GPU Computing on the FASRC Cluster

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Objectives

- To advise you on the best practices for running GPU applications on the FASRC cluster
- To provide the basic knowledge required for building your own GPU apps

FAS Research Computing (FASRC)

Faculty of Arts and Sciences (FAS) department that handles non-enterprise IT requests from researchers.

- **RC Primary Services:**
  - Cannon Supercomputing Environment
  - Lab Storage
  - Instrument Computing Support
  - Hosted Machines (virtual or physical)
- **RC Staff:**
  - 20+ staff with backgrounds ranging from systems administration to development-operations to PhD research scientists
  - Supporting 600+ research groups and 5500+ users across FAS, SEAS, HSPH, HBS, GSE, CfA, Kempener, HKS, etc.
  - For Bioinformatics researchers the Harvard Informatics group is closely tied to RC and is there to support the specific problems for that domain

Cannon Cluster

Compute:

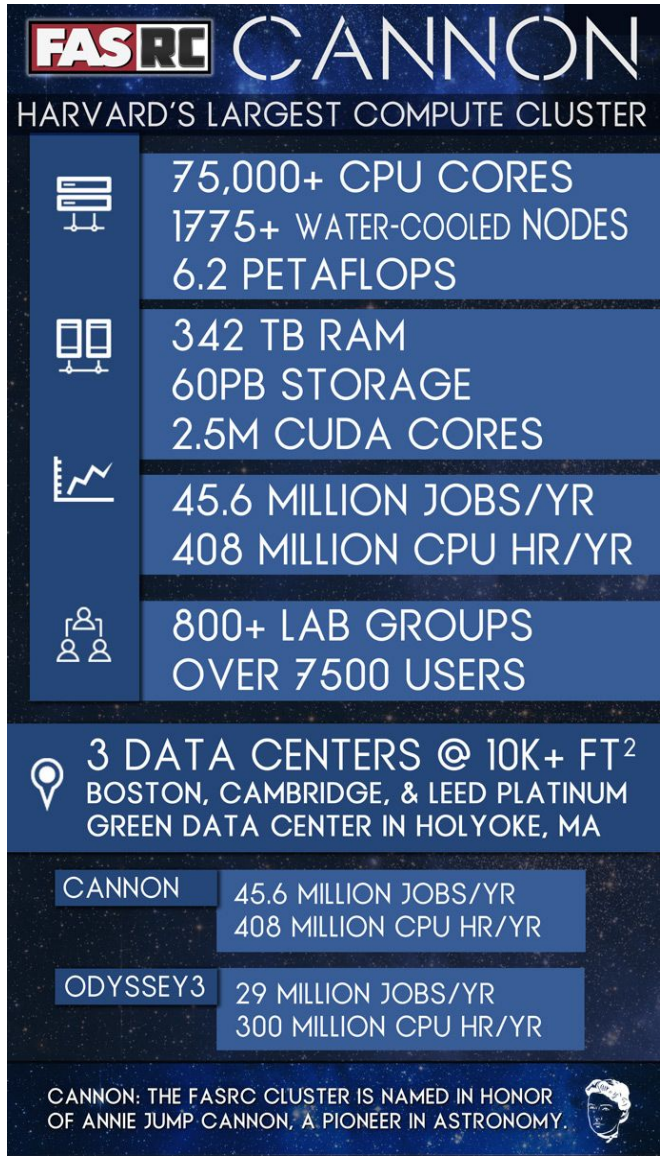
- 100,000+ compute cores + 220 Intel's latest Sapphire nodes
- Cores/node: 32 to 112
- Memory/node: 12GB to 512GB (4GB/core)
- 2,500,000+ NVIDIA GPU cores + 144 new A100 80GB GPUs (36 nodes)

Software:

- Operating System Rocky 8
- Slurm job manager
- Spack software package manager

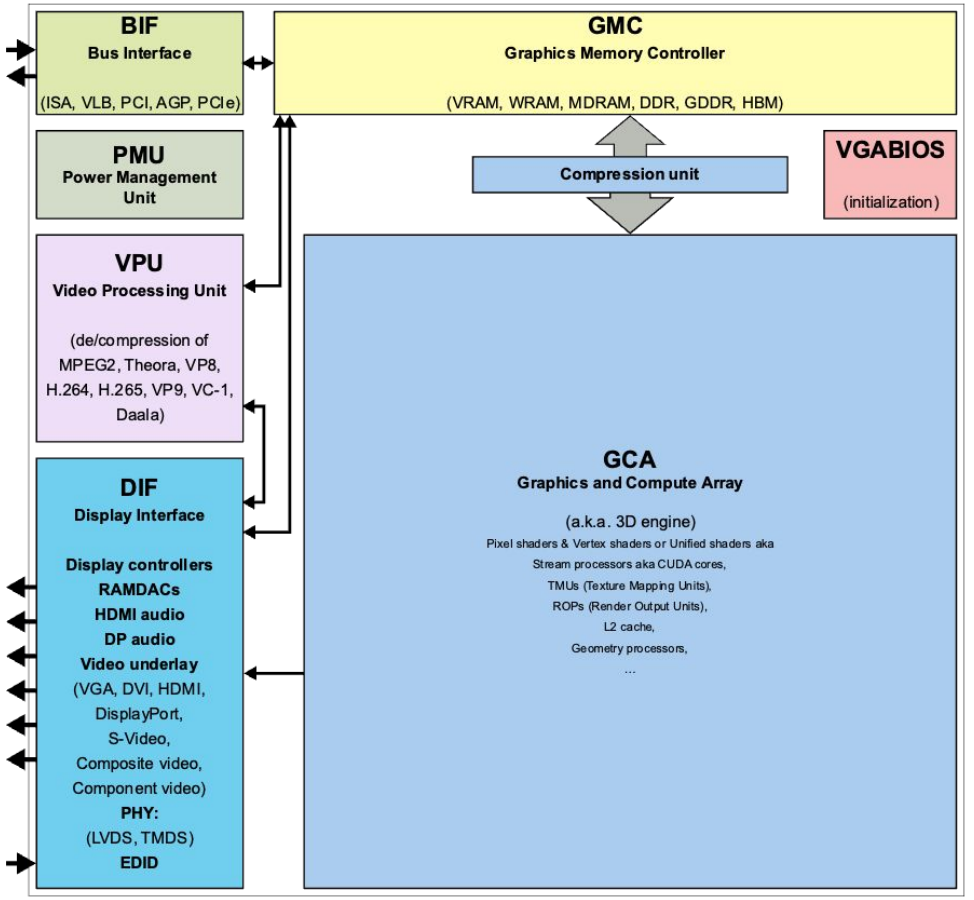
Interconnect:

