ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

A PARALLEL FLUID FLOW SIMULATION WITH EXTERNAL SOLVERS

Marcos Antonio de Souza Lourenço
Elie Luis Martínez Padilla
Aristeu da Silveira Neto
Federal University of Uberlândia
lourenco@mecanica.ufu.br, epadilla@mecanica.ufu.br, aristeus@mecanica.ufu.br

Andre Leibsohn Martins
CENPES/Petrobras
aleibsohn@petrobras.com

Abstract. *In the present work, a parallel, distributed-memory implementation, of a rectilinear Cartesian mesh solver, is described. It is based on the Navier-Stokes equations with a Newtonian, viscous incompressible fluid with constant coefficients. We used the Finite Volume Method, with the central-differences and the Adams-Bashforth methods, with second order accuracy in both space and time, respectively. To solve the Poisson equation, from the pressure correction of the fractional-step method, we applied a parallel external solver. The numerical results are compared with numerical and experimental data, and the agreement is found to be good.*

Keywords: *Finite volume method, Taylor-Couette flow, Navier-Stokes equations, Parallelization, External solver.*

1. INTRODUCTION

The research in the field of computational fluid dynamics (CFD) has grown in recent years, mainly due the development of new mathematical models, algorithms and computational power available. This way, its possible to engineers to simulate the physics behind increasing problem sizes. However, in the simulations of problems like the deep and ultra-deep exploration of water oilfields by *Petrobras*, as well as in the pre-salt oilfields, complex models and high computational power are required, even with simplifications. Also, in the recent years, there has been an impressive increase in the number of multi-core processors together with small to medium computational clusters. This happened as the high speed networks becomes cheaper and therefore more accessible, mainly to scientific institutions. Furthermore, microprocessors were highly improved in the last few decades, particularly with regard to floating-point performance. These hardware performance improvements have provided a basis to overcome some challenges in the simulation of problems large proportions. In a cluster, a big number of interconnected processors nodes can be used to achieve a common goal. However, subdivide the computational solution of a continuous physical problem into sub-applications is not a straightforward task. The inherent difficulty is due the fact of problems are generally inherently not fully parallelizable. Moreover, there is currently a large number of numerical libraries available of scientific computing, both open source and commercial ones. Consequently, there is an increasing number of scientific frameworks, with dozens of tools that can be directly or indirectly applied in CFD. Thus, the aim of the present work is to make use of these numerical libraries in an optimized and flexible way, in order to improve our application.

1.1 LOAD BALANCING

Generally, the physical problem is discretized in a mesh or grid using schemes like the Finite Volume Method (FVM), Finite Difference Method (FDM) or Finite Element Method (FEM). Perhaps the most frequent strategy adopted to parallelize problems in this way is using the *Domain Decomposition Method*, where a certain number of nodes or volumes of the computational mesh, is assigned to each processor in the cluster. Similarly, in a matrix-vector multiplication for example, the multiplication blocks can be assigned to different nodes and the final result is then summed to a root node or to all nodes in the cluster. Although it seems intuitive, in practice this is not a simple task. Fortunately, there are computational libraries and frameworks, both commercial and free(generally open source) ones, with the only purpose of distribute the nodes or volumes forming a problem domain, in order to perform load balancing.

Such framework is Zoltan (Catalyurek *et al.*, 2007), a collection of data management services for unstructured, adaptive and dynamic applications, used to perform the load balancing in all cases considered in the present work. Here, the Eulerian, rectilinear mesh is passed, together with another variables, as input parameters to Zoltan. In this case, the output are the definitions of the blocks/domains assigned to each processor utilized. In the dynamic case, its also possible to utilize Zoltan to manage the migration of data between processors. The new blocks are created not only in order to distribute the load evenly among the processors, but also to optimize the data transfer between partitions.

ISSN 2176-5480

2. MATHEMATICAL AND NUMERICAL MODELING

The equations of mass conservation and balance of momentum are used to model the cases simulated in this work, considering an incompressible flow with a Newtonian fluid. These equations are given, in dimensional form and Cartesian coordinates, respectively as:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{f_i}{\rho} \tag{2}$$

were u_i and p are the velocity components and pressure field respectively, ρ is the density and ν is the kinematic viscosity.

