Parallel Thinking

CSCI 4239/5239

Advanced Computer Graphics

Spring 2018

Objective

- To provide you with a framework based on the techniques and best practices used by experienced parallel programmers for
  - Thinking about the problem of parallel programming
  - Discussing your work with others
  - Addressing performance and functionality issues in your parallel program
  - Using or building useful tools and environments
  - understanding case studies and projects

The Goal

- Speedup $S = T_1 / T_n \sim n$
- Efficiency $E = T_1 / nT_n \sim 1$
- Very hard to achieve
  - Instead of solving the problem in *1/n*'th the time, solve a problem *n* times larger in the same amount of time

Fundamentals of Parallel Computing

- Parallel computing requires that
  - The problem can be decomposed into sub-problems that can be safely solved at the same time
  - The programmer structures the code and data to solve these sub-problems concurrently
- The goals of parallel computing are
  - To solve problems in less time, and/or
  - To solve bigger problems, and/or
  - To achieve better solutions

The problems must be large enough to justify parallel computing and to exhibit exploitable concurrency.

A Recommended Reading

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

- We draw quite a bit from the book
- A good overview of challenges, best practices, and common techniques in all aspects of parallel programming

Key Parallel Programming Steps

- **To find the concurrency in the problem**
- To structure the algorithm so that concurrency can be exploited
- To implement the algorithm in a suitable programming environment
- To execute and tune the performance of the code on a parallel system

Unfortunately, these have not been separated into levels of abstractions that can be dealt with independently.

Challenges of Parallel Programming

- Finding and exploiting concurrency often requires looking at the problem from a non-obvious angle
  - Computational thinking (J. Wing)
- Dependences need to be identified and managed
  - The order of task execution may change the answers
    - Obvious: One step feeds result to the next steps
    - Subtle: numeric accuracy may be affected by ordering steps that are logically parallel with each other
- 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

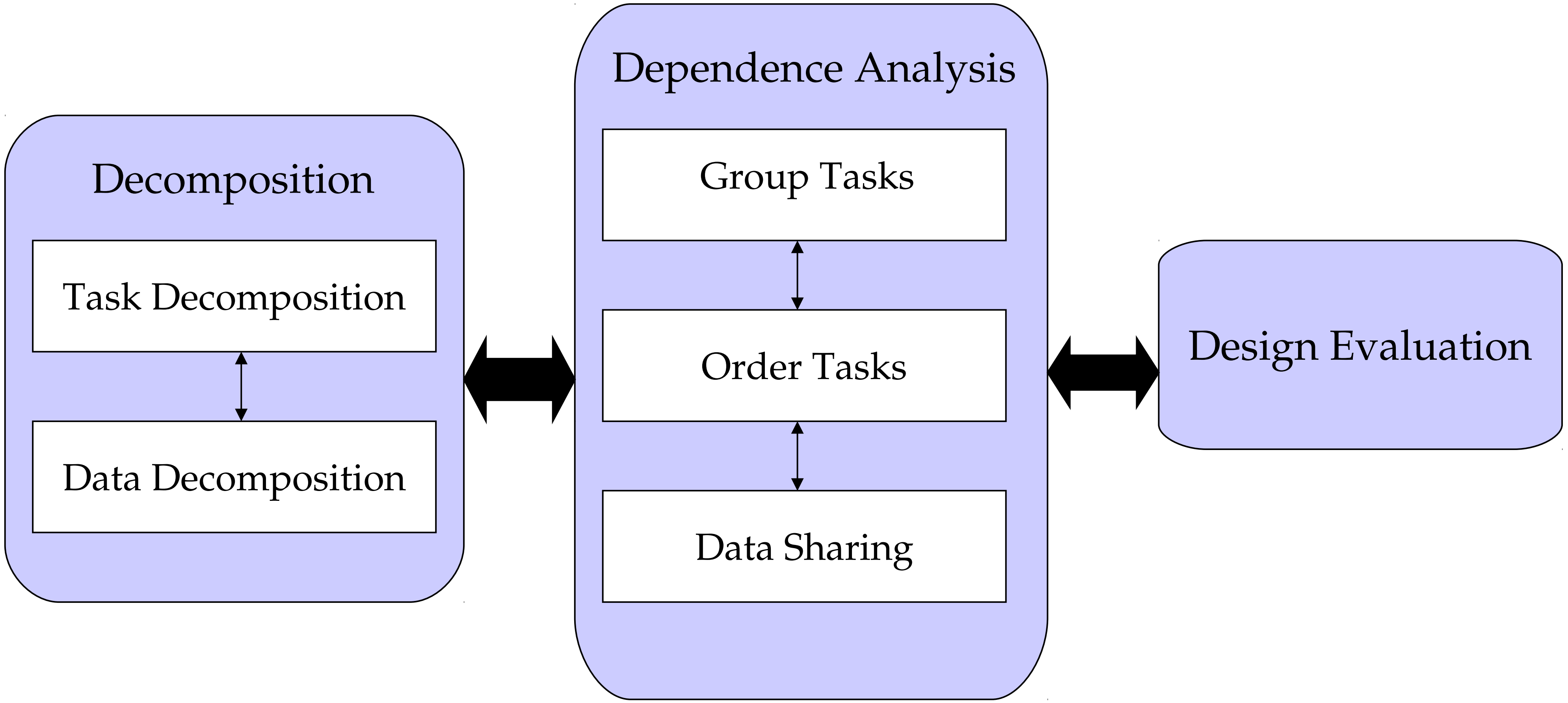
Shared Memory vs. Message Passing

- We will focus on shared memory parallel programming
  - This is what CUDA is based on
  - Future massively parallel microprocessors are expected to support shared memory at the chip level
- The programming considerations of message passing model is quite different!
  - Look at MPI (Message Passing Interface) and its relatives such as Charm++

Finding Concurrency in Problems

- Identify a decomposition of the problem into sub-problems that can be solved simultaneously
  - A task decomposition that identifies tasks for potential concurrent execution
  - A data decomposition that identifies data local to each task
  - A way of grouping tasks and ordering the groups to satisfy temporal constraints
  - An analysis on the data sharing patterns among the concurrent tasks
  - A design evaluation that assesses of the quality the choices made in all the steps

Finding Concurrency – The Process



This is typically a iterative process.
Opportunities exist for dependence analysis to play earlier role in decomposition.

