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Iteration error estimation in Computacional Fluid Dynamics using a new Empirical Estimator

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Abstract. This study aims to improve the techniques for estimates of iteration errors, through the use of a new estimator. The new estimator provides estimates of iteration errors based on variables convergence rate. Its performance was tested in two one-dimensional steady-state mathematical models: Poisson's equation and advection-diffusion equation, discretized through the Finite Difference Method (FDM). The numerical schemes used were CDS and CDS-2 (Central Difference Scheme), for first and second order derivatives, respectively. The systems of equations resulting from the discretizations were solved by the TriDiagonal Matrix Algorithm (TDMA) and Gauss-Seidel (GS). The solver TDMA was used to obtain the exact solution and the solver GS to estimate the errors at each iteration. Two variables were chosen to evaluate the results: function value at the central grid point (local) and the average value of the function (global). The codes were implemented in Fortran 95, with quadruple precision, in the Microsoft Visual Studio Community 2013. The results showed that the proposed estimator has a performance similar to the ones already existing in the literature and that it is necessary to improve the estimates in the initial ranges of the iterative process and in the final ranges, where the rounding error becomes more significant.

Keywords: Iteration Error, Computacional Fluid Dynamics, Verification.

1 Introduction

According to Fortuna [1], the Computacional Fluid Dynamics (CFD) studies computacional methods to simulate fluid moviments phenomena with or without heat exchange. However, these simulations are subjected to numerical errors of different sources, e.g., discretization, round-off, programming and iteration. Then, for Roache [2], verification techniques are used to assess the accuracy and reliability of solutions obtained by numerical simulations. These techniques include ways to estimate and reduce numerical errors.

The iteration errors are mainly caused by the use of iterative solvers, multigrid methods, nonlinearities present in the equations and the use of segregated methods to solve systems of equations. In this work, a new iteration error estimator is proposed and its effectiveness is evaluated with respect to its accuracy. The new estimator is convergence rate based and it is tested in two mathematical models: one-dimensional Poisson's equation and one-dimensional advection-diffusion equation. The FDM was employed to solve this equations with second order schemes. The TDMA solver was used to obtain the direct solution of the variables of interest and the GS solver was used to estimate the errors at each iteration. Two variables of interest were chosen: function value at the domain central point (local) and averaged function value (global).

2 Methodolgy

This section presents the mathematical models characteristics, the numerical schemes used to discretize it and the new empirical estimator used to estimate the iteration errors.

2.1 Mathematical models and discretization

The first model is a one-dimensional heat diffusion equation, in a steady state with heat generation, called Poisson's equation, given by

$$\frac{d^2T}{dx^2} = 12x^2, \tag{1}$$

with Dirichlet-type boundary conditions $T(0) = 0$ e $T(L) = 1$, and $L = 1$.

This model was discretized using FDM, with second order approximations (Central Difference Scheme - CDS-2) and a uniform grid (Fig. 1),

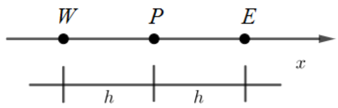

Figure 1. One-dimensional uniform grid.

which resulted in

$$\frac{(T_W + T_E - 2T_P)}{h^2} = 12x_P^2, \tag{2}$$

that represents the discretized form of the mathematical model of the eq. (1). The comparision with

$$a_P T_P = a_W T_W + a_E T_E + b_p \tag{3}$$

provides the coefficients (a_P, a_W, a_E) and the source therm (b_p) of the interior grid points. The border points coefficients and source therm are obtained by applying the boundary conditions.

The second model consists of one-dimensional advection-diffusion, in a steady state, which equation is given by

$$Pe\frac{dT}{dx} = \frac{d^2T}{dx^2}, \tag{4}$$

where Pe is the Peclet number, with the same Dirichlet-type boundary conditions of the first problem, $T(0) = 0$ e $T(L) = 1$, $L = 1$. This equation was also discretized using the FDM, with second order schemes, namely, central difference (CDS and CDS-2) and a uniform grid:

$$Pe\frac{(T_E - T_W)}{2h} = \frac{(T_W + T_E - 2T_P)}{h^2}. \tag{5}$$

Once again, by comparing eq. (5) with the eq. (3), it is obtained the coefficients (a_P, a_W, a_E) and the source therm (b_p) of the interior grid points. The boarder points coefficients and source therm are obtained by applying the boundary conditions.

The variable of interest function value at the central point of the grid $(T(1/2))$ was obtaneid from the above procedure and the averaged function value (T_m) was obtained from the trapezoidal rule.

