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# VC3

## Virtual Clusters for Community Computation



Ben Tovar <[btovar@nd.edu](mailto:btovar@nd.edu)> for the VC3 team

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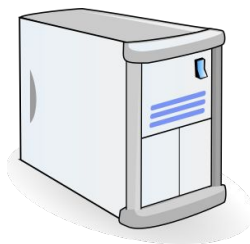
# Where our users are



A scientist that knows how to scale their computation in a particular site.



one  
task



submit node  
campus cluster,  
HPC center, etc.

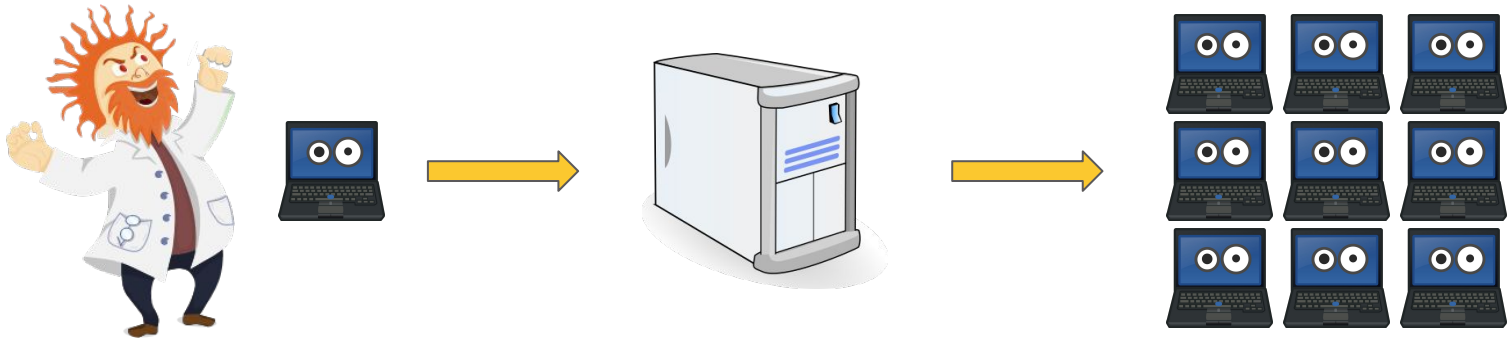
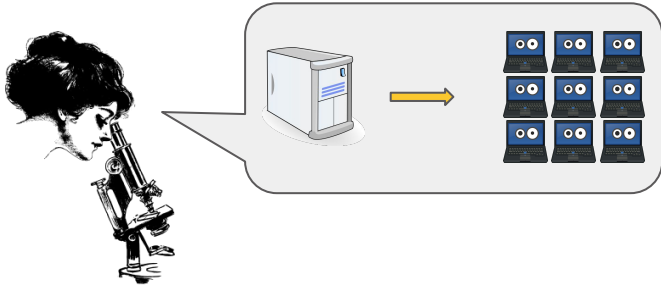


many task running on many  
computational nodes

# Where our users want to be



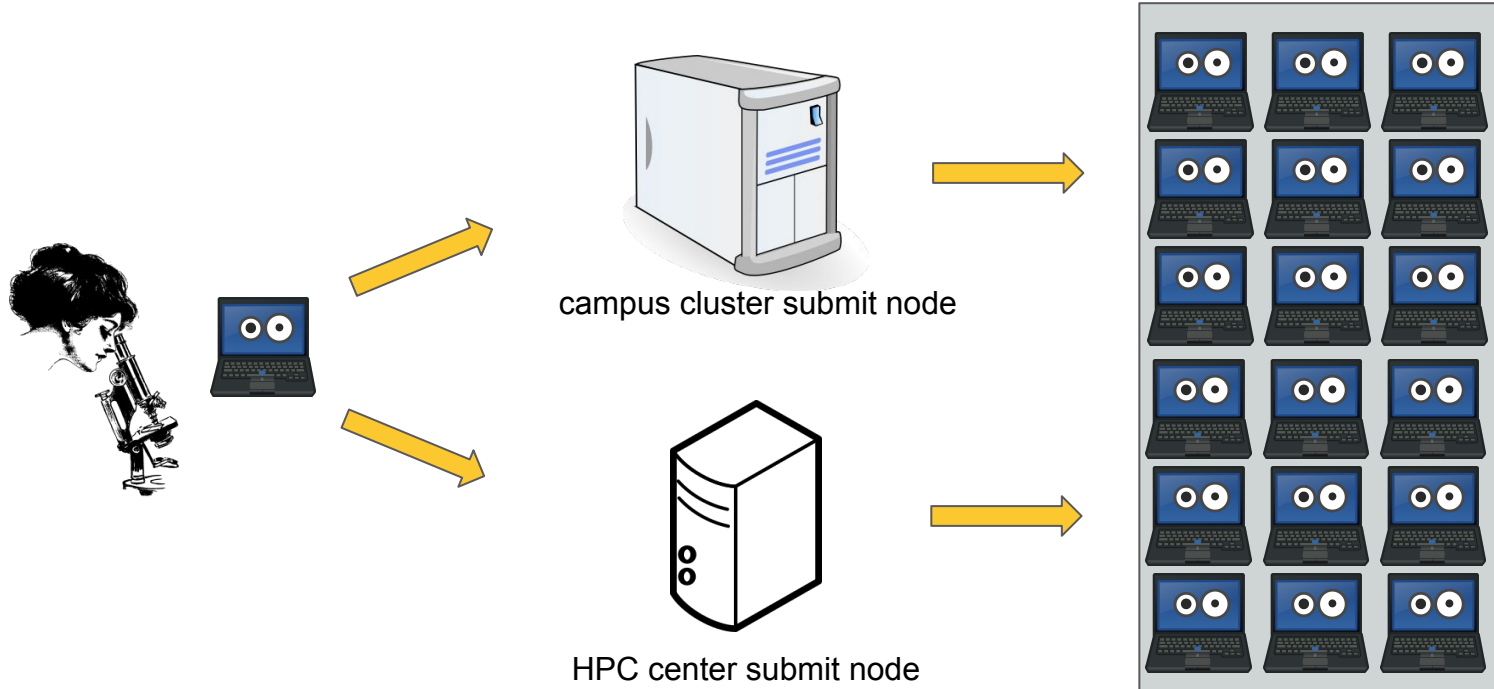
Communicate working setups to colleagues.



