NERSC NEWS

News from the National Energy Research Scientific Computing Center

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ORNL's David Dean Elected to Lead NERSC Users Group

NERSC Division Director Horst Simon announced this month that David Dean, a nuclear physicist from Oak Ridge National Lab, has been elected chair of the NERSC Users Group. Stephane Ethier, a fusion energy researcher from the Princeton Plasma Physics Lab, has been elected vice chair.

"Both are long term users of NERSC with an excellent understanding of the issues facing NERSC users," Simon wrote in his announcement. "I am looking forward to working with them for the benefit of all NERSC users in the future."

Simon also acknowledged the long service and consistent support of the outgoing chair and vice-chair, Rob Ryne of LBNL and Doug Rotman of LLNL, adding "I want to thank Rob and Doug for always being available to help and support NERSC and being excellent representatives of the user community."

In his message to NERSC users, Dean wrote, "I am honored to work over the next three years as the new chair of the NERSC Users Group. Stephane Ethier, the newly elected vice-chair, and I will work to ensure the continued excellence of NERSC computing for the various scientific and computational endeavors of the Office of Science. During the next years, NERSC will likely see an upgraded computational capability. Our main challenges in the coming years will be to work with NERSC staff to ensure a smooth transition to the next major platform at NERSC, to ensure that NERSC continues its key role in providing an excellent national resource for scientific computing, and to ensure that the user community is well represented by the executive committee. We are looking forward to the task. We also want to thank the outgoing chair, Rob Ryne, and vice-chair, Doug Rotman, for their efforts during the last three years."

NERSC News

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NERSC's Storage Strategy Paying Off in Savings

Since relocating to Berkeley Lab almost 10 years ago, one of NERSC's goals has been to consistently introduce new technologies without creating bottlenecks. In a program of planned upgrades to tapes with greater density, the Mass Storage Group has not only achieved this goal, but will save $3.7 million over the course of five years. Over that same time, from 2003 to 2007, the amount of data stored will grow from just over 1 terabyte (TB) to 11.3 TB.

As computational science becomes increasingly data intensive, the need for storage has ballooned. When the NERSC Center moved into the Oakland Scientific Facility in 2000, the archival data were stored on 8,000 tape cartridges. Four years later, the silos housed 35,000 cartridges. While this increase is dramatic, the real growth indicator is that the amount of data stored on each cartridge has also risen by a factor of 10.

It is this planned switch to higher density cartridges that is at the heart of the Mass Storage Group's investment strategy. The strategy of saving money by adopting the latest technology as soon as it is available flies in the face of conventional wisdom, which holds that by waiting for the technology to become pervasive, the price will drop.

Yet NERSC's investment strategy is already paying off, saving an estimated $135,000 in 2004. By 2007, the annual saving is estimated at $2.3 million. In all, the program is expected to save $2,694,754 over five years. Here's how it works.

At the start of the plan, data was stored on a mix of cartridges, each capable of holding either 20 or 60 gigabytes (GB). To keep up with data growth, the group could either stick with the current cartridges — and buy a lot of them — or adopt the newly available 200 GB cartridges. While this switch would also require the center to buy new tape drives to read the denser tapes, the long-term costs showed that higher density meant lower overall costs.

For example, in 2004, data grew by 832,000 TB. Buying enough new lower-density (60 GB) cartridges would have cost $497,952. Switching to the higher-density tapes cost $262,000. Buying new tape drives to read the denser cartridges cost another $100,000, but the strategy resulted in savings of $135,872. In 2005, when the group expects to upgrade to 500 GB cartridges, the estimated savings will be $308,000 — even after accounting for new tape drives.

"It's important to note that these savings only reflect the cost of the tapes," said Nancy Meyer, leader of the Mass Storage Group. "It doesn't include the money saved by not adding more silos or moving other systems to create more adjacent floor space."

Fusion Researchers Use 4,096 Processors to Study Electron Collisions

As NERSC moves to allocate more resources to larger jobs, researchers are making greater use of the opportunity to run on more processors and combine this with NERSC's well-established reliability.

In March, Connor Ballance of Rollins College, a research scientist in a collaborative research effort between Rollins College, Auburn University, and Oak Ridge National Laboratory, undertook a large R-matrix scattering calculation on an iron ion. He used 4,096 processors for a twelve-hour period to calculate a total of 9,591 electron-impact excitations, at hundreds of thousands of electron energies. Such a calculation would be intractable on any machine available to this group other than Seaborg, according to Ballance.

"We simply could not have completed this calculation in a reasonable amount of time." Ballance said.

