Balsam Workflows and Ensemble Jobs

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Overview

- When can Balsam be useful?
- What is Balsam?
- Starting on Theta
- Case study: managing a large campaign of simulations
- Data dependencies and dynamic workflows
- Case study: hyperparameter optimization

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What is a workflow?

- **Strategy for executing your application runs**
  - **Job scheduling**
  - **“Packing” small runs into larger ensemble jobs**
  - **Data movement**
  - **Pre- and post-processing**

In some cases, a few command line tools is enough
(20 jobs) (1024 nodes) (12 hours) = 245,760 node-hours

Other cases demand a more careful approach
(2,457,600 jobs) (1 node) (6 minutes) = 245,760 node-hours

Theta Ensemble Jobs: Quick Solution

- Up to 1000 concurrent apruns per Cobalt job
- Easy way to achieve throughput, given the ALCF queueing policies

```
-----myjob.sh------
#!/bin/sh
echo "Starting Cobalt job script"
aprun -n 128 -N 64 run1.exe arg1 &
sleep 1
aprun -n 256 -N 64 run1.exe arg1 &
sleep 1
aprun -n 512 -N 64 run1.exe arg1 &
wait


-----end myjob.sh---
```

This approach needs help to scale

- Large number of application runs
- Dependencies in workflow
- Maintaining high resource utilization
- Tracking finished/failed/timed-out runs, modifying inputs, and dispatching new batches of work becomes cumbersome

Write your own scripts?
Invest in a workflow manager?

Why workflow management?

- Organize large compute campaigns
- Automate scheduling & job dispatch
- Maximize concurrency to exploit LCF resources
- Improve robustness with error-handling and retry capabilities
- Record provenance data for:
    - Faster detection of errors
    - Workflow execution statistics (e.g. throughput over time)

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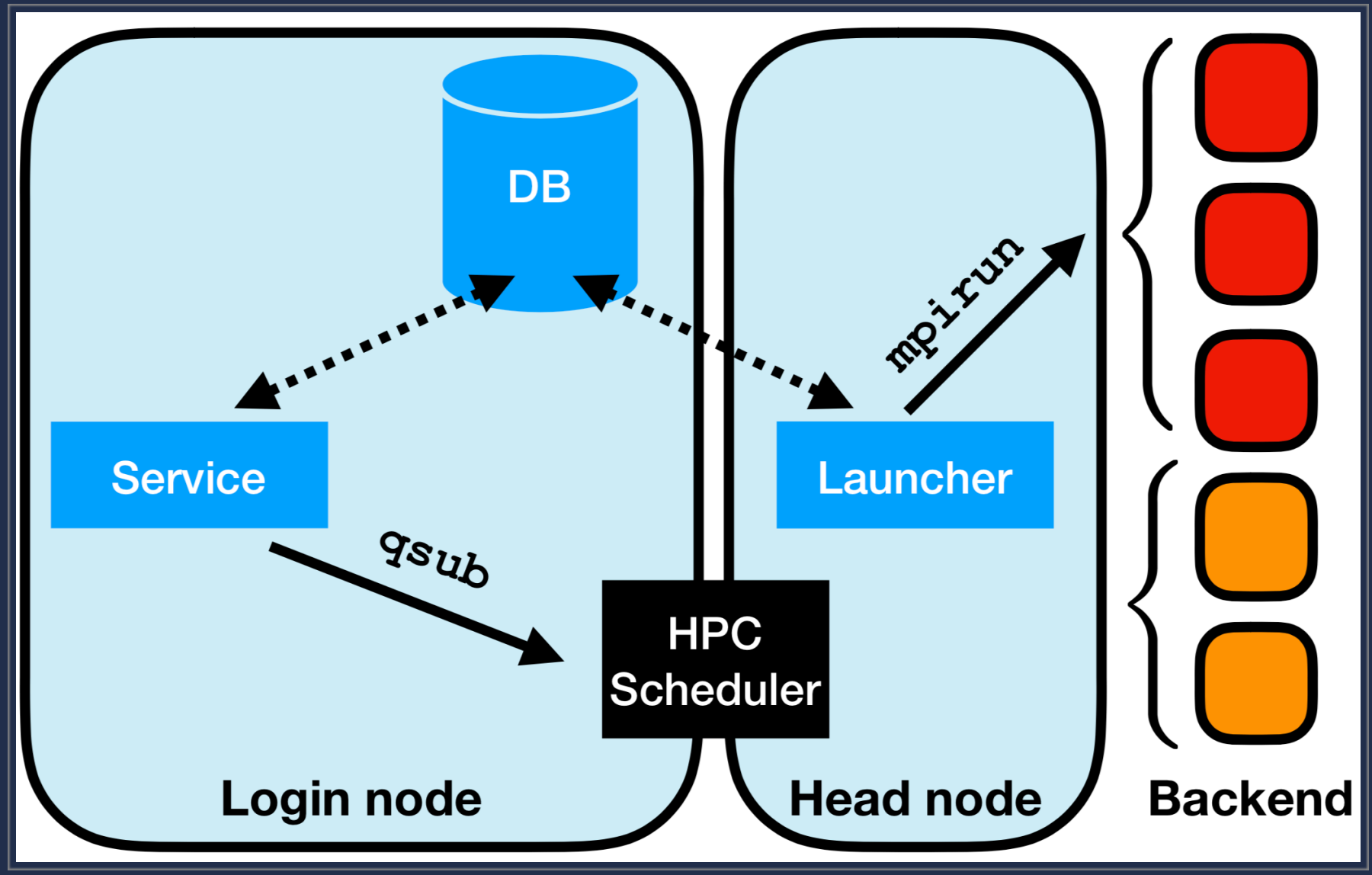
Balsam components

