High Performance Computing

4. Design Patterns for Parallel Programming

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Credits:
Roberto Cavicchioli, Università di Modena e Reggio Emilia
Luca Benini, Università di Bologna, 2018
Marwedel, Embedded System Design, Springer 2018,
Wolf, Computers as Components 4th Ed. Morgan Kaufmann 2016
Wolf, High-Performance Embedded Computing 2nd Ed. Morgan Kaufmann 2014
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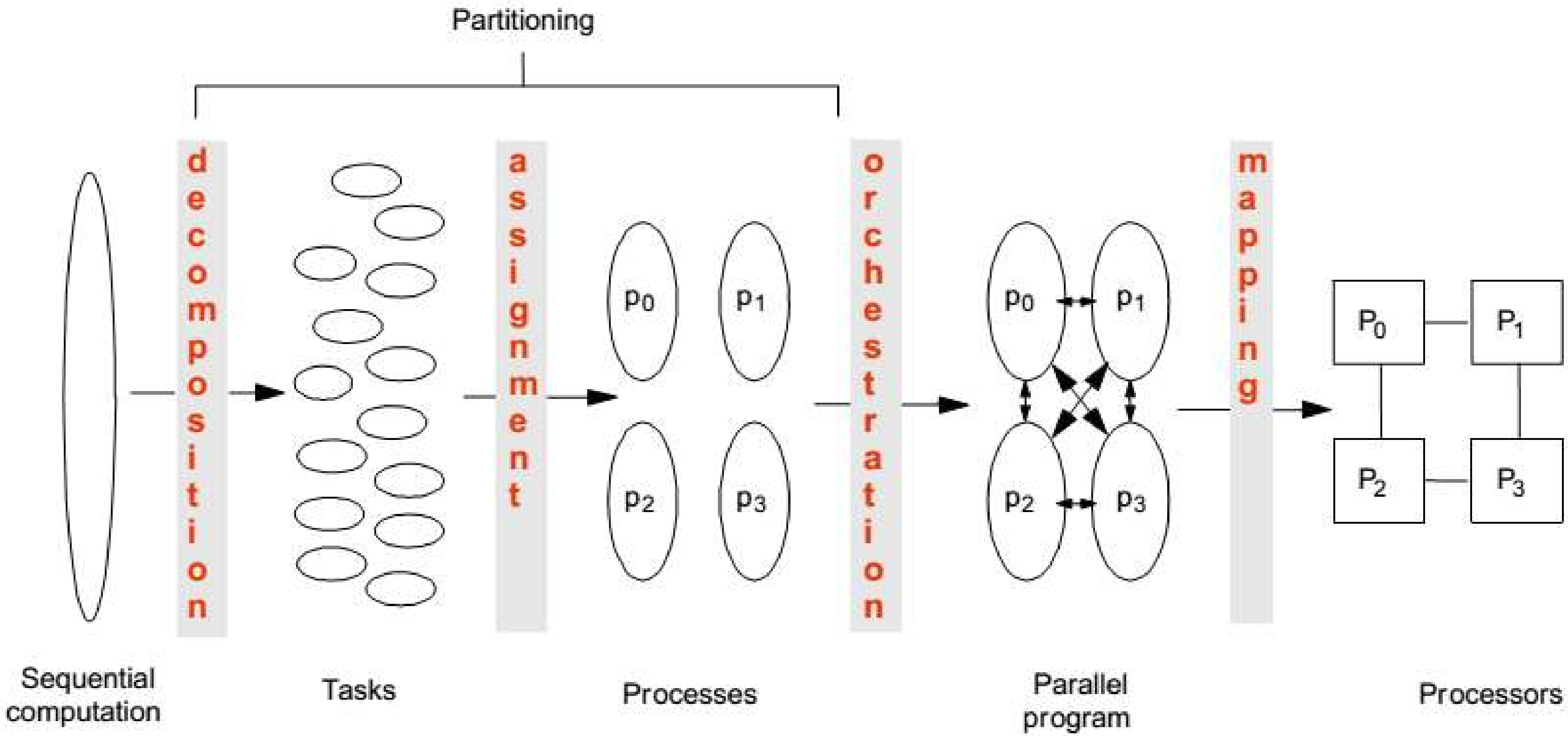
Understanding performance

What factors affect performance of parallel programs?

