Advanced Research Computing

Justin Krometis
Advanced Research Computing
Information Technology
Virginia Tech
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.

Provide Virginia Tech students and faculty with the Research Computing software, hardware and support required to advance their research programs (provide a competitive edge in external research funding)
Who We Are

- **Associate VP for Research Computing:** Terry Herdman (herd88@vt.edu)
- **Director, Visualization:** Nicholas Polys (npolys@vt.edu)
- **Director, Archival Data Management:** Gary Worley (gworley@vt.edu)
- **Assist. Director, Development and Fiscal Admin:** Alana Romanella (aromanel@vt.edu)
- **Network Research Manager:** Mark K. Gardner (mkg@vt.edu)
- **Computational Scientists/Software Engineers:**
  - Justin Krometis (jkrometis@vt.edu), James McClure (mcclurej@vt.edu)
  - Srijith Rajamohan (srijithr@vt.edu), Bob Settlage (rsettlage@vt.edu)
  - Mathew Brown (brownm12@vt.edu), Nathan Liles (nml5566@vt.edu)
- **Visualization and Virtual Reality Systems Specialist:** Lance Arsenault (lanceman@vt.edu)
- **NI&S provides systems support, Lead:** Matt Stricker (mdstrick@vt.edu)
# Hardware (20k cores, 1.8 PFLOPS)

<table>
<thead>
<tr>
<th>System</th>
<th>Usage</th>
<th>Description</th>
<th>Special Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cascades</td>
<td>Large-scale CPU, GPU</td>
<td>194x 32 cores, 128 GB&lt;br&gt;39x 24 cores, 276 GB&lt;br&gt;2x 72 cores, 3 TB</td>
<td>78 V100 GPU&lt;br&gt;8 K80 GPU&lt;br&gt;2 3TB nodes</td>
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<tr>
<td>Huckleberry</td>
<td>Deep Learning</td>
<td>12x IBM Power8 (Minsky), 256 GB</td>
<td>96 P100 GPU with NVLink</td>
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<tr>
<td>NewRiver</td>
<td>Large-scale CPU, GPU, Data Intensive</td>
<td>124x 24 cores, 128 GB (Haswell)&lt;br&gt;39x 28 cores, 512 GB (Broadwell)&lt;br&gt;2x 60 cores, 3 TB (Ivy Bridge)</td>
<td>78 P100 GPU&lt;br&gt;8 K80 GPU&lt;br&gt;16 “big data” nodes&lt;br&gt;24 512GB &amp; 2 3TB nodes</td>
</tr>
<tr>
<td>DragonsTooth</td>
<td>Single-node</td>
<td>96x 24 cores, 256 GB (Haswell)</td>
<td>OpenStack on 48 nodes</td>
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<tr>
<td>BlueRidge</td>
<td>Large-scale CPU</td>
<td>408x 16 cores, 64 GB (Sandy Bridge)</td>
<td>4 K40 GPU&lt;br&gt;18 128GB nodes</td>
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Visualization

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

• Understand the Applications
• Provide Research Domain Expertise
• Offer Classes, Short Courses and Workshops
• Optimization of Codes
• Provide ARC HPC Cloud Environment
• Provide HPC Investment Computing Program
ARC Course Offerings

• ARC Personnel offer or guest lecture in regular courses (Math, CS, AOE, Statistics, CMDA)
• ARC Personnel offer short courses and workshops
  • Examples:
    • 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
IBM “Minsky” compute node: higher performance per node, increase research productivity per unit time from a physical rack

Fourteen nodes, IBM Power8 CPU + 4 NVIDIA P100 GPU per node

Data movement limits performance for most applications — NVLINK accelerates data transfers within a node

Deep learning applications have the largest performance advantages

IBM Power AI software supports major open source deep learning frameworks optimized for POWER + NVIDIA architecture
How We Implement DoIT’s Core Values

• Trust: We invest in developing partnerships and strive to deliver sustainable support for the communities that we serve

• Inclusion: We actively search for new tools and means of engagement to enable non-traditional HPC users to use our resources

• Care: We actively listen to our users and students while remembering to ask the question "how can we support and help you.”

• Service: We are always available for our users both walk-in and through appointments and strive to rapidly and proactively address users’ needs

• Striving for Excellence: We work to provide cutting-edge hardware and end-to-end support to enable users to leverage it.