BLUE WATERS

SUSTAINED PETASCALE COMPUTING

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Installation, Configuration and Performance Tuning of Shifter V16 on Blue Waters

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GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

Outline

- Background and Challenges
- Installation
- Configuration
- Integration with Workload Manager
- Scaling Performance
- Operational Issues

Background

- Shifter enables execution of container-based applications on HPC systems.
- Shifter Version 1.0 was deployed on Blue Waters since 2016.
- Limited scaling capability of Shifter V1.
- 2016 version (V16) is made available through CLE release 6.0 (but not available to Blue Waters).
- Security concerns and demand for better scalability prompted a need for upgrade on Blue Waters.

Challenges

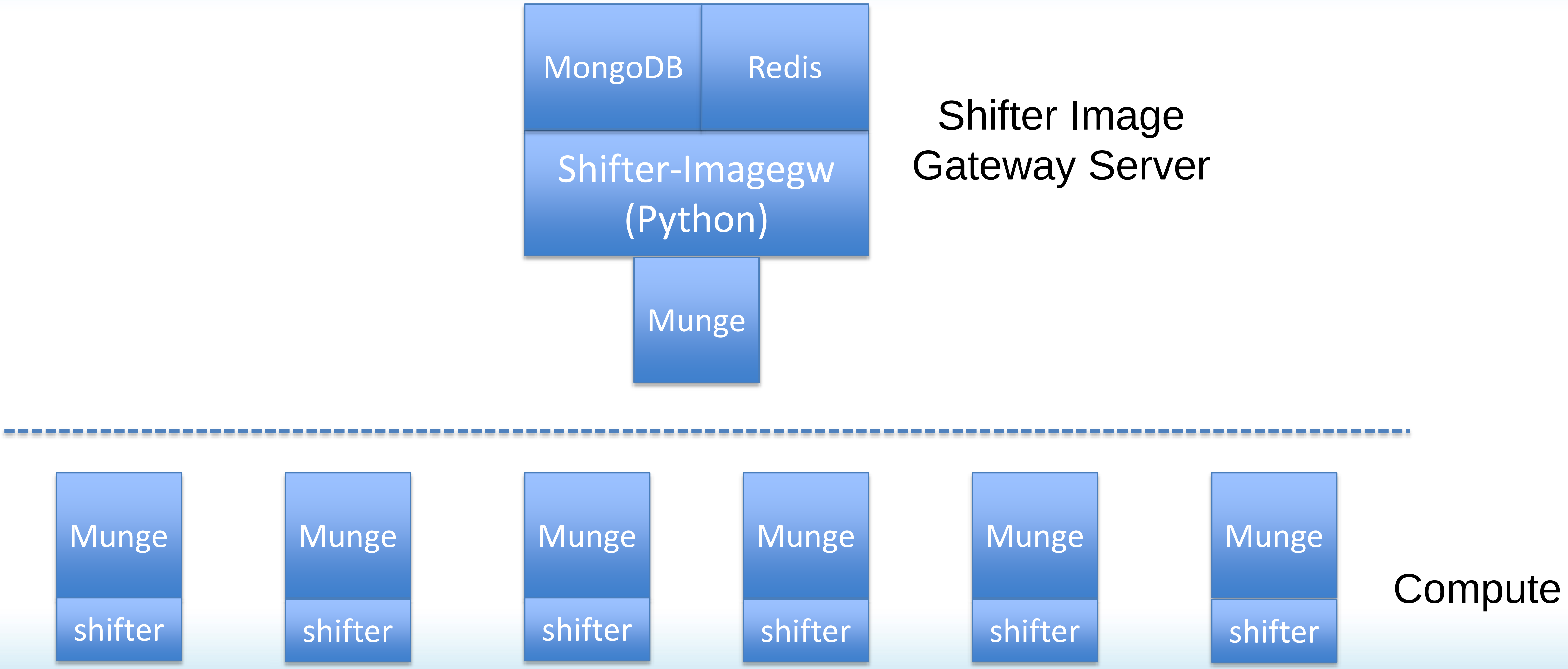
- Official installation procedure provided by Cray is not designed for CLE 5.2.
- Ongoing integration and testing on boot image require tedious and time consuming efforts.
- “It ain’t broken, don’t fix it” rules of thumb for a five-year-old seasoned system.

