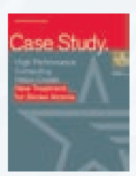
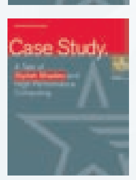
A BETTER STROKE BUSTER & SMART SHADES

PSC's corporate partnerships lead to improved high-tech sunglasses and a rapid feasibility decision for a catheter design

Through PSC's corporate affiliates program, the same computational resources and expertise that help university scientists advance knowledge in many fields are available to business. Since its beginnings in 1986, PSC has worked with a number of corporations in new product research and design. These include more efficient power turbines by Westinghouse, better mixing of molten steel in "tundishes" for continuous casting by U.S. Steel, and improvements in lightweight beverage cans and aluminum car parts by ALCOA.

Two recent PSC corporate projects — one involving PPG Industries and another involving Medrad, Inc. — were recognized by the Council on Competitiveness, a Washington, DC organization of business, labor, academic and governmental leaders who focus on private-sector competitiveness. PPG worked with PSC to improve a state-of-the-art technology for eyewear — sunglasses that automatically change from clear to dark in the presence of ultraviolet rays. Medrad, an Indianola, Pennsylvania company, collaborated with PSC and Carnegie Mellon University to study the feasibility of a novel catheter for safe, efficient removal of deep-vein blood clots.

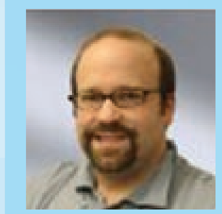




Through its High Performance Computing (HPC) Initiative, which facilitates usage of HPC across the private sector, the Council on Competitiveness recognized both projects as success stories — demonstrating how HPC drives corporate innovation and productivity. The Council's case studies about these projects were made possible by a National Science Foundation grant and are available on the Council website at **http://www.compete.org**

Both projects highlight how the availability of sophisticated HPC technologies can reduce costly trial-and-error design and accelerate time-to-market for innovative ideas.

A WINDOW OF TIME FOR FEASIBILITY



John Kalafut, *principal research scientist, Medrad, Inc.*

The leading cause of death in industrialized nations is blood clots — "thromboembolic disease" — a piece of blood clot (thrombus) blocking a vessel (embolism). Ruptured clots that lodge in a vessel can cause heart attack, pulmonary embolism or stroke.

For all these conditions, time is a factor. The sooner there's treatment, the better the chance of recovery without serious consequences. Recently, a patented but unmarketed, deep-vein catheter technology that could speed-up treatment of blocked vessels came to the attention of Medrad.

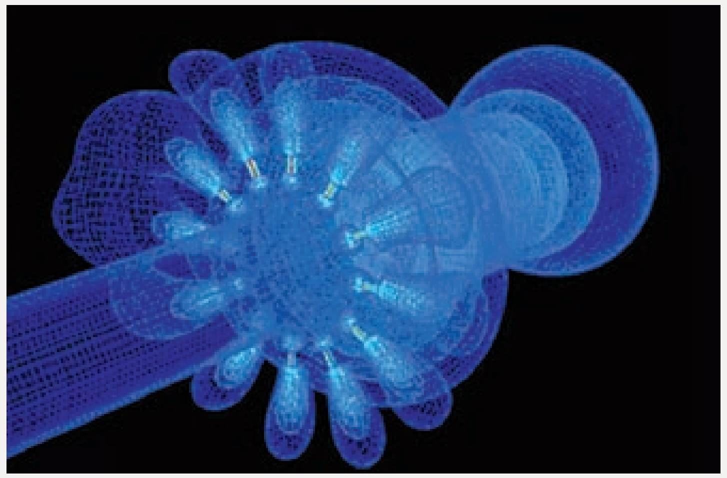
"The patented prototype device seemed like a good fit with Medrad's growth objectives, so we purchased the rights," says John Kalafut, principal research scientist at Medrad. "But before we could give the go-ahead to proceed with product development, we had a number of practical questions that needed answers, and we needed them quickly."

