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Parallel Programming Concepts

2021 HPC Workshop: Parallel Programming

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Research Computing

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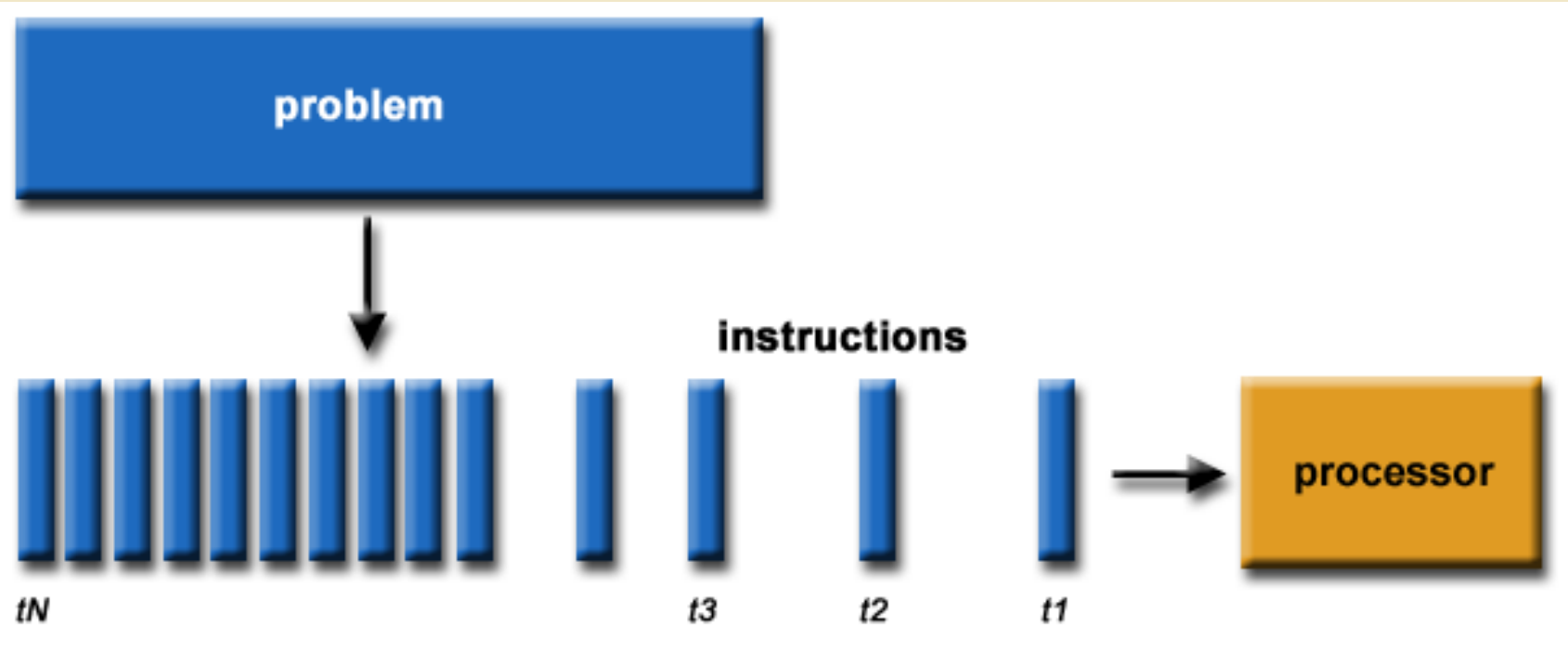
Outline

Outline

What is Serial Computing?

- 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

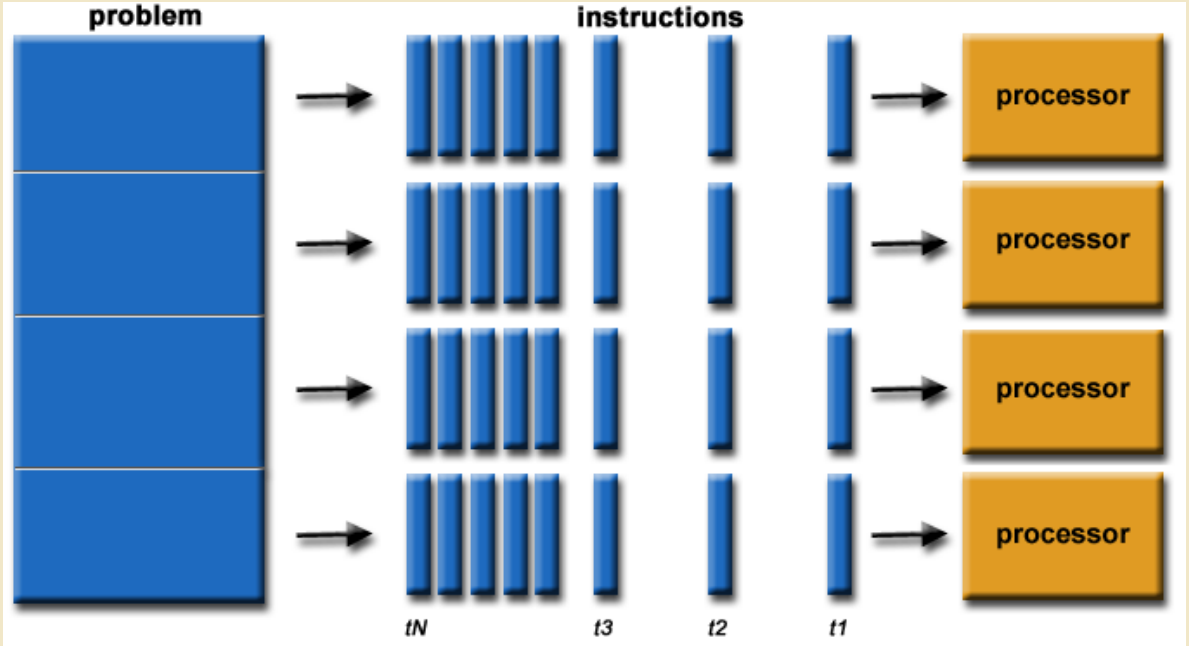


What is Parallel Computing?

- 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, · · ·

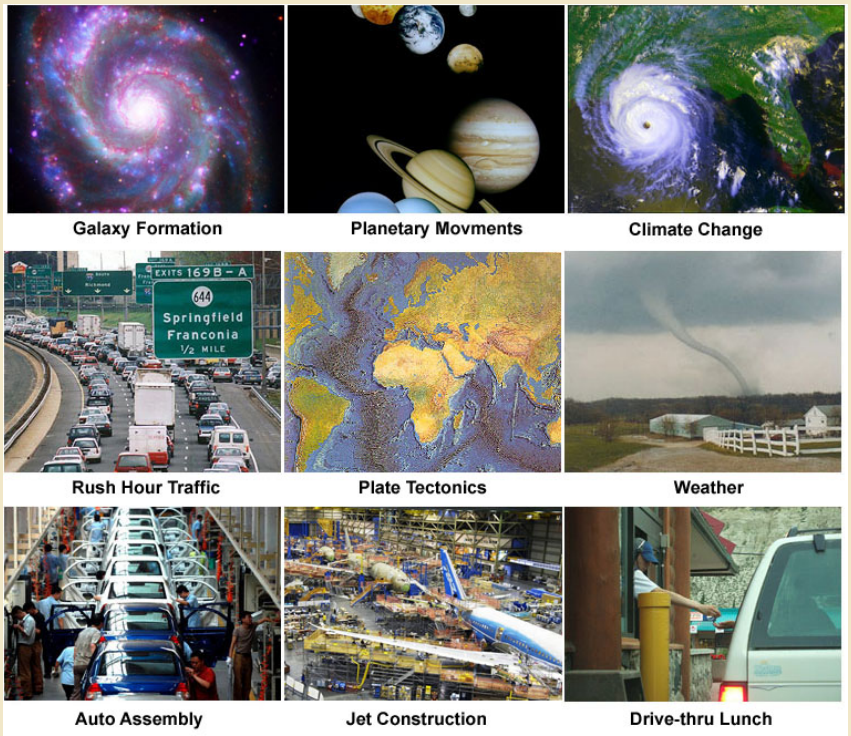


What are Parallel Computers?

