VC3

Virtual Clusters for Community Computation

Ben Tovar <btovar@nd.edu> for the VC3 team

UNIVERSITY OF NOTRE DAME

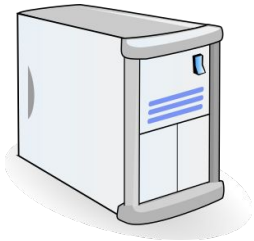
THE UNIVERSITY OF CHICAGO

BROOKHAVEN NATIONAL LABORATORY

Where our users are

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

one task

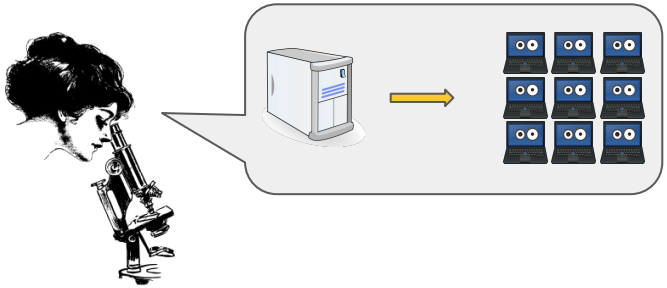


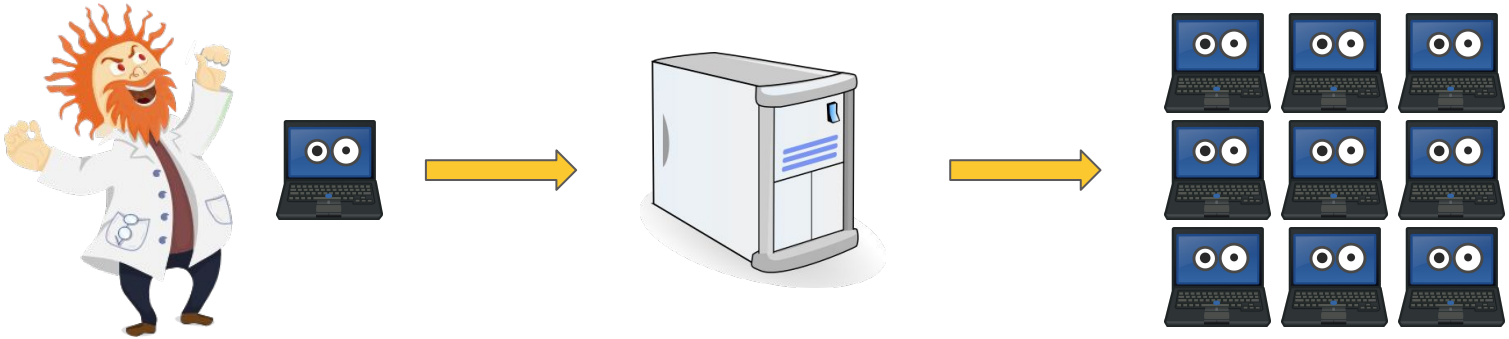
submit node campus cluster, HPC center, etc.

many task running on many computational nodes

Where our users want to be

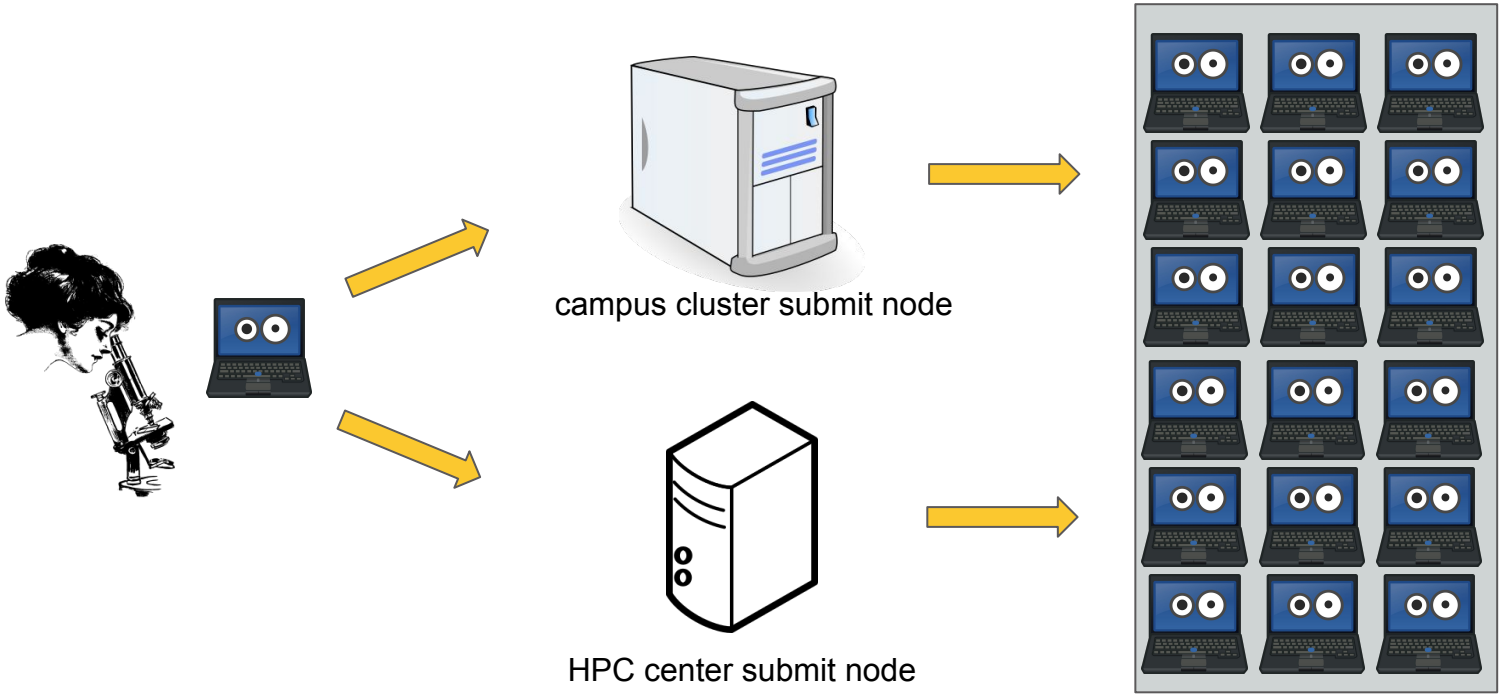
Communicate working setups to colleagues.





