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 “tundish” 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 Indiana, 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

The leading cause of death in industrialized nations is blood clots — “thromboembolic disease” — a piece of blood clot (thrombus) blocking a vessel (embolism). Battered 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 catheter 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.”

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“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, 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 development of successive generations of photochromic lenses has been based in large part on PPG research. Beginning several years ago, Jun Dong 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 block 100-percent of harmful UV light and block 100-percent of harmful UV light. The transition is the result of photochromic dyes. When exposed to ultraviolet light, the dye’s 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.

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

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 UV light. The transition is the result of photochromic dyes. When exposed to ultraviolet light, the dye’s 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. The development of successive generations of photochromic lenses has been based in large part on PPG research. Beginning several years ago, Jun Dong 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.”

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