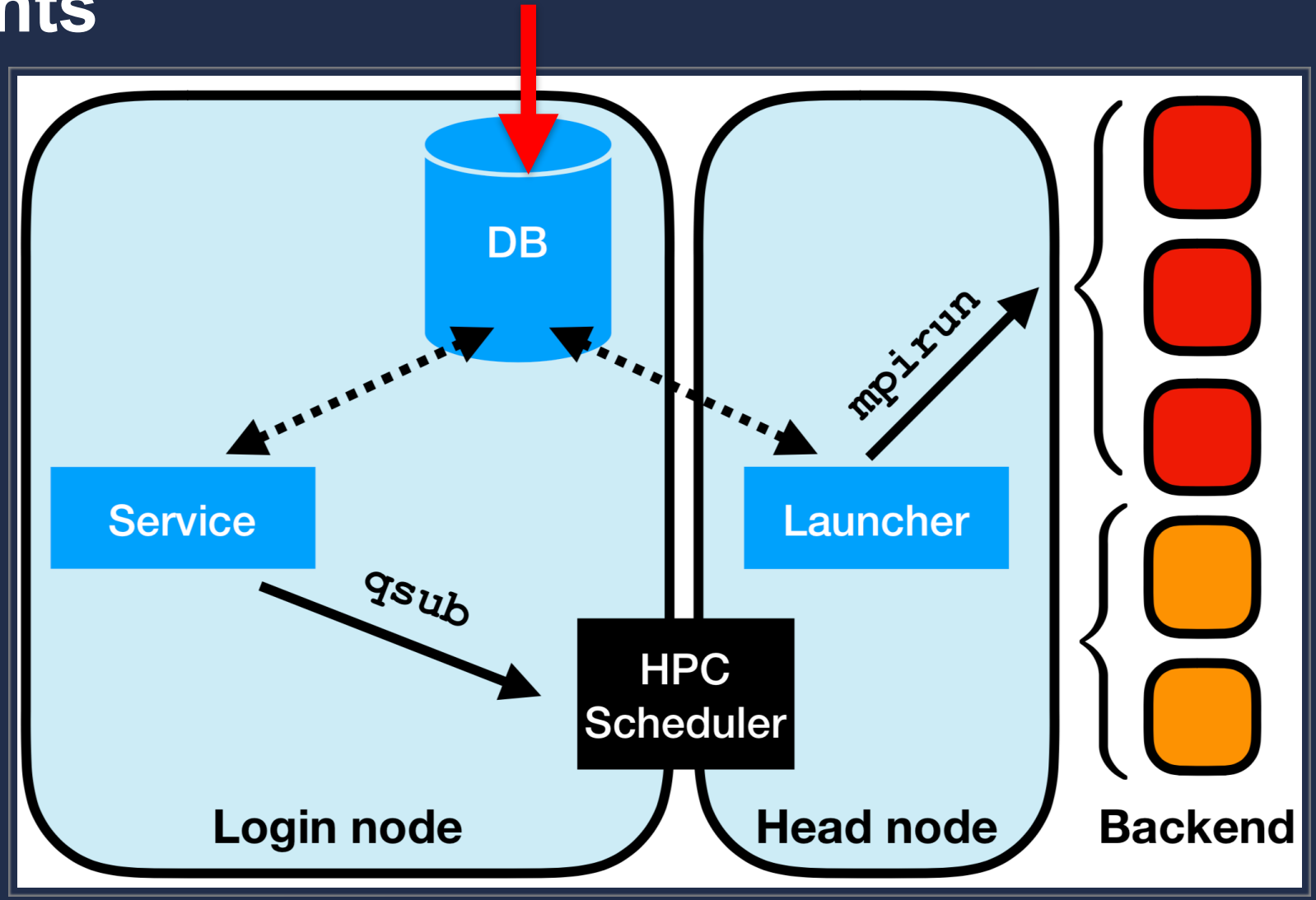


Balsam components

Database

BalsamJob table stores workflow state

One row for each planned application run

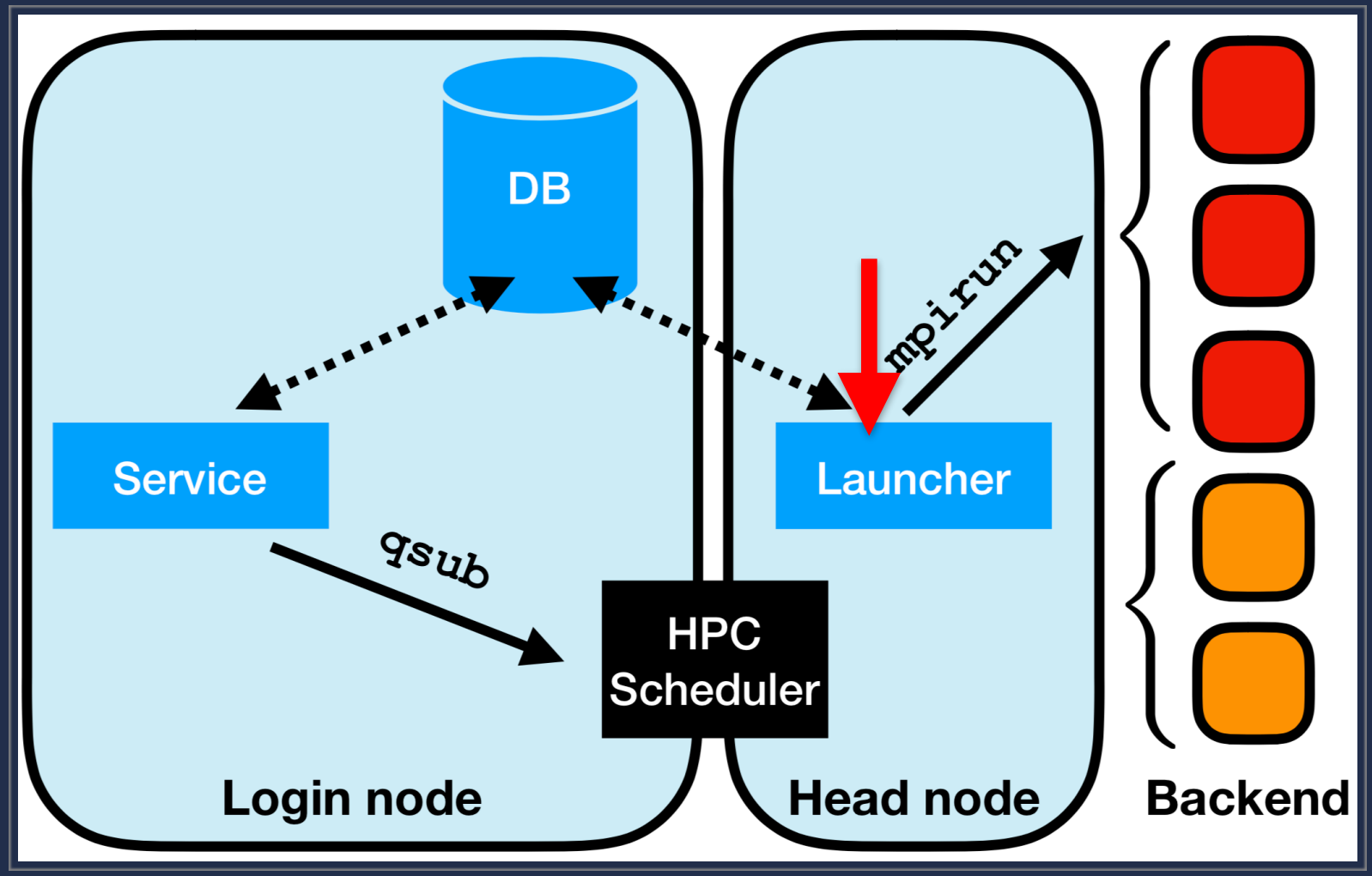


Balsam components

Launcher

