Hello World

This script will print "Hello World", sleep for 10 seconds, and then print the time and date. The output will be written to a file in your current directory.

```
#!/bin/sh
#
# Simple "Hello World" submit script for Slurm.
#
#SBATCH --account=ACCOUNT        # Replace ACCOUNT with your group account name
#SBATCH --job-name=HelloWorld    # The job name
#SBATCH -c 1                     # The number of cpu cores to use (up to 32 cores per server)
#SBATCH --time=0-0:30            # The time the job will take to run in D-HH:MM
#SBATCH --mem-per-cpu=5G         # The memory the job will use per cpu core

echo "Hello World"
sleep 10
date
```

Running Precompiled Binaries

To submit a precompiled binary to run on Ginsburg, the script will look just as it does in the Hello World example. The difference is that you will call your executable file instead of the shell commands "echo", "sleep", and "date".

C, C++, Fortran MPI

Intel Parallel Studio

Ginsburg supports Intel Parallel Studio which is a highly optimized compiler that builds software with the highest performance. It also supports MPI for applications that require communication between multiple nodes. All the nodes on the cluster have Infiniband transport and that is the fabric that MPI jobs avail themselves of - which is another reason for a substantial boost of efficiency on the cluster.

To use Intel MPI, you must load the Intel module first:
In order to take advantage of Ginsburg architecture, your program should be (re)compiled on the cluster even if you used Intel for compiling it on another cluster. It is important to compile with the compiler provided by the module mentioned above. Note that you may have to set additional environment variables in order to successfully compile your program.

These are the locations of the C and Fortran compilers for Intel Studio:

```
$ module load intel-parallel-studio/2020
(...) 
$ which mpiicc
/burg/opt/parallel_studio_xe_2020/compilers_and_libraries_2020.4.304/linux/mpi/intel64/bin/mpicc

$ which ifort
/burg/opt/parallel_studio_xe_2020/compilers_and_libraries_2020.4.304/linux/bin/intel64/ifort
```

For programs written in C, use mpiicc in order to compile them:

```
$ mpiicc -o <MPI_OUTFILE> <MPI_INFILE.c>
```

The submit script below, named pi_mpi.sh, assumes that you have compiled a simple MPI program used to compute pi, (see mpi_test.c), and created a binary called pi_mpi:

```
#!/bin/sh

#SBATCH --account ACCOUNT  # Replace ACCOUNT with your group account name
#SBATCH -N 2                # Number of nodes
#SBATCH --mem-per-cpu=5800  # Default is 5800
#SBATCH --time=0:30         # Runtime in D-HH:MM
#SBATCH --ntasks-per-node=32 # Max 32 since Ginsburg has 32 cores per node

module load intel-parallel-studio/2020

mpiexec -bootstrap slurm ./pi_mpi
```

```
Job Submission

$ sbatch pi_mpi.sh
```

**OpenMPI**

Ginsburg supports also OpenMPI from the GNU family.

To use OpenMPI, you must load the openmpi module instead:

```
#!/bin/sh

#SBATCH --account ACCOUNT  # Replace ACCOUNT with your account name
#SBATCH -N 2                # Number of nodes
#SBATCH --mem-per-cpu=5800  # Default is 5800
#SBATCH --time=0:30         # Runtime in D-HH:MM
#SBATCH --ntasks-per-node=32 # Max 32 since Ginsburg has 32 cores per node

module load openmpi/gcc/64

mpiexec myprogram
```

Your program must be compiled on the cluster. You can use the the module command as explained above to set your path so that the corresponding mpicc will be found. Note that you may have to set additional environment variables in order to successfully compile your program.
$ module load openmpi/gcc/64
$ which mpicc
/cm/shared/apps/openmpi/gcc/64/1.10.7/bin/mpicc

Compile your program using mpicc. For programs written in C:

$ mpicc -o <MPI_OUTFILE> <MPI_INFILE.c>

GPU (CUDA C/C++)

The cluster includes 18 Nvidia RTX 8000 nodes and 4 Nvidia V100S GPU nodes each with 2 GPU modules per server.

To use a GPU server you must specify the --gres=gpu option in your submit request, followed by a colon and the number of GPU modules you require (with a maximum of 2 per server).

Request a gpu, specify this in your submit script. If the colon and number are omitted, as shown below, the scheduler will request 1 GPU module.

#SBATCH --gres=gpu

Not all applications have GPU support, but some, such as MATLAB, have built-in GPU support and can be configured to use GPUs.

To build your CUDA code and run it on the GPU modules you must first set your paths so that the Nvidia compiler can be found. Please note you must be logged into a GPU node to access these commands. To login interactively to a GPU node, run the following command, replacing <ACCOUNT> with your account.

$ srun --pty -t 0-01:00 --gres=gpu:1 -A <ACCOUNT> /bin/bash

Load the cuda environment module which will add cuda to your PATH and set related environment variables.

$ module load cudall1.1/toolkit

You then may need to compile your program using nvcc if you are compiling cuda code directly.

$ nvcc -o <EXECUTABLE_NAME> <FILE_NAME.cu

You can compile hello_world.cu sample code which can be built with the following command:

$ nvcc -o hello_world hello_world.cu

For non-trivial code samples, refer to Nvidia’s CUDA Toolkit Documentation.