2.2 Iteration Error Estimation

An important feature of the iteration error is that, if the iterative process has monotonic convergence, the iteration error $(E(\phi_k))$ of any variable ϕ decreases on a logarithmic scale and it tends to a constant slope as the number of iterations increases $(k \to \infty)$ [3]. This slope is called asymptotic order (p_L). It can be represented by the equation

$$E(\phi_k) = C10^{-kp_L}, \tag{6}$$

where C is a constant.

It is known that the iteration error estimation $U(\phi_k)$ is given by the difference

$$U(\phi_k) = \phi_\infty - \phi_k, \tag{7}$$

where ϕ_∞ is the exact solution of the discretized equations for the chosen grid and ϕ_k is the numerical solution in the k-th iteration.

In order to obtain the error estimates, the eq. (6) is compared to the eq. (7) and three consecutive iterative levels are considered k_1, k_2, e k_3, with com $k_1 < k_2 < k_3$. Solving the resulting system and manipulating the terms algebraically, it obtains the expression of the new empirical estimator

$$U(\phi_{k_2}) = \frac{(\phi_{k_2} - \phi_{k_1})}{\psi - 1}, \tag{8}$$

where ψ is the convergence rate given by

$$\psi = \frac{\phi_{k_2} - \phi_{k_1}}{\phi_{k_3} - \phi_{k_2}}. \tag{9}$$

Initially, the numerical value of the converged solution Φ (exact solution of the discretized system) was calculated using the TDMA solver. Then, using the GS solver, the estimates were obtained, iteration by iteration, using the estimators of Roy e Blottner [4], Martins and Marchi [5], Ferziger and Perić [6] and the empirical (this work), to be compared with the iteration error, given by the difference between the exact solution of the discretized system and the solution in the present iteration, as follows

$$E(\phi_k) = \Phi - \phi_k. \tag{10}$$

Numerical solutions were obtained for grids with $N = 64, 256$ and 1024 elements. The convergence criterion chosen to end the iterative process was the machine error for each problem size. The effectiveness θ given by

$$\theta = \frac{U(\phi_k)}{E(\phi_k)} \tag{11}$$

was used to measure the reliability of the estimators. For Zhu [7], if this value is close to 1, the estimate is said to be accurate and if it is greater than or equal to the unit, it says that the estimator is reliable.

The computacional codes were implemented in the Fortran 95 language, with quadruple precision in the Microsoft Visual Studio Community community 2013 and were executed on a PC with a 64-bit processor, Intel(R) Core(TM) i7-6700, 3.40 GHz and 16 GB of RAM, with Windows 10 Pro operating system.

3 Results and discussion

This section contains the results of applying the new estimator to the proposed problems. The results presented are the case of $N = 1024$ grid elements. The results for cases of $N = 64$ and $N = 256$ were similar to those presented.

For the one-dimensional Poisson's equation, the results obtained for the local variable ($T(1/2)$) are shown in Fig. 2. According to this figure, it is possible to observe that, in general, all the estimators presented similar performance when predicting the iteration error for this case. However, the proposed estimator proved to be reliable ($\theta \geq 1$) in only 56% of iterations, which suggests a further study of the estimates obtained.

Thus, when separating the estimates into intervals, it is possible to observe, still in Fig. 2, that the inicial and the final ranges of iterations have inaccurate estimates. At the final range, it is due to the more significant presence of the round-off error in these iterations. Observing the initial range of iterations (about 10% of the total iteration number), represented in Fig. 3, it can see that the estimators also do not present good predictions of the iteration error, sometimes overestimating it, sometimes underestimating it. And once again, at the initial range of about 13% of the total iterations, all the estimators underestimate the iteration error, as shown in Fig. 5.

The results for the averaged function value (T_m) were similar. Figure 4 shows the error and the estimatives for all iterations needed until the machine error is achieved. In this case, it is also possible to notice that the presence of round off-errors undermines the error predictions at the end of the iterative procedure.

