## CENTER FOR COMPUTATIONAL RESEARCH: OVERVIEW

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## **CCR Overview:**

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## **CCR's Mission**

- Enable research and scholarship among UB faculty
  - High-performance computing and data services, sponsored funding support, faculty recruitment and retention
- Provide hi-tech workforce training
  - Partner with applicable coursework, IAD/ICDS/CDSE programs
- Foster economic development and job creation among area industries
  - Work closely with faculty engaged in industrial collaboration, and the Office of Economic Development











## About CCR:

- CCR provides UB researchers and affiliated partners, including industry, with access to advanced computing resources and services
  - 24 years experience delivering HPC and related services to UB
- UB CCR serves all decanal units at UB
  - ~1300 active users (~350 PI groups)
  - Involved in >470 proposals >90M\$ awarded in external funding since 2017
  - >2000 CCR-related publications since reporting started in 2016.
- Personnel
  - CCR operations: Computational Scientists (2), Sys Admins (5), Admin+Vis (2)
  - Research support (XDMoD/ACCESS MMS): Computational Scientists (3), Software Engineers (6)
- National Recognition

#### \$27M 15-year NSF Metrics Service award (3x 5y awards)

- <u>XDMoD</u> software used by academic and industrial HPC centers worldwide
- Measure and optimize system and application performance

#### Open Source projects (ColdFront, Grendel/Heorot, Mokey, Open XDMoD)

Conference presentations/papers/tutorials and collaborations with other academic HPC centers

## **Research Services: High Performance Computing/Data**

- Academic cluster:
  - Approximately 1200 servers (some include GPUs) and 4PB of storage
  - Resources requested via jobs through batch scheduler (SLURM)
  - High-performance networking for parallel applications
  - Accessed remotely via command line SSH or Open OnDemand web portal
- No cost for faculty groups to access CCR compute resources
  - 1TB of free shared group storage (cost recovery for >1TB)
  - 10TB of free shared group scratch storage (60 day limit)
- Faculty/project specific server hosting
  - CCR provides quotation and order assistance, installation, and on-going maintenance for up to 7 years
  - Small cost recovery charged as a one-time fee for rack space, network switches, and cabling
  - Made available for preemptable "scavenger" jobs when otherwise idle

Academic cluster details Faculty cluster details









### **Research Services: Private On-Premise Cloud**

- Designed, procured, installed, and managed in-house
- Your data stays at UB!
- Useful for non-HPC research needs such as websites, databases, long-running services, proof of concept tests
- Users have full control (and responsibility) for virtual instances
- Built on Openstack cloud software
  - 24 nodes (768 CPU cores & 8.8TB RAM) and growing
  - 1.7PB Ceph storage (object-oriented), NVME ephemeral storage & PMEM (persistent memory) storage
  - Nvidia V100 vGPUs
- Eventually burst to commercial cloud capability
- Unlike HPC resources, cloud does have a cost recovery model, see link below for current rates



More LakeEffect cloud details

#### **Moving and Sharing Data: Globus**

- Easily and securely move data from/to your PC to CCR, UB Box, or other institutions with Globus collections (including NIH)
- Globus Personal Connect software available for Linux, MacOS, & Windows
- Browser-based & Command line tools available for scripting regular data transfers
- Set and forget: Will resume failed transfers, distributes large transfers across multiple servers, brokers direct transfers between remote computing centers
- Performs MD5-checksum at completion of transfer to verify data transferred
- Easy way to share data on CCR's storage with external collaborators without a CCR/UB account!
- Currently only available for CCR users but in the works for all of UB

#### More Globus Details



### **Sponsored Research/Grant Support**

- CCR actively seeks funding opportunities both on its own and in active collaboration with others
- CCR funds almost all of its infrastructure (and more than half of its staff) via sponsored research
- Direct support of HPC activities (development, administration, engineering, etc.)
- Support for collaborative research platforms (web, etc.)
- Software engineering support
- Scientific computing/modeling

#### More details





#### **Economic Outreach**

- UB CCR provides local industry partners with access to a 650 TFlop/s (5544 cores) cluster
- Including nodes with Nvidia A100 GPUs and larger memory (1TB) capability
- Since 2013, CCR has assisted over 42 companies
- Can be direct engagement or faculty-led collaborations



#### More Details



#### **Account Policies & Requirements for Use:**

- No cost to use academic (UB-HPC) cluster queue priority is based on contribution level (more info on <u>Supporters Boost</u>)
- Publications: Acknowledge CCR support in publications (<u>citation format</u>)
- Grants: Include a percent credit to CCR (at least a 5%) on the Sponsored Programs Approval Form (though this can be larger for grants requiring significant CCR resources)
- Communicate with CCR about the nature of your research, publications and any funding that you have using **ColdFront allocations portal** 
  - Use ColdFront to manage your project: add/remove users, request allocations to resources, provide research information (publications, grant info, other reportable data)
  - You may add students, postdocs, external collaborators
  - Required to review and update this information annually
  - Allocations usually last one year and if you wish to continuing access the resource you
    request renewal
- Classes may be able to be supported contact CCR Help to discuss class size and requirements – all access is managed through ColdFront with allocations good for the current semester







# **QUESTIONS?**

RESOURCES: <u>https://buffalo.edu/ccr</u> Help Desk: <u>https://ubccr.freshdesk.com</u> Documentation: <u>https://docs.ccr.buffalo.edu</u> Email: ccr-help@buffalo.edu