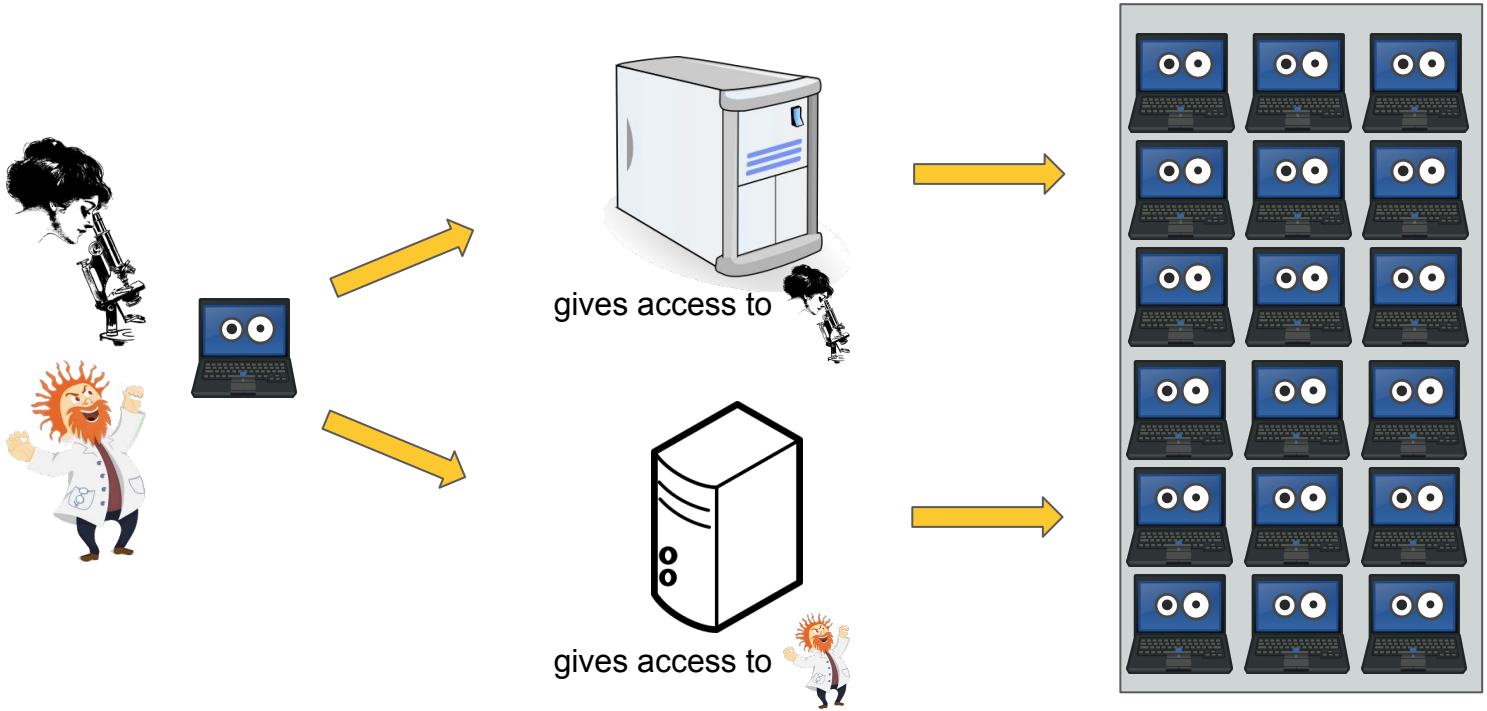
Where our users want to be

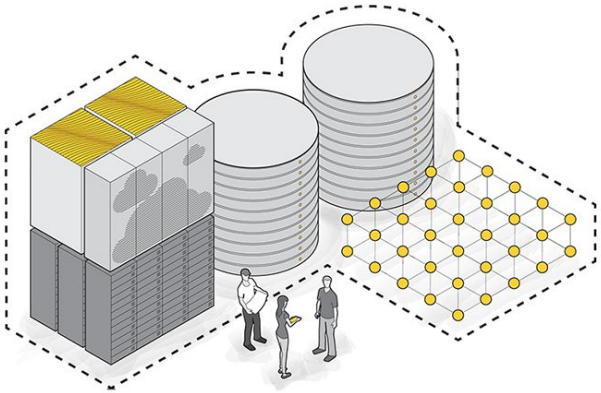
Pool resources together



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

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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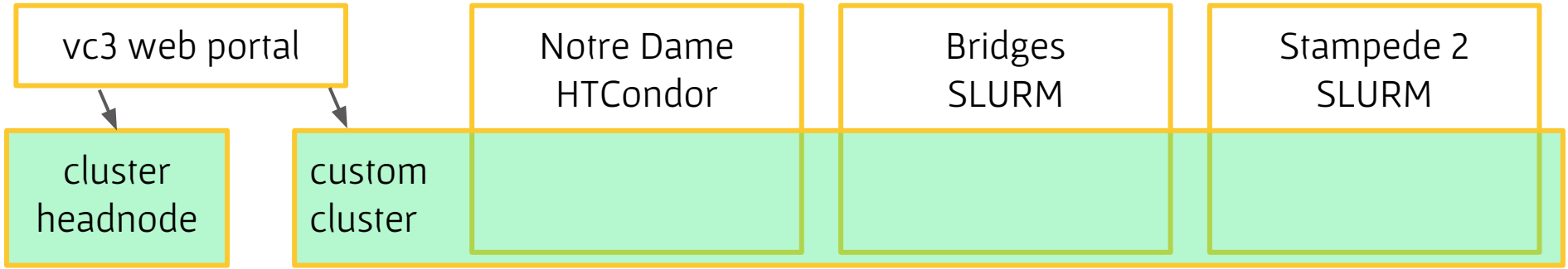

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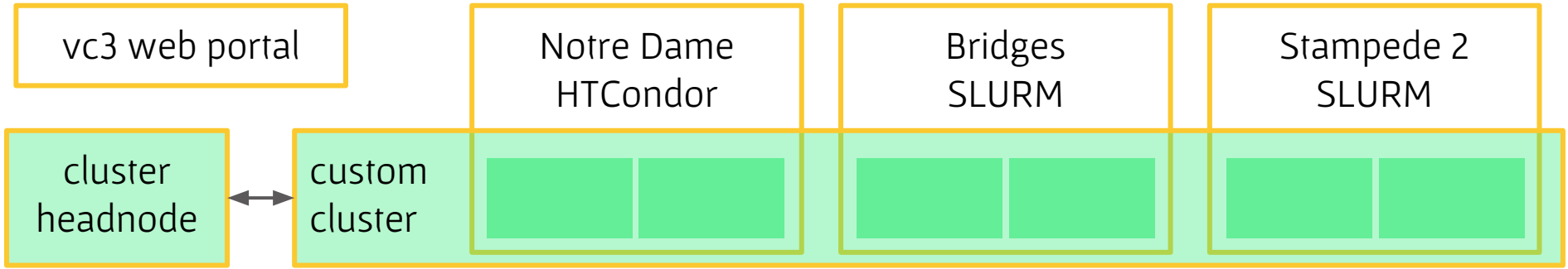

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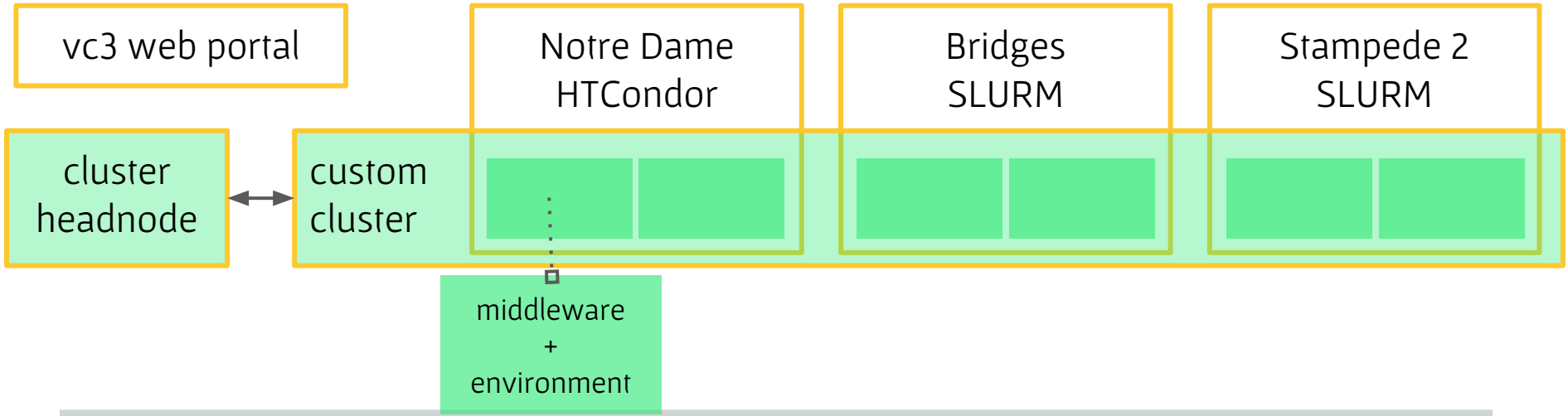

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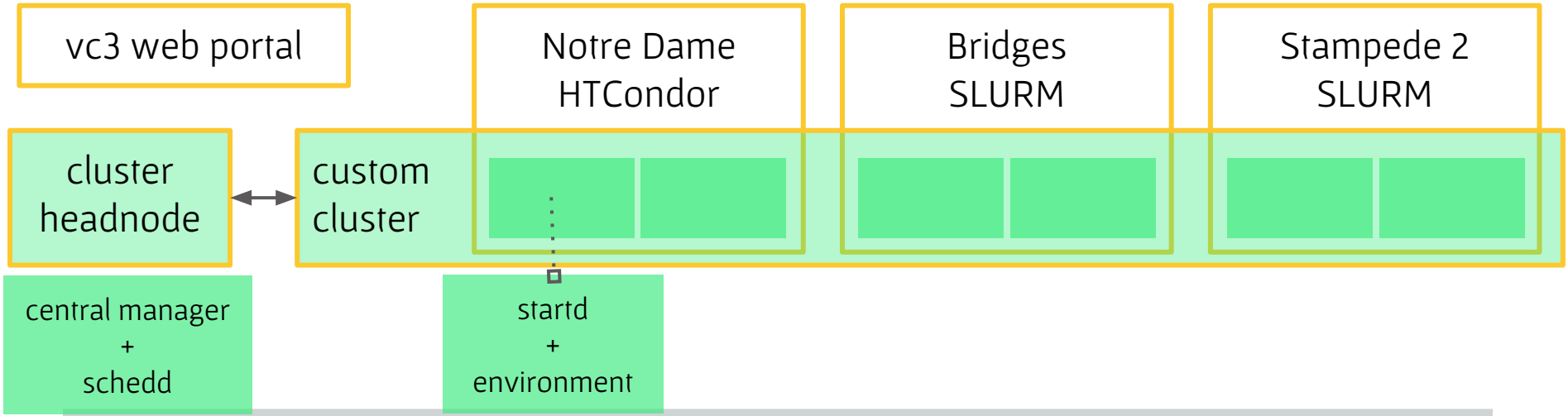

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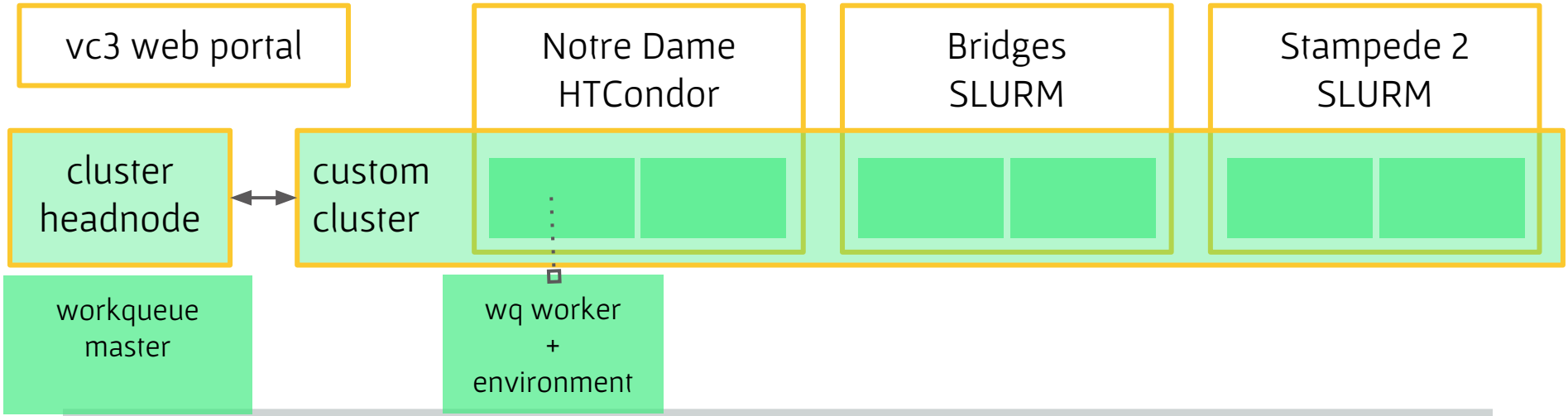


What is a Virtual Cluster?

