# ECE408 / CS483/CSE408 Fall 2022

# Applied Parallel Programming

## Lecture 23: Alternatives to CUDA

# Accelerated Computing is no longer a question

GPU vendors include:
Nvidia
AMD
Intel
Samsung
Apple
Qualcomm
ARM
Etc….

## CUDA is just one model for Compute Acceleration

OpenGL (1992)
DirectX (1995)

GPGPU (2002)

CUDA (2007)

OpenCL (2008)

OpenACC (2012)
C++AMP (2013)
RenderScript (2013)

Metal (2014)
SYCL (2014)
Vulkan (2016)
ROCm HIP (2016)

Existing frameworks such as MPI, TBB, OpenCV adapted to provide support.
New frameworks such as Caffe, TensorFlow, R, PyCUDA natively support acceleration.

# OpenCL, OpenACC, MPI

- OpenCL: An Open Standard Acceleration API
- OpenACC: A “Low-Code” Acceleration API
- MPI: A Large Scale, Multi-Node Parallel API

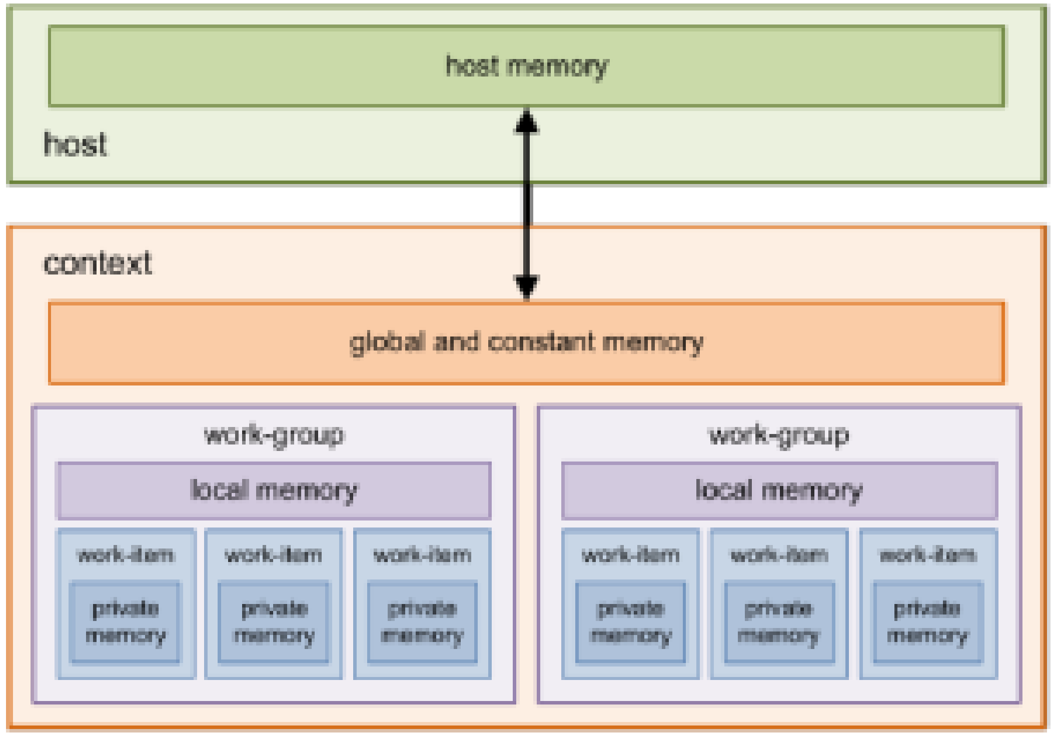
# Common Traits for Acceleration APIs

- HARDWARE
  - Hierarchy of lightweight cores
  - Local scratchpad memories
  - Lack of HW coherence
  - Slow global atomics
  - Threading
- SOFTWARE
  - Kernel oriented acceleration
  - Device memory vs. Host memory
  - Software managed memory
  - Grids, Blocks, Threads
  - Bulk Synchronous Parallelism

# OpenCL

- Framework for CPUs, GPUs, DSPs, FPGAs, etc (not just Nvidia GPUs)
- Initially developed by Apple with support from AMD, IBM, Qualcomm, Intel, and Nvidia. OpenCL 1.0 launched in 2008.
- OpenCL 2.2 launched in May 2017
- Apple announces dropping of OpenCL in 2018

# OpenCL Memory Model



# OpenCL MatMult

- Notice similarity to CUDA
- WorkGroup similar to Block
- WorkItem similar to Thread
- __local similar to __shared

```
// Tiled and coalesced version
__kernel void myGEMM2(int M, int N, int K, __global float* A, __global float* B, __global float* C) {

   // Thread identifiers
   const int row = get_local_id(0); // Local row ID (max: TS)
   const int col = get_local_id(1); // Local col ID (max: TS)
   const int globalRow = TS*get_group_id(0) + row; // Row ID of C (0..M)
   const int globalCol = TS*get_group_id(1) + col; // Col ID of C (0..N)

    // Local memory to fit a tile of TS*TS elements of A and B
    __local float Asub[TS][TS];
    __local float Bsub[TS][TS];

    // Initialise the accumulation register
    float acc = 0.0f;
    // Loop over all tiles
    const int numTiles = K/TS;
    for (int t=0; t<numTiles; t++) {

       // Load one tile of A and B into local memory
       const int tiledRow = TS*t + row;
       const int tiledCol = TS*t + col;
       Asub[col][row] = A[tiledCol*M + globalRow];
       Bsub[col][row] = B[globalCol*K + tiledRow];

       // Synchronise to make sure the tile is loaded
       barrier(CLK_LOCAL_MEM_FENCE);

       // Perform the computation for a single tile
       for (int k=0; k<TS; k++)
          acc += Asub[k][row] * Bsub[col][k];

       // Synchronise before loading the next tile
       barrier(CLK_LOCAL_MEM_FENCE);
    }

    // Store the final result in C
    C[globalCol*M + globalRow] = acc;
}
```