Pilot application running inside Cobalt job

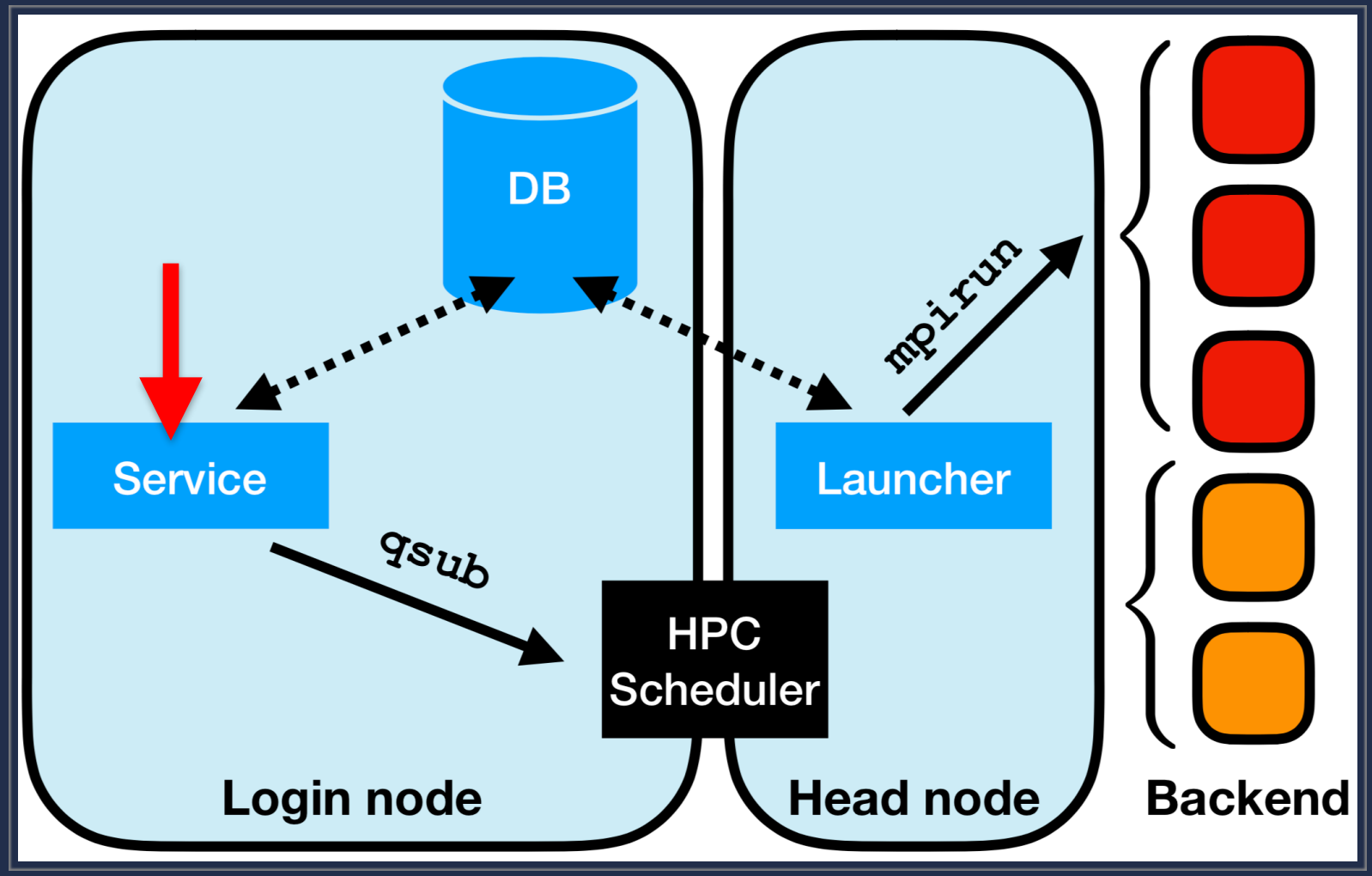
Dynamic task pull and execution



Balsam components

Service

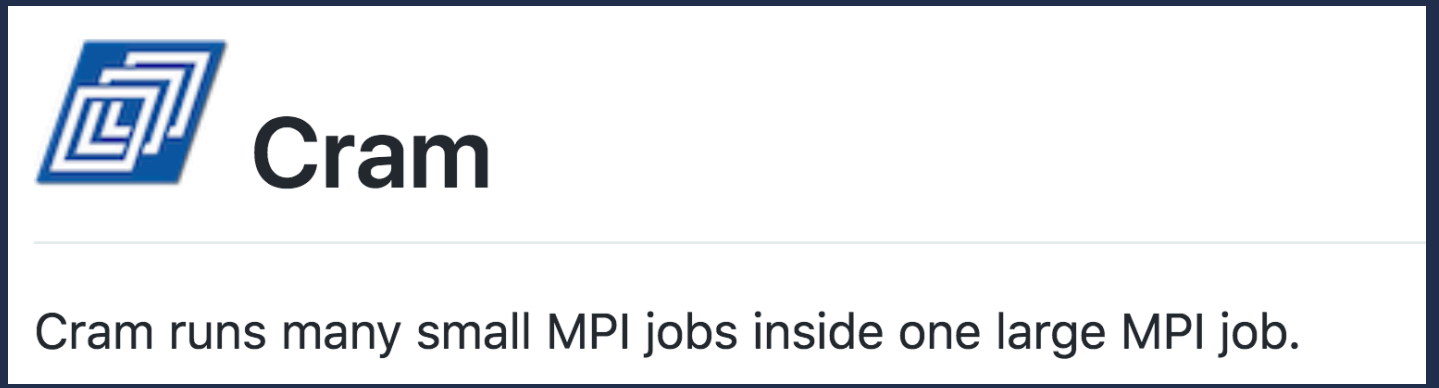
Elastic scheduling of launcher jobs under varying workload



