Proposal for a new FET Proactive topic

Title: Value creation through mathematical modeling, simulation and optimization

Keywords: innovation, mathematical modeling, computer simulation, optimization, applications of high performance computing

Scientific and technological topics to be addressed

Future challenges for innovation in industry and society exhibit increasing complexity and at the same time have to obey to ever-shorter innovation cycles. One of the key technologies in this permanent fight is the use of computers at peak performance in an appropriate way, i.e. in the integrated modeling, simulation and optimization (MSO) frame. In the competitive industry and in the top scientific research projects a full holistic approach is to be applied (e.g. to MSO of a complete vehicle, a full digital factory, human heart and the complete vascular system). To be able to fulfil the needs of the holistic approach we need the planning and the operation by a mathematical model which allows to simulate and optimize the real product on virtual product via the use of high performance computing (HPC) tools.

Although there are many success stories of the use of MSO (see "European success stories in Industrial Mathematics", Springer, 2011, ISBN 978-3-642-23848-2), the full potential of MSO as an integrated discipline is not yet realized and hence the potential creation of value is still severely overlooked. Often, MSO is taken on board only in the final stages of a project. In order to create real value from MSO, it must be an essential part of every innovation project, and urges also developments in new mathematical methodologies, e.g. in:

- multi-physics and multi-scale systems,
- combined discrete and continuous non-linear systems,
- non-deterministic stochastic influences,
- approximating systems too large to be dealt with via adequate model reduction schemes,
- dealing with inhomogeneous uncertainties among the various parts of the model,
- management of big data.

All these fields (and many others) are of high importance in order to deal with problems arising in areas like nanotechnology, medicine and health, the environment, energy production and transport image and data processing, etc. Moreover, the MSO technology itself faces challenges, e.g. sensitivity analysis of and adjoint methods for the full, integrated model.

In order to create real value, many disciplines need to be involved. Clearly, mathematics is the basic discipline here, integrated to computer science, especially associated with HPC, and all disciplines of engineering and natural sciences.

In Europe several research groups with excellent researchers work on the scientific research and application of MSO in industry and innovations. Numerous of them formed the international network EU-MATHS-IN, the European Service Network of Mathematics for Industry and Innovations (see http://www.eu-maths-in.eu/). This international network currently consists of a dozen of national networks representing dozens of research groups each to boost mathematics for industry in Europe.

Many recent top scientific and innovation projects make use of the MSO technology. A true success case is the virtual paint shop: initiated by Volvo Car Corporation in 2006, the Fraunhofer-Chalmers Research Centre for Industrial Mathematics developed mathematical software for virtual spray painting in 2009. Since then even more painting technologies have been involved into the virtual paint shop and the number of top manufacturers using the methodology and software has increased above twenty. Use of the virtual paint shop reduced the environmental impact and increased the product quality as well.

Highlighting MSO as a FET Proactive initiative would provide both the scientific and industrial research communities with the proper way of using advanced mathematical technology combined with high performance computer resources and give a tool for them to systematically achieve new results of high impact in their fields. Establishing MSO as a future emerging technology will enable Europe to capitalize on the current European leadership in application-driven MSO, to strengthen European competitiveness in industrial innovation in allowing industry with tools of higher precision within the same time scale, and to meet important future societal challenges. Moreover, there exist many significant research projects also among granted projects that could be brought into the breakthrough level.

No doubt that continuous multi- and interdisciplinary research and novel mathematical and computational methods are needed to provide the necessary tools for industrial innovation and European competitiveness. It has become widely recognized that the approach of mathematical modeling, simulation and optimization (MSO) is the third, and indispensable, pillar for scientific progress and technological innovation, besides experiments and theory building. When full scale simulation is no more possible, mathematical modeling and simulation and optimization can do it!
This viewpoint is supported by the Forward Look on Mathematics and Industry of the European Science Foundation (http://www.esf.org/index.php?id=6264) and in further reports:

- *Mathematical sciences work is becoming an increasingly integral and essential component of a growing array of areas of investigation in biology, medicine, social sciences, business, advanced design, climate, finance, advanced materials, and many more – crucial to economic growth and societal well-being ("The Mathematical Sciences in 2025", report of the National Research Council in the USA, 2013)*
- *The GVA attributable to the direct application and generation of mathematical science research in the UK in 2010 was around 16 percent of total UK GVA (Deloitte report on "Measuring the Economic Benefits of Mathematical Science Research in the UK", November 2012 and a similar report issued in The Netherlands in 2014)*