# OpenACC

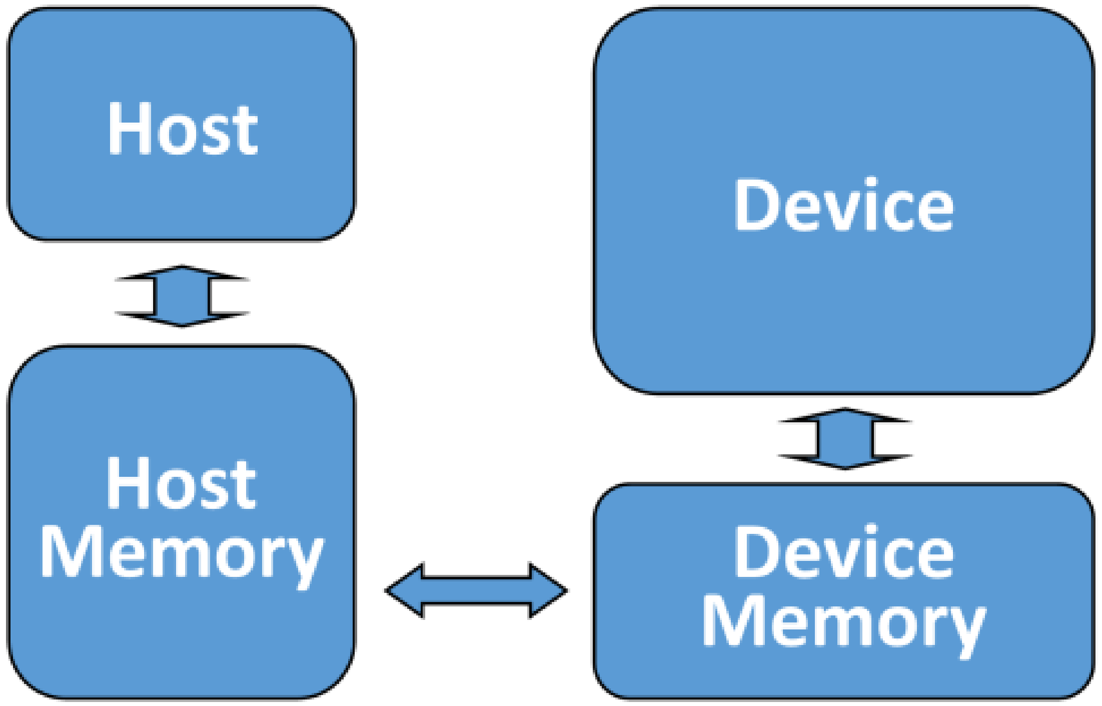
- The OpenACC Application Programming Interface (API) provides a set of
  - compiler directives (pragmas)
  - library routines and
  - environment variables

  that can be used to write data parallel FORTRAN, C and C++ programs that run on accelerator devices including GPUs and CPUs

## OpenACC Pragmas

- In C and C++, the #pragma directive is the means to provide, to the compiler, information that is not specified in the standard language.

# The OpenACC Abstract Machine Model



# Simple Matrix-Matrix Multiplication in OpenACC

```
void computeAcc(float *P, const float *M, const float *N, int Mh, int Mw, int Nw)
{

 #pragma acc parallel loop copyin(M[0:Mh*Mw]) copyin(N[0:Nw*Mw]) copyout(P[0:Mh*Nw])
 for (int i=0; i<Mh; i++) {
     #pragma acc loop
     for (int j=0; j<Nw; j++) {
         float sum = 0;
         for (int k=0; k<Mw; k++) {
             float a = M[i*Mw+k];
             float b = N[k*Nw+j];
             sum += a*b;
         }
         P[i*Nw+j] = sum;
     }
  }
}
```

## Some Observations

- The code is almost identical to the sequential version, except for the two lines with #pragma at line 4 and line 6.
- OpenACC uses compiler directives to extend the base language.
  - #pragma at line 4 tells the compiler to generate code for the 'i' loop at line 5 through 16 so that the loop iterations are executed in parallel on the accelerator.
  - The copyin clause and the copyout clause specify how the matrix data should be transferred between the host and the accelerator. The #pragma at line 6 instructs the compiler to map the inner 'j' loop to the second level of parallelism on the accelerator.

