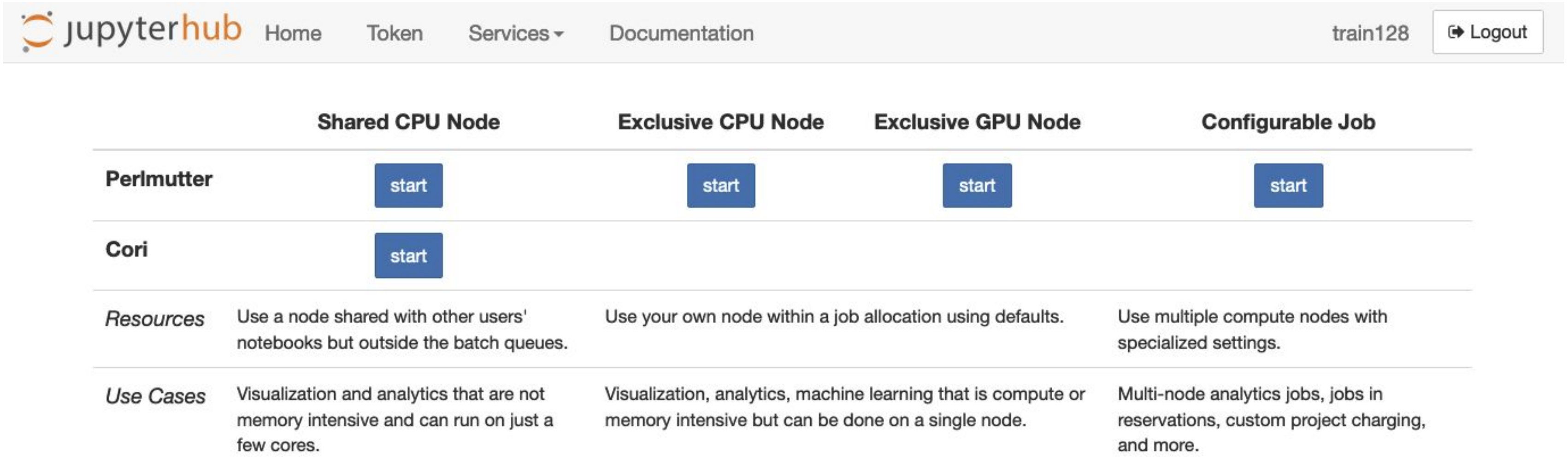
Parsl

https://parsl-project.org/

Bjoern Enders (NERSC) & Tyler Skluzacek (OLCF)

The Parsl demo at NERSC will be run via Jupyter

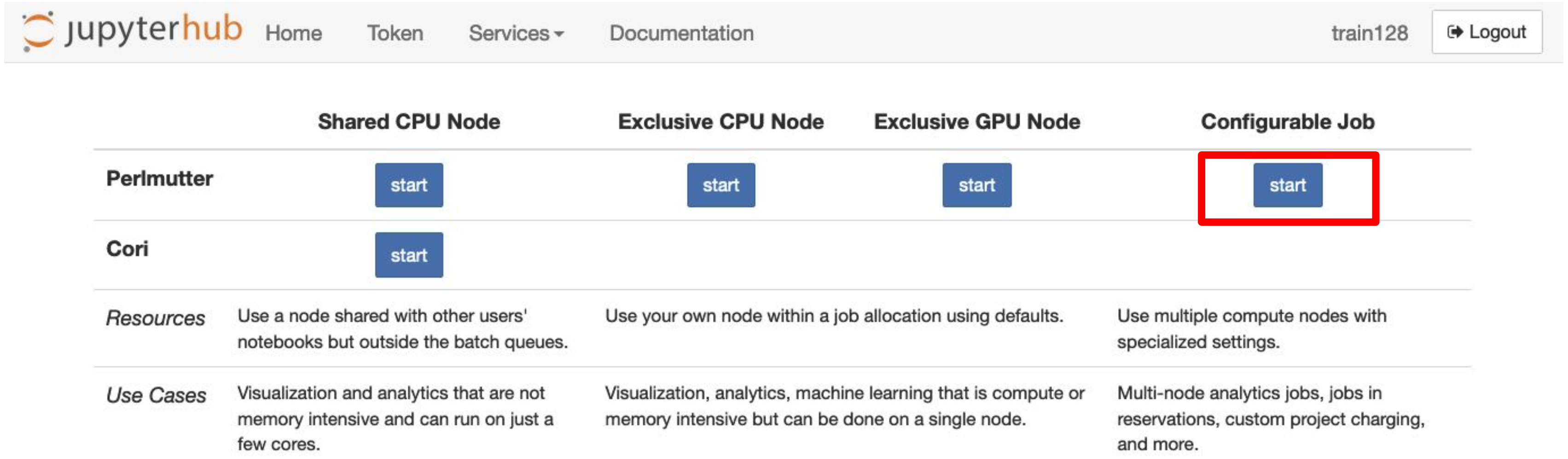
- Go to https://jupyter.nersc.gov
- Sign in using your training account credentials
- Select your preferred jupyter instance:



	Shared CPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable Job
Perlmutter	start	start	start	start
Cori	start			
Resources	Use a node shared with other users' notebooks but outside the batch queues.	Use your own node within a job allocation using defaults.		Use multiple compute nodes with specialized settings.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.		Multi-node analytics jobs, jobs in reservations, custom project charging, and more.

Using Reservations in Tutorials

- Go to https://jupyter.nersc.gov and select: "Configurable Job" in the "Perlmutter" row



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Jupyter Options:

Leave defaults, except:

Constraint:

`cpu`

Account:

