

Computational Science – What’s the Status of this New Science?

EDITORIAL

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In 2005, there was a wake up call sent to the President of the United States by PITAC that warned of our information technology decline over the last 3 decades and decreasing high technology exports in the face of Asia’s rising exports. America was slipping and our technological prowess was being questioned and threatened all over the world. The PITAC believes that

we must come to grips with both the broad science and technology challenge we face and the reality that the 21st century scientific and engineering enterprise is computational and multidisciplinary, requiring the collaborative scientific skills of diverse disciplines. This country led the world in developing the advanced information technologies that are transforming research, commerce, and communications. These capabilities place us on the threshold of revolutionary discoveries, such as in the treatment of disease, atom-by-atom construction of materials with previously unimaginable properties, miniaturization of devices down to the quantum level, and new energy sources and fuel technologies. But we are not minding the store of U.S. intellectual resources needed to capitalize on the scientific opportunities of the new century. A dangerous consequence of our current complacency is that, as on the eve of Sputnik’s launch, we have not marshaled and focused our efforts to elevate computational science and the computing infrastructure to their appropriate status as a long-term, strategic

national priority in education as well as R&D. Without such a commitment and focus, the PITAC believes, we cannot sustain U.S. scientific leadership, security, and economic prosperity in the decades ahead. (pp. 9-10).

NSF (2007) has responded with its Information Technology Research (ITR) priority area that “sowed the seeds of broad and intensive collaboration among the computational, computer, and domain research communities” (p. 6). NSF is broadening access to state-of-the-art resources wherever computational science is an emerging movement to reduce the time-to-solution of computationally-intensive problems by applying computational techniques to extract new knowledge and obtain results in hours rather than days, weeks, months or years. Computational needs have been discussed and delineated (NSF). These needs must be met through this highly supported labor.

Hence the birth of computational science, a field that is in its infancy. It is stated by many in this new field that there is not a precise definition that everyone can wrap their arms around (Krell Institute, 2008). So, what is computational science? The PITAC (2005)

recognizes the diverse components, ranging from algorithms, software, architecture, applications, and infrastructure that collectively represent computational science. Computational science a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems. Computational science fuses three distinct elements:

- Algorithms (numerical and non-numerical) and modeling and simulation software developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems
- Computer and information science that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems
- The computing infrastructure that supports both the science and engineering problem solving and the developmental computer and information science (p. 10)

Now, in 2008, 3 years after the PITAC report, we are seeing graduates from computational science programs such as the Computational Science Interdisciplinary Graduate Minor program at Penn State University (Long, 2008). These pioneers will be forging the path to the next frontier, computational science.

This begs the question, how will we capitalize on advances in computational science to enhance nursing informatics and nursing?

References

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Computational Science Programs*:

Old Dominion University	http://www.math.odu.edu/~keyes/cse_announcement.htm
Penn State University	http://www.csci.psu.edu/
TU München (TUM)	http://www.cse.tum.de/index.html
University of Amsterdam	http://www.science.uva.nl/research/scs/edu/imcs/
University of California, SD	http://csme.ucsd.edu/
University of Iowa	http://www.amcs.uiowa.edu/
University of Waterloo	http://www.computational.uwaterloo.ca/

*All of these web sites were accessed on October 2, 2008.