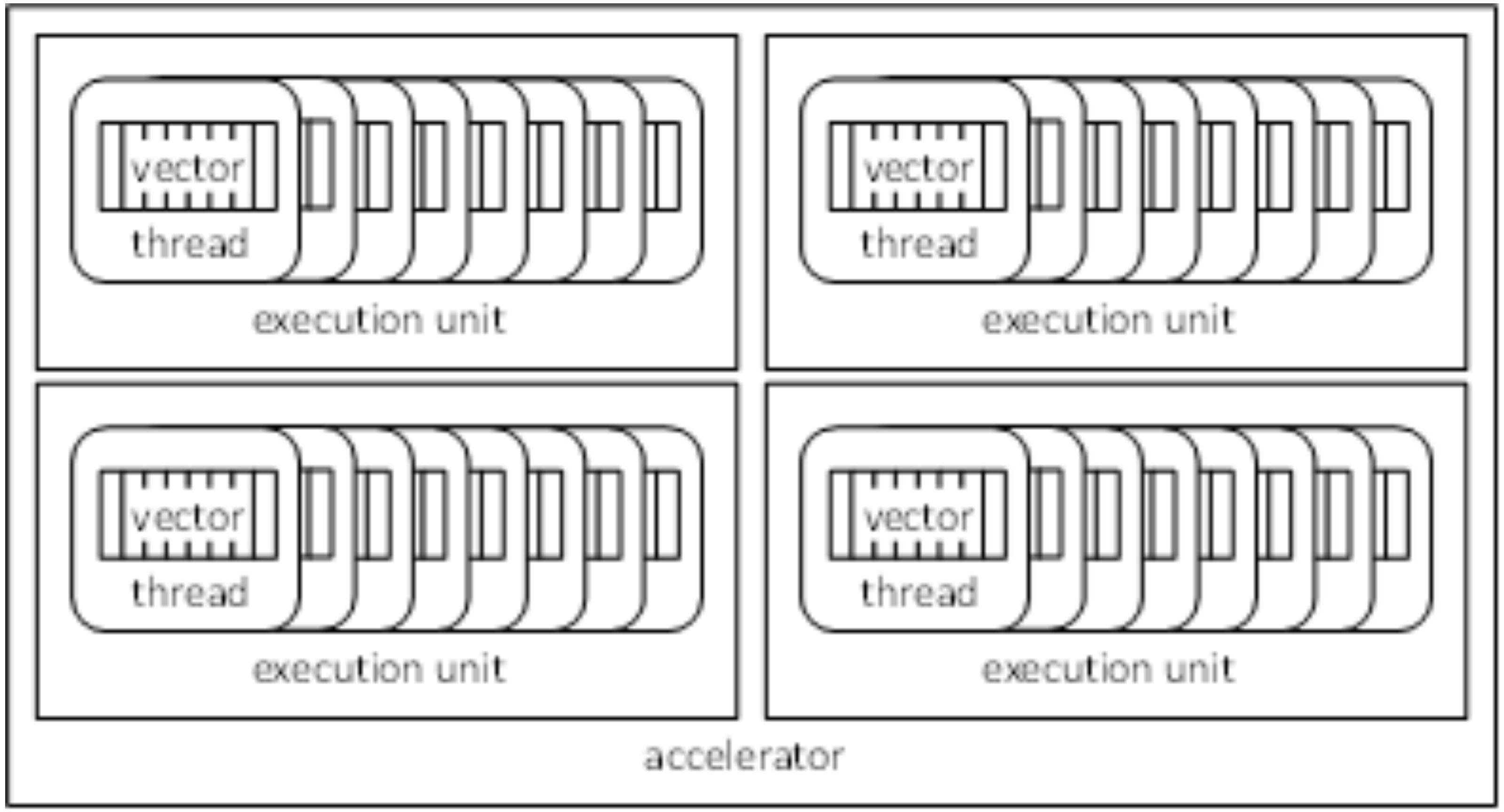
## Motivation

- OpenACC programmers can often start with writing a sequential version and then annotate their sequential program with OpenACC directives.
  – leave most of the details in generating a kernel and data transfers to the OpenACC compiler.
- OpenACC code can be compiled by non-OpenACC compilers by ignoring the pragmas.

## Frequently Encountered Issues

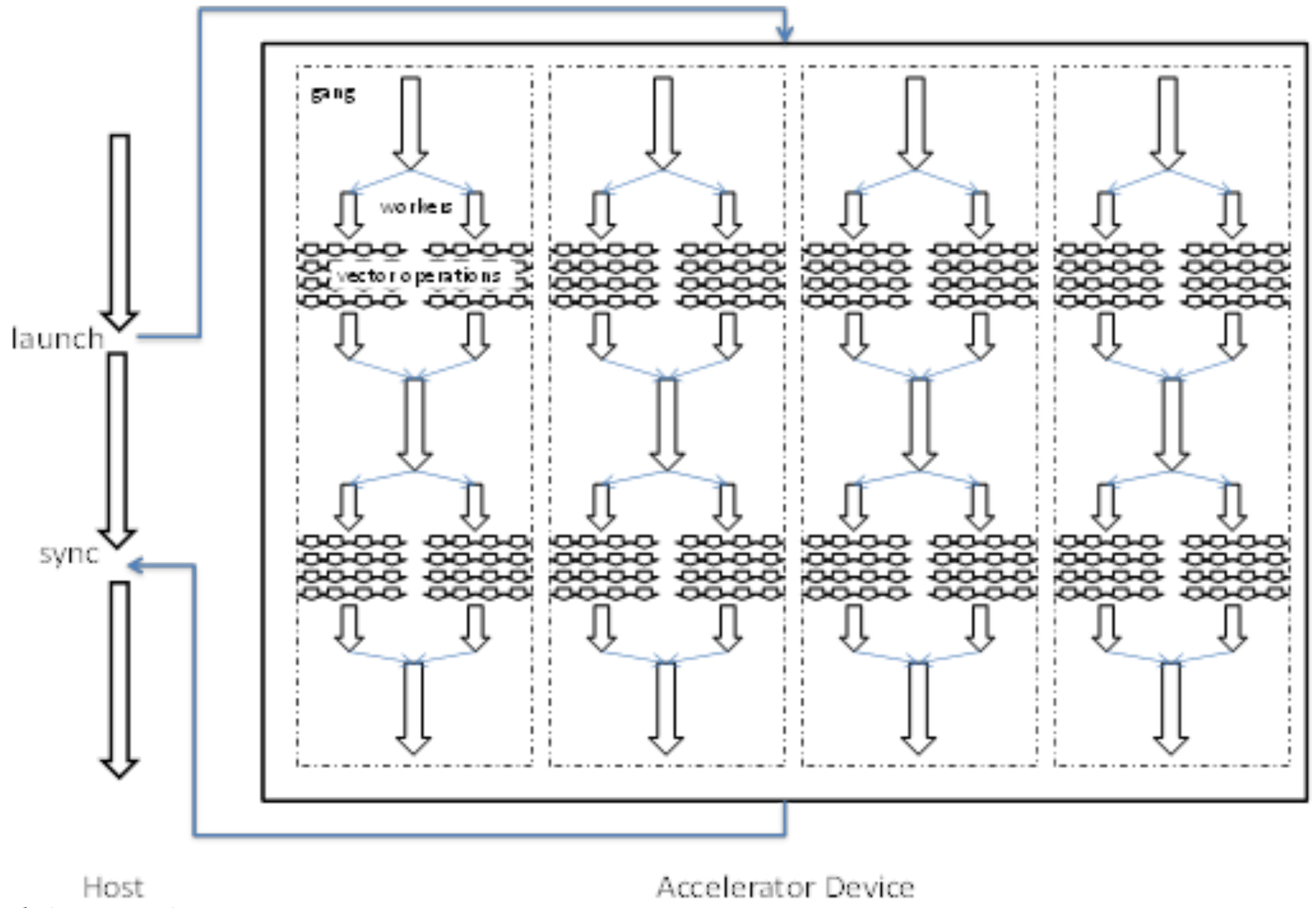
- Some OpenACC pragmas are hints to the OpenACC compiler, which may or may not be able to act accordingly
  - The performance of an OpenACC depends heavily on the quality of the compiler.
  - Much less so in CUDA or OpenCL, which are explicit
- Some OpenACC programs may behave differently or even incorrectly if pragmas are ignored

# OpenACC Device Model



There are is also a minimal set of APIs in OpenACC, for things like synchronization, memory management, etc

# OpenACC Execution Model (Terminology: Gangs and Workers)



# Parallel vs. Loop Constructs

```
#pragma acc parallel loop copyin(M[0:Mh*Mw]) copyin(N[0:Nw*Mw]) copyout(P[0:Mh*Nw])
for (int i=0; i<Mh; i++) {
…
}
```

is equivalent to:

```
#pragma acc parallel copyin(M[0:Mh*Mw]) copyin(N[0:Nw*Mw]) copyout(P[0:Mh*Nw])
{
      #pragma acc loop
      for (int i=0; i<Mh; i++) {
          …
      }
}
```

(a parallel region that consists of just a loop)

## Parallel Construct

- A parallel construct is executed on an accelerator
- One can specify the number of gangs and number of workers in each gang
- Programmer's directive

```
#pragma acc parallel copyout(a) num_gangs(1024) num_workers(32)
{
      a = 23;
}
```

