GETTING STARTED WITH HIGH-PERFORMANCE COMPUTING ON PURDUE COMMUNITY CLUSTERS

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Agenda

- Intro to HPC
- Intro to Purdue clusters
- Clusters overview
- Storage overview
- How to log in
- Login vs. compute nodes
- Submitting a job
    - Monitoring a job
- Useful commands
- Open OnDemand
- Globus
- Application modules
- Engineering applications and licensing
- User support
- Questions

Introduction to HPC

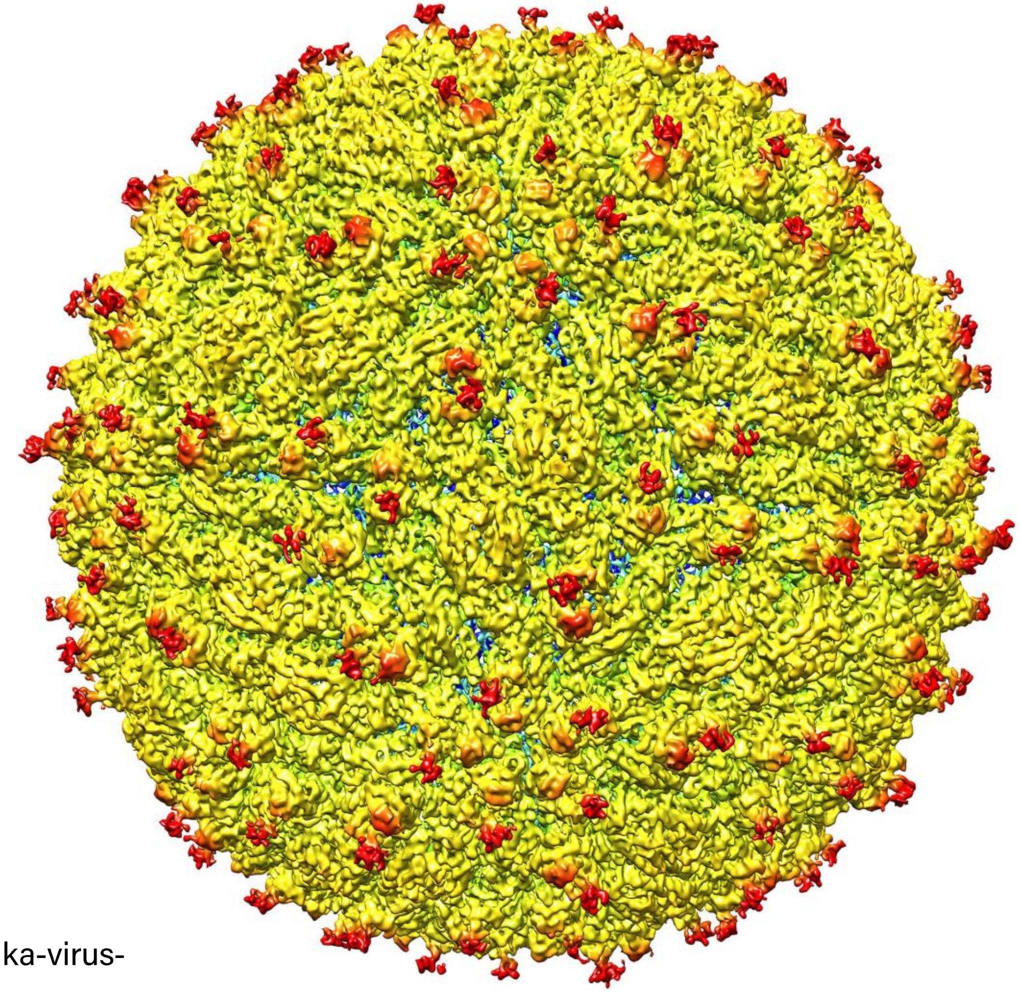
- High-performance computing (HPC) is technology that uses clusters of powerful processors that work in parallel to process massive multi-dimensional data sets, also known as big data, and solve complex problems at extremely high speeds.

www.ibm.com/topics/hpc

- World’s fastest supercomputer
  - Frontier (ORNL)
  - 1.102 exaflops

Structure of Zika Virus

- Kuhn, Rossmann, *et al.*
- Combined Cryo-EM images of many Zika virus particles using RCAC clusters to create a 3-D structural map of the Zika virus.
- Work done on Snyder cluster.

