ME964
High Performance Computing for Engineering Applications

Parallel Programming Patterns

One Slide Summary of ME964

April 7, 2011

"Part of the inhumanity of the computer is that, once it is competently programmed and working smoothly, it is completely honest."
Isaac Asimov

Before We Get Started…

- Last Time
  - OpenMP wrap up
    - Variable scoping
    - Synchronization issues
- Today
  - Parallel programming patterns
  - One slide summary of ME964
- Other issues:
  - No class on April 12
  - Assignment 7 due tonight
  - Assignment 8 (last ME964 assignment) posted on the class website, due next Th
  - Midterm exam on April 19
    - Review session the evening before
  - From now on only guest lectures and such, time to concentrate on your projects

Recommended Reading

Mattson, Sanders, Massingill, *Patterns for Parallel Programming*, Addison Wesley, 2005, ISBN 0-321-22811-1.

- Used for this presentation
- A good overview of challenges, best practices, and common techniques in all aspects of parallel programming
- Book is on reserve at Wendt Library

Objective

- Get exposed to techniques & best practices that have emerged as useful in the parallel programming practice
- They are expected to facilitate and/or help you with
  - Thinking/Visualizing your problem as being solved in parallel
  - Addressing functionality and performance issues in your parallel program design
  - Discussing your design decisions with others
  - Selecting an appropriate platform that helps you express & implement the parallel design for the solution you identified

Parallel Computing: When and Why.

- Parallel computing, prerequisites
  - The problem can be decomposed into sub-problems that can be independently solved at the same time
  - The part of the problem that is concurrent is large enough to justify an approach that exploits this concurrency
    - Recall Amdhal's law

- Parallel computing, goals
  - Solve problems in less time

    and/or
  - Solve bigger problems

Parallel Computing, Caveats

- Performance can be drastically reduced by many factors
  - Overhead of parallel processing
  - Load imbalance among processor elements
  - Inefficient data sharing patterns
  - Saturation of critical resources such as memory bandwidth

Implementing a Parallel Solution to Your Problem: Key Steps

1) **Find the concurrency in the problem**

2) Structure the algorithm so that concurrency can be exploited

3) Implement the algorithm in a suitable programming environment

4) Tune the performance of the code on the target parallel system

NOTE: The reality is that these have not been separated into levels of abstractions that can be dealt with independently.

What's Next?

Focus on this for a while

Finding Concurrency

Algorithm Structure

Supporting Structures

Implementation Mechanisms

From *"Patterns for Parallel Programming"*

Finding and Nurturing Concurrency

- Dependence kills concurrency. Dependencies need to be identified and managed
  - Dependencies prevent parallelism, at least the "embarrassingly parallel" flavor
  - Often times, dependencies end up requiring synchronization barriers (not good…)

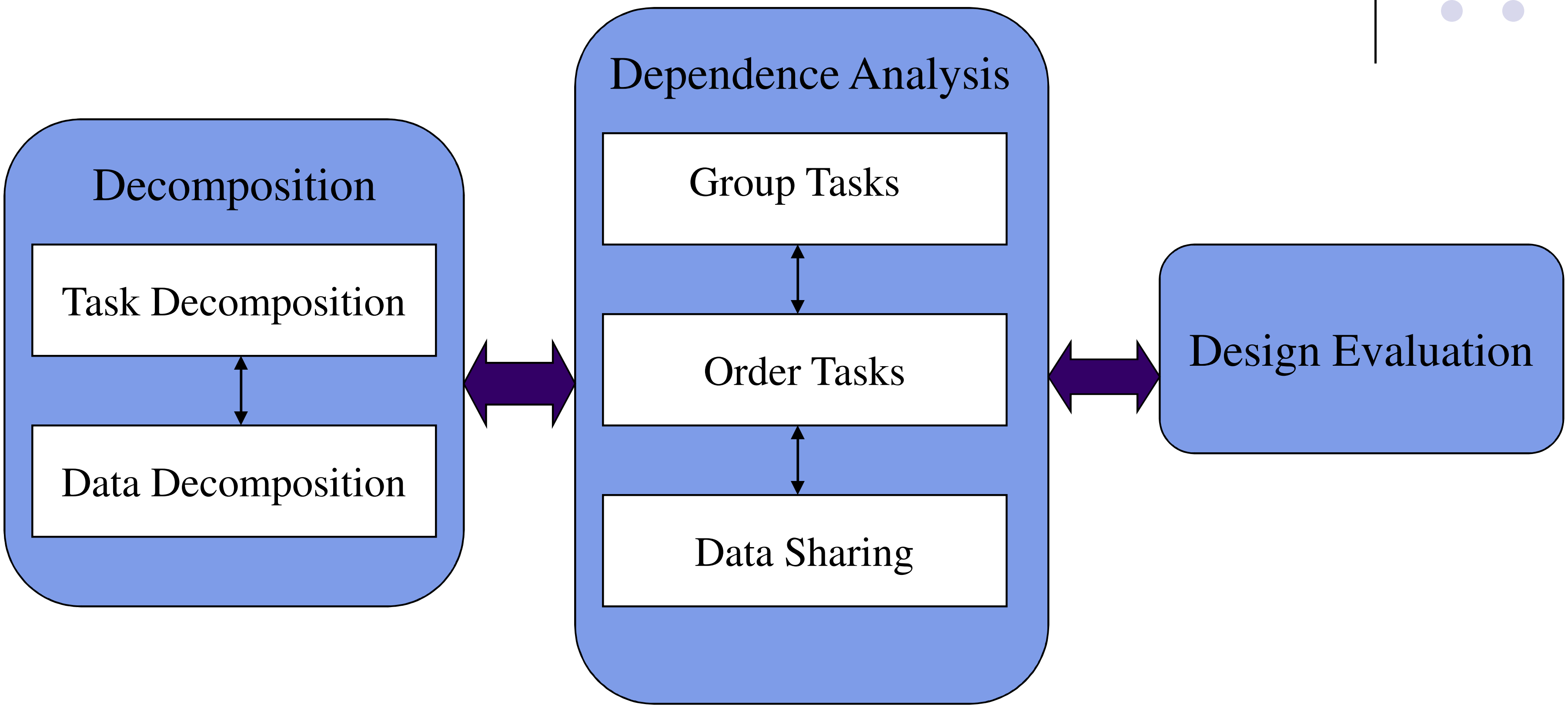
- Concurrency has some caveats
  - In sequential execution: One step feeds result to the next steps $\Rightarrow$ a unique way moving from A to Z
  - In parallel execution: numeric accuracy may be affected by ordering steps that parallel with each other $\Rightarrow$ platform dependent, OS dependent possibly even dependent on the state of the system

