User Forum

NASA Center for Climate Simulation
High Performance Science

June 26, 2018
Agenda

• CISTO and NCCS Changes
• Discover Linux Cluster
• ADAPT Virtualization Environment
• Storage/Analytics Architecture and Data Management Plans
CISTO and NCCS Changes

Dan Duffy,
Chief, Computational and Information Sciences and Technology Office (CISTO)
HPC Lead and NCCS Lead Architect
June 2018: Staff Additions

Welcome to New Members of the NCCS and CISTO Team:

Kerman Bime/IT Coalition, System Administration
Jim Carlisi/GDIT, System Administration
Luli Laulu/Inuteq, Office Administrative Assistant
Elizabeth Nerdig/GDIT, Facilities Engineer
Jason Robbins/ GDIT, System Administration
George Roros, Kiosk Technology Consultant
Darryl Smallwood/ IT Coalition, Data Services
Colton Weinman, Graphics Design Consultant
Gabe Borroni, Disasters GIS Analyst
Garrett Layne, Disasters GIS Analyst
Buchi Oraegbu, AIST Managed Cloud Environment
Dan Sherman, AIST Managed Cloud Environment
Welcome to New Members of the NCCS and CISTO Team:

Jordan Caraballo-Vega
Thomas Favata
August Morin
Paulo Paz
Carly Robbins
Matt Stroud
Donovan Murphy (working with Craig)
Chris Culver (working with Craig)
Deadline for Oct. 1 allocation requests is August 1, 2018.
Principal Investigators can submit eBooks requests now!
Webinar on the revised SMD HEC allocation process: 4 pm ET today!
- Slides and webinar recording will be available later

If you have questions about the new eBooks process, or an existing allocation or request, email support@nccs.nasa.gov to talk to Nancy Carney.
Scientific Visualization Studio
Visualizers working closely with scientists to create new ways of viewing massive amounts of data.

Contact Horace Mitchell for more information: horace.g.mitchell@nasa.gov

All content available at https://svs.gsfc.nasa.gov
Discover Linux Cluster
Dan Duffy
Discover 12-Month Utilization Percentage Trend

Discover Monthly Utilization (Including Dedicated Partitions)
June 2017 - May 2018

Month

June, July, August, September, October, November, December, January, February, March, April, May

Percent Capacity

SBUs Used
75% capacity
Discover Expansion Factors – 12-Month Trend

Discover Expansion Factors
June 2017 - May 2018

Expansion Factor
- 90% User Expansion
- All Users Expansion Factor

Month
- June
- July
- August
- September
- October
- November
- December
- January
- February
- March
- April
- May
Discover FY17 Compute Upgrade Summary

- Scalable Unit 14 (SCU14)
  - First single NCCS system with >1.5 PF
  - First OPA system in NASA
- Edge Solutions and SuperMicro
- 520 Compute Nodes
  - Dual-socket with 20-core Intel Skylake 2.4 GHz processors
  - 20,800 total cores
  - 1,560 TF peak computing
  - 192 GB of RAM per node
- 24 Service Nodes
- 20 I/O Nodes
- Intel OmniPath (OPA) Interconnect
  - 100 Gbps
  - 2-to-1 blocking
  - Interconnect designed to easily scale to 2x the number of compute nodes

Come visit during the Science Jamboree: July 25th
## Discover Scalable Unit Evolution

