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Parallel Programming Concepts

HPC Workshop: Parallel Programming

Alexander B. Pacheco

Research Computing

Outline

Outline

What is Serial Computing?

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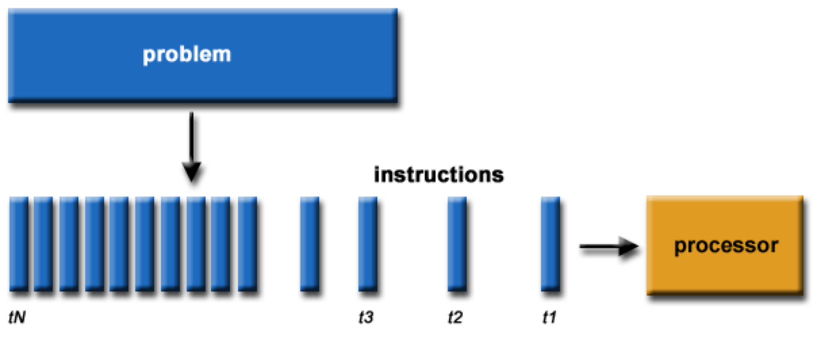
- Traditionally, software has been written for serial computation:
  - A problem is broken into a discrete series of instructions
  - Instructions are executed sequentially one after another
  - Executed on a single processor
  - Only one instruction may execute at any moment in time



What is Parallel Computing?

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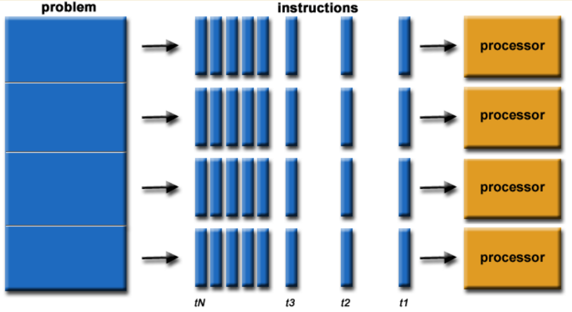
- In the simplest sense, parallel computing is the simultaneous use of multiple compute resources to solve a computational problem:
  - A problem is broken into discrete parts that can be solved concurrently
  - Each part is further broken down to a series of instructions
  - Instructions from each part execute simultaneously on different processors
  - An overall control/coordination mechanism is employed
  - The computational problem should be able to:
    - Be broken apart into discrete pieces of work that can be solved simultaneously;
    - Execute multiple program instructions at any moment in time;
    - Be solved in less time with multiple compute resources than with a single compute resource.
  - The compute resources are typically:
    - A single computer with multiple processors/cores
    - An arbitrary number of such computers connected by a network

Why Parallel Computing?

- Parallel computing might be the only way to achieve certain goals
  - Problem size (memory, disk etc.)
  - Time needed to solve problems
- Parallel computing allows us to take advantage of ever-growing parallelism at all levels
  - Multi-core, many-core, cluster, grid, cloud, $\cdots$

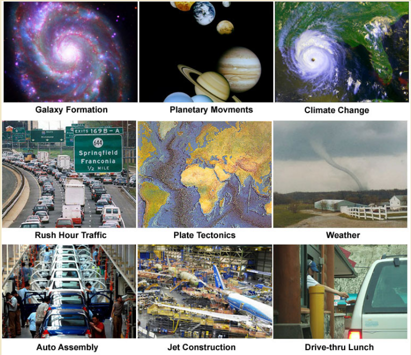


What are Parallel Computers?

- Virtually all stand-alone computers today are parallel from a hardware perspective:
  - Multiple functional units (L1 cache, L2 cache, branch, prefetch, decode, floating-point, graphics processing (GPU), integer, etc.)
  - Multiple execution units/cores
  - Multiple hardware threads
  - Networks connect multiple stand-alone computers (nodes) to make larger parallel computer clusters.

