INTERACTIVE SUPERCOMPUTING WITH

jupyter DASK

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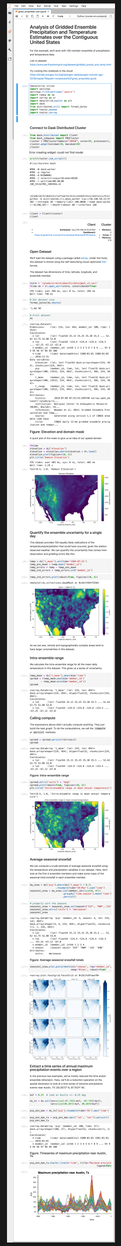
National Center for Atmospheric Research (NCAR)

SciPy 2019, Austin, TX.

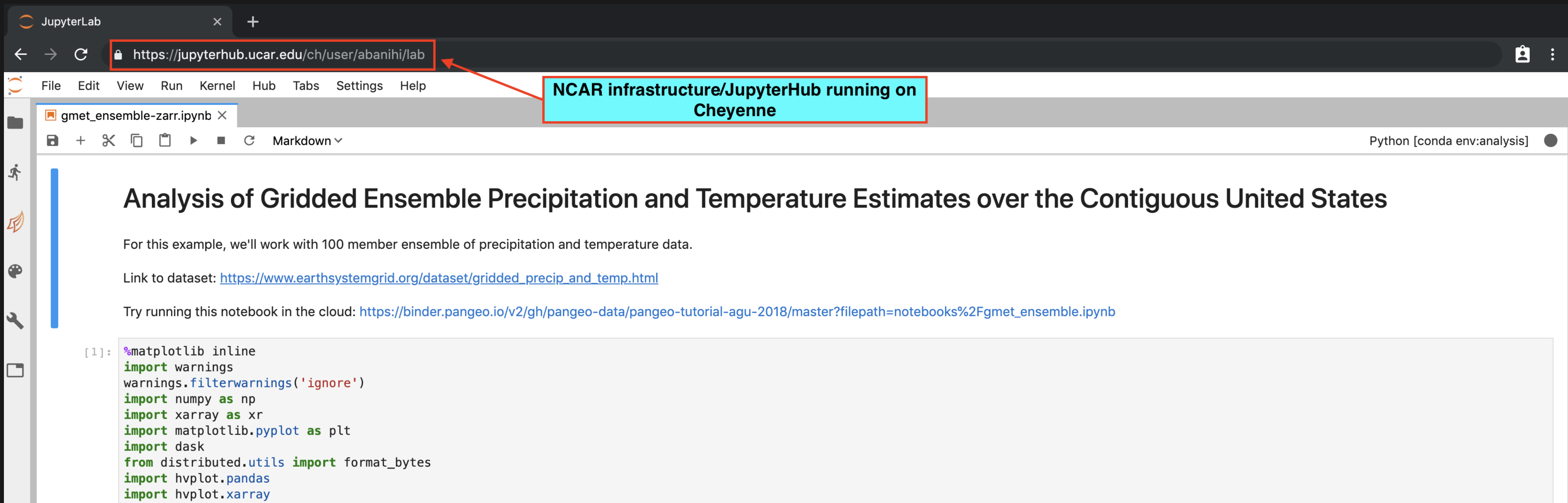
Slides: https://andersonbanihirwe.dev/talks/dask-jupyter-scipy-2019.html



- Alice, project scientist @ NCAR
- Field of Expertise: Hydrology/Hydrometeorolgy

3 INTERESTING THINGS ABOUT ALICE'S NOTEBOOK

1) NCAR INFRASTRUCTURE



2) DISTRIBUTED COMPUTING RESOURCES

Connect to Dask Distributed Cluster

[2]:
```python
from dask.distributed import Client
from dask_jobqueue import PBSCluster
cluster = PBSCluster(memory="109GB", cores=12, processes=12, walltime="00:30:00",
                     queue="economy")
# Scale adaptively (minimum of 10 nodes = 120 dask workers )
cluster.adapt(minimum=12*10, maximum=12*20, wait_count=60)
cluster
```

PBSCluster

Workers	120
Cores	120
Memory	1.09 TB

▸ Manual Scaling

▸ Adaptive Scaling

3) ACTUAL SCIENCE

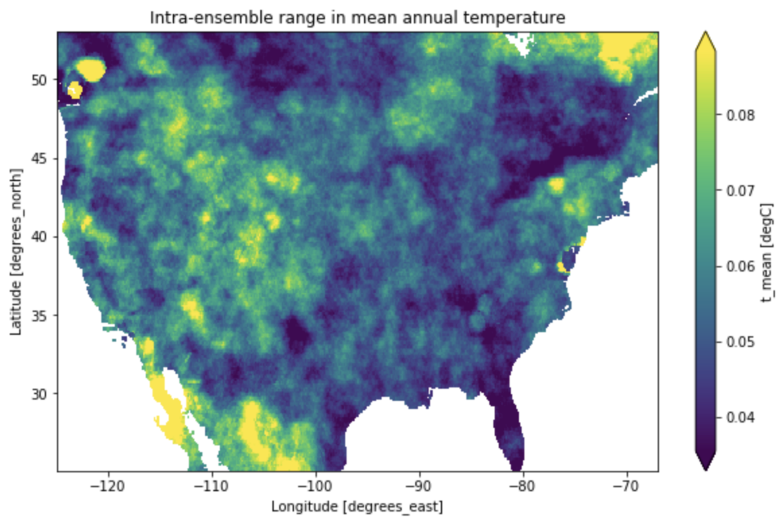
[13]:
```
spread = spread.persist(retries=2)
spread
```

[13]:
```
<xarray.DataArray 't_mean' (lat: 224, lon: 464)>
dask.array<shape=(224, 464), dtype=float32, chunksize=(224, 464)>
Coordinates:
  * lat      (lat) float64 25.12 25.25 25.38 25.5 ... 52.62 52.75 52.88 53.0
  * lon      (lon) float64 -124.9 -124.8 -124.6 -124.5 ... -67.25 -67.12 -67.0
```

Figure: Intra-ensemble range

[14]:
```
spread.attrs['units'] = 'degC'
spread.plot(robust=True, figsize=(10, 6))
plt.title('Intra-ensemble range in mean annual temperature')
```

[14]:
```
Text(0.5, 1.0, 'Intra-ensemble range in mean annual temperature')
```



[18]:
```
buf = 0.25  # look at Austin +/- 0.25 deg

ds_tx = ds.sel(lon=slice(-97.7431-buf, -97.7431+buf),
               lat=slice(30.2672-buf, 30.2672+buf))
```

