Green computing as an emerging technology claims to lower operational costs as well as its obvious benefits to the environment. What are some of the other benefits of green computing?

Energy-smart, or "green," HPC systems are impacting more and more pharmaceutical companies, and for reasons that some may find surprising. Pharmaceutical data centers are running out of room as applications such as Gaussian, AMBER and BLAST increasingly require more compute power. This has led to a growing reliance on high-density rack-systems, which pack multi-core processors into tall racks stacked with dense servers and even denser blade systems.

Without energy-efficient designs, more powerful systems would produce soaring energy bills. And they would produce something else: heat. Excessive heat drives up cooling costs and causes computer components to wear out faster. Because server cooling can add 50 to 100 percent to power consumption costs, so-called green computers equate to significant savings for customers who face rapidly compounding costs as they try to supply power to their data centers, while keeping them cool enough to maximize product life. For a large deployment, these efficiencies can mean hundreds of thousands of dollars in cost savings every year.

Energy-efficient systems address these challenges. For instance, the recently unveiled SGI Altix ICE line of HPC blade systems features an energy-smart power architecture that realizes more than 90 percent efficiency on its 12-volt DC front-end power supply, up to 87 percent efficiency on compute blades, and up to 76 percent efficiency at the rack level. The new platform also boasts SGI’s water-cooled door design for large and dense configurations. Chilled water running through the unique hinged door carries away up to 95 percent of the heat generated by the system.

Innovations like these will someday be commonplace as more corporations, universities and research institutions adopt initiatives to reduce their environmental footprint. Furthermore, many experts predict that federal regulations mandating the purchase of energy-efficient computers are not far off. Both of these trends show that purchasing green HPC solutions is not only beneficial today, but will likely be a strategic decision for the future.

High Performance Computing (HPC) creates efficiency by utilizing an interlinked network. What are some ways that you see HPC being implemented? The current supercomputing environment is evolving and is more commonly referred to as High Productivity Computing. What has been the catalyst for this shift? Where will this technology go in the future?

HPC is about productivity, and the perception among many users that HPC means “High Productivity Computing” was more or less inevitable. The catalyst for this has been the ability of HPC to do two things. First, it accelerates existing research. Second, it allows researchers to new avenues of study that previously were not reasonable to pursue.

New, more powerful systems have an immediate impact on productivity by delivering results faster than ever before. For instance, scientists at the National Cancer Institute’s (NCI’s) Pediatric Oncology Branch are using a powerful SGI Altix system to mine vast public databases of genomic information for potential new medical discoveries. Owned and managed by NCI’s Advanced Biomedical Computing Center (ABCC), the HPC system allows them to dramatically accelerate the process of genomic profiling. Using a specialized software application called CORR4DB, researchers correlate one genomic array against a database of 100,000 probe pieces of a gene in search of specific DNA components or attributes. Correlations previously took nearly a week on a desktop system to complete. But by taking advantage of the 256GB of memory available on ABCC’s 64-processor SGI Altix system, correlations are now completed up to 200 times faster – sometimes in as little as 15 minutes – allowing researchers to run multiple correlations in a single day. The same type of productivity improvements are witnessed every day in organizations around the world with search-and-compare applications like BLAST.

Scientists not only are working faster, they are breaking new ground. A research team led by Professor Klaus Schulten at the University of Illinois at Urbana-Champaign is just one example. Using SGI Altix systems, they created the first atomic-level simulation of a complete, functioning organism – a breakthrough they hope will speed development of new drugs to combat viruses in plants, animals and even people. The team simulated a plant virus with as many as 1 million moving atoms. The achievement is historic due to the sheer complexity of the problem. Had the researchers relied on today’s desktop computer systems, they wouldn’t have finished until 2041. However, using an SGI Altix system housed at the National Center for Supercomputing Applications (NCSA), they were able calculate how all the atoms interact every femtosecond, or one-millionth-of-a-billionth of a second. Best of all, they accomplished the simulation in only 50 days.

Other examples abound, and all of them illustrate how HPC systems, whether in-house or shared by large institutions, are transforming the productivity of life sciences research.

In recent years HPC has been utilized extensively among R&D departments in their Genomics Research. How has HPC furthered the productivity and understanding of Genomics? Have you witnessed any breakthroughs in Genomics that have been a direct result of HPC?

HPC environments have created a framework in which high-end research is defining the leading edge of genomics. Until recently, certain problems have been simply untouchable because researchers lacked access to the kinds of systems powerful enough to enable real-time simulations, or large-scale genomic searches.

A prime example of this can be found at Stony Brook University in New York. There, working on an SGI Altix system located at NCSA, researchers have achieved computer simulations that
offer insight into the mechanics of HIV protease, a molecule that slices the pre-HIV protein chain into pieces that ultimately evolve into a mature virus. By modeling how HIV protease works across time, researchers hope to determine how best to target it with medicines that could stop the molecule from doing its job and thus prevent the HIV virus from developing altogether.

