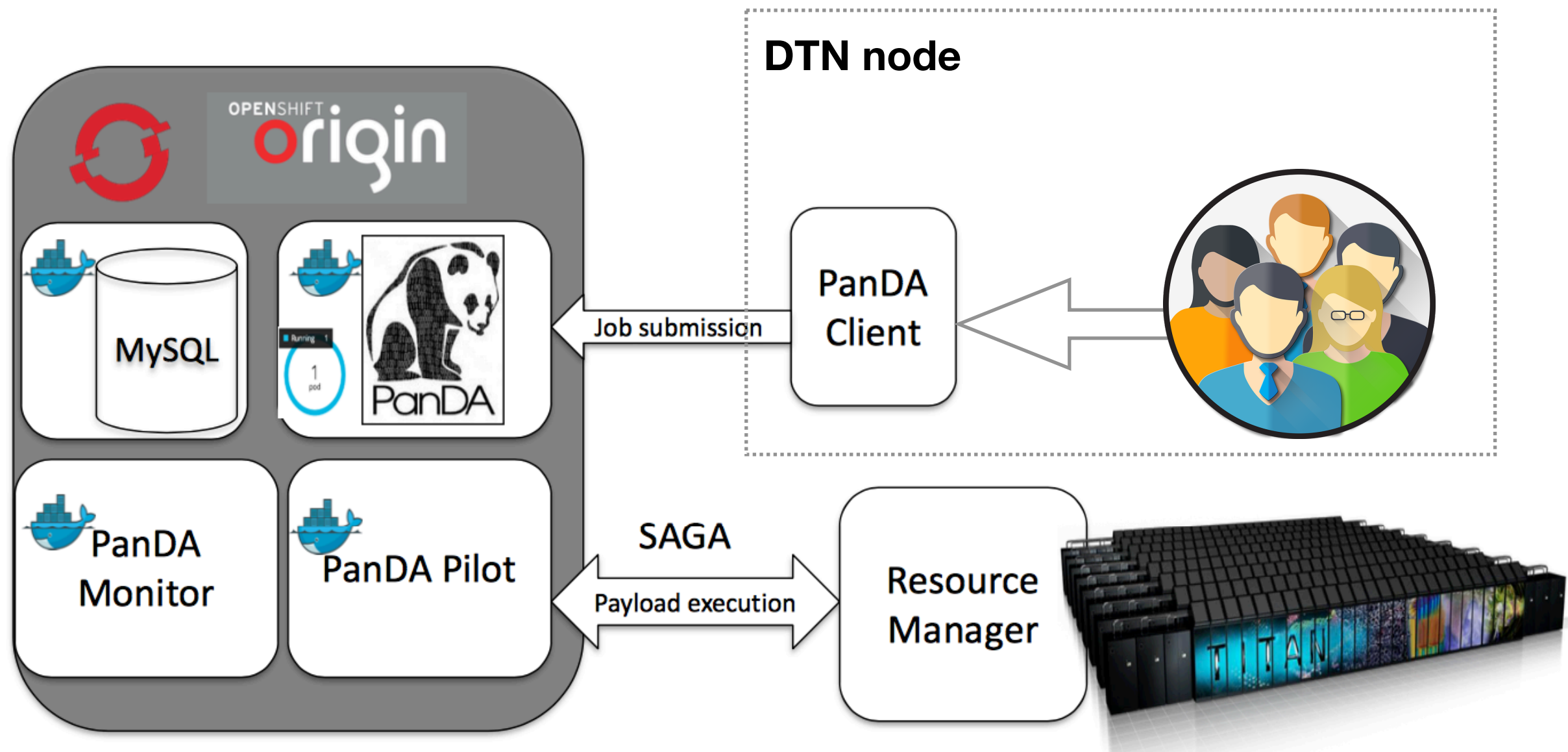


LQCD and other payloads/PanDA status update

P. Svirin, S. Panitkin

BigPaDA Technical Interchange Meeting, Arlington
February 17, 2018

PanDA infrastructure at OLCF



Original slide by: Ruslan Mashinistov

PanDA Monitor@OLCF

Job attribute summary Sort by count , alpha	
computingsite (1)	ANALY_ORNL_Titan_LQCD (2)
destinationse (1)	local (2)
eventservice (1)	ordinary (2)
jobstatus (1)	running (2)
outputfiletype (1)	? (2)
priorityrange (1)	900:999 (2)
prodsourcelabel (1)	user (2)
produsername (1)	/ST=TXRuslan Mashinistov (2)
transformation (1)	#json# (2)