- 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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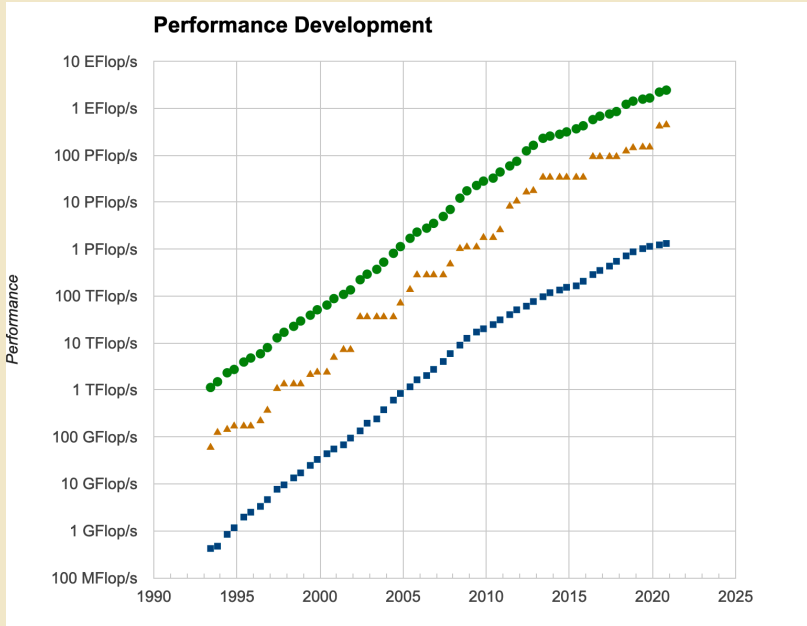
- TAKE ADVANTAGE OF NON-LOCAL RESOURCES:
  - Using compute resources on a wide area network, or even the Internet when local compute resources are scarce or insufficient.
  - Example: SETI@home (setiathome.berkeley.edu) over 1.5 million users in nearly every country in the world. Source: www.boincsynergy.com/stats/ (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.

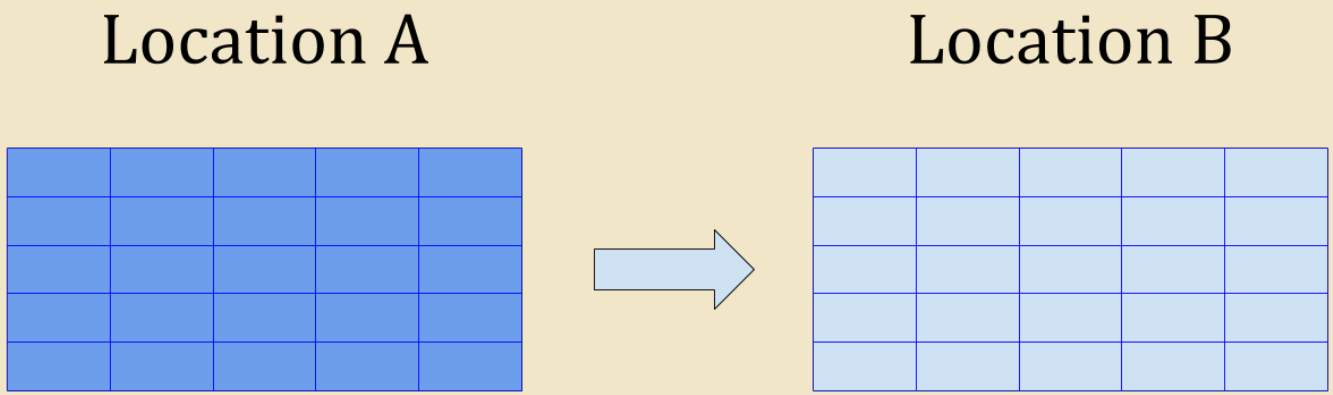
Why Use Parallel Computing?

- 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!

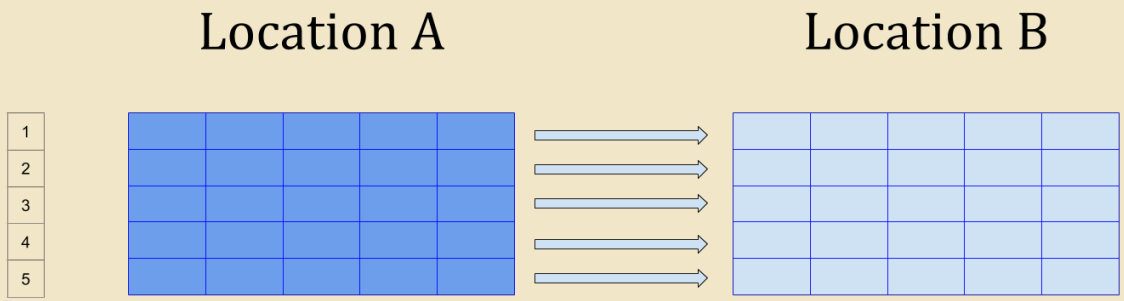
  Exaflop = 10^{18} calculations per second



- 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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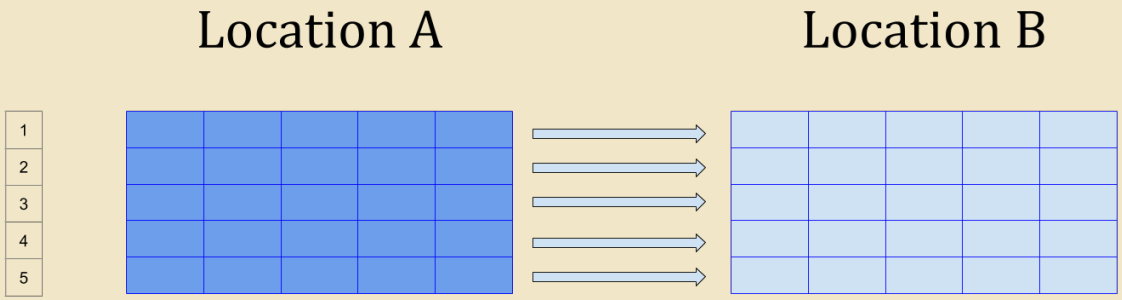


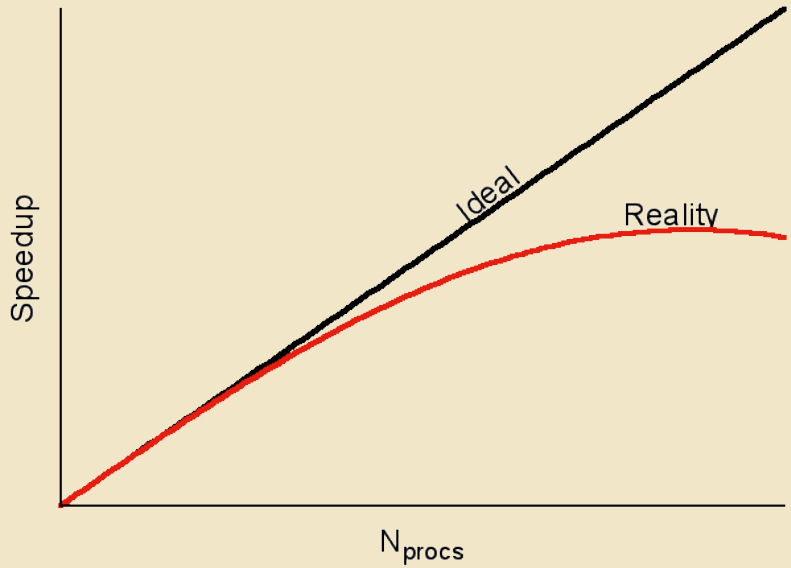
Number of People	Time (mins)
2	13x
3	9x
4	7x
5	5x
6	5x
7-8	4x
9-12	3x
13-24	2x
≥25	1x

