Fall Talon User Group Meeting

September 23, 2020

North Texas Scientific Computing

Sponsored by
The Office of the Chief Information Officer, UNT and UNT System

Chris McCoy
Chris.McCoy@untsystem.edu

Opening Remarks

Chris McCoy, M.B.A.
Chief Information Officer
UNT and UNT System

Partnerships

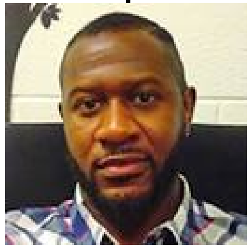
Change: Full Research Support

Chris McCoy, M.B.A
Chief Information Officer
UNT and UNT System

Larry Mendez, Ed.D.
Chief Technology Officer, ITSS

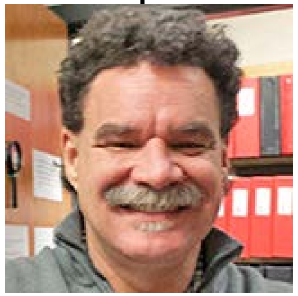
- System Administration
- Data Center Operations

Michael Heredia
System Administration Manager
Enterprise Systems Support



DaMiri Young
System Administration Lead

Ravi Vadapalli, Ph.D.
Senior Director
North Texas Scientific Computing



Richard Herrington, Ph.D.

Yuguang Ma, Ph.D.

Charles Peterson, Ph.D.

Agenda

- Talon3 Computing Environment
- North Texas Scientific Computing
  - Purpose
  - Talon Resource Allocation Management
  - Usage Analytics: Improvement Opportunities
  - Data Science and Analytics: Capabilities & Services
- Interactive Data Exploration and Analytics
- New Directions
- Key Takeaways
- Q & A

Talon3 HPC Environment

New Ticketing System

ServiceNow (to replace OTRS)

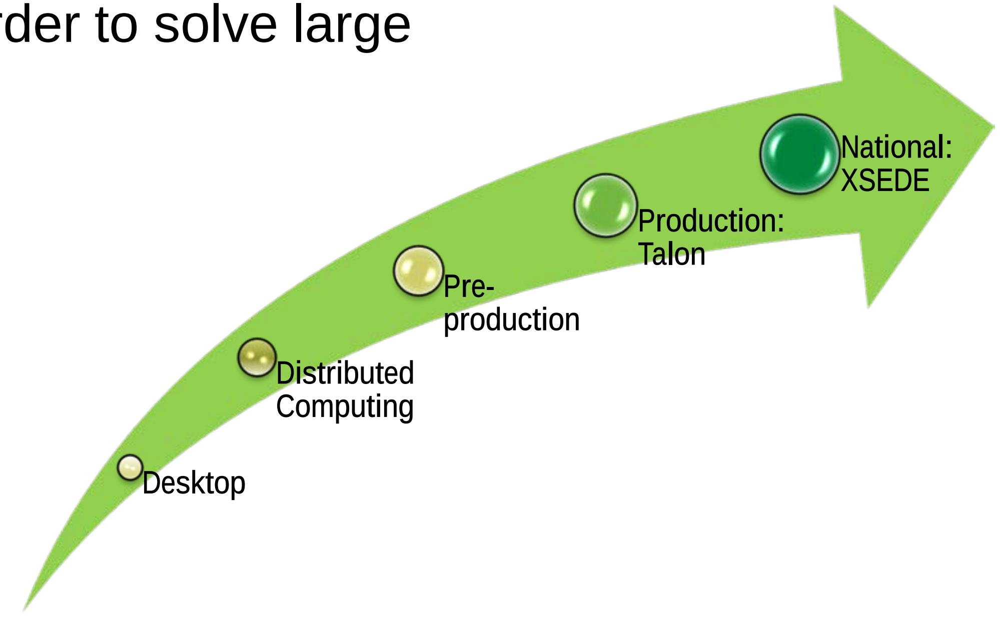
Scicomp-Support@unt.edu

- 8,300 CPU (Broadwell and Sandy Bridge) cores.
- GPUs
  - 16 Dell R730 servers, each with two NVIDIA Tesla K80 GPUs (4992 cores/card), 28 cores/node.
  - Two servers with one V100 32GB card per server, 18cores/node
  - Three newer servers with one V100S 32GB card per server, 40cores/node.
- Connected through 56 Gbps Mellanox fourteen data rate (FDR) InfiniBand network
- 570TB DDN Web Object Storage, 1.4PB DDN SFX7K Lustre parallel file system for SCRATCH
- 10TB NFS for Shared Apps and HOME areas
- SLURM workload manager job scheduling and resource management.
- Open Ticket Request System (ORTS 5.x) for customer support. Write to hpc-admin@unt.edu

What is HPC & Why Should I Care?

What is High-Performance Computing?

- HPC aggregates computing power and techniques in order to solve large or *intractable* problems—fast computing.
- Enables model size to scale manifold.



Scientific Computing Continuum

Why should I care?

- ❑ Is your scientific computing taking hours or days to complete on a desktop?
- ❑ Are you limited by model size due to its run-time limitations? memory or storage issues?
- ❑ Is your research data growing or disparate across sources and potentially unmanageable with current tools?
- ❑ Do you anticipate scaling the problem beyond what you currently work with?

Purpose

To help the researcher unlock the wide range of computational resources to solve the most challenging science problems.

TRAIN> SCOPE> SCALE> SECURE

Incremental pattern of success

1. **Train** emerging researchers
2. **Scope** and prototype application
3. **Scale** problems across computing platforms
4. **Secure** grants and build partnerships

Change: Reactive → Proactive Support

The Team: Computing Support

Ravi Vadapalli, Ph.D.
Joined UNT in May 2018
Senior Director, North Texas Scientific Computing
CAAAM Strategic Initiatives Coordinator | ***caaam.unt.edu***
Site Director, NSF IUCRC Cloud and Autonomic Computing Center Affiliate Site at UNT | ***cac.unt.edu***

Academic Preparation
Andhra University, Visakhapatnam, India
M.Sc., Nuclear Physics, 1988
Ph.D., Nuclear Physics, 1994
Mississippi State Univ., Starkville, Miss.
M.S., Computational Engineering, 2002

Research & Professional Summary

- 18+ years of experience in high-performance scientific computing and applications.
- Collaborative research in many areas in science, engineering, liberal arts, and medicine.
- Helped and collaborated in over $20MM in external funding with a high success rate, and
- Secured $230MM+ in-kind across disciplines.
- Helped develop new program opportunities, sustainable industry-research partnerships, and workforce development.

Position Summary — 18 years

- **2019 – present:** Sr. Director, RITS
- **2018 – 2019:** Director, RITS
- **2006 – 2018:** Sr. Research Scientist, HPCC@TTU: Curtsey Professor of Petroleum Engineering
- **2003-2005:** Asst. Research Physicist in Computational Nanomaterials
- **2002-2003**: Postdoc, Scientific Computing

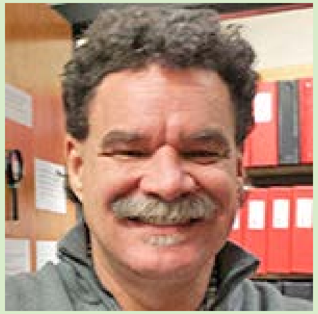
Meet the Team: Computing Support

Yuguang Ma, Ph.D.
Research Scientist-II
Liaison for College of Engineering

- Computational Chemistry
- High-Performance Computing
- Code Optimization
- Machine Learning
- Algorithms

Charles Peterson, Ph.D.
Research Scientist-II
Liaison for College of Science

- Computational Chemistry
- High-Performance Computing
- Application Support Services
- Workforce Training and Outreach



Richard Herrington, Ph.D.
Research Scientist-III
Liaison for all Colleges except CoS and CENG

- Data Analytics
- Research Methodology
- Machine Learning and AI
- Distributed Computing
- Technology Evaluation

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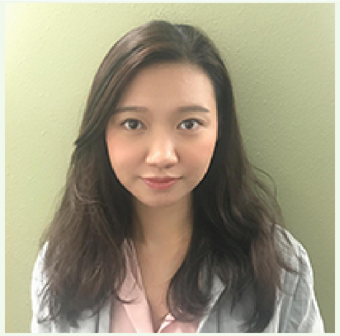
Support Staff

Change: Shared GRAs and Postdocs!

