Enabling computational research and education in North Dakota

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<u>C</u>enter for <u>C</u>omputationally <u>A</u>ssisted <u>S</u>cience and <u>T</u>echnology (**CCAST**), Information Technology Division

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What is CCAST?

The <u>C</u>enter for <u>C</u>omputationally <u>A</u>ssisted <u>S</u>cience and <u>T</u>echnology (CCAST; pronounced "*c-cast*"), a part of NDSU IT, provides advanced cyberinfrastructure for computational research and education at NDSU and beyond.

CCAST (i) develops, manages, brokers, and operates high-performance, cloud, and interactive computing resources, and (ii) educates researchers on proper and efficient use of the resources and on other topics of interest to the computational science and engineering community.

Basic services are provided at no charge. Dedicated services available at cost.

CCAST resources: Hardware, software, data transfer, cloud...

- Hardware: purchased almost entirely with external/non-appropriated funds
 - o 12,564 Intel and AMD CPU cores and 55TB of RAM, incl. big-memory compute nodes
- o **2.2PB** high-performance storage; **6PB** tape/archive tape storage; **1PB** research data archive...
- o 70 general-purpose GPU cards, including NVIDIA A100s

Basic level of services is FREE to NDSU researchers and certain external collaborators

Researchers can purchase "condo" (i.e., researcher-owned) compute or storage units

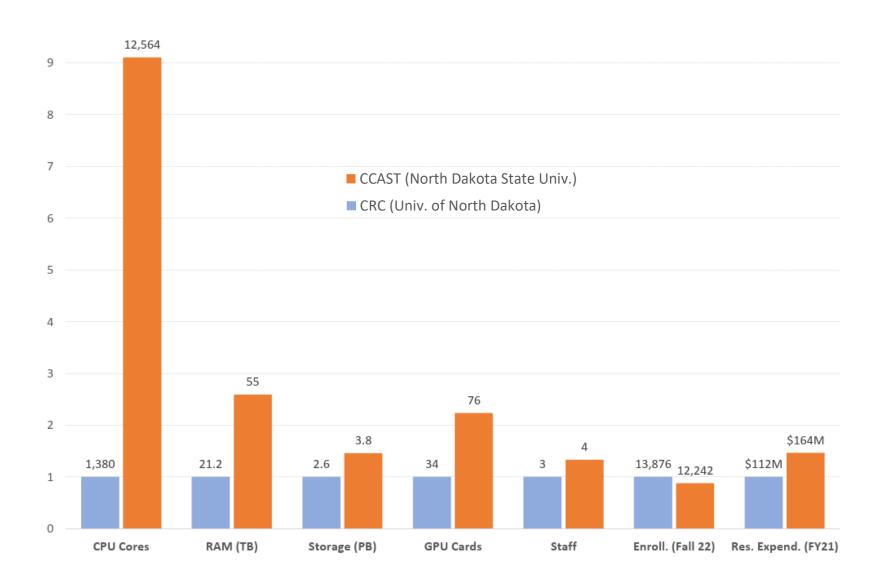
- **Software**: various
 - General libraries/compilers
 - Specific applications in different areas
- Fast data transfer

via Globus & ScienceDMZ

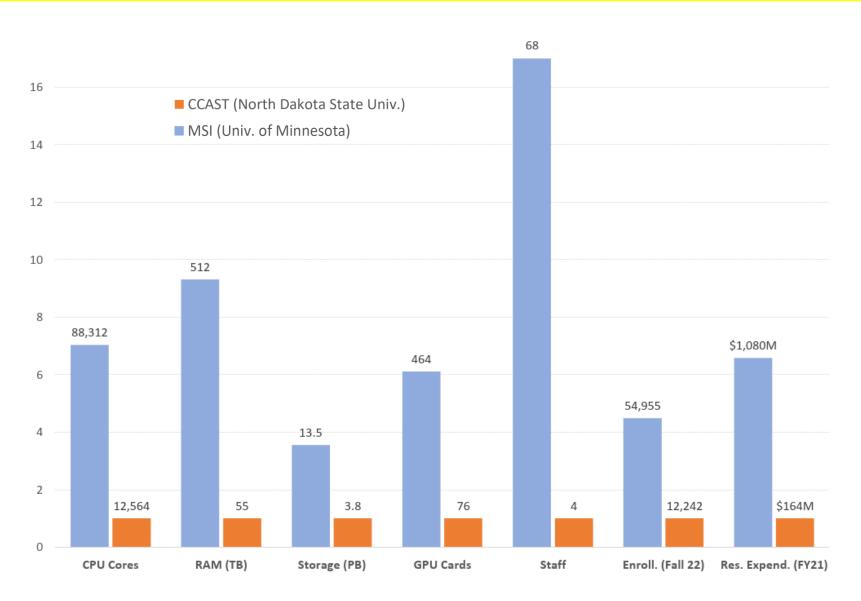
Cloud services via external partners



How is CCAST compared to its peers?



