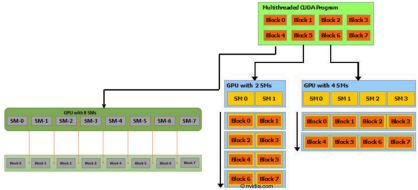


8. GPU (GRAPHICS PROCESSING UNIT)

End of Moores Law: We can no longer gain performance by "growing" sequential processors. Instead, we *improve performance* by running code in *parallel* on *multiple CPUs* (*low latency*) and many cores are *optimally parallel* (*co-processors*) (*high throughput*).
GPU's are specialized electronic circuits designed to accelerate the computation of *computer graphics*. They are faster than CPUs for suitable algorithms on large datasets. *Useful* for calculations which consist of *multiple independent sub-calculations*, not very useful for calculations where the results rely on the previous results (*like Fibonacci*).
High Parallelism: A CPU offers few cores (4, 8, 16, 64) and is very fast. Programming is easier. A GPU offers a very large number of cores (512, 1024, 3284, 5760) and has very specific slower processors. It is optimized for throughput. Programming is more difficult.
GPU Structure: A GPU consists of multiple *Streaming Multiprocessors (SM)* which in turn consist of multiple *Streaming Processors (SP)* (e.g. 1-30 SMs, 8-192 SPs per SM).
SIMD: Single Instruction Multiple Data. *The same instruction* is executed simultaneously on *multiple cores* working on *different data elements* (Vector parallelism). Saves fetch & decode instructions.
SISD: Single Instruction Single Data. Purely *sequential* calculations.
SIMT: Single Instruction Multiple Threads. The same instruction is executed in different threads over different data.



8.1. LATENCY VS. THROUGHPUT

Latency: *Elapsed time* of an event, *measuring from point A to B* takes one minute, the latency is one minute.
Throughput: *The number of events* that can be executed *per unit of time* (*bandwidth*).
There is a *tradeoff* between latency and throughput. Increasing throughput by pipelined processing, latency must often also increase. All pipeline stages must operate in *lockstep*. The *rate of processing* is determined by the *slowest step*.
Pipelining: Run processes in an overlapping manner.
Example: A program consists of two operations: Transfer data from CPU memory to GPU memory (*T_{cpu}* units = 20ms), execute computation on the device (*T_{gpu}* units = 60ms).
What is the latency (non-pipelined)? 20 + 60 = 80ms.
What is the throughput (pipelined)? Every 60ms an operation is finished.
Throughput = 1/60 operations/ms.

8.2. CPU VS GPU

CPUs	GPUs
<ul style="list-style-type: none">Low latencyFew but <i>optimized cores</i>General purpose	<ul style="list-style-type: none">Can execute <i>highly parallel</i> data operationsSimple but a lot of cores with cache per coreVery useful for problems which consist of a <i>lot of independent data elements</i>Efficiency must be achieved by <i>optimizing the program</i>
Aim: low latency per thread	Aim: high throughput

8.3. NUMA MODEL

NUMA stands for *Non-Uniform Memory Access*. CPUs on host and GPU devices each have local memory. There is *no common main memory* between the two, so *explicit transfer* between CPU and GPU is needed. There is also *no garbage collector* on the GPU.

8.4. CUDA

Computer Unified Device Architecture. Is a *parallel computing platform* and an *API* for Nvidia GPU that allows the host program to use GPUs for general purpose processing.

CUDA Execution steps

1. *cudaInit*: GPU memory allocate
2. *cudaMemcpy*: Transfer results from GPU to CPU (*Devicehost*)
3. *KernelExec*: Kernel execution
4. *cudaFree*: Deallocate GPU memory

Example: Array addition

```
C = 0; N = 3; for (i = 0; i < N; i++) { C[i] = A[i] + B[i]; } // sequential  
C = 0; N = 3; for (i = 0; i < N; i++) { C[i] = A[i] + B[i]; } // parallel using n threads
```

CUDA Kernel

A kernel is a function that is executed *n* times in parallel by *m* different CUDA threads.

```
// kernel definition on GPU  
__global__  
void VectorAddKernel(float* A, float* B, float* C, int N) {  
    int i = threadIdx.x; C[i] = A[i] + B[i];  
}  
// kernel invocation on CPU  
VectorAddKernel<<1, N>>>(A, B, C); // N is amount of threads  
// The GPU knows when the task is finished.
```

