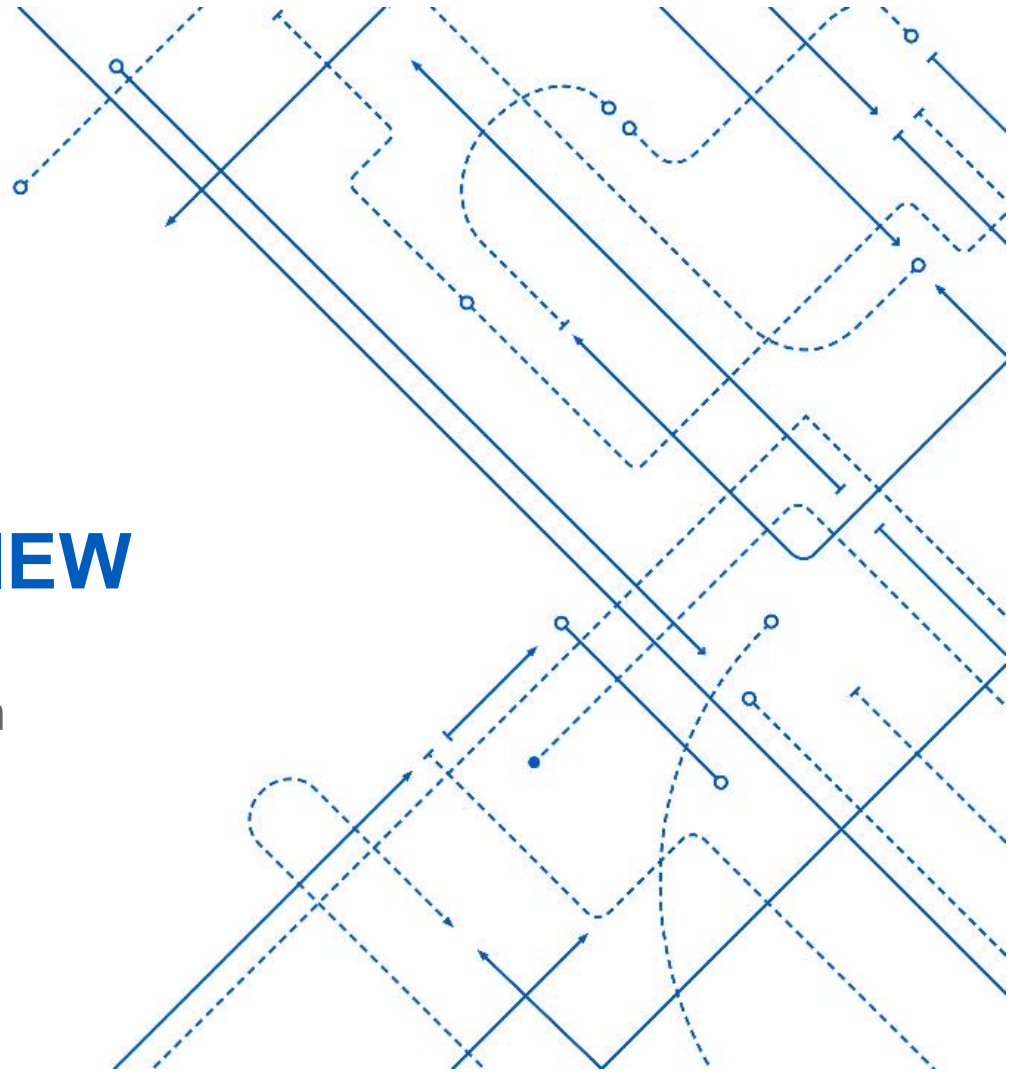# CENTER FOR COMPUTATIONAL RESEARCH: OVERVIEW

Matthew D. Jones, Ph.D.

Center for Computational Research

University at Buffalo

UB Geology 2021-04-22

Center for Computational Research

- Leading Academic Research Computing Center:
  - 20+ years delivering research computing and related services to UB

- National Recognition:
  - $17M 10-year NSF XD Metrics Service award (2x 5y awards)
    - XDMoD (XD Metrics on Demand) for NSF HPC resource/service portfolio
    - Open XDMoD software used by academic and industrial HPC centers worldwide
    - Monitor, measure and optimize system and application performance

- Personnel:
  - 19 total: Operational (10) and Research Support (9) : Computational Scientists (5), Software Engineers (7), Sys Admin (5), Admin (2)
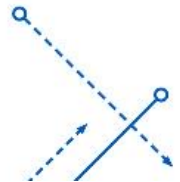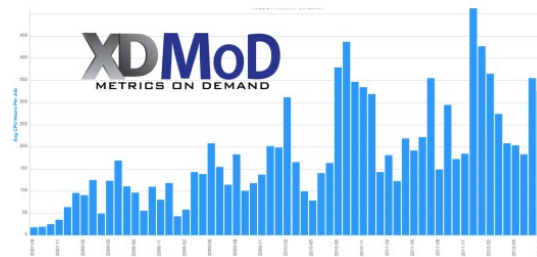
What is UB CCR?