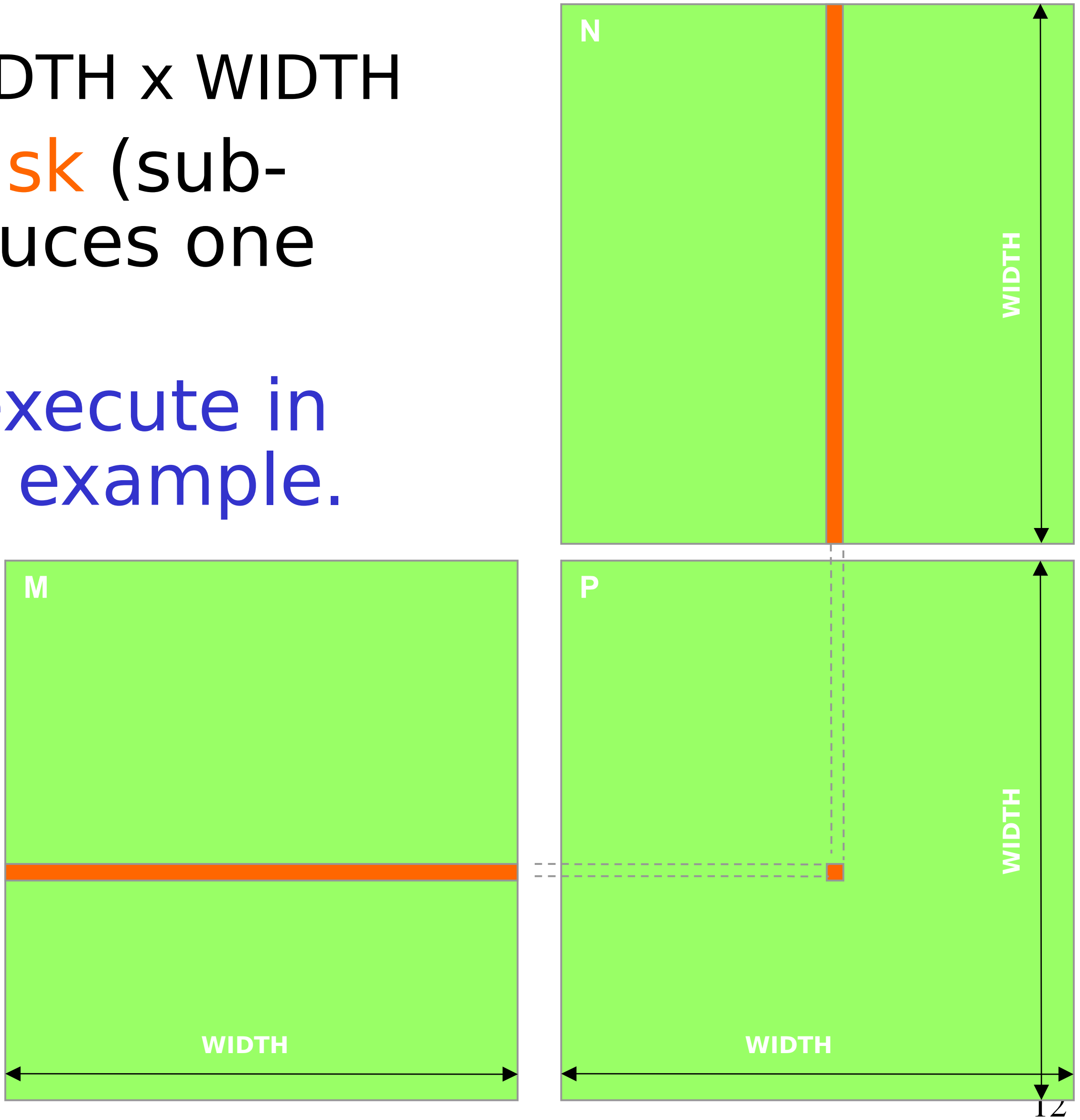
Task Decomposition

- Many large problems can be naturally decomposed into tasks – CUDA kernels are largely 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 effort.

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

Task Decomposition Example - Square Matrix Multiplication

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

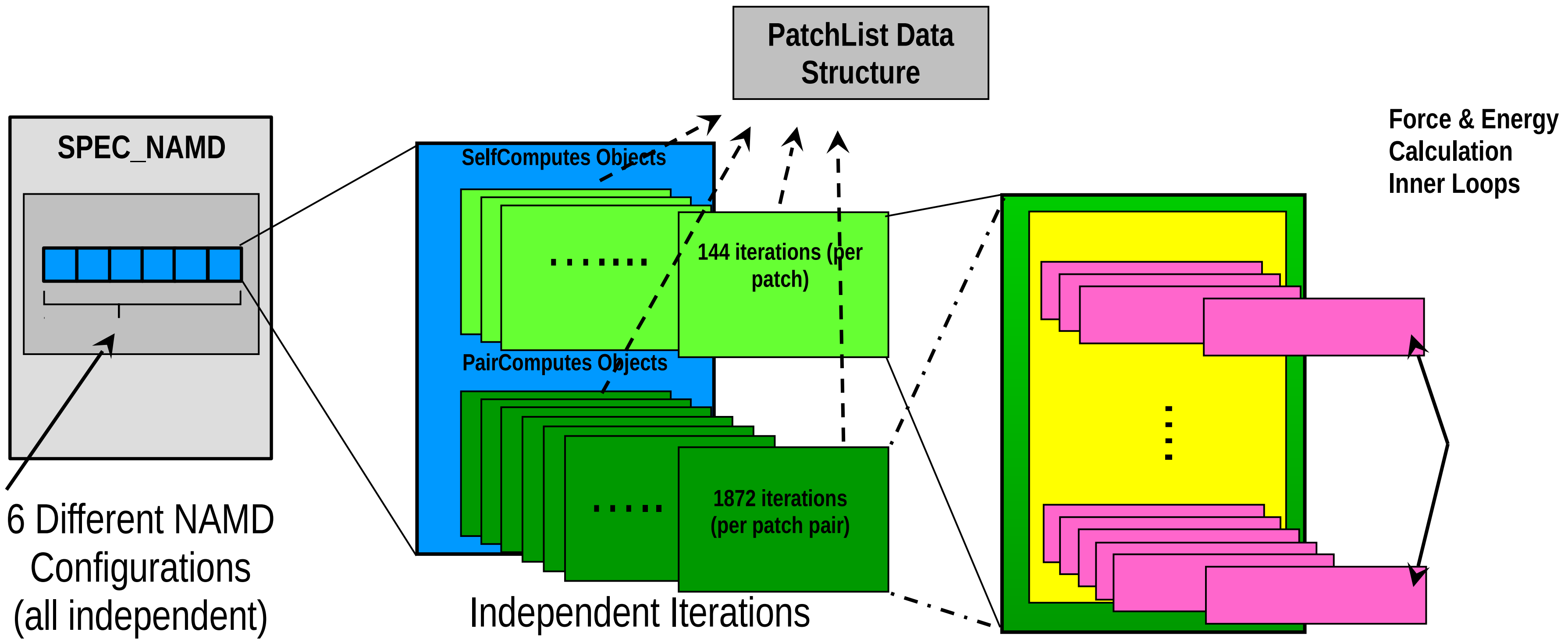


Task Decomposition Example – Molecular Dynamics

- Simulation of motions of a large molecular system
- For each atom, there are natural tasks to calculate
  - Vibrational forces
  - Rotational forces
  - Neighbors that must be considered in non-bonded forces
  - Non-bonded forces
  - Update position and velocity
  - Misc physical properties based on motions
- Some of these can go in parallel for an atom

It is common that there are multiple ways to decompose any given problem.