- Finding and exploiting concurrency often requires looking at the problem from a non-obvious angle

Finding Concurrency in Problems

- Goal: Identify a decomposition of the problem into sub-problems that can be solved simultaneously
- In order to meet this goal:
  - Perform a task decomposition to identify tasks that can execute concurrently
  - Carry out data decomposition to identify data local to each task
  - Identify a way of grouping tasks and ordering the groups to satisfy temporal constraints
  - Carry out an analysis of the data sharing patterns among the concurrent tasks to avoid any race condition issues and optimize memory access
  - Perform a design evaluation that assesses the quality of the choices made in all the steps

Finding Concurrency – The Process



This is typically an iterative process, like an optimization process that has to negotiate several constraints

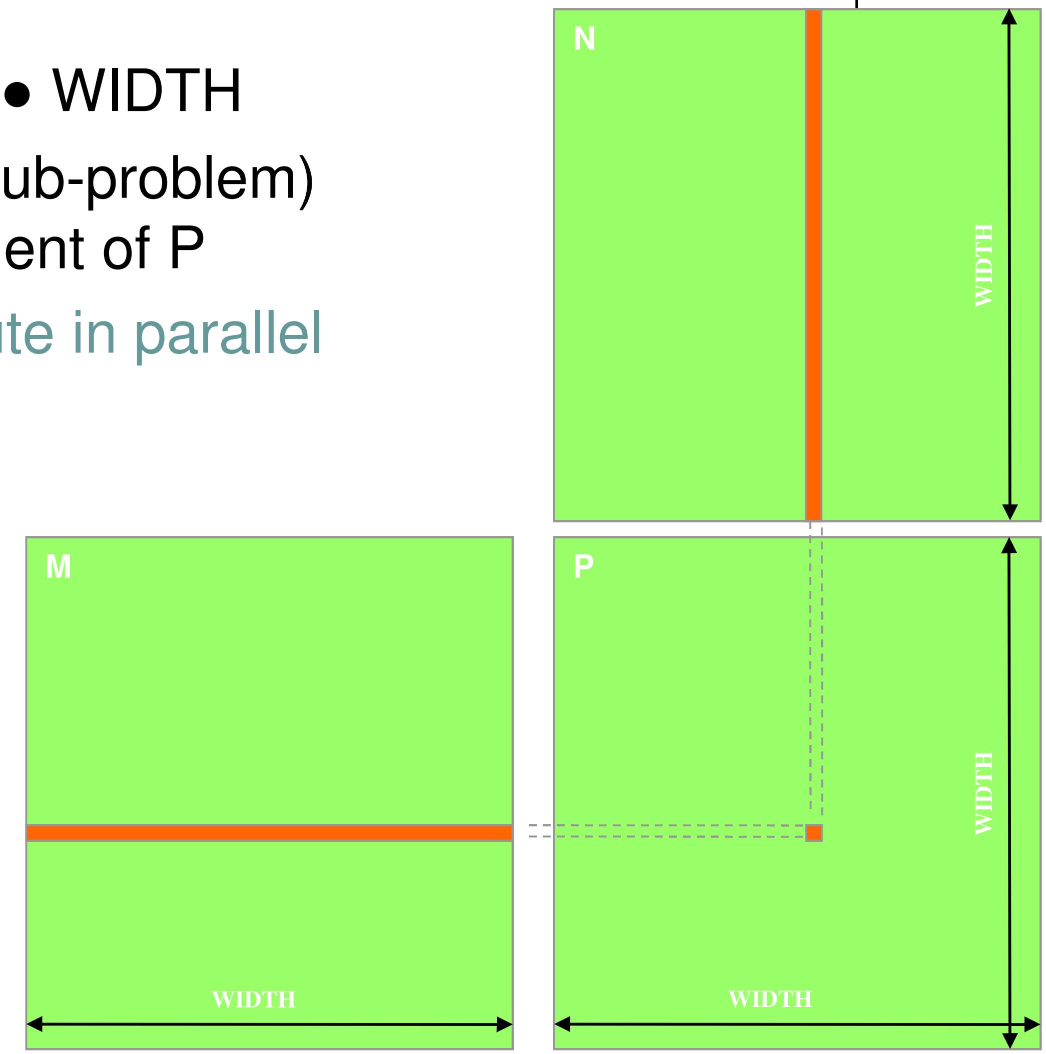
Find Concurrency 1:
Decomp. Stage: Task Decomposition

- Many large problems have natural independent tasks
  - The number of tasks used should be adjustable to the execution resources available.
  - Each task must include sufficient work in order to compensate for the overhead of managing their parallel execution.
  - Tasks should maximize reuse of sequential program code to minimize design/implementation effort.

> "In an ideal world, the compiler would find tasks for the programmer. Unfortunately, this almost never happens."
> - Mattson, Sanders, Massingill

Example: Task Decomposition Square Matrix Multiplication

- P = M * N of WIDTH • WIDTH
  - One natural task (sub-problem) produces one element of P
  - All tasks can execute in parallel



Find Concurrency 2: Decomp. Stage: Data Decomposition

- The most compute intensive parts of many large problems manipulate a large data structure
  - Similar operations are being applied to different parts of the data structure, in a mostly independent manner.
  - This is what CUDA is optimized for.