The Stony Brook researchers’ simulations are the most extensive ever done on HIV protease. Led by award-winning structural biologist Dr. Carlos Simmerring, the team successfully simulated how the HIV protease changes between two forms that already have been determined through experiments. More importantly, the group was able to capture the protease in a fully open state – one that had previously been hypothesized but never directly observed. The researchers note that without access to the right HPC resources, such a breakthrough would have been simply too time-consuming to pursue.

New technologies are also helping genomic researchers break through common productivity logjams. Consider innovations surrounding the performance of BLAST-n (Basic Local Alignment Search Tool for nucleotides), the worlds most widely used bioinformatics application. The accelerating pace of genomics research means scientists are running more and larger nucleotide sequence queries. As traditional servers fail to keep up, SGI and Mitronics, Inc. have developed a turnkey BLAST appliance that transforms long-running batch jobs into interactive scientific investigation. The appliance relies on powerful and energy-efficient Field Programmable Gate Array technology designed to accelerate often-repeated routines that are common in BLAST-n queries. Leveraging the Mitron Virtual processor, the appliance completes complex BLAST-n queries up to 16 times faster than a standard server based on Intel Itanium 2 processors, and 10 times faster than a server based on AMD Opteron processors. Clearly, HPC is enabling breakthroughs on many levels.

As there is an influx of technological advances, there is also better information sharing, file transportation and increased strain on data storage facilities. What are R&D professionals doing in order to empower themselves with ample amounts of storage? What are some suggestions you can offer in order to ensure data is managed properly? How can biopharmaceutical organizations ensure the sanctity of their information remains intact?

For scientists and researchers in the pharmaceutical field, data is a problem that just keeps on growing. Some genome sequencing research generates between 1 and 10 Terabytes of information every day. In just seven days, the most intensive genomics sequencing research could generate a volume of data that is equivalent to the entire U.S. Library of Congress print collection.

Forward-thinking HPC solution providers have known for some time that this “data tsunami” was underway, and they have developed solutions to strategically manage it. For its part, SGI has developed a unique data-centric storage architecture that addresses the challenges faced by organizations involved in both basic research and applied science.

A key element of the SGI solution is the SGI InfiniteStorage Shared File System CXFS. CXFS avoids the bottlenecks associated with manual copying and dramatically streamlines workflow. The ability to concurrently access data without copying delays significantly improves productivity. More work can be completed in the same amount of time – or the scale and complexity of individual simulations can be increased.

Organizations should be careful not to overlook data migration. In the typical data life cycle, new genomic and bioinformatics data is accessed intensively. As data ages, it is accessed less frequently and may remain dormant for many months or even years, although it may occasionally undergo brief periods of renewed intense access. SGI helps pharmaceutical companies and research institutions flexibly and economically adapt to changing data access patterns with SGI InfiniteStorage Data Migration Facility (DMF). DMF transparently migrates files from online storage to near-line storage based on user-defined criteria such as time of last access.

Today’s powerful HPC computers certainly deliver productivity improvements, but effectively managing data within the scientific workflow is essential to realizing those improvements day in and day out.

What do you envisage for the future of SGI’s work in the life sciences arena?

HPC systems are no longer the sole domain of large companies and institutions with seemingly limitless budgets. The class of HPC solution that once took months or even years to bring on line now can be fully productive within a week. Last year, SGI delivered an update to NASA’s storied Columbia system. Packed with 512 processor cores, the new system was available to researchers just five days after its arrival. A growing reliance on industry-standard components has also made the systems more affordable, so more institutions can deploy them. Life sciences organizations can expect SGI to ensure that this trend continues.

In addition, we will continue our view of HPC products from a solutions perspective. We realize that scientists need to focus on their research, not on determining how to modify their gene sequencing routines so they will run on a cluster with 68 instances of Linux. Rather than force-fitting all applications and workflows onto a single computing architecture, scientists are far better served by an HPC solution that provides a uniform end-user view, but can be easily customized to the needs of each user and field of study.

To that end, we will continue our focus on providing solutions that integrate disparate source data (genomics, proteomics, chemistry, biology, clinical data, regulatory data, financial and competitive data) into a unified virtual environment to compare, use, and apply this data. In partnership with scientists, ISVs and technology partners, we will also continue to develop solutions that address specific portions of the scientific workflow.

We will continue our efforts to bring to market solutions that accelerate key processes for genomics, proteomics, chem informatics, and other disciplines that address specific productivity-sapping bottlenecks. Our new BLAST-n appliance developed with Mitronics is an excellent example of this.

Finally, you can count on SGI to continue its leadership in the scientific discovery environment by developing targeted solutions to address specific scientific processes. By leveraging our in-house expertise in key scientific fields, these solutions will be clearly differentiated from more generic HPC offerings that populate the market today.