EMMC-CSA

European Materials Modelling Council

Report

Sessions on

Industrial Software Deployment

within the

EMMC International Workshop 2019

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TABLE OF CONTENT

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1. Executive summary

1.1 Description of the deliverable content and objectives

At the EMMC International Workshop 2019, WP5 organised sessions 11, 14, and 17 related to its main objectives in the present EMMC-CSA, namely "Professional Software Deployment". Session 11 reviewed the progress in the industrial deployment of materials modelling software drawing on the ample expertise of software owners. Session 14 addressed the issue of business models for materials modelling software and session 17 shed light on the complicated topic of the synergy and conflicts between open source and commercial software for industrial deployment of materials modelling software. In the following, the each of the sessions is reviewed in detail.

1.2 Major outcome

The following points summarise the major outcome of sessions 11, 14 and 17:

- The European industry is catching up in using materials modelling software. An increasing number of companies including new players in the field integrate materials modelling into their research efforts. This is related to both growth and accessibility of compute resources and the increased maturity level of the software.
- Industry is expecting robust solutions provided by reliable partners in form of commercial software companies, who can guarantee long-term support. In addition, confidentiality is becoming more and more important. Open source software without support is not attractive for industry.
- At present, cloud solutions and SaaS are not finding much interest from industrial users.
- There is continuous demand for improved education and training both by universities and the software companies.
- More success stories are needed to motivate even more companies to include materials modelling as part of their research and development processes.
- Combination of physics-based and data-driven models can create new business value.
- SME's should not be neglected as customers.
- Marketplaces need to be made attractive to SWO's.
- License models using GPL can cause problems.
- Validated software solutions employing discrete models need to be standardised to become valuable for technicians, as has happened with software based on continuum models.

2. Progress report (main activities)

2.1 Session 11: Progress in the Industrial Deployment of Materials Modelling Software

2.1.1 Overview

Chair

Erich Wimmer (MDS, FR)

Impulse 1

Anders Engström (Thermo-Calc, SE)

Progress in the industrial deployment of thermodynamic modelling software

Impulse 2

Brian Dron (MDS, DE)

Drivers for the industrial deployment of atomic-scale materials modelling software

Impulse 3

Stan van Gisbergen (SCM, NL)

Opportunities and challenges in the industrial usage of chemistry modelling software

Rapporteur

Volker Eyert (MDS, FR)

Session presenter at Podium Discussion

Erich Wimmer (MDS, FR)

Introduction

This session addressed the present status of industrial deployment of materials modelling software especially in Europe. Examples of both successful implementations of atomistic simulations in the industrial context and the barriers to overcome were discussed. Focus was also on measures to be taken by all stakeholders to promote the integration of materials modelling in industrial processes.

Objectives

- The key objective of this session was an assessment of the progress of the industrial deployment of materials modelling software.
- Related objectives are
  - An understanding of the main drivers of this progress
  - A comparison of the European, American, and Asian companies in terms of the deployment of materials modelling software
  - Assessment of the impact of different business models
- Recommendations were given to promote the uptake of materials modelling by industry

Background information and documents

- The progress in the industrial deployment of materials modelling can be seen from trends such as the number of industrial patents citing materials modelling and the growth in the number of employees being hired in modelling groups.
- About a decade ago, a series of workshops organized by the University of Vienna titled "Theory Meets Industry" illustrated global trends and the growing interest of industrial R&D laboratories in materials modelling and simulations. A summary of such a workshop was published by Erich Wimmer in 2008 (see below). At that workshop, Toyota, General Motors, and Ford were present showing their materials modelling activities while European car manufacturers were absent.

Together with DuPont in the USA and Sumitomo Chemical in Japan, BASF is one of leaders in the industrial deployment of quantum chemical methods. DuPont installed a supercomputer in 1985 and a few years later Sumitomo Chemical inaugurated its supercomputer. At that time, BASF pioneered the use of quantum chemical calculations on workstation clusters. A milestone in the industrial deployment of materials modelling was the installation of a supercomputer at BASF in 2017, clearly demonstrating the growing relevance of computational modelling in industry.
(see: https://www.basf.com/global/en/who-we-are/innovation/our-way-to-innovations/supercomputer.html and https://www.youtube.com/watch?v=t3pDRyXMizI).
Further information on the current industrial deployment of materials modelling can be found on the websites of the leading software providers.
Additional articles related to this subject are:

