Resource Allocation Policy

Center for Research Computing
University of Notre Dame

Updated For Academic Year: 2023-2024

1. **Introduction**

   This document provides guidance for preparing requests to use Notre Dame's research computing resources at the Center for Research Computing (CRC). All interested persons are encouraged to review this guide prior to making requests; questions regarding these policies should be directed to CRC User Support (crcsupport@nd.edu). Additional information about the CRC and other services provided are located on the CRC website.

   The CRC has finite centrally funded resources to leverage either in cooperation with funded projects or in support of Notre Dame's priority unfunded projects. Separate mechanisms exist for the provisioning of different resources. Allocation requests exceeding available 'fair share' resources will be met through the annually approved CRC charge models. Examples of 'fair share' resources and those provided in conjunction with the charge model follow:

   - Example no cost 'fair share' resources:
     o CRC general access compute cycles where job priority is based on consumption
     o One day of support profiling user code for runtime performance
     o Consulting on hardware/software for unique computational requirements
     o Software infrastructure design and planning consultations
   - Example charge model 'dedicated' resources:
     o Hardware acquisition and operation for dedicated use by an individual faculty member
     o One year of scientific software or web portal development services
     o Data formatting for geospatial analysis
     o Data visualization and analytics support

   Recharge services are provided based on a service level agreement (SLA) between a project principal investigator and the CRC. An SLA defines the scope of work, time, and cost. The CRC uses hourly charging fees, which are approved every June for the next fiscal year.

2. **CRC Resources**

   The CRC makes available a set of cyberinfrastructure resources for allocation. In general, these resources can be categorized into computational, storage, specialized, and advanced user support resources. The following bullet summary and narrative for inclusion in grant proposals will be updated annually with this policy.

   Bullet Summary of Resources

- Computational resources are typically HPC systems oriented toward batch job submission. The CRC manages ~45,000 CPU cores in systems of various architectures and interconnects.
- Storage resources (~4,000TB) including disk based systems for medium term storage of data and tape based systems for backup storage.
- Specialized resources include dedicated GPU systems, systems for virtual hosting, large memory systems and high-throughput HTCondor pools.
- Access and interface to ACCESS and Open Science Grid (OSG) resources
- Advanced User Support
  - Software Development and Profiling.
  - System Administration/Design and Acquisition.
  - Cyberinfrastructure/eScience Portal and Gateway Development.
  - Collaborative Research/Grant Development.
  - Machine Learning and GenAI Algorithm Development and Implementation Support.

Narrative of CRC Resources for Insertion into Grant Proposals

The CRC operates a state of the art High Performance Computing (HPC) facility providing advanced computing support to researchers within Notre Dame, the local community, and industry. The facility is highly secure and reliable and can be accessed securely and seamlessly. The CRC systems have a wide range of software, including applications for: Computational Chemistry, CFD & Engineering, Climate Modeling & Earth Systems, Computational Physics, Computational Social Sciences, Bioinformatics, Statistics, and Mathematical Modeling. This diverse portfolio enables CRC to address the needs of faculty, students and other customers in new or unique areas of research and development.

The HPC team manages parallel supercomputers, clusters, grid networks and storage (around 45,000 cores and 4,000 TB of storage) which provide exceptional levels of processing speed and power compared to desktop and monolithic mainframe systems. Any task which can be most effectively resolved by segmenting the problem into a number of parallel tasks can be efficiently carried out by a CRC cluster. HPC systems at the CRC are highly optimized to ensure maximum performance. At present there are more than 2,000 researchers from the University of Notre Dame making use of the CRC's resources for calculation-intensive tasks.

The CRC has extensive experience in designing, purchasing and managing HPC solutions for operations ranging from small to large scale and offers assistance to users who wish to integrate HPC into their current operations. The CRC conducts a full requirements analysis to determine areas that may benefit from HPC and to improve current in-house processes around the management and use of compute servers.

The CRC is the perfect partner for any scientific or technically-focused software project; with broad software development experience across a wide range of research areas, and technologies. Accomplished software developers (around 20), and domain experts and computational scientists (around 10); including proficient mathematicians, scientists, engineers and designers, can design parallel software tailored to research needs. The CRC values open standards, maintainability, extensibility and agile development with continual client feedback and thorough

testing. For maximum utility, software is supported by comprehensive documentation, sample data, tutorials and training.

The CRC also hosts specialized teams of technical subject matter experts in the areas of visualization, interactive collaborative environments (eScience and gateway development), data integration and management, and geographical information systems. The teams function in active collaboration with new and ongoing research projects supported or enabled through the use of developing cyberinfrastructure technologies.

4. **Requests and Allocation Policies for Specific Resources**

PIs should submit requests for allocations of those resources identified above to crcsupport@nd.edu. Individual policies detailing the allocation of specific resources are posted on the CRC website. Current individual policies for the 2024 academic year include: Software, Storage, Cluster Partnership Program, and Virtual Machines.

5. **Guest Collaborator Accounts**

Full-time ND faculty can sponsor non-ND guest collaborator accounts for research collaborators with whom they are actively pursuing co-authored and/or co-funded research. Non-ND accounts must be renewed annually and may have full access to resources funded/owned by the faculty sponsor. Access to all other shared campus computational resources will be on a limited and lowest priority basis as resource availability dictates.

6. **Acknowledging Support**

An acknowledgement of support from the CRC and the University of Notre Dame should appear in any publication of material, whether copyrighted or not, that describes work which benefited from access to CRC cyberinfrastructure resources.

PIs should include a bibliography of articles or other manuscripts —*published, accepted, submitted or in preparation*— that benefited from support by CRC resources as part of their annual reports. The following statement should be placed in the acknowledgments section or in the footnote of each paper:

> "This research was supported in part by the Notre Dame's Center for Research Computing through [CRC resources]. We specifically acknowledge the assistance of [relevant CRC staff members' names]"