Why Use Parallel Computing?

- The Real World is Massively Parallel:
  - In the natural world, many complex, interrelated events are happening at the same time, yet within a temporal sequence.
  - Compared to serial computing, parallel computing is much better suited for modeling, simulating and understanding complex, real world phenomena.



Why Use Parallel Computing?

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- SAVE TIME AND/OR MONEY:
  - In theory, throwing more resources at a task will shorten its time to completion, with potential cost savings.
  - Parallel computers can be built from cheap, commodity components.
- SOLVE LARGER / MORE COMPLEX PROBLEMS:
  - Many problems are so large and/or complex that it is impractical or impossible to solve them on a single computer, especially given limited computer memory.
  - Example: "Grand Challenge Problems" (en.wikipedia.org/wiki/Grand_Challenge) requiring PetaFLOPS and PetaBytes of computing resources.
  - Example: Web search engines/databases processing millions of transactions every second
- PROVIDE CONCURRENCY:
  - A single compute resource can only do one thing at a time. Multiple compute resources can do many things simultaneously.
  - Example: Collaborative Networks provide a global venue where people from around the world can meet and conduct work "virtually".

Why Use Parallel Computing?

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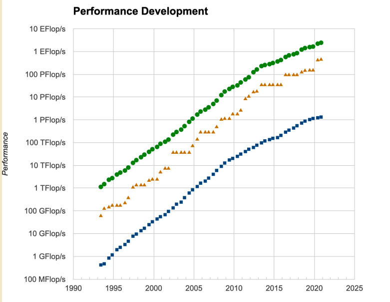
- TAKE ADVANTAGE OF NON-LOCAL RESOURCES:
  - Using compute resources on a wide area network, or even the Internet when local compute resources are scarce or insufficient.
  - Example: SETI@home (setiathome.berkeley.edu) over 1.5 million users in nearly every country in the world. Source: www.boincsynergy.com/stats/ (June, 2015).
  - Example: Folding@home (folding.stanford.edu) uses over 160,000 computers globally (June, 2015)
- MAKE BETTER USE OF UNDERLYING PARALLEL HARDWARE:
  - Modern computers, even laptops, are parallel in architecture with multiple processors/cores.
  - Parallel software is specifically intended for parallel hardware with multiple cores, threads, etc.
  - In most cases, serial programs run on modern computers "waste" potential computing power.

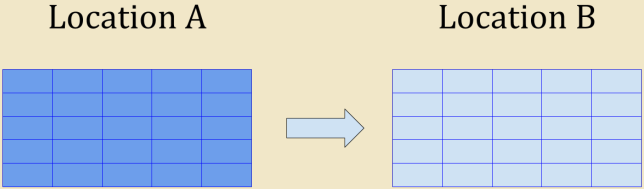
Why Use Parallel Computing?

- The Future:
- During the past 20+ years, the trends indicated by ever faster networks, distributed systems, and multi-processor computer architectures (even at the desktop level) clearly show that parallelism is the future of computing.
- In this same time period, there has been a greater than 500,000x increase in supercomputer performance, with no end currently in sight.
- The race is already on for Exascale Computing!

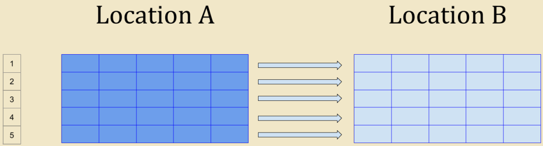
  Exaflop = 10^{18} calculations per second



- Consider an example of moving a pile of boxes from location A to location B
- Lets say, it takes x mins per box. Total time required to move the boxes is 25x.
- How do you speed up moving 25 boxes from Location A to Location B?



- You enlist more people to move the boxes.
- If 5 people move the boxes simultaneously, it should theoretically take 5x mins to move 25 boxes.



