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UF Scientist Finds Attractive Solutions on SP2

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Discontinued Offering

The "Research Computing Initiative" (RCI) referenced in this article was discontinued as of January 2005. RCI accounts are no longer available. The article is being preserved only for its historical value. <editor@cns.ufl.edu>

UF Scientist Finds Attractive Solutions on SP2

Marian Lech Buszko had a vexing computing problem, and no attractive solution was in sight.

The superconducting magnet in his laboratory, and others like it, could break new ground in high-resolution magnetic resonance imaging and spectroscopy -- if only it had more accurate coils!

Dr. Buszko holds the newly designed gradient coil. The uniformity of its magnetic field is shown on the monitor of his workstation.

The Polish Ph.D. scientist was prepared to design these magnet coils himself; it was one of his research specialties, as director of the UF-IFAS Nuclear Magnetic Resonance (NMR) Facility.

The problem was not with the fixed coils built into superconducting magnets, which, in the case of the IFAS machine, generated 7 Tesla, a field some 140,000 times stronger than the Earth's magnetic field. The problem lay with small "gradient" coils which were wound around the chamber where samples to be imaged were placed.

Attached to a cylindrical probe, the gradient coils slide into the hollow bore of the fixed magnet. There, during imaging experiments, the gradient coils encode spatial information needed to create images.

The fields generated by the gradient coils were the critical element in obtaining accurate, undistorted, high-resolution images. Buszko and his collaborators, Dr. E. Raymond Andrew of the UF Physics Department and two visiting Polish scientists, knew what was needed: gradient coils with excellent linearity, a large volume of homogenous field with respect to coil size, low inductance, and efficient use of small currents. These could all be obtained if longitudinal
distribution of individual coil windings were optimized. This was the goal. The problem was that the "ideal" distribution had to be found among a virtually unlimited number of possible arrangements.

Buszko and graduate student Daniel Wang wrote a C program to evaluate the coil configurations and optimize them, using publicly available code for simulated annealing. This scientifically hailed code would simulate the repeated heating and cooling of countless coil distributions in order to discover the global minimum, a theoretical state of minimum energy corresponding to the most uniform magnetic fields.

If only he could find a platform where he could successfully run his experiments! Simulated annealing is not a brute-force method, but the computational requirements for Buszko's implementation turned out to be extremely high.

He'd begun, with high hopes, at the workstation on his desk, a Sun SPARC IPC-model with 8MB of RAM. But the job, he quickly realized, would take many months to complete -- at best. Buszko's experiments floundered on this and three other platforms until he discovered CNS's RS/6000 SP (SP2) supercomputer.

On an Indigo2 workstation at the UF Center for Structural Biology, his program began, but never completed, the lengthy calculations needed. He tried the N-Cube, a 64-node system at UF's Parallel Research Lab in CSE, with similar results. He even attempted to use a DEC Alpha 7000 via the Internet. While this was useful to test his code, Digital Corporation, which provided the service, didn't allow long-running jobs, so no runs were completed.

Supercomputer services were needed, Buszko decided. The scientist applied for and received a Research Computing Initiative (RCI) grant at CNS in August 1994. He began modifying his program to run on NERIX, the primary UNIX-research platform at CNS prior to the arrival of the SP2 computer.

"NERIX just didn't have the resources available for what I wanted," recalls Buszko.

"Because of the great amount of CPU time it required, the program had to run as a low-priority job, so smaller jobs in the system could get through. My program would run continuously, one week, two weeks, and never find the global minimum. Before the run would finish, NERIX would be put off-line for maintenance, or the system would need to be reset, and I had to start all over again. Part of the problem was that NERIX allowed multiple jobs to run on its single computational node. If a lot of people submitted jobs at the same time (they often did), the processor got swamped."

It was at this time that Buszko joined the CNS Instruction and Research Users' Committee. At one meeting, he heard about the Data Day home page the committee had created on a pre-production UNIX system at CNS called "NERSP."

"NERSP was new to me," recalls Buszko, "I was curious. Back at the office, I tried logging on. It accepted my NERIX password, and after looking around this RISC-based computing environment, I saw some exciting possibilities. I exchanged e-mail with Bill Kirchhoff, CNS system administrator for NERSP, and was invited to become the SP2's first external user. For a while, I had the whole computer to myself."

To his great pleasure, Buszko discovered that the C program he'd run on his UNIX Sun workstation did not have to be altered in any way to run on AIX/6000, IBM's implementation of UNIX for the RS/6000 SP. Furthermore, NERSP was configured to limit the number of jobs
per computational node. "Once you get a program started-mine runs 50,000 to 200,000 loops-you've got performance. Nothing slows you down."

The results?

After several trial-and-error attempts-needed to adjust annealing parameters-NERSP successfully optimized an eight-winding coil in three hours!

"This prompted me to try more complex designs, for even more efficient coils-I knew the computer could handle the calculations," Buszko said. "So, we modified the code to accommodate new designs, one of which, in addition to having 16 individual windings, added variables on the radii of individual windings."

NERSP successfully completed this numerically-intensive experiment in six days. These results have been submitted for publication in the Journal of Magnetic Resonance, but the quest for ever-better designs continues.

In the meantime, the UF Department of Physics machine shop constructed a set of coils, one of which was used by the Center for Structural Biology (CSB) to obtain the first very-high quality micro-images of the human spinal cord. These and other NMR images are available on-line at:http://csbnmr.health.ufl.edu/~binglis/index.html.

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