Job list Sort by PandaID , time since last state change, ascending mod time , descending mod time , priority , attemptnr , ascending duration , descending duration											
PanDA ID Attempt#	Owner / VO Group	Request Task ID	Transformation	Status	Created	Time to start d:h:m:s	Duration d:h:m:s	Mod	Site	Priority	Job info
165 Attempt 0	/ST=TXRuslan Mashinistov	2	#json#	running	2017-10-11 14:45	0:0:00:33	86:8:39:50	10-11 19:51	ANALY_ORNL_Titan_LQCD	970	
	Job name: 33f01ce0-c561-49a0-b51f-f9d7f9b42a2e #0										
	Datasets: Out: panda.destDB.c23944ef-8169-4c00-b13c-e71i34ae9733										
191 Attempt 0	/ST=TXRuslan Mashinistov	2	#json#	running	2017-10-17 20:59	0:0:00:58	80:2:24:58	10-18 02:06	ANALY_ORNL_Titan_LQCD	965	
	Job name: 04a262fd-fabe-4295-88d7-8fe1e756a8e6 #0										
	Datasets: Out: panda.destDB.d0166def-1484-411c-aebc-8c872f580884										

Job submission

- Grid proxy recognized by PanDA Server was provided by Ruslan Mashinistov in order to submit LQCD jobs
- A dedicated pilot launcher was installed
 - in order to make this process easier in the future we created a scripted installer
- Job submission and execution succeeded

PanDA Monitor@OLCF

monitor-bigpanda.apps.ccs.ornl.gov/job?pandaid=164									
PanDA Dash Tasks Jobs Errors Users Sites Incidents Search Admin VO Help									
Job details for PanDA job 164 monitor-4-zbgk3 Built 17:30, cache 3' Actual version									
PandaID Attempt#	Owner	Request Task ID	Status	Created	Time to start d:h:m:s	Duration d:h:m:s	Modified	Site	Priority
164 Attempt 10	/ST=TXRuslan Mashinistov	2	finished	2017-10-10 23:11	0:0:01:31	0:1:28:22	10-11 00:44	ANALY_ORNL_Titan_LQCD	970
Job name: b2caad75-00d0-4ada-9eba-e4ffde7fc604 transformation: #json#									
Datasets: Out: panda.destDB.c7939fdb-0fb1-4a83-b1fe-e88f0c36839a									
Dataset summary: log: 1									

This is attempt number 10 for this job. To see a history of job attempts click on the job name above.

Show script to re-create job for offline debugging: 164

Job information	job stdoutoutputs	payload stdout	job cache tarball	pilot records	JEDI action logger	child jobs
-----------------	-------------------	----------------	-------------------	---------------	--------------------	------------

1 job files					
Filename (Type)	Scope	Size (MB)	Status	Attempt (max)	Dataset
b2caad75-00d0-4ada-9eba-e4ffde7fc604.job.log.tgz (log)	None	0	ready		panda.destDB.c7939fdb-0fb1-4a83-b1fe-e88f0c36839a (destination block: panda.destDB.c7939fdb-0fb1-4a83-b1fe-e88f0c36839a rucio)

Other key job parameters	
Last state change	to finished at 2017-10-11 00:44
Attempt number	10 of a maximum 2
Output destination	local
Job parameters	{ "nodes": 10, "command": "ncd /lustre/atlas1/nph109/proj-shared/forPSV\nnecho \"-----\nnecho \\\nStart job: `date`\nnecho \"-----\nnecho \\\naprun -n 10 -N 1 ./wrapper\nnaprun -n 10 -N 1 ./wrapper\nnecho \"-----\nnecho \\\nEnd job: `date`\nnecho \"-----\n\n", "name": "lqcd-test", "walltime": "02:00:00" }
Pilot ID	xtestP001 PR PICARD 59aRC2 (Titan)

Sequential jobs

- A simple workflow management system was developed only by means of PanDA Server (Adder/Setuppper modules), no extension to database has been done
- Tested on EC2 instance as well as at OLCF instance
- Can be reused for other experiments

Sequential jobs, workflow representation in command line

```
[psvirin@54 LQCD]$ python sequential-test.py
+----+      +----+      +----+      +----+
|  A  | --> |  C  | --> |  D  | <-- |  E  |
+----+      +----+      +----+      +----+
              ^
              |
              |
          +----+
          |  B  |
          +----+

Now submitting.....
```

- all jobs from the workflow set are submitted at the same time, then labels are turned into real PanDA jobid numbers