[19]:
```
pcp_ann_max = ds_tx['pcp'].resample(time='AS').max('time')
```

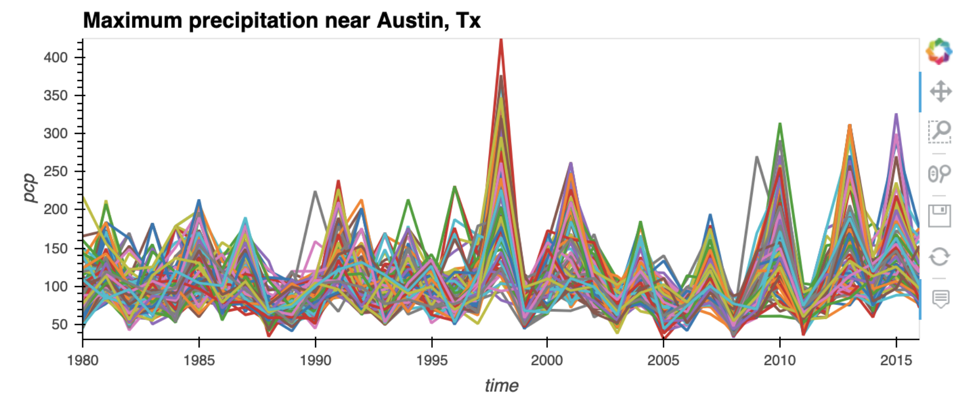
[20]:
```
pcp_ann_max_ts = pcp_ann_max.max(('lat', 'lon')).persist()
pcp_ann_max_ts
```

[20]:
```
<xarray.DataArray 'pcp' (member_id: 100, time: 37)>
dask.array<shape=(100, 37), dtype=float32, chunksize=(1, 1)>
Coordinates:
  * time       (time) datetime64[ns] 1980-01-01 1981-01-01 ... 2016-01-01
  * member_id  (member_id) int64 1 2 3 4 5 6 7 8 9 ... 93 94 95 96 97 98 99 100
```

Figure: Timeseries of maximum precipitation near Austin, Tx.

[21]:
```
pcp_ann_max_ts.hvplot.line(x='time', title='Maximum precipitation near Austin, Tx',
                           legend=False)
```

[21]:

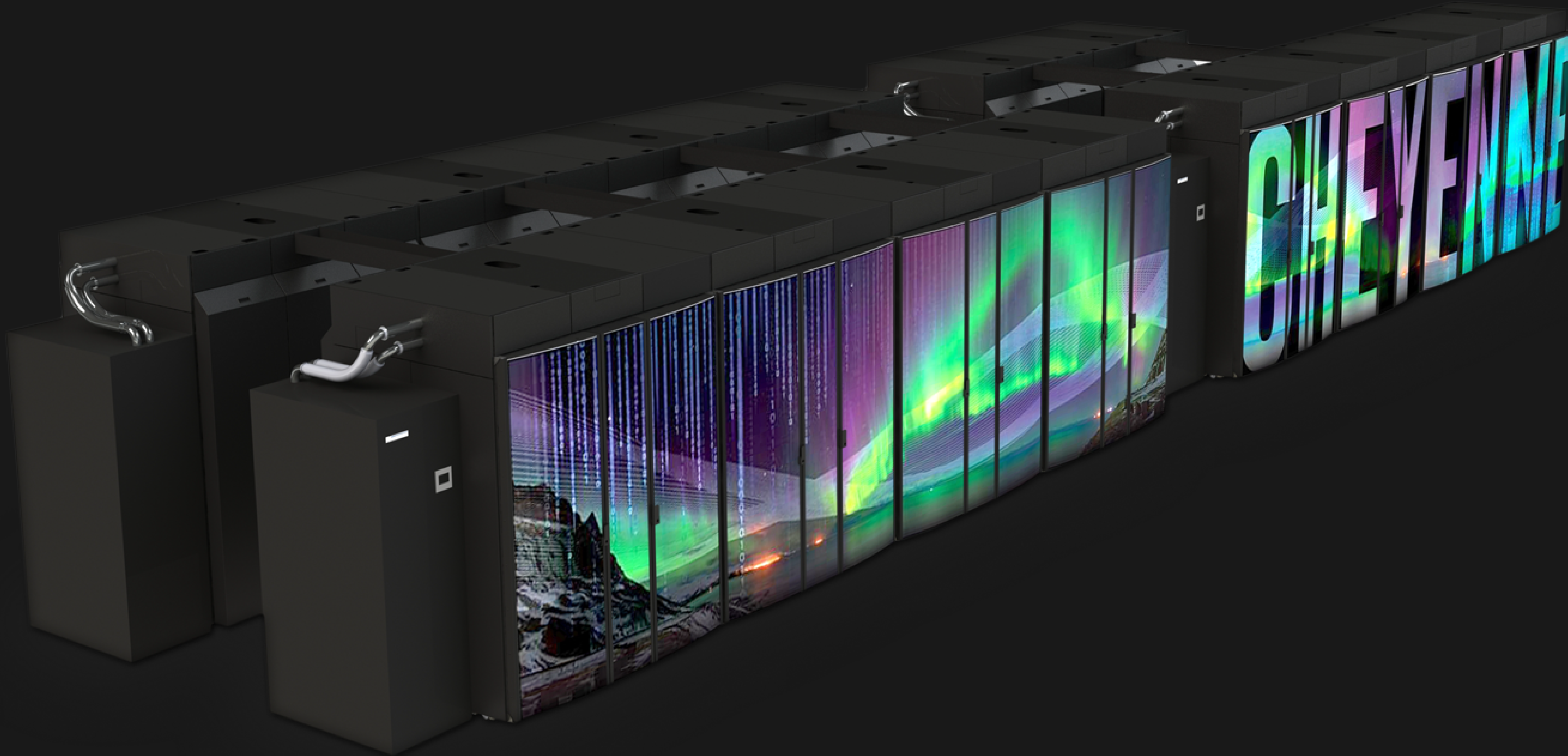


WHAT DO WE MEAN BY SUPERCOMPUTING?

WHAT DO WE MEAN BY SUPERCOMPUTING?

- MPI, batch processing...
- Lots of heavy machines managed by sysadmins...

Cheyenne is a 5.34-petaflops, high-performance computer operated by NCAR.