Balsam Highlights

- No modification of user applications
- Command line and Python interfaces
- Performance tested up to 1.2M jobs in database
- Strengths & limitations of launcher on Theta are well-understood
- Strong task-level fault tolerance
    - even fatal errors do not interrupt workflow
- Concurrent execution of serial and MPI applications across one or many Cobalt jobs

Other approaches



- https://github.com/llnl/cram
- SPMD approach: link your application against libcram
- Create a “CramFile” with args for each application instance
- Unlimited MPI jobs can be packed into one; no strain on head node
- All instances start concurrently; job takes as long as the the slowest instance
- All tasks run under MPI_COMM_WORLD; one fault can abort the entire run

Other approaches

- http://swift-lang.org/Swift-T/index.php http://parsl-project.org/
- Express workflow as code with dataflow constructs
- Tasks eligible for concurrent execution automatically distributed
- Concise and flexible language for defining workflows
- Swift/T backend provides high performance, scalable MPI runtime environment for workflow
- Running “MPI-inside-MPI” becomes a technical hurdle
- Lack of resource isolation between Swift/T tasks hampers fault tolerance
- No notion of centralized database; may be less appropriate for extended computational campaigns

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Balsam on Theta — Walkthrough

- https://balsam.alcf.anl.gov/index.html — documentation undergoing major update
- Up-to-date module available on Theta:

```
msalim@thetalogin6:~> module load balsam
msalim@thetalogin6:~> balsam
Balsam requires Python version >= 3.6
```

Command line interface

Load 3.6

```
msalim@thetalogin6:~> module load cray-python/3.6.1.1
msalim@thetalogin6:~> balsam
usage: balsam [-h]
              {app,job,dep,ls,modify,rm,killjob,mkchild,launcher,submit-launch,
mmies,which,log,server}
              ...

Balsam command line interface

optional arguments:
  -h, --help            show this help message and exit

Subcommands:
  {app,job,dep,ls,modify,rm,killjob,mkchild,launcher,submit-launch,init,service
log,server}
    app                 add a new application definition
    job                 add a new Balsam job
    dep                 add a dependency between two existing jobs
    ls                  list jobs, applications, or jobs-by-workflow
    modify              alter job or application
    rm                  remove jobs or applications from the database
    killjob             Kill a job without removing it from the DB
    mkchild             Create a child job of a specified job
    launcher            Start a local instance of the balsam launcher
```

CLI subcommands

Start a new Balsam DB

Use `balsam init` to create a new database directory

```
msalim@thetalogin6:~> balsam init ~/test-db
```

```
**********************************************************************
  Successfully created Balsam DB at: /home/msalim/test-db
  Use `source balsamactivate test-db` to begin working.
**********************************************************************
```

Start a new Balsam DB

`source balsamactivate <db-name>` **: starts server, if not already running, sets environment for Balsam**

```
msalim@thetalogin6:~> . balsamactivate test-db
Launching Balsam DB server
waiting for server to start.... done
server started
[BalsamDB: test-db] msalim@thetalogin6:~>
```

Hello World

`balsam app` :

Register new applications with Balsam

```
[BalsamDB: test-db] msalim@thetalogin6:~> balsam app --name say-hello --executable "echo Hello,"
Application 1:
----------------------------
Name:           say-hello
Description:
Executable:     echo Hello,
Preprocess:
Postprocess:

Added app to database
```

Hello World

`balsam job` :

Add a new run (or task) to the database

```
[BalsamDB: test-db] msalim@thetalogin6:~> balsam job --name test1 --workflow test \
> --app say-hello --args "world!"
```

Hello World

Confirmation shows task details and names of adjustable fields

```
BalsamJob 7df86c8b-f94b-4349-8ab6-a8afc85d8a9f
-----------------------------------------------
workflow:                       test
name:                           test1
description:
lock:
parents:                        []
input_files:                    *
stage_in_url:
stage_out_files:
stage_out_url:
wall_time_minutes:              1
num_nodes:                      1
coschedule_num_nodes:           0
ranks_per_node:                 1
cpu_affinity:                   none
threads_per_rank:               1
threads_per_core:               1
node_packing_count:             1
environ_vars:
application:                    say-hello
args:                           world!
user_workdir:
wait_for_parents:               True
post_error_handler:             False
post_timeout_handler:           False
```

Hello World

Confirmation shows task details and names of adjustable fields

```
auto_timeout_retry:          True
state:                       CREATED
queued_launch_id:            None
data:                        {}
  *** Executed command:      echo Hello, world!
  *** Working directory:     /gpfs/mira-home/msalim/test-db/data/test/test1_7df86c8b
```

Hello World

Adding 9 more jobs…

```
[BalsamDB: test-db] msalim@thetalogin6:~> for i in {2..10}
> do
> balsam job --name test${i} --workflow test --app say-hello \
> --args "world ${i}!" --yes
> done
```

Hello World

`balsam ls` :

View tasks in database

```
[BalsamDB: test-db] msalim@thetalogin6:~> balsam ls
                                  job_id |   name | workflow | application |   state
-------------------------------------------------------------------------------------
7df86c8b-f94b-4349-8ab6-a8afc85d8a9f | test1  | test     | say-hello   | CREATED
ab58c816-0665-4cd3-b3f2-e16312e77887 | test2  | test     | say-hello   | CREATED
ff23e57b-6829-4abc-966d-82e2c6a90d9e | test3  | test     | say-hello   | CREATED
5bee0827-99bb-4bbb-ac7a-a7dd15e4bda3 | test4  | test     | say-hello   | CREATED
d4705a0a-bf6d-4f7e-a4fb-146a9bfe55a1 | test5  | test     | say-hello   | CREATED
b830798e-a4f8-45b1-b7bd-dd62adfb92ac | test6  | test     | say-hello   | CREATED
51e23e81-0655-436e-a1f0-550b6a1b3102 | test7  | test     | say-hello   | CREATED
6a87c9cf-19d5-4796-8d3b-1c6115067ad5 | test8  | test     | say-hello   | CREATED
cac08656-8056-452f-b709-bdadd21ccf46 | test9  | test     | say-hello   | CREATED
14f94e50-9076-4db5-ac3f-de7977717b8c | test10 | test     | say-hello   | CREATED
```