In this paper, the discretization of the governing equations Eqs. (1-5), for the Eulerian field uses the finite volume method (Patankar, 1980) in a staggered computational grid, using the Adams-Bashforth (Bashforth and Adams, 1883) scheme in time and central-differences scheme in space, both of second order. The velocity pressure coupling uses a two step fractional step method of Kim and Moin (1985).

2.1 Poisson's equation

The time discretization of Eq. 2 is made using a modification of the Adams-Bashforth method by Lilly (1965), an explicit extrapolation from the preceding time step, avoiding an additional linear system of equations to solve. The Eq. 2 then becomes:

$$\frac{u_i^{t+1} - u_i^t}{\Delta t} = \frac{3}{2}U^t - \frac{1}{2}U^{t-1} - P_i^{t+1} \tag{3}$$

where U^t and U^{t-1} are the discretized RHS of the momentum equation, in the current and from the previous time steps respectively. The velocity component u_i^{t+1} in the equation above needs the discretized pressure gradient evaluated in next time step $t+1$, P_i^{t+1}. Applying the classical fractional step method, using two steps, one for prediction and another for correction, its possible to find the equations Eq. 4 and Eq. 5.

$$\frac{u_i^* - u_i^t}{\Delta t} = \frac{3}{2}U^t - \frac{1}{2}U^{t-1} - P_i^t \tag{4}$$

$$\frac{u_i^{t+1} - u_i^*}{\Delta t} = -\nabla \phi_i \tag{5}$$

where ϕ is the pressure correction variable. In the first step, u_i^* is estimated using the pressure in the current time t. Then, u_i^{t+1} and p are corrected using the pressure correction variable (Ferziger and Peric, 2002), respectively as:

$$u_i^{t+1} = u_i^{*t} - (\nabla \phi_i)\, \Delta t \tag{6}$$

$$p^{t+1} = p^t + \phi \tag{7}$$

The greater the complexity of a problem, generally greater will be the number of degrees of freedom to be solved. The solution of the Poisson equation arising from Eq. 5, is a serious computational bottleneck, mainly in unsteady simulations. In this study, we used the scientific computation framework *Trilinos* (Heroux *et al.*, 2003) to solve the linear system of equations in parallel, using the libraries *ML* and *AztecOO*, provided by framework. We used the Bi-Conjugated Gradient Stabilized (BiCGStab) and Generalized Minimum Residual methods (Saad and Schultz, 1986), both of them preconditioned by Algebraic Multigrid (AMG). In the sequential solver used previously by the authors, the *Strongly Implicit Procedure* SIP Stone (1968) was used as the Poisson pressure correction solver.

3. PROBLEM DESCRIPTION

Here we used the classical lid-driven cavity fluid flow as a test case, due to the simplicity of implementation and by the great number of available data for comparison. The problem is depicted in Fig. 1.

ISSN 2176-5480

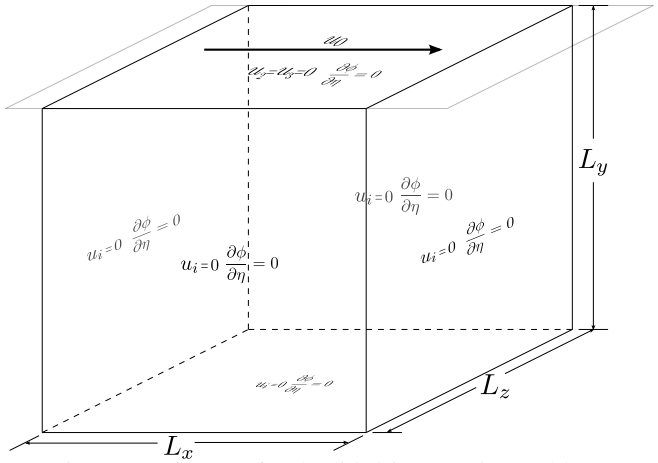


Figure 1: Diagram for the lid-driven cavity problem.