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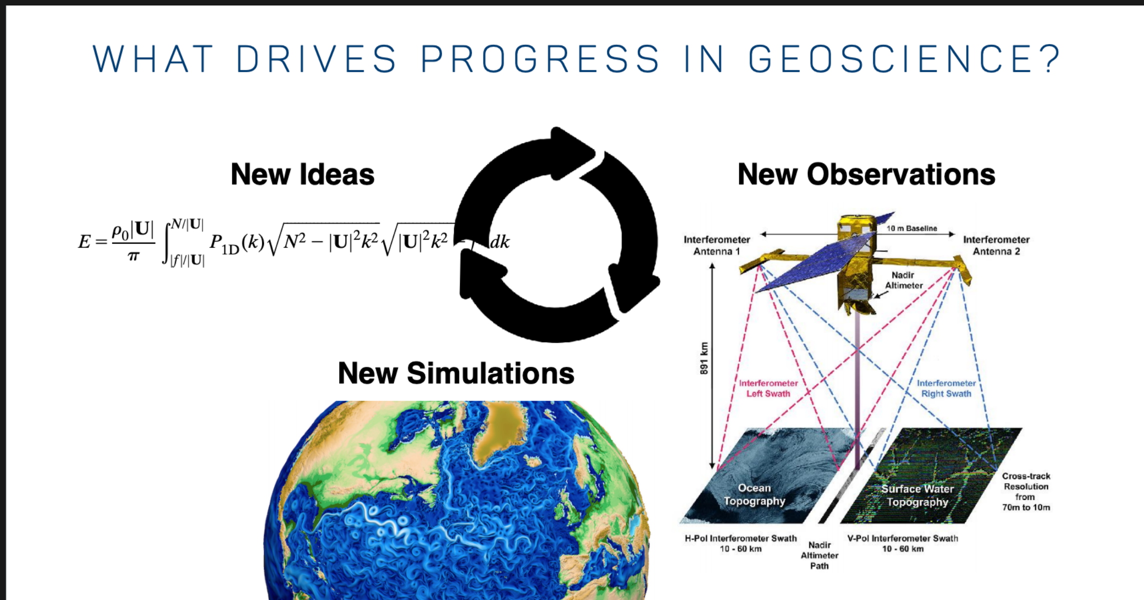
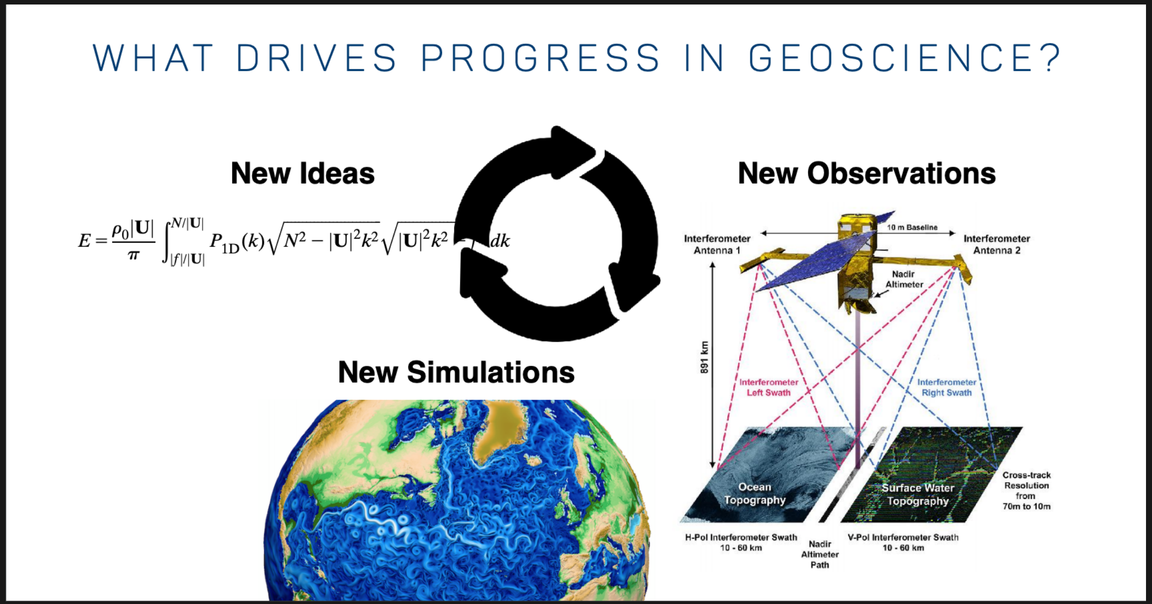


- Need for more "human-in-the-loop" workflows, rapid iteration due to huge growth in data creation
- Jupyter notebooks, interactive visualization, etc
- Adaptive scaling of computing resources based on the load

WHAT DO WE MEAN BY INTERACTIVE SUPERCOMPUTING?



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This combination would be powerful...

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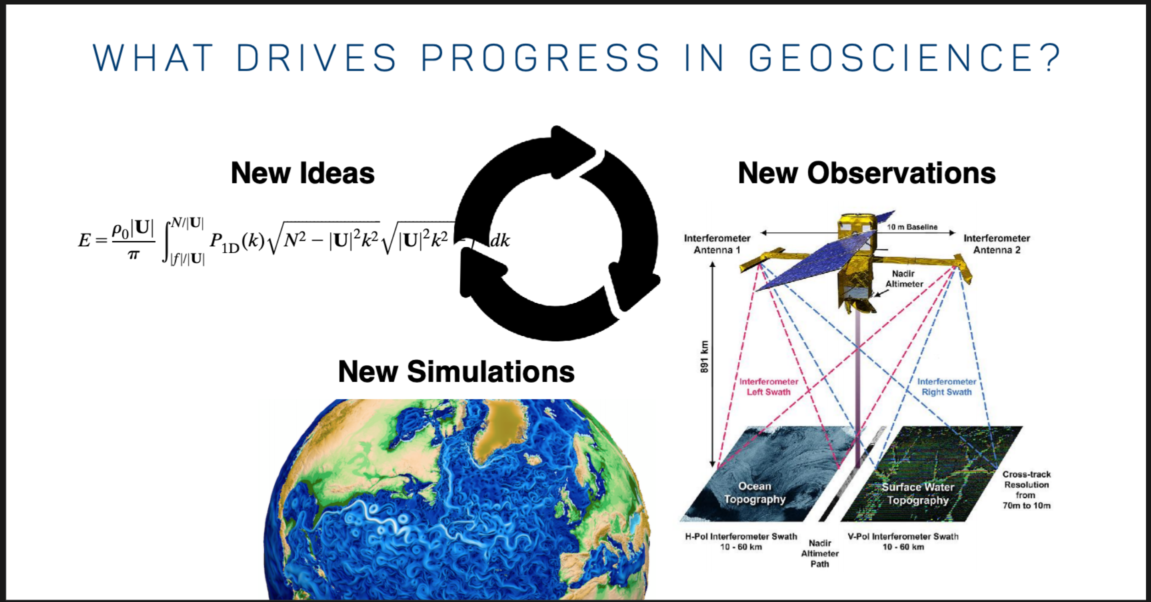

- Need for more "human-in-the-loop" workflows, rapid iteration due to huge growth in data creation
- Jupyter notebooks, interactive visualization, etc
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This combination would be powerful...