Sequential jobs, workflow representation in Monitor

PandaID Attempt#	Owner / VO	Request Task ID	Status	Created
426 Attempt 10	/ST=TXRuslan Mashinistov / lqcd	10	defined	2018-01-05 23:25

transformation	#json#
vo	lqcd
cmtconfig	{"prev": [424, 425], "name": "C", "next": 427}
computingsite	ANALY_ORNL_Titan_LQCD

Job parameters	<pre>{ "nodes": 1, "command": "\nncd /lustre/atlas1/nph109/proj-shared/forPSV\n\nnecho \"-----\n\nnecho \"Start job: `date`\n\nnecho \n\n-----\n\nnaprun -n 10 date\nnecho \"-----\n\nnecho \"End job: `date`\n\nnecho \n\n-----\n\n\", \"name\": \"lqcd-test\", \"walltime\": \"00:10:00\"} }</pre>
-----------------------	--

- if job has one or more predecessors it stays in “defined” state until all of them finish successfully

A simpler job description

- we introduced job description in Yet Another Markup Language (YAML)
- a simple Bash syntax check feature is also available for command description

```
seqname: Test_Seq_LQCD

jobs:
  JOB1:
    walltime: "20:00:00"
    nodes: "8000"
    command: |+
      export PMI_NO_FORK=1
      export CRAY_CUDA_MPS=1

      cd $PBS_O_WORKDIR

      conf_num=0

      for i in {0..31}; do
        aprun -n 12 -N 1 ./wrapper1.sh \
          $((i*12+conf_num*396)) &
        sleep 2s
      done

  JOB2:
    ...
```

Sequential jobs description

- it is also possible to specify a list of jobs, which have to be executed in a necessary order

```
seqname: Test_Seq_LQCD
```

```
jobs:
```

```
  A:
```

```
    ...
```

```
  B:
```

```
    ...
```

```
  C:
```

```
    ...
```

```
  D:
```

```
    ...
```

```
  E:
```

```
    ...
```

```
sequence:
```

```
  A: B
```

```
  C: B
```

```
  B: D
```

```
  E: D
```

Sequential jobs description

- problem: job B will never start as it depends on job D which is a successor of job B
- cycle detection feature will be introduced (a simple Depth-first search algorithm)

```
seqname: Test_Seq_LQCD
```

```
jobs:
```

```
...
```

```
sequence:
```

