High Performance Computing

Case Study.

Procter & Gamble's Story of Suds, Soaps, Simulations and Supercomputers

Compete.
Council on Competitiveness

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Procter & Gamble's Story of Suds, Soaps, Simulations and Supercomputers

In the highly competitive world of consumer products, Procter & Gamble (P&G) has a new imperative: ensuring that current and new products are environmentally sustainable without sacrificing product performance and market share. This requires cutting edge research at the molecular level of materials that make up P&G products, a supercomputing challenge that demands the most powerful systems. Through a grant from the Department of Energy's INCITE program, P&G research scientists have enlisted the help of the leadership class high performance computing resources at the Argonne National Laboratory. Using the Argonne system, P&G molecular dynamists are studying the complex interactions of billions of atoms and creating simulations at the atomic level to determine how tiny submicroscopic structures impact the characteristics of the ingredients in their soaps, detergents, lotions and shampoos. The excellent results have prompted P&G management to beef up the company's own supercomputer clusters, and dedicate the new processors to computational chemical research.

If someone said to you, "Surfactants are substances that, when dissolved in water, lower the surface tension of the water and increase the solubility of organic compounds," you might understandably reply "Huh?"

But for research scientists at P&G investigating the fundamental nature of matter at the molecular level, this kind of talk is their daily lingua franca.

How surfactants—the dominant ingredient in soaps, detergents, lotions and shampoos—behave at the molecular level can have a profound impact on a product's properties, and ultimately, its acceptance by consumers. But new imperatives centered on environmental sustainability have researchers pushing their investigatory limits. With unprecedented oil prices, limited water in third world countries, and a global push for products that are more environmentally friendly, P&G must rethink many of the products that consumers have come to depend on around the world. The scale of the research challenge is experimentally overwhelming. To address this, P&G has invested in high performance computing (HPC), but this too presents sophisticated challenges in both theoretical and computational capabilities.

Sustainable Surfactants

P&G had revenues of $76.4 billion in 2007 and employs 138,000 people working in 80 countries. This includes some 9,000 R&D staff who tackle high tech challenges and foster innovation to keep the company competitive. They produce many of the popular brands of cleaning products that are in homes around the world including Tide®, Cascade®, Dawn®, Cheer®, Pantene®, Downy®, Head and Shoulders®, and Oil of Olay®.

Says Tom Lange, P&G's director of modeling and simulation, corporate research and development, "Because of the sustainability movement, the drive to use natural ingredients, and P&G's desire to reduce its dependency on the use of petroleum in its products, we are now investigating a whole host of new materials. In order to understand the properties of these materials and how they interact with other ingredients, we have to be a lot smarter from the molecule up."

Lange notes that in the past, products introduced by various companies as being environmentally friendly often did not perform as well as their more traditional competitors. The attrition rate for these less effective green products has been fairly high. He says that at P&G, researchers are not willing to lower quality to achieve sustainability. Instead they are conducting research at the molecular level to enhance existing products and develop new ones that meet environmental and sustainability goals while retaining the top performance that customers have come to expect from P&G products.

"This can be a difficult process," he comments. "Discovery is fundamentally an unpredictable business. You have to keep trying different approaches, some of them highly counterintuitive, until you get a winner. Molecular dynamics provides the framework for our investigations

and allows our researchers to understand the complex and sometimes unusual interactions that occur at these submicroscopic levels."

Science of Surfactants and the Fundamentals of Foam

Kelly Anderson, a senior scientist specializing in molecular dynamics in Lange's department, is one of those investigators. Anderson conducts fundamental research into the nature of surfactants and polymers at the molecular and mesoscale levels. Surfactants, such as soaps and detergents, create self-organizing structures. These structures are so small and dynamic that they cannot be seen even with very powerful microscopes—a typical micelle is three to five nanometers (one nanometer is one-billionth of a meter). Unlike the nanoparticles used in electronics, these tiny micelles are soft; they are constantly forming and breaking up.

"Even though we cannot see these structures, we are able to observe the effect they have on the surfactants or other materials we are studying," says Anderson. "And their impact is considerable. The fundamental properties of our soaps, lotions, detergents and shampoos that you use every day are determined by these tiny structures—for example, how thick something is, how it feels in your hand, how well it mixes with water, how it pours, how foamy is it, does it coat the sides of a container, will it separate into two or three liquids…all these properties and more depend on these submicroscopic micelles and vesicles."

Foaming, in particular, is an important characteristic that is not well understood. Sometimes a product is designed to foam to meet customer expectations—if soap or shampoo does not produce enough suds, consumers may think it isn't cleaning. But foam in the wrong places can be a household nightmare. Dawn, P&G's liquid dishwashing soap, creates mounds of foam; Cascade, a detergent made for automatic dishwashers, generates very little. Anyone who has accidentally put Dawn in the dishwasher knows the clean-up challenge when bubbles come oozing out on to the floor. And in areas of the world where water is scarce, achieving an effective clean with a surfactant that requires fewer rinses to wash out suds is important for basic resource sustainability.

