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PURIFICATION OF CONVERGENCE AN APPROACH TOWARDS RELIABLE ERROR EVALUATION

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In view of the everyday increasing size and complicatedness of structural systems, implementation of approximate computations and specifically computational mechanics methods are essential in the study of structural systems behaviours. The quality of the computations would rather be evaluated, in order to prevent computational shortcomings and lack of sufficient accuracies in the consequent engineering designs, and scientific/engineering decision makings. Accuracy is the major issue defining the quality of approximate computations; and in this regard, it is decades that convergence is broadly accepted as computations most important necessity, guaranteeing asymptotic approach to the exact results. Nevertheless, for many practical cases, e.g. analysis and design of nuclear power plants, besides reliable approach to the exact results, an idea, about the amount of the approximations, would rather be available. In spite of the many *a posteriori* and *a priori* error estimators, introduced in the last decades, a conventional simple approach to evaluate the computational errors is repeating the analyses with smaller values of the algorithmic parameters, e.g. element size, integration step size, etc. (generally half), and comparing the results, considering the difference of the results as an indicator for the inaccuracies. This approach and many *a priori* estimations are successful, when convergence occurs in a proper manner, i.e. the logarithm of errors decrease with respect to the logarithm of the algorithmic parameter, as a line with positive integer slope (see Fig. 1). Considering the fact that for real computations, convergence may occur improperly, i.e. either the above mentioned line does not exist in the convergence plot, or the slope is not precisely equal to a positive integer, the objective of this paper is to study the reasons of improper convergence and introduce an approach to eliminate them.

The nature of the problem at hand (for instance the nonlinearity and discontinuity) and the features of the computational method can cause the linear section of the convergence occur in regions of the convergence plot affected by round-off, where, the proper convergence disappears. Accordingly, by forcing the convergence to occur properly for larger values of the algorithmic parameter, improper convergence can be prevented, and proper convergence would be practically achievable.

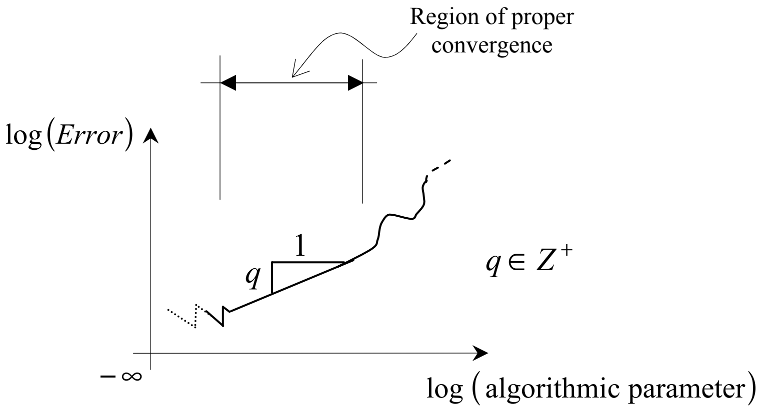

Figure 1. Typical convergence of approximate responses, with proper convergence apparent for practical values of the algorithmic parameter

Based on the Taylor series expansion of an arbitrary approximate computation with respect to the algorithmic parameter, and Richardson extrapolation, an approach, to guarantee proper convergence will be proposed for the first time in this paper (in view of the mathematical details, the approach is addressed as a *purification* methods). The effects of the proper convergence on the evaluation of errors will also be discussed, via examples from finite element and time integration analyses, and finally, reliable enhancements of analyses results towards desired accuracies would be briefly addressed. Though the study is not finalized yet, the proposed approach seems successful from the points of view of reliability of error estimation and the computational costs.

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