NAMD

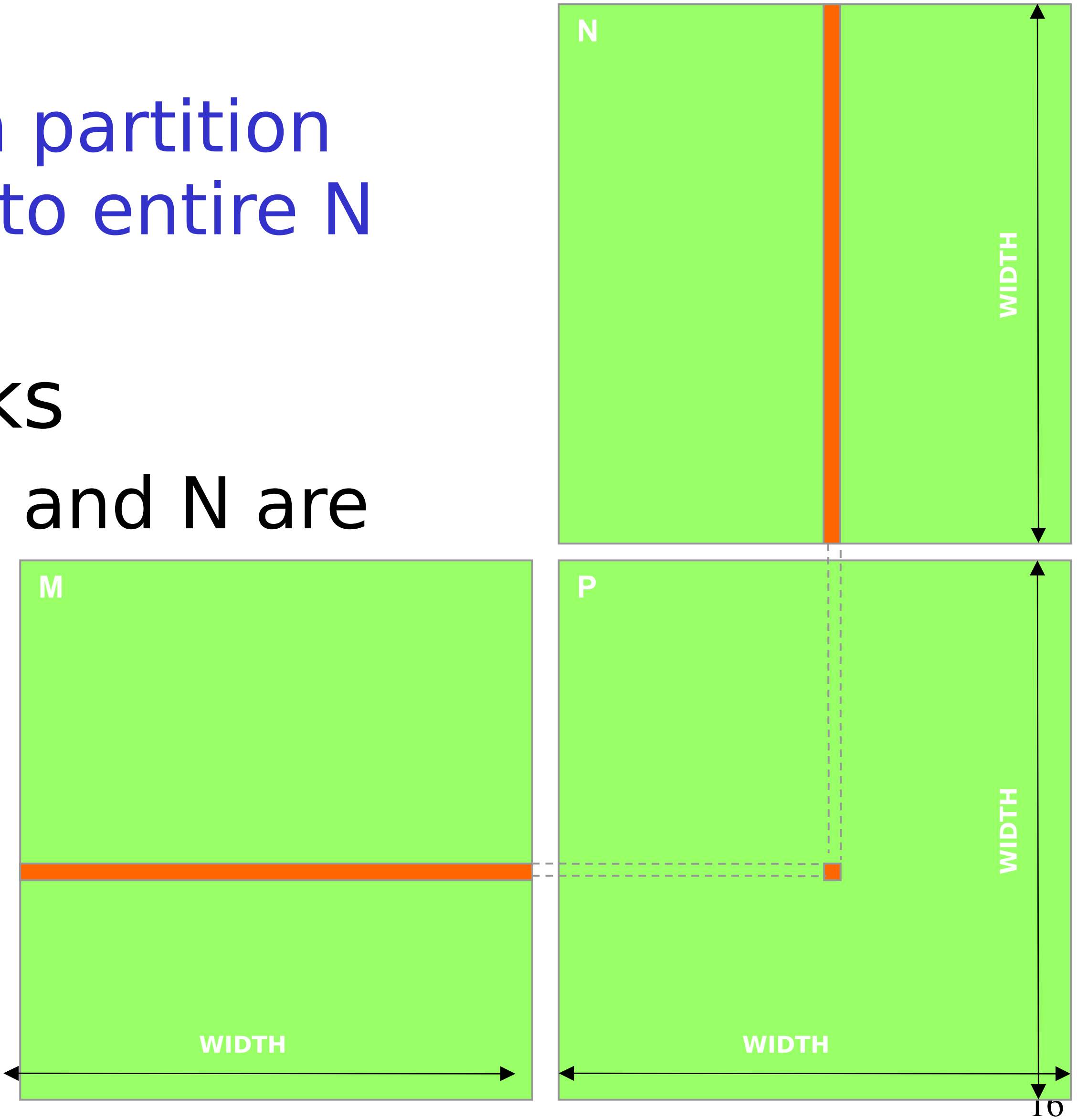

PatchList Data Structure
SPEC_NAMD
Force & Energy Calculation Inner Loops
SelfComputes Objects
144 iterations (per patch)
PairComputes Objects
1872 iterations (per patch pair)
6 Different NAMD Configurations (all independent)
Independent Iterations

Data Decomposition

- The most compute intensive parts of many large problem 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 tasks within the partition
  - Few dependencies across the tasks that work on different partitions
  - Adjustable partitions that can be varied according to the hardware characteristics

Data Decomposition Example - Square Matrix Multiplication

- Row blocks
  - Computing each partition requires access to entire N array
- Square sub-blocks
  - Only bands of M and N are needed