Anderson explains that foams have been studied at the physical level for hundreds of years. But there has been no real understanding of what is happening at the molecular and atomic level. "Molecular dynamics allows us to make approximations about the interactions—the chemical potentials—that are occurring," he says. "By investigating the molecular composition of these materials, we are better able to predict what properties a formulation will exhibit—not only its immediate characteristics, but what will happen to the mix six months from now. By mixing and matching different molecules containing different configurations of atoms, we can create the most desirable characteristics for our consumer products such as detergents and shampoos and, at the same time, ensure they are safe and environmentally friendly. That's really the magic of what we are trying to do."

To meet these goals, Anderson and his colleagues needed a window into the complex interactions that are occurring in this essentially invisible submicroscopic world. They knew that even though they cannot actually see the soft nanoparticles as they interact, they could simulate their effects using HPC.

Searching for Computer Cycles

P&G has a HPC cluster made up of about 2,000 processors. But there is a problem. The P&G supercomputing environment is primarily allocated to tackling routine production tasks and other classic HPC jobs, such as computational fluid dynamics, testing virtual rather than physical prototypes, and solving last minute design problems associated with products being readied for release into the marketplace. This limits the amount of time and the number of processors available to Anderson and his team, making their investigations into the complex world of self-assembling molecules even more difficult.

"Given the limited scope of the in-house computing resources available to us, we can only simulate a few thousand molecules at a time," he says. "This provides some interesting results, but we really need to be simulating billions of atoms—just a few errant molecules can make major changes in the product. However, I can imagine the reaction I'd get if I went to our IT guys and said, 'Well, I need to do some calculations involving one or two billion atoms, and the job will tie up 1,000 of our processors for a month.' That's the entire computing environment dedicated to providing support for 50 of our businesses. They'd either laugh or recommend that I provide business justification for such."

Assistance from INCITE and Argonne

Fortunately help has arrived in the form of access to the leadership-class supercomputers at Argonne National Laboratory. Argonne, located about 25 miles from Chicago, is one of the U.S. Department of Energy's (DOE) largest research centers. It is also the nation's first national laboratory, chartered in 1946. P&G applied

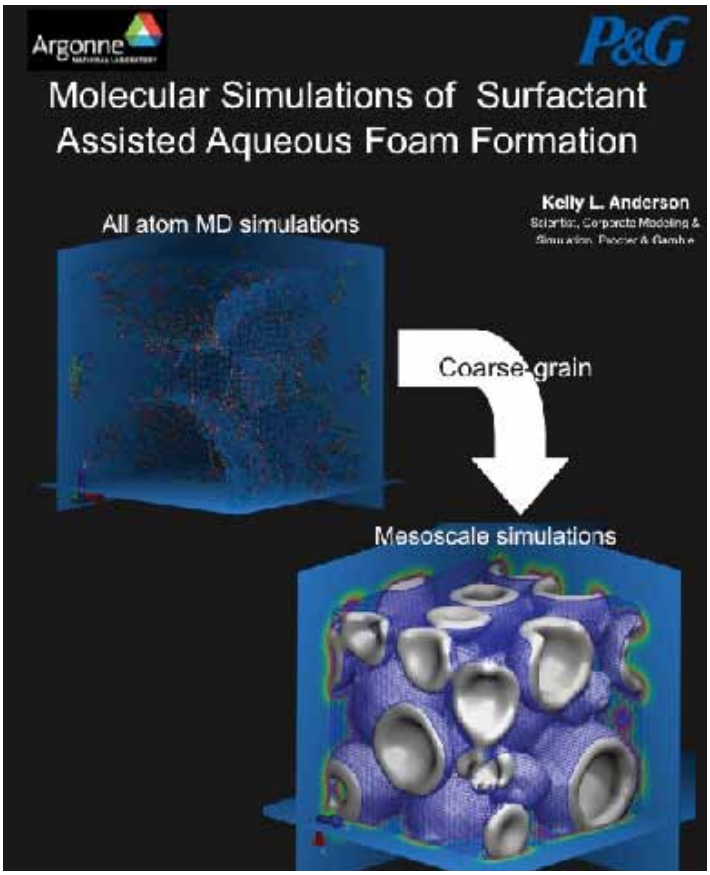

Figure 1: Simulations of bubble formation, from all atom detail to the mesoscale level. All atom simulations allow exploration of fine detail, while mesoscale simulations allow simulations of many bubbles forming simultaneously.

for and was awarded access to the lab's HPC system through the DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The program provides computing time on some of the world's most powerful supercomputers at Oak Ridge National Laboratory, Argonne, Lawrence Berkeley National Laboratory and the Pacific Northwest National Laboratory. The program supports innovative, large-scale science projects that enable scientific advancements. And it has given Anderson the computational horsepower he needs to tackle investigations involving billions of atoms.

"We're just at the very beginning," he says. "We are doing basic research trying to understand the fundamental nature of materials. When we run the simulations, we can see what happens to the molecular structure based on the interaction of all those invisible atoms—particles are aggregating, clumping, accumulating and moving through various phases, such as separating or transitioning from a solid to a liquid.

