E-CAM Scoping Workshop: From the Atom to the Material

Date: 18 – 20 September 2017, University of Cambridge

Organisers: Mike Payne (University of Cambridge, UK), Victor Milman (Biovia, UK)

1. State of the Art

One of the buzz phrases currently in fashion is 'From the atom to the material'. It is one of the major drivers of the Materials Genome Initiative which has, amongst its objectives, the aim of reducing the time to market for materials from the current value of 20 years or more through increased use of modelling, simulation and data. It is also one of the objectives of the European Materials Modelling Council, and there are many calls from industry for such capability. The Workshop aimed to bring a sense of reality and achievability to the field by discussing and reviewing:

i. Examples of use case requirements from industry for modelling and simulation under the general objectives of 'From the atom to the material' and the timescales for these requirements;
ii. Which of these requirements can already be fulfilled by current simulation and modelling capabilities;
iii. Which of these requirements will be fulfilled by methods and technologies currently under development;
iv. Gaps in capability.

The primary aim of the Workshop was to open up dialogue between modellers and industrial users of modelling with the intention that:

- current modelling and simulation capability is used to its maximum effect;
- future development of modelling and simulation capability is aligned closely with fulfilling the objectives of 'From the atom to the material';
- we jointly educate and lobby Funding Councils to ensure that research is funded to address the gaps in the capability ecosystem which will thus allow us to achieve the ultimate goal of designing, testing and verifying real world materials using modelling and simulation and thus realise the ambition of 'From the atom to the material'.

2. Programme of the workshop

Day 1, Monday 18th September

13.00 – 14.00 Lunch
14.00 – 14.10 Welcome and outline of objectives of meeting, Mike Payne (University of Cambridge)

Session: Industry challenges and requirements
14.10 – 15.00 David Rugg (Rolls Royce)
15.00 – 15.45 Stephen Todd (Biovia)
15.45 – 16.15 Break
16.15 – 17.00 Detlef Hohl (Shell)
17.00 – 17.45 Filip Sorin (BP)

Day 2, Tuesday 19th December

Session: Virtual materials design
09.00 – 09.45 Marek Hytha (Atomera)
09.45 – 10.30 Gareth Conduit (University of Cambridge)
10.30 – 11.00 Break

Session: Emerging methods
11.00 – 11.45 David Quigley (University of Warwick)
11.45 – 12.30 Gabor Csanyi (University of Cambridge)
12.30 – 13.15 William Curtin (Ecole Polytechnique Fédérale de Lausanne)
13.15 – 14.00 Lunch

14.00 – 14.30 Discussion session 1 – 'Reconciling Capability and Industry Requirements'

Session: 'Poacher turned gamekeeper'
14.30 – 15.15 Chris Wolverton (Northwestern University)
15.15 – 16.00 Sadasivan Shankar (Harvard University)
16.00 – 16.30 Break

Session: Materials modelling initiatives
16.30 – 17.15 MARVEL/MAX, Nicola Marzari (Ecole Polytechnique Fédérale de Lausanne)
17.15 – 18.00 MicCom, Peter Littlewood (University of Chicago)

Day 3, Wednesday 20th September

Session: Materials modelling initiatives (continued)
09.00 – 09.45 E-CAM, Sara Bonellla (Ecole Polytechnique Fédérale de Lausanne)
09.45 – 10.30 EMMC, Gerhard Goldbeck (Goldbeck Consulting Ltd)
10.30 – 11.00 Break
11.00 – 11.45 The Materials Project, Joseph Montoya (Georgia Institute of Technology)
11.45 – 12.30 NoMAD, Matthias Scheffler (Fritz Haber Institute)

12.30 – 13.00 Discussion session 2 – "Gaps in modelling capability"

13.00 – 13.10 Closing comments, Victor Milman (Biovia)

3. List of Participants

Group	First Name Last Name	Affiliation
Industry	Stephen Todd	Biovia
	Victor Milman	Biovia
	David Rugg	Rolls Royce
	Detlef Hohl	Shell
	Filip Sorin	BP
	Marek Hytha	Atomera
	Gerhard Goldbeck	Goldbeck Consulting Ltd
	Woomin Kyoung	Hyundai
Academics	Gareth Conduit	University of Cambridge
	David Quigley	University of Warwick
	Gabor Csanyi	University of Cambridge
	William Curtin	Ecole Polytechnique Fédérale de Lausanne

	Chris Wolverton	Northwestern University
	Sadasivan Shankar	Harvard University
	Nicola Marzari	Ecole Polytechnique Fédérale de Lausanne
	Peter Littlewood	University of Chicago
	Joseph Montoya	Georgia Institute of Technology
	Matthias Scheffler	Fritz Haber Institute
	Matt Probert	York University
E-CAM	Mike Payne	University of Cambridge
	Sara Bonella	Ecole Polytechnique Fédérale de Lausanne
	Christoph Dellago	University of Vienna
	Leon Petit	STFC Daresbury Laboratory
	Ignacio Pogonabarra	Ecole Polytechnique Fédérale de Lausanne
	Dominic Tildesley	University of Southampton
	Valerio Vitale	University of Cambridge

4. Major outcomes

The meeting was divided into themes with clear steers given to the speakers:

Industry requirements – review some of your industry's materials challenges, existing applications of modelling which have been helpful and provide a 'wish list' for future modelling capability.

Virtual materials design – be positive about your achievements, but at the same time be realistic about the limits of an entirely 'in-silico' approach to creating materials.

Emerging methods – please talk about the materials modelling methods you are developing and how they can address challenges in virtual materials design.