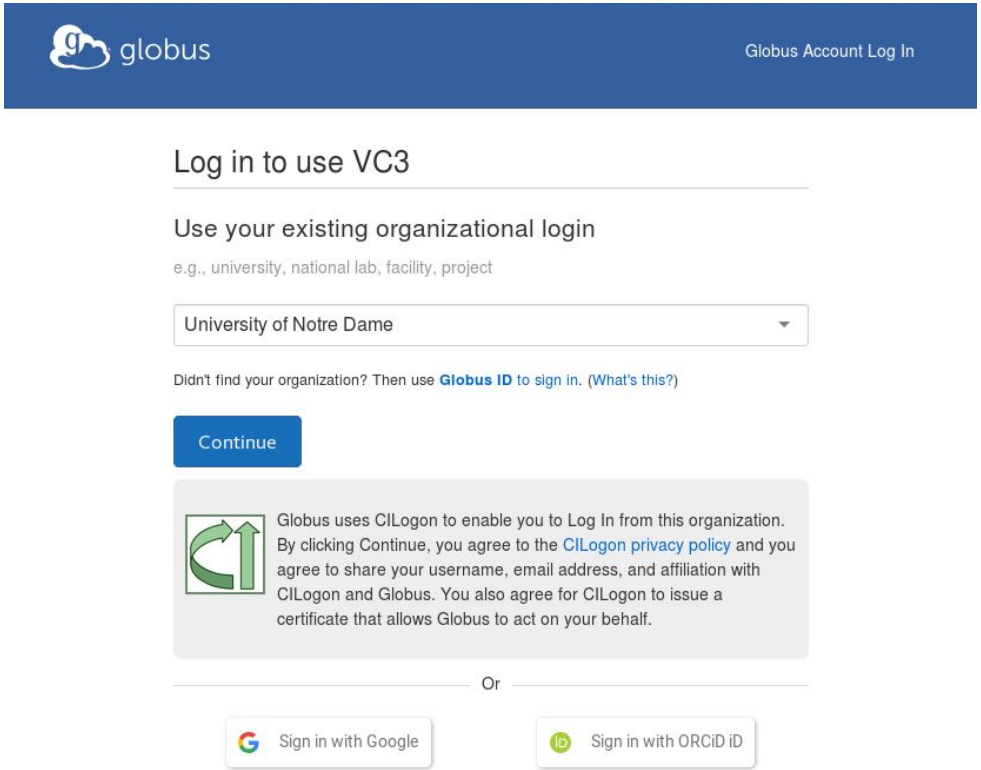
- `1` headnode
- `n` middleware workers running on `m` sites
- `k` environments to run user tasks

Web portal

www.virtualclusters.org

login with a vc3 account

Globus login authentication



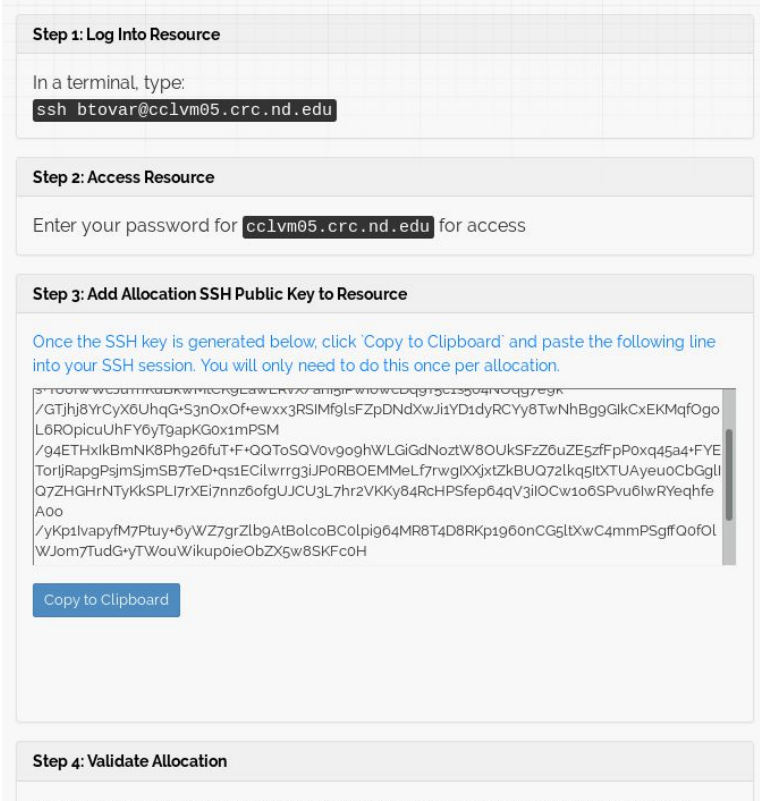
Curated Resources

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



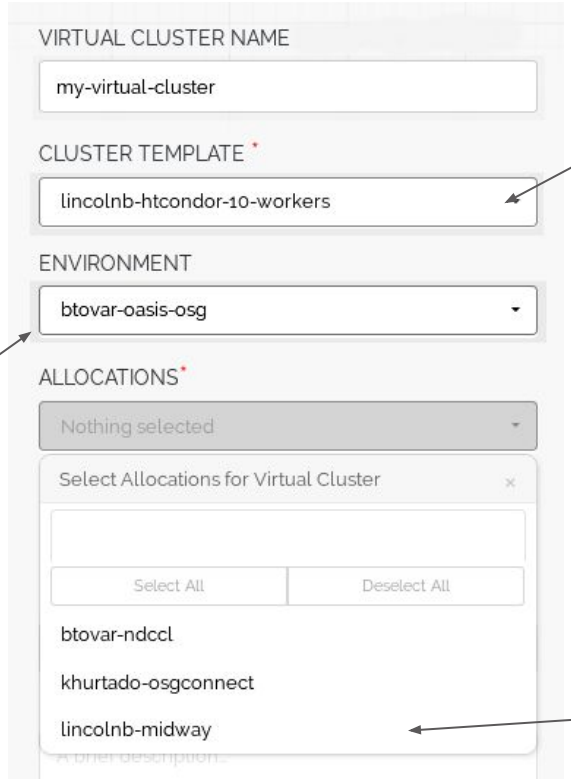
Projects

Project Profiles

Filter

Name	Members	Allocations	Description
vc3-team	**Benjamin Tovar (Owner) - btovar@nd.edu** 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	**Benjamin Tovar (Owner) - btovar@nd.edu** Benjamin Tovar (University of Notre Dame)	btovar-ndccl	Currently no description

