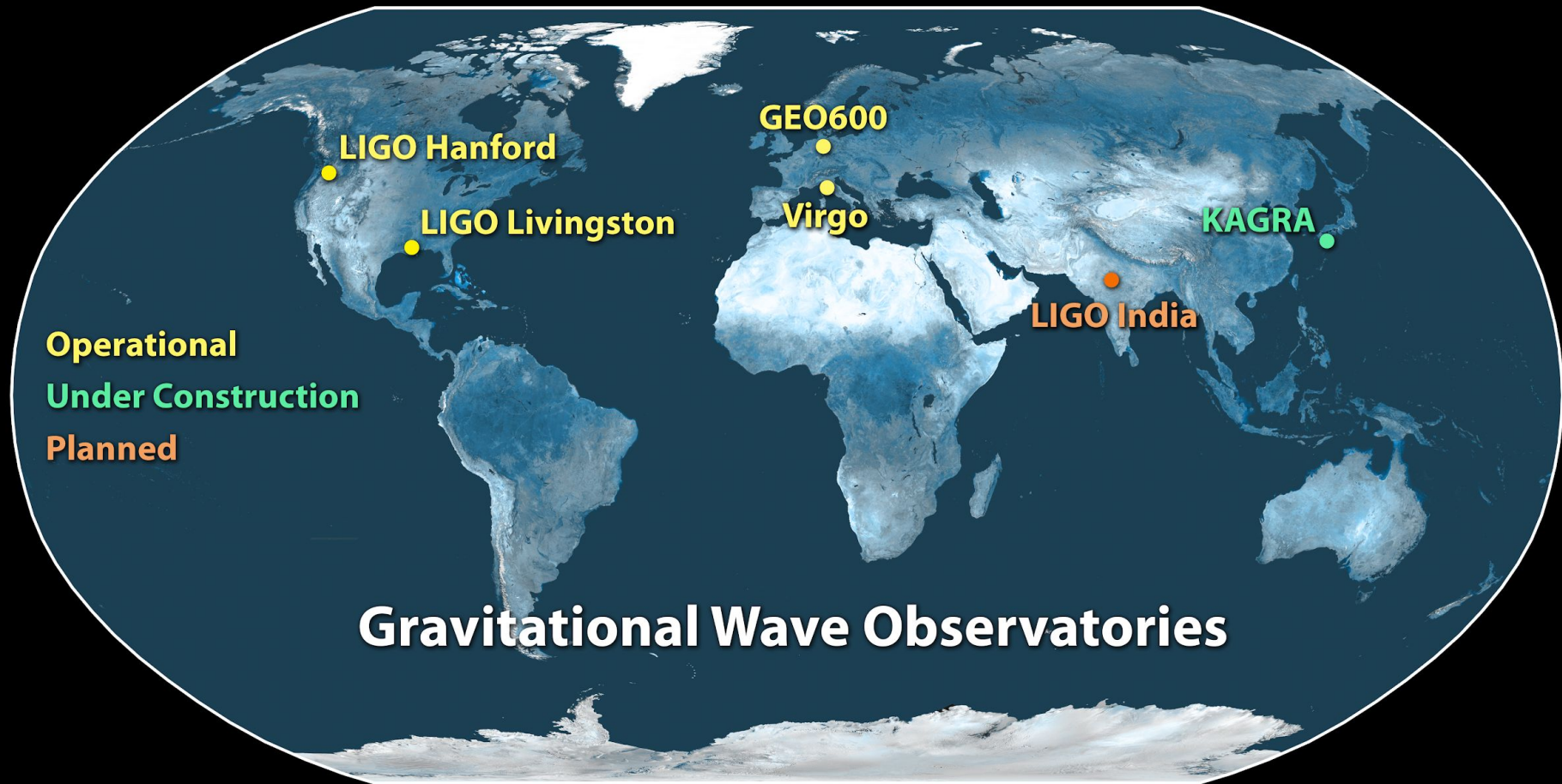


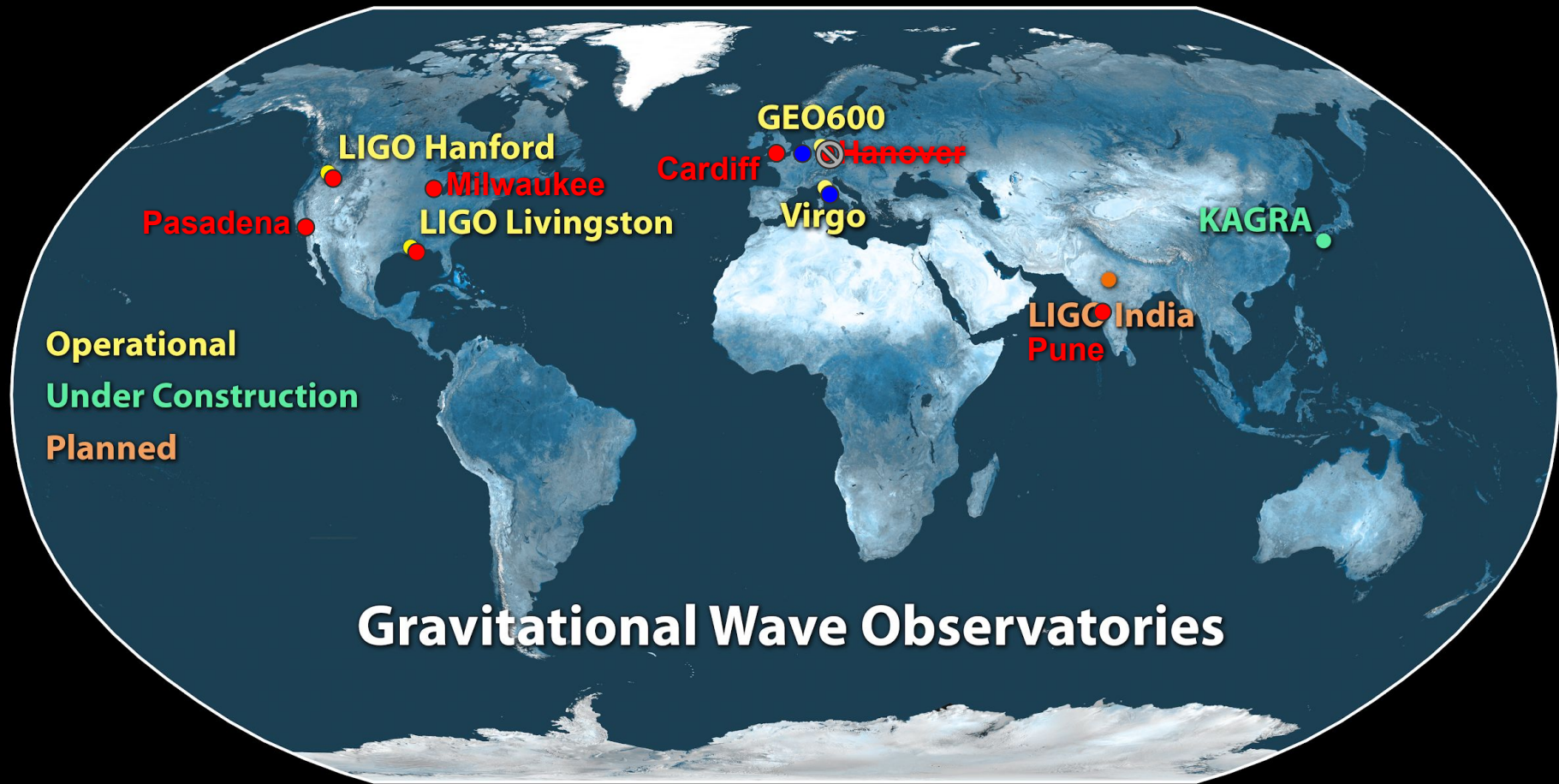
Building a LIGO HTCondor site on top of a shared HPC cluster

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Gravitational Wave Observatories