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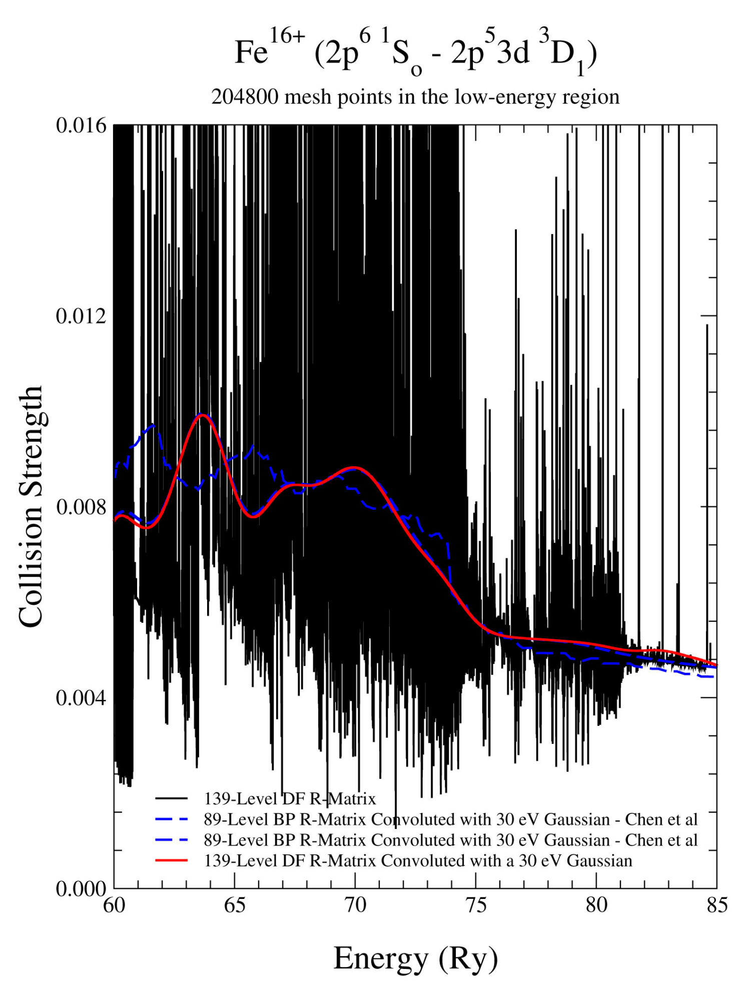
Large-Scale Job Models Electron Collisions (continued from p.1)

From a fusion perspective, this research is important for the design of a fusion reactor. Since reactor walls are made of metal, the intense energy inside the reactor will eject atoms from the walls, and once inside the plasma, collisions of free electrons with these atoms can cause ionization (the removal of bound electrons) and excitation (the promotion of the bound electrons to higher energies). The calculation described here is on a particular iron ion that would be expected to be present, in any fusion devices with steel in the reactor walls.

Metal ions act as impurities in the plasma, which must be heated to extreme temperatures in order to achieve fusion. When electrons in the plasma collide with ions of impurity atoms, there is a certain probability that they will be excited to higher energy states. After excitation, they will relax to lower energy states and emit the excess energy as electromagnetic radiation, primarily in the X-ray region. Such radiation from impurities is the primary energy loss mechanism inside a fusion plasma. If enough energy is lost through X-ray radiation, the plasma will never reach the temperature necessary for fusion to occur. To understand and prevent this, researchers must develop collisional-radiative models based on accurate electron-impact excitation calculations.

However, applications of this research go beyond fusion; it is also directly applicable to the diagnostics of astrophysical plasmas. In the particular iron ion considered in the present calculation, 16 of its 26 electrons have been removed, leaving it in a state that is stable over a relatively wide temperature range. Therefore it is very useful for diagnostics of both fusion and astrophysical plasmas. However, discrepancies exist between the observed intensity ratios of the X-rays emitted from this ion of iron and those determined from previous theoretical calculations. Since these ratios are critical to the determination of density and temperature in both astrophysical and laboratory plasmas, an attempt to understand these discrepancies is quite important.

This particular calculation employed a suite of parallel programs developed primarily at Rollins College for the determination of electron-impact excitation and ionization. They employ a theory referred to as the R-matrix method, which has been used in a variety of serial computer programs and is particularly well suited to systems such as this iron ion in which the probability is dominated by complex resonance structures. These resonances are due to the colliding electron being temporarily captured by the ion, before being re-emitted; they are very narrow in electron energy and must be calculated at many thousands of energies in order to obtain accurate results. The resonance structures can in turn have a pronounced effect on the intensity of emitted X-rays, and this is a possible source of the discrepancy between experiment and theory.



This graph for a particular excitation of this sixteen times ionized species of iron illustrates the complex resonance structure involved in many of the 9,591 excitations studied. It has also been numerically averaged over a wider energy range to more clearly illustrate the enhancement of the probability of excitation due to resonances.

At each electron energy, the calculation took five to 10 minutes, and over the course of the run, each processor on Seaborg calculated results at 50 different energies. The calculation was distributed over processors by energy in order to achieve the best load balance between processors. During the 12-hour run, 204,800 energies were calculated.

"At NERSC, our research group uses the available ScaLAPACK and ESSL libraries to add further performance to our existing codes, and also gets support from the NERSC User Services Group. The NERSC staff provide a robust supercomputing environment," Ballance said. "They have offered advice about I/O issues beyond Seaborg that have proved to also work on our local Beowulf cluster."