Launching a Virtual Cluster

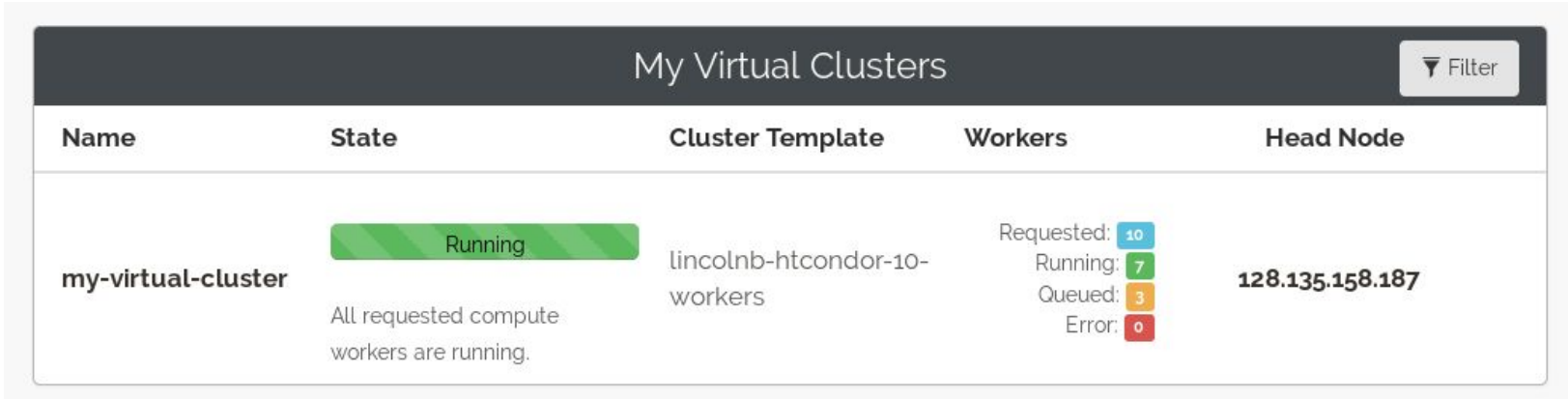


shared cluster definition

workers will have this environment installed

allocations available in this project

Cluster status



Workers from many sites

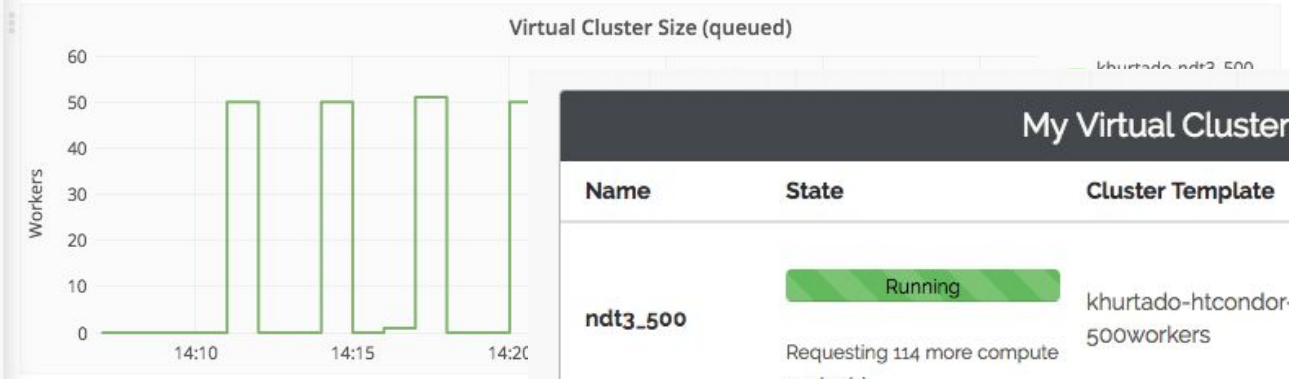
```
[btovar@btovar-my-virtual-cluster ~]$ ip addr | grep 128.135.158.187
    inet 128.135.158.187/25 brd 128.135.158.255 scope global dynamic eth0
[btovar@btovar-my-virtual-cluster ~]$ condor_status
Name                                     OpSys      Arch   State     Activity LoadAv Mem   ActvtyTime

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 ~]$
```