Di Wu, Ph.D.
Postdoctoral Associate
Center for Agile and Adaptive Additive Manufacturing (CAAAM)

- High-Performance Computing
- Machine Learning and AI
- Multi-scale modeling & optimization
- Algorithms and Numerical Analysis



Bailu Zhang • Ph.D. Candidate
Graduate Assistant
Computer Science & Engineering

- Biocomputing
- Machine Learning, R, Python
- Data Science & Analytics
- High-Performance Computing


WE ARE
HIRING!

NTSC: ASSUR^{2}E*

- Application Support Services for User Recruitment and Retention
- Supports student-leveraged research development and grant collaborations

Funding

- Supports one graduate and one understand student costs
- Faculty and NTSC Staff co-mentor students & share student costs

Metrics for Success

- Results in new research development / interdisciplinary collaborations
- At least one grant application submitted with a potential to generate 3x or more ROI
- Author/co-author at least one peer-reviewed publication to a reputed journal or conference

*Jointly funded through support from Offices of the Provost and Research & Innovation.

Talon3 Resource Usage Policy Changes

- SLURM Resource Allocation Management
- Tiered Computing Support
- Storage Management

Charles Peterson, Ph.D.

Liaison for College of Science

NSF XSEDE Campus Champion

UTK Institute for Nuclear Security Scientific Fellow https://insfellows.utk.edu/people/

XSEDE: e**X**treme **S**cience and **E**ngineering **D**iscovery **E**nvironment, https://www.xsede.org

Talon3 Resource Management Policies & Practices

- Talon3 compute resources have several policies in place to help guarantee fair resource utilization.
- These policies are currently implemented via SLURM Workload Manager. SLURM provides three key functions:
  - Allocates exclusive and/or non-exclusive access to resources for predefined duration.
  - Provides a framework for starting, executing, and monitoring work (typically a parallel job such as MPI) on a set of allocated compute nodes.
  - Arbitrates contention for resources by managing a queue of pending jobs according to a set of administrator defined priorities*.

*Policies determined in consultation with the Division of Research and Innovation.

SLURM Quality of Service, QoS

- Each SLURM partition supports three types of QoS

- Debug QOS for running quick test computations for debugging purposes. Limit is 2 hours and 2 compute nodes per user.
- General Default QOS for submitting jobs that take 72 hours or less. Limit is 72 hours and 616 CPUs per user.
- Large QOS for large jobs that consume > 72 hours of wall time. Limit 22 compute nodes and allows exclusive jobs.

Goal is to provide an efficient resource engagement that allows debugging, testing, and production computing.

Talon3 Allocation Management (Past)

Factors: fair share, running jobs, age of the job, starvation, QOS priority, etc.

If all variables are equal, jobs submitted by users with higher priority are scheduled first.

Fair share factor is determined by the Activity Type outlined in descending order below.

- Funded Research
- Eagle (Awards >= $100k)
- Eaglet (Awards < $100k >= $10k)
- Hatchling (Awards < $10k)

Categories

- Grant Initiated
- Doctoral Dissertation
- Class Instruction
- Undergraduate Research
- Scholarly/Creative Research

ISSUES

- Grant status update during FY
- Monopoly by user group size
- Competition with exploratory users (starvation scheduling)
- Efficacies: Node request-to-utilization
- Queuing process frustration
- Long-term compute versus On-demand

Talon3 Resource Policies

Change: Tiered Support

Production Partition

- Used 300K CPU-core hours per year OR Active Grant

Resources

Access to all Nodes
C6320 (192), R420 (139), 8 Big Mem, K-80, V100 nodes

Ad hoc Allocations for On-Demand Computing

Advanced Support

Preproduction Partition

- Used < 300K CPU-core hours per year

Resources

All Nodes except C6320

Basic Support

More to come…

Collaborating with DRI for additional improvisations on ISSUES

Talon3 Storage Policies

Change: $HOME Backed up

Area	Purpose	Allocation	Policies
$HOME	Login and critical files	20GB per user	• NFS mount, • Daily incremental backup
$WORK	Research Data Management	2TB per user	• DDN WOS • No backup • No purge
$SCRATCH Quota Enforced	Data staging & Intermediate Data Management	25TB per Faculty	• DDN Lustre PFS • No backup • Purge at 75% usage

Talon3 Usage Analytics With XALT 2.8*

(Sample: 3 months, June 10 – Sept 10)

- Applied Computing
- Collaborative Opportunities

Yuguang Ma, Ph.D.
Liaison for College of Engineering

*XALT 2.8. https://xalt.readthedocs.io/en/latest/
Developed at Texas Advanced Computing Center for accounting for cluster resource utilization

XALT Job Statistics on Talon3

	CPU Hours	Jobs*	Adjusted Jobs*
Submitted to SLURM	4,178,757	11,044	31,649
Directly Running**	34,155	1,020	1,020
CPU Jobs	4,180,242	11,719	32,196
GPU Jobs	32,670	345	473
Serial Jobs (1 core)	92,844	1,701	5,745
Parallel Jobs (1 node)	697,101	4,058	19,935
Parallel Jobs (multi nodes)	3,422,967	6,305	6,989
Jobs with RITS Maintained Apps	2,765,092	5,830	9,035
Jobs with User Installed Apps	1,442,474	6,138	23,229
Others (gzip, cmsh, system python scripts, etc)	5,346	96	585
All	4,212,912	12,064	32,849

**Jobs are counted by SLURM job ids and interactive jobs; Adjusted jobs were statisticized by XALT, as some SLURM jobs include independent sub-jobs.*

***Directly running jobs include those not submitted to SLURM and running on the login, visualization and Dr. Liu nodes.*

