Institute for Advanced Computational Science (IACS) at Stony Brook University

The Institute for Advanced Computational Science at Stony Brook University was established in 2012 with a $20M private endowment. With a core of thirteen faculty in a variety of computational disciplines (chemistry, materials, atmospheric science, geoscience, social science, applied mathematics, and computer science), the institute will grow to circa 20 faculty including at least two new endowed chairs. The institute seeks to make sustained advances in the fundamental techniques of data, computation and in high-impact applications.

Our state-of-the-art new facility is located next to the Laufer Center for Physical and Quantitative Biology. This new space houses the institute's faculty, students/postdocs (circa 45), and technical/administrative staff. There is 10Gigabit networking throughout the building (optical fiber within the building to major hubs across campus). The institute provides to its members' office space, office materials and supplies, administrative support, commonly used software packages including select compilers and libraries, technical assistance with computer administration and software installation, and use of the institute's computer clusters.

IACS Cluster: The initial IACS high-performance cluster HANDY includes 40 compute nodes (each with dual socket 2.6 GHz Xeon E5-2670 processors, 16 cores per node, and 128 GB of memory), and two high-performance file servers direct attached to a total of 350 TB of storage. In addition, there are two "fat" nodes configured with more memory (256 GB) to support data analysis and software development.

Stony Brook University Research Computing Clusters: A second high-performance cluster (**LIred**) is a **100 TFLOP/s** Cray cluster outfitted with 100 compute nodes each with two Intel Xeon E5-2690v3 CPUs. These Intel CPUs offer 12 cores each, and operate at a base speed of 2.6 Gigahertz. The system also highlights a large memory node that spotlights 3 TB of DDR4 RAM and 4 Intel E7-8870v3 processors with 18 cores each operating at 2.1 Gigahertz, for a total of 72 cores and 144 threads (via Hyper-Threading). Additionally, the system also includes a login node and a management node. A third cluster (**SeaWulf**) was installed in fall 2016. The SeaWulf system was purchased by IACS as a result of a Major Research Instrumentation grant from the National Science Foundation and is a 4,592 core cluster consisting of 164 compute nodes with a peak performance of **~240 TFLOP/s**. Each node is equipped with 128 gigabytes of memory and interconnected via a 40 Gbps network link. Eight of the compute nodes are GPU nodes, with 32 Nvidia K80 GPUs. The 40 Gbps interconnects also attach the nodes to a Petabyte shared storage array running the GPFS file system.

The LI-red and SeaWulf clusters are managed as a single logical high-performance cluster to provide a seamless user experience for Stony Brook researchers. In April of 2019, the SeaWulf cluster was further expanded via the purchase of 64 compute nodes each with two Intel Xeon Gold 6148 CPUs with 20 cores each that operate at a base speed of 2.4 Ghz and have 192 GB of RAM. This upgrade adds **196 TFLOP/s**. **In total**, the Stony Brook University computing clusters include 328 nodes and 9,552 cores, with a peak performance of ~ **536 TFLOP/s** available for research computation. The cluster is available for use by all Stony Brook University faculty and students.

Ookami, the newest of the Stony Brook computing clusters, is one of the first computers outside of Japan to be powered by the HPE Apollo 80 system, which was originally developed by Cray and Fujitsu, and uses the Fujitsu A64FX processor, the same processor technology as the fastest and most power efficient supercomputer in the world, the Fugaku system at the RIKEN Center for Computational Science, in Japan.

The ARM-based processor includes multiple innovations integrated with very fast, low-latency memory that together make it easier for science and engineering applications to reach both high performance and

high power efficiency, therefore “greener” technology. Ookami is made up of 176 compute nodes with 48 cores each, for a total of 8,448 cores, and it is coupled with a petabyte of Lustre shared storage.

Networking at SBU is provided by a redundant 100 Gigabit connection to Internet2, connecting to ESNET, as well as Amazon, Microsoft, & Google, at 100 Gigabits/sec at 32 Avenue of the Americas in New York City. The Campus Data Center and the campus network operations center are connected via single-mode fiber, with 2 links providing redundant connectivity at not less than 40 Gbit/s with 100 Gbit/s in the campus network plan. Cybersecurity is provided through a layered approach, including a high-availability pair of firewalls that can support up to 40 Gigabits/sec.