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Rosen Center for Advanced Computing: Facilities, Equipment, and Resources

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The RCAC (Rosen Center for Advanced Computing, http://www.rcac.purdue.edu) is the research computing arm of the Information Technology at Purdue (ITaP), the University’s central IT organization. RCAC provides a large and diverse set of computation and data resources, high-speed networks, and to researchers at Purdue and elsewhere. It also provides resources, services, and support, such as science gateways, through partnership with national cyberinfrastructure such as the XSEDE (formerly TeraGrid) and the Open Science Grid to researchers nationwide.

RCAC offers a broad range of technical support services to researchers, including user support, consulting, training, and documentation; software installation; program design and optimization; large-scale data management; distributed computing; capacity planning and cluster deployment. RCAC researchers and software engineers also collaborate with faculty and students in creating solutions and tools through software development, integration and hosting services. The RCAC staff are provided with office space at Young Hall, Purdue University.

The paragraphs below provide additional details of the Purdue centrally supported research computing resources.

**Computing and Data Resources**

Purdue’s RCAC operates several large, state-of-the-art computing clusters as well as data storage and other resources to serve the research and education community at Purdue campuses and nationwide. These systems support scientific computation and data analysis in many research domains ranging from science, engineering and social sciences. The RCAC operated systems include:

**High-performance computing:**

- **Halstead cluster:** This is the newest community cluster to be deployed in December 2016. This system will consist of approximately 400 nodes at the initial installation with more nodes to be added according to demand. Each node has two 10-core Intel Xeon E5 processor (20 cores total per node) and 128 GB memory. All nodes will be connected through the EDR Infiniband interconnect and to a Lustre parallel file system built on Data Direct Networks' SFA12KX EXAScaler storage platform. This cluster will be in operation from 2016 through December 2021.

- **Rice cluster:** the newest community cluster at Purdue, Rice was built through a partnership with HP and Intel in April 2015. Rice consists of HP compute nodes with two 10-core Intel Xeon-E5 processors (20 cores per node) and 64 GB of memory. Rice has a total of 13,200 processor cores, and in testing, clocked in with a sustained, measured maximum speed of 407.1 teraflops and a peak performance of 549.1 teraflops. All nodes have Mellanox 56 Gb FDR Infiniband interconnect and a Lustre parallel file system built on Data Direct Networks' SFA12KX EXAScaler storage platform. The cluster has a five-year warranty.

- **Snyder cluster:** one of the systems in the latest community cluster build, Snyder is a big-memory system optimized for data intensive applications requiring large amounts of shared memory per node, such as life sciences. Snyder consists of HP compute nodes with two 10-core Intel Xeon-E5 processors (20 cores per node) and 256 GB of memory. All nodes have 40 Gbps Ethernet connections.

- **Conte cluster:** Conte, deployed in Oct. 28, 2013, is the newest campus HPC cluster at Purdue. Developed in a collaboration with HP, Intel, and Mellanox, Conte consists of 580 HP ProLiant SL250 Generation 8 (Gen8) servers, each with two Intel Xeon processors and two Intel Xeon Phi
Coprocessors (for a total of 77,520 processor cores), integrated with Mellanox 56Gb/S FDR InfiniBand. In testing, Conte clocked in with a sustained, measured maximum speed of 943.38 teraflops and a peak performance of 1.342 petaflops. In testing, Conte clocked in with a sustained, measured maximum speed of 943.38 teraflops and a peak performance of 1.342 petaflops, placing it 28th in the June 2013 Top500.org list of international supercomputers.

- **Carter cluster**: Carter was built in partnership with Intel in November 2011. Carter primarily consists of HP compute nodes with two 8-core Intel Xeon-E5 processors (16 cores per node), either 32 GB or 64 GB of memory, and a 500 GB system disk. A few NVIDIA GPU-accelerated nodes are also available. All nodes have 56 Gbps FDR Infiniband connections. Carter ranked 54th on the November 2011 TOP500 list of the world's most powerful supercomputers and was among the half dozen most powerful machines at U.S. academic institutions.

- **Hammer cluster**: Also part of latest new build, Hammer is a high-throughput system optimized for scientific applications running loosely-coupled computation tasks. Hammer was initially built through a partnership with HP and Intel in April 2015, consisting of HP DL60 compute nodes with two 10-core Intel Xeon-E5 processors (20 cores per node) and 64 GB of memory. All nodes have 10 Gbps Ethernet connections. The number of nodes in Hammer will be expanded annually.

- **Purdue HTCondor Pool**: A production distributed computing system that provides opportunistic computing cycles to users. Linking computers in the Purdue community clusters, labs, desktops around the campus, as well as distributed resources at partner institutions (diagrid.org), this resource utilizes the HTCondor (http://research.cs.wisc.edu/htcondor/) job management system to run computation codes on the otherwise idle computers. The Purdue HTCondor pool can provide a large quantity of cycles for researchers who need to run thousands of short computation jobs within a short period of time (aka high-throughput computing). Purdue’s HTCondor pool is the largest academic pool in the world and has more than 40,000 processor cores to date with an aggregate peak performance of 170 teraflops.

- **Scholar cluster**: The Scholar cluster is open to Purdue instructors from any field whose classes include assignments that could make use of supercomputing, from high-end graphics rendering and weather modeling to simulating millions of molecules and exploring masses of data to understand the dynamics of social networks. The hardware of Scholar consists of HP compute nodes with two 8-core Intel Xeon-E5 processors (16 cores per node), 32 GB of memory, and a 500 GB system disk. All nodes have 56 Gbps FDR Infiniband connections.