But it is hard...

INTERACTIVE SUPERCOMPUTING CHALLENGES

- Every high performance computing (HPC) system is unique:
  - Security policies
  - Container experience/policy
  - Queue configuration
  - External node access policies
- Tension between interactive availability and machine utilization (HPC centers often measured on this)...
- Lack of "elastic scaling" support in HPC workload managers...

ENABLING TECHNOLOGIES FOR INTERACTIVE SUPERCOMPUTING

jupyter

...back to oxygen

Set contour levels to non-uniform intervals and make the colormap centered at the hypoxic threshold using `DivergingNorm`.

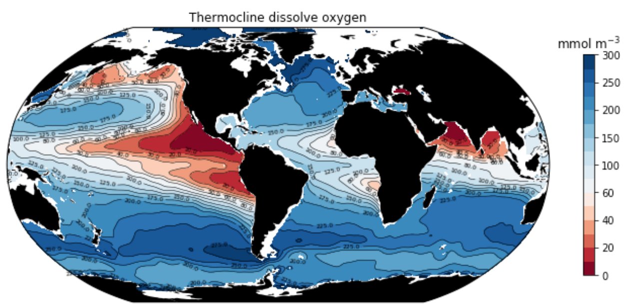
In [7]:
```
levels = [0, 10, 20,  30, 40, 50, 60, 80, 100, 125, 150, 175, 200, 225,
          250, 275, 300]

norm = colors.DivergingNorm(vmin=levels[0], vmax=levels[-1], vcenter=60.)
```

Add a cyclic point to accomodate the periodic domain.

In [8]:
```
from cartopy.util import add_cyclic_point
field, lon = add_cyclic_point(ds.O2, coord=ds.lon)
lat = ds.lat
```

Putting it all together...

In [9]:
```
fig = plt.figure(figsize=(12, 8))
ax = fig.add_subplot(1, 1, 1, projection=ccrs.Robinson(central_longitude=305.0))

# filled contours
cf = ax.contourf(lon, lat, field, levels=levels, norm=norm, cmap='RdBu',
                 transform=ccrs.PlateCarree());

# contour lines
cs = ax.contour(lon, lat, field, colors='k', levels=levels, linewidths=0.5,
                transform=ccrs.PlateCarree())

# add contour labels
lb = plt.clabel(cs, fontsize=6, inline=True, fmt='%r');

# land
land = ax.add_feature(
    cartopy.feature.NaturalEarthFeature('physical','land','110m', facecolor='black'))

# colorbar and labels
cb = plt.colorbar(cf, shrink=0.5)
cb.ax.set_title('mmol m$^{-3}$')
ax.set_title('Thermocline dissolve oxygen');
```



- Interactive, web browser-based computing environment
- Reproducible document format.
  - Code
  - Prose
  - Equations (LaTeX)
  - Visualizations

JUPYTER NOTEBOOKS ON HPC SYSTEMS

Q: But isn't Jupyter already usable on HCP systems?

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A: Yes, But......

- SSH-in

```
$ ssh <remote_user>@<remote_host>
```

- Launch Jupyter on a remote machine

```
$ jupyter lab --no-browser --ip=`hostname` --port=<port>
```

- Set up SSH-tunnel to the remote machine

```
$ ssh -N -L <port>:<hostname>:<port> <remote_user>@<remote_hos
```

- Open the notebook in a browser on the local machine

```
$ open http://localhost:<port>/
```

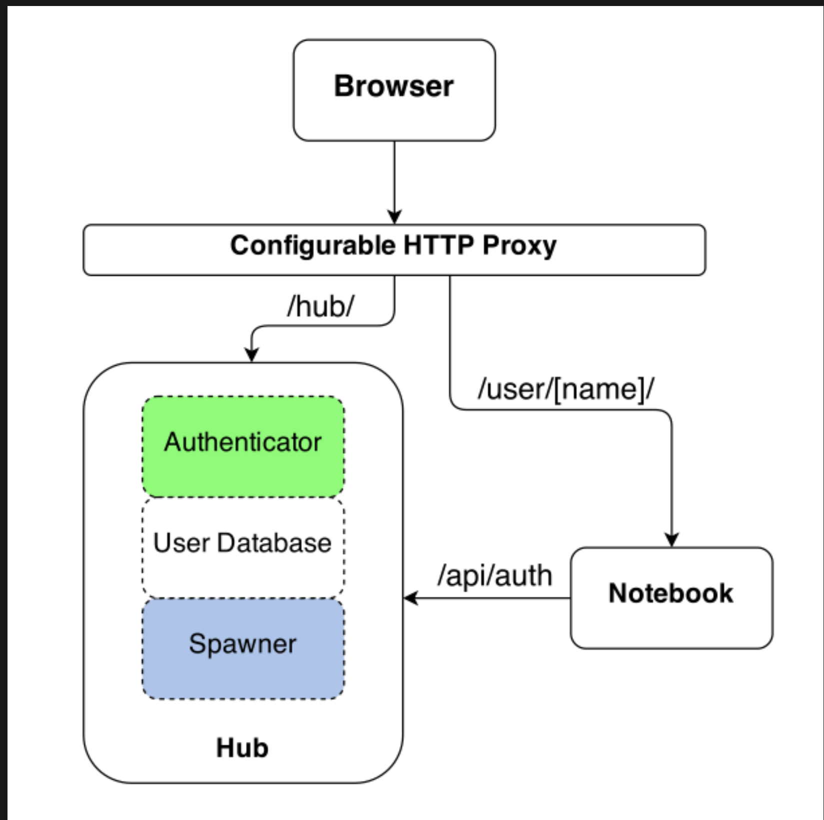
JUPYTER NOTEBOOKS ON HPC SYSTEMS

What is missing?