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



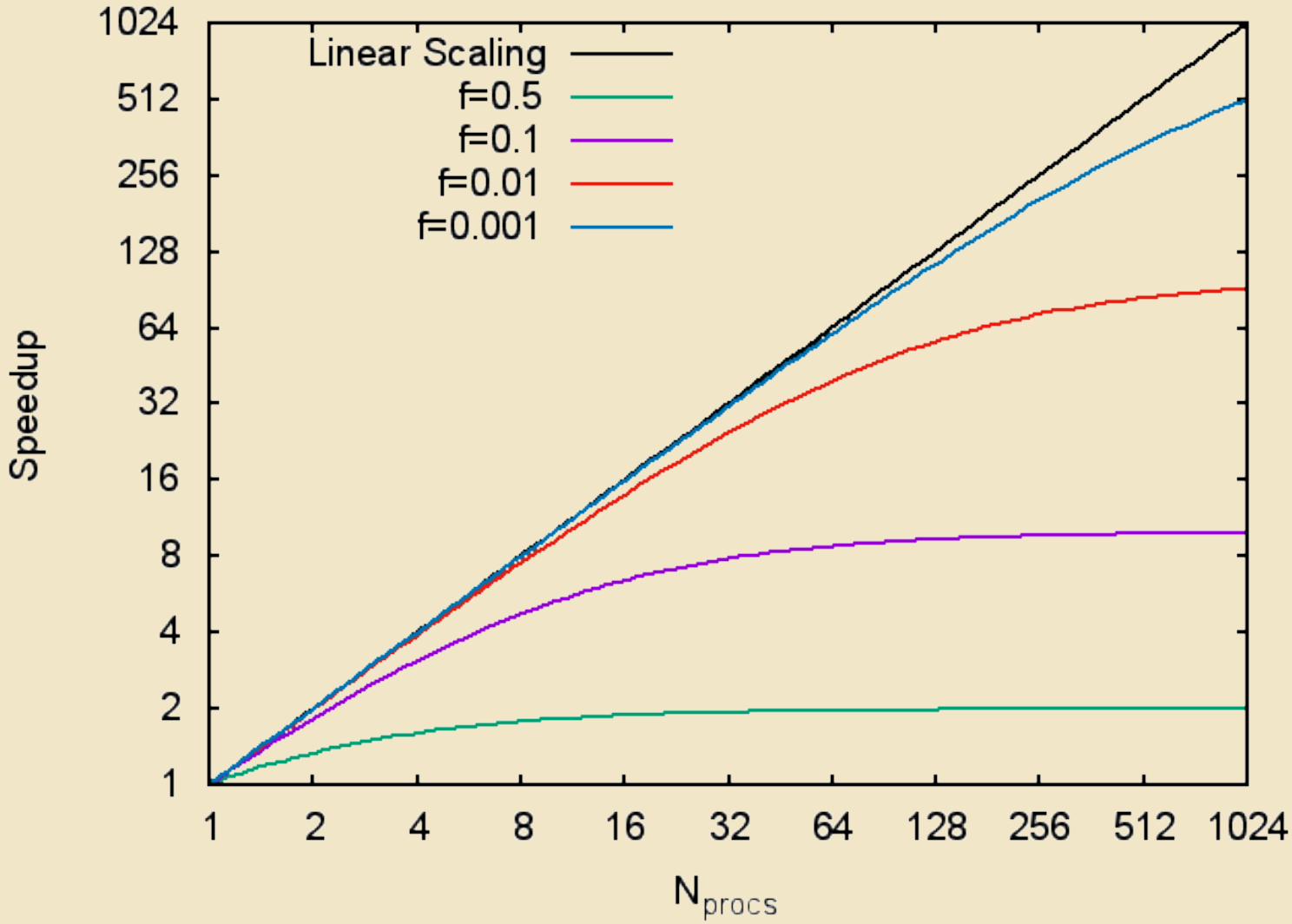
- Let f be the fraction of the serial program that cannot be parallelized
- Assume that the rest of the serial program can be perfectly parallelized (linear speedup)

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

- Or

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

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

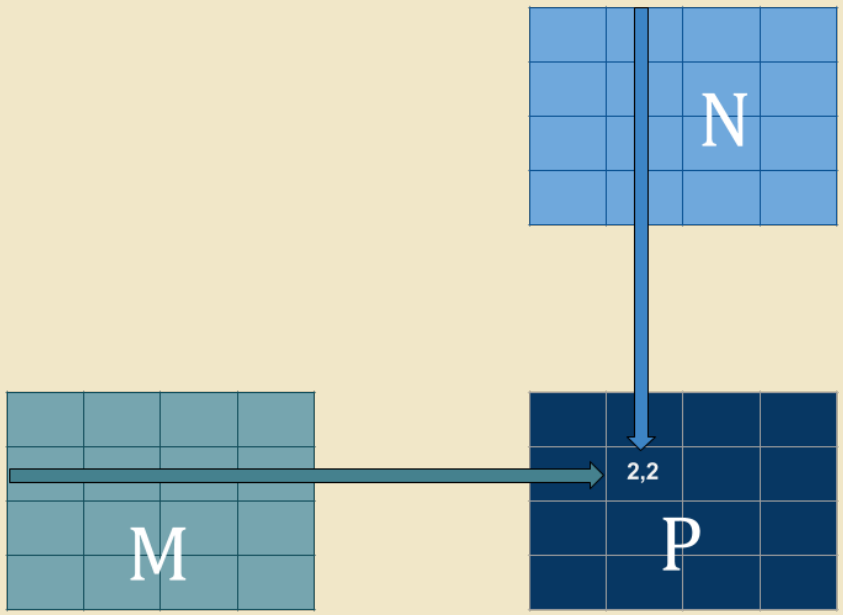
1. Start from serial programs as a baseline
   - Something to check correctness and efficiency against
2. Analyze and profile the serial program
   - Identify the "hotspot"
   - Identify the parts that can be parallelized
3. Parallelize code incrementally
4. Check correctness of the parallel code
5.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

A REAL example of parallel computing

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

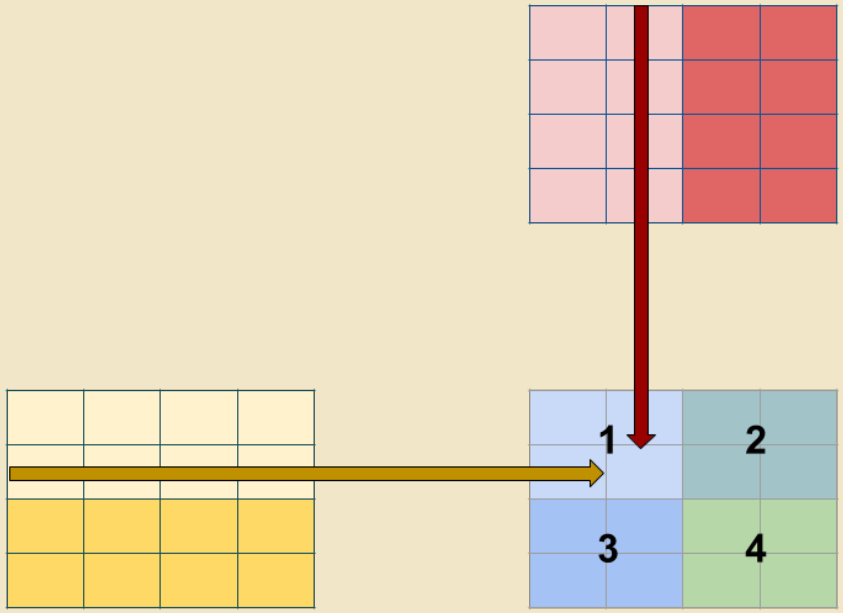
$$P_{m,n} = \sum_{k=1}^{d} M_{m,k} \times N_{k,n}$$

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



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

Single Program Multiple Data (SPMD)

