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# OSG Connect

Thursday 9:00 AM

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University of Chicago, OSG User Support Team (former)

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# Overview

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- What is OSG Connect
- OSG Connect Services
  - Help Desk and User Support
  - Software Support
  - Data Management: Storage and Transfer

# Open Science Grid (OSG)



A **framework** for large scale distributed resource sharing addressing the technology, policy, and social requirements of sharing computing resources.

Integrates computing and storage resources from over 120 sites in the U.S. These resources are owned by virtual organizations (VOs)



A Virtual Organization (VO) is a set of groups or individuals defined by some common cyber-infrastructure need. This can be a scientific experiment, a university campus or a distributed research effort.

# Open Science Grid (OSG)



- OSG supports a default virtual organization (VO) called "OSG"
- If you are not already part of a VO, you can join OSG via [OSG Connect](#)
- OSG welcomes any researcher affiliated with an U.S. institution!



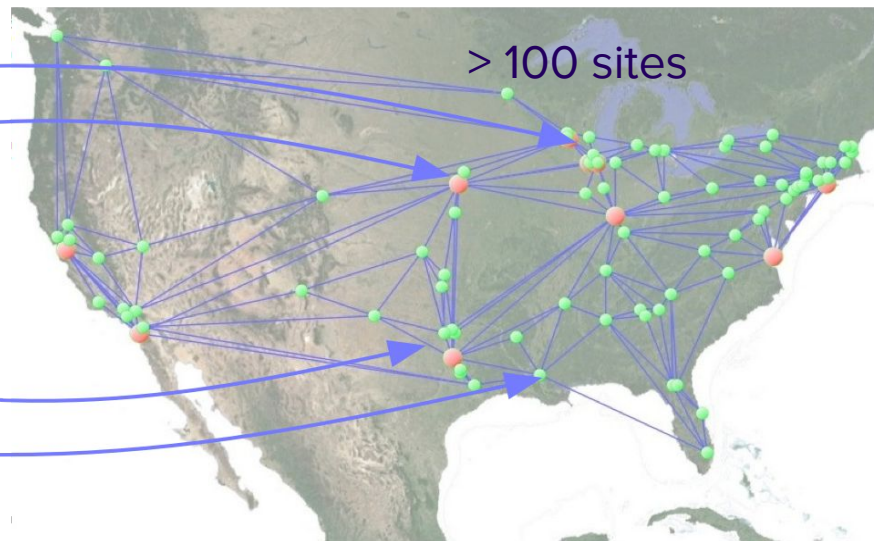
*Tell colleagues who don't have a local VO!*

# Open Science Grid (OSG)



Local VO  
(Campus or group specific)

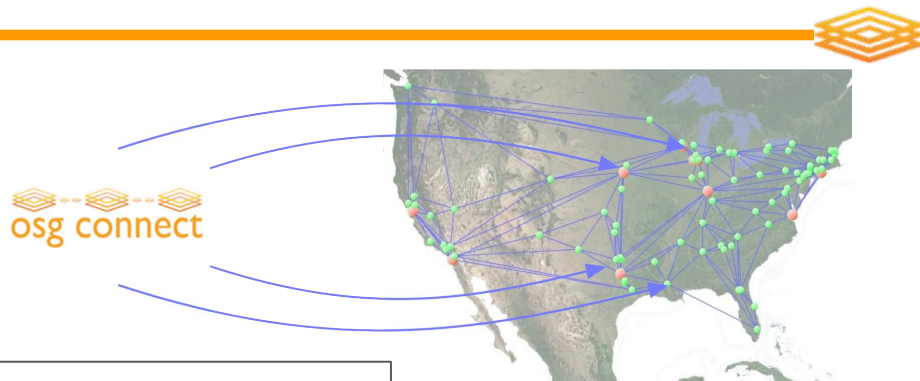
OSG VO  
(OSG Connect, XD Connect)



- Local VO: Users with Campus/Org
- OSG Connect: Affiliated with U.S. research university/institute
- XD Connect: Users with XSEDE allocations