'**Poacher turned gamekeeper**' – please talk about both your experience of materials design/discovery in an industrial context and in an academic context and how the two sides could most effectively work.

International initiatives – in addition to outlining the activity you are presenting please could you explain how this activity can respond to the various materials design challenges described in the meeting.

The talks and comments from industry-based participants showed that there is a very broad range of requirements from industry for materials modelling, in terms of types of material, properties of interest and, interestingly, the level of accuracy needed. This ranged from one extreme of a requirement for quantitatively accurate predictive simulations to, in the middle, not being worried about the absolute value of a predicted quantity but only about trends under change of composition to only using modelling and simulation to provide insight into complex physical problems without requiring quantitative accuracy. It became apparent that even in large companies in most cases materials modelling is a very small scale activity at present and in many companies, it does not exist at all. It is also not unusual to have no company-wide view of modelling activities, so that there is no information exchange between different divisions of the same organisation.

The first talk in the Virtual Materials Design section showed how a novel material had been not only designed using ab initio calculations but how the same calculations helped to guide the fabrication process for this new material and were also used to demonstrate a wider range of improved properties possessed by the new material. The second talk showed how a data led approach based on the application of advanced neural networks and taking companies existing data sets had successfully predicted materials with improved properties. A particularly interesting feature of this talk was the ability of this advanced neural network approach to fill in missing data in datasets – a feature that is particularly relevant for materials data, which are rarely complete.

The emerging technologies talks covered a number of methods that should become important tools for materials modelling with a strong emphasis on machine learning approaches. The talks emphasised that many materials properties require large numbers of modest size calculations that collectively require peta to exascale resources; owners of such resources should be made aware of such needs.

The 'Poacher turned Gamekeeper' session reiterated many of the points raised in the Industry talks but also clearly demonstrated how the value of materials modelling was, in these cases, only realised when these tools were integrated into the entire design process. This is something that academics cannot do alone and, hence, there is a significant challenge to making a real economic impact from academic research unless it leaves the academic sphere. There was some related discussion about Open Source software; there was a view that very few companies would use Open Source software though they would be willing to use a supported version of the same software. This session also helped to stress the importance of the 'translator' – the individual who can connect (in both directions) a complex product challenge to a set of feasible materials modelling tasks.

The Materials Modelling Initiative session showed just how large an investment is being made in research in this field. Most of the initiatives are under pressure to show industry engagement and take up. In some cases, this is with a view to creating long term sustainable efforts – a goal that, historically, has rarely been fulfilled.

5. Community needs

There was a general feeling that there are many initiatives in this area on the academic side. There is also a profusion of computational resources becoming available though there are issues about the suitability of proposed exascale machines for running most materials codes. At the meeting, the industrial participants were asked whether they felt that exascale machines (as opposed to exascale resources) were of interest to them and the answer was universally 'no'. The issues in this area focussed around two major subjects:

- In every example of significant impact of materials modelling presented at the meeting, the role of the Translator was seen as absolutely crucial. There was significant concern that even at companies where very successful materials modelling project had run, subsequent re-organisations had often led to the loss of such translators and/or the loss of critical mass in materials modelling

- Despite (or because of) the large number of well-funded research projects in this area, there is a problem of lack of connectivity and continuous re-invention of the wheel many times over. This is wasteful of resources but, particularly on the data/informatics side it is positively dangerous as it significantly reduces the possible impact of big data – particularly in a field

where the amount of data available is very modest bearing in mind the complexity of materials space.

6. Funding

As mentioned previously, this field of research is very well supported in academia with numerous initiatives. It was encouraging to hear that the European Materials Modelling Council had recognised the role of the translator and that there will probably be an EC call for funding in this area in due course. However, it is important that any such call is inclusive and does not just fund a tiny fraction of the community of translators. It was agreed that it is important to provide more easily accessible case studies of successful materials modelling projects which could be used to encourage further adoption of such methods in industry. Along similar lines, it was pointed out that providing Cloud access to materials modelling tools could have a significant impact in allowing companies to experiment with these tools without incurring a significant start-up cost. Perhaps the biggest challenge, as illustrated in the examples presented at the meeting, is that materials modelling from the atomistic scale will only have significant impact if it is embedded within in an entire suite of product development tools. This currently requires a scale of investment within a company and a degree of expertise in using such tools that is way beyond the reach of most companies though it should be emphasised that some of this can be outsourced to academic groups. Clearly, there are significant requirements for funding to address this issue though current mechanisms for supporting research would struggle to find mechanisms of doing this in an inclusive fashion – (inclusive of both researchers and of modelling methods).

7. Potential benefits

Just the small number of examples presented at this meeting give some indication of the potential impact of materials modelling though the fact that significant gains require a broad raft of tools and methods means that it is difficult to quantify the benefits that result from any one method alone. However, it is stated that Ford's 'Virtual Aluminum Castings' project has provided $millions of benefit to the Company and it was also stated that materials modelling has played a significant role in the continuation of Moore's Law for at least the last decade.

If we were truly to realise the promise of 'From the atom to the material' the economic benefit would be many $billions per year with numerous further benefits, such as reduction of toxicity. However, this goal is still many years away. There was a general consensus at the meeting that even with its current limitations, materials modelling has significant economic impact (as evidenced in the various reports from Goldbeck Consulting) and that this impact would be much higher if more companies used this modelling where appropriate – common problems being that too often companies do not know when modelling is appropriate and that academics are prone to overselling their methods and do not give sufficient advice about which methods are appropriate.