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Letter to the Editor

Comment on "A procedure for the estimation of the numerical uncertainty of CFD calculations based on grid refinement studies" (L. Eça and M. Hoekstra, Journal of Computational Physics 262 (2014) 104–130)

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Eça and Hoekstra [1] proposed a procedure for the estimation of the numerical uncertainty of CFD calculations based on the least squares root (LSR) method. We believe that the LSR method has potential value for providing an extended Richardson-extrapolation solution verification procedure for mixed monotonic and oscillatory or only oscillatory convergent solutions (based on the usual systematic grid-triplet convergence condition R). Current Richardson-extrapolation solution verification procedures [2–7] are restricted to monotonic convergent solutions $0 < R < 1$. Procedures for oscillatory convergence simply either use uncertainty estimate based on average maximum minus minimum solutions [8,9] or arbitrarily large factors of safety (F_S) [2]. However, in our opinion several issues preclude the usefulness of the presented LSR method: five criticisms follow.

1. The solution verification literature needs technical discussion in order to put the LSR method in context. The LSR method has many options making it very difficult to follow. Fig. 1 provides a block diagram, which summarizes the LSR procedure and options, including some of which we are in disagreement. Compared to the grid-triplet and three-step procedure followed by most solution verification methods (convergence condition followed by error and uncertainty estimates), the LSR method follows a four-grid (minimum) and four-step procedure (error estimate, data range parameter Δ_ϕ, F_S, and uncertainty estimate).
2. Equation (2) provides the definition of R, although not used in the LSR method. The LSR method uses un-weighted and weighted LSR estimates of the order of accuracy p [equations (8) and (12), respectively] to define three possible convergence condition options, as shown in Fig. 1. Convergence condition options [P2] and [P3] are unacceptable since

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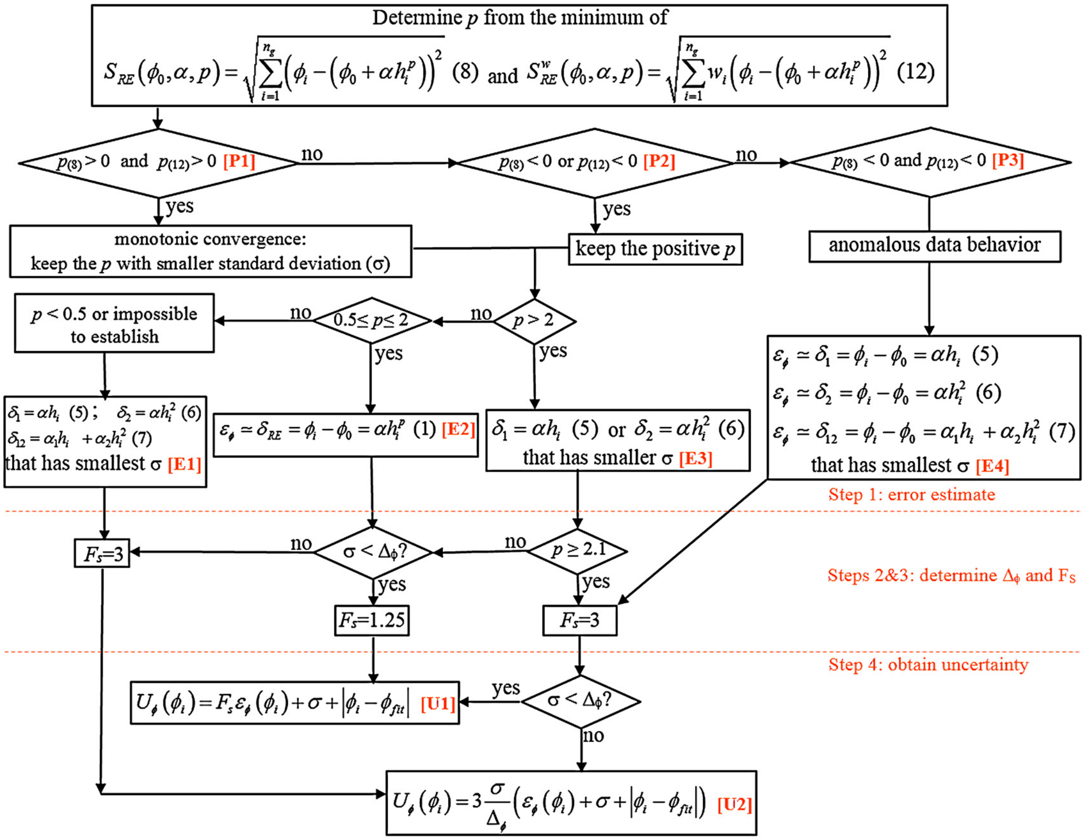