"One of the main reasons we need access to a leadership class HPC system like the one at Argonne is that it takes a lot of processors a long time to simulate a microsecond of these interactions in the real world," Anderson continues. "For example, in the actual world, it might take a month for salad dressing to separate. But, through simulation, I can speed up the process and observe what happens. In other cases, the interactions we are interested in occur far too fast to ever observe. Molecules interact at the femtosecond level. (A femtosecond is one quadrillionth (10^{15}) of a second.) Simulation allows me to slow those processes down so they can be studied. These kinds of simulations require an enormous amount of processing power—far more than P&G has available. At Argonne, I have been able to run simulations using up to 16,000 processors. What would have taken a month on P&G's system, if it had been available, now takes a few hours."

Benefiting the Scientific and Global Communities

The research that the P&G scientists are conducting—discovering how to work at the atomic level to create larger particles that either exhibit predetermined properties or open new avenues of investigation—will be published in refereed scientific journals. To that end, they are working with Professor Michael Klein from the University of Pennsylvania, one of the world's leading molecular dynamicists. The research is also a major part of a Ph.D. student's thesis and will be published in his dissertation.

Says Lange, "We're adding to the methodology of studying materials at their molecular scale through computer simulation, something that has very broad application. Internally we use the methodologies Kelly and his team are developing for our own proprietary processes and competitive advantage—we get the "first look." But we are also making these methodologies public in order to advance understanding in other important fields. For example, foams are used in separation processes such as municipal and industrial water and wastewater treatment. Foams are used for fire extinguishers, building insulation materials, and oil companies use surfactants and polymers to increase the amount of oil they can recover. The applications for these materials are seemingly endless."

HPC Competitive Impact: Improved, More Sustainable Products

Anderson says that participating in DOE's INCITE program has provided significant benefits. He and his research team have already been able to produce virtual (i.e. computer generated) "phase diagrams" that examine the behavior of materials at various concentrations.

They can now predict at what concentration these materials will make a phase change into a different structure.

This information is then passed on to the P&G formulators who mix and match the ingredients to create a new or improved product. Which ingredients they choose determines how well the product will perform– e.g. amount of sudsing, shelf life, color, ability to remove stains and a myriad of other characteristics. Formulators also must balance cost and availability of ingredients with the wants and desires of the consumer. Anderson's access to HPC at Argonne allows him to simulate and capture information that the formulators cannot access using physical experiments. This data helps make their work that much easier and more productive.

Anderson says that the advances they are making have inspired some additional changes within the firm. "Increasingly, others want me to train them in how to conduct the kinds of investigations that I'm doing. So our work at Argonne is also stimulating the development of the workforce of the future. In addition, our highly positive experience with INCITE and supercomputing on the scale provided by Argonne has motivated senior management to add to our internal computing capabilities. We are proceeding to purchase an additional 512 processors to add to the P&G supercomputer cluster and dedicate the increased capacity to computational chemistry."

In the not too distant future, HPC simulations will allow P&G to create "designer" molecules that will exhibit new and sometimes unexpected properties. This research will permit the company to improve existing products and create new products that are not only highly effective, but are consumer safe, have minimal environmental impact, and, in general, help meet the goals of a sustainable human ecological system. And of course, keep P&G ahead of the competition. "That's the ultimate value proposition," says Lange, "making something that delights our customers, meeting our sustainability goals without sacrificing product performance or profitability, and maintaining our competitive edge." It is no wonder P&G's top management considers HPC hardware and software a strategic asset. Says Anderson, "It's really our next-generation laboratory."

In Brief

Key Challenges

- Enhance existing P&G products and create new ones that are environmentally sustainable without sacrificing performance, particularly surfactants such as detergents and shampoos
- Investigate computationally at the molecular and atomic levels the fundamental nature of the ingredients in these products in order to meet these goals
- Obtain access to sufficient computing capacity to conduct this research

Solutions

- Applied for and was awarded access to the leadership class high performance computer at the Argonne National Laboratories
- Gain access through INCITE to an order-of-magnitude more computational capability than available within P&G

Key HPC Benefits

- Reduces simulation time from months to hours, dramatically accelerating the research process
- Simulates billions of atoms, providing researchers with significant new understanding as to how molecules behave as they aggregate, clump and move through various phases
- Adds to the broader scientific community's methodology of studying materials at the molecular level through computer simulation
- Creates a new "workforce of the future" as other P&G researchers are inspired to request training in modeling and simulation with HPC
- Validates high performance computing as a company strategic asset
- Motivates top management to significantly enhance P&G's internal computing resources, creating a "next-generation laboratory"

Web Site

- www.pg.com

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

XX trees preserved for the future
XX gal of water flow saved
XX lbs of solid waste not generated
XX lbs of greenhouse gasses prevented
XX million BTUs of energy not consumed

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Council on Competitiveness
1500 K Street, NW, Suite 850, Washington, D.C. 20005 T 202 682 4292
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