- **Coverage** or extent of parallelism in algorithm
- **Granularity** of partitioning among processors
- **Locality** of computation and communication

Remember from previous class

Common steps to creating a parallel program



Decomposition (Amdahl’s Law)

- Identify concurrency and decide at what level to exploit it
- Break up computation into tasks to be divided among processes
  - Tasks may become available dynamically
  - Number of tasks may vary with time
- Enough tasks to keep processors busy
  - Number of tasks available at a time is upper bound on achievable speedup

Assignment (Granularity)

- Specify mechanism to divide work among core
  - Balance work and reduce communication
- Structured approaches usually work well
  - Code inspection or understanding of application
  - Well-known design patterns
- As programmers, we worry about partitioning first
  - Independent of architecture or programming model
  - But complexity often affect decisions!

Orchestration and Mapping (Locality)

- Computation and communication concurrency
- Preserve locality of data
- Schedule tasks to satisfy dependences early

Parallel Programming with Patterns

- Provides a cookbook to systematically guide programmers
  - Decompose, Assign, Orchestrate, Map
  - Can lead to high quality solutions in some domains
- Provide common vocabulary to the programming community
  - Each pattern has a name, providing a vocabulary for discussing solutions
- Helps with software reusability, malleability, and modularity
  - Written in prescribed format to allow the reader to quickly understand the solution and its context
- Otherwise, too difficult for programmers, and software will not fully exploit parallel hardware