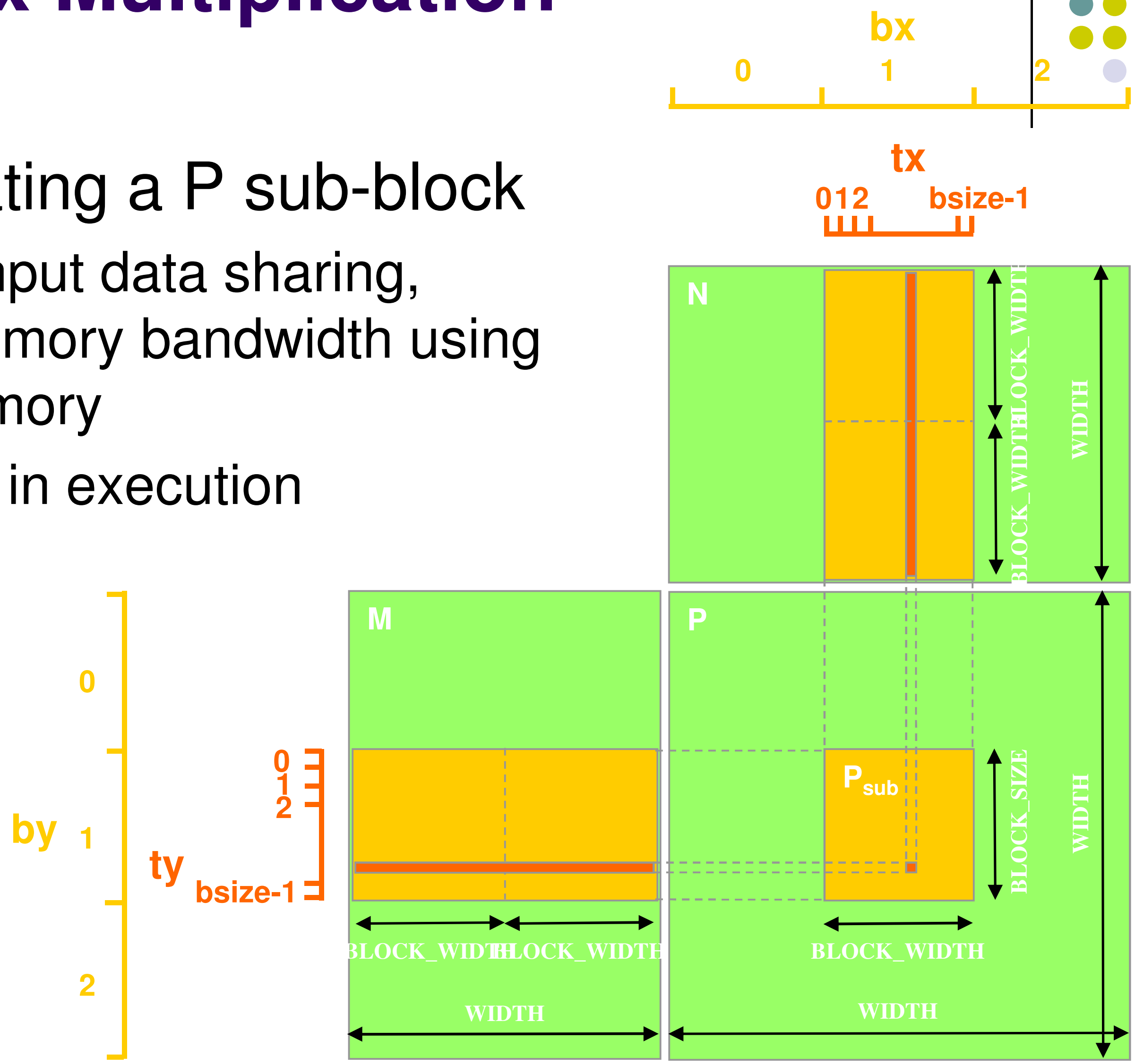
- The data decomposition should lead to
  - Efficient data usage by each Unit of Execution (UE) within the partition
  - Few dependencies between the UEs that work on different partitions
  - Adjustable partitions that can be varied according to the hardware characteristics

Find Concurrency 3: Dependence Analysis - Tasks Grouping

- Sometimes several tasks in problem can be grouped to improve efficiency
  - Reduced synchronization overhead – because when task grouping there is supposedly no need for synchronization
  - All tasks in the group efficiently share data loaded into a common on-chip, shared storage (Shared Memory)