- Erich Wimmer, Summary of workshop 'Theory Meets Industry'—the impact of ab initio solid state calculations on industrial materials research, J. Phys.: Condens. Matter 20 (2008) 064243.
- Erich Wimmer, Reza Najafabadi, George A Young, Jake D Ballard, Thomas M Angeliu, James Vollmer, James J Chambers, Hiroaki Niimi, Judy Shaw, Clive Freeman, Mikael Christensen, Walter Wolf and Paul Saxe, Ab initio calculations for industrial materials engineering: successes and challenges, J. Phys.: Condens. Matter 22 (2010) 384215.
- Volker Eyert, Mikael Christensen, Walter Wolf, David Reith, Alexander Mavromaras, Clive Freeman, and Erich Wimmer, Unravelling the Potential of Density Functional Theory through Integrated Computational Environments: Recent Applications of the Vienna Ab Initio Simulation Package in the MedeA® Software, Computation 6, 63 (2018).

Specific questions addressed in this session:

- What progress has been achieved during the past decades?
- Which measures should be taken to increase the uptake of materials modelling in industry?
- How does the investment in materials modelling in European industry compare with American and Asian companies?

Opening this session, the chairman pointed out the importance of materials modelling for industrial research and development. He compared materials modelling to the role of vitamins for the body: One does not need much, but their availability in high quality is essential. In addition, he emphasized the important role that materials modelling is playing already in a large variety of industries including automotive, aerospace, chemicals, energy, metals and alloys, and electronics/semiconductors to specialty materials. Underpinning the urgent need of continuous deployment of materials modelling in the European industry, the chairman presented a slide on the

increase of worldwide R&D spending between 2000 and 2016, which clearly revealed the outstanding role of China.
The session focused on the following two key questions: What is needed to strengthen the role of materials modelling for industrial innovation? What strategy gives Europe the greatest economic advantage?

2.1.2 Summary and collected feedback

Impulse 1

Anders Engström (Thermo-Calc, SE)

Progress in the industrial deployment of thermodynamic modelling software

Highlights

The speaker started by introducing the company Thermo-Calc and presenting the first example of the use of Thermo-Calc software in 1983 by scientists at SANDVIK, who had developed a new duplex steel (ferritic and austenitic phases) aided by CALPHAD-based calculations. According to his experience materials modelling in industry is mainly driven by the ability of predictive calculations to cut development times and increase quality. Success factors for the use of materials modelling software are functionality, access to relevant data, the fact that such calculations need only few assumptions as well as close collaboration with academia. Gaps affecting the deployment may arise from the fact that industry is mainly interested in applications and production, whereas the original development of materials modelling software is rooted rather in theoretical foundations and fundamental research. Yet, the gap can be bridged by increasing efforts in education, training, marketing, functionality, interoperability as well as the spread of success stories. In addition, emphasis should be put on improving the user experience (documentation, ease of use, robustness, reliability, speed, support). Education and training will cause deeper understanding of the calculated results, which in turn leads to improved patent applications.

Interestingly, according to the speaker’s experience, perpetual licenses are mostly preferred over annual licenses, with the latter having the largest fraction in North America. No strong request for Cloud computing or SaaS is observed. The customers of Thermo-Calc usually have large global R&D units. However, on increasing decentralization of modelling, ICME and AM drive more cross-team modelling involving more non-materials scientists.

Questions, Remarks

How is training at Thermo-Calc organized? - Training courses are held both in Thermo-Calc’s offices and at customer’s sites. In addition, Thermo-Calc offers free download of their software as well as teaching materials for academia.

Is the software adapted to changing needs? - Yes

Does more decentralized modelling introduce licensing problems? - No, since the licenses are site specific.

Why is SaaS not so much requested? - Customers of Thermo-Calc are large companies, which have high interest in securing their data and IP.

Impulse 2

Brian Dron (MDS, DE)

Drivers for the industrial deployment of atomic-scale materials modelling software

Highlights

This speaker focused on the business aspects of industrial material modelling. After briefly reporting on his personal career and long-year experience in the field he summarized the present state of the art with atomistic simulations used in many different industries ranging from automotive, aerospace, fluids, oil and gas, polymers, metals and alloys, and energy storage, to catalysts and specialty chemicals. The impact of materials modelling was demonstrated with the example of materials research to continuously increase the safety of nuclear reactors.