ND

OSG

UChicago

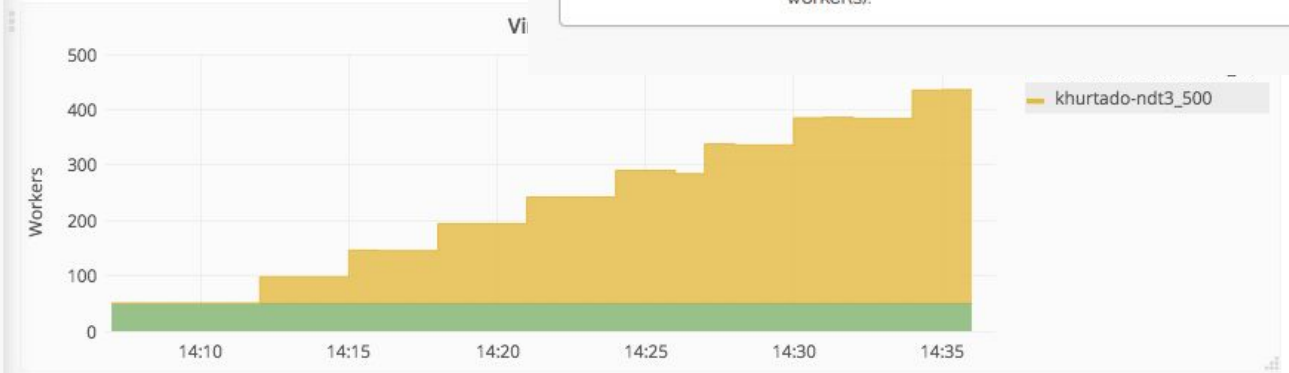
VC3 Monitoring



My Virtual Clusters

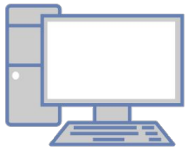
Filter

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

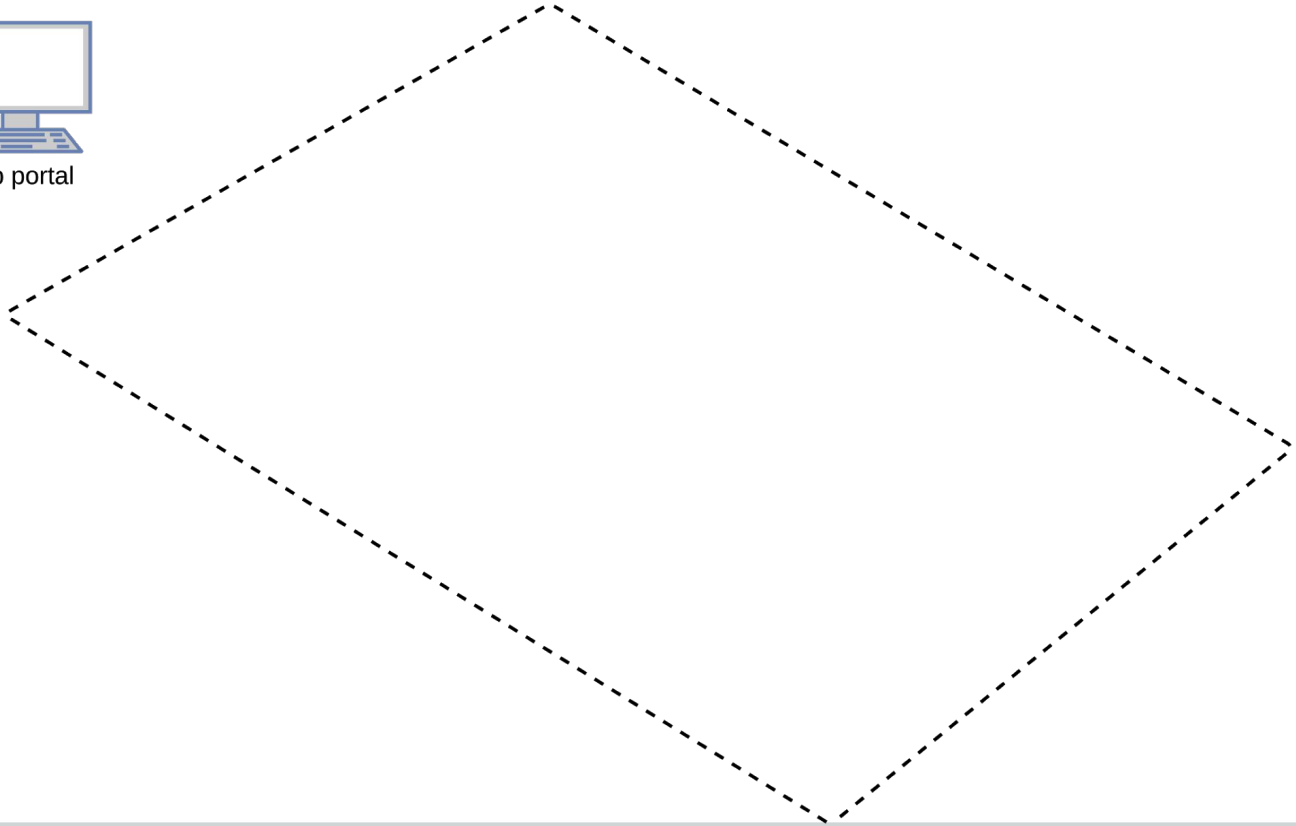


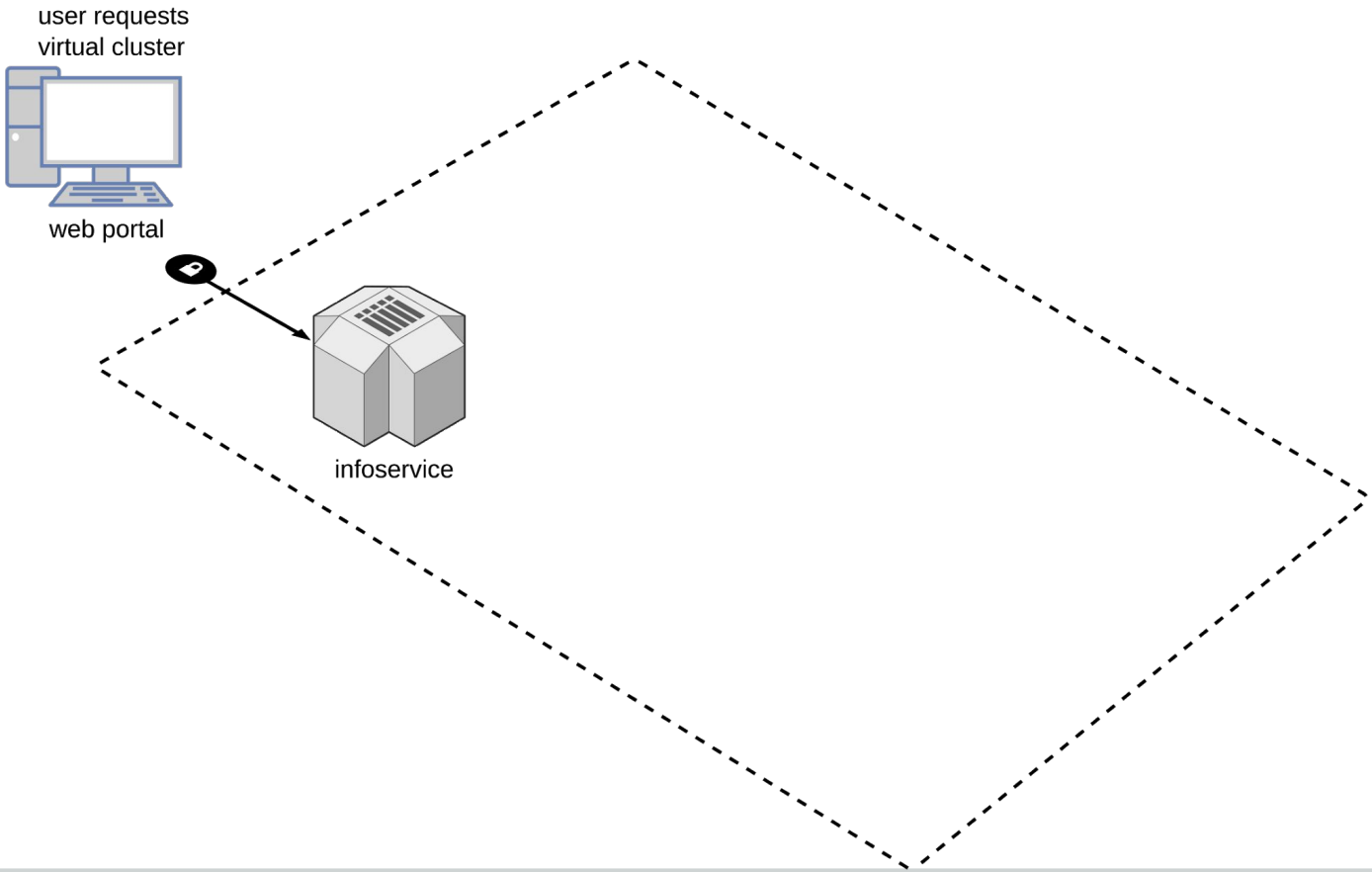
Architecture

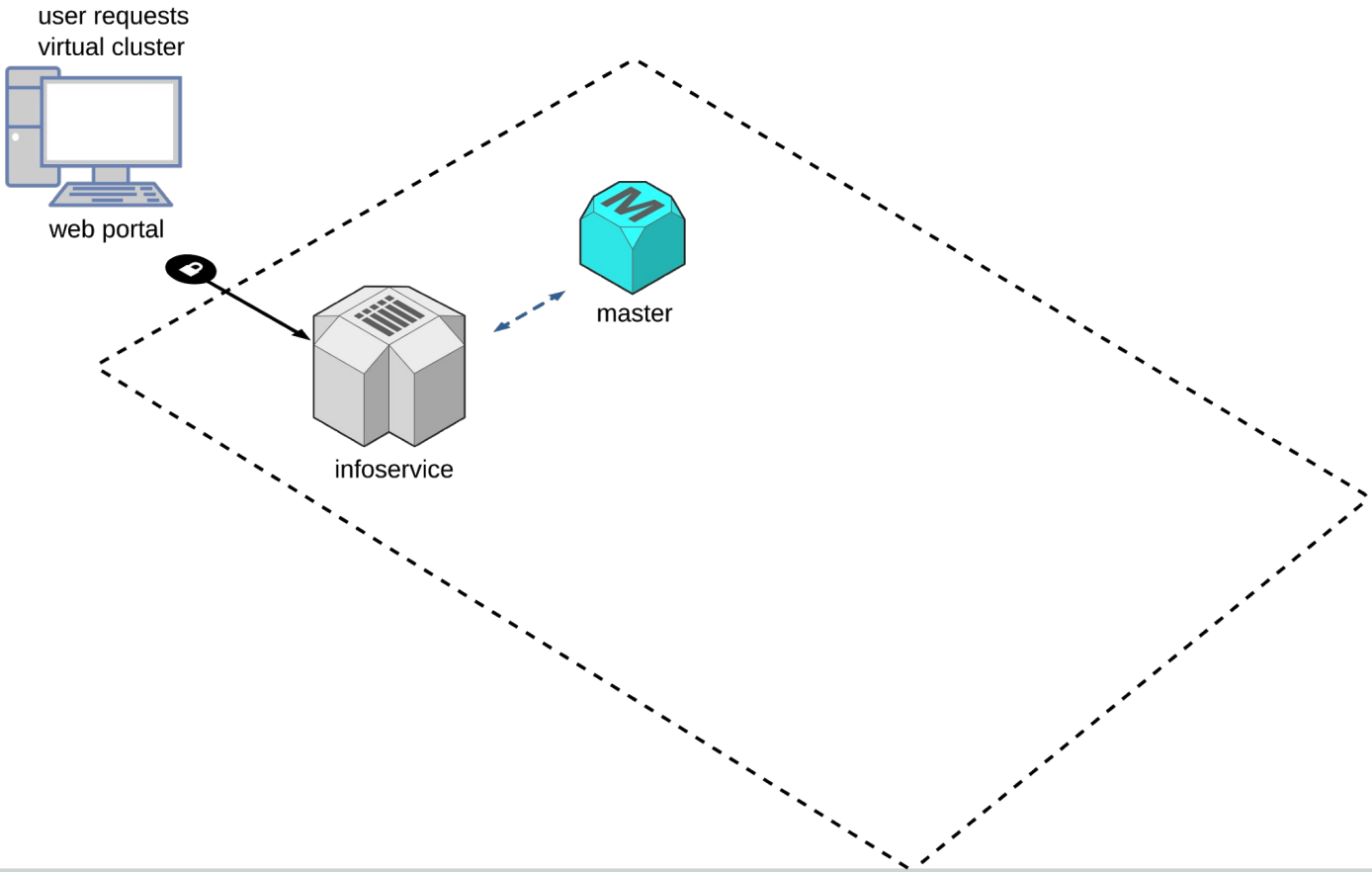
user requests