# Where our users want to be



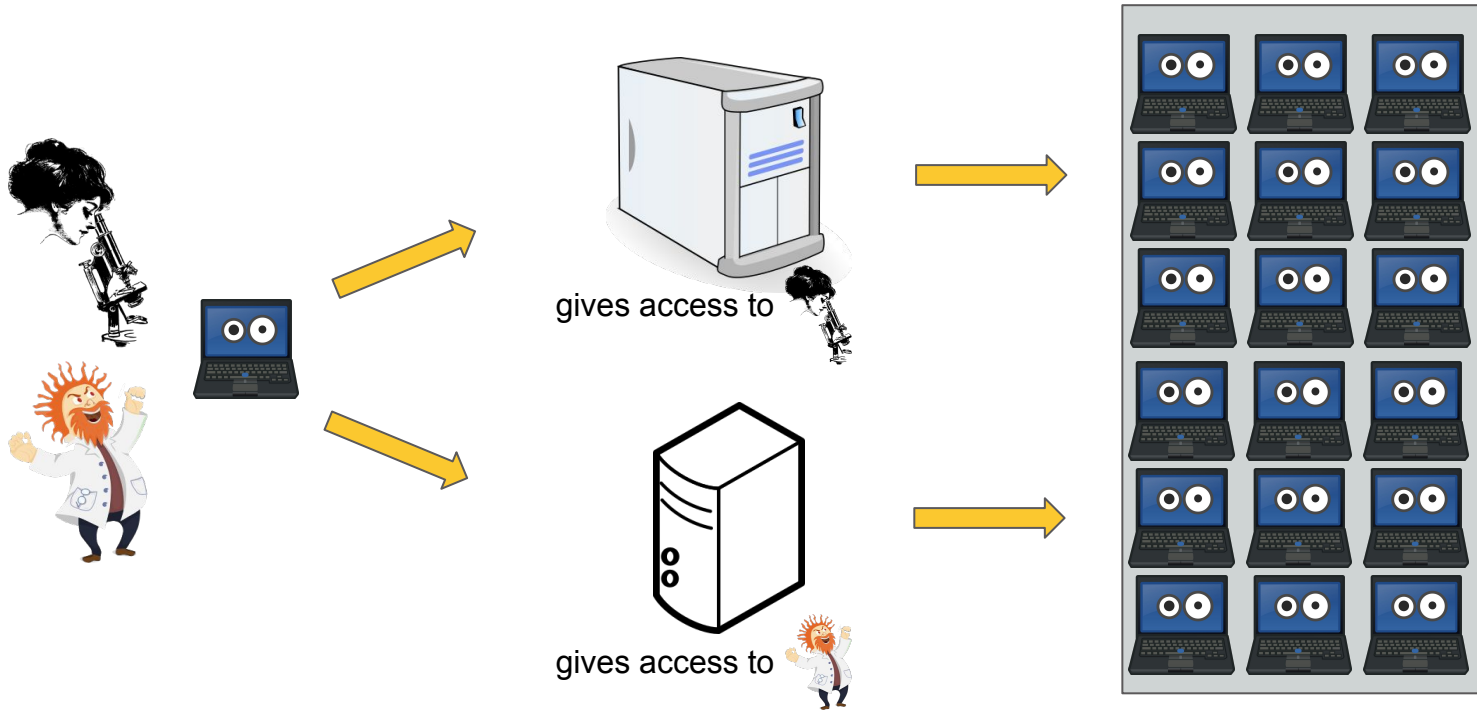
Pool resources together

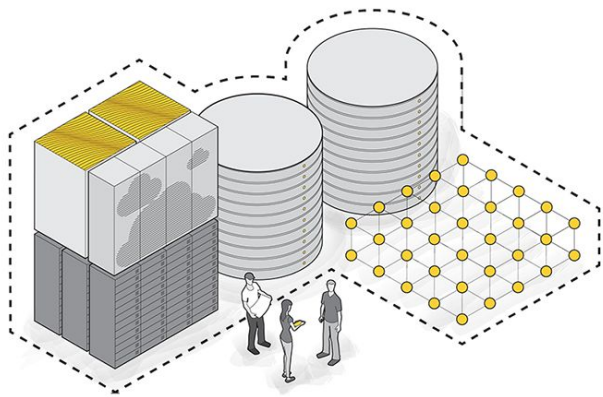


# Where our users want to be



## Share resources





VC3: A platform for provisioning customized short-lived clusters over heterogeneous resources for collaborative science teams

# VC3 in a nutshell

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Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.

vc3 web portal

Notre Dame  
HTCondor

Bridges  
SLURM

Stampede 2  
SLURM

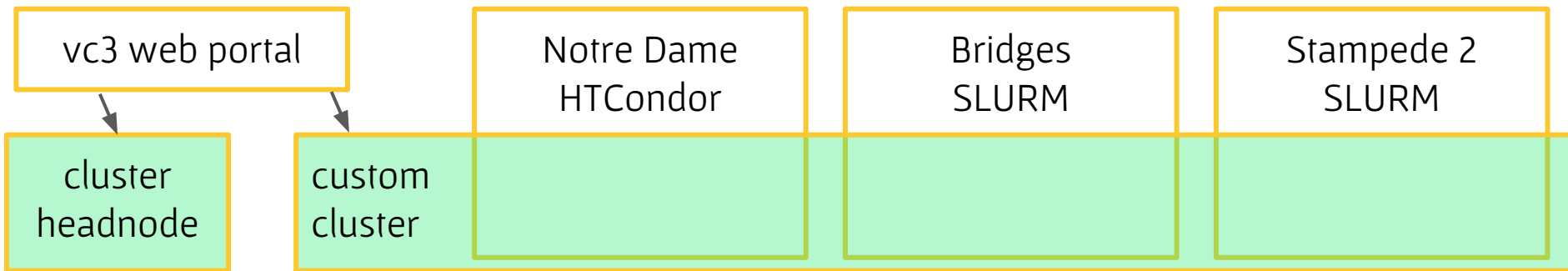
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# VC3 in a nutshell

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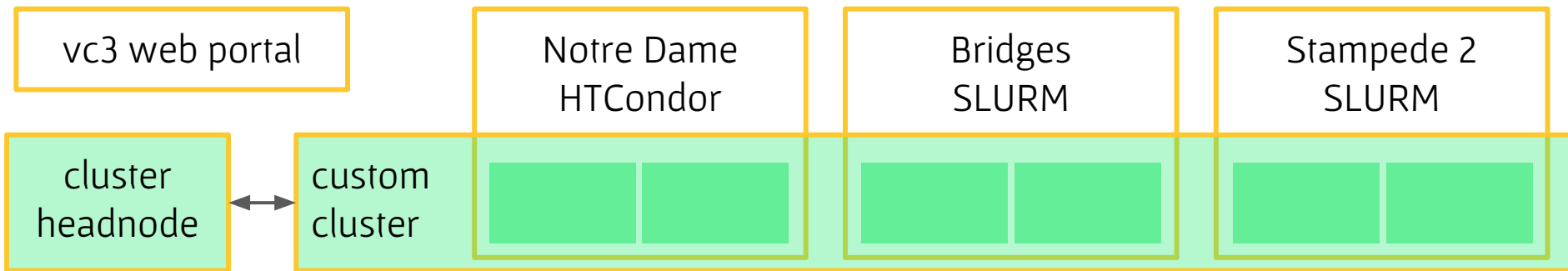
Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.



# VC3 in a nutshell



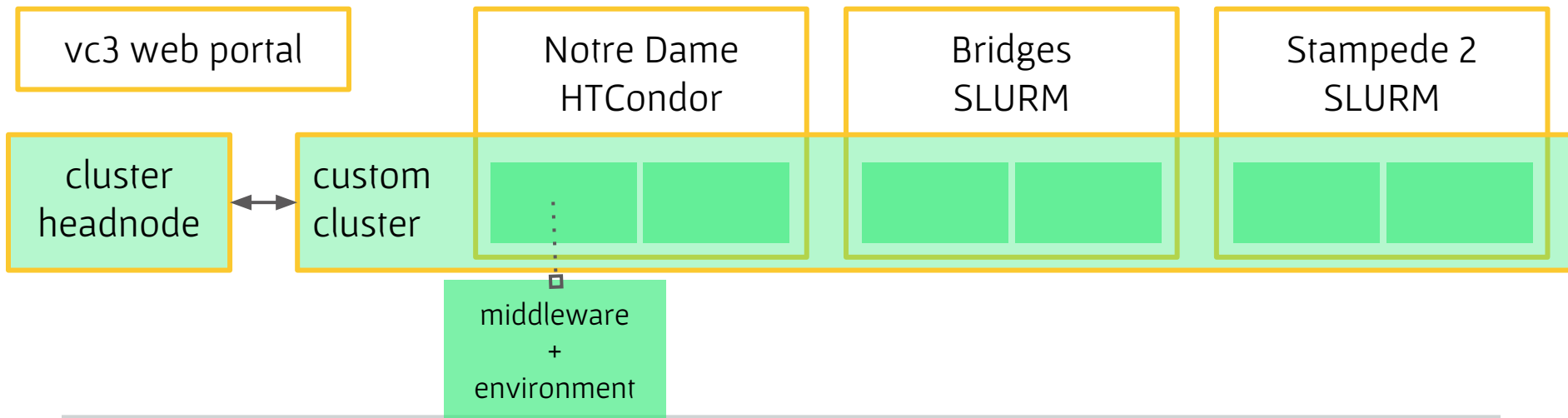
Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.



