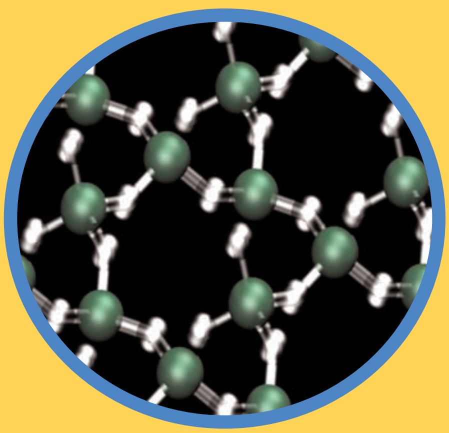
COMPOSE

THE DOE CSGF ANNUAL ESSAY CONTEST JOURNAL

DOE CSGF



THE SIMULATED SIMULATOR,
OR WHY I STOPPED DELETING MY FILES

CHANGING THE WORLD
ONE ATOM AT A TIME

THE DOE CSGF ESSAY CONTEST WINNING ESSAYS

2008

The DOE CSGF Annual Essay Contest was launched in 2005 as an exciting opportunity for DOE CSGF participants to hone their writing skills. This contest requires fellows to write a popular science essay on a topic of personal importance directed at a non-science audience.

The DOE CSGF is proud to recognize outstanding fellows and alumni who have completed a non-technical writing composition on a topic in computational science. In addition to recognition and a cash prize, the winners received the opportunity to work with a professional science writer to critique and copy-edit their essays.

These copy-edited winning essays are published here, in this issue of Compose Magazine.

FOR MORE INFORMATION ON THE DOE CSGF ANNUAL ESSAY CONTEST, VISIT http://www.krellinst.org/csgf/compose/index.shtml

Many interesting essay submissions were received in 2008 and two were selected as finalists. Selections were made based upon which essays clearly conveyed the complexity of computational science to a lay audience. Carolyn Phillips' essay "The Simulated Simulator, or Why I Stopped Deleting My Files" was awarded first place for its creativity and ability to illustrate computational science. Jack Deslippe won Honorable Mention for his interesting essay "Changing the World One Atom at a Time."

Both Ms. Phillips and Mr. Deslippe are third-year fellows in the DOE CSGF program.

The Simulated Simulator, or Why I Stopped Deleting My Files

Carolyn L. Phillips – 2008 DOE CSGF Essay Contest Winner

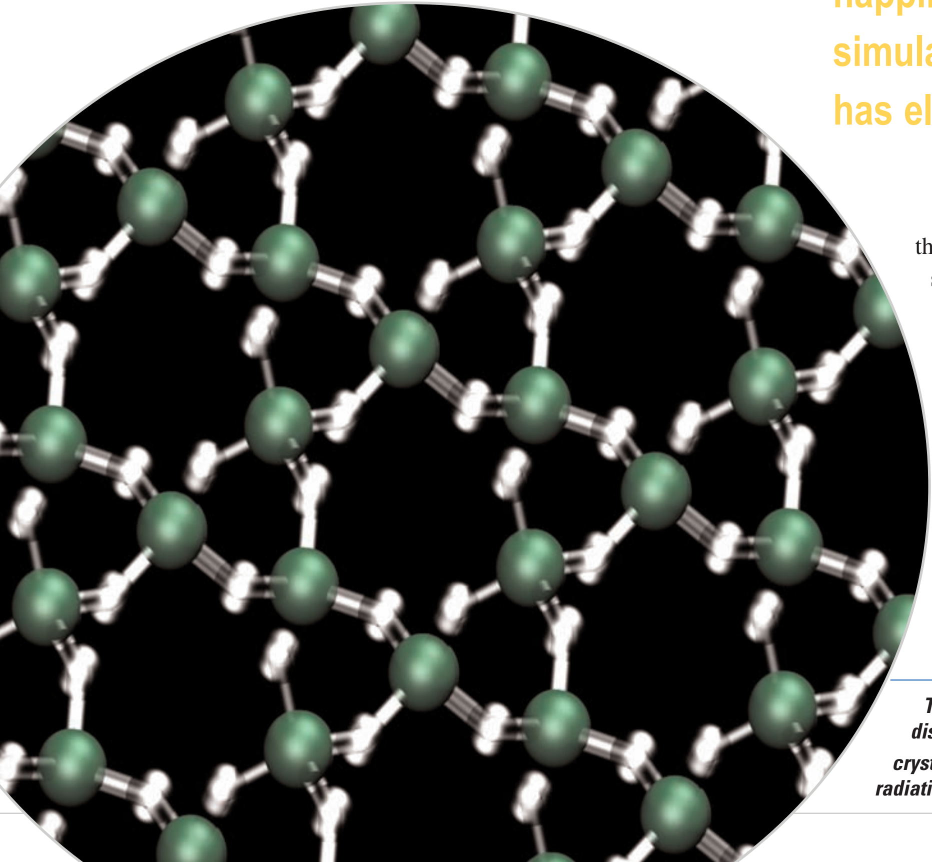
An article in the *New York Times* recently discussed the work of Dr. Nick Bostrum, a philosopher from Oxford University. Dr. Bostrum imagines that some day, computer simulations will grow so powerful that we will simulate little versions of ourselves in completely artificially constructed universes. The corollary of that notion, as discussed by Dr. David J. Chalmers, a philosopher from the University of Arizona, is that there is a high probability that's exactly what we are right now. We could be a simulation, a stream of 1s and 0s in a massive computer, like Neo in "The Matrix," but unfortunately lacking the ability to wake to a real body, as we have none.