According to the speaker's experience, industrial deployment of materials modelling software is driven by a number of factors including senior-management commitment, vendor selection, IT deployment in-house/via cloud, central R&D or business units, licensing (tokens, annual, perpetual, open-trust), ROI (cost of simulation vs. experiment, opportunity cost, headcount). Success achieved at different levels, corporate, departmental, and personal, is also vital to further dissemination.

The speaker also shared more general insight gained over the last years. In particular, he mentioned that

- atomistic materials modelling has come of age (advances in software, hardware, awareness),
- industry expects robust commercial solutions (proven partners, not open source),
- Europe is catching up with US/Asian investments (new companies),
- cloud is not that cost effective,
- compute resources have increased and are dedicated much better than before,
- commercial software companies receive sufficient funding.

Finally, the speaker summarized the lessons learned in his business career:

- In-house industrial software development doesn't work, it is too expensive, and companies prefer to focus on their core strength,
- Industry expects robust commercial solutions,
- Confidentiality is becoming more important.

Questions, Remarks

If materials modelling software plays an increasing role in production as compared to the original exclusive use in R&D department, what does that mean for the software? - This impacts mainly licensing schemes and contract research.

How important is understanding vs. predictive power? - Both play a role as quantitative prediction is coming more and more into reach.

Impulse 3

Stan van Gisbergen (SCM, NL)

Opportunities and challenges in the industrial usage of chemistry modelling software

Highlights

This speaker also started out presenting his company. The main product is the Amsterdam Modelling Suite (AMS), which allows to perform DFT, semi-empirical, and forcefield calculations using ReaxFF forcefields. In addition, it gives access to the COSMO-RS software and offers a graphical interface, python scripting, driver routines, and a graphical user interface. Application areas include spectroscopy, catalysis, pharma, solubility, polymers, batteries, etc.

The speaker also shared his observations regarding the industrial usage of materials modelling software:

- Cloud computing/SaaS not much requested,
- Each type of modelling needs its own expert/full-time specialist,
- The cost of switching to other software is high due to license fees, learning barriers, software infrastructure and integration and depends on the type of modeling (interactive vs. long execution time, expertise needed, human time vs. computer time, human time limiting factor in industry, discrete and continuous modelling done in different groups),
- The complexity of materials and simulations is increasing and requires more support, consultancy as well as interoperability,
- Companies have a tendency to outsource research to academia especially in Europe.

Questions, Remarks

According to your experience, do you see a stronger tendency in industry to improve materials or to replace existing materials? - Both strategies are followed.

Discussion points and questions

The discussion centered especially about the following topics and questions:

Deployment of materials modelling in different industrial sectors including automotive & aerospace, chemical & petrochemical, electronics, specialty materials, pharmaceutical

- What are the main drivers of industrial uptake of materials modelling?
  The experts agreed that industrial uptake of materials modelling is driven by the competitive advantage over competitors it offers and the fear of falling behind, respectively ("you don't want to be left behind", old example of crash simulation in automotive industry). Being the first, being the innovator is indeed a strong motivation even though the role of innovation may be different in different industries.
- Which industry is most sensitive to be susceptible to modelling?
  This applies to the semiconductor industry and the chemical industry.
- What type of software is being used and most effective?
  In industry the preference of open-source vs. commercially supported software is guided by the strong need of robust software. Long-term support and maintenance are also of special importance. Electronic notebooks integrating different software were also mentioned in this context.
- International comparison
  As Brian Dron pointed out in his talk "Europe is catching up". The experts stated that not much commercial software has been developed in Far East so far and no software developments are visible at the horizon.
- Software as a service

There was general agreement that SaaS is not much requested. The same applies to cloud computing except for use in peak times, when computing demands exceed the in-house resources. CDD Vault was mentioned as a viable example in pharma.

- Organizational aspects, e.g. central modelling groups, modelling embedded in business units, budget, staffing
  The organization of materials modelling in companies is domain and industry specific and depends very much on company size. Beyond the company level, the role of international centers of excellence is increasing. In addition, a need for sustainable industrial engagement strategies, e.g. in forms of consortia was stated. However, consortia may be faced with IP issues, they take a lot of time. Since certain industries are less interested in consortia and centers of excellence, European funding should support collaborations.