# VC3 in a nutshell



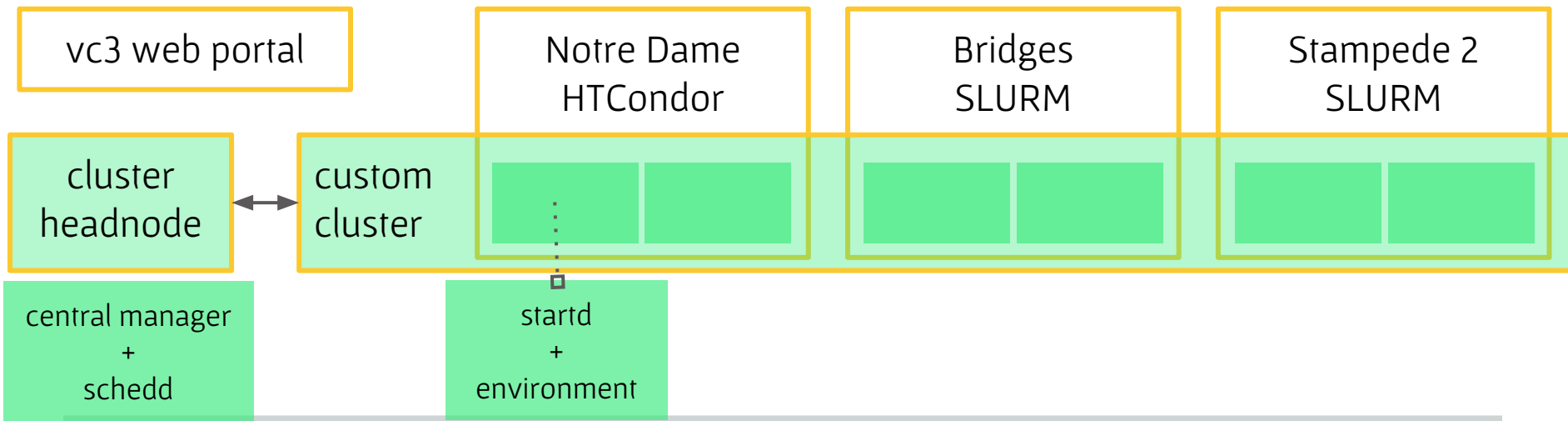
Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.



# VC3 in a nutshell



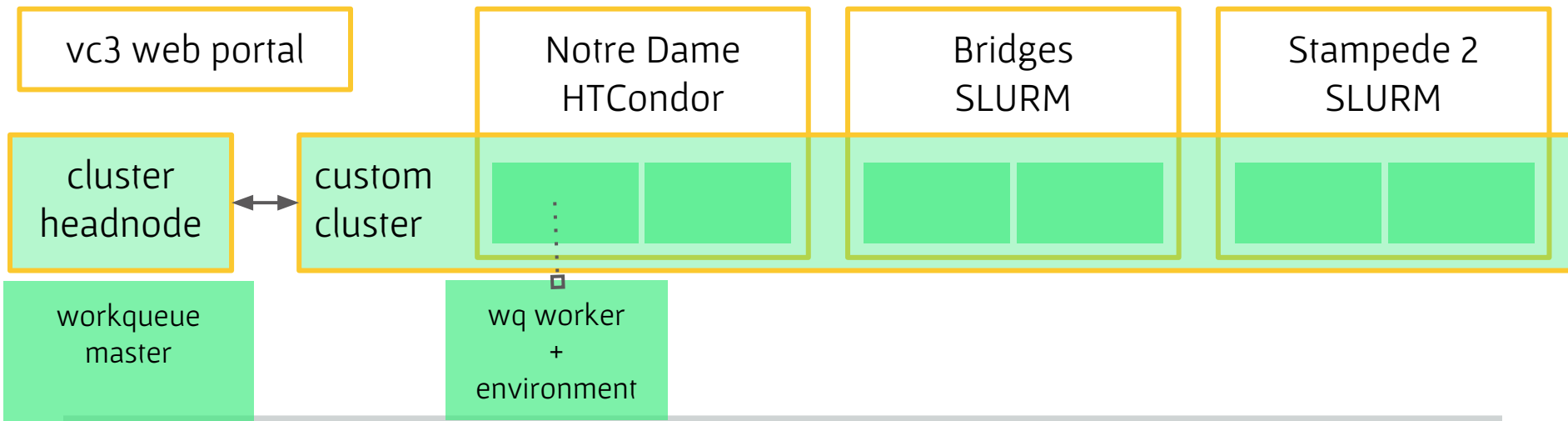
Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.



# VC3 in a nutshell



Users go to a **website** and create **short lived clusters** across **heterogeneous resources**.



# What is a Virtual Cluster?

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- 1 headnode
  - + n middleware workers running on  $m$  sites
  - k environments to run user tasks
-

Web portal



# www.virtualclusters.org



login with a vc3  
account

# Globus login authentication



globus

Globus Account Log In

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							
Filter							
Name	Organization	Description	Cores	Memory	Storage	Native OS	Features
Cori	National Energy Research Scientific Computing Center (NERSC)	Cori Supercomputer at NERSC	32	4000 MB	10000 MB	suse.v12	Shifter
MWT2	Midwest Tier 2	ATLAS Midwest Tier 2 Center job gateway (UChicago)	4	1000 MB	1000 MB	scientificlinux.v6.9	N/A
Midway	University of Chicago Research Computing Center (RCC)	Midway cluster at the University of Chicago Research Computing Center (RCC)	64	4000 MB	10000 MB	scientificlinux.v6.7	N/A
Stampede 2	Texas Advanced Computing Center (TACC)	Stampede 2 Super Computer	96	2000 MB	10000 MB	centos.v7.4	Singularity
CoreOS	University of Chicago	CoreOS Cluster	4	1000 MB	1000 MB	scientificlinux.v6.9	Singularity
UCT3	University of Chicago	UChicago ATLAS Tier 3	4	1000 MB	1000 MB	scientificlinux.v6.9	N/A
ND CCL	University of Notre Dame Cooperative Computing Lab	ND-CCL login none	4	1000 MB	10000 MB	redhat.v7	Singularity
Bridges	Pittsburgh Supercomputing Center	Bridges Supercomputer at PSC	28	4000 MB	35000 MB	centos.v7.3	Singularity
VC3 Test Pool	VC3	VC3 Test Pool	4	1000 MB	1000 MB	centos.v6.9	N/A
UCLA Hoffman2	University of California, Los Angeles	UCLA Hoffman2	8	1000 MB	10000 MB	centos.v6.9	N/A
OSG Connect	Open Science Grid	Open Science Grid (SL7)	4	1000 MB	1000 MB	Unknown	N/A

# Allocations



## Step 1: Log Into Resource

In a terminal, type:

```
ssh btovar@cc1vm05.crc.nd.edu
```

## Step 2: Access Resource

Enter your password for `cc1vm05.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.

```
S*00rWwCjUmRudKwMlCngCawCRVx7anGfRwIowCdq9t9c13g04r0qg7e9K  
/GTjh8YrCyX6UhqG+S3nOxOf+ewxx3RSIMfglsFZpDNdXwJl1YD1dyRCYy8TwNhBg9GkCxEKmqfOgo  
L6ROpicuUhfY6yT9apKGox1mPSM  
/g4ETHxIkBmNK8Ph926fuT+F+QQTosQVovgoghW/LGiGdNoztW/8OUkSFzZ6uZE5zfPp0xq45a4*FYE  
TorlJRapgPsjmSjmSB7TeD+qs1ECilwrrg3JP0RBOEMMeL7rwgDxjxtZkBUQ72lkq5lXTUAYeu0CbGgll  
Q7ZHGHRnTyKkSPLl7rXEi7nnz6ofgUJCU3L7hr2VKKy84RcHPsfep64qV3ilOCw1o6SPvu6lwRYeqhfe  
Aoo  
/yKp1lvapyfM7Ptuy+6yW/Z7grZlb9AtBolcoBColpig64MR8T4D8RKp1960nCG5ltXwC4mmPSgffQofOl  
WJom7TudG+yTWouWikupoieObZX5w8SKFcoH
```