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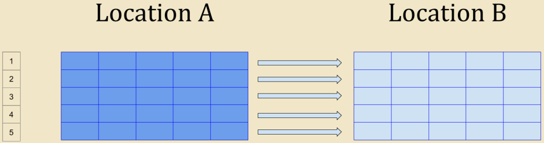


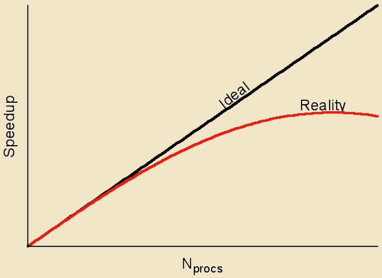
Number of People	Time (mins)
2	13x
3	9x
4	7x
5	5x
6	5x
7-8	4x
9-12	3x
13-24	2x
≥ 25	1x

Evaluating Parallel Programs

- Speedup
  - Let N_{Proc} be the number of parallel processes
  - $\text{Speedup}(N_{\text{Proc}}) = \dfrac{\text{Time used by best serial program}}{\text{Time used by parallel program}}$
  - Speedup is usually between 0 and N_{Proc}
- Efficiency
  - $\text{Efficiency}(N_{\text{Proc}}) = \dfrac{\text{Speedup}(N_{\text{Proc}})}{N_{\text{Proc}}}$
  - Efficiency is usually between 0 and 1

Speedup as a function of N_{Proc}

- Ideally
  - The speedup will be linear
- Even better
  - (in very rare cases) we can have superlinear speedup
- But in reality
  - Efficiency decreases with increasing number of processes



Amdahl's Law

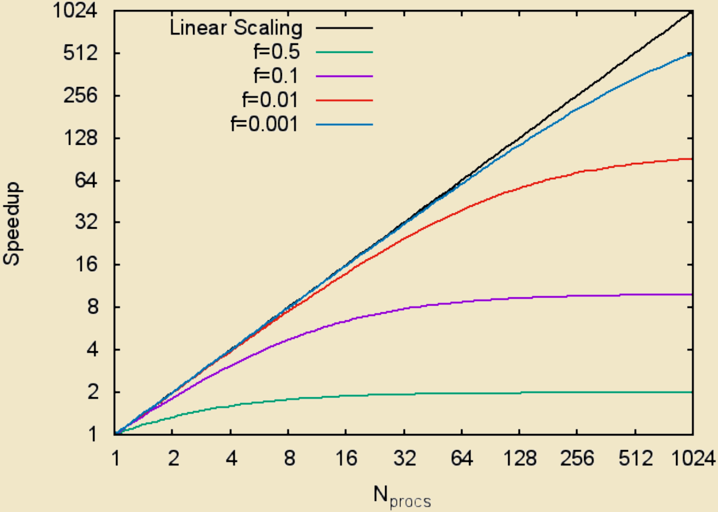
- Let f be the fraction of the serial program that cannot be parallelized
- Assume that the rest of the serial program can be perfectly parallelized (linear speedup)

$$\text{Time}_{\text{parallel}} = \text{Time}_{\text{serial}} \cdot \left(f + \frac{1-f}{N_{\text{proc}}} \right)$$

- Or

$$\text{Speedup} = \frac{1}{f + \frac{1-f}{N_{\text{proc}}}} \leq \frac{1}{f}$$

Maximal Possible Speedup



Amdahl's Law

- What Amdahl's law says
  - It puts an upper bound on speedup (for a given f), no matter how many processes are thrown at it
- Beyond Amdahl's law
  - Parallelization adds overhead (communication)
  - f could be a variable too
    - It may drop when problem size and N_{proc} increase
  - Parallel algorithm is different from the serial one

