Lecture 11 - GPGPU (The Easy Parts) Part 1

DSE 512

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From Last Time

- Homework is out --- due Saturday
- Slack channel
- ISAAC help
- Questions?

Structure

- Part 1
  - GPGPU Basics
  - NVBLAS
- Part 2
  - Python (CuPy)
  - R (gpuR, fmlr)

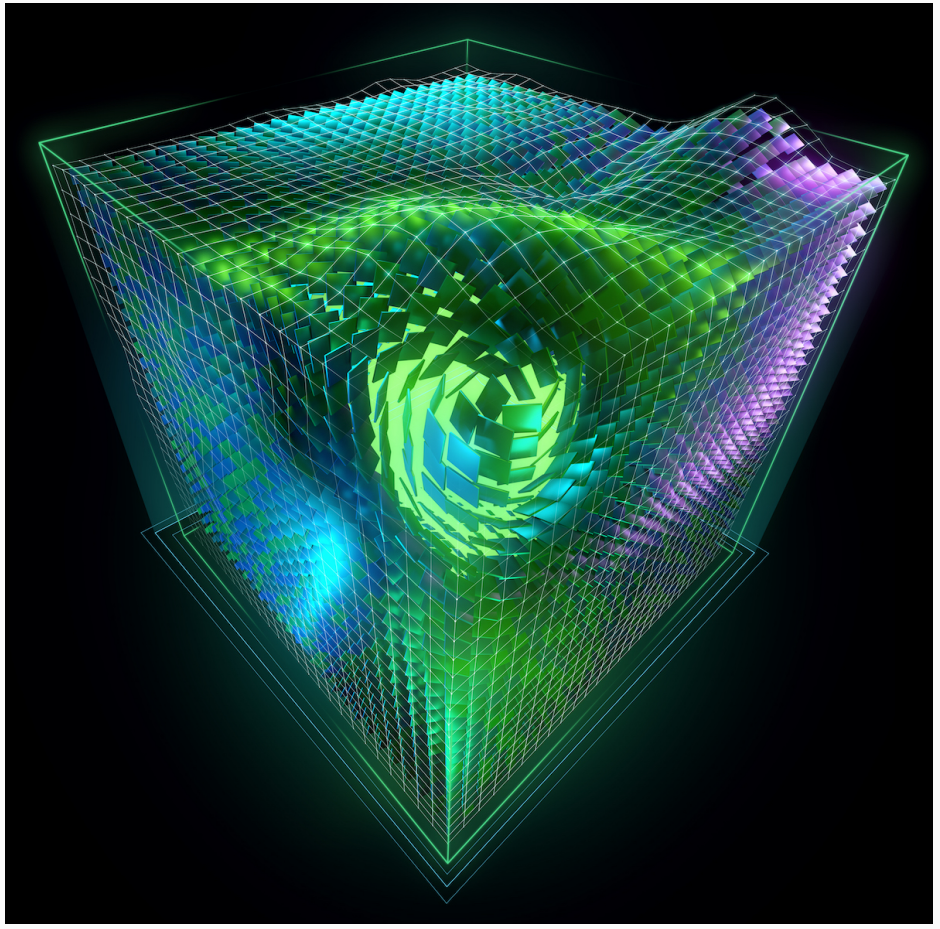
GPGPU

GPGPU

- General Purpose GPU
- Using Video Game Hardware to Multiply Matrices
- Major players
  - NVIDIA
  - AMD
  - Intel

"Low-Level" GPGPU Technologies

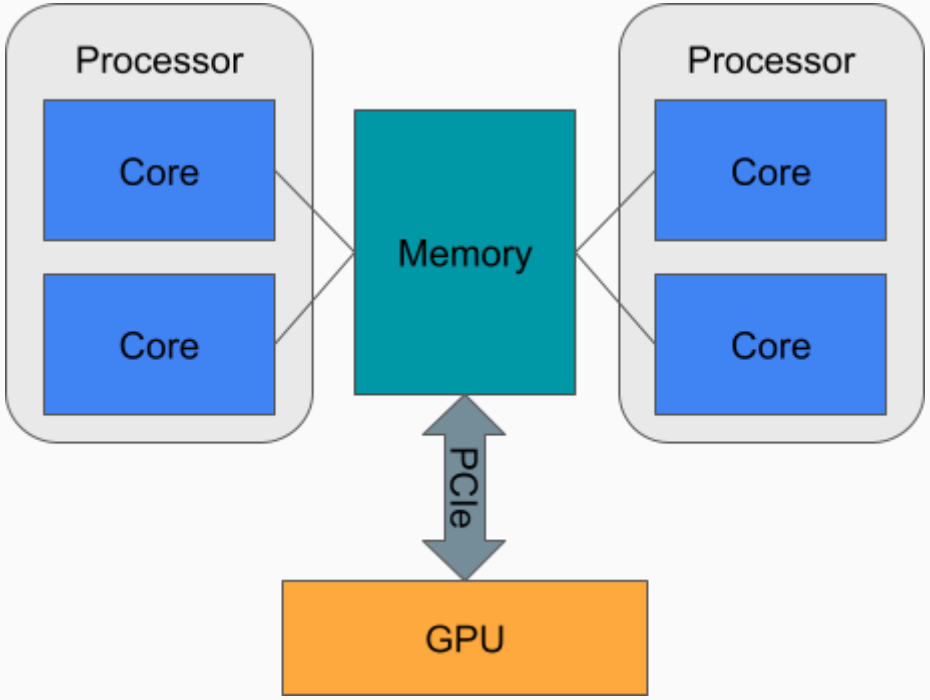
- ~~Shaders~~
- CUDA
- OpenCL
- OpenACC
- OpenMP



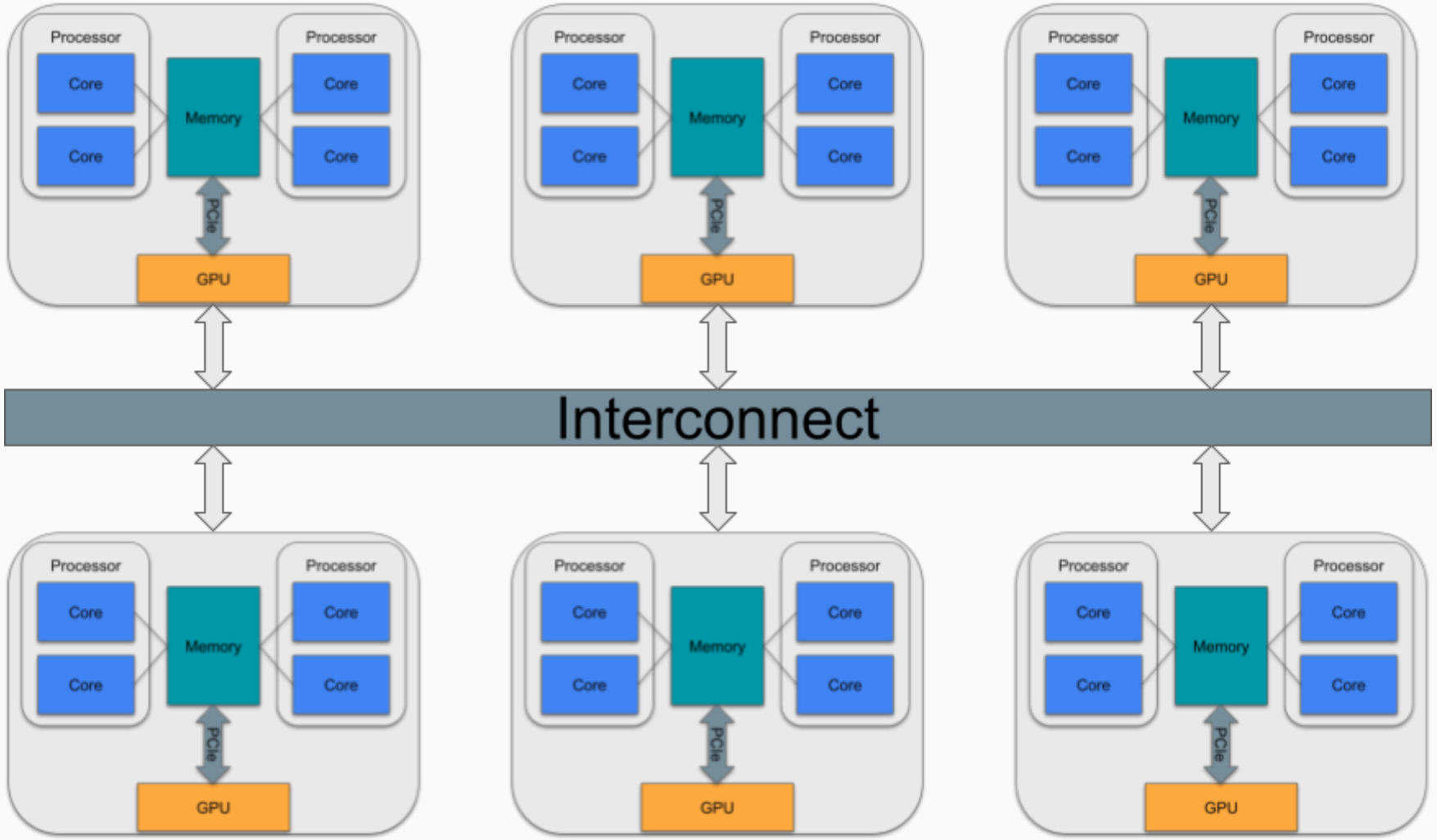
"High-Level" GPGPU Technologies

- NVBLAS
- Python
  - CuPy
- R
  - fmlr
  - gpuR
- Deep Learning frameworks

Hardware

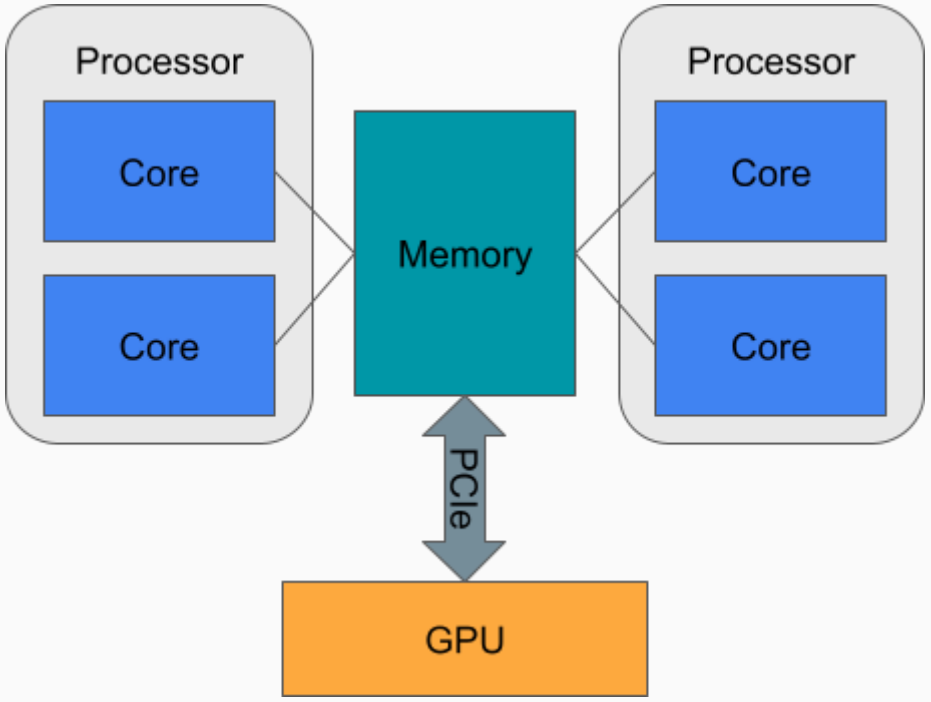


Hardware


Processor
Core
Core
Memory
Processor
Core
Core
PCIe
GPU
Interconnect

Using a GPU

- GPUs have their own (HB) memory
- Transferring data is very expensive
- Leave data on GPU as long as possible



So How Does a GPU Work?

SIMD Parallelism

- GPUs use Single Instruction Multiple Data
- SIMD aka vectorization

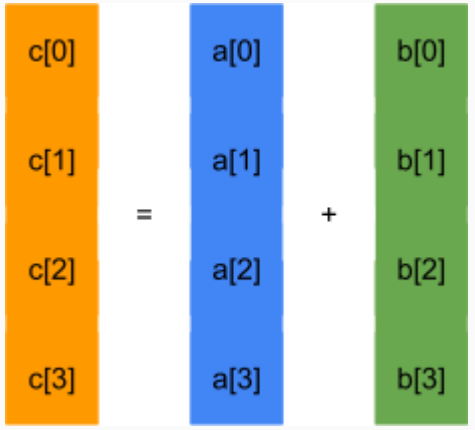
> SIMD describes computers with multiple processing elements that perform the same operation on multiple data points simultaneously.

https://en.wikipedia.org/wiki/Single_instruction,_multiple_data

SIMD Parallelism

Serial

SIMD



SIMD Kernel

```
template <typename REAL>
__global__ void kernel_vec_vec_add(const int n, const REAL *a, const REAL *b, REAL *c)
{
  c[i] = a[i] + b[i];
}

template <typename T>
Vec vec_vec_add(const Vec a, const Vec b)
{
  static const int BLOCK_SIZE = 16;
  dim3 dim_block(BLOCK_SIZE);
  dim3 dim_grid((len + BLOCK_SIZE - 1) / BLOCK_SIZE);

  Vec c(a.size());
  kernel_vec_vec_add<<<dim_grid, dim_block>>>(a.size(), a.data(), b.data(), c.data());
  this->c->check();
}
```

GPGPU Myth vs Reality

Myth

- Easy to use!
- Libraries work well!
- SO FAST 2000x OMG!!!

Reality

- ***IMPOSSIBLE TO USE***
- Libraries are buggy garbage
- Some operations are fast; many are ***SLOW***

CUDA OS Support

- Linux - Full support; works best
- Windows - Mostly works; dll problem even worse than usual
- MacOS - Not supported; will not work

NVBLAS

BLAS and LAPACK on a GPU

- MAGMA https://icl.cs.utk.edu/magma/
- AMD ROCm
  https://rocmdocs.amd.com/en/latest/Installation_Guide/HIP.html
- NVIDIA
  - cuBLAS https://docs.nvidia.com/cuda/cublas/index.html
  - cuSOLVER https://docs.nvidia.com/cuda/cusolver/index.html
  - NVBLAS https://docs.nvidia.com/cuda/nvblas/index.html

gemm

```
NAME
     dgemm - perform one of the matrix-matrix operations    C  :=
     alpha*op( A )*op( B ) + beta*C

SYNOPSIS
     SUBROUTINE DGEMM(TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB,
           BETA, C, LDC)

     CHARACTER * 1 TRANSA, TRANSB
     INTEGER M, N, K, LDA, LDB, LDC
     DOUBLE PRECISION ALPHA, BETA
     DOUBLE PRECISION A(LDA,*), B(LDB,*), C(LDC,*)

     SUBROUTINE DGEMM_64(TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB,
           BETA, C, LDC)

     CHARACTER * 1 TRANSA, TRANSB
     INTEGER*8 M, N, K, LDA, LDB, LDC
     DOUBLE PRECISION ALPHA, BETA
     DOUBLE PRECISION A(LDA,*), B(LDB,*), C(LDC,*)
```

gemm

```
dgemm_(
  const char *transa, const char *transb,
  int *m, int *n, int *k,
  const double *alpha,
  const double *a, int *lda,
  const double *b, int *ldb,
  const double *beta,
  double *c, int *ldc)
```

```
cublasStatus_t cublasDgemm(
  cublasHandle_t handle,
  cublasOperation_t transa, cublasOperation_t transb,
  int m, int n, int k,
  const double *alpha,
  const double *A, int lda,
  const double *B, int ldb,
  const double *beta,
  double *C, int ldc)
```

Can We Offload Computations to GPU Automatically?

NVBLAS

- Uses `LD_PRELOAD` trick
- BLAS calls get hijacked
- Data transfer handled automatically
- Pros
  - easy to use
  - somewhat configurable
  - problems can exceed GPU memory
- Cons
  - Uses `LD_PRELOAD` trick
  - Some environments just not set up for it
  - ***DOES NOT WORK WELL FOR SMALL PROBLEMS***

Supported Routines

Routine	Types	Operation
gemm	S,D,C,Z	Multiplication of 2 matrices
syrk	S,D,C,Z	Symmetric rank-k update
herk	C,Z	Hermitian rank-k update
syr2k	S,D,C,Z	Symmetric rank-2k update
her2k	C,Z	Hermitian rank-2k update
trsm	S,D,C,Z	Triangular solve with multiple right-hand sides
trmm	S,D,C,Z	Triangular matrix-matrix multiplication
symm	S,D,C,Z	Symmetric matrix-matrix multiplication
hemm	C,Z	Hermitian matrix-matrix multiplication

Matrix Products Benchmark

Matrix Products Benchmark

Matrix Products Benchmark

Configuring NVBLAS

- Create `nvblas.conf` file
- Set `NVBLAS_CONFIG_FILE`

```
export NVBLAS_CONFIG_FILE=${HOME}/nvblas.conf
```

- Set `LD_PRELOAD`

```
CUDA_HOME=/sw/isaac/applications/cuda/11.4.2/rhel8_binary/
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so
```

- READ THE DOCS https://docs.nvidia.com/cuda/nvblas/index.html

Configuring NVBLAS

```
NVBLAS_LOGFILE nvblas.log
NVBLAS_TRACE_LOG_ENABLED

NVBLAS_CPU_BLAS_LIB /spack/spack-0.16.3/apps/linux-rhel8-cascadelake/gcc-10.2.0/openblas-0.3.12-c4x3

# NVBLAS_GPU_LIST 0
NVBLAS_GPU_LIST ALL

NVBLAS_TILE_DIM 2048
NVBLAS_AUTOPIN_MEM_ENABLED

# Disable routines
# NVBLAS_GPU_DISABLED_DSYRK

# Set CPU/GPU compute ratio
# NVBLAS_CPU_RATIO_DGEMM 0.07
```

NVBLAS on ISAAC

It Doesn't Go Well

Test Scripts

test.r

```
set.seed(1234)
n = 10000 # set to 10 for testing
x = matrix(runif(n*n), n, n)
y = matrix(runif(n*n), n, n)
system.time({x %*% y})[3]
```

test.py

```
import numpy as np
import random
import time

np.random.seed(1234)
n = 10000 # set to 10 for testing
x = np.random.rand(n, n)
y = np.random.rand(n, n)
t0 = time.perf_counter()
z = np.dot(x, y)
t1 = time.perf_counter()
print(t1 - t0)
```

R - OpenBLAS

```
singularity exec r.simg Rscript test.r
```

```
elapsed
   1.26
```

R - NVBLAS

```
module load openblas
module load cuda
export CUDA_HOME=/sw/isaac/applications/cuda/11.4.2/rhel8_binary/

export NVBLAS_CONFIG_FILE=$HOME/nvblas.conf
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so singularity exec --bind /sw:/sw r.simg Rscript
```

```
[NVBLAS] NVBLAS_CONFIG_FILE environment variable is set to '/nfs/home/mschmid3/nvblas.conf'

 *** caught segfault ***
address 0xc0, cause 'memory not mapped'

Traceback:
 1: system.time({    x %*% y})
An irrecoverable exception occurred. R is aborting now ...
```

Python - MKL

```
python3 test.py
```

```
1.4268960766494274
```

Python - NVBLAS???

```
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so python3 test.py
```

```
1.3604787662625313
```