- CCR provides UB researchers and affiliated partners, including industry, with access to advanced computing resources.
  - Academic, Industrial, and Faculty Compute Nodes
  - High Performance Storage and Networking
  - Cloud Computing Resources
  - Associated Services
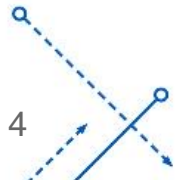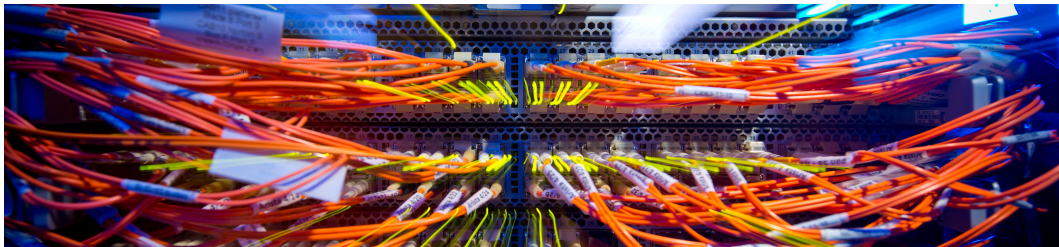
Who is UB CCR for?

- UB CCR serves all decanal units at UB
  - ○ >1000 total users in 2020, >150 research groups
  - ○ >1600 CCR-related publications since reporting started in 2016
    - ○ >250 publications in 2018.

- **No cost for faculty groups to use CCR compute resources (cost recovery cloud and for addditional /projects storage beyond 1TB)**

- Online account requests:
  buffalo.edu/ccr/support/ccr-help/accounts.html

- Online account/access management:
  https://coldfront.ccr.buffalo.edu

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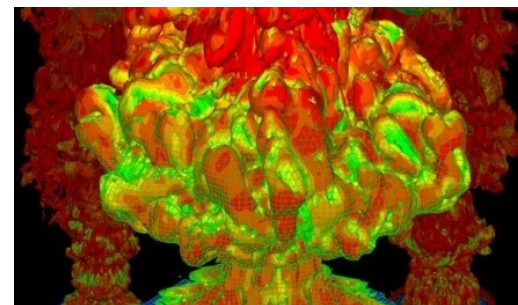
CCR Infrastructure Resources

General Compute:
- ~800 nodes, >15000 cores: 48 dual-GPU nodes (V100)

Faculty Compute:
- ~500 nodes, >11000 cores, "condo" model

Industry Compute:
- ~200 nodes, >3000 cores, various use cases intended for economic outreach
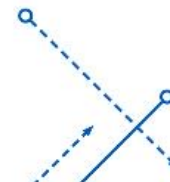- Upgrade in progress, expected 2021Q2/2021Q3

Storage:
- 1.2 PB Panasas PanFS parallel scratch
- 2 PB VAST Data flash network file system

Networking:
- 40gigE core networking (and edge)
 - 2022 100gigE planned

Cloud:
- OpenStack, >1000 vCPUs, >700GB Ceph object storage

Education, Outreach and Training

- Workshop instruction
  - [Virtual workshop series](#) last year during COVID
- Group training and Q&A sessions
- Individual training and help sessions
- Classroom instructional support
  - >20 classes per year, from computational chemistry to bioinformatics and parallel computing
- ICDS/CDSE support
  - Institute for Computational and Data Sciences (ICDS), university wide umbrella program including CCR and CDSE (Computational and Data-Enabled Sciences and Engineering) degree programs
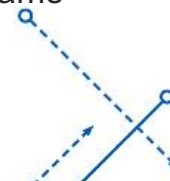
Sponsored Research/Grant Support

CCR actively seeks funding opportunities both on its own and in collaboration with others, some examples:

- Direct support of HPC activities (development, administration, engineering, etc.)
  - XDMoD (NSF 1445806)
    - OpenOnDemand (NSF 1835725), Ookami A64FX Testbed (NSF 1927880)
  - NSF MRI (1724891 in 2018), NIH S10 (1S10OD024973-01A1 in 2019)
  - DOE PSAAP CHREST
- Support for collaborative platforms (web, gateway, etc.)
  - Ghub, Community-Driven Data-Model Framework for Ice-Sheet Science, doi.org/10.1002/cpe.6130, NSF 2004826