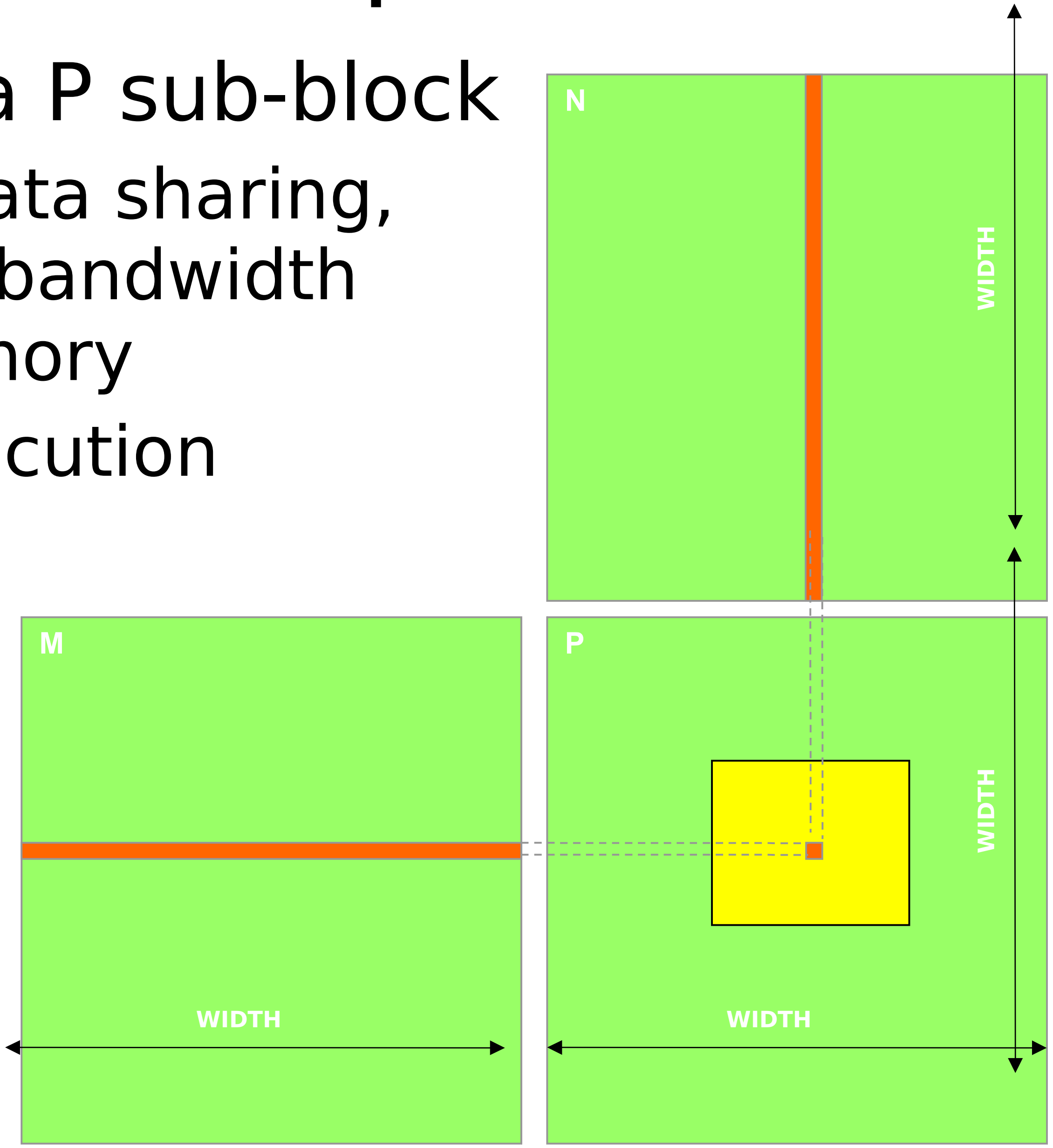


Tasks Grouping

- Sometimes natural tasks of a problem can be grouped together to improve efficiency
  - Reduced synchronization overhead – all tasks in the group can use a barrier to wait for a common dependence
  - All tasks in the group efficiently share data loaded into a common on-chip, shared storage (Shard Memory)
  - Grouping and merging dependent tasks into one task reduces need for synchronization
  - CUDA thread blocks are task grouping examples.

Task Grouping Example - Square Matrix Multiplication

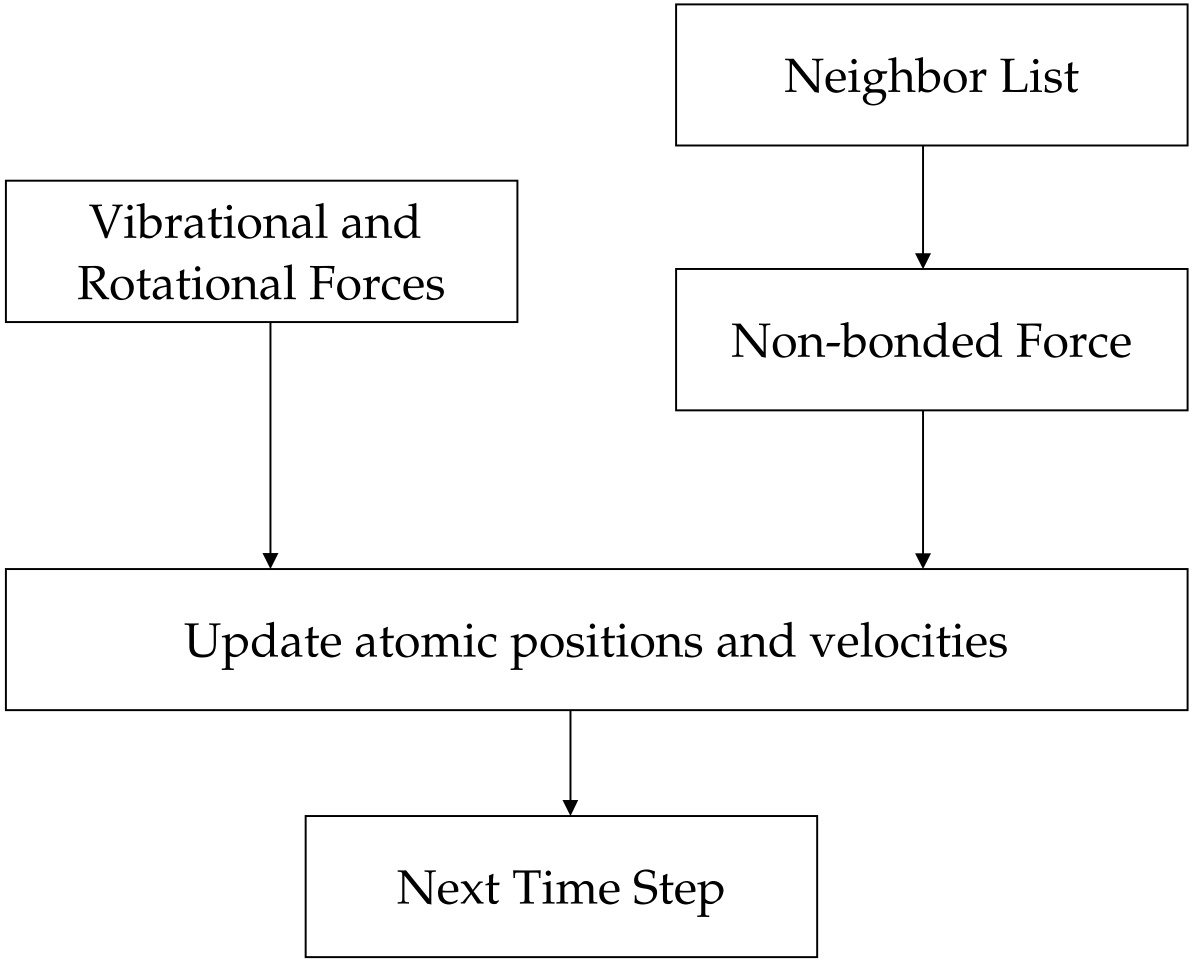
- Tasks calculating a P sub-block
  - Extensive input data sharing, reduced memory bandwidth using Shared Memory
  - All synched in execution



Task Ordering

- Identify the data and resource required by a group of tasks before they can execute them
  - Find the task group that creates it
  - Determine a temporal order that satisfy all data constraints

Task Ordering Example: Molecular Dynamics



Neighbor List
Vibrational and Rotational Forces
Non-bonded Force
Update atomic positions and velocities
Next Time Step

