Numerical flow simulation - Assessment 1 Report

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***Abstract*—The SIMPLE method is an algorithm widely used in CFD to solve steady incompressible problems. In the present work, it is applied to a 1D steady incompressible problem consisting of a converging nozzle. The numerical solution obtained for a number of grid nodes $N = 21$ and a tolerance $tol = 1e-6$ on the residuals was compared to the closed-form solution of the problem. Relative errors obtained for both velocity and pressure fields are around 7% and 8%. A further study on the under-relaxation coefficients α_u and α_p aimed to maximize the convergence speed led to halve the number of required iterations, from an initial value of 249 to 105.**

I. Introduction

The solution of a steady incompressible flow in a 2D planar converging nozzle was found by means of the SIMPLE algorithm. Firstly, the flow was supposed to be frictionless: neglecting the viscous effects leads to a uniform velocity distribution on each section of the nozzle; furthermore, the absence of the gravitational field effect (or of other forces per unit volume) makes the pressure uniform as well. Therefore, all the variables of interest are uniformly distributed throughout every cross section, and consequently the 2D problem could be solved as a 1D problem. The numerical results were then compared with the exact solution of the problem, in order to assess the accuracy of the solution.

A further insight into the convergence speed is presented: initially through a coarse grid search, and eventually through the Nelder-Mead algorithm, an optimization problem was solved to find α_p and α_u that ensure the fastest convergence speed.

II. Models and methods

A. Problem data

The nozzle is shown in fig. 1. For what concerns its geometry, its length is equal to $L = 2\,\mathrm{m}$, the area of the inlet is $A_{in} = 0.5\,\mathrm{m}^2$, while the area of the outlet is $A_{out} = 0.1\,\mathrm{m}^2$. The area change rate is a linear function of the distance from the inlet. The boundary conditions are the stagnation pressure upstream the nozzle, which is $p_0 = 10\,\mathrm{Pa}$, and the pressure on the outlet, which is $p_{out} = 0\,\mathrm{Pa}$.

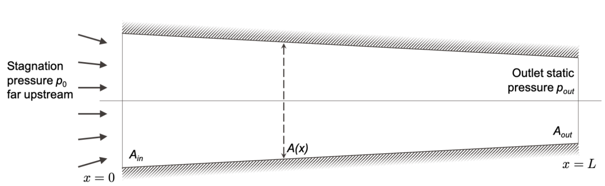


Fig. 1: Converging nozzle.

B. Governing equations and exact solution

The governing equations for the flow are the 1D steady inviscid Navier-Stokes equations (also known as Euler's equations). They consist of the continuity equation and the 1D momentum equation:

$$\frac{d}{dx}\left(\rho A(x)u(x)\right) = 0 \tag{1}$$

$$\rho u(x)A(x)\frac{du}{dx} = -A(x)\frac{dp}{dx} \tag{2}$$

The exact solution to the problem is obtained through Bernoulli's equation[1]:

$$p_0 = p(x) + \frac{1}{2}\rho u(x)^2 \tag{3}$$

Furthermore, the mass flow rate is equal to:

$$\dot{m} = \rho A(x)u(x) \tag{4}$$

Combining Eq. 3 and 4 at $x = x_{inlet} = 0$, $A = A_{inlet}$ yields the value of $\dot{m} = 0.447\,\mathrm{kg/s}$. Through Eq. 3, velocity and pressure fields $u(x)$ and $p(x)$ are immediately obtained:

$$u\left(x\right) = \frac{A_{out}}{A_{in} - \left(\frac{A_{out}-A_{in}}{L}\right)\cdot x}\cdot\sqrt{\frac{2\,p_0}{\rho}} \tag{5}$$

$$p\left(x\right) = p_0\cdot\left[1-\left(\frac{A_{out}}{A_{in} - \left(\frac{A_{out}-A_{in}}{L}\right)\cdot x}\right)^2\right] \tag{6}$$

C. The SIMPLE algorithm

The SIMPLE method is a guess-and-correct procedure for the calculation of pressure on a staggered grid [2]. The method makes use of a guessed velocity field to evaluate the convective fluxes through cell faces, and a guessed pressure field (or the pressure field at previous iteration) is used to solve the momentum equations. Then, a pressure correction equation is derived from the continuity and momentum equation: such equation is solved in order to obtain the new pressure distribution, which is used to correct and update the velocity and pressure fields that satisfy the continuity equation. The momentum equation is solved with the updated pressure and velocity field and the process is iterated until convergence.

[1]The hypothesis that must be satisfied for the applicability of Bernoulli's equation are: inviscid, irrotational, steady and barotropic flow. For the given problem, they are all verified.