Strategy

- Implemented Shifter on `/dsl`.
- Faster turnaround time in testing and troubleshooting.
- Installed and conducted functional tests on Test and Development System (TDS), then replicated the installation procedure on Blue Waters.
- Installation on `/dsl` provides agility for performance tuning on Blue Waters.

Shifter V16 Software Stack

- Shifter 16.08.3
- Squashfs Linux kernel modules
- MongoDB 3.4.7
- Redis 3.2.8
- Python 2.7.13
- Python modules: Celery, PyMongo, Flask, redis, gunicorn
- Munge


MongoDB
Redis
Shifter-Imagegw (Python)
Munge
Shifter Image Gateway Server
Munge
shifter
Munge
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Compute

Installation

- All installations are done in /dsl through xtopview utility on the boot node.

```
boot: ~# xtopview
default/:/ #
```

- Dependencies: *fdupes*, *json*, *squashfs*. Only needed for building the RPM packages of Shifter, not required for Shifter installation.
- Compilation of Shifter software also requires newer version of *Autoconf* and *Automake* tools.

Installation of Shifter 16.08.3

- The Shifter source distribution was cloned from NERSC's *github* repository.

```
# git clone https://github.com/NERSC/shifter.git shifter-16.08.3
```

- At the time when we cloned the repository, the source distribution came with GPU support, but it is now removed from the master branch.
- Source modification: Added user definable `MountCmd` parameter into `UdiRootConfig.h`, `UdiRootConfig.c` and `shifter_core.c` source files. This parameter is configurable in `UdiRoot.conf`.
- Linux kernel module lookup path: `kmodBasePath + `uname -r` + kernel`

Installation of Shifter 16.08.3

- RPM spec files:
  a) Shifter binaries
  b) Linux kernel modules: `squashfs.ko`, `loop.ko`
- Added “Prefix” macro to the spec files, to make installation of the binaries relocatable.
- We modified the given sample spec file (initially written for CLE6) to build Linux kernel modules for CLE5.

Installation of Shifter 16.08.3

- Build procedure - Shifter RPM packages:

```
# pwd
/software/shifter-16.08.3
# ./autogen.sh
# cd ..
# tar czvf shifter-16.08.3.tar.gz shifter-16.08.3
# cp shifter-16.08.3.tar.gz /usr/src/packages/SOURCES
# cd shifter-16.08.3
# rpmbuild -ba shifter.spec
```

- Build procedure - Linux kernel modules:

```
# cd extra
# rpmbuild -bb shifter_cle5_gem-c_kmod.spec
```

Installation of Shifter 16.08.3

```
# cd /usr/src/packages/RPMS/x86_64
# rpm -ivh --prefix=/opt/cray/shifter/16.08.3 \
shifter_cle5_kmod_deps-cray_gem_c-1.0-3.x86_64.rpm

# rpm -ivh --prefix=/opt/cray/shifter/16.08.3 \
shifter-16.08.3-1.nersc.x86_64.rpm

# rpm -ivh --relocate /usr=/opt/cray/shifter/16.08.3 \
shifter-imagegw-16.08.3-1.nersc.x86_64.rpm

# rpm -ivh --prefix /opt/cray/shifter/16.08.3 \
shifter-runtime-16.08.3-1.nersc.x86_64.rpm
```

Installation of MongoDB

- Download RPM packages from *https://repo.mongodb.org*.
- Import MongoDB PGP key.

```
# wget --no-check-certificate \
https://www.mongodb.org/static/pgp/server-3.4.asc
# rpm --import server-3.4.asc
```

- Install procedure:

```
# rpm -ivh --prefix=/opt/mongodb/3.4.7 \
mongodb-org-3.4.7-1.suse11.x86_64.rpm \
mongodb-org-server-3.4.7-1.suse11.x86_64.rpm \
mongodb-org-shell-3.4.7-1.suse11.x86_64.rpm \
mongodb-org-mongos-3.4.7-1.suse11.x86_64.rpm \
mongodb-org-tools-3.4.7-1.suse11.x86_64.rpm
```

Installation of Redis

- Download and extract source package from http://download.redis.io.
- Install procedure:

```
# export CC=gcc
# make PREFIX=/opt/redis/3.2.8 install
```

Installation of Python modules

- Installation of Python modules using *pip* tool in a *virtualenv* isolated Python environment.
- *PyPI* enforces SSL enabled client connections (TLSv1.2 is mandatory now).
- Python with SSL support is required.

```
# virtualenv.py /opt/cray/shifter/16.08.3/imagegw_venv \
  --python=/opt/python/2.7.13/bin/python

# source /opt/cray/shifter/16.08.3/imagegw_venv/bin/activate

(imagage_venv) # pip install \
                 -r /opt/cray/shifter/16.08.3/share/shifter/requirements
```

Munge

- Munge is provided by cray-munge RPM package.
- The PRM package provides a `/etc/munge.key` file.
- All compute nodes and the Shifter image manager gateway node use the same key for authentication.