It is a cubic cavity, with no-slip boundary conditions in all of the six faces. All faces are static, with the exception of the upper face, which moves with prescribed velocity u_0 only in the x direction and with the respective dimensions shown in the figure. For all the faces, the boundary condition of null derivative is imposed for the pressure correction $\left(\frac{\partial \phi}{\partial \eta}=0\right)$. The Reynolds number is the non-dimensional factor governing the flow, given by:

$$Re = \frac{u_0 L}{\nu} \tag{8}$$

where L is the side length of the cavity and ν is the cinematic viscosity of the fluid. In the first numerical investigations of the problem, in two-dimensions, there are (Kawaguti, 1961; Bozeman and Dalton, 1973). Another two-dimensional simulation are the work of Ghia *et al.* (1982), for Reynolds numbers in the range of $Re = 10^2$ to $Re = 10^4$, using high resolution meshes with a vorticity-stream function formulation (de Vahl Davis and Mallinson, 1976). An overview on the subject can be found in the work of Shankar and Deshpande (2000).

4. RESULTS

4.1 Lid-driven cavity flow

The comparisons are made with the numerical works Ku *et al.* (1987) Kato *et al.* (1990), Babu and Korpela (1994), Sheu and Tsai (2002), Deshpande and Milton (1998) and Padilla and da Silveira Neto (2005). The works of Kato *et al.* (1990) and Sheu and Tsai (2002) are based on the FEM, while the work of Babu and Korpela (1994) uses a FDM formulation. In the last one, to take advantage on the plane of symmetry of the problem in the z direction, was utilized a mesh of $63 \times 63 \times 33$ nodes. Ku *et al.* (1987) shows high resolution simulations, determined by a pseudo-spectral method for Reynolds numbers of $Re = 100$, $Re = 400$ e $Re = 1000$. The FDM is also used in the work of Deshpande and Milton (1998), and they present solutions for various aspect ratios and Reynolds numbers.

ISSN 2176-5480

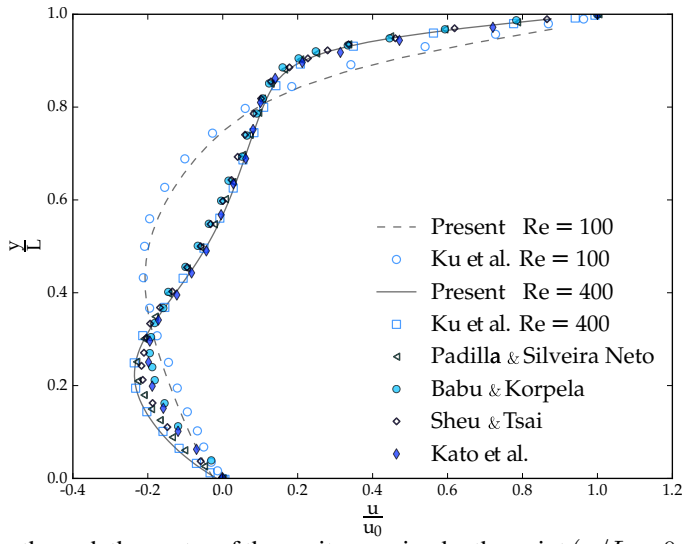


Figure 2: Velocity profile of u through the center of the cavity, passing by the point $(x/L = 0.5; z/L = 0.5)$. Comparisons are made to $Re = 100$ and $Re = 400$.