Boilerplate Orchestration Code

```
void CudaVectorAdd(float* h_A, float* h_B, float* h_C, int N) {  
    size_t size = N * sizeof(float);  
    float* d_A, *d_B, *d_C; // data on GPU  
    cudaMalloc(&d_A, size); cudaMalloc(&d_B, size); cudaMalloc(&d_C, size);  
    cudaMemcpy(d_A, h_A, size, cudaMemcpyHostToDevice);  
    cudaMemcpy(d_B, h_B, size, cudaMemcpyHostToDevice);  
    VectorAddKernel<<1, N>>>(d_A, d_B, d_C, N);  
    cudaMemcpy(h_C, d_C, size, cudaMemcpyDeviceToHost);  
    cudaFree(d_A); cudaFree(d_B); cudaFree(d_C);  
}
```

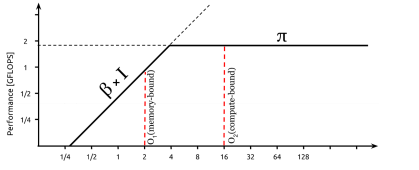
8.5. PERFORMANCE METRICS

The performance is either limited by *memory bandwidth* or *computation*.
Compute Bound: Throughput is limited by calculation (Cores are at the limit, but the memory bus could transfer more data).
This is better and reached if AI Kernel = AI GPU.
Memory Bound: Throughput is limited by data transfer (Memory bus bandwidth is at limit, but cores could process more data).
Arithmetic intensity: Defined as FLOPS (Floating Point Operations per second) per Byte. The higher, the better.
Number of operations / FLOPS
Number of transferred bytes / Bytes

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8.5.1. Roofline model

Provides performance estimates of a kernel running on differently sized architectures. Has three parameters: Peak performance, peak bandwidth vs. arithmetic intensity.
Peak performance is derived from benchmarking FLOPS or GFLOPS (*single FLOPS*, *10⁹ FLOPS*). The *peak bandwidth* from manuals of the memory subsystems. The *ridge point* where the horizontal and diagonal lines meet = minimum AI required to achieve the peak performance.



9. GPU ARCHITECTURE

Because there are *so many cores* on GPUs, it is possible to run many threads in parallel *without context switches*. This allows better parallelism without a performance penalty.

9.1. COMPIATION

Just-in-time Compilation: The *NVCC compiler* compiles the non-CUDA code with the host C compiler and translates code written in CUDA into *PTX instructions* (assembly language represented as ASCII text). The graphics driver compiles the PTX into *executable binary code*. The assembly of PTX code is *postponed until application runtime*, at which time the target GPU is known. The *disadvantage* of this is the *increased application startup delay*. However, thanks to cache this only happens once (*warmup*).
Programming Interface: *Runtime* (The cuda runtime provides functions that execute on the host to de-allocate device memory, transfer data etc.) or *Driver API* (The CUDA driver API is implemented in the cuda.dll or so which is copied on the system during installation of the driver. This provides an additional level of control by exposing lower-level concepts such as CUDA contexts. Often overkill).

Asynchronous Execution: The command pipeline in CUDA works asynchronous, commands and data can be transferred from/to the GPU at the same time.

9.2. CUDA SIMT EXECUTION MODEL

Single instruction, multiple Threads. The kernel is executed *N* times in parallel by *N* different CUDA threads.
Blocks: Threads are *grouped* in blocks. The host can define how many threads each block has (*up to 512*). Threads in one block can interact with each other but not with threads in other blocks.
Execution Model: *One thread* runs on *one virtual scalar processor* (one GPU core). *One block* runs on *one virtual multiprocessor* (one GPU Streaming Multiprocessor). *Blocks must be independent*.
Thread Pool Abstraction: The compiled CUDA program has e.g. 8 CUDA blocks. The *runtime* can choose how to *allocate* these blocks to multiprocessors. For a larger GPU with 8 SMs, each SM gets one CUDA block. This enables performance scalability without code changes.