# OSG Connect

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- OSG VO
- Jobs are submitted via HTCondor
- Provides online guides, remote human support, software, and data support
- Submit locally, run globally

# Overview

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# Help Desk and User Support

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- Knowledge Base
  - User guides/tutorials
  - HTC Recipes
- Forums
- “How do I...?” articles
- Interactive online chat
- Workshops and outreach
- Help Desk: <https://support.opensciencegrid.org>
- Support email: [user-support@opensciencegrid.org](mailto:user-support@opensciencegrid.org)



# Help Desk Tickets




 **opensciencegrid** help desk


Welcome  
Login Sign up

Home Solutions

## How can we help you today?

Enter your search term here... **SEARCH**


 New support ticket


 Check ticket status

## Knowledge base


### Overview

Getting Started (4)


 A welcome from the User Support Team

 Communicate with us via Twitter

OSG XSEDE Users (1)

 OSG XSEDE User Guide

Leave us a message!



Create  
Ticket

Online Chat

# Help Desk Articles - Basic Topics



## OSG Connect User Guide

### Getting Started with OSG Connect (5)

- Registration and Login for OSG Connect
- OSG Connect Quickstart
- Start a Project with OSG Connect
- The "tutorial" Command
- Generate SSH key pair and add the public key to your account

### Choosing Resources for Jobs (5)

- Steer your jobs with HTCondor job requirements
- Large Memory Jobs
- GPU Jobs
- Multicore Jobs
- Singularity Containers

### Running applications on OSG Connect (6)

- Accessing Software using Distributed Environment Modules
- Software modules catalog
- Troubleshooting Condor errors
- Requesting a software installation
- Software transfer via HTCondor or HTTP
- >> See all 6 articles

Getting started info and how-to's for serial HTC jobs, multicore jobs, containers, and more

## Data Management

### Introduction to data management on OSG (1)

- Guidelines for data management in OSG - Storage and Transfer

### Data storage (1)

- Storage Solutions on OSG: home, local, scratch, stash, and public

Leave us a message!



# Help Desk Articles - HTC Recipes



## High Throughput Computing Recipes

### Molecular Dynamics (4)

- [A Simple NAMD Application](#)
- [NAMD with input data from Stash using HTTP](#)
- [Pegasus - NAMD example](#)
- [GROMACS](#)

### Quantum Chemistry (1)

- [Electronic Structure Calculations with CP2K](#)

### Workflow solutions (5)

- [Makeflow - Quickstart](#)
- [Makeflow - Running GROMACS simulations in sequence of steps](#)
- [DAGMan - NAMD example](#)
- [Pegasus](#)
- [Swift](#)

### R (3)

- [Calculating Pi using R](#)
- [Adding external packages to your R jobs](#)
- [Scaling up compute resources](#)

### Using FreeSurfer on OSG (9)

- [What's New in Fsurf 2.0](#)

### Drug Discovery (2)

- [AutoDock Vina](#)
- [Managing AutoDock Vina Tasks with Pegasus](#)

### Bioinformatics (3)

- [Sequence Search with BLAST](#)
- [Blast Similarity Search with Pegasus](#)
- [StashCache-Blast](#)

### MATLAB Runtime (4)

- [Basics of compiled MATLAB applications - He](#)
- [RandomMatrix and Wigner's semi-circle law](#)
- [Parameter sweep: Resonance in a driven-damped harmonic oscillator](#)
- [Optimization Tool box: Simulated Annealing](#)

### Python (1)

- [Virtualenv in Python](#)

### Machine Learning (1)

- [TensorFlow](#)

The tutorial command quickly prepares files to launch an HTC recipe.

There are a number of recipes for common workloads available.

[Leave us a message!](#)

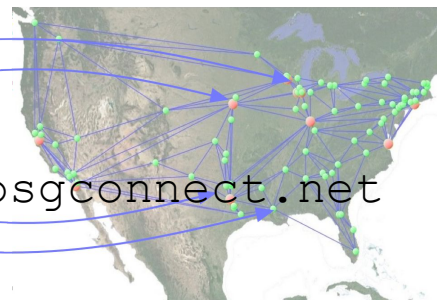
# OSG Connect Submit Hosts



Submit Host for this workshop: `training.osgconnect.net`

For permanent accounts: `login.osgconnect.net`

- Today you need to be able to ssh to: `username@training.osgconnect.net`
- Please let an instructor know if you are not able to log in.
- The workshop account is valid for a month. If you are interested in a long-term account, please signup: <http://osgconnect.net/signup>



# OSG Connect Submit Hosts

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- Job Manager: HTCondor
- Workflow Managers: DAGMan, Pegasus, and, Makeflow
- Use `condor` commands and submit files as usual!
- One exception: `condor_status`

```
condor_status -pool
```

```
flock.opensciencegrid.org
```

# Tutorials on OSG Connect: tutorial Command



- Tutorials are maintained in [Github](#) and downloaded on demand
- Each tutorial's README is in the OSG Support site
  - <http://osg.link/connect/userguide>
  - <http://osg.link/connect/recipes>
- These are recommended for learning new techniques on OSG Connect

# tutorial Command



```
sh$ tutorial
```

```
tutorial
```

```
usage: tutorial list          - show available tutorials
      tutorial info <tutorial-name> - show details of a tutorial
      tutorial <tutorial-name>    - set up a tutorial
```

Currently available tutorials:

```
AutoDockVina ..... Ligand-Receptor docking with AutoDock Vina
R ..... Estimate Pi using the R programming language
R-addlibSNA ..... Shows how to add R external libraries for the R
jobs
ScalingUp-Python ..... Python example to optimize a function on grid
points
```

# tutorial Command



```
sh$ tutorial quickstart
```

```
Installing quickstart (master)...
```

```
Tutorial files installed in ./tutorial-quickstart.
```

```
Running setup in ./tutorial-quickstart...
```

```
sh$ cd tutorial-quickstart/
```

```
sh$ ls
```

```
Images      osg-template-job.submit  short.sh      tutorial02.submit
```

```
log  README.md          tutorial01.submit  tutorial03.submit
```



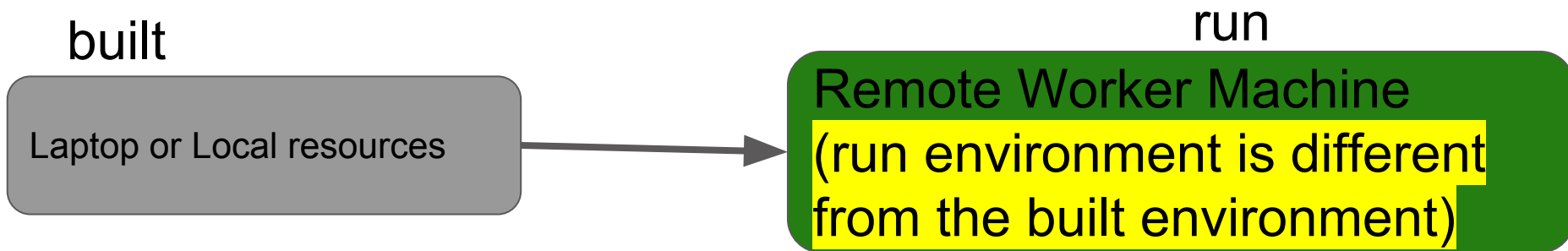
# Overview

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- What is OSG Connect
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  - Software Support
  - Data Management: Storage and Transfer

# Software Support: OASIS



There are several ways to build and run software on OSG.  
(See Christina's talk). We will focus on two approaches.

- **OASIS (OSG Application Software Installation Service)**
- Singularity containers (Time permitting)

- 
- A word cloud in the shape of a heart, composed of various open-source project names and software tools. The most prominent words include GROMACS, STASHC, BOOST, PYTHON, and MATLAB. Other visible words include GGC, client, PROTEIN, FFMPEG, FSL, NVIDIA, CUDA, and many others. The words are arranged in a circular pattern within the heart shape, with varying font sizes and colors (primarily green, yellow, and red) to create a visually appealing effect.

# Accessing OASIS on the Submit Host

([training.osgconnect.net/login.osgconnect.net](http://training.osgconnect.net/login.osgconnect.net))



## See the available packages in OASIS

module avail

```
sh$ module avail
----- /cvmfs/oasis.opensciencegrid.org/osg/modules/modulefiles/Core-----
  ANTS/1.9.4          ectools          lapack/3.5.0          python/2.7          (D)
  ANTS/2.1.0          (D)          eemt/0.1             lapack/3.6.1          (D)  python/3.4
  MUMmer/3.23         elastix/2015      libXpm/3.5.10         python/3.5.2
  OpenBUGS/3.2.3      entropy/2017.03.16  libgfortran/4.4.7     qhull/2012.1
  R/3.1.1             (D)          espresso/5.1          libtiff/4.0.4        root/5.34-32-py34
  R/3.2.0             espresso/5.2      (D)          llvm/3.6             root/5.34-32
  R/3.2.1             ete2/2.3.8        llvm/3.7             root/6.06-02-py34 (D)
[...]
```

# Accessing OASIS on the Submit Host

([training.osgconnect.net/login.osgconnect.net](http://training.osgconnect.net/login.osgconnect.net))



```
sh$ module load R
```

```
sh$ which R
```

```
/cvmfs/oasis.opensciencegrid.org/osg/modules/R/3.1.1/bin/R
```

```
sh$ Rscript --version
```

```
R scripting front-end version 3.1.1 (2014-07-10)
```

```
sh$ module list
```

```
Currently Loaded Modules:
```

```
1) R/3.1.1
```

# Accessing OASIS for your job

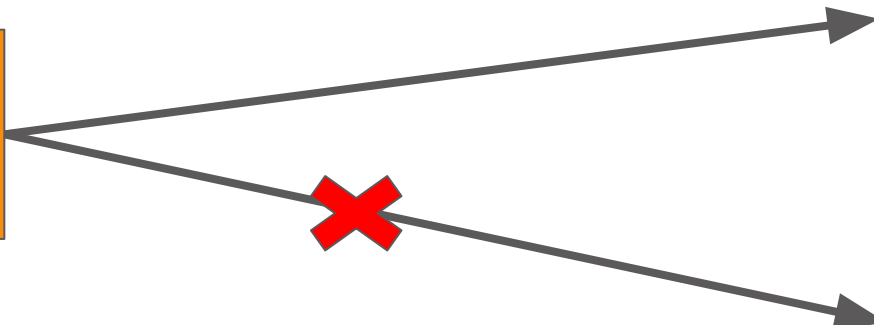
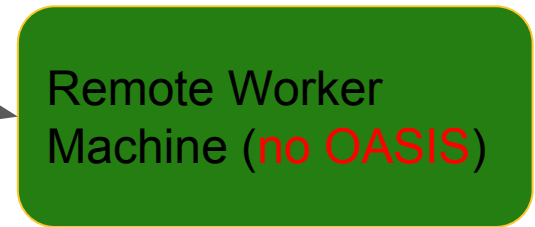
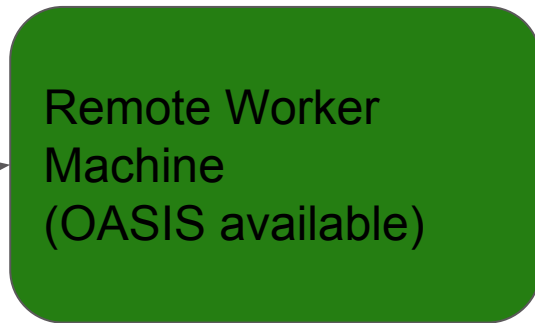
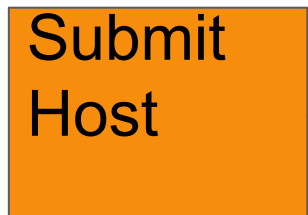


In your execution script file:

```
module load package-name
```

In your job description:

```
requirements = (HAS_MODULES == true)
```



# Basic OASIS Commands

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- Load a software module:  
`module load package-name`
- List loaded modules:  
`module list`
- Unload a module (to prepare for another)  
`module unload package-name`



# Overview

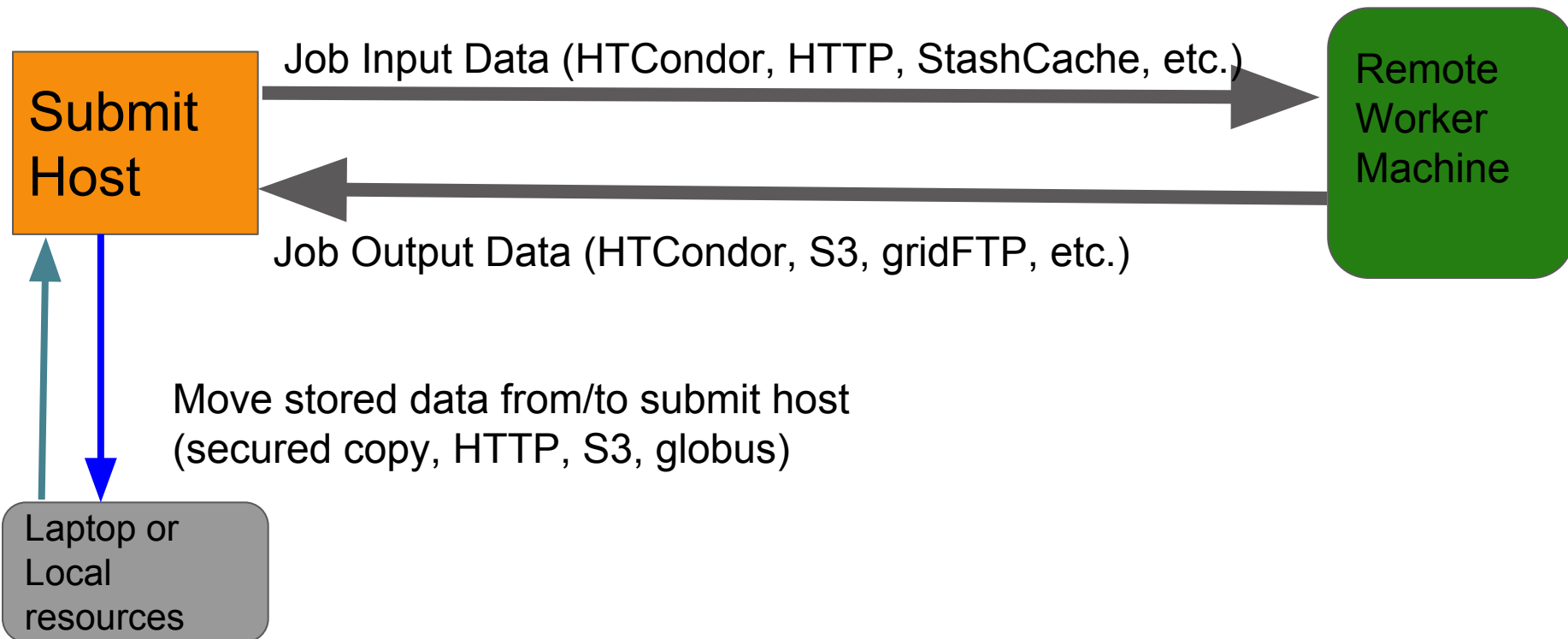
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- What is OSG Connect
  - OSG Connect Services
    - Help Desk and User Support
    - Software Support
    - Data Management: Storage and Transfer
- (we cover some basics, more details in Derek's talk)



# Data Transfer from OSG Connect



# Data Storage on OSG Connect



System	Default Limit	Purpose	Network mounted	Backed Up
home	20 GB	Quick data access and not for submitting jobs	Yes	Yes
local-scratch	25 GB	Large temporary storage and I/O for your jobs. Files older than 30 days are automatically removed.	No	No
stash	200 GB	Large storage and accessible via Globus to/from your campus or laptop	Yes	No
public	10 GB	Sharing data and transfer input data via HTTP or stashcp	Yes	No

- Both **stash** and **public** are on the same filesystem.
- Public directory has an http interface and the files are world readable.
- Let us know if you need more!

# Transferring Input Data for your Job

Method	Recommended File Size	Command	Purpose
HTCondor	< 100 MB	<code>transfer_input_files</code>	Input data from home, local-scratch, public or stash
HTTP and UNIX tools	< 1 GB	<code>wget</code> , <code>curl</code> , or <code>rsync</code>	Input data from <code>~/public</code> for HTTP tools ( <code>wget</code> , <code>curl</code> ), or home, local-scratch, public or stash ( <code>rsync</code> )
StashCache	> 1 GB, < 50 GB	<code>stashcp</code>	Input data from <code>~/public</code>
GridFTP	> 1 GB < 50 GB	<code>gfal-copy</code>	Experts with large workflows. Contact us if you want to use it.

**Submit Host**

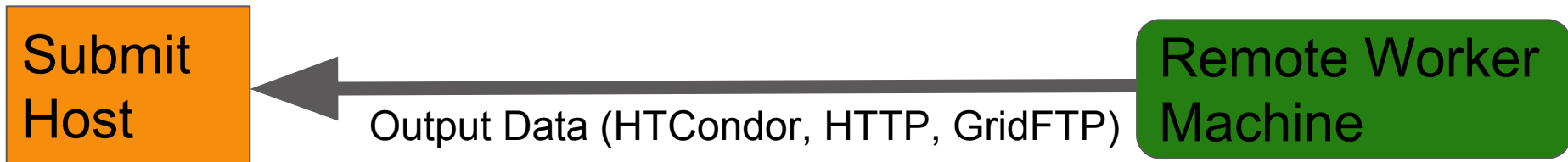
Input Data (HTCondor, HTTP, StashCache, etc.)

**Remote Worker Machine**

# Transferring Output Data from your Job



Method	Recommended File Size	Command	Purpose
HTCondor	< 100 MB	<code>transfer_output_files</code>	Transfer data to submit directory
UNIX Tools	< 1 GB	<code>rsync</code> , <code>scp</code> , etc.	Transfer data to home, local-scratch, stash, etc.
GridFTP	> 1 GB, < 50 GB	<code>gfal_copy</code>	Experts with large workflows. Contact us if you want to use it.

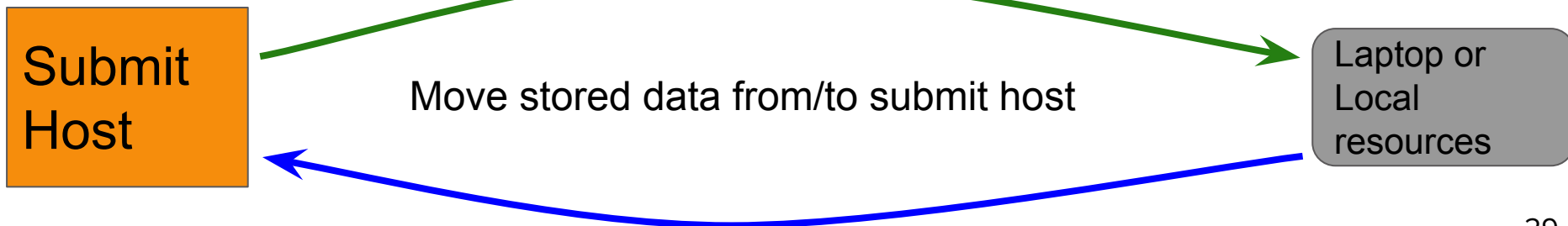


# Data Transfer from OSG Connect



Method	Data Size	Tools
Secure Copy Protocol	< 1GB	scp, putty, WinSCP, gFTP, etc.
Globus	> 1GB	Globus web service or globus CLI

NOTE: Globus transfer is available through the OSG Connect Globus “endpoint”. You will need to a Globus personal endpoint to transfer to your laptop.