`ntrain7`

Reservation

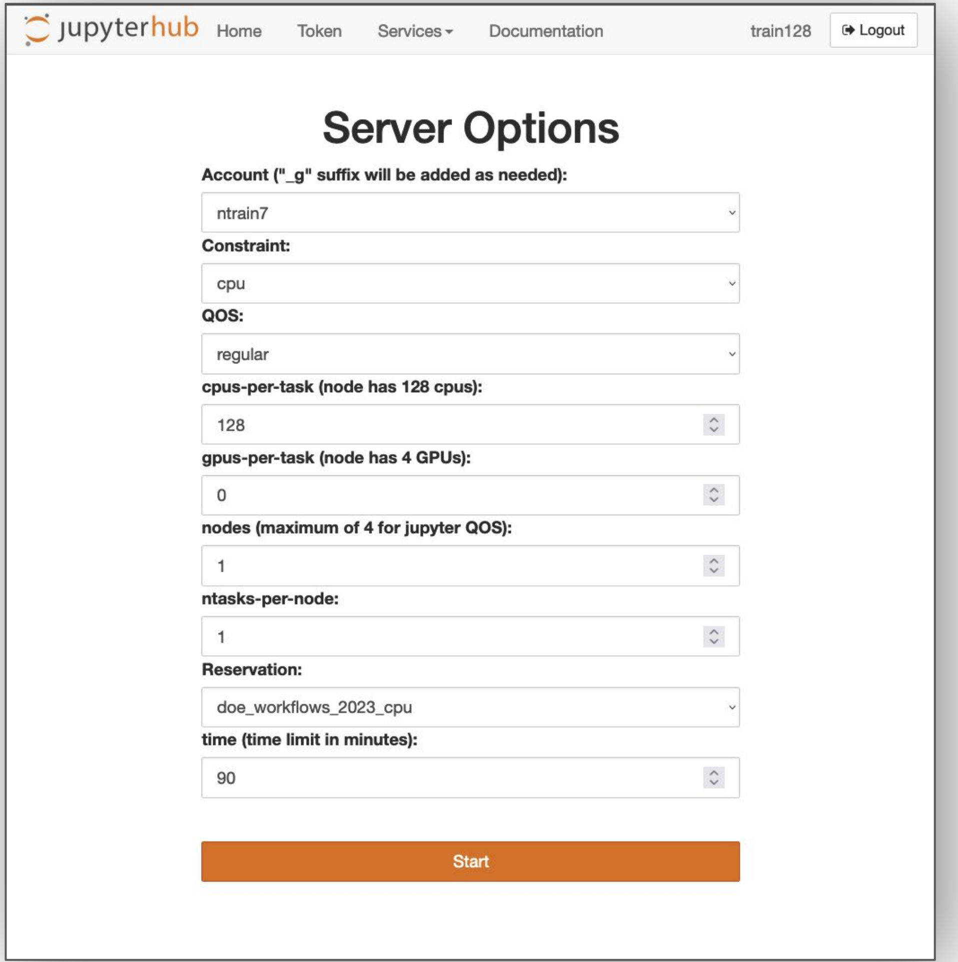
`doe_workflows_2023_cpu`

Time

`90`

QOS

`regular`



Server Options

Account ("_g" suffix will be added as needed): ntrain7

Constraint: cpu

QOS: regular

cpus-per-task (node has 128 cpus): 128

gpus-per-task (node has 4 GPUs): 0

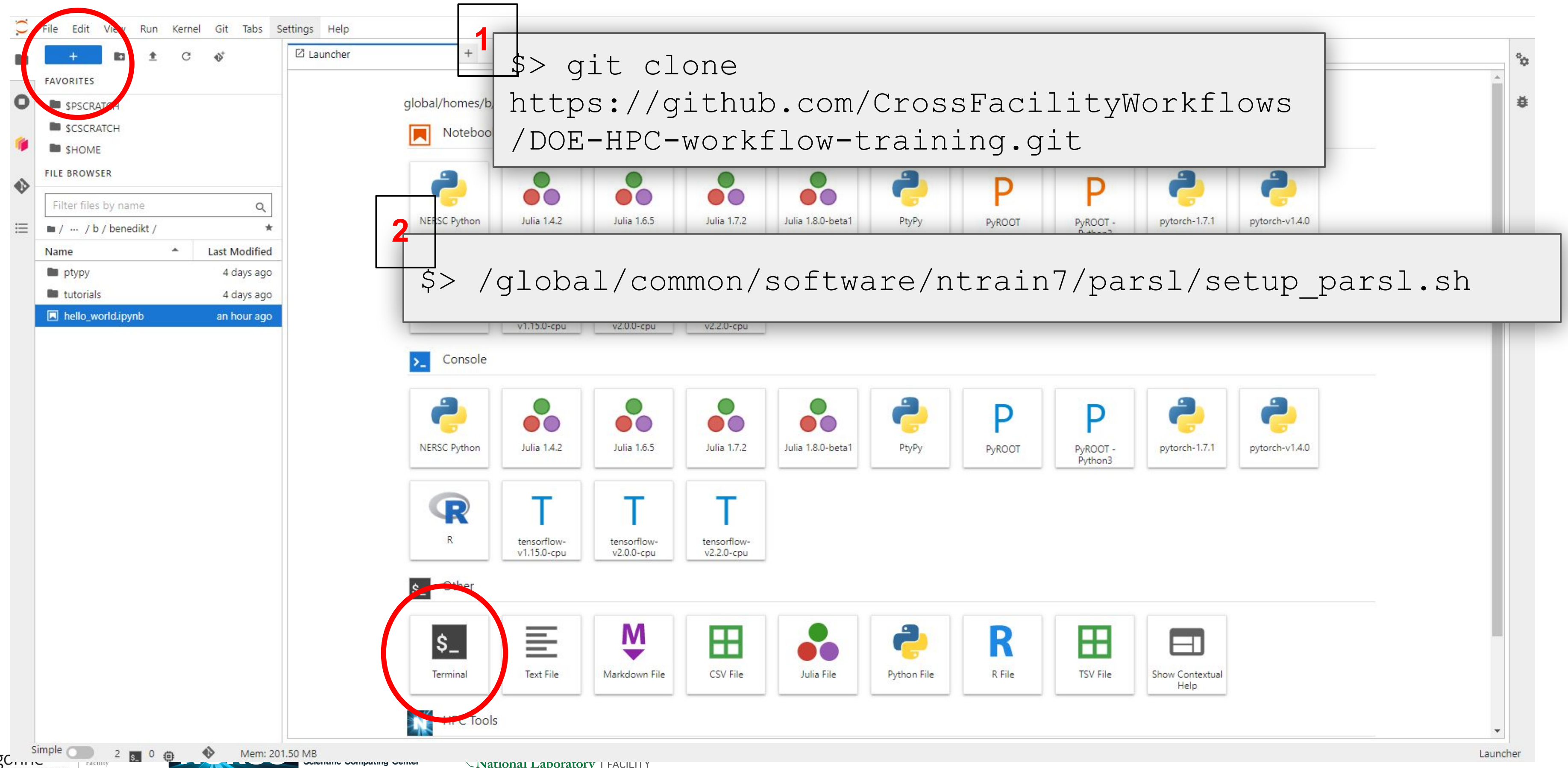
nodes (maximum of 4 for jupyter QOS): 1

ntasks-per-node: 1

Reservation: doe_workflows_2023_cpu

time (time limit in minutes): 90

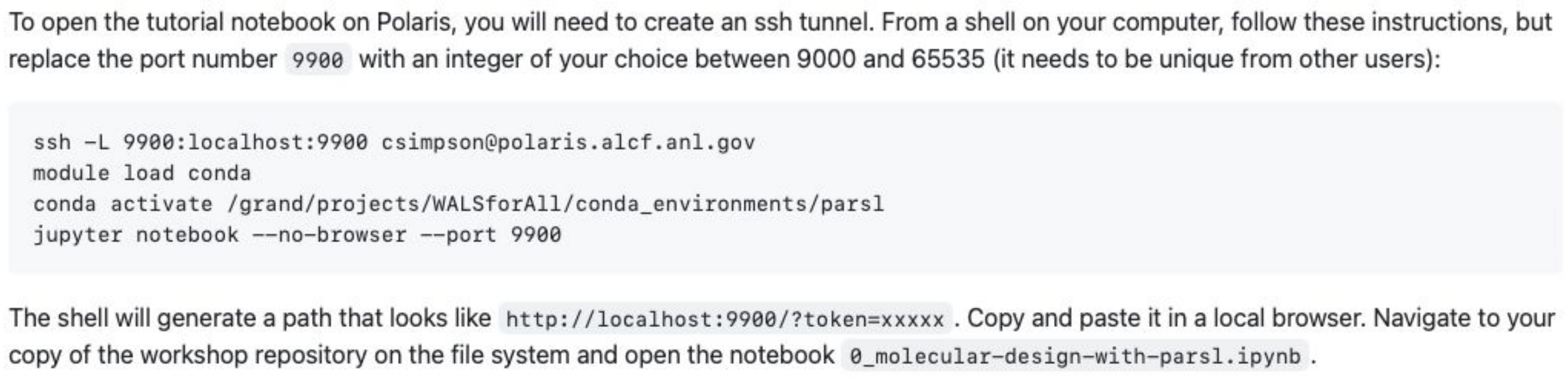
Open Terminal, download tutorials, setup



```
$> git clone
https://github.com/CrossFacilityWorkflows
/DOE-HPC-workflow-training.git
```

```
$> /global/common/software/ntrain7/parsl/setup_parsl.sh
```

Instructions for ALCF



To open the tutorial notebook on Polaris, you will need to create an ssh tunnel. From a shell on your computer, follow these instructions, but replace the port number `9900` with an integer of your choice between 9000 and 65535 (it needs to be unique from other users):

```
ssh -L 9900:localhost:9900 csimpson@polaris.alcf.anl.gov
module load conda
conda activate /grand/projects/WALSforAll/conda_environments/parsl