Operational

Under Construction

Planned

Gravitational Wave Observatories

LIGO Accounting

	Cluster	SU HOURS (7 days)	SU HOURS (52 weeks)	SU HOURS (total)	SU HOURS (since O2) ▼
0	Total	4,090,733	263,041,029	570,800,210	395,855,806
1	ATLAS-AEI	17,057	127,801,704	278,258,904	179,066,042
2	LIGO-CIT	2,464,169	87,174,828	149,071,732	135,476,858
3	LIGO-LHO	659,423	14,995,694	20,067,524	18,932,514
4	NEMO-UWM	196,382	8,414,530	38,849,419	16,235,290
5	LIGO-LLO	183,902	9,291,258	13,717,300	12,008,455
6	ARCCA-CDF	94,178	8,197,247	20,603,810	11,238,248
7	IUCAA	17,849	4,354,131	7,014,275	6,390,264
8	VIRGO.CNAF	0	256,317	10,960,224	4,166,846
9	SUGAR-SU	0	264,573	10,265,547	2,817,724
10	OSG-LIGO-CIT-->OSG.Unknown	0	266,049	1,771,775	1,771,775
11	OSG-SUGAR-SU-->OSG.SU-OG	0	17,939	1,276,126	1,276,126
12	OSG-SUGAR-SU-->OSG.NIKHEF	0	17,224	866,375	866,375
35	OSG-SUGAR-SU-->OSG.RAL	0	10,245	67,842	67,842
49	OSG-LIGO-CIT-->OSG.RAL	0	9,568	12,095	12,095

What does a LIGO Data Grid site need?

- Access cluster using LIGO credentials
- ★ Software
- Data
- ★ HTCondor Scheduler
- Web Server to view results with LIGO Shibboleth authentication
- JupyterLab Service with “LIGO” kernels
- Shared File System!

Running HTCondor at Cardiff

- Standard RHEL 6.4 head node and compute nodes
- PBSPro scheduler
- Filesystems: /home, /software (NFS); /scratch (Lustre) and /tmp (local)

- Virtual and Physical head nodes under my control
- HTCondor Central Manager and Submit run on dedicated head nodes
- Only minor modifications allowed on the compute nodes
 - How do deliver them to HTCondor?

HTCondor “Glideins”

- HTCondor borrows whole nodes from PBSPro using custom glidein script:
 - ```
if $idle_jobs_in_condor ; then
 submit_glidein_jobs_to_pbs_queue()
fi
```
- PBSPro then runs jobs on a dedicated queue using an operational user:
  - ```
#!/bin/bash  
#PBS -q ligo-condor  
source /software/tools/condor/8.6.11/condor.sh  
sudo -E $(which condor_master) -d -f
```
- `sudo` necessary to switch user to allow access to shared file system
- HTCondor is given whole node, 12 or 24 cores, depending on hardware.
- PBS maximum wall time is 5 or 10 days.

Glidein Config

```
DAEMON_LIST = MASTER STARTD
```

```
LOCAL_DIR = /tmp
```

```
LOG = $(LOCAL_DIR)/Condor-log
```

```
SPOOL = $(LOCAL_DIR)/Condor-spool
```

```
EXECUTE = $(LOCAL_DIR)/Condor-execute
```

```
UID_DOMAIN = arcca.cf.ac.uk
```

```
FILESYSTEM_DOMAIN = arcca.cf.ac.uk
```

```
TRUST_UID_DOMAIN = True
```

```
STARTD_NOCLAIM_SHUTDOWN = 300
```

```
slot_type_1_partitionable = true
```

```
slot_type_1 = cpus=$(DETECTED_CORES), mem=$(DETECTED_MEMORY)
```

```
num_slots_type_1 = 1
```


Pros / Cons of whole node glidein

- PROS:
 - Can use HTCondor to manage whole node:
 - condor_drain, reservation for development and testing
 - Due to PBS walltime has a natural de-fragmentation and reassignment to faster nodes.
-
- CONS:
 - Harder for HPC admins to monitor usage and job efficiency

Glidein Alternatives?