Guarantees: CUDA guarantees that *all threads* in a block run on the *same SM at the same time* and that the blocks in a kernel *finish* before any block from a new, *dependent kernel* is started.
Mapping: One SM can run several *concurrent blocks* depending on the resources needed. Each kernel is executed on *one device*. CUDA supports running *multiple kernels* on a device at one time.

9.3. CUDA KERNEL SPECIFICATION

Specifying Kernel: VectorAddKernel <<gridDim, blockDim, blockDim>>>(A, B, C);
Dimensions can be 1D, 2D or 3D and specified via dim3 which is a structure designed for storing block and grid dimensions: struct dim3 {x, y, z};
dim3 dimGrid(2, 1, 1) (Unassigned components are set to 1)
VectorAddKernel<<dimGrid, dimBlock>>>(A, B, C);
Number of blocks in a grid: dimGrid.x * dimGrid.y * dimGrid.z
Number of threads in a block: dimBlock.x * dimBlock.y * dimBlock.z
Grids: VectorAddKernel<<gridDim, blockDim, blockDim>>>(A, B, C);
2D Grid: dim3 grid(5, 3); dim3 block(5, 3); VectorAddKernel<<gridDim, blockDim>>>(A, B, C);
3D Grid: dim3 grid(3, 2, 1); dim3 block(3, 2, 1); VectorAddKernel<<gridDim, blockDim>>>(A, B, C);
Device Limits: Max threads per block: 1024, Max thread dimensions per block: (1024, 1024, 64)
Max grid size: (2147483647, 65535, 65535)

Calculation Examples

```
VectorAddKernel<<dim3(8, 4, 2), dim3(16, 16)>>>(d_A, d_B, d_C);  
Amount of blocks: 4 * 2 = 64  
Amount of threads per block: 16 * 16 = 256  
Threads in total: 64 * 256 = 16384
```

If we have 1024 threads in a block, how many blocks are needed to launch N threads?
int blocksPerGrid = (N + threadPerBlock - 1) / threadPerBlock;

if we have 1024 threads in a block, how many blocks are needed to launch N threads?
int blocksPerGrid = (N + threadPerBlock - 1) / threadPerBlock;

9.4. DATA PARTITIONING WITHIN THREADS

Data Access: Each kernel defines a block to data to work on. The programmers decide data partitioning scheme. threadid.x / y / z (Thread no. in block), blockDim.x (Block no.), blockDim.x (Block size)
Partitioning in Blocks:
__global__
void VectorAddKernel(float* A, float* B, float* C) {
 int i = blockDim.x * blockDim.y + threadIdx.x; // index based on blockDim, threadIdx
 if (i < N) {
 C[i] = A[i] + B[i]; // without this if, some threads will be idle
 }
 // kernel invocation
 N = 4097; int blockSize = 1024; int gridSize = (N + blockSize - 1) / blockSize;
 VectorAddKernel<<gridSize, blockDim>>>(A, B, C);
}

Boundary Check: More threads than necessary work on the data. If N = 4097, 5 blocks with 1024 threads are needed which results in 1023 *unused threads*. Threads with i > N must not be allowed to write to array C because they might corrupt the *working memory* of some other thread.

9.5. ERROR HANDLING

Some functions have return type cudaError. Need to check for cudaSuccess, it's best to write your own helper function and wrap *every fucking line* in it. E.g. handLetCudaError() which prints the error and exits the program.
9.6. UNIFIED MEMORY
Unified memory allows automatic transfer from CPU to GPU and vice versa. No explicit Memory Copy needed, but has other new rules.
cudaMallocManaged(&A, size); // ... same for B and C
A[0] = B; // ... Initialize A and B assuming they reside on the host
// A and B are automatically transferred to the device
VectorAddKernel<<1, N>>>(A, B, C);
cudaDeviceSynchronize(); // ... wait for the GPU to finish
// C is transferred automatically to the host and can be read directly
std::cout << C[0]; ...
cudaFree(A); cudaFree(B); cudaFree(C);

10. GPU PERFORMANCE OPTIMIZATIONS

Hardware: A scalable array of multithreaded *Streaming Multiprocessors (SMs)*, the *threads* of a thread block execute *concurrently* on one multiprocessor, *multiple thread blocks* can execute *concurrently* on one multiprocessor. When thread blocks *terminate*, new blocks are launched on the free multiprocessors.

10.1. MATRIX ADDITION

```
__global__  
void MatAddKernel(float* A, float* B, float* C) {  
    int col = blockDim.x * blockDim.y + threadIdx.x;  
    int row = blockDim.y * blockDim.y + threadIdx.y;  
    if (row < A_ROWS && col < A_COLS) { // boundary checking  
        C[row * A_COLS + col] = A[row * A_COLS + col] + B[row * A_COLS + col];  
    }  
    const int A_COLS, B_COLS, C_COLS = 4;  
    const int A_ROWS, B_ROWS, C_ROWS = 4;  
    dim3 block(2, 2); dim3 grid(8, 8);  
    MatAddKernel<<grid, block>>>(A, B, C);  
}
```

10.2. MATRIX MULTIPLICATION

Parallelization: Every thread computes one element of the result matrix C. Can be parallelized because results do not depend on each other.

```
__global__  
void multiply(float* A, float* B, float* C) {  
    int i = blockDim.x * blockDim.y + threadIdx.x;  
    int j = blockDim.y * blockDim.y + threadIdx.y;  
    if (i < N && j < M) { // boundary checking  
        float sum = 0;  
        for (int k = 0; k < K; k++) {  
            sum += A[i * K + k] * B[k * M + j];  
        }  
        C[i * M + j] = sum;  
    }  
}
```

10.3. MAPPING THREADS / BLOCKS TO GPU WARPS

Warps: Blocks are split into *warps* (Warp = 32 Threads) and all threads within execute the same code. If there aren't enough threads to fill a warp, "empty" threads are launched. A number of warps constitutes a *thread block*. A number of *thread blocks* are assigned to a *Streaming Multiprocessor*. The whole GPU consists of several SM.
Thread blocks are scheduled in *parallel* or *sequentially*. Once a thread block is *launched* on a SM, *all of its warps are resident* until their execution finishes. Therefore, a *new block* on a SM is *not launched* until there is a *sufficient number* of free registers and shared memory for *all warps* of the new block.
Warp Execution: All threads in a warp execute the same instruction (same) ASM can accommodate all warps of a block, but only a *subset is running* in parallel at the same time (i to 24).
Divergence: Not all threads of a warp may *branch the same way*. The branches do *not run simultaneously*, so the other threads need to wait until one branch is finished. So branches within one warp should be *avoided* because of *performance problems* (Branches are born at if / switch ->)
// bad case, divergence in same warp // good case, all in warp in same branch
if (threadid.x > 0) { else { } if (threadid.x / 32 > 1) { else { }

DRAM (Dynamic Random Access Memory): *Global memory of a CUDA device* is implemented with DRAMs: A GPU kernel accesses data from *consecutive locations*, the DRAMs can supply the data at a *much higher rate* than if a random sequence of locations were accessed.
Memory Coalescing: Thread access patterns are critical for performance. If the threads in a warp *simultaneously access consecutive memory locations*, their reads can be combined into a single access (*burst*). Otherwise there are *expensive individual accesses*.
Coalesced Accesses: Read/Write the burst in one transaction per warp burst section, swapped read/write within the same 0 and using NPI_SUM as the reduction operation. The four numbers are added and stored on the root process. B is done in a *distributed manner*.

Not Coalesced Access: Read/Write in different warp bursts, one action that spans multiple bursts. *Interprocessor, avoid!*
Coalesced in Use: Use of Expression without threadid.x + threadid.y
Coalescing with Matrices: Matrices get linearized to a 1D array. The row of the matrix should be the longer side so that there are as many coalescing accesses as possible.

10.4. MEMORY MODEL

All threads have the access to the same *global memory*. Each thread block has *shared memory* visible to all threads of the block and with the same lifetime as the block (its higher bandwidth and lower latency than global or local memory but longer latency and lower bandwidth than registers which are private to a thread). Each thread has *private local memory* (in device memory, high latency and low bandwidth, same as global). Constant, texture and surface memory also reside in device memory.

Memory Hierarchy: Shared Memory (per SM, fast, shared between threads in 1 block, 16 KB, shared), Local Memory (per SM, fast, shared between threads in 1 block, 16 KB, shared), Registers (private to a thread, fastest but very limited storage).
Constant memory: Constant variables are stored in the *global memory* but are *cached*.
Shared Memory Declaration: With keyword __shared__. A static array size is necessary. Limited memory, around 48KB. Multidimensionality is allowed.