jupyter notebook --no-browser --port 9900
```

The shell will generate a path that looks like `http://localhost:9900/?token=xxxxx`. Copy and paste it in a local browser. Navigate to your copy of the workshop repository on the file system and open the notebook `0_molecular-design-with-parsl.ipynb`.

Instructions for OLCF

To open the tutorial notebook on Summit, you will need to create an ssh tunnel. From a shell on your computer, follow these instructions, but replace the port number `9900` with an integer of your choice between 9000 and 65535 (it needs to be unique from other users):

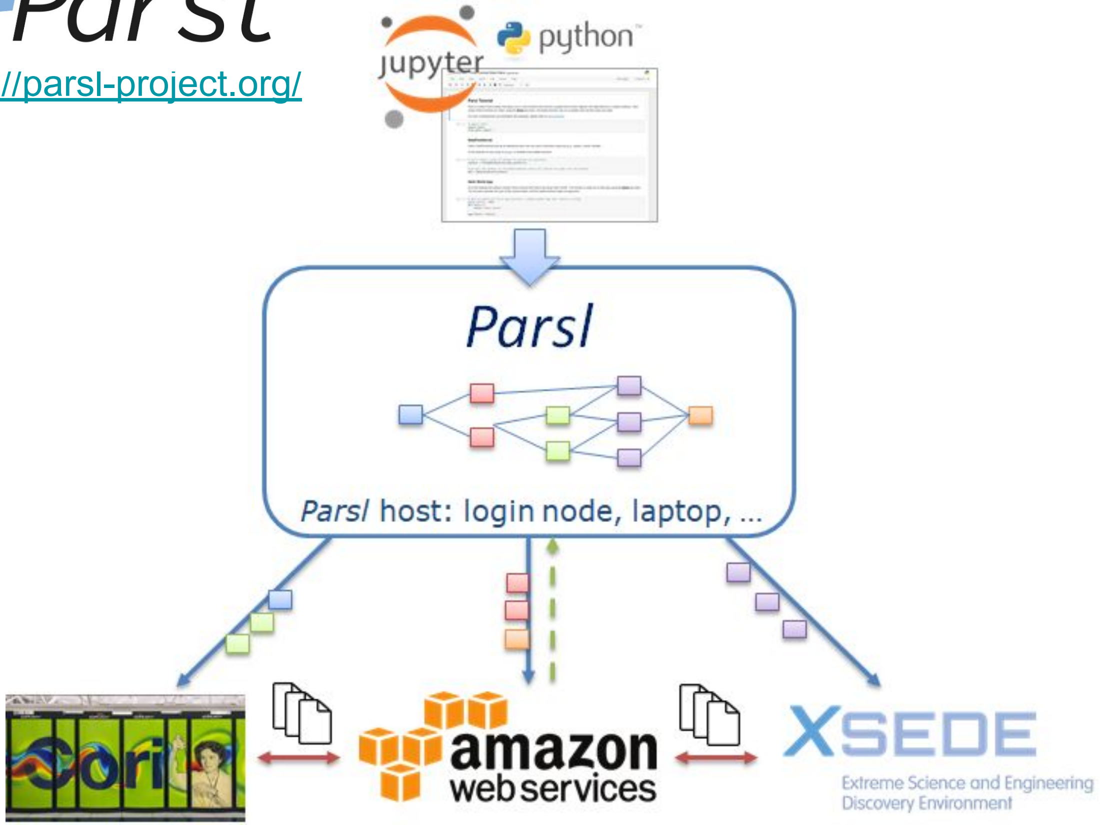
```
$ ssh -L 9900:localhost:9900 tskluzac@summit.olcf.ornl.gov

$ git clone https://github.com/CrossFacilityWorkflows/DOE-HPC-workflow-training.git

$ module load python

$ source activate /gpfs/alpine/world-shared/stf001/parsl_tutorial

$ jupyter notebook --no-browser --port 9900
```

The shell will generate a URL that looks like `http://localhost:9900/?token=xxxxx`. Copy and paste it in a local browser. Navigate to your copy of the workshop repository on the file system and open the notebook `mol-design-demo.ipynb`.