<table>
<thead>
<tr>
<th>Year</th>
<th>SCU1</th>
<th>SCU2</th>
<th>SCU3</th>
<th>SCU4</th>
<th>SCU7</th>
<th>SCU8</th>
<th>SCU9</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014</td>
<td>258 Nodes</td>
<td>258 Nodes</td>
<td>258 Nodes</td>
<td>258 Nodes</td>
<td>1,200 Nodes</td>
<td>480 Nodes</td>
<td>480 Nodes</td>
</tr>
<tr>
<td></td>
<td>3,096 Cores</td>
<td>3,096 Cores</td>
<td>3,096 Cores</td>
<td>3,096 Cores</td>
<td>14,400 Cores</td>
<td>7,680 Cores</td>
<td>7,680 Cores</td>
</tr>
<tr>
<td></td>
<td>2.8 GHz, 24 GB</td>
<td>2.8 GHz, 24 GB</td>
<td>2.8 GHz, 24 GB</td>
<td>2.8 GHz, 24 GB</td>
<td>2.8 GHz, 32 GB</td>
<td>2.6 GHz, 64 GB</td>
<td>2.6 GHz, 64 GB</td>
</tr>
<tr>
<td></td>
<td>Westmere DDR IB</td>
<td>Westmere DDR IB</td>
<td>Westmere DDR IB</td>
<td>Westmere DDR IB</td>
<td>Westmere QDR IB</td>
<td>SandyBridge QDR IB</td>
<td>SandyBridge QDR IB</td>
</tr>
<tr>
<td></td>
<td>34.7 TF</td>
<td>34.7 TF</td>
<td>34.7 TF</td>
<td>34.7 TF</td>
<td>161.3 TF</td>
<td>Xeon Phi 606 TF</td>
<td>FDR IB 160 TF</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Year</th>
<th>SCU10</th>
<th>SCU11</th>
<th>SCU12</th>
<th>SCU13</th>
<th>SCU14</th>
<th>SCU15</th>
</tr>
</thead>
<tbody>
<tr>
<td>2015</td>
<td>1,080 Nodes</td>
<td>612 Nodes</td>
<td>612 Nodes</td>
<td>1,080 Nodes</td>
<td>648 Nodes</td>
<td>1,080 Nodes</td>
</tr>
<tr>
<td></td>
<td>30,240 Cores</td>
<td>17,136 Cores</td>
<td>17,136 Cores</td>
<td>30,240 Cores</td>
<td>18,144 Cores</td>
<td>30,240 Cores</td>
</tr>
<tr>
<td></td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
</tr>
<tr>
<td></td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
</tr>
<tr>
<td></td>
<td>683 TF</td>
<td>683 TF</td>
<td>683 TF</td>
<td>683 TF</td>
<td>723 TF</td>
<td>683 TF</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Year</th>
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<th>SCU14</th>
<th>SCU15</th>
</tr>
</thead>
<tbody>
<tr>
<td>2016</td>
<td>648 Nodes</td>
<td>612 Nodes</td>
<td>612 Nodes</td>
<td>648 Nodes</td>
<td>520 Nodes</td>
<td>648 Nodes</td>
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<tr>
<td></td>
<td>18,144 Cores</td>
<td>17,136 Cores</td>
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<td>18,144 Cores</td>
<td>20,800 Cores</td>
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<td></td>
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<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.6 GHz, 128 GB</td>
<td>2.4 GHz, 192 GB</td>
<td>2.6 GHz, 128 GB</td>
</tr>
<tr>
<td></td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Skylake OPA</td>
<td>Haswell FDR IB</td>
</tr>
<tr>
<td></td>
<td>723 TF</td>
<td>683 TF</td>
<td>683 TF</td>
<td>723 TF</td>
<td>1,560 TF</td>
<td>80 TF</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Year</th>
<th>SCU10</th>
<th>SCU11</th>
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<th>SCU14</th>
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</tr>
</thead>
<tbody>
<tr>
<td>2017</td>
<td>520 Nodes</td>
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<td>240 Nodes</td>
<td>612 Nodes</td>
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<tr>
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<td>Haswell FDR IB</td>
<td>Haswell FDR IB</td>
<td>Skylake OPA</td>
<td>Haswell FDR IB</td>
</tr>
<tr>
<td></td>
<td>1,560 TF</td>
<td>683 TF</td>
<td>683 TF</td>
<td>723 TF</td>
<td>1,560 TF</td>
<td>80 TF</td>
</tr>
</tbody>
</table>
Current NCCS HPC Platform Summary