Hello World

`balsam submit-launch` :

Shortcut for Cobalt job submission (template in ~/.balsam)

```
[BalsamDB: test-db] msalim@thetalogin6:~> balsam submit-launch -n 2 -t 5 -q debug-cache-quad \
> -A SDL_Workshop -q training --job-mode=serial
Submit OK: Qlaunch {   'command': '/gpfs/mira-home/msalim/test-db/qsubmit/qlaunch1.sh',
    'from_balsam': True,
    'id': 1,
    'job_mode': 'serial',
    'nodes': 2,
    'prescheduled_only': False,
    'project': 'SDL_Workshop',
    'queue': 'training',
    'scheduler_id': 278079,
    'state': 'submitted',
    'wall_minutes': 5,
    'wf_filter': ''}
```

Hello World

If successful, jobs eventually marked JOB_FINISHED

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db/qsubmit> balsam ls
                              job_id |   name | workflow | application |          state
-------------------------------------------------------------------------------------
cac08656-8056-452f-b709-bdadd21ccf46 | test9  | test     | say-hello   | JOB_FINISHED
b830798e-a4f8-45b1-b7bd-dd62adfb92ac | test6  | test     | say-hello   | JOB_FINISHED
ff23e57b-6829-4abc-966d-82e2c6a90d9e | test3  | test     | say-hello   | JOB_FINISHED
ab58c816-0665-4cd3-b3f2-e16312e77887 | test2  | test     | say-hello   | JOB_FINISHED
7df86c8b-f94b-4349-8ab6-a8afc85d8a9f | test1  | test     | say-hello   | JOB_FINISHED
6a87c9cf-19d5-4796-8d3b-1c6115067ad5 | test8  | test     | say-hello   | JOB_FINISHED
51e23e81-0655-436e-a1f0-550b6a1b3102 | test7  | test     | say-hello   | JOB_FINISHED
14f94e50-9076-4db5-ac3f-de7977717b8c | test10 | test     | say-hello   | JOB_FINISHED
d4705a0a-bf6d-4f7e-a4fb-146a9bfe55a1 | test5  | test     | say-hello   | JOB_FINISHED
5bee0827-99bb-4bbb-ac7a-a7dd15e4bda3 | test4  | test     | say-hello   | JOB_FINISHED
```

Hello World

`balsam ls –hist` :

View state history metadata

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db/qsubmit> balsam ls --name test5 --history
Job test5 [d4705a0a-bf6d-4f7e-a4fb-146a9bfe55a1]
------------------------------------------

[10-03-2018 19:04:00.143928 CREATED]
[10-03-2018 19:21:59.293648 PREPROCESSED]
[10-03-2018 19:22:27.183762 RUNNING] Not scheduled by Balsam service
[10-03-2018 19:22:28.200423 RUN_DONE]
[10-03-2018 19:22:29.354333 JOB_FINISHED]
```

Where did the output go?

By default, everything goes into DB directory

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db> ls
balsamdb  data  log  qsubmit  server-info
```

Job working directories are created as:

`data/<workflow>/<name>_<id>`

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db> ls data/test/
test10_14f94e50  test2_ab58c816  test4_5bee0827  test6_b830798e  test8_6a87c9cf  testfail_fab575a3
test1_7df86c8b   test3_ff23e57b  test5_d4705a0a  test7_51e23e81  test9_cac08656
```

Error States

Balsam handles failed runs gracefully

```python
from mpi4py import MPI

rank = MPI.COMM_WORLD.Get_rank()
if rank == 0:
    raise RuntimeError("simulated error")
else:
    print("Hello from rank", rank)
```

fail.py

Error States

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db/qsubmit> balsam app --name failer --exec fail.py
Application 2:
--------------------------
Name:           failer
Description:
Executable:     /opt/python/3.6.1.1/bin/python /gpfs/mira-home/msalim/test-db/qsubmit/fail.py
```

Error States

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db/data/test/testfail_fab575a3> balsam ls
                              job_id |     name | workflow | application |        state
-----------------------------------------------------------------------------------------
fab575a3-01db-41b5-b70d-c396c17ef10d | testfail | test     | failer      | FAILED
cac08656-8056-452f-b709-bdadd21ccf46 | test9    | test     | say-hello   | JOB_FINISHED
b830798e-a4f8-45b1-b7bd-dd62adfb92ac | test6    | test     | say-hello   | JOB_FINISHED
ff23e57b-6829-4abc-966d-82e2c6a90d9e | test3    | test     | say-hello   | JOB_FINISHED
ab58c816-0665-4cd3-b3f2-e16312e77887 | test2    | test     | say-hello   | JOB_FINISHED
7df86c8b-f94b-4349-8ab6-a8afc85d8a9f | test1    | test     | say-hello   | JOB_FINISHED
6a87c9cf-19d5-4796-8d3b-1c6115067ad5 | test8    | test     | say-hello   | JOB_FINISHED
51e23e81-0655-436e-a1f0-550b6a1b3102 | test7    | test     | say-hello   | JOB_FINISHED
14f94e50-9076-4db5-ac3f-de7977717b8c | test10   | test     | say-hello   | JOB_FINISHED
d4705a0a-bf6d-4f7e-a4fb-146a9bfe55a1 | test5    | test     | say-hello   | JOB_FINISHED
5bee0827-99bb-4bbb-ac7a-a7dd15e4bda3 | test4    | test     | say-hello   | JOB_FINISHED
```

Error States

`balsam ls –state :`
Filter jobs by state

```
[BalsamDB: test-db] msalim@thetalogin6:~/test-db/data/test/testfail_fab575a3> balsam ls --state FAILED --history
Job testfail [fab575a3-01db-41b5-b70d-c396c17ef10d]
------------------------------------------------

[10-03-2018 19:34:38.379895 CREATED]
[10-03-2018 19:38:24.490910 PREPROCESSED]
[10-03-2018 19:38:24.701099 RUNNING] Not scheduled by service
[10-03-2018 19:38:30.618931 RUN_ERROR]    Traceback (most recent call last):
    Hello from rank 2
    Hello from rank 1
      File "/gpfs/mira-home/msalim/test-db/qsubmit/fail.py", line 5, in <module>
        raise RuntimeError("simulated error")
    RuntimeError: simulated error
    Hello from rank 4
    Hello from rank 3
    Hello from rank 5
    Application 5762994 exit codes: 1
    Application 5762994 resources: utime ~2s, stime ~4s, Rss ~19956, inblocks ~22664, outblocks ~0

[10-03-2018 19:38:34.516193 FAILED]
```