- Multi-user support
- Pure web-access to HPC resources

jupyterhub

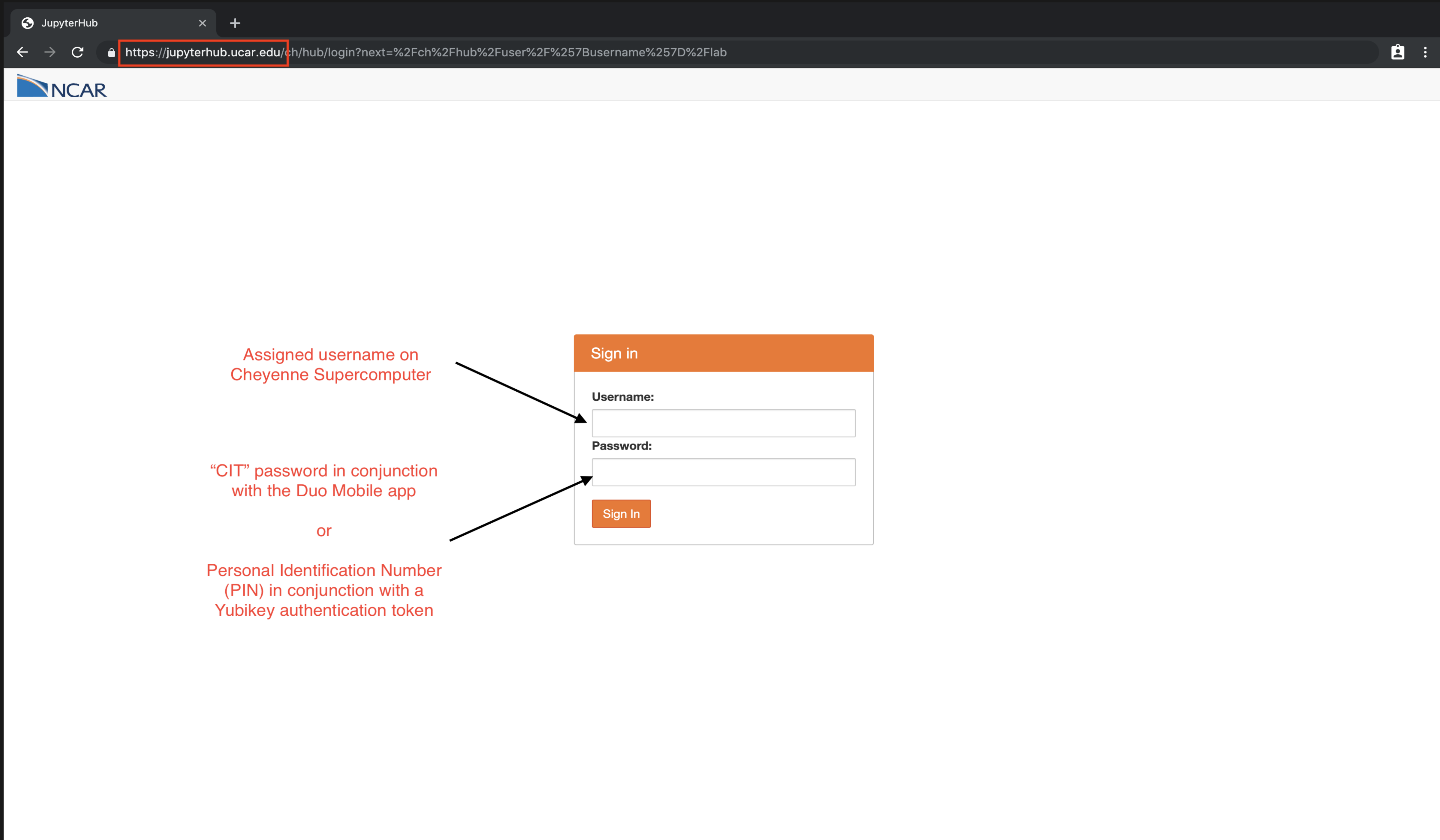
to the rescue...



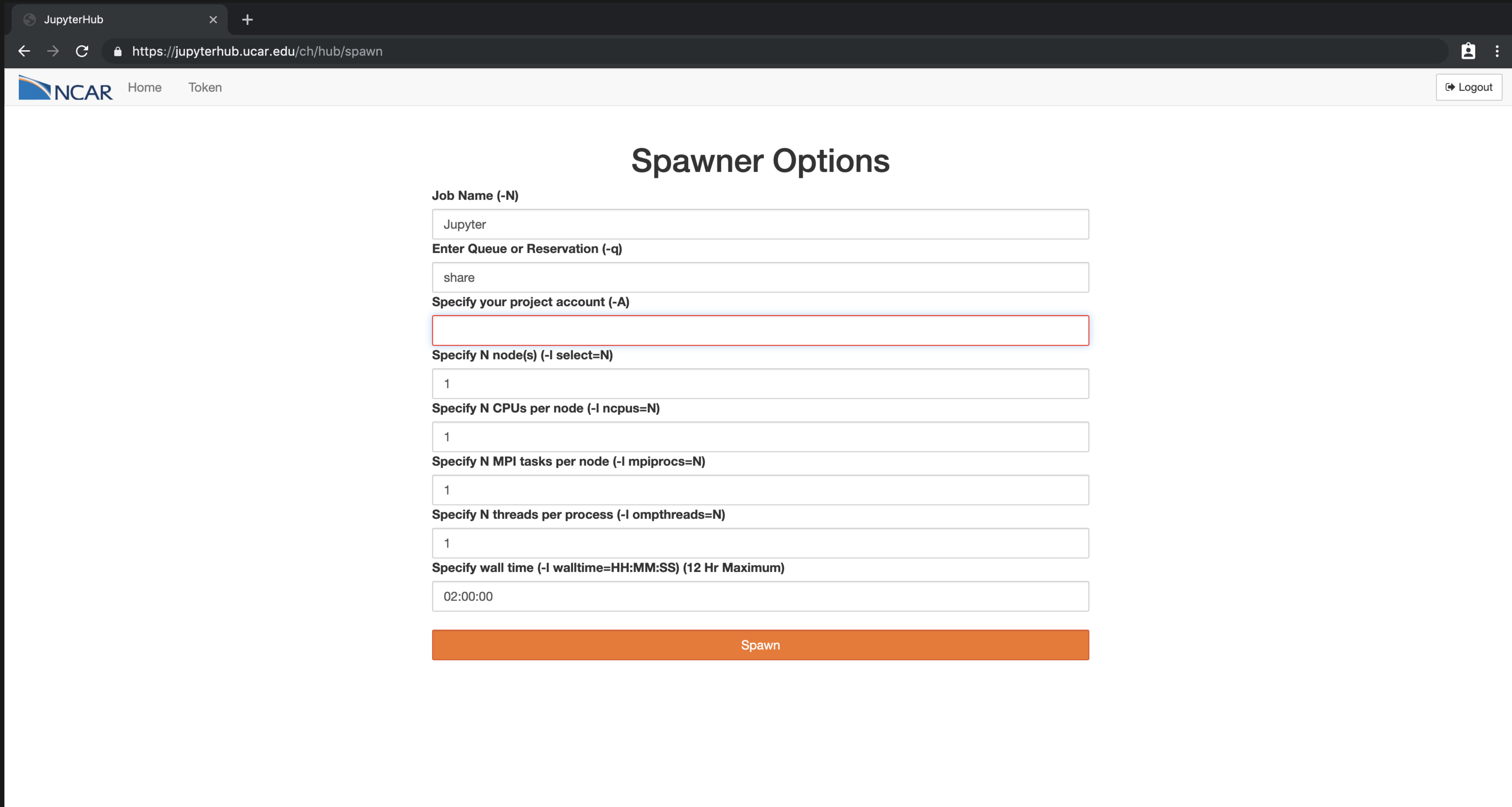
- Manages authentication
- Spawns single-user servers on-demand
- Each user gets a complete notebook server