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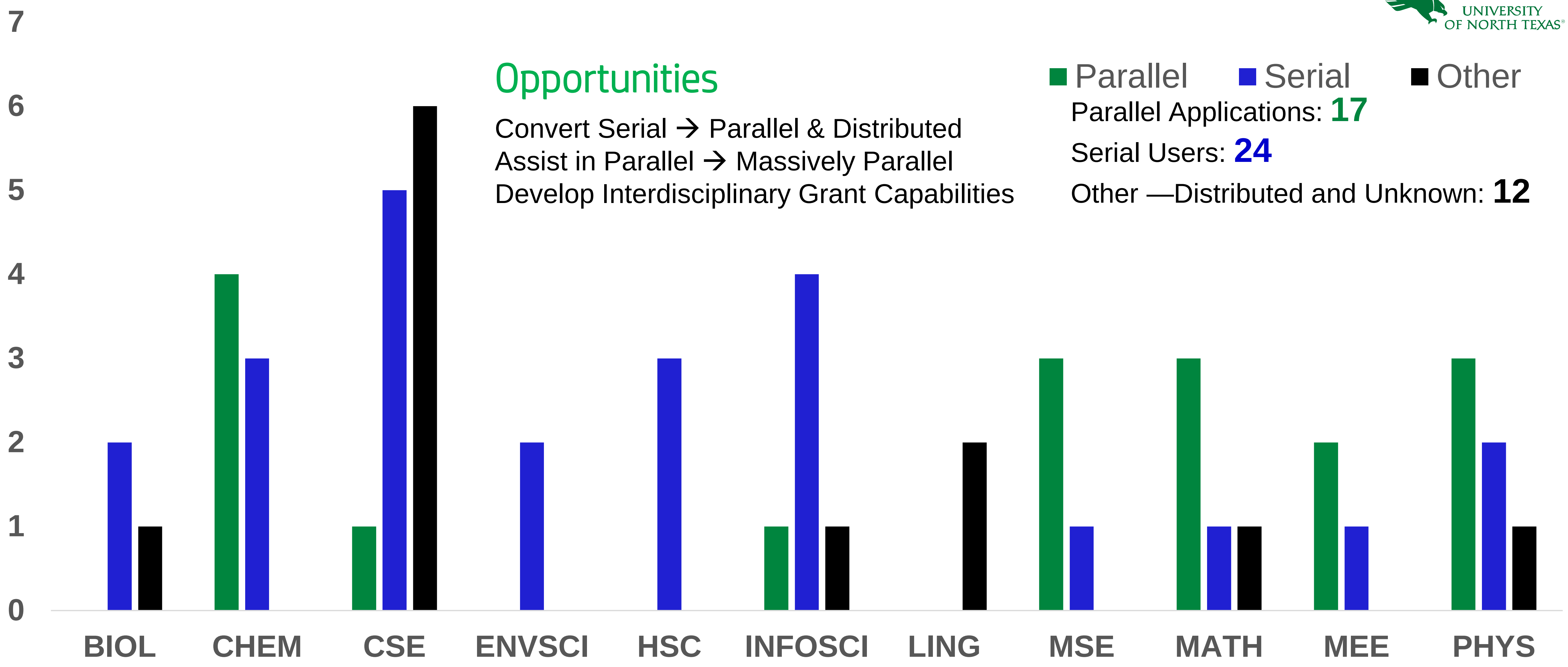
Active Users: Talon-Usage Profile Across Domains



Opportunities

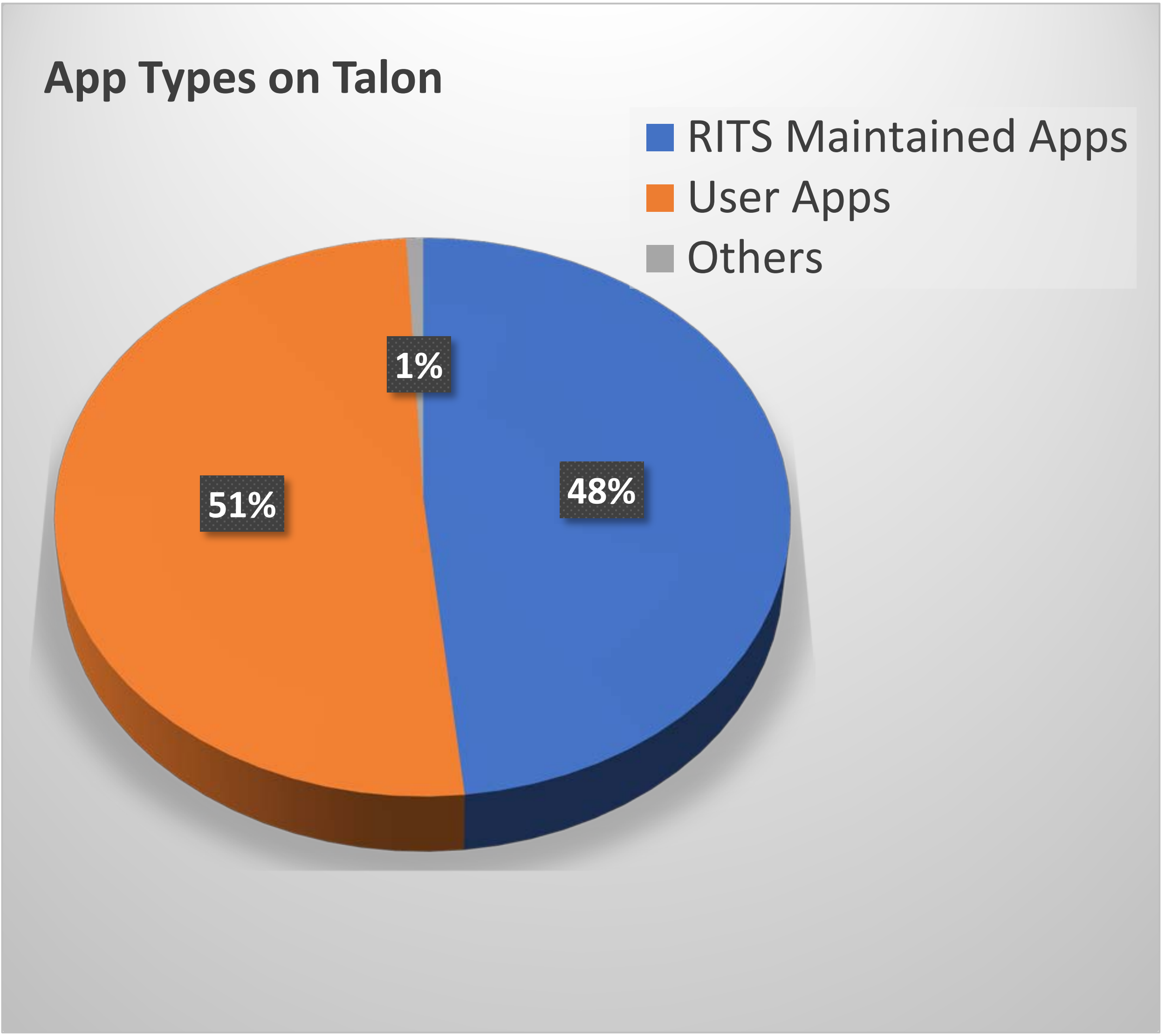
Convert Serial → Parallel & Distributed
Assist in Parallel → Massively Parallel
Develop Interdisciplinary Grant Capabilities

