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# Scaling Up Research Computing: ARC Systems and Services

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# Some Common Scenarios

*“Our team just completed the first run of our analysis and found that it took four hours to run on a laptop. The results are perfect, but we have 8,500 more of these to run and need finish in a few months. Even if we all had our laptops running 24x7, it would take more than a year!”*

*“I have a 80GB data set that I need to process using a colleague’s program. I have done this with 3GB data sets in the past, but my computer crashes when I try to process the larger data set. I think I need more memory.”*

*“I want to try out using this neural network to see if it provide insights into my problem. But training it on my data is taking weeks.”*

# Overview

- What is ARC?
- What does ARC have?
- What services does ARC provide?
- How to get started

# What is ARC?



# ARC's Mission

*Advanced Research Computing (ARC) provides centralized support for research computing by building, operating and promoting the use of advanced cyberinfrastructure at Virginia Tech.*

*ARC delivers a comprehensive ecosystem consisting of advanced computational systems, large-scale data storage, visualization facilities, software, and consulting services.*

*ARC provides education and outreach services through conferences, seminars, and scientific computing courses.*

*ARC seeks to help maximize research productivity at Virginia Tech through interdisciplinary collaborations that connect researchers to new opportunities in computing and data driven research as they occur.*

*By fostering strategic partnerships with the public and private sector, ARC serves to cultivate an entrepreneurial spirit around advanced computing infrastructure as a platform for collaboration and helps secure the position of Virginia Tech as a leader in education and research.*

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# ARC's Mission

In a nutshell our goals are to:

- Engage with researchers across all colleges, centers, and disciplines at Virginia Tech

... and to ...

- Advance the research programs of Virginia Tech faculty and students by providing the Research Computing systems (hardware, software, integration) and support (helpdesk, consultation, collaboration) that will help them excel.



# Who We Are

**Associate VP for Research Computing:**

Terry Herdman

**Assist. Director, Development and Fiscal Admin:  
Network Research Manager:**

Alana Romanella  
Mark K. Gardner

**Director, Visualization:  
Visualization and Virtual Reality Systems Specialist:**

Nicholas Polys  
Lance Arsenault

**Computational Scientists/Software Engineers:**

Justin Krometis, James McClure,  
Bob Settlage, Matt Brown, Nathan Liles

**Director of ARC Operations:  
Systems Engineers/HPC System Administrators:**

Kevin Shinpaugh  
Miles Gentry, Jeremy Johnson,  
Doug McMaster, William Marmagas,  
Jessie Bowman, Ben Sandbrook

**Plus our student interns and Helpdesk GRAs!**





# Division of IT Inter-Connections

- ARC systems are connected to and integrated with VT infrastructure and services
  - Networks and data centers
  - Authentication, directory services, 4Help, hosting
  - Logging, monitoring, alerting
- Deliver courses/workshops via TLOS's Prof. Development Network
- Direct or indirectly make use of wide range of DoIT systems/services

# ARC Systems

## TinkerCliffs - Flagship CPU Cluster

tc-hm[001-008]  
largemem\_q



tc[001-308]  
dev\_q, preemptable\_q  
tc[001-307]  
  
normal\_q  
tc[001-302]  
  
interactive\_q  
tc308



tc-cl[001-016]



316 Nodes w/ 128 cores (AMD EPYC Rome)  
16 Nodes w/ 96 cores (Intel Cascade Lake-AP)  
41,984 CPU cores

## Infer - Accelerating ML/DL and Inference

inf[001-016]  
t4\_normal\_q



inf[021-060]  
p100\_normal\_q



16 Nodes w/ 32 cores (Intel Skylake) + 1 NVIDIA T4 GPU (2560 CUDA + 320 tensor cores)  
40 Nodes w/ 28 cores (Intel Broadwell) + 2 NVIDIA P100 GPUs (3580 CUDA cores)  
1,632 CPU cores  
96 GPU accelerators  
184,160 CUDA cores  
5,120 Tensor cores