Python - NumPy config

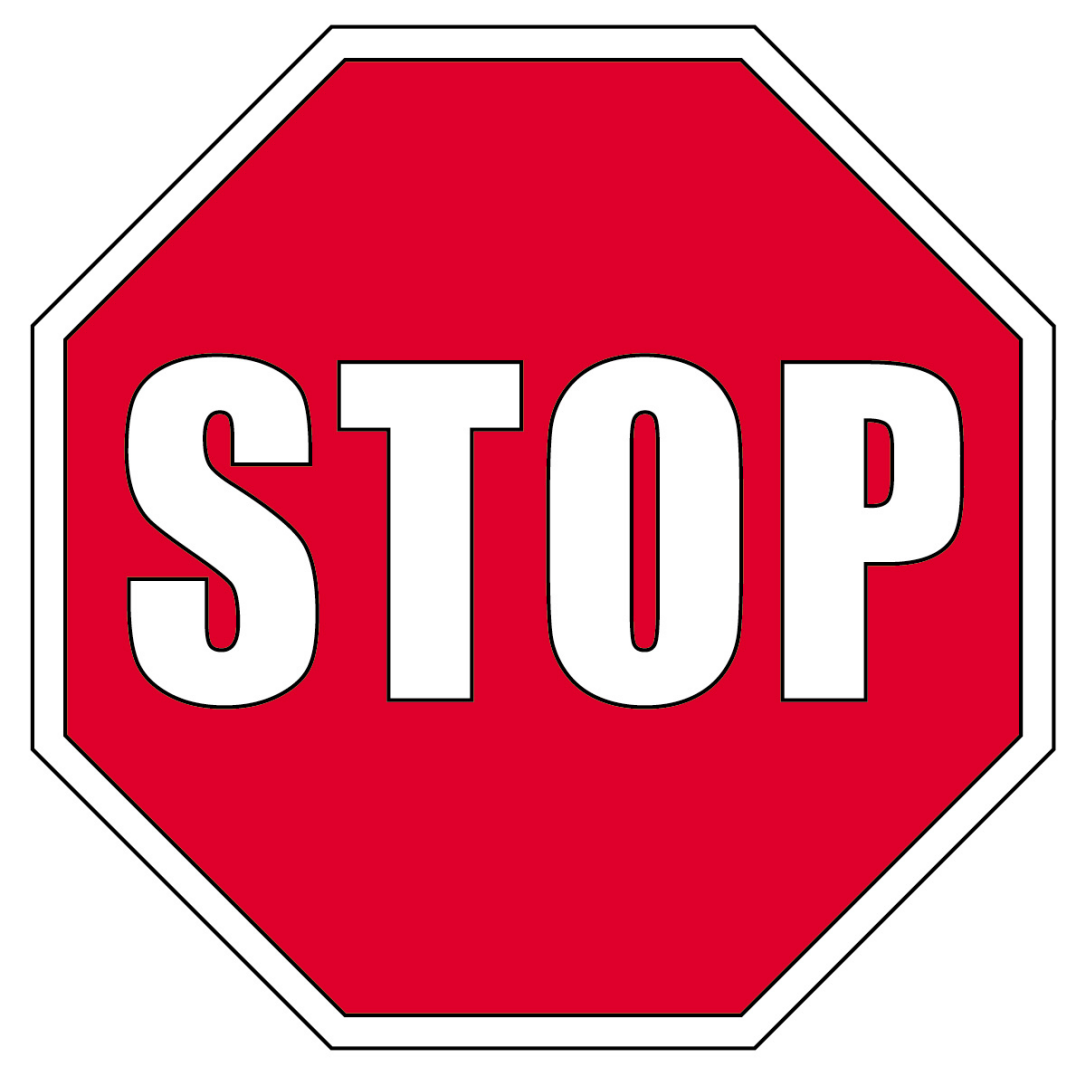
```
Python 3.8.8 (default, Apr 13 2021, 19:58:26)
[GCC 7.3.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> np.show_config()
blas_mkl_info:
    libraries = ['mkl_rt', 'pthread']
    library_dirs = ['/sw/isaac/applications/anaconda3/2021.05/rhel8_gcc10.2.0/anaconda3-2021.05/lib'
    define_macros = [('SCIPY_MKL_H', None), ('HAVE_CBLAS', None)]
    include_dirs = ['/sw/isaac/applications/anaconda3/2021.05/rhel8_gcc10.2.0/anaconda3-2021.05/incl
```

