

The Scientific Computing Resource (SCR) at SCSBMB was begun in January 2012 to fill a growing need for scientific hardware and software support on which all scientific research increasingly relies. The majority of modern scientific IT applications are Unix based, and are usually written by research groups at other Universities and Institutes. While these applications are provided free, they come with little or no support. They are often difficult to install and run without significant special knowledge of the software and hardware on which it is run. The scientific computation resource provides this expertise so each individual research group does not have to hire a scientific IT specialist of their own. There is no other support for Unix based software, or scientific software on campus at UTMB.

### **General Request Policy**

Any Sealy Center member or UTMB campus research group with an ongoing funded research program may request help from the Scientific Computing Resource. Initial requests must come from a research project's PI and are directed to the SCR managers. The managers then assign the projects to staff members based on expertise and availability. Once the project's needs and scope have been evaluated and assigned, individual researchers work directly with SCR staff members as the ongoing project's course requires.

Many research projects require collaboration between UTMB researchers and those from other Universities and Institutes. The SCR accepts requests for help with any such collaborations, such as porting applications to or from UTMB, as projects require.

The SCR also initiates and accepts ongoing direct collaborations with other Institutions where a need for expertise is warranted.

Requests for help will generally fall into the following categories:

#### **1) Research Group Owned Scientific Computational Hardware**

For researchers who have the need to purchase scientific computing platforms for their labs, the SCR offers help for all stages of this process, from helping to choose the appropriate hardware configuration for a given application, to negotiating a good price with a vendor. When a new system arrives we offer operating systems installation and configuration. We also offer ongoing support, hardware upgrades, component failure replacements, OS upgrades, and the setting up of cost effective backup systems.

#### **2) Research Group Scientific Software Installations**

For researchers who require scientific software on their own equipment the SCR offers installation, setup and initial usage training. Since this is our area of expertise, we can also offer advice as to which of several choices may be optimal for a given research project. Since new applications are being released regularly we are able and willing to install these applications for evaluation purposes. No applications will be installed on any equipment unless proper licensing requirements have been met.

#### **3) Use of the SCR Development Cluster**

The SCR has just deployed a small cluster designed as a staging, development and software testing platform for new software applications. It is a heterogeneous cluster with two types of GPUs installed to allow for the porting of existing codes to take advantage of the speed and multiparallel aspects of leading edge GPU systems. This cluster is not designed to run long computational projects, but rather to develop codes and scripting systems to ultimately be ported to larger computing platforms, but ongoing production jobs will be allowed as availability of the cluster permits. Short projects and test projects that are not worth the effort of porting to larger machines will be allowed, again as availability permits. Restrictions on job submissions, including but not limited to resource allocation, CPU and GPU time limits and number of jobs submitted are adjusted and enforced to optimize project completion as well as to promote fair use among multiple users.

For long computational projects the SCR, whose members have over 20 years of experience in High Performance Computing, works as the liaison between the research group and the computing center, e.g., the Texas Advanced Computing Center (TACC), whose resources are available to faculty and staff at UT System institutions. The SCR provides support in identifying the appropriate resource for the project, helps with the allocation process and allocation management, transfer of data to and from the computing center, and, if needed, installation of project specific software on the computing resource.

#### **4) Use of the SCR JBOD**

The SCR has recently deployed a scalable expandable disk storage JBOD primarily for the support of large data producing projects such as those associated with the SCSBMB CryoEM resource. While it is primarily for Center use, there will be ongoing research projects that require a large amount of available storage for a fixed time period. Requests to house large data sets temporarily will be honored as space permits. For long term storage needs the SCR is willing to expand the JBOD to accommodate the need. Most projects would simply need to buy the number of hard disk drives necessary to house their data and the SCR will create a contiguous file space for the project and make it available across the network.

#### **5) Use of SCR Scientific Software**

The SCR has a large and continuously expanding list of scientific software titles available on SCR owned servers, workstations and the development cluster. The SCR administers all SCSBMB paid-for titles. The SCSBMB is the UTMB campus license holder for the Mathematica program (Unix, Windows, and MAC). The center also holds a 6 seat license for MATHLAB which includes the Bioinformatics and Statistics toolboxes, Amber, and Imagic that are available to all SCSBMB researchers on both the SCSBMB compute resources as well as the compute resources in the individual PIs' labs. Requests to use the software, or to add to the titles will be accepted as resources permit. No titles will be installed on SCR equipment unless proper licensing requirements have been met. The following is a list of specialty titles currently available: EMAN, EMAN2, Spider, Direx, Haddock, ARIA, CCPNMR, NMR Pipe, Phenix, O, COOT, CNS, CCP4, DINO, XDS, DPS, Chimera, VMD, NAMD, APBS, Modeller, PyMol, 3DNA, MPSA

#### **6) Use of the SCR 3D-Printing Facility**

The SCR has deployed a 3D-Printing facility with two printers, a 3D-Systems Projet 660Pro and a Makerbot Replicator 2X. The Projet is a powder core epoxy system and is capable of full color printing with a resolution of 300dpi. It has a print volume of 10x15x8 inches. The Replicator is a two

color plastic extrusion system capable of printing in both ABS and PLA filaments and has a print volume of 10x6x6 inches. Requests for printing by on campus users are accepted but researchers should be advised that we may need significant lead time in order to get the model built. Currently we recommend models be requested at least a week in advance.

The SCR will accept requests from collaborators at other research institutions but researchers should be advised that the raw materials for 3D printing are expensive and if a large amount of printing is required they should be prepared to replace the materials used on their behalf.

To utilize the services/resources above, contact: for hardware: John Perkyns, [jperkyn@utmb.edu](mailto:jperkyn@utmb.edu); and for software, Gillian Lynch, [gclynch@utmb.edu](mailto:gclynch@utmb.edu).