Writing a parallel program step by step

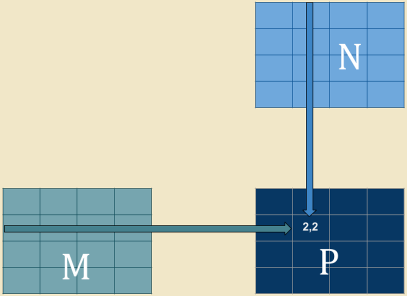
1. Start from serial programs as a baseline
   - Something to check correctness and efficiency against
2. Analyze and profile the serial program
   - Identify the "hotspot"
   - Identify the parts that can be parallelized
3. Parallelize code incrementally
4. Check correctness of the parallel code
5. Iterate step 3 and 4

A REAL example of parallel computing

- Dense matrix multiplication $M_{md} \times N_{dn} = P_{mn}$

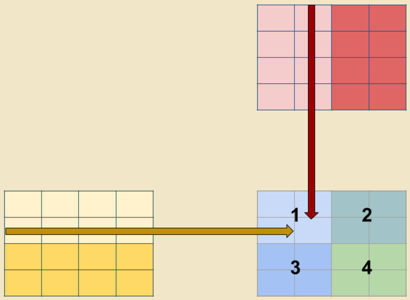
$$P_{m,n} = \sum_{k=1}^{d} M_{m,k} \times N_{k,n}$$

$$P_{2,2} = M_{2,1} * N_{1,2} + M_{2,2} * N_{2,2} + M_{2,3} * N_{3,2} + M_{2,4} * N_{4,2}$$



Parallelizing matrix multiplication

- Divide work among processors
- In our 4x4 example
  - Assuming 4 processors
  - Each responsible for a 2x2 tile (submatrix)
  - Can we do 4x1 or 1x4?



Pseudo Code

Serial

```
for i = 1, 4
  for j = 1, 4
    for k = 1, 4
      P(i,j) += M(i,k)*N(k,j);
```

Parallel

```
for i = istart, iend
  for j = jstart, jend
    for k = 1, 4
      P(i,j) += M(i,k)*N(k,j);
```

Outline

1. Introduction
2. Parallel programming models
3. Parallel programming hurdles
4. Heterogeneous computing

Single Program Multiple Data (SPMD)

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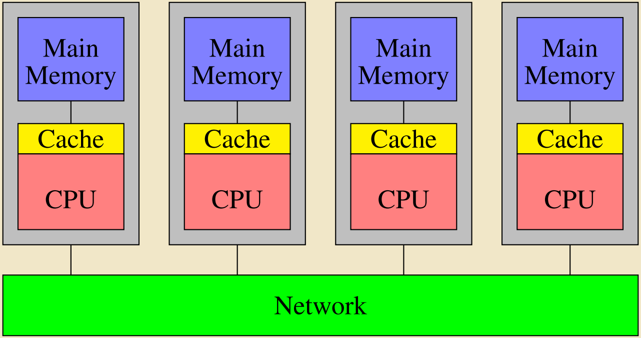
- All program instances execute same program
- Data parallel - Each instance works on different part of the data
- The majority of parallel programs are of this type
- Can also have
  - SPSD: serial program
  - MPSD: rare
  - MPMD

Memory system models

- Different ways of sharing data among processors
  - Distributed Memory
  - Shared Memory
  - Other memory models
    - Hybrid model
    - PGAS (Partitioned Global Address Space)

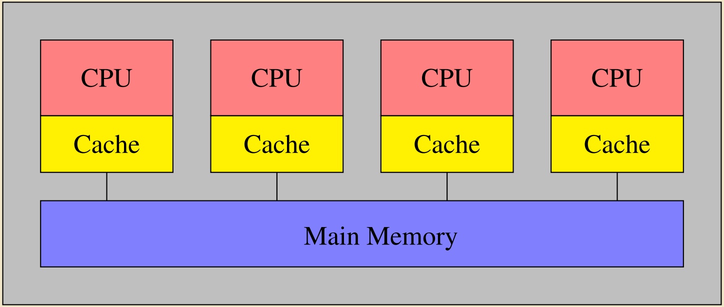
Distributed Memory Model

- Each process has its own address space
  - Data is local to each process
- Data sharing is achieved via explicit message passing
- Example
  - MPI