- 2 underlying networks connecting 3 data centers
- TCP/IP network
- Low-latency 200 GB/s HDR InfiniBand (IB) and 56 GB/s FDR IB network:
  - inter-node parallel computing
  - fast access to Lustre mounted storage



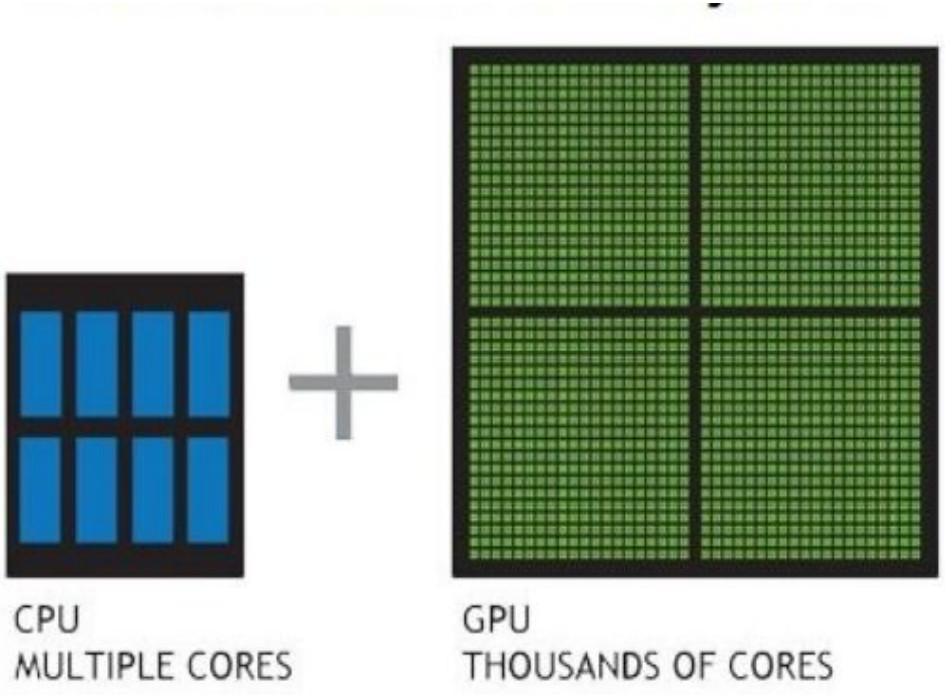
GPU (Graphics Processing Unit)?

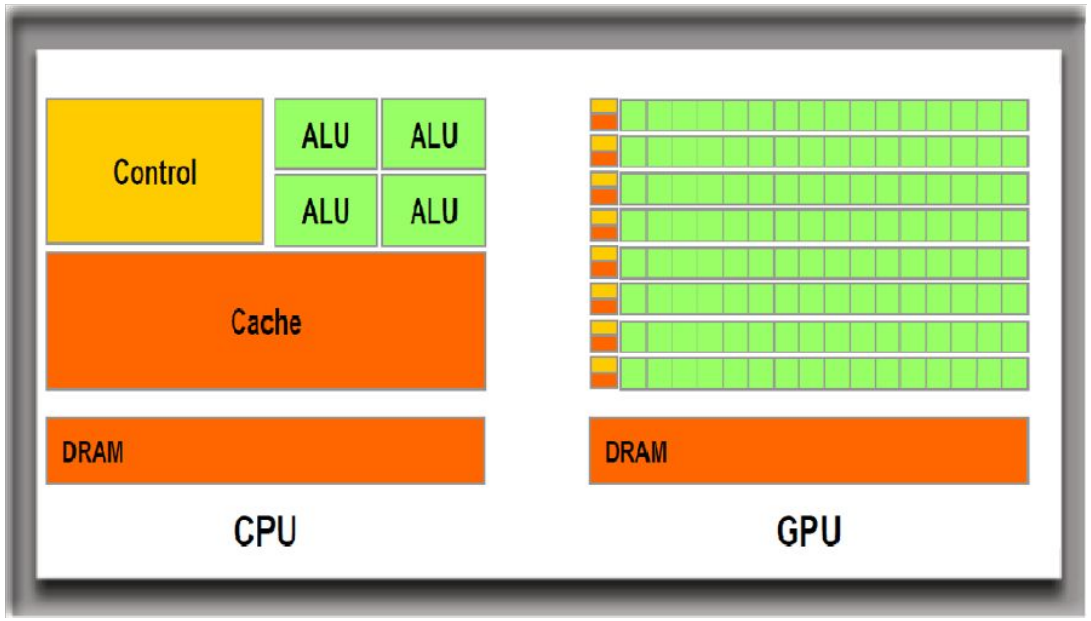
- Specialized microprocessor designed to accelerate graphics rendering to a display device.
- Highly parallel structure, process large blocks of data **simultaneously**
- Integrated into computer's central processing unit (CPU) [embedded systems] or offered as a discrete hardware unit
- Applications ranging from scientific computing, ML/DL/AI to gaming, laptops, cell phones, etc.



By ScotXW - Own work, CC0, https://commons.wikimedia.org/w/index.php?curid=61055349

What is a GPGPU?





General-Purpose Graphics Processing Unit (**GPGPU**) - GPU programmed for purposes *beyond* graphics processing, such as performing computations typically conducted by a CPU.