Patterns for Parallelizing Programs

4 Design Spaces

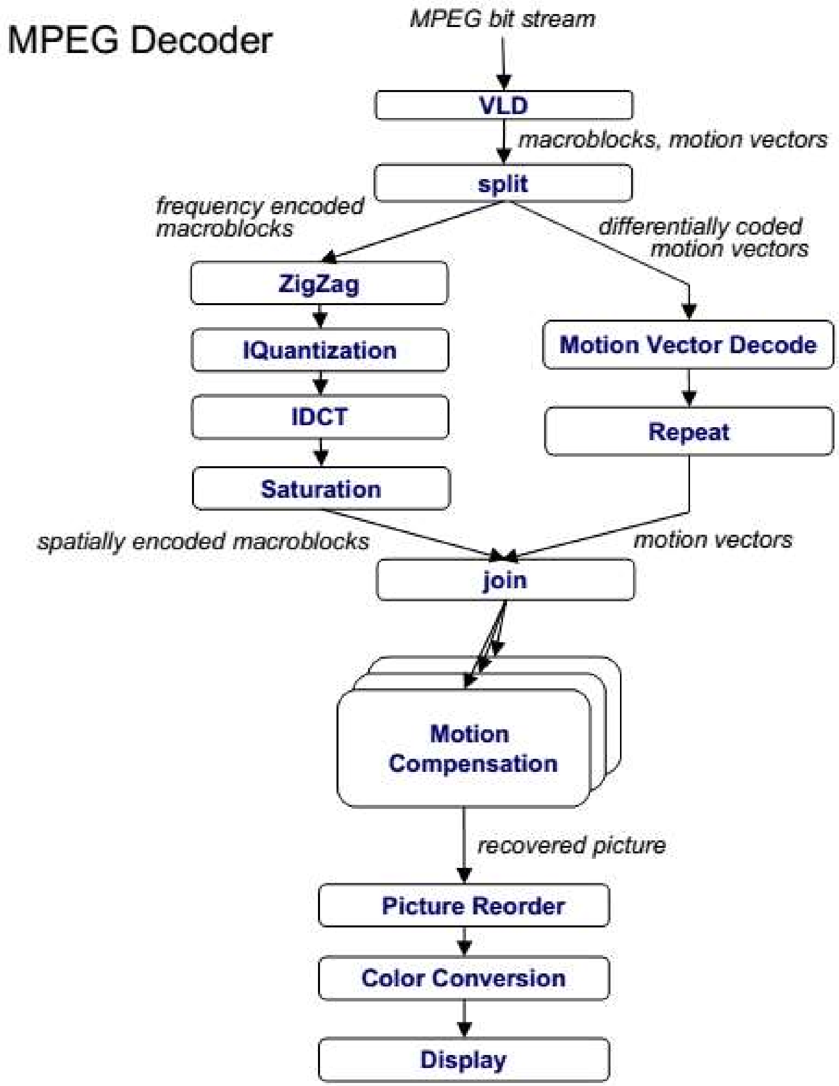
Algorithm Expression

- Finding Concurrency
  - Expose concurrent tasks
- Algorithm structure
  - Map tasks to processes to exploit parallel architecture

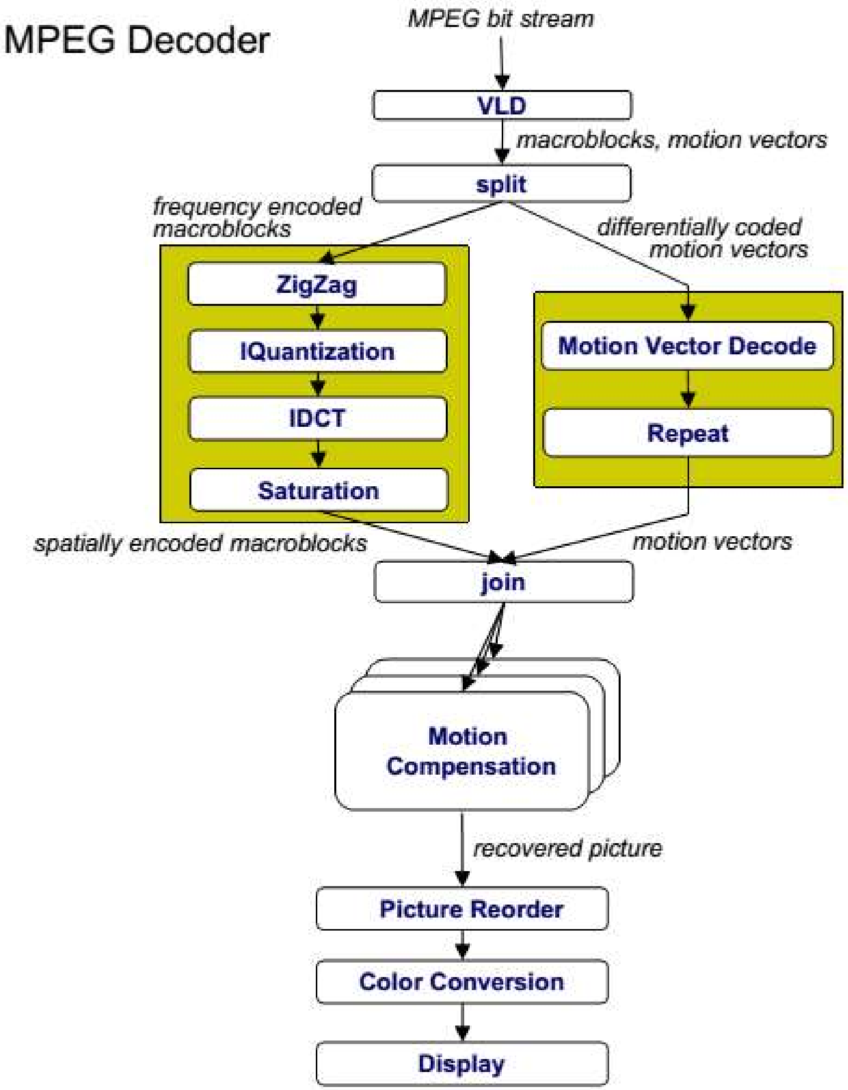
Software Construction

- Supporting Structures
  - Code and data structuring patterns
- Implementation Mechanisms
  - Low level mechanisms used to write parallel programs

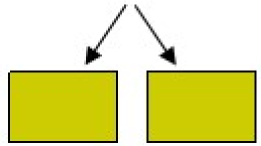
Where is the parallelism?