Shared Memory Model

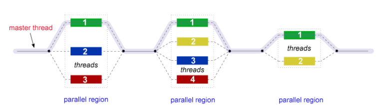
- All threads can access the global memory space.
- Data sharing achieved via writing to/reading from the same memory location
- Example
  - OpenMP
  - Pthreads



Shared vs Distributed

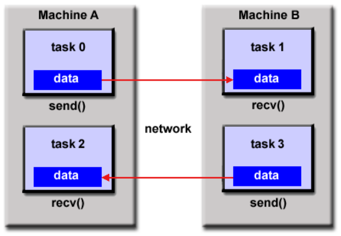
Shared

- Pros
  - Global address space is user friendly
  - Data sharing is fast
- Cons
  - Lack of scalability
  - Data conflict issues



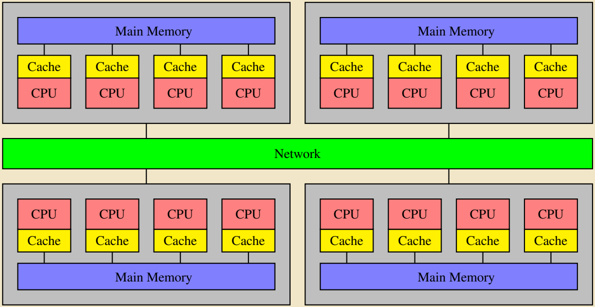
Distributed

- Pros
  - Memory scalable with number of processors
  - Easier and cheaper to build
- Cons
  - Difficult load balancing
  - Data sharing is slow



Hybrid model

- Clusters of SMP (symmetric multi-processing) nodes dominate nowadays
- Hybrid model matches the physical structure of SMP clusters
  - OpenMP within nodes
  - MPI between nodes



Potential benefits of hybrid model

- Message-passing within nodes (loopback) is eliminated
- Number of MPI processes is reduced, which means
  - Message size increases
  - Message number decreases
- Memory usage could be reduced
  - Eliminate replicated data
- Those are good, but in reality, (most) pure MPI programs run as fast (sometimes faster than) as hybrid ones $\cdots$

Reasons why NOT to use hybrid model

- Some (most?) MPI libraries already use internally different protocols
  - Shared memory data exchange within SMP nodes
  - Network communication between SMP nodes
- Overhead associated with thread management
  - Thread fork/join
  - Additional synchronization with hybrid programs

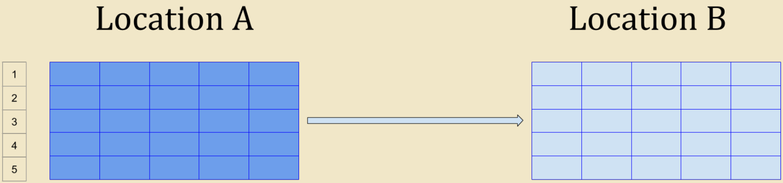
Outline

Parallel Programming Hurdles

- Hidden serializations
- Overhead caused by parallelization
- Load balancing
- Synchronization issues

Hidden Serialization

- Back to our box moving example
- What if there is a very long corridor that allows only one work to pass at a time between Location A and B?



Hidden Serialization

- It is the part in serial programs that is hard or impossible to parallelize
  - Intrinsic serialization (the f in Amdahl's law)
- Examples of hidden serialization:
  - System resources contention, e.g. I/O hotspot
  - Internal serialization, e.g. library functions that cannot be executed in parallel for correctness

Communication overhead

- Sharing data across network is slow
  - Mainly a problem for distributed memory systems
- There are two parts of it
  - Latency: startup cost for each transfer
  - Bandwidth: extra cost for each byte
- Reduce communication overhead
  - Avoid unnecessary message passing
  - Reduce number of messages by combining them