Post Installation

- After exiting from `xtopview`, copy files to Shifter service node persistent `/var` space.

```
# cd /rr/current/var/lib
# cp -Rp mongo /snv/<nid_id>/var/lib
# cd ../log
# cp -Rp mongodb shifter_imagegw* /snv/<nid_id>/var/log
# cd ../run
# cp -Rp mongodb /snv/<nid_id>/var/run
```

Configuration

- Shifter image manager gateway: `imagemanager.json`
- Shifter runtime: `udiRoot.conf`
- Redis: `redis.conf`
- MongoDB: `mongod.conf`
- Service init scripts: `munge, mongod, redisd, shifter-imagegw`

Redis

- `/etc/shifter/redis.conf`

```
dir /var/lib/redis
requirepass P@55w0rd
```

- `/etc/init.d/redisd` is written to read from `/etc/shifter/redis.conf` file.
- Set permission of files to be accessible only by root user.

```
# chown root: /etc/shifter/redis.conf
# chmod 640 /etc/shifter/redis.conf
# chown root: /etc/init.d/redisd
# chmod 750 /etc/shifter/redisd
```

MongoDB

- Listen to localhost only (set in `/etc/mongod.conf`).

```
net:
  port: 27017
  bindIp: 127.0.0.1
```

- Create admin user.

```
# mongo
> use admin
> > db.createUser(
... {
... user: "mongodbadmin",
... pwd: "<P@55w0rd>",
... roles: [ { role: "root", db: "admin" } ]
... }
... )
```

MongoDB

- Restart MongoDB with `--auth` option in init script (`/etc/init.d/mongod`).

```
CONFIGFILE="/etc/mongod.conf"
OPTIONS=" -f $CONFIGFILE --auth "
```

- Create Shifter DB owner.

```
# mongo admin -u mongodbadmin -p
> use Shifter
switched to db Shifter
> db.createUser(
... {
... user: "shifteradmin",
... pwd: "<P@55w0rd>",
... roles: [ { role: "dbOwner", db: "Shifter" } ]
... }
... )
```

Shifter Image Manager Gateway Init Script

- `/etc/init.d/shifter-imagegw`

```
command=/opt/cray/shifter/16.08.3/sbin/shifter-imagegw
start() {
  lockfile -r 0 $lockfile || \
  { echo shifter-imagegw service is already running. && exit -1; }
  echo -n "Starting ${util}: "
  ulimit -S -n 8192; ulimit -H -n 16384
  startproc -u shifter ${command} >> /var/log/${util}.log 2>&1
  pidofproc $command > $PIDFILE 2>/dev/null
  rc_status -v
}
```

- /opt/cray/shifter/16.08.3/sbin/shifter-imagegw

```
#!/bin/bash
ROOT_TREE='/opt/cray/shifter/16.08.3'
PYTHON_VENV='imagegw_venv'
SHIFTER_SYSTEM_NAME='bluewaters'
QA="${SHIFTER_SYSTEM_NAME}"
cd ${ROOT_TREE}
source ${PYTHON_VENV}/bin/activate
echo "Starting Celery Queue $QA"
celery -A shifter_imagegw.imageworker worker -Q $QA --loglevel=WARNING –n \
    worker.queue.$QA -E --concurrency=24 &
echo "Starting imagegw API"
python lib64/shifter/imagegwapi.py &
python lib64/shifter/imagegwapi1.py &
python lib64/shifter/imagegwapi2.py &
wait
```

Shifter Image Manager

- `/etc/shifter/imagemanager.json`

```
"MongoDBURI":"mongodb://shifteradmin:<P@55w0rd>@
              localhost/Shifter?authMechanism=SCRAM-SHA-1",
"MongoDB":"Shifter",
"Broker":"redis://:<P@55w0rd>@localhost/",
```

- Owned by “shifter” user. Accessible by “shifter” and root user only.
- Specialized to utility class service nodes.