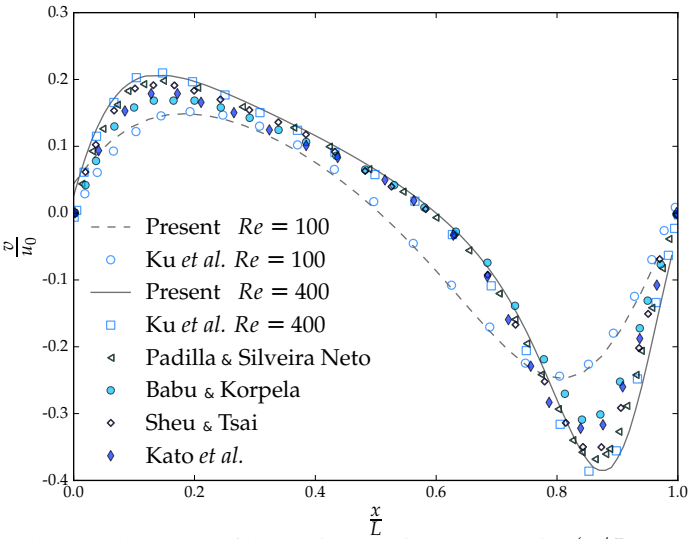


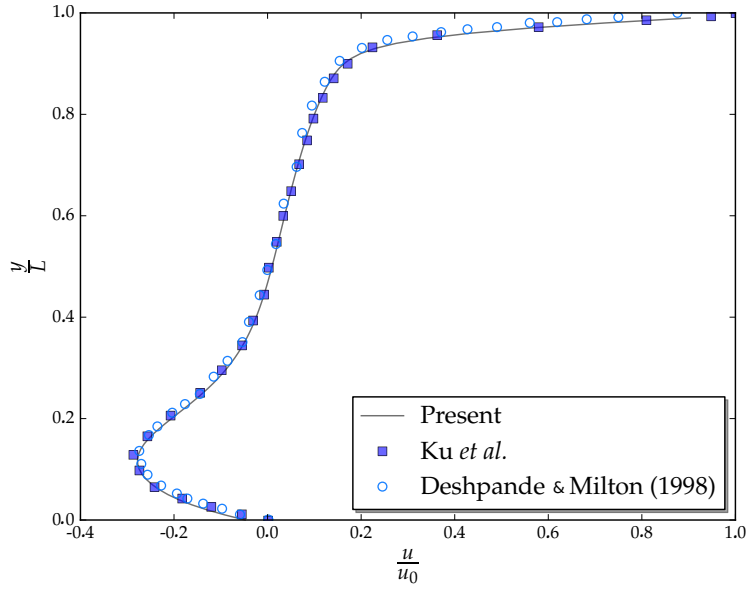
Figure 3: Velocity profile of v through the center of the cavity, passing by the point $(y/L = 0.5; z/L = 0.5)$. Comparisons are made to $Re = 100$ and $Re = 400$.

In Fig. 2 is presented the x velocity distribution over the vertical line $(x/L = 0.5; z/L = 0.5)$ for $Re = 100$ and $Re = 400$. Also for Reynolds numbers of $Re = 100$ and $Re = 400$, the y velocity component, v, is presented in the Fig. 3, over the horizontal line, trough the point $(y/L = 0.5; z/L = 0.5)$. The results for $Re = 100$ are compared only with the results of Ku *et al.* (1987), showing good agreement, except in regions near the cavity walls. This can be due the coarse mesh ($32 \times 32 \times 32$) in these regions, or by influence of linear interpolations used in the post-processing.

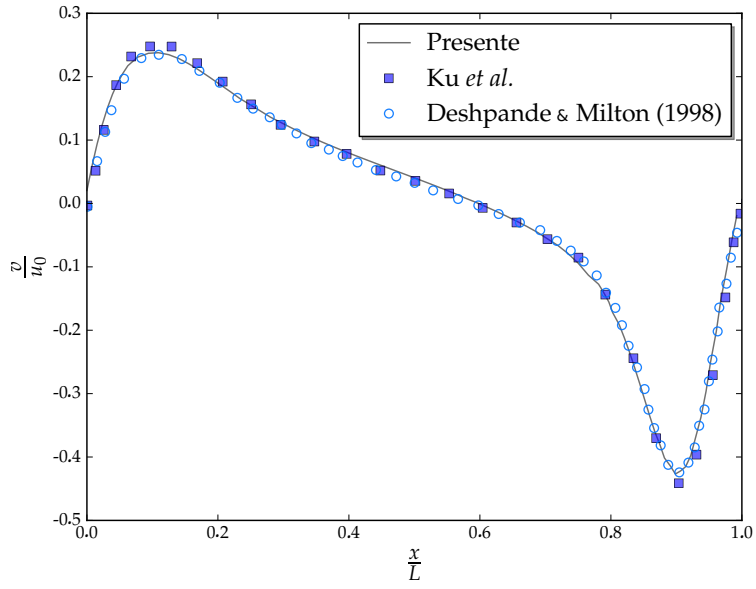
For $Re = 400$, the results are also in agreement with the spectral based solutions of Ku *et al.* (1987). The small difference observed with the results of Padilla and da Silveira Neto (2005) is probably due to different mesh resolutions of ($50 \times 50 \times 50$) and ($60 \times 60 \times 60$) of the present work.

