# E-CAM Scoping Workshop: “Building the bridge between theories and software: SME as a boost for technology transfer in industrial simulative pipelines”

**Location: Fondazione Istituto Italiano di Tecnologia (IIT), Genoa, Italy**
**Dates: May 23, 2018 to May 25, 2018**
**Organizers: Sergio Decherchi (IIT, IT), Andrea Cavalli (IIT, IT), Sara Bonella (EPFL, CH)**

# 1 State of the art

Statistical mechanics, electronic structure and multiscale modelling are three of the theoretical tools that enable understanding and modelling of physicochemical processes in computational chemistry/physics. Several theoretical/computational methods have emerged over the last decades. Despite their remarkable value in terms of novel ideas and theories, however, such approaches are often far from a practical applicability within industrial settings. This is mainly due to the fact that: i) these algorithms are often written in rather inefficient programming languages and therefore not fully optimized for new generation hardware architectures; ii) these methods can be very accurate from the physics standpoint, but quite far away from the industrial needs of finding a suitable trade-off between speed and accuracy. Therefore, companies in different areas are actively seeking more reliable, still rather fast, computational methods to reduce the overall costs of industrial R&D pipelines. This is, for example, the case in drug discovery, where companies are looking for innovative approaches to accurate kinetics and thermodynamics predictions, and in the material industry, where designing new nanostructures with improved features could greatly benefit from computational simulations. There exists, however, a clear and long-lasting gap between the theoretical chemistry/physics community and industries, which are looking for efficient, user-friendly, and professional software solutions to be utilized in many different areas. Against this scenario, small/medium enterprises (SMEs) that develop simulative software can play an increasingly key role not only in translating the science developed in academia into a proper technological transfer process, but also in building a scientific bridge between the industry requirements in terms of automation and the new theories and algorithms developed at an academic level. It is crucial to remark that transforming academic algorithms into usable software is not only a matter of software engineering, but often also means reconsidering the original theories and formalisms. In this context, software development SMEs, which have a clear mission towards top level science suitable for

industrial settings, may represent the missing link in the pipeline from-theory-to-software.

# 2 Major outcomes

In this E-CAM workshop, we addressed in particular the following question: (1) which is the most appropriate propelling element of innovation, top-level academic science or industrial needs of accelerating R&D towards novel and cheaper products? Traditionally, the approach to technology is conceiving technology as a corollary of scientific research. However, there is compelling evidence that for several mid-term projects an industry-requirements-driven approach is largely feasible if not best suited. A tightly connected topic regards on how to match and synchronize curiosity driven research with industrial needs and how to manage the resulting, possibly academic/industrial mixed, intellectual property. This led us to consider the further question (2) can this 'engineering' or 'politechnique' approach to science/technology transfer be the way to boost the technological SMEs European tissue?

Talks from academia and industry were interleaved in the meeting. This allowed to complement and contrast experiences and knowledge coming from academia and industry.

Industrial requirements, expressed in particular by scientists from the drug discovery field, emerged quite clearly and consisted in the need of fast albeit approximate methods for analysing ligands. This analysis should include both thermodynamic and kinetic properties with very high efficiency (overnight production of results). It was also stated that pharma companies are quite sceptical about the real effectiveness of machine learning when applied to docking or thermodynamics prediction.

The role of SME also emerged quite clearly. The underlined how, even though fundamental methodologies such the creation of an interaction field comes from academia, commercial products need to re-elaborate and recast methods to be effective. This observation created a certain consensus on the audience for which while the idea is coming from academia, the innovation, the application to the real-world problem often comes from the SME, whose success is tightly linked to its ability to address real industrial needs.

The role of software developers in SME and academia was also discussed. Different points of view emerged in the discussion. For some participants, software engineering is a fundamental component to any success in the computational field either commercial or academic software. For others, even for SME it is more important to hire personnel with a strong background in chemistry or physics, than in software developments.

There was also a consensus that EU funded Centers of Excellence for Computing Applications can provide an opportunity to enhance the expertise and scope of software vendors SMEs.

# 3 Community needs

The following needs were highlighted by the academia and the industry participants.

Academia: (1) include in the research group software engineers able to properly code methods or ensure access to sustained consultancy and assistance in this area.; (2) identify means to ensure a certain degree of time continuity in the code development and maintenance; (3) identify and assist to assess the potential for technology transfer of in-house activities. The EU centers of excellence might provide an environment to systematize, host and enhance in-house software developments and foster technology transfer.

Industry: (1) increase the dialog between industry and academy; (2) seed academia with real world problems whose solution industry could benefit also in economic terms. There was unanimous consensus that SMEs are playing a significant role in bridging the two worlds. However, this can only work with a proper “feedback-cycle”: academy talks with SME/Industry and vice-versa in a not interrupted loop to foster high level science that on the long term could be applied to industrial problems. Opportunities to create and sustain this cycle were indicated as still insufficient and absolutely crucial. In the discussion industrial participants, and in particular software vendors SMEs, raised the point that activities that are, or can be perceived, as establishing EU funded Centers of Excellence as competitors of SMEs should be avoided. The promotion of collaborative efforts was also indicated as a necessity.

# 4 Funding

From the academy side, there are several European initiatives that found computational methods ranging from material science to biological systems. Even if not a grant deliverer, CECAM constitutes a key resource to centralize in a common framework/place various research efforts in Europe and beyond and all the audience acknowledged the importance of such initiatives as E-CAM.
From an industrial perspective, it emerged that it is rare to have an internal “methods development unit”. Software vendors SMEs can play an important role benefitting from industrial funding targeted not only at software development, but also at outsourcing the development of new protocols and approaches.

# 5 Will these developments bring societal benefits?

The potential benefit of the technologies and methods discussed is notable. For instance, in drug discovery, considering that the overall time needed to start from the target and arrive to a marketable drug is about 10 years and 1 billion of dollars of capitalization, it's then clear how computational methods, the ones presented at the meeting, can remarkably impact in economic terms. There are technological realities such as FEP as presented by Schrodinger and newer methods such as those delivered by BiKi Technologies. Also out of equilibrium method (Hummer's talk) and path sampling methods (D. Swenson) if properly tuned for the drug discovery requirements might have the potential to accelerate the drug discovery, hence impacting at an economical level.

# 6 Participant list

**Organizers**

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