# OSG Connect Exercises ([SchoolPage](#))



```
ssh username@training.osgconnect.net
```

1.1 Get acquainted with OSG Connect

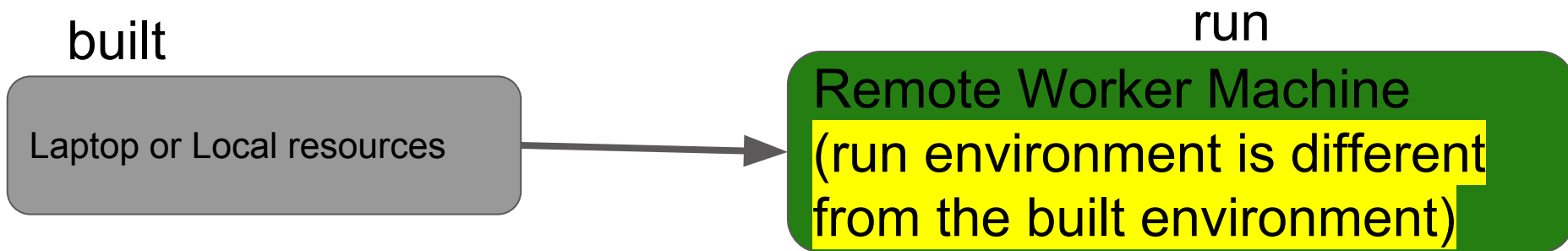
1.2 Do the “OSG Connect Quickstart”

1.3 Run ‘Gromacs’ via the OASIS module

BONUS: submit jobs from **osg-learn** using other software in OASIS (matlab, python, etc)

1.4 Submit the tensorflow example “tf-matmul.py” on the OSG and see how it works.

# Software Support - Containers



There are several ways to build and run software on OSG.  
(See Christina's talk yesterday). We will focus on two approaches.

- OASIS (**O**SG **A**pplication **S**oftware **I**nstallation **S**ervice)
- Singularity containers

# Software portability



- Build with compiler tools (make, cmake, etc.)
- OASIS - portable modules via CVMFS
- Containers (Dockers, Singularity, Rockers, etc.)
- Virtual Machines

How much to pack?

	Containers
Size	Small (about 10 - 20 times) compared to VM
Speed	Starts in milliseconds
Overhead	negligible



# Singularity

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## Singularity:

- can run either a Docker or a Singularity image.

- does not need a daemon process to run an image

- can run workloads as MPI or OpenMP jobs

## Singularity in OSG:

- available in 75% of OSG machines

- user defined images are supported

# Software support on OSG



	User	OSG support team
Compilation	Builds the package on submit host or remote workers.	May help to resolve software dependency questions on local or remote workers.
OASIS	Sends a software installation request to OSG team.	Installs the requested package in OASIS which are available on the OSG (~ 90% machines)
Container	Builds the required image on personal machine (laptop/desktop), publish on docker hub, and give the dockerID to the OSG team.	Distributes the images on the OSG (~75% machines). Also, helps to build the image.
VM	(I have not seen any production runs)	May have some support for special cases on some sites

# User created images



**You** Build image and send the docker id to OSG team **OSG Team**

Laptop or Desktop

Build and publish

Docker Hub

Synced

Replicated

OSG

OSG Image Repo (similar to OASIS model)

- User can't build on Submit Host.
- Build on a personal machine.
- Docker is recommended for building the image.

[/cvmfs/singularity.opensciencegrid.org/...](https://cvmfs/singularity.opensciencegrid.org/...)

# Build image with docker: a simple example



```
#  
# Dockerfile - Simple example  
FROM ubuntu:latest  
MAINTAINER Bala Desinghu "bala.desinghu@rutgers.edu"
```

```
RUN apt-get update  
RUN apt-get install -y python python-pip wget  
RUN pip install nltk
```

```
ADD hello.py /home/hello.py
```

```
WORKDIR /home
```

```
sh$ docker build -t my-python-image .
```

```
sh$ docker push $DOCKER_ID_USER/my-python-image
```

