Case Study.

A Tale of Stylish Shades and High Performance Computing

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To advance the state of the art of its proprietary photochromic technology used in Transitions® eyewear and speed its time-to-market, PPG Industries enlisted the help of high performance computing. Advancing photochromic technology, which allows lenses to change from clear to dark and block harmful ultraviolet rays, involves complex modeling and simulation of molecules at the atomic and quantum levels. By enlisting the help of the NSF-funded Pittsburgh Supercomputing Center and its powerful high performance computing capabilities, PPG's R&D organization was able to rapidly create the next generation of photochromic dyes and move out in front of its competition.

If you own eyewear made with Transitions® lenses, you are wearing the coolest shades in town. But they are cooler than you think. Riding on your nose is a product made with the help of quantum physics, advanced photochromic technology and the high performance computing (HPC) capabilities of a massive supercomputer.

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 applied to the lenses. When exposed to ultraviolet light, the dyes' molecular bonds break to change the molecular structure – this 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 is based in large part on research conducted at PPG. With annual revenues in 2006 of $11 billion, PPG is a global leader in the diversified manufacture of paints, coatings, chemicals, optical products, specialty materials, glass and fiberglass. The company has 32,000 employees worldwide. At the heart of the company is the research and development organization, where a group of chemists use HPC to conduct advanced modeling and simulation. One of them is Michael Makowski, group leader, whose staff members use HPC to tackle the difficult task of advancing photochromic technology, a move that keeps PPG out in front of its competition.

Building the Business

"About five years ago, a major challenge the company faced was meeting market demands for providing improved photochromic technologies for a high growth segment within the ophthalmic lens market using new impact-resistant, high-index and polycarbonate materials," recalls Makowski.

One of the main competitive differentiators between 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, you want to differentiate yourself from your competition by developing a product that has better performance, is very robust to various substrates and processing, and has a lower price tag," Makowski notes.

"This was, and continues to be, essentially a science problem," he explains. "In order to advance the science of making photochromic dyes and coatings, we had to understand what was going on not only at the molecular level (between dyes and their matrix), but also at the quantum level (i.e. electronic structure) which dictates the dyes' behavior when interacting with light. In fact, one of our chief researchers working with photochromic dyes, Dr. Jun Deng, has spent the majority of her time at PPG developing expertise in the area of quantum chemistry."

But the experimental process of physically synthesizing and testing a new material can take weeks to months, and PPG needed to examine many materials. Intensive new computational research was required to speed up time-to-market for the next generation product. PPG soon found that the quantum chemistry problems it had the desire to tackle were too rigorous – too computationally intensive – for their in-house HPC systems. The problems took just too long to run, if they could be run at all. "At the time, we simply couldn't do the modeling and simulation that was required to advance the photochromic state of the art," Makowski recalls.

BigBen to the Rescue

PPG determined that adding more processors to their existing HPC systems was not cost effective because it would increase their capital costs and overhead in the form of additional staffing. So they began to look for an external resource to meet their HPC needs more cost effectively and found it at the nearby Pittsburgh Supercomputing Center (PSC). PSC is a joint effort of Carnegie Mellon University and the University of Pittsburgh together with Westinghouse Electric Company, and is supported by the National Science Foundation along with the Commonwealth of Pennsylvania.

PPG became a member of PSC's industrial affiliates program and began to access the center's high-end supercomputer and the expertise of its personnel.

The PSC system known as "BigBen", with it's thousands of high-speed processors, has an order of magnitude more capacity compared to PPG's in-house systems. Using parallel processing, the PSC HPC machine can run massive jobs that are simply beyond the reach of resources available within PPG.

Makowski estimates that a complex calculation that might have taken a week on their in-house machines – if it could be run at all – now takes only four to eight hours on the center's machine. This permits PPG to predict many of the performance characteristics of molecular structures and how they will behave under a variety of conditions, without having to construct a physical prototype. "Using the PSC supercomputer, we can computationally screen a whole series or family of new molecular structures proposed by our organic chemists and weed out the 80 percent that will ultimately fail when they are tested experimentally. This allows us to focus our physical testing on the candidates which have the highest probability of success and those whose behavior we can predictably understand," Makowski says.

HPC Competitive Impact: Lower Costs, Better Science, Faster Time-to-Market

Makowski says that the business case for using HPC has been made without a doubt. PPG's work with PSC has allowed it to accelerate the R&D process, which translates into faster product development and more new products – in this case the fifth generation

Transitions® lenses are the #1-recommended photochromic lenses in the world. More information can be found at www.transitions.com. Photos courtesy of Transitions Optical, Inc.

of photochromic materials (Gen 5). The HPC work on the PSC supercomputer allowed PPG to bring the Gen 5 technology to market in advance of its competitors and has allowed PPG to continue to gain market share and increase its sales and earnings. Ongoing work now continues and PPG's sixth generation product is slated for launch within the next year.

By using the PSC system to perform sophisticated modeling, the PPG research team is able to gather information that they would not be able to obtain experimentally. The research also adds to PPG's fundamental understanding of the science and physics of its photochromic materials, and allows the researchers to continually fine tune the models used to investigate these materials at the molecular and quantum levels. This provides insights into the material's properties that would not be possible with physical observation and testing.

In addition to speeding up time-to-market with new photochromic products, PPG knows it is reducing costs, although exactly how much is hard to quantify.

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

"Overall, having access to these supercomputing resources provides us with the competitive edge we need to be successful in our marketplace," he concludes.

"(Using high performance computing at PSC) not only means a more efficient R&D process, it also speeds up the time-to-market for the next generation of Transitions® lenses and enhances PPG's competitive position."

Michael Makowski, a group leader with PPG's research and development organization

In Brief

Key Challenges

- Grow the mature photochromic ophthalmic lens market segment while maintaining a competitive lead
- Overcome the limitations of the R&D laboratories in-house entry-level high performance computing systems
- Speed up time-to-market for next generation photochromic products

Solutions

- Advance the state-of-the-art photochromic technology by modeling and simulating photochromic dyes at both the molecular and quantum levels
- Access high-end supercomputers and the expertise at the Pittsburgh Supercomputing Center to screen these new chemical structures and their interactions computationally rather than use time-consuming and expensive physical experiments and/or less powerful in-house computing systems

Key HPC Benefits

- Performs leading edge computational tasks in hours that would have taken weeks using PPG's in-house systems
- Investigates computationally new chemical structures and culls the 80 percent that will ultimately fail in the physical testing phase in order to focus on the candidates that have the highest chance of success
- Reduces substantially the number of physical experiments that must be performed
- Positions the company to become more competitive, including speeding up time-to-market
- Adds to the R&D organization's basic understanding of the science and physics involved with developing new photochromic materials

Web Site

- www.ppg.com

FSC
Mixed Sources
Product group from well-managed forests, controlled sources and recycled wood or fiber
www.fsc.org Cert no. SW-COC-002557
© 1996 Forest Stewardship Council
30%

Instead of using 100% virgin paper, we used paper that has been 30% Post-Consumer Recycled and made with 100% wind-generated electricty. We saved:

5 trees preserved for the future
1667 gal of water flow saved
276 lbs of solid waste not generated
509 lbs of greenhouse gasses prevented
3 million BTUs of energy not consumed

Environmental impact statements were made using the Environmental Defense Fund Paper Calculator.

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