Copy to Clipboard

## Step 4: Validate Allocation

# Projects



## Project Profiles

Filter

Name	Members	Allocations	Description
vc3-team	<b>Benjamin Tovar (Owner) - btovar@nd.edu</b> Lincoln Bryant (UChicago) Jeremy Van (UChicago) Robert Gardner (UChicago) Kenyi Hurtado (University of Notre Dame)	btovar-ndccl khurtado-osgconnect lincolnb-midway	Currently no description
btovar	<b>Benjamin Tovar (Owner) - btovar@nd.edu</b> Benjamin Tovar (University of Notre Dame)	btovar-ndccl	Currently no description

# Launching a Virtual Cluster



VIRTUAL CLUSTER NAME

my-virtual-cluster

CLUSTER TEMPLATE \*

lincolnb-htcondor-10-workers

ENVIRONMENT

btovar-oasis-osg

ALLOCATIONS \*

Nothing selected

Select Allocations for Virtual Cluster

Select All Deselect All

btovar-ndccl

khurtado-osgconnect

lincolnb-midway

shared cluster  
definition

workers will  
have this  
environment  
installed

allocations  
available in this  
project

# Cluster status



My Virtual Clusters <span>Filter</span>				
Name	State	Cluster Template	Workers	Head Node
my-virtual-cluster	<div>Running</div> <p>All requested compute workers are running.</p>	lincolnb-htcondor-10-workers	Requested: 10 Running: 7 Queued: 3 Error: 0	128.135.158.187

# 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
```

Name	OpSys	Arch	State	Activity	LoadAv	Mem	ActvtyTime
slot1@glidein_21791@camd01.crc.nd.edu	LINUX	X86_64	Unclaimed	Idle	5.120	4013	0+00:19:37
slot1@glidein_29106@camd01.crc.nd.edu	LINUX	X86_64	Unclaimed	Idle	5.120	4013	0+00:19:37
slot1@glidein_91802@camd05.crc.nd.edu	LINUX	X86_64	Unclaimed	Idle	5.260	4013	0+00:19:37
slot1@glidein_39133@iut2-c257.iu.edu	LINUX	X86_64	Unclaimed	Idle	34.620	3223	0+00:19:48
slot1@glidein_61297@lnxfarm275.colorado.edu	LINUX	X86_64	Unclaimed	Idle	6.990	3002	0+00:14:36
slot1@glidein_28373@midway091.rcc.local	LINUX	X86_64	Unclaimed	Idle	8.170	2013	0+00:19:36
slot1@glidein_71179@midway098.rcc.local	LINUX	X86_64	Unclaimed	Idle	7.480	2013	0+00:19:36
slot1@glidein_46364@midway260.rcc.local	LINUX	X86_64	Unclaimed	Idle	8.040	2013	0+00:19:35
slot1@glidein_39282@midway324.rcc.local	LINUX	X86_64	Unclaimed	Idle	8.750	2013	0+00:19:36
slot1@glidein_39133@uct2-c373.mwt2.org	LINUX	X86_64	Unclaimed	Idle	34.080	2415	0+00:19:33

```
Machines Owner Claimed Unclaimed Matched Preempting Drain
```

```
X86_64/LINUX      10      0      0      10      0      0      0
```

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

