Exciting Advances: Growth of HPC in the Life Sciences

Andrew Purcell

Manuel Peitsch, co-founder of the Swiss Institute of Bioinformatics [1]*, will chair a* session *[2] on high-performance computing (HPC) in the life sciences at ISC'14* [3]*in Leipzig, Germany, in June. Peitsch is also a professor of bioinformatics at the University of Basel* [4] *in Switzerland and is vice president of biological systems research at Philip Morris International* [5]*. In addition, Peitsch has previously worked at Novartis* [6]*, GlaxoSmithKline* [7]*, and the Geneva Institute for Biomedical Research* [8]*.*

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 [9]' 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 [10]) to advance our understanding of biomolecular reactions and aid 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.

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.

ISC'14 [3] *will be held in Leipzig, Germany, from 22-26 June, 2014.*

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