Before we get too nervous about our current state of existence, I'll mention that this theory has its practical rebuttals. Could the complexity of the universe ever fit inside any arbitrarily sized but finite computer? For comparison, at the current state of technology, most computational engineers working in molecular dynamics would be ecstatic to model a single protein for as much as a microsecond.

But as a computational scientist, I happily confess that the idea of the simulated universe on a microchip has elements of truth for me. This philosopher's treatise captures my attitude toward what I do and why I love what I do. For me, each simulation on my computer is a tiny artificial world that I control. I graciously populate my simulation with simple computational entities (*particles, cells, molecules, heat flows, radiation, etc.*), give them a simple rule set to follow (*electrostatics, transport equations, Newton's laws*) and then see what transpires. It's a world where I control time. It can be sped up, slowed down and even reversed. An event can be played over and over again, with small modifications. Occasionally it can be convenient to turn off physics in a little corner of that world to adjust local conditions to a more favorable state. (*Would my entities consider these miracles?*) It's also a world fully capable of surprising me with its behavior. Computational scientists periodically find themselves scratching their heads in response to something a simulation suddenly did, and asking themselves whether they just unmasked a true phenomenon or simply some silly glitch in their code. (*Free will or a cosmic accident?*)

But as a computational scientist, I happily confess that the idea of the simulated universe on a microchip has elements of truth for me.

What I enjoy about computational simulation is how the simulation space becomes a scratch pad for my imagination. An idea becomes a hypothesis, becomes a model and provides an answer in a relatively short time. Maybe a molecular scientist imagines a new drug design that may bind better with a virus. An auto



The internal structure of alpha-quartz, with its distinctive tetrahedral SiO_4 units. Little does this crystal know that it is about to be subjected to a radiation event and transformed into glass.

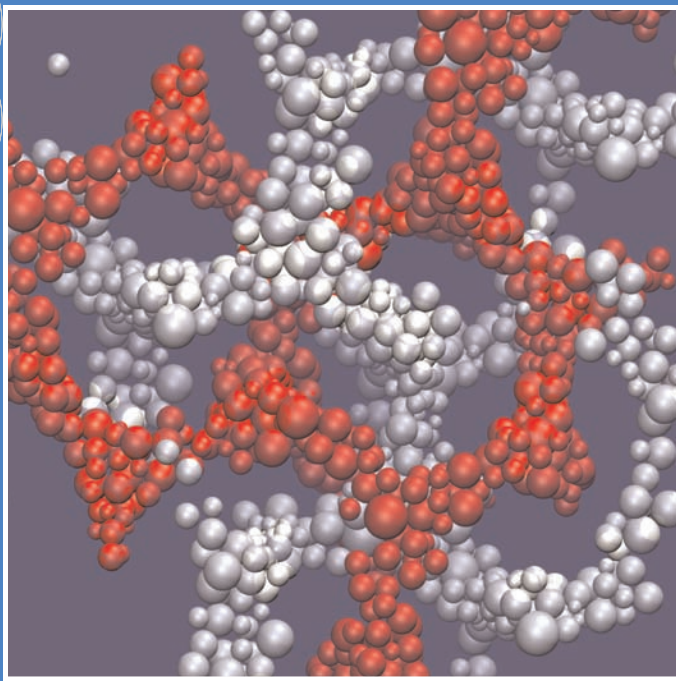
engineer might conceive of a new bumper design that dissipates energy by crumpling more effectively. A physicist may consider a network design that tolerates errors better. A neuroscientist may theorize on how the behavior of a collection of neurons might be related to memory formation. In some of these cases, the scientist or engineer could laboriously construct their idea in a lab and test it. In other cases, the idea is utterly resistant to physical construction. (*Can supernovae be ordered from a scientific catalog?*) Instead, the idea can be constructed and tested inside a simulation on a computer. Good hypotheses can be winnowed from bad hypotheses rapidly. An event that occurs in a simulation can be poked, prodded, turned upside down and run again 20 times to test its sensitivity. Through this process, a good idea can suggest an even better one that can be modeled just as rapidly. The innovator's imagination becomes unshackled from material and physical constraints.