```
[btovar@btovar-my-virtual-cluster ~]$
```

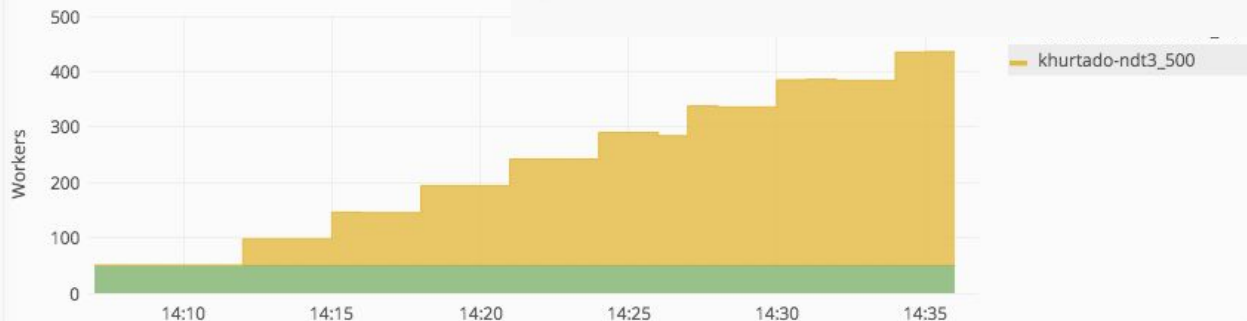


## VC3 Monitoring

Virtual Cluster Size (queued)



Vi



### My Virtual Clusters

Filter

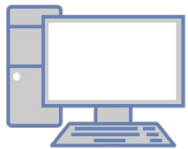
Name	State	Cluster Template	Workers	Head Node
ndt3_500	<div>Running</div> <div>Requesting 114 more compute worker(s).</div>	khurtado-htcondor-500workers	Requested: 500 Running: 386 Queued: 48 Error: 0	128.135.158.178

# Architecture

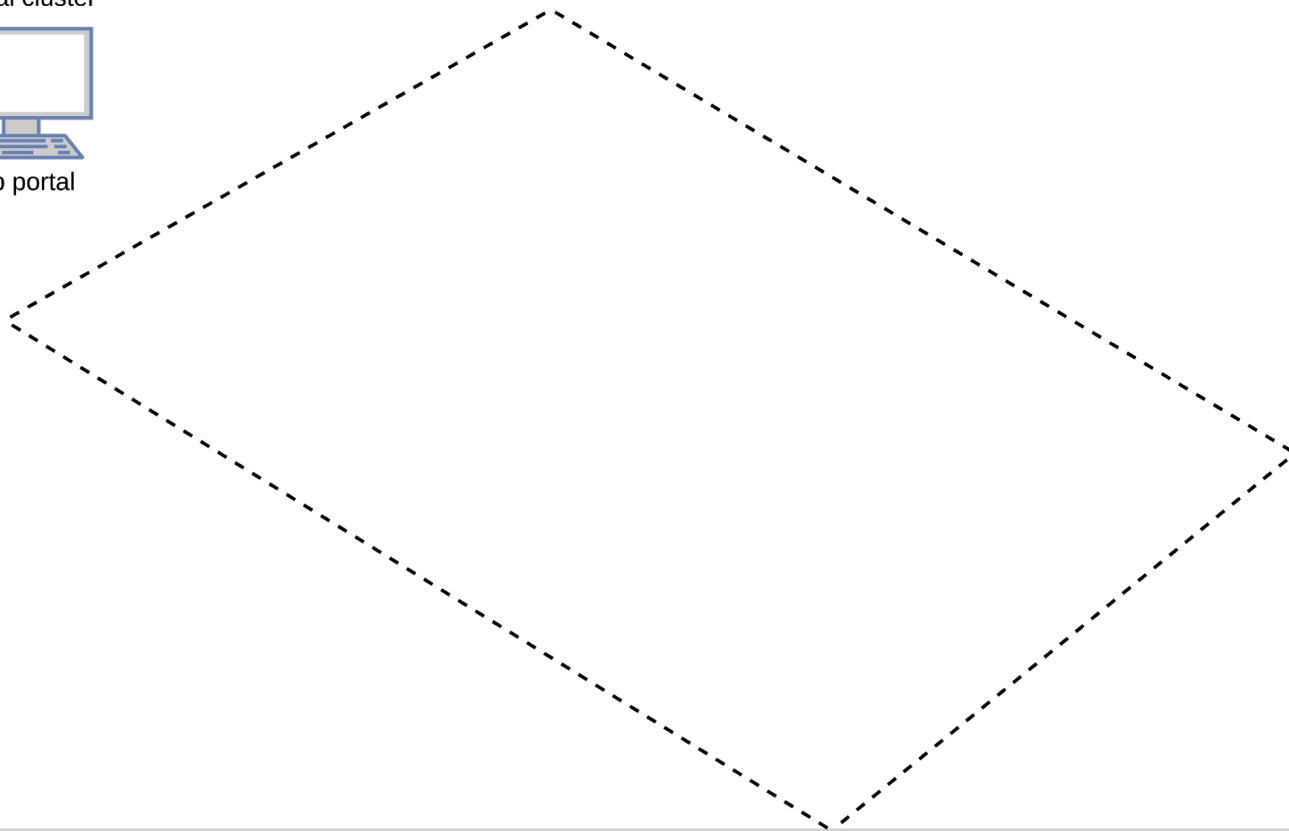


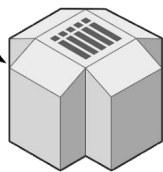


user requests  
virtual cluster

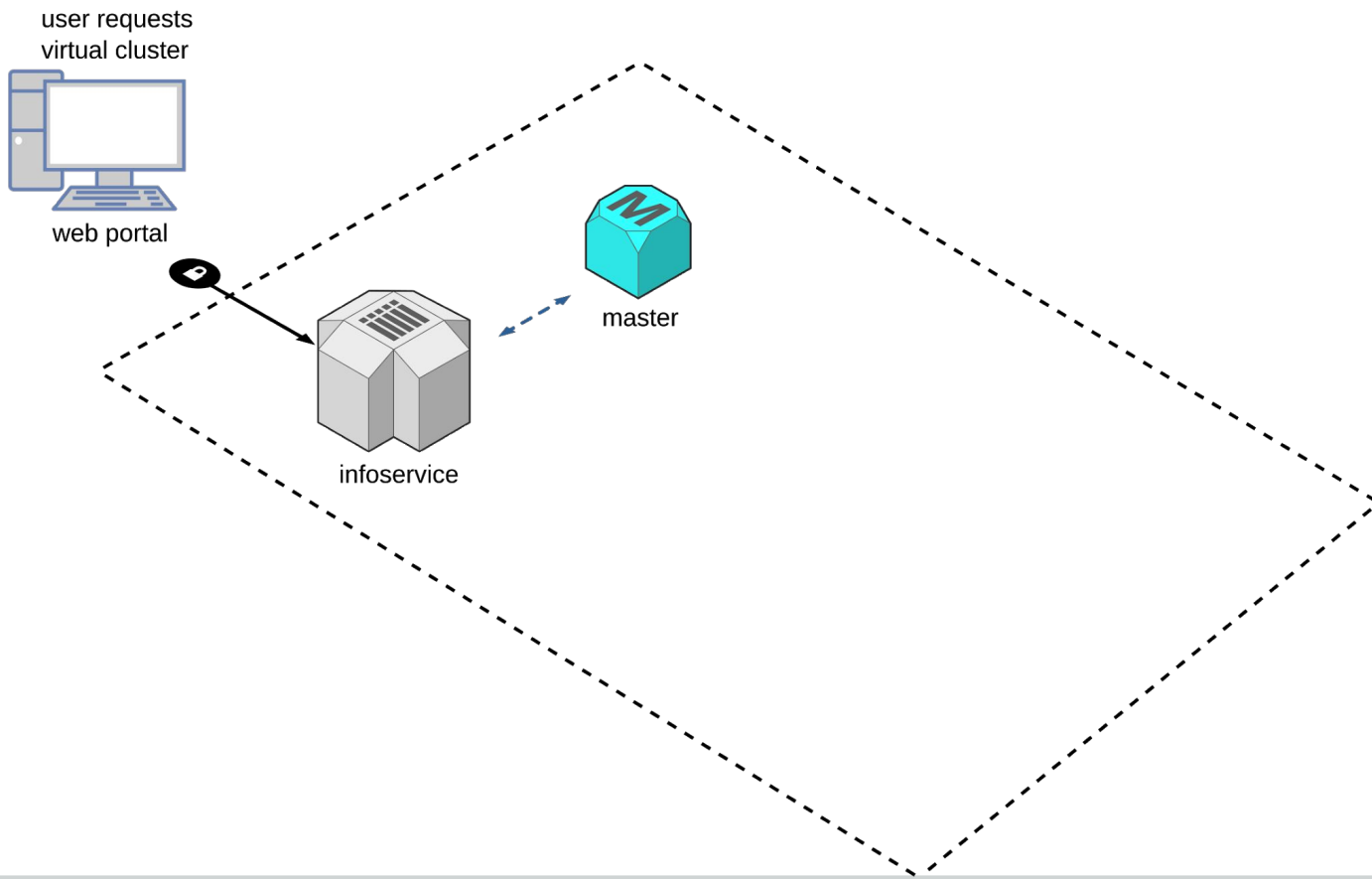


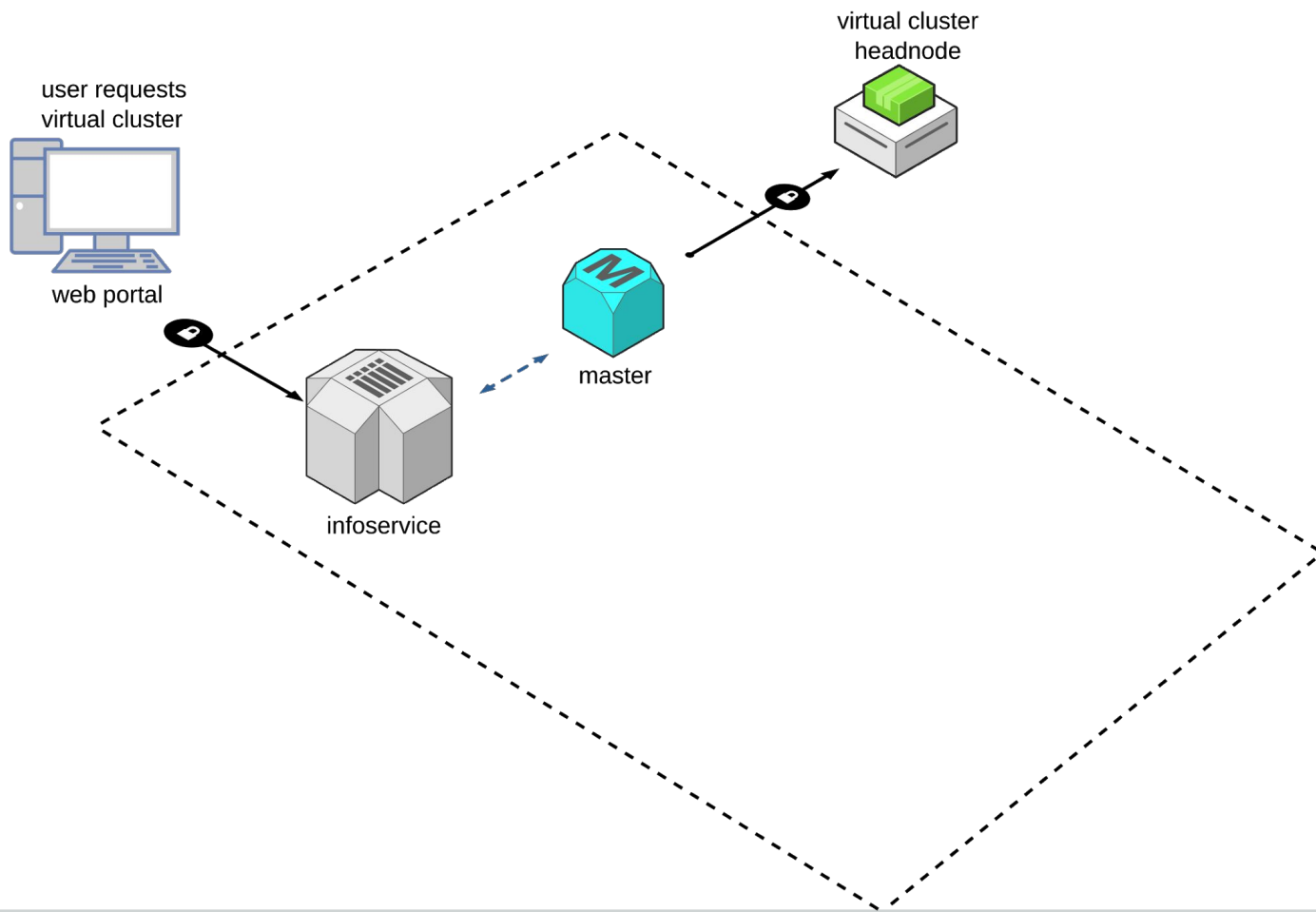
web portal

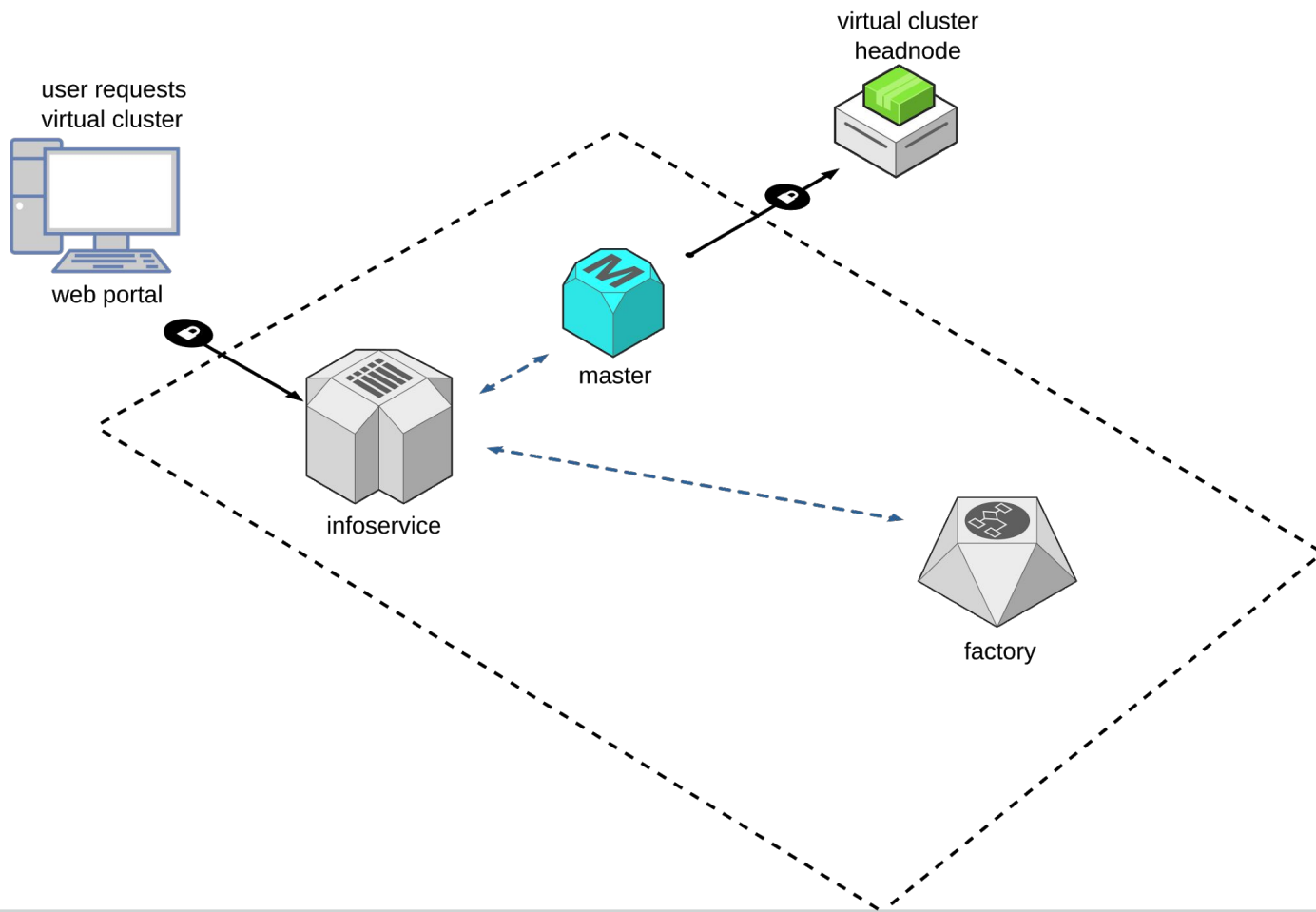


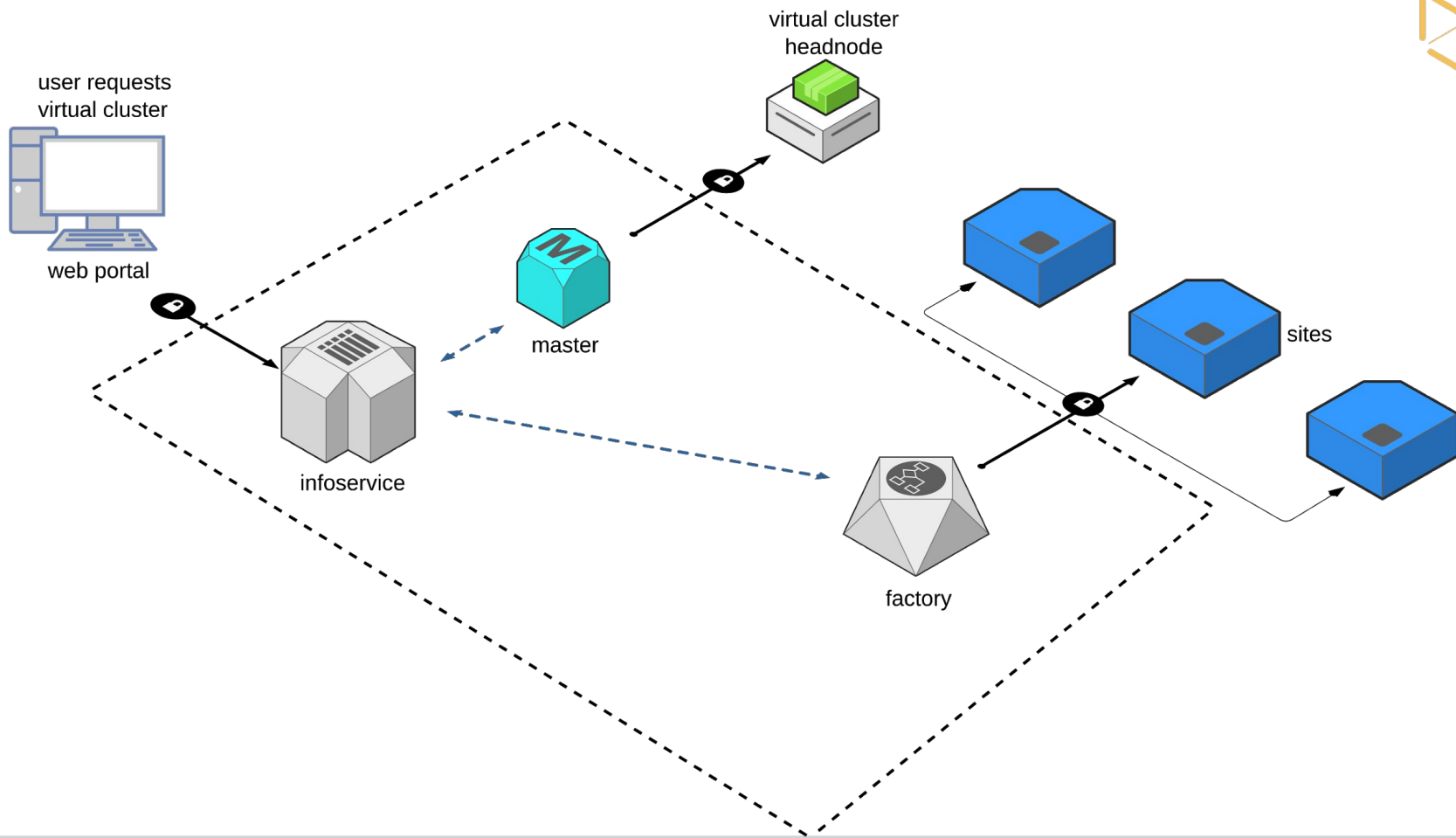


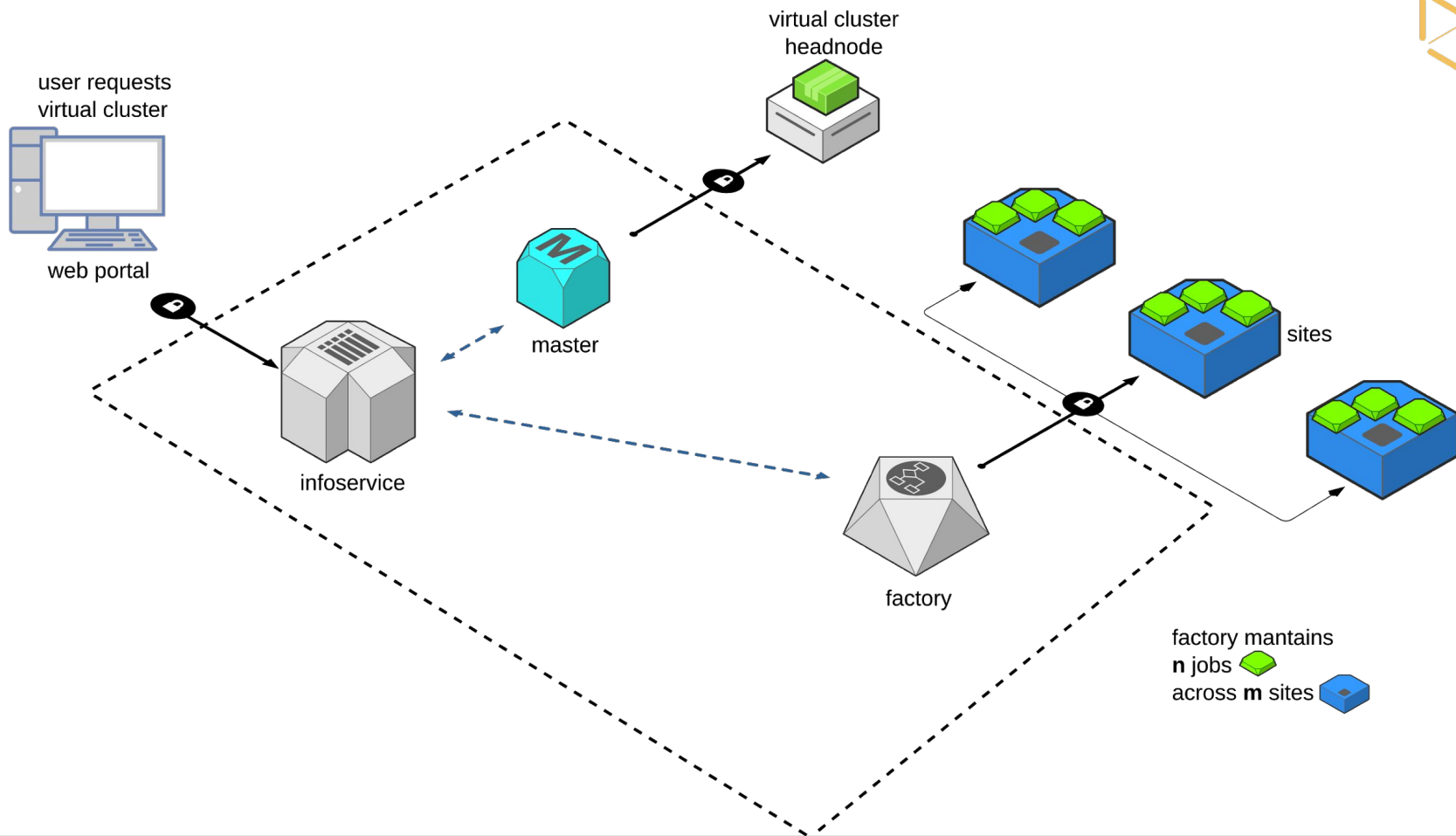
infoservice