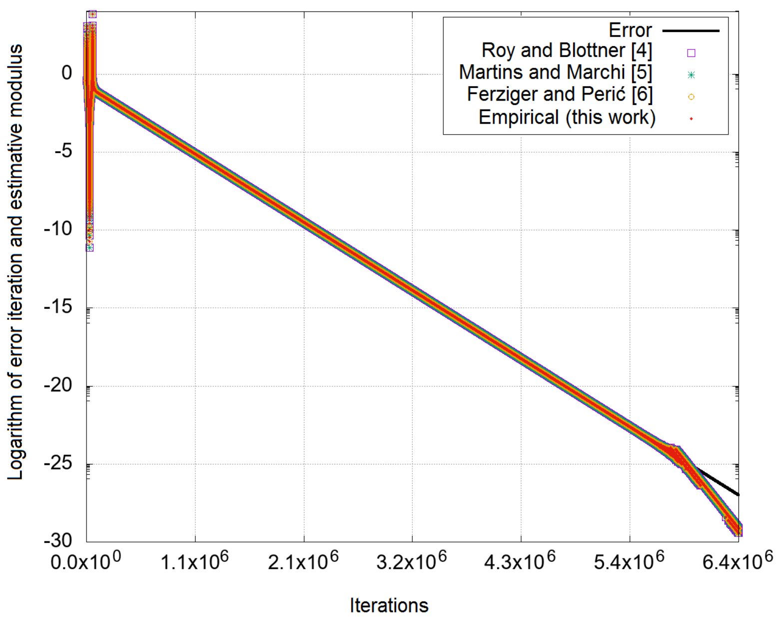

Figure 2. Estimations and iteration error at each iteration for the variable $T(1/2)$, Poisson's equation, with $N = 1024$, for all the iterations needed to achieve the machine error.

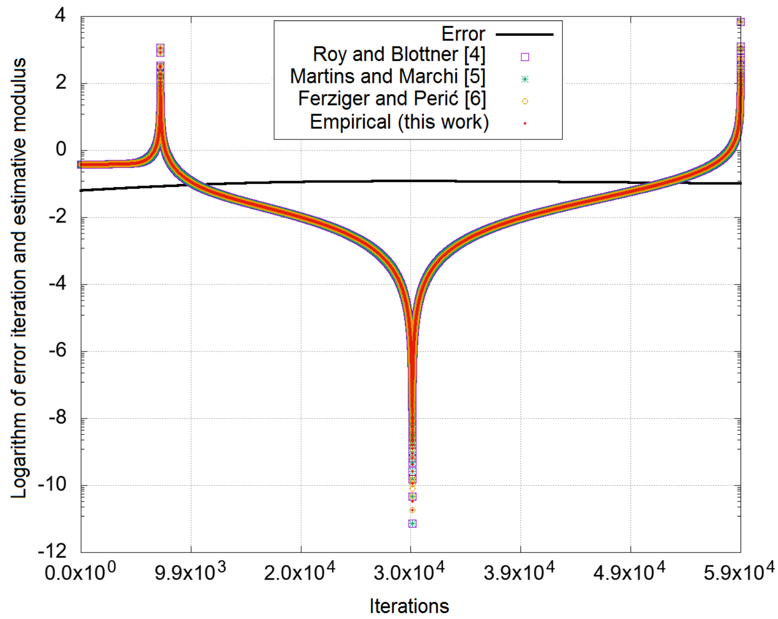

Figure 3. Estimations and iteration error at each iteration for the variable $T(1/2)$, Poisson's equation, with $N = 1024$, for the initial range of iterations.

For the second model, the advection-diffusion equation, similar results were found. Analyzing the totality of iterations necessary to achieve the machine error, for both the $T(1/2)$ variable and the T_m variable, the estimates obtained were considered accurated, as shown in Figs. 6 and 7.

For this problem the proposed estimator proved to be reliable ($\theta \geq 1$) in 64% of the total iterations. Considering the final range of the iterative process, it was observed that, for the variable T_m, (Fig. 7) the round-off errors are more significant, interfering in the calculations of the estimates and in its accuracy.

In the case of the variable $T(1/2)$, when observing the initial range of iterations, it can be noticed that the estimators underestimate the iteration error, as shown in Fig. 8. The same was not observed for the variable T_m.