## Coming 2021: Dense GPU for AI

ai[001-04]  
a1\_q



4 Nodes w/ 128 cores (AMD Epyc Rome 7742)  
+ 8 NVIDIA A100-80GB GPUs (6912 CUDA)  
512 CPU cores  
32 GPU accelerators  
221,184 CUDA cores

## Cascades - Heterogeneous HPC + GPU

ca[001-002]  
largemem\_q



ca[003-006]  
k88\_q



tc[007-196]  
dev\_q, preemptable\_q  
tc[007-196]  
normal\_q  
tc[007-195]



ca[197-236]  
v100\_normal\_q



2 Nodes w/ 72 cores (Intel Broadwell)  
4 Nodes w/ 32 cores (Intel Broadwell) + 2 NVIDIA K80 GPUs (4,992 CUDA cores)  
190 Nodes w/ 32 cores (Intel Broadwell)  
40 Nodes w/ 24 cores (Intel Skylake) + 2 NVIDIA V100 GPUs (5,120 CUDA cores, 640 tensor cores)  
7,168 CPU cores  
88 GPU accelerators  
449,536 CUDA cores

## Dragonstooth - HTC

dt[003-048]  
normal\_q



48 Nodes w/ 24 cores (Intel Haswell)  
1,152 CPU cores

Scheduler permits very long jobs (30 days)  
Scheduler permits large volumes of small jobs

## Huckleberry - Power for Deep Learning

hu[001-014]  
normal\_q



14 Nodes w/ 120 cores (IBM Power8) and 4 NVIDIA P100 GPUs w/ NVLINK  
1,680 CPU cores  
56 GPU accelerators  
200,704 CUDA cores



# Systems

## Aggregated resources:

690	Compute nodes
54,128	CPU cores
272	GPU accelerators
1,055,584	NVIDIA Cuda cores

- + high speed Ethernet and low-latency Infiniband interconnecting networks
- + large scale and high-performance parallel storage (~10PB total)
- + various boutique/custom architecture systems



# Systems

## Aggregated resources:

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54,128	CPU cores
272	GPU accelerators
1,055,584	NVIDIA Cuda cores



ARC has diverse architectures and capacity to meet the demands of a wide variety of projects and scale them up.