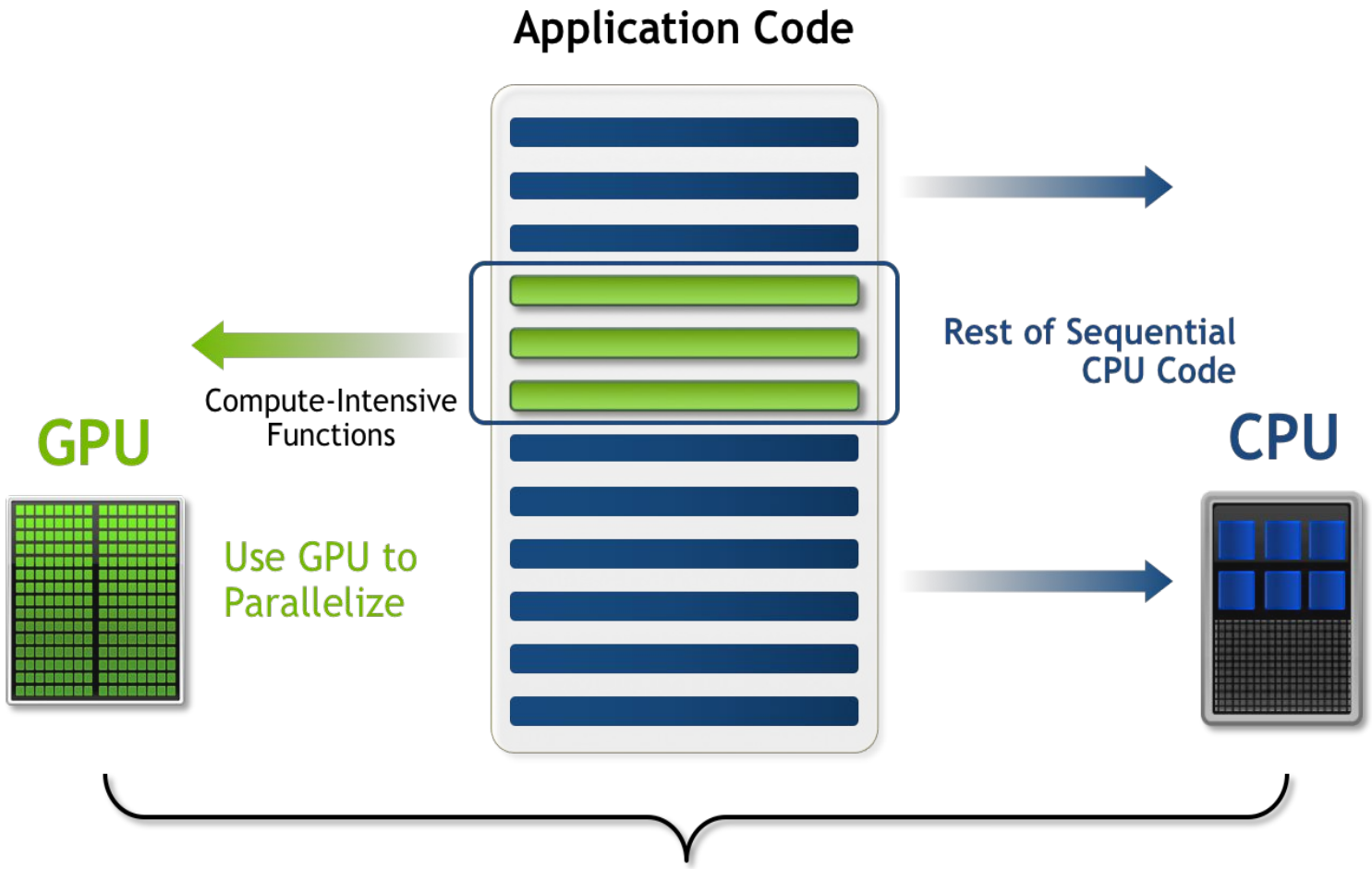
GPU vs CPU

CPU	GPU
Central Processing Unit	Graphics Processing Unit
Several (~4-8) cores	Many (100s) cores [Arithmetic Logic Unit]
Low latency	High throughput
Good for serial processing	Good for parallel processing
Can do a handful of operations at once	Can do thousands of operations at once

Check out: https://www.youtube.com/watch?v=ZrJeYFxpUyQ

https://blogs.nvidia.com/blog/2009/12/16/whats-the-difference-between-a-cpu-and-a-gpu/

Heterogeneous Computing



Using GPGPUs

- GPU enabled applications requires a parallel computing platform and application programming interface (API) that allows software developers and software engineers to build algorithms to modify their application and map compute-intensive kernels to the GPU

- GPGPU supports several types of memory in a memory hierarchy for designers to optimize their programs

- GPGPU memory is used for transferring data between device and host - shared memory is an efficient way for threads in the same block to share their runtime and data

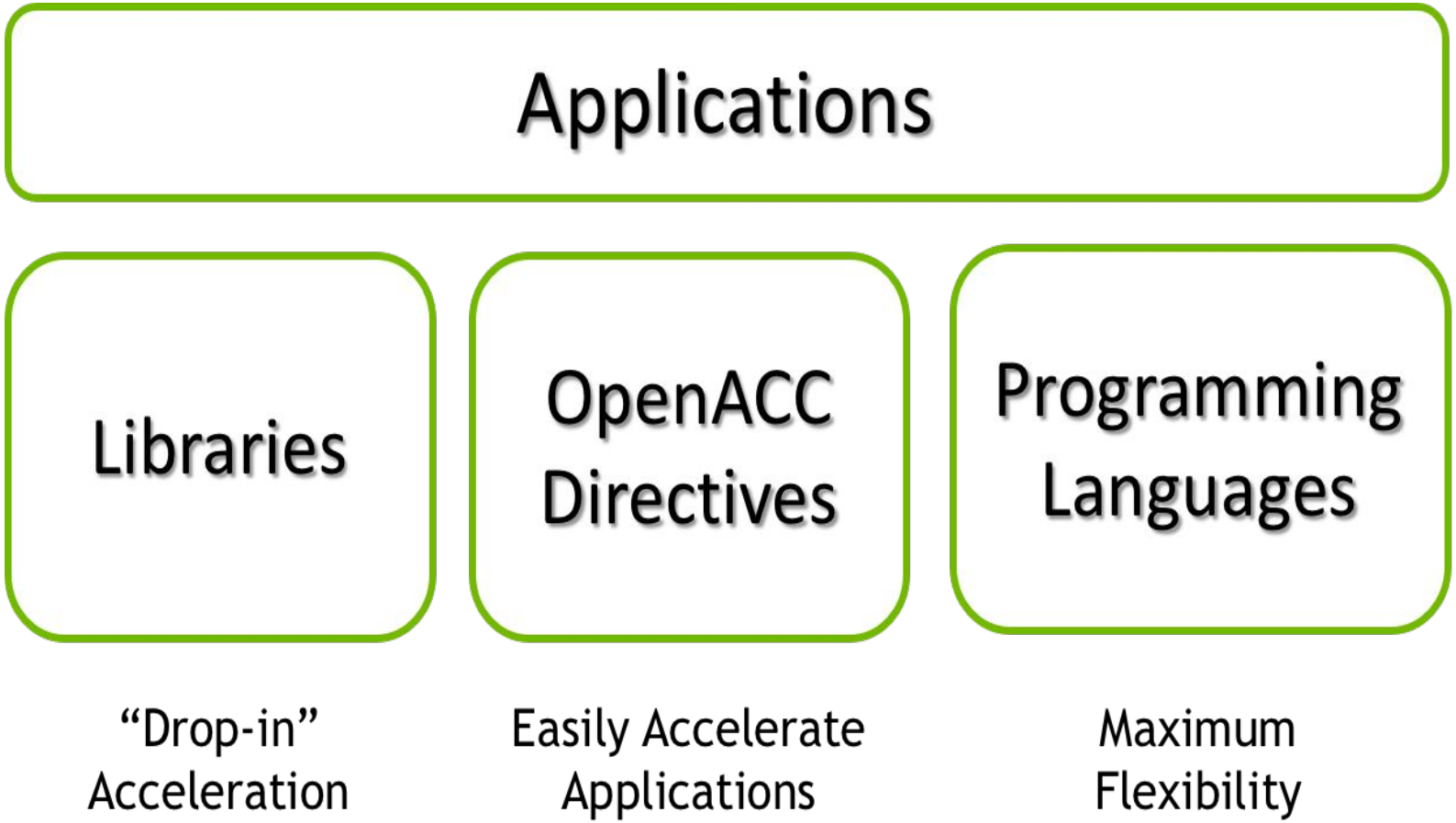
GPU accelerated applications

Large number of applications and frameworks in different scientific and engineering domains have been adapted to take advantage of GPUs.

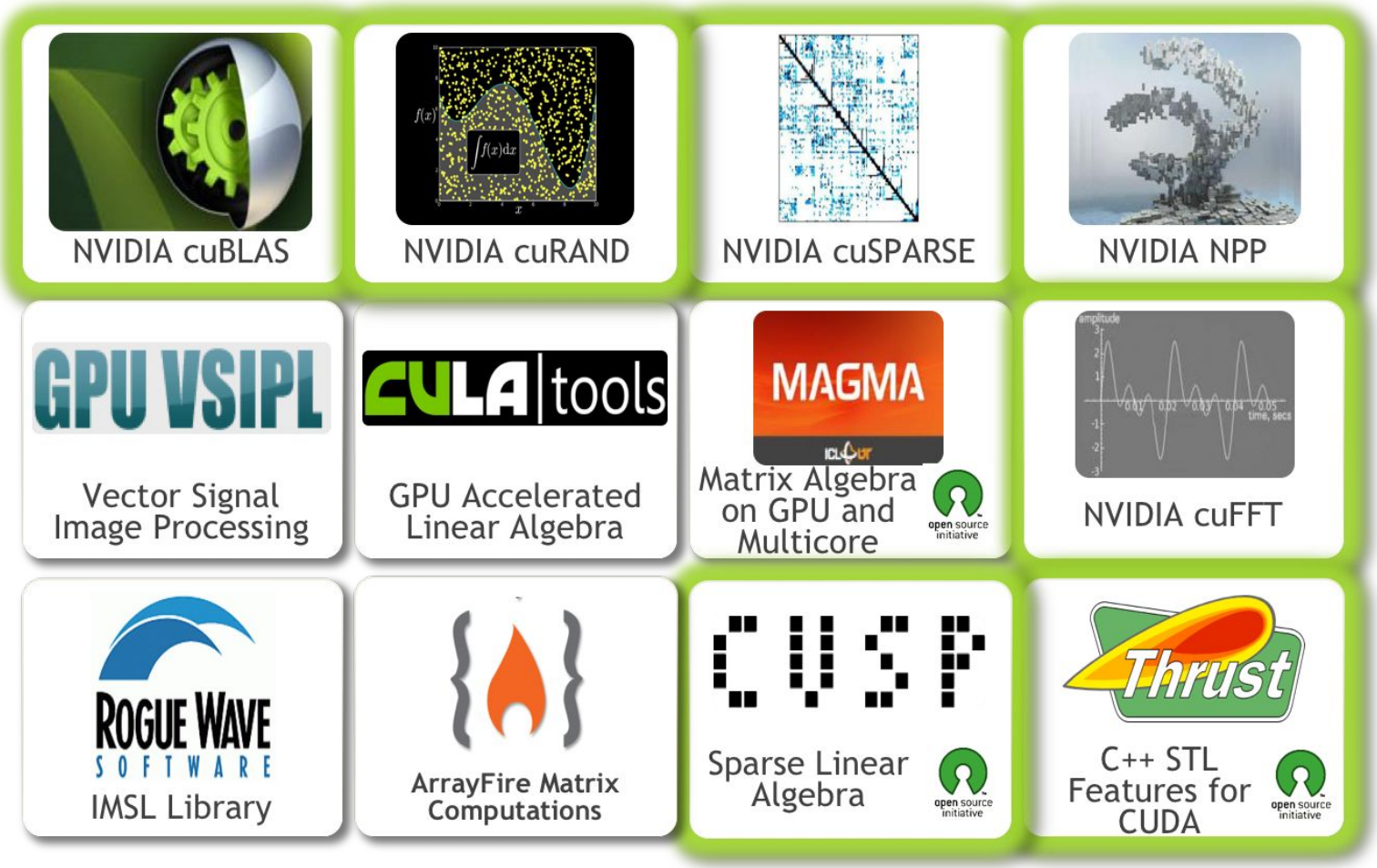
Examples:

- Deep Learning frameworks (TensorFlow, PyTorch, MXNet, etc.) have transparent Python APIs
  Typically, these can be easily installed via pip or `conda/mamba`
- MATLAB supports GPU computing via PCT
- Specific applications built with CUDA
- Containers available via Nvidia Cloud Computing platform
  https://ngc.nvidia.com/catalog/all

Three Ways to Accelerate Your Applications

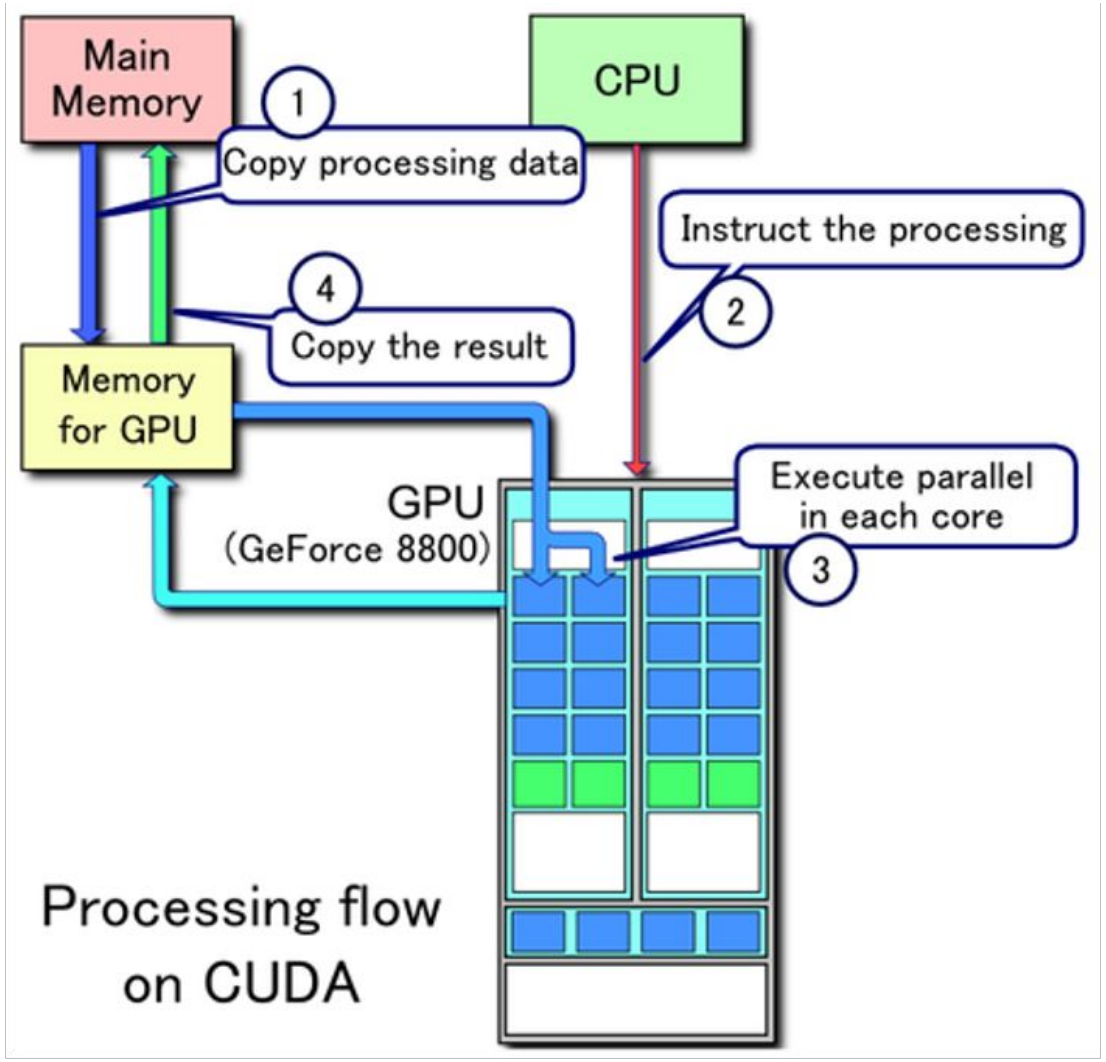


Some GPU-Accelerated Libraries



Processing Flow

- Copy input from CPU to GPU
- Load GPU program & execute it
- Copy back from GPU to CPU



Drop-in Library: cuBLAS (1)

Example: SAXPY
Stands for "Single-Precision A*X Plus Y" (a function in the standard BLAS library)

CPU version:

```
#include <stdio.h>
#include <gsl/gsl_cblas.h>

int main(){
    const int n = 5;
    const float alpha = 2.0;
    float x[] = {1.0, 2.0, 3.0, 4.0, 5.0};
    float y[] = {2.0, 4.0, 6.0, 8.0, 10.0};

    // Perform SAXPY operation
    cblas_saxpy(n, alpha, x, 1, y, 1);

    // Print final values
    printf("SAXPY result: ");
    for (int i = 0; i < n; i++) {
        printf("%f ", y[i]);
    }
    printf("\n");

    return 0;
}
```

Drop-in Library: cuBLAS (2)

Example: SAXPY
Stands for "Single-Precision A*X Plus Y" (a function in the standard BLAS library)

GPU version:

```
#include <stdio.h>
#include <cuda_runtime.h>
#include <cublas_v2.h>

int main(){
    ...
    // Initialize cuBLAS context
    cublasHandle_t handle;
    cublasCreate(&handle);

    // Allocate memory on device
    float *d_x, *d_y;
    cudaMalloc(&d_x, n*sizeof(float));
    cudaMalloc(&d_y, n*sizeof(float));

    // Copy data to device
    cudaMemcpy(d_x, x, n*sizeof(float), cudaMemcpyHostToDevice);
    cudaMemcpy(d_y, y, n*sizeof(float), cudaMemcpyHostToDevice);

    // Perform SAXPY operation
    cublasSaxpy(handle, n, &alpha, d_x, 1, d_y, 1);

    // Copy data back to host
    cudaMemcpy(y, d_y, n*sizeof(float), cudaMemcpyDeviceToHost);

    // Destroy cuBLAS context
    cublasDestroy(handle);

    // Free memory on device
    cudaFree(d_x);
    cudaFree(d_y);
    ...
```

Drop-in Library: cuBLAS (3)

Compiling

CPU version: saxpy_blas.c

```
# Load software modules
$ module load gcc/13.2.0-fasrc01

# Compile the code
$ gcc -o saxpy_blas.x saxpy_blas.c -lgslcblas
```

GPU version: saxpy_cublas.c

```
# Load software modules
$ module load cuda/12.2.0-fasrc01 gcc/13.2.0-fasrc01

# Compile the code
$ gcc -o saxpy_cublas.x saxpy_cublas.c -lcudart -lcublas
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/GPU/Libs

OpenACC

- **OpenACC** (for Open Accelerators) is a programming standard for parallel computing on accelerators (mostly on NIVDIA GPU)
- It is designed to simplify GPU programming
- The basic approach is to insert special comments (directives) into the code to offload computation onto GPUs and parallelize the code at the level of GPU (CUDA) cores
- It is possible for programmers to create an efficient parallel OpenACC code with only minor modifications to a serial CPU code

OpenACC

OpenACC COMPILER DIRECTIVES

Parallel C Code

```
void saxpy(int n,
           float a,
           float *x,
           float *y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

Parallel Fortran Code

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
!$acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$acc end kernels
end subroutine saxpy


...
! Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

http://developer.nvidia.com/openacc or http://openacc.org

Slide from Jeff Larkin - Nvidia
https://www.bu.edu/tech/files/2017/04/OpenACC-2017Spring.pdf

OpenACC

Compiling

GPU version: `example_acc.f90`

```
# Load software modules (NVIDIA HPC SDK)
$ module load nvhpc/23.7-fasrc01

# Compile command
$ nvfortran -o example_acc.x example_acc.f90 -acc
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/GPU/OpenACC

Using Programming Languages

- **Numerical frameworks:** MATLAB, Mathematica
- **Fortran:** OpenACC, CUDA Fortran, OpenCL/CLFORTRAN
- **C:** OpenACC, CUDA C, OpenCL
- **C++:** CUDA C++, Thrust, OpenCL C++
- **Python:** PyCUDA / Numba, Copperhead, PyOpenCL

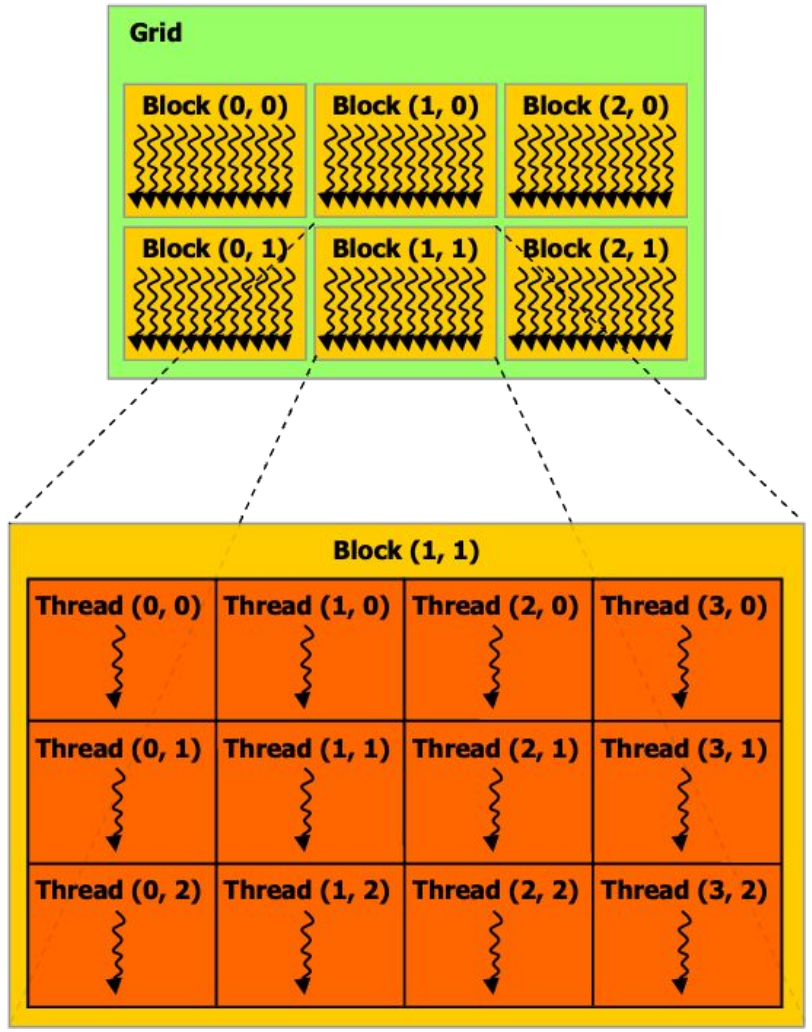
Compute Unified Device Architecture (CUDA)

- CUDA platform is a software layer that gives direct access to the GPU's virtual instruction set and parallel computational elements for the execution of compute kernels
- Designed to work with programming languages such as C, C++, and Fortran
- CUDA is an accessible platform, requiring no advanced skills in graphics programming, and available to software developers through CUDA-accelerated libraries and compiler directives
- CUDA-capable devices are typically connected with a host CPU and the host CPUs are used for data transmission and kernel invocation for CUDA devices
- The CUDA Toolkit includes GPU-accelerated libraries, a compiler, programming guides, API references, and the CUDA runtime

  https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/index.html

GPU computing with CUDA

- Threads
  - Execute kernels (simple C programs)
  - Executed by GPU cores
  - Each thread has its own ID
- Warp: Group of 32 threads
- Blocks:
  - Group of threads.
  - Threads in a block can synchronize execution
  - Executed by multiprocessors
- Grids: Group of blocks



By NVIDA Cuda programming

Using Programming Languages

CUDA C

```
void saxpy(int n, float a,
      float *x, float *y)
{
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

int N = 1<<20;



// Perform SAXPY on 1M elements
saxpy(N, 2.0, x, y);
```

```
__global__
void saxpy(int n, float a,
     float *x, float *y)
{
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n) y[i] = a*x[i] + y[i];
}

int N = 1<<20;
cudaMemcpy(d_x, x, N, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, N, cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements
saxpy<<<4096,256>>>(N, 2.0, d_x, d_y);

cudaMemcpy(y, d_y, N, cudaMemcpyDeviceToHost);
```

Slide from Jeff Larkin - Nvidia
https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/index.html

Using Programming Languages

Compiling

CUDA C

```
# Load software modules
$ module load nvhpc/23.7-fasrc01

# Compile command
$ nvcc -o saxpy.x saxpy.cu
```

CUDA Fortran

```
# Load software modules
$ module load nvhpc/23.7-fasrc01

# Compile command
$ nvfortran -o saxpy.x saxpy.cuf
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/GPU/CUDA

Using Programming Languages

PYTHON

Standard Python

```
import numpy as np


def saxpy(a, x, y):
  return [a * xi + yi
          for xi, yi in zip(x, y)]

x = np.arange(2**20, dtype=np.float32)
y = np.arange(2**20, dtype=np.float32)



cpu_result = saxpy(2.0, x, y)
```

http://numpy.scipy.org

Numba Parallel Python

```
import numpy as np
from numba import vectorize

@vectorize(['float32(float32, float32,
float32)'], target='cuda')
def saxpy(a, x, y):
  return a * x + y

N = 1048576

# Initialize arrays
A = np.ones(N, dtype=np.float32)
B = np.ones(A.shape, dtype=A.dtype)
C = np.empty_like(A, dtype=A.dtype)

# Add arrays onGPU
C = saxpy(2.0, X, Y)
```

https://numba.pydata.org

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/GPU/Numba

GPU Computing on the FASRC Cluster

The FASRC cluster has nodes with NVIDIA general purpose graphics processing units (GPGPU).