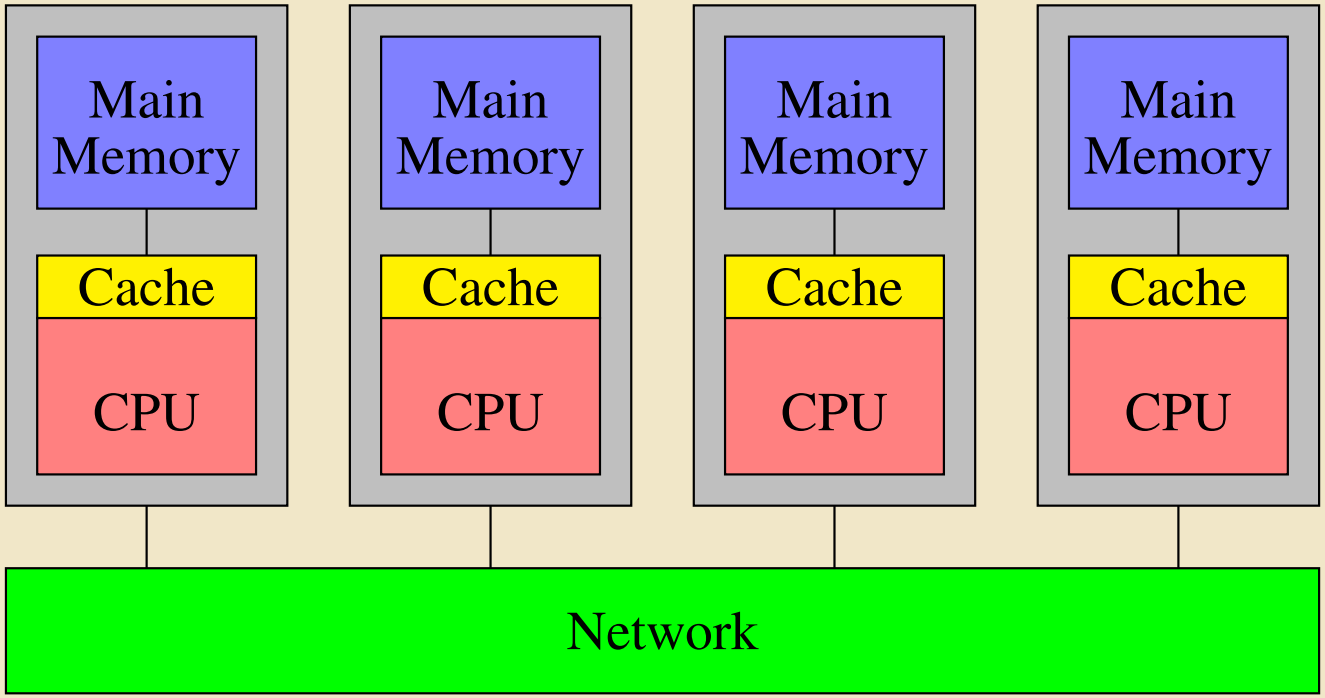
- All program instances execute same program
- Data parallel - Each instance works on different part of the data
- The majority of parallel programs are of this type
- Can also have
  - SPSD: serial program
  - MPSD: rare
  - MPMD

Memory system models

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

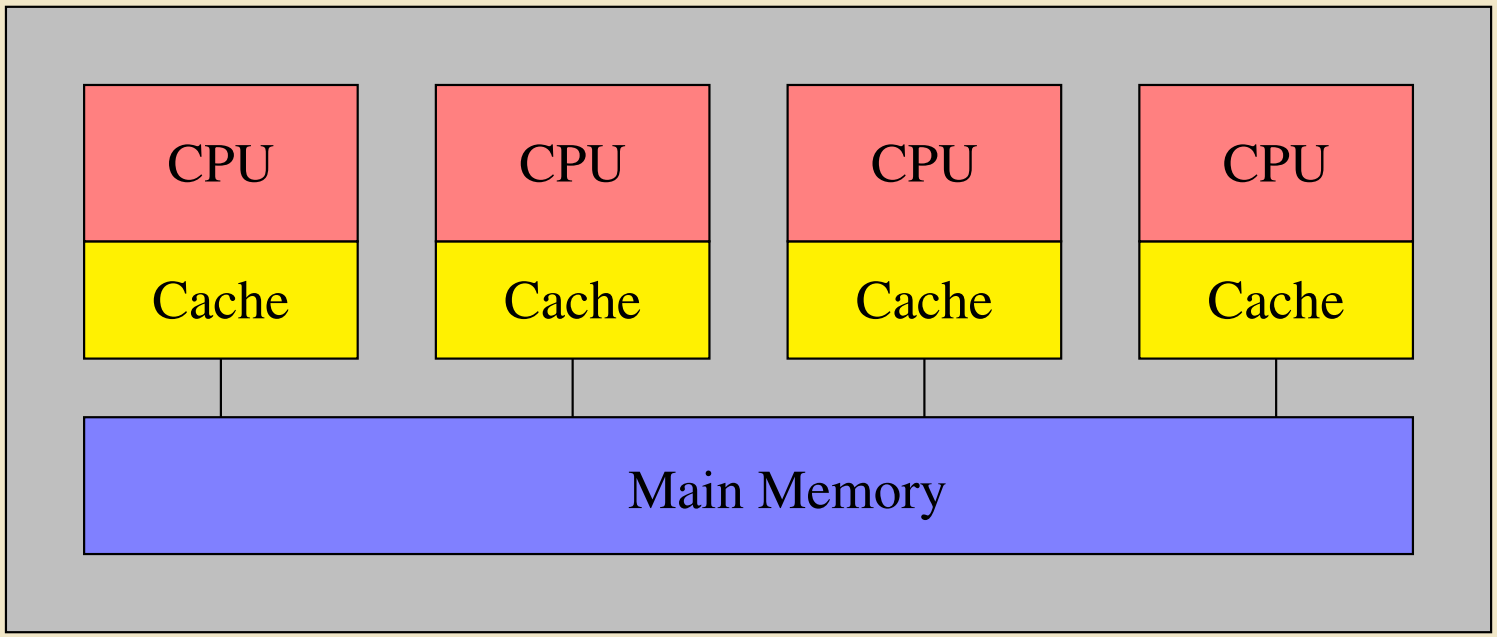
Distributed Memory Model

- 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

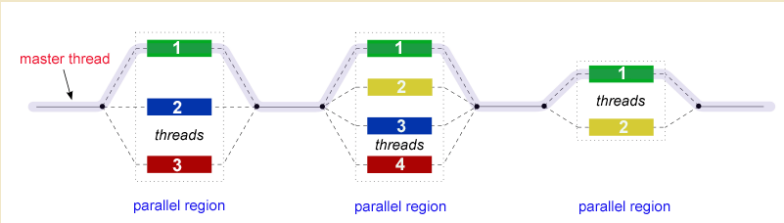
- All threads can access the global memory space.
- Data sharing achieved via writing to/reading from the same memory location
- Example
  - OpenMP
  - Pthreads



