SimBest

High Value Manufacturing

Modelling and Simulation
Best Practices Knowledge Transfer Project

Simulation and Modelling for Life Sciences:
Exploring the State-of-the-Art

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01	22-Mar-16	*Dr Jim Wood / David Calder*	

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SimBest

0 Summary

This document provides a review of the workshop "**Simulation and Modelling for Life Sciences**" held at Glasgow University on 9th March 2016.

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2 Introduction to SimBest

SimBest is an Innovate UK funded project delivered by KTN (http://www.ktn-uk.co.uk/) and NAFEMS (http://www.nafems.org/) which aims to reveal the present industrial best practice in the use of simulation and modelling techniques within the UK across several industry sectors. It is also to investigating the state-of-the-art for these technologies by engaging with leading academic institutions. A key driver is to improve the UK's productivity and competitiveness (time to market, R&D costs, innovation capacity).

The state-of-the-art study will produce reports that aim to provide a vision for what might be possible in the future and how to help industry 'raise its game' in using these techniques. Information for the report was generated in several ways, by direct industrial and academic input (1:1 interviews) working in the field, an EPSRC conference hosted by KTN and via bespoke workshops.

The report will be a key input to future Innovate UK activity across several sectors, which it is hoped will emphasis the role for modelling and simulation in future innovation activities.

3 Workshop

This particular workshop aimed to explore modelling and simulation techniques, and potential translation of techniques between sectors, with an emphasis on the life sciences/health. However, it also looked at the underpinning technologies, techniques and resource requirements.

In the spirit of the KTN model for innovation networking the intention was to see what alternative approaches might offer to the HVM sector.

Whereas previous workshops and interviews engaging academic colleagues had focussed on 'health' with the emphasis on the aspects of that sector that are part of 'high value manufacturing' (HVM) the workshop hosted at the University of Glasgow covered the broader remit of 'life sciences'.

The broad objective for the workshop was to discuss Current and Future applications for simulation and modelling in the life/health science sector:

- What tools and techniques are available now?
- What is under development?
- What is needed to enhance the development of these techniques (connections to users / HPC resources etc)?
- Is the life science/health sector exploiting the opportunity offered by these techniques?
- How might the industry benefit in future – what needs to be done (future funding etc)?
- What can be learned from or transferred to other sectors beyond life sciences/Health? What can other sectors learn from Life Sciences/Health?

The workshop also explored the main topics generated during the industry analysis which were simulation and modelling applied to:

- Materials Technologies
- Coupled and Multi – Physics
- Multi-Scale
- Optimisation
- High Performance Computing
- Uncertainty Quantification
- Verification and Validation
- Simulation Process and Data Management

There were 19 registrations (with 14 attendees).
The registrations and presentations are stored in http://bit.ly/SimBestLifeSciencesWorkshop

3.1 Workshop Agenda

11:45	Registration tea and coffee
12:00	KTN and SimBest Overview
12:15	Presentations – examples of the advanced use of modelling and simulation in the Life sciences/Health sector
13:00	Networking Lunch
13:45	Workshop discussion
14:45	Wrap-up, next steps and close
15:00	Venue closes

4 Workshop Feedback

4.1 Overview

The presentations made were diverse and covered state of the art in this sector. The research teams were clearly using simulation and experimentation to good effect in addressing the challenges in their field. International and national networking was much in evidence, as was access to state of the art facilities.

There was clear evidence of engagement with industry and clinicians; although engagement with industry was recognised as a challenge and there was clearly a desire to build on the current levels of collaboration. Finding suitable collaborators appears to be a challenge and business appears to need support in developing a vision of the potential benefits offered by applying these techniques to product realisation pathways.

IP barriers (business commercial sensitivity vs academic drive to publish findings) can also throw up some barriers to engagement with state-of-the-art techniques.

Perhaps not surprisingly, the University environment provided a ready source of expert support across other relevant disciplines such as chemistry, physics, mathematics, statistics, computer science, mechanical engineering and electrical & electronic engineering. This ready engagement with other disciplines no doubt provides a basis for inter-disciplinary cross-fertilisations. University structures were certainly not seen as a barrier to this process.

The software used ranged from industry standard general purpose simulation systems, through specialist pre and post-processing software, to bespoke systems developed within departments. Use included open-source software – and in some instances was a pre-requisite for grant-funded projects. Business partners (software vendors) often develop code to enhance their offer where their platforms are used in research but are not typically funded to do so and some learning is lost as a result.

4.2 Additional Comments

The event very obviously provided a platform for sharing of ideas between institutional colleagues with several connections established on the day for follow-up.