What is Parsl?

https://parsl-project.org/

- Started in 2017 by Y. Babuji, K. Chard, et al. at UChicago/ANL
- Parsl "provides an intuitive, pythonic way of parallelizing codes by annotating 'apps' "
- Apps execute concurrently while respecting data dependencies.
- "Write once, run anywhere" philosophy


jupyter
python
Parsl
Parsl host: login node, laptop, ...
Cori
amazon web services
XSEDE
Extreme Science and Engineering Discovery Environment

Motivation: The modern research computing landscape

Software is increasingly *assembled* rather than written

- High-level language to integrate components from many sources

Parallel and distributed computing is ubiquitous

- Increasing data sizes & plateauing sequential processing

Resources are increasingly heterogeneous (distributed)

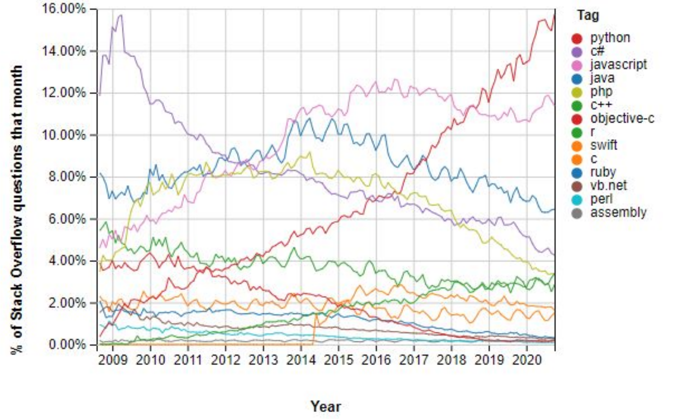
- Application components best run in different places

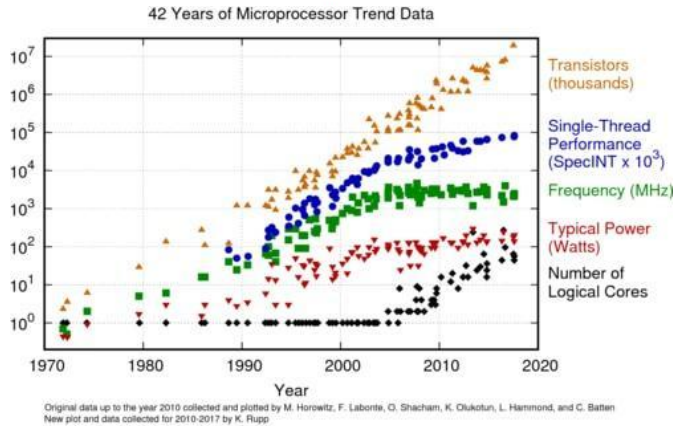
Python (& SciPy ecosystem) de facto standard language

- Libraries, tools, Jupyter, etc.

Parsl allows for the natural expression of parallelism in Python

funcX enables fire-and-forget remote and distributed execution of Python functions





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OAK RIDGE National Laboratory LEADERSHIP COMPUTING FACILITY

Parsl programs can be executed in different ways on different systems

Parsl

Executors (`concurrent.futures.Executor` interface)

- 🟩 HTEX
- 🟩 Work Queue
- 🟧 Flux
- 🟧 EXEX
- 🟧 RADICAL-Cybertools
- 🟧 funcX
- 🟥 IPyParallel

IP[y]:

🟩 Production
🟧 Prototype
🟥 Deprecated

Providers

Slurm	LSF	GridEngine	Kubernetes	AWS
PBS	Cobalt	HTCondor	Google	Ad hoc

Why Parsl?

- Easy to install, no database dependencies.
- Designed for large scale computing.
- Strong documentation and community support.
- Entirely Python orchestration: No bash scripts for workflows, no explicit slurm calls in the workflow.
- Not dependant on external infrastructure (i.e. like a DB)

- Most issues with running Parsl arise from its preferred setup of a master process trying to orchestrate resources with NERSC's busy slurm instance.
- How executor, provider and launcher parameters relate to slurm parameters is a learning process.
- Workers are stateless.

Parsl was made with HPC in mind.

- Parsl can schedule up to 1000-2000 apps/tasks per second.
- As a rule of thumb, in a high throughput case, the ideal duration of a task is larger than 0.01s times the number of nodes, i.e. for 100 nodes the duration of a task shall be longer than a second.
- Parsl has been tested to scale up to 250K workers on 8000 nodes. (Y. Babuji et al. https://doi.org/10.1145/3307681.3325400)
- For logging, Parsl will create one directory for each node, and 1 manager and N workers will write separate logs to this directory. Logging is pretty minimal at two lines per task unless debug logging is turned on.
- Bash apps communicate via files only. This may add to or suffer from file system congestions

Parsl executors scale to 2M tasks/256K workers

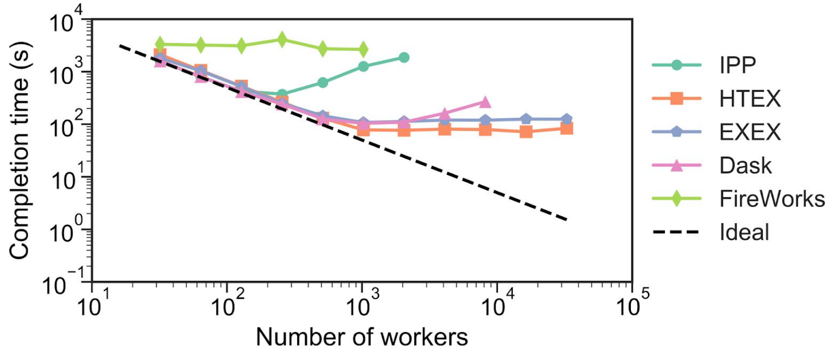
HTEX and EXEX outperform other Python-based approaches

Parsl scales to more than 250K workers (8K nodes) and ~2M tasks

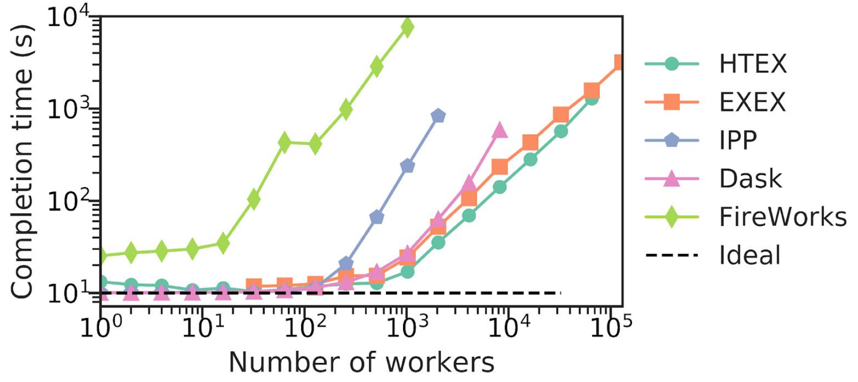
Framework	Maximum # of workers[†]	Maximum # of nodes[†]	Maximum tasks/second[‡]
Parsl-IPP	2048	64	330
Parsl-HTEX	65 536	2048*	1181
Parsl-EXEX	262 144	8192*	1176
FireWorks	1024	32	4
Dask distributed	4096	128	2617

Babuji et.al. "Parsl: Pervasive Parallel Programming in Python." ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC). 2019.