The convective term was discretized through the upwind differencing scheme, while the Picard's method was employed to linearize it.

Initially, the guessed velocity field was calculated from a guessed mass flow rate value $\dot{m} = 1\,\text{kg/s}$, while the initial pressure field adopted was a linear field between the two boundary conditions. The number of grid nodes considered was $N = 21$, the chosen tolerance on the residuals, defined in the following section, was $tol = 1e-6$, and the maximum number of iterations allowed was $\texttt{maxiter} = 1e3$. Under-relaxation was used as well, in order to stabilize the algorithm. At every iteration, let $\boldsymbol{p}^{(n-1)}$ be the guessed pressure field (or the pressure field computed at previous iteration)[2], $\boldsymbol{p}$ the computed and corrected pressure field, $\boldsymbol{u}$ the computed and corrected velocity field, $\boldsymbol{u}^{(n-1)}$ the velocity field computed at the previous iteration, we compute:

$$\boldsymbol{p}^{new} = \alpha_p \boldsymbol{p} + (1-\alpha_p)\boldsymbol{p}^{(n-1)} \tag{7}$$

$$\boldsymbol{u}^{new} = \alpha_u \boldsymbol{u} + (1-\alpha_u)\boldsymbol{u}^{(n-1)} \tag{8}$$

The α_p coefficient is required since the pressure correction equation especially is susceptible to divergence. For the stability of the pressure solution, Eq. 8 requires $\alpha_p < 1$, while α_u may take values greater the 1, depending on the given flow. Initially, $\alpha_p = \alpha_u = 0.1$ were the values considered.

D. Convergence and errors

The algorithm was stopped either by the maximum number of iterations allowed `maxiter` or the value of at least one of the residuals smaller than a given tolerance tol. Two different residuals were used as convergence indicators: r_u, the relative residual of the momentum equation and r_p, the absolute RHS of the pressure correction equation. They are defined as follows:

$$r_u = \frac{||\boldsymbol{M}_u \boldsymbol{u}^{calc} - \boldsymbol{b}_u||}{||diag(\boldsymbol{M}_u)\boldsymbol{u}^{calc}||} \tag{9}$$

$$r_p = ||\boldsymbol{b}_p|| \tag{10}$$

where $\boldsymbol{M}_u$ is the matrix associated with the linear system of the discretized momentum equation, $\boldsymbol{b}_u$ is the right-hand-side of the linear system itself and $\boldsymbol{b}_p$ indicates the right-hand-side of the linear system associated with the discretized pressure correction equation.
Additionally, once the converged solution is obtained, it is possible to define the relative error between the numerical solution and the exact one. The i-th element of such vector is defined as:

$$\Delta e_{(.),i} = \frac{|(.)_i^{calc} - (.)_{ex,i}|}{(.)_{ex,i}} \cdot 100 \tag{11}$$

Finally, the value of final global mass balance (FMB) is computed as well as the relative error of the flow rate compared to the analytical one:

$$FMB = \frac{\dot{m}_{in}^{calc} - \dot{m}_{out}^{calc}}{\text{mean}(\dot{m}^{calc})} \tag{12}$$

$$\Delta e_{\dot{m}} = \frac{|\dot{m}^{calc} - \dot{m}_{ex}|}{\dot{m}_{ex}} \cdot 100 \tag{13}$$

In order to compute FMB, the values of the numerical velocity vector (defined on the staggered grid) are to be used.

E. About the under-relaxation coefficients

As previously stated, the stability and speed convergence of the method are controlled by the under-relaxation coefficients α_p and α_u. The optimal values depend on what goal one would like to reach and on the particular problem considered. This part of the project was focused on finding the values of α_p and α_u that lead to the minimum number of iterations, keeping $N = 21$ and for $tol = 1e-6$. In order to do that, the entire SIMPLE algorithm was implemented in a function that takes the two αs as inputs and returns the number of iterations required to reach the given tolerance on both the indicators previously described. This function was later minimized using the Nelder-Mead algorithm [1], a derivative-free optimization algorithm. To find a suitable guess value, a coarse grid search was implemented: the minimum value of the function on a grid of αs was used as initial condition for the Nelder-Mead method.

The results of this analysis are presented in the following sections.

III. RESULTS

The velocity and pressure trends for $N = 21$ are shown in figure 2a and are compared with the exact solution. In fig. 2b r_u and r_p are plotted as a function of the i-th iteration until convergence.