- **Diagrid.org**: DiaGrid.org is a web-based system that delivers computation and data resources to scientists via a web browser. Built on the HUBzero™ Scientific Collaboration Platform software package, DiaGrid.org provides “Science-as-a-Service”, online applications delivered to user’s web browser with graphical user interfaces while accessing large-scale computing and data resources behind the scene. It is also an open platform for researchers and students to share their own scientific applications following a do-it-yourself process. Current applications on DiaGrid include tools for bioinformatics, molecular dynamics, structural biology, climate modeling, and statistical analysis and parameter sweeps using R language. DiaGrid.org also provides many social networking capabilities built for research and learning, including projects, groups, discussion forums, review, tagging, citation, and so on.

- **Hathi Hadoop Cluster**: Hathi is a Hadoop cluster deployed in September 2014. Hathi consists of six Dell compute nodes with two Intel E5-2650v2 CPUs, 64 GB of memory, and 48TB of local storage per node for a total cluster capacity of 288 terabytes. All nodes have 40 Gigabit Ethernet interconnects. Hathi has two main components: the Hadoop Distributed File System (HDFS) and a MapReduce framework for job and task tracking. A number of open source software for Hadoop are supported, including the Apache Pig for large data analysis, the Apache Hive data warehouse software for querying and managing large datasets in distributed storage, the Apache HBase for distributed, non-
relational databases, and the Apache Spark for in-memory computation of large data analytics work, especially well-suited for machine learning algorithms and similar tasks.

**Network connectivity**

All Purdue clusters and storage systems are connected with redundant 160 Gigabits per second (Gbps) Ethernet links to the research network core. The campus systems’ wide-area connection to the Indiana GigaPOP and major research networks including XSEDE, OmniPOP, and ESNET is 100 Gbps.

**Data Storage and Collections**

Purdue operates and maintains a multi-tier storage system to meet the needs of researchers conducting computation, data analysis, data management and sharing, and data archiving.

- **Research Data Depot:** The Data Depot is a high-capacity, fast, reliable and secure data storage service designed, configured and operated for the needs of Purdue researchers in any field and shareable with both on-campus and off-campus collaborators. The Data Depot uses an enterprise-class GPFS storage solution with an initial total capacity of over 2 PB and will continue to expand to meet growing demands. This storage is non-purging, redundant and reliable, features regular snapshots, and is accessible from all Purdue research systems. Built on Data Direct Networks' SFA12k storage platform, the Data Depot has redundant storage arrays in multiple campus datacenters for maximum availability. Multiple data transfer methods are supported, including SCP/SFTP, CIFS/SMB (as Windows drive), and Globus data transfer for fast and easy unattended transmission of large amounts of data between local systems or to/from national resources and labs.

- **Scratch Storage:** Each computing cluster has a default Lustre parallel file system to provide work-area storage optimized for a wide variety of job types, and are designed to perform well with data-intensive computations, while scaling well to large numbers of simultaneous connections. Scratch storage currently consists of 1.9PB of redundant, high-availability disk space. All scratch tier resources are high-performance, large capacity, and subject to scheduled purging of old files.

- **Home storage:** Designed for use by individual researchers to hold files permanently. It is being served from the DDN GPFS appliance and uses a quota system for space management. Snapshots of user data are regularly taken and accessible from all Purdue research systems.

- **Archive storage:** The Fortress Archive (HPSS) system is a large, long-term, multi-tiered file caching and storage system utilizing both online disk and robotic tape drives. This archival system consists of 400 TB of disk cache, 1.2 TB of SSD for file metadata storage, and two tape libraries currently totaling 11PB in storage capacity which can be expanded to provide additional archival storage according to user demands.

- RCAC also supports various scientific data collections, including real-time satellite images, multispectral and hyperspectral remote sensing data, real-time Doppler radar data, climate simulation data, and social science data (e.g., Wikipedia data), stored in distributed data repositories and managed and accessed via web and command interfaces.

- **Globus data transfer:** Data transfer and sharing

**Visualization and Graphics:**

RCAC is home to the Purdue Envision Center, a facility that provides novel solutions to effectively communicate complex research concepts through computer graphics, advanced visualization, auditory (sound), haptic (touch), and multimodal interaction integrated with state-of-the-art high performance computation. The Envision Center is staffed by project manager, technical lead, developers and students to assist researchers, instructors, and leaders in their quest for new knowledge and innovative products. Recent and ongoing research supported by center staff includes projects in the life sciences, audiology, engineering, communications, theatre, computer science, geology, and management.
National Cyberinfrastructure Resource Provider
Purdue University is a resource provider (RP) to the NSF-funded national high-end computational cyberinfrastructure XSEDE (http://xsede.org) and a member of the XD Service Provider Forum (https://www.xsede.org/web/sp-forum/spf-membership). Purdue’s research computing systems are connected to the XSEDE resources via 100 Gbps network links. Purdue’s Condor pool of ~40,000 computer processors, a distributed computation resource for high-throughput computing, is available to XSEDE users. Purdue’s DiaGrid, a HUBzero web-enabled platform with online scientific applications backed up by high-performance and high-throughput computing resources, supports XSEDE researchers through hosting of their scientific applications and gateways. DiaGrid is also available to the broader research community, educators and students.

As a partner to the XSEDE project, Purdue staff provides in-depth advanced consulting services to help researchers nationwide to effectively utilize the XSEDE resource. Their expertise areas include optimization, scientific application development, and science gateway development and operations. Purdue staff also participate in the XSEDE Campus Champion program, helping to connect campus research needs to advanced digital resources on XSEDE and other national cyberinfrastructures.

Purdue is a resource provider to the Open Science Grid with its Condor pool for high-throughput computing applications. Purdue provides computing and storage resources to the OSG, supporting the CMS (Compact Muon Solenoid) project as a Tier-2 site and other OSG virtual organizations.