Session 4 Discussion Notes

Verification and validation as tools for promoting discrete models in industry

Introduction

In many industrial applications, materials modelling is not trusted as a predictive tool at small scale: Modelling is often seen just as a qualitative tool, useful for pre-screening. There are many reasons for this situation: besides the theoretical and computational limits of the existing models, industries suffer from a knowledge gap and a communication gap between experimentalists and modellers. In other to overcome these limits, we envision a more systematic verification and comparison with experiments (validation), e.g. by means of benchmarking and round-robin tests, blind tests and simulation challenges. This would lead to making available success stories and identifying dead ends.

Common practices that are prevailing among expert and even novice modellers include already a form of de facto V&V process. Normally this consists of relying on existing reference cases that are available publicly (e.g., in professional literature) on which the materials models have been already tested or applied by others as baseline cases. The Verification is then performed by comparing the results of one's own modelling workflows done with one's own set of tools and settings on one of these available baseline systems and comparing the results. Additionally, it is common practice to perform simulations on limiting cases for which theoretical or analytical solutions exists, or even to compare with select validation experimental results extracted from existing literature or even performed specifically for the validation. In all cases, the researcher (modeller) is interested in gaining confidence in the applied set of tools and models for a specific application window. Once such validation and verification process is done satisfactory, the models are then applied to other cases expecting (hoping) that they deliver accurate enough results.

With the increasing application of computational models in materials and device design in an industrial context the requirement for formal V&V procedures becomes increasingly urgent. In the two stages of V&V we find that verification is a first step which is driven by the model developers: testing assumptions and solution techniques by comparison with analytic results in limiting cases (where appropriate) and with known experimental data. Validation is a more outward looking stage, where the model is further tested against independent experimental data. As a result of the industrial need for materials model development there is a burgeoning literature in V&V including a significant amount related to materials modelling. However these treat the process in a somewhat academic way, with exemplars which involve close feedback between model output and experiments which may not be applicable in the case that industrial data is proprietary. In summary, if there is to be an improved uptake of materials models by European industry the V&V process needs to be formalised along with ways to overcome any lack of detailed feedback, which is currently done on a case-by-case basis.

Objectives

The objective of this session is to present the current state of the art in V&V.

The session will focus on the basis of verification and validation and their use in an industrial context and will thereby focus on, but not be restricted to, the following topics:

- Beyond academic perspectives: The role of V&V in the promotion of the use of advanced materials models in an industrial context. How does V&V function in an industrial environment where data for validation may be undefined for commercial reasons? What is the effect of limited feedback on the validation process?
- New challenges for V&V: new approaches for
  a. Multiscale models
  b. V&V for AI and machine learning

Background information and documents

- Los Alamos Model V&V approach (Ben H Thacker et.al LA-14167-MS (2004) https://www.osti.gov/servlets/purl/835920/.

Discussion points and questions

The following questions summarize the issues for this session.

- To what extent is a formal V&V process likely to enhance the uptake of materials models by European industry?
- How realistic is this in validating model performance in the case that initial and boundary conditions and input data are provided by the customer, and relate to a commercially sensitive application?
- To what extent is the V&V process limited by such incomplete feedback due to testing against proprietary information?
- This problem is often solved on a case-by-case basis, is it possible to formalize this process or at least define best practice?
- Comments please on the following roadmap
  - Initial V&V workflows validation & Verification
  - Towards ISO and formalized standards
  - CEN-Workshop on terminology…