Fast Matrix Multiplication: By reducing *global memory traffic*. Partition data into subtasks called tiles which fit into shared memory (the row & column that must be multiplied and the result cell). The kernel computation on these tiles must be able to run independently of each other. Because the shared memory is *limited*, load the tiles in several steps and calculate the *intermediate result* from this.

```
__global__ float MatMulKernel(float* d_M, float* d_N, float* d_P, int Width) {  
    __shared__ float Ms[TileWidth][TileWidth];  
    __shared__ float Ns[TileWidth][TileWidth];  
    int tx = blockDim.x; int ty = blockDim.y;  
    int tx = threadIdx.x; int ty = threadIdx.y;  
    // Identify row and column of the d_P element to work on  
    int Row = tileWidth * ty;  
    int Col = tx * tileWidth + ty;  
    float PValue = 0;  
    // Loop over m and n tiles required to compute d_P element  
    for (int m = 0; m < M; m++) {  
        // collaborative loading of d_M and d_N tiles into shared memory  
        Ms[ty][tx] = d_M[Row * Width + m * tileWidth + tx];  
        Ns[ty][tx] = d_N[(m * tileWidth + ty) * Width + Col];  
        __syncthreads(); // CUDA equivalent to wait() for (int k = 0; k < tileWidth; ++k) {  
            PValue += Ms[ty][tx] * Ns[ty][tx];  
        }  
        __syncthreads();  
    }  
    d_P[Row * Width + Col] = PValue;  
}
```

__syncthreads() is only allowed in if/else if all threads of a block choose the same branch, otherwise undefined behavior.

11. HIGH PERFORMANCE COMPUTING (HPC) CLUSTER PARALLELIZATION

Cluster programming is the *highest possible parallel acceleration* (factor 100 and more). Used for *very general purpose programming*, lots of CPU cores. Combination of CPUs and GPUs possible.
Computer Cluster: Network of powerful computing nodes, linearly connected at one location. *Every fast interconnect* (the 100Gb/s), used by big simulations (Fluids, Weather, traffic, etc.)
SPMD: This is the most commonly used programming model, "high level".
Single Program (All tasks execute their copy of the same program simultaneously), **Multiple Data** (all tasks may use different data). The MPI program is started in several processes. All processes start and terminate synchronously. Synchronization is done with barriers.

MPMD: Also a "high level" programming model. **Multiple Program** (Tasks may execute different programs simultaneously), **Multiple Data** (all tasks may use different data).

Hybrid Memory Model: All processors in a machine can *share* the memory. They also can *request* data from other computers. (non-uniform memory access: not all accesses take the same time)
Message Passing Interface (MPI): Distributed programming model. Is a common choice for Parallelization on a cluster. Industry-Standard libraries for multiple programming languages.

MPI Model: Node of Processes (Process is the running program plus its data), parallelism is achieved by running *multiple processes*, co-operating on the *same task*. Each process has *direct access* only to its own data (variables are private). Inter-Process-Communication by sending and receiving messages.
SPMD in MPI: All processes run their *own local copy* of the program & data. Each process has a *unique identifier*, processes can take *different paths* through the program depending on their IDs.
Message Passing Interface (MPI): Distributed programming model. Is a common choice for Parallelization on a cluster. Industry-Standard libraries for multiple programming languages.
Formalizing Message: A message transfer data a number of data items from the memory of one process to the memory of another process (Typically contains data ID of sender and receiver, data type to be sent, number of data items, data itself, message type identifier).

Communication modes: *Point to Point* (very simple, one sender and one receiver. Relies on matching send and receive calls) and *Collective communications* (between groups of processes. Broadcast: one to all, Scatter: Split data and send each chunk to different nodes. Gather: Collect the chunks back at the originating node).