Where is the parallelism?

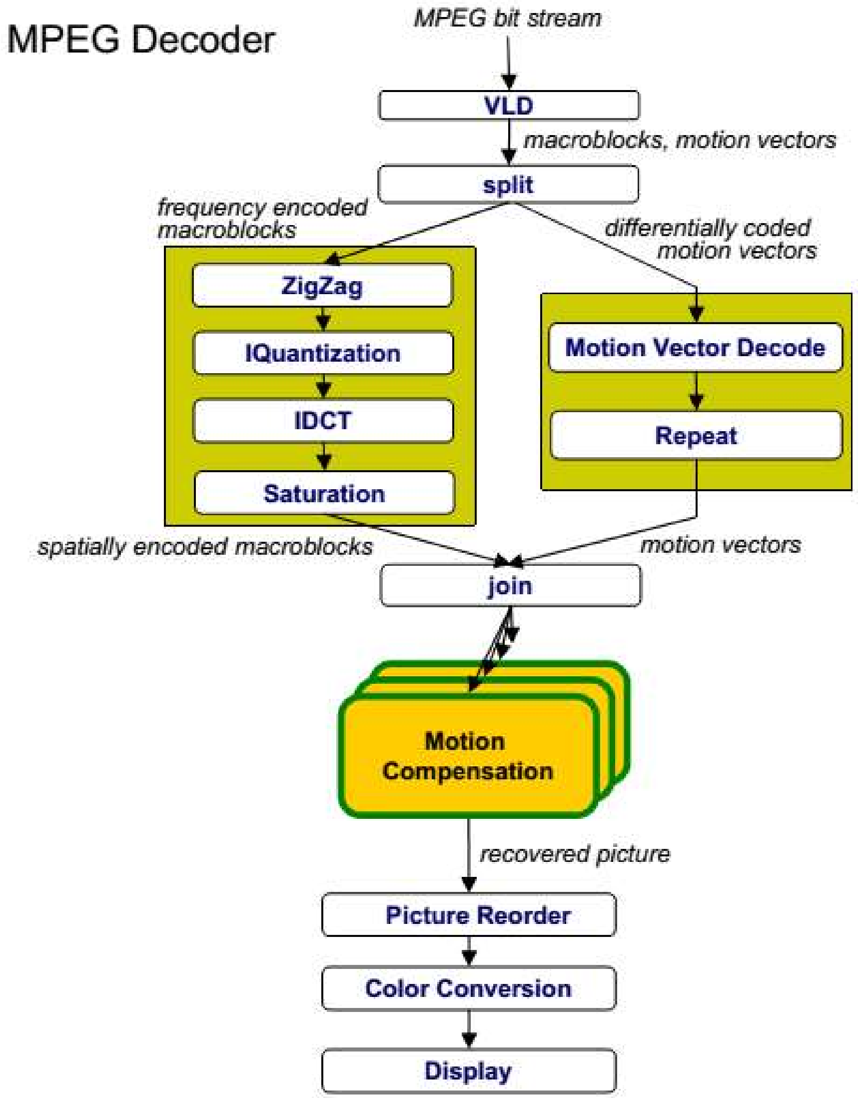


- Task decomposition

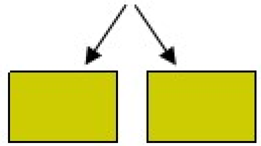


  - Independent coarse-grained computation
  - Inherent to algorithm
- Sequence of statements (instructions) that operate together as a group
  - Corresponds to some logical part of program
  - Usually follows from the way programmer thinks about a problem

Where is the parallelism?

