

JupyterHub on Scientific OpenStack

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StackHPC

Jupyter Ecosystem

- “Classic” Jupyter Notebook
- JupyterLab Notebook (replaces classic)
- JupyterHub (multi-user, creates both notebooks)
- Others: BinderHub, Pangeo, Conda, Voila



Jupyter Notebooks @ DiRAC

- Performance Tips
- File and I/O Management
- Data Transfer Guide
- Policies
- References and further reading
- APPLICATIONS
 - ABAQUS
 - CASTEP
 - Gaussian
 - GROMACS
 - ANSYS Fluent
 - LAMMPS Molecular Dynamics Simulator
 - MATLAB
 - PyTorch
- ☰ Jupyter Notebooks
 - Setup Jupyter on CSD3
 - Running Jupyter
 - Running Jupyter on a compute node
 - Running jobs from within Jupyter
- OpenFOAM
- OpenMM
- Tensorflow

```
$ pip install kiwisolver
```

Running Jupyter

- activate the virtual environment:

```
$ source ~/jupyter-env/bin/activate
```

- start notebook server:

```
$ jupyter notebook --no-browser --ip=127.0.0.1 --port=8081
```

this will print out lots of messages, finishing with a web address. Copy this web address into the clipboard and make a note of which login node you have used.

Then from your local machine, forward a port to be able to connect to the notebook server:

```
$ ssh -L 8081:127.0.0.1:8081 -fN login-e-1.hpc.cam.ac.uk
```

and ensure that you pick the same login node (here we are assuming login-e-1) that you started the notebook server on. You can then open the web address and connect to your notebook server.