Task Grouping Example - Square Matrix Multiplication

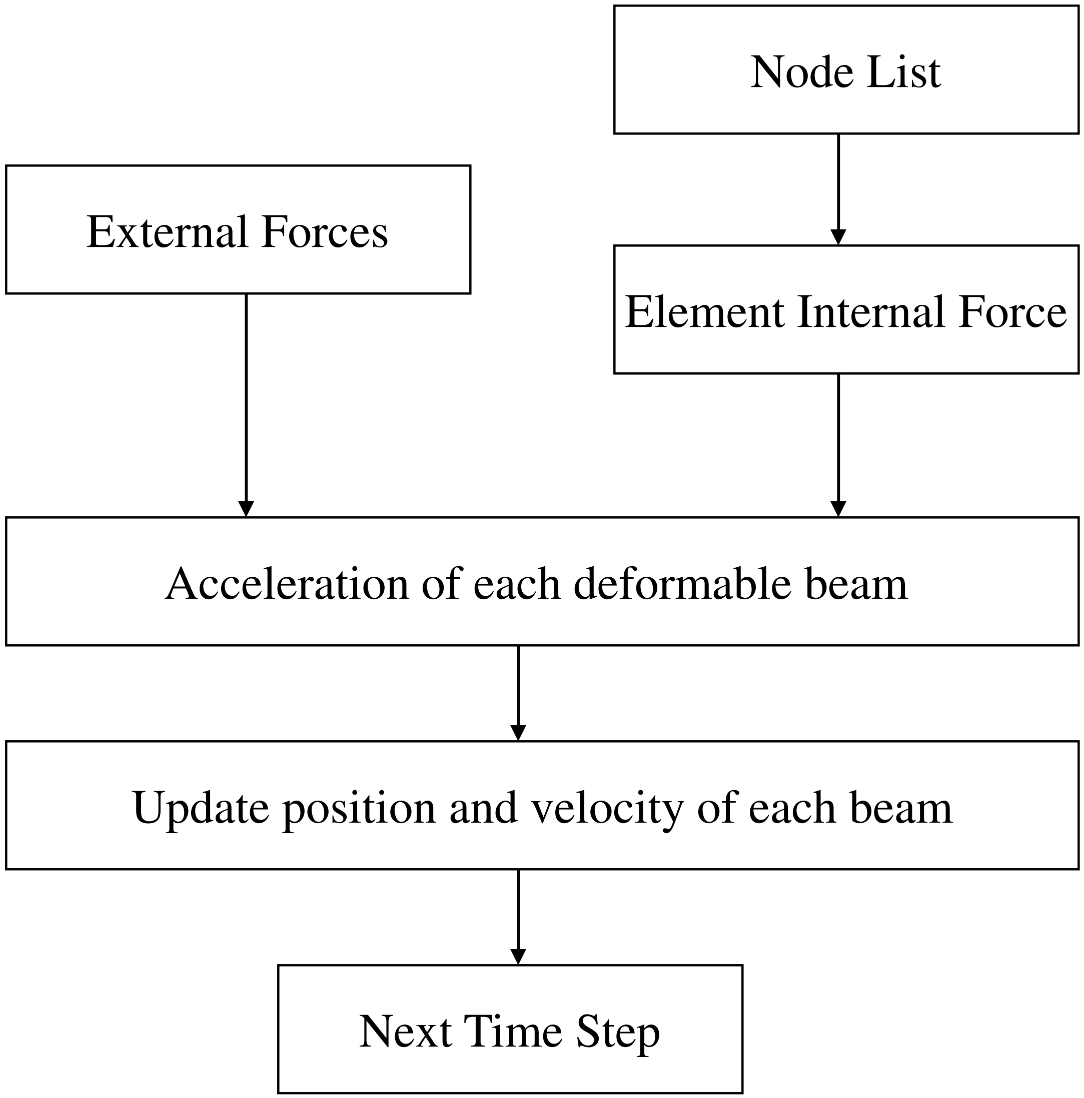
- Tasks calculating a P sub-block
  - Extensive input data sharing, reduced memory bandwidth using Shared Memory
  - All synched in execution



Find Concurrency 4: Dependence Analysis - Task Ordering

- Identify the data required by a group of tasks before they can execute
  - Find the task group that creates it (look upwind)
  - Determine a temporal order that satisfy all data constraints

Task Ordering Example: Finite Element Analysis



Find Concurrency 5: Dependence Analysis - Data Sharing

- Data sharing can be a double-edged sword
  - An algorithm that calls for excessive data sharing can drastically reduce advantage of parallel execution
  - Localized sharing can improve memory bandwidth efficiency
  - Use the execution of task groups to interleave with (mask) global memory data accesses
- Read-only sharing can usually be done at much higher efficiency than read-write sharing, which often requires a higher level of synchronization

Data Sharing Example
Matrix Multiplication on the GPU

- Each task group will finish usage of each sub-block of N and M before moving on
  - N and M sub-blocks loaded into Shared Memory for use by all threads of a P sub-block
  - Amount of on-chip Shared Memory strictly limits the number of threads working on a P sub-block
- Read-only shared data can be efficiently accessed as Constant or Texture data (on the GPU)
  - Frees up the shared memory for other uses

Find Concurrency 6: Design Evaluation

- Key questions to ask
  - How many Units of Execution (UE) can be used?
  - How are the data structures shared?
  - Is there a lot of data dependency that leads to excessive synchronization needs?
  - Is there enough work in each UE between synchronizations to make parallel execution worthwhile?

Implementing a Parallel Solution to Your Problem: Key Steps

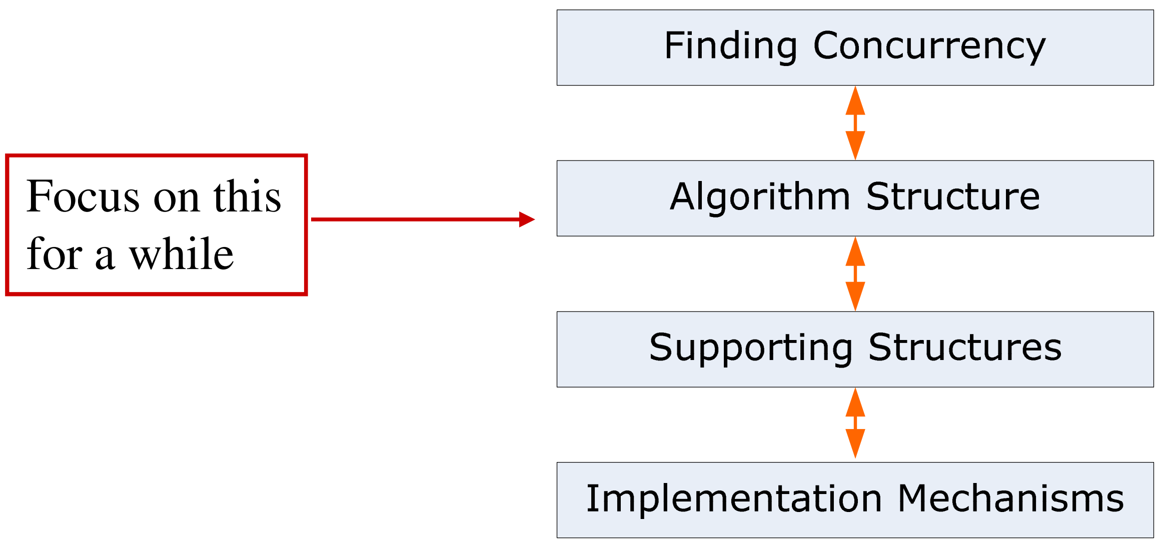
1) Find the concurrency in the problem

2) **Structure the algorithm so that concurrency can be exploited**

3) Implement the algorithm in a suitable programming environment

4) Execute and tune the performance of the code on a parallel system

What's Next?