Conclusions

The state of materials modelling in the European industry is probably best reflected by the statement of the second impulse speaker that "Europe is catching up". An increasing number of companies including new players in the field integrate materials modelling into their research efforts. This is related to both growth and accessibility of compute resources and the increased maturity level of the software. At the same time, industry is expecting robust solutions provided by reliable partners in form of commercial software companies, who can guarantee long-term support. In addition, confidentiality is becoming more and more important. For this reason, as well as because of lack in cost effectiveness, cloud solutions and SaaS are not finding much interest of industrial users. In contrast, there is continuous demand for improved education and training both by universities and the software companies. Finally, more success stories are needed to motivate even more companies to include materials modelling as part of their research and development processes. However, overall the European industry is increasingly aware of the high value of materials modelling.

2.3 Session 14: Business Models for Materials Modelling Software

2.2.1 Overview

Chair

Alexandra Simperler (GCL, UK)

Impulse 1

Hans Fraaije (Culgi, NL)

Software, Service, Data

Impulse 2

Thomas Schrefl (Danube University Krems, AT)

Magnetic materials modelling – Bridging the gap between academic software and industry needs

Impulse 3

Zlatan Stanojevic (Global TCAD Solutions GmbH, AT)

How to Fail Commercially in Materials Modeling

Rapporteur

Natalia Konchakova (HZG, DE)

Session presenter at Podium Discussion

Alexandra Simperler (GCL, UK)

Introduction

Successful software for materials modelling has an expected lifetime of many decades. This long-term nature requires a sound legal and business foundation: the ownership of software must be clearly established, and the license models need to be carefully thought through to ensure a sustainable development and maintenance of the software and impactful exploitation by both academic and industrial end-users. Different business models carefully need to be considered when developing a strategy for long term sustainability of software and sustainment of the operation.

Objectives

The objectives of Session 14 are to uncover business models already in place and raise awareness of novel strategies. We will discuss in particular how Business Models relevant to materials modelling software are evolving and what future contribution digital marketplaces can make. For further background, see the recent White Paper published by EMMC.

Background information and documents

- Goldbeck, Gerhard and Simperler, Alexandra. Business models and sustainability for materials modelling software.
- https://emmc.info/wp-content/uploads/2019/01/EMMC-CSA-D5.5_M22_vfinal2-PU-WEBa.pdf
- Goldbeck, Gerhard. The scientific software industry: a general overview. Goldbeck Consulting, 2017. http://doi.org/10.5281/zenodo.260408

Discussion points and questions

The following questions summarize the issues for this session.

- What do you consider the “perfect” ratio of services vs software sales?
  That depends on the needs of the customer. Experienced customers will need less service (consulting, support ...) than beginners do. Services can be prevalent whenever the demand of data is popular and comes from a basis that is not enough proficient in the field to manage software autonomously. Software becomes prevalent whenever the demand comes from consultants or industry researcher who are competent and have the necessity to have complete control on the product.
  30% service vs 70% software: seems a good ratio to provide a stimulus for software development and services to keep educating software developers in industrial needs. Software sales is the main part as services (consulting) are seen as supporting the software sales. In addition, annual maintenance including support and providing new version could be important.
- What can be done to use SaaS more as it regarded as a potentially way to attract customers who have not the means to get infrastructure and skilled staff in place?
  If a customer does not have skilled staff the most important need is not software (be it SaaS or not) but service in the form of consulting, education, and support. This could enable easier use, ensuring

confidentiality of data and bringing in confidence about modelling. Offering more detailed manuals could help, and also freemium plans where the software can be trialled initially. This can be followed on with online workshops offering training to use the software. It also may be beneficial to set up modelling centres certified by a trusted public body. SaaS should comply to well defined ontologies, well understood by the audience and adopt standard formats for data exchange in order to allows efficient queries from client applications. Modellers should prepare the documentation for SMEs related to modelling process and workflow. They could provide a case studies, which help SMEs. However, investors will be required to pay for marketing and realisation of a product.