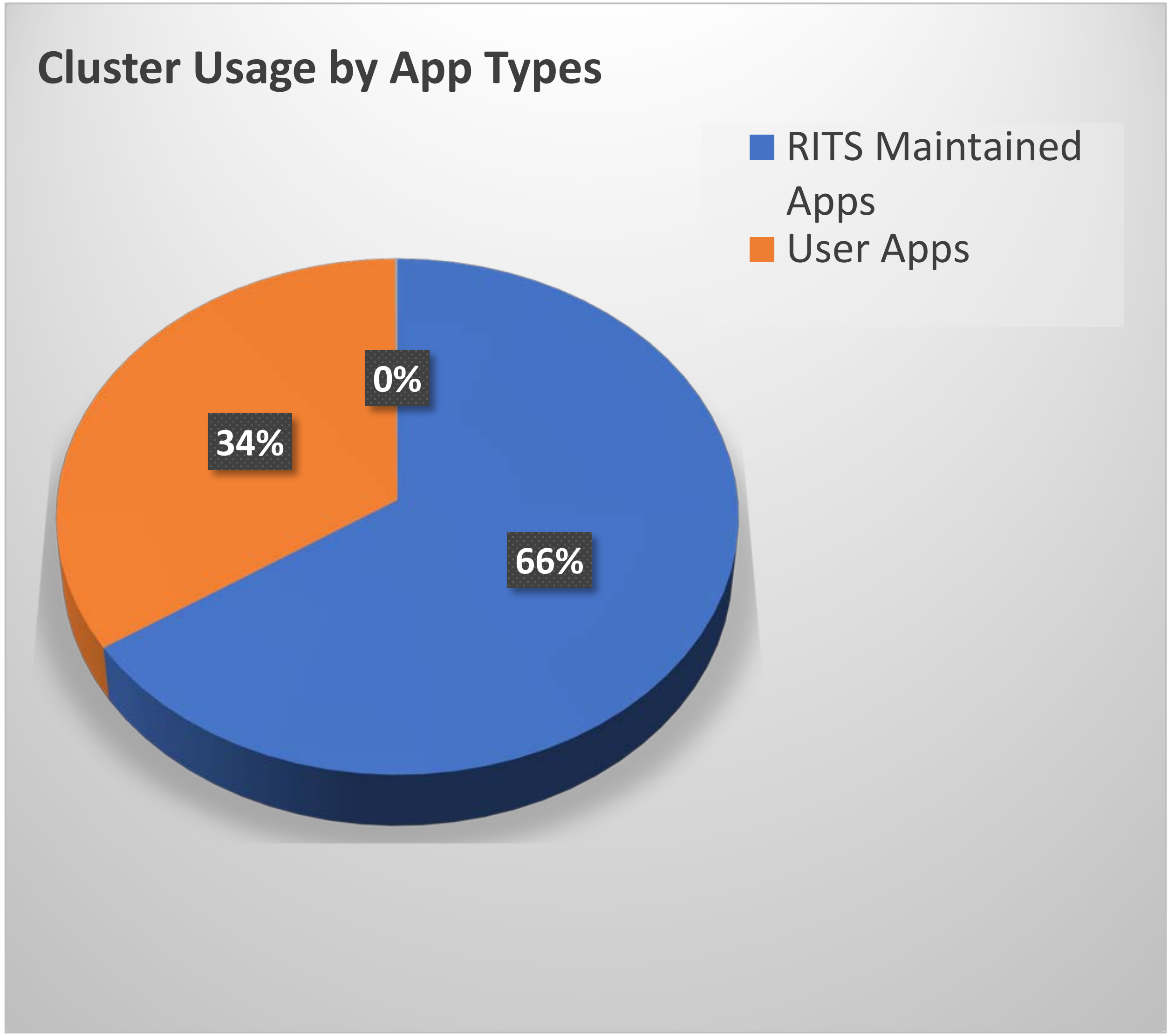
Parallel Applications: **17**

Serial Users: **24**

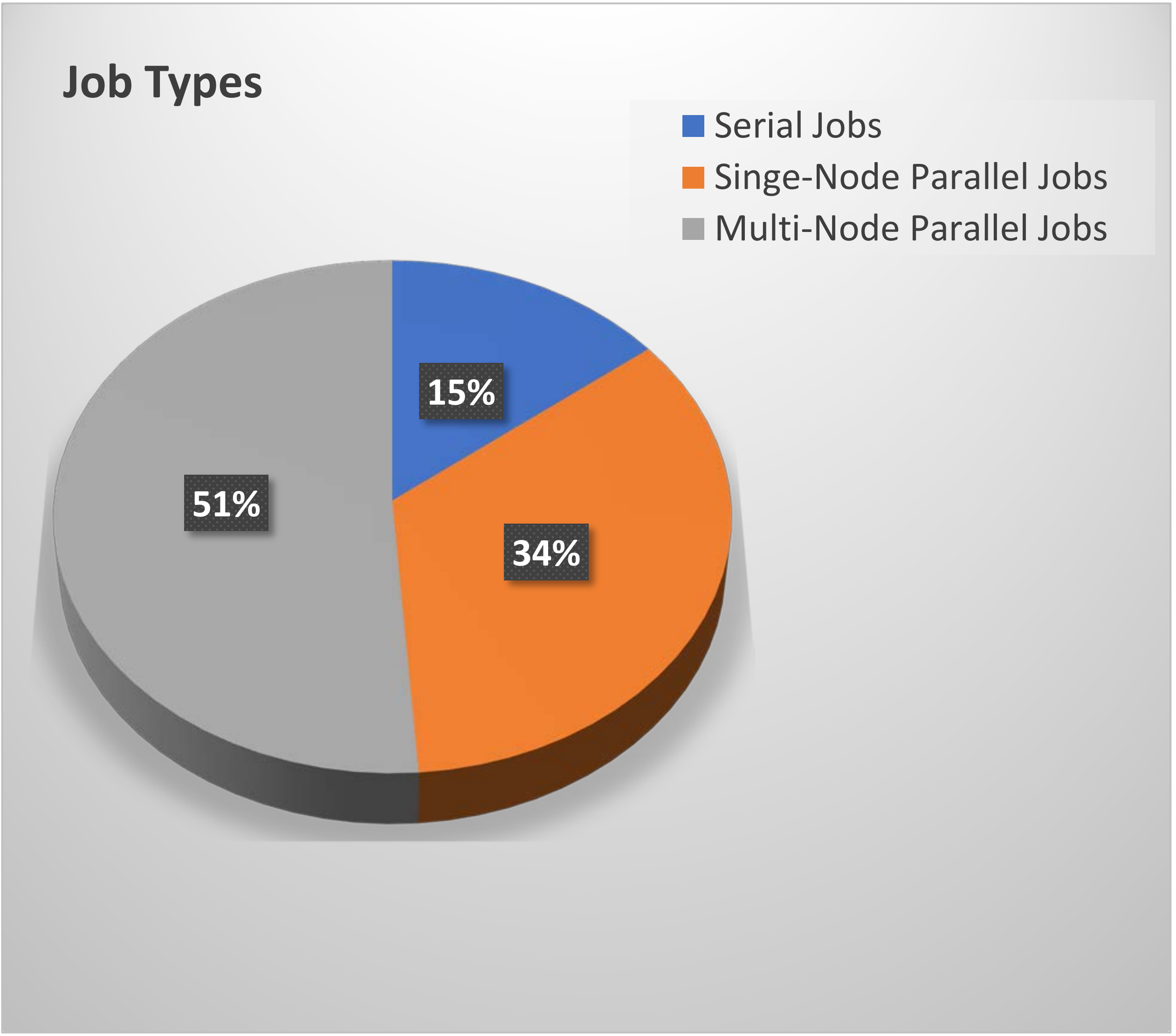
Other —Distributed and Unknown: **12**

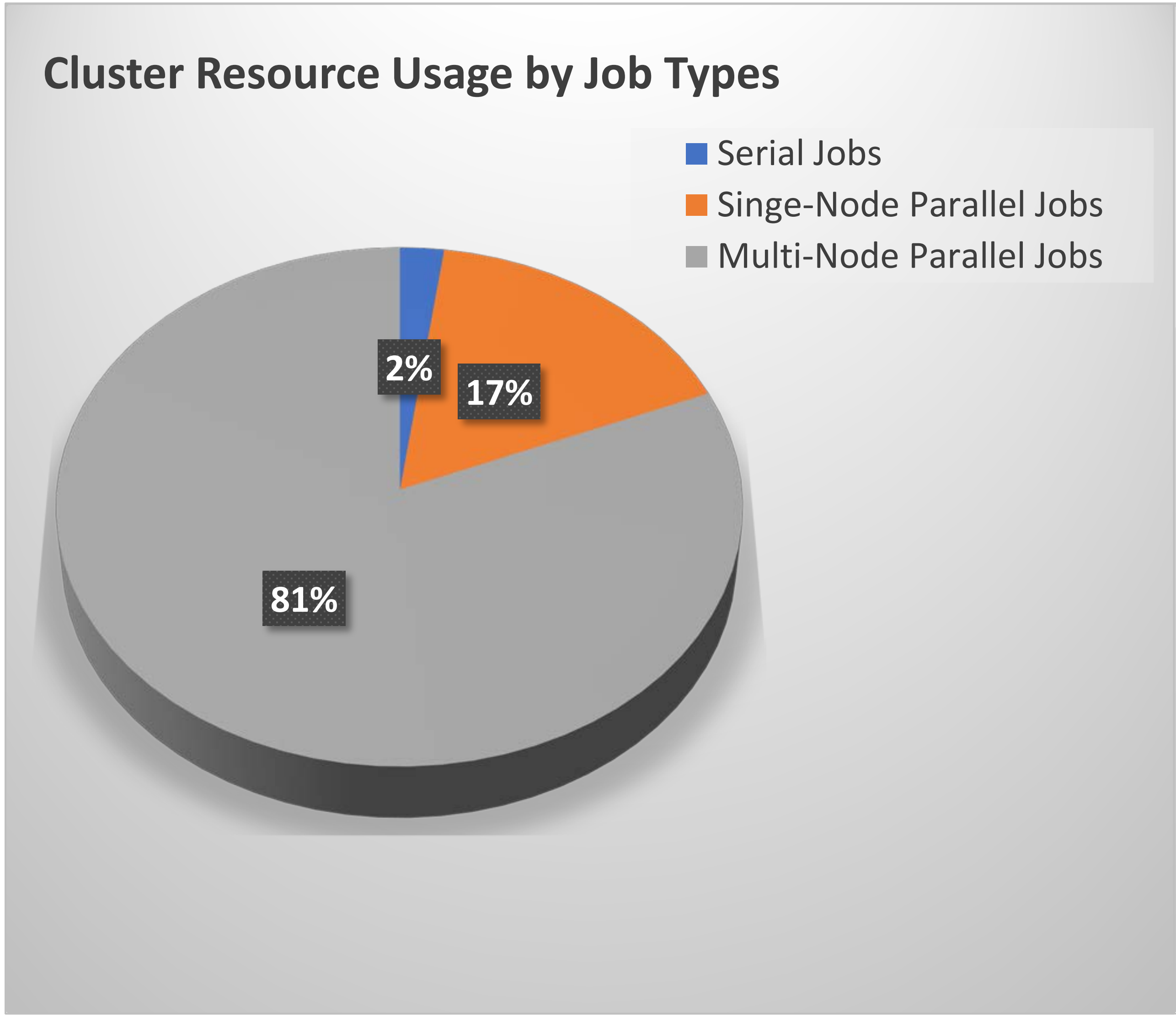
App Types on Talon



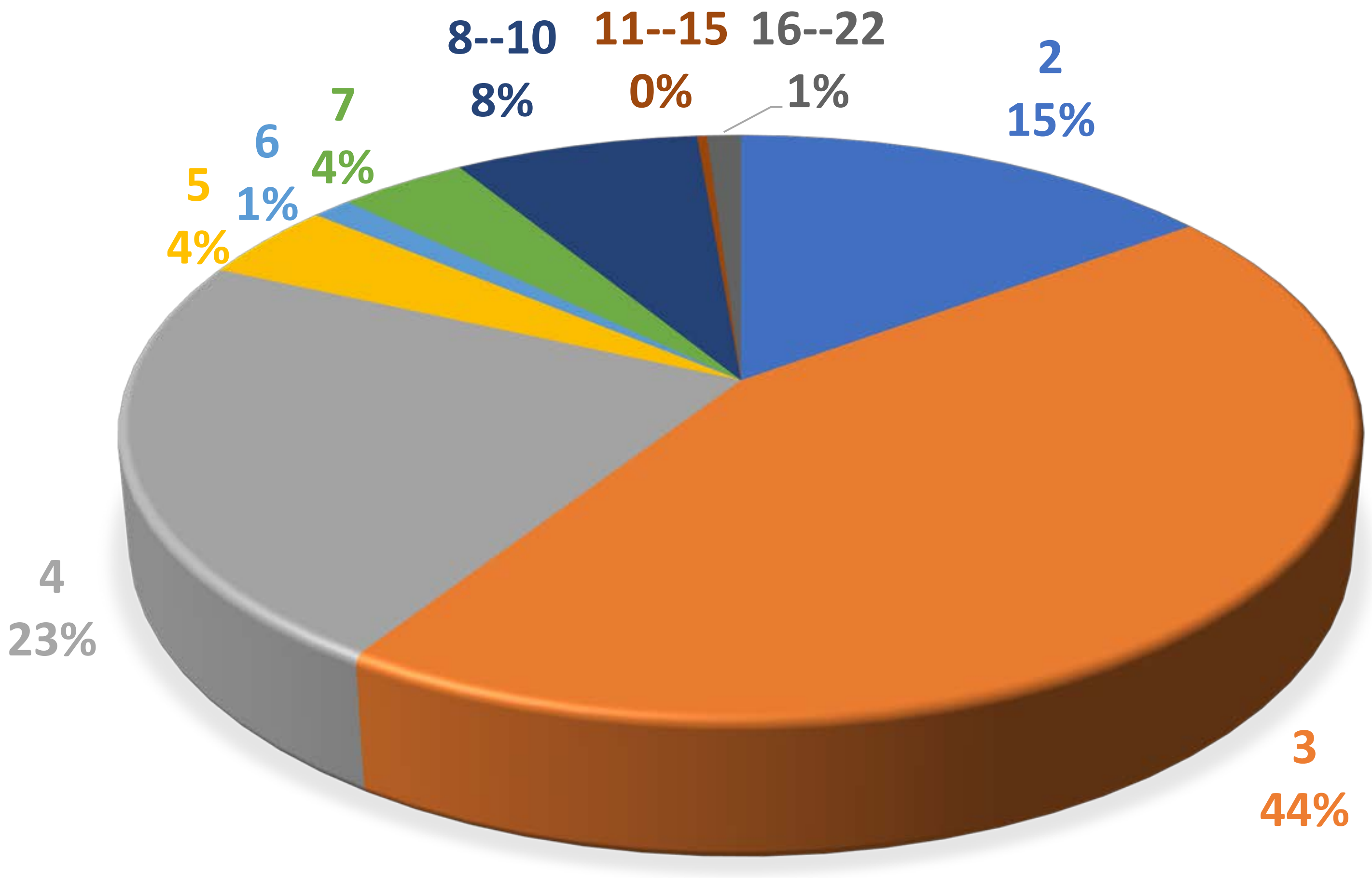