JUPYTERHUB @ NCAR

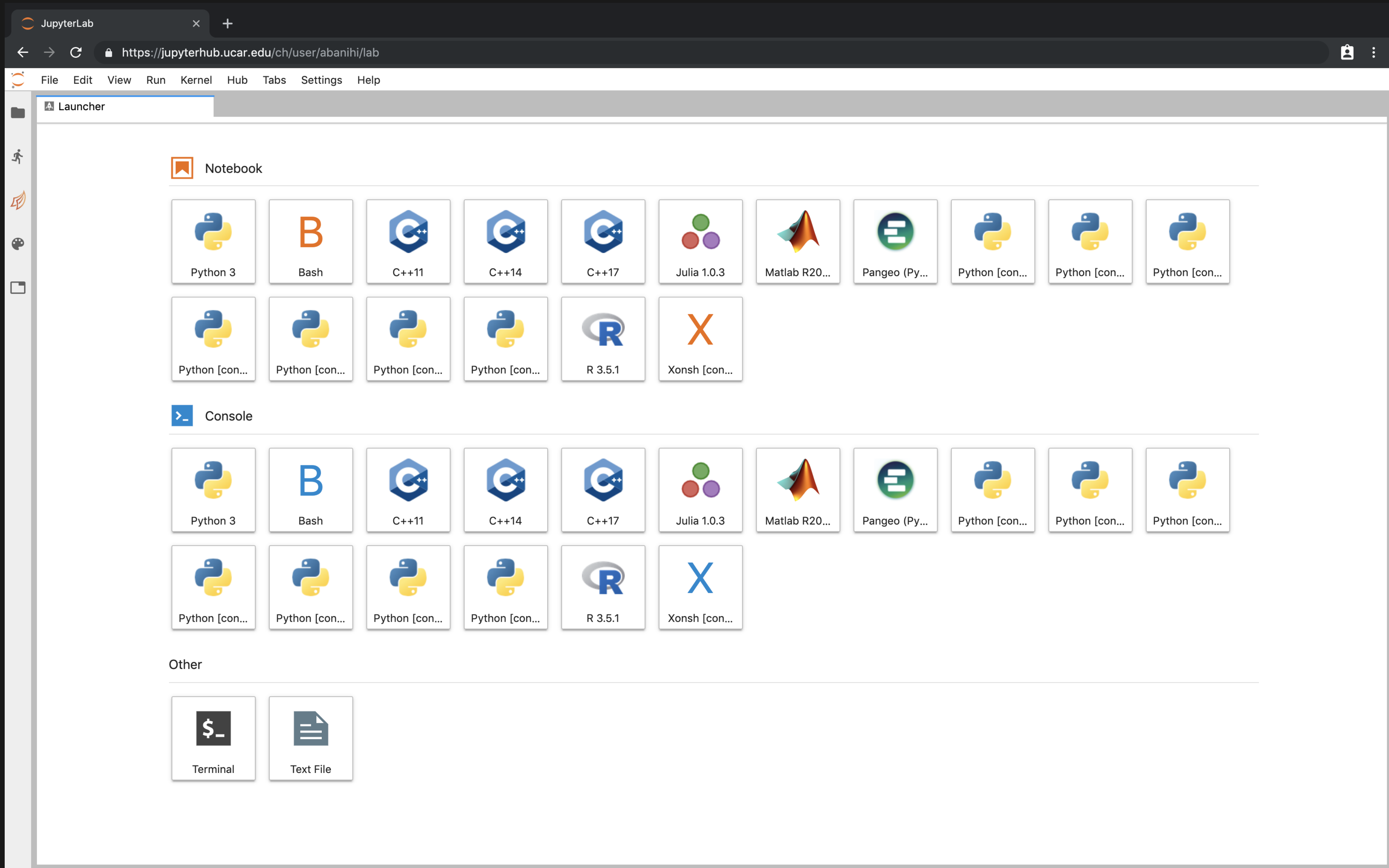
JupyterHub @ NCAR: Login


JupyterHub
https://jupyterhub.ucar.edu/ch/hub/login?next=%2Fch%2Fhub%2Fuser%2F%257Busername%257D%2Flab
NCAR
Sign in
Username:
Password:
Sign In
Assigned username on Cheyenne Supercomputer
"CIT" password in conjunction with the Duo Mobile app
or
Personal Identification Number (PIN) in conjunction with a Yubikey authentication token

