance of the fully-coupled technique followed, again, by the SIMPLE method. Based on both graphics of Figure 2, it can be said there is no advantage in solving a laplacian equation for pressure as it is done by the PRIME and SIMPLER methods.
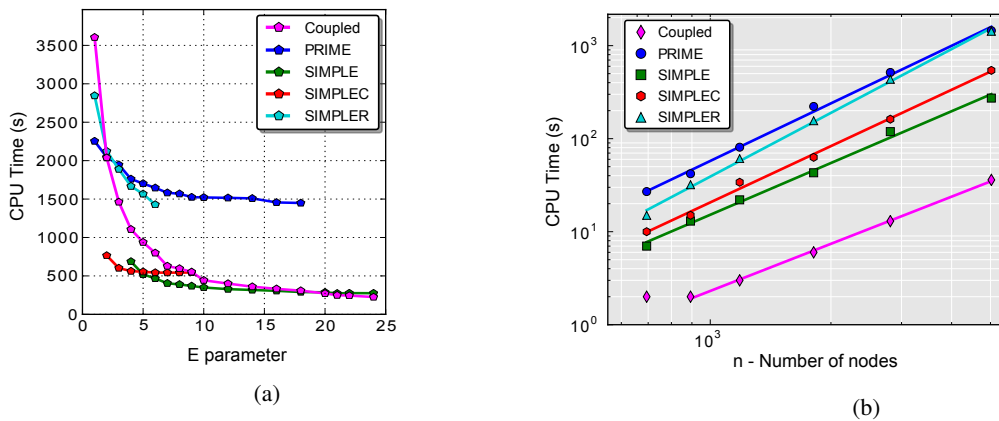

Figure 2: These figures show the CPU time behavior of all methods with respect to (a) the E parameter (which is proportional to time step) and (b) the grid refinement.

Also, the methods' robustness were analyzed through the same problem with $Re = 3200$, which is a highly advective-dominated flow. Again, Figure 3 shows expressive oscillations in pressure residue of both PRIME and SIMPLER, which should not happen since they solve a system of equations exclusively for pressure. At this time, the SIMPLE method took less iterations to reach the convergence criteria (which is when the euclidean norm of $|U - U^o|$ and $|V - V^o|$ reaches a value below 10^{-4}) than the fully-coupled one. The most important fact observed was the SIMPLEC's lack of stability and robustness, as shown by Figures 2a and 3. It was found that this method never converge when in momentum equations $A_p + \sum_{nb} A_{nb} < 0$ in at least one control volume. This causes a bad conditioning in the pressure correction system of equations that prevents its solution. It can be overcome by choosing a small time step in a way that $A_p > - \sum_{nb} A_{nb}$. However, it considerably slows down the convergence rate, as it can be expected when small time steps are employed. This is the cause of the slow convergence observed in Figure 3 for SIMPLEC. The detailed reasons for this to happen will
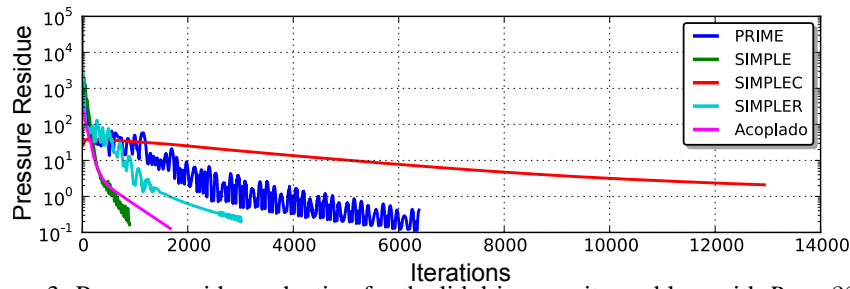
be addressed soon in another paper.

Figure 3: Pressure residue reduction for the lid driven cavity problem with $Re = 3200$.

The bidimensional flow inside a ball valve was also solved. The grid employed and the boundary conditions imposed are shown in Figure 4. Despite not having a reference solution, this problem is of interest because it represents a case where there is mass flux in and out of the domain and it has a complex flow pattern, with some regions of recirculation. Also, the irregular geometry illustrates a domain that would be difficult to be discretized using structured grids.
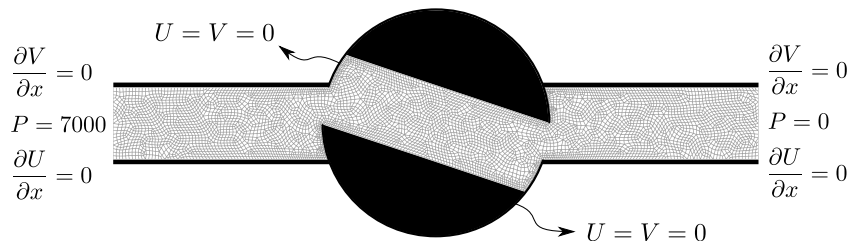

Figure 4: Pressure residue reduction for all methods as the iterative process goes on.

This problem was also solved by all the methods presented before. The convergence criteria was the same for the lid driven cavity. Figure 5 shows the pressure residue drop for each method. As expected, the convergence rate of the PRIME methods was lower than the other methods, except for SIMPLE. At this time, the SIMPLE method was very unstable and required a small time step (causing the slow convergence rate) to reach the convergence criteria. As it can be seen, the SIMPLEC and SIMPLER methods took the same number of iterations and showed the best performances among the segregated methods. The coupled solution took only 9 iterations to reach the convergence criteria, showing excellent robustness and stability.
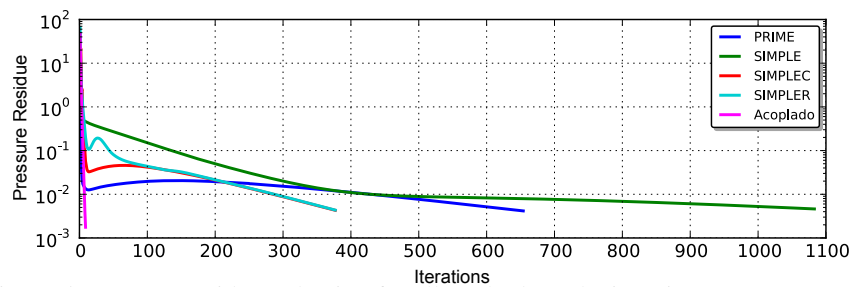

Figure 5: Pressure residue reduction for all methods as the iterative process goes on.

5. CONCLUSIONS

The most known segregated techniques and the fully-coupled solution were tested and compared on the element based finite volume method (EbFVM) framework. For the mathematical model considered, it was found that taking the pressure-velocity coupling implicitly in the system of equations, as it is done by the fully-coupled technique, brings great robustness and stability for the iterative process. Despite having a system of equations three times bigger, the coupled solution is usually less time consuming than the segregated methods and, therefore, more efficient. The SIMPLE method was the

most efficient among the segregated methods, except for the ball valve problem. It was not expected the instabilities presented by the SIMPLEC method. These instabilities are caused by the way the mass fluxes are calculated at the control volume faces, but only the SIMPLEC method was affected by that. Both methods that solved a linear system to obtain the pressure field (PRIME and SIMPLER) did not show a good performance most of the time. In general, it could be observed that the segregated methods' efficiency has a certain dependency on the problem to be solved. In this sense, the fully-coupled technique is more consistent and reliable than the segregated ones, since its performance did not decrease drastically in any situation.

6. ACKNOWLEDGEMENTS

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