From the Staff

Computing Technology Update

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Frank Labonte, designer and builder of FEYNMAN, the next generation supercomputer, with his creation.

Overview: The rapid evolution of computer technology has affected all those who use it. Institutions everywhere are struggling to keep up as their machines and infrastructure decay into obsolescence. At CHESS and MacCHESS we have implemented several ambitious initiatives to propel us to the forefront of computer technology. Our HP 700s, the heart of each station's data acquisition and systems control, were overwhelmed by the demands of modern beam lines and in desperate need of upgrade. Replacements that could handle the current workload, yet allow growing room, were clearly needed. We also opted for large RAID arrays and supercomputers to handle storage and processing of the enormous volumes of data generated by our detectors. Many network infrastructure upgrades were also required to enable us to seamlessly transfer data from place to place. Additionally, we have upgraded much of our software to complement the new hardware, and, in several instances, enhanced it or developed our own software to meet our requirements.

New CHESS Station Computers: The old HP 700s ran the SPEC software package from Certified Scientific Software. SPEC provides the basic movement and data collection functions as well as a versatile macro language for defining complex scans and other data collection procedures. To address the HP's shortcomings, we replaced them with modern Linux PC's. These computers are based on a dual AMD Athlon processor configuration and run the latest version of the Red Hat operating system. These computers will provide the computing power, storage, and software compatibility needed to enhance data collection, visualization, and processing. These systems interface with PCI, CAMAC, VME, RS-232, and USB devices, and have the option of USB 2.0 and Firewire (IEEE 1394) support.

Backside view of the next generation supercomputer.

MacCHESS Super Computer: Data processing in crystallography is an extremely difficult task. The experimental process frequently yields many gigabytes of complex data, overwhelming ordinary desktop computers. MacCHESS opted for a Linux cluster to deal with this issue, the prototype for which was SIRIUS. SIRIUS is based on 64 1.2 GHz Athlon MP processors and Myrinet two Gbit/sec high-speed low latency networking. SIRIUS has been a tremendous success, posting some remarkable benchmarks. Users are now competing for computing time and our design has been cloned by other institutions in order to satisfy their computing needs. This success has spurred the design of a second, even more powerful machine. This next generation supercomputer, which is already under development and has been dubbed FEYNMAN, will have twice the number of processors as SIRIUS, more than twice the memory and even faster networking. Furthermore, each CPU will be 600 MHz faster than those of SIRIUS. For data storage, four 2.0 Terabyte RAID arrays were constructed and all of these systems are linked together via Gigabit networking.

In developing appropriate software for use with SIRIUS, MacCHESS scientists ported several key software packages to function in its highly parallel environment. Structure phasing codes such as FSEARCH and SnB are already in use and other packages such as webXDS and DPS, which are used for data reduction, are under development. Other codes such as SHELXL are also being considered for parallel development. On the CHESS side, software such as SPEC 5, IDL, MatLab, TV6/TVX and SimPA are in use or under development.