Modifying Tasks

Modify BalsamJob fields from command line:

```
balsam modify fab5 state RESTART_READY
```

Or with more flexible Python API:

```
>>> from balsam.launcher.dag import BalsamJob
>>> BalsamJob.objects.filter(num_nodes__lte=128, name__contains="test", state="JOB_FINISHED").update(
... state="RESTART_READY")
10
```

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Populating the Database

- **“Constructing and Navigating Polymorphic Landscapes of Molecular Crystals” ADSP** (PI: Alexandre Tkatchenko)
- **High-throughput characterization of ~1.2M structures by DFT**
- **How do we get all of these jobs into Balsam?**

Populating the Database

```
for (dirpath, dirnames, filenames) in os.walk(inbox_path):
    xyz_files = [f for f in filenames if f.endswith('.xyz')]
    new_jobs = []
    for f in xyz_files:
        name = os.path.splitext(f)[0]
        workflow = os.path.basename(dirpath)
        xyz_path = os.path.join(dirpath, f)
        job = prep_job(name, workflow, xyz_path)
        new_jobs.append(job)
    BalsamJob.objects.bulk_create(new_jobs)
    print("Created", len(new_jobs), "new jobs in DB")
```

Populating the Database

```
def prep_job(name, workflow, xyz_path):
    return BalsamJob(name=name,
                     workflow = workflow,
                     stage_in_url = xyz_path,
                     application = 'fhi-aims',
                     ranks_per_node=64,
                     cpu_affinity='depth',
                     environ_vars="OMP_NUM_THREADS=1",
                     )
```

Submitting Jobs

- Use “submit-launch” shortcut to enqueue ~10-20 large jobs
- Each launcher job consumes as much available work as it can
- Concurrent launcher jobs work cooperatively by means of application-enforced locks acquired in the database

- Alternatively, Balsam service can manage job packing and flow into scheduler

The Launcher job template

~/.balsam/settings.json

```
"SCHEDULER_CLASS": "CobaltScheduler",
"SCHEDULER_SUBMIT_EXE": "/usr/bin/qsub",
"SCHEDULER_STATUS_EXE": "/usr/bin/qstat",
"DEFAULT_PROJECT": "datascience",
"SERVICE_PERIOD": 1,

"NUM_TRANSITION_THREADS": 5,
"MAX_CONCURRENT_MPIRUNS": 1000,

"LOG_HANDLER_LEVEL": "INFO",
"LOG_BACKUP_COUNT": 5,
"LOG_FILE_SIZE_LIMIT": 104857600,

"QUEUE_POLICY": "theta_policy.ini",
"JOB_TEMPLATE": "job-templates/theta.cobaltscheduler.tmpl"
```

The Launcher job template

```
#!/bin/bash -x
#COBALT -A {{ project }}
#COBALT -n {{ nodes }}
#COBALT -q {{ queue }}
#COBALT -t {{ time_minutes }}
#COBALT --attrs ssds=required:ssd_size=128
```

...

```
source balsamactivate {{ balsam_db_path }}
sleep 2

balsam launcher --{{ wf_filter }} --job-mode={{ job_mode }} --time-limit-minutes={{ time_minutes-2 }}

source balsamdeactivate
```

Configurable Queue Submission Policy

```
[debug-flat-quad]
submit-jobs = on
max-queued = 1
policy =  [
            {"min-nodes": 1,
             "max-nodes": 16,
             "min-time": 0,
             "max-time": 1
            }
          ]
```

Monitoring Progress

`balsam ls –by-states` :

Group by state

```
msalim@thetalogin6:/projects/CrystalsADSP/msalim> BALSAM_LS_LIMIT=2 balsam ls --by-states
```

Monitoring Progress

```
JOB_FINISHED  (573989 BalsamJobs)
                            job_id |                 name |         workflow | application |        state
-----------------------------------------------------------------------------------------------------------
7cceb07b-ea1b-4567-8dbc-6d0b4f8ba51e | gdb7-m4101-i2-c1-d67 | gdb7-m4101-i2-c1 | fhi-aims    | JOB_FINISHED
02b806d7-ddf4-42e8-9367-e6676541da55 | gdb7-m4012-i1-c6-d57 | gdb7-m4012-i1-c6 | fhi-aims    | JOB_FINISHED
(573993 more BalsamJobs not shown...)

PREPROCESSED  (72409 BalsamJobs)
                            job_id |                 name |         workflow | application |        state
-----------------------------------------------------------------------------------------------------------
91725337-6226-4302-8ddd-f97044612b1a | gdb7-m4002-i1-c6-d43 | gdb7-m4002-i1-c6 | fhi-aims    | PREPROCESSED
91827748-7550-41a4-bdb9-88ac1d2b131d | gdb7-m3492-i7-c1-d52 | gdb7-m3492-i7-c1 | fhi-aims    | PREPROCESSED
(72402 more BalsamJobs not shown...)

RESTART_READY  (5396 BalsamJobs)
                            job_id |                  name |          workflow | application |         state
-----------------------------------------------------------------------------------------------------------
2c03e5cd-2c94-4376-8c1c-5cd8abb6adbf | gdb7-m4449-i2-c7-d97  | gdb7-m4449-i2-c7  | fhi-aims    | RESTART_READY
2c0325ac-3135-424c-b332-17909e4e6c13 | gdb7-m5074-i1-c10-d70 | gdb7-m5074-i1-c10 | fhi-aims    | RESTART_READY
(5394 more BalsamJobs not shown...)

RUN_DONE  (17 BalsamJobs)
                            job_id |                 name |         workflow | application |    state
-----------------------------------------------------------------------------------------------------------
34020491-3c31-4dc2-a9a4-5aa622fc517d | gdb7-m4960-i2-c4-d75 | gdb7-m4960-i2-c4 | fhi-aims    | RUN_DONE
251ac1f1-566f-446b-9245-0a1079a701f0 | gdb7-m3695-i1-c5-d96 | gdb7-m3695-i1-c5 | fhi-aims    | RUN_DONE
(10 more BalsamJobs not shown...)

RUNNING  (797 BalsamJobs)
```