Job Types on Talon





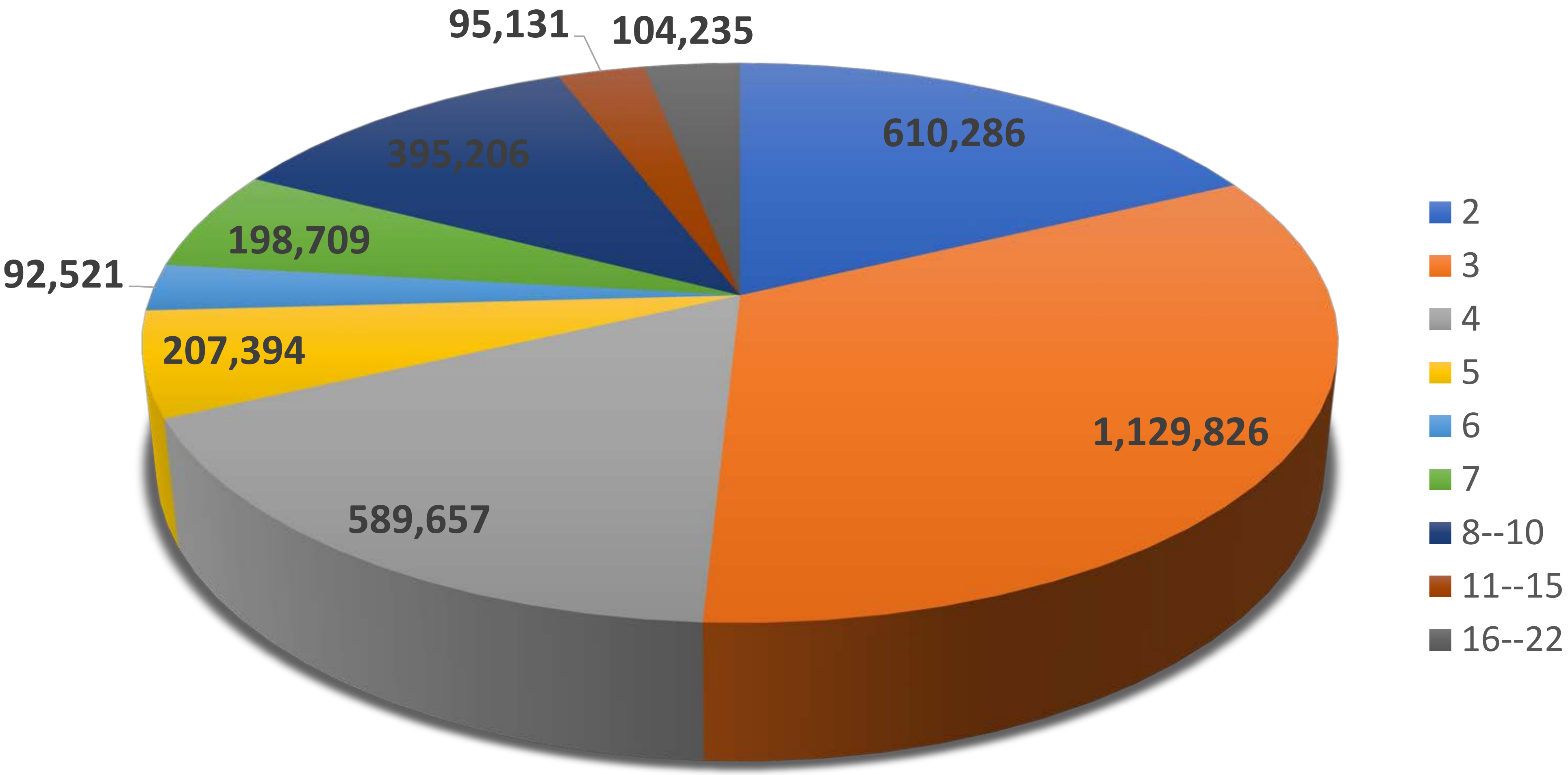
Node Distribution of MPI Jobs



Major MPI Apps Running On Talon

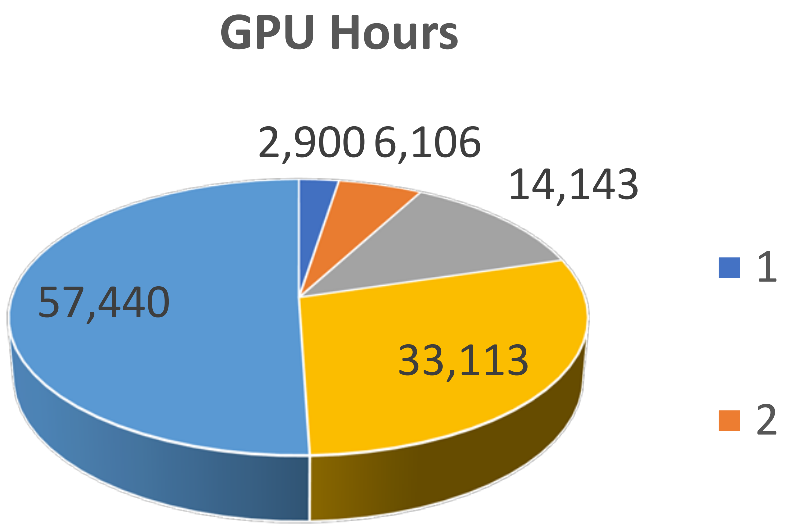
VASP
Quantum Espresso
LAMMPS
DLPOLY
NWChem
Amber
OpenFOAM

CPU Hours Used Across the MPI Jobs