Strong scaling (50K 1s tasks)



Weak scaling (10 1s tasks per worker)



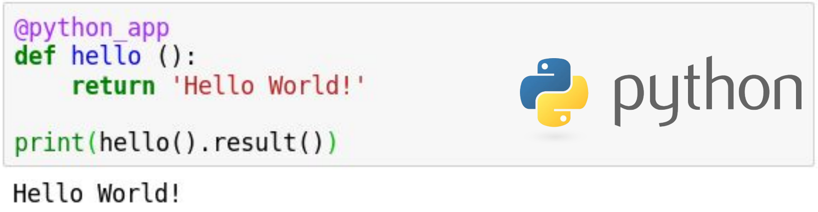
Parsl: parallel programming in Python

Apps define opportunities for parallelism

- Python apps call Python functions
- Bash apps call external applications

```
pip install parsl
```

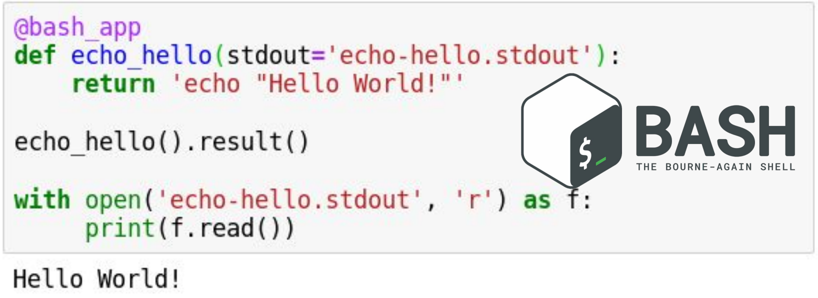
Apps return “futures”: a proxy for a result that might not yet be available



```
@python_app
def hello ():
    return 'Hello World!'

print(hello().result())
```

```
Hello World!
```

Apps run concurrently respecting dataflow dependencies. Natural parallel programming!



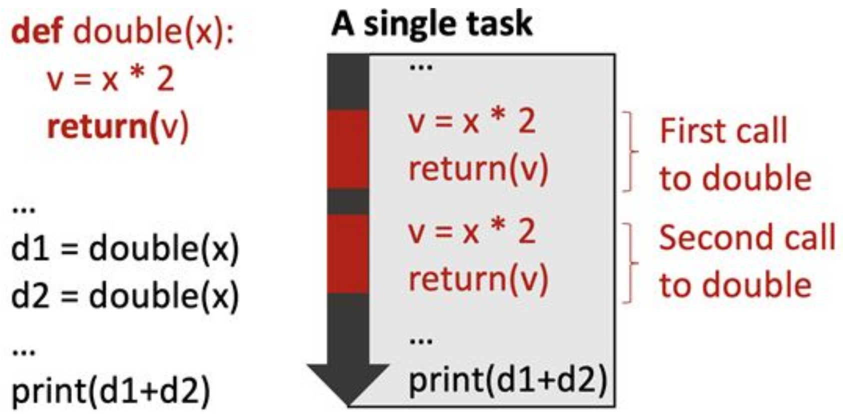
```
@bash_app
def echo_hello(stdout='echo-hello.stdout'):
    return 'echo "Hello World!"'

echo_hello().result()

with open('echo-hello.stdout', 'r') as f:
    print(f.read())
```

```
Hello World!
```

Parsl scripts are independent of where they run. Write once run anywhere!

Try Parsl: https://parsl-project.org/binder

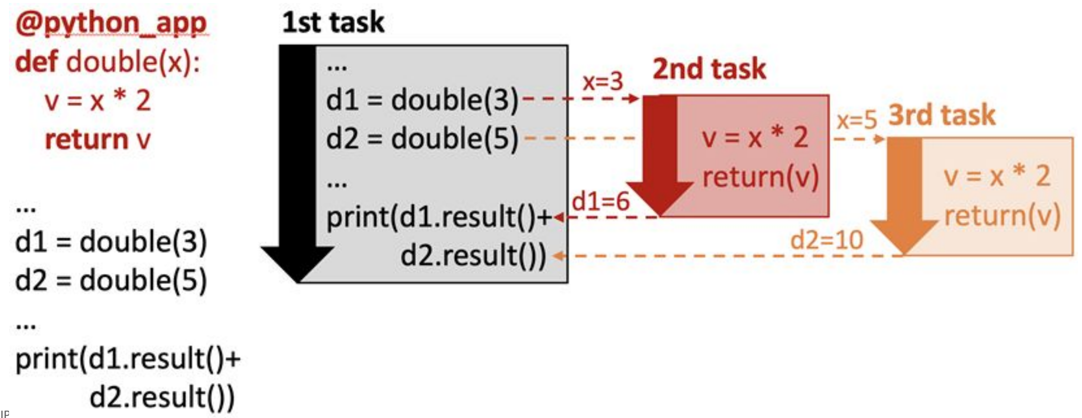
How does it work?



```
def double(x):
   v = x * 2
   return(v)

...
d1 = double(x)
d2 = double(x)
...
print(d1+d2)
```

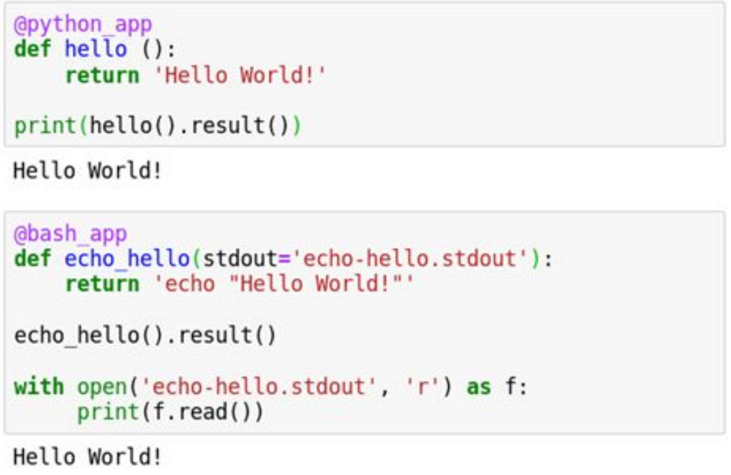
Python

Parsl



```
@python_app
def double(x):
   v = x * 2
   return v

...
d1 = double(3)
d2 = double(5)
...
print(d1.result()+
       d2.result())
```

