Ramsay Maunder
ASSOCIATES
Finite Element Specialists and Engineering Consultants

Prepared: 31rd May 2016

Raising your Game with Good Simulation Governance

Angus Ramsay

1. Introduction

As anyone who attended last year's NAFEMS World Congress (NWC2015) will have observed, the sophistication of computational simulation software and hardware is moving ahead at an extremely rapid pace. In watching presentations and speaking to delegates, a new variant on a familiar phrase was heard for the first time by the author - ***'the democratisation of simulation'***.

There are obvious significant commercial advantages for engineering companies to embrace and utilise numerical simulation in their design processes. If the democratisation of simulation means the development of bespoke software tools for the design of a particular product that encodes sound simulation governance principles then this is a laudable aim. If, on the other hand, it means the selling of cheap and cheerful generalist finite element software then that is another matter and raises the spectre of all sorts of verification issues with the software and the possibility of finite element malpractice by the user.

Peter Bartholomew's interesting article, [1], reminded readers of John Robinson's thoughts of some 40 years ago. John, one of the founders of NAFEMS, noted in the early 1970s *"… that both coding and modelling errors were commonplace and only time separated the [simulation] community from computer-aided catastrophe [CAC]"*. Just such an incident of CAC occurred in the early 1990s when the Sleipner Platform A sank in a Norwegian Fjord, [2]. There is an idea, expressed elegantly by Henry Petroski, [3], that major failures (at least for bridges) have been observed to be spaced at approximately thiry year intervals. The reason for this is postulated as being the result of a ***'communication gap'*** between one generation of engineers and the next; the *raison d'être* why structural members or components were designed in the way they were, is lost. It is for this reason that the author has chosen to revisit the Sleipner incident in the sixth NAFEMS Benchmark Challenge.

In the simulation industry we are facing a somewhat more severe example of Petroski's generation gap. The simulation 'experts' of today are, often as not (as pointed out in the NAFEMS overview of democratisation [4]) either early [simulation] pioneers or direct disciples of them. They have often written finite element software and are familiar with the practices of good simulation governance. Such specialists are becoming rarer as the opportunities to conduct research is declining. For this reason alone the development of bespoke software tools that encode not only sound simulation governance principles, but also a company's design knowhow, is certainly a safe and efficient way forward for the industry.

In this environment, the practising engineer needs to exercise great care in his/her work. The engineer may have little background in simulation beyond a vendor's training course. His/her manager may well not have any background in numerical simulation either and in some cases might not even be an engineer! Whilst the ***European Court of Human Rights*** would, no doubt, baulk at such a retrograde idea, the practising engineer might best be served by adopting the Napoleonic Code of Jurisprudence for the results of a numerical simulation:

Guilty until Proven Innocent!

2. Verification and Validation

A sound engineering design is supported on the 'three pillars' of *numerical simulation*, *mathematical models* and *physical experiments* - figure 1. The goal of good *simulation governance,* [5], is to match numerical simulation with physical experiments. This cannot be done in any rational manner without consideration of the mathematical models that govern the physics of the problem. Whilst the two terms, at first sight, may appear to be almost synonymous, the processes of verification and validation have distinct meanings, [6]. They provide the foundations for engineering design by tying together the three pillars of engineering design. Although equally important processes, this article concentrates on the process of verification which lies in the control of the simulation engineer.

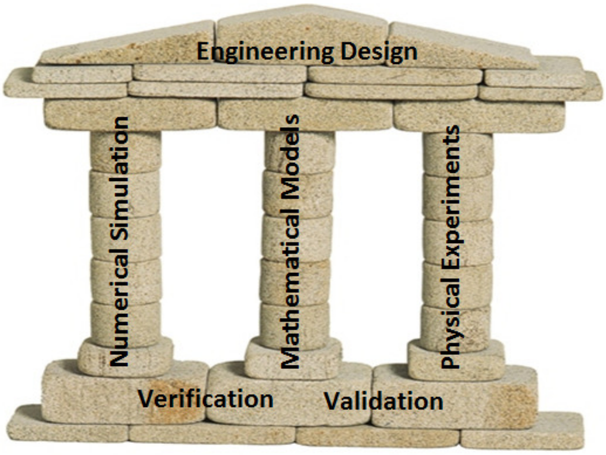


Figure 1: Three pillars of engineering design on the foundations of Verification and Validation