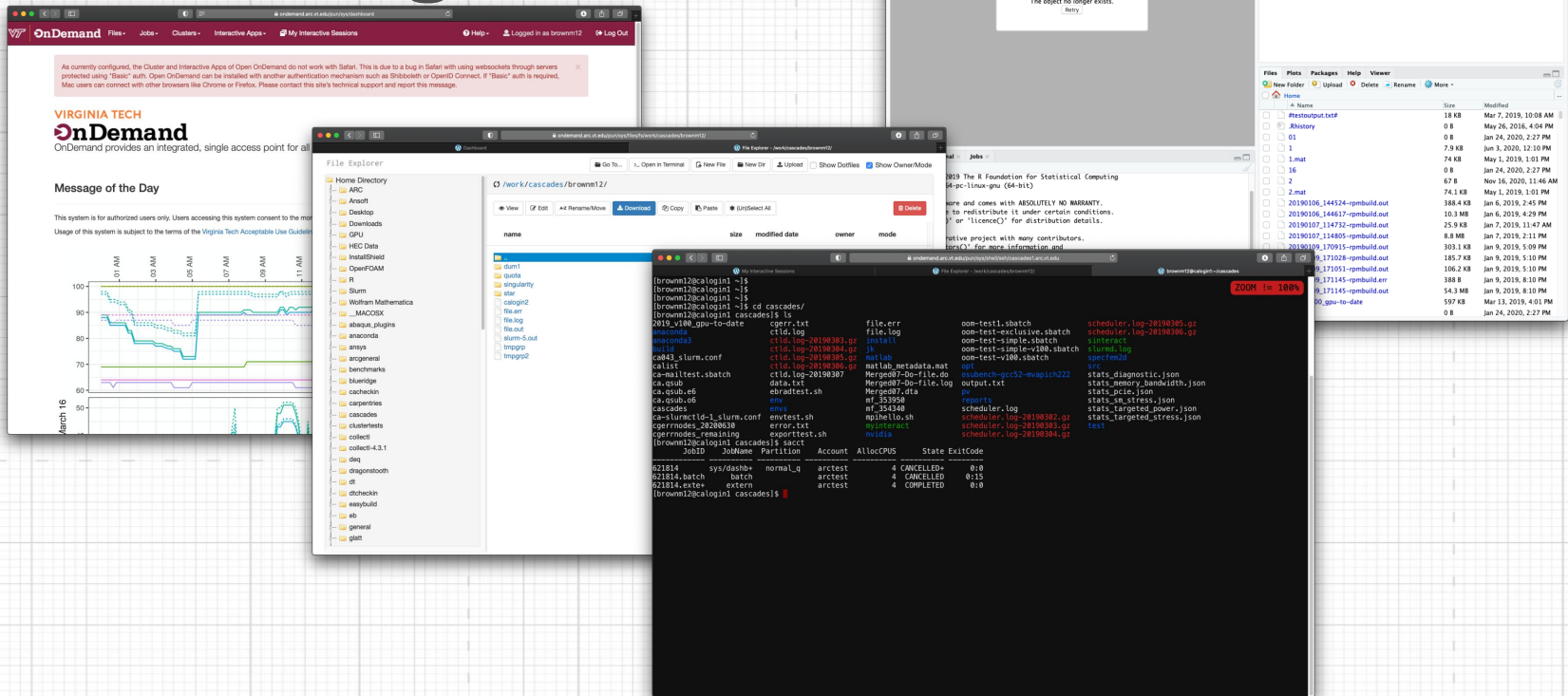
# Industry standard usage model

- Linux clusters, SLURM scheduler, Infiniband interconnect
- Connect to “login node” using SSH client, upload/download files
- Compose job script, submit to scheduler, job runs in batch mode on compute nodes

This is still a very productive model and the dominant mode of usage for many researchers, but has presented barriers to entry for others.



# Removing barriers





# ARC Services

# Use of Systems

## Free Tier (Subsidized by VT/DoIT)

- Unlimited use (subject to availability) of older systems
- Generous monthly compute allowances on newer system
- 1TB storage per person, 25TB per principle investigator
- Support via ARC Helpdesk, consultation with Computational Scientists
- Archival data storage

## ARC Cost Center

- Compute capacity and priority beyond the free tier
- More storage capacity available

# Consulting and Collaboration

## **ARC Computational Scientists**

- Understand the Applications
- Provide Research Domain Expertise
- Offer Classes, Short Courses and Workshops
- Optimization of Codes

## **ARC Helpdesk (via 4Help)**

- Getting started with ARC
- Basic questions and troubleshooting



# Visualization













- Desktop Visualization
- HyperCube in the Visionarium Lab
- User support and consulting
- Research collaboration
- Trainings and classes
- Tours and field trips





