VC3

A Virtual Cluster Service for Community Computation

Lincoln Bryant, Jeremy Van, Benedikt Riedel, Robert Gardner, Jose Caballero Bejar, John Hover, Ben Tovar, and Douglas Thain

http://www.virtualclusters.org
VC3: A platform for provisioning cluster frameworks over heterogenous resources for collaborative science teams
You have developed a complex workload which runs successfully at one site, perhaps your home university.

Now, you want to migrate and expand that application to national-scale infrastructure. And allow others to easily access and run similar workloads.
**Concept: Virtual Cluster**

- 200 nodes of 24 cores and 64GB RAM
- 100GB local disk per node
- CMS software 8.1.3 and python 2.7
- CentOS 6 Operating System
- Running the HTCondor batch system.
- Shared between Alice, Bill, and Charles.

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Virtual Cluster Service

Virtual Cluster Head Node

Virtual Cluster Head Node

Virtual Cluster Head Node

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Deploy Software

Deploy Software

Deploy Software

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Leadership HPC Facility

Distributed Computing Facility

Commercial Cloud
Concept: Virtual Cluster

Share with collaborators.

SSH Access

Deploy Software

Virtual Cluster Head Node

Virtual Cluster Service

Virtual Cluster Head Node

Virtual Cluster

Leadership HPC Facility

Distributed Computing Facility

Commercial Cloud
VC3: Virtual Clusters for Community Computation

- VC3 is an interactive service for creating/sharing/using virtual clusters.
- A virtual cluster consists of:
  - 1 x head node for interactive access to the cluster.
  - N x worker nodes for executing your workload.
  - Middleware to manage the cluster. (HTCondor, Makeflow, Spark, ...)
  - Application software to do real work. (BLAST, Python, etc...)
- A virtual cluster is created using:
  - Your standard accounts/credentials on existing facilities.
  - Plain ssh/qsub access on each facility.
  - Container technology (if available) or user-level software builds (otherwise).
  - (No special privileges or admin access required on the facility.)
Limited Beta Release

Current status: **limited beta release!** We are **looking** for **collaborators** to help us work through bugs and offer feedback.

[http://virtualclusters.org](http://virtualclusters.org)

If you have an ambitious goal and feel VC3 may help you get there, please fill out the form below and we’ll send an invite:

www.virtualclusters.org

login with a vc3 account
Globus Authentication

Log in to use VC3

Use your existing organizational login
e.g., university, national lab, facility, project

University of Notre Dame

Didn't find your organization? Then use Globus ID to sign in. (What's this?)

Continue

Globus uses CILogon to enable you to Log In from this organization. By clicking Continue, you agree to the CILogon privacy policy and you agree to share your username, email address, and affiliation with CILogon and Globus. You also agree for CILogon to issue a certificate that allows Globus to act on your behalf.

Or

Sign in with Google

Sign in with ORCID iD
## Curated Resources

### Resource Profiles

<table>
<thead>
<tr>
<th>Name</th>
<th>Organization</th>
<th>Description</th>
<th>Cores</th>
<th>Memory</th>
<th>Storage</th>
<th>Native OS</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cori</td>
<td>National Energy Research Scientific Computing Center (NERSC)</td>
<td>Cori Supercomputer at NERSC</td>
<td>32</td>
<td>4000 MB</td>
<td>10000 MB</td>
<td>susev12</td>
<td>Shifter</td>
</tr>
<tr>
<td>MWT2</td>
<td>Midwest Tier 2</td>
<td>ATLAS Midwest Tier 2 Center job gateway (UCichicago)</td>
<td>4</td>
<td>1000 MB</td>
<td>1000 MB</td>
<td>scientificlinuxv6.9</td>
<td>N/A</td>
</tr>
<tr>
<td>Midway</td>
<td>University of Chicago Research Computing Center (RCC)</td>
<td>Midway cluster at the University of Chicago Research Computing Center (RCC)</td>
<td>64</td>
<td>4000 MB</td>
<td>10000 MB</td>
<td>scientificlinuxv6.7</td>
<td>N/A</td>
</tr>
<tr>
<td>Stampede 2</td>
<td>Texas Advanced Computing Center (TACC)</td>
<td>Stampede 2 Super Computer</td>
<td>96</td>
<td>2000 MB</td>
<td>10000 MB</td>
<td>centosv7.4</td>
<td>Singularity</td>
</tr>
<tr>
<td>CoreOS</td>
<td>University of Chicago</td>
<td>CoreOS Cluster</td>
<td>4</td>
<td>1000 MB</td>
<td>1000 MB</td>
<td>scientificlinuxv6.9</td>
<td>Singularity</td>
</tr>
<tr>
<td>UCT3</td>
<td>University of Chicago</td>
<td>UChicago ATLAS Tier 3</td>
<td>4</td>
<td>1000 MB</td>
<td>1000 MB</td>
<td>scientificlinuxv6.9</td>
<td>N/A</td>
</tr>
<tr>
<td>ND CCL</td>
<td>University of Notre Dame Cooperative Computing Lab</td>
<td>ND-CCL login node</td>
<td>4</td>
<td>1000 MB</td>
<td>10000 MB</td>
<td>redhatv7</td>
<td>Singularity</td>
</tr>
<tr>
<td>Bridges</td>
<td>Pittsburgh Supercomputing Center</td>
<td>Bridges Supercomputer at PSC</td>
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<td>35000 MB</td>
<td>centosv7.3</td>
<td>Singularity</td>
</tr>
<tr>
<td>VC3 Test Pool</td>
<td>VC3</td>
<td>VC3 Test Pool</td>
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<td>1000 MB</td>
<td>1000 MB</td>
<td>centosv6.9</td>
<td>N/A</td>
</tr>
<tr>
<td>UCLA</td>
<td>University of California, Los Angeles</td>
<td>UCLA Hoffman2</td>
<td>8</td>
<td>1000 MB</td>
<td>10000 MB</td>
<td>centosv6.9</td>
<td>N/A</td>
</tr>
<tr>
<td>OSG Connect</td>
<td>Open Science Grid</td>
<td>Open Science Grid (SL7)</td>
<td>4</td>
<td>1000 MB</td>
<td>1000 MB</td>
<td>Unknown</td>
<td>N/A</td>
</tr>
</tbody>
</table>
Allocations