virtual cluster

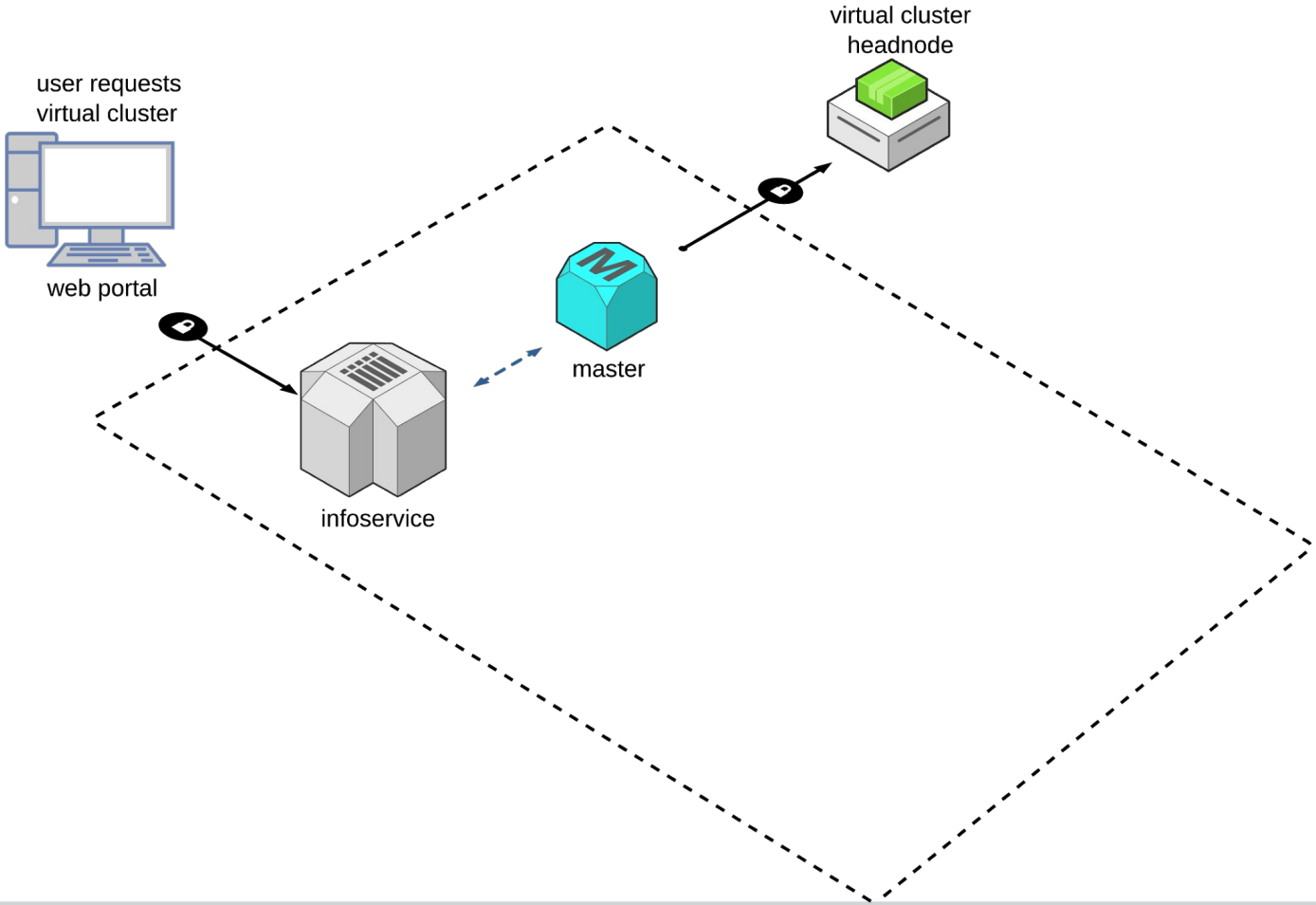


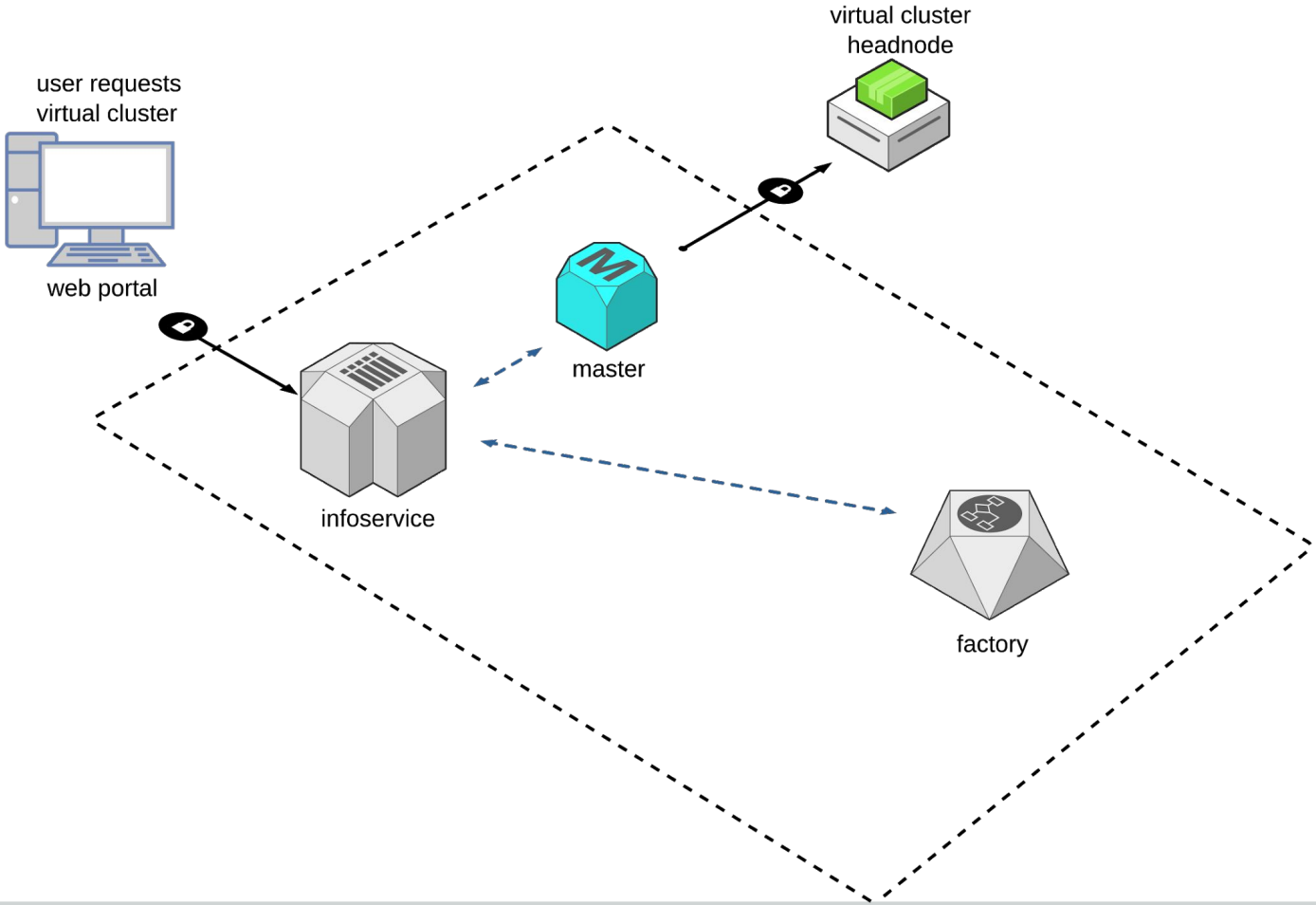
web portal

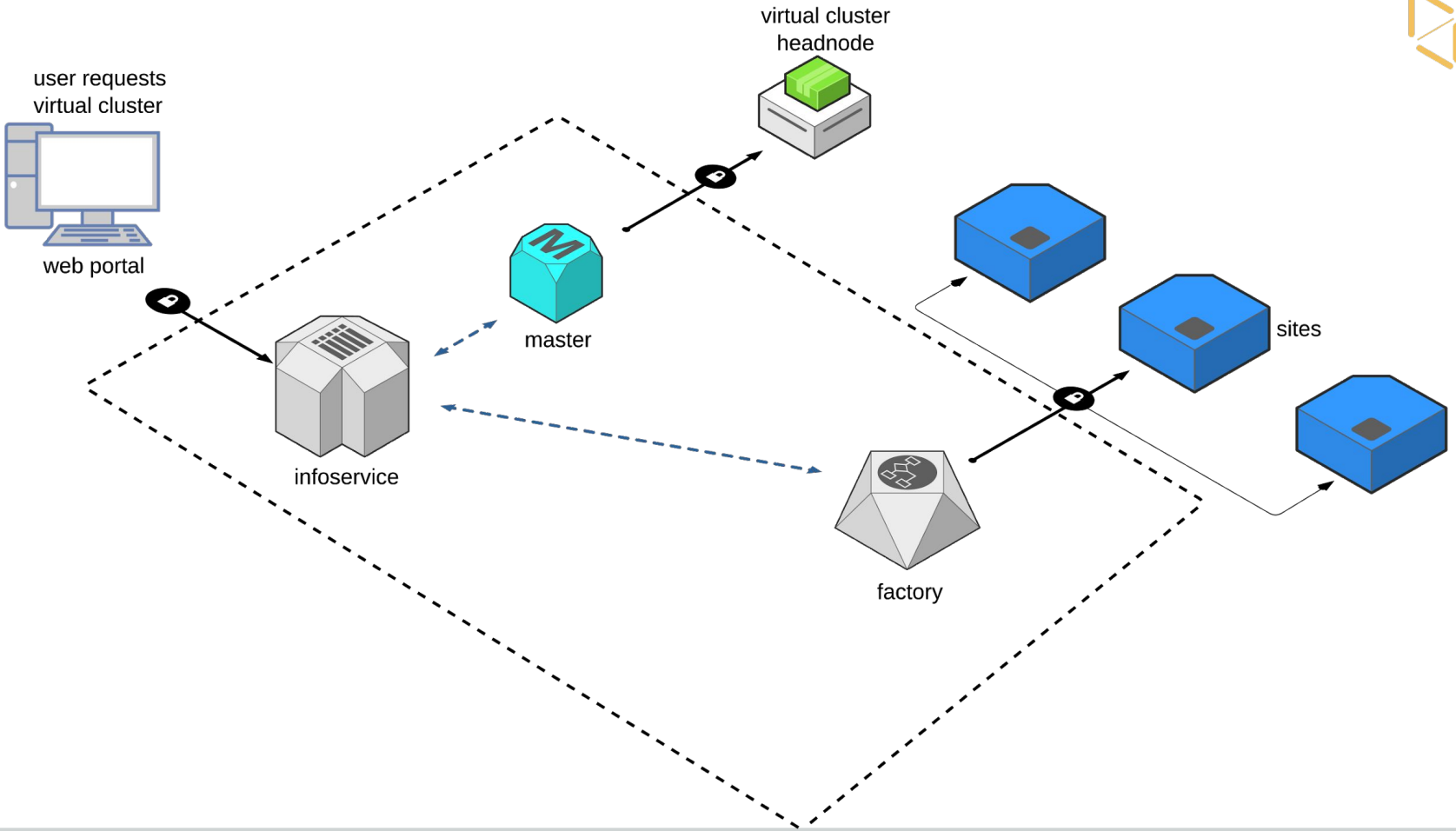


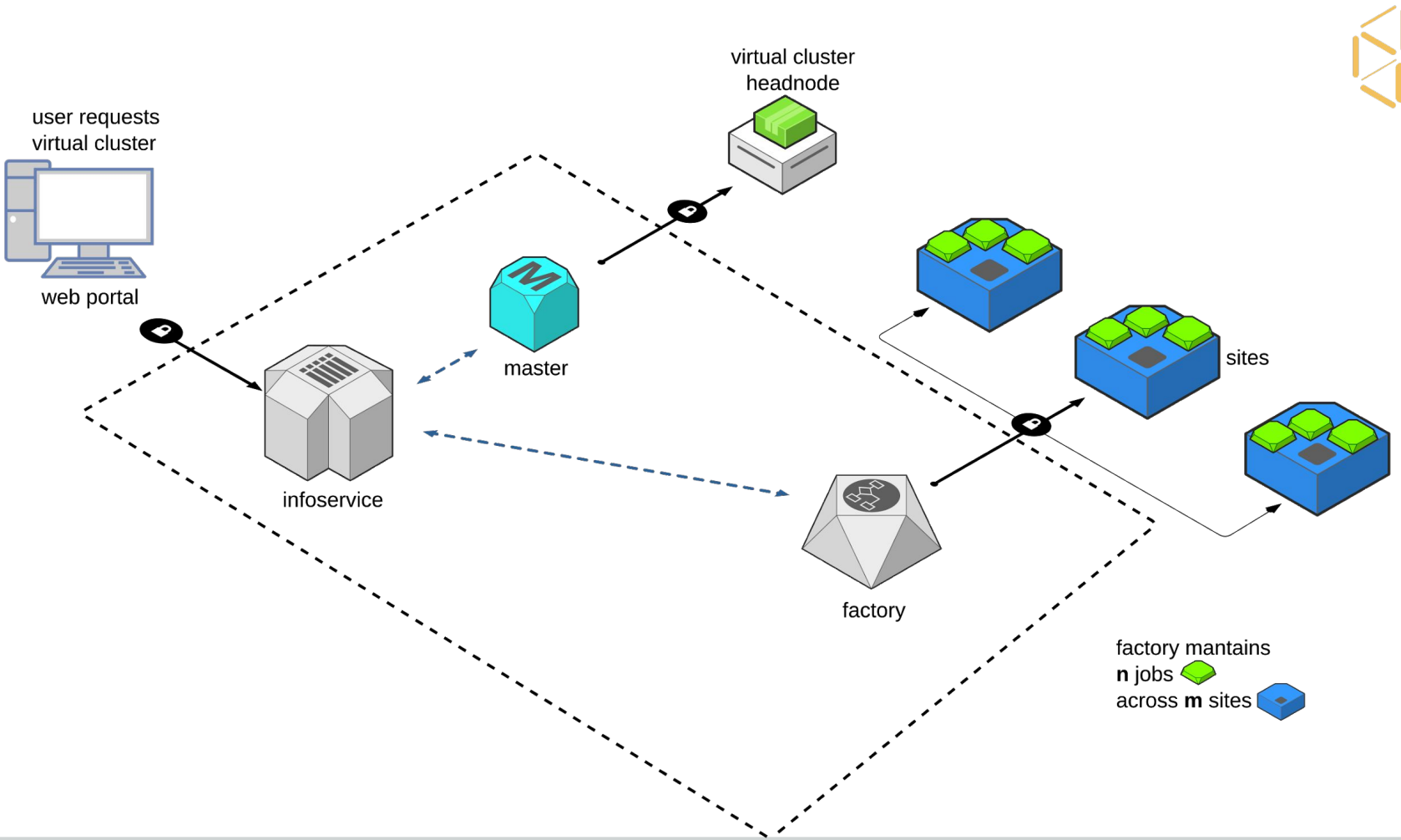

user requests
virtual cluster
web portal
infoservice


user requests
virtual cluster
web portal
master
infoservice


virtual cluster
headnode
user requests
virtual cluster