Shifter Runtime

- `/etc/shifter/udiRoot.conf`

```
udiMount=/var/udiMount
loopMount=/var/udiLoopMount
udiRootPath=/opt/cray/shifter/16.08.3
sitePreHookMount=/opt/cray/shifter/16.08.3/sbin/premount.sh
mountCmd=/opt/cray/shifter/16.08.3/lib64/shifter/mount
kmodBasePath=/opt/cray/shifter/16.08.3/modules
imageGateway=http://shifter:5000 http://shifter:5001 http://shifter:5002
siteResources=/opt/shifter/site-resources
allowLibcPwdCalls=1
```

- sitePreHookMount=/opt/cray/shifter/16.08.3/sbin/premount.sh

```
#!/bin/bash
mkdir -p mnt/a
mkdir -p mnt/b
mkdir –p mnt/c

mount --bind /mnt/a mnt/a
mount --bind /mnt/b mnt/b
mount --bind /mnt/c mnt/c

mkdir -p ufs
mount --bind /ufs ufs

mkdir -p var/opt/cray/alps
mount --bind /var/opt/cray/alps var/opt/cray/alps

mkdir -p dsl/opt
mount --bind /dsl/opt dsl/opt
```

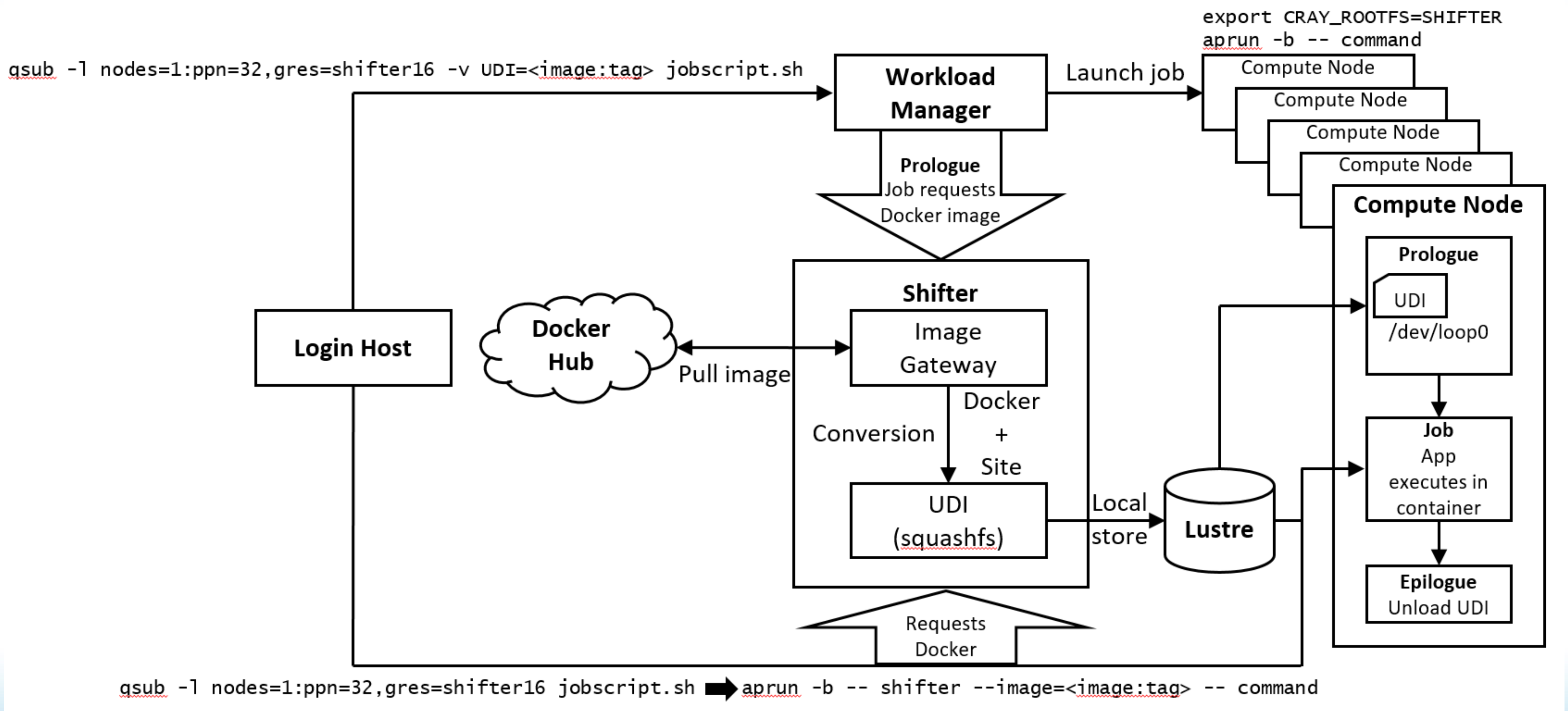
```
ln -s mnt/a/u u
ln -s mnt/b/projects projects
ln -s mnt/c/scratch scratch
```