1024*32 workers will be created. a=23 will be executed redundantly by all 1024 gang leads

# What does each "Gang Loop" do?

```
#pragma acc parallel num_gangs(1024)
{
     for (int i=0; i<2048; i++) {
          …
     }
}
```

The for-loop will be redundantly executed by 1024 gangs

```
#pragma acc parallel num_gangs(1024)
{
#pragma acc loop gang
     for (int i=0; i<2048; i++) {
          …
     }
}
```

The 2048 iterations of the for-loop will be divided among 1024 gangs for execution

## Worker Loop

```
#pragma acc parallel num_gangs(1024) num_workers(32)
{
     #pragma acc loop gang
     for (int i=0; i<2048; i++) {
          #pragma acc loop worker
          for (int j=0; j<512; j++) {
              foo(i,j);
         }
     }
}
```

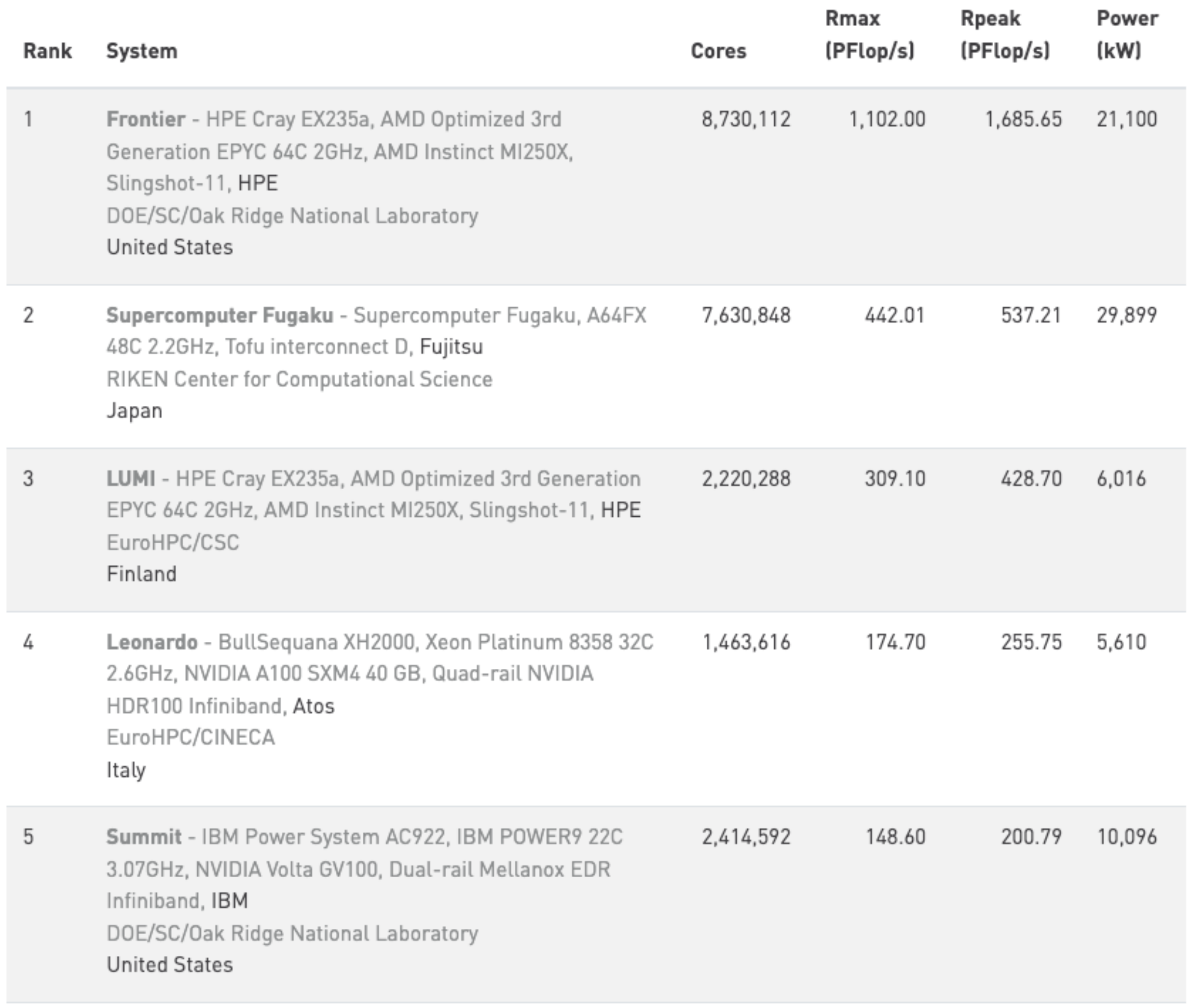
1024*32=32K workers will be created, each executing 1M/32K = 32 instance of foo()

# A More Complex Example

```
#pragma acc parallel num_gangs(32)
{
     Statement 1; Statement 2;
     #pragma acc loop gang
     for (int i=0; i<n; i++) {
         Statement 3; Statement 4;
     }
     Statement 5;  Statement 6;
     #pragma acc loop gang
     for (int i=0; i<m; i++) {
         Statement 7;  Statement 8;
     }
     Statement 9;
     if (condition)
        Statement 10;
}
```

- Statements 1 and 2 are redundantly executed by 32 gangs
- The n for-loop iterations are distributed to 32 gangs

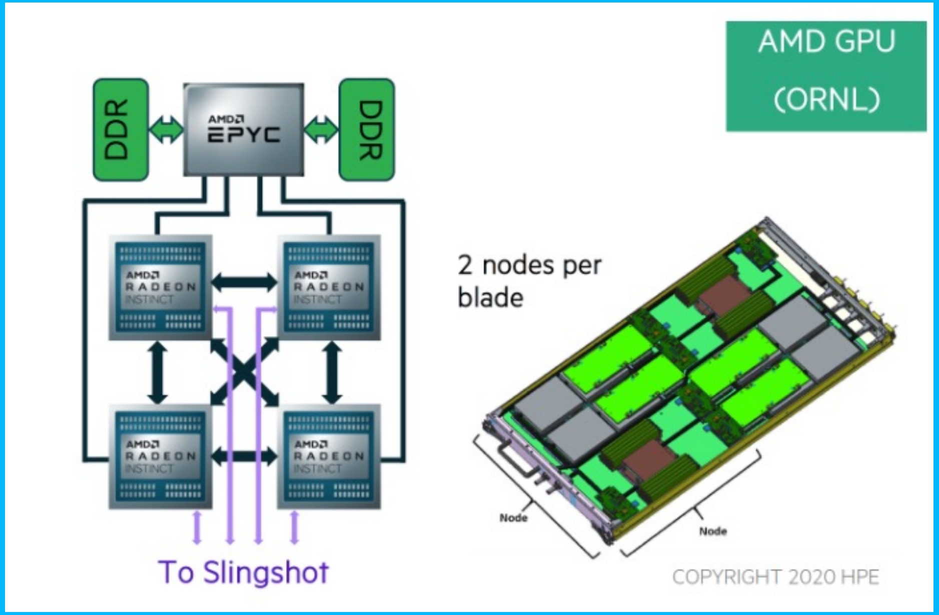
# Top 5 Supercomputers (Fall 2022)