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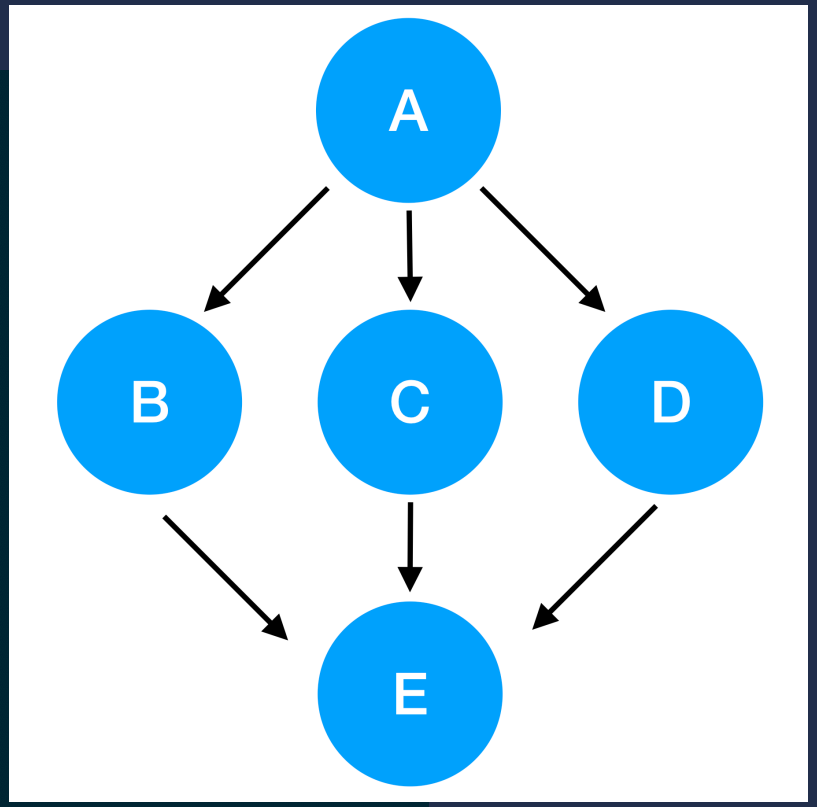
Defining Dependencies

```
from balsam.launcher.dag import (
        add_job, add_dependency)

A = add_job(name="A", application="generate")
B,C,D = [
        add_job(
            name=name,
            application="simulate",
            input_files=name+".inp"
        )
        for name in "BCD"
        ]
E = add_job(name="E", application="reduce", input_files="*.out")

for job in B,C,D:
    add_dependency(A, job)
    add_dependency(job,E)
```



Dynamic Workflows

- `balsam.launcher.dag` **enables context-aware processing**
  - `dag.current_job`

- **Attach pre/post-processing scripts to application**
  - **Inspect** `dag.current_job`
  - **Modify DB in response to workflow outcomes**

- `dag.kill(job)`
  - **terminate and replace launcher tasks in near-realtime**

Dynamic Workflows

- **In more tightly-coupled workflows, a “master” app running under Balsam may itself spawn tasks for parallel, asynchronous execution**

- `balsam.launcher.async` **facilitates programmatic polling/ processing of BalsamJobs**
    - **borrow heavily from** `concurrent.futures` **API**
    - **reduces DB polling logic in user code**

Dynamic Workflows

```
from balsam.launcher.dag import add_job
from balsam.launcher.async import wait, FutureTask
```

```
def on_done(job):
    return job.read_file_in_workdir(f'{job.name}.out')

futures = []
for i in range(10):
    j = add_job(name=f'task{i}',
                application='say-hello',
                args=f'world {i}!'
                )
    futures.append(FutureTask(j, on_done))

results = wait(futures, return_when='ANY_COMPLETED', timeout=30)
```

Overview

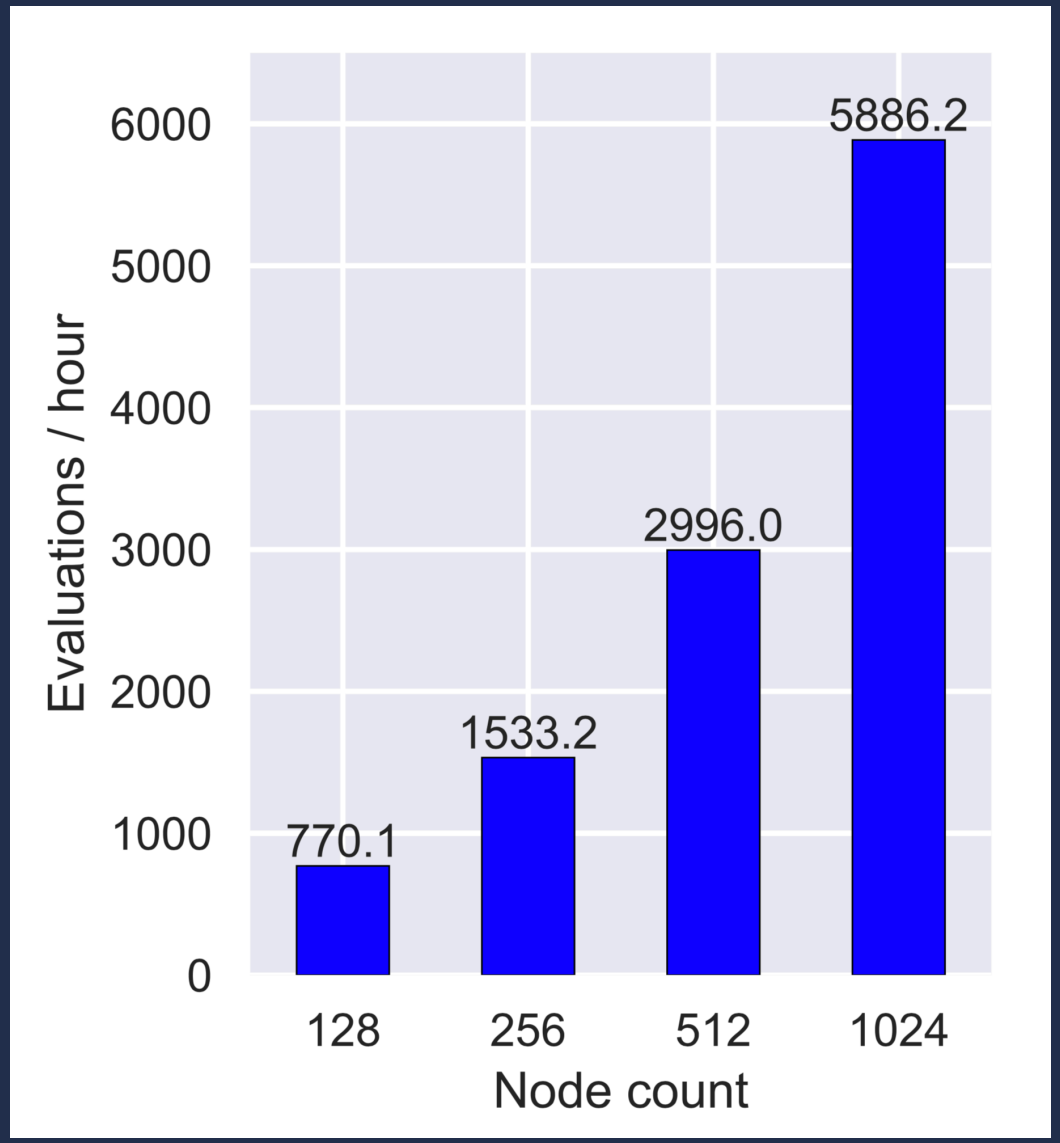
- When can Balsam be useful?
- What is Balsam?
- Starting on Theta
- Case study: managing a large campaign of simulations
- Data dependencies and dynamic workflows
- **Case study: hyperparameter optimization**