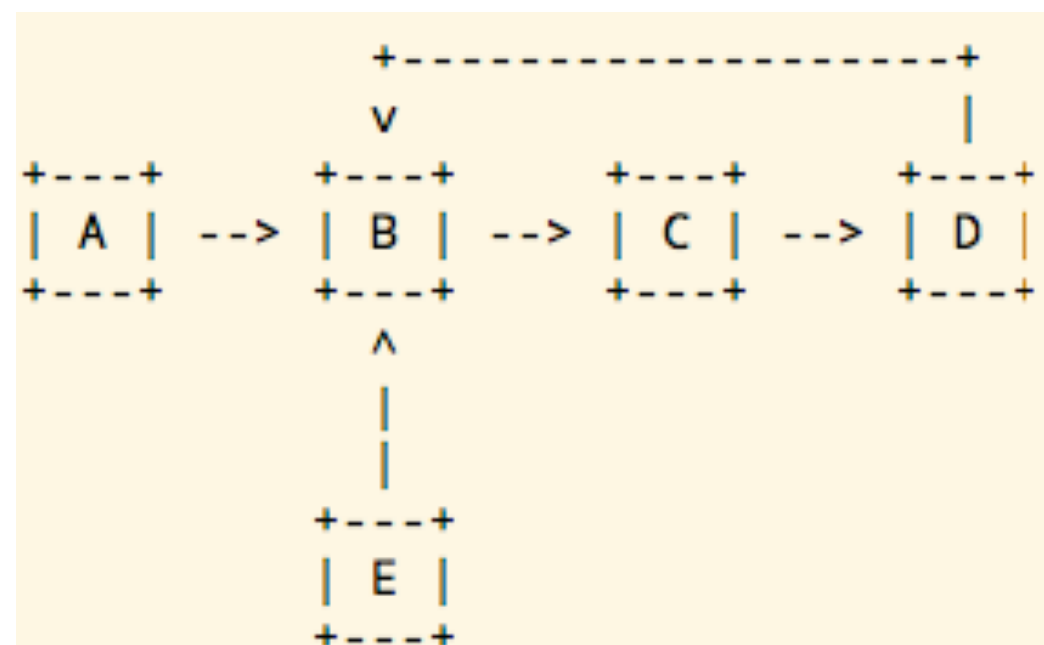
```
A: B
```

```
B: C
```

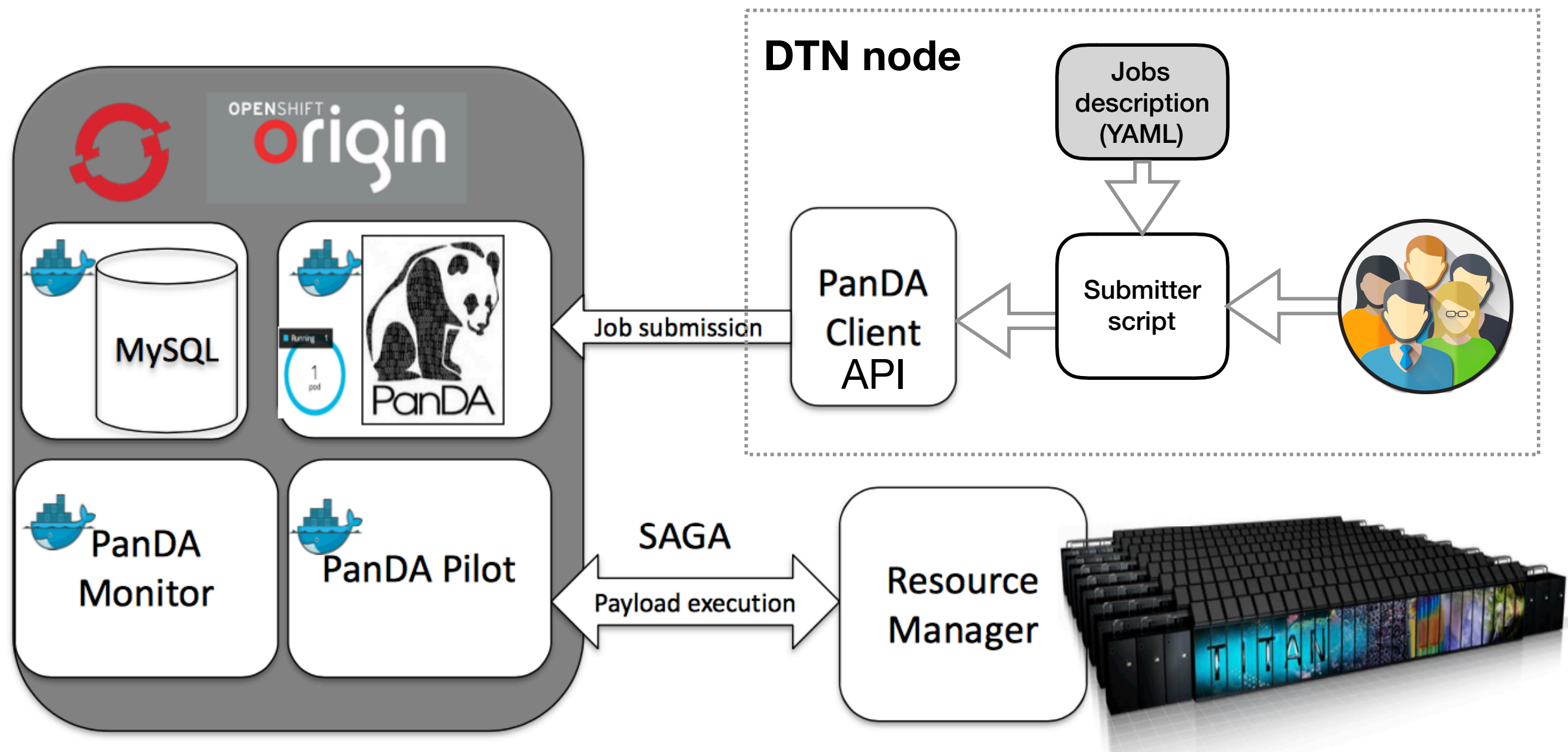
```
C: D
```

```
E: B
```

```
D: E
```