# Build image with docker: a simple example



## What you need?

- Docker installed on your personal machine
- Create an account on docker hub (DOCKER\_USER\_ID)
- Docker file (FROM, RUN, etc.)
- Learn basic docker commands (build, push, pull, search, etc.)

```
sh$ $ cat Dockerfile
# Dockerfile - Simple example
FROM ubuntu:latest
MAINTAINER Bala "bala.desinghu@rutgers.edu"
RUN apt-get update
RUN apt-get install -y python python-pip wget
RUN pip install numpy
sh$ $ docker build -t my-python-image .
sh$ docker push $DOCKER_USER_ID/my-python-image
```

# Singularity on OSG: Documentation

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- Further details:
  - Help Desk articles:
    - <https://goo.gl/FmVkKN>
    - <https://bit.ly/2IUzWAZ>
  - Derek's Blog: <https://goo.gl/LBtBbw>



A brief discussion about an example use case (TensorFlow)

# Running TensorFlow Jobs using Singularity

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TensorFlow

An open-source software library for Machine Intelligence



- TensorFlow Installation
  - TensorFlow is a very active project which requires up-to-date Python modules and system libraries - Makes it a difficult installation on long-term supported Red Hat Enterprise Linux distributions
- TensorFlow Singularity Solution - OSG provides vetted TensorFlow images
  - CPU version: directly imported from Docker image release by TensorFlow project
  - GPU version: based on NVIDIA's CUDA image, with TensorFlow added

# Getting TensorFlow Tutorial



```
sh$ $ tutorial tf-matmul
```

```
Installing tf-matmul (master)...
```

```
Tutorial files installed in ./tutorial-tf-matmul.
```

```
Running setup in ./tutorial-tf-matmul...
```

```
sh$ cd ./tutorial-tf-matmul
```

```
sh$ ls
```

```
README.md  tf_matmul.py  tf_matmul.submit  tf_matmul_wrapper.sh
```



# Using Singularity to run TensorFlow



## Running the singularity container on the submit host

```
sh$ python tf_matmul.py
```

```
Traceback (most recent call last):
```

```
  File "tf_matmul.py", line 3, in <module>
```

```
    import tensorflow as tf
```

```
ImportError: No module named tensorflow
```

```
sh$ singularity shell /cvmfs/singularity.opensciencegrid.org/tensorflow/tensorflow:latest
```

```
sh$ python tf_matmul.py
```

```
result of matrix multiplication
```

```
=====
```

```
[[ 1.00000000e+00  0.00000000e+00]
```

```
 [ -4.76837158e-07  1.00000024e+00]]
```

```
=====
```

Throws error because tensorflow is only available in the container environment and not as a regular package.

Start a container and a shell inside the container

Inside the container, the job execution is successful.

# Requesting TensorFlow Containers on OSG



## Running on the remote worker machine

- Take a look at the job description file
- `Requirements = HAS_SINGULARITY == True` (Find a machine that has singularity installed)
- `+SingularityImage =`  
`"/cvmfs/singularity.opensciencegrid.org/tensorflow/tensorflow:latest"`  
(use the container image on cvmfs)

# OSG Connect Exercises ([twiki](#))

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`ssh username@training.osgconnect.net`

1.1 Get acquainted with OSG Connect

1.2 Do the “OSG Connect Quickstart”

1.3 Run ‘Gromacs’ via the OASIS module

1.4 Submit the tensorflow example “tf-matmul.py” on the OSG and see how it works.

BONUS: submit jobs from **osg-learn** using other software in OASIS (matlab, python, etc)



# Thank You

# Review: OSG Submit Locations



	Local	OSG Connect	XD Connect
Available to:	Researchers affiliated with institution	Affiliates of U.S. research orgs	Users with XSEDE allocation
Compute resource	Opportunistic + Allocations	Opportunistic	Allocations
Limit on CPU hrs	Unlikely	No	Yes (per allocation)
User support	Local staff	Help Desk, Documentation, Support chat, email, and tickets	OSG Connect Support and, if available, campus champion
Submit location	Local submit server	login.osgconnect.net (user-training.osgconnect.net)	xd-login.opensciencegrid.org