In Fig. 4, the comparison results are presented for $Re = 1000$. Also in the other cases, for Reynolds numbers of $Re = 100$ and $Re = 400$, shown a good agreement with the references. The profiles for the x velocity component, u, was get in the line passing trough $(x/L = 0.5; z/L = 0.5)$. The distribution for the y velocity component, v, lies over $(y/L = 0.5; z/L = 0.5)$. The values are quite the same for both parallel and sequential simulations.

ISSN 2176-5480



(a)



(b)

Figure 4: Velocity profiles in the lid-driven cavity flow. Comparison with the works of Ku *et al.* (1987); Deshpande and Milton (1998) with $Re = 1000$: *(a)* Component u over the vertical line y and passing trough the point $(x/L = 0.5; z/L = 0.5)$ and; *(b)* Component v over the horizontal line in x, crossing the point $(y/L = 0.5; z/L = 0.5)$.

4.2 Computational aspects

In the tests performed, we used meshes of $32 \times 32 \times 32$, $60 \times 60 \times 60$ and $100 \times 100 \times 100$ volumes, for simulations with the Reynolds numbers of $Re = 100$, $Re = 400$ and $Re = 1000$, respectively. For $Re = 1000$, was used a non-uniform mesh, with a stretching of about 6% near the walls. Was found that the number of iterations of solution are highly dependent on the parameters passed to the AMG precondition. Furthermore, this number of iterations is inversely proportional to the time spent in each iteration and of the number of processors utilized. The number of iterations of solution are shown in Table 1.

ISSN 2176-5480

Table 1: Iterations of solution for 3 test cases analyzed in the lid-driven cavity flow.

Re	100	400	10^3
Mesh	Uniforme	Uniforme	Refinada
Resolution	$32 \times 32 \times 32$	$60 \times 60 \times 60$	$100 \times 100 \times 100$
N° of processors	2	8	16
N° of iterations of solution	4	5	5

We have partitioned a mesh between 64 processors, and the load balancing for the test is depicted in Fig. 5. The mesh have $128 \times 128 \times 128$ volumes, and can be seen by the results a small difference of 0.5% in the distribution.

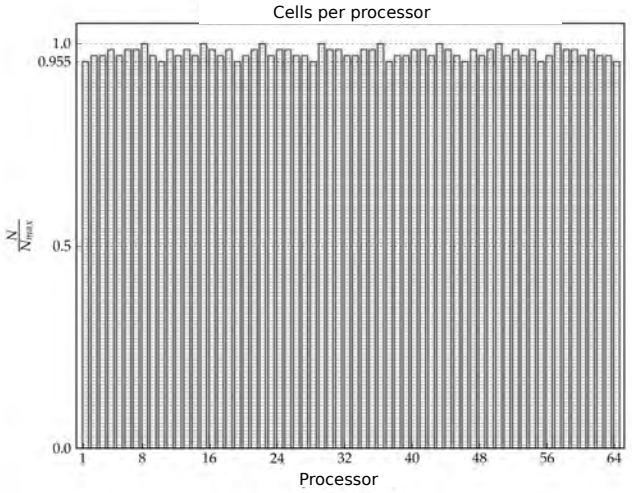


Figure 5: Load balance for the lid-driven cavity flow at $Re = 400$.

The Fig. 6 shows the speedup for the simulation of the lid-driven cavity flow with $Re = 1000$, mesh of $256 \times 256 \times 256$ volumes in the x,y and z, respectively, partitioned on 2, 4, 8, 16, 32, 64 and 128 processors. Only the case with 128 processors used *Hyperthreading*[1]. In the test, was performed 25 iterations of solution using the *BiCGStab* method to solve the Poisson equation.