Memory Heirarchy

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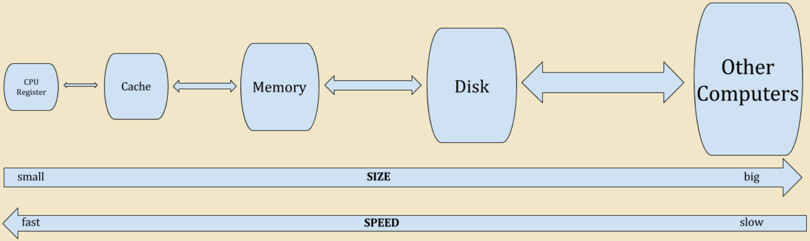
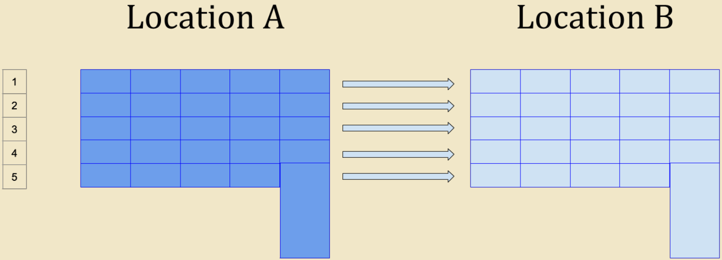


- Avoid unnecessary data transfer
- Load data in blocks (spatial locality)
- Reuse loaded data (temporal locality)
- All these apply to serial programs as well

Load balancing

- Back to our box moving example, again
- Anyone see a problem?



Load balancing

- Work load not evenly distributed
  - Some are working while others are idle
  - The slowest worker dominates in extreme cases
- Solutions
  - Explore various decomposition techniques
  - Dynamic load balancing
- Hard for distributed memory
- Adds overhead

Synchronization issues - deadlock

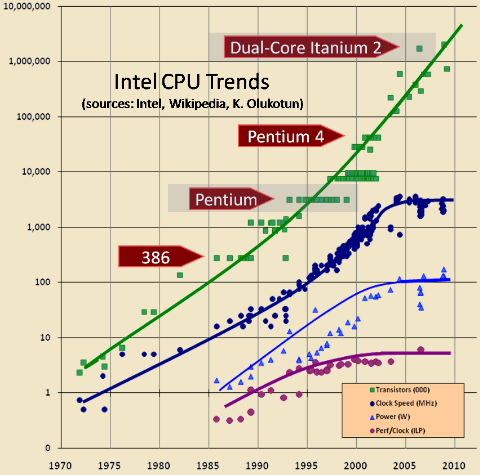
- Often caused by "blocking" communication operations
  - "Blocking" means "I will not proceed until the current operation is over"
- Solution
  - Use "non-blocking" operations
  - Caution: trade-off between data safety and performance

Outline

Heterogeneous computing

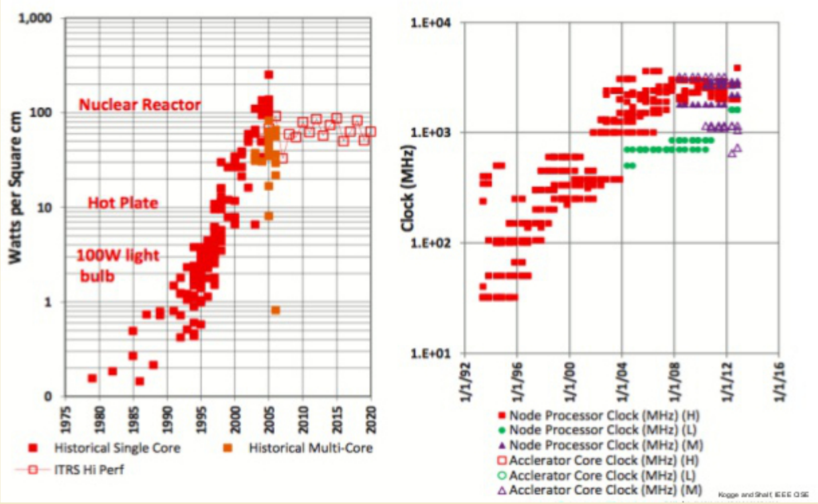
- A heterogeneous system solves tasks using different types of processing units
  - CPUs
  - GPUs
  - DSPs
  - Co-processors
  - $\cdots$
- As opposed to homogeneous systems, e.g. SMP nodes with CPUs only