How does it work?



```
@python_app
def hello ():
    return 'Hello World!'

print(hello().result())
```

```
Hello World!
```

```
@bash_app
def echo_hello(stdout='echo-hello.stdout'):
    return 'echo "Hello World!"'

echo_hello().result()

with open('echo-hello.stdout', 'r') as f:
    print(f.read())
```

```
Hello World!
```

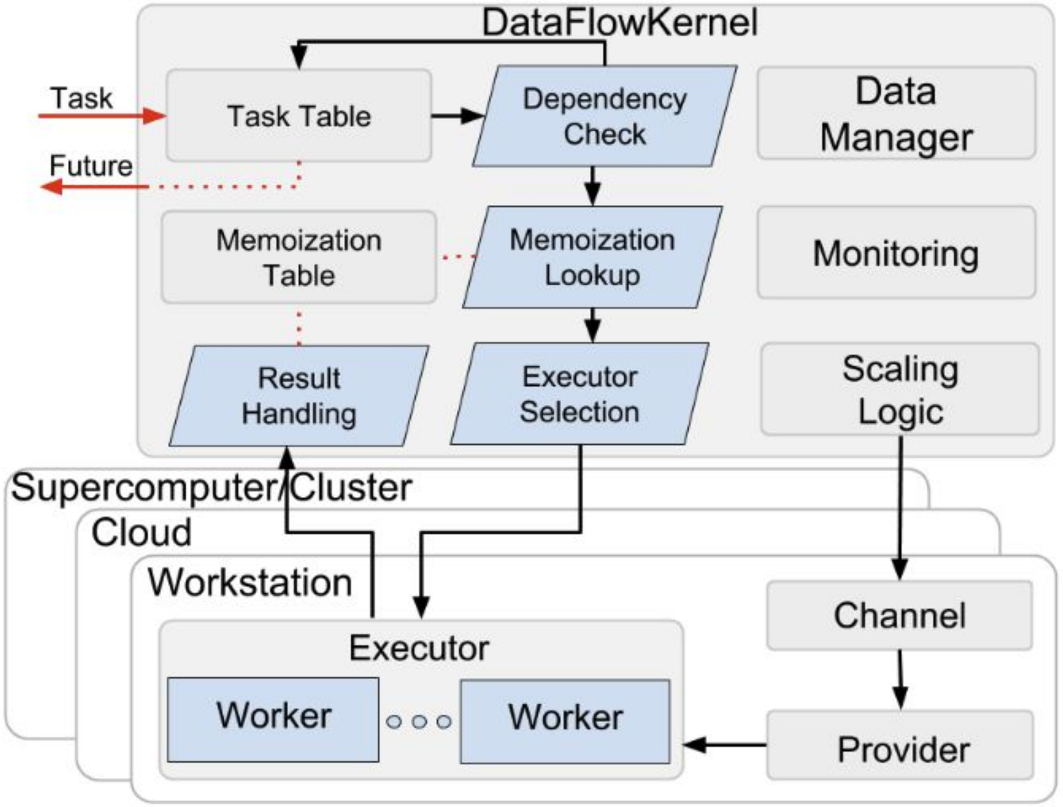
Developing a workflow is a two-step process:

- Annotate functions that can be executed in parallel as Parsl apps.
- Specify dependencies between functions using standard Python code.

- An App call returns immediately, generates a *task* in the DataFlowKernel (Parsl's task management engine) and a Future in the Python script.
- Futures can be passed to other apps as inputs, establishing a dependency.
- Dependencies are assembled implicitly into **directed acyclic graphs**
- Dependency graph is not computed in advance but dynamically built and updated while the Parsl script executes. It complete when the script finishes executing.

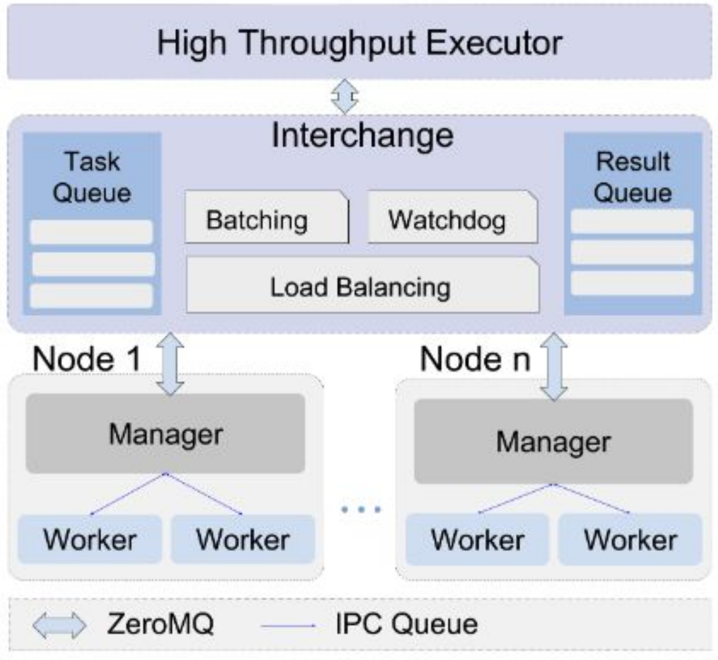
High Level Architecture

- ***DataFlowKernel (DFK)*** is responsible for constructing and orchestrating the execution of the task graph.
- Uses one or more connected ***Executors***.
- ***Tasks*** are dispatched to Executor(s) which run in blocks of nodes from Providers.
- *Tasks* are executed concurrently if their (data-)dependencies are met
- *Tasks* will run in parallel if the Executor has enough resources/workers.



High Throughput Executor (HTEX)

- Engineered to support up to 2000 nodes, millions of sub-second tasks, and multi-day workflow campaigns with high fault tolerance.
- Manager is a multi-threaded agent responsible for a single node, initializing workers based on HTEX configuration (i.e., *workers_per_node*).
- Task & results are prefetched and batched to minimize communication overhead.
- Managers and the interchange exchange periodic heartbeat messages.