It is possible to use Nvidia CUDA tools for running computational work, and in certain use cases achieve very significant speedups.

GPU partitions:

- `gpu` partition: 36 nodes with 4 A100 80 GB GPUs per node
- `gpu_test` partition: 14 nodes with 4 A100 40 GB GPUs per node (MIG mode)
- `gpu_requeue` partition: nodes are owned by various research groups and are available when idle

Your lab may have access to other partitions with GPUs

https://docs.rc.fas.harvard.edu/kb/gpgpu-computing-on-the-cluster/

Running GPU jobs

Interactive Jobs:

```
# --- Start an interactive session on a partition with GPUs, e.g.,
[login-node ]$ salloc -p gpu_test --gres=gpu:1 --mem=4G -N 1 -t 60

# --- Check CUDA runtime (use nvidia-smi or nvtop)
[gpu-compute-node]$ nvidia-smi
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 535.54.03              Driver Version: 535.54.03    CUDA Version: 12.2     |
|-------------------------------+----------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-PCIE-32GB           On  | 00000000:06:00.0 Off |                    0 |
| N/A   35C    P0              25W / 250W |      0MiB / 32768MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

Running GPU jobs

```
# --- Check available CUDA versions
$ module available cuda/

---------------------------------- /n/sw/helmod-rocky8/modulefiles/Core ----------------------------
   cuda/9.1.85-fasrc01    cuda/11.8.0-fasrc01    cuda/12.2.0-fasrc01 (D)
   cuda/11.3.1-fasrc01    cuda/12.0.1-fasrc01
...

# --- Load required modules, e.g.,
$ module load cuda/12.2.0-fasrc01
$ which nvcc
/n/sw/helmod-rocky8/apps/Core/cuda/12.2.0-fasrc01/cuda/bin/nvcc

# --- Using CUDA-dependent software modules, e.g.,
$ module load cuda/12.2.0-fasrc01 cudnn/8.9.2.26_cuda12-fasrc01
```

Running GPU jobs

Example: Running tensorflow on a GPU node with Singularity:

```
# --- Start an interactive session on a partition with GPUs, e.g.,
[login-node  ]$ salloc -p gpu_test --gres=gpu:1 --mem=4G -N 1 -t 60
# --- cd to your SCRATCH folder ---
[compute-node]$ cd $SCRATCH/your_lab/your_user/
# --- Pull the latest TF GPU version from the Docker registry ---
# We could use a local installation of python and TF, but we'll use singularity
[compute-node]$ singularity pull --name tf213_gpu.simg \
> docker://tensorflow/tensorflow:2.13.0-gpu
# --- Get examples from keras.io ---
[compute-node]$ git clone https://github.com/keras-team/keras-io.git
# --- Execute the code ---
[compute-node]$ singularity exec --nv tf213_gpu.simg python  \
./keras-io/examples/vision/mnist_convnet.py
… (omitted output)
Test loss: 0.023846622556447983
Test accuracy: 0.9919000267982483
```

https://docs.rc.fas.harvard.edu/kb/singularity-on-the-cluster/

https://github.com/fasrc/User_Codes/tree/master/AI/TensorFlow#gpu-version

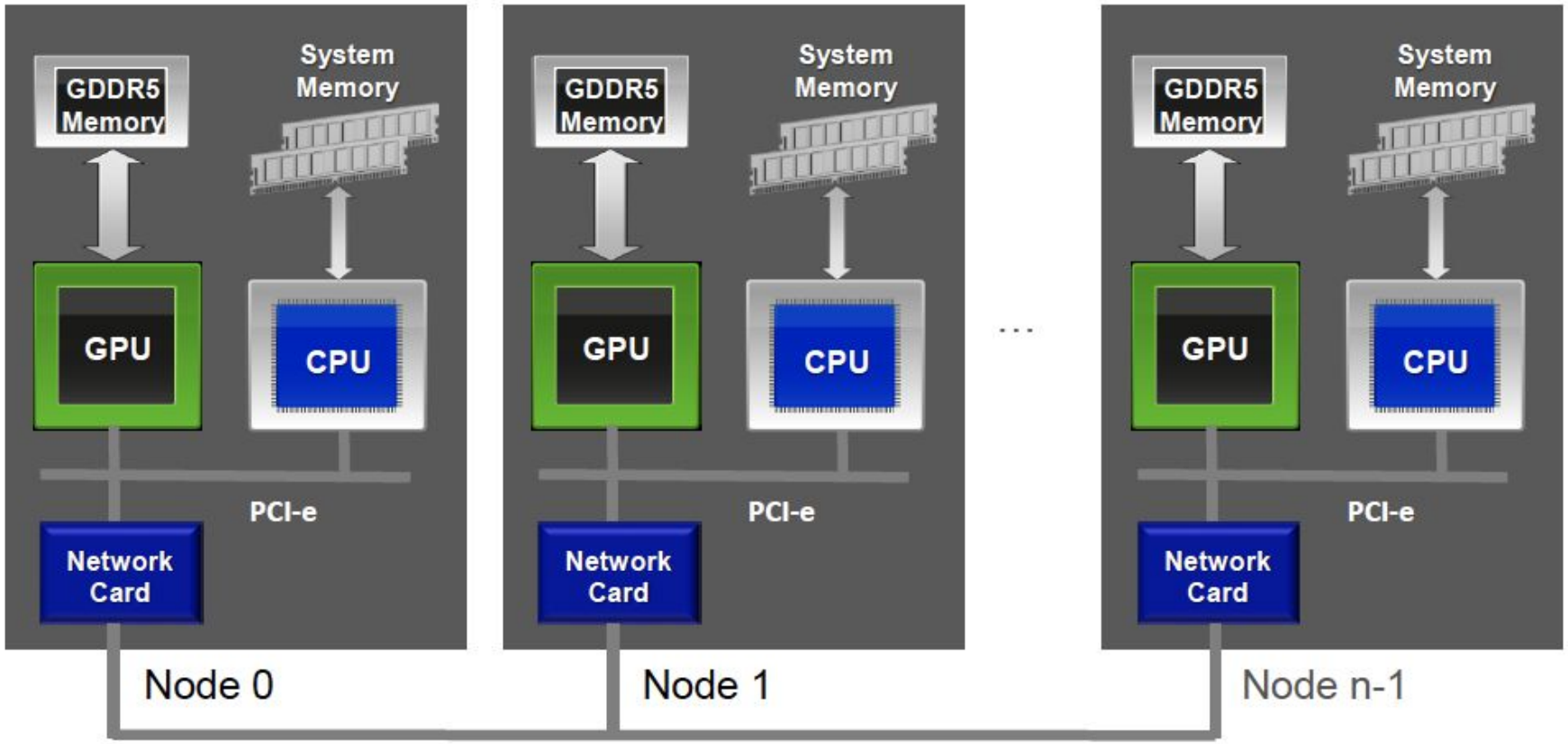
Running GPU batch jobs