Values of the converged solution and the exact one may be compared, by means of the relative error computed for velocity and pressure field. The i-th element of such vectors of errors is defined as follows:

$$\Delta e_{u,i} = \frac{|u_i^{calc} - u_{ex,i}|}{u_{ex,i}} \cdot 100 \tag{14}$$

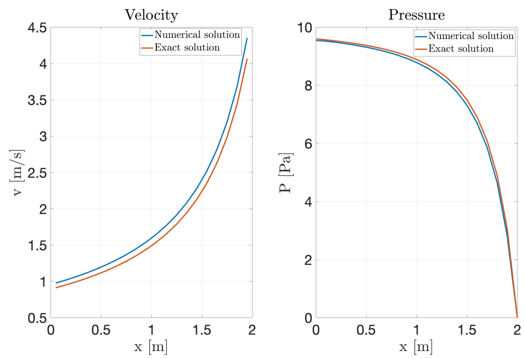
$$\Delta e_{p,i} = \frac{|p_i^{calc} - p_{ex,i}|}{p_{ex,i}} \cdot 100 \tag{15}$$

Finally, FMB and $\Delta e_{\dot{m}}$ were computed as well, according to the previous definitions. The above defined numerical errors are presented in table I.

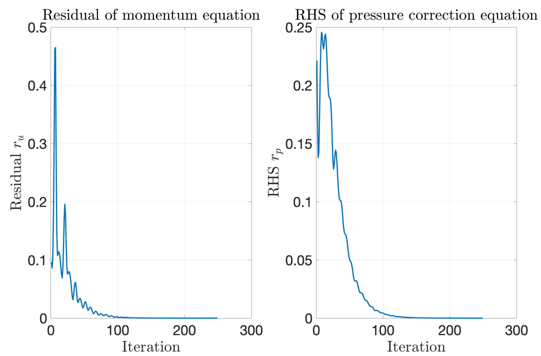
Quantity	Value
$\boldsymbol{\Delta e}_u$	$\approx 7.1\%$
$\boldsymbol{\Delta e}_p$	$\approx 0.6 - 8.3\%$
$\Delta e_{\dot{m}}$	$\approx 2.7\%$
FMB	$\approx -2.32e-16$

TABLE I: Relative errors and FMB

[2]Numerical pressure and velocity fields are vectors, and therefore will be indicated in bold.



(a) Velocity and pressure trend against the exact solution



(b) Residuals trend as function of iterations number

Fig. 2: Plots of results obtained with $N = 21$ and under-relaxation coefficients $\alpha_u = \alpha_p = 0.1$.

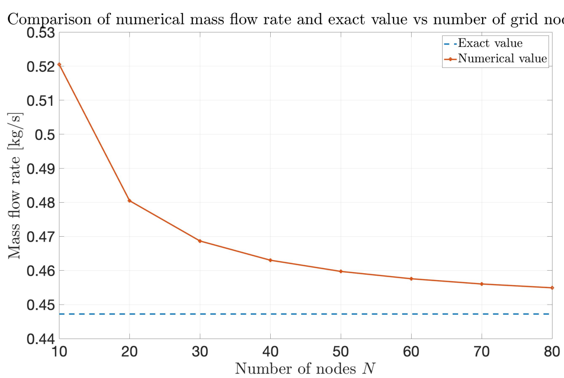


Fig. 3: Mass flow rate: numerical value vs number of grid nodes N (the exact value is plotted for reference). $\alpha_p = 0.01$, $\alpha_u = 0.1$.

The algorithm was subsequently run varying the value of N, and the predicted value of $\dot{m}$ was plotted against the exact value. The resulting graph is shown in figure 3.

Figure 4 shows empirically the order of accuracy of the method: as the theory predicts, since the upwind scheme has a 1^{st} order accuracy, the error of the numerical solution decreases as $1/N$. It has to be noted that both figures were obtained using $\alpha_p = 0.01$ (and $\alpha_u = 0.1$): this was necessary to ensure the stability of the solution when increasing N.

For what concerns the study of α_p and α_u and the consequently required number of iterations for the algorithm to converge, fig. 5 shows how the algorithm behaves under the

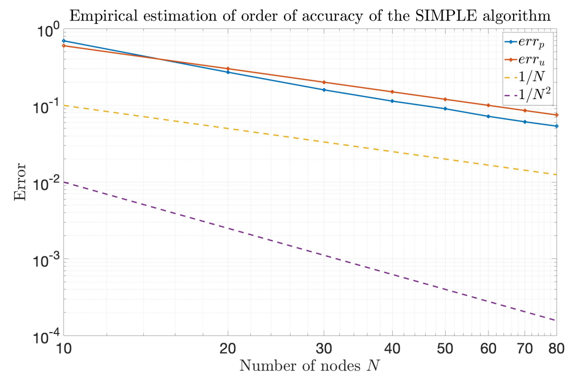


Fig. 4: Error on pressure and velocity as function of N. Both axis are in logarithmic scale. The trend of $1/N$ and $1/N^2$ is plotted in order to estimate visually the order of accuracy. $\alpha_p = 0.01$, $\alpha_u = 0.1$.

given conditions. The yellow area denotes pairs of α values that made the algorithm reach `maxiter` $= 1e3$ or that led to an ill-conditioned matrix $\boldsymbol{M_p}$, the matrix associated with the discretized pressure correction equation. When $\boldsymbol{M_p}$ was ill-conditioned, the SIMPLE algorithm was stopped, and the function used for the optimization problem returned a number of iterations equal to `maxiter` to account for this situation.