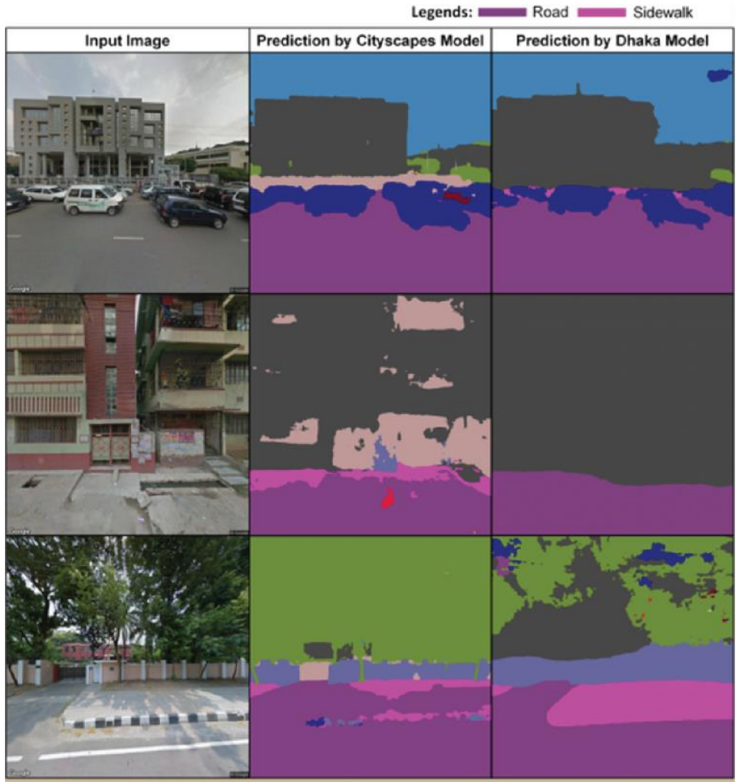


https://www.purdue.edu/newsroom/releases/2016/Q1/researchers-reveal-zika-virus-structure,-a-critical-advance-in-the-development-of-treatments.html

Automated Sidewalk Mapping

- Hamim, Kancharla, and Ukkusuri (Civil Engineering, Purdue)
- Used deep learning to create sidewalk maps from Google street view images.
- Work done on Anvil cluster.

https://www.rcac.purdue.edu/news/6424



Semantic segmentation model examples. From left to right: Input image; pre-trained model prediction; revised, locally trained model prediction.