Is It Using CBLAS?

```
nm /sw/isaac/applications/anaconda3/2021.05/rhel8_gcc10.2.0/anaconda3-2021.05/lib/libmkl_
```

```
00000000001a10c0 T cblas_dgemm_
00000000001a1210 T cblas_dgemm_batch
00000000001a1210 T cblas_dgemm_batch_
00000000001a1390 T cblas_dgemm_batch_strided
00000000001a1390 T cblas_dgemm_batch_strided_
00000000001a1520 T cblas_dgemm_compute
00000000001a1520 T cblas_dgemm_compute_
00000000001a1660 T cblas_dgemm_pack
00000000001a1660 T cblas_dgemm_pack_
00000000001a1780 T cblas_dgemm_pack_get_size
00000000001a1780 T cblas_dgemm_pack_get_size_
```

NVBLAS DOESN'T WORK WITH CBLAS



Retry With OpenBLAS

```
module load openblas
pip install --force-reinstall numpy
```

```
>>> import numpy as np
>>> np.show_config()
openblas64__info:
    libraries = ['openblas64_', 'openblas64_']
    library_dirs = ['/usr/local/lib']
    language = c
    define_macros = [('HAVE_CBLAS', None), ('BLAS_SYMBOL_SUFFIX', '64_'), ('HAVE_BLAS_ILP64', None)]
    runtime_library_dirs = ['/usr/local/lib']
```

Python - NVBLAS???

```
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so python3 test.py
```

```
1.5831096079200506
```

Retry With Netlib BLAS

```
module unload openblas
module load netlib-lapack
export NETLIB_HOME=/spack/spack-0.16.3/apps/linux-rhel8-cascadelake/gcc-10.2.0/netlib-lap
BLAS=$NETLIB_HOME/libblas.so LAPACK=$NETLIB_HOME/liblapack.so pip install --force-reinsta

LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so python3 test.py
```

```
1.6391727197915316
```

Building R from Source

```
module unload PE-intel
module load gcc
wget https://tukaani.org/xz/xz-5.2.5.tar.gz
tar zxf xz-5.2.5.tar.gz
cd xz-5.2.5
./configure --prefix=`pwd`/build && make -j && make install
export LD_LIBRARY_PATH=${LD_LIBRARY_PATH}:${HOME}/R/xz-5.2.5/build/lib
export PATH=$PATH:${HOME}/R/xz-5.2.5/build/bin

module load bzip2
module load openblas
cd ${HOME}/R/
wget https://cran.r-project.org/src/base/R-4/R-4.1.2.tar.gz
tar zxf R-4.1.2.tar.gz
cd R-4.1.2
OBPATH=/spack/spack-0.16.3/apps/linux-rhel8-cascadelake/gcc-10.2.0/openblas-0.3.12-c4x3eo
LDFLAGS="-L${HOME}/R/xz-5.2.5/build/lib/ -llzma" CFLAGS="-I${HOME}/R/xz-5.2.5/build/inclu
  ./configure --with-x=no --enable-R-shlib=yes \
  --with-blas=${OBPATH} --with-lapack=${OBPATH}
make -j16
```

NVBLAS

```
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so ${HOME}/R/R-4.1.2/bin/Rscript test.r
```

```
[NVBLAS] No Gpu available
[NVBLAS] NVBLAS_CONFIG_FILE environment variable is set to '/nfs/home/mschmid3/nvblas.conf'
```

```
cat nvblas.log
```

```
[NVBLAS] Problem parsing line 7
[NVBLAS] Config parsed
[NVBLAS] No device selected
[NVBLAS] dgemm[cpu]: ta=N, tb=N, m=10000, n=10000, k=10000
```

Running a GPU Job?

```
#!/bin/bash
#SBATCH --account UTK0011
#SBATCH --job-name=nvblas_test
#SBATCH --nodes=1
#SBATCH --time=00:05:00
#SBATCH --partition=campus-gpu
#SBATCH --qos=campus

module load bzip2
module load openblas
module load cuda

CUDA_HOME=/sw/isaac/applications/cuda/11.4.2/rhel8_binary/
LD_PRELOAD=${CUDA_HOME}/lib64/libnvblas.so ${HOME}/R/R-4.1.2/bin/Rscript test.r
```

```
sbatch: error: Batch job submission failed: Invalid account or account/partition combination specifi
```

What To Do?

Questions?