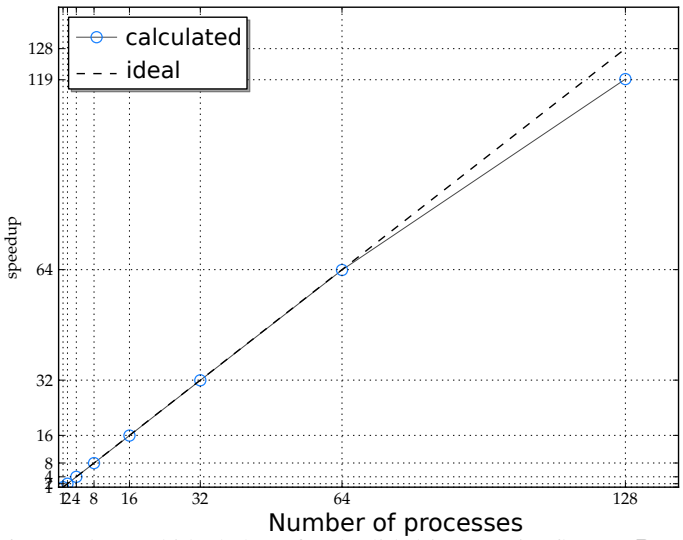


Figure 6: Speedup and ideal slope for the lid-driven cavity flow at $Re = 1000$.

[1]Computer system that processes two or more tasks simultaneously, best known as SMT (*Simultaneous Multi Threading*), with the intent to make better use of computer resources.

ISSN 2176-5480

5. CONCLUSIONS

In this work was described a distributed-memory parallel implementation of a rectilinear solver, based on the Navier-Stokes equations with a Newtonian, viscous, incompressible fluid with constant coefficients. We used the Finite Volume Method, with second order accuracy methods central-differences and the Adams-Bashforth, in both space and time, respectively. The numerical results are compared with numerical data in the literature and the agreement between is found to be good. We conclude that it seems feasible to use an external library to solve critical parts in the simulation, since the huge background of these libraries are difficult to achieve in terms of performance in a short term.

6. ACKNOWLEDGEMENTS

The authors like to tank the Support and Research of Minas Gerais State (FAPEMIG), the CNPq and the Research Center of PETROBRAS (CENPES) for the financial support.

7. REFERENCES

Babu, V. and Korpela, S.A., 1994. "Numerical solution of the incompressible three-dimensional navier-stokes equations". *Computers & Fluids*, Vol. 23, No. 5, pp. 675 – 691. ISSN 0045-7930. doi:10.1016/0045-7930(94)90009-4. URL http://www.sciencedirect.com/science/article/pii/0045793094900094.

Bashforth, F. and Adams, J., 1883. *An attempt to test the theories of capillary action: by comparing the theoretical and measured forms of drops of fluid. With an explanation of the method of integration employed in constucting the tables which give the theoretical forms of such drops*. University Press.

Bozeman, J.D. and Dalton, C., 1973. "Numerical study of viscous flow in a cavity". *Journal of Computational Physics*, Vol. 12, No. 3, pp. 348 – 363. ISSN 0021-9991. doi:10.1016/0021-9991(73)90157-5. URL http://www.sciencedirect.com/science/article/pii/0021999173901575.

Catalyurek, U., Boman, E., Devine, K., Bozdag, D., Heaphy, R. and Riesen, L., 2007. "Hypergraph-based dynamic load balancing for adaptive scientific computations". In *Proc. of 21st International Parallel and Distributed Processing Symposium (IPDPS'07)*. IEEE. Best Algorithms Paper Award.

de Vahl Davis, G. and Mallinson, G., 1976. "An evaluation of upwind and central difference approximations by a study of recirculating flow". *Computers & Fluids*, Vol. 4, No. 1, pp. 29 – 43. ISSN 0045-7930. doi:10.1016/0045-7930(76)90010-4. URL http://www.sciencedirect.com/science/article/pii/0045793076900104.

Deshpande, M. and Milton, S., 1998. "Kolmogorov scales in a driven cavity flow". *Fluid Dynamics Research*, Vol. 22, No. 6, pp. 359 – 381. ISSN 0169-5983. doi:10.1016/S0169-5983(97)00043-9. URL http://www.sciencedirect.com/science/article/pii/S0169598397000439.

Ferziger, J.H. and Peric, M., 2002. *Computational methods for fluid dynamics*. Springer, 3rd edition.

Ghia, U., Ghia, K. and Shin, C., 1982. "High-re solutions for incompressible flow using the navier-stokes equations and a multigrid method". *Journal of Computational Physics*, Vol. 48, No. 3, pp. 387 – 411. ISSN 0021-9991. doi:10.1016/0021-9991(82)90058-4. URL http://www.sciencedirect.com/science/article/pii/0021999182900584.