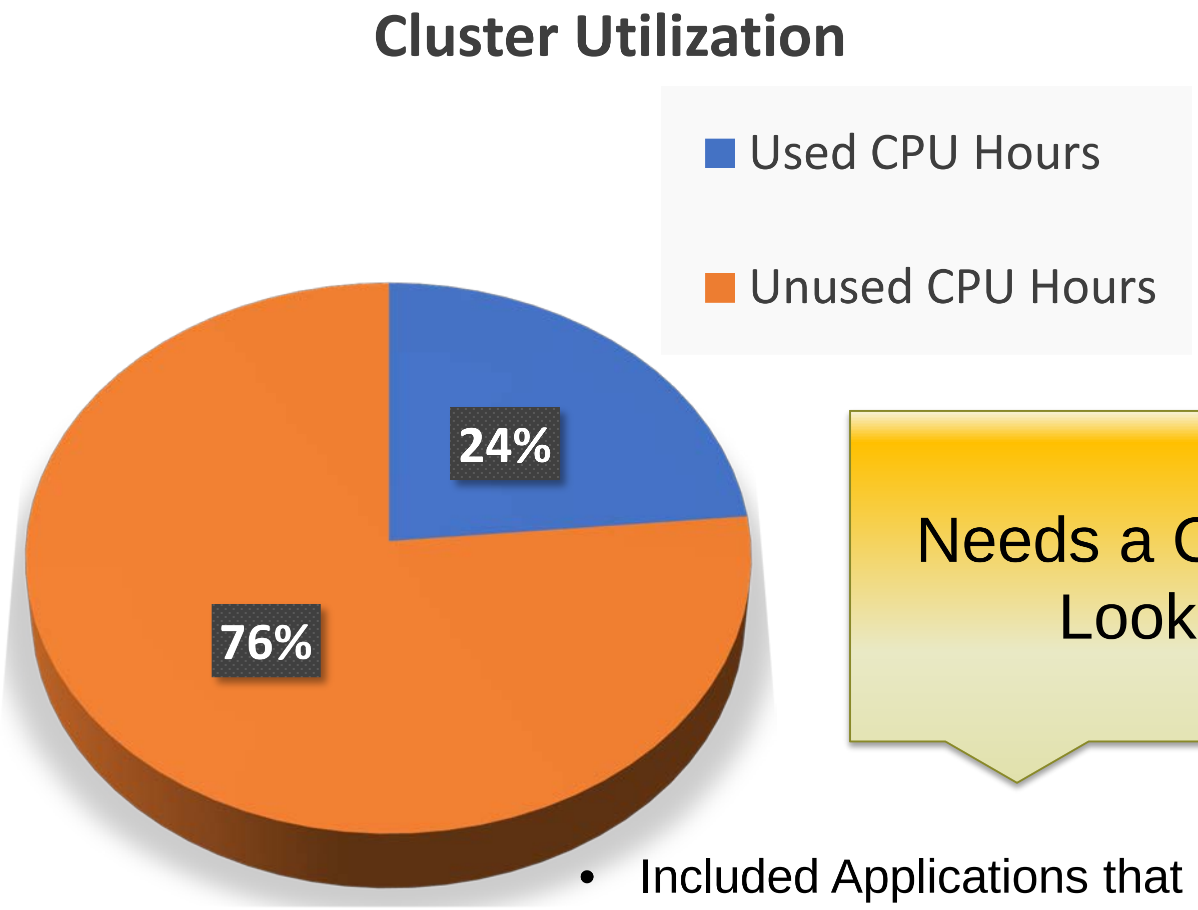
GPU Jobs Running on Talon

		GPU Hours	Jobs	Adjusted Jobs
Number of GPUs	1	2,900	55*	105
	2	6,106	50*	54
	3	14,143	39*	64
	4	33,113	123*	147
	5-8	57,440	103*	103
Amber		80,344	219	254
Python based GPU applications		33,358	125	219
All		113,702	344	473