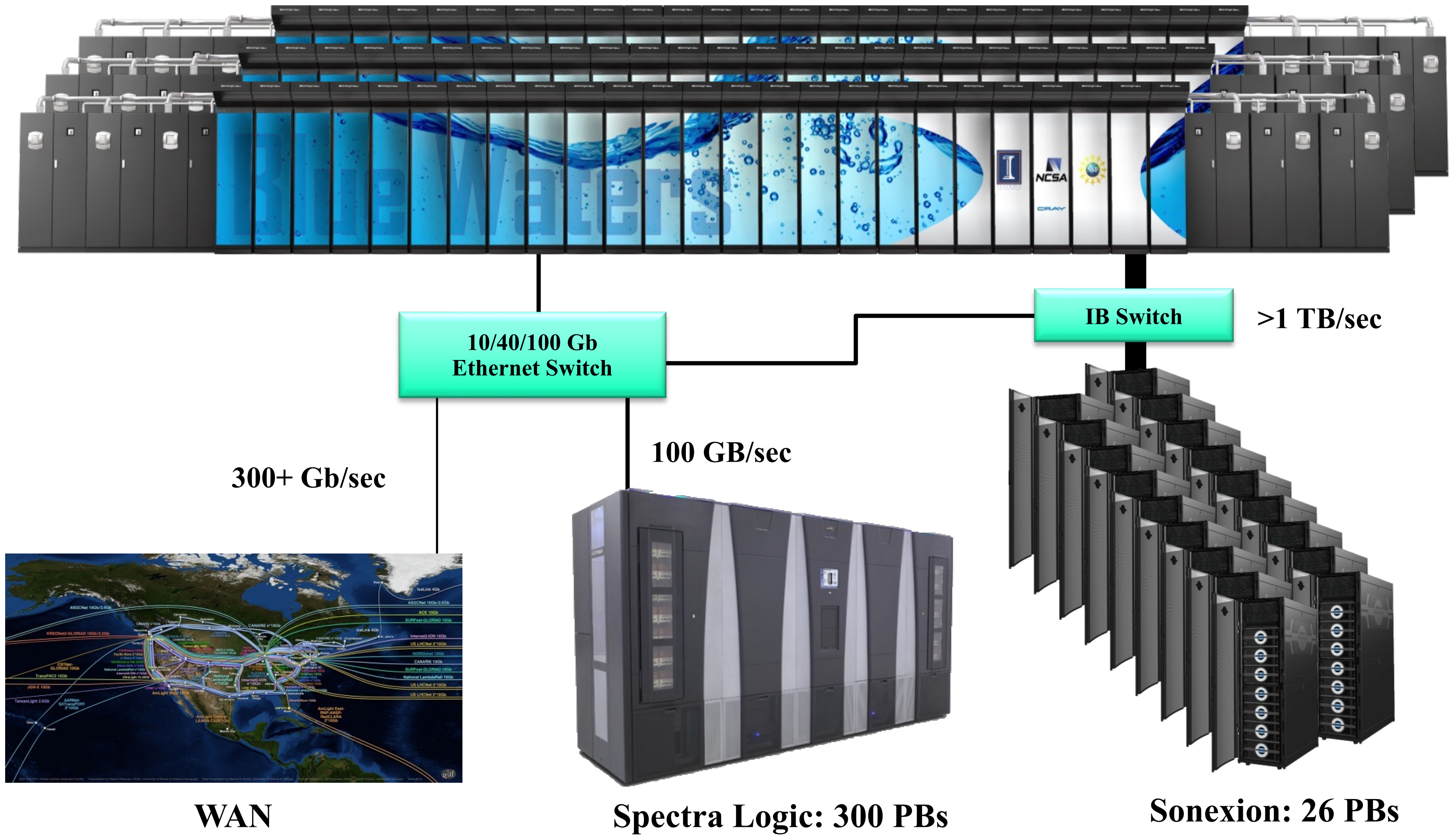
| Rank | System | Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) |
|---|---|---|---|---|---|
| 1 | **Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE<br>DOE/SC/Oak Ridge National Laboratory<br>United States | 8,730,112 | 1,102.00 | 1,685.65 | 21,100 |
| 2 | **Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu<br>RIKEN Center for Computational Science<br>Japan | 7,630,848 | 442.01 | 537.21 | 29,899 |
| 3 | **LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE<br>EuroHPC/CSC<br>Finland | 2,220,288 | 309.10 | 428.70 | 6,016 |
| 4 | **Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 40 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos<br>EuroHPC/CINECA<br>Italy | 1,463,616 | 174.70 | 255.75 | 5,610 |
| 5 | **Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM<br>DOE/SC/Oak Ridge National Laboratory<br>United States | 2,414,592 | 148.60 | 200.79 | 10,096 |