Heroux, M., Bartlett, R., Hoekstra, V.H.R., Hu, J., Kolda, T., Lehoucq, R., Long, K., Pawlowski, R., Phipps, E., Salinger, A., Thornquist, H., Tuminaro, R., Willenbring, J. and Williams, A., 2003. "An Overview of Trilinos". Technical Report SAND2003-2927, Sandia National Laboratories.

Kato, Y., Kawai, H. and Tanahashi, T., 1990. "Numerical flow analysis in a cubic cavity by the gsmac finite-element method : In the case where the reynolds numbers are 1000 and 3200". *JSME international journal. Ser. 2, Fluids engineering, heat transfer, power, combustion, thermophysical properties*, Vol. 33, No. 4, pp. 649–658. ISSN 09148817. URL http://ci.nii.ac.jp/naid/110002492540/.

Kawaguti, M., 1961. "Numerical solution of the navier-stokes equations for the flow in a two-dimensional cavity". *Journal of the Physical Society of Japan*, Vol. 16, No. 11, pp. 2307–2315. doi:10.1143/JPSJ.16.2307. URL http://jpsj.ipap.jp/link?JPSJ/16/2307/.

Kim, J. and Moin, P., 1985. "Application of a fractional-step method to incompressible navier-stokes equations". *Journal of Computational Physics*, Vol. 59, No. 2, pp. 308 – 323. ISSN 0021-9991. doi:DOI: 10.1016/0021-9991(85)90148-2. URL http://www.sciencedirect.com/science/article/B6WHY-4DD1VRS-146/2/a3d27f0031b262180e467036ab03e9db.

Ku, H.C., Hirsh, R.S. and Taylor, T.D., 1987. "A pseudospectral method for solution of the three-dimensional incompressible navier-stokes equations". *Journal of Computational Physics*, Vol. 70, No. 2, pp. 439 – 462. ISSN 0021-9991. doi:10.1016/0021-9991(87)90190-2. URL http://www.sciencedirect.com/science/article/pii/0021999187901902.

Lilly, D.K., 1965. "On the computational stability of numerical solutions of time-dependent non-linear geophysical fluid dynamics problems". *Monthly Weather Review - American Meteorological Society*, Vol. 93, p. 24.

Padilla, E.L.M. and da Silveira Neto, A., 2005. "Desenvolvimento de um cÃşdigo computacional tridimensional para soluÃğÃčo de escoamentos em transiÃğÃčo e turbulÃłncia". In *Proceedings of the XXVII Iberian Latin-American Congress on Computational Methods in Engineering (CILAMCE)*. Brazilian Assoc. for Comp. Mechanics & Latin American Assoc. of Comp. Methods in Engineering.

Patankar, S., 1980. *Numerical Heat Transfer and Fluid Flow*. Series in computational and physical processes in mechanics and thermal sciences. Hemisphere Publishing Company. ISBN 9780891165224. URL http://books.google.com.br/books?id=5JMYZMX3OVcC.

Saad, Y. and Schultz, M.H., 1986. "Gmres: a generalized minimal residual algorithm for solving nonsymmetric linear systems". *SIAM J. Sci. Stat. Comput.*, Vol. 7, No. 3, pp. 856–869. ISSN 0196-5204. doi:10.1137/0907058. URL http://dx.doi.org/10.1137/0907058.

Shankar, P.N. and Deshpande, M.D., 2000. "Fluid Mechanics in the Driven Cavity". *Annual Review of Fluid Mechanics*, Vol. 32, pp. 93–136. doi:10.1146/annurev.fluid.32.1.93.

Sheu, T. and Tsai, S., 2002. "Flow topology in a steady three-dimensional lid-driven cavity". *Computers & Fluids*, Vol. 31, No. 8, pp. 911 – 934. ISSN 0045-7930. doi:10.1016/S0045-7930(01)00083-4. URL http://www.sciencedirect.com/science/article/pii/S0045793001000834.

Stone, H.L., 1968. "Iterative solution of implicit approximations of multidimensional partial differential equations". *SIAM Journal on Numerical Analysis*, Vol. 5, pp. 530 – 558.

8. RESPONSIBILITY NOTICE

The author(s) is (are) the only responsible for the printed material included in this paper.