Journal of Computational Science 14 (2016) 69–73

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Editorial

# Education and training for exascale

ARTICLE INFO

*Keywords:*
Computational Science research methods
HPC curricula
University studies
Professional training
HPC skills gap
Exascale computing

ABSTRACT

This editorial focuses on education and training approaches on the route to exascale. In a wider context the editorial outlines how the Computational Science research methods can be used in university studies and professional training in HPC in order to narrow the HPC and Computational Science skills gap. It provides short analysis of the HPC and Computational Science research context and analyses the current state. It also describes and proposes the relevant curricula structure covering not only mathematics, computer science and supercomputing areas but also natural and life sciences domains. It is aimed at enhancing student's and professional's research profiles developing their abilities to investigate complex problems, build and apply advanced mathematical models, analyze the resulting data and use adequately HPC environments and tools for computation and visualization all so needed on the route to exascale. It also gives examples how this approach can be applied in Higher Education setting in case of specific scientific domains with explicitly taught and embedded Computational Science subjects and in case of professional training and outlines the differences and similarities in both cases as well as links the proposed approach with the papers in the special section.

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## 1. Research context

Computational Science and High-Performance Computing (HPC) are key strategic assets for the EU and its innovative capacity [8,14,15]. Large scale computing in science and industry has become an indispensable way to tackle societal and scientific grand challenges, and to address the needs of industry to innovate in products and services. Computational approaches to scientific grand challenge problems such as the detection and treatment of diseases like cancer, modelling of the human brain, and climate forecasting are beginning to bear fruit. Computational Science, an interdisciplinary field that melds basic sciences, mathematical modelling, quantitative analysis techniques and HPC techniques, is integral in addressing the big problems in industries ranging from manufacturing and aerospace, to drug design and risk management.

According to the latest IDC Report [13], in Europe, 97% of companies that adopted HPC stated that they "could no longer compete or survive without it." From the study it is also evident that Computational Science and HPC are of increasing importance for manufacturing, especially enabling smart manufacturing (automotive, etc.), resource exploration such as oil and gas, health and medicine, drug design, weather forecasting and global climate change [13]. The areas according to IDC where Europe has an advantage, provide substantial contribution and can provide leadership, can be identified as: weather and climate research, clean and sustainable energy, automotive and aerospace design, bio-life sciences, particle physics and related fields, modeling of materials/molecular dynamics. It is also evident that Computational Science and HPC advances are integral for scientific and industrial advances in other developed economies such as USA, Canada, Japan, etc [1].

Many of the above areas represent also **major societal drivers/challenges** such as Energy, Climate Change, Urbanization, etc. [16] and scientific methods, in particular Computational Science and HPC are crucial to address these challenges.

Computational Science as an interdisciplinary field is undergoing rapid change. Scientific instruments from particle accelerators to DNA sequencers are generating petabytes of data faster than our current capacity to analyze it. 'Big Data' approaches to grand challenges are increasingly involving the integration of massive and many sources of data. Hardware designers, backed by governments from the EU and US to India and China, are in a global race to create supercomputers capable of exascale performance (1000 times the performance of the very large supercomputers of today). New computational models such as CPU-GPUs and many-core architectures, and software models such as clouds and highly virtualized infrastructures, and data models such as schema-less unstructured data and high-throughput sensor streams, are increasing the number of design approaches and are fundamentally changing the range of problems that can be effectively addressed.

"By 2020 the computing power available in today's most performant HPC systems will be available on desktop systems. A well

http://dx.doi.org/10.1016/j.jocs.2016.04.013
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trained workforce capable of efficiently using this computing power is essential.” [8]

The direction of most change is positive. Key societal and scientific grand challenges have been identified and in many areas there are tools for amassing the required analytical data, as our computing capacity continues to scale-up. However, there is an important ingredient lacking, namely an adequate supply of highly trained computational scientists with the ability to understand complex scientific problems and the skills in mathematical modelling, simulation, Big Data techniques, and HPC to address them. Indeed the focus on training capable scientists and capable workforce with the right mix of skills to address the above challenges is growing both in Europe and the USA. The latest executive order of the US President Obama (July 2015) has focused on long term National Strategic Computing Initiative [20] that in addition to focusing on ensuring US leadership in HPC also states as key component education and training in order to educate and train scientists for the “next generation of HPC systems, covering fundamental concepts in modeling, simulation and data analytics, as well as the ability to formulate and solve problems using advanced computing [21].