ORNL Frontier

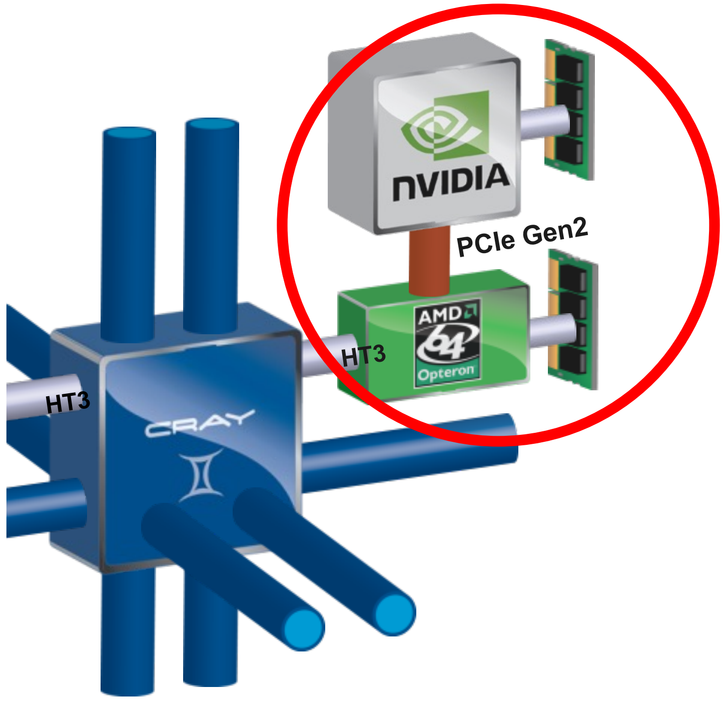
9472 AMD CPUs
37,888 AMD GPUs



# Blue Waters @ UIUC (2013-2021)



# Cray XK7 Nodes



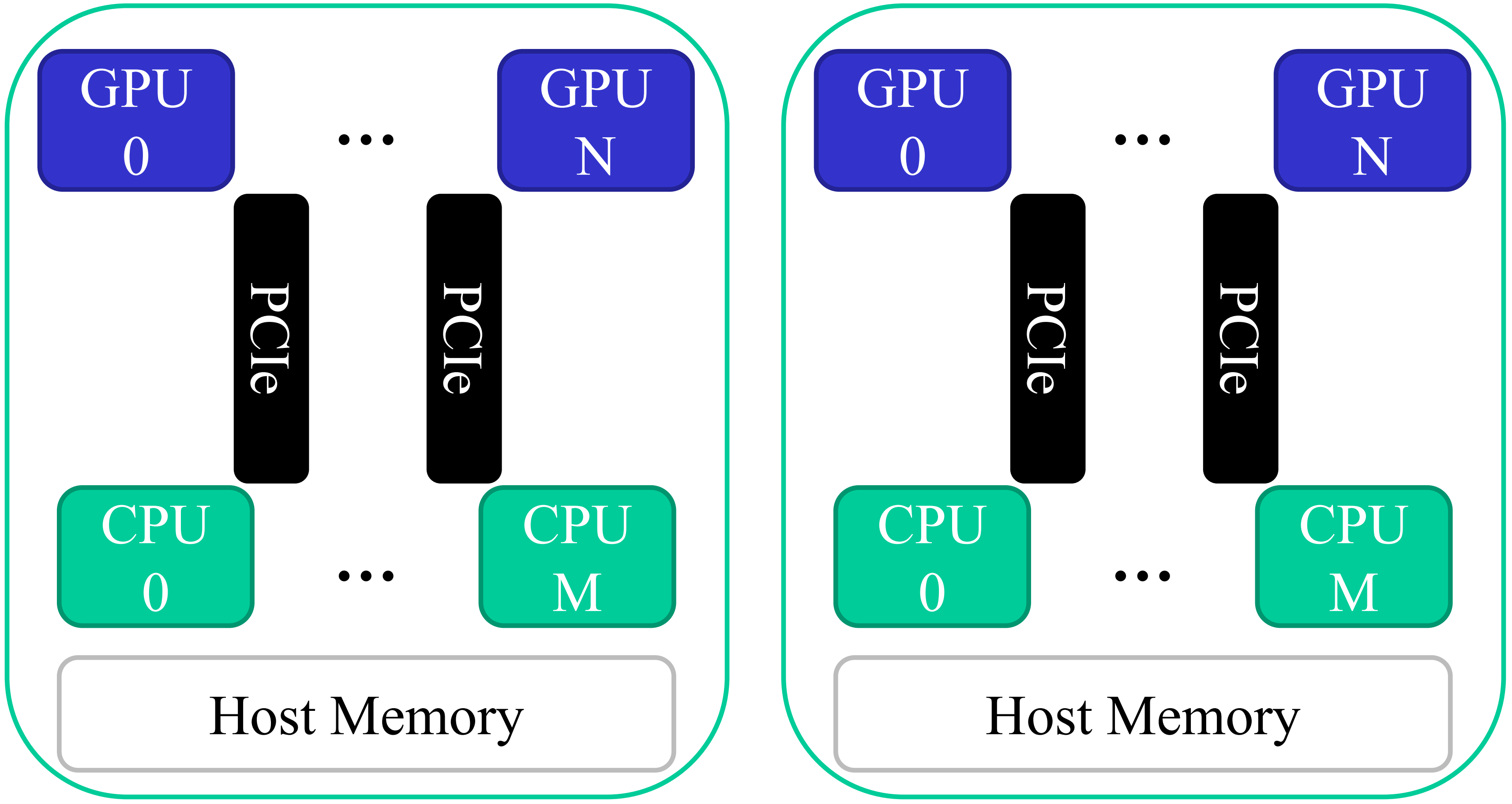
- Dual-socket Node
  - One AMD Interlagos chip
    - 8 core modules, 32 threads
    - 156.5 GFs peak performance
    - 32 GBs memory
      - 51 GB/s bandwidth
  - One NVIDIA Kepler chip
    - 1.3 TFs peak performance
    - 6 GBs GDDR5 memory
      - 250 GB/sec bandwidth
  - Gemini Interconnect
    - Same as XE6 nodes

**Blue Waters contains 4,224 Cray XK7 compute nodes.**

| Science Area | Number of Teams | Codes | Struct Grids | Unstruct Grids | Dense Matrix | Sparse Matrix | N-Body | Monte Carlo | FF T | PIC | Signific ant I/O |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Climate and Weather | 3 | CESM, GCRM, CM1/WRF, HOMME | X | X |  | X |  | X |  |  | X |
| Plasmas/Magnetosphere | 2 | H3D(M),VPIC, OSIRIS, Magtail/UPIC | X |  |  |  | X |  | X |  | X |
| Stellar Atmospheres and Supernovae | 5 | PPM, MAESTRO, CASTRO, SEDONA, ChaNGa, MS-FLUKSS | X |  |  | X | X | X |  | X | X |
| Cosmology | 2 | Enzo, pGADGET | X |  |  | X | X |  |  |  |  |
| Combustion/Turbulence | 2 | PSDNS, DISTUF | X |  |  |  |  |  | X |  |  |
| General Relativity | 2 | Cactus, Harm3D, LazEV | X |  |  | X |  |  |  |  |  |
| Molecular Dynamics | 4 | AMBER, Gromacs, NAMD, LAMMPS |  |  |  | X | X |  | X |  |  |
| Quantum Chemistry | 2 | SIAL, GAMESS, NWChem |  |  | X | X | X | X |  |  | X |
| Material Science | 3 | NEMOS, OMEN, GW, QMCPACK |  |  | X | X | X | X |  |  |  |
| Earthquakes/Seismology | 2 | AWP-ODC, HERCULES, PLSQR, SPECFEM3D | X | X |  |  | X |  |  |  | X |
| Quantum Chromo Dynamics | 1 | Chroma, MILC, USQCD | X |  | X | X |  |  |  |  |  |
| Social Networks | 1 | EPISIMDEMICS |  |  |  |  |  |  |  |  |  |
| Evolution | 1 | Eve |  |  |  |  |  |  |  |  |  |
| Engineering/System of Systems | 1 | GRIPS,Revisit |  |  |  |  |  | X |  |  |  |
| Computer Science | 1 |  |  | X | X | X |  |  | X |  | X |

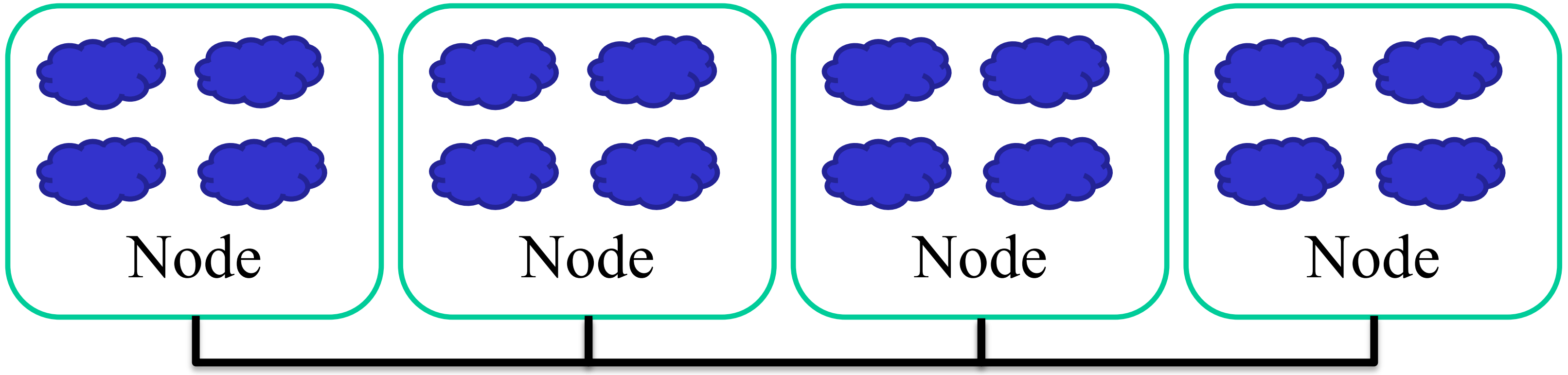
# Abstract CUDA-based Node

- Each node contains *N* GPUs



# MPI Model

- Many processes distributed in a cluster



- Each process computes part of the output
- Processes communicate with each other through message passing (not global memory)
- Processes can synchronize through messages

# MPI Initialization, Info

- `User launches an MPI job with X processes by executing in the command shell`
  - `MPIrun -np X`
- `int MPI_Init(int *argc, char ***argv)`
  - Initialize MPI
- `MPI_COMM_WORLD`
  - MPI group formed with all allocated nodes
- `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Rank of the calling process in group of comm
- `int MPI_Comm_size(MPI_Comm comm, int *size)`
  - Number of processes in the group of comm

# Vector Addition: Main Process

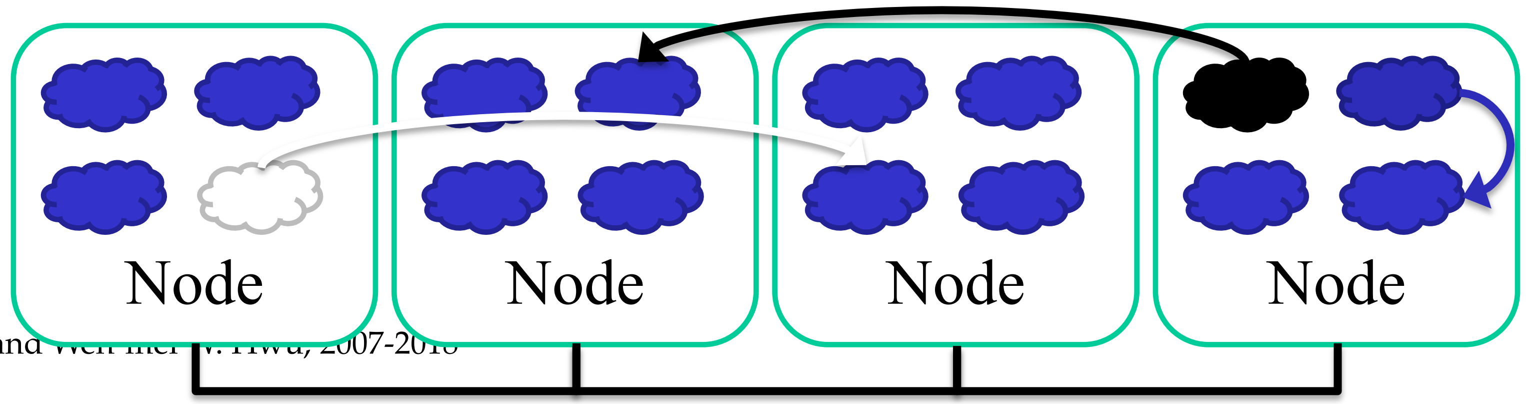
```
int main(int argc, char *argv[]) {
    int vector_size = 1024 * 1024 * 1024;
    int pid=-1, np=-1;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    if(np < 3) {
        if(0 == pid) printf(“Nedded 3 or more processes.\n");
        MPI_Abort( MPI_COMM_WORLD, 1 ); return 1;
    }
    if(pid < np - 1)
        compute_node(vector_size / (np - 1));
    else
        data_server(vector_size);

    MPI_Finalize();
    return 0;
}
```

## MPI Sending Data

- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
  - buf: Starting address of send buffer
  - count: Number of elements in send buffer (nonnegative integer)
  - datatype: Datatype of each send buffer element
  - dest: Rank of destination (integer)
  - tag: Message tag (integer)
  - comm: Communicator (handle)