Shared vs Distributed

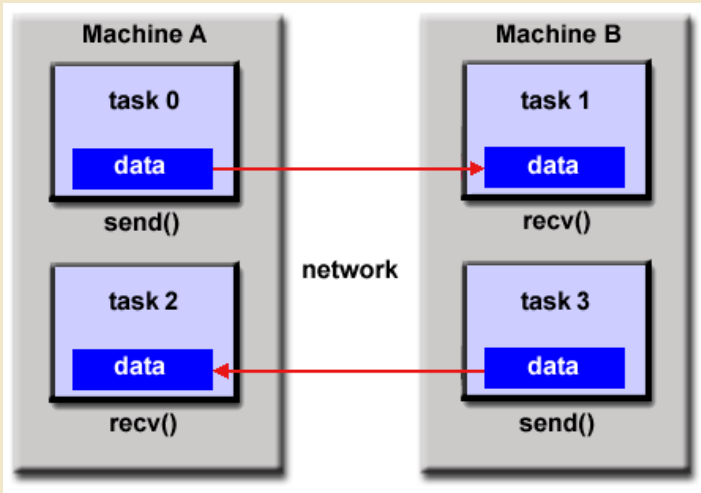
Shared

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



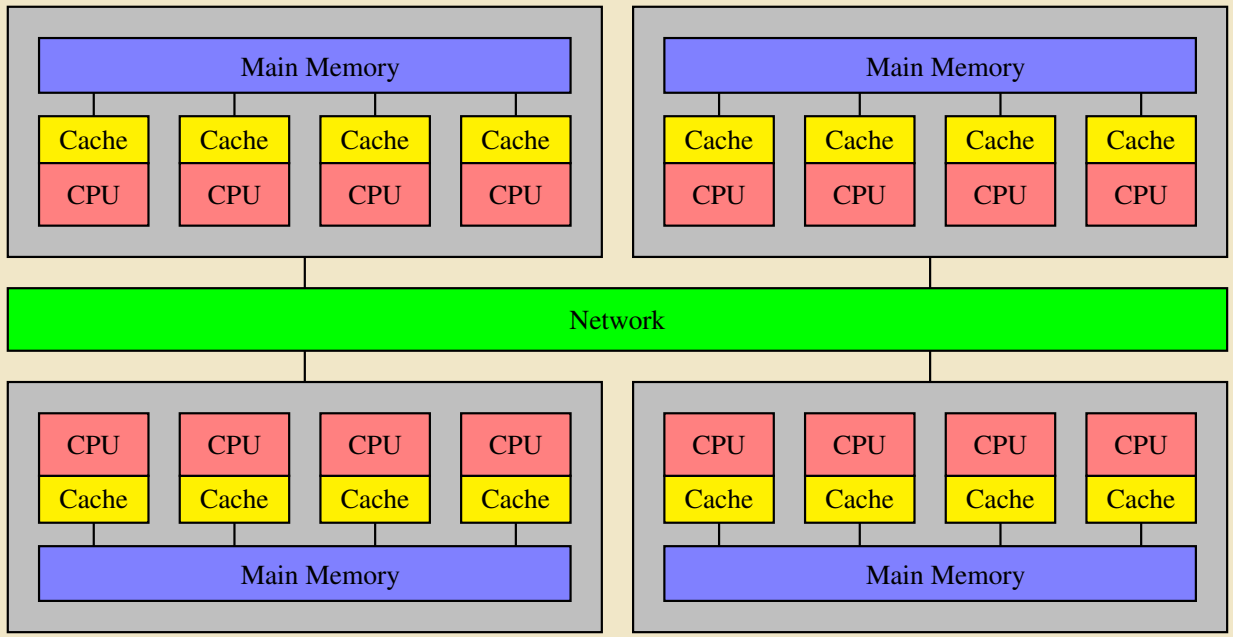
Distributed

- 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 · · ·

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

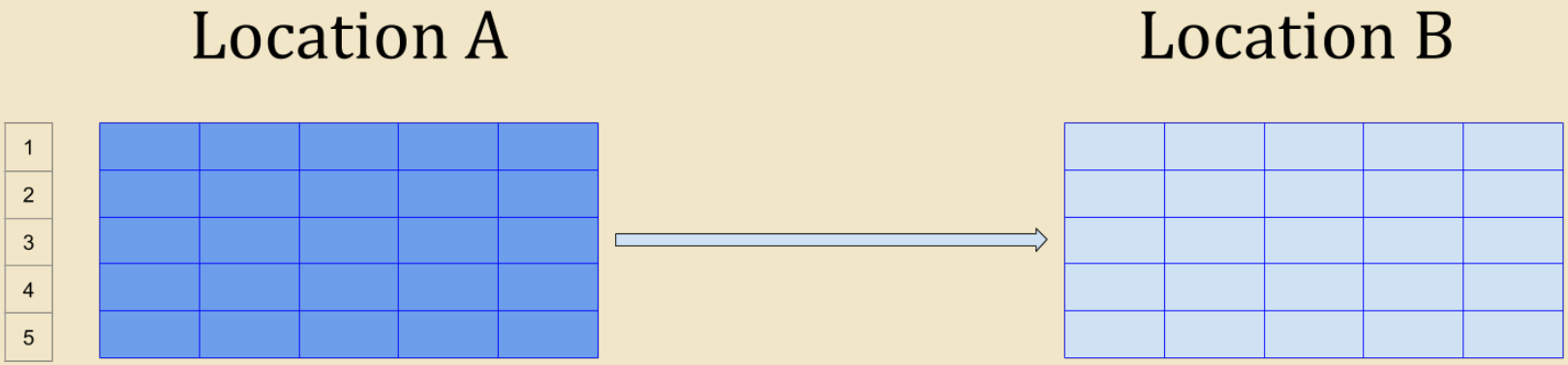
Outline

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?