Verification

Verification can be considered as two distinct parts:

1) **Software Verification** – here problems with known theoretical solutions are analysed with the software to ensure that it can recover the theoretical solution. This uncovers software bugs and educates the engineer on how the solution procedure used in the software performs, e.g., what level of mesh refinement is required to obtain good engineering accuracy.
2) **Solution Verification** – here the actual problem, which generally has no known theoretical solution, is studied to see how the solution quantities of interest converge with mesh refinement.

Assuming the mathematical models to be correct and all else being equal, then verification is a matter of controlling discretisation error.

3. Error Estimation

The ideal situation, when conducting numerical simulation, would be able to predict the exact error. Clearly, however, this would require the exact solution, and if one had that one would not need to conduct numerical simulation in the first place! Error estimation is a set of ideas and techniques, aimed at providing an estimate of the discretisation error and it is often considered as two distinct topics; ***a priori*** error estimation, which is conducted before a simulation and, ***a posteriori*** error estimation, which is conducted after a simulation has taken place and when the results are available.

A Priori Error Estimation

It might seem rather paradoxical that one can even attempt to predict the error before one has even conducted an analysis, but it is often possible to make sensible predictions prior to an actual simulation and some of these ideas are listed below.

- Experience gained from previous work
- Appropriate degree of element, e.g., lower or higher degree elements
- Quality of mesh
- Rate of Convergence – Theoretical

A Posteriori Error Estimation

This form of error estimation occurs once the simulation has been completed and the results are thus available. The first question one might ask is, in the absence of the exact solution, how can one expect to improve on the simulation results such that a sensible error estimate is possible?

One way in which this may be done is to make use, where possible, of super-convergent properties exhibited in some element formulations. The super-convergent patch (SPR) scheme, [7], is such a method and has been demonstrated as effective in driving adaptive schemes to refine the mesh where the error is greatest. As an example of this, the adapted mesh for the supersonic flow around an ogive (nose cone) with a 10-degree incident angle is shown in figure 2, [8].

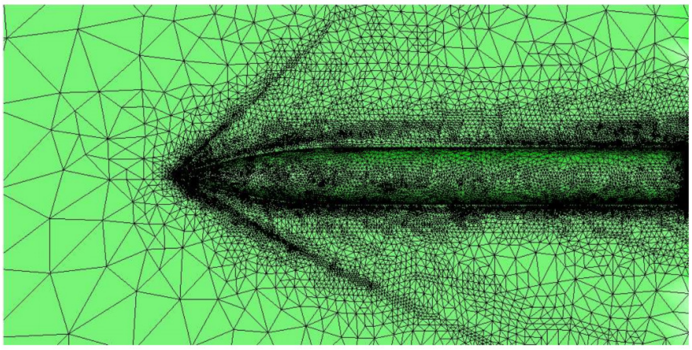


Figure 2: Adapted mesh obtained through Error Estimation (SPR) and Adaptivity

However, such a 'brute-force approach' is not always of much help to the practising engineer who might be more interested in bounding the error in a local quantity of interest, e.g., a point stress or stress resultant across a section of the model. This idea is expressed clearly in the conclusion to a 2004 paper, [9]:

"Hence, while the theory of error estimation has provided much valuable insight into the finite element solution process, many of the proposed techniques are at present only valuable to a limited extent in engineering practice."