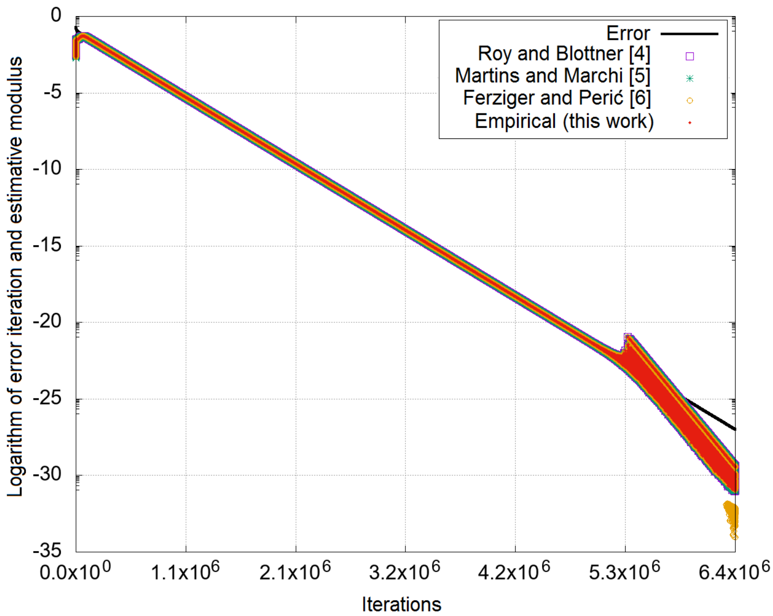

Figure 4. Estimations and iteration error (in logarithmic scale) at each iteration for the variable T_m, Poisson's equation, with $N = 1024$, for all the iterations necessary to achieve the machine error.

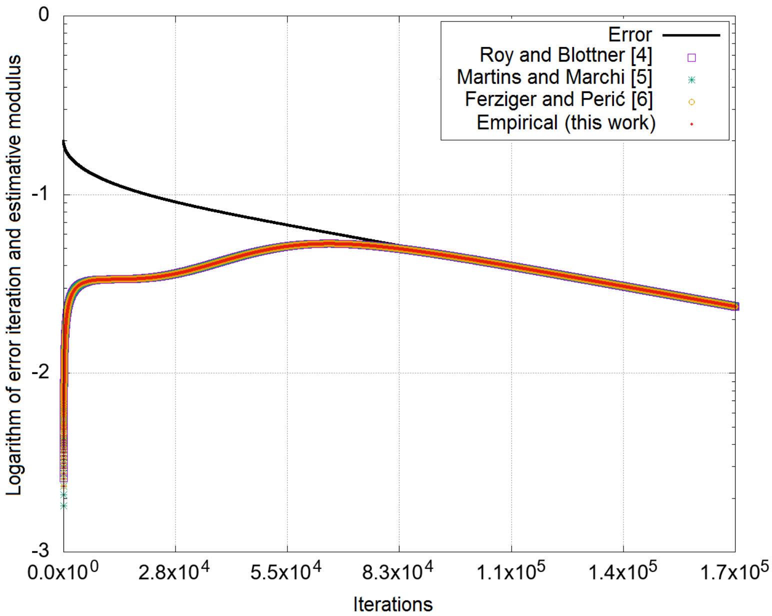

Figure 5. Estimations and iteration error (in logarithmic scale) at each iteration for the variable $T(1/2)$, Poisson's equation, with $N = 1024$, for the initial range of iterations.

4 Conclusions

In this work, a new empirical estimator for iteration errors was proposed. This estimator is based on the ψ convergence rate and was tested on two proposed models: Poisson's equation and advection-diffusion equation. The models were discretized using FDM and central numerical approximations of the first and second order derivatives of the differential equations with central difference, CDS and CDS-2, respectively. The trapezoidal rule was used to calculate the global variable. The solver used to obtain the exact solution was TDMA, while for the iterative process and calculation of estimates the Gauss-Seidel solver was used.

For both models proposed, it was observed that, for the variable $T(1/2)$, the estimates at the initial and at the final ranges are less accurate when compared to the estimates obtained for the variable T_m, at the same ranges. As

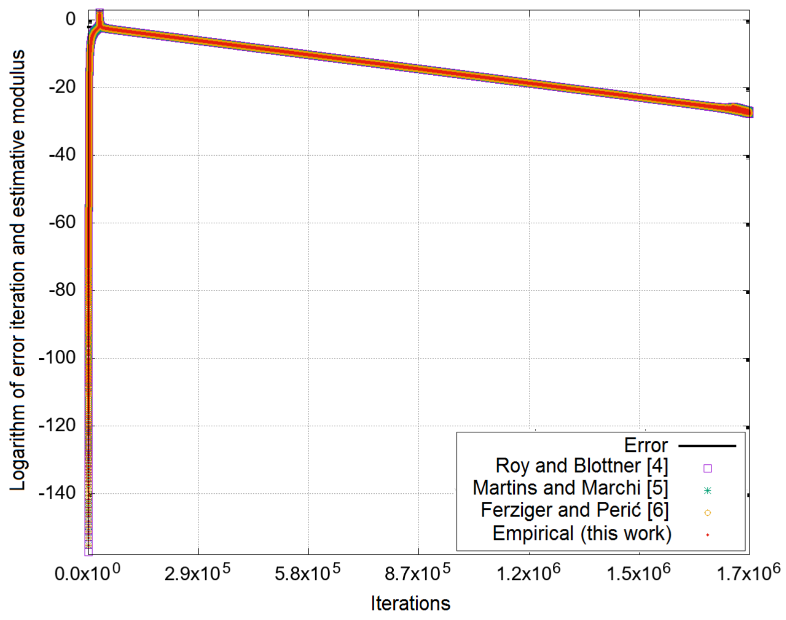

Figure 6. Estimations and iteration error (in logarithmic scale) at each iteration for the variable $T(1/2)$, of the advection-diffusion equation, with $N = 1024$, for all the iterations necessary to achieve the machine error

