FROM THE EDITORS

Computational Science, Demystified … the Future, Revealed … and *CiSE*, 2013

By George K. Thiruvathukal, Editor in Chief

ONE OF THE THINGS I TRULY HAD HOPED TO DO AS THE INCOMING AND NOW EDITOR IN CHIEF OF *CISE* IS DEEPEN OUR CONNECTIONS TO "COMPUTATIONAL SCIENCE AND ENGINEERING." WE ALL KNOW THAT THESE ARE THE KEYWORDS OF OUR PUBLICATION'S TITLE—A TITLE THAT'S becoming more important by the minute, with interdisciplinary education and research increasingly at the forefront of everything in this millennium.

It's an interesting exercise to ponder what we actually mean when we say *computational science*. (I also plan to take on the subject of engineering in a future message.) It's instructional to look at what *Wikipedia* has to say on the subject (see http://en.wikipedia.org/wiki/computational_science):

> *Computational science (or scientific computing) is concerned with constructing mathematical models and quantitative analysis techniques and using computers to analyze and solve scientific problems. In practical use, it is typically the application of computer simulation and other forms of computation from numerical analysis and theoretical computer science to problems in various scientific disciplines.*
>
> *The field is different from theory and laboratory experiment which are the traditional forms of science and engineering. The scientific computing approach is to gain understanding, mainly through the analysis of mathematical models implemented on computers.*
>
> *Scientists and engineers develop computer programs and application software that model systems being studied and run these programs with various sets of input parameters. Typically, these models require massive amounts of calculations (usually floating-point) and are often executed on supercomputers or distributed computing platforms.*
>
> *Numerical analysis is an important underpinning for techniques used in computational science.*

Armed with this definition, I think we have a firm grip on what computational science actually *is*. (It's hard to argue with *Wikipedia* on this definition. My other source, *Encyclopedia Britannica Online*, offers definitions for computational biology and linguistics, but alas, it lacks entries for the rest of us.)

A Representational Checklist

In looking at our 2013 editorial calendar, we've recently published articles on digital manufacturing and general-purpose graphics processing unit (GPGPU) programming. On the docket are medical simulation, scientific data management, cloud computing, machine learning, and exascale computing. This editorial calendar, which was put together by my esteemed predecessor, Isabel Beichl, with some input from me (being the co-editor for the upcoming cloud topic), reflects our continued efforts to address computational science in our content.

Viewing the *Wikipedia* definition as a bit of a checklist, we're continuing our efforts to move beyond the domain of computational physics (without forgetting or abandoning our roots). Many topics are only getting hotter when it comes to computational and data-driven thinking, especially computational biology/proteomics, medical/healthcare simulation and informatics, social computing/analytics, and machine learning (an area many people think is pure computer science, but is actually an intersection with neuroscience, psychology, and biochemistry, among others). More importantly, the tradition of computational physics is instrumental in supporting many of these topics (it's well known that many physicists/computational physicists have played a major role in the formation and evolution of these fields).

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Thus, it's a daunting challenge, but one that's an unprecedented opportunity for *CiSE*: to be one of the premiere destinations for interdisciplinary computing, mathematical, and scientific content. Sometimes I drool at this possibility, because there's a seemingly infinite well of ideas that we can publish. The challenge, however, is twofold: how to cover a meaningful set of topics in a timely matter, and how to remain coherent. (That's my job as the editor in chief—in theory.)

Looking further at what *Wikipedia* has to say, the computational part requires a great deal of care. It should include simulation, mathematical modeling, computation, and theoretical computer science. The methods, typically, require massive amounts of floating-point calculations that would benefit from supercomputing or distributed-computing platforms. Without a doubt, *CiSE* has many of these elements covered. Where could we improve? We offer columns in simulation and modeling and cover scientific programming (part of computation). We could do more with theoretical computer science, although this topic does occasionally surface in the "Scientific Programming" department. In terms of computational scale, it seems like we can do a lot more with large-scale computation and data (for example, things happening at the national labs) without losing coverage of the immense amount of computation that can be done without supercomputers.

Deeper Connections and Future Relevance

In the years ahead, I'm hoping to take the "good thing" I've inherited and tweak it to ensure our relevance for decades to come. Several ideas began to emerge when I was at the Supercomputing 2012 Conference in November, where it was abundantly clear that we can do more. I spoke with the leaders of a major national laboratory about how to deepen connections between *CiSE* and the large-scale computing facilities. The idea would be to add a department that's reminiscent of the "notes" concept that's often associated with the mainstream science publication *Scientific American*. It's also the subject of several successful science education and outreach reality shows such as *Mythbusters* and *How It's Made*, where an initial problem is given and the details unfold for how to solve that problem. I think such a column would go a long way toward enhancing *CiSE*.

Also at this year's Supercomputing conference, one of the most interesting sessions featured *electronic posters*. In contrast to the traditional approach of making posters on poster board, the electronic posters were done on high-end visualization displays, often incorporating a compelling visualization. In one visualization, created by a group from NASA, the electronic poster featured a whole-earth model that showed aerosol dispersion and how it moves around the globe. Clearly, the group used a precomputed model to generate an MPEG or similar video. As I was watching this, I kept wondering how did they actually do that? I would like to think that our readers would like to know.

As everyone knows by reading my recent musings on the subject, I'm also keenly interested to see us produce more value-added content that goes beyond print and desktop PDF viewing. So much of what we do in *CiSE* is already aimed at being compelling, not just in computational science, but also in an interactive and visual sense. If you're at all contemplating a submission to *CiSE*—as a regular or theme-oriented article, I encourage you to think about how your article could have more impact by including supplemental materials similar to what I described from the NASA Supercomputing poster. I can't promise that your article will be guaranteed acceptance, but *CiSE*'s board will be on the lookout for articles that have value-added content that can be repurposed for more public-facing situations, especially our collaboration with our co-sponsoring society's *Computing Now* initiative, where we've seen evidence that featured *CiSE* content does extremely well (in an analytics sense). If you're planning a submission where you have compelling visual materials, I would like to hear from you.

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I want to close by letting everyone know that on a personal note, a more coherent view of my social strategy is beginning to emerge. I've decided to go with Google Plus as my primary focal point for social outreach. You can find me by visiting http://gplus.to/gkt.