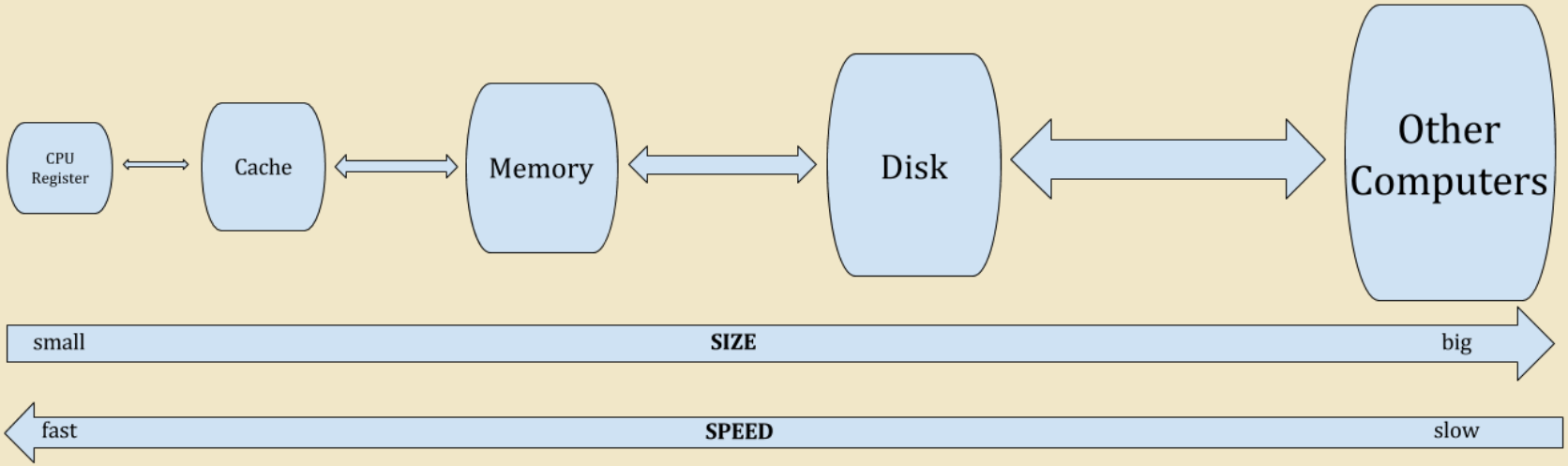
Hidden Serialization

- 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

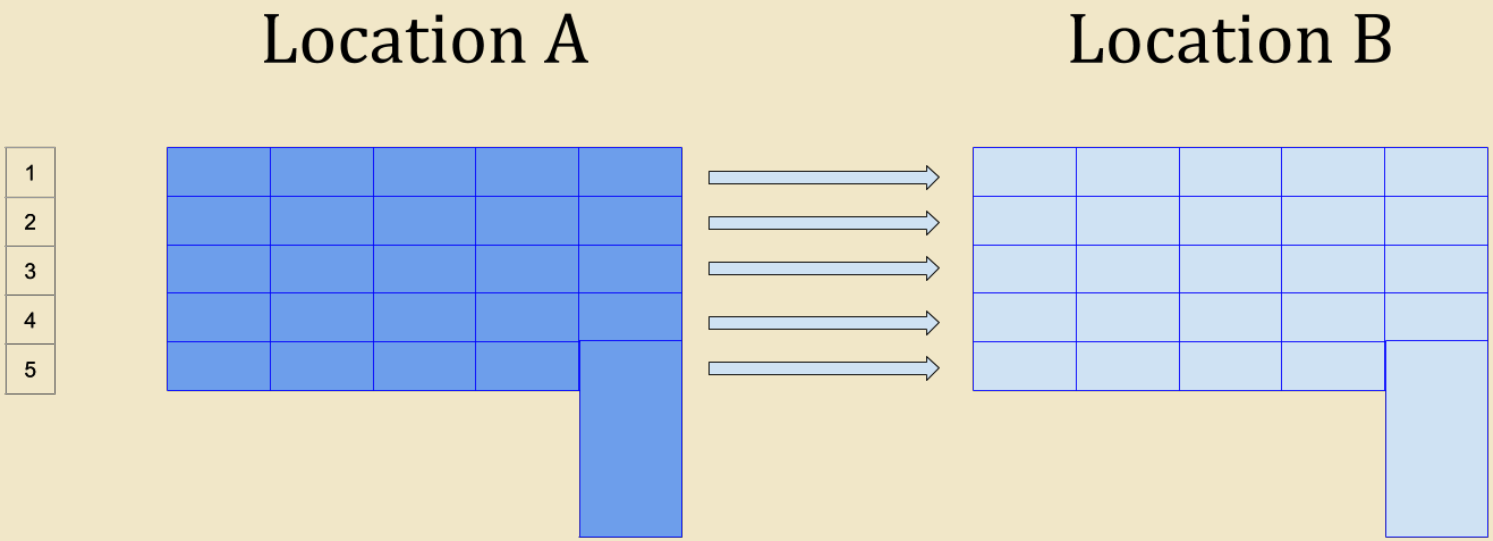
Memory Heirarchy



- 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

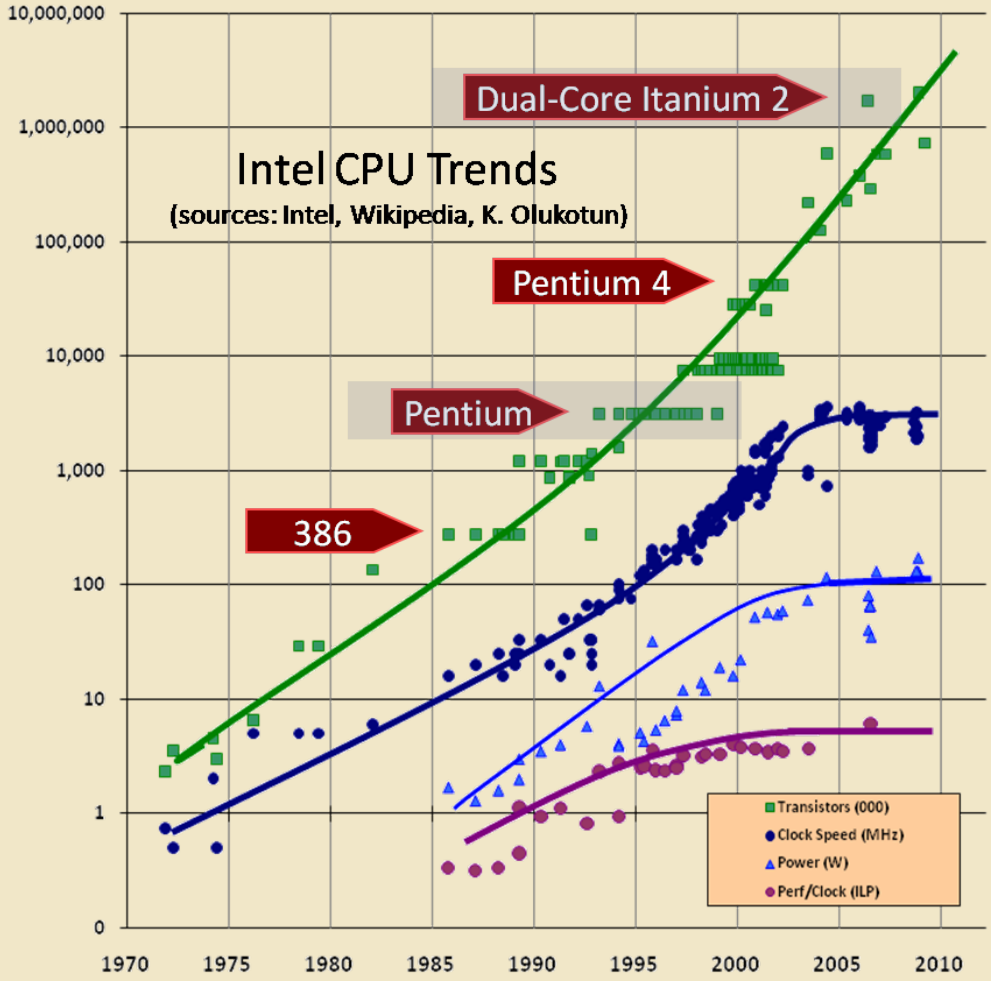
- Often caused by "blocking" communication operations
  - "Blocking" means "I will not proceed until the current operation is over"
- Solution
  - Use "non-blocking" operations
  - Caution: trade-off between data safety and performance

Outline

Heterogeneous computing

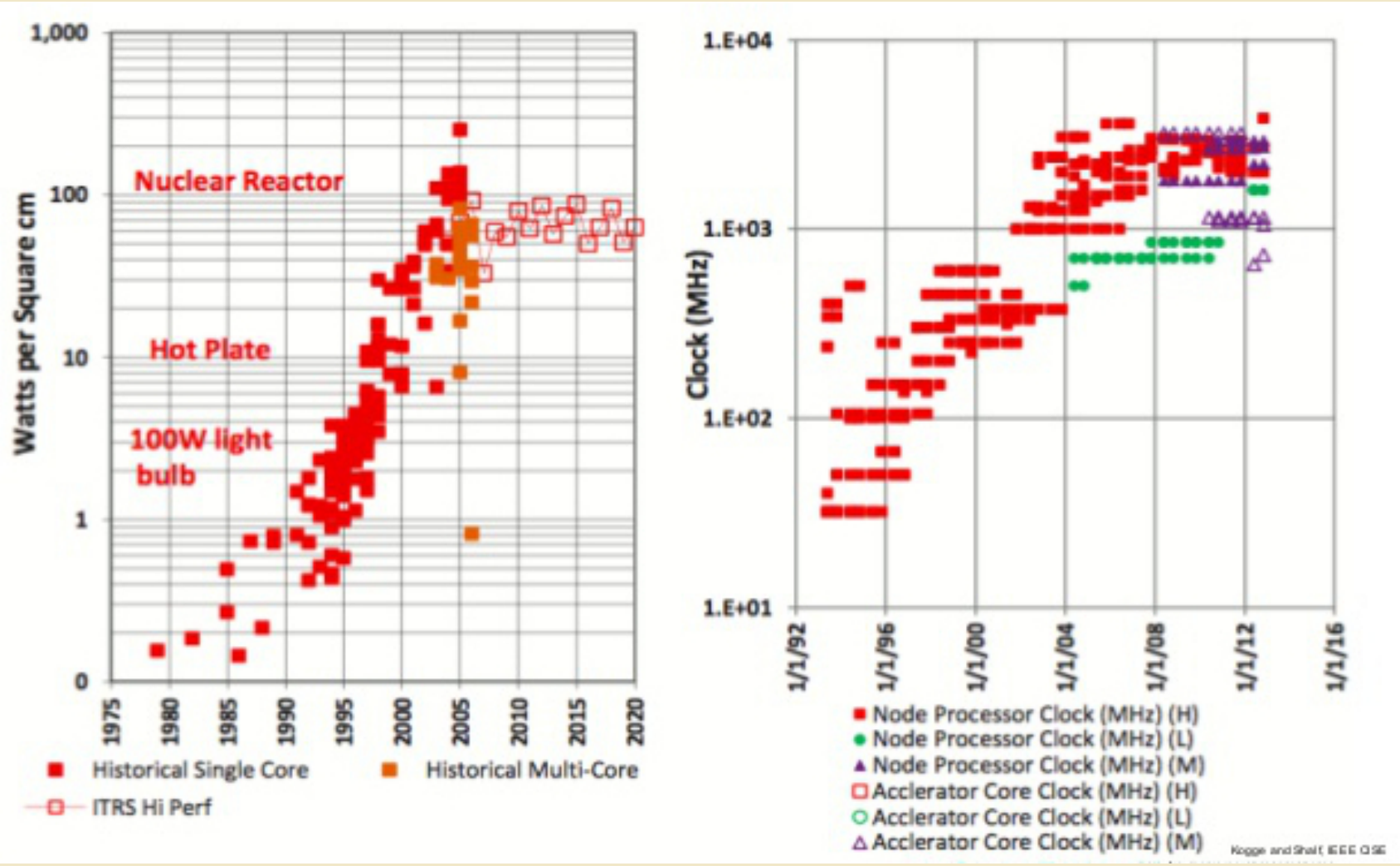
- A heterogeneous system solves tasks using different types of processing units
  - CPUs
  - GPUs
  - DSPs
  - Co-processors
  - ...
- As opposed to homogeneous systems, e.g. SMP nodes with CPUs only