Our sole industrial participant – Ethos Health Partnerships - was also connected with one of the researchers so from a knowledge transfer perspective the event was an obvious success.

The group discussed the concept of a 'simulation engineer' as a new professional occupation.

The emerging field of precision medicine requires emphasis across several areas described below: V&V, optimisation and the development of the mathematics to support new diagnostic tools. The group could foresee an integrated approach which might be explored via simulation techniques.

The idea of a capability / maturity model for these techniques was also proposed.

4.3 Main Topics (SimBest)

4.3.1 Materials Technologies

This is a particularly challenging area for simulation in this sector, ranging from bio-compatible metallic, polymers and ceramics, through to natural materials (both healthy and diseased individuals) with unique properties of growth, adaptation and repair – and where nonlinearities and time-dependencies abound. The use and development of state-of-the-art constitutive models was evident.

The interaction of living cells with medical grade materials is an area for further research in order to generate better models. Bio-compatible and bio-materials are key in the progression of implantable and wearable medical technology.

Key research centres were named: Imperial, Nottingham, UCL and KCL with Sheffield strong on bio-mechanics.

(Cancer centres at Oxford, St Andrews and Dundee were also mentioned)

4.3.2 Coupled & Multi-physics

Many problems in this sector are clearly in this category and this was evident from the presentations, which covered both loosely and highly coupled physics.

4.3.3 Multi-scale

Multi-scale simulation was also apparent from the presentations and discussions. This appeared to be an inherent challenge in this sector. Living tissue presents macro-micro (nano?) scale challenges as fibres / muscle sheets are so dependant on cellular factors to determine their characteristics. As mentioned above these vary with time.

4.3.4 Optimisation

Sensitivity studies would appear to be common, with interest in tailoring solutions to individuals.

4.3.5 High Performance Computing

Research groups were accessing various national HPC facilities. This is essential for molecular and cellular level research. Awareness of local regional facilities appeared to be lacking. Difficulties were expressed with respect to obtaining access to these "in-demand" facilities. Installing bespoke software on these facilities was also seen as a challenge. Current software licensing was identified as a barrier. Locally the 'Archer' system offered an accessible model - £500 PA per user.

In research environments the need to access HPC to develop the model as opposed to running tests makes the prevalent licensing models problematic.

Present emphasis from funders (e.g. EPSRC) is still on provision of hardware whereas the pressing need is funded access to the facilities and code development. In addition, funding the expert developers rather than allowing academic teams to write code themselves was seen as a more effective approach.

Data systems are key to successful use of complex models.

SME's have theoretical access (noting that SME uptake of modelling in health is typically via local University collaborations) however few make any use of this.

An opportunity exists for greater collaboration between imaging and modelling centres.

4.3.6 Uncertainty Quantification

This appeared to be a topic that researchers in this area were familiar with, both from a simulation and experimental viewpoint. It was also an area that the group saw as growing in importance as regulators increasingly require justified use of modelling to reduce human risk and to reduce reliance on animal testing as below.

The impact of environmental factors on basic physiology – disease impacts muscle elasticity etc – makes this a very complex area where modelling an individual patient is concerned.

New methods are needed to support research applications in this space. Life science models are open systems adding another layer of complexity

4.3.7 Verification and Validation

In-vitro experimental validation would appear to be common and established regulatory frameworks governed testing using animals and humans. The researchers appeared to be well aware of the requirements of regulatory bodies with respect to V&V. However as above, the present body of knowledge in vendor solutions is weak regarding tissue properties.

In life sciences the opportunity to diverge from the model concept via its eventual expression in code and on to potential process errors (e.g. compiler errors) is also exaggerated in life-science applications requiring more extensive V&V activity.

4.3.8 Simulation Process & Data Management

This was the only area that appeared to lack relevance, to some extent, to the work of research teams in this sector. It was seen more of an issue for the industrial enterprise. That being said, there was simulation being carried out on disease and life-expectancy within large population data sets, which no doubt was moving forward capability in utilising large data in an effective manner, within an ethical regulatory framework.

4.4 Additional Topics

The following concepts were outside the main headings generated within the SimBest project to date:

- Perturbation – short and long timescales for life-science models
- Coupled models - for drug release
- Diffusion and Advection – non-linear

- Modelling and Simulation in the design phase for drug releasing systems
- Regulatory engagement approaches (FDA / MHRA)
- COMSOL
- Large Scale socio-technical systems with ‘fuzzing’
- Testing simulations of the above (totally new area?)