A leader in providing medical devices and services for diagnostic and therapeutic imaging of the human body, Medrad is an affiliate of Bayer Schering Pharmaceutical AG, Germany with annual revenues of around $500 million and 1,700 employees. Their products have captured 70 to 80-percent market share.

The task for Kalafut and Medrad's R&D group was to determine if the potential technology was actually feasible — will it work and, if so, what are its limitations? "Because we examine many different opportunities each year," says Kalafut, "we need to be able to quickly gauge the technology's efficacy and either start the development process, or turn it down and move on to the next. If the technology looks promising, we make an initial commitment and then, several years later, launch a multimillion-dollar project to commercialize it."

The classic approach for a biomedical product involves building bench-top models, subjecting each one to a variety of trial conditions and then moving into animal and human testing. For a catheter, this costly, time-consuming approach had serious limitations in the ability to efficiently capture the complicated interactions between blood cells, vessel walls, the clot and the catheter.

Kalafut felt the cath eter was an opportunity to try numerical simulations. "Not only did we need to understand the physics, we also wanted to explore different design and manufacturing approaches. We felt that doing this computationally would be both more cost-efficient and faster than building lots of different physical prototypes."



Simulated flow field from the prototype catheter as computed by 3D computational fluid dynamics software at PSC.

Supercomputing cut eight-to-ten months — a huge savings in time and money — off the feasibility decision.

The physics involved with a blocked circulatory system and the catheter includes complex fluid dynamics that can be represented mathematically — via techniques associated with a field of HPC called computational fluid dynamics (CFD). The R&D group's high-end workstations, however, lacked the horsepower for these complex simulations. They also didn't have the in-house expertise to develop or use detailed CFD codes.

Other challenges facing Kalafut's group had less to do with technology than with tradition and individual mindsets. Some of the company's engineers who had been building prototypes for decades felt that computer simulation wouldn't work — you had to build something real, something tangible, not just work with a bunch of equations. Kalafut and the R&D group convinced management that HPC was essential to capture first-to-market advantage if Medrad wanted to move forward.

Kalafut consulted with the Institute for Complex Engineered Systems at Carnegie Mellon University (CMU), and PSC supercomputing was enlisted in the R&D process. Medrad's work with PSC consultants Jun-Woo Lim and Dave O'Neal and its HP shared-memory systems, Jonas and Rachel, focused first on the physics — using CFD software to simulate the process of the catheter destroying clots, adjusting the parameters again and again to ensure that the phenomenon was repeatable. This work validated that the patent's theory was solid and that the device would do what its inventors claimed.

Medrad and PSC then did more modeling to refine the prototypes by simulating many different combinations of changes to arrive at the best design.

"Using PSC's systems," says Kalafut, "we have been able to look at multiple iterations of different design parameters without building numerous, expensive prototypes."

With the CFD studies as a foundation, a Medrad and CMU team demonstrated the physical principles of the catheter technology. Subsequent animal studies validated the operational principles and the CFD results, but clinical validation wasn't proven. Kalafut estimates that supercomputing cut eight-to-ten months off feasibility determination, a huge savings in time and money.

"If we weren't partnering with PSC and CMU," says Kalafut, "we'd probably be a year away from determining feasibility. It is critical to quickly and accurately evaluate new medical devices with numerical, bench-top and animal models. The resources at PSC allowed us to fully explore a concept months before expensive animal testing." In a competitive global market, a year can be the difference between market success or failure. And for victims of thromboembolic disease, it can be the difference between life and death.

THE QUANTUM SCIENCE OF STYLISH EYEWEAR

Michael Makowski, *leader of the computational chemistry research group, PPG Industries*

Jun Deng, *PPG Industries, specializes in quantum chemistry.*

If you wear eyewear made with Transitions® lenses, you have the coolest shades in town — maybe even cooler than you realize. Riding on your nose is a product created with help from quantum chemistry and PSC's parallel supercomputing resources — mainly Rachel, PSC's shared-memory HP system, and some use of BigBen.