Services

- Start services

```
# service munge start
# service mongod start
# service redisd start
# service shifter-imagegw start
```

Integration with Moab/Torque



Shifter Job Submission

- Invoking "`shifter`" command in job script.

```
$ cat jobscript.sh
#!/bin/bash
#PBS -l nodes=1:ppn=32
#PBS -l gres=shifter16

cd $PBS_O_WORKDIR
module load shifter/16.08.3

aprun -n 1 -b -- shifterimg pull <image:tag>
aprun -n 1 -b -- shifter --image=<image:tag> -- command

$ qsub jobscript.sh
```

Shifter Job Submission

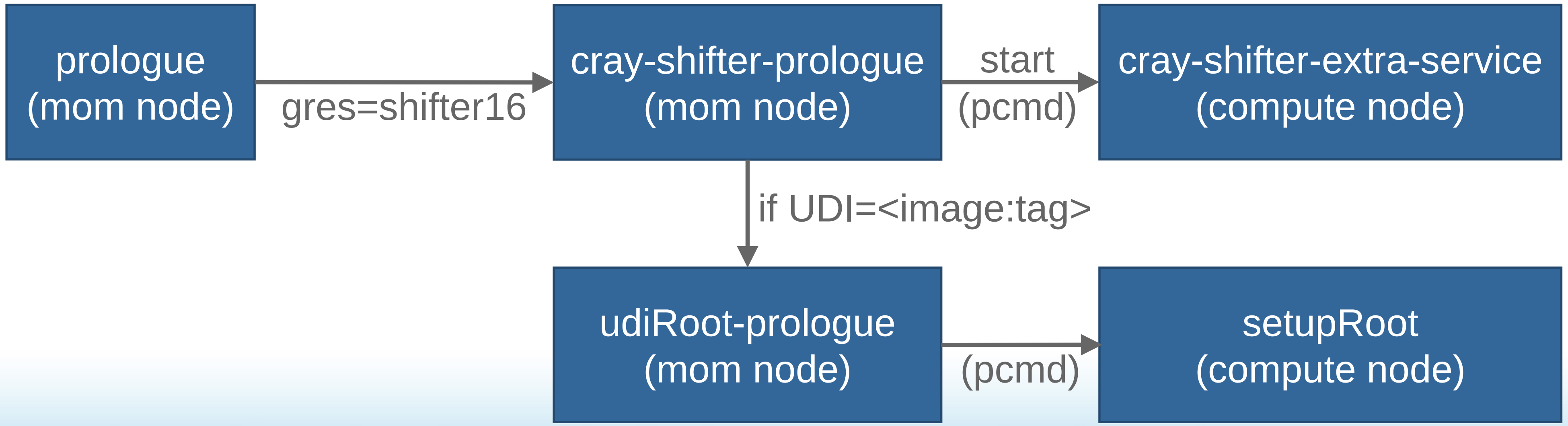
- Invoking "`setupRoot`" command through Torque prologue script.

```
$ cat jobscript.sh
#!/bin/bash
#PBS -l nodes=1:ppn=32
#PBS -l gres=shifter16
#PBS -v UDI=<image:tag>

cd $PBS_O_WORKDIR

export CRAY_ROOTFS=SHIFTER

aprun -n 1 -b -- command

$ qsub jobscript.sh
```