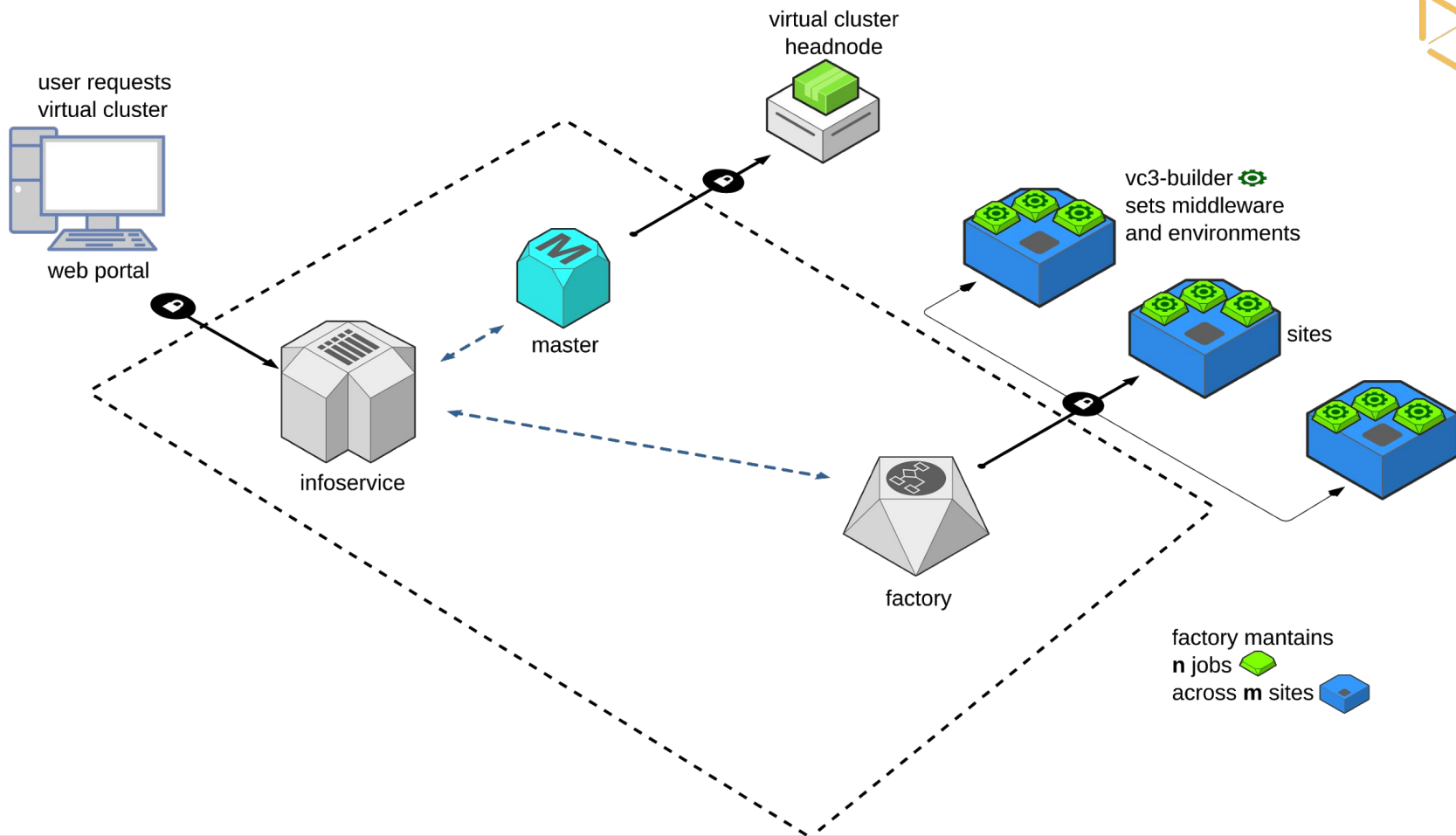


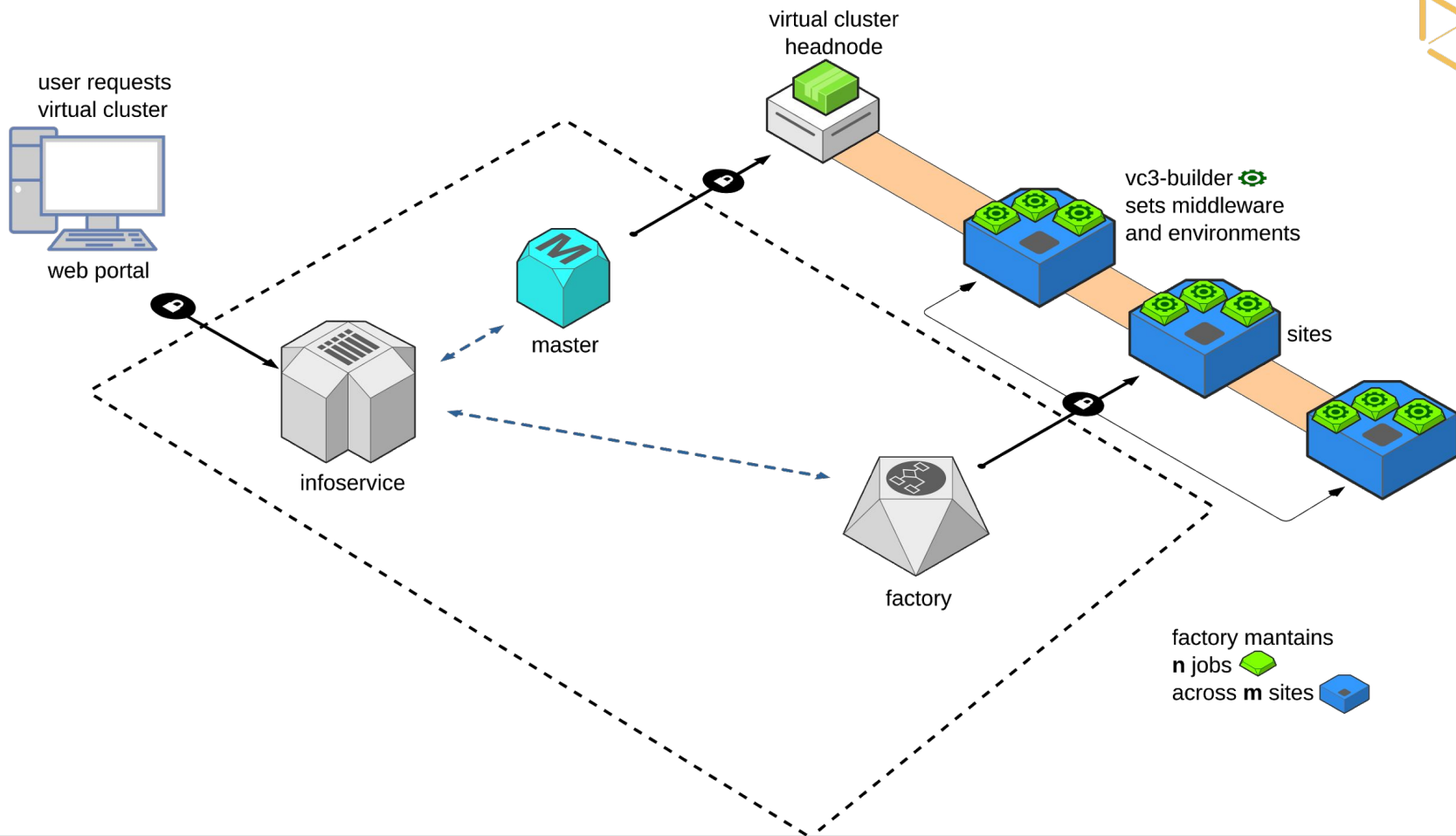














# VC3 builder

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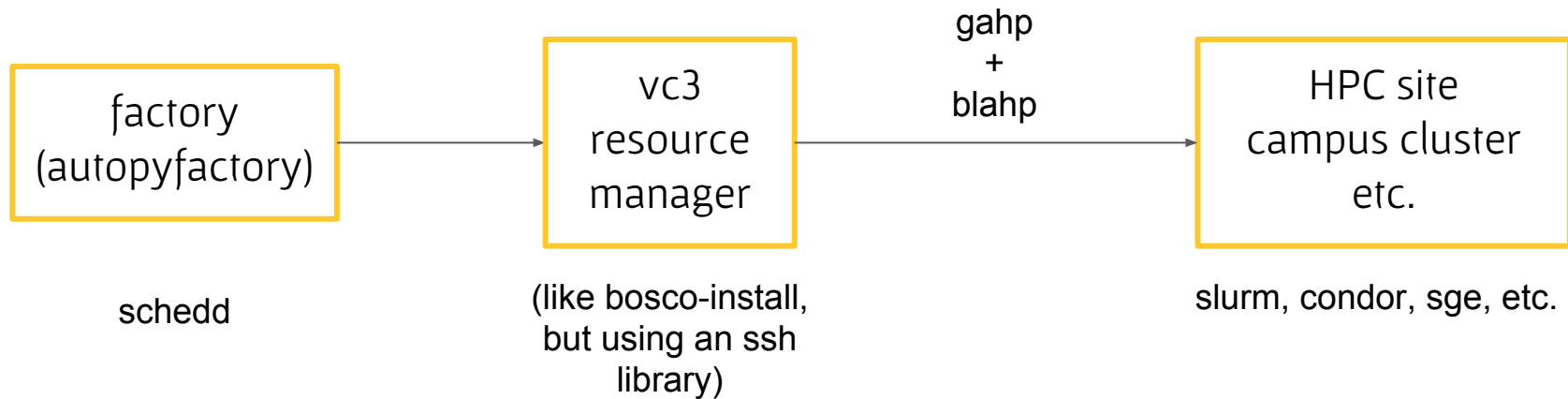
The **vc3-builder**, a command-line tool for deploying software environments on clusters.

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

<https://github.com/vc3-project/vc3-builder>

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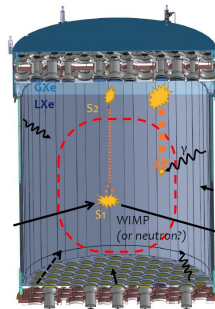
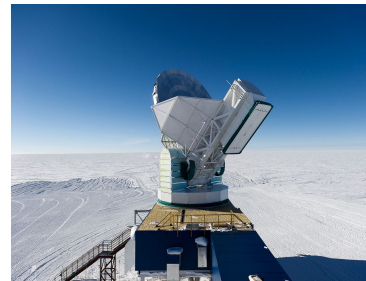
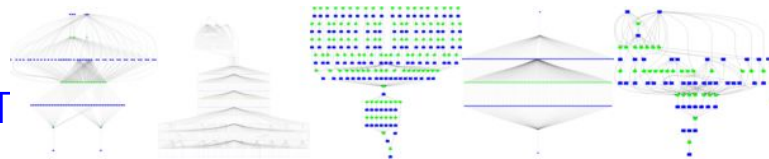
# How Condor makes VC3 possible



# 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**



# Major challenges

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Idiosyncrasies of each site



Multi-factor authentication



