

UC SANTA BARBARA engineering and the sciences





California NanoSystems Institute offers High Preformance Computing with the Center for Scientific Computing facility

The demand for high performance computing research has been significantly increasing over the past few years. Various centers have been created in an attempt to address an aspect of this increasing demand, with a select few truly making an impact. The Center for Scientific Computing (CSC) at UCSB is one of these select few. The CSC, located in the California NanoSystems Institute (CNSI), was formed to promote the effective use of High Performance Computing in the research environment. In addition to providing resources, the CSC has incorporated training into their mission as well by sponsoring classes, tutorials, and individual training.

According to Chris Van de Walle, professor of materials, the CSC facility has enabled cutting-edge computations material research, "Having a high-performance computing environment available right here on campus has allowed us to directly impact a number of research projects." One such area of investigation is the effect of impurities on the electronic properties of semiconductors. Using "first-principles calculations", Van de Walle's group found that hydrogen impurities significantly affect the electrical conductivity of semiconducting oxides. "The ability offered by the CSC facility to run large-scale calculations on a number of candidate qubit centers has significantly contributed to our success in this field", concluded Van de Walle.

Eckart Meinburg, professor of mechanical engineering, also recognizes the importance of the CSC, "The CSC provides an excellent test bed facility for developing, validating and executing massively parallel computer codes for flow simulations. In particular, it allows for fine-tuning and optimizing the performance of these codes on



Eckart Meinburg Professor, ME

many processors. For fluid flows exhibiting a large range of temporal and spatial scales, along with complex nonlinear

dynamics, the CSC allows us to perform high-resolution simulations based on first principles, with a minimum of empirical modeling assumptions."



In 2009, 3.5 million hours of computer time were accrued. These figures have already been surpassed in 2010, and are expected to grow dramatically in 2011.

Since CNSI started sponsoring campus High Performance Computing, the program has grown to 300 users, with 50% being graduate students, 25% postdocs, and the remaining 25% split between faculty, visiting researchers, and undergrads.

The CSC is going to be an enabling resource to drive new collaborations between industry and UCSB faculty. The partnership between CNSI and Hewlett-Packard is a perfect example of industry collaboration furthering the mission of CNSI. HP Labs partnered with the CNSI's at UCLA and UCSB to collaborate on research in nanoscience, and provide some funding for HPC infrastructure. These funds enabled the creation of 'condo clusters' where researchers, spanning several departments, collaborate to build larger HPC systems, thus enabling more productive research. The cross disciplinary nature of the center encourages interaction amongst computational researchers in a wide variety of fields, such as Chemistry, Physics, Materials, Engineering, Earth Sciences, Biology, and more. We hope to expand these interactions beyond UCSB and to other industry partners.

To learn more about how your company can work with UC Santa Barbara, contact Leslie Edwards (805-893-3944/edwards@ engineering.ucsb.edu) or Chris Russo (805.893.5544/crusso@ engineering.ucsb.edu) in the Corporate Affiliates Programs Office.