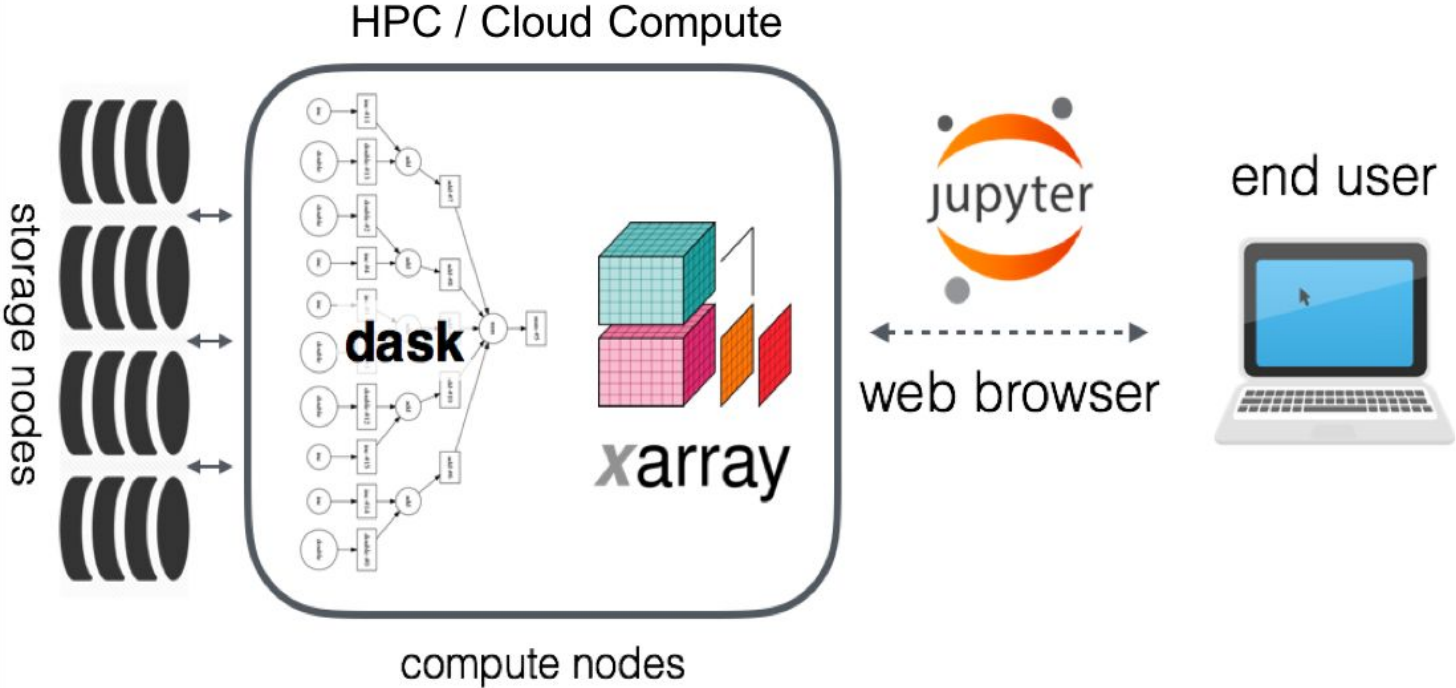
Running Jupyter on a compute node

- On Wilkes-2 submit a GPU job by running the following or setting the appropriate SLURM variables in a submission script:

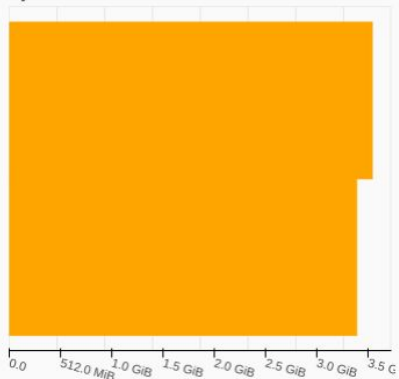
```
$ srun -t 02:00:00 --nodes=1 --gres=gpu:1 --ntasks-per-node=1 --cpus-per-task=3 --partition:
```

<https://docs.hpc.cam.ac.uk/hpc/software-packages/jupyter.html>

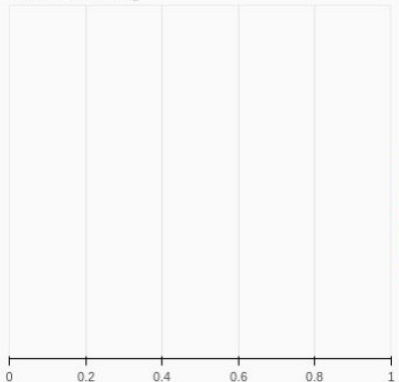
Pangeo



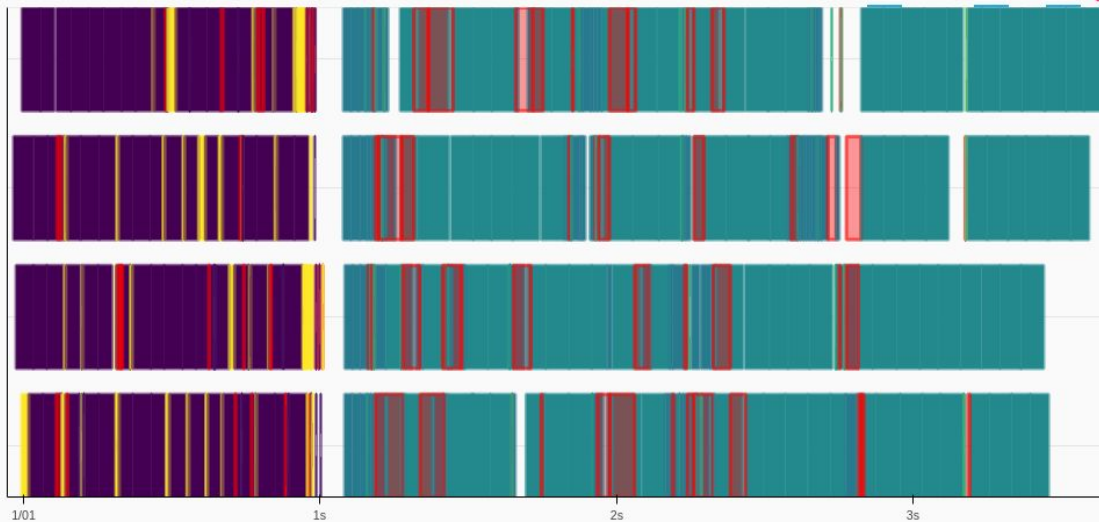
Bytes stored: 7.43 GB



Tasks Processing



Task Stream



Progress -- total: 340, in-memory: 200, processing: 0, erred: 0

random_sample	100 / 100
mean_chunk	100 / 100
sub	100 / 100
mean_combine...	30 / 30
mean_agg-agg...	10 / 10