- What attractive new ways are there to enable new materials modelling businesses?
  There is some scepticism if "attractive new ways" could have been missed by commercial SWOs. We would for sure have already heard about them. However, some participants are fond of creating a platform as this could encourage participation of modelling businesses in all publicly funded projects; provide funding for initial purchasing of software libraries (graphical, mathematical, …) and stimulate interest of students in modelling. This platform could permit to make material models commercially available, with a defined ontology to ensure that it would be compatible with the tools that an end-user would be using in conjunction with a material model. Also, academic SWOs could show there the impact of their tools concerning up-to-date research questions.
- How is software sustainability best achieved?
  This needs a lot of emphasis on software design from the very beginning including the right design decisions, early and well-thought decisions regarding layout, licensing, purpose, etc. Also, a certain level of funding for small modelling business or open source software development would be beneficial. There could be initiatives such as "buy European", to encourage that European software is used by European industry. One could also encourage employment of university graduates at small modelling businesses to train them to become proficient in sustainability.
  It could be beneficial if the original authors of software remain connected with the software developments and also keep a tight relationship with customers. Moderators could be put in place to oversee and curate software, particularly in terms of identifying bugs, managing updates, building FAQs for users, etc.
- How can we enable a change in education and better recognition of the efforts involved in software sustainability?
  There are several examples of software sustainability available right now, and hence it would be a case of providing these as case studies to highlight the value of this kind of approach. People could then be made aware of the importance of early (explicit or implicit) decisions. If this step is not well taken, it hits back at a later time. Curricula could be influenced to shift from "zero and unities" to "thinking and modelling". A broader use of modelling software in academic teaching could be encouraged and students could be “recruited” as testers of new software versions – so they learn about sustainability by contributing to it.
- What role can Marketplaces play to facilitate a more dynamic materials modelling software ecosystem?
  Some SWOs see marketplaces as a hype that may pass. Some others see them as a way of sharing and reaching out globally. They could be key to share models, tools and engineering protocols. Marketplaces can facilitate global availability of models, as well as providing a commercial route to motivate researchers and modellers to share and upload their work. They can make it easier for industry to evaluate different software solutions.
  A marketplace would be very useful for small companies who know their customers very well and the existence of marketplaces with small domains could help a lot for specialised SWO SMEs.

- How can Marketplaces be made sustainable, i.e. self-sustaining?
  Active promotion of the marketplace to attract new contributors and users as well as assigning moderators or establishing frameworks to maintain the high quality and standard of the marketplace.
- What role could/should government support/EC play in sustaining marketplaces as a key facility for research and industry?
  They could fund student education in modelling, software maintenance at universities and co-fund employment of university graduates who choose modelling businesses (rather than financial services). Also, initial funding for platform development and maintenance could be provided. Funding can be made available in the form of research grants that revolve around marketplaces and their expansion. Additionally, a consortium could be setup to monitor and support the marketplaces as required.

2.2.2 Summary and collected feedback

Impulse 1

Hans Fraaije (Culgi, NL)

Software, Service, Data

Key Points

Robotics and chemical analytics are going to create a lot more of data. Manufacturers in the age of circular economics will require more knowledge of chemical ingredients. So far, companies would buy chemicals without considering “what’s in” but when a product instead of turning into waste becomes a new resource one has to care about details. Digitalisation of R&D in chemical industry will happen and there is a new market developing where computational chemistry can tap into. There is a good case for combining computational chemistry with continuum models.

We need to start thinking that modelling can mean “interpreting knowledge” and deduct a value for the customer. We need to change our vocabulary from “better insight” to “faster IP to process”. The word “better” is not strong enough anymore to emphasise what modelling is capable of.

- Current market size of materials modelling is small: how do we leave this ‘small island’?
- Need to emphasize value much more strongly: e.g. faster to IP/patent.
- Serve chemist/end user more directly (e.g. with protocols/apps). Example of marketplace SpecialChem: https://www.specialchem.com/about-specialchem. It includes a number of science-based articles, i.e. training to help people select e.g. additive and even one on Science based Formulation that links to Hansen Parameter site where you can get a software tool for these solubility calculations. https://coatings.specialchem.com/tech-library/article/hsp-science-based-formulation-for-coatings
- If software serves non-modeller, where does that leave the materials modeller?
- Discussion: Materials Modeller shifts more to CAE and CAE shifts more to CAD.?

Continuum field more and more requires chemistry/material detail: new market developing in CAE domain (see also above).

Conclusion, Questions, Remarks

- The combination of computational chemistry and continuum modelling will be important when industry wants to tap into the chemistry underneath continuum level problems.

- It will be important to find collaborators who are willing to join forces and cover the wider spectrum of multiscale modelling for as many fields as possible.
- Modellers should prepare the documentation for SMEs related to modelling process and workflow. They provide the case studies, which help SMEs. However, investors will pay for marketing and realisation of a product.
- The modellers/practitioner should feature on the start of the chain Computer-aided Engineering → Design →Product. Otherwise the starter is missing and a whole ecosystem is shifting.