## 2. Curricula development

At the start of the 21st century Career Space Consortium established a working group comprising of representatives of 20 EU universities and companies to establish ICT curricula development guidelines. The resulting guidelines [12] were based on the industry’s needs that the graduate skills profiles reflect the ICT generic job profiles. The working group conducted a wide ranging analysis of the existing university degree routes related to ICT and the corresponding graduate specializations. The guidelines suggested the implementation of block-build modularized curriculum content in order to ensure the right scope of competences relevant to the ICT industry. The recommendations of the group were to provide a broad foundation of science and technology in order to ensure a balanced overview of the broader subject areas of relevance, including mathematical, scientific and technical knowledge. These have to be pared with broad overview of the various technologies available and in-depth specialized knowledge to ensure professional competence of the graduates. Students should also be equipped with sound understanding of workplace context, as well as the needed personal skills for collaboration, communication and project management.

The standard taught MSc program in EU is usually 120 ECTS (European Credit Transfer System) which comprises four semesters consisting usually of three main blocks:

- one to two semesters of core subject modules with a few or in some cases no electives,
- at least one semester of specialization where the elective subjects are clustered,
- between half and one semester consisting of a final project and a dissertation.

The available credits for taught modules are about 90 ECTS. Depending on the structure and the subject area, that usually means teaching between nine and twelve separate modules with electives rarely being more than two to three modules (between 1/3 and ¼ of the modules).

In EU there are several established Computational Science MSc degrees with the possibility to specialise in a certain scientific discipline such as ETH Zurich “Diploma in Computational Science and Engineering”, KTH Sweden “International Master Program in Scientific Computing”, University of Amsterdam “MSc in Computational Science” as well as few emerging joint Computational Science

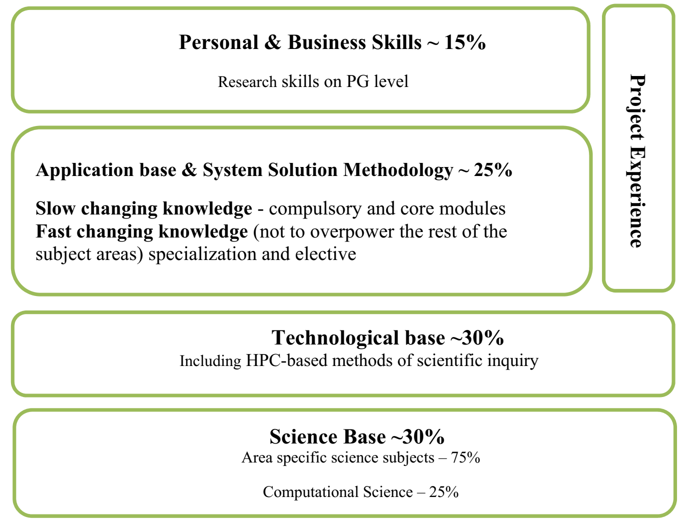


**Fig. 1.** Optimization of the curricula route for inclusion of Computational Science research methods and HPC-based methods of scientific inquiry.

degrees such as, for example, the one between the University of Amsterdam and ITMO University, Russia [9]. On the other hand the US experience shows two currently predominant models of Computational Science programs at PG level: one delivered at computer science or mathematics departments and another in scientific disciplines departments with the participation of computer science and engineering where the Computational Science subjects are given as a specialisation [6]. The issue both in EU and US, seems to be the low numbers of graduates which are by no means adequate to answer the need of required specialists. Both [1] and [6] outline the need and the skills shortage of specialists in exascale computing area. Additionally with the advent of Big Data this shortage becomes even more acute on the interface of Data Science and Computational Science [6,7,10].

If the skills gap is to be bridged, the way forward should be introducing Computational Science research skills as a part of the core subject block in the majority of the MSc science degrees. The proposal is to embed several taught modules delivering the core theoretical knowledge and introduce at the dissertation module project specific practical skills training.

Building on 15 years of experience in creating multidisciplinary postgraduate degrees based on the Career Space curriculum development model, an integration of Computational Science research methods and HPC technology and tools into science postgraduate courses is proposed where Computational Science subject modules are part of the science base block and HPC-based methods of scientific inquiry are becoming an integral part of the technological base. These are complemented by the inclusion of both functional skills at university level and advanced research methodology with emphasis on explicit and embedded teaching of personal skills and introduction of near real life project experiences in collaborative environment (see Fig. 1).

The taught modules could be in a block of five or as a “lighter version” in a block of three [5]. Significant Computational Science element, a combined degree in its essence, with five modules (at least 25 ECTS) would include: **introduction to mathematical modelling** (introduction to PDEs and ODEs, discretization approaches, linear algebra, introduction to parallel algorithms); **advanced mathematical modelling** (complex systems and systems approach to modelling, multi-level, multi-scale methods, elements of optimization, advanced linear algebra, advanced parallel algorithms and parallelization techniques); **introduction to programing environments and tools** (introduction to parallel

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