**Mass Storage System**
- ~90 PB robotic tape library
- Data Management Facility (DMF) space management
- 4.4 PB disk

**Centralized Storage (evolved from DASS)**
- 11 HP Apollo Intel Xeon nodes
- 15 PB disk

**Discover**
- Intel Xeon nodes
- 3,752 nodes
- 107,936 cores
- Peak 5,129 TFLOPS general purpose
- 42 PB disk

**ADAPT**
- Intel Xeon nodes
- 554 nodes
- 12,148 cores
- Peak 232.2 TF
- 8 PB disk

**SCU9**
- 280 Nodes
- 4,480 Cores
- 2.6 GHz
- 64 GB
- Sandy Bridge
- FDR IB
- 93.2 TF

**SCU10**
- 1,080 Nodes
- 30,240 Cores
- 2.6 GHz
- 128 GB
- Haswell
- FDR IB
- 1,258.0 TF

**SCU11**
- 612 Nodes
- 17,136 Cores
- 2.6 GHz
- 128 GB
- Haswell
- FDR IB
- 712.9 TF

**SCU12**
- 612 Nodes
- 17,136 Cores
- 2.6 GHz
- 128 GB
- Haswell
- FDR IB
- 712.9 TF

**SCU13**
- 648 Nodes
- 18,144 Cores
- 2.6 GHz
- 128 GB
- Haswell
- FDR IB
- 754.8 TF

**SCU14**
- 520 Nodes
- 20,800 Cores
- 2.4 GHz
- 192 GB
- Skylake
- OPA 100
- 1,597.4 TF
Discover Upgrades: Omnipath/OPA, SLES 12 and Slurm17

• All three are being refined and tested in the more isolated SCU14 environment first, with measured deployment to the rest of Discover later.

• A number of changes, especially for Omnipath/OPA and SLES 12.

• Look for upcoming Brown Bags and Documentation!
Discover Upgrades for FY19 – Plans

• Compute
  – SCU15 (specific details TBD)
  – Compute nodes only, to be integrated with SCU14 to approximately double the total number of cores and peak computing capability

• Storage
  – High speed disk
  – Minimum of 15 PBs RAW (prior to RAID)
Advanced Data Analytics Platform (ADAPT)

Dan Duffy
## Advanced Data Analytics Platform (ADAPT) - High-Performance Science Cloud

<table>
<thead>
<tr>
<th>Capability and Description</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Persistent Data Services</strong></td>
<td>128 GB of RAM, 10 GbE, and FDR IB</td>
</tr>
<tr>
<td>Virtual machines or containers deployed for web services,</td>
<td></td>
</tr>
<tr>
<td>examples include ESGF, GDS, THREDDS, FTP, etc.</td>
<td></td>
</tr>
<tr>
<td><strong>DataBase</strong></td>
<td>128 GB of RAM, 3.2 TB of SSD, 10 GbE, and FDR IB</td>
</tr>
<tr>
<td>High available database nodes with solid state disk.</td>
<td></td>
</tr>
<tr>
<td><strong>Remote Visualization</strong></td>
<td>128 GB of RAM, 10 GbE, FDR IB, and GPUs</td>
</tr>
<tr>
<td>Enable server side graphical processing and rendering of data.</td>
<td></td>
</tr>
<tr>
<td><strong>High Performance Compute and Machine Learning</strong></td>
<td>~300 nodes with between 24 and 256 GB of RAM; Small set of nodes with 6 TB of</td>
</tr>
<tr>
<td>More than ~10,000 cores coupled via high speed networks for</td>
<td>SSD; 16 Nvidia Tesla V100s</td>
</tr>
<tr>
<td>elastic or itinerant computing requirements.</td>
<td></td>
</tr>
<tr>
<td><strong>High-Speed/High-Capacity Storage</strong></td>
<td>Storage nodes configured with ~10 PB’s of usable capacity</td>
</tr>
<tr>
<td>Petabytes of storage accessible to all the above capabilities</td>
<td></td>
</tr>
<tr>
<td>over the high speed Infiniband network.</td>
<td></td>
</tr>
<tr>
<td><strong>High Performance Networks</strong></td>
<td>External: 10 and 40 GbE</td>
</tr>
<tr>
<td>Internal networks enable high speed access to storage, while</td>
<td>Internal: 10 GbE and Infiniband</td>
</tr>
<tr>
<td>external networks provide high performance data movement.</td>
<td></td>
</tr>
</tbody>
</table>
ADAPT, Current and Coming Soon

