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Guest Editorial

Transforming medical sciences with high-performance computing, high-performance data analytics and AI

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Abstract. The advance of high-performance computing (HPC), high-performance data analytics (HPDA) and AI and their synergetic integration into workflows has revolutionized numerous industries, amongst others the medical and pharmaceutical sectors. In this special section of *Technology and Health Care*, we delve into the remarkable advancements and potential of HPC, HPDA and AI (together termed *HPC+*) in driving innovation, improving patient outcomes, and accelerating drug discovery. The articles in this issue shed light onto the potential of HPC+ in addressing several critical areas, including medical imaging, personalized medicine, drug discovery, and clinical as well as political decision support.

Keywords: Computer simulation, big data, image processing, computer-assisted diagnosis, drug development, computer-assisted decision making, precision medicine

The rapid advancements in high-performance computing (HPC) and high-performance data analytics (HPDA) together with AI (jointly called *HPC+*) have paved the way for revolutionary transformations in the field of medicine and pharmaceuticals. These cutting-edge technologies have shown immense potential to accelerate research, enhance clinical decision-making, optimize treatments, and ultimately improve patient outcomes. In this issue of *Technology and Health Care*, we delve into the remarkable utilization of HPC, HPDA and AI in the medical and pharmaceutical domains and present success stories from the application in the medical sciences and health sector, and provide background information on the important role of HPC+ competence development, as well as an example of current technological and support capabilities within the European network of National Competence Centres (NCCs) in HPC.[1]

The convergence of HPC and HPDA has brought forth an era of unprecedented opportunities in healthcare. With the ability to process vast amounts of data and perform complex computations in real-time, HPC+ empowers researchers, clinicians, medical technology providers and pharmaceutical experts

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to extract meaningful insights, discover novel patterns, and drive innovation across various medical disciplines.

An extremely crucial step forward through the advent of HPC+ methods has been made in medical imaging: HPC+ has revolutionized medical imaging by enabling faster and more accurate analysis of complex images and also allowing for real-time usage, such as augmented reality applications during surgical procedures or the usage of Digital Twins already in pre-op planning. Algorithms powered by HPC+ can also detect subtle patterns, assist in diagnosing diseases at earlier stages, and even predict treatment responses. Furthermore, the integration of artificial intelligence (AI) and machine learning (ML) algorithms with HPC has led to remarkable advancements in automated image analysis, for instance aiding radiologists in interpreting medical images with increased accuracy and efficiency.

HPC+ serves as an enabler and accelerator of personalized medicine. HPC enables the integration and analysis of vast datasets, including genomics, electronic health records, and medical imaging, to develop personalized treatment plans and also develop medical solutions and technology such as implants, tailored to individual patients' needs. This approach enhances the accuracy and effectiveness of diagnoses, prognoses, and therapies, ultimately leading to improved patient outcomes.

Among the most transformative use cases has been the impact of HPC+ in the field of genomics and precision medicine. By analysing massive volumes of genomic data, researchers can unravel the complexities of human genetics, identify disease risk factors, and develop targeted therapies. This breakthrough technology has paved the way for personalized medicine, where treatments can be tailored towards an individual, enhancing both efficacy and safety. Furthermore, HPC+ significantly accelerated the drug discovery process. Researchers can leverage the immense computing power to analyse vast chemical libraries, simulate drug-target interactions, and optimize drug candidates. This expedites the identification of potential therapeutic agents and reduces the time and cost associated with traditional trial-and-error approaches.

The integration of HPC+ into clinical workflows empowers healthcare professionals to make more informed decisions in a timely matter and with greater precision. By leveraging real-time data analytics, clinicians can, for instance, access comprehensive patient records, identify potential risks, predict disease progression, and tailor treatment plans accordingly. This approach enables proactive and personalized care, ultimately improving patient outcomes. Having access to large-scale simulations fed with daily data updates on, e.g., the number of patients newly admitted to hospitals or specialized hospital units can also help optimize clinical capacity planning on a day-to-day basis, thereby improving patient care. At the same time, HPC in this example can also deliver important information for fast political decision-making in the health care sector – the more so in emergency situations, such as the recent COVID-19 pandemic.

While the benefits of HPC, HPDA and AI in healthcare are undeniable, the application of the technologies is not without its challenges. A successful collaboration between researchers, clinicians and pharmaceutical experts with the HPC+ world depends largely on the availability of both highly-trained (medical) domain experts and HPC+ technology experts, which is paramount to harnessing the full potential of these technologies and translating them into real-world solutions. Furthermore, availability of data sets, e.g. to train AI, is of utmost importance but still a legal challenge in a variety of countries. Therefore, accessing the data and building up the necessary expertise in the HPC domain and matching this with specialized domain experts in the medical, medical technology and the pharmaceutical field is a prerequisite for providing tailored HPC services and conducting research in this area. Last but not least, special attention also needs to be devoted to ensuring a maximum data security level for the sensitive medical data, and also to uncovering and addressing potential biases within algorithms.

As already mentioned, a necessary prerequisite for the usage of HPC+ in any scientific or technological domain including the medical sciences, is the uptake of skills in HPC+ by future experts in the field.

Malisic and Tinaj in the current issue shed light on this matter by discussing the importance of competence development in HPC to be able to provide the necessary support to different scientific domains and also businesses, to allow the adoption and application of AI, HPDA and HPC technologies. They describe the current endeavours, status quo and future plans in the Montenegrin National Competence Centre (NCC) which allow them to act as a facilitator in bridging the gaps between domain-specific expertise and technological know-how. In another article of this issue, Martensson provides insight into solutions for healthcare innovations and the skills and support the NCC Luxembourg can provide to healthtech companies.

Central to this issue are also several success stories from the collaboration of HPC+ technology providers from the EuroCC project network and medical and pharmaceutical domain experts. The overview article by Koch et al. provides case studies from various National Competence Centres in HPC+ established within the H2020 project EuroCC (01.09.2020 – 31.12.2022) which present their successful collaboration with medical sciences, ranging from applications in medical imaging (Svobodova, Sethia and Strakos), algorithm development for medical technology and simulation of the behaviour of a drug target for immunotherapy (Beaujean, Mensch and Bex), prosthesis design for aortic valve replacement (Drescher et al.), the development of a tool for personalised medicine – namely for pediatric dosimetry (Papadimitroulas et al.[2]) and finally a cloud-based solution to support medical procedures with the help of a Digital Twin (Vignali et al.).

Within the area of precision medicine, Schnabel et al. present in their standalone paper results of a biomechanical simulation study for bone-implant-systems, and deliver valuable insights into their benefits for personalized medicine and how they can achieve clinical-readiness. Another use case study of an HPC application is presented by Zečević, Filipović and Marčev where high-resolution models for the timely forecast of dangerous meteorological phenomena and the potential provision of HPC services within emergency situations are discussed.

This special section of *Technology and Health Care* provides valuable insights into the ground-breaking potential of HPC+ in fast-tracking medical and pharmaceutical solutions. With continued advancements in computing power, data analytics, and AI, HPC+ holds tremendous promise for enhancing patient care, enabling precision medicine, and expediting drug discovery and development. As we move forward, it is crucial to foster interdisciplinary collaboration and also address ethical considerations. Together, we can harness the transformative power of HPC, HPDA and AI to shape a future where technology truly enhances the well-being of individuals and communities, and allows us to benefit from not only safer, and better-targeted solutions, but also to gain access to these improvements much faster than what was thought to be possible.

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