The Forge

System Information

Software

The Forge was built with rocks 6.1.1 which is built on top of CentOS 6.5. With the Forge we made the conversion from using PBS/Maui to using SLURM as our scheduler and resource manager.

Hardware

Management nodes

The head node and login node are Dell commodity servers configured as follows.

Dell R430: Dual 8 core Haswell CPUs with 64GB of DDR4 ram and dual 1TB 7.2K rpm drives in RAID 1

Compute nodes

The newly added compute nodes are all SuperMicro super servers TP-2028 chassis configured as follows.

SuperMicro TP-2028: 4 node chassis with each node containing dual 16 core Haswell CPUs with 256 GB DDR4 ram and 6 300GB 15K SAS drives in raid 0.

Storage

The Forge home directory storage is a Dell NSS high availability storage solution. This storage will provide 480 TB of raw storage, 349 TB of that is available for users, limited to 50GB per user, which can be expanded upon request with proof of need. This volume is not backed up, we do not provide any data recovery guarantee in the event of a storage system failure. System failures where data loss occurs are rare, but they do happen. All this to say, you should not be storing the only copy of your critical data on this system.

Policies

Under no circumstances should your code be running on the login node.

You are allowed to install software in your home directory for your own use. Know that you will *NOT* be given root/sudo access, so if your software requires it you will not be able to use that software. Contact ITRSS about having the software installed cluster-wide.
User data on the Forge is **not backed up** meaning it is your responsibility to back up important research data to a location off site via any of the methods in the **moving data** section.

If you are a student your jobs can run on any compute node in the cluster, even the ones dedicated to researchers, however if the researcher who has priority access to that dedicated node then your job will stop and go back into the queue. You may prevent this preemption by specifying to run on just the general nodes in your job file, please see the documentation on how to submit this request.

If you are a researcher who has purchased priority access for 3 years to an allocation of nodes your jobs will primarily run on those nodes, if your job requires more resources than you have available in your priority queue your job will run in the general queue at the same priority as student jobs. You may add users to your allocation so that your research group may also benefit from the priority access.

If you are a researcher who has purchased an allocation of CPU hours you will run on the general nodes at the same priority as the students. Your job will not run on any dedicated nodes and will not be susceptible to preemption by any other user. Once your job starts it will run until it fails, completes, or runs out of allocated time.

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**Partitions**

The Hardware in the Forge is split up into separate groups, or partitions. Some hardware is in more
than one partition, for the most part you won't have to define a partition in a job submission file as we have a plugin that will select the best partition for your user for the job to run in. However there are a few cases that you will want to assign a job to a specific partition. Please see the table below for a list of the limits or default values given to jobs based on the partition. The important thing to note is how long you can request your job to run.

<table>
<thead>
<tr>
<th>Partition</th>
<th>Time Limit</th>
<th>Default Memory per CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>short</td>
<td>4 hours</td>
<td>1000MB</td>
</tr>
<tr>
<td>requeue</td>
<td>7 days</td>
<td>1000MB</td>
</tr>
<tr>
<td>free</td>
<td>14 days</td>
<td>1000MB</td>
</tr>
<tr>
<td>any priority partition</td>
<td>30 days</td>
<td>varies by hardware</td>
</tr>
</tbody>
</table>

Quick Start

Logging in

SSH (Linux)

Open a terminal and type

```bash
ssh username@forge.mst.edu
```

replacing username with your campus sso username, Enter your sso password

Logging in places you onto the login node. Under no circumstances should you run your code on the login node.

If you are submitting a batch file, then your job will be redirected to a compute node to be computed.

However, if you are attempting use a GUI, ensure that you do not run your session on the login node (Example: username@login-44-0). Use an interactive session to be directed to a compute node to run your software.

```bash
sinteractive
```

For further description of sinteractive, read the section in this documentation titled Interactive Jobs.

Putty (Windows)

Open Putty and connect to forge.mst.edu using your campus SSO.
Off Campus Logins

Our off campus logins go through a different host, forge-remote.mst.edu and use public key authentication only, password authentication is disabled for off campus users. To learn how to connect from off campus please see our how to on setting up public key authentication

Submitting a job

Using SLURM is very similar to using PBS/Maui to submit jobs, you need to create a submission script to execute on the backend nodes, then use a command line utility to submit the script to the resource manager. See the file contents of a general submission script complete with comments.

Example Job Script

batch.sub

#!/bin/bash
#SBATCH --job-name=Change_ME
#SBATCH --ntasks=1
#SBATCH --time=0-00:10:00
#SBATCH --mail-type=begin,end,fail,requeue
#SBATCH --export=all
#SBATCH --out=Forge-%j.out

# %j will substitute to the job's id
# now run your executables just like you would in a shell script, Slurm
will set the working directory as the directory the job was submitted from. # e.g. if you submitted from /home/blspcy/softwaretesting your job would run in that directory.

# (executables) (options) (parameters)
  echo "this is a general submission script"
  echo "I've submitted my first batch job successfully"

Now you need to submit that batch file to the scheduler so that it will run when it is time.

```
sbatch batch.sub
```

You will see the output of sbatch after the job submission that will give you the job number, if you would like to monitor the status of your jobs you may do so with the `squeue` command.

**Common SBATCH Directives**

<table>
<thead>
<tr>
<th>Directive</th>
<th>Valid Values</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-job-name=</td>
<td>string value no spaces</td>
<td>Sets the job name to something more friendly, useful when examining the queue.</td>
</tr>
<tr>
<td>-ntasks=</td>
<td>integer value</td>
<td>Sets the requested CPUs for the job</td>
</tr>
<tr>
<td>-nodes=</td>
<td>integer value</td>
<td>Sets the number of nodes you wish to use, useful if you want all your tasks to land on one node.</td>
</tr>
<tr>
<td>-time=</td>
<td>D-HH:MM:SS, HH:MM:SS</td>
<td>Sets the allowed run time for the job, accepted formats are listed in the valid values column.</td>
</tr>
<tr>
<td>-mail-type=</td>
<td>begin,end,fail,requeue</td>
<td>Sets when you would like the scheduler to notify you about a job running. By default no email is sent</td>
</tr>
<tr>
<td>-mail-user=</td>
<td>email address</td>
<td>Sets the mailto address for this job</td>
</tr>
<tr>
<td>-export=</td>
<td>ALL, or specific variable names</td>
<td>By default Slurm exports the current environment variables so all loaded modules will be passed to the environment of the job</td>
</tr>
<tr>
<td>-mem=</td>
<td>integer value</td>
<td>number in MB of memory you would like the job to have access to, each queue has default memory per CPU values set so unless your executable runs out of memory you will likely not need to use this directive.</td>
</tr>
<tr>
<td>-mem-per-cpu=</td>
<td>integer</td>
<td>Number in MB of memory you want per cpu, default values vary by queue but are typically greater than 1000Mb.</td>
</tr>
<tr>
<td>-nice=</td>
<td>integer</td>
<td>Allows you to lower a job's priority if you would like other jobs set to a higher priority in the queue, the higher the nice number the lower the priority.</td>
</tr>
<tr>
<td>-constraint=</td>
<td>please see sbatch man page for usage</td>
<td>Used only if you want to constrain your job to only run on resources with specific features, please see the next table for a list of valid features to request constraints on.</td>
</tr>
</tbody>
</table>
| -gres=      | name:count                    | Allows the user to reserve additional resources on the node, specifically for our cluster gpus. e.g. 
  -gres=gpu:2 will reserve 2 gpus on a gpu enabled node |
-p partition_name

Not typically used, if not defined jobs get routed to the highest priority partition your user has permission to use. If you were wanting to specifically use a lower priority partition because of higher resource availability you may do so.