JupyterHub @ NCAR: Specifying Job Configuration

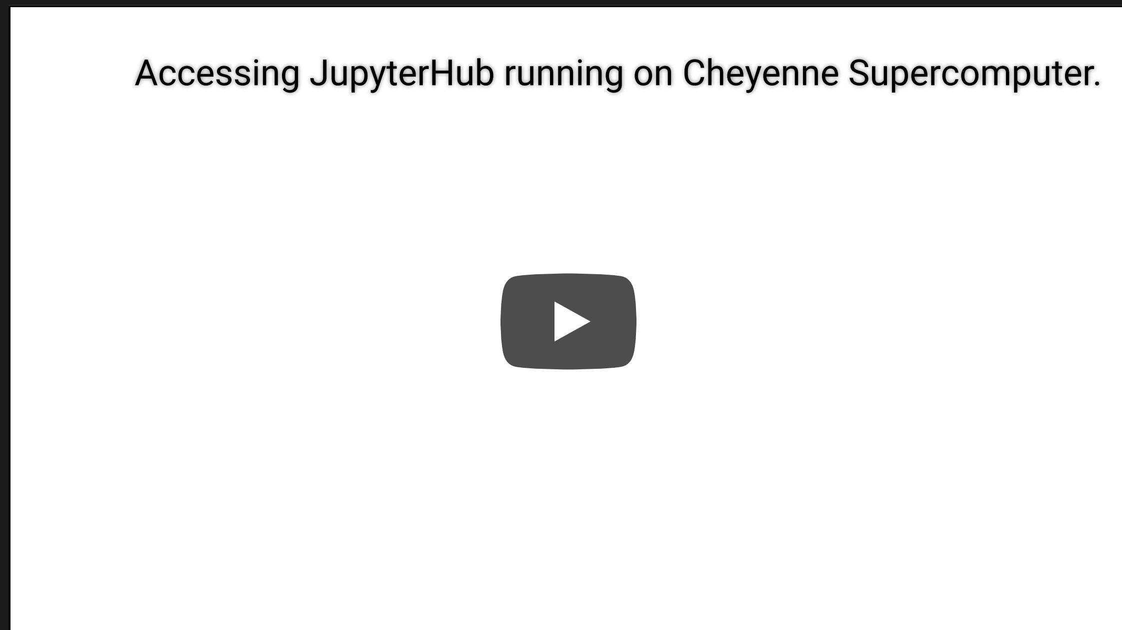

JupyterHub
https://jupyterhub.ucar.edu/ch/hub/spawn
NCAR
Home
Token
Logout
Spawner Options
Job Name (-N)
Jupyter
Enter Queue or Reservation (-q)
share
Specify your project account (-A)
Specify N node(s) (-l select=N)
1
Specify N CPUs per node (-l ncpus=N)
1
Specify N MPI tasks per node (-l mpiprocs=N)
1
Specify N threads per process (-l ompthreads=N)
1
Specify wall time (-l walltime=HH:MM:SS) (12 Hr Maximum)
02:00:00
Spawn

JupyterHub @ NCAR: A Running Jupyter Server


JupyterLab
https://jupyterhub.ucar.edu/ch/user/abanihi/lab
File Edit View Run Kernel Hub Tabs Settings Help
Launcher
Notebook
Python 3
Bash
C++11
C++14
C++17
Julia 1.0.3
Matlab R20...
Pangeo (Py...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
R 3.5.1
Xonsh [con...
Console
Python 3
Bash
C++11
C++14
C++17
Julia 1.0.3
Matlab R20...
Pangeo (Py...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
Python [con...
R 3.5.1
Xonsh [con...
Other
Terminal
Text File

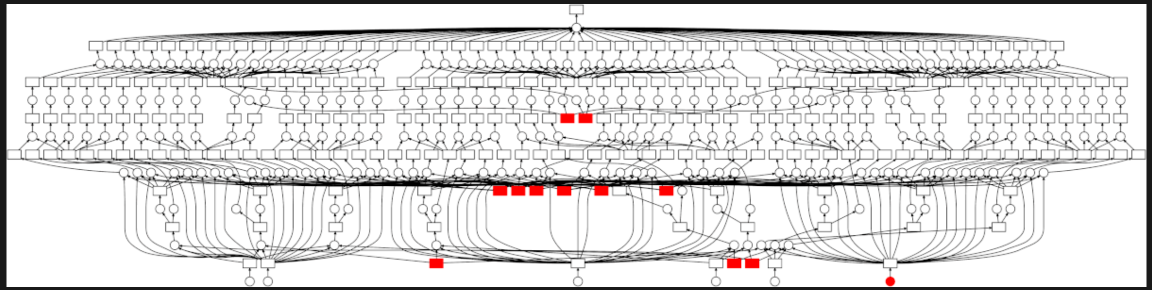
JUPYTERHUB LIVE DEMO

(if live demo gods are in a good mood...)



DASK

- Parallel programming library for Python
- Scales data libraries like Numpy, Pandas, Scikit-Learn, Xarray...
- Deploys on HPC systems
- Culturally native to Scientific Computing
- Provides schedulers for executing task graphs



DASK-JOBQUEUE

DASK-JOBQUEUE

- Easily deploy Dask on job queuing systems like PBS, Slurm, MOAB, SGE, and LSF, etc...
- Created as a spinoff of the Pangeo project.
- Pythonic user interface that manages dask workers/clusters

DASK-JOBQUEUE

```
from dask_jobqueue import PBSCluster
from distributed import Client
cluster = PBSCluster(project=..,
  queue=.., cores=1, processes=1,
  memory="100GB", walltime=...)
# Ask for 10 nodes
cluster.scale(10)
# OR scale adaptively based on load
cluster.adapt(minimum=1, maximum=100,
            wait_count=60)
# Connect to remote workers
client = Client(cluster)
```

Note: The cluster object stores a configuration for a block of worker nodes that you will be requesting...

DASK-JOBQUEUE

```python
from dask_jobqueue import PBSCluster
from distributed import Client
cluster = PBSCluster(project=..,
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# Ask for 10 nodes
cluster.scale(10)
# OR scale adaptively based on load
cluster.adapt(minimum=1, maximum=100,
              wait_count=60)
# Connect to remote workers
client = Client(cluster)
```
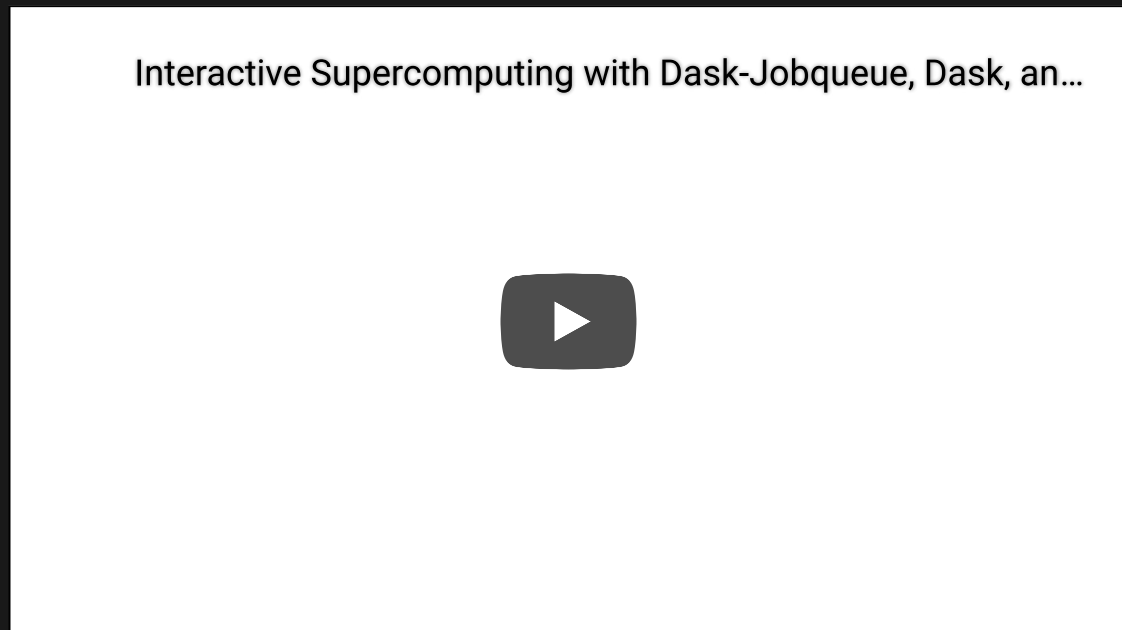

```python
from dask_jobqueue import SLURMCluster
from distributed import Client
cluster = SLURMCluster(project=..,
  queue=.., cores=1, processes=1,
  memory="100GB", walltime=...)
# Ask for 10 nodes
cluster.scale(10)
# OR scale adaptively based on load
cluster.adapt(minimum=1, maximum=100,
              wait_count=60)
# Connect to remote workers
client = Client(cluster)
```

Note: The cluster object stores a configuration for a block of worker nodes that you will be requesting...