Step 1: Log Into Resource

In a terminal, type:

```
ssh btovar@cclvm05.crc.nd.edu
```

Step 2: Access Resource

Enter your password for `cclvm05.crc.nd.edu` for access.

Step 3: Add Allocation SSH Public Key to Resource

Once the SSH key is generated below, click 'Copy to Clipboard' and paste the following line into your SSH session. You will only need to do this once per allocation:

```
/p09d5W1WYcXYW/0tnQG7mYF3iP0YwBn0mVw0V04fW2B2nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/s8h5YF3iP0YwBn0mVw0V04fC4/28ns62B37nYKQ47/...```

Also:

```
/ykptv/savy7fNh7Ply76yW/Z3glb21b943aAC4BC01G1q5dW4B8T4D08R6ps39060CCgJXuxUc4mmP5gWb67bF0cL
/WqJcm7UdcWY/Wou/Zlkup00cOb2X6jw855Fcd4H
```

Step 4: Validate Allocation
## Projects

### Project Profiles

<table>
<thead>
<tr>
<th>Name</th>
<th>Members</th>
<th>Allocations</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>vc3-team</td>
<td>Benjamin Tovar (Owner) - <a href="mailto:btovar@nd.edu">btovar@nd.edu</a>&lt;br&gt;Lincoln Bryant (UChicago)&lt;br&gt;Jeremy Van (UChicago)&lt;br&gt;Robert Gardner (UChicago)&lt;br&gt;Kenyi Hurtado (University of Notre Dame)</td>
<td>btovar-ndccl&lt;br&gt;khurtado-osgconnect&lt;br&gt;lincolnb-midway</td>
<td>Currently no description</td>
</tr>
<tr>
<td>btovar</td>
<td>Benjamin Tovar (Owner) - <a href="mailto:btovar@nd.edu">btovar@nd.edu</a>&lt;br&gt;Benjamin Tovar (University of Notre Dame)</td>
<td>btovar-ndccl</td>
<td>Currently no description</td>
</tr>
</tbody>
</table>
Launching a Virtual Cluster

- **Shared Cluster Definition**
- **Environment**
- **Allocations Available in This Project**

Workers will have this environment installed.
## Cluster Status

### My Virtual Clusters

<table>
<thead>
<tr>
<th>Name</th>
<th>State</th>
<th>Cluster Template</th>
<th>Workers</th>
<th>Head Node</th>
</tr>
</thead>
<tbody>
<tr>
<td>my-virtual-cluster</td>
<td>Running</td>
<td>lincoln-b-hetcondor-10-workers</td>
<td>Requested: 10, Running: 7, Queued: 3, Error: 0</td>
<td>128.135.158.187</td>
</tr>
</tbody>
</table>

All requested compute workers are running.
Workers from many sites

```
[btovar@btovar-my-virtual-cluster ~]$ ip addr | grep 128.135.158.187
   inet 128.135.158.187/25 brd 128.135.158.255 scope global dynamic eth0
[btovar@btovar-my-virtual-cluster ~]$ condor_status