# MPI Sending Data

- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
  - Buf: Initial address of send buffer
  - Count: Number of elements in send buffer (nonnegative integer)
  - Datatype: Datatype of each send buffer element
  - Dest: Rank of destination (integer)
  - Tag: Message tag (integer)
  - Comm: Communicator (handle)



# MPI Receiving Data

- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`
  - Buf: Starting address of receive buffer
  - Count: Maximum number of elements in receive buffer (non-negative integer)
  - Datatype:  Datatype of each receive buffer element
  - Source: Rank of source (integer)
  - Tag: Message tag (integer)
  - Comm: Communicator (handle)
  - Status: Status object

# MPI Receiving Data

- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`
  - Buf: Initial address of receive buffer
  - Count: Maximum number of elements in receive buffer (non-negative integer)
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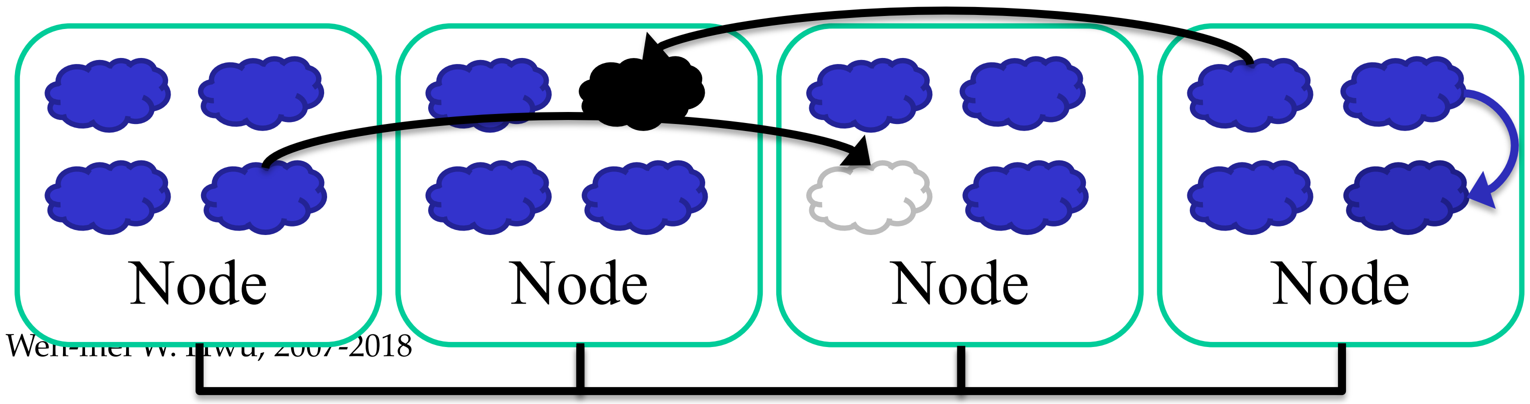
  - Source: Rank of source (integer)
  - Tag: Message tag (integer)
  - Comm: Communicator (handle)
  - Status: Status object (Status)



# Vector Addition: Server Process (I)

```
void data_server(unsigned int vector_size) {
    int np, num_nodes = np – 1, first_node = 0, last_node = np - 2;
    unsigned int num_bytes  = vector_size * sizeof(float);
    float *input_a = 0, *input_b = 0, *output = 0;

    /* Set MPI Communication Size */
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    /* Allocate input data */
    input_a = (float *)malloc(num_bytes);
    input_b = (float *)malloc(num_bytes);
    output = (float *)malloc(num_bytes);
    if(input_a == NULL || input_b == NULL || output == NULL) {
        printf("Server couldn't allocate memory\n");
        MPI_Abort( MPI_COMM_WORLD, 1 );
    }
    /* Initialize input data */
    random_data(input_a, vector_size , 1, 10);
    random_data(input_b, vector_size ,
```

## Vector Addition: Server Process (II)

```
/* Send data to compute nodes */
float *ptr_a = input_a;
float *ptr_b = input_b;

for(int process = 1; process < last_node; process++) {
    MPI_Send(ptr_a, vector_size / num_nodes, MPI_FLOAT,
            process, DATA_DISTRIBUTE, MPI_COMM_WORLD);
    ptr_a += vector_size / num_nodes;

    MPI_Send(ptr_b, vector_size / num_nodes, MPI_FLOAT,
            process, DATA_DISTRIBUTE, MPI_COMM_WORLD);
    ptr_b += vector_size / num_nodes;
}
```

## Vector Addition: Server Process (III)

```
    /* Wait for compute to complete*/
    MPI_Barrier(MPI_COMM_WORLD);

    /* Collect output data */
    MPI_Status status;
    for(int process = 0; process < num_nodes; process++) {
        MPI_Recv(output + process * num_points / num_nodes,
            num_points / num_comp_nodes, MPI_REAL, process,
            DATA_COLLECT, MPI_COMM_WORLD, &status );
    }

    /* Store output data */
    store_output(output, dimx, dimy, dimz);

    /* Release resources */
    free(input);
    free(output);
}
```

## Vector Addition: Compute Process (I)

```
void compute_node(unsigned int vector_size ) {
    int np;
    unsigned int num_bytes = vector_size * sizeof(float);
    float *input_a, *input_b, *output;
    MPI_Status status;

    MPI_Comm_size(MPI_COMM_WORLD, &np);
    int server_process = np - 1;

    /* Alloc host memory */
    input_a = (float *)malloc(num_bytes);
    input_b = (float *)malloc(num_bytes);
    output = (float *)malloc(num_bytes);

    /* Get the input data from server process */
    MPI_Recv(input_a, vector_size, MPI_FLOAT, server_process,
            DATA_DISTRIBUTE, MPI_COMM_WORLD, &status);
    MPI_Recv(input_b, vector_size, MPI_FLOAT, server_process,
            DATA_DISTRIBUTE, MPI_COMM_WORLD, &status);
```

# Vector Addition: Compute Process (II)

```
    /* Compute the partial vector addition */
    for(int i = 0; i < vector_size; ++i) {
        output[i] = input_a[i] + input_b[i];
    }

    /* Or, can offload to GPU here */
    /* cudaMalloc(), cudaMemcpy(), kernel launch, etc. */

    MPI_Barrier(MPI_COMM_WORLD);

    /* Send the output */
    MPI_Send(output, vector_size, MPI_FLOAT,
            server_process, DATA_COLLECT, MPI_COMM_WORLD);

    /* Release memory */
    free(input_a);
    free(input_b);
    free(output);
}
```

## ANY MORE QUESTIONS?
## READ CHAPTER 15