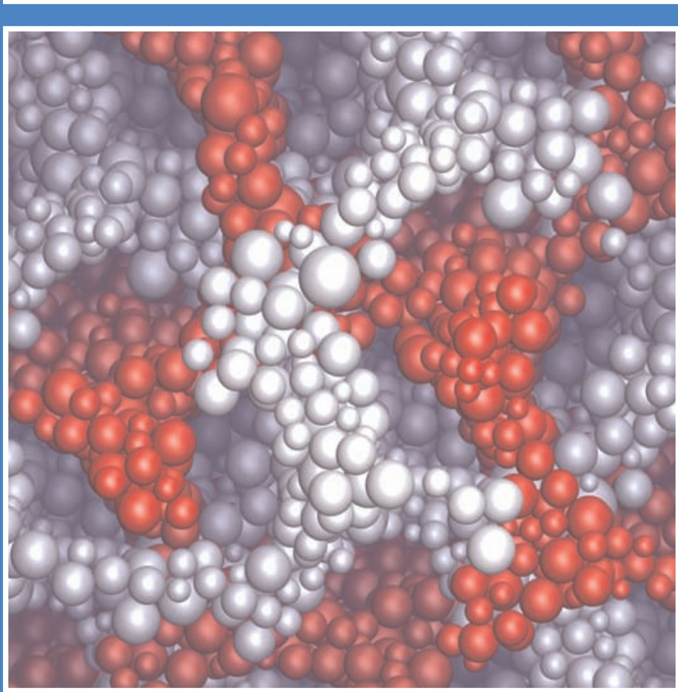
As faithful stewards of our simulations, we computational scientists must connect our results back to the real world (*such as it may be*). We carefully argue our numbers are repeatable and stable, our model assumptions are sufficient and our code has been tested and found true, all to convince our peers that our conclusions are worth believing.

And what do we gain from this exercise? We gain insight into the critical economic variables causing a bank failure to happen. We provide direction as to what families of drugs a biochemist should manufacture for testing. We predict how an environmental regulation will actually affect net carbon dioxide release 50 years in the future to help politicians make good choices now.

Our little simulation worlds exist, therefore, for only the noblest of purposes. We wield our power inside them to extract a greater understanding of the world outside them. We recognize they are but poor shadows of what they are meant to represent. But they let us surmount those real-world barriers — the limits of time, materials, physical access, personal safety and repeatability, to name a few — that would block us from insight. Is that not a worthy reason for existence?

So if it should turn out that I am nothing but a stream of 1s and 0s, the trace of an electron, or a small dip or rise in voltage across a sea of tiny capacitors, then I look around and I am impressed. Consider the atomistic and even sub-atomistic detail, the 14 billion years of simulation time, the 78 billion light-year diameter simulation cell, and several billion irrational independently acting agents. I conclude that we are no mere dissertation project. We must be part of something big!





Above, polymer-tethered nanoparticles have self-assembled into a Double Gyroid (polymers not shown). The two intertwining lattices have been colored red and white, but are chemically identical. This feat of self-organization occurs only at a particular system density, a suitably low temperature, and for nanoparticles manufactured to a sufficiently high tolerance.