From *"Patterns for Parallel Programming"*

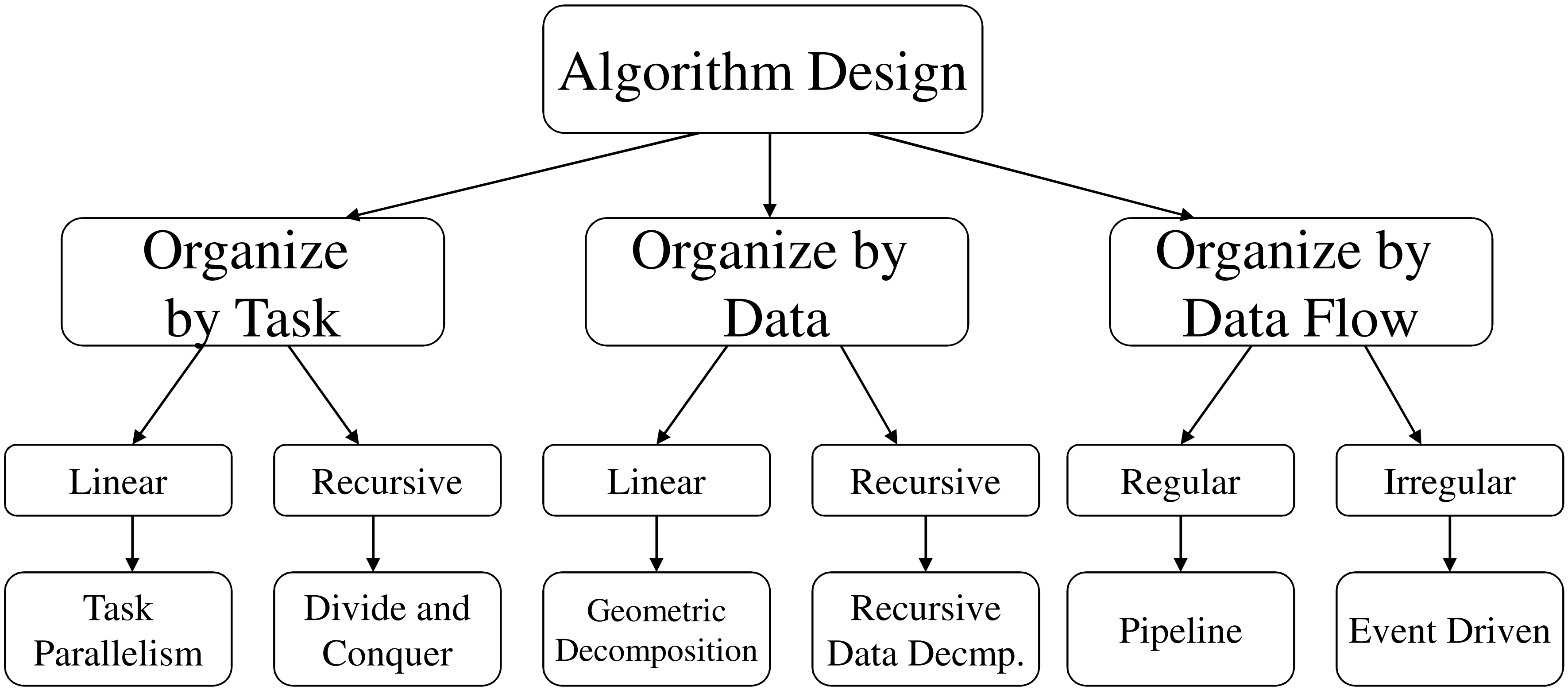
Algorithm: Definition

- A step by step procedure that is guaranteed to terminate, such that each step is precisely stated and can be carried out by a computer
  - Definiteness – the notion that each step is precisely stated
  - Effective computability – each step can be carried out by a computer
  - Finiteness – the procedure terminates
- Multiple algorithms can be used to solve the same problem
  - Some require fewer steps and some exhibit more parallelism

Algorithm Structure - Strategies

Organize by Tasks	Organize by Data	Organize by Flow
Task Parallelism	Geometric Decomposition	Pipeline
Divide and Conquer	Recursive Data Decomposition	Event Condition

Choosing Algorithm Structure



Alg. Struct. 1: Organize by Structure Linear Parallel Tasks

- Common in the context of distributed memory models

- These are the algorithms where the work needed can be represented as a collection of decoupled or loosely coupled tasks that can be executed in parallel
  - The tasks don't even have to be identical
  - Load balancing between UE can be an issue (dynamic load balancing?)
  - If there is no data dependency involved there is no need for synchronization: the so called "embarrassingly parallel" scenario

Alg. Struct. 1: Organize by Structure Linear Parallel Tasks [Cntd.]

- Examples
  - Imagine a car that needs to be painted:
    - One robot paints the front left door, another one the rear left door, another one the hood, etc.
    - The car is parceled up with a collection of UEs taking care of subtasks
  - Other: ray tracing, a good portion of the N-body problem, Monte Carlo type simulation