Deploying JupyterHub

- Ground up install
<https://jupyterhub.readthedocs.io>
- The Littlest JupyterHub (single server)
<https://tljh.jupyter.org>
- Zero to JupyterHub (for Kubernetes)
<https://z2jh.jupyter.org>



[Kubernetes on Google Cloud \(GKE\)](#)[Kubernetes on Microsoft Azure Kubernetes Service \(AKS\)](#)[Kubernetes on Microsoft Azure Kubernetes Service \(AKS\) with Autoscaling](#)[Kubernetes on Amazon Web Services \(AWS\)](#)[Kubernetes on Amazon Web Services \(AWS\) with Elastic Container with Kubernetes \(EKS\)](#)[Kubernetes on Red Hat OpenShift](#)[Kubernetes on IBM Cloud](#)[Kubernetes on Digital Ocean](#)

Setup Kubernetes

Kubernetes' documentation describes the many [ways to set up a cluster](#). We attempt to provide quick instructions for the most painless and popular ways of setting up a Kubernetes cluster on various cloud providers and on other infrastructure.

Choose one option and proceed.

- [Kubernetes on Google Cloud \(GKE\)](#)
- [Kubernetes on Microsoft Azure Kubernetes Service \(AKS\)](#)
- [Kubernetes on Microsoft Azure Kubernetes Service \(AKS\) with Autoscaling](#)
- [Kubernetes on Amazon Web Services \(AWS\)](#)
- [Kubernetes on Amazon Web Services \(AWS\) with Elastic Container with Kubernetes \(EKS\)](#)
- [Kubernetes on Red Hat OpenShift](#)
- [Kubernetes on IBM Cloud](#)
- [Kubernetes on Digital Ocean](#)

Note

- During the process of setting up JupyterHub, you'll be creating some files for configuration purposes. It may be helpful to create a folder for your JupyterHub deployment to keep track of these files.

FY19 Digital Assets

StackHPC

OpenStack Magnum

- Kubernetes Cloud Provider OpenStack
 - Storage: Cinder, Manila
 - Load Balancer: Octavia
 - Cluster Autoscaler and Auto-healing
- Monitoring via Prometheus and Grafana
- Improved documentation:
 - Terraform to create/re-size Kubernetes
 - Ingress via Nginx, Terraform to add a Router to CephFS
 - JupyterHub on Kubernetes, with IRIS IAM (using Helm 3)
 - Apache Spark (using Helm 3)



<https://github.com/RSE-Cambridge/iris-magnum>

Example: Terraform for K8s

```
terraform {  
  required_version = ">= 0.12, < 0.13"  
}  
  
module "cluster" {  
  source = "../../modules/cluster"  
  
  cluster_name = "my-test"  
  cluster_template_name = "kubernetes-1.15.9-20200205"  
  master_flavor_name = "general.v1.tiny"  
  flavor_name = "general.v1.tiny"  
  master_count = 1  
  node_count = 1  
  max_node_count = 2  
}
```



Cinder Volumes in K8s

Assuming your magnum templated enabled the built in cinder volumes, you can use them for PVCs by create a new storage class:

```
cat <<END | kubectl apply -f -
kind: StorageClass
apiVersion: storage.k8s.io/v1
metadata:
  name: cinder
  annotations:
provisioner: kubernetes.io/cinder
END
```

You can make it the default by applying:

```
kubectl patch storageclass cinder -p \
'{"metadata": {"annotations":{"storageclass.kubernetes.io/is-default-class":"true"}}}'
```

Note: the above uses the in-tree cinder driver that is deprecated. We are looking to change OpenStack Magnum to rely on the more supported setup of using the cloud-provider-openstack based driver. But for now, this seems to be the best way to use cinder volumes.

Zero to Jupyterhub

At this point you will have Helm installed and kubectl pointing at your kubernetes cluster created by OpenStack Magnum.