Transitions lenses are made by Transitions Optical Inc., a joint venture formed in 1990 by PPG Industries of Pittsburgh and Essilor International of Paris. Based on proprietary photochromic technology, the lenses quickly change from clear to dark in the presence of ultraviolet light and block 100-percent of harmful UVA and UVB rays. The transition is the result of photochromic dyes. When exposed to ultraviolet light, the dyes' molecular bonds break and the molecular structure changes, which in turn changes the lens color and provides UV protection. Remove the UV, and the lenses quickly return to a colorless state.

A calculation that might have taken a week on in-house machines runs in a matter of hours at PSC.

The development of successive generations of photochromic lenses has been based in large part on PPG research. Beginning several years ago, Jun Deng and Michael Makowski, scientists in PPG's computational-chemistry research group, faced a challenge in eyewear. "About five years ago, a major challenge we faced was meeting market demands for improved photochromic technologies for a high-growth segment within the ophthalmic lens market using new impact-resistant, high-index and polycarbonate materials."

One of the main differentiators among lenses that "transition" is the performance of the photochromic dyes — how fast the lenses shift from light to dark and back again, how dark the lenses can become when exposed to UV light and the color itself — brown and gray are good, hot pink or dark purple not so good. How long the product will last before the photochromic coating begins to lose its effectiveness is also key to product success. "With each successive generation," says Makowski, "you want to develop a product that has better performance, is robust to various substrates and processing, and has a lower price tag."

Essentially, it's a scientific problem. In order to advance photochromic dyes and coatings, PPG had to understand what was going on not only at the molecular level (between dyes and their matrix), but also at the quantum level (electronic structure), which dictates the dyes' behavior when they interact with light.

To physically synthesize and test a new dye can take weeks to months, and PPG needed to examine many materials. Computational research was key to fast time-to-market, but PPG soon found that the quantum-chemistry problems it wanted to tackle were too computationally intensive for their in-house systems.

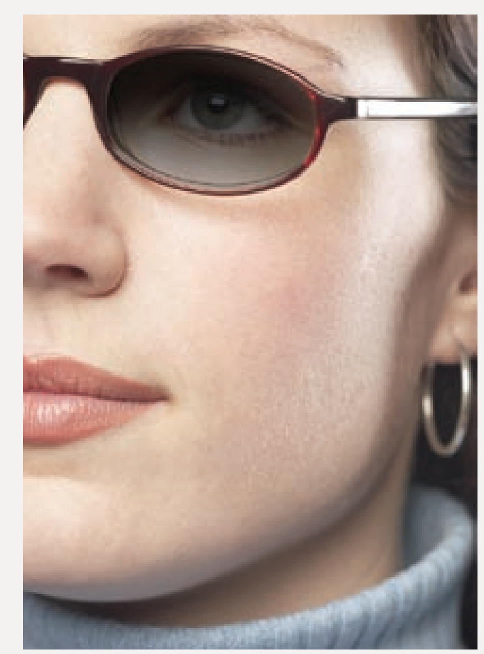
By joining PSC's industrial affiliates program, PPG gained access not only to PSC computational resources but also to the expertise of PSC personnel. A complex calculation that might have taken a week on PPG's in-house machines — if it could be run at all, says Makowski, now takes only several hours.

This permits PPG to predict many performance characteristics of molecular structures under a variety of conditions, without having to construct a physical prototype. "We can computationally screen a whole series or family of new structures proposed by our organic chemists," says Makowski, "and weed out the 80-percent that will ultimately fail when they are tested experimentally."

With PSC resources doing quantum calculations, PPG brought its new fifth-generation photochromic technology to market ahead of competitors, gaining market share and increased sales and earnings. Ongoing work now continues and PPG's sixth-generation product is slated for launch within the next year.

"It's very difficult to calculate just how much time and money we are saving by working with PSC," says Makowski, "but the return has been very evident. We achieve faster, more accurate results with far fewer physical prototypes, which reduces cost. This not only means a more efficient R&D process, it also speeds up the time-to-market and enhances PPG's competitive position.

MORE INFORMATION
http://www.psc.edu/science/2008/stroke_shades.html



Transitions® lenses shift from dark to light automatically in the presence of harmful UV light.