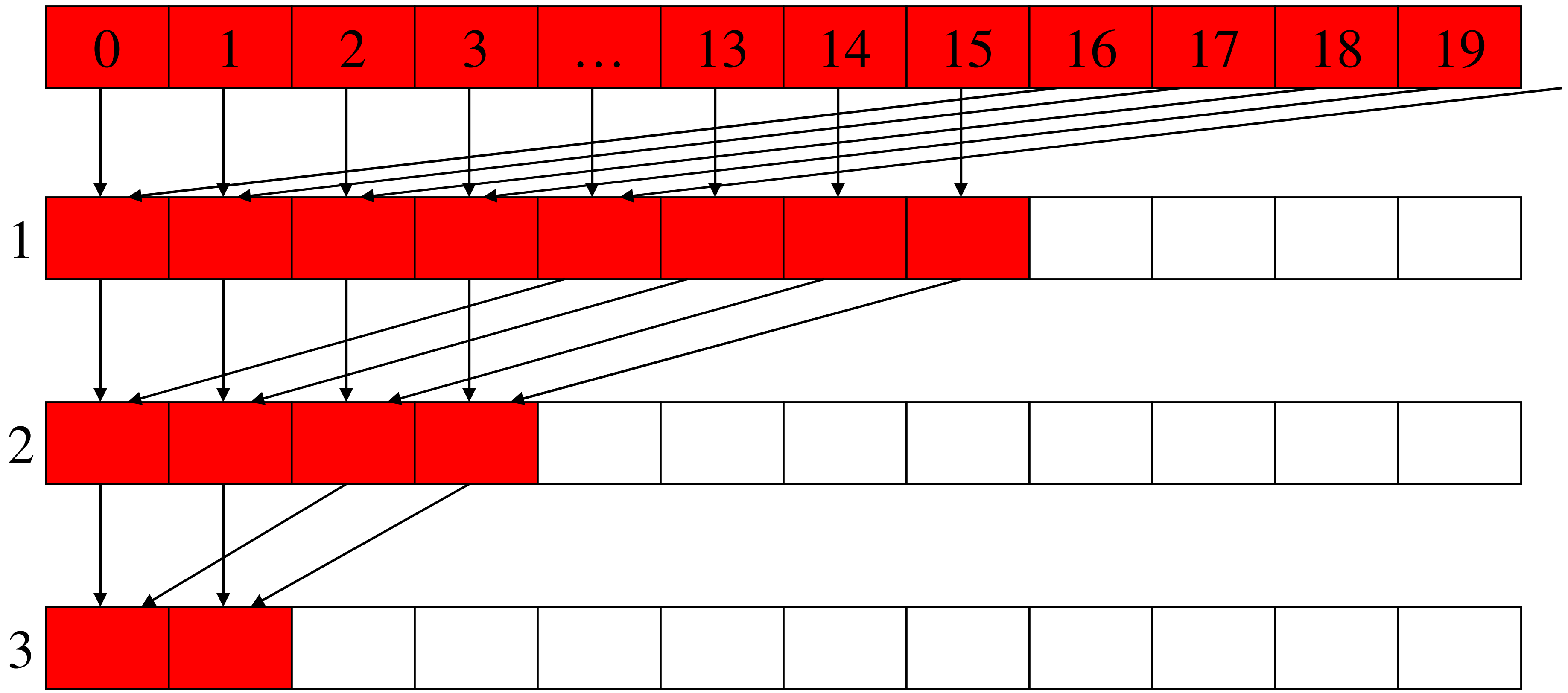
Alg. Struct. 2: Organize by Structure Recursive Parallel Tasks (Divide & Conquer)

- Valid when you can break a problem into a set of decoupled or loosely coupled smaller problems, which in turn can be broken etc…
  - This pattern is applicable when you can solve concurrently and with little synchronization the small problems (the leafs)

- In some case you need synchronization when dealing with this balanced tree type algorithm
  - Often required by the merging step (assembling the result from the "subresults")

- Examples: FFT, Linear Algebra problems (see FLAME project), the vector reduce operation

Computational ordering can have major effects on memory bank conflicts and control flow divergence.



Alg. Struct. 3: Organize by Data ~ Linear (Geometric Decomposition) ~

- This is the case where the UEs gather and work around a big chunk of data with little or no synchronization
- This is exactly the algorithmic approach enabled best by the GPU & CUDA
- Examples: Matrix multiplication, matrix convolution, image processing

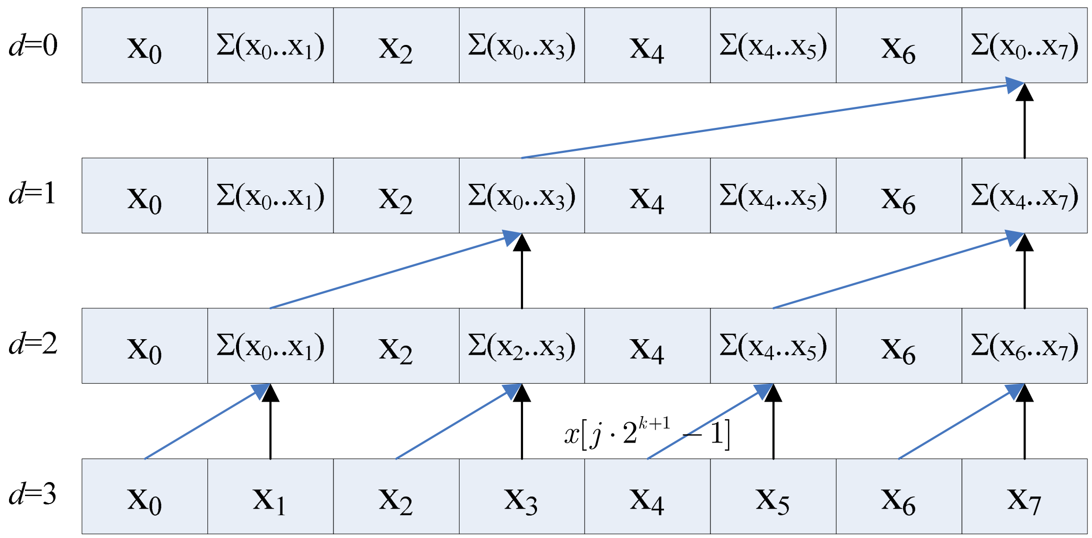
Alg. Struct. 4: Organize by Data
~ Recursive Data Scenario ~

- This scenario comes into play when the data that you operate on is structured in a recursive fashion
  - Balanced Trees
  - Graphs
  - Lists

- Sometimes you don't even have to have the data represented as such
  - See example with prefix scan
  - You choose to look at data as having a balanced tree structure