<table>
<thead>
<tr>
<th>Name</th>
<th>OpSys</th>
<th>Arch</th>
<th>State</th>
<th>Activity</th>
<th>LoadAv</th>
<th>Mem</th>
<th>ActvtyTime</th>
</tr>
</thead>
<tbody>
<tr>
<td>slot1@<a href="mailto:glidein_21791@camd01.crc.nd.edu">glidein_21791@camd01.crc.nd.edu</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>5.120</td>
<td>4013</td>
<td>0:00:19:37</td>
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<tr>
<td>slot1@<a href="mailto:glidein_29106@camd01.crc.nd.edu">glidein_29106@camd01.crc.nd.edu</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
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<td>0:00:19:37</td>
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<tr>
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<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>5.260</td>
<td>4013</td>
<td>0:00:19:37</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_39133@iut2-c257.iu.edu">glidein_39133@iut2-c257.iu.edu</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>34.620</td>
<td>3223</td>
<td>0:00:19:48</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_61297@lnxfarm275.colorado.edu">glidein_61297@lnxfarm275.colorado.edu</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>6.990</td>
<td>3002</td>
<td>0:00:14:36</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_28373@midway091.rcc.local">glidein_28373@midway091.rcc.local</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>8.170</td>
<td>2013</td>
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<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>7.480</td>
<td>2013</td>
<td>0:00:19:36</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_46364@midway260.rcc.local">glidein_46364@midway260.rcc.local</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>8.040</td>
<td>2013</td>
<td>0:00:19:35</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_39282@midway324.rcc.local">glidein_39282@midway324.rcc.local</a></td>
<td>LINUX</td>
<td>X86_64</td>
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<td>Idle</td>
<td>8.750</td>
<td>2013</td>
<td>0:00:19:36</td>
</tr>
<tr>
<td>slot1@<a href="mailto:glidein_39133@uct2-c373.mwt2.org">glidein_39133@uct2-c373.mwt2.org</a></td>
<td>LINUX</td>
<td>X86_64</td>
<td>Unclaimed</td>
<td>Idle</td>
<td>34.080</td>
<td>2415</td>
<td>0:00:19:33</td>
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</table>

<table>
<thead>
<tr>
<th>Machines</th>
<th>Owner</th>
<th>Claimed</th>
<th>Unclaimed</th>
<th>Matched</th>
<th>Preempting</th>
<th>Drain</th>
</tr>
</thead>
<tbody>
<tr>
<td>X86_64/LINUX</td>
<td>10</td>
<td>0</td>
<td>0</td>
<td>10</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Total | 10    | 0       | 0         | 10      | 0          | 0     |
```

ND: University of Notre Dame
OSG: Open Science Grid
UChicago: University of Chicago
VC3 Monitoring

Virtual Cluster Size (queued)

My Virtual Clusters

<table>
<thead>
<tr>
<th>Name</th>
<th>State</th>
<th>Cluster Template</th>
<th>Workers</th>
<th>Head Node</th>
</tr>
</thead>
<tbody>
<tr>
<td>ndt3_500</td>
<td>Running</td>
<td>khurtado-htcondor-500</td>
<td>48</td>
<td>128.135.158.178</td>
</tr>
</tbody>
</table>

Requested: 500
Running: 48
Queued: 40
Error: 0

Requesting 44 more compute workers!
Details: System Monitoring
Deploying Software Environments

The **vc3-builder**, a command-line tool for deploying software environments on clusters.

```
vc3-builder
   --require-os centos:7
   --mount /scratch=/data
   --require /cvmfs
   --require python:2.7 -- myapp ...my args...
```

[GitHub](https://github.com/vc3-project/vc3-builder)
Custom docker container in Jetstream took weeks to install pieces by hand. Converted to vc3-builder, successfully ported to Stampede in a single automated install.
Working **Middleware** and **Applications**

- Various Bioinformatics Workflows
  - Makeflow + HTCondor + BWA, Shrimp, BLAST
- Lobster CMS Data Analysis
  - Work Queue + Builder + CVMFS
- South Pole Telescope (SPT–3G) Analysis Framework
  - HTCondor Jobs + Docker/Shifter + CVMFS
- XENON1T Analysis Framework
  - Pegasus + HTCondor + CVMFS
- MAKER Bioinformatics Pipeline
  - Work Queue + Builder
- IceCube **Simulation** Framework
  - HTCondor
In Progress...

Current Work

- Dynamic reconfiguration of cluster.
- Adding new middleware: Jupyter, Spark, Parsl.

Perennial Challenges

- Idiosyncrasies of each site
- Multi-factor authentication
- Communicate delays/errors from sites to portal
Collaborators and Connections

AutoPyFactory

XENON Dark Matter Project

CMS

ATLAS Experiment

Makeflow

HTCondor

Science Gateways Community Institute

globus

Open Science Grid

ci connect
VC3 Funding and Team

Funded by DOE Office of Advanced Scientific Computing Research (ASCR) and NSF Next Generation Networking Services (NGNS)

PIs: Rob Gardner (UC), Douglas Thain (ND), and John Hover (BNL)

c−PIs:  David Miller (UC), Paul Brenner (ND), Mike Hildreth (ND), Kevin Lannon (ND)

dev−team: Lincoln Bryant (UC), Benedikt Riedel (UC), Suchandra Thapa (UC), Jeremy Van (UC), Kenyi Hurtado Anampa (ND), Ben Tovar (ND), Jose Caballero Bejar (BNL).
Virtual Clusters for Community Computation

https://www.virtualclusters.org
@virtualclusters


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