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Quasi-*a priori* truncation error estimation and higher order extrapolation for non-linear partial differential equations

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A B S T R A C T

In this paper, we show how to accurately estimate the local truncation error of partial differential equations in a quasi-*a priori* way. We approximate the spatial truncation error using the τ-estimation procedure, which aims to compare the discretisation on a sequence of grids with different spacing. While most of the works in the literature focused on an *a posteriori* estimation, the following work develops an estimator for non-converged solutions. First, we focus the analysis on one- and two-dimensional scalar non-linear test cases to examine the accuracy of the approach using a finite difference discretisation. Then, we extend the analysis to a two-dimensional vectorial problem: the Euler equations discretised using a finite volume vertex-based approach. Finally, we propose to analyse a direct application: τ-extrapolation based on non-converged τ-estimation. We demonstrate that a solution with an improved accuracy can be obtained from a non-*a posteriori* error estimation approach.

1. Introduction

In the past decades, due to the increasing demand for complex fluid flow simulations, great effort has been done by the Computational Fluid Dynamics (CFD) community in order to increase the accuracy and reduce the calculation costs. It is now well understood that numerical errors play a crucial role in the balance between accuracy and computational time.

The errors committed in solving numerically a set of Partial Differential Equations (PDE) can be broadly classified into three categories:

- Discretisation errors (DE). These errors arise when the mathematical problem is solved numerically on discrete domains. The discretisation error is defined as the difference between the exact solution to the PDE and the exact solution to the discretised PDE.
- Truncation errors (TE). They act as a source for the DE through the *discretisation error transport equation* (DETE, see Roy [1]). The truncation error is defined as the difference between the discrete and continuous PDE both applied to the exact solution of the mathematical model.
- Iteration errors (IE). Iterative error is present in a solution when an iterative procedure is used to solve the discrete equations. The iteration error is defined as the difference between the exact solution to the discrete equations and the solution at the current iteration.

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The estimation of the numerical error provides valuable information that can be used in different applications. The truncation/discretisation errors are directly related to the mesh distribution, and thus, a careful estimation might be employed in mesh generation/mesh adaptation. These estimations might also be used to increase the accuracy of the partial differential equation solution. However, the accurate evaluation of numerical errors is a challenging task.

The most commonly used strategy to study discretisation errors is based on Richardson extrapolation [2]. Richardson extrapolation is derived from a power series expansion of the numerical solution expanded about the exact solution to the PDE, thus, it assumes a smooth solution in the asymptotic range. The success of Richardson extrapolation [3–8] is due to its generality as it can be applied to any set of PDE independently of the numerical scheme. Because it is an *a posteriori* error estimator, the method is not code intrusive and relatively easy to implement. However, this approach requires the computation of at least three numerical solutions, on grid of different spacing, in order to obtain the expression of the leading term of the Taylor series. Therefore, this makes this method hardly suitable for complex three-dimensional industrial applications. Another family of discretisation error estimators comes from the solution of auxiliary equations like the DETE (Shih [9]) or the adjoint equations [10,11]. While these methods proved to be very reliable estimators, they however suffer from a very high computational cost and are code intrusive.

The analysis of truncation error can be done in two manners. First, by deriving analytically the Taylor series expansions [12–16]. This approach allows for an *a priori* analysis and gives very valuable information on the quality of the mesh and on the accuracy of the numerical scheme. However, the complexity of the related expressions for general three-dimensional non-linear problems together with the dependence on the numerical scheme have prevented the expansion of this approach. The second way of studying the truncation error arised from the multigrid theory [5] and is known as τ-estimation. Given an exact (converged) solution to the discrete PDE, this method relies on the evaluation of the discrete PDE operator on a coarser mesh [4,17–20]. Because of its strong relation to mesh quality and accuracy, a careful estimation can yield an increase in the order of the scheme (procedure known as τ-extrapolation) and/or a reliable mesh adaptation indicator [21,22]. However, truncation error estimation by τ-estimation has always been used *a posteriori*, from converged solutions.

Here, we propose to extend the work of Bernert [18], Fulton [19] and Fraysse et al. [20,23], who focused their study on converged solutions, to non-converged solutions. We develop a truncation error estimator and derive all of the necessary conditions to ensure accuracy. We discuss the conditions for an accurate estimation as follows: the order of the transfer operators acting in the truncation error estimator formula as a function of the order of the numerical scheme, the influence of distortion and the influence of the iteration error on the accuracy of the estimation. In a second step, a τ-extrapolation formula is presented accounting for the above conditions. Whereas non-converged τ-estimation/τ-extrapolation are performed on one- and two-dimensional scalar equations using a finite difference method, a concrete application using the finite volume vertex-based DLR TAU-Code [24] for the Euler equations is subsequently presented.

The present paper is organised as follows. First, we derive in Section 2 the mathematical formulation and the conditions to be fulfilled for an accurate τ-estimation/τ-extrapolation for non-converged solutions. In Sections 3.1 and 3.2, we study the accuracy of the τ-estimation/τ-extrapolation for non-converged solutions of one-dimensional and two-dimensional reference problems. We present the difficulties associated with this methodology as well as different solutions. Finally, in Section 4, we address more realistic configurations with Euler equations on quadrilateral- and triangle-based grids.

2. Problem formulation

Let us consider the discretisation of a partial differential equation on a grid Ω^h indexed by a mesh size parameter h of the following form:

$$\mathcal{A}^h(u^h) = f^h := \mathcal{I}^h f \tag{1}$$

where, $\mathcal{I}^h$ represents a continuum-to-grid Ω^h transfer for the specified f (e.g., pointwise restriction) and u^h represents the converged numerical solution. The discretisation error ϵ^h and the local truncation error τ^h corresponding to Eq. (1) are defined as follows:

$$\begin{aligned} \epsilon^h &= \mathcal{I}^h u - u^h \\ \tau^h &= \mathcal{A}^h(\mathcal{I}^h u) - \mathcal{I}^h \mathcal{A}(u) \end{aligned} \tag{2}$$

In addition to the discrete equation Eq. (1) and considering a full approximation storage multigrid algorithm [5], the coarse grid equation may be written as follows:

$$\mathcal{A}^H(\hat{u}^H) = \mathcal{A}^H(\hat{\mathcal{I}}_h^H \tilde{u}^h) + \mathcal{I}_h^H(f^h - \mathcal{A}^h(\tilde{u}^h)), \qquad \hat{u}^H \approx \hat{\mathcal{I}}_h^H(\epsilon_{it}^h + \tilde{u}^h) \tag{3}$$

corresponding to the discrete equation on a coarser mesh Ω^H, with a mesh ratio of $\rho = h/H < 1$. In Eq. (3), $\tilde{u}^h$ is the current approximation of the solution (relaxed on the fine grid and not necessarily converged), $\epsilon_{it}^h = u^h - \tilde{u}^h$ is the fine grid iteration error, for which its high frequencies must be smoothed, $\hat{I}_h^H$ represents the fine to coarse transfer operator of the solution, whereas I_h^H represents the fine to coarse transfer operator of the residual. Note that these restriction operators are not necessarily identical. Similarly, introducing the *relative truncation error* τ_h^H, Eq. (3) may be written as follows: