

Geoscientific Data Distribution in the XSEDE Jetstream Cloud

Unidata on the Jetstream Cloud

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1 Introduction

This guide is a companion document (available in HTML, Markdown, text, PDF)¹ to a 2017 American Meteorological Society oral presentation, *Geoscientific Data Distribution in the XSEDE Jetstream Cloud*². It describes how to configure the LDM³, TDS⁴, RAMADDA⁵, and McIDAS ADDE⁶ on XSEDE Jetstream VMs⁷. It assumes you have access to Jetstream resources though these instructions should be fairly similar on other cloud providers (e.g., Amazon). These instructions also require familiarity with Unix, Docker, and Unidata technology in general. We will also be making use of the Jetstream API⁸. Obtain permission from the XSEDE Jetstream team to use Jetstream API. You must be comfortable entering commands at the Unix command line. We will be using Docker images available at the Unidata Github account⁹ in addition to a configuration specifically planned for an AMS 2017 demonstration¹⁰.

2 Obtain Jetstream Resources

Apply for cloud resource allocations on Jetstream¹¹.

3 Configure Jetstream to Run Unidata Docker Containers

3.1 Clone the Unidata-Dockerfiles Repository

We will be making heavy use of the Unidata/Unidata-Dockerfiles git repository. Install git¹² and clone that repository first:

```
git clone https://github.com/Unidata/Unidata-Dockerfiles
```

3.2 Build and Start the Jetstream API Docker Container

We will be using the Jetstream API directly and via convenience scripts. Install Docker (e.g., docker-machine¹³) on your local computing environment because we will be interacting with the Jetstream API in a Docker container.

```
cd Unidata-Dockerfiles/jetstream/openstack
```

3.2.1 Create ssh Keys

Create an .ssh directory for your ssh keys:

```
mkdir -p .ssh && ssh-keygen -b 2048 -t rsa -f .ssh/id_rsa -P ""
```

¹<https://github.com/Unidata/Unidata-Dockerfiles/tree/master/jetstream/readme>

²<https://ams.confex.com/ams/97Annual/webprogram/Paper315508.html>

³<http://www.unidata.ucar.edu/software/ldm/>

⁴<http://www.unidata.ucar.edu/software/thredds/current/tds/>

⁵<http://sourceforge.net/projects/ramadda/>

⁶<https://www.ssec.wisc.edu/mcidas/>

⁷<https://www.xsede.org/jump-on-jetstream>

⁸<https://iujetstream.atlassian.net/wiki/display/JWT/Using+the+Jetstream+API>

⁹<https://github.com/Unidata>

¹⁰<http://jetstream.unidata.ucar.edu>

¹¹<https://www.xsede.org/jump-on-jetstream>

¹²<https://www.git-scm.com/book/en/v2/Getting-Started-Installing-Git>

¹³<https://docs.docker.com/machine/>

3.2.2 Download openrc.sh

Download the `openrc.sh` file into the `Unidata-Dockerfiles/jetstream/openstack` directory according to the Jetstream API instructions¹⁴. In the Jetstream Dashboard, navigate to Access & Security, API Access to download `openrc.sh`.

Edit the `openrc.sh` file and supply the TACC resource `OS_PASSWORD`:

```
export OS_PASSWORD="changeme!"
```

Comment out

```
# echo "Please enter your OpenStack Password: "
# read -sr OS_PASSWORD_INPUT
```

3.2.3 Build the openstack-client Container

Build the `openstack-client` container, here done via `docker-machine`.

```
docker-machine create --driver virtualbox openstack
eval "$(docker-machine env openstack)"
docker build -t openstack-client .
```

3.3 Set Up Jetstream API to Create VMs

Start the `openstack-client` container with

```
sh os.sh
```

You should be inside the container which has been configured to run `openstack nova` and `neutron` commands. Go through the following Jetstream API sections¹⁵:

- Create security group
- Upload SSH key
- Setup the network

At this point, you should be able to run `glance image-list` which should yield something like:

ID	Name
fd4bf587-39e6-4640-b459-96471c9edb5c	AutoDock Vina Launch at Boot
02217ab0-3ee0-444e-b16e-8fbdae4ed33f	AutoDock Vina with ChemBridge Data
b40b2ef5-23e9-4305-8372-35e891e55fc5	BioLinux 8

If not, check your setup.

3.4 Working with Jetstream API to Create VMs

3.4.1 IP Numbers

We are ready to fire up VMs. First create an IP number which we will be using shortly:

```
nova floating-ip-create public
nova floating-ip-list
```

or you can just `nova floating-ip-list` if you have IP numbers left around from previous VMs.

¹⁴<https://iujetstream.atlassian.net/wiki/display/JWT/Setting+up+openrc.sh>

¹⁵<https://iujetstream.atlassian.net/wiki/display/JWT/OpenStack+command+line>

3.4.2 Boot VM

Now you can boot up a VM with something like the following command:

```
boot.sh -n unicloud -s m1.medium -ip 149.165.157.137
```

The `boot.sh` command takes a VM name, size, and IP number created earlier. See `boot.sh -h` and `nova flavor-list` for more information.

3.4.3 Create and Attach Data Volumes

Also, create and attach `/data` and `/repository` volumes which we will be using shortly via the openstack API:

```
cinder create 750 --display-name data
cinder create 100 --display-name repository

cinder list && nova list

nova volume-attach <vm-uid-number> <volume-uid-number> auto
nova volume-attach <vm-uid-number> <volume-uid-number> auto
```

3.4.4 ssh Into New VM

ssh into that newly minted VM:

```
ssh ubuntu@149.165.157.137
```

If you are having trouble logging in, you may try to delete the `~/.ssh/known_hosts` file. If you still have trouble, try `nova stop <vm-uid-number>` followed by `nova start <vm-uid-number>`.

3.5 Set up VM to Run LDM, TDS, RAMADDA, ADDE

3.5.1 VM Maintenance and Install git

As root (`sudo su -`), update, upgrade and install git:

```
apt-get update && apt-get -y upgrade && apt-get -y dist-upgrade && apt-get -y install git ntp
```

Create a git directory for the Unidata-Dockerfiles project.

```
mkdir -p ~/git
```

3.5.2 Clone Unidata-Dockerfiles

Clone the the Unidata-Dockerfiles project.

```
git clone https://github.com/Unidata/Unidata-Dockerfiles ~/git/Unidata-Dockerfiles
```

3.5.3 Run the VM Set Up Script and Reboot

Install Docker and docker-compose and get the ubuntu user set up to run docker.

```
bash ~/git/Unidata-Dockerfiles/docker-vm-setup/ubuntu/setup-ubuntu.sh -u ubuntu \
    -dc 1.8.1
```

Reboot

```
reboot now
```

3.5.4 Check Docker Installation

Log back in to the VM as user ubuntu. Test docker with

```
docker run hello-world
```

If docker gives an error

```
docker: An error occurred trying to connect: Post http://%2Fvar%2Frun%2Fdocker.sock/v1.24/containers/create: dial unix /var/run/docker.sock: connect: no such file or directory
See 'docker run --help'.
```

Try as root

```
service docker stop
rm -rf /var/lib/docker/aufs #always think hard before rm -rf
service docker start
```

If the hello-world container runs smoothly, continue.

3.5.5 Mount Data Volumes

As root, run some convenience scripts to mount the data volumes for data being delivered via the LDM (/data) and RAMADDA (/repository).

```
bash ~/git/Unidata-Dockerfiles/jetstream/openstack/mount.sh -m /dev/sdb \
    -d /data
bash ~/git/Unidata-Dockerfiles/jetstream/openstack/mount.sh -m /dev/sdc \
    -d /repository

# ensure disks reappear on startup
echo /dev/sdb /data ext4 rw 0 0 | tee --append /etc/fstab > /dev/null
echo /dev/sdc /repository ext4 rw 0 0 | tee --append /etc/fstab > /dev/null
```

3.5.6 Clone Unidata-Dockerfiles and TdsConfig Repositories

We will again be cloning the Unidata-Dockerfiles repository, this time as user ubuntu.

```
mkdir -p ~/git
git clone https://github.com/Unidata/Unidata-Dockerfiles \
    ~/git/Unidata-Dockerfiles
git clone https://github.com/Unidata/TdsConfig ~/git/TdsConfig
```

3.5.7 Create Log Directories

Create all log directories

```
mkdir -p ~/logs/ldm/ ~/logs/ramadda-tomcat/ ~/logs/ramadda/ ~/logs/tds-tomcat/ \
    ~/logs/tds/ ~/logs/traefik/ ~/logs/tdm/
```

3.5.8 Configure the LDM

Grab the ldm etc directory

```
mkdir -p ~/etc
cp -r ~/git/Unidata-Dockerfiles/jetstream/etc/* ~/etc/
```

In the `~/etc` you will find the usual LDM configuration files (e.g., `ldmd.conf`, `registry.xml`). Configure them to your liking.

1. NTP As root, you also want to ensure the network time protocol configuration file accesses `timeserver.unidata.ucar.edu`.

```
sed -i \
    s/server\ 0.ubuntu.pool.ntp.org/server\ timeserver.unidata.ucar.edu\\nserver\ 0.ubuntu.pool.ntp
    /etc/ntp.conf
```

3.5.9 Configure the TDS

In the `ldmd.conf` file we copied just a moment ago, there is a reference to a `pqact` file; `etc/TDS/pqact.forecastModels`. We need to ensure that file exists by doing the following instructions. Specifically, explode `~/git/TdsConfig/idd/config.zip` into `~/tdsconfig` and `cp -r` the `pqacts` directory into `~/etc/TDS`. **Note** do NOT use soft links. Docker does not like them. Be sure to edit `~/tdsconfig/threddsConfig.xml` for contact information in the `serverInformation` element.

```
mkdir -p ~/tdsconfig/ ~/etc/TDS
cp ~/git/TdsConfig/idd/config.zip ~/tdsconfig/
unzip ~/tdsconfig/config.zip -d ~/tdsconfig/
cp -r ~/tdsconfig/pqacts/* ~/etc/TDS
```

1. Edit `ldmfile.sh`

Examine the `etc/TDS/util/ldmfile.sh` file. As the top of this file indicates, you must change the logfile to suit your needs. Change the

```
logfile=logs/ldm-mcidas.log
```

line to

```
logfile=var/logs/ldm-mcidas.log
```

This will ensure `ldmfile.sh` can properly invoked from the `pqact` files.

We can achieve this change with a bit of `sed`:

```
# in place change of logs dir w/ sed
```

```
sed -i s/logs\\ldm-mcidas.log/var\\logs\\ldm-mcidas\\.log/g \
    ~/etc/TDS/util/ldmfile.sh
```

Also ensure that `ldmfile.sh` is executable.

```
chmod +x ~/etc/TDS/util/ldmfile.sh
```

3.5.10 Configure RAMADDA

When you start RAMADDA for the very first time, you must have a `password.properties` file in the RAMADDA home directory which is `/repository/`. See RAMADDA documentation¹⁶ for more details on setting up RAMADDA. Here is a `pw.properties` file to get you going. Change password below to something more secure!

```
# Create RAMADDA default password
```

```
echo ramadda.install.password=changeme! | tee --append \
    /repository/pw.properties > /dev/null
```

¹⁶<http://ramadda.org/repository/userguide/toc.html>

3.5.11 Configure McIDAS ADDE

```
cp ~/git/Unidata-Dockerfiles/jetstream/mcidas/pqact.conf_mcidasA ~/etc
mkdir -p ~/mcidas/upcworkdata/ ~/mcidas/decoders/ ~/mcidas/util/
cp ~/git/Unidata-Dockerfiles/mcidas/RESOLV.SRV ~/mcidas/upcworkdata/
```