• Access available now for NCCS users, email support@nccs.nasa.gov

• Coming Soon:
  • Additional compute nodes (modular container)
  • New NVIDIA V100 GPU systems (more detail on next slides), K40 GPU nodes available now
  • Convert InfiniBand network to Ethernet
    – Better utilization of container-based hypervisors
  • Fold ADAPT 1.0, where feasible, into OpenStack (ADAPT 2.0) control
    – Future user portal for self-provisioning
  • Introduce Cloud Bursting
    – Leverage commercial clouds to augment processing
### Three New Systems in ADAPT for Machine Learning/Deep Learning (ML/DL)

<table>
<thead>
<tr>
<th></th>
<th>2 @ 4 GPU Systems</th>
<th>8 GPU System</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total Cores</strong></td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td><strong>Speed of Core</strong></td>
<td>2.3 GHz</td>
<td>2.3 GHz</td>
</tr>
<tr>
<td><strong>RAM</strong></td>
<td>512 GB</td>
<td>512 GB</td>
</tr>
<tr>
<td><strong>GPUs</strong></td>
<td>4 by V100</td>
<td>8 by V100</td>
</tr>
<tr>
<td><strong>Network Interface</strong></td>
<td>2 by 50 Gbps</td>
<td>2 by 50 Gpbs</td>
</tr>
<tr>
<td><strong>Local Storage</strong></td>
<td>2 by 800 GB SSD</td>
<td>2 by 800 GB SSD</td>
</tr>
<tr>
<td></td>
<td>2 by 3.2 TB NVMe</td>
<td>2 by 3.2 TB NVMe</td>
</tr>
<tr>
<td><strong>Operating System</strong></td>
<td>CentOS</td>
<td>CentOS</td>
</tr>
<tr>
<td><strong>Software</strong></td>
<td>Python, Caffe, TensorFlow, Custom</td>
<td>Python, Caffe, TensorFlow, Custom</td>
</tr>
</tbody>
</table>

Accessible by NASA credentialed users; must have an NCCS account. Email support@nccs.nasa.gov to inquire about getting access.
## NVidia Tesla V100 Specifications

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Double Precision Performance (64-bit)</td>
<td>7.8 teraFLOPS</td>
</tr>
<tr>
<td>Single Precision Performance (32-bit)</td>
<td>15.7 teraFLOPS</td>
</tr>
<tr>
<td>Tensor Performance (16-bit)</td>
<td>125 teraFLOPS</td>
</tr>
<tr>
<td>High Bandwidth Memory (HBM)</td>
<td>16 GB</td>
</tr>
<tr>
<td>HBM Throughput</td>
<td>900 GB/sec</td>
</tr>
<tr>
<td>Interconnect Bandwidth (NVLink)</td>
<td>300 GB/sec</td>
</tr>
</tbody>
</table>

Two Systems with 4 GPUs

Specifications

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Total Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Double Precision Performance (64-bit)</td>
<td>31.2 teraFLOPS</td>
</tr>
<tr>
<td>Single Precision Performance (32-bit)</td>
<td>62.8 teraFLOPS</td>
</tr>
<tr>
<td>Tensor Performance (16-bit)</td>
<td>500 teraFLOPS</td>
</tr>
</tbody>
</table>
One Systems with 8 GPUs

