

A reoriented Theory Center: Renewed focus on Cornell research



University Photography

The Cornell Theory Center is located in Frank H.T. Rhodes Hall on Hoy Road.

Sometimes adverse circumstances give rise to promising opportunities. Such was the situation that led to the reinvention of the Cornell Theory Center (CTC) in the winter of 1997. As the sunset of its funding as a National Science Foundation-supported supercomputing center approached, CTC discovered widespread faculty and administration support for maintaining its high-performance computing resources.

At the heart of this support was the recognition that a significant computational science community had grown at Cornell because of the existence of CTC. In fields from drug design to black-hole collisions, from crack formation in materials to quark interactions in subnuclear science, from protein folding to earthquake prediction, the ability to carry out large-scale simulations and to manipulate large amounts of data has revolutionized Cornell research.

Thus, the phase out of CTC as a national center supporting thousands of users across the country coincided with the rebirth of CTC, with a mission to sustain Cornell's prominence in research by providing a high-performance computing environment to advance and facilitate research and education in all areas of computational science and engineering across campus.

Faculty committees and CTC members

CTC has a new faculty executive committee to advise center Director Thomas F. Coleman on direction and opportunities. The members are Susan Holmes (biometrics), Tony Ingraffea (civil and environmental engineering), David Shalloway (biochemistry, molecular and cell biology), Steven Tanksley (plant breeding) and Saul Teukolsky (physics). An allocations committee chaired by Paulette Clancy (chemical engineering) meets monthly to review proposals for time on the supercomputer, a 160-processor IBM RS/6000 POWERparallel System (SP). A broader faculty advisory committee will meet twice a year to review CTC progress and to give input to the executive committee.

CTC invites faculty to become CTC members. Currently, more than 150 faculty are considered to be members of the center. These faculty are either users of the SP or have expressed interest in becoming involved in CTC programs. CTC has created a new "Members" page on its web site <http://www.tc.cornell.edu/> to provide timely information.

Interdisciplinary emphasis

CTC's director is already strengthening the interdisciplinary nature of the center. Coleman is himself a computer scientist who applies his algorithmic research to a variety of scientific and engineering fields.

"The cross-fertilization of ideas and techniques that results from interdisciplinary research is a proven approach to achieving advances in computational science and engineering," said Coleman. "Over the next year we will pursue a number of large-scale collaborations that eliminate departmental walls."

Examples of such projects include computational finance -- an initiative in which Coleman is directly involved -- computational genomics and high-temperature systems and materials.

As new federal initiatives, such as NSF's recently announced Knowledge and Distributed Information program, become available, CTC encourages faculty to meet with CTC staff to discuss how a collaboration with the center might strengthen proposals.

"CTC is offering to coordinate, write and edit large-scale interdisciplinary proposals, develop budgets and provide administrative assistance to faculty," said Linda Callahan, CTC associate director. To qualify for such assistance, she said, projects should include a strong computational component and be submitted through CTC. In addition to SP access, CTC can contribute expertise in a number of areas, such as visualization (including virtual reality), parallelization and optimization of codes, algorithm development, web-based science communication and development of complex web sites. Callahan, at cal@tc.cornell.edu, is the initial contact person for faculty interested in exploring proposal collaborations.

Education in high-performance computing

CTC offers help to faculty interested in integrating high-performance computing into the classroom in two ways. First, CTC offers education accounts (<http://www.tc.cornell.edu/Edu/CTC/EduAccts.html>) for courses in which students can benefit from access to the SP. Second, CTC has developed a virtual workshop for training in high-performance computing that is entirely web-based. The framework of this self-paced, modular workshop can be adapted to web-assisted classes and for distance learning courses. An innovative companion to the virtual workshop is an interface that uses point-and-click features to run programs on the SP.

"The interface is appropriate for faculty who do not necessarily want to teach students how to program for the SP," said Callahan, "but who want to take advantage of the SP's capabilities to allow students to run simulations."

A virtual workshop covering "Introduction to High-Performance Computing at CTC" will be offered this summer, beginning July 6. The Cornell community is invited to register for this free workshop, which is intended to get new users started computing on the SP. Information is available at <http://www.tc.cornell.edu/Edu/VW/Summer98/>. This introduction will be followed in the fall by an "Introduction to Parallel Computing on the SP."

Smart Node infrastructure

Because of CTC's experience operating a national supercomputing center, the organization is able to adapt successful programs to benefit Cornell. An example is CTC's Smart Node program, which will be launched this spring.

"Our goal is to create closer integration of CTC into departments, centers and colleges," said Dan Dwyer, Smart Node coordinator. "Campus Smart Nodes will provide information about CTC and will be able to allocate training and small research accounts on the SP."

Each Smart Node will have a consultant designated by the department or center. CTC plans to provide training in high-performance computing to the Smart Node consultants so that they can then provide consulting to their community of users. Regular meetings between CTC staff and Smart Node consultants will provide an information channel to get news and updates dispersed quickly. An organizational meeting for the Smart Nodes will be held on May 11.

Increased corporate emphasis

The new CTC will move to an operating model where approximately 25 percent of its computing resources are dedicated to corporate partners, with an emphasis on New York state-based companies. In addition to providing CTC with additional funds, the center's Corporate Partnership Program (CPP) "helps us fulfill our mission of applying our expertise in high-performance computing, visualization and computational algorithms and methodologies to large-scale problems," said Jay Blaire, CTC deputy director. "Understanding and applying parallel applications to real-world problems will benefit not only our corporate partners, but also Cornell's research environment."

According to Blaire, CTC has successfully retained its CPP membership, expanded current partnerships and added new clients. Among the latter are Abbott Laboratories, Algorithmics, Nichols Research and IBM Japan.

New opportunities

The rebirth of the Cornell Theory Center presents opportunities for faculty who have not previously used high-performance computing to become familiarized with how these capabilities can be applied to new research fields.

Said Coleman, "We encourage faculty to take advantage of the Theory Center's new orientation. We have the infrastructure, the expertise and the commitment to make computational science and engineering flourish at Cornell through the next decade."

At the heart of CTC's resources is the 160-processor IBM RS/6000 POWERparallel System. Now is a good time for Cornell faculty to apply for time on the system, since remaining national users will be phased out this spring. For information on applying for an allocation, see <http://www.tc.cornell.edu/Allocations/>.

To help inaugurate the next decade of computational science and engineering, the university will host a symposium and reception on Sept. 1 to showcase leading-edge research in a variety of fields. The public is invited.

Recaping upcoming CTC events:

May 11: Smart Node organizational meeting

July 5: Virtual Workshop: Introduction to High Performance Computing at CTC

Sept. 1: Symposium and reception

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