A Slurm script template, gpu.sh, that can be used to submit this job is shown below:

#!/bin/sh
#SBATCH --account=<ACCOUNT> # The account name for the job.
#SBATCH --job-name=HelloWorld # The job name.
#SBATCH --gres=gpu:1 # Request 1 gpu (Up to 2 gpus per GPU node)
#SBATCH --constraint=rtx8000 # You may specify rtx8000 or v100s or omit this line for either
#SBATCH --c 1 # The number of cpu cores to use.
#SBATCH --time=0-01:00 # The time the job will take to run in D-HH:MM
#SBATCH --mem-per-cpu=5gb # The memory the job will use per cpu core.

module load cudall1.1/toolkit
./hello_world

# End of script
Job submission

```
$ sbatch gpu.sh
```

This program will print out "Hello World!" when run on a gpu server or print "Hello Hello" when no gpu module is found.

Ocean Climate Physics OCP GPU Partition ("For OCP members only")

Members of OCP have access to a separate GPU partition which accesses only OCP gpu nodes. This directs jobs to first request the 4 GPU servers that OCP owns and guarantees priority access as well as allowing running up to 5 day jobs on those gpu nodes. If no OCP GPU servers are available, the scheduler will fall back to request non-OCP gpu nodes across the cluster.

To submit to this gpu partition, ocp members must specify the partition explicitly in their submit scripts as shown below.

```
#SBATCH --partition=ocp_gpu       # Request ocp_gpu nodes first. If none are available, the scheduler will
#SBATCH --gres=gpu:1             # Request 1 gpu (Up to 2 gpus per GPU node)
#SBATCH --constraint=rtx8000    # You may specify rtx8000 or v100s or omit this line for either
```

If `--partition=ocp_gpu` is omitted, the scheduler will request any gpu across the cluster by default.

Singularity

Singularity is a software tool that brings Docker-like containers and reproducibility to scientific computing and HPC. Singularity has Docker container support and enables users to easily run different flavors of Linux with different software stacks. These containers provide a single universal on-ramp from the laptop, to HPC, to cloud.

Users can run Singularity containers just as they run any other program on our HPC clusters. Example usage of Singularity is listed below. For additional details on how to use Singularity, please contact us or refer to the Singularity User Guide.

Downloading Pre-Built Containers

Singularity makes it easy to quickly deploy and use software stacks or new versions of software. Since Singularity has Docker support, users can simply pull existing Docker images from Docker Hub or download docker images directly from software repositories that increasingly support the Docker format. Singularity Container Library also provides a number of additional containers.

You can use the `pull` command to download pre-built images from an external resource into your current working directory. The `docker://` uri reference can be used to pull Docker images. Pulled Docker images will be automatically converted to the Singularity container format.

```
$ singularity pull docker://ubuntu
```

Running Singularity Containers

Here’s an example of pulling the latest stable release of the Tensorflow Docker image and running it with Singularity. (Note: these pre-built versions may not be optimized for use with our CPUs.)

First, load the Singularity software into your environment with:

```
$ module load singularity
```

Then pull the docker image. This also converts the downloaded docker image to Singularity format and save it in your current working directory:

```
$ singularity pull tensorflow.sif docker://tensorflow/tensorflow
```

Done. Container is at: ./tensorflow.sif
Once you have download a container, you can run it interactively in a shell or in batch mode.

**Singularity - Interactive Shell**

The `shell` command allows you to spawn a new shell within your container and interact with it as though it were a small virtual machine:

```bash
$ singularity shell tensorflow.sif
Singularity: Invoking an interactive shell within container...
```

From within the Singularity shell, you will see the Singularity prompt and can run the downloaded software. In this example, python is launched and tensorflow is loaded.

```sh
Singularity> python
>>> import tensorflow as tf
>>> print(tf.__version__)
2.4.1
>>> exit()
```

When done, you may exit the Singularity interactive shell with the "exit" command.

```sh
Singularity> exit
```

**Singularity: Executing Commands**

The `exec` command allows you to execute a custom command within a container by specifying the image file. This is the way to invoke commands in your job submission script.

```bash
$ module load singularity
$ singularity exec tensorflow.sif [command]
```

For example, to run python example above using the exec command:

```bash
$ singularity exec tensorflow.sif python -c 'import tensorflow as tf; print(tf.__version__)'
```

**Singularity: Running a Batch Job**

Below is an example of job submission script named `submit.sh` that runs Singularity. Note that you may need to specify the full path to the Singularity image you wish to run.
#!/bin/bash
# Singularity example submit script for Slurm.
#
# Replace <ACCOUNT> with your account name before submitting.
#
#SBATCH -A <ACCOUNT>           # Set Account name
#SBATCH --job-name=tensorflow  # The job name
#SBATCH -c 1                   # Number of cores
#SBATCH -t 0-0:30              # Runtime in D-HH:MM
#SBATCH --mem-per-cpu=5gb      # Memory per cpu core

module load singularity

singularity exec tensorflow.sif python -c 'import tensorflow as tf; print(tf.__version__)'

Then submit the job to the scheduler. This example prints out the tensorflow version.

$ sbatch submit.sh

Using MAKER in a Singularity container

MAKER is an easy-to-use genome annotation pipeline designed to be usable by small research groups with little bioinformatics experience. It has many dependencies, especially for Perl and using a container is a convenient way to have all the requirements in one place. The BioContainers website maintains a Singularity container as of Dec. 2023, version 3.01.03. Here is a sample tutorial.

module load singularity

Note that the environment variable LIBDIR needs to be set and since export is a Builtin command that needs to be called via the bash command:

```
singularity run https://depot.galaxyproject.org/singularity/maker:3.01.03--pl5262h8f1cd36_2 bash -c 'export LIBDIR=/usr/local/share/RepeatMasker && maker --help'
```

You can ignore the warning:

```
Possible precedence issue with control flow operator at /usr/local/lib/site_perl/5.26.2/Bio/DB/IndexedBase.pm line 805. ERRO:`
```

There are two options to maker that can be used, as Ginsburg uses the Lustre parallel file system:

```
# * -nolock reduces file creation overhead (lock files not needed when using MPI)
# * -nodatastore is suggested for Lustre, as it reduces the number of directories created
```

Using example 03 legacy from the MAKER Tutorial for WGS Assembly and Annotation Winter School, you will be using the model_gff option to pass in legacy gene models. The full tutorial files can be downloaded here.

```
wget http://weatherby.genetics.utah.edu/data/maker_tutorial.tgz
tar -zxvf maker_tutorial.tgz
cd maker_tutorial/example_03_legacy
singularity run https://depot.galaxyproject.org/singularity/maker:3.01.03--pl5262h8f1cd36_2 bash -c 'export LIBDIR=/usr/local/share/RepeatMasker && maker --CTL'
cp opts.txt maker_opts.ctl
nano maker_opts.ctl
```

Add a label:

```
est=pyu_est.fasta:hypoxia
ctl-c ctl-x
singularity run https://depot.galaxyproject.org/singularity/maker:3.01.03--pl5262h8f1cd36_2 bash -c 'export LIBDIR=/usr/local/share/RepeatMasker && maker --CTL'
```

Possible precedence issue with control flow operator at /usr/local/lib/site_perl/5.26.2/Bio/DB/IndexedBase.pm line 805.
STATUS: Parsing control files...
STATUS: Processing and indexing input FASTA files...
STATUS: Setting up database for any GFF3 input...
A data structure will be created for you at:
/burg/home/you/maker_tutorial/example_03_legacy/legacy_contig_maker.output/legacy_contig_datastore

To access files for individual sequences use the datastore index:
/burg/home/you/maker_tutorial/example_03_legacy/legacy_contig_maker.output/legacy_contig_master_datastore_index.log

STATUS: Now running MAKER...
examining contents of the fasta file and run log

[...]

To use Maker with OpenMPI, e.g., requesting 8 CPU `ntasks` (which are processes that a job executes in parallel in one or more nodes), you can use the following suggested options, which will help reduce warnings:

```
srun --pty --ntasks 8 -t 0-04:00 -X -A <account-name> /bin/bash
module load openmpi/gcc/64/4.1.5a1 singularity
mpirun -np 2 --mca btl '^openib' --mca orte_base_help_aggregate 0 singularity run https://depot.galaxyproject.org/singularity/maker:3.01.03--pl5262h8f1cd36_2 bash -c "export LIBDIR=/usr/local/share/RepeatMasker && maker"
```

Additionally `samtools` (used for reading/writing/editing/indexing/viewing SAM/BAM/CRAM format) is available in the container:

```
Singularity> samtools --version
samtools 1.7
Using htslib 1.7-2
Copyright (C) 2018 Genome Research Ltd.
```

Note, if you are testing `maker` and kill jobs/processes look out for `.NFSLock` files, which you will likely need to delete for subsequent runs of `maker`. You will need to use the `--a` option with `ls` as files that start with a dot/period are hidden from the `ls` command by default.

### Using GATK in a Singularity container

GATK, the Genome Analysis Toolkit has several dependencies and can run inside a container. Here is a sample tutorial:

```
module load singularity
singularity pull docker://broadinstitute/gatk
```

Using Step 4 at the GATK Best Practices page, download the suggested .bam file:

```
wget https://raw.githubusercontent.com/broadinstitute/gatk/master/src/test/resources/org/broadinstitute/hellbender/tools/BQSR/NA12878.chr17_69k_70k.dictFix.bam
```

Then run:

```
singularity shell gatk_latest.sif
```

In the container run:

```
gatk PrintReads -I NA12878.chr17_69k_70k.dictFix.bam -O output.bam
```

The output should end with (timestamp removed for clarity):

```
INFO PrintReads - Done initializing engine
WARN IntelDeflaterFactory - Intel Deflater not supported, using Java.util.zip.Deflater
INFO ProgressMeter - Starting traversal
INFO ProgressMeter - Current Locus Elapsed Minutes Reads Processed Reads/Minute
INFO ProgressMeter - unmapped 0.0 493 896363.6
INFO ProgressMeter - Traversal complete. Processed 493 total reads in 0.0 minutes.
INFO PrintReads - Shutting down engine
org.broadinstitute.hellbender.tools.PrintReads done. Elapsed time: 0.00 minutes.
Runtime.totalMemory()=285212672
```

To quit the container press `ctl-D`.

These 2 files were created:

```
-rw-r--r-- 1 rk3199 user 128 Nov 28 16:48 output.bai
-rw-r--r-- 1 rk3199 user 62571 Nov 28 16:48 output.bam
```

### Using GeoChemFoam in a Singularity container

GeoChemFoam is open source code, based on the OpenFoam CFD toolbox developed at the Institute of GeoEnergy Engineering, Heriot-Watt University.

After converting one of the available Docker containers to Singularity 3.x.sif, some additional steps/tweaks are needed to get all of the features working. For this tutorial we assume GeoChemFoam version 5.0 and use the Test Case 01 Species transport in a Ketton Micro-CT image tutorial. You can choose your version of Anaconda Python. Note there are some changes in the tutorial from earlier versions of GeoChemFoam, e.g., 4.8. For this tutorial we assume the name of the Singularity container is geochemfoam-5.0.sif and we'll use an interactive job with `srun`, to request 8 `ntasks` for use with OpenMPI in the Ketton tutorial.

```
srun --pty -t 0-08:00 --ntasks 8 --mem=10gb -X -A <your-account> /bin/bash
module load singularity/3.7.1 anaconda/3-2022.05 openmpi/gcc/64/4.1.5a1
```

Singularity offers a few ways to set/pass environment variables, we'll use `SINGULARITYENV_PREPEND_PATH` as the container needs to know where the S run command is.
export SINGULARITYENV_PREPEND_PATH=$PATH
singularity shell --bind /path/to/your-directory/runs:/home/gcfoam/works/GeoChemFoam-5.0/runs:rw geochemfoam-5.0.
sif

--bind connects whatever is to the left of the colon, in this case, a new directory called 'runs'. The right side of the colon is a path that exists in the container. rw is read/write

All files written to the /runs directory will remain and that's the only directory that files can be written to when the container is bound.

Change the value of $HOME:
export HOME=/home/gcfoam

Copy the multiSpeciesTransportFoam directory from /home/gcfoam/works/GeoChemFoam-5.0/tutorials/transport to /path/to/your-directory/runs, e.g.,
cp -a /home/gcfoam/works/GeoChemFoam-5.0/tutorials/transport /path/to/your-directory/runs/

Install 5 Python libraries using Python from within the container. Specify where to install these (--t option as follows is one way).
/usr/bin/pip3 install --t /home/gcfoam/works/GeoChemFoam-5.0/runs matplotlib numpy scikit-image numpy-stl h5py

Note this will populate the ~/runs directory where the results from the tutorial are so you may want to put these in a different directory.

Set 2 additional environment variables:
export PYTHONPATH=/home/gcfoam/works/GeoChemFoam-5.0/runs
export MPLCONFIGDIR=/home/gcfoam/works/GeoChemFoam-5.0/runs

Source the .bashrc file in the container:
source $HOME/works/GeoChemFoam-5.0/etc/bashrc

Run the scripts in the tutorial in your ~/runs directory.
cd transport/multiSpeciesTransportFoam/Ketton/
./createMesh.sh

To avoid seeing a couple of warnings from OpenMPI, you can add the following options to the mpirun command in the scripts (using vi) that use them:
--mca btl '^openib' --mca orte_base_help_aggregate 0

For the next script, runSnappyHexMesh.sh, that would change as follows:
mpirun -np $NP --mca btl '^openib' --mca orte_base_help_aggregate 0 snappyHexMesh -overwrite -parallel > snappyHexMesh.out
./runSnappyHexMesh.sh
./initCaseFlow.sh

The next two scripts have mpirun, which you can add --mca btl '^openib' --mca orte_base_help_aggregate 0
./runCaseFlow.sh

Check the simpleFoamFlow.out file for 'SIMPLE solution converged in <X> iterations'
./processFlow.sh

cat poroPerm.csv
time poro perm Lpore Re UD
0 0.133986 5.71129e-12 1.84664e-05 0.0220027 0.00239467
./initCaseTransport.sh

The next two scripts contain mpirun:
./runCaseTransport.sh
./processTransport.sh
To run the tutorial again make sure to run one of the delete scripts, e.g., `deleteAll.sh`

For additional details on how to use Singularity, please contact us or refer to the Singularity User Guide.

Using Couenne in a Singularity container

Couenne (Convex Over and Under ENvelopes for Nonlinear Estimation) is a branch-and-bound algorithm to solve Mixed-Integer Nonlinear Programming (MINLP) problems. It includes a suite of programs with several dependencies. Fortunately there is a Docker container which can be used to access these programs, e.g., bonmin, couenne, Ipopt, Cgl, and Cbc, via Singularity. You can use these sample .nl files to test with Couenne.
singularity pull docker://coinor/coin-or-optimization-suite
singularity shell coin-or-optimization-suite_latest.sif
Singularity> couenne hs015.nl
Couenne 0.5 -- an Open-Source solver for Mixed Integer Nonlinear Optimization
Mailing list: couenne@list.coin-or.org
Instructions: http://www.coin-or.org/Couenne

NLP0012I Num Status Obj It time Location
NLP0014I 1 OPT 306.49998 22 0.004007
Couenne: new cutoff value 3.0649997900e+02 (0.009883 seconds)
Loaded instance "hs015.nl"
Constraints: 2
Variables: 2 (0 integer)
Auxiliaries: 8 (0 integer)

Coin0506I Presolve 29 (-1) rows, 9 (-1) columns and 64 (-2) elements
Clp0006I 0 Obj 0.25 Primal inf 473.75936 (14)
Clp0006I 13 Obj 0.31728151
Clp0000I Optimal - objective value 0.31728151
Clp0032I Optimal objective 0.3172815065 - 13 iterations time 0.002, Presolve 0.00
Clp0000I Optimal - objective value 0.31728151
Cbc0012I Integer solution of 306.49998 found by Couenne Rounding NLP after 0 iterations and 0 nodes (0.00 seconds)
NLP Heuristic: NLP0014I 2 OPT 306.49998 5 0.001228
solution found, obj. 306.5
Clp0000I Optimal - objective value 0.31728151
Optimality Based BT: 3 improved bounds
Probing: 2 improved bounds
Cbc0031I 1 added rows had average density of 2
Cbc0013I At root node, 4 cuts changed objective from 0.31728151 to 306.49998 in 1 passes
Cbc0014I Cut generator 0 (Couenne convexifier cuts) - 4 row cuts average 2.0 elements, 3 column cuts (3 active)
Cbc0001I Search completed - best objective 306.4999790004336, took 0 iterations and 0 nodes (0.00 seconds)
Cbc0035I Maximum depth 0, 0 variables fixed on reduced cost

couenne: Optimal
"Finished"

Linearization cuts added at root node: 30
Linearization cuts added in total: 30 (separation time: 2.4e-05s)
Total solve time: 0.003242s (0.003242s in branch-and-bound)
Lower bound: 306.5 (gap: 0.00%)
Branch-and-bound nodes: 0
Performance of FBBT: 2.75 2ubd: 0.5 inffeas: 0
Performance of ORBT: 0.000742s, 1 runs. fix: 0 shrnk: 6.70203

Example of R run

For this example, the R code below is used to generate a graph "Rplot.pdf" of a discrete Delta-hedging of a call. It hedges along a path and repeats over many paths. There are two R files required:

hedge.R
BlackScholesFormula.R

A Slurm script, hedge.sh, that can be used to submit this job is presented below:
#!/bin/sh
#hedge.sh
#Slurm script to run R program that generates graph of discrete Delta-hedging call option

#SBATCH -A ACCOUNT               # Replace ACCOUNT with your group account name
#SBATCH -J DeltaHedge            # The job name
#SBATCH -c 4                     # The number of cpu cores to use. Max 32.
#SBATCH -t 0-0:30                # Runtime in D-HH:MM
#SBATCH --mem-per-cpu 5gb        # The memory the job will use per cpu core

module load R

#Command to execute R code
R CMD BATCH --no-save --vanilla hedge.R routput

#End of script

Batch queue submission

$ sbatch hedge.sh

This program will leave several files in the output directory: slurm-{jobid}.out, Rplots.pdf, and routput (the first one will be empty).

Running LAMMPS in a Singularity Container with a GPU

Nvidia provides prebuilt Singularity LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) GPU-enabled containers in its New General Catalogue (NGC). Using the tutorial provided you can use:

$ docker://nvcr.io/hpc/lammps:29Sep2021

Here is a modified tutorial for Ginsburg, starting with an interactive session requesting one GPU, 10 GB of memory and note the extra option for the wget commands:

```bash
srun --pty --mem=10gb -t 0-2:00 --gres=gpule1 -A <your-account> /bin/bash
module load singularity/3.7.1
wget https://lammps.sandia.gov/inputs/in.lj.txt --no-check-certificate
export BENCHMARK_DIR=$PWD
cd $BENCHMARK_DIR
chmod +x run_lammps.sh
cd $BENCHMARK_DIR
singularity run --nv -B $PWD:/host_pwd --pwd /host_pwd docker://nvcr.io/hpc/lammps:29Sep2021 ./run_lammps.sh
```

You should start seeing this response:

```
Running Lennard Jones 8x4x8 example on 1 GPUs...
LAMMPS (29 Sep 2021)
KOKKOS mode is enabled (src/KOKKOS/kokkos.cpp:97)
will use up to 1 GPU(s) per node
using 1 OpenMP thread(s) per MPI task
Lattice spacing in x,y,z = 1.6795962 1.6795962 1.6795962
```

You can combine the commands for use with directly with a Slurm interactive session as suggested in the original tutorial

```bash
srun --pty --mem=10gb -t 0-4:00 --gres=gpus:1 -A <your-account> -v --mi=pmi2 -c 4 singularity run --nv -B $PWD:/host_pwd --pwd /host_pwd docker://nvcr.io/hpc/lammps:29Sep2021 ./run_lammps.sh
```

The same container can be used for non-GPU jobs but still requires requesting a GPU node. You can test with a tutorial that provides polymer_plus_bridge.s.lam. Download the .lam and initial configuration files. With srun, -v will show more verbose output.
wget https://cbrackley.github.io/simple_lammps_tutorial/lammps_tutorial/tutorial5/polymer_plus_bridges.lam
wget https://cbrackley.github.io/simple_lammps_tutorial/lammps_tutorial/tutorial5/initial_configuration.txt


Reading data file ...
  orthogonal box = (-25.000000 -25.000000 -25.000000) to (25.000000 25.000000 25.000000)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
   220 atoms
  reading velocities ...
   220 velocities
  scanning bonds ...
   1 = max bonds/atom
  scanning angles ...
   1 = max angles/atom
  reading bonds ...
   199 bonds
  reading angles ...
   198 angles
  Finding 1-2 1-3 1-4 neighbors ...

Installing R Packages on Ginsburg

HPC users can install R packages locally in their home directory or group's scratch space (see below).

Local Installation

After logging in to Ginsburg, start R:

```bash
$ module load R

$ R
```

You can see the default library paths (where R looks for packages) by calling `.libPaths()`:

```r
> .libPaths()
[1] "/burg/opt/r-4.0.4/lib64/R/library"
```

These paths are all read-only, and so you cannot install packages to them. To fix this, we will tell R to look in additional places for packages.

Exit R and create a directory `rpackages` in `/burg/<GROUP>/users/<UNI>/`.

```bash
$ mkdir /burg/<GROUP>/users/<UNI>/rpackages
```

Go back into R and add this path to `.libPaths()`

```r
$ R

> .libPaths("/burg/<GROUP>/users/<UNI>/rpackages/")
```

Call `.libPaths()` to make sure the path has been added

```r
> .libPaths()
[1] "/burg/rcs/users/UNI/rpackages" "/burg/opt/r-4.0.4/lib64/R/library"
```

To install a package, such as the "sm" package, tell R to put the package in your newly created local library:
install.packages("sm", lib="/burg/<GROUP>/users/<UNI>/rpackages")

Select appropriate mirror and follow install instructions.

Test to see if package can be called:

> library(sm)
Package `sm`, version 2.2-3; Copyright (C) 1997, 2000, 2005, 2007 A.W.Bowman & A.Azzalini
type
help(sm) for summary information

In order to access this library from your programs, make sure you add the following line to the top of every program:

.libPaths("/burg/<GROUP>/users/<UNI>/rpackages/")

Since R will know where to look for libraries, a call to library(sm) will be successful (however, this line is not necessary per se for the install.packages(...) call, as the directory is already specified in it).

MATLAB

MATLAB atlab (single thread)

The file linked below is a MATLAB M-file containing a single function, simPoissGLM, that takes one argument (lambda).

simPoissGLM.m

A Slurm script, simpoiss.sh, that can be used to submit this job is presented below.

#!/bin/sh
#
# Simple MATLAB submit script for Slurm.
#
#SBATCH -A ACCOUNT               # Replace ACCOUNT with your group account name
#SBATCH -J SimpleMLJob           # The job name
#SBATCH -c 1                     # Number of cores to use (max 32)
#SBATCH -t 0-0:30                # Runtime in D-HH:MM
#SBATCH --mem-per-cpu=5G         # The memory the job will use per cpu core

module load matlab
echo "Launching a MATLAB run"
date
#define parameter lambda
LAMBDA=10

#Command to execute MATLAB code
MATLAB -nosplash -nodisplay -nodesktop -r "simPoissGLM($LAMBDA)" # > matoutfile

# End of script

Batch queue submission

$ sbatch simpoiss.sh

This program will leave several files in the output directory: slurm-<jobid>.out, out.mat, and matoutfile.

MATLAB with Parallel Computing Toolbox
Parallel Computing Toolbox (PCT), formerly known as Distributed Computing Engine, is installed within MATLAB. It lets you solve computationally and data-intensive problems using multicore processors, but limited to one compute/execute node. The compute nodes on Ginsburg have 32 CPUs, over 2 sockets, with 16 cores per socket. In order to use PCT you will have to incorporate MATLAB functions such as distributed or parfor. Note in order to use all 32 CPUs the best practice is to use the --exclusive option to srun in order to assure no other users are running jobs on the requested node and it may take a while to get a free node, depending on how many users are running jobs. As in the previous section, the -c option option can be used to specify the number of cores, with 16 being the maximum

- To configure PCT, from the Home tab, under Environment, select the down arrow next to Parallel and select Create and manage a cluster.
- This opens up Cluster Profile Manager. Click Add cluster profile and choose Local (use the cores on your machine).
- Click Set as default.
- Click Edit, which is within the Manage Profile section.
- Add a Description
- Set Number of workers to start on your local machine, with the maximum being 16.
- The rest of the fields can be left to their default value, unless you want to change them.
- Click Validate, it can take a minute to complete.

Once validation completes you can use the example for Use Distributed Arrays to Solve Systems of Linear Equations with Direct Methods, you can paste the following into MATLAB's Editor and click Run. A graph labeled System of Linear Equations with Full Matrices will pop up. In the bottom left corner under ondemand (Folder) you will see Connected to the parallel pool (number of workers: ##). ## is the number of cores you configured earlier. Assuming you opened MATLAB in the background, you can also run the top -i command to see the number of CPUs being used during the calculation.

```matlab
n = 1e3;
A = randi(100,n,n);
ADist = distributed(A);
b = sum(A,2);
bDist = sum(ADist,2);
xEx = ones(n,1);
xDistEx = ones(n,1,'distributed');
x = A\b;
err = abs(xEx-x);

xDist = ADist\bDist;
errDist = abs(xDistEx-xDist);

figure
subplot(2,1,1)
semilogy(err,'o');
title('System of Linear Equations with Full Matrices');
ylabel('Absolute Error');
xlabel('Element in x');
ylim([10e-17,10e-13])
subplot(2,1,2)
semilogy(errDist,'o');
title('System of Linear Equations with Distributed Full Matrices');
ylabel('Absolute Error');
xlabel('Element in x');
ylim([10e-17,10e-13])
```

MATLAB with Parallel Server

Running MATLAB via X11 Forwarding

MATLAB Parallel Server is now configured on Ginsburg for R2022b and R2023a. X11 Forwarding is available and for Apple Mac computers, XQuartz is recommended and for Windows, MobaXterm. The first time you run MATLAB via X11, it can take a few minutes to fully open, especially over WiFi. You can run one simple command to enable the Toolbox:

```matlab
>> configCluster
You should see:
Must set AccountName before submitting jobs to GINSBURG. E.g.
```n
```matlab
>> c = parcluster;
>> c.AdditionalProperties.AccountName = 'group-account-name';
>> c.saveProfile
Complete. Default cluster profile set to "Ginsburg".
```

Running MATLAB From Your Desktop/Laptop
You can now also install MATLAB on your laptop/desktop and download it from MathWorks Columbia page, where students can download it for free. You will need to download and install a zip file which contains all the necessary integration scripts including the license. You will also need to be on the Columbia WiFi or VPN and copy the network.lic file into your device's MATLAB directory or running the userpath command. On a Mac, you would use Finder, Applications, MATLAB, click the mouse, Show Package Contents, then licenses. In MATLAB, navigate to the Columbia-University.Desktop folder. In the Command Window type configCluster. You will be prompted for Ginsburg and Terremoto, select 1, for Ginsburg. Enter your UNI (without @columbia.edu). You should see:

```
>> c = parcluster;
    >> c.AdditionalProperties.AccountName = 'group-account-name';
    >> c.saveProfile
```

Complete. Default cluster profile set to "Ginsburg".

Inside the zip file is a Getting Started tutorial in a Word document. An example interactive pool job follows:

```
>> c = parcluster;
```

Submission to the remote cluster requires SSH credentials. You will be prompted for your SSH username and password or identity file (private key). The username and location of the private key will be stored in MATLAB for future sessions. Jobs will now default to the cluster rather than submit to the local machine.

Configuring Jobs

Prior to submitting the job, we can specify various parameters to pass to our jobs, such as queue, e-mail, walltime, etc. See AdditionalProperties for the complete list. AccountName and MemPerCPU are the only fields that are mandatory.

```
>> % Specify the account
>> c.AdditionalProperties.AccountName = 'group-account-name';

>> % Specify memory to use, per core (default: 4gb)
>> c.AdditionalProperties.MemPerCPU = '6gb';
```

Python and JULIA

To use python you need to use:

```
$ module load anaconda
```

Here's a simple python program called "example.py" – it has just one line:

```
print("Hello, World!")
```

Save as example.py.

To submit it on the Ginsburg Cluster, use the submit script "example.sh"

```
#!/bin/sh
#
# Simple "Hello World" submit script for Slurm.
#
#SBATCH --account=ACCOUNT    # Replace ACCOUNT with your group account name
#SBATCH --job-name=HelloWorld  # The job name.
#SBATCH -c 1                  # The number of cpu cores to use
#SBATCH -t 0-0:30             # Runtime in D-HH:MM
#SBATCH --mem-per-cpu=5gb     # The memory the job will use per cpu core

module load anaconda

#Command to execute Python program
python example.py

#End of script
```

If you use "ls" command you should see 2 programs:

```
example.sh
example.py
```
To submit it - please use:

```
$ sbatch example.sh
```

To check the output use:

```
$ cat slurm-463023.out
Hello, World!
```

Similarly, here is the "julia_example.jl" with just one line

```
$ cat julia_example.jl
println("hello world")
```

and

```
$ cat julia_example.sh
```

```shell
#!/bin/sh
#
# Simple "Hello World" submit script for Slurm.
#
#SBATCH --account=ACCOUNT             # Replace ACCOUNT with your group account name
#SBATCH --job-name=HelloWorld         # The job name
#SBATCH -c 1                          # The number of cpu cores to use
#SBATCH --time=1:00                   # The time the job will take to run
#SBATCH --mem-per-cpu=5gb             # The memory the job will use per cpu core

module load julia

#Command to execute Python program
julia julia_example.jl

#End of script
```

After you finish creating those two files, if you use "ls" command you should see:

```
julia_example.jl
julia_example.sh
```

To submit it use:

```
$ sbatch julia_example.sh
Submitted batch job 463030
```

To check the output

```
$ cat slurm-463030.out
hello world
```

Julia Interactive Session Usage:

Step 1 >> start an interactive session (*** replace ACCOUNT with your slurm group account name below):
$ srun --pty -t 0-04:00 -A ACCOUNT /bin/bash
$ module load julia
$ julia julia_example.jl
hello world
$ julia

_ _ _(_)_ | A fresh approach to technical computing
{() | () (}_ | Documentation: http://docs.julialang.org
-- --|--|--|-- | Type "?help" for help.
_/|_ _  | Official http://julialang.org/ release
__/|_ _ | x86_64-pc-linux-gnu

julia>

To quit Julia use "CTRL +D"

Julia packages can be installed with this command (for example "DataFrames" package):

julia> using Pkg
julia> Pkg.add("DataFrames")

Please check this website:
https://julialang.org/packages/

to see the full list of the official packages available.