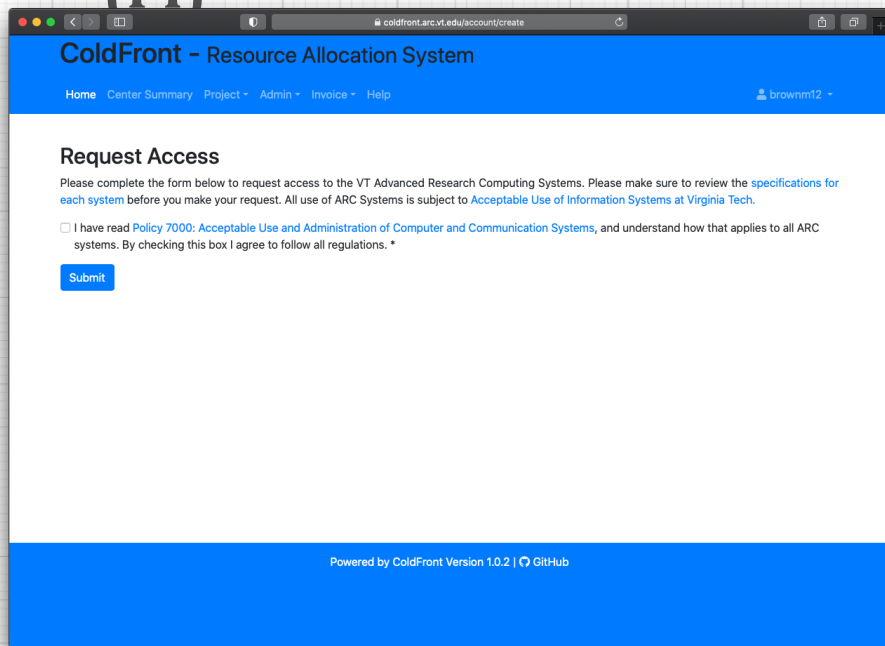
# ARC Course Offerings

- ARC Personnel offer or guest lecture in regular courses (Math, CS, AOE, Statistics, CMDA)
- ARC Personnel offer short courses and workshops
  - Introduction to ARC systems
  - Introduction to High Performance Computing
  - Deep learning with NVIDIA Digits
  - Python for scientific computing
  - Parallel R
  - Numerical computing in Julia
  - Visual computing
  - Virtual Reality

 <p>Research &amp; Discovery</p> <p> Introduction to Visualization at ARC</p> <p>Thu Mar 28 / 10:00-11:30a / Torg 1100</p> <p>Mar 28 - Mar 28, 2019   2 credits</p> <p></p>	 <p>Research &amp; Discovery</p> <p> Intro to ARC</p> <p>Fri Feb 22 / 11:00a-12:00p / Torg 1100</p> <p>Feb 22 - Feb 22, 2019   1 credit</p> <p></p>
 <p>Research &amp; Discovery</p> <p> Intro To HPC</p> <p>Fri Feb 22 / 1:00-3:00p / Torg 1100</p> <p>Mar 5 - Mar 5, 2019   2 credits</p> <p></p>	 <p>Research &amp; Discovery</p> <p> Parallel R Tutorial</p> <p>Tues Apr 2 / 10:00-11:30am / Torg 1100</p> <p>Self-paced   2 credits</p> <p></p>

# Getting Started

# Getting Started: Create an account (all) & project (PI)



The screenshot shows the 'ColdFront - Resource Allocation System' interface for account creation. The browser address bar shows 'coldfront.arc.vt.edu/account/create'. The page has a blue header with navigation links: Home, Center Summary, Project, Admin, Invoice, and Help. The user 'brownm12' is logged in. The main content area is titled 'Request Access' and contains instructions to complete the form for requesting access to VT Advanced Research Computing Systems. It includes a checkbox for agreeing to the 'Policy 7000: Acceptable Use and Administration of Computer and Communication Systems'. A 'Submit' button is at the bottom of the form. The footer indicates 'Powered by ColdFront Version 1.0.2 | GitHub'.

