GuestEditorial

BY RUSS ALTMAN, MD, PhD

Biomedical Computation Review: The Simbios Fifth Anniversary Issue

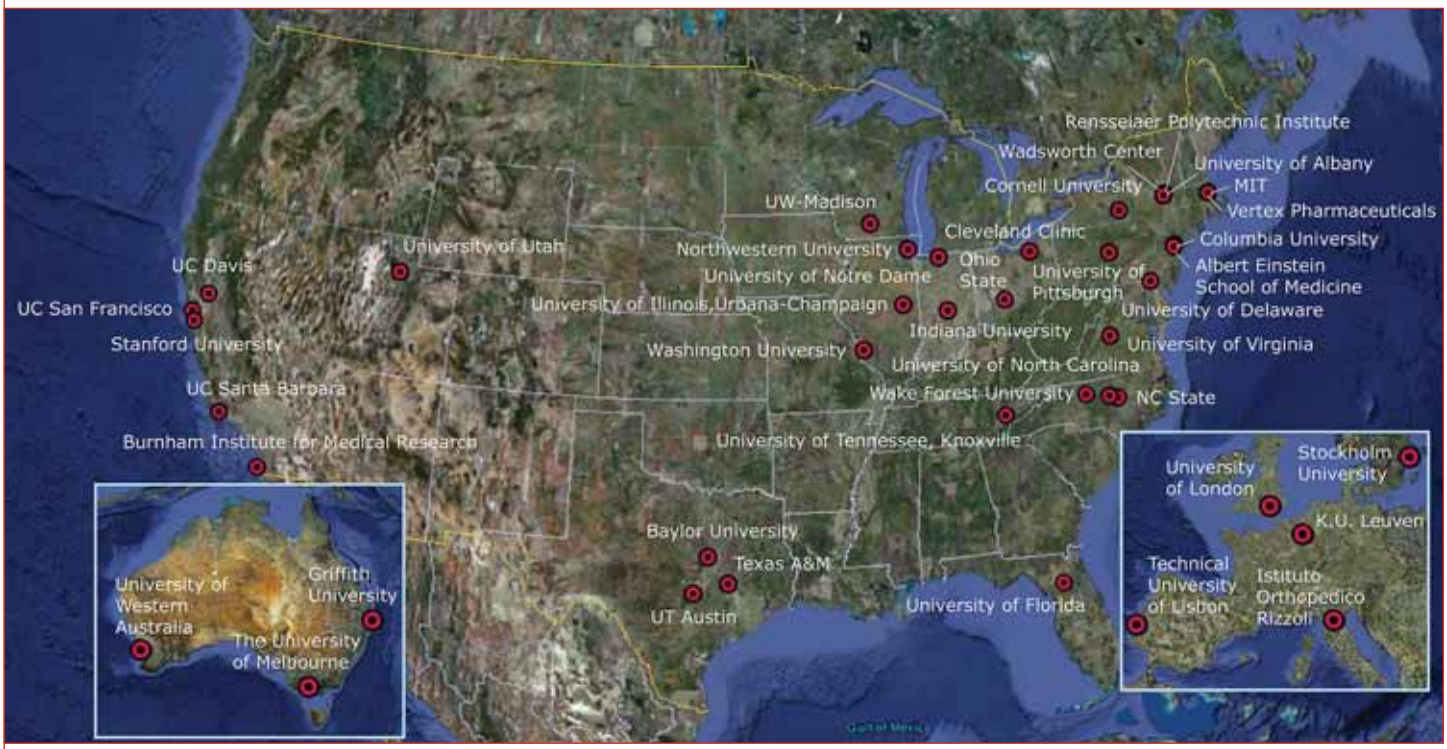
Dear Reader,

In this eighteenth issue of Biomedical Computation Review (BCR), we bring you a special edition devoted to the work of the magazine's publisher: the Simbios National Center for Physics-Based Simulation of Biological Structures (http://simbios.stanford.edu/).

The magazine itself is one of the innovations Simbios introduced to help build a national community of biomedical investigators with a devotion to computation. But Simbios' national presence is also being built in other ways. The initial Simbios team, formed in 2004, was based at Stanford and included biologists, biomedical computation and informatics scientists, and computer scientists. We therefore made special attempts to grow from the strong core at Stanford to the national and international community. Taking our "national center" mandate seriously, we set out to serve a much larger community of biomedical scientists who could benefit from software technologies that brought easier and better ways to use simulation in the pursuit of new knowledge.