Specifications

<table>
<thead>
<tr>
<th>Performance</th>
<th>Total Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Double Precision Performance (64-bit)</td>
<td>62.4 teraFLOPS</td>
</tr>
<tr>
<td>Single Precision Performance (32-bit)</td>
<td>125.6 teraFLOPS</td>
</tr>
<tr>
<td>Tensor Performance (16-bit)</td>
<td>1,000 teraFLOPS</td>
</tr>
</tbody>
</table>

NCCS User Forum June 26, 2018
Storage/Analytics Architecture
Evolution
and
Data Management Plans

Dan Duffy and Laura Carriere
NCCS Mass Storage
October 2009 – May 2018

NCCS Mass Storage, October 2009 - May 2018

- Unique File Data Stored
- Unique Plus User-Specified Duplicate File Data Stored
- Total Data Stored (Managed)
Evolution of Major NCCS Systems

Future: How will the GSFC climate affect my health over time?

Now: What is the temperature anomaly for GSFC during the month of February?

Past: What climate data can I download that has surface temperature for GSFC?

Compute
Data Services

FY15

Mass Storage
HPC - Discover

Data Portal

Cloud Virtualization

Combining Compute and Storage

Analytic Centric

Inference

EDAS ADAPT (cloud)

Mass Storage
Centralized Storage
HPC - Discover

FY18

FY17

FY16

ADAPT (cloud)

Mass Storage
Centralized Storage
HPC - Discover
FY19-FY20 Centralized Storage Concept

ADAPT
Analytics and Inference Based Services

High Performance Science Cloud

Current capacity: 9 PB
Planned capacity: 25 PB

Centralized Storage
Data Lake Concept
Tiered Storage

Tier 1 – Spinning Disk and Compute

Tier 2 – Object Store (future)

Discover
High Performance Computing

Mass Storage
Legacy System
Becomes Read Only
What Goes into the Centralized Storage?

- Not an archive, not a scratch space
- Long term **curated** data sets, e.g.
  - Final data product, either public or private, optionally with an official or second copy at another location, e.g. a NASA archive, or on different media
  - Suitable for use as input by other projects
- Require a Data Management Plan – coming up next
- Write once/read many data sets
-Sharable through services
- Examples:
  - Model input data
  - Reanalysis and forecast data
  - Model Intercomparison and IPCC runs
  - Research runs, Nature Runs, high resolution simulations
  - Digital Globe
  - Other relevant observation data sets
Draft Data Management Plans

• Manage input data, intermediate files, in-house software, final products
• Plan for disposition of each data type
• Tied to allocation process in the future
  – Will submit along with allocation requests
  – No automatic centralized storage allocation
• Advantages: easier to locate, share, and delete
• NCCS will provide help developing plans
Data Management Tools – in Progress

- Track storage usage of running jobs
- Track trends in disk usage, both in MSS and online
- Identify duplication
- Provide usage within group quotas
- Find and delete within MSS – (data older than x days)
- Improved public usage statistics
Downsizing Your Mass Storage Data

- Know what you have in Mass Storage (see Tools, previous slide)
- Review & remove unneeded data, e.g.
  - Experiments no longer needed
  - Data already archived elsewhere
- Thanks for some recent large deletions:
  - Lena Marshak (1.6 PB)
  - dao_it (GMAO) (0.5 PB)
- Prize – Pizza for Petabytes (Deleted)!
- Email support@nccs.nasa.gov if you’d like to be included
Be a Part of the Conversation

- Make sure we understand your requirements
- Help influence the process
- We’ll meet with your group or one-on-one
- Contact support@nccs.nasa.gov, Laura.Carriere@nasa.gov, Ellen.Salmon@nasa.gov
Questions & Answers