Fig. 1. Block diagram of the LSR method.

one or both p are negative and not considered in following discussion. If p is negative, the equation (1) power series expansion used for the error estimate is divergent and unusable. Since the LSR method uses at least four solutions, a minimum of two grid-triplet convergence conditions are available. Convergence based on R and restricted to monotonic or oscillatory convergent solutions is required along with positive p. Otherwise finer or better quality grids are required for acceptable solutions and solution verification. In addition, the use of equation (12) without providing validation is questionable as the weights defined in equation (16) depend on grid refinement ratio: larger grid refinement ratio leads to larger and smaller weights for the finer and coarser grids, respectively.

3. For $p > 0$, three error-estimate options are used depending on $p < 0.5$ or impossible to establish [E1], $0.5 \le p \le 2$ [E2] or $p > 2$ [E3], as shown in Fig. 1. Option [E2] uses the usual one-term Richardson extrapolation for the error estimate δ_{RE}. Options [E1] and [E3] discard the estimated p and use equations (5)–(7) and equations (5) or (6) for the error estimate, respectively, depending on which one has the smallest LSR standard deviation σ. Options [E1] and [E3] assume that the order of accuracy is one or two or mixed one and two. Equation (5) is equation (1) with $p = 1$, equation (6) is equation (1) with $p = 2$ and equation (7) seems to be a form of the two-term Richardson extrapolation error estimate with $p^{(1)} = 1$ and $p^{(2)} = 2$ [9]. These error estimates are not derived or sufficiently validated. References [3,4] show the usefulness of the effectivity index (absolute value true error/error estimate) in deriving and validating alternative error estimates. Reference [3] shows that δ_{RE} times P (the ratio of the estimated to theoretical orders of accuracy) provides a better error estimate than δ_{RE}.
4. For [E1] and [E3] if $p \ge 2.1$, $F_S = 3$. For [E2], $F_S = 1.25$ or 3 depending on whether $\sigma < \Delta_\phi$ or not. The uncertainty estimate has two options depending on whether $\sigma < \Delta_\phi$ or not, as shown in Fig. 1. These uncertainty estimates are not derived or sufficiently validated. Unlike the factor of safety [3] and grid convergence index [2] methods, the LSR uncertainty estimate options are not proportional to F_S, which makes validation difficult using the actual factor of safety F_{SA} (ratio of uncertainty estimate to the magnitude of true error) approach [3]. Including uncertainties due to σ and Δ_ϕ may make the uncertainty estimate overly conservative, as indicated by the analytical benchmark test cases. The error and uncertainty estimates are not continuous and therefore have undesirable jumps in values depending on p and on p, σ and Δ_ϕ, respectively.
5. Validation uses three analytical benchmarks and three numerical test cases. The analytical benchmark test cases are useful for validation. The exact error ratio evaluated similarly as F_{SA} for 144 LSR studies has averages of about 1.6 and 5.5 for grid refinement ratio $h_i/h_1 = 1$ and 4, respectively, which are undesirably large such that the LSR method

achieves 100% reliability. The numerical test cases need to demonstrate achievement of the asymptotic range to be useful for validation. Monotonic convergence of all solution and verification variables for several multiple grid triplets is a possible criterion [10]. Some numerical test case variables do not converge and many uncertainty estimates show oscillatory convergence; therefore, the results cannot be used for validation. Alternatively, the LSR method calculates reliability based on the consistency of uncertainty estimates for different grid sets but similar grid refinement ratios. For their 268 LSR integral variable numerical test case studies, our estimate is 88% consistency; however, consistency of uncertainty estimates does not provide evidence of validation.

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