To make it easy to tidy up and separate your work, we create a new namespace to contain all the work on JupyterHub:

```
kubectl create namespace jhub
```

We can now follow this tutorial: <https://zero-to-jupyterhub.readthedocs.io/en/latest/setup-jupyterhub/setup-jupyterhub.html>

```
helm repo add jupyterhub https://jupyterhub.github.io/helm-chart/  
helm repo update  
  
cat >config.yml <<END  
proxy:  
  secretToken: "`openssl rand -hex 32`"  
END  
  
helm install jhub jupyterhub/jupyterhub --values config.yml --namespace jhub  
  
kubectl --namespace jhub get service
```

Once the external IP appears you can now login as any username and password. This is clearly an unsafe default for a

Example: JupyterHub with IRIS IAM

```
jupyterhub:  
  hub:  
    extraEnv:  
      OAUTH2_AUTHORIZE_URL: https://iris-iam.stfc.ac.uk/authorize  
      OAUTH2_TOKEN_URL: https://iris-iam.stfc.ac.uk/token  
      OAUTH_CALLBACK_URL: http://128.232.227.125/hub/oauth_callback  
  auth:  
    type: custom  
    custom:  
      className: oauthenticator.generic.GenericOAuthenticator  
      config:  
        login_service: "IRIS IAM"  
        client_id: "75dc9e2a-3c08-436e-b110-d710d1e3c530"  
        client_secret: "xxxx"  
        token_url: https://iris-iam.stfc.ac.uk/token  
        userdata_url: https://iris-iam.stfc.ac.uk/userinfo  
        userdata_method: GET  
        userdata_params: {'state': 'state'}  
        username_key: preferred_username  
        oauth_callback_url: "http://128.232.227.125/hub/oauth_callback"
```

```
proxy:  
  service:  
    type: LoadBalancer  
    loadBalancerIP: 128.232.227.125
```



Demo: *JupyterHub via Pangeo*

StackHPC

Sign in with IRIS IAM



Welcome to IRIS IAM

Sign in with your IRIS IAM credentials

[Forgot your password?](#)

Or sign in with

Not a member?

[About Us, Contact information and Privacy Policy](#)

JupyterLab

Not secure | 128.232.227.125/user/jmfg2@cam.ac.uk/lab?redirects=1

Incognito

jupyter Home Token Logout

Your server is starting up.
You will be redirected automatically when it's ready for you.

Server ready at /user/jmfg2@cam.ac.uk/

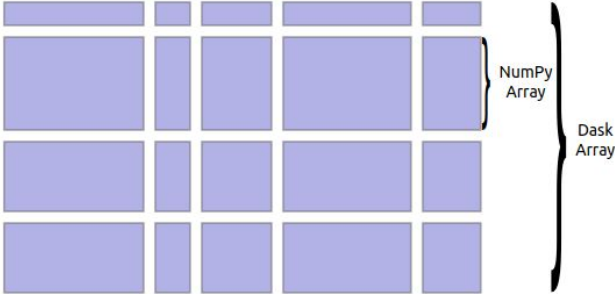
► Event log

Waiting for 128.232.227.125...

JupyterLab interface showing a file browser on the left and a code editor on the right. The file browser lists files: lost+found, dask-array.ipynb (13 minutes ago), and dask.yaml (16 minutes ago). The code editor displays the following content:

Dask Array scales NumPy

Dask array implements the NumPy API. It is composed of many small NumPy arrays



```
[1]: from dask_kubernetes import KubeCluster
cluster = KubeCluster(n_workers=2)
cluster
```

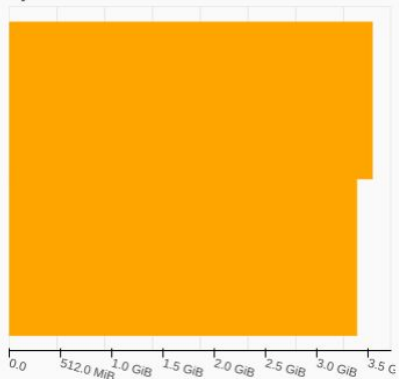
Error creating widget: could not find model

```
[2]: from dask.distributed import Client
client = Client(cluster)
client
```

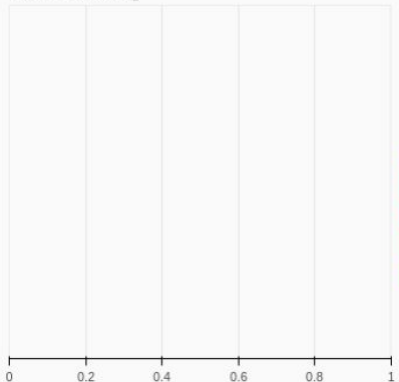
```
[2]:
```

	Client	Cluster
• Scheduler:	tcp://192.168.3.6:37753	• Workers: 0
• Dashboard:	/user/jmfg2@cam.ac.uk/proxy/8787/status	• Cores: 0
		• Memory: 0 B