The Free Lunch Is Over



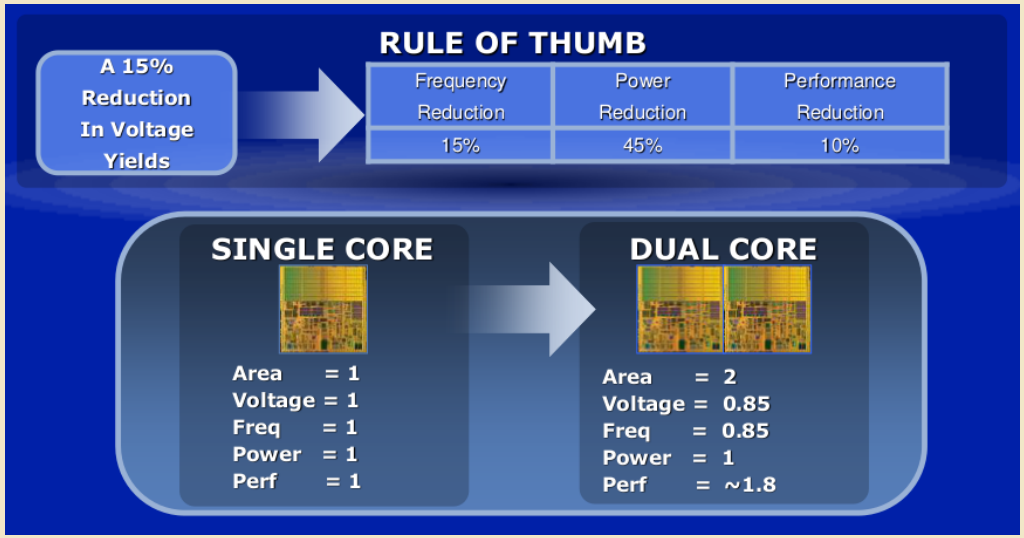
Source: Herb Sutter
http://www.gotw.ca/publications/concurrency-ddj.htm

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

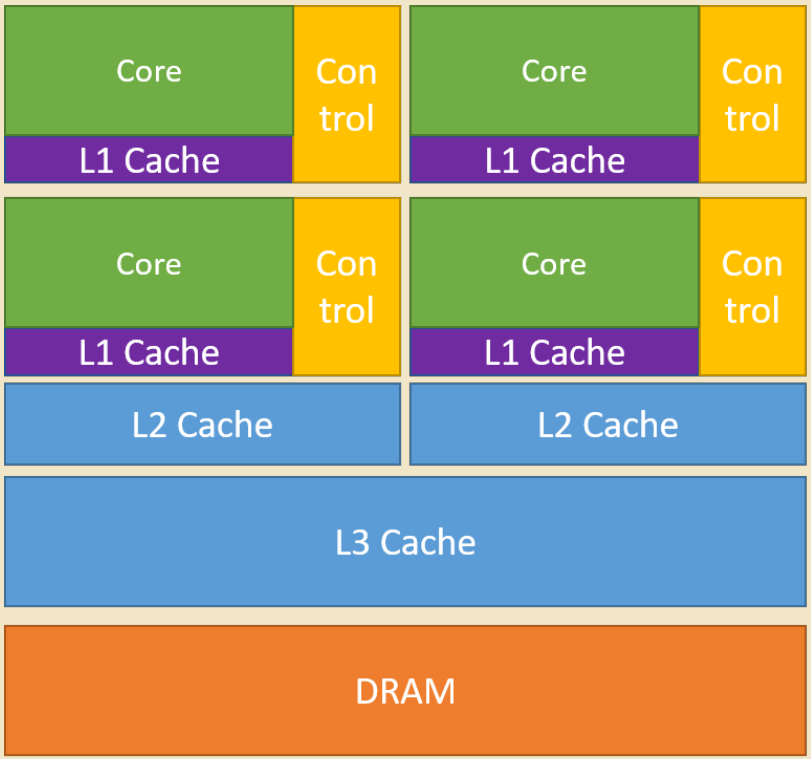


Source: John Urbanic, PSC

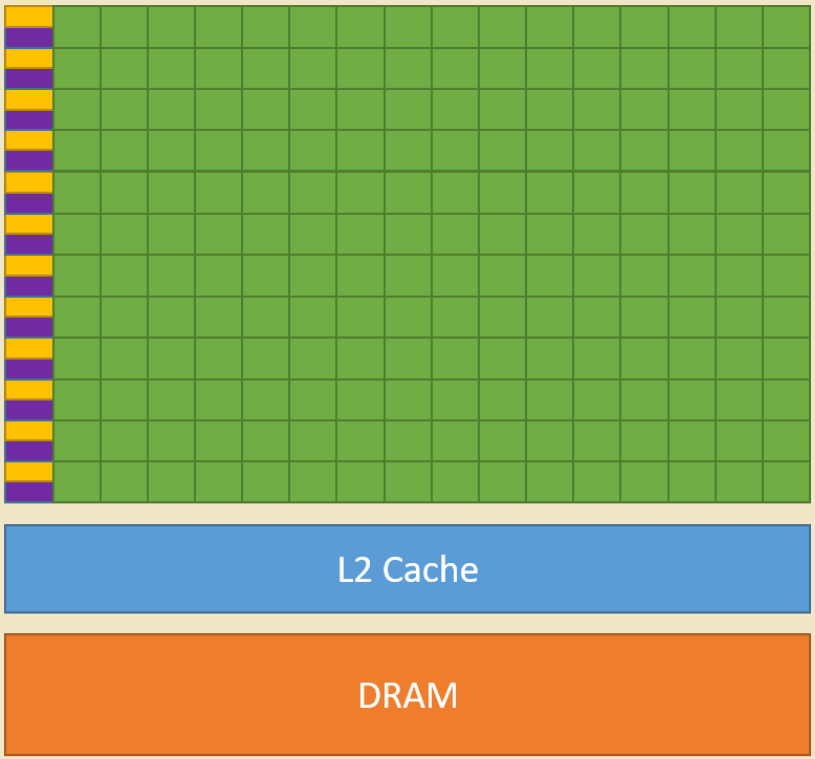
Graphic Processing Units (GPUs)