web portal
master
infoservice


virtual cluster
headnode
user requests
virtual cluster
web portal
master
infoservice
factory


virtual cluster
headnode
user requests
virtual cluster
web portal
master
infoservice
sites
factory


virtual cluster
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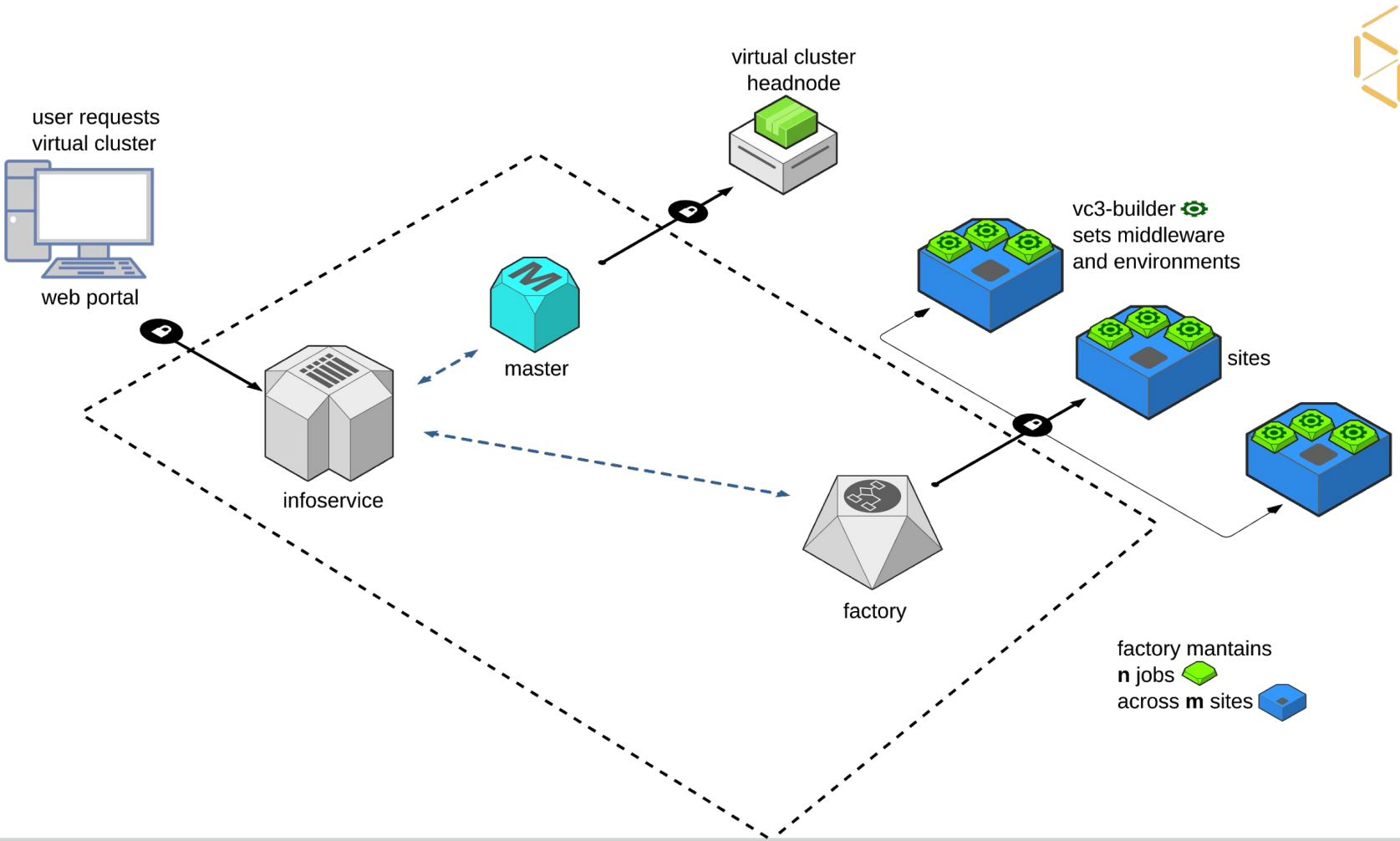
across **m** sites