Communicate delays/errors  
from sites to portal



# Limited Beta Release

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Today we are announcing our **limited beta release!** We are **looking** for **collaborators** to help us work through the bugs and offer feedback.

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:

<http://bit.ly/vc3-signup>

[btovar@nd.edu](mailto:btovar@nd.edu)  
[khurtado@nd.edu](mailto:khurtado@nd.edu)

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# VC3 Funding and Team

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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)

co-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** (BNL).



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

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**Rich Carlson, Program Manager**

# VC3 thanks



Thank you to other sponsors and the technology providers that made this possible.



Science Gateways  
Community Institute

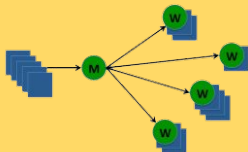


globus



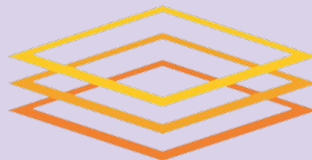
AutoPyFactory

*Work Queue*



ci c•nnect

**HTC**condor  
High Throughput Computing



Open Science Grid



# VC3



## Virtual Clusters for Community Computation

<https://www.virtualclusters.org>

<https://www.virtualclusters.org/community>

@virtualclusters

Limited beta signup: <http://bit.ly/vc3-signup>



Supported by the Department of Energy Office of Advanced Scientific Computing Research and Next Generation Networking Services, Solicitation DE--FOA-0001344 (DDRM), Proposal 0000219942.

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