

## Success Story

## Dalhousie University



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– Dr. Randall Martin, scientific researcher,  
Dalhousie University

## Global Numerical Model, Now Tracking Pollutant Emissions In Up to 35 Atmosphere Levels Around the World, Runs 3-to-4 Times Faster On SGI® Altix® 350

Located in Halifax, Nova Scotia, Canada, Dalhousie University is one of Canada’s leading universities. It attracts more than \$93 million dollars in research awards and grants yearly. In 2003, *The Scientist* magazine named Dalhousie the best place in the world to work, outside the United States, as a scientific researcher. Two of Dalhousie’s researchers in its Physics and Atmospheric Science department are immersed in solving intense computational problems requiring the speed and expandability of SGI® high performance compute (HPC) power and storage, and both agree SGI® Altix® computers turned out to be the best choice for the large data sets they run.

Dr. Randall Martin is currently conducting global pollution studies—including how pollutants react in the atmosphere and how pollution spreads across the globe—as well as developing tools to monitor emissions for international agreements, such as the Kyoto Protocol, on two SGI Altix systems with heavy duty SGI storage support.

Dr. Jordan Kyriakidis is researching theoretical quantum nano-electronics, with a long-term goal to develop quantum materials as replacements for transistors in computers and other electronics, using another pair of SGI Altix systems linked to SGI RAID storage via fiber optics.

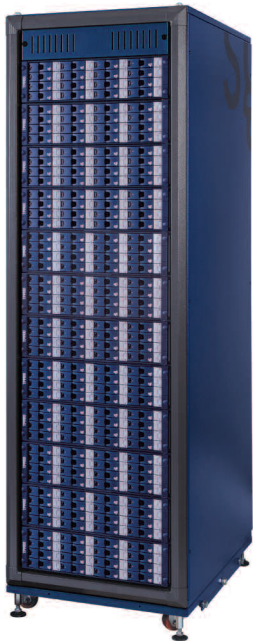
### Global Pollution Studies

No stranger to the power of SGI high performance computers, Dr. Martin, a Research Associate at the Harvard-Smithsonian Center for Astrophysics in addition to his role at Dalhousie, previously assisted in the design of a global numerical model at Harvard, GEOS-CHEM, which is now used at a number of universities. A UNIX® OS-based application originally developed on an SGI® Origin® family system running SGI® IRIX® OS, GEOS-CHEM uses simulated meteorological fields from NASA and other models to divide the atmosphere into a grid and solve for chemical composition. The application was already in the process of being ported to a variety of other platforms including 32-bit



Linux® operating system when Dr. Martin considered the Linux OS-based SGI Altix for his work at Dalhousie. SGI technicians easily ported GEOS-CHEM to the 64-bit Altix system. Dr. Martin reported the SGI Altix system runs his global atmospheric data sets at 3 to 4 times the speed of computers he used at Harvard University a little over two years ago.

To track global emissions, Dr. Martin receives satellite data from NASA and the European Space Agency (ESA), as well as data from aircraft and other sources. During the summer of 2004, Dr. Martin completed his first satellite retrieval using



the two SGI® Altix® 350 systems, each with 16 Intel® Itanium® 2 processors, linked via gigabit Ethernet to an SGI® InfiniteStorage TP9100 with 3TB of RAID storage. Taking raw spectra data of the earth's atmosphere and of the sun, he assessed pollutant concentrations around the globe and is now providing that data to NASA for analysis as part of an integrated satellite aircraft campaign. The campaign, called ICARTT, is designed to investigate the outflow of pollution from North America into the global atmosphere. The aircraft take samples of a whole range of atmospheric constituents, including aerosols and trace gases; some of these are toxic and some are greenhouse gases.

"SGI Altix is much, much faster than anything I've ever used before," said Dr. Martin, "probably three to four times faster, which is just phenomenal. Altix also enables us to run our simulations at higher resolutions and therefore provide a more accurate picture of the atmosphere, and it enables us to examine results more quickly: In my work, time is of the essence. It's important to have a fast computer. Otherwise, we'd have to restrict what we could do, the type of sensitivity studies we could perform, the resolution at which features can be examined and the number of pollutants that we can put into our model."

Resolution currently runs at two degrees by two and a half degrees (approximately

several hundred kilometers) on Dr. Martin's SGI Altix system running GEOS-CHEM software. GEOS-CHEM divides the atmosphere up into about a million boxes—and within those boxes there are roughly 30 to 35 layers in the atmosphere—and solves for all of those attributes, simultaneously, every three hours. "Thanks to the SGI Altix systems, we're contemplating the possibility of running at one by one degree globally, which is something we never would have even considered beforehand, but I believe we can do it with the SGI system," added Dr. Martin. "Understand: one by one increases the number of 'boxes' by a factor of five and in each of those boxes we have maybe 45 different pollutants that we advected (transported from one box to the other, either vertically or horizontally) around between boxes, so all of these numbers all multiply and you can get a very large array of data very quickly."

Not only can SGI Altix handle the one by one degree calculations, said Dr. Martin, but, "Most importantly, SGI InfiniteStorage TP9100 with 3TB of RAID can expand to support one by one resolution."

By using satellites to observe the abundance of pollutants in the atmosphere, and combining the satellite data and the models, Dr. Martin said he could infer what the emissions from various countries had to have been. He is expecting to develop

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techniques towards enforcing protocols, such as the Kyoto Protocol, to monitor emissions from various countries from space using the SGI Altix 350 system running the GEOS-CHEM model. Dr. Martin will also be investigating the use of the GEM-AQ model, currently being developed in Canada, to similarly examine surface air quality and climate issues.