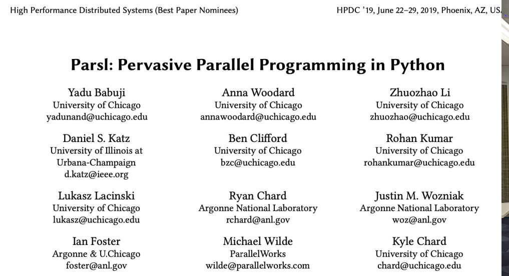
(a) HTEX: High Throughput Executor

Parsl++

You

I'm interested in learning more about Parsl!

I'm becoming proficient in Parsl!



High Performance Distributed Systems (Best Paper Nominees) HPDC '19, June 22–29, 2019, Phoenix, AZ, US

Parsl: Pervasive Parallel Programming in Python

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Read the Parsl paper! [HPDC '19]

Attend Parsl Fest

funcX

Federated function as a service

Check out funcX (FaaS system built atop Parsl)

Launching Parsl Project

Join the Parsl community on Slack!

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Parsl is commonly installed via conda

```
$ module load python
$ conda create --name parsl
$ source activate parsl
(parsl) $
```

Install parsl or with pip or through conda forge:

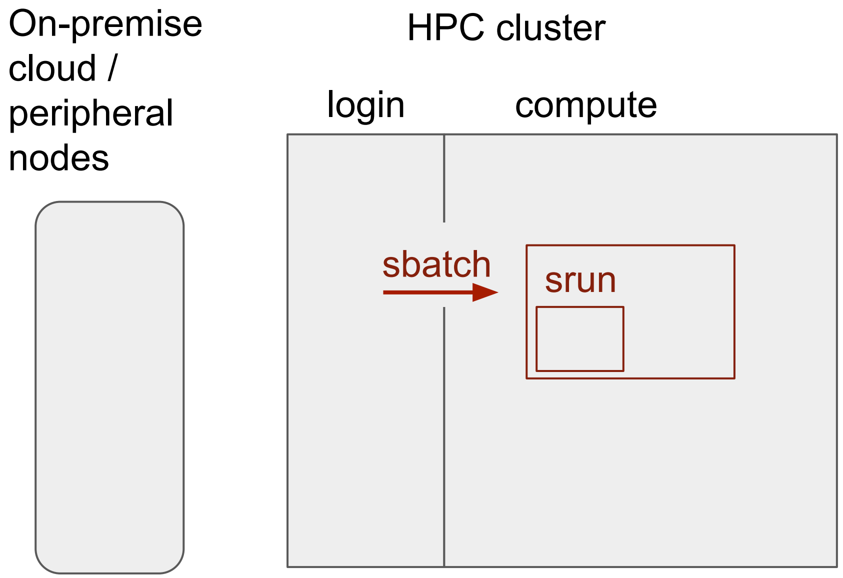
```
(parsl) $ python -m pip install parsl
```

or

```
(parsl) $ conda install -c conda-forge parsl
```

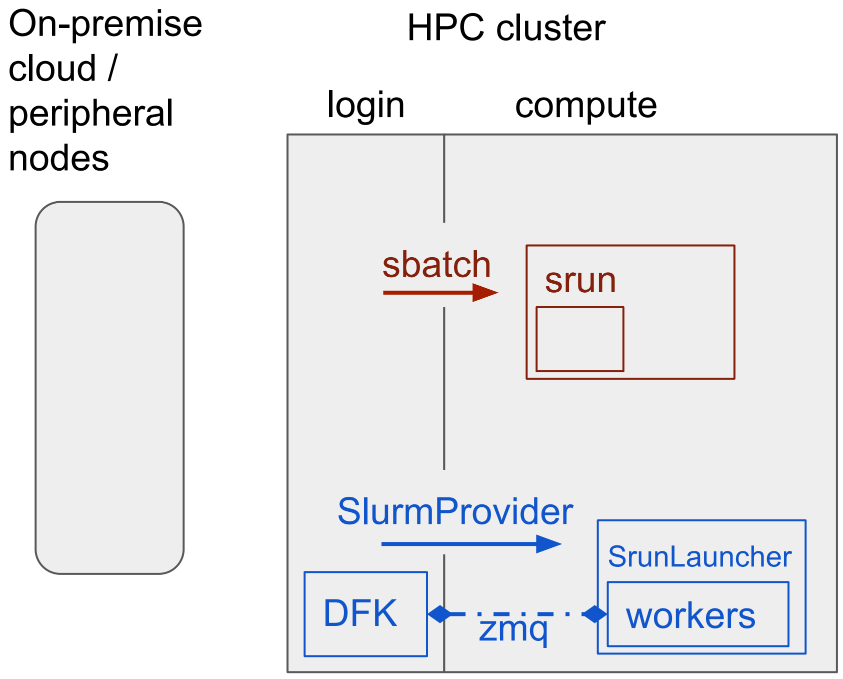
Configuring Parsl for your HPC system

- For Parsl to work as expected it is crucial to set up the config properly.
- The DFK will run in the process where the config is loaded, i.e. the main script



(Semi)permanent "Pilot" process hosts the DFK

- For long or semipermanent workflows that may react on external commands/data.
- DFK process placed on login nodes (or workflow nodes) or in SCRONTAB/workflow qos (NERSC).
- Must keep DFK process alive after logout.
- Parsl needs to use LRM provider (e.g. SlurmProvider) to get resources for the workers.



SlurmProvider = sbatch

(Semi)permanent "Pilot" process hosts the DFK

```
import parsl
from parsl.config import Config
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher
from parsl.executors import HighThroughputExecutor

config = Config(
     executors=[
     HighThroughputExecutor(
          label='PM_HTEX_multinode',
          cores_per_worker=2,
          provider=SlurmProvider(
                    #'regular',  # Partition / QOS (NERSC doesn't use partitions though)
                    nodes_per_block=2,
                    scheduler_options=' #SBATCH -C cpu',
                    worker_init='module load python; source activate parsl',
                    launcher=SrunLauncher(overrides='-c 128 -q regular'),
                    walltime='00:10:00',
                    # Slurm scheduler on Cori can be slow at times, increase the command timeouts
                    cmd_timeout=120, # Increase timeout for unresponsive schedulers
          ),
     )]
)
parsl.load(config)
```

https://docs.nersc.gov/jobs/workflow/parsl/#example-creating-a-parsl-script-for-a-high-throughput-scenario

