Oxford Materials Engineering – Microstructural digital twin test bed

Digital didactic platform for virtual micromechanical materials engineering

Simone Falco, Daniel Eakins, and Nik Petrinic

Introduction

This document outlines a software technology test bed proposal to develop an educational platform to explore the study of micromechanical behaviour of materials, by linking already existing numerical tools for the generation of microstructural models into a user-friendly and interactive graphical interface aimed primarly to STEM undergraduate (towards the end of their studies) and graduate students.
Although the numerical platform does not rely on data management for its functioning, the intrinsically probabilistic nature of the problem addressed makes the software extremely well suited to use *machine learning* to contribute to data science environments as part of a *performance-driven material design* tool.

The continuous rise in available computational power has led to increased efforts towards the generation of a "digital twin" of real materials with ever-increasing resolution at multiple scales. Significant effort is being made towards the refinement of macroscopic models to reduce the simplistic approximations underlying the classical mechanical simulations [1], and towards the development of accurate models of microstructural [2] and atomistic features of solid materials [3].
At the microstructural scale, in particular, the combination of improved micrography techniques with increased computational power has stimulated the development of several algorithms to create virtual microstructures, either reproducing specific experimental measurements [4] or generating statistically representative models the material [5]. Notable examples of the ongoing efforts are algorithms for the generation of virtual microstructures of polycrystalline ceramics [6] and metals [7], polymers [8], fibre composites [9], granular reinforced materials [10], and granular media [11].
The flourishing of algorithms to reproduce each specific material is reflecting in large research to increase the understanding and optimise materials at the microstructural level. There is, however, still limited use of virtual microstructures in commercial pieces of software used by industry, and even less in didactic tools to train the next generation of engineers on how to effective use numerical simulation for *material design* applications.

This test bed proposal is supported by the pump-priming funding of the Oxford-Singapore Human-Machine Collaboration Programme (HMC) – Innovation Pillar – Test Beds 2022. It is utilising the innovation ecosystem development budget line which supports pilots, test beds, proof-of-concepts in collaborative platform development. The test bed enables cloud-based data lake establishments and cross-departmental/cross-divisional, Oxford lab-driven research collaborations.

Motivations

The nature of the research work has led to the development of sophisticated algorithms to model specific materials and/or behaviour that most often remain as standalone codes with limited scope beyond the highly specialistic use for which they are coded.

The insularity of the algorithms also hinders the development of stochastic approaches to the micromechanical modelling of materials as it requires the combination of relatively complex algorithms for the generation of statistically representative microstructures with probabilistic properties distribution in non-deterministic simulations.

As the available computational power has increased exponentially, lack of integration between complementary pieces of software can be argued as the main obstacle to widespread use of micromechanical models combined with probabilistic approach, as the field is still dominated by deterministic modelling of macroscopic models.

The integration of standalone algorithms into an interactive graphical interface to generate, visualise, and modify virtual microstructures, alongside the capability to generate micromechanical models compatible with the main commercial FE pieces of software, would provide a novel *material design* platform that can be used both as an interactive didactic tool and as a research instrument for the design of materials tailored to the specific desired application.

Goal of the test bed

The final aim of the testbed is to develop a platform to integrate multiple, separate but complementary, algorithms for the generation, visualisation, and manipulation of microstructural models.

The user-friendly and interactive graphical interface aims to provide didactic tools to explore different topology related phenomena in a wide range of solid materials, offering a direct and effective link to commercial and in-house pieces of software for the simulation of the micromechanical response of the structures. As the correct usage of the platform requires basic knowledge of microstructural topology and micromechanics, the envisaged target of the platform is primarily STEM undergraduate students toward the end of their degree and graduate students. However, the links to commercial software render it also useful for training within engineering focused industrial organisations.

The implementation of the novel platform will offer the possibility to exploit the potential of stochastic virtual microstructures both for material design applications, and as didactic tools for the training of the next generation of engineers and material scientists.

The project will also explore in-kind technical support opportunities of industrial partners to link the platform for the generation of virtual microstructures to open data management (for microstructural characterisation) and applied ML technologies[1]

Research scope

At the core of this endeavour are several algorithms implemented to generate representative models of the microstructure of a wide range of materials developed within the Impact Engineering group in the past 10 years.

Starting from the implementation of a method for the generation of virtual polycrystalline microstructures [6], several algorithms have been implemented and used to successfully reproduce the micromechanical behaviour of a wide range of materials (e.g. polycrystalline ceramics [6], sand [11], polymer fibre [8] presented in Figure 1).