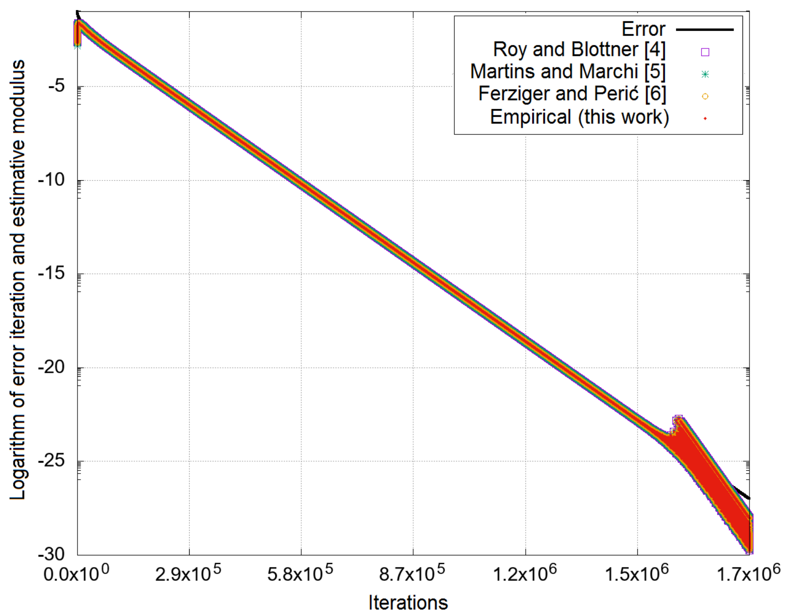

Figure 7. Estimations and iteration error (in logarithmic scale) at each iteration for the variable T_m, of the advection-diffusion equation, with $N = 1024$, for all the iterations necessary to achieve the machine error

for the parameter θ, the estimator proved to be more reliable ($\theta \geq 1$) at the second model (in 64% of iterations) than at the first one (56% of iterations).

The results also show that, for the two proposed problems, the new empirical estimator performed similarly to the estimators found in the literature. And, because it is easier to formulate and implement than others, it can be chosen to estimate iteration errors of these problems. In general, the estimates obtained were accurated for the most part of the iterations, however, it is suggested to improve the estimates in the initial and final ranges of the iterative process. In the mentioned ranges, none of the tested estimators had accurate estimates.

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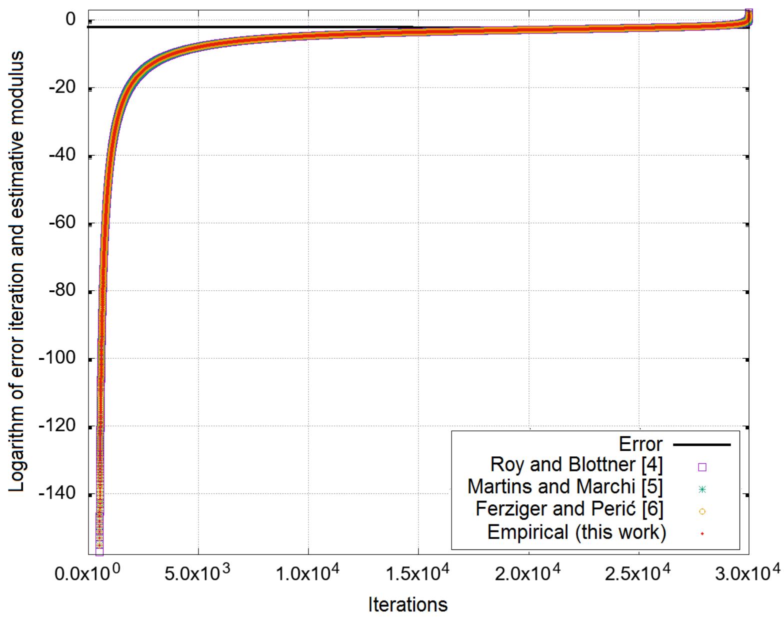

Figure 8. Estimations and iteration error (in logarithmic scale) at each iteration for the variable $T(1/2)$, advection-diffusion equation, with $N = 1024$, for the initial range of iterations.

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