Jack Deslippe – 2008 DOE CSGF Essay Contest Honorable Mention

Changing the World
One Atom at a Time

"This is going to be embarrassing." That was my thought after knocking a full glass of water onto my lap. But wait! These were no ordinary pants. They were nanopants, incorporating hydrophobic nanofibers to repel water and avoid stains. As I casually wiped the pooled water off the fabric and left the restaurant, dignity intact, I thought to myself, "This must be what the future is like."

In some sense, it really is what the future is like. Human history has always been shaped and characterized by the types of materials used during each period of development. There was the Stone Age, the Bronze Age, the Iron Age, the Steel Age and the Silicon Age — the current period in which the microchip has revolutionized the world. What materials will characterize the 21st century? It's a safe bet that it's the class of substances we now call nanomaterials. You might be thinking, "That must be what's in my iPod, right?" And, while there are undoubtedly some nanomaterials in an iPod, the "iPod Nano" gets its trendy name not from what it's made of, but because it's smaller than the regular iPod. The Nano version of the iPod is approximately a quarter the size of the full version, but when scientists use the word nano to describe an object, we're describing materials that have a dimension on the order of a nanometer — 10,000 times smaller than the width of a human hair, or just a few atoms wide. For example, graphene is a single atom-thick sheet of graphite, the flaky carbon substance that makes up what is incorrectly termed pencil lead. It's the thinnest sheet ever created, and if it's rolled up, you get a one-dimensional tube whose diameter is the size of a nanometer: a carbon nanotube.

Using HPCs, I get to play with materials that might be fabricated in the coming months or years. Computer simulations can tell us whether the particular arrangement of atoms we suggest will form a stable structure or if it will disintegrate.

What's so exciting about nanomaterials is they can be designed literally each individual atom at a time. The different arrangements, patterns (or defects in patterns), yield structural, electronic and optical properties that are unique from those of nanostructures and traditional three-dimensional materials. Because these materials live on nanometer-length scales, they are the ideal place to study and harness the effects of quantum mechanics, the physical theory that replaces Newton's laws of motion for very small objects. Nanomaterials may be small in size, but the equations involved in studying them are extremely complex because the motion of every electron is correlated with the motion of every other electron (and there are still a lot of them). It's difficult to understand the unique quantum effects and predict the types of systems that will yield the best materials for new devices. Only computational "nanoscientists" working on the world's biggest and most powerful high-performance computers (HPCs) can meet this challenge.

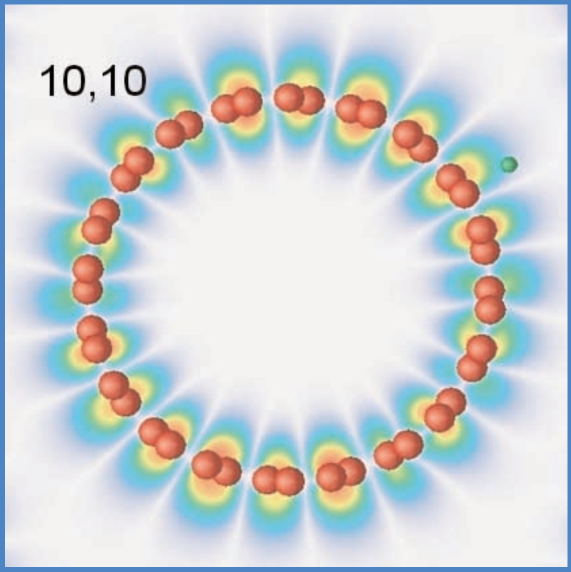
Using HPCs, I get to play with materials that might be fabricated in the coming months or years. Computer simulations can tell us whether the particular arrangement of atoms we suggest will form a stable structure or if it will disintegrate. We can make this determination more quickly and for many more configurations than are feasible to try in the lab.

Despite having benefited directly from how the nanofibers in my pants interact with water, I am most interested in understanding the unique way these materials interact with light. For example, nanomaterials absorb light in unique ways. When light hits an object, the object captures that energy by promoting an electron into a higher energy state. This leaves a "hole" in the low-energy state that acts like an oppositely charged particle. We have discovered that when confined on the nanoscale, the electron and the hole interact very strongly. This dramatically changes the ranges of the optical spectrum at which these materials will absorb light and how efficiently they do so.