Prologue

- /var/spool/torque/mom_priv/prologue

```
if [ $(qstat -f ${BATCH_JOB_ID} | grep Resource_List.gres | grep -c \
'\bshifter16\b') -gt 0 ];then
    shifter_prologue=/opt/cray/shifter/16.08.3/wlm/torque/cray-shifter-prologue
    if [[ -x $shifter_prologue ]]; then
        $shifter_prologue ${BATCH_JOB_ID} $USER $GROUP ${RESV_ID} ${NIDS}
    fi
fi
```



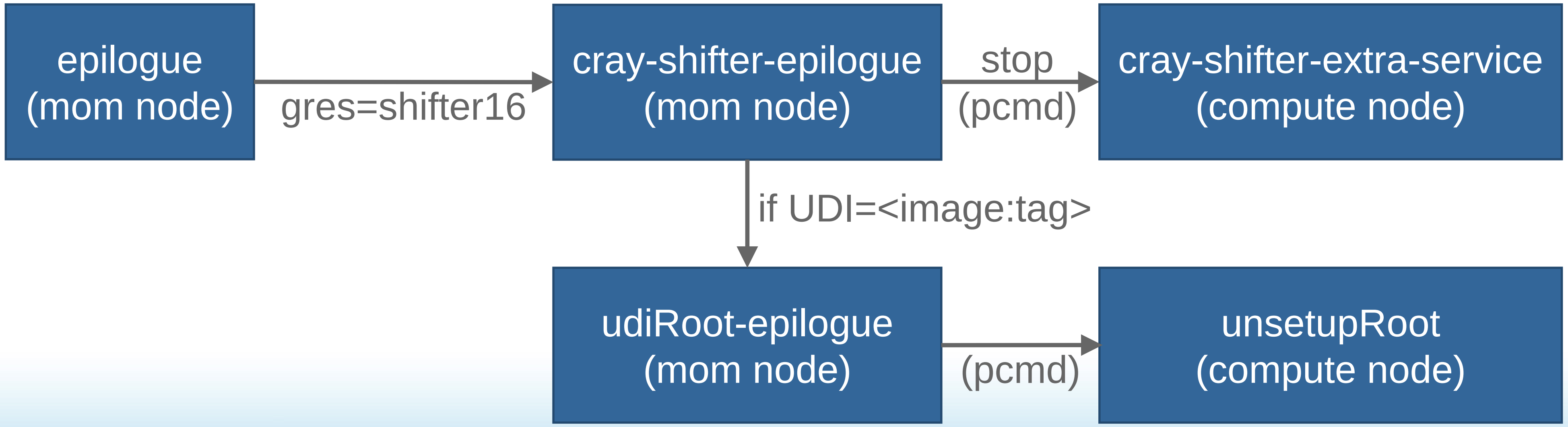
cray-shifter-prologue

- Start munge and nscd services on compute nodes (invoking `cray-shifter-extra-service start`)
- If UDI is defined in job submission, execute `setupRoot` on compute nodes to mount UDI (invoking `udiRoot-prologue`).

Epilogue

- /var/spool/torque/mom_priv/epilogue

```
if [ $(qstat -f ${BATCH_JOB_ID} | grep Resource_List.gres | grep -c \
'\bshifter16\b') -gt 0 ];then
    shifter_epilogue=/opt/cray/shifter/16.08.3/wlm/torque/cray-shifter-epilogue
    if [[ -x $shifter_epilogue ]]; then
        $shifter_epilogue ${BATCH_JOB_ID} $USER $GROUP ${RESV_ID} ${NIDS}
    fi
fi
```



cray-shifter-epilogue

- Stop munge and nscd services on compute nodes (invoking `cray-shifter-extra-service stop`)
- If UDI is defined in job submission, execute `unsetupRoot` on compute nodes to un-mount UDI (invoking `udiRoot-epilogue`).