PanDA infrastructure at OLCF

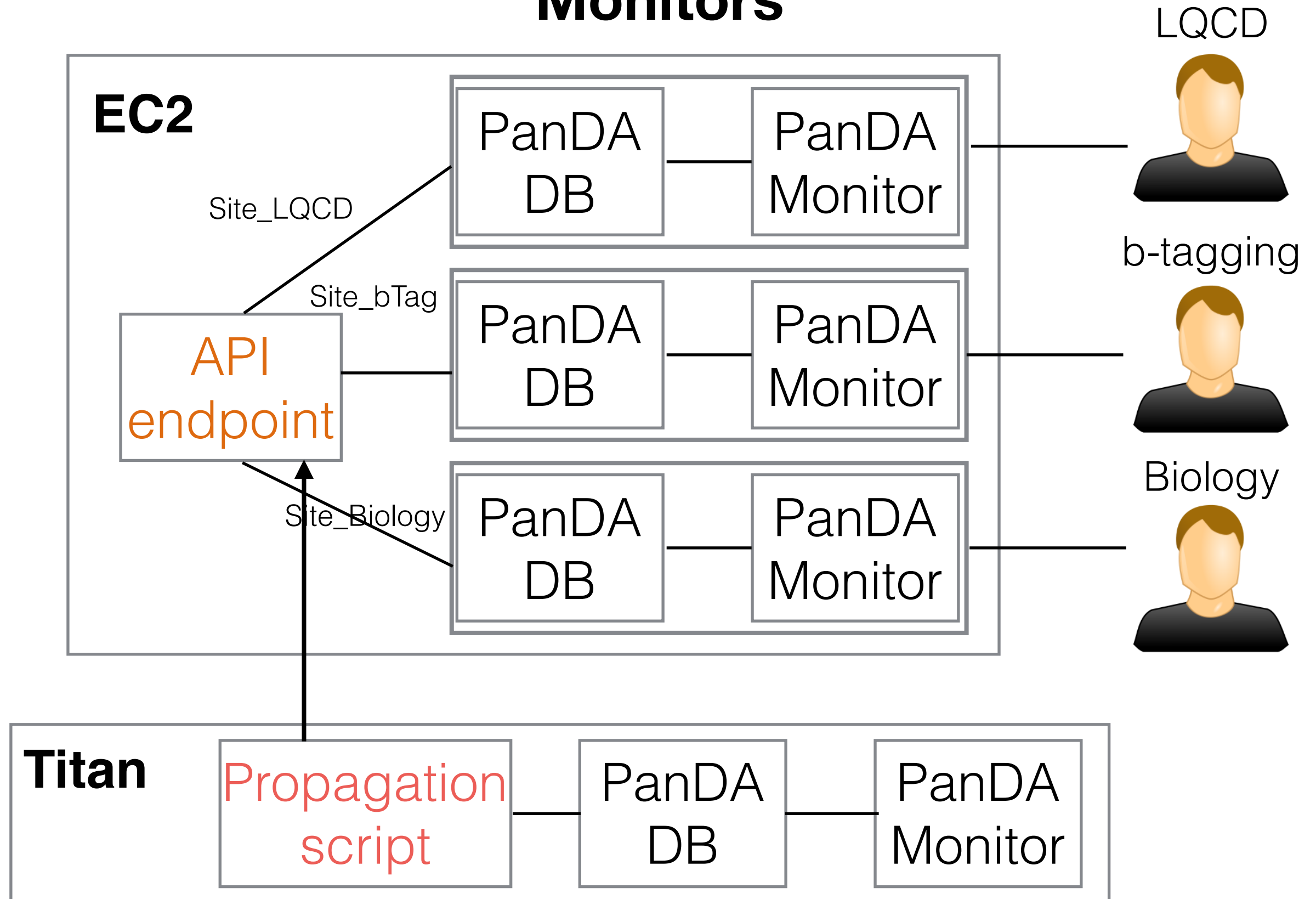


Original slide by: Ruslan Mashinistov

Open questions and suggestions

- Notifications on job start/end?
- Could it be possible to introduce a feature to modify job before it starts?
- Right now LQCD team can use only self-signed certificates to submit jobs
- We will need different certificates/proxies for different experiments, right now it is possible to submit to any site defined at OLCF PanDA instance
- Make pretty output for client tools; now in case of error cURL error code is shown

Job information propagation to external Monitors



Closest events and plans

- Meetings:
 - Meeting with people from Thomas Jefferson Lab
 - Meeting with BNL LQCD team - we will have one next week
- New candidates for LQCD computing infrastructure
 - TJLab cluster
 - GPU cluster at BNL

Other payloads

- nEDM:
 - pilot launcher ready on Titan
 - queue created in PanDA instance @OLCF
 - job submission and execution succeeded
 - nEDM team was informed about the status and we asked about the possible time frame for data challenge
- ATLAS b-tagging:
 - expect more news from them in spring 2018

Summary

- Queue in OLCF PanDA instance created
- Realistic LQCD jobs can be submitted and run through PanDA instance@OLCF
- Sequential jobs submission tested and executing in correct order, all of the necessary modules to run LQCD jobs were installed and tested
- Improvements to user interface have been done to provide an easier job definition to users