```
#!/bin/bash
#SBATCH -p gpu
#SBATCH -n 1
#SBATCH -c 1
#SBATCH --gres=gpu:1
#SBATCH --mem=12000
#SBATCH -J example_tf
#SBATCH -t 30

## you could use a local installation of python and tensorflow,
## but we'll use singularity

singularity exec --nv docker://tensorflow/tensorflow:latest-gpu \
                        python myCNN.py  > output.tf
```

NOTE: Use `nvidia-smi` or `nvtop` to monitor GPU usage in real-time on the execution host

Multi-GPU jobs with MPI

MPI+CUDA

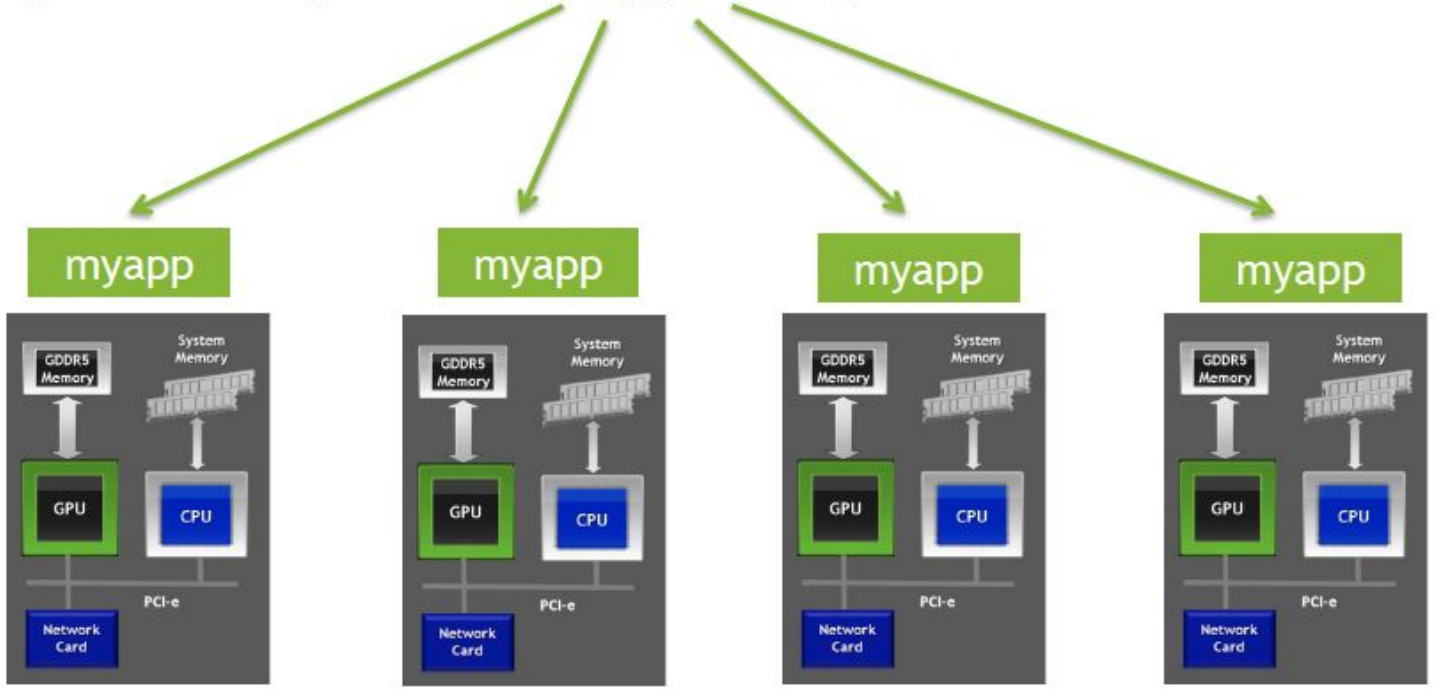


Slide by Jiri Kraus and Peter Messmer
https://on-demand.gputechconf.com/gtc/2014/presentations/S4236-multi-gpu-programming-mpi.pdf

Multi-GPU jobs with MPI

Compiling and Launching

```
$ mpicc -o myapp myapp.c
$ mpirun -np 4 ./myapp <args>
```



Slide by Jiri Kraus and Peter Messmer
https://on-demand.gputechconf.com/gtc/2014/presentations/S4236-multi-gpu-programming-mpi.pdf

Multi-GPU jobs with MPI

Example: 2 nodes with 4 MPI tasks and 4 GPUs per node

```
#!/bin/bash
#SBATCH -N 2
#SBATCH --ntasks-per-node=4
#SBATCH --gres=gpu:4
#SBATCH --mem-per-cpu=8G
#SBATCH -J gpu_mpi_test
#SBATCH -t 1:00:00
#SBATCH -p gpu_test
#SBATCH -o gpu_mpi_test.out
#SBATCH -e gpu_mpi_test.err

# --- Load required modules
module load gcc/12.2.0-fasrc01
module load openmpi/4.1.5-fasrc02 # built against cuda/12.2.2-fasrc01 and ucx/1.14.1-fasrc02

# --- Launch application
srun -n 8 --mpi=pmix ./app.mpi.cuda
```

Request Help - Resources

- https://docs.rc.fas.harvard.edu/kb/support/
  - Rocky 8 Transition Guide
    - https://docs.rc.fas.harvard.edu/kb/rocky-8-transition-guide/
  - Portal
    - http://portal.rc.fas.harvard.edu/rcrt/submit_ticket
  - Email
    - rchelp@rc.fas.harvard.edu
  - Office Hours
    - Wednesday noon-3pm https://harvard.zoom.us/j/255102481
  - Training Calendar
    - https://www.rc.fas.harvard.edu/upcoming-training/

Thank you! Questions? Comments?

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