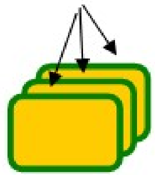


- Task decomposition



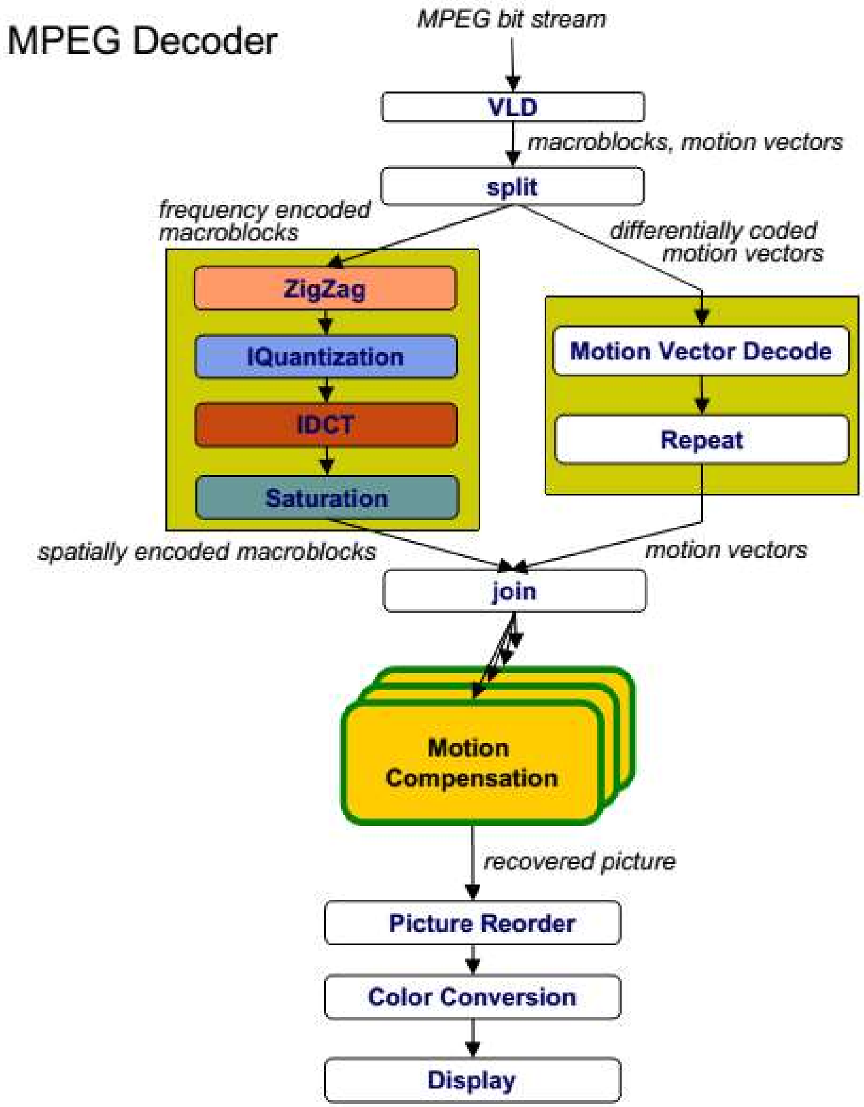
  - Parallelism in the application

- Data decomposition

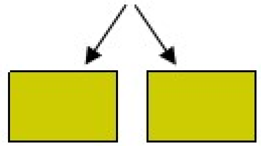


  - Same computation is applied to small data chunks derived from large data set

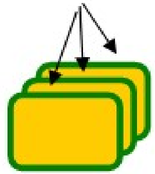
Where is the parallelism?



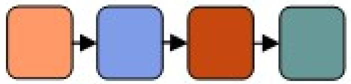
- Task decomposition



  - Parallelism in the application
- Data decomposition



  - Same computation is applied to small data chunks derived from large data set
- Pipeline decomposition
  - Data assembly lines
  - Producer-consumer chains



Guidelines for Task Decomposition

- Algorithms start with a good understanding of the problem being solved
- Programs often naturally decompose into tasks
  - Two common decompositions are
    - Function calls and
    - Distinct loop iterations
- Easier to start with many tasks and later fuse them, rather than too few tasks and later try to split them

