

Mathematica on HPC cluster:

What is Mathematica?

Mathematica is a powerful and elegant mathematical computational tool available natively on all modern desktops as well as on the cloud. It boasts intuitive- English like – code, fast algorithms, a vast integrated system, seamless cloud integration, and its versatility.

Academic uses for Mathematica include teaching simple concepts in the classroom to doing high-level research using some of the world's largest clusters. Mathematica can be used by faculty as an interactive teaching tool – classroom lectures, assignments and exams can all be created within Mathematica. Additionally, High Performance Computing and data analysis can be performed in Mathematica.

More info on Mathematica:

<https://www.wolfram.com/mathematica/pricing/students/>

<https://oit.ua.edu/software/mathematica/>

Versions Available:

Mathematica - 10.4.0

Mathematica – 12.3.1

How to load a version of Mathematica?

To load a version of Mathematica on the HPC on current terminal session, use the following command:

```
module avail math/mathematica
```

The version will be listed. To a version of software, use following command:

```
module load math/mathematica/12.3.1
```

Verify by using this command:

```
module list
```

The loaded software and dependencies will be shown.

How to use Mathematica on the cluster?

There are three main ways to run mathematica on the cluster- Interactive method, Terminal run, or Script.

Terminal Run:

```
# Load the module and start a terminal session on compute node
srun -p main --qos main -n 1 -c 12 --mem 10G --pty bash

# Use this terminal session to open mathematica
math

#This opens a mathematica session on the terminal.
Integrate[E^(-1*x^2), {x, -2,2}]
```

The Interactive Mode (GUI):

```
# Load the module and start a terminal session on compute node
srun -p main --qos main -n 1 -c 18 --mem 10G --pty bash

#To open a GUI, use the following command
mathematica
```

```

#####NOTE#####
#NOTE THIS ONLY WORKS IF THE TERMINAL HAS X11 FORWARDING ENABALED
#To enable X-11 FW, use this command to ssh.
ssh -X username@domain-name
#####

#Now make a script file and open it
Plot3D[Sin[x + y^2], {x, -3, 3}, {y, -1, 1}]

#This will render a graph of the function on the screen

```

The Script:

```

#!/bin/bash
#SBATCH -J Jobname # Jobname
#SBATCH -n 1      # Nodes per task
#SBATCH --mem=10G # Must need to allocate memory to run Mathematica - at least 4G
#SBATCH -p main  # Partition
#SBATCH --qos main # Quality of service
#SBATCH -o Mathematica_out-%J.txt # STDOUT Out file
#SBATCH -e Mathematica_out-%J.txt # Error file
#SBATCH -t 30      # Time in minutes

module load math/mathematica/12.3.1 # load the module

cd $SLURM_SUBMIT_DIR # Moving to the test directory
wget https://rcc.uchicago.edu/docs/downloads/math-simple.m #Download a test file

#Runs a mathematica script on the cluster

```

```
math -run < math-simple.m > out.txt
```

Schedule the job with the following sbatch command.

```
sbatch myscript.sh
```

All the processed files will be written in the same directory as the script. The results will be written in the out.txt file.

Where to find help?

If you are stuck on some part or need help at any point, please contact OIT at the following address.

<https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp>

Resources:

<https://www.wolfram.com/mathematica/>

<https://reference.wolfram.com/language/ref/Parallelize.html>