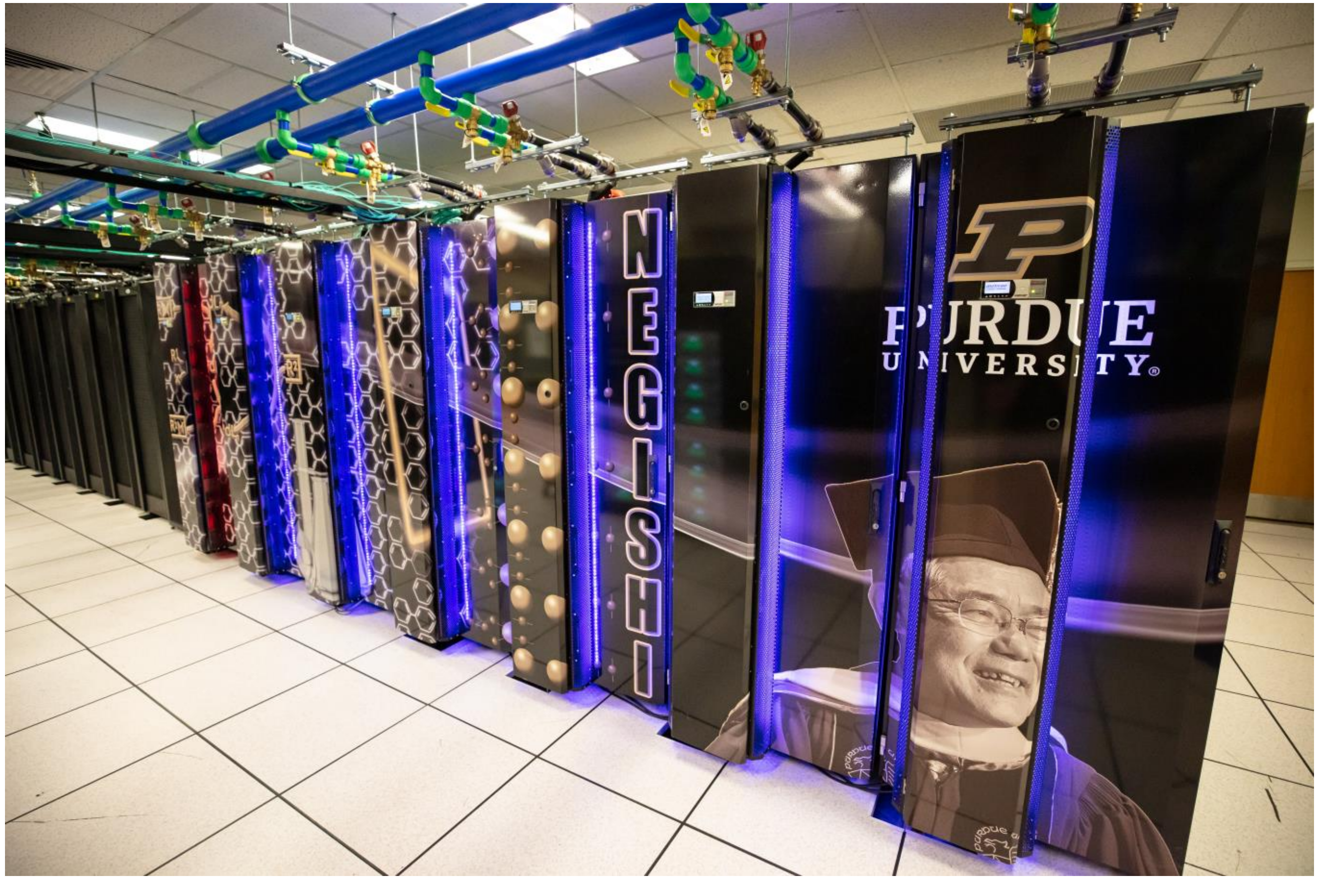
RCAC Services

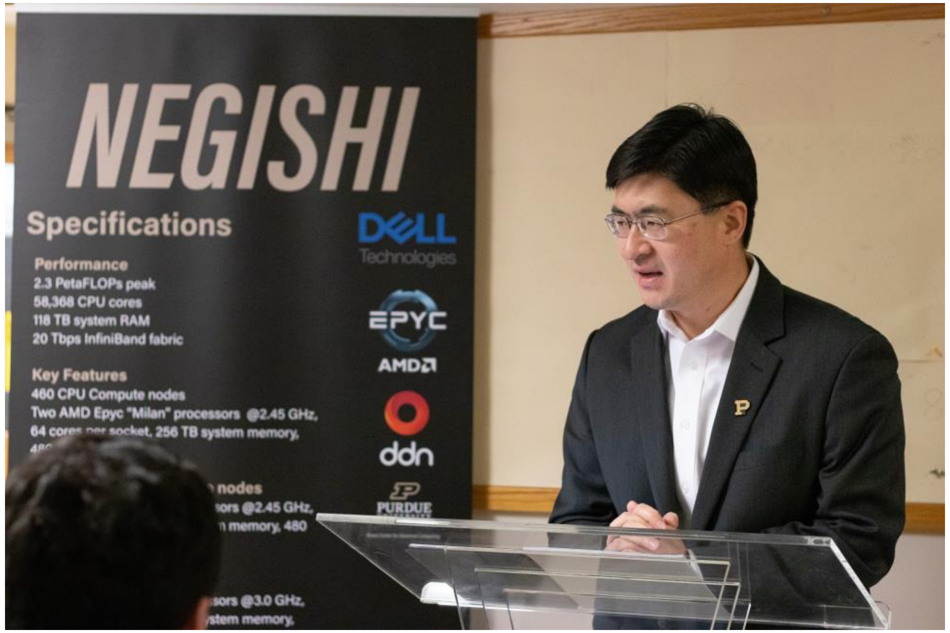
- **Compute**
- **Storage**
- **Visualization**
- **Grant collaboration**
- **Training**

Community Cluster

- Faculty A needs 10 x 64-core nodes
- Faculty B needs 5 x 64-core nodes
- Faculty C needs 2 x 64-core nodes
- … … …
- Build a 100-node cluster for all the faculties
  - Ease of maintenance
  - Cost effective
  - Node failures do not lead to work stoppage
  - Use additional burst capacity when others are not using their nodes
  - Faculties buy “shares” on the cluster

Negishi Cluster at Purdue





List of Community Clusters

Name	Purpose	Hardware	Access
Negishi	CPU community cluster	CPU + AMD GPU	Community cluster purchase
Gilbreth	GPU community cluster	Nvidia GPU	Community cluster purchase
Anvil	NSF ACCESS resource	CPU + Nvidia GPU	NSF ACCESS allocations
Bell	CPU community cluster	CPU + AMD GPU	Community cluster purchase
Scholar	Teaching cluster	CPU + Nvidia GPU	Free
Weber	Export controlled research	CPU + Nvidia GPU	Community cluster purchase
Hammer	High-energy physics	CPU + Nvidia GPU	Community cluster purchase

Technical Specifications

Negishi

- 450+ nodes