The Free Lunch Is Over



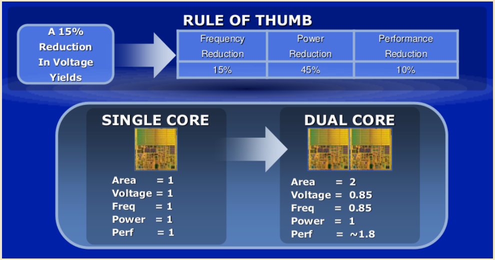
Source: Herb Sutter
http://www.gotw.ca/publications/concurrency-ddj.htm

Power and Clock Speed



Power efficiency is the key

- We have been able to make computer run faster by adding more transistors
  - Moore's law
- Unfortunately, not any more
  - Power consumption/heat generation limits packing density
  - Power $\sim$ speed^2
- Solution
  - Reduce each core's speed and use more cores - increased parallelism

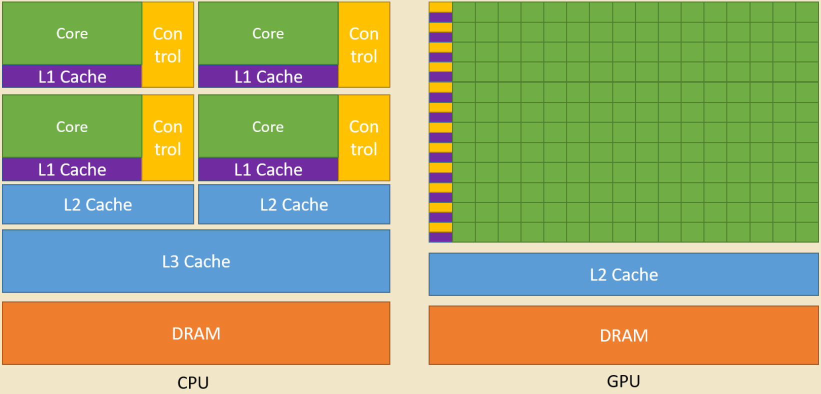


Source: John Urbanic, PSC

Graphic Processing Units (GPUs)

- Massively parallel many-core architecture
  - Thousands of cores capable of running millions of threads
  - Data parallelism
- GPUs are traditionally dedicated for graphic rendering, but become more versatile thanks to
  - Hardware: faster data transfer and more on-board memory
  - Software: libraries that provide more general purposed functions
- GPU vs CPU
  - GPUs are very effectively for certain type of tasks, but we still need the general purpose CPUs

CPU vs GPU


Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
L2 Cache
L2 Cache
L3 Cache
DRAM
CPU
L2 Cache
DRAM
GPU

NVIDIA Tesla T4

- GPU Architecture: NVIDIA Turing
- Tensor Cores: 320
- CUDA Cores: 2560
- Performance:
  - Single Precision: 8.1 TFLOPS
  - Mixed Precision (FP16/FP32): 65 TFLOPS
  - INT8: 130 TOPS
  - INT4: 260 TOPS
- Memory (GDDR5): 16GB
- Memory (Bandwidth): 320GBs