3.5.12 Create a Self-Signed Certificates

In the ~/git/Unidata-Dockerfiles/jetstream/files/ directory, generate a self-signed certificate with openssl (or better yet, obtain a real certificate from a certificate authority).

```
openssl req -new -newkey rsa:4096 -days 3650 -nodes -x509 -subj \
  "/C=US/ST=Colorado/L=Boulder/O=Unidata/CN=tomcat.example.com" \
  -keyout ~/git/Unidata-Dockerfiles/jetstream/files/ssl.key \
  -out ~/git/Unidata-Dockerfiles/jetstream/files/ssl.crt
```

3.5.13 TDS Host and TDM User

Ensure the TDS_HOST URL (with a publicly accessible IP number of the docker host or DNS name) is correct in /git/Unidata-Dockerfiles/jetstream/docker-compose.yml.

In the same docker-compose.yml file, ensure the TDM_PW corresponds to the SHA digested password of the tdm user /git/Unidata-Dockerfiles/jetstream/files/tomcat-users.xml

```
docker run tomcat /usr/local/tomcat/bin/digest.sh -a "SHA" mysupersecretpassword
```

3.5.14 Configure TDM

TDM logging will not be configurable until TDS 5.0¹⁷. Until then:

```
curl -SL \
  https://artifacts.unidata.ucar.edu/content/repositories/unidata-releases/edu/ucar/tdmFat/4.6.6/tdmFat.jar \
  -o ~/logs/tdm/tdm.jar
curl -SL https://raw.githubusercontent.com/Unidata/thredds-docker/master/tdm/tdm.sh \
  -o ~/logs/tdm/tdm.sh
chmod +x ~/logs/tdm/tdm.sh
```

3.6 chown for Good Measure

As root ensure that permissions are as they should be:

```
chown -R ubuntu:docker /data /repository ~ubuntu
```

4 Start Everything

Fire up the whole kit and caboodle with docker-compose.yml which will start:

- LDM
- Traefik¹⁸, a reverse proxy that will channel ramadda and tds http request to the right container
- NGINX web server
- RAMADDA

¹⁷<https://github.com/Unidata/thredds-docker#capturing-tdm-log-files-outside-the-container>

¹⁸<https://traefik.io/>

- THREDDS
- TDM
- McIDAS ADDE

As user ubuntu:

```
docker-compose -f ~/git/Unidata-Dockerfiles/jetstream/docker-compose.yml up -d
```

4.1 Bootstrapping

The problem at this point is that it will take a little while for the LDM to fill the /data directory up with data. I don't believe the TDS/TDM can "see" directories created after start up. Therefore, you may have to bootstrap this set up a few times as the /data directory fills up with:

```
cd ~/git/Unidata-Dockerfiles/jetstream/  
docker-compose stop && docker-compose up -d
```

5 References

Stewart, C.A., Cockerill, T.M., Foster, I., Hancock, D., Merchant, N., Skidmore, E., Stanzione, D., Taylor, J., Tuecke, S., Turner, G., Vaughn, M., and Gaffney, N.I., Jetstream: a self-provisioned, scalable science and engineering cloud environment. 2015, In Proceedings of the 2015 XSEDE Conference: Scientific Advancements Enabled by Enhanced Cyberinfrastructure. St. Louis, Missouri. ACM: 2792774. p. 1-8. <http://dx.doi.org/10.1145/2792745.2792774>

John Towns, Timothy Cockerill, Maytal Dahan, Ian Foster, Kelly Gaitner, Andrew Grimshaw, Victor Hazlewood, Scott Lathrop, Dave Lifka, Gregory D. Peterson, Ralph Roskies, J. Ray Scott, Nancy Wilkins-Diehr, "XSEDE: Accelerating Scientific Discovery", Computing in Science & Engineering, vol.16, no. 5, pp. 62-74, Sept.-Oct. 2014, [doi:10.1109/MCSE.2014.80](https://doi.org/10.1109/MCSE.2014.80)

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