11.1. MPI BOILERPLATE CODE

```
int main(int argc, char* argv[]) {  
    MPI_Init(&argc, &argv); // MPI Initialization  
    int rank; int len;  
    MPI_Comm_rank(MPI_COMM_WORLD, &rank); // Process Identification  
    char name[MPI_MAX_PROCESSOR_NAME];  
    MPI_Get_processor_name(name, &len);  
    printf("MPI process %i on %s\n", rank, name);  
    MPI_Finalize(); // MPI Finalization  
    return 0;  
}
```

NPI_Init: Must be the *first MPI call*. Allows the mpi_init to broadcast to all the processes. Does not create processes, they are only created at launch time. All MPI *global and internal variables* are *constructed*. A *communicator* is formed around all the processes that were spawned and *unique ranks* (ids) are assigned to each process. **MPI_COMM_WORLD** encompasses all processes in the job.
Communicator: Group of MPI processes, allows inter-process communication.
MPI_Comm_rank: Returns the rank of a process in a communicator. Used for sender/receiver IDs.
MPI_Comm_size: Returns the total number of processes in a communicator.
MPI_Finalize: Is used to *clean up* the environment. No more MPI calls after that.
MPI_Barrier: Blocks until all processes in the communicator have reached the barrier.
Compilation & Execution: mpicc HelloCluster.c -o mpiexec -x c24 a.out -x sbatch -hi.su
Process Identification: Rank = number within a group, incremental numbering from 0.
Unique Identification = (Rank, Communicator)

```
MPI_Send(void* data, int count, MPI_Datatype datatype, int destination, int tag, MPI_Comm comm); // tag: freely selectable number for msg type (2-0)  
MPI_Recv(void* data, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm communicator, MPI_Status* status); // status: error information
```

Each send should have a matching receive.

Example direct communication:

```
MPI_Send(&value, 1, MPI_INT, receiverRank, tag, MPI_COMM_WORLD);  
MPI_Recv(&value, 1, MPI_INT, senderRank, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
Array send: int array[LENGTH];  
MPI_Send(array, LENGTH, MPI_INT, receiverRank, tag, MPI_COMM_WORLD);  
MPI_Recv(array, LENGTH, MPI_INT, senderRank, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
MPI_Bcast: Is efficient, because the root node does not send the signal individually to each node, the other nodes help spread the message to others, signal spreads like a caracol: MPI_Bcast(&data, 1, MPI_INT, root, MPI_COMM_WORLD);  
MPI_Reduce: Reduction is a classic concept: reducing a set of numbers into a smaller set of numbers via a function (e.g. 1, 2, 3, 4, 5) sum = 15). Each process contains one integer, MPI_Reduce is called with a root process of 0 and using NPI_SUM as the reduction operation. The four numbers are added and stored on the root process. B is done in a distributed manner.
```

MPI_Reduce: void* send_data, void* recv_data, int count, MPI_Datatype datatype, int op, int root, MPI_Comm comm; // op: MPI_Op: array of elements of type datatype to reduce from each process, root: data: data to be reduced, contain the reduced result and has a size of sizeof(datatype)
// op: the operation you wish to apply to your data: MPI_MAX, MPI_MIN, MPI_PROD, multiplies all MPI_BAND/ MPI_LAND: bitwise/Logical AND, MPI_LOR: Logical OR, MPI_NXCLUSIVE: Same as max plus rank of process that owns B
MPI_AllReduce: Many parallel applications require accessing the reduced results across all processes. This function reduces the values and distributes the result to all processes. Does not need a root node. This is an implicit broadcast to all processes.
MPI_AllReduce(&send_data, &recv_data, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)

MPI_Gather: Gather together multiple values from different processors.
MPI_Gather(&input_value, 1, MPI_INT, &output_array, 1, MPI_INT, 0, MPI_COMM_WORLD)

11.2. APPROXIMATION OF π VIA MONTE CARLO SIMULATION

Draw a circle inside of a square and randomly place dots in the square. The ratio of dots inside the circle to the total number of dots will approximately equal π/4.
// Sequential
long count_hits(long trials) { long hits = 0; for (i = 0; i < trials; i++) { double x = (double)rand() / RAND_MAX; double y = (double)rand() / RAND_MAX; if (x * x + y * y <= 1) hits++; } // distance to center bigger than radius } return hits; }