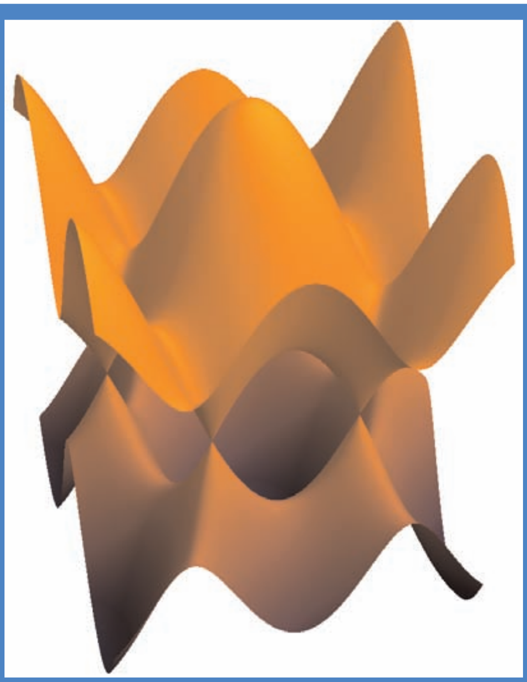
Utilizing the optical properties of nanomaterials to create inexpensive and efficient solar cells may prove to be the way these materials come to characterize the new era. It seems strange that, in the first decade of the 21st century, almost all of our energy is still generated from the same basic technique that was used in the dawn of the industrial revolution: by turning a turbine. Even in nuclear power plants, the energy comes from heating water to generate steam that rotates a turbine. Solar energy could change this trend since solar cells generate energy with no moving parts. However, besides representing a paradigm shift, solar energy is clean and renewable and represents a solution to the long-term energy and environmental crisis.

Computational scientists such as myself are studying an emerging branch of solar cells based on nanomaterials like polymers, nanotubes and fullerenes that has the possibility of providing cheap solar energy devices. Using the world's most powerful computers, we are working on predicting the types of materials that will absorb the most sunlight and understanding the absorption process in these devices.

By simulating nanomaterials with HPCs, we are beginning to understand and harness nanosystems for uses beyond saving the dignity of spill-prone graduate students. The nano-age is beginning and HPCs are the tools that will usher it in. Which is why, when someone asks me what I do, I say I'm changing the world one atom at a time.



Schematic of an optically excited correlated electron-hole state known as an exciton. When a material absorbs light, an electron in the material is promoted to a higher energy state, leaving a hole behind in the lower energy state. In nanosystems, the excited electron and the hole interact strongly.



The bandstructure, or energy state diagram, for a 2D graphene sheet. The structure is unique due to the conical points that connect the upper (unoccupied) and lower (occupied) energy states.

Meet the Judges ...

This year the essay submissions were judged by a three-person panel consisting of Christine Chalk, Jacob Berkowitz, and David Brown.

Christine Chalk has been with the U.S. Department of Energy's Office of Science for more than 15 years in a variety of science policy positions. Ms. Chalk has degrees in Economics and Physics and experience on Capitol Hill. She is currently on a long-term detail to the Office of Advanced Scientific Computing Research from the Office of Budget and Planning — Division of Planning and Analysis. In addition, she has served on the screening panels for the American Association for the Advancement of Science's Science Journalism Awards. This is Ms. Chalk's third year reviewing DOE CSGF essay submissions.

Jacob Berkowitz is a Canadian writer, journalist and playwright. He popularizes the work of leading scientists at major research-based organizations in Canada and the United States and is a long-standing contributor to DEIXIS, the DOE CSGF annual magazine. Mr. Berkowitz spoke about science writing at the 2006 DOE CSGF Annual Meeting in a talk titled, "Starting from the End: The Power of Turning Science into Story." His first book, "Jurassic Poop: What Dinosaurs and Others Left Behind," was published in 2006 and he's presently at work on a 50th anniversary follow-up to C.P. Snow's classic book on science and society "The Two Cultures." Mr. Berkowitz has been a DOE CSGF essay reviewer for four years.

David Brown is deputy department head for science & technology in the Computing Applications & Research (CAR) Department at Lawrence Livermore National Laboratory. He is responsible for overseeing science and technology planning, execution and new initiatives in CAR. He is also principal point of contact for the Office of Advanced Scientific Computing Research in the DOE Office Of Science. Dr. Brown earned his Ph.D. in Applied Mathematics from the California Institute of Technology in 1982. He also holds a B.S. in Physics and an M.S. in Geophysics from Stanford University. He joined Lawrence Livermore National Laboratory in 1998. This is Dr. Brown's first year as a DOE CSGF essay reviewer.

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