Charter for EMMC team on Open Simulation Platforms

Background – Status Assessment

Materials' modeling is recognized as one of the strongly developed capabilities of Europe and is certainly a strong domain of competence. Academia is continuously working both on expanding the fundamental capabilities of the software, the size of problems and not at least smarter and faster algorithms that enable the user to solve larger and larger problems of higher complexity and better predictive capabilities. Industry is increasingly asking for the simulation of a variety of complex materials, to predict a variety of properties and to model a production processes with the goal to eventually define the relevant properties along the complete life cycle of plant and material. This requires a modular, configurable system of models and equally modular software tools replacing the current monolithic approaches.

Scope

Scope of the EMMC team on "Open Simulation Platforms" is to elaborate concepts for an open simulation platform allowing plug & play type combinations of different software tools – academic and commercial - across different length and time scales and along the entire value chain and to promote the development of a meta information that makes it possible to raise the level of abstraction and thereby to eliminate the majority of communication problems. A further objective of the team is the specification/definition of the wordings used in the field and often being interpreted differently by different communities.

The basic ingredients of a strategic approach towards such an integrated computational materials engineering (ICME)-platform and their implications for the concept (*in italics*) are:

- allow for use of existing and verified models to a maximum extent: *extendable, modular,*
- allow for use in existing environments: *support existing established operating systems and programming languages*, *interactive*
- close existing gaps in the present manifold of models mapping the materials and the process chain aiming at the provision of a *comprehensive* concept building on *meta information*.
- speed-up individual models by data-reduction where applicable: *adaptable*
- speed-up individual models by efficient programming: *efficient, parallelized/distributed*
- enable and speed-up information exchange between different models: *standardized, metadata*
- integrate different process scales (length, time): *comprehensive, adaptable*
- useful for different types of materials and processes: *generic and/or adaptable*
- use only models being relevant to describe/predict the process: *modular, interactive*
- model-refinement or –reduction where necessary and/or beneficial : *extendable, modular*

- facilitate creation of simulation chains by drawing on prior knowledge: s*elf-learning, knowledge integrative*
- account for changes and evolution of the underlying software/models/tools : *dynamic, generic*
- allow for networking and for easy use by different communities: *open*
- provide interfaces to open and free visualization/post-processing tools: *open*
- provide persistent data storage and retrieval: *sustainable, knowledge integrative*
- allow for secure commercial applications: *industrially relevant*

An *open architecture* will be a key ingredient of a strategic approach toward integrated computational materials engineering. Anybody interested in profiting from ICME by performing respective simulations must be able to do so without major barriers. In the same spirit anybody willing and capable to provide models or simulation tools should be able to easily include them into the ICME framework. Even if an open architecture is highly desirable one has to account for the interests of commercial providers of simulation software as well. The easiest way and probably the fast lane to integrate academic and commercial model worlds thus seems to be the definition of a common language in the sense of an information exchange between different models being based upon a *common, open standard format*. This should be done exploiting metadata concepts, since different codes have very different requirements for data representation and access (file formats, databases, etc.).

Working domain

Currently the main challenge is to have a large variety of programs to be organized in integrated computational materials engineering “ICME” procedures and workflows involving a family of different codes. In a first step this requires the identification of available solutions and stakeholders to a maximum extent. In a second step, co-ordination and organized communication of data, models and workflows, has to be specified. This also implies the specification of methods to generate and store data, models and workflows in a form making it easy to store and to retrieve these data.

First steps already taken by the team on “Open Platforms” are the launch of a market survey of materials & process simulations and their use in industry and academia and identify all relevant stakeholders– (https://docs.google.com/forms/d/130ajVA_b5_tqUf9DCixhzX0tIg0Ieo6MWLU_wDYMAAQ/viewform) and the creation of a structured inventory of globally available commercial and academic software solutions especially comprising details about I/O formats and interoperability of the tools – (https://docs.google.com/forms/d/186kvoljlLdUZ0tr4PANkJYbhau9tAQ67xnqTUX1P3M8/viewform)

The first stage thus is to collect information on what is to be communicated and stored. Having a catalog of “sand box scenarios” should then serve as a basis for the unification and finally standardization of data representation, models and workflows. It is apparent that a respective standard will help to reduce the workload associated with linking software together. Standardization on the one hand is required for a weak coupling of different models by e.g. file exchange but especially for strong in-line coupling of codes requiring high-level user interfaces (APIs). It should be noted that APIs can be also beneficial for weak coupling. Their use naturally allows for data format independent data exchange as communication and data exchange is defined by means of services and not by means of data itself. In view of established and validated commercial software being a mandatory component, the realization of such standardized protocols will most probably require implementation of adaptors. The conceptualization of such adaptors accordingly forms another core activity of the "Open Platform Team".

In summary, the development of "Open Platforms" will require input from people defining the models, thus from the domain of physics and materials science/engineering, theoretical system theory and the application domains of industrial users as well as computer science for the structuring and implementation. It is envisioned that on a long time horizon the subject of restructuring the software domain should evolve as a core subject, namely the separation of model generation, both on the abstract algebraic level and the automatically compiled version, from the tools to instantiate the mathematical problems from the solvers and the data bases. Anybody willing and capable to contribute is invited.

Objectives

Find and define platform type approaches to structure the information associated with defining a set of models and solving ICME-types of problems formulated utilizing the set of models such that the platform system becomes very flexible and efficient in use also by non-specialists in the particular fields of expertise involved.

Goals/Steps to be taken

1. Establish a core team
2. Define a work approach and context for addressing the defining challenges associated with the objective
3. Develop a (representative) social network related to (open-source) modeling and simulation software.
4. Identify, define and articulate specific objects that need to be included in the standardization.
5. Define standards for communication, data exchange, models and workflow information representation, handling and storing.
6. Specify an implementation to demonstrate feasibility and validity of the approach providing input into the future funding programs.

Desired outcome

A model-centered and object-oriented computational environment for Integrated Computational Materials Engineering being applicable to a very broad range of materials, processes and properties.

Timeline

- Continuously: expand representative network of stakeholders with active core (the team)
- Continuously: collect information about available software tools
- Sept 2014: Request for sharing of ideas sent to existing list of companies using the Charter
- October 2014 Invitation to Nov meeting of active contributors by EC
- Nov 2014: Report on outcome of the consultation in Brussels
- Dec 2014: draft Road Map

Team members

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