Interacting with Blue Waters

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Agenda

1. Connecting to Blue Waters
2. Moving data to/from Blue Waters
3. Running applications on Blue Waters
Connecting to Blue Waters
Connecting to Blue Waters

Required tools

Terminal*

SSH Client
Connecting to Blue Waters

1. ssh username@bw.ncsa.illinois.edu

2. Enter your NCSA password

3. Confirm with NCSA DUO
Connecting to Blue Waters

Hands-on practice

Let's try it out!
The end of "Connecting to Blue Waters" section

Questions?

Next up "Moving data to/from Blue Waters"
Moving data to/from Blue Waters
Moving data to/from Blue Waters

Blue Waters supports data transfers via:

- scp, rsync, wget, curl, git (git clone)

Globus (https://www.globus.org)

We recommend using Globus!
Data transfer with Globus

(1/3) create

(2/3) connect to

(3/3) initiate transfer
(1/3) Creating personal Globus storage endpoint
Creating personal Globus storage endpoint

**STEP 1**

Create a Globus ID at globusid.org/create

You can skip this step if you have either Google or ORCiD accounts and plan on using one of them.
Creating personal Globus storage endpoint

**STEP 2**

Log in to 
app.globus.org
Creating personal Globus storage endpoint

**STEP 3**

**Navigate to ENDPOINTS**

app.globus.org/endpoints

**Click on Create a personal endpoint**

app.globus.org/file-manager/gcp
Creating personal Globus storage endpoint

**STEP 4**
Specify endpoint name

Click "Generate Setup Key"

Be sure to copy/save generated Setup Key

**STEP 5**
Install Globus Connect Personal

https://www.globus.org/globus-connect-personal
Creating personal Globus storage endpoint

**STEP 6** Launch Globus Connect Personal...

...enter the Setup Key from **STEP 4**

press "Ok"
(2/3) Connecting to Blue Waters Globus storage endpoint
Connecting to Blue Waters Globus storage endpoint

**STEP 1**

Navigate to **app.globus.org**

**STEP 2**

Search for **ncsa#BlueWaters**

**STEP 3**

Click on **ncsa#BlueWaters**

You will be asked to authenticate to access the endpoint.

Click **Continue** to proceed.
Connecting to Blue Waters Globus storage endpoint

STEP 4

Your browser should be redirected to https://cilogon.org/...

In the Select an Identity Provider section click on current provider name, type NCSA and click on National Center for Supercomputing Applications

Click Log On
Connecting to Blue Waters Globus storage endpoint

**STEP 5**
Login with your NCSA Username and Password

**STEP 6**
When prompted, confirm your identity with NCSA DUO
Connecting to Blue Waters Globus storage endpoint

Once the sign in step completes, Globus opens a **FILE MANAGER** tab showing your Blue Waters home folder. This indicates that you have successfully connected to the Blue Waters Globus storage endpoint. 🎉
(3/3) Transferring files between Globus endpoints
Transferring files between Globus endpoints

**STEP 1** Navigate to app.globus.org

After the last step in **Connecting to Blue Waters Globus storage endpoint** section, the **FILE MANAGER** tab should have Blue Waters Globus storage endpoint open.

**STEP 2** Click on Transfer or Sync to... icon in the right-hand side toolbar
Transferring files between Globus endpoints

**STEP 3**

In the second panel, select the Globus storage endpoint you wish to transfer data to or from. It can be any endpoint, including the one we created in *Creating personal Globus storage endpoint* section or some other endpoint (on another HPC or data center, etc).
Transferring files between Globus endpoints

**STEP 4**
Select the files and folders on the sender you wish to transfer to another endpoint.

**STEP 5**
Navigate to the destination directory in the recipient's panel.

**STEP 6**
Click on Transfer & Sync Options at the bottom of the page and choose transfer option you wish to use.

We recommend using:
- sync - only transfer new or changed files
- preserve source file modification times
- verify file integrity after transfer
- encrypt transfer
Transferring files between Globus endpoints

**STEP 7** Click on the Start button in the Sender's panel on the bottom of the page.

Globus will initiate data transfer and send you an email when the transfer is complete or if there is a problem.
The end of "Moving data to/from Blue Waters" section

Questions?

Next up "Running applications on Blue Waters"
Running applications on Blue Waters
Running applications on Blue Waters

So, can we go ahead and...  

```
mpirun -n 20000 ./application
```
Running applications on Blue Waters

User

ssh

qsub

aprun

Blue Waters

Nodes:

Login

MOM

Compute
Running applications on Blue Waters

To run an application on Blue Waters, we need bundle it into a **job script**.

**Job script example**

```bash
#!/bin/bash
PBS -l nodes=2:ppn=32:xe
PBS -l walltime=00:10:00
PBS -q normal
PBS -N myjob

cd $PBS_O_WORKDIR
aprun -n 2 -N 1 -- ./application
```

- **Special PBS comments** must come first in the script.
- **PBS: Portable Batch System** job scheduler.
- **2 XE nodes**
- **10 minutes of walltime**
- "normal" queue
- call it "myjob"
Running applications on Blue Waters

Once we have a job script, we can submit it for execution to a queue with

\[
\text{qsub } \text{job_script}
\]

\text{qsub} returns a job identifier that looks something like \textbf{12312312.bw}

Using this identifier, we can manipulate submitted job:

Delete: \texttt{qdel <jobid>}

Put on hold: \texttt{qhold <jobid>}

Check status: \texttt{qstat -u $USER}

Release a hold: \texttt{qrls <jobid>
Running applications on Blue Waters

PORTAL ➔ USING BLUE WATERS ➔ User Guide ➔ Running Your Jobs

PORTAL ➔ USING BLUE WATERS ➔ User Guide ➔ Running Your Jobs ➔ Batch Jobs - sample scripts

PORTAL ➔ USING BLUE WATERS ➔ User Guide ➔ Running Your Jobs ➔ Queue, Scheduling and Charging Policies

PORTAL ➔ USING BLUE WATERS ➔ User Guide ➔ Running Your Jobs ➔ Monitoring Jobs

PORTAL ➔ USING BLUE WATERS ➔ User Guide ➔ Running Your Jobs ➔ Using aprun

Need help / training? help+bw@ncsa.illinois.edu
The end of "Running applications on Blue Waters" section

Questions?

The end of "Interacting with Blue Waters" presentations