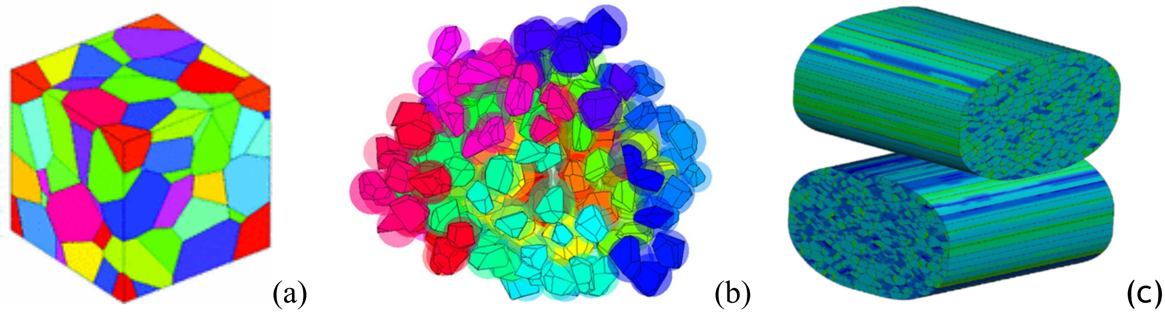

Figure 1: Examples of microstructures generated with different algorithms: (a) polycrystalline ceramic [6], (b) sand [11], and (c) polymer fibres [8].

The objective of the pilot study is to develop a learning platform to link, as a preliminary stage, the in-house algorithms for the generation of four broad classes of materials:

- densely packed polycrystalline materials (ceramics, metals),
- loosely packed granular media (sand),
- columnar materials (polymer fibres, sea-ice),
- granular reinforced composites (asphalt, construction materials).

In its first implementation, the platform will provide a user-friendly environment to generate, visualise, and edit virtual microstructures representative of the vast majority of materials used for structural applications, and it is being implemented to allow the integration of additional algorithms (e.g. for fibre composite materials [9]) in the future to further increase the range reproducible materials.
Basics meshing approaches will be included to allow for the spatial discretisation of the Computer Aided Design (CAD) structures into Finite Elements (FE) models, enabling their immediate use with the major FEM commercial pieces of software (e.g. LS-Dyna, ABAQUS, Pegasus).

[1] AWS Data Lab: https://aws.amazon.com/aws-data-lab/;
AWS Lake Formation; https://aws.amazon.com/lake-formation;
Open Data on AWS: https://aws.amazon.com/opendata;
Registry of Open Data on AWS: https://registry.opendata.aws/;
AWS Innovate – AI and Machine Learning: https://aws.amazon.com/events/aws-innovate/machine-learning/
AWS AI & ML capabilities https://aws.amazon.com/about-aws/whats-new/machine-learning/

The modularity at the core of the implementation approach leaves the platform open to further integrations with additional in-house or commercial algorithms, which include the already mentioned increased range of reproducible materials, the development of more sophisticated discretisation techniques, and the introduction of constitutive properties for bulk and interface behaviour.

The proposed objective of implementing a user-friendly platform for the generation of statistically representative microstructures requires a number of coordinated tasks that can be summarised as follows:

1) Homogenisation of the format of input and output files for the array of algorithms developed to generate microstructural models.
2) Develop a user-friendly graphical interface to define the input parameters and automatically generate the required input files using the newly defined format.
3) Develop a user-friendly graphical interface to visualise the output models, both in their CAD and FE formats.
4) Implement numerical tools to evaluate statistical properties of virtual micro-structures, thus allowing the direct comparison against experimental measurements.
5) Write a user manual to provide the users with the fundamental know-how.
6) Create video tutorials of relevant benchmark problems to offer practical examples of applications for different types of materials.

Schedule, activities, and owners

1 February – 31 May 2022

Outcome and impact

The direct outcome of the project will be a standalone software for the generation, visualisation, and manipulation of virtual microstructures, a user-manual, and a set of video tutorials to provide users with step-by-step instructions for relevant benchmark problems.

The software is envisaged as an interactive didactic tool for graduate students, to increase understanding and stimulate research efforts in the field of *material design* by strengthening the contribution of stochastic micromechanical modelling.

The interactive platform will provide students and researchers with direct access to a wide range of already implemented methods both for the generation of virtual microstructures and to build corresponding FE models, as well as offer the possibility to link additional in-house and commercial algorithms, thus growing the scope of the software.

Looking for

The interactive platform being developed and implemented is a fundamental tool for the generation of virtual microstructures, but it still requires reliable characterisation data to provide representative models. Therefore, it links with *Open Data AWS* initiative will be sought to support the creation of characterisation database for different materials by providing visualisation and analysis tools for the equivalent virtual microstructures.

Additionally, the final product will be particularly well suited to be part of machine learning platform, and the researchers involved in the project plan to join *AWS innovate* to explore pathways to include *performance driven material design* into the education tool developed.

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