Impulse 2

Thomas Schrefl (Danube University Krems, AT)

Magnetic materials modelling – Bridging the gap between academic software and industry needs

Key Points

Once software bridges the gap from academia to industry it becomes a tool for the latter and thus, demands for this tool are emerging. Industry wants updates, new features, customisations, support and they are very product driven and work to a strict time line. This requires the academic SWO to think industrial and trying to understand the underling market and how fast "hot topics" can change. When this point is reached the SWO requires a more commercial setup and provide the demanded support and development activities.

One also has to understand the geographical preferences of the market. US based customers are keen on consultancy, whereas Asian based customers like to embark on university – joint research projects.

It is important to keep visibility and exposure to potential customers and find answers to new industrial questions frequently; thus, monitoring the current state of industry is pertinent.

Conclusion, Questions, Remarks

- The dissemination of software at conferences (both scientific and industrial) helps to attract clients. Thus, presentations should comprise state of the art industrial application of the respective software. The dissemination at the focused conferences is extremely important.
- Industry drives the universities to develop effective solutions for industrial relevant problems.
- A marketplace would be very useful for small companies who know their customers very well. However, the existing of marketplaces with small domains could help a lot for SMEs. E.g. magnetic materials modelling, a very small area with very limited market could profit from a marketplace.
- To make a software venture successful it is necessary to control the time effort that leads to a solution. This should go hand in hand with preparing a software manual and demo version as well as providing customer support.
- The customization process is the driving force for an SME, based on the confidentiality and long-term guarantee.
- Service agreements become important with an increasing number of customers. This comprises services after sales, provision of training courses, updates and technical support as well as the information regarding new features or workflows according to customer needs.
- The market is characterized by a wide range of SME SWOs specialized on particular applications and market niches, i.e. it is quite fragmented. Business and marketing models tend to be strongly dependent on the specific market served.

Impulse 3

Zlatan Stanojevic (Global TCAD Solutions GmbH, AT)

How to Fail Commercially in Materials Modelling

Key Points

Software SMEs are presented as very exciting ventures that have to ingeniously conquer a market full of competitors. They have to beat software monopolies and established in-house solutions.

They are very attractive for employees who are looking for a wide job spectrum as each individual has to take on different roles. This must be enabled by a rigorous project management and optimised workflows and a good offering of CPD – it is very hard to replace versatile skilled staff. SMEs would profit from feedback, but it is not easily given by customers due to confidential research to which the software is applied. The SMEs have to gather intelligences elsewhere. They would be very interested in research funding as development needs stability. They could be interested in projects and international matchmaking events.

Conclusion, Questions, Remarks

- In reality, SMEs have pressure from a client to provide a software product. Customers do not give time for validation. That is why sometimes SMEs need to provide the product without validation and verification of models. However, it is possible to solve the problem by research co-operations and involving SMEs for research funding.
- Chemistry needs big impulse to develop focused software and integrate A.I. to analyse the experimental data. Computational chemistry has a great potential. Moreover, multi -physics problems are the open field for materials modelling. It could be possible to find the solution on the academia-industrial (SMEs) collaboration.
- Marketplaces should be a home to both large enterprise and SME SWOs. The market scaling supports high specialization of solutions, which fosters emergence of oligopolies and de-facto monopolies. Beating a monopoly is extremely difficult for SMEs. Marketplaces should therefore foster SMEs and open opportunities and communication with potential clients. To increase the success of the marketplaces feedback should be improved.
- Validation of a software can be very customer specific as their data might be pertinent to it. SWOs should cover generic verification and validation and instruct customers how to perform validation using their proprietary data.

Expected outcome and future activities

- Monitor the ongoing digitalisation projects closely as new data can mean new business
- Be visionary and demonstrate how software can solve/aid with industrial projects.
- Let’s not neglect SMEs as a customer
- Keep working on SaaS business models and remove barriers for its adoption.
- Assure that marketplaces are attractive to SWOs and can offer something for both the established and new SWOs

2.3 Session 17: Open source and commercial software for Industrial Deployment of Materials Modelling Software

2.2.1 Overview

Chair

Kurt Stokbro (Synopsys, DK)

Impulse 1

Georg Kresse (University Vienna, AT)

The VASP Software GmbH: why did we go commercial

Impulse 2

Michael Haverty (Applied Materials, US)

Materials Integration: An All-Of-The-Above Approach

Impulse 3

Laurent Adam (e-Xstream engineering, BE)

Multi-scale continuum modeling with Digimat : 15 years journey from academia to industrial application

Rapporteur

Umberto Martinez (Synopsys, DK)

Session presenter at Podium Discussion

Kurt Stokbro (Synopsys, DK)

Introduction

This session will address the role of open source and commercially distributed software in the advancement of industrial usage of materials modelling software. The meeting is intended to be inspired by concise impulse talks addressing the following objectives, which are complemented by in-depth discussions on the points below.