Data Sharing

- Data sharing can be a double-edged sword
  - Excessive data sharing can drastically reduce advantage of parallel execution
  - Localized sharing can improve memory bandwidth efficiency
- Efficient memory bandwidth usage can be achieved by synchronizing the execution of task groups and coordinating their usage of memory data
  - Efficient use of on-chip, shared storage
- Read-only sharing can usually be done at much higher efficiency than read-write sharing, which often requires synchronization

Data Sharing Example – Matrix Multiplication

- 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 more efficiently accessed as Constant or Texture data

Data Sharing Example – Molecular Dynamics

- The atomic coordinates
  - Read-only access by the neighbor list, bonded force, and non-bonded force task groups
  - Read-write access for the position update task group
- The force array
  - Read-only access by position update group
  - Accumulate access by bonded and non-bonded task groups
- The neighbor list
  - Read-only access by non-bonded force task groups
  - Generated by the neighbor list task group

Key Parallel Programming Steps

- To find the concurrency in the problem
- **To structure the algorithm to translate concurrency into performance**
- To implement the algorithm in a suitable programming environment
- To execute and tune the performance of the code on a parallel system

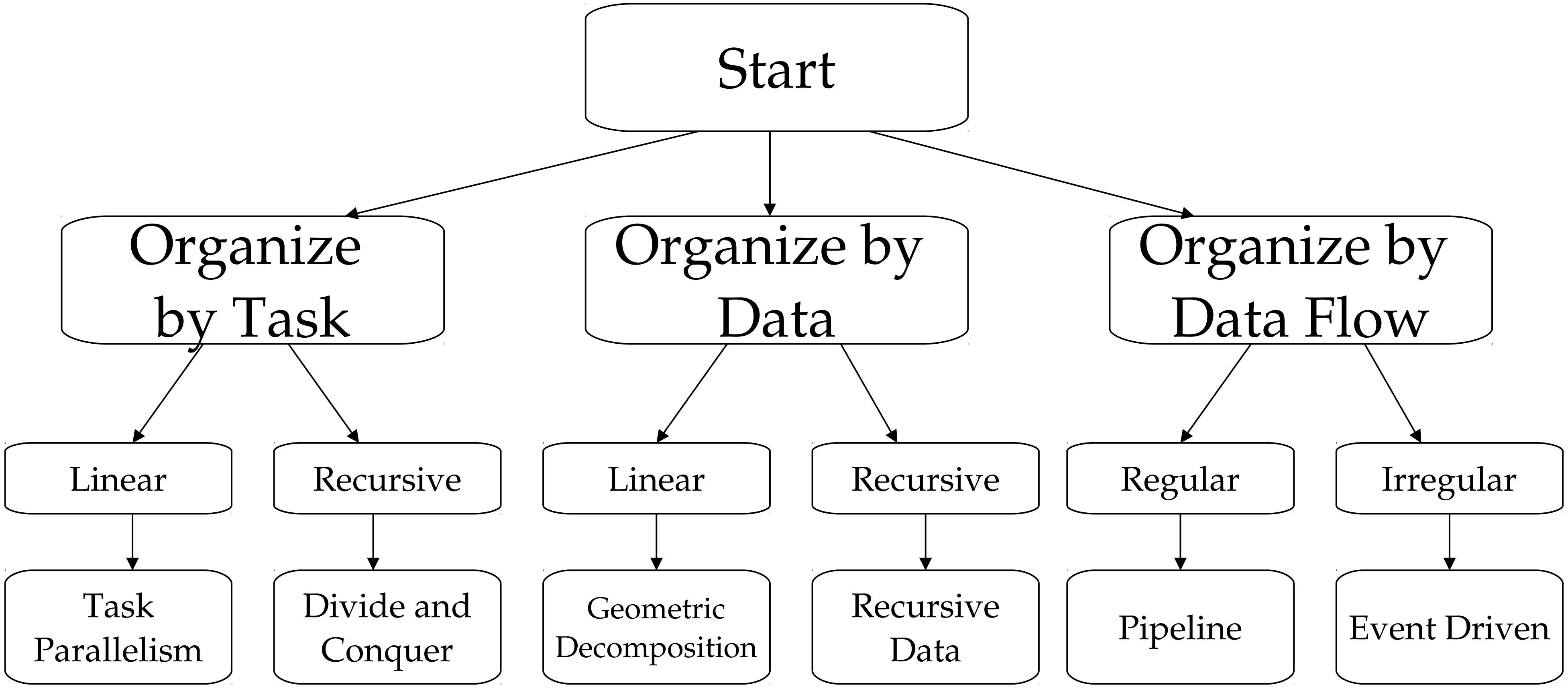
Unfortunately, these have not been separated into levels of abstractions that can be dealt with independently.

Algorithm

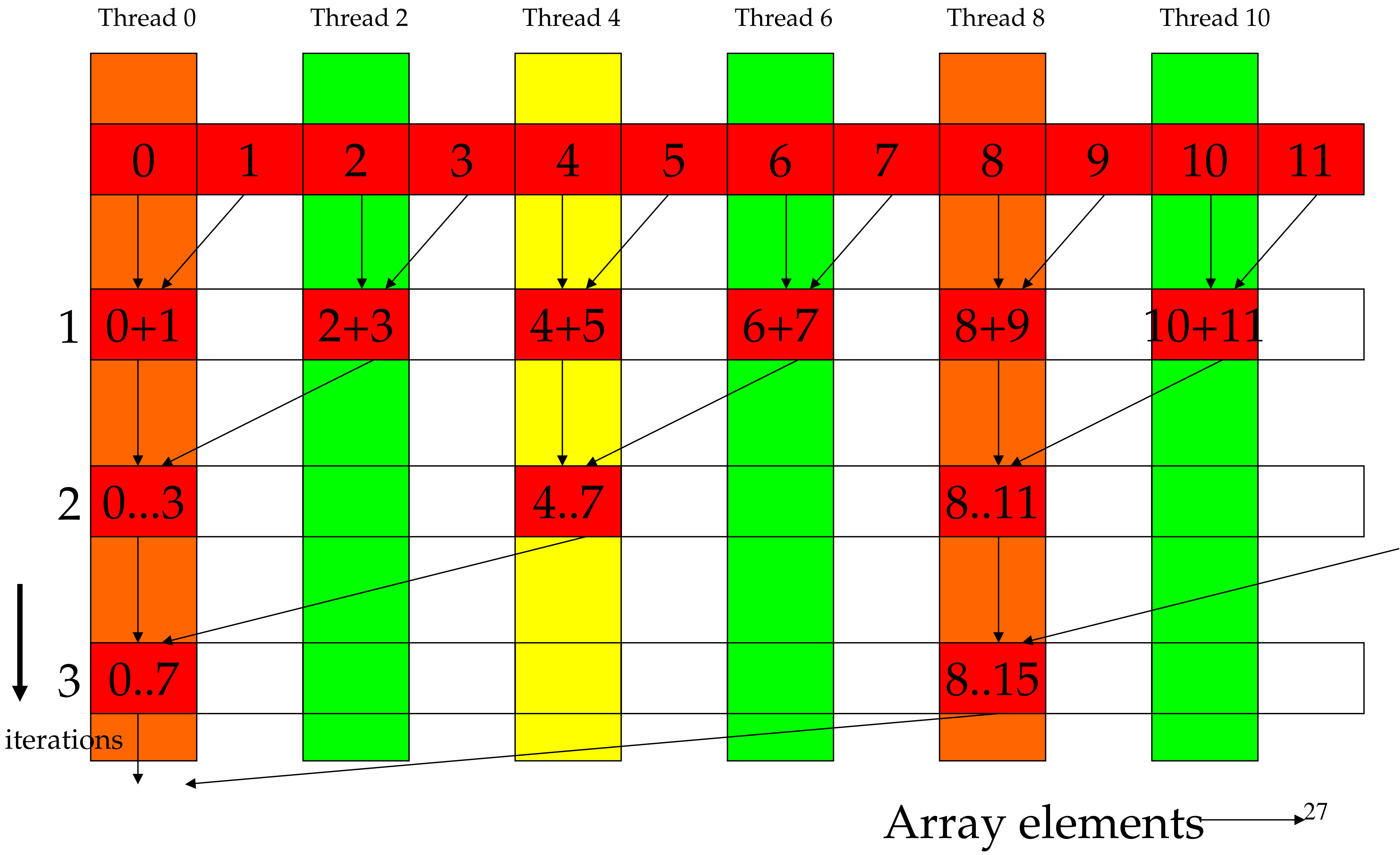
- A step by step procedure that is guaranteed to terminate, such that each step is precisely stated and can be carried out by a computer
  - Definiteness – the notion that each step is precisely stated
  - Effective computability – each step can be carried out by a computer
  - Finiteness – the procedure terminates