- 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



CPU



GPU

NVIDIA Tesla T4

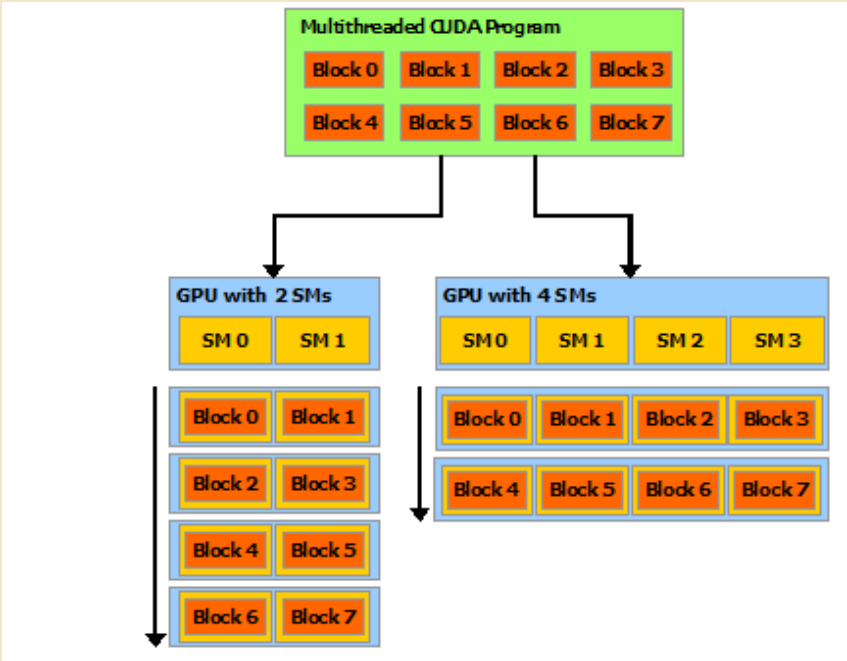
- GPU Architecture: NVIDIA Turing
- Tensor Cores: 320
- CUDA Cores: 2560
- Performance:
  - Single Precision: 8.1 TFLOPS
  - Mixed Precision (FP16/FP32): 65 TFLOPS
  - INT8: 130 TOPS
  - INT4: 260 TOPS
- Memory (GDDR5): 16GB
- Memory (Bandwidth): 320GBs

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.



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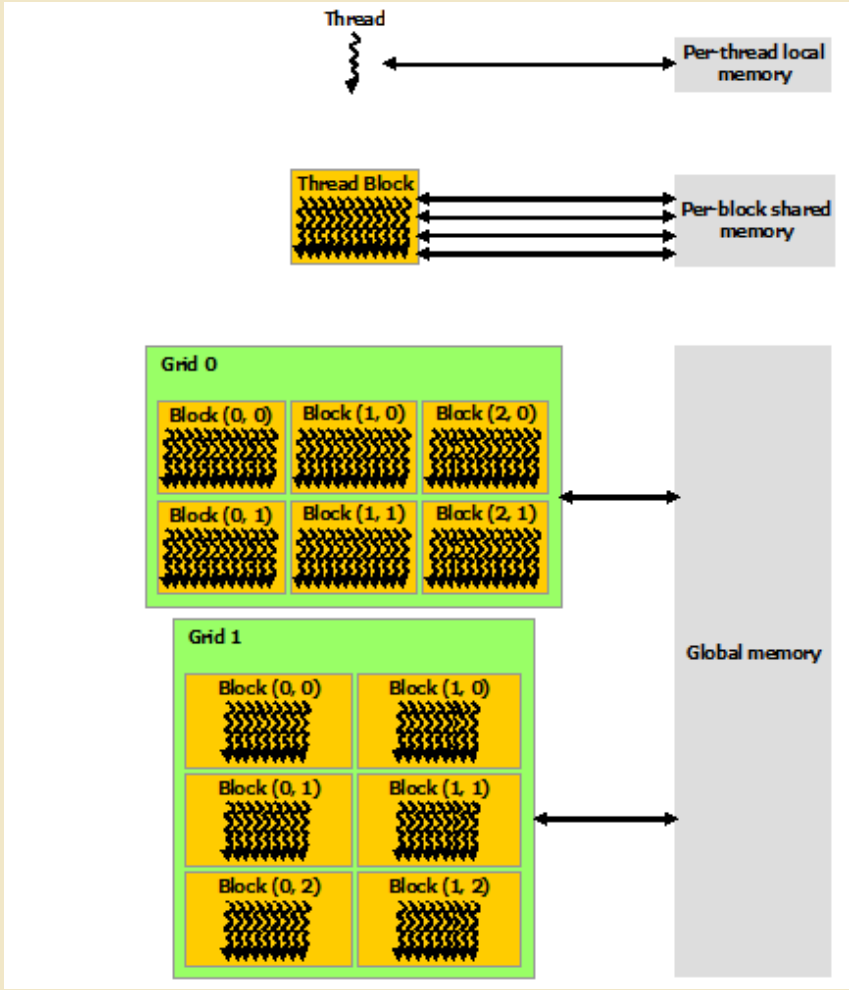
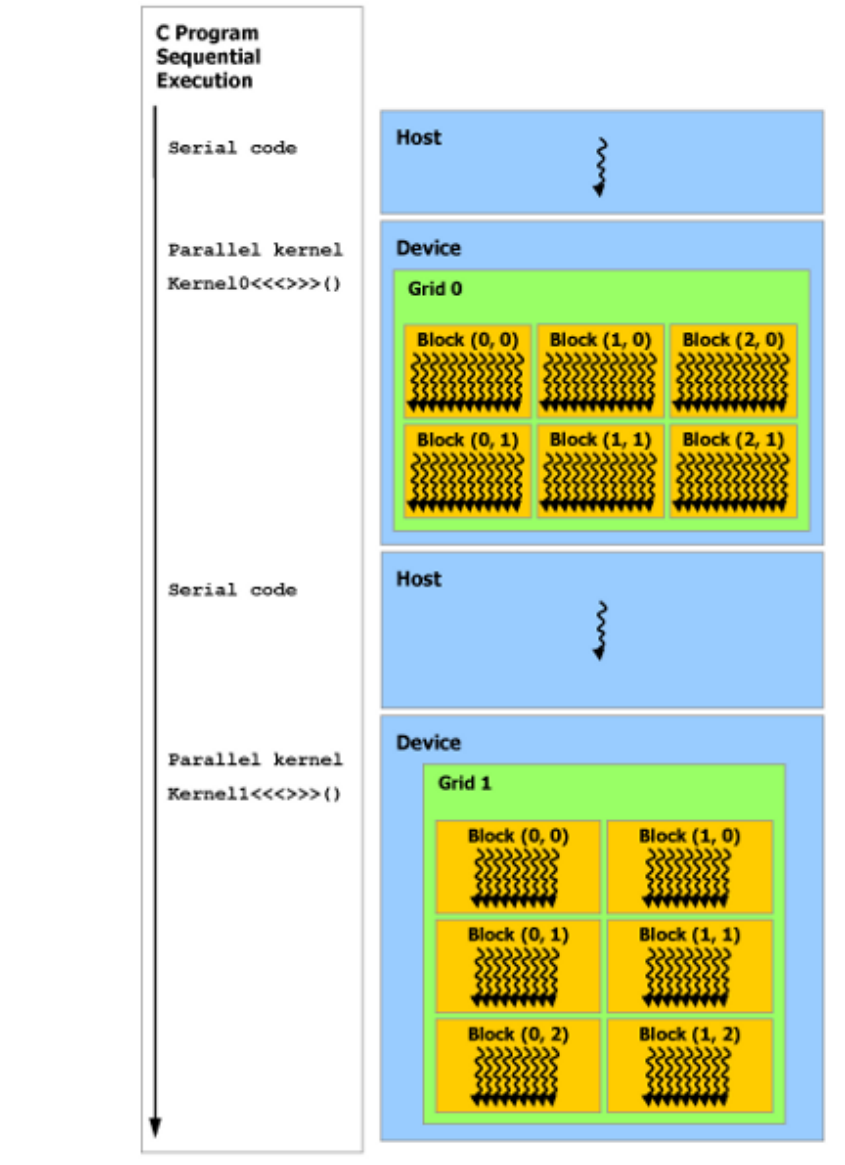


GPU Program


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