Guidelines for Task Decomposition

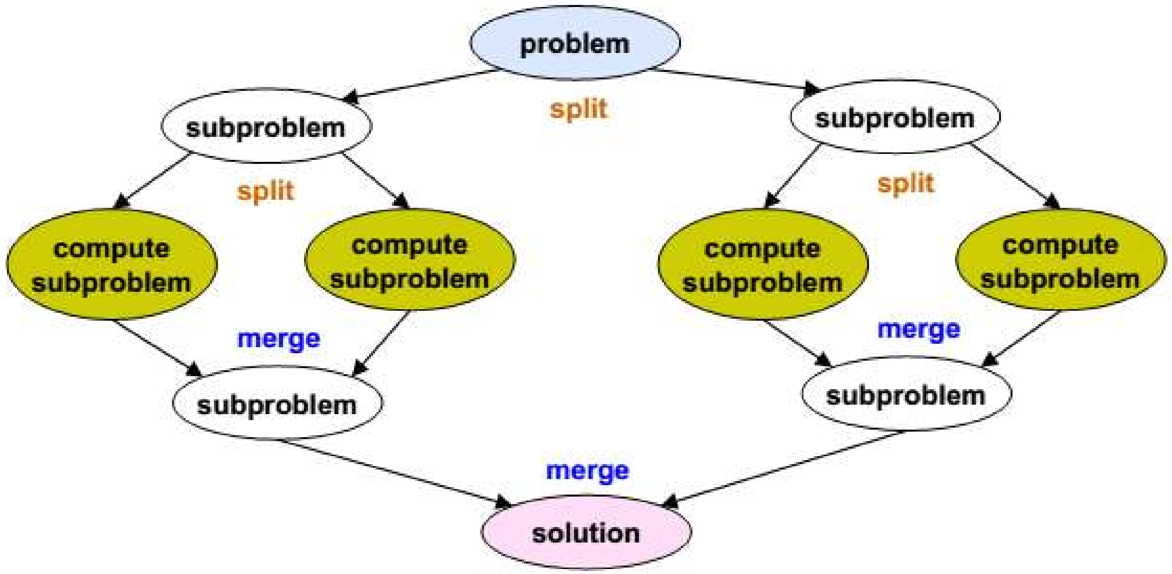
- Flexibility
  - Program design should afford flexibility in the number and size of tasks generated
    - Tasks should not tied to a specific architecture
    - Fixed tasks vs. Parameterized tasks
- Efficiency
  - Tasks should have enough work to amortize the cost of creating and managing them
  - Tasks should be sufficiently independent so that managing dependencies doesn’t become the bottleneck
- Simplicity
  - The code has to remain readable and easy to understand, and debug

Guidelines for Data Decomposition

- Data decomposition is often implied by task decomposition
- Programmers need to address task and data decomposition to create a parallel program
  - Which decomposition to start with?
- Data decomposition is a good starting point when
  - Main computation is organized around manipulation of a large data structure
  - Similar operations are applied to different parts of the data structure

Common Data Decompositions

- Array data structures
  - Decomposition of arrays along rows, columns, blocks
- Recursive data structures
  - Example: decomposition of trees into sub-trees



Guidelines for Data Decomposition

- Flexibility
  - Size and number of data chunks should support a wide range of executions
- Efficiency
  - Data chunks should generate comparable amounts of work (for load balancing)
- Simplicity
  - Complex data compositions can get difficult to manage and debug

Case for Pipeline Decomposition

- Data is flowing through a sequence of stages
  - Assembly line is a good analogy
- What's a prime example of pipeline decomposition in computer architecture?
  - Instruction pipeline in modern CPUs
- What's an example pipeline you may use in your UNIX shell?
  - Pipes in UNIX: `cat foobar.c | grep bar | wc`
- Other examples
  - Signal processing
  - Graphics

Re-engineering for parallelism

Reengineering for Parallelism

- Parallel programs often start as sequential programs
  - Easier to write and debug
  - Legacy codes
- How to reengineer a sequential program for parallelism:
  - Survey the landscape
  - Pattern provides a list of questions to help assess existing code
  - Many are the same as in any reengineering project
  - Is program numerically well-behaved?
- Define the scope and get users acceptance
  - Required precision of results
  - Input range
  - Performance expectations
  - Feasibility (back of envelope calculations)