- Multiple algorithms can be used to solve the same problem
  - Some require fewer steps
  - Some exhibit more parallelism
  - Some have larger memory footprint than others

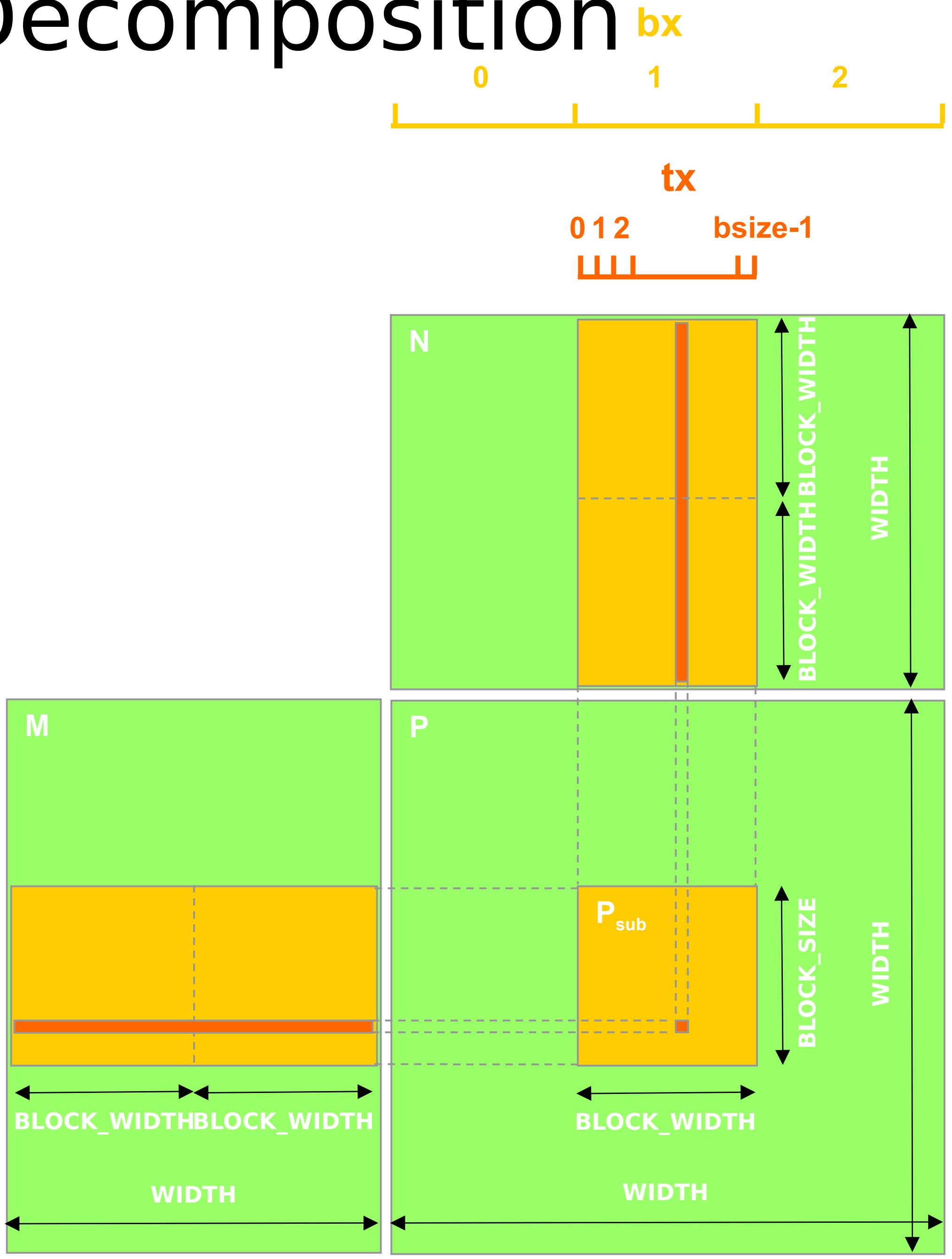
Choosing Algorithm Structure



Mapping a Divide and Conquer Algorithm



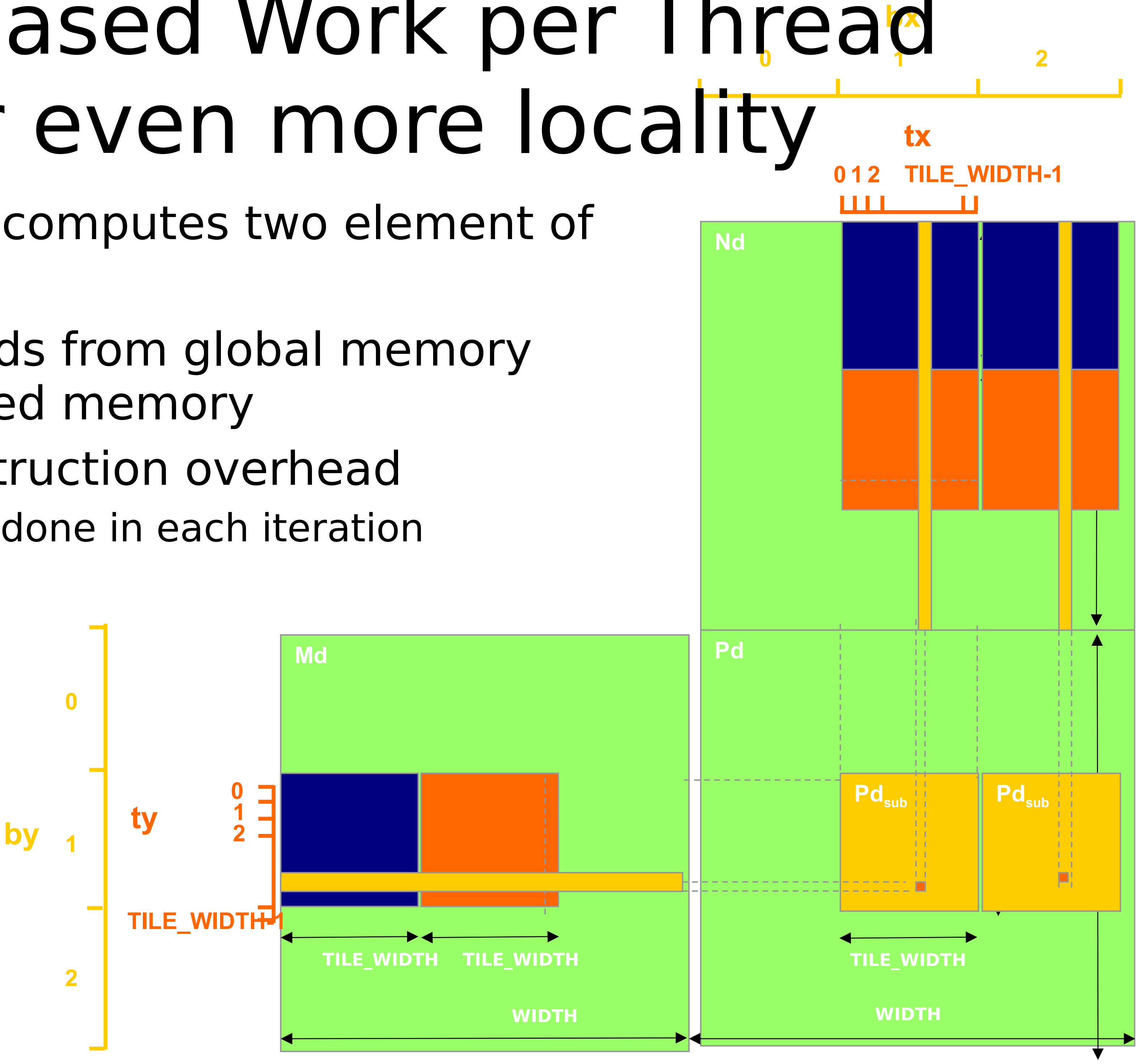
Tiled (Stenciled) Algorithms are Important for Geometric Decomposition



- A framework for memory data sharing and reuse by increasing data access locality.
  - Tiled access patterns allow small cache/scartchpad memories to hold on to data for re-use.
  - For matrix multiplication, a 16X16 thread block perform 2*256 = 512 float loads from device memory for 256 * (2*16) = 8,192 mul/add operations.
- A convenient framework for organizing threads (tasks)

Increased Work per Thread for even more locality

- Each thread computes two element of Pd$_{sub}$
- Reduced loads from global memory (Md) to shared memory
- Reduced instruction overhead
  - More work done in each iteration



Double Buffering - a frequently used algorithm pattern

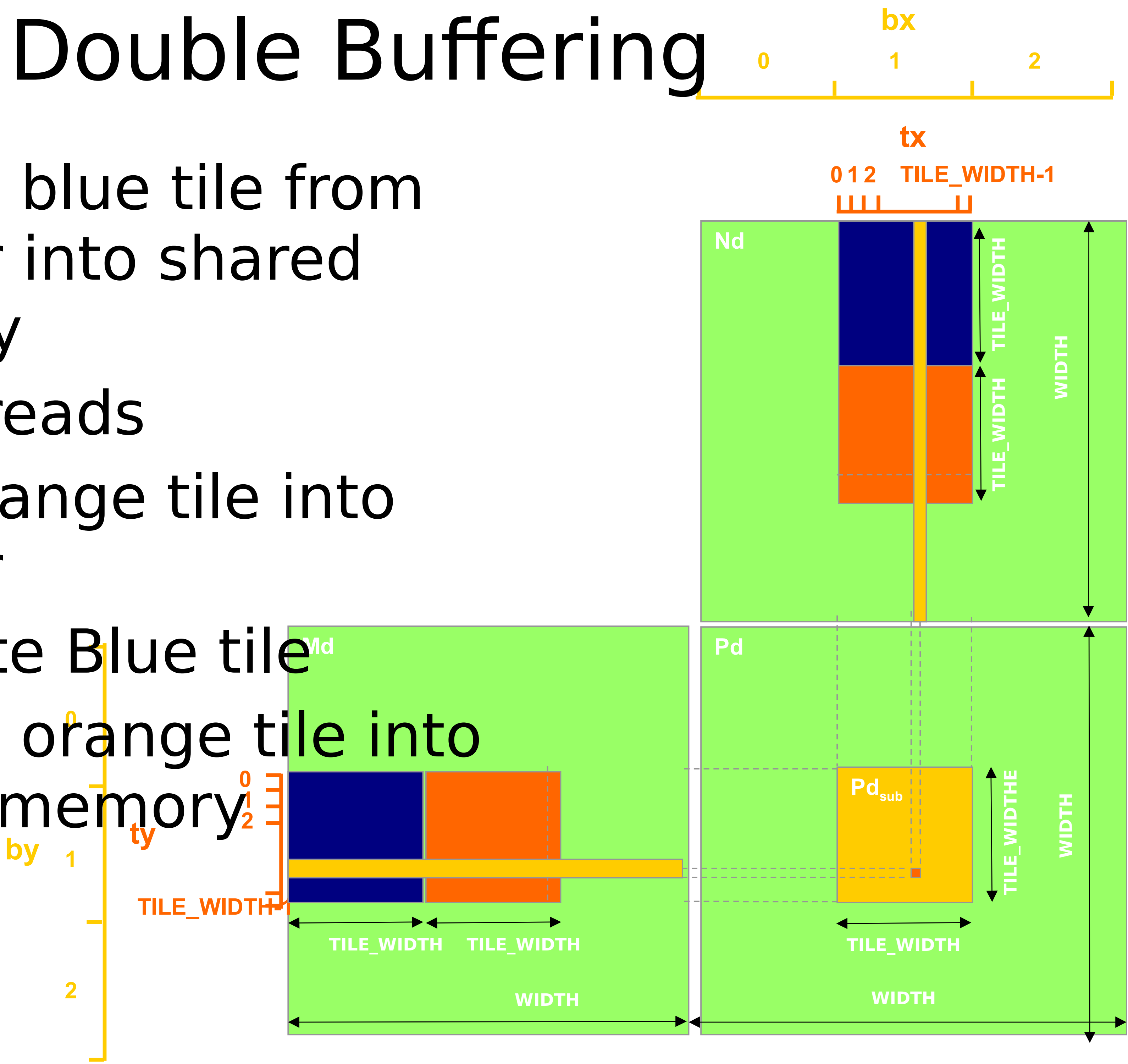
- One could double buffer the computation, getting better instruction mix within each thread
  - This is classic software pipelining in ILP compilers