  - 2 x 64-core AMD Milan processors
  - 256 GB memory
- 100 Gbps infiniband interconnect
- 6 x 1TB nodes
- 5 x 3 AMD MI210 GPUs
- 6.7 PB scratch storage

Gilbreth

- Heterogeneous cluster
- 100 Gbps infiniband interconnect
- 4.5 PB scratch storage
- Generations of Nvidia GPUs
  - V100
  - A100
  - H100
  - A10
  - A30

List of Storage Resources

Storage	Purpose	Capacity per user	Access	Access methods
Home	Persistent files, codes	25 GB	With community cluster	Terminal, network drive, Globus
Scratch	Temporary files, data, results	200 TB	With community cluster	Terminal, network drive, Globus
Data Depot	Persistent files, data, software (group shared)	On Demand	Purchased in units of 1 TB	Terminal, network drive, Globus
Fortress	Data archival	Unlimited	Free	SCP, HSI/HTAR, Globus
DBGAP	dbGaP-compliant storage	On Demand	With Negishi cluster	Terminal, Globus

Data Depot

- 6.5 PB GPFS file system
- Shared workspace for research groups
- **Data owned by faculty/PI**
- **Fault tolerant**
  - All data duplicated at independent “sites”
- Regular snapshots for recovering old files
- Accessible from all clusters
- Use Globus for bulk data transfers
- Can be mounted as a network drive on laptop
- $70/TB per year