### Valid Constraints

<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>intel</td>
<td>Node has intel CPUs</td>
</tr>
<tr>
<td>amd</td>
<td>Node has amd CPUs</td>
</tr>
<tr>
<td>EDR</td>
<td>Node has an EDR (100Gbit/sec) infiniband interconnect</td>
</tr>
<tr>
<td>FDR</td>
<td>Node has a FDR (56Gbit/sec) infiniband interconnect</td>
</tr>
<tr>
<td>QDR</td>
<td>Node has a QDR (36Gbit/sec) infiniband interconnect</td>
</tr>
<tr>
<td>DDR</td>
<td>Node has a DDR (16Gbit/sec) Infiniband interconnect</td>
</tr>
<tr>
<td>serial</td>
<td>Node has no high speed interconnect</td>
</tr>
<tr>
<td>gpu</td>
<td>Node has GPU acceleration capabilities</td>
</tr>
</tbody>
</table>

### Monitoring your jobs

```
squeue -u username
```

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>STATE</th>
<th>TIME</th>
<th>CPUS</th>
<th>NODES</th>
</tr>
</thead>
<tbody>
<tr>
<td>719</td>
<td>requeue</td>
<td>Submit</td>
<td>blspcy</td>
<td>RUNNING</td>
<td>00:01</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

### Cancel your job

```
scancel <jobnumber>
```

### Viewing your results

Output from your submission will go into an output file in the submission directory, this will either be slurm-jobnumber.out or whatever you defined in your submission script. In our example script we set this to Forge-jobnumber.out, this file is written asynchronously so it may take a bit after the job is complete for the file to show up if it is a very short job.

### Moving Data

Moving data in and out of the forge can be done with a few different tools depending on your operating system and preference.

### DFS volumes

Missouri S&T users can mount their web volumes and S Drives with the...
mountdfs

command. This will mount your user directories to the login machine under /mnt/dfs/$USER. The data can be copied over with command line tools to your home directory, **your data will not be accessible from the compute nodes so do not submit jobs from these directories.** Aliases “cds” and “cdwww” have been created to allow you to cd into your s drive and web volume quickly and easily.

**Windows**

**WinSCP**

Using winSCP connect to forge.mst.edu using your SSO just as you would with ssh or putty and you will be presented with the contents of your home directory. Now you will be able to drag files into the winscp window and drop them in the folder you want them in and the copying process should begin. It should also work the same in the opposite direction to get data back out.

**Filezilla**

Using Filezilla you connect to forge.mst.edu using your SSO and you will have the contents of your home directory displayed, drag and drop works with Filezilla as well.

**Git**

git is installed on the cluster and is recommended to keep track of code changes across your research. See [getting started with git](https://git.mst.edu) for usage guides, Campus offers a hosted private git server at [https://git.mst.edu](https://git.mst.edu) at no additional cost.

**Linux**

**Filezilla**

See windows instructions

**scp**

scp is a command line utility that allows for secure copies from one machine to another through ssh, scp is available on most Linux distributions. If I wanted to copy a file in using scp I would open a terminal on my workstation and issue the following command.

```
scp /home/blspcy/batch.sub blspcy@forge.mst.edu:/home/blspcy/batch.sub
```
It will then ask me to authenticate using my campus SSO, then copy the file from my local local location of /home/blspcy/batch.sub to my forge home directory. If you have questions on how to use scp I recommend reading the man page for scp, or check it out online at SCP man page.

rsync

rsync is a more powerful command line utility than scp, it has a simpler syntax, and checks to see if the file has actually changed before performing the copy. See the man page for usage details or online documentation.

git

See git for windows for instruction, it works the same way.

Modules

An important concept for running on the cluster is modules. Unlike a traditional computer where you can run every program from the command line after installing it, with the cluster we install the programs to a main “repository” so to speak, and then you load only the ones you need as modules. To see which modules are available for you to use you would type “module avail”. Once you find which module you need for your file, you type “module load <module>” where <module> is the module you found you wanted from the module avail list. You can see which modules you already have loaded by typing “module list”.

Here is the output of module avail as of 06/26/2017

--------------------------------------------------
/share/apps/modulefiles/mst-mpi-modules
--------------------------------------------------

intelmpi

openmpi/1.10.6/intel/2013_sp1.3.174 openmpi/2.1.0/intel/2015.2.164
(D) openmpi/2.0.2/gnu/4.9.3
mvapich2/gnu/4.9.2/eth
mvapich2/intel/11/eth
mvapich2/intel/11/ib
openmpi/intel/11/backup
openmpi/intel/11/eth
mvapich2/intel/13/eth
openmpi/intel/11/ib
mvapich2/intel/12/ib
openmpi/intel/13/backup
mvapich2/intel/15/eth
(D) openmpi/intel/12/eth
mvapich2/intel/15/ib
(D)
openmpi/2.0.2/intel/2011_sp1.11.339

mvapich2/pgi/11.4/eth

openmpi/2.0.2/intel/2013_sp1.3.174

mvapich2/pgi/11.4/ib

openmpi/2.0.2/intel/2015.2.164

openmpi

openmpi/pgi/11.4/eth

openmpi/1.10.6/gnu/4.9.3

openmpi/1.10.6/ib

rocks-openmpi

rocks-openmpi_ib

openmpi/2.1.0/intel/2011_sp1.11.339

openmpi/2.1.0/intel/2013_sp1.3.174

---

/share/apps/modulefiles/mst-lib-modules

--------------

arpack

python/modules/argparse/1.4.0

atlas/gnu/3.10.2

python/modules/decorator/4.0.11

BOOST/gnu/1.55.0

python/modules/kwant/1.0.5

hdf/5/mvapich2_ib/gnu/1.8.14

hdf/5/mvapich2_ib/intel/1.8.14

hdf/5/mvapich2_ib/pgi/1.8.14

cgns/openmpi_ib/gnu

cgns/openmpi_ib/intel

cgns/openmpi_ib/intel/1.8.14

fftw/mvapich2_ib/gnu4.9.2/2.1.5

python/modules/mkl/2011_sp1.11.339

python/modules/numpy/1.10.0

fftw/mvapich2_ib/intel2015.2.164/2.1.5

fftw/mvapich2_ib/pgi11.4/2.1.5

fftw/mvapich2_ib/intel2015.2.164/3.3.4

fftw/mvapich2_ib/pgi11.4/2.1.5

netcdf/mvapich2_ib/gnu/3.6.2
fftw/mvapich2_ib/pgi11.4/3.3.4 (D)
netcdf/mvapich2_ib/gnu/4.3.2 (D)
python/modules/scipy/0.16.0
fftw/openmpi_ib/gnu4.9.2/2.1.5
netcdf/mvapich2_ib/intel/3.6.2
python/modules/sympy/1.0
fftw/openmpi_ib/gnu4.9.2/3.3.4 (D)
netcdf/mvapich2_ib/intel/4.3.2 (D)
python/modules/theano/0.8.0

lines 1-79

/share/apps/modulefiles/mst-app-modules ------------------------------------
-------------
AnsysEM/17/17 cp2k maple/2015
(D) qe
cst/2014 (D) cplot maple/2016
qmcpack/3.0
cst/2015 cpmd matlab/2012
qmcpack/2014
cst/2016 dirac matlab/2013a
qmcpack/2016 (D)
cst/2017 dock/6.6eth matlab/2014a
(D) rum
dock/2.3.1 (D) dock/6.6ib matlab/2016a
samtools
dock/6.6ib (D) espresso matlab/2017a
scipy
dock/2.3.x (D) espresso matlab/2017a
siesta
dock/6.6ib (D) espresso matlab/2017a
spark
dock/6.6ib (D) espresso matlab/2017a
sparta
fun3d/custom (D) mcnp
molpro/2010.1.nightly
fun3d/12.2 mctdh
molpro/2010.1.3
fun3d/12.2 mctdh
molpro/2010.1.25
fun3d/12.2 mctdh
molpro/2012.1.nightly (D)
gamess
abacus/6.11-2
gamess
molpro/2012.1.9
abacus/6.11-2
gamess
molpro/2015.1.source.block
abacus/6.11-2
gamess
molpro/2015.1.source.s
abacus/2016
gamess
molpro/2015.1.source
geos
accelrys/material_studio/6.1
gmp
amber/12
geos
molpro/2015.1
amber/13
gmp
molpro/2015.1
amber/13
gmp
molpro/2015.1
amber/13
gmp
tecplot/2013
amd/14.0
amd/14.0
amd/14.0
gmp
tecplot/2014 (D)
mobo-3.6.4
amd/14.0
gmp
tecplot/2014 (D)
mobo-3.6.4
amd/14.0
gmp

ansys/15.0  (D) gridgen                   mpc
tecplot/2016.old   gromacs
ansys/17.0
msc/adams/2015   tecplot/2016
ansys/18.0  hadoop/1.1.1
msc/nastran/2014  trinity
apbs              hadoop/1.2.1
msc/patran/2014  valgrind/3.12
bowtie            hadoop/2.6.0  (D) namd/2.9
vasp/4.6          lammps/9Dec14  namd/2.10
casino            lammps/17Nov16  namd/2.12b
(D) vasp/5.4.1  (D)
cmg
visit/2.8.2
comsol/4.3a
visit/2.9.0  (D)
comsol/4.4  (D)
linpack
vmd
comsol/5.2a_deng
vulcan
comsol/5.2a_park
parmetis/4.0.3
comsol/5.2a_yang
comsol/5.2a_zaeem
lammps/30July16  (D) octave
lammps/17Nov16
lammps/30July16  (D)
lammps/30July16
visit/2.9.0  (D)
comsol/5.2a_deng
comsol/5.2a_park
comsol/5.2a_yang
comsol/5.2a_zaeem
lsdyna/8.0
packmol
lsdyna/8.1.hybrid
lsdyna/8.1  (D) proj
maple/16
psi4

---------------------------------------------- /share/apps/modulefiles/mst-
compiler-modules -----------------------------------------------
cilk/5.4.6         gnu/4.9.3    gpi2/1.0.1
intel/2015.2.164  (D) python/2.7.9
cmake/3.2.1  (D) gnu/5.4.0    gpi2/1.1.1  (D) mono/3.12.0
python/3.5.2_GCC  gnu/6.3.0    intel/2011_sp1.11.339  pgi/11.4
cmake/3.6.2
python/3.5.2  (D) gnu/7.1.0    intel/2013_sp1.3.174
pgi/RCS/11.4,v

Where:
L: Module is loaded
D: Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules
matching any of the "keys".

Compiling Code

There are several compilers available through modules, to see a full list of modules run

module avail
the naming scheme for the compiler modules are as follows.

MPI_PROTOCOL/COMPILER/COMPILER_VERSION/INTERFACE e.g openmpi/intel/15/ib is the 2015 intel compiler built with openmpi libraries and is set to communicate over the high speed infiniband interface.

After you have decided which compiler you want to use you need to load it.

```
module load openmpi/intel/15/ib
```

Then compile your code, use mpicc for c code and mpif90 for fortran code. Here is an MPI hello world C code.

```
/* C Example */
#include <stdio.h>
#include <mpi.h>

int main (argc, argv)

    int argc;
    char *argv[];

{
    int rank, size;

    MPI_Init (&argc, &argv); /* starts MPI */
    MPI_Comm_rank (MPI_COMM_WORLD, &rank); /* get current process id */
    MPI_Comm_size (MPI_COMM_WORLD, &size); /* get number of processes */

    printf( "Hello world from process %d of %d\n", rank, size );
    MPI_Finalize();
    return ;
}
```

Use mpicc to compile it.

```
mpicc ./helloworld.c
```

Now you should see a a.out executable in your current working directory, this is your mpi compiled code that we will run when we submit it as a job.

**Submitting an MPI job**

You need to be sure that you have the same module loaded in your job environment as you did when you compiled the code to ensure that the compiled executables will run correctly, you may either load them before submitting a job and use the directive
in your submission script, or load the module prior to running your executable in your submission script. Please see the sample submission script below for an mpi job.

```
#!/bin/bash
#SBATCH --export=all
#SBATCH -J MPI_HELLO
#SBATCH --ntasks=8
#SBATCH --export=all
#SBATCH --out=Forge-%j.out
#SBATCH --time=0:00:10:00
#SBATCH --mail-type=begin,end,fail,requeue
module load openmpi/intel/15/ib
mpirun ./a.out
```

Now we need to submit that file to the scheduler to be put into the queue.

```
sbatch helloworld.sub
```

You should see the scheduler report back what job number your job was assigned just as before, and you should shortly see an output file in the directory you submitted your job from.

**Interactive jobs**

Some things can't be run with a batch script because they require user input, or you need to compile some large code and are worried about bogging down the login node. To start an interactive job simply use the

```
sinteractive
```

command and your terminal will now be running on one of the compute nodes. The hostname command can help you confirm you are no longer running on a login node. Now you may run your executable by hand without worrying about impacting other users. The sinteractive script by default will allot a 1 cpu for 1 hour, you may request more by using SBATCH directives, e.g.

```
sinteractive --time=02:00:00 --cpus-per-task=2
```

will start a job with 2 CPUs on one node for 2 hours.

If you will need a GUI Window for whatever you are running inside the interactive job you will need to connect to The Forge with X forwarding enabled. For Linux this is simply adding the -X switch to the ssh command.

```
ssh forge.mst.edu -X
```
For Windows there are a couple X server software's available for use, x-ming and x-win32 that can be configured with putty. Here is a simple guide for configuring putty to use xming.

**Job Arrays**

If you have a large number of jobs you need to start I recommend becoming familiar with using job arrays, basically it allows you to submit one job file to start up to 10000 jobs at once.

One of the ways you can vary the input of the job array from task to task is to set a variable based on which array id the job is and then use that value to read the matching line of a file. For instance the following line when put into a script will set the variable PARAMETERS to the matching line of the file data.dat in the submission directory.

```
PARAMETERS=$(awk -v line=${SLURM_ARRAY_TASK_ID} '{if (NR == line) { print $0; };};' ./data.dat)
```

You can then use this variable in your execution line to do whatever you would like to do, you just have to have the appropriate data in the data.dat file on the appropriate lines for the array you are submitting. See the sample data.dat file below.

```
data.dat

"I am line number 1"
"I am line number 2"
"I am line number 3"
"I am line number 4"
```

you can then submit your job as an array by using the -array directive, either in the job file or as an argument at submission time, see the example below.

```
array_test.sub

#!/bin/bash
#SBATCH -J Array_test
#SBATCH --ntasks=1
#SBATCH --out=Forge-%j.out
#SBATCH --time=0-00:10:00
#SBATCH --mail-type=begin,end,fail,requeue

PARAMETERS=$(awk -v line=${SLURM_ARRAY_TASK_ID} '{if (NR == line) { print $0; };};' ./data.dat)

echo $PARAMETERS
```

I prefer to use the array as an argument at submission time so I don't have to touch my submission file again, just the data.dat file that it reads from.
sbatch --array=1-2,4 array_test.sub

Will execute lines 1, 2, and 4 of data.dat which echo out what line number they are from my data.dat file.

You may also add this as a directive in your submission file and submit without any switches as normal. Adding the following line to the header of the submission file above will accomplish the same thing as supplying the array values at submission time.

#SBATCH --array=1-2,4

Then you may submit it as normal

sbatch array_test.sub

Converting From Torque

With the new cluster we have changed resource managers from PBS/Maui to Slurm. We have provided a script to convert your submission files from PBS directives to slurm. This script, pbs2slurm.py, should be in your executable path and can be used as follows.

pbs2slurm.py < batch.qsub > batch.sbatch

Where batch.qsub is the name of your old submission script file and batch.sbatch is the name of your new submission script file. Please see the table below for commonly used command conversions.

<table>
<thead>
<tr>
<th>PBS/Maui Command</th>
<th>Slurm Equivalent</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>qsub</td>
<td>sbatch</td>
<td>Submit a job for execution</td>
</tr>
<tr>
<td>qdel</td>
<td>scancel</td>
<td>Cancel a job</td>
</tr>
<tr>
<td>showq</td>
<td>squeue</td>
<td>check the status of jobs</td>
</tr>
<tr>
<td>qstat</td>
<td>squeue</td>
<td>check the status of jobs</td>
</tr>
<tr>
<td>checkjob</td>
<td>scontrol show job</td>
<td>check the detailed information of a specific job</td>
</tr>
<tr>
<td>checknode</td>
<td>scontrol show node</td>
<td>check the detailed information of a specific node</td>
</tr>
</tbody>
</table>

Checking your account usage

If you have purchased a number of CPU hours from us you may check on how many hours you have used by issuing the

userreport

command from a login node, this will show your account's CPU hour limit and the total amount used.

**Note this is usage for your account, not your user.**
Applications

The applications portion of this wiki is currently a Work in progress, not all applications are currently here, but they will eventually be.

Abaqus

- Default Version = 6.12
- Other versions available - 6.13 & 6.14

This example is for 6.12

The SBATCH commands are explained in the Forge Documentation.

You will need a *.inp file from where you built the model on another system. This .inp file needs to be in the same folder as the jobfile you will create.

Example jobfile:

```
abaqus.sub

#!/bin/bash
#SBATCH --job-name=sbatchfilename.sbatch
#SBATCH --nodes=1
#SBATCH --ntasks=2
#SBATCH --mem=4000
#SBATCH --time=00:60:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=joeminer@mst.edu

input=inputfile.inp

/share/apps/ABAQUS/Commands/abq6123 job=$input analysis cpus=2
interactive
```

- Replace the sbatchfilename.sbatch with the name of your jobfile.
- Replace the email address with your own.
- Replace the inputfile.inp with the *.inp file that you want to analyze.
- Keep ntasks and cpu equal to the same amount of processors

This job will run on 1 node with 2 processors and allocate 4GB of memory per processor. These node/processor values can change, but be aware that the Abaqus licensing is limited and the job may queue for hours or days before licenses are available, depending on the quantities you selected.

Simple breakdown of Abaqus Licensing:
<table>
<thead>
<tr>
<th>Parallel License</th>
<th>Number of Processors used</th>
<th>Tokens Allocated</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>40</td>
</tr>
<tr>
<td>3</td>
<td>16</td>
<td>60</td>
</tr>
<tr>
<td>4</td>
<td>32</td>
<td>80</td>
</tr>
<tr>
<td>5</td>
<td>64</td>
<td>100</td>
</tr>
</tbody>
</table>

**Abaqus 2016**

module load abaqus/2016

`abaqus2016.sbatch`

```
#!/bin/bash
#SBATCH --job-name=sbatchfilename.sbatch
#SBATCH --nodes=1
#SBATCH --ntasks=20
#SBATCH --mem=4000
#SBATCH --partition=requeue
#SBATCH --time=10:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=joemin@mst.edu

unset SLURM_GTIDS

input=inputfile.inp
time abaqus2016hf3 job=$input analysis standard_parallel=all cpus=20
interactive

unset SLURM_GTIDS
```

This is a new variable that must be in place for 2016 to run with MPI.

Chain loading jobs for Abaqus 2016.

`abaqus2016chain.sbatch`

```
#!/bin/bash
#SBATCH --job-name=sbatchfilename.sbatch
#SBATCH --nodes=1
#SBATCH --ntasks=20
#SBATCH --mem=4000
#SBATCH --partition=requeue
#SBATCH --time=10:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
```
Ansys

- Default Version = 15.0
- Other versions available
  - 14.0

Running the Workbench

Be sure you are connected to the Forge with X forwarding enabled, and running inside an interactive job using command

```bash
sinteractive
```

before you attempt to launch the work bench. Running sinteractive without any switches will give you 1 cpu for 1 hour, if you need more time or resources you may request it. See Interactive Jobs for more information.

Once inside an interactive job you need to load the ansys module.

```bash
module load ansys
```

Now you may run the workbench.

```bash
runwb2
```

Job Submission Information

Fluent is the primary tool in the Ansys suite of software used on the Forge. Most of the fluent simulation creation process is done on your Windows or Linux workstation. The 'Solving' portion of a simulation is where the Forge is utilized. Fluent will output a lengthy file, based on the simulation being run and that lengthy output file would be used on your Windows or Linux Workstation to do the final review and analysis of your simulation.
The basic steps

1. Create your geometry
2. Setup your mesh
3. Setup your solving method
4. Use the .cas and .dat files, generated from the first three steps, to construct your jobfile
5. Copy those files to the Forge, to your home folder
6. Create your jobfile using the slurm tools on the Forge Documentation page
7. Load the Ansys module
8. Submit your newly created jobfile with sbatch

Serial Example.

I used the Turbulent Flow example from Cornell's SimCafe.
On the Forge, I have this directory structure for this example. Please create your own structure that makes sense to you.

```
TurbulentFlow/
|-- flntgz-48243.cas
|-- flntgz-48243.dat
|-- output.dat
|-- slurm-8731.out
|-- TurbulentFlow_command.txt
|-- TurbulentFlow.sbatch
```

The .cas file is the CASE file that contains the parameters define by you when creating the model. The .dat file is the data result file used when running the simulation. The .txt file, is the actual, command equivalent, of your model, in a form that the Forge understands. The .sbatch file, is the slurm job file that you will use to submit your model for analysis. The .out file is the output from the run. The .dat file is the binary (ansys specific) file created during the solution, that could be imported into Ansys back on the Windows/Linux workstation for further analysis.

Jobfile Example.

```
#!/bin/bash
#SBATCH --job-name=TurbulentFlow.sbatch
#SBATCH --ntasks=1
#SBATCH --nodes=1
#SBATCH --time=01:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=rlhaffer@mst.edu
#SBATCH -o Forge-%j.out
```
fluent 2ddp -g <
/home/rlhaffer/unitests/ANSYS/TurbulentFlow/TurbulentFlow_command.txt

The SBATCH commands are explained in the Forge Documentation.

The job-name is a name given to help you determine which job is which.
This job will be in the — partition=requeue queue.
It will use 1 node — nodes=1.
It will use 4 processors in one node — ntasks=4.
It has a wall clock time of 1 hour — time=01:00:00.
It will email the user when it begins, ends, or if it fails. -mail-type & -mail-user

fluent is the command we are going to run.
2ddp is the mode we want fluent to use

Modes The [mode] option must be supplied and is one of the following:
* 2d runs the two-dimensional, single-precision solver
* 3d runs the three-dimensional, single-precision solver
* 2ddp runs the two-dimensional, double-precision solver
* 3ddp runs the three-dimensional, double-precision solver
-g turns off the GUI
Path to the command file we are calling in fluent. <
/home/rlhaffer/unitests/ANSYS/TurbulentFlow/TurbulentFlow_command.txt

Contents of command file
This file can get long. As it contains the .cas file & .dat file information as well as saving frequency
and iteration count

NOTE, this is all in one line when creating the command file

/file/rcd /home/rlhaffer/unitests/ANSYS/TurbulentFlow/flntgz-48243.cas
/file/autosave/data-frequency 20000 /solve/iterate 150000 /file/wd
/home/rlhaffer/unitests/ANSYS/TurbulentFlow/output.dat /exit

When the simulation is finished, you will have a Forge-#####.out file that looks something like this:

/share/apps/ansys_inc/v150/fluent/fluent15.0.7/bin/fluent -r15.0.7 2ddp -g
/share/apps/ansys_inc/v150/fluent/fluent15.0.7/cortex/lnamd64/cortex.15.0.7
-f fluent -g (fluent "2ddp -alnamd64 -r15.0.7 -
path/share/apps/ansys_inc/v150/fluent")
Loading
"/share/apps/ansys_inc/v150/fluent/fluent15.0.7/lib/fluent.dmp.114-64"
Done.
/share/apps/ansys_inc/v150/fluent/fluent15.0.7/bin/fluent -r15.0.7 2ddp -
alnamd64 -path/share/apps/ansys_inc/v150/fluent -cx
edrcompute-43-17.local:56955:53521
Starting
/share/apps/ansys_inc/v150/fluent/fluent15.0.7/lnamd64/2ddp/fluent.15.0.7 -
cx edrcompute-43-17.local:56955:53521
   Welcome to ANSYS Fluent 15.0.7
Loading
"/share/apps/ansys_inc/v150/fluent/fluent15.0.7/lib/flprim.dmp.1119-64"
Done.

This is an academic version of ANSYS FLUENT. Usage of this product license is limited to the terms and conditions specified in your ANSYS license form, additional terms section.

Cleanup script file is /home/rlhaffer/unittests/ANSYS/TurbulentFlow/cleanup-fluent-edrcompute-43-17.local-17945.sh

> Reading "/home/rlhaffer/unittests/ANSYS/TurbulentFlow/flntgz-48243.cas"
  3000 quadrilateral cells, zone 2, binary.
  5870 2D interior faces, zone 1, binary.
    30 2D velocity-inlet faces, zone 5, binary.
    30 2D pressure-outlet faces, zone 6, binary.
  100 2D wall faces, zone 7, binary.
  100 2D axis faces, zone 8, binary.
  3131 nodes, binary.
  3131 node flags, binary.

Building...
  mesh
  materials,
  interface,
  domains,
  mixture
    zones,
  pipewall
  outlet
  inlet
    interior-surface_body
  centerline
  surface_body
Done.

Reading "/home/rlhaffer/unittests/ANSYS/TurbulentFlow/flntgz-48243.dat"
Done.
  iter continuity x-velocity y-velocity k epsilon
time/iter
Parallel Example

To use fluent in parallel please you need set the PBS_NODEFILE environment variable inside your job. Please see example submission file below.

TurbulentFlow.sbatch

```bash
#!/bin/bash

#SBATCH --job-name=TurbulentFlow.sbatch
#SBATCH --ntasks=32
#SBATCH --time=01:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=rlhaffer@mst.edu
#SBATCH -o Forge-%j.out

#generate a node file
export PBS_NODEFILE=generate_nodefile

#run fluent in parallel.
fluent 2ddp -g -t32 -pinfiniband -cnf=$PBS_NODEFILE -ssh <
/home/rlhaffer/unittests/ANSYS/TurbulentFlow/TurbulentFlow_command.txt
```

Interactive Fluent

If you would like to run the full GUI you may do so inside an interactive job, make sure you've connected to The Forge with X Forwarding enabled. Start the job with.

```
sinteractive
```

This will give you 1 processor for 1 hour, to request more processors or more time please see the documentation at Interactive Jobs.

Once inside the interactive job you will need to load the ansys module.

```
module load ansys
```
Then you may start fluent from the command line.

```
fluent 2ddp
```

will start the 2d, double precision version of fluent. If you've requested more than one processor you need to first run

```
export PBS_NODEFILE=`generate_nodefile`
```

Then you need to add some switches to fluent to get it to use those processors.

```
fluent 2ddp -t## -pethernet -cnf=$PBS_NODEFILE -ssh
```

You need to replace the ## with the number of processors requested.

**Ansys Mechanical**

Tested for version 18.1

**Simple tutorial**

`round.sbatch`

```bash
#!/bin/bash
#SBATCH --job-name=round
#SBATCH --ntasks=10
#SBATCH --mem=20000
#SBATCH -p=requeue
#SBATCH --time=00:60:00
--comment
#SBATCH --mail-type=begin
--comment
#SBATCH --mail-type=end
#SBATCH --export=all
#SBATCH --out=Forge-%j.out
module load ansys/18.1

time ansys181 -j round -b -dis -np 10 <
/home/rlhaffer/unittests/ANSYS/roundthing/round.log
```

ansys mechanical log file

`round.inp`

```
/INPUT,'round','inp',,,
/SOLU
SOLVE
```
AnsysEM

- Default Version = 17.0
- Also Called Ansys Electronics Desktop

```bash
#!/bin/bash
#SBATCH --job-name=jobfile.sbatch
#SBATCH --partition=requeue
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=20
#SBATCH --time=01:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=joe miner@mst.edu
module load AnsysEM/17

time ansysedt -ng -batchsolve Model_Cluster_Test_v2.aedt
```

CMG

Computer Modeling Group - This is a WORKING SECTION - Edits are actively taking place.

Default version = 2015

**Constructing the jobfile**

From the Windows installation the `.dat` model will be needed.

Please follow the general Forge documentation for submission techniques.

After logged into The Forge, run:

```bash
module load cmg
```

This loads environment variables needed to for CMG to function.

Copy your `.dat` file from your Windows system to your cluster home folder. This is explained in the Forge documentation.
Example sbatch jobfile

```bash
#!/bin/bash
#SBATCH --job-name=batchfilename.sbatch
#SBATCH --nodes=1
#SBATCH --ntasks=7
#SBATCH --mem=17000
#SBATCH --time=10:00:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=joeminer@mst.edu
#SBATCH --export=ALL

RunSim.sh gem 2015.10 GasModel4P.dat -parasol 7
```

| RunSim.h | the CMG sim script that allows the simulation to run on multiple processors |
| gem | the solver specified |
| 2015.10 | version of the software used |
| GasModel4P.dat | the model to be analyzed |
| -parasol 7 | this is the command switch to tell CMG there are processors to use. In this example, 7 processors were allocated. |

**CMG licensing**

When running the above example, we discovered how CMG's licensing really works. We have varying quantities of licenses for different features and each seat of those licenses equates to 20 solver tokens that will be allocated to jobs on the cluster.

For this example..

- **20** tokens of the **solve-stars** solver are being used, because we have an instance of the solver open.
- **35** tokens of the **solve-parallel** solver are being used, because we have asked for 7 processors.

We currently have 8 seats for **Stars** and 8 seats for **Parallel**. This equates to **160** tokens of each. Out of that **160** tokens, your job can take at least **20** tokens from the stars solver, and up to **160** tokens of the parallel solver.

**160** tokens of the parallel solver actually equates to 32 processors when building the job file.

So, the max processors requested is **32**.

**Token Scenario example**

If a student submits a parallel job asking for 32 processors (all 160 tokens) and all 160 are free, the job will begin running.
If a second student then submits a job asking for 10 processors (50 tokens) but all 160 are currently in use, the job will fail. In the output file of the failed job, it will indicate that the job failed because it did not have enough licenses to run.

If this happens, the best suggestion is to modify your jobfile with a smaller number of processors. This may take a few iterations until you find a number of processors that will work.

There is no efficient way to know how many licenses are in use.

Licensing for CMG is limited. Some features have 2160 tokens, some only 100. Please be patient when submitting jobs as they could fail in this no license manner.

The jobs tested only indicate the solve-star and solve-parallel are being used. We have not seen a test case using these other features:

```
gem_forgas
gem_gap
imex_forgas
imex_gap
imex_iam
stars_forgas
stars_gap
winprop
builder
cmost_studio
dynagrid
solve_university
rlm_roam
```

CST

- (Computer Simulation Technology)
- Default version = 2014
- Other versions available = 2015

Job Submission information

CST is an electromagnetic simulation solver, primarily used by the EMCLab.

Steps.

1. Build your simulation on one of the Windows workstations available to you.
2. Copy your .cst file to your home directory on the Forge.
3. Write you job submission file.
4. Either use the default CST version of 2014 or use 2015 by loading its module file.

```
module load CST/2015
```

Example Job File

CST.sub
```bash
#!/bin/bash
#SBATCH --job-name=CST_Test
#SBATCH --nodes=1
#SBATCH --ntasks=2
#SBATCH --mem=4000
#SBATCH --partition=cuda
#SBATCH --gres=gpu:2
#SBATCH --time=08:00:00
#SBATCH --mail-type=FAIL
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-user=joeminer@mst.edu

cst_design_environment /home/userID/path/to/.cst/file/example.cst --r -withgpu=2
```

This job will use 1 node, 2 processors from that node, 4GB of memory, the cuda queue, 2 gpus, 8 hours of wall clock time and email the user when the job starts, ends, or fails.

This will output the results in the standard CST folder structure:

```
/path/to/.cst/file/example
|-- DC
|-- Model
|-- ModelCache
|-- Model.lok
|-- Result
|-- SP
   -- Temp
```

**Cuda**

If you would like to use CUDA programs or GPU accelerated code you will need to use our GPU nodes. Access to our GPU nodes is granted on a case by case basis, please request access to them through the help desk or submit a ticket at [http://help.mst.edu](http://help.mst.edu).

Our login nodes don't have the CUDA toolkit installed so to compile your code you will need to start an interactive job on these nodes to do your compilation.

```
sinteractive -p cuda --time=01:00:00 --gres=gpu:1
```

This interactive session will start on a cuda node and give you access to one of the GPUs on the node, once started you may compile your code and do whatever testing you need to do inside this interactive session.

To submit a job for batch processing please see this example submission file below.

`cuda.sub`
This file requests 1 cpu and 1 gpu on 1 node for 1 hour, to request more cpus or more gpus you will need to modify the values related to ntasks and gres=gpu. It is recommended that you at least have 1 cpu for each gpu you intend to use, we currently only have 2 gpus available per node. Once we incorporate the remainder of the GPU nodes we will have 7 gpus available in one chassis.

**Espresso**

- Espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.
- Default version - 5.2.1

All of the available pseudopotential files `.UPF` as of 12/14/2015, are copied into the pseudo install folder.

Before running an Espresso job, run:

```
module load espresso
```

Example:

The `sbatch` file is the job file you will run on the Forge HPC.
The `.pw.in` is the input file you create, that you will reference in the jobfile.
In the job file, change the path to your input file.
In the `.pw.in` file, change the paths of `outdir`, `wfcdir` to a location in your Forge home directory and change the `pseudo_dir` path as in the example below.

**FeGeom2BU.sbatch**

```
#!/bin/bash
#SBATCH --job-name=FeGeomBU
#SBATCH --ntasks=20
#SBATCH --time=0-04:00:00
#SBATCH --mail-type=begin,end,fail,requeue
#SBATCH --out=forge-%j.out

./a.out
```
mpirun pw.x -procs 20 -i /path/to/your/inputfile/FeGeom2BU.pw.in

FeGeom2BU.pw.in

```xml
&CONTROL
    title = 'Na3FePO4CO3 geom+U',
    calculation = 'vc-relax',
    outdir = '/path/to/your/inputfile',
    wfcdir = '/path/to/your/inputfile',
    pseudo_dir =
        '/share/apps/ espresso/ espresso-5.2.1/pseudo',
    prefix = 'Na3FePO4CO3Geom',
    verbosity = 'high',
/
&SYSTEM
    ibrav = 12,
        A = 8.997 ,
        B = 5.163 ,
        C = 6.741 ,
        cosAB = -0.0027925231 ,
        nat = 11,
        ntyp = 5,
        ecutwfc = 40 ,
        ecutrho = 400 ,
        lda_plus_u = .true. ,
        lda_plus_u_kind = ,
        Hubbard_U(1) = 6.39,
        space_group = 11 ,
        uniqueb = .false. ,
/
&ELECTRONS
    conv_thr = 1d-6 ,
    startingpot = 'file' ,
    startingwfc = 'atomic' ,
/
&IONS
    ion_dynamics = 'bfgs' ,
/
&CELL
    cell_dynamics = 'bfgs' ,
    cell_dofree = 'all' ,
/
ATOMIC_SPECIES
    Fe   55.93300   Fe.pbe-sp-van_mit.UPF
    P   30.97400   P.pbe-van_ak.UPF
    C  12.01100   C.pbe-van_ak.UPF
    O  15.99900   O.pbe-van_ak.UPF
    Na 22.99000   Na.pbe-sp-van_ak.UPF

ATOMIC_POSITIONS crystal_sg
    Fe  0.362400000  0.279900000  0.250000000
```

IT Research Support Team - https://wiki.mst.edu/itrst/
Lammps

To use lammps you will need to load the lammps module

```
module load lammps
```

and use a submission file similar to the following

```
lammps.sub

#SBATCH -J Zn-ZnO-rapid
#SBATCH --ntasks=4
#SBATCH --mail-type=FAIL
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --time=02:00:00
#SBATCH --export=ALL

module load lammps/23Oct2017

mpirun lmp_forge < in.heating
```

Other options may be configured. please refer to the lammps documentation.

Version 23Oct2017 has support for the following packages

```
asphere body class2 colloid compress coreshell dipole granular kspace
manybody mc mean misc molecule mpiio opt peri python qeq replica rigid shock
snap srd user-cgdna user-cgsdk user-diffraction user-dpd user-drude user-eff
user-fep user-lb user-manifold user-meamc user-meso user-mgpt user-misc
user-molfile user-netcdf user-omp user-phonon user-qtb user-reaxc user-smtbq
```
Maple

Default version = 2015

Example:

This is a simple polynomial and the goal is to find the roots of the polynomial.

Open Maple on your Windows or Linux workstation and start a new project:

```
findroots.mpl
```

```
# Solve a simple polynomial equation
f(x):=(x^9-x^8+x^7-x^6+x^5-x^4+x^3-x^2+x^4+9*x^3-2.4^2+.5*x)/(x-1);
myroots:=solve(f(x)=148596);

# Save the results into a Maple input file for later post-processing.
save myroots, "myroots.mpl";
```

When this runs, it will save the output to the myroots.mpl file.

As seen in Maple:

Now, you need to SSH into the Forge with your MST userID/password.

Once connected, you need to copy the findroots.mpl file from your local system to your home directory on the cluster.
You can build your folder structure on the Forge how you wish, just use something that is meaningful.

Once copied, you can return to your terminal on Forge and create your jobfile to run your findroots.mpl project.

Open vi to create your job file.

Since this example is simple, it is assigned 1 node, with 2 processors and 15 minutes wall time. The job will email when it begins, ends or fails.

First:

```
module load maple/2015
```

Then write your jobfile:

```
maple.sub
```

```bash
#!/bin/bash

#SBATCH --job-name=maple_example
#SBATCH --nodes=1
#SBATCH --ntasks=2
#SBATCH --mem=2000
#SBATCH --time=00:15:00
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-type=FAIL
#SBATCH --mail-user=rlhaffer@mst.edu

maple -q findroots.mpl
```

Then run:

```
sbatch maple.sbatch
```

When the job finishes, you will have a

```
slurm-jobID.out
```

This contains the output of the finished job.

**Matlab**
Matlab is available to run in batch form or interactively on the cluster, we currently have versions 2012, 2013a, and 2014a installed through modules.

**Interactive Matlab**

The simplest way to get up and running with matlab on the cluster is to simply run

```
matlab
```

from the login node. This will start an interactive job on the backend nodes, load the 2014a module and open matlab. If you have connected with X forwarding you will get the full matlab GUI to use however you would like. This method however limits you to 1 core for 4 hours maximum on one of our compute nodes. To use more than 1 core, or run for longer than 4 hours, you will need to submit your job as a batch submission and use Matlab's Distributive Computing Engine.

**Batch Submit**

If you want to use Batch Submissions for Matlab you will need to create a submission script similar to the ones above in quick start, but you will want to limit the nodes your job runs on 1, please see the sample submission script below.

```
#!/bin/bash

#SBATCH --nodes=1
#SBATCH --ntasks=12
#SBATCH -J Matlab_job
#SBATCH -o Forge-%j.out
#SBATCH --time=01:00:00
module load matlab
matlab < helloworld.m
```

This submission asks for 12 processors on 1 node for an hour, the maximum per node we currently have is 64. If you load the any version older than 2014a your matlab can't use more than 12 processors as that is what mathworks limited you to using on one machine, however Mathworks lifted this limitation to 512 processors in 2014a.

**Distributive Computing Engine**

Mathworks has developed a parallel computing product that the campus has purchased licenses for, We have developed a parallel cluster profile that must be loaded on a user to user basis. To begin using the distributive computing profile you must open an interactive matlab session with X forwarding so you get the matlab GUI.
[blspcy@login-44-0 ~]$ matlab

Once the GUI is open you need to open the parallel computing options menu, noted simply by parallel.

Now open the Parallel profile manager and import the Forge.settings profile from the root directory of the version of matlab you are using, e.g. for 2014a /share/apps/matlab/matlab-2014/
You will now have a Forge_IMPORT profile in your profile list, select this profile and set it as default.

If you would like you may validate the imported profile and see that it is indeed working.

The validation will run a series of five tests which it should pass, if for any reason the profile doesn't pass any test please contact the helpdesk or create a ticket at http://help.mst.edu
To modify how many workers the pool will try to use when you call

```
matlabpool open
```

**in your matlab script** you may edit the profile and set the NumWorkersRange value to the number you wish to use, or simply specify when you call the pool open

```
matlabpool open 24
```

will open a pool of 24 workers.

You may now use `matlabpool open` in your code and it will call the Forge cluster profile configured above. These steps must be followed for every version of Matlab you wish to use before calling the pool. The parallel profiles are only built for versions newer than 2014a.

To make use of this new found power you must implement

```
matlabpool open
```

calls in your matlab script then run it using either the interactive method or batch submit method listed above, make sure to close the pool when you are finished with your work with

```
matlabpool close
```

Keep in mind that the University only has 160 of these licenses and your job may fail if someone else is using the licenses when your job runs.

**METIS**

\*\*\*Under Construction/\*\*\*

METIS and parMETIS are installed as modules, to use the software please load the modules with either

```
module load metis
```

or

```
module load parmetis
```

Once loaded you may submit jobs using the METIS or parMETIS binaries as defined in the METIS [user manual](https://wiki.mst.edu/itrst/pub/forge) or the parMETIS [user manual](https://wiki.mst.edu/itrst/pub/forge)

**MSC**

**Nastran**

MSC nastran 2014.1 is available through the module `msc/nastran/2014`
module load msc/nastran/2014

Here is an example job file.

msc.sub

#!/bin/bash

#SBATCH -J Nastran
#SBATCH -o Forge-%j.out
#SBATCH --ntasks=1
#SBATCH --time=01:00:00

nast20141 test.bdf
#you should also be able to use .dat files with nastran this way.

Submit it as normal.

NAMD

This article is under development. Things referenced below are written as we make progress and some instruction may not work as intended.

Below is an example file for namd, versions prior to 2.12b have not been tested as of yet and may not function in the same way as 2.12b.

namd.sub

#SBATCH -J NAMD_EXAMPLE
#SBATCH --ntask=16
#SBATCH --time=01:00:00
#SBATCH -o Forge-%J.out

module load namd/2.12b

charmrun +p16 namd2 [options]

You will need to give namd2 whatever options you would like to run, user documentation for what those may be is available from the developers at http://www.ks.uiuc.edu/Research/namd/2.12b1/ug/.

Gamess

To use gamess you will need to load the gamess module

module load gamess
and use a submission file similar to the following

gamess.sub

```bash
#!/bin/bash

#SBATCH -J Gamess_test
#SBATCH --time=01:00:00
#SBATCH --ntasks=2
#SBATCH -o Forge-%J.out

rungms -i ./test.inp
```

We have customized the rungms script extensively for our system and have introduced several useful switch options.

<table>
<thead>
<tr>
<th>Switch</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>-i</td>
<td>defines the path to the input file, no default value</td>
</tr>
<tr>
<td>-d</td>
<td>defines the path to the data folder, default value is the submission directory</td>
</tr>
<tr>
<td>-s</td>
<td>defines the path to the scratch folder, default value is ~/gamess/scr-$input-$date this folder gets removed once the job completes.</td>
</tr>
<tr>
<td>-b</td>
<td>defines the binary that will be used, default is /share/apps/gamess/gamess.00.x useful if you've compiled your own version of gamess.</td>
</tr>
<tr>
<td>-a</td>
<td>defines the auxdata folder, default is /share/apps/gamess/auxdata useful if you've compiled your own version of gamess.</td>
</tr>
</tbody>
</table>

**OpenFOAM**

First load the module

```
module load OpenFOAM
```

then source the bash file,

```
source $FOAMBASH
```

or the csh file if you are using csh as your shell

```
source $FOAMCSH
```

Then you may use open foam to work on your data files, anything that needs to be generated interactively needs to be done in an interactive job

```
sinteractive
```

You can create a job file to submit from the data directory to do anything that needs more processing, please see the example below.
foam.sub

#!/bin/bash

#SBATCH -J FOAMtest
#SBATCH --nodes=1
#SBATCH --ntasks=2
#SBATCH --time=01:00:00

blockMesh

This will execute blockMesh on the input files in the submission directory on 1 node with 2 CPUs for 1 hour.

**Python**

**Python 2**

Python modules are available through system modules as well. To see what python modules have been installed issue

```bash
module avail python
```

These are the site installed python modules and can be used just like any other module.

```bash
module load python
```

will load all python modules,

```bash
module load python/matplotlib
```

will load the matplotlib module and any module it depends on.

**Python 3**

There are many modules available for Python 3. However, unlike Python 2.7, all of the python modules are installed in the python directory rather than being separate modules. Currently, the newest Python 3 version available on the Forge is Python 3.6.4. To see a current list of available python versions, run the command

```bash
module avail python
```

To see a list of all available Python modules available for a particular Python version, load that Python version and run

```bash
pip list
```
Users are welcome to install additional modules on their account using

```
pip install --user <package name>
```

**QMCPack**

Start by loading the module.

```
module load qmcpack
```

Then create your submission file in the directory where your input files are, see example below.

```
qmcpack.sub

#!/bin/bash

#SBATCH -J qmcpack
#SBATCH -o Forge-%j.out
#SBATCH --ntasks=8
#SBATCH --time=1:00:00
#SBATCH --constraint=intel

mpirun qmcapp input.xml
```

**Note:** QMCPack is compiled to run only on intel processors, you need to add

```
--constraint=intel
```

to make sure that your job doesn't run on a node with amd processors.

This should run qmcpack on 8 cpus for 1 hour on your input file. If you want to run multiple instances, in parallel, in the same job you may pass an input.list file in place of the input.xml which contains all the input xml files you wish to run.

For more information on creating the input files please see QMCPack's [user guide](https://wiki.mst.edu/itrst/pub/forge).

**SAS 9.4**

**Notes:**
SAS can be run from the login node, with an X session, or from command line.
SAS is node-locked to only forge.mst.edu, so it won't work in a jobfile. You must run it interactively on forge.mst.edu.

For both methods, you need to load the SAS module.

```
module load SAS/9.4
```
Interactive:

Steps:

1. Start a local X Server XWin 32
2. SSH to forge.mst.edu
3. On our Linux builds, type the command “ssh -XC forge.mst.edu”
4. Once logged in onto the Forge, run

   sinteractive -p=free

   - the sinteractive command will open a new SSH tunnel on a compute node with free resources.

5. One this new SSH command line, run the

   sas_en

   and it will open the interface on the compute node that sinteractive has set.

6. Remember to close all your windows when you're finished

This series of Windows will appear.
Jobfile

sas.sub

```bash
#!/bin/bash
#SBATCH --job-name=job_name
#SBATCH --ntasks=1
#SBATCH --time=23:59:59
#SBATCH --mem=31000
#SBATCH --mail-type=begin,end,fail,requeue
#SBATCH --export=all
#SBATCH --out=Forge-%j.out

module load SAS/9.4
sas_en -nodms sas_script.sas
```

Command line:

`sas_en -nodms`

runs the command line version of sas. (type endsas; to get out)

```
[rlhaffer@login-44-0 apps]$ sas_en -nodms
NOTE: Copyright (c) 2002-2012 by SAS Institute Inc., Cary, NC, USA.
NOTE: SAS (r) Proprietary Software 9.4 (TS1M3)
Licensed to THE CURATORS OF THE UNIV OF MISSOURI - T&R, Site 70084282.
NOTE: This session is executing on the Linux 2.6.32-431.11.2.el6.x86_64 (LIN
X64) platform.
SAS/QC 14.1

NOTE: Additional host information:

Linux LIN X64 2.6.32-431.11.2.el6.x86_64 #1 SMP Tue Mar 25 19:59:55 UTC
2014
x86_64 CentOS release 6.5 (Final)

You are running SAS 9. Some SAS 8 files will be automatically converted
by the V9 engine; others are incompatible. Please see
http://support.sas.com/rnd/migration/planning/platform/64bit.html

PROC MIGRATE will preserve current SAS file attributes and is
recommended for converting all your SAS libraries from any
SAS 8 release to SAS 9. For details and examples, please see
http://support.sas.com/rnd/migration/index.html

This message is contained in the SAS news file, and is presented upon
initialization. Edit the file "news" in the "misc/base" directory to display site-specific news and information in the program log. The command line option "-nonews" will prevent this display.

NOTE: SAS initialization used:

real time 0.11 seconds
cpu time 0.04 seconds

PRINTING:

- Select File | Print.
- This will create a postscript file, “sasprt.ps”, in the directory you started SAS from. You can download it to your computer and use ps2pdf to print it.

StarCCM+

Engineering Simulation Software

Default version = 10.04.011

Other working versions: 11.02.009

- module load starccm/11.02
- module load starccm/10.06
- module load starccm/8.04
- module load starccm/7.04
- module load starccm/6.04

Job Submission Information

Copy your .sim file from the workstation to your cluster home profile. The Forge documentation explains how to do this.
Once copied, create your job file.

Example job file: First

```bash
module load starccm/10.04

starccm.sub
```

```bash
#!/bin/bash
#SBATCH --job-name=starccm_example
#SBATCH --nodes=1
#SBATCH --ntasks=12
#SBATCH --partition=queue
#SBATCH --time=08:00:00
#SBATCH --mail-type=FAIL
#SBATCH --mail-type=BEGIN
#SBATCH --mail-type=END
#SBATCH --mail-user=joeminer@mst.edu

module load starccm/10.04

time starccm+ -power -batch -np 12 -licpath 1999@flex.cd-adapco.com -podkey AABBCCDDee112234455
/path/to/your/starccm/simulation/example.sim
```

**It's preferred that you keep the ntasks and -np set to the same processor count.**

Breakdown of the script:
This job will use 1 node, asking for 12 processors, for a total wall time of 8 hours and will email you when the job starts, finishes or fails.

The StarCCM commands:

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-power</td>
<td>using the power session and power on demand key</td>
</tr>
<tr>
<td>-batch</td>
<td>tells Star to utilize more than one processor</td>
</tr>
<tr>
<td>-np</td>
<td>number of processors to allocate</td>
</tr>
<tr>
<td>-licpath</td>
<td><a href="mailto:1999@flex.cd-adapco.com">1999@flex.cd-adapco.com</a> - Since users of StarCCM at S&amp;T must have Power On Demand keys, we use CD-Adapco's license server</td>
</tr>
<tr>
<td>-podkey</td>
<td>Enter your PoD key....AABBCCDDee112234455 This is given to you when you sign up for Star, or someone from the FSAE team provides it.</td>
</tr>
<tr>
<td>/path/to/your/starccm/simulation/example.sim</td>
<td>use the true path to your .sim file in your cluster home directory</td>
</tr>
</tbody>
</table>

**Vasp**

To use our site installation of Vasp you must first prove that you have a license to use it by emailing your vasp license confirmation to it-research-support@mst.edu.
Once you have been granted access to using vaspr you may load the vaspr module

```
module load vaspr
```

and create a vaspr job file, in the directory that your input files are, that will look similar to the one below.

```
vasp.sub

#!/bin/bash

#SBATCH -J Vasp
#SBATCH -o Forge-%j.out
#SBATCH --time=1:00:00
#SBATCH --ntasks=8

mpirun vaspr
```

This example will run the standard vaspr compilation on 8 cpus for 1 hour.

If you need the gamma only version of vaspr use

```
mpirun vaspr_gam
```

in your submission file.

If you need the non-colinear version of vaspr use

```
mpirun vaspr_ncl
```

in your submission file.

There are some globally available Psudop potentials available, the module sets the environment variable $POTENDIR to the global directory.

From:
https://wiki.mst.edu/itrst/ - IT Research Support Team

Permanent link:
https://wiki.mst.edu/itrst/pub/forge

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