*Jobs may use different number of GPUs in sub jobs.

XALT 2.8: Node Allocation / Utilization



Needs a Closer Look!

- Included Applications that use DLL
- Nodes allocated for Memory
- Aborted jobs don't count
- Job runtime under 30min not included

SLURM Report

hpc.unt.edu

System Status and Alerts

	Talon3
System Status	UP/Healthy
Number of Jobs	94 Running / 99 Queued
Allocated C6320	99.5 %
Allocated R420	99.3 %
Allocated R720	12.5 %
Allocated R730	100 %

- Statically linked apps not included
- Legacy Codes?
- Asking for more and using less?
- Mixed node issues (C6320, R420)

Data Science & Analytics

Richard Herrington, Ph.D.

Liaison for All Colleges — except CoS and CENG

We can help in convergence research!

Research(er) Challenges

- **Typical data are messy and modelling with messy data is problematic**
  - Small data or large data — so-called “curse of dimensionality”
  - Missing data — drop-out, unit non-response — and outlying data
  - Unidentified mixtures in the data — multiple modes or “bumps”
  - Unidentified sources of hidden correlation in the data
  - Complex data structures or data collection designs — hierarchical, unbalanced, and non-replicated designs
  - Non-random sampling and assignment designs — observational data versus experimental
  - Correlational versus causal modeling research goals — the mismatch
  - Selection bias and measurement error
- **Software algorithms can be fragile**
  - Many software algorithms can fail to converge or fail to provide satisfactory solutions
  - We will either find resolutions to these software convergence issues or suggest alternatives that are more robust and meet your goals

DSA Software Services

- **General purpose software**
  - R, Python (general purpose statistical programming language and statistical analysis environment – like MATLAB or Octave); SAS, SPSS
  - RStudio (a desktop and server-based R and Python IDE for browser-based analysis and visualization); JupyterLab and Jupyter Notebooks

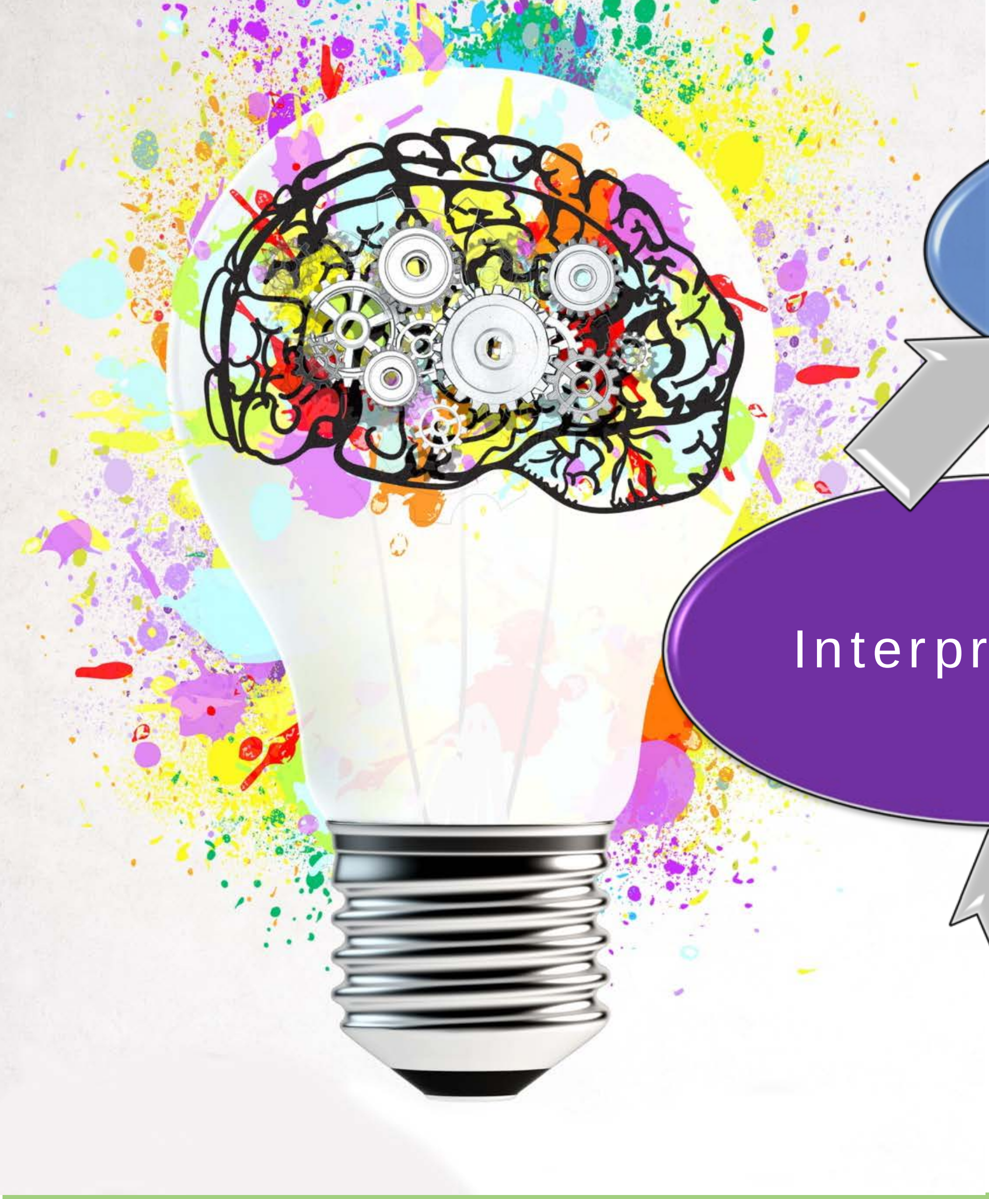
- **Specialized software**
  - MATLAB, Mathematica (numerical and symbolic analysis)
  - Mplus, LISREL, AMOS (structural equations)