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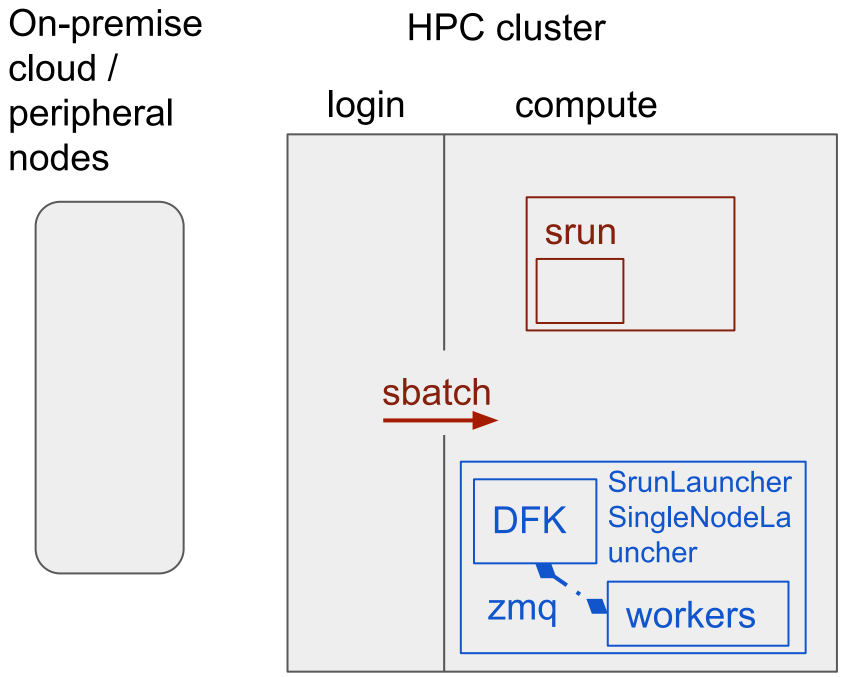
Headless config with DFK inside allocation

- For "boxed" workflows or Jupyter kernels on compute nodes.
- DFK process runs in head node of preallocated block of resources.
- Can run unattended.
- No need to use a LRM provider class, only needs LRM launcher for multi node access.


On-premise cloud / peripheral nodes
HPC cluster
login
compute
srun
sbatch
DFK
SrunLauncher SingleNodeLauncher
zmq
workers

Headless config with DFK inside allocation

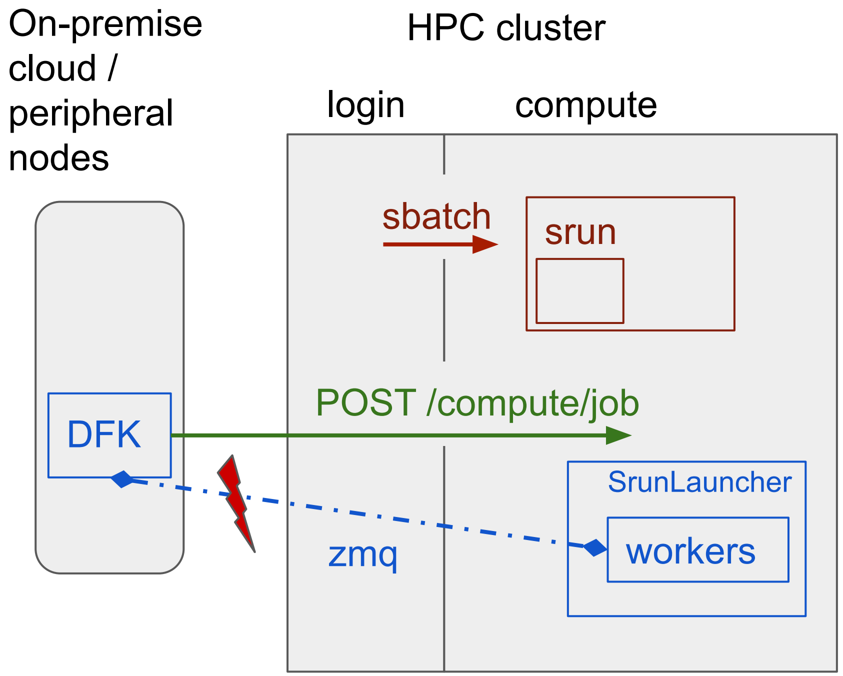
```
import parsl
from parsl.config import Config
from parsl.providers import LocalProvider
from parsl.launchers import SrunLauncher
from parsl.channels import LocalChannel
from parsl.executors import HighThroughputExecutor

config = Config(
      executors=[HighThroughputExecutor(
            label='PM_HTEX_headless',
            max_workers=1,  # one worker per manager / node
            provider=LocalProvider(
                  channel=LocalChannel(script_dir='.'),
                  nodes_per_block=2,
                  launcher=SrunLauncher(overrides='-c 32'),
                  cmd_timeout=120,
                  init_blocks=1,
                  max_blocks=1
            ),
      )],
      strategy=None,
)
parsl.load(config)
```

https://docs.nersc.gov/jobs/workflow/parsl/#example-headless-workflow-launched-from-node-0

Why not put the DFK on cloud/peripheral nodes?

- For permanent workflows with a web frontend.
- DFK process runs in on on-premise Cloud (i.e. Spin at NERSC).
- If LRM isn't exposed, it needs a new provider that wraps facility APIs for job execution.
- Can be problematic with all the ports that the zmq communication needs.

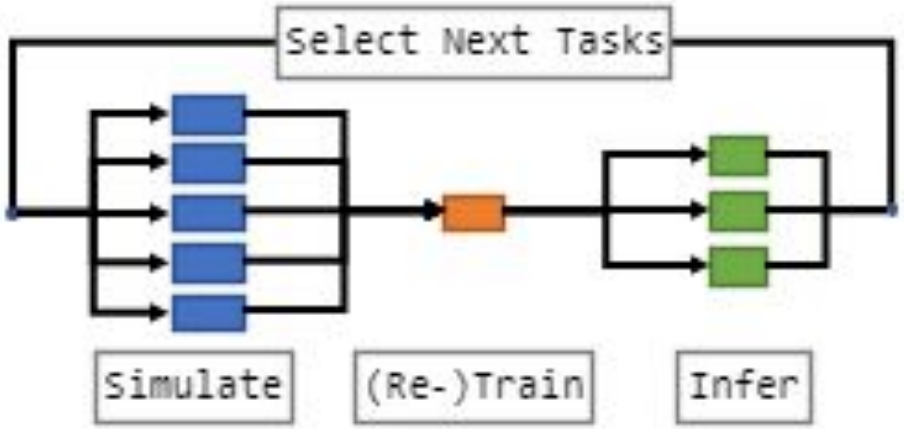


Tutorial example: ML-in-the-loop materials design

Aim: identify high value molecules (high ionization energy) among a search space of billions of candidates

Problem: Simulation is expensive

Solution: Create an active learning loop that couples simulation with machine learning to simulate only high value candidates



https://github.com/ExaWorks/molecular-design-parsl-demo

If you can't get the notebook up at NERSC | ALCF | OLCF, go there and use binder.