virtual cluster
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sets middleware
and environments
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infoservice
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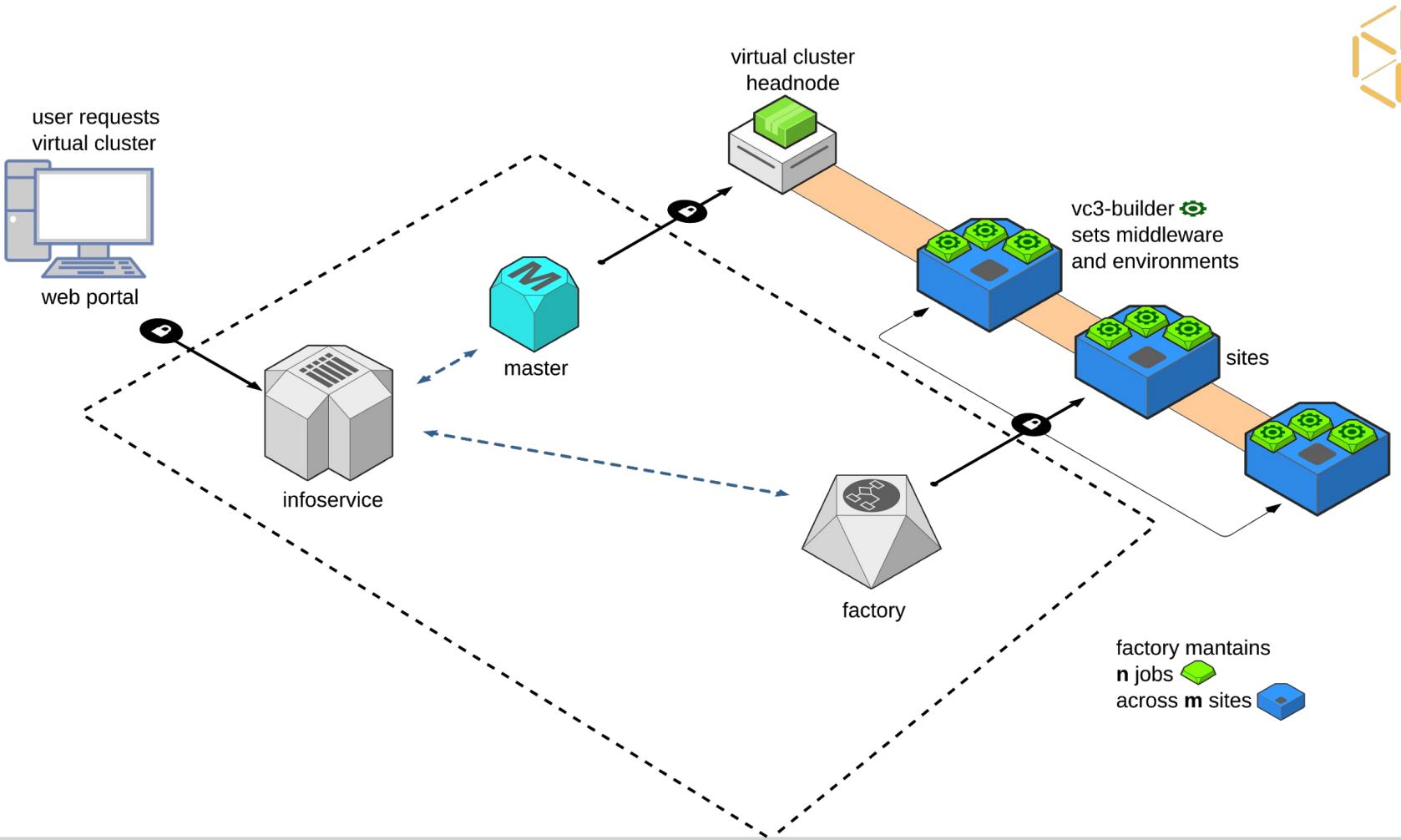
user requests
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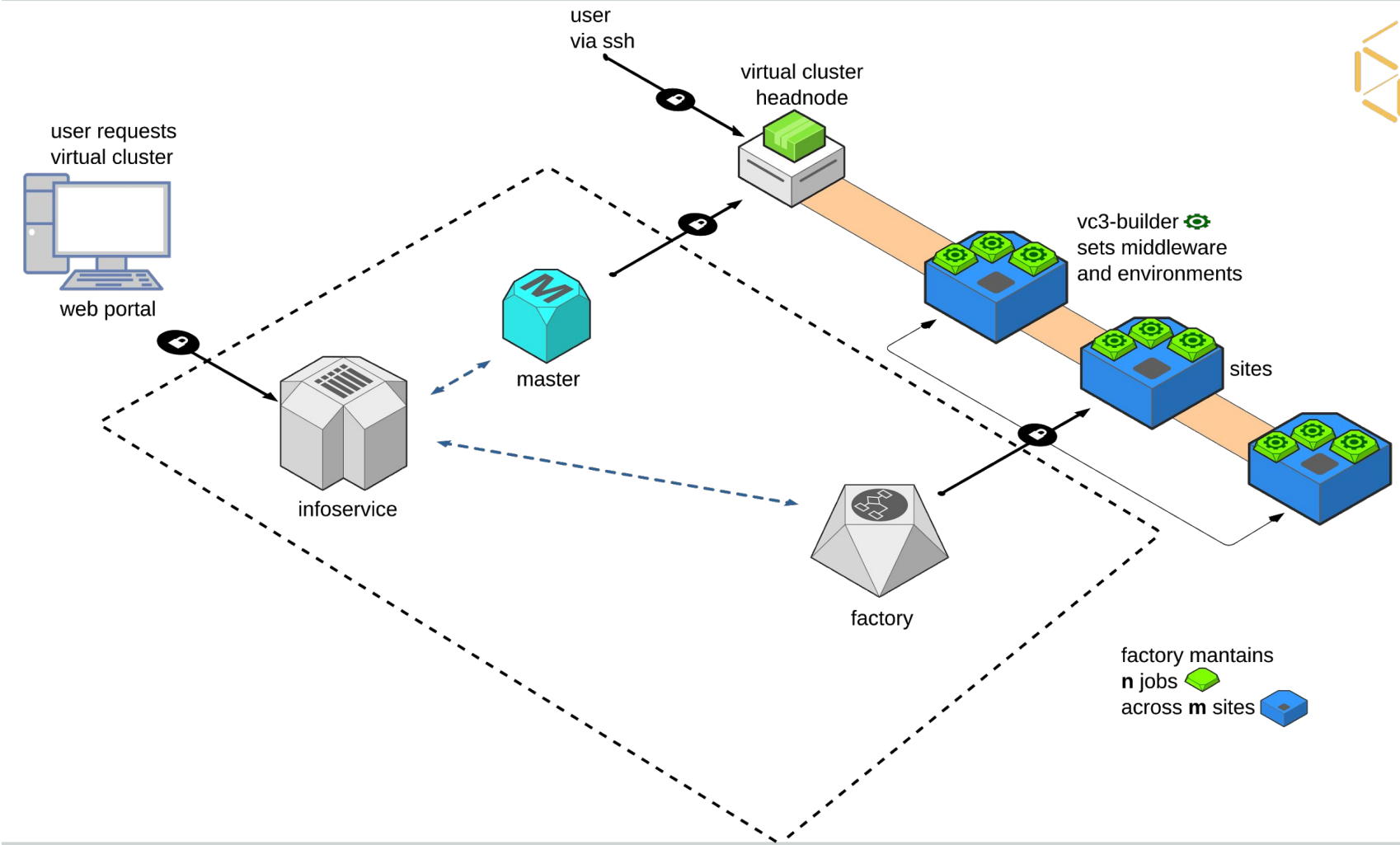

user
via ssh
virtual cluster
headnode
user requests
virtual cluster
web portal
vc3-builder
sets middleware
and environments
sites
master
infoservice
factory
factory mantains
n jobs
across m sites

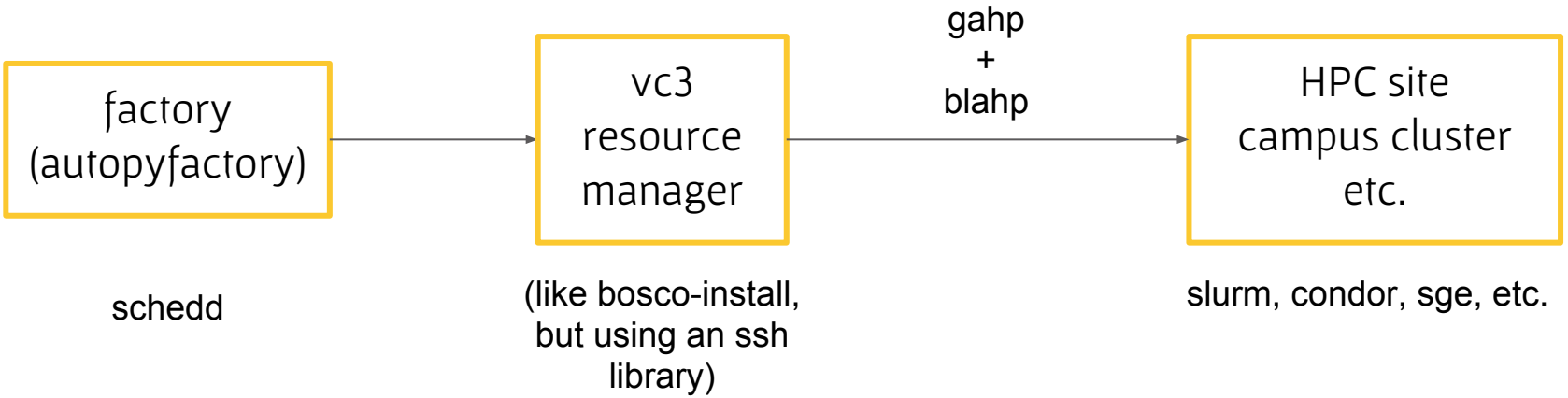
VC3 builder

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

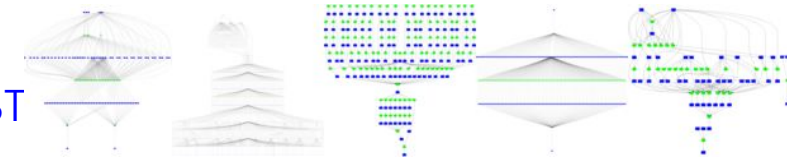
```
vc3-builder
    --require-os centos:7
    --mount /scratch=/data
    --require /cvmfs
    --require python:2.7 -- myapp ...my args...
```

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

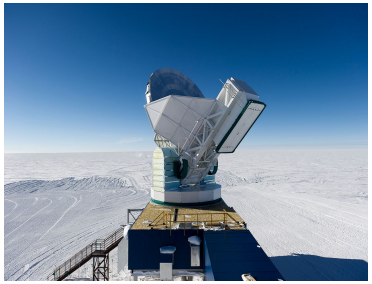
How Condor makes VC3 possible

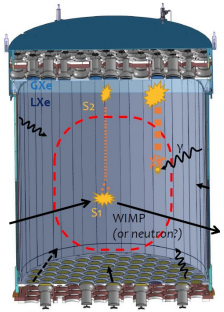


Working Middleware and Applications



- 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

Idiosyncrasies of each site

Multi-factor authentication

Communicate delays/errors from sites to portal

Limited Beta Release

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
khurtado@nd.edu

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)

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

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

VC3 thanks

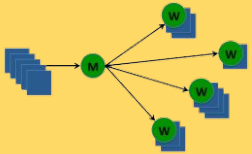
Thank you to other sponsors and the technology providers that made this possible.

SGCI Science Gateways Community Institute

globus

AutoPyFactory

Work Queue



ci connect

HTCondor High Throughput Computing

Open Science Grid

NSF

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.

btovar@nd.edu