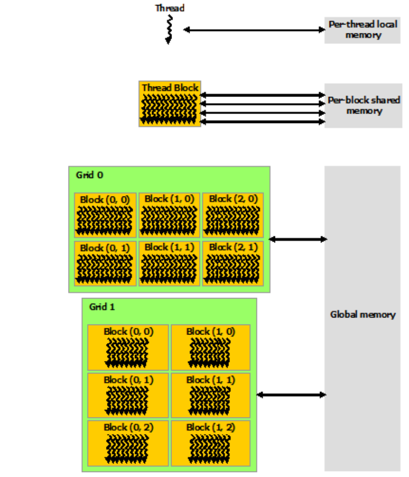
GPU Programming

- a hierarchy of thread groups, shared memories, and barrier synchronization exposed to programmer as a minimal set of language extensions
- provide fine-grained data parallelism and thread parallelism, nested within coarse-grained data parallelism and task parallelism
- guide programmer to partitionthe problem into coarse sub-problems
- solved independently in parallel by blocks of threads, and each sub-problem into finer pieces that can be solved cooperatively in parallel by all threads within the block

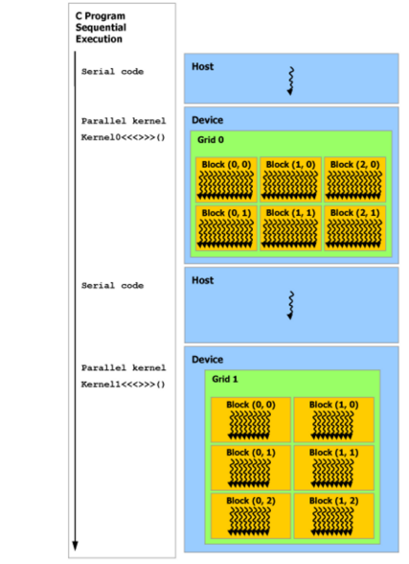
Streaming Multiprocessors

- A GPU is built around an array of Streaming Multiprocessors (SMs).
- A multithreaded program is partitioned into blocks of threads that execute independently from each other.
- a GPU with more multiprocessors will automatically execute the program in less time than a GPU with fewer multiprocessors.

Memory Heirarchy



GPU Program



C Program Sequential Execution
Serial code
Host
Parallel kernel
Kernel0<<<>>>()
Device
Grid 0
Block (0, 0)
Block (1, 0)
Block (2, 0)
Block (0, 1)
Block (1, 1)
Block (2, 1)
Serial code
Host
Parallel kernel
Kernel1<<<>>>()
Device
Grid 1
Block (0, 0)
Block (1, 0)
Block (0, 1)
Block (1, 1)
Block (0, 2)
Block (1, 2)

GPU programming strategies

- GPUs need to copy data from main memory to its onboard memory and copy them back
  - Data transfer over PCIe is the bottleneck, so one needs to
- Avoid data transfer and reuse data
- Overlap data transfer and computation
- Massively parallel, so it is a crime to do anything antiparallel
  - Need to launch enough threads in parallel to keep the device busy
  - Threads need to access contiguous data
  - Thread divergence needs to be eliminated
- Fine Grained Parallelism: relatively small amounts of computational work are done between communication events

Recommended Further Reading

- "Designing and Building Parallel Programs", Ian Foster - from the early days of parallel computing, but still illuminating.
- "Introduction to Parallel Computing", Ananth Grama, Anshul Gupta, George Karypis, Vipin Kumar.
- University of Oregon - Intel Parallel Computing Curriculum
- UC Berkeley CS267, Applications of Parallel Computing, Prof. Jim Demmel, UCB Spring 2021
- "Programming on Parallel Machines", Norm Matloff, UC Davis.
- Cornell Virtual Workshop: Parallel Programming Concepts and High-Performance Computing
- Introduction to High Performance Scientific Computing", Victor Eijkhout, TACC
- COMP 705: Advanced Parallel Computing (Fall, 2017), SDSU, Prof. Mary Thomas
- Slides based on material from https://hpc.llnl.gov/training/tutorials