4. Convergence and Extrapolation

Error estimation, useful though it is in its current state of development, is not of much practical use to engineers because it does not provide the essential verification quantities of an accurate error bound. One technique that can help here, and which the author has found invaluable in his simulation career, is that of convergence and extrapolation. For a numerical simulation tool to be verifiable, then it must converge to the theoretical solution of the mathematical model with mesh refinement.

Mathematical treatment of numerical simulation techniques will generally provide theoretical convergence rates for the various quantities involved in the simulation. The observed rate of convergence, in practical engineering problems, may differ from these theoretical rates but, in the limit, as the mesh is refined, these theoretical rates will be seen. Richardson Extrapolation, [10], makes use of the convergent properties of a simulation by extrapolating (from the results of two successively uniformly refined meshes) to an estimate of the theoretical solution that possesses a higher order of accuracy than that of the simulations.

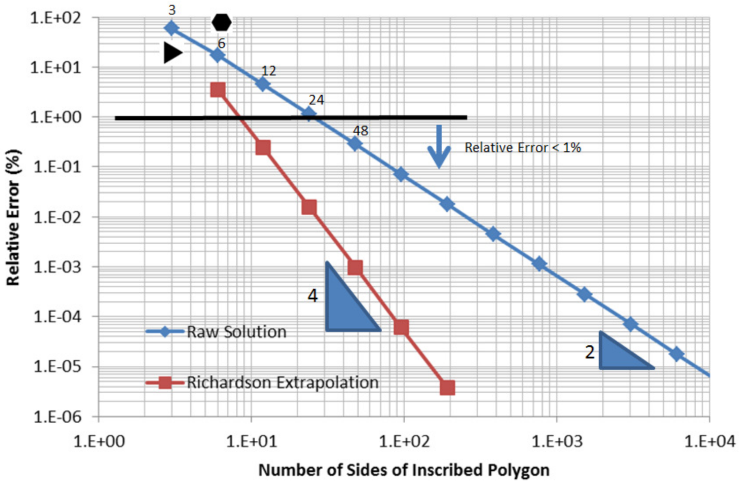
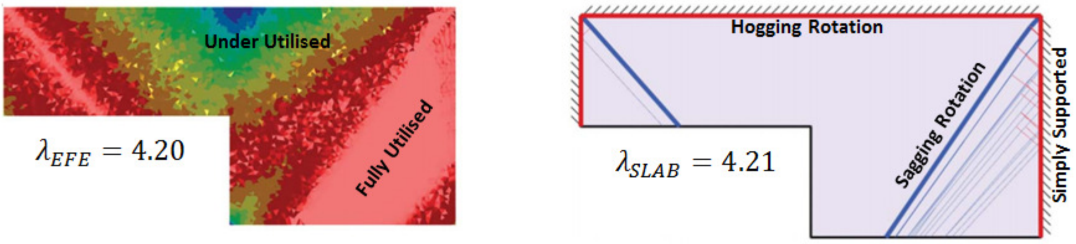


Figure 3: Convergence of the area of inscribed regular polygons

An example of Richardson Extrapolation is given in figure 3 for the area of regular inscribed polygons. The convergence is well behaved and as the number of sides is increased, the rate of convergence tends to the theoretical value of two. Richardson Extrapolation, in its basic form, assumes the theoretical rate of convergence and uses two successive approximate values of the area to extrapolate to an estimate of the theoretical solution. As seen, the rate of convergence of the extrapolated solution is double that of the raw solution. Thus, if we require an error of less than 1% in the area, whereas this would require 24 sides for the raw solution, it can also be achieved with only 12 sides for the extrapolated solution.

5. Dual Analysis

If, in the previous example, a solution using a circumscribed regular polygon had also been available, then we would have had results converging from both *below* and *above* the theoretical solution. This enables the placing of exact bounds on the error and the ideas of so-called *dual analysis* may be applied to engineering problems where *pure (dual) solutions* are available.