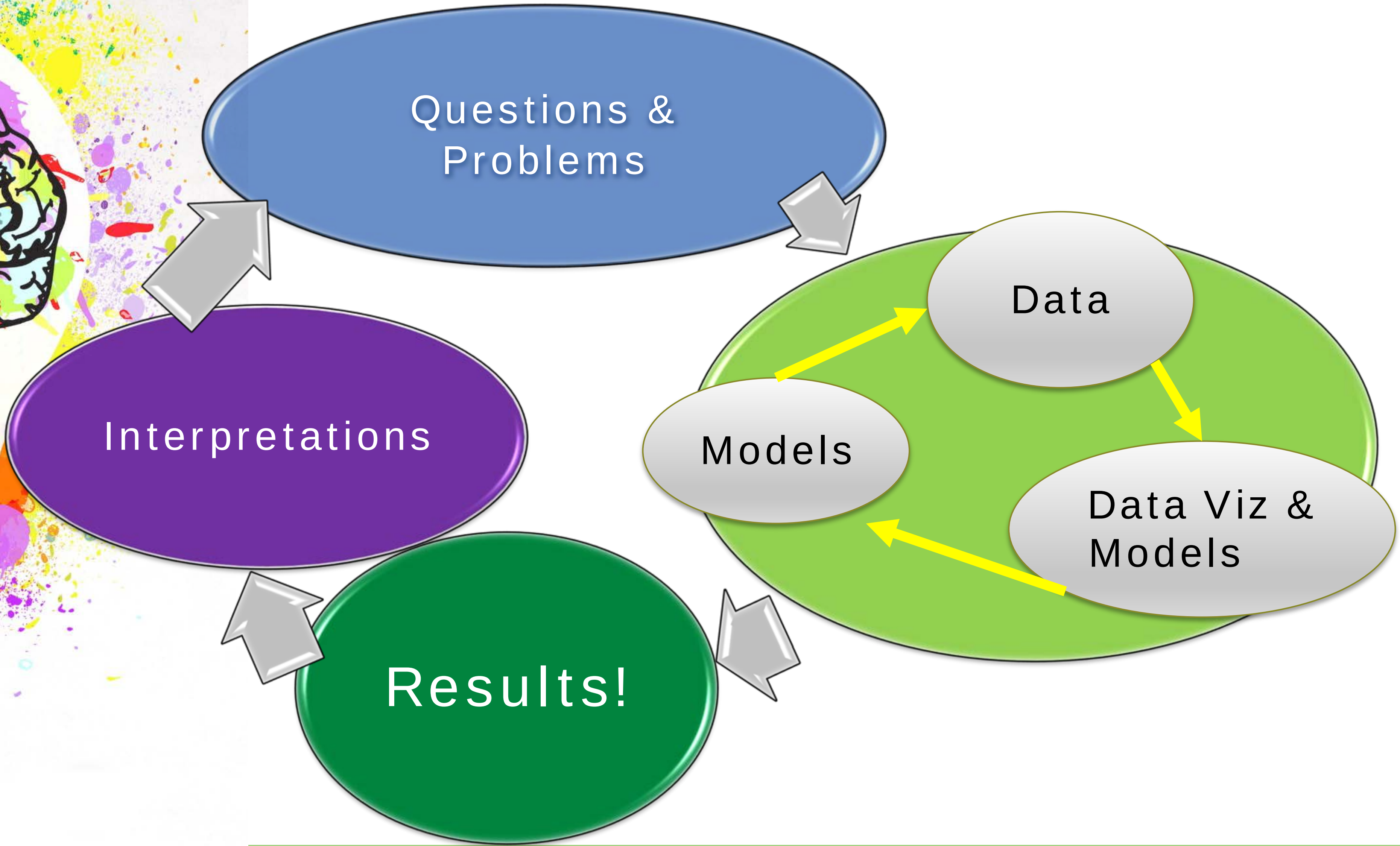
Interactive Data Exploration and Analytics on Talon (IDEA)

Let's have an IDEA together!

North Texas Scientific Computing

IDEATION for Agile Analytics





IDEA

- Framework for on-demand collaborations: engage with data and models
- Hardware:
  - Five visualization nodes with 2 NVIDIA V100 GPU cards, and 3 NVIDIA V100S GPU cards, and a total of 156 CPU-cores.
  - Support batch submission and interactive logins
  - Access these nodes through SSH login and through web API's
- These nodes are equipped with:
  - X11 windowing capability
  - Authentication into RStudio IDE (port 8787) and JupyterHub Platform (port 8000)
  - Access to customize-able Shiny Web Applications (port 3838)

Video of this introduction will be posted on our NTSC website (no more than 5 minutes)

- Quick introduction to RStudio IDE (demonstrate main capabilities)
- Quick introduction to Shiny Web Application Server (give quick example)
- Quick Introduction to JupyterHub Server and Jupyter Notebooks

New Directions

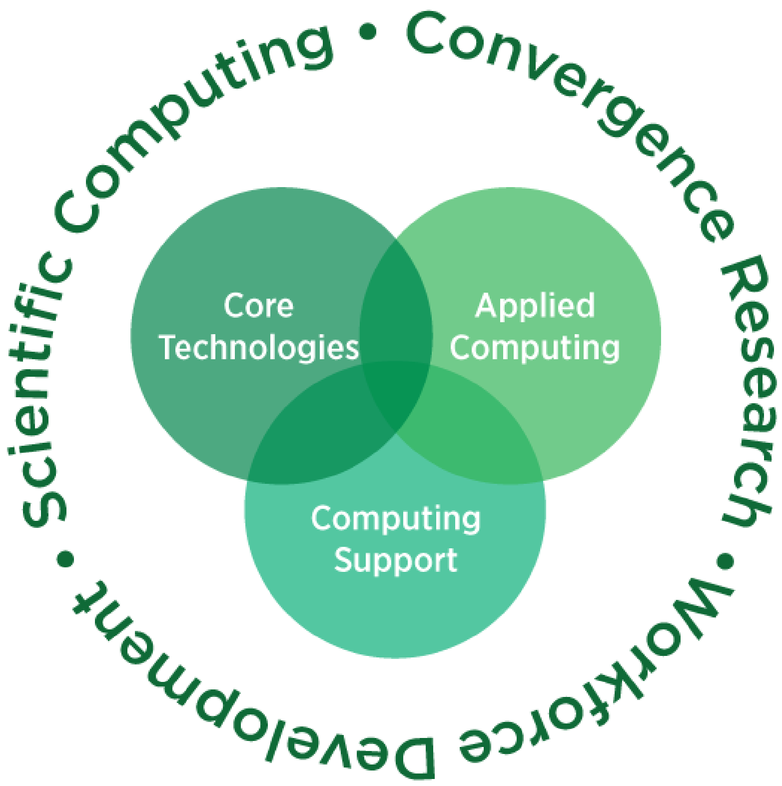
Campus CI:
Extended Collaborative Support Services*

Core Technologies. Faculty and staff engaged in high-performance computing, cloud computing, data analytics, algorithms, machine learning, artificial intelligence, and embedded systems, etc.

Applied Computing. Faculty and staff with research and interests in science, engineering, liberal arts, and medicine.

Computing Support. The NTCSC staff with advanced degrees in domain areas. Deploy scientific computing technologies and provide application support services.

Convergence research. Sharing scientific methods and ideas across a broad range of varied disciplines to untangle complex problems focusing on societal needs.



Paradigm for
ECSS at UNT

*Campus-level deployment of XSEDE ECSS

Key Takeaways

- Our purpose is to help you unlock the wide range of computational resources to expedite science and innovation through incremental pattern of success.
- We fully engage in research support and our partnerships with ITSS provide widespread engagement opportunities across UNT System.
- College liaisons serve as your point of contact in your research journey throughout the scientific computing continuum.
- Establishing Extended Collaborative Support Services, ECSS@UNT, to accelerate applied computing and convergence research opportunities.
- *Talon3 customer support management is moving to ServiceNow. For support, please write to us at* **SciComp-Support@unt.edu**.

Thank you!

Questions?

email: SciComp-Support@unt.edu
Web: it.unt.edu/ntsc