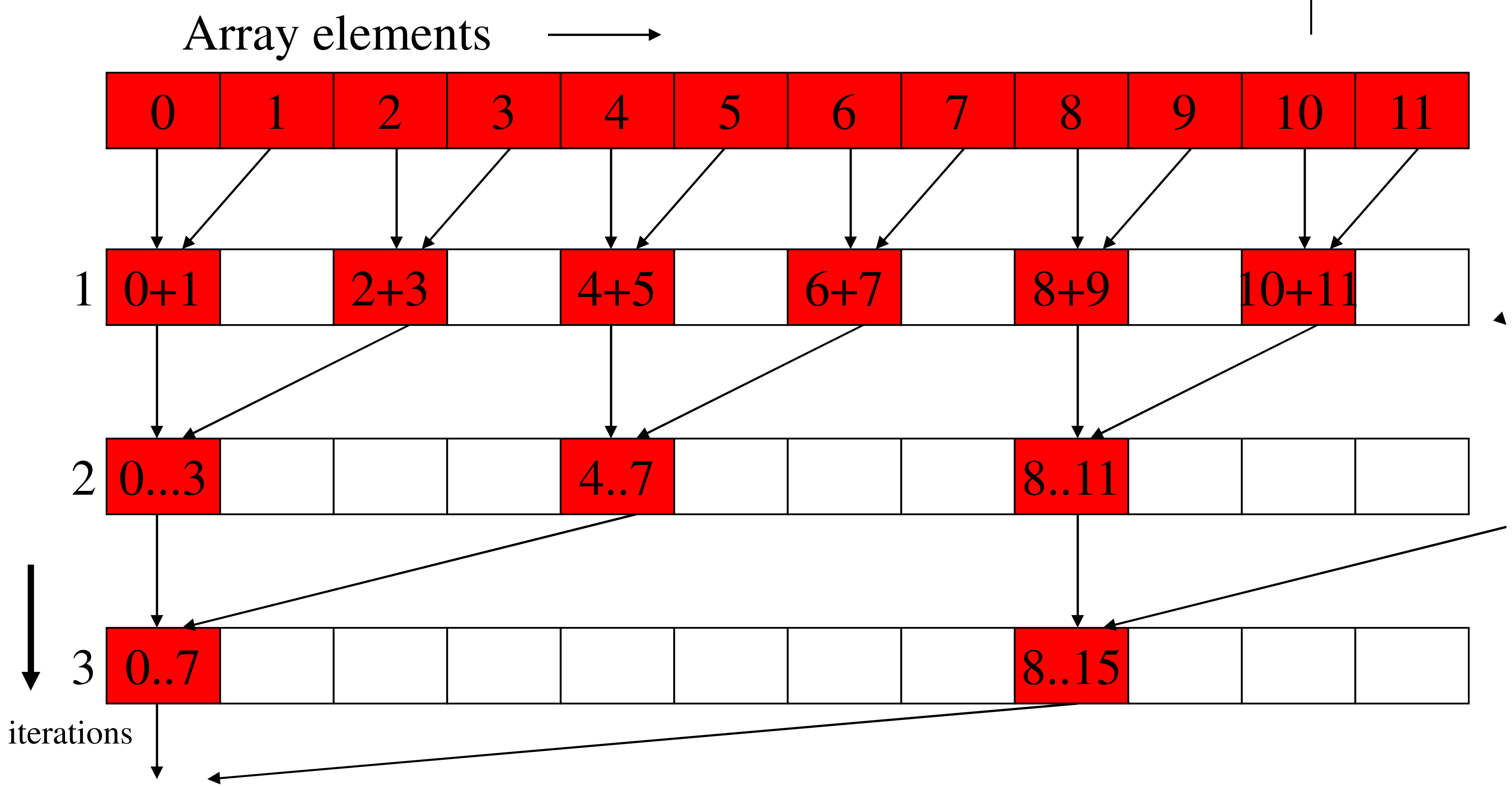
- Problems that seem inherently sequential can be approached in this framework
  - This is typically associated with an net increase in the amount of work you have to do
  - Work goes up from O(n) to O(n log(n)) (see for instance Hillis and Steele algorithm)
  - The key question is whether parallelism gained brings you ahead of the sequential alternative

Example: The Prefix Scan ~ Reduction Step~




```
for k=0 to M-1
        offset = 2^k
        for j=1 to 2^(M-k-1) in parallel do
                x[j·2^(k+1)-1] = x[j·2^(k+1)-1] + x[j·2^(k+1)-2^k-1]
        endfor
endfor
```

Example: The array reduction (the bad choice)



Alg. Struct. 5: Organize by Data Flow
~ Regular: Pipeline ~

- Tasks are parallel, but there is a high degree of synchronization (coordination) between the UEs
  - The input of one UE is the output of an upwind UE (the "pipeline")
  - The time elapsed between two pipeline ticks dictated by the slowest stage of the pipeline (the bottleneck)

- Commonly employed by sequential chips

- For complex problems having a deep pipeline is attractive
  - At each pipeline tick you output one set of results

- Examples:
  - CPU: instruction fetch, decode, data fetch, instruction execution, data write are pipelined.
  - The Cray vector architecture drawing heavily on this algorithmic structure when performing linear algebra operations

Alg. Struct. 6: Organize by Data Flow ~ Irregular: Event Driven Scenarios ~

- The furthest away from what the GPU can support today
- Well supported by MIMD architectures
- You coordinate UEs through asynchronous events
- Critical aspects:
  - Load balancing – should be dynamic
  - Communication overhead, particularly in real-time applications
- Suitable for action-reaction type simulations
- Examples: computer games, traffic control algorithms, server operation (amazon, google)

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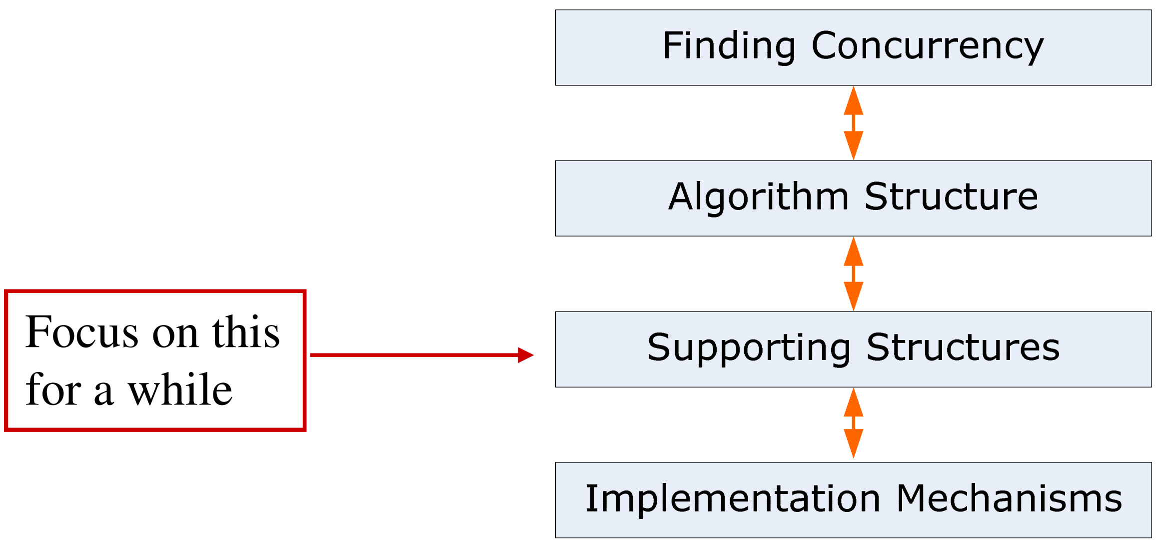
What's Comes Next?



Supporting Structures
~ Data and Program Models~

Data Models

- Shared Data
- Shared Queue
- Distributed Array

Program Models

- SPMD
- Master/Worker
- Loop Parallelism
- Fork/Join

Above are the models for which parallel software/hardware combos provide good support nowadays. If you don't fall in one of the above there'll be no sailing, you'll have to row.

Data Models

- Shared Data
  - All threads share a major data structure
  - This is what CUDA and GPU computing support the best
- Shared Queue
  - All threads see a “thread safe” queue
  - Very relevant in conjunction with the Master/Worker scenarios
  - OpenMP is very helpful here if your problem fits on one machine
    - If not, MPI can help
- Distributed Array
  - Decomposed and distributed among threads
  - Limited support in CUDA Shared Memory but the direction where libraries are going (thrust, for instance)
  - Good library support under MPI (this is how things get done in PETSc)
  - OpenMP: doesn’t apply

Program Models

- Master/Worker
  - A Master thread sets up a pool of worker threads and a bag of tasks
  - Workers execute concurrently, removing tasks until done
  - Common in OpenMP
- Loop Parallelism
  - Loop iterations execute in parallel
  - FORTRAN do-all (truly parallel), do-across (with dependence)
  - Very common in OpenMP
- Fork/Join
  - Most general way of creation of threads (the POSIX standard)
  - Can be regarded as a very low level approach in which you use the OS to manage parallelism

Program Models

- SPMD (Single Program, Multiple Data)
  - All PE's (Processor Elements) execute the same program in parallel
  - Each PE has its own data
  - Each PE uses a unique ID to access its portion of data
  - Different PE can follow different paths through the same code

SPMD is by far the most commonly used pattern for structuring parallel programs.

More on SPMD

- Dominant coding style of scalable parallel computing
  - MPI code is mostly developed in SPMD style
  - Almost exclusively used as the pattern in GPU computing
  - Much OpenMP code is also in SPMD
  - Particularly suitable for algorithms based on data parallelism, geometric decomposition, divide and conquer.

- Main advantage
  - Tasks and their interactions visible in one piece of source code, no need to correlated multiple sources

Typical SPMD Program Phases

- Initialize
  - Establish localized data structure and communication channels
- Obtain a unique identifier
  - Each thread acquires a unique identifier, typically in the range from 0 to N-1, where N is the number of threads.
    - OpenMP, MPI, and CUDA have built-in support for this
- Distribute Data
  - Decompose global data into chunks and localize them, or
  - Sharing/replicating major data structure using thread ID to associate subset of the data to threads
- Run the core computation
  - More details in next slide…
- Finalize
  - Reconcile global data structure, prepare for the next major iteration

Core Computation Phase

- Thread IDs are used to differentiate behavior of threads
  - CUDA: Indx.x, Indx.y, Indx.z (also block ids)
  - MPI: rank of a process
  - OpenMP: get_thread_num() – gets id associated with a specific thread in a parallel region
- Use thread ID in loop index calculations to split loop iterations among threads
- Use conditions based on thread ID to branch to their specific actions

Algorithm Structures [in columns]
vs.
Program Models [in rows]

	Task Parallel.	Divide/Conquer	Geometric Decomp.	Recursive Data	Pipeline	Event-based
SPMD	☺ ☺ ☺ ☺	☺ ☺ ☺	☺ ☺ ☺ ☺	☺ ☺	☺ ☺ ☺	☺ ☺
Loop Parallel	☺ ☺ ☺ ☺	☺ ☺	☺ ☺ ☺			
Master/ Worker	☺ ☺ ☺ ☺	☺ ☺	☺	☺	☺	☺
Fork/ Join	☺ ☺	☺ ☺ ☺ ☺	☺ ☺		☺ ☺ ☺ ☺	☺ ☺ ☺ ☺

Four smilies is the best (Source: Mattson, et al.)

Parallel Programming Support [in columns] vs. Program Models [in rows]

	OpenMP	MPI	CUDA
SPMD	☺ ☺ ☺	☺ ☺ ☺ ☺	☺ ☺ ☺ ☺
Loop Parallel	☺ ☺ ☺ ☺	☺	
Master/ Slave	☺ ☺	☺ ☺ ☺	
Fork/Join	☺ ☺ ☺		

ME964 On One Slide

- Sequential computing hit three walls: power, memory, and ILP walls
- Moore's law scales at least for one more decade
  - Parallel computing poised to pick up where sequential computing left
- Moore's law brought us powerful CPUs and GPUs
  - Use OpenMP and/or CUDA (or OpenCL) to leverage this hardware
- Large problems do not always fit inside one workstation
  - Not enough memory, or if enough memory not enough crunching number power
- Large problem handled well by clusters or massively parallel computers
  - MPI helps you here
- When possible, use parallel libraries (thrust, PETSc, TBB, MKL, etc.)
  - However, writing your own code for your own small problem sometimes pays off nicely