DeepHyper: Hyperparameter Optimization

- *Prasanna Balaprakash (MCS)*
- **Framework for defining hyperparameter search problems**
    - **Repository has ~20 ML benchmarks and growing…**
- **Variety of generic optimization methods**
- **Optimizers use `Evaluator` abstraction for asynchronous model training/validation with Balsam**
- **Theta release forthcoming…**

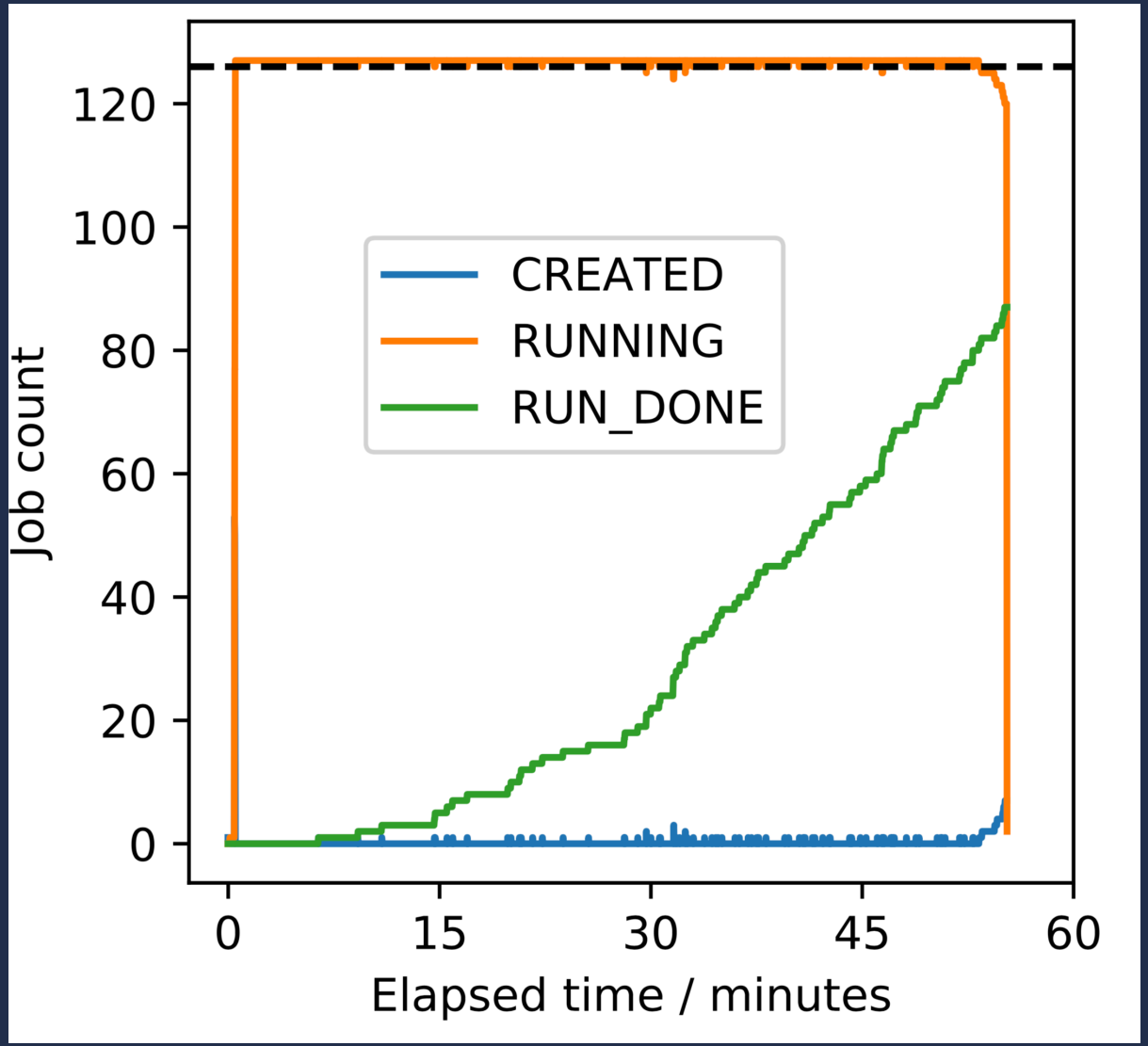
DeepHyper+Balsam: Throughput on Theta

- Random Search over 8 h.p.s
- rnn2 (question-answering) model benchmark
- **96% weak-scaling efficiency** from 128 to 1024 nodes



Utilization Profiles from Balsam

- BalsamJob metadata from a Bayesian surrogate model-based search run on 64 Cooley nodes
- Balsam provides convenience functions to parse state history and generate throughput/ utilization profiles



Summary

- Balsam is under active development and in rapidly growing use for ADSP projects and beyond
- Facilitates large campaigns of ensemble jobs, with task-level fault tolerance and persistent provenance data
- Tools for automatic scheduling and dynamic workflows facilitate complex use cases