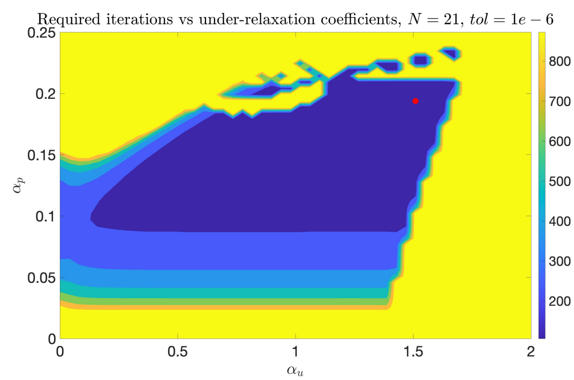


Fig. 5: Number of iterations required for convergence as function of α_p and α_u. The minimum is highlighted with a red dot. The yellow region denotes divergence or very slow convergence

Since the gradient of the function is approximately null near its minimum (dark blue region in the figure), a grid search on a 10×10 values of αs yields an initial guess for the Nelder-Mead which is approximately the very same minimum later found by the optimization method.

IV. Discussion

The SIMPLE algorithm proves to be sufficiently accurate to yield a reliable solution even on a grid made up of $N = 21$ nodes. With a tolerance of $tol = 1e-6$, it took 249 iterations to reach convergence. In fig. 2 it is noticeable how the method converges rapidly after 100 iterations circa. Additionally, despite using a coarse grid, the numerical solution does not differ significantly from the exact one. Nevertheless, the algorithm showed a certain instability: with $\alpha_p = \alpha_u = 0.1$, for $N > 50$, the numerical solution is no longer stable and diverges. The under-relaxation coefficients need to be consequently re-tuned. In particular, as figure 5 shows, the range of α_p values that leads to convergence of the algorithm is significantly narrower than the range of possible α_u values[3]. It is therefore the value of α_p that must be chosen accurately in order to avoid divergence of the solution. The run of the algorithm varying N showed that the initial values of $\alpha_p = 0.1$ is too large to control the stability, and that the greater N, the smaller α_p needs to be to ensure stability of the solution.

The errors in table I are restrained: the vector $\boldsymbol{\Delta e}_u$ has practically constant values from the first to last grid node. On the contrary, the $\boldsymbol{\Delta e}_p$ has increasing values: this is partially owed to the fact that the boundary condition on the outlet is $p = 0\,\mathrm{Pa}$, and hence in Eq. 15 the denominator tends to 0 for the nodes near the outlet. Nevertheless, the error $\boldsymbol{\Delta e}_p$ never exceeds 8.3%, which is an acceptable result for such a small N. The value of FMB is negligible (order of the $\varepsilon_{machine}$), according to the fact that the SIMPLE method implemented is conservative.

The study of the under/over-relaxation coefficients produced the values $\alpha_p = 0.1944$ and $\alpha_u = 1.556$ to reach the usual tolerance in only 105 iterations. In this case α_u is then called an *over*-relaxation coefficient: for the given problem, it increases the convergence speed, without affecting stability.

V. Summary

The errors obtained comparing the numerical solution and the exact solution demonstrate the accuracy of the SIMPLE algorithm in such a simple case. It could be argued that the computational cost of the optimization problem concerning the two under-relaxation coefficients greatly exceeds the benefit of the reduced number of iterations. However, the found values may be of use for a further work on the same flow geometry or on a similar one and thus it could be possible to benefit from the results obtained from the present discussion.

References

[1] M. H. W. Jeffrey C. Lagarias James A. Reeds and P. E. Wright, "Convergence properties of the nelder-mead simplex method in low dimensions," *Society for Industrial and Applied Mathematics*, vol. 9, Dec. 1998.

[2] H. Versteeg and W. Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*. Pearson Education Limited, 2007, ISBN: 9780131274983. [Online]. Available: https://books.google.ch/books?id=RvBZ-UMpGzIC.

[3] Note the different range for the two axes in figure.