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Current status of advanced research computing

- Advances in high-performance computing (HPC)
 - o Petaflops (10¹⁵) to exaflops (10¹⁸), hybrid CPU/GPU nodes...
 - o Numerical and parallel algorithms, code development...
- More powerful computers allow solving more complex and bigger problems (and usually enable better science)



NERSC/LBNL/DOE

But... "Law of Constancy of Pain"! (Craig Good, original Pixar employee)



CCAST/NDSU

- Hardware and software have become have become more complex/usually harder to use
 - o HPC is parallel computing!
 - o HPC resources are shared resources, and ALWAYS limited
- HPC knowledge/skills are required...
 - ... to use the resources properly and efficiently and to improve research productivity

CCAST resources: Research computing (RC) facilitation

- Goal: to advance researchers' capabilities and hence accelerate scholarly discovery
- Engagement with researchers to understand their needs and advise on RC strategies
- Ongoing support researchers of executing projects on computing resources
- Education and training: trained >600 faculty, staff, and students (since 2019), provided internships to >40 students (since 2018); guest lecturing...
- Consulting on computational tools/approaches, infrastructure for research and teaching

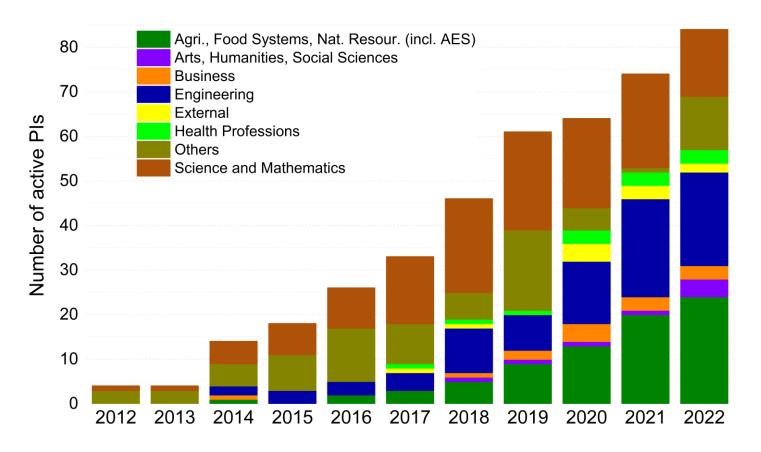


- Proposal writing assistance, proposal writing and collaboration...
- Advocating for the needs of researchers to inform RC design and institutional support

CCAST user community: Growing rapidly and getting more diverse

Number of active PIs by year and research fields

(i.e., approx. number of research groups actively use CCAST resources)



Campuses with <u>active</u> CCAST users: North Dakota State University, University of North Dakota, Cankdeska Cikana Community College, Dickinson State University, Valley City State University...

CCAST staff

Current open positions: Scientific Software Specialist and Systems Engineer



Khang Hoang
Interim Executive Director
Research Facilitator



Nick Dusek Research Facilitator



Samuel Saula HPC Systems Admin



Ryan Anderson HPC Systems Admin

- CCAST staff has...
 - ... decades of combined experience in high-performance and scientific computing.
 - ... research experience in multiple areas: bioinformatics, chemistry, computer science, materials science, microbiology, physics, and statistics.

Summary

- Research computing (incl. HPC) resources are available for your research and teaching
- HPC resources are <u>shared</u> and ALWAYS <u>limited</u>. HPC knowledge/skills are required to use the resources properly and efficiently and to improve research productivity
- As a PI, HPC knowledge and familiarity with computing facilities is needed to design and plan your research, and to supervise your group members effectively
- Consider integrating advanced computing into your teaching.

Mark your calendar! Conference on Computational Science and Engineering (October 18, 2023, NDSU Memorial Union)

Contact CCAST at ndsu.ccast.support@ndsu.edu

