[Template for Duke Compute Cluster. If this template is used for a grant, please consult with Duke Research Computing so that assurances and descriptions put forth in this document are well suited for the research you intend to conduct. Duke Research Computing can in many cases also provide a letter of support to explain commitments and suitability of the computational/storage infrastructure for your research. Contact rescomputing@duke.edu.

This template includes information on Duke Research Computing and on the Duke Compute Cluster.

Revised 18 September 2018; https://rc.duke.edu/grant-resources/]

Duke Research Computing

The success of today's research depends on a computational infrastructure that provides essential computational services while at the same time meeting ever evolving demands of changing technology. Duke offers researchers centralized “core” resources for computing that meet the great majority of researchers’ computing needs. These services are developed, managed, and offered by Duke Research Computing, a group reporting to the Office of the Provost and to the University's Office of Information Technology and charged with providing useful research computing services that take best advantage of current information technology. Because the services are shared across the University, wasted expense on redundant, poorly managed, or ill-fit computer technology has been cut to a minimum. Researchers can spend more time conducting research and less time fretting about computational infrastructure.

Duke Compute Cluster

The Duke Compute Cluster consists of machines that the University has provided for community use and that researchers have purchased to conduct their research. At present, the cluster consists of nearly 12,000 CPU-cores comprised mostly of Cisco Systems UCS blades as well as host machines for GPUs. The cluster itself is a project of the University community, with the hardware provided by individual researchers and the University. The University, through Duke Research Computing and the Office of Information Technology, maintains and administers the equipment for its useful life (designated to be four years) and provides support for cluster users. As a result of the incremental purchases, the cluster is heterogenous, with a narrow range of Intel chipsets and RAM capacities, though purchases of equipment are organized and channeled by Duke Research Computing in order to ease maintenance and exploit economies of scale. New nodes have 768 GB of RAM and 36 CPU-cores under a “standard” configuration; the oldest machines are configured with 256 GB RAM and 24 CPU-cores. The cluster does have a small number of large memory machines (up to 2 TB RAM) that are used for certain memory-hungry processes. Recent additions to the cluster have favored GPU-accelerated machines, and the cluster has an array of Nvidia GPU devices including V100, P100, K80, TitanXP, and GTX1080 cards. The features of these GPU devices differ, and some are better suited than others for certain tasks. Of the nearly 100 GPUs on the cluster, over half have been supplied by researchers with intensive computational requirements. A "gpu-common" partition on the cluster is available to all users.

The University has provided high performance data storage to serve as "scratch" space for data under analysis. This storage volume has a 500 TB capacity. To increase speed and efficiency of the storage, a large SSD installation provides data caching. Also available to mount on the cluster is capacity from the Duke Data Commons, a large 1.5 PB storage installation made available to all Duke researchers. This installation was begun in 2014 and targeted NIH-sponsored researchers and researchers using several molecular-data-producing and light microscopy cores. The Duke Data Commons was initiated by an NIH S10 grant (1S10OD018164-01), and the University has continued to offer the service with newly purchased equipment.
Researchers who have provided equipment have “high priority” access to their nodes and have “low priority” (or “common”) access to others' nodes, including those purchased by the University, when idle cycles are available. Since researchers tend not to use 100 percent of the CPU of nodes they have purchased, “low priority” consumption of cycles greatly increases the efficiency of the cluster overall, while also providing all users the benefit of being able to access more than their own nodes' cycles when they might need it. Jobs submitted with high priority run only on the nodes that members have bought, and low priority jobs on the machines yield to high priority jobs. Additional flexibility is afforded the entire system because of the use of VMWare ESX hypervisors on all machines. This system allows for the dynamic moving of computing jobs, resizing of machines, flexibility during maintenance and repair, and even the use of different operating systems or presentation of machines to different networks.

The Duke Compute Cluster is a general purpose high performance/high-throughput installation, and it is fitted with software used for a broad array of scientific projects. For the most part, applications on the cluster are Free and Open Source Software (FOSS), though some researchers have arranged for proprietary licenses for software they use on the cluster. The operating system and software installation and configuration is standard across all nodes (barring license restrictions), with Red Hat Enterprise Linux 7 the operating system (with the move taking place in January 2017). SLURM is the scheduler for the entire system. The entire system is professional managed by systems administrators in the Office of Information Technology and the equipment is housed in enterprise-grade data centers on Duke's West Campus. Software installations and user support, including training on using the system, is provided by experienced staff of Duke Research Computing.

The great advantage of cluster computing is that many CPUs can be put on task in parallel. A task that can be broken up into discrete tasks and run simultaneously on many machines completes much more quickly than if the large task was run serially on a single machine. Thus, months of computational work can be completed in a couple of days – or even hours – on a cluster. Computation times can be brought down by orders of magnitude, and that advantage of cluster computing will greatly speed progress on the proposed project.