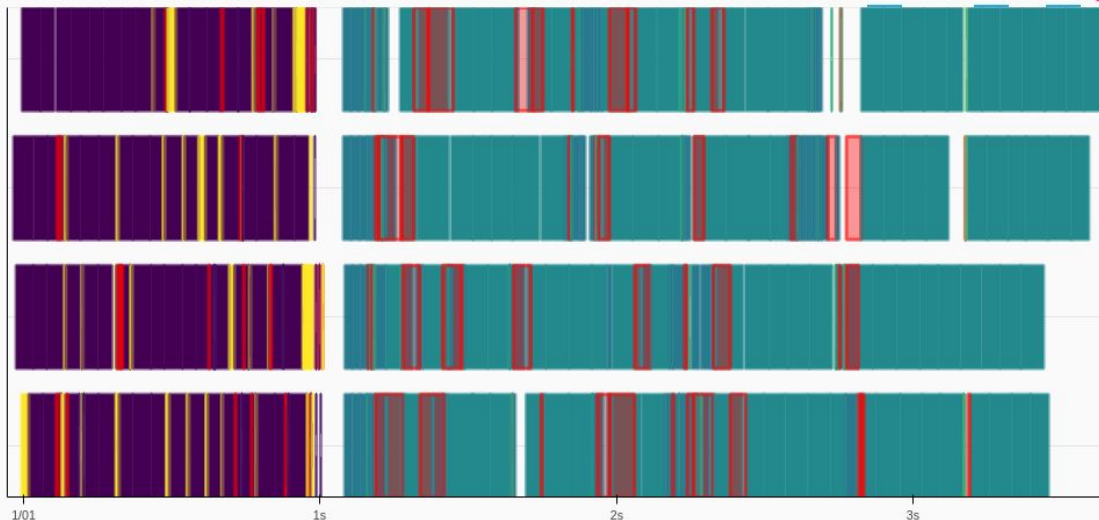
Bytes stored: 7.43 GB



Tasks Processing



Task Stream



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mean_chunk	100 / 100
sub	100 / 100
mean_combine...	30 / 30
mean_agg-agg...	10 / 10

JupyterLab Container Infra - Clusters

cumulus.openstack.hpc.cam.ac.uk/ngdetails/OS::Magnum::Cluster/29f11ac7-f5d9-4139-bbca-9382a5b68c6e

openstack demo johng-admin

Project / Container Infra / Clusters

API Access

Compute Back

Volumes

Container Infra

k8s-atomic

Show Certificate

Cluster Template

Name	k8s-atomic
ID	04245965-3dea-4202-9e58-70b389985059
COE	kubernetes
Image ID	Fedora-AtomicHost-29-20191126.0

Miscellaneous

Discovery URL	https://discovery.etcd.io/297112308d6686a1665b847f5b1e0dca
Cluster Create Timeout	Infinite
Keypair	default
Docker Volume Size	- GB
Master Flavor ID	general.v1.tiny
Node Flavor ID	general.v1.small
COE Version	v1.15.7
Container Version	1.12.6

Nodes

Master Count	2
Node Count	2
API Address	https://128.232.221.138:6443
Master Addresses	10.0.0.17 10.0.0.9
Node Addresses	10.0.0.12

Labels

kube_tag	v1.15.7
tiller_tag	v2.16.0
nginx_ingress_controll...	1.24.7
max_node_count	2
prometheus_operator_...	8.2.2
etcd_tag	
monitoring_enabled	true
heat_container_agent t...	train-stable
tiller_enabled	true
min_node_count	1
nginx_ingress_controll...	0.26.1
master_lb_floating_ip_...	true
use_podman	false
ingress_controller	
auto_healing_enabled	true

```
I1216 15:53:27.616349 1 ledelection.go:227] successfully acquired lease kube-system/cluster-autoscaler
I1216 15:53:30.912732 1 magnum_manager_heat.go:293] For stack ID f864efb5-ceec-45b1-a660-a987f482d0ac, stack name is k8s-atomic-j7g2o2g55jsz
I1216 15:53:31.111256 1 magnum_manager_heat.go:310] Found nested kube_minions stack: name k8s-atomic-j7g2o2g55jsz-kube_minions-pdtyqdas7jho, ID bae86ecf-7b61-446f-830e-a30cf9b0e01d
I1216 16:29:07.348067 1 scale_up.go:689] Scale-up: setting group default-worker size to 2
I1216 16:29:12.250370 1 magnum_nodegroup.go:101] Increasing size by 1, 1->2
I1216 16:29:48.614285 1 magnum_nodegroup.go:67] Waited for cluster UPDATE_IN_PROGRESS status
I1216 16:33:34.949178 1 magnum_nodegroup.go:67] Waited for cluster UPDATE_COMPLETE status
I1216 17:16:27.410946 1 scale_down.go:882] Scale-down: removing empty node k8s-atomic-j7g2o2g55jsz-node-1
I1216 17:16:34.387762 1 magnum_manager_heat.go:344] Resolved node k8s-atomic-j7g2o2g55jsz-node-1 to stack index 1
I1216 17:16:35.804520 1 magnum_manager_heat.go:280] Waited for stack UPDATE_IN_PROGRESS status
I1216 17:17:06.289528 1 magnum_manager_heat.go:280] Waited for stack UPDATE_COMPLETE status
```