Objectives

- What is the current situation for funding the development of open source, commercial and closed software in electronic, atomistic and continuum modelling?
- Who is pursuing the development of new methodologies, what is the role of commercial and open source software for progressing the field?
- What is the role of open source and commercial software for the industrial exploration?
- What are the barriers for commercializing open source software?
- New business models for making simulation tools available, for instance cloud-based tools.
- What are the trends in industrial usage, which industries are using electronic or atomistic modelling, do we see an expansion in the usage?

- What kind of problems are investigated, do we see new trends, for instance high throughput screening?

Background information and documents

BUSINESS MODELS AND SUSTAINABILITY FOR MATERIALS MODELLING SOFTWARE, White paper for the EMMC, Gerhard Goldbeck, Alexandra Simperler; Goldbeck Consulting Ltd 2018

https://emmc.info/emmc-csa-white-paper-for-business-models-and-sustainability-for-materials-modelling-software/

Discussion points and questions

- How can open source software models be sustainable and benefit from industrial usage?
- Can the more immature fields of electronic and atomistic models learn from other fields (for instance continuum models) to progress industrial usage?
- Will we see new business models in the future, for instance cloud based?

Within the EMMC-CSA, an expert meeting was held in October 2018 in Paris about Open source, free software, and commercially supported software. This outcome of this earlier expert meeting provided a basis for the present session.

2.2.2 Summary and collected feedback

Impulse 1

Georg Kresse (University Vienna, AT)

The VASP Software GmbH: why did we go commercial

GK gave a brief background info of VASP software (most widely used for solids, estimated user base 5k-15k users, hybrid license model -> proprietary license but they distribute the source code)
GK finds that the usage of all atomic scale codes is growing. The reasons of the success of VASP are the following:

1. Ready to use pseudopotentials
2. Unprecedented robustness – PRB 54, 11169 (1996)
3. Stat of the art: first to introduce hybrid functionals, beyond DFT

Less than 1% of the users examine and study the code (tiny developer base)
Complex codes:

- 500k lines of Fortran 90 legacy code
- refactoring will be extremely expensive

Funding situation: not good for code development, mainly for engineering (in US, EU slightly better). Code refactoring and rewriting is not funded. Support is not funded.

Today in Science code development, support and maintenance relies on funding for fundamental research. Infrastructure funding, e.g. ETSF, Psi-k, MaX, NOMAD. However, infrastructure funding of software is difficult. Let the market (users) and not the referees of research grants decide what should be funded. Physics community is very against paying for software, however, license payment by the end users is the only sustainable model.

VASP hybrid marketing model: until 2018 developed at University of Vienna. 4k permanent license allow for robust and constant stream of income. VASP had problems having long term commitment from university, overwhelmed by support. Only long time solution is to make a private company (with same license model). VASP Software GmbH is now a team of six.

Conclusion, Questions, Remarks

Conclusions:

1. Funding problem for refactoring
2. Progress in the field: keep open source but commercial exploitation is required
3. Barriers: EU physics community believe in open source, not sustainable. Good software is never free or cheap
4. Usage of the codes: large user base 10k+ users. Industry is behind in the usage of atomic-scale modelling - like 10 years

Questions:

- If 1% only check source code, why making it open source?
  It is a matter of fairness, we want to give the opportunity to people to learn.
- Questions about the plot showed on slide 11 which compare the speed of VASP to Quantum Espresso *[Slides can be found on EMMC website at https://emmc.info/emmc-international-workshop-2019-workshop-presentations/].* There was a technical discussion about the fairness of the comparison.
- Can you give some figures about your customers?
- Erich Wimmer from Materials Design gives few names of commercial customers including the world's major automotive companies.
- How to include changes in the code from the user base? Hard to maintain support with huge user base.