Compute Node Root Runtime Environment (CNRTE)

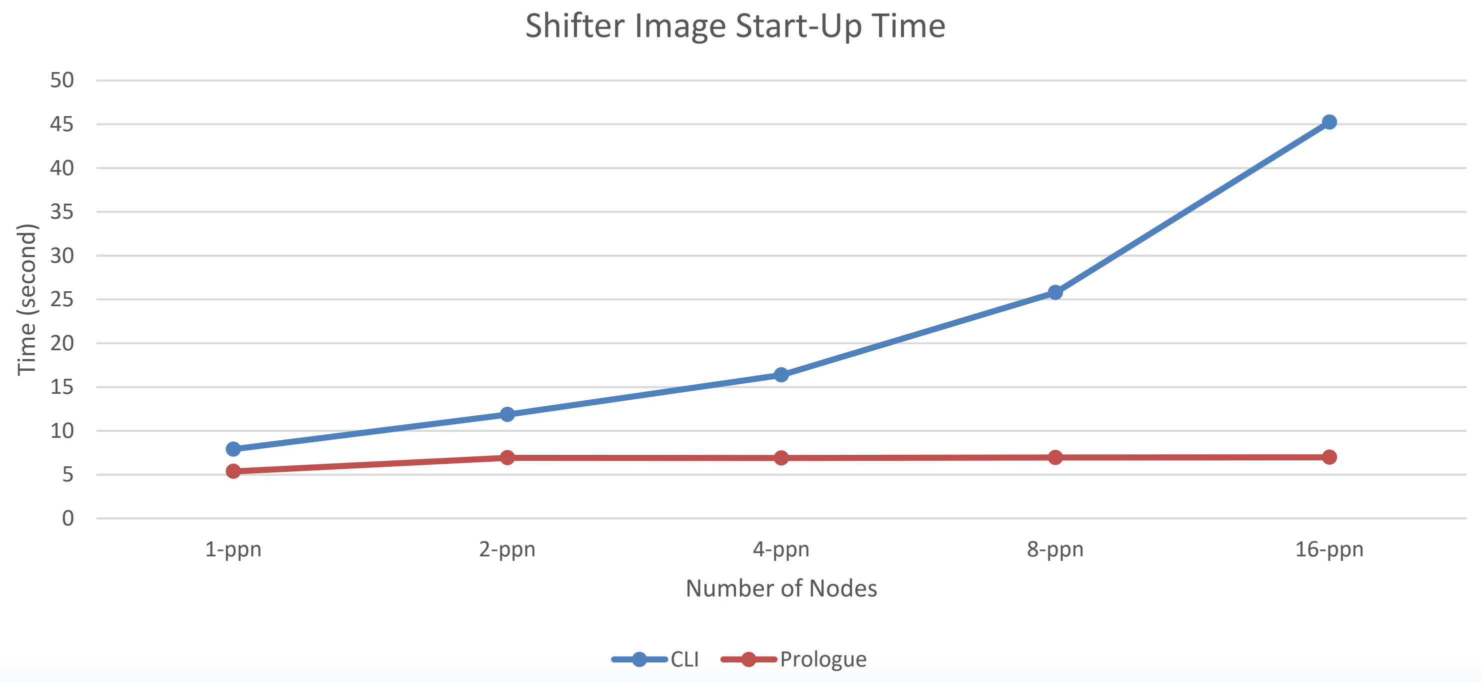
- Shifter is installed in `/dsl` and executes from `/dsl`.
- In `udiRoot.conf`, `udiMount=/var/udiMount`
- Absolute root path as seen from compute node => `/dsl/var/udiMount`
- `/etc/opt/cray/cnrte/roots.conf`

```
    SHIFTER=/dsl/var/udiMount
```

- When using `setupRoot` in job prologue and setting `CRAY_ROOTFS=SHIFTER` in job script, alps tasks land on `/dsl/var/udiMount`.

shifter vs. setupRoot (80 nodes)

```
aprun -n 1280 -N 16 -- shifter --image=centos:latest -- cat /etc/centos-release
aprun -n 1280 -N 16 -- cat /etc/centos-release
```



Initial Scaling Test Results - shifter

```
$ qsub -l nodes=4096:ppn=16,gres=shifter16

> aprun -n 4096 -N 1 -b -- shifter --image=centos:latest -- cat /etc/centos-release
```

- 2000+ nodes success.
  - `FAILED to lookup docker image`
  - `Failed to lookup username or attempted to run as root`

Initial Scaling Test Results - setupRoot

```
$ qsub -l nodes=2048:ppn=16,gres=shifter16 -v UDI=centos:latest,CRAY_ROOTFS=SHIFTER

> aprun -n 2048 -N 1 -b -- cat /etc/centos-release
```

- 700+ nodes success.
  - `FAILED to get groups correctly`
  - `FAILED to lookup auxiliary gids. Exiting`

Username, groups, gids related issues

- Scalability issue with LDAP.
- Too many query requests to LDAP server.
- Workarounds:
  - Start NSCD service on compute nodes => random caching
  - Perform “`id $USER`” on compute nodes => taking too long

Resolution

i. Perform “`id $USER`” on mom node.
ii. Copy `/var/run/nscd/passwd` and `/var/run/nscd/group` files from the mom node to a cluster shared location.