DASK-JOBQUEUE LIVE DEMO

(if live demo gods are in a good mood...)



ADAPTIVE/ELASTIC SCALING, RESILIENCE, ETC...

ADAPTIVE/ELASTIC SCALING

Challenges:

- Balancing cluster resources and performance
  - is challenging
  - requires a lot of experimentation...
- Computational workloads fluctuate throughout the analysis...

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- Balancing cluster resources and performance
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- Computational workloads fluctuate throughout the analysis...

Dask thinks about ...

- Scaling up and down
- Resilience
- Load balancing

ADAPTIVE/ELASTIC SCALING ON HPC SYSTEMS

Solution:

1. Start your Jupyter Notebook
2. Instantiate your dask cluster
3. Let dask determine when to scale up and/or down
4. **Do science**

ADAPTIVE/ELASTIC SCALING ON HPC SYSTEMS

Benefits:

- Adaptive scaling improves HPC systems' occupancy / utilization...
- Resilience against the death of all or part of computing resources provides new ways of leveraging job preemption...

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Benefits:

- Adaptive scaling improves HPC systems' occupancy / utilization...
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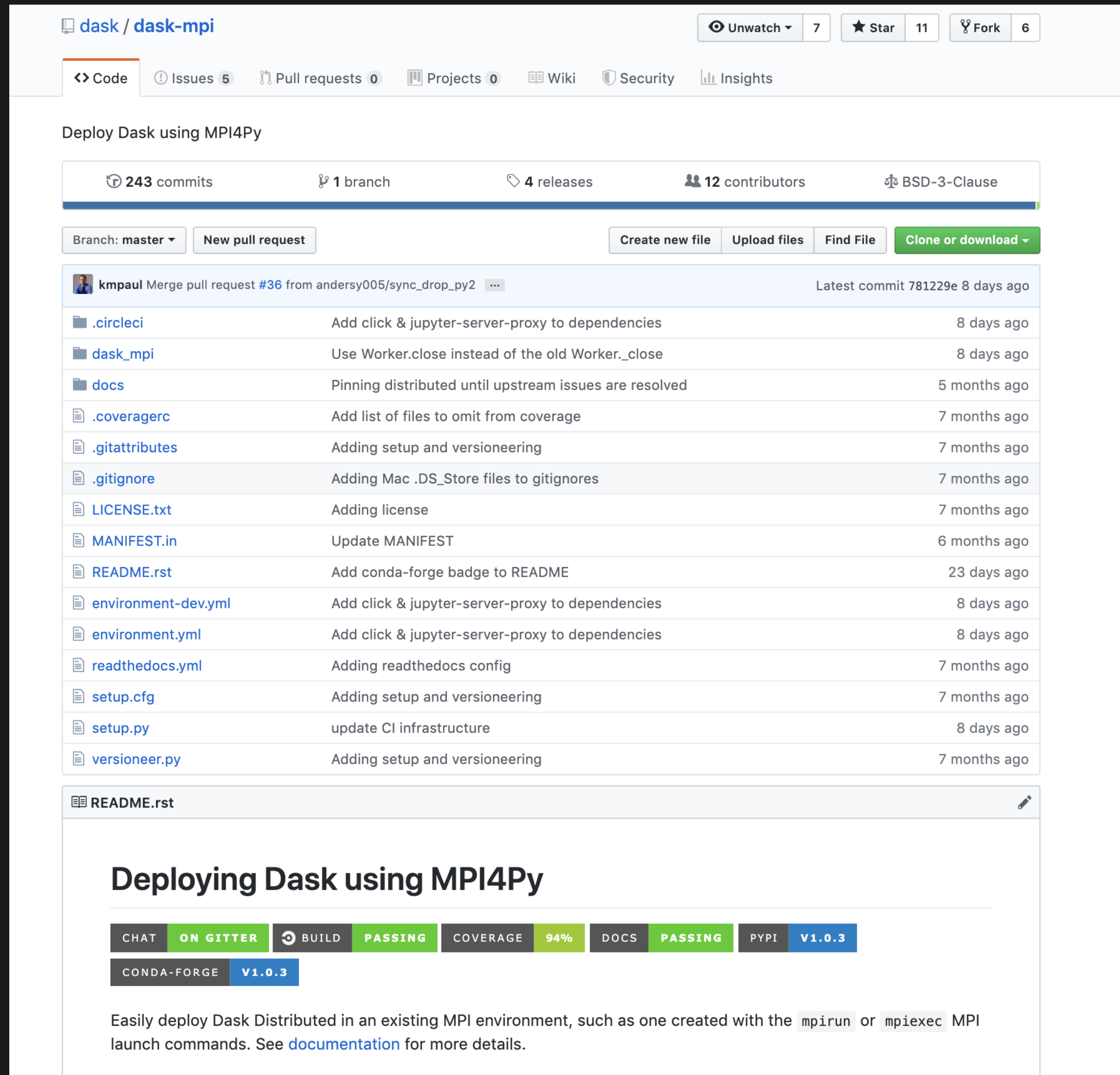
Dask thinks about these benefits...

NOT ALL JOBS ARE INTERACTIVE



FUTURE

- Heterogeneous resources handling
- Coarse-Grained Diagnostics and History
- Scheduler Performance on Large Graphs

RESOURCES

- https://jobqueue.dask.org/
- https://mpi.dask.org
- Dask-jobqueue workshop materials
- Jupyter for Science User Facilities and High Performance Computing workshop

Participate

- https://github.com/dask/dask-jobqueue/issues
- https://github.com/dask/dask-mpi/issues

ACKNOWLEDGMENTS

- Jupyter/JupyterHub development teams
- NCAR/CISL Supercomputer Systems, Consulting Services Groups
- Pangeo collaborators