Impulse 2

Michael Haverty (Applied Materials, US)

Materials Integration: An All-Of-The-Above Approach

Material modeling in industry is maturing, new capabilities being developed, cloud a viable alternative in some cases

Four types of typical materials modeling projects:

1- Screening
2- Optimization
3- Mechanism (understand why)
4- Parametrization

Mike highlights successful applications in Semiconductors. Many technical challenges in atomic-scale modelling methods are solved or «good enough», e.g. electronic properties, mechanical properties, chemical properties. The still remaining open challenges in atomic-scale simulation software are:

Practical: workflows, reliable and easy-to-use software. Computational resources. Realistic interfaces. Bridging realistic time scales

Technical: some requires 10x computing

Capability SW drives. Commercial codes start to be quite similar in capabilities, i.e. many similar provides. Why Cloud computing? To have state of the art hardware. It is competitive in some cases. Security is a big roadblock however it is mainly irrational, and Michael expects that this roadblock will disappear with time when companies get more used to cloud based solutions. Potential value-added feature, to add scalability.

Conclusion, Questions, Remarks

Conclusions:

Currently no commercial, academic, or open-source set of tools provide all that is needed. Future may involve hybrid supported open source models.

Ideal state/software. 1) Stable and comprehensive core engine(s) 2) Simple automated workflows (for non-experts) 3) Ability/flexibility to leverage open-source development 4) Databasing and analysis 5) Cloud + on-premises hybrid options

Questions:

1- Workflows are written by experts to non-expert. Somehow what AiiDA is doing [AiiDA is a flexible and scalable informatics' infrastructure to manage, preserve, and disseminate the simulations, data, and workflows of modern-day computational science. http://www.aiida.net/]
2- How about multiscale modeling? Multiscale modeling can mean many things and it is today practical only across specific scale ranges. Sometimes people talking about multiscale modeling refers to the wider range going from atomistic to macroscale within one single framework/solutions. This is not achieved in practice yet.

Impulse 3

Laurent Adam (e-Xstream engineering, BE)

Multi-scale continuum modeling with Digimat : 15 years journey from academia to industrial application

Conclusion, Questions, Remarks

Overview of Digimat and e-Xstream. Highlighted how they can help improving R&D providing multi-scale material modelling, customizable, with state-of-the-art models and methodologies, with proven applicability in industrial environment. They have 500+ customers in various industries.

Keep funding R&D also via public funding.

e-Xstream also offers services to drive revenue e.g. strong education, support.

Hexagon overview

Questions:

1. Questions about applications on electromagnetics. 95% applications are mechanical or thermomechanical.
2. Technical question about long fibers.
3. What has been the main challenge in building vertical solutions for non-experts? Understand the mindsets and needs.
4. 80% revenue from licenses, 20% other.

Discussion points and questions

The following questions summarize the issues for this session.

- How can open source software models be sustainable and benefit from industrial usage?
  Discussion about license models, problems with GPL and how to go back to it, MIT licenses …
- Can the less industrial deployed fields of electronic and atomistic models learn from other fields (for instance continuum models) to progress industrial usage?
  Many continuum tools have been so standardized such that they can be used by technicians and other non modelling experts. Similar evolution can expand the industrial uptake of atomic-scale modelling.
- Will we see new business models in the future, for instance cloud based?
  Importance to distribute source code, but there is a fear of doing that. Few big companies going open source, e.g. red hat.
  Mike stresses that for industry it is tough to go open source without support
  Danger of user wrongly compiling and getting wrong results. Possible to distribute executable but difficult to provide scalable and universal executable.
  Providing source code is important for example for force fields which allows verification and validation. However, cases like Schrodinger that invested 20M $ to develop their own force field.
  In physics community is hard to establish your code if it is not open source, the market dictates it.

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Consortium		
TU WIEN	Technische Universität Wien	Austria
FRAUNHOFER	Fraunhofer Gesellschaft	Germany
GCL	Goldbeck Consulting Limited	United Kingdom
POLITO	Politecnico di Torino	Italy
UU	Uppsala Universitet	Sweden
DOW	Dow Benelux B.V.	Netherlands
EPFL	Ecole Polytechnique Federale de Lausanne	Switzerland
DPI	Dutch Polymer Institute	Netherlands
SINTEF	SINTEF AS	Norway
ACCESS e.V.	ACCESS e.V.	Germany
HZG	Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GMBH	Germany
MDS	Materials Design S.A.R.L	France
Synopsys / QW	Synopsys (former QuantumWise A/S)	Denmark
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