Fortress Data Archive

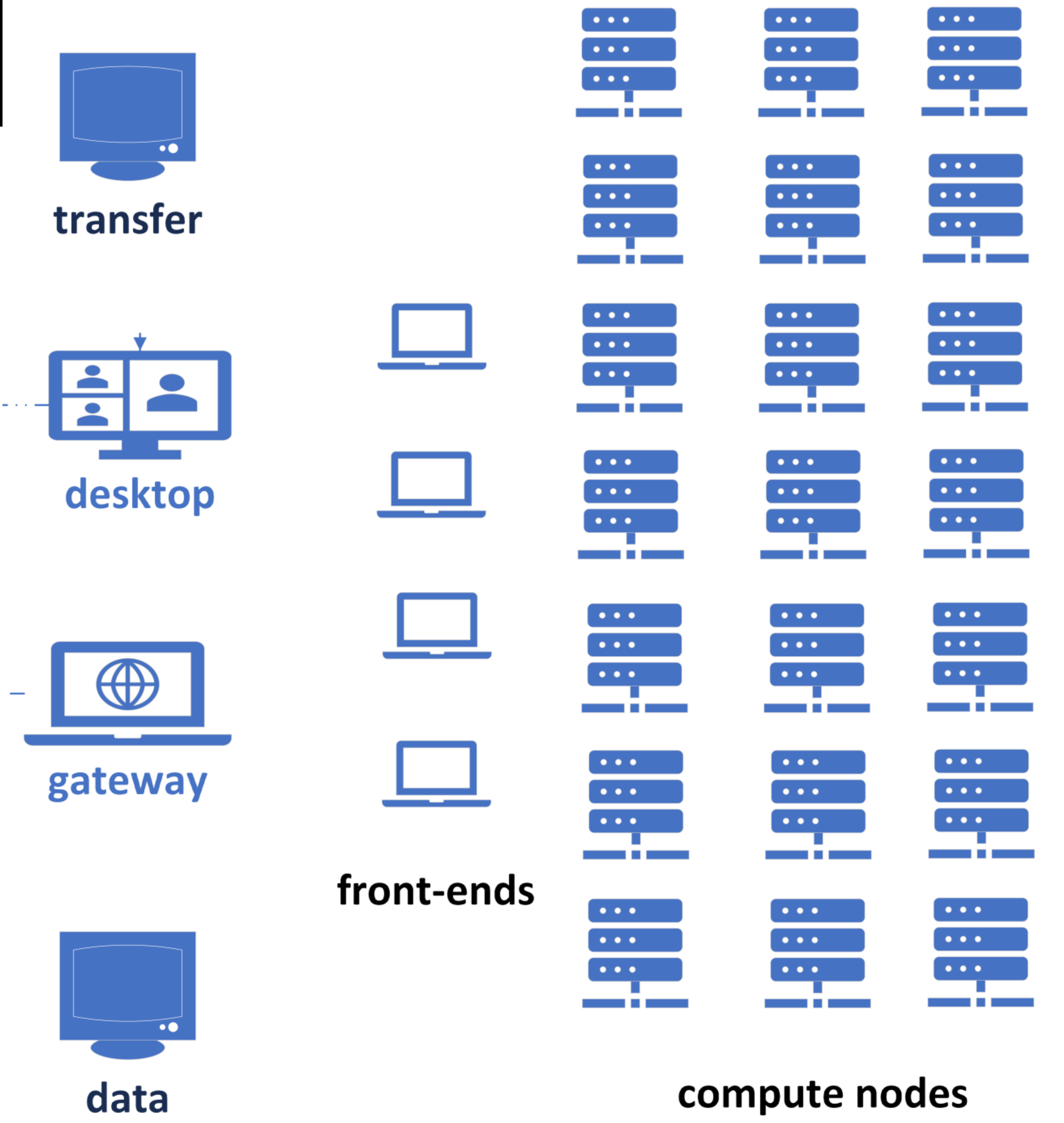
- 200 PB HPSS tape archive
- Free for all Purdue researchers
- Practically unlimited storage
- Not for interactive work
- Data can be transferred using Globus or HSI/HTAR