- Pyglidein
- ~~Job Transforms to grid universe~~
- ~~Gender Annex~~



LSC Software on Dedicated Sites

- All other LSC sites are dedicated to LIGO so software is installed as system packages, e.g. `/usr/bin/python`
- Two reference OSes; Scientific Linux 7 and Debian 8/9
- Sites carefully updated to ensure library versions are similar
- Software can be easily installed at another dedicated site:
 - `yum install lscsoft-all`
- Some disadvantages:
 - Only one version of package can exist
 - Users are forced to upgrade
 - 3rd party packages within repository often quite old

LSC Software on ARCCA

- Software must be installed from source packages:
 - `./configure`
`make`
`make install`
 - Software then loaded via environment modules
- From 2012-2016 software was managed by hand
- From 2016-2018 I used [Spack](https://spack.io/) (<https://spack.io/>)
 - Many libraries already packaged (2771), adding packages very easy
 - Allows users to install different versions and “variants” simultaneously
 - Creates modules to load environment
 - `spack install lscsoft-all`

Spack - Disadvantages

- By default installs ALL dependencies
- For a large number of packages this can be too cumbersome
- Extra work needed to combine into a single installation directory
- Ultimately could not recommend to users
- If I restarted today then I would begin with Anaconda....

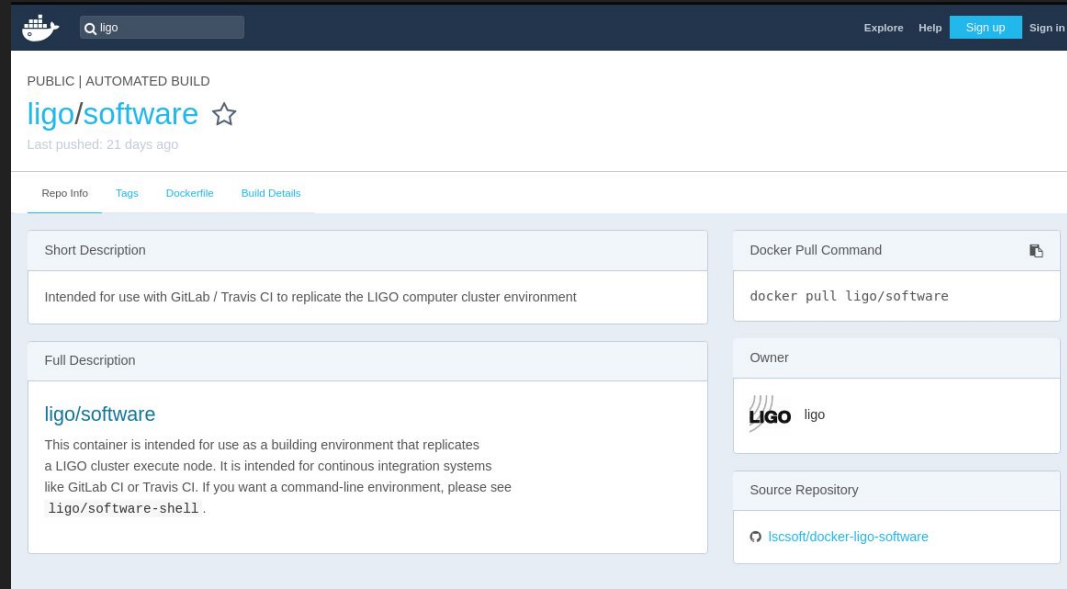


Singularity + CVMFS

- As well as containing processes, Singularity presents a complete software environment
- Can be efficiently distributed using CVMFS
- How should I allow users to make use of it?

LIGO + Docker Hub

- LIGO already provide various OS and application images on Docker Hub
- These are unpacked onto CVMFS



The screenshot shows the Docker Hub interface for the repository `ligo/software`. The page is titled "PUBLIC | AUTOMATED BUILD" and includes a search bar with "ligo" entered. The repository name "ligo/software" is displayed with a star icon and a note "Last pushed: 21 days ago". Navigation tabs include "Repo Info", "Tags", "Dockerfile", and "Build Details".

Short Description

Intended for use with GitLab / Travis CI to replicate the LIGO computer cluster environment

Full Description


[ligo/software](#)

This container is intended for use as a building environment that replicates a LIGO cluster execute node. It is intended for continuous integration systems like GitLab CI or Travis CI. If you want a command-line environment, please see `ligo/software-shell`.