ColdFront - Resource Allocation System

Home Center Summary Project Admin Invoice Help brownm12

## Request Access

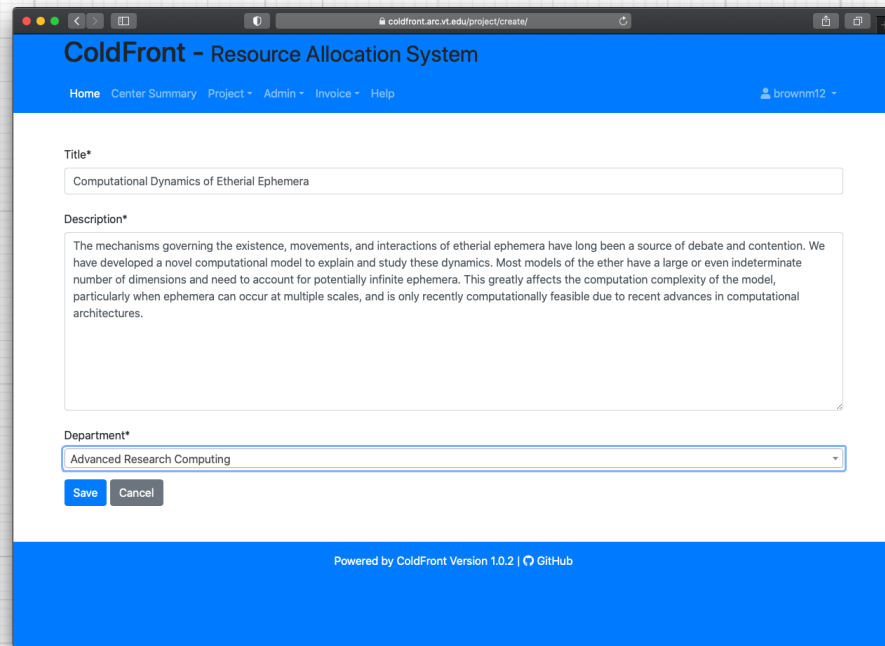
Please complete the form below to request access to the VT Advanced Research Computing Systems. Please make sure to review the [specifications for each system](#) before you make your request. All use of ARC Systems is subject to [Acceptable Use of Information Systems at Virginia Tech](#).

☐ I have read [Policy 7000: Acceptable Use and Administration of Computer and Communication Systems](#), and understand how that applies to all ARC systems. By checking this box I agree to follow all regulations. \*

Submit

Powered by ColdFront Version 1.0.2 | GitHub

<https://coldfront.arc.vt.edu/account/create>



The screenshot shows the 'ColdFront - Resource Allocation System' interface for project creation. The browser address bar shows 'coldfront.arc.vt.edu/project/create/'. The page has a blue header with navigation links: Home, Center Summary, Project, Admin, Invoice, and Help. The user 'brownm12' is logged in. The main content area is titled 'Title\*' and 'Description\*'. The 'Title\*' field contains 'Computational Dynamics of Etherial Ephemera'. The 'Description\*' field contains a paragraph about the mechanisms governing the existence, movements, and interactions of etherial ephemera. Below the description is a 'Department\*' dropdown menu with 'Advanced Research Computing' selected. 'Save' and 'Cancel' buttons are at the bottom of the form. The footer indicates 'Powered by ColdFront Version 1.0.2 | GitHub'.

ColdFront - Resource Allocation System

Home Center Summary Project Admin Invoice Help brownm12

Title\*

Computational Dynamics of Etherial Ephemera

Description\*

The mechanisms governing the existence, movements, and interactions of etherial ephemera have long been a source of debate and contention. We have developed a novel computational model to explain and study these dynamics. Most models of the ether have a large or even indeterminate number of dimensions and need to account for potentially infinite ephemera. This greatly affects the computation complexity of the model, particularly when ephemera can occur at multiple scales, and is only recently computationally feasible due to recent advances in computational architectures.

Department\*

Advanced Research Computing

Save Cancel

Powered by ColdFront Version 1.0.2 | GitHub

<https://coldfront.arc.vt.edu/>

# References

- ARC Website resources: <https://arc.vt.edu/>
- ARC has [video tutorials](#)
- OnDemand web interface for ARC systems <https://ondemand.arc.vt.edu>
- ColdFront - Account creation and management <https://coldfront.arc.vt.edu>
- ARC Training opportunities via TLOS PDN <https://profdev.tlos.vt.edu>
- General questions or help with ARC systems: <https://arc.vt.edu/help>
- Me (Matthew Brown): [brownm12@vt.edu](mailto:brownm12@vt.edu)