Hemez, Francois, 2020, Robust estimation of truncation-induced numerical uncertainty, Proceedings of the Society for Experimental Mechanics Series, IMAC, A Conference and Exposition on Structural Dynamics, Houston, 10 February 2020 through 13 February 2020, Code 245349, pp.223–232.

Abstract Truncation error is ubiquitous in computational sciences, yet, rarely quantified and often ignored altogether. By definition, it is the difference between the exact-but-unknown solution of continuous equations that one wishes to solve, such as conservation laws, and what the computational software (finite elements, finite volumes, etc.) calculates. We contend that the commonly-accepted representation of truncation error as a single-term power-law (i.e., $\varepsilon(\Delta x) = \beta \cdot \Delta x p$ where Δx is the level of mesh resolution in the calculation and p is the accuracy of the numerical method) is inadequate and can lead to an erroneous quantification. The remedy proposed is to model this error as a series expansion of integer-valued powers (i.e., $\varepsilon(\Delta x) = \beta_1 \cdot \Delta x_1 + \beta_2 \cdot \Delta x_2 + \cdots + \beta_N \cdot \Delta x_N$ where the expansion order N is unknown and potentially infinite). This representation is consistent with the theoretical form of truncation error derived from Modified Equation Analysis. Because N and the regression coefficients β_k are not known, we further propose to use an info-gap model to numerically derive bounds of truncation error. These bounds, $\|y_{\text{Exact}} - y(\Delta x)\| \leq U(\Delta x)$, would express the worst-case error between what is calculated at resolution Δx) and what is exact but unknown. Reporting such bounds is essential to assess the quality of a numerical simulation, much like an experimental uncertainty should accompany a measurement. The discussion proposed is, for the most part, conceptual and future efforts will focus on the numerical implementation of these ideas.

Keywords Mesh refinement; Robust bounds; Solution uncertainty; Truncation error.

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