The growth of HPC in the life sciences

Manuel Peitsch, co-founder of the Swiss Institute of Bioinformatics, will chair a session on high-performance computing in the life sciences at ISC'14 in Leipzig, Germany, in June. He tells iSGTW about the exciting advancements being made in this field. Peitsch argues that bioinformatics — enabled by advances in high-performance computing — has a major role to play in tackling the grand challenges of the 21st century, such as environmental protection, energy supply, public health, and sustainable food production.

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Manuel Peitsch, co-founder of the Swiss Institute of Bioinformatics, will chair a session on high-performance computing (HPC) in the life sciences at ISC'14in Leipzig, Germany, in June. Peitsch is also a professor of bioinformatics at the University of Basel in Switzerland and is vice president of biological systems research at Philip Morris International. In addition, Peitsch has previously

"A new 'systems mindset' needs to permeate the life sciences," says Peitsch. Image courtesy Manuel Peitsch.

worked at Novartis, GlaxoSmithKline, and the Geneva Institute for Biomedical Research.

What, in your opinion, are the most exciting advancements being made in the life sciences today thanks to HPC?

HPC has contributed to spectacular advancements in the life sciences on four levels. First, HPC is playing a crucial role in making sense of the massive amounts of data generated by modern 'omics' and genome sequencing technologies. Second, HPC is key to modeling increasingly large biomolecular systems using approaches such as quantum mechanics/molecular mechanics and molecular dynamics (see, for instance, the 2013 Noble Prize in Chemistry) to advance our understanding of biomolecular reactions and aid

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the discovery of new therapeutic molecules. Third, HPC is essential to modeling biological networks and simulating how network perturbations lead to adverse outcomes and disease. Finally, the simulation of organ function, such as the heart or the brain, not only depends on HPC, but also drives its development.

University of Basel

The use of HPC for research in the life sciences is often perceived to be less advanced than within the physical sciences: do you think this notion is justified? What can be done about it?

There is certainly truth in this perception. Historically, the physical sciences have embraced computational approaches much earlier. The reasons for this are both scientific and cultural.

Describing biological processes with mathematical equations is a tall order, because one first needs to 'reverse engineer' these processes experimentally using very sensitive and quantitative measurement methods. Indeed, the human genome was sequenced little more than a decade ago, but we are still very far from understanding how this code leads to a living organism of such complexity. I have great hope that systems biology, an approach which integrates the most advanced experimental methods with computational approaches, will allow us to elucidate these biological processes and build the models necessary to understand disease and drive advancements in medicine.

Another reason is that biomedicine has long been a purely observational and experimental science, whereas engineering, physics, mathematics, and chemistry integrated theoretical approaches long ago. Our educational system is still fostering this difference and too few programs are driving for a more integrative scientific education. A new 'systems mindset' needs to permeate the life sciences: they have their roots in the physicochemical laws that govern the interactions between molecular entities, which can in turn be described mathematically and modeled computationally.

What role does HPC play in the work you do at Philip Morris International?

Philip Morris International is developing candidate modified-risk tobacco products. To conduct the non-clinical assessment of these potentially reduced-risk tobacco products and determine whether they are indeed reducing the risk of disease, we have implemented a systems toxicology-based approach. Systems toxicology is the integration of classical toxicology with quantitative analysis of large networks of molecular and functional changes occurring across multiple levels of biological organization. HPC enables our data analysis processes and biological network models, which are used to compare mechanism-by-mechanism the biological impact of novel product candidates with that of conventional cigarettes.

You've also been a professor of bioinformatics at the University of Basel for

the last 12 years. How have developments in HPC caused the field of bioinformatics to evolve over this time?

In the last decade, we have witnessed an unprecedented development in 'omics' technologies, driving the need for new methods in bioinformatics, which in turn are impossible to implement without HPC. It is, therefore, the interplay between the needs of data analysis and the opportunities provided by advancements in HPC that drive evolution in bioinformatics. These developments in HPC have not only enabled a far deeper analysis of the data, but also testing of many hypotheses which we could only dream about a decade ago. For instance, at the end of the nineties it took several days of computing time to compare two mammalian genomes (e.g. Genecrunch) or build molecular models for every protein in the human genome (e.g. 3D-Crunch). Today, we can do these things in just a few hours and with far more accuracy. This enables biologists to test several hypotheses and design more targeted experiments.

And, I believe that as well as being a co-founder of the Swiss Institute of Bioinformatics, you also serve as the chairperson of its executive board. According to the organization's website, its vision is 'to help shape the future of life sciences through excellence in bioinformatics'. How can this be achieved?

This can be achieved by bringing bioinformaticians closer to the experimentalists and providing excellent information resources, analytical software tools, and computing infrastructure. Taking an active role in education and federating bioinformatics scientists across Switzerland is also an important part of our mission. Furthermore, The Swiss Institute of Bioinformatics also serves as an organizational model for other federated scientific organizations in Switzerland and abroad.

How do you think HPC is likely to change bioinformatics over the next decade?

Modern society is facing some major challenges in the 21st century. These include the improvement of health, the sustainable production of food and energy, and the protection of our environment. The life sciences have a major role to play in all these areas and bioinformatics, enabled by HPC, is a key to finding solutions. For instance, increasingly affordable genome sequencing and 'omics' technologies drive new developments in bioinformatics and computational systems biology, with applications ranging from personalized medicine to the development of improved crops for food and green energy production.

Finally, what topics are you most excited to learn more about at ISC'14?

The two sessions which I am most interested in are 'Supercomputing solving real life problems' and The Human Brain Project. As I am much focused on solving real life problems, I am keen to see where and how scientists are applying HPC to come up with innovative approaches to address meaningful challenges. Furthermore, The Human Brain Project is of particular interest to the life sciences, as it integrates levels of complexity spanning molecular, structural, and functional levels of the brain. At the same time, The Human Brain Project will also help drive new developments in HPC to cope with the demands of such a project.

ISC'14 will be held in Leipzig, Germany, from 22-26 June, 2014.

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