This issue's feature story, appropriately titled "Simbios: Bringing Biomedical Simulation to Your Fingertips," describes some of the technologies and projects that Simbios created in its first five years and how Simbios tools are being adopted by the research community well beyond Stanford.

The story focuses primarily on three of the center's "driving biological problems" or DBPs—the problems that drove us to develop tools that would matter for bioscience. Each of these DBPs—neuromuscular, protein-folding, and cardiovascular—introduced at least one key open-source computational tool during Simbios' first five years. These include OpenSim, a neuromuscular simulation package for simulating human movement; Open Molecular Mechanics (OpenMM), which permits the use of very fast GPUs for molecular dynamics simulations, including pro-



Map of Simbios collaborators. Red markers indicate institutions that have worked with Simbios during the last five years: some collaborated on a driving biological project; others received a collaborative R01 grant or seed funding from Simbios; others have made significant contributions to our software offerings; and still others were lead or senior authors on a Simbios publication.

tein-folding; and SimVascular, for simulating blood flow velocities and pressures in deformable vessels.

Simbios researchers are using these tools to advance their own research goals, but Simbios' reach extends much farther, as you'll see from the feature's focused stories about 13 people who are Simbios collaborators, tool users and/or alumni. These individuals describe how they are using Simbios tools to further their biomedical research goals. We hope their stories inspire more of you to sample Simbios' wares.

Also within these covers you'll find our regular Point/Counterpoint column where Vijay Pande highlights key issues in the debate between Supercomputers and Superclusters and which is better suited to the needs of molecular simulations.

And in this issue's "Under the Hood" column, our chief software architect, Michael Sherman, provides insight into how the incredibly complex technologies required for fast, accurate simulations can be bundled into software packages that are usable by domain experts.

Some basic principles that have guided much of the Simbios software development include the following:

- Simulations must be fast, in order to yield results of potential interest on a timescale compatible with scientific progress. Accuracy must be measured and documented, but given a specification of tolerances in accuracy and precision, simulation is all about speed.
- "General purpose" applications are nice for software engineers to create, but are not generally useful to domain scientists who want narrowly defined tools with narrowly defined capabilities, tuned to their domain. This means that an underlying toolkit must be available, so that narrow applications can be created quickly to address this need, while not causing the software team to endlessly reinvent the wheel.
- Putting the above two rules together is the special sauce: the very complex technologies required to make simulations fast and accurate must be totally hidden from the users, who must be presented with application-specific, easy to use software

At the end of the day, the National Centers for Biomedical Computing are charged with catalyzing high-impact research in biomedicine, and with making tools available for the community to use. To that end, Simbios created Simtk.org, a repository for software, data and models related to physics-based simulation. On Simtk.org, we distribute the open source software products we've developed. And any other biomedical investigator may do the same. Simtk.org is intended to gain momentum and have a sustainable life even after the end of the Simbios center. As of this writing, Simtk.org had nearly 350 (348 to be exact) software projects, including eight that are actively being disseminated in our workshop and tutorial program. Over 6500 users have registered on the site to download our software, and that number continues to grow. In fact, for each of the last few years, we have seen a doubling in the membership growth rate and currently have an average of 400 new users signing up each month.

Simbios has made great strides in our key missions. Our scientists have made important, high-impact contributions to their domains of research, while also creating software, data, and models that can be used by others in the field.

As you can see, I am thrilled to report that in its first five years, Simbios has made great strides in our key missions. Our scientists have made important, high-impact contributions to their domains of research, while also creating software, data, and models that can be used by others in the field. We have hardened key software (such as those described above) in order to guarantee utility to the community. We have engaged in a blitz of workshops and tutorial sessions in order to disseminate these programs, and show the target audience how to use them. Our singular devotion to physics-based simulation has also attracted a network of collaborators (see map) who are co-developing software projects, using them in their research or engaging as serious "alpha" testers to see if the software is performing well.

The task of becoming a National Center is not an easy one. It is not sufficient simply to post a sign and declare national center-dom. Instead, a national center must start with service. By building a core of useful technologies, generating compelling scientific results, and then making the technologies available along with training materials, we can best serve the scientific community. We begin generating the core on the inside, but we make our impact by bringing it outside. □