// Parallel, the trials are split across different nodes
int rank, size;
MPI_Comm_rank(MPI_COMM_WORLD, &rank); MPI_Comm_size(MPI_COMM_WORLD, &size);
rand((rank * 4711)); // each process receives a different seed
long hits = count_hits(TRIALS / size); // Each process computes a subtask
long total;
MPI_Reduce(&hits, &total, 1, MPI_LONG, MPI_SUM, 0, MPI_COMM_WORLD);
if (rank == 0) { double pi = 4 * ((double)total / TRIALS); }

12. OPENMP

Model: A standalone "computer in a box". Usually comprised of multiple CPU/processors/cores, memory, network interfaces etc. Nodes are *networked together* to comprise a supercomputer. Each node consists of 20 cores. The processes do *not share memory* and must use messages.
Threads: Default are 24 on a single Node in OST cluster. Can be set with omp_set_num_threads() or with the OMP_NUM_THREADS environment variable. Threads range from 0 (master thread) to N-1.
HPC Hybrid Parallelism: Run a program on multiple nodes. No shared memory (NUMA).
OpenMP: Is a programming model for different languages. Allows to run *multiple threads*, distribute working using synchronization and reduction constructs. **Shared Memory** (shared memory process, consists of multiple threads), **Explicit Parallelism** (Programmer has full control over parallelization) and **Compiler Directives** (Most OpenMP parallelism is specified through use of compiler directives (pragmas) in the source code).

Fork and Join

```
#include <stdio.h>  
#include <omp.h>  
int main(int argc, char* argv[]) {  
    const int n = omp_get_num_threads(); // executed by initial thread  
    printf("OpenMP with threads %d\n", n); // executed by initial thread  
    #pragma omp parallel {  
        // pragma spawns multiple threads (fork)  
        const int n = omp_get_num_threads(); // executed in parallel  
        printf("Hello from thread %d\n", omp_get_thread_num()); // executed in paral.  
        // thread order not fixed, after execution, threads synchronize & terminate  
        return 0;  
    }
```

For loops

```
#pragma omp parallel for  
for (i=0; i<n; i++) { ... }
```

Each thread executes one *loop-iteration* at a time. Execution returns to the initial threads. **OverSubscription** (too many threads for a problem) is handled by OpenMP. The iteration variable (i.e. i) is implicitly made private for the duration of the loop.

Memory Model

int A, B, C; // automatically global because outside of pragma
#pragma omp private (A, B, C) shared (B) firstprivate (C)
for(...)

Each thread has a *private copy* of A and use the *same memory location* for B, C is also private, but gets its initial value from the global variable. After the loop is over, threads die and both A and B will be cleared/removed from memory.

```
#pragma omp parallel  
int A = 0; // automatically private because inside of pragma  
#pragma omp for ...
```

Avoiding Race conditions: Mutex

```
int sum = 0;  
#pragma omp parallel for  
for (int i = 0; i < n; i++)  
#pragma omp critical { sum += i; } // only one thread at a time
```

This is *extremely slow* due to serialization, slower than single threading. Critical section is *overkill* for this code, with a heavy weight mutex the performance overhead is large.

Lightweight mutex: Atomic

```
int sum = 0; int i;  
#pragma omp parallel for  
for (i = 0; i < n; i++)  
#pragma omp atomic { sum += i; }
```

Reduction across threads

When using reduction(operator: variable), a *copy* of the reduction variable per thread is created, initialized to the identity of the reduction operator (e.g. +=, *). Each thread will then *reduce* into its local variable. At the end of the parallel region, the local results are *combined into the global variable*. Any associative operators allowed (+, *, not -, /).

```
// Code using the reduction clause  
int sum = 0;  
#pragma omp parallel for reduction(+: sum)  
for (int i = 0; i < n; i++) { sum += i; }
```

```
// The same code without the reduction clause  
int sum = 0;  
#pragma omp parallel {  
    int intermediate_sum = 0; // private  
    #pragma omp for  
    for (int i = 0; i < n; i++) { intermediate_sum += i; } // thread partial sum  
    #pragma omp atomic { sum = sum + intermediate_sum; }  
}
```

Hybrid: OpenMP & MPI

```
int numprocs, rank; int ian = 0, np = 1;  
MPI_Init(&argc, &argv);  
MPI_Comm_rank(MPI_COMM_WORLD, &rank);  
MPI_Comm_size(MPI_COMM_WORLD, &size);  
#pragma omp
```