NCCS User Services:

support@nccs.nasa.gov
301-286-9120

https://www.nccs.nasa.gov
Contact Information

NCCS User Services:

support@nccs.nasa.gov
301-286-9120

https://www.nccs.nasa.gov

http://twitter.com/NASA_NCCS

Thank you
SUPPLEMENTAL SLIDES
Discover System Availability

**Discover Total System Availability**
June 2017 - May 2018

**Discover System Scheduled Availability**
June 2017 - May 2018
Data Analytics Storage System (DASS) Concept

Read access from all nodes within the ADAPT system
- Portals and web services
- Purpose built virtual machines for scientific analysis
- User driven science and applications
- Flexible and extensible
- Mixing model and observations

Climate Analytics as a Service
Analysis request is sent to a service. Answer is returned.

ADAPT

DASS (~15PB)

Tier 1 – Spinning Disk and Compute

Tier 2 – Object Store (future)

Mass Storage
Read and write access from the mass storage
- Stage data into and out of the centralized storage environment as needed

HPC - Discover
Source of Much of the Data: Write and Read from all nodes within Discover – models write data into GPFS which is then staged into the centralized storage (burst buffer like).

Note that all the services will still have local file systems to enable local optimized writes and reads as needed within their respective security domains.
Discover Scratch Disk Evolution

- Usable capacity differs from raw capacity for two reasons. First, the NCCS uses RAID6 (double parity) to protect against drive failures. This incurs a 20% overhead for the disk capacity. Second, the file system formatting is estimated to also need about 5% of the overall disk capacity. The total reduction from the RAW capacity to usable space is about 25%.

<table>
<thead>
<tr>
<th>Calendar</th>
<th>Description</th>
<th>Decommission</th>
<th>Total Usable Capacity (TB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012</td>
<td>Combination of DDN disks</td>
<td>None</td>
<td>3,960</td>
</tr>
<tr>
<td>Fall 2012</td>
<td>NetApp1: 1,800 by 3 TB Disk Drives; 5,400 TB RAW (prior to RAID protection)</td>
<td>None</td>
<td>9,360</td>
</tr>
<tr>
<td>Fall 2013</td>
<td>NetApp2: 1,800 by 4 TB Disk Drives; 7,200 TB RAW (prior to RAID protection)</td>
<td>None</td>
<td>16,560</td>
</tr>
<tr>
<td>Early 2015</td>
<td>DDN10: 1,680 by 6 TB Disk Drives, 10,080 TB RAW (prior to RAID protection)</td>
<td>DDNs 3, 4, 5</td>
<td>~26,000</td>
</tr>
<tr>
<td>Mid 2015</td>
<td>DDN11: 1,680 by 6 TB Disk Drives, 10,080 TB RAW (prior to RAID protection)</td>
<td>DDNs 7, 8, 9</td>
<td>~33,000</td>
</tr>
<tr>
<td>Mid 2016</td>
<td>DDN12: 1,680 by 6 TB Disk Drives, 10,080 TB RAW (prior to RAID protection)</td>
<td>None</td>
<td>~40,000</td>
</tr>
<tr>
<td>Early 2017</td>
<td>13+ PB RAW (prior to RAID protection)</td>
<td>TBD</td>
<td>~50,000</td>
</tr>
</tbody>
</table>
Data Management Plans & Centralized Storage

Motivation

• Increasing costs due to uncontrolled growth in Mass Storage
  – 94 PB and growing by 1.5 PB/month
• Duplication of data due to individual storage practices
• Slow access to data in MSS, e.g. GMAO input data

Working towards the goal of a sustainable storage environment that embodies analytics
ADAPT Use Cases

- Arctic Boreal Vulnerability Experiment (ABoVE)
- CALET (CALorimetric Electron Telescope)
- High Mountain Asia Terrain (HiMAT)
- Asteroid Hunters – Near Earth Objects
- Biomass in South Sahara
- NCCS Data Services
- Laser Communications Relay Demonstration (LCRD) Project - FPGA simulations