

# High Performance RESEARCH COMPUTING

HPRC is a dedicated computing resource used for cutting-edge, collaborative, and transformative research and discovery at Texas A&M University.

#### **ADMINISTERS 4 CLUSTERS**

TOTAL PEAK PERFORMANCE WITH 18 PB OF HIGH-PERFORMANCE STORAGE

### A DEDICATED RESOURCE For Research and Discovery

Since 1989, the High Performance Research Computing (HPRC) has been a dedicated resource for research and discovery at Texas A&M. HPRC, formerly known as the Supercomputing Facility, has been transformed from a mere service facility to an interdisciplinary research center advancing computational and data-enabled science and engineering with a broad mission for advancing research, education, outreach, training and service since January 2016. HPRC supports more than 2,500 users, including more than 450 faculty members. Computing resources are used for cutting-edge, collaborative, and transformative research including, but not limited to, materials development, quantum optimization, and climate prediction. HPRC promotes emerging computing technology to researchers and assists them in using it for research and discovery.

#### HPRC HARDWARE, SOFTWARE, AND TRAINING RESOURCES

New users can apply for accounts at *hprc.tamu.edu*. The website offers training and documentation for HPRC systems and software. HPRC provides a broad range of regularly scheduled training sessions and workshops for our users. These sessions may be included in formal classes that have a technical and scientific computing focus. HPRC also hosts the Summer Computing Academy to promote computing among middle and high school students.

# Electrostatic potential map for Si cluster and solvent decomposition products by *Perla albuena*.

## SUPPORTS MORE THAN **25000** USERS, INCLUDING 450 FACULTY MEMBERS

## CONTACTS

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hprc.tamu.edu

## **RESOURCES AVAILABLE**

#### GRACE

Grace is the university's new flagship supercomputer, a heterogeneous HPC cluster replacing the Ada. The new cluster provides a minimum



aggregate peak performance computing capacity of 6 PFLOPS. The Grace cluster is composed of 800 regular compute nodes, 100 A100 GPU compute nodes, 17 single precision T4/ RTX6000 GPU compute nodes, 8 large memory (3 TB) compute nodes, 5 login nodes, and 6 management servers. The Grace cluster has an HDR 3:1 InfiniBand interconnect and 5+ PB of usable high-performance storage running Lustre parallel filesystem.

#### TERRA

The 320-node heterogeneous cluster with 8,520 Intel Broadwell cores, 48 NVIDIA K80 dual-GPU accelerators,16 Intel Knights



Landing processor, and an Intel Omni-Path Architecture (OPA) interconnect.

#### LONESTAR

Lonestar-6, a Lonestar cluster hosted at the Texas Advanced Computing Center at The University of Texas at Austin, employs Dell Servers



with AMD's EPYC Milan processor, Mellanox's HDR Infiniband technology, and 8 PB of BeeGFS based storage on Dell storage hardware. Total of 74,368 core with a peak performance of 5TFlops per compute node. Jointly funded by The University of Texas System, Texas A&M University, Texas Tech University, and the University of North Texas, Lonestar provides additional resources to Texas A&M researchers. Allocation requests are made through the HPRC request page.

## **UPCOMING SYSTEMS**

#### ACES

Accelerating Computing for Emerging Sciences (ACES) is a dynamically composable high-performance data analysis and computing platform funded by NSF. Ninety percent of ACES resources will be made available to national research community via NSF ACCESS program. ACES leverage Liqid's composable framework on Intel's Sapphire Rapid processors to offer a rich of accelerators testbed containing Intel Ponte Vecchio GPUs (Graphics Processing Units), NVIDIA H100 GPUs, Intel FPGAs (Field Programmable Gate Arrays), NEC Vector Engines, NextSilicon co-processors, Graphcore IPUs (Intelligence Processing Units) coupled with Intel Optane memory and DDN Lustre storage interconnected with Mellanox NDR 400Gbps (gigabit-per second) InfiniBand to support workflows that benefit from optimized devices. ACES will allow researchers to creatively develop new programming models and workflows that utilize these architectures while simultaneously advancing HPC, Artificial Intelligence(AI), and data science projects. The phase I & II of ACES with new accelerators such as NVIDIA H100 GPUs, Intel FPGAs, NEC Vector Engines, and Graphcore IPUs is available to the national research community and Texas A&M researchers now.

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#### FASTER

FASTER (Fostering Accelerated Scientific Transformations, Education, and Research) is a novel composable highperformance data-analysis



and computing instrument funded by the NSF MRI program. FASTER adopts the innovative Ligid composable software-hardware approach combined with cutting-edge technologies such as Intel Ice Lake 32-core 2.2GHz CPUs, NVIDIA A100/ A40/A30/A10/T4 GPUs, NVMe based storage, and high-speed Infiniband HDR interconnect. FASTER is a 184-node cluster built by Dell and has 40 A100, 200 T4, 8 A40, 8 A10, and 4 A30 GPUs. Each compute node can compose more than 16 GPUs of various types via Liqid PCIe fabrics. The FASTER platform removes significant bottlenecks in research computing by leveraging composable technology that can dynamically integrate disaggregated GPUs to a single node, allowing HPC/AI workflows to flexibly choose the type and number of GPUs to fit their needs. Thirty percent of FASTER's computing resources are allocated to researchers nationwide by NSF ACCESS program. FASTER is in production and open to NSF ACCESS and Texas A&M users.

#### Vidal

A 24-node secure and compliant computing environment supports data intensive research using



sensitive person level data or proprietary licensed data to meet the myriad legal requirements of handling such data (e.g., HIPAA, Texas HB 300, NDA). It has 16 compute nodes with 192 GB Ram each and 4 large memory nodes with 1.5 TB Ram each, and 4 GPU nodes with 192 GB Ram and two NVIDIA V100 GPUs each.



### ADVANCED SUPPORT Program (ASP)

HPRC provides technical assistance to research teams across campus that goes beyond general consulting.

HPRC offers collaborations in research projects with a large computational component. Under the ASP, one or more HPRC analysts will contribute expertise and experience in several areas of high performance computing.

#### OUR COLLABORATIVE CONTRIBUTIONS INCLUDE:

- porting applications to our clusters
- analyzing and optimizing code performance
- developing parallel code from serial versions and analyzing performance
- bioinformatics and genomics
- optimizing serial and parallel
  I/O code performance
- optimal use of mathematical libraries
- code development and design