Tensorflow

Tensorflow computations can use CPUs or GPUs. The default is to use CPUs which are more prevalent, but typically slower than GPUs.

Anaconda Python makes it easy to install Tensorflow, enabling your data science, machine learning, and artificial intelligence workflows.
https://docs.anaconda.com/anaconda/user-guide/tasks/tensorflow/

Tensorflow

First, load the anaconda python module.

$ module load anaconda

You may need to run "conda init bash" to initialize your conda shell.
$ conda init bash
==> For changes to take effect, close and re-open your current shell. <==

To install the current release of CPU-only TensorFlow:

$ conda create -n tf tensorflow
$ conda activate tf

Or, to install the current release of GPU TensorFlow:

$ conda create -n tf-gpu tensorflow-gpu
$ conda activate tf-gpu

Test tensorflow

$ python
Python 3.7.1 (default, Dec 14 2018, 19:28:38)
>>> import tensorflow as tf
>>> print(tf.__version__)
1.13.1

Test tensorflow gpu support (you must be on a GPU)
$ python
>>> import tensorflow as tf
>>> print("Num GPUs Available: ", len(tf.config.list_physical_devices('GPU')))

NetCDF

NetCDF (Network Common Data Form) is an interface for array-oriented data access and a library that provides an implementation of the interface. The NetCDF library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data.

To load the NetCDF Fortran Intel module:

```
$ module load netcdf-fortran-intel/4.5.3
```

To see all available NetCDF modules run:

```
$ module avail netcdf

netcdf-fortran-intel/4.5.3     netcdf/gcc/64/gcc/64/4.7.3
netcdf-fortran/4.5.3          netcdf/gcc/64/gcc/64/4.7.4 (D)
```

Jupyter Notebooks

This is one way to set up and run a jupyter notebook on Ginsburg. As your notebook will listen on a port that will be accessible to anyone logged in on a submit node you should first create a password.

Creating a Password

The following steps can be run on the submit node or in an interactive job.

1. Load the anaconda python module.

```
$ module load anaconda
```

2. If you haven't already done so, initialize your jupyter environment.

```
$ jupyter notebook --generate-config
```

3. Start a python or ipython session.

```
$ ipython
```

4. Run the password hash generator. You will be prompted for a password, prompted again to verify, and then a hash of that password will be displayed.

```
In [1]: from notebook.auth import passwd; passwd()
Enter password:
Verify password:
Out[1]: 'sha1:60bdb1:306fe0101ca73be2429edbab0935c545'
```

5. Cut and paste the hash into ~/.jupyter/jupyter_notebook_config.py

(Important: the following line in the file is commented out by default so please uncomment it first)
Running a Jupyter Notebook

1. Log in to the submit node. Start an interactive job.

   $ srun --pty -t 0-01:00 -A <ACCOUNT> /bin/bash

   Please note that the example above specifies time limit of one hour only. That can be set to a much higher value, and in fact the default (i.e. if not specified at all) is as long as 5 days.

2. Get rid of XDG_RUNTIME_DIR environment variable

   $ unset XDG_RUNTIME_DIR

3. Load the anaconda environment module.

   $ module load anaconda

4. Look up the IP of the node your interactive job is running on.

   $ hostname -i
   10.43.4.206

5. Start the jupyter notebook, specifying the node IP.

   $ jupyter notebook --no-browser --ip=10.43.4.206

6. Look for the following line in the startup output to get the port number.

   The Jupyter Notebook is running at: http://10.43.4.206:8888/

7. From your local system, open a second connection to Ginsburg that forwards a local port to the remote node and port. Replace UNI below with your uni.

   $ ssh -L 8080:10.43.4.206:8888 UNI@burg.rcs.columbia.edu

8. Open a browser session on your desktop and enter the URL 'localhost:8080' (i.e. the string within the single quotes) into its search field. You should now see the notebook.

Getting Python libraries JAX and JAXLIB to work with GPUs

JAX, a Just-In-Time (JIT) compiler focused on harnessing the maximum number of FLOPs to generate optimized code while using the simplicity of pure Python. It is frequently updated with strict version requirements for minimum versions of CUDA and CUDNN. The following combination of modules and libraries will work:

```
module load anaconda/3-2022.05 cuda11.8/toolkit/11.8.0 cudnn8.6-cuda11.8/8.6.0.163
pip install --U jax[cudal12]==0.4.7 -f https://storage.googleapis.com/jax-releases/jax_cuda_releases.html
https://storage.googleapis.com/jax-releases/cudal1/jaxlib-0.4.7+cudal11.cudnn86-cp39-cp39-manylinux2014_x86_64.whl
```

```
Python 3.9.12 (main, Apr 5 2022, 06:56:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> from jax.lib import xla_bridge
>>> print(xla_bridge.get_backend().platform)
gpu
```
Running FSL from a Mac with multiple monitors

Running FSL on a Mac with multiple monitors causes the application to open too large to view. One of the developers/maintainers of FSL provided RCS with a PKL file ("A PKL file is a serialized object created with the pickle module in Python 2.x. It contains binary strings representing an object used in a Python project"). A copy is located in /burg/rcs/projects/files/config.pkl. In order for it to work you need to put it in your $HOME/.config/fsleyes/ directory. This has been preset to open at a reasonable size on the leftmost monitor.