“SGI Altix offered the best price/performance of any vendor,” concluded Dr. Martin. “We looked at IBM, Sun and HP but SGI had a much better price/performance. By price/performance, I mean relating to the number of computations it can do within a shared memory framework and the RAM that could be provided as well. Plus, I’d had a lot of good experience with SGI beforehand on their Origin platform. SGI has a strong history of shared memory systems and that was important as well.”

More information on Dr. Randall Martin’s work can be found on the Web at <http://fizz.phys.dal.ca/~atmos/>.

### Exploring Quantum Nano-Electronics Theory on SGI Altix

Dr. Jordan Kyriadis’ work is taking him into uncharted territory. As he points out, he is “a theorist, not an experimentalist.” His work revolves around a simple fact: the world has relied on transistors (which replaced vacuum tubes) for more than 40 years. And while electronic devices grow

ever smaller, there has been no essential change in the original transistor. Many scientists, especially in nanotechnology, feel a replacement – a new technology – will soon be needed. Dr. Kyriakidis uses his two 16-processor SGI Altix 350 systems, with 54GB RAM and SGI Infinite Storage TP9100, with one TB of storage, to work with quantum dots – “think of them as artificial atoms” – which can be designed and engineered to have properties a scientist wants them to have, i.e. artificial hydrogen, artificial helium, etc.

“Nanotechnology is a gigantic field. Within that, the small piece that we’re looking at is called quantum nano-electronics,” explained Dr. Kyriakidis. “This field is relatively new but it’s moving very rapidly. The bottleneck in all of nanotechnology is that we don’t have any good way to control the systems. We know we can do things — place atoms one at a time — but we can’t do it very well or very quickly. And part of the issue that needs to be resolved before the field can progress is that we have to find new and innovative techniques that will enable us to control these systems far beyond the current levels. What I do is look at what kinds of controls we can have on these systems, and how fine a level of control can we have. We have a theory of how these artificial atoms should behave and we use the SGI Altix systems to do quantum simulations — calculations to figure out if they do actually have the properties that we think they should have.”



*Although researching two very different subjects, Jordan Kyriakidis (left) and Randall Martin began collaborating even before Martin arrived at Dalhousie, to acquire this cluster of SGI Altix computers.*

This is the first time Dr. Kyriakidis has done serious research on SGI computers, and a high performance Linux OS-based system was exactly what he was looking for. "I've had lots of experience with Linux," he added. "We write a lot of our own software because there is no generally accepted software: everything is very leading edge. The fact that SGI has these 64-bit Altix machines, which are Linux OS with such huge processing power in a very professional, high performance grade of machine, was very attractive to us because it meant we could start being productive right away. We didn't have to spend time writing software again on some specialized operating system."

In addition to 64-bit performance on SGI Altix, powerful storage is essential for quantum simulations. "We have a huge database that we need to store somewhere," explained Dr. Kyriakidis. "In a sense, we can't handle the data that our software produces all in one shot, so we have to store it somewhere and then we have to go back and look through the data and see what it's trying to tell us. The storage is an integral part. We have an SGI TP9100 — a big storage array — and it's connected via fiber optics to one of our two Altix systems. With fiber optics from the processor, we can really, very quickly write the data to the hard drive, which is a collection of about 10 or 15 hard drives, and then read the data back again."

Dr. Kyriakidis chose SGI as a company, and Altix in particular, because, "It represented the best value in pure processing

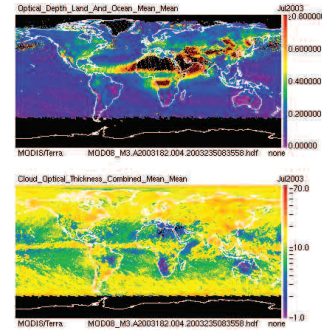
power, operating system and storage requirements and price," he concluded. "Combine all those things together and SGI Altix far and away became the best option for us. And so far, we've been bang-on in our decisions. We're quite, quite happy with it. Because we now have SGI Altix, I'm able to do things that just were not possible before. SGI Altix systems will clearly enable us to move the science forward — more forward than we've ever been able to do before."

More information on Dr. Jordan Kyriakidis' work can be found on the Web at <http://soliton.phys.dal.ca/>.

#### Collaboration Key To Best SGI Solution

Both Dr. Martin and Dr. Kyriakidis applied for Canada Foundation for Innovation (CFI) funding, through a program called the New Opportunities Grant, for the monies to acquire super-fast computers and storage to further their research. Both received their funding grants and — in an unusual collaboration — decided to pool their money to get more together than they would have individually.

"Dalhousie is Nova Scotia's leading research university and our researchers and graduate students have used SGI high-performance computer and visualization systems for many years," said Dr. Carl Breckenridge, vice-president of research at Dalhousie University. "We're very pleased with this collaborative initiative by these new researchers, which led to this acquisition of state-of-the-art SGI Altix systems under the CFI grant. We encourage



our researchers to consider the benefits of pooling funding when approaching companies like SGI. It can give researchers great strategic advantages. We look forward to the results of their research."

"SGI's cost-effective 64-bit Altix systems continue to be of huge importance to atmosphere, weather, and physics researchers around the world as the migration to Linux continues among many disciplines in the scientific community," said Martin Pinard, president of SGI Canada. "Dalhousie University experienced first-hand how easy it is to port code written in SGI IRIX over to what is simply the highest performance Linux OS-based computer system in the world: SGI Altix, backed by the most solid and reliable storage in the world, the SGI InfiniteStorage family."

Installed in early July 2004, the Dalhousie University installation includes four SGI Altix 350 systems with 16 processors in each system and two SGI InfiniteStorage TP9100 systems — one with 3TB of storage, the other with 1TB storage — plus assorted networking hardware enabling a gigabit Ethernet connection in one department and fiber optic connectivity in the other.