JupyterLab Instances - OpenStack Dashboard

cumulus.openstack.hpc.cam.ac.uk/project/instances/

openstack demo johng-admin

Project / Compute / Instances

Instances

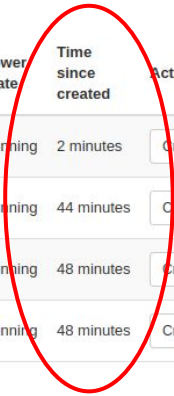
Instance Name = k8s* Filter Launch Instance Delete Instances More Actions

Displaying 4 items

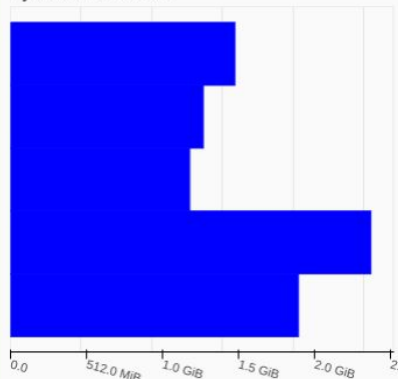
<input type="checkbox"/>	Instance Name	Image Name	IP Address	Flavor	Key Pair	Status	Availability Zone	Task	Power State	Time since created	Actions
<input type="checkbox"/>	k8s-atomic-j7g2o2g55jsz-node-1	Fedora-AtomicHost-29-20191126.0	10.0.0.18	general.v1.small	default	Active	nova	None	Running	2 minutes	Create Snapshot
<input type="checkbox"/>	k8s-atomic-j7g2o2g55jsz-node-0	Fedora-AtomicHost-29-20191126.0	10.0.0.12	general.v1.small	default	Active	nova	None	Running	44 minutes	Create Snapshot
<input type="checkbox"/>	k8s-atomic-j7g2o2g55jsz-master-0	Fedora-AtomicHost-29-20191126.0	10.0.0.17	general.v1.tiny	default	Active	nova	None	Running	48 minutes	Create Snapshot
<input type="checkbox"/>	k8s-atomic-j7g2o2g55jsz-master-1	Fedora-AtomicHost-29-20191126.0	10.0.0.9	general.v1.tiny	default	Active	nova	None	Running	48 minutes	Create Snapshot

Displaying 4 items

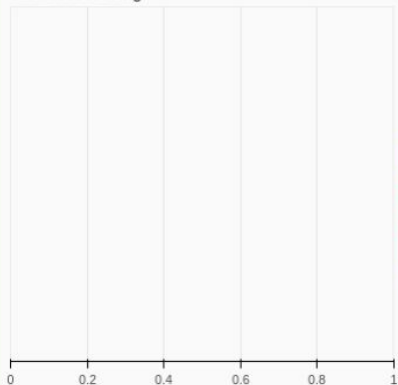
Admin Identity



Bytes stored: 8.80 GB



Tasks Processing



Task Stream



Progress -- total: 340, in-memory: 200, processing: 0, erred: 0

random_sample	100 / 100
mean_chunk	100 / 100
sub	100 / 100
mean_combine...	30 / 30
mean_agg-agg...	10 / 10

Plans for FY20

StackHPC

Plans for FY2020

- Clusters with multiple node types
- GPU support
- Upgrading kubernetes in-place
- More Magnum automation of common setups

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