RMA:EFE - Utilisation LimitState:SLAB – Yield Lines (Rotations)

The load factor, λ, is the ratio collapse load / applied load.
(EFE provides a lower-bound and SLAB provides an upper-bound to the theoretical solution, i.e., $\lambda_{EFE} \leq \lambda \leq \lambda_{SLAB}$
Yield lines show rotation and the thickness is proportional to the rotation of the yield line

Figure 4: Limit analysis solutions for a landing slab

The results from just such a dual analysis using a pure equilibrium and a pure kinematic formulation to predict the collapse of a reinforced concrete landing slab are shown in figure 4, [11]. The collapse load is presented in terms of the load factor λ (this scales the applied load to give the collapse load). The lower-bound solution, and the upper-bound solution bound the theoretical solution extremely tightly, and provide a high degree of confidence for the practising engineer.

6. Closure

Good simulation governance, which enables the practising engineer to have confidence in his/her results, is all about matching the results from numerical simulation with, where possible, those of physical experiment, and must take place with reference to a mathematical model. For the engineer working in the field of numerical simulation it is the process of verification that ensures the quality of the match between his/her simulation results and the mathematical model. Verification takes two forms in which the software first needs to be verified using problems with known exact or manufactured solutions. Once this form of verification has been demonstrated then the engineer may safely use the software to simulate his/her particular problem and conduct verification to ensure that the discretisation error is sufficiently small and the result is presented with sufficient engineering accuracy.

This article is an abridged version that, it is hoped, captures the essence of a more detailed article that may be found at the following address:

www.ramsay-maunder.co.uk

7. Acknowledgements

The author would like to acknowledge the input to this article of John Robinson and Edward Maunder.

8. References

[1] Peter Bartholomew, *'NAFEMS: the early days'* NAFEMS Benchmark Magazine, January 2016.

[2] Bernt Jakobsen, *'The Sleipner Accident and its Causes'*, Engineering Failure Analysis, Vol. 1, No. 3, pp 193-199, 1994.

[3] Henry Petroski, *'Design Paradigms: Case Histories of Error and Judgement in Engineering'*, Cambridge University Press, 1994.

[4] Democratization (NAFEMS) https://www.nafems.org/about/regional/americas/events/2020vision/democratization/

[5] Barna Szabo, *'A Case for Simulation Governance'*, Desktop Engineering, February 2015.
http://www.deskeng.com/de/case-simulation-governance/

[6] William L Oberkampf & Christopher J Roy, *'Verification and Validation in Scientific Computing'*, Virginia Polytechnic Institute and State University, 2010.

[7] O C Zeinkiewicz & J Z Zhu, *'The Superconvergent Patch Recovery (SPR) and Adaptive Finite Element Refinement'*, Computer Methods in Applied Mechanics and Engineering, Vol. 101, Issues 1-3, pp207-224, 1992.
http://www.sciencedirect.com/science/article/pii/004578259290023D

[8] C.L. Bottasso , G. Maisano , S. Micheletti , S. Perotto, *'New recovery based a posteriori error estimators'*, COFIN Project, 2003.
https://www.mate.polimi.it/biblioteca/add/qmox/mox52.pdf

[9] Thomas Grätsch & Klaus-Jürgen Bathe, *'A Posteriori Error Estimation Techniques in Practical Finite Element Analysis'*, Computers and Structures, 83, 235-265, 2005.

[10] Lewis F Richardson, *'The approximate arithmetical solution by finite differences of physical problems including differential equations, with an application to the stresses in a masonry dam'*, *Philosophical Transactions of the Royal Society A* Vol. **210**, Issue: 459-470, pp307–357, January 1911.
http://rsta.royalsocietypublishing.org/content/210/459-470/307

[11] Angus Ramsay, Edward Maunder & Matthew Gilbert, *'Yield Line Analysis of Reinforced Concrete Slabs: is the 10% Rule Safe?'*, NAFEMS Benchmark Magazine, January 2015.
http://www.ramsay-maunder.co.uk/downloads/Yield-Line_Article_for_Benchmark_Magazine.pdf