Docker Pull Command

```
docker pull ligo/software
```

Owner

 ligo

Source Repository

[lscsoft/docker-ligo-software](#)

```
singularity shell
```

```
/cvmfs/ligo-containers.opensciencegrid.org/dockerhub/ligo/software:e17
```

```
singularity exec
```

```
/cvmfs/ligo-containers.opensciencegrid.org/dockerhub/ligo/software:e17 python
```

Automatic Singularity Environment

- Intend to give normal users an automatic Singularity LIGO environment
- But, allow power users to opt out, or to use own custom environment.
- Singularity image path stored in `$HOME/.singularity_image`:
 - `SINGULARITY_IMAGE=$(cat $HOME/.singularity_image)`
- When users login automatically launch shell:
 - `singularity shell -s /bin/bash $SINGULARITY_IMAGE`

Example Shell Login

```
paul@HopkinsThinkpad:~$ gsissh ligo.arcca.cf.ac.uk
```

```
....
```

```
Singularity: Invoking an interactive shell within container...
```

```
ligo-headnode/latest spxph@raven14:~$
```

```
python -c "import lalapps; print lalapps.__file__"
```

```
/usr/lib/python2.7/dist-packages/lalapps/__init__.pyc
```

3.17 Singularity Support

Note: This documentation is very basic and needs improvement!

Here's an example configuration file:

```
# Only set if singularity is not in $PATH.
#SINGULARITY = /opt/singularity/bin/singularity

# Forces _all_ jobs to run inside singularity.
SINGULARITY_JOB = true

# Forces all jobs to use the CernVM-based image.
SINGULARITY_IMAGE_EXPR = "/cvmfs/cernvm-prod.cern.ch/cvm3"

# Maps $_CONDOR_SCRATCH_DIR on the host to /srv inside the image.
SINGULARITY_TARGET_DIR = /srv

# Writable scratch directories inside the image. Auto-deleted after the job exits.
MOUNT_UNDER_SCRATCH = /tmp, /var/tmp
```

This provides the user with no opportunity to select a specific image. Here are some changes to the above example to allow the user to specify an image path:

```
SINGULARITY_JOB = !isUndefined(TARGET.SingularityImage)
SINGULARITY_IMAGE_EXPR = TARGET.SingularityImage
```

Then, users could add the following to their submit file (note the quoting):

```
+SingularityImage = "/cvmfs/cernvm-prod.cern.ch/cvm3"
```

Possible Issues and Workarounds

- Care must be taken to ensure HTCondor configuration is the same inside the environment as outside
- Can using `_CONDOR_*` environment variables or bind mount configuration files
- Note that Singularity is executed with `--containall` option:
 - Use minimal `/dev` and empty other directories (e.g. `/tmp` and `$HOME`) instead of sharing filesystems on your host.
 - Contain not only file systems, but also PID, IPC, and environment
- Alternative solution is to use HTCondor `USER_JOB_WRAPPER`:

```
#!/bin/sh
```

```
if [ -n "${_CONDOR_JOB_AD}" ]; then
```

```
    owner=$( grep -E '^Owner' $_CONDOR_JOB_AD | cut -d ' ' -f 3 | tr -d "'" )
```

```
    SINGULARITY_IMAGE_FILE=$( getent passwd $owner | \
```

```
        cut -d: -f6 )/.singularity_image
```

```
fi
```

The Pegasus Problem - Scheduler Universe

- Pegasus is used by some LIGO workflows; it is a high-level workflow manager that runs in the scheduler universe.
- BUT, scheduler universe does not support `SINGULARITY_JOB` or `USER_JOB_WRAPPER`!?
- Tried, local universe, but Pegasus fails. Need to add environment variable:

```
JOB_TRANSFORM_NAMES = SchedulerUniverse
JOB_TRANSFORM_SchedulerUniverse @=end
```

```
[
```

```
    Requirements = JobUniverse == 7;
```

```
    SET_JobUniverse = 12;
```

```
    EVAL_SET_Env = strcat("CONDOR_ID=", ClusterId, " ", Env);
```

```
] @end
```

Paul's Lament

- Doing lots of work to give users what they have elsewhere
- Shared file systems and dedicated sites prevent LIGO users from making use of Grid Resources, e.g. OSG and IRIS
- Trying to wean users off it via CVMFS, Singularity, Large scale CVMFS for data, including standard file locations.
- Would like to get Cardiff to accept GRID jobs, but need to convince HPC admins....

Suggestions welcome