`shifter-cray-prologue`

```
id $USER
cp /var/nscd/run/passwd /scratch/system/shifter/jobs/passwd.$JOBID
cp /var/nscd/run/group /scratch/system/shifter/jobs/group.$JOBID
pcmd -r -q -n $NIDS "/dsl/usr/bin/chroot /dsl cray-shifter-extra-service start $JOBID"
```

iii. On each compute node, copy nscd passwd and group files from cluster shared location to local `/var/run/nscd` directory.

iv. Start nscd service on compute node.

```
cray-shifter-extra-service start $JOBID
```

```
cp /scratch/system/shifter/jobs/passwd.$JOBID /var/run/nscd
cp /scratch/system/shifter/jobs/group.$JOBID /var/run/nscd
/etc/init.d/nscd start
```

Failed to lookup docker image

- Too many query requests sent to Shifter image manager gateway.
- Six *celery* threads were started by default.
- imagegwapi.py listen to port 5000.

shifter-imagegw

```
celery -A shifter_imagegw.imageworker worker -Q $QA -n worker.queue.$QA &
python imagegwapi.py
```

Workarounds

- Increase number of threads to 24.
- Duplicate `imagegwapi.py`, listing to port 5000, 5001 and 5002.

`shifter-imagegw`

```
celery -A shifter_imagegw.imageworker worker -Q $QA -n worker.queue.$QA -E \
    concurrency=24 &
python imagegwapi.py &
Python imagegwapi1.py &
python imagegwapi2.py &
```

Improved Scaling Performance

- 4096 nodes using `shifter` CLI.
- 2048 nodes using `setupRoot` through job prologue.
- `setupRoot` is limited to 2048 nodes due to prologue timeout duration set at 300 seconds.

aprun -N >1

```
$ qsub -l nodes=256:ppn=16,gres=shifter16

> aprun -n 4096 -N 16 -b -- shifter --image=centos:latest -- cat /etc/centos-release
```

- Preload `loop.ko` and `squashfs.ko` in job prologue.
- Set `max_loop=128`

`cray-shifter-extra-service start $JOBID`

```
/sbin/insmod $KMODPATH/drivers/block/loop.ko max_loop=128
/sbin/insmod $KMODPATH/fs/squashfs/squashfs.ko
```

Encoding and Decoding Issues

${SHIFTER_ROOT_DIR}/lib64/python2.6/site-packages/sitecustomize.py

```
import sys
reload(sys)
sys.setdefaultencoding('utf8')
```

${SHIFTER_ROOT_DIR}/lib64/python2.6/site-packages/shifter_imagegw/dockerv2.py

```
@@ -625,6 +625,9 @@
     tfp = tar_file_refs[layer_idx]
     members = layer_paths[layer_idx]
+
+    # Change encoding to 'utf8' to take care of unicode character in file paths.
+    base_path = base_path.encode('utf8')
     tfp.extractall(path=base_path, members=members)
```

Untracked process in SSH session

```
user@mom:~> cat .shifter/config
Host *
Port 1204
IdentityFile ~/.shifter/id_rsa
StrictHostKeyChecking no
UserKnownHostsFile /dev/null
LogLevel error

user@mom:~> ssh -F .shifter/config nidxxxxx
```

- Background/daemon processes are left running on compute nodes even after job ends.
- An epilogue script is written to cleanup these stray processes

/etc/shifter/shifter_etc_files

- Files under `/etc/shifter/shifter_etc_files` directory are copied from host into container.
- `passwd, group, nsswitch.conf`
- Some applications (e.g. spark) validates user/group information of execution user before launching.
- A `cron` script is written to update the `passwd` and `group` files in the directory regularly.

Conclusions

- Lots of works needed to maintain Shifter software stack.
- To do:
  - Use distributed MongoDB servers for scale-out performance.
  - Use multiple service nodes to host Shifter image manager gateways.
- Shifter on Blue Waters provides an platform for researchers to develop and test container-based applications, in preparation for next generation HPC systems.

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