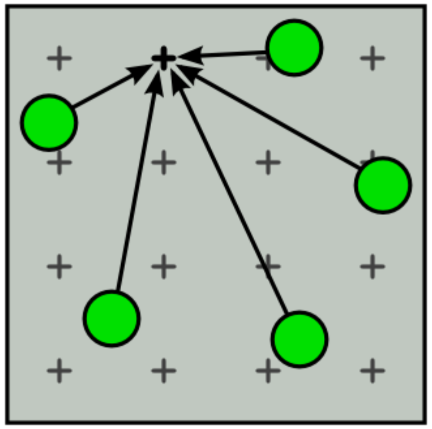
```
Loop {

  Load current tile to shared memory

  syncthreads()

  Compute current tile

  syncthreads()
}
```

```
Load next tile from global memory

Loop {
  Deposit current tile to shared memory

  syncthreads()

  Load next tile from global memory

  Compute current tile

  syncthreads()
}
```

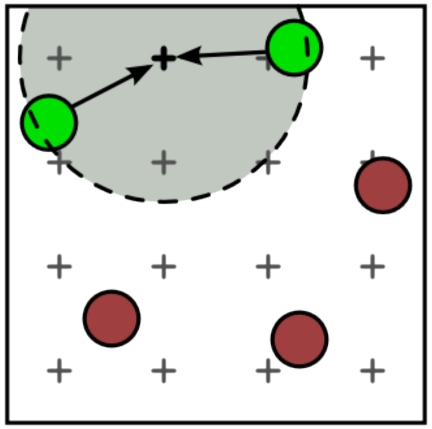
Double Buffering

- Deposit blue tile from register into shared memory
- Syncthreads
- Load orange tile into register
- Compute Blue tile
- Deposit orange tile into shared memory
- ….

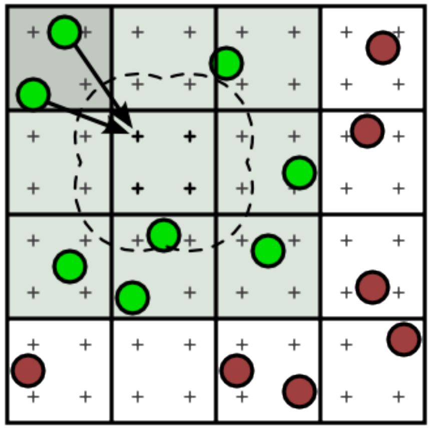




(a) Direct summation
At each grid point, sum the electrostatic potential from all charges



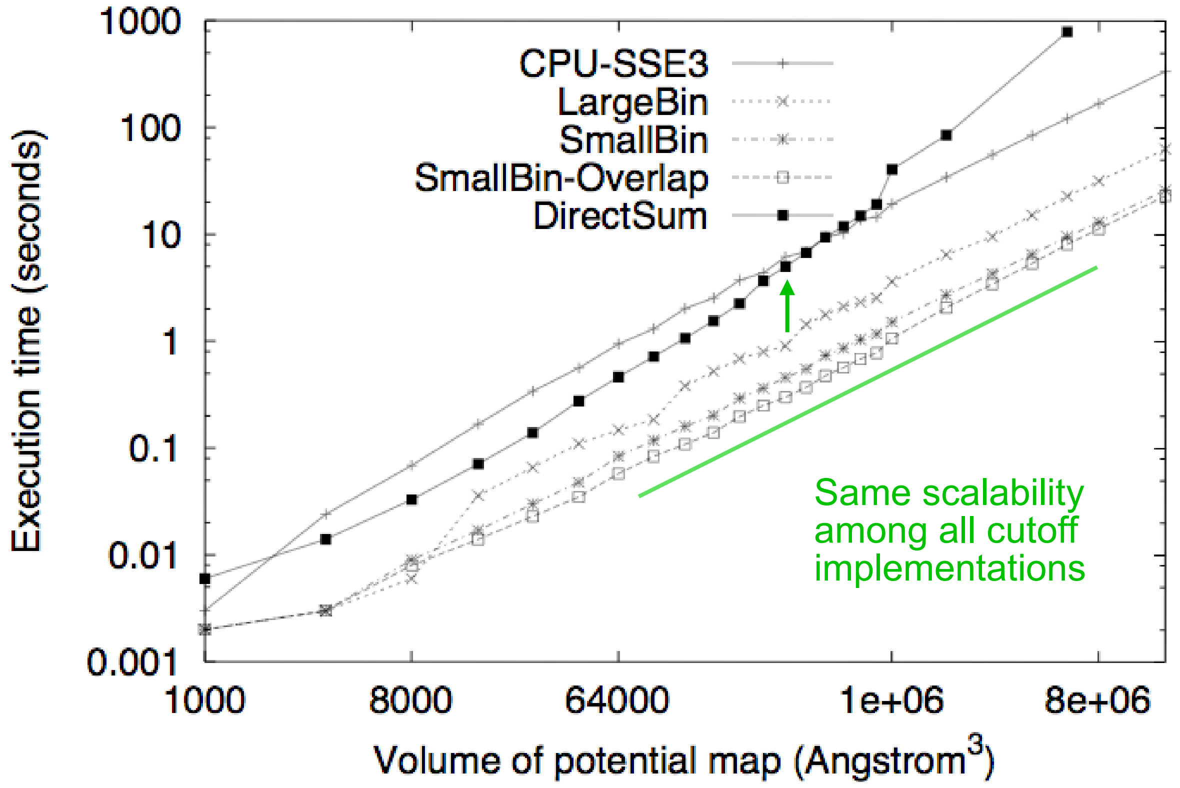
(b) Cutoff summation
Electrostatic potential from nearby charges summed; spatially sort charges first



(c) Cutoff summation using direct summation kernel
Spatially sort charges into bins; adapt direct summation to process a bin

Figure 10.2 Cutoff Summation algorithm

Cut-Off Summation Restores Data Scalability



Scalability and Performance of different algorithms for calculating electrostatic potential map.