How to Login to Purdue HPC Clusters

- Thinlinc desktop
  - `desktop.clustername.rcac.purdue.edu`
- SSH client
  - `clustername.rcac.purdue.edu`
- Open OnDemand gateway
  - `gateway.clustername.rcac.purdue.edu`

Quick Glance at a Cluster

- Login to the front-ends
  - Shared among all users
  - User for coding, data transfer, etc.
- Heavy computational work must be submitted to the back end nodes
- Submitting jobs
  - Command line and batch scripts
  - Graphical
  - Ondemand portal
- To find applications
  - Use the module command
  - Extensive listing on RCAC website



How to Submit a Job

- A “job” is a request for compute resources for a specific duration
- “Job request” is submitted using Slurm commands
  - Which queue
  - How many cores
  - How long
- Jobs are of two types
  - Batch: Submit a script
  - Interactive: Enter commands in the terminal

Demo: Submitting a job

- Batch job
  - `sbatch myscript.sh`
- Interactive job
  - `sinteractive -N 1 -n 128 -A rcac -t 1:00:00`
  - Request an interactive job with 1 node and 128 cores for 1 hour under the queue “`rcac`”

Useful Commands

- How do I find out which queues I can submit to?
  - `slist`
- How do I find out which jobs are currently running?
  - `squeue –u myusername`
- List details about a job
  - `jobinfo jobid`
- Show my storage usage
  - `myquota`

Open OnDemand

- An easy web-based GUI for submitting jobs
  - `gateway.clustername.rcac.purdue.edu`
- Great for running GUI/interactive applications
  - Jupyterhub
  - Rstudio server
  - Matlab
  - VMD
  - Cryosparc/Relion
  - ...

Data Transfer

- How do I transfer my files from my desktop to the HPC cluster?
  - SCP/SFTP
  - **Globus**
- Advantages of using **Globus**
  - Fast
  - Reliable
  - Intuitive web-based GUI
  - Can transfer to/from any location that supports Globus
- Login to `transfer.rcac.purdue.edu`

Scientific Applications

- Compilers: GCC, Intel, AMD, Nvidia
- MPI libraries: OpenMPI, Intel, MVAPICH2
- Numerical libraries
- Data formats
- Popular applications
  - Chemistry, Physics, Biology, Statistics, etc.
  - ~280 application modules
- 600+ biocontainers
- Most engineering applications
  - Matlab, Ansys, Abaqus, Tecplot, Comsol, etc.
- `https://www.rcac.purdue.edu/knowledge/applications`

Application Modules

- Scientific applications can be loaded using the “`module`” commands
- “`module`” is a software that updates your environment to make it easier to run applications
- Typical workflow
  - Load a module
  - Run application
  - Unload the module

Module Commands

- Load an application module
  - `module load appname`
  - `module load matlab`
- Unload an application module
  - `module unload matlab`
- Search for an application
  - `module spider matlab`
- Find out application dependencies
  - `module spider paraview`

Engineering Applications and Licensing

Sundeep Rao
Engineering IT
Executive Director, Information Technology

Application list: https://slic.ecn.purdue.edu/
Engineering support: https://engineering.purdue.edu/ECN/AboutUs/ContactUs

Resources

- RCAC website: www.rcac.purdue.edu
- Cluster user guides: https://www.rcac.purdue.edu/knowledge
- Trainings: https://www.rcac.purdue.edu/training
- Coffee hour consultations: https://www.rcac.purdue.edu/coffee
- Purchase: https://www.rcac.purdue.edu/purchase
- User management: https://www.rcac.purdue.edu/account/groups
- PURR (data publishing): https://purr.purdue.edu
- RCAC facilities document: https://docs.lib.purdue.edu/gendes/4/

Contacts

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- **RCAC user support**
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Questions

THANK YOU