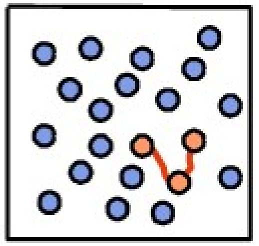
Reengineering for Parallelism

- Define a testing protocol
- Identify program hot spots: where is most of the time spent?
    - Look at code
    - Use **profiling** tools

- Parallelization
    - Start with **hot spots** first
    - Make sequences of small changes, each followed by **testing**
    - Pattern provides guidance

Example: Molecular dynamics

- Simulate motion in large molecular system
  - Used for example to understand drug-protein interactions
- Forces
  - Bonded forces within a molecule
  - Long-range forces between atoms



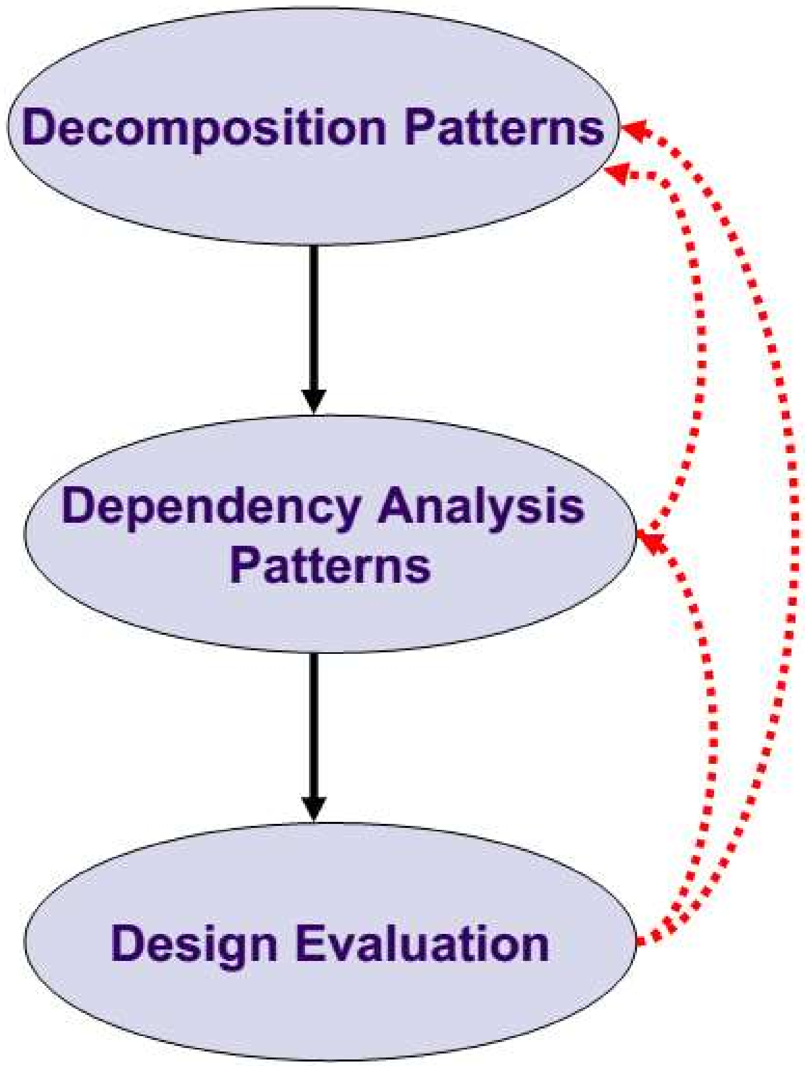
- Naïve algorithm has n^2 interactions: not feasible
- Use cutoff method: only consider forces from neighbors that are "close enough"

Sequential Molecular Dynamics Simulator

```
// pseudo code
real[3,n] atoms
real[3,n] force
int [2,m] neighbors

function simulate(steps)
  for time = 1 to steps and for each atom
      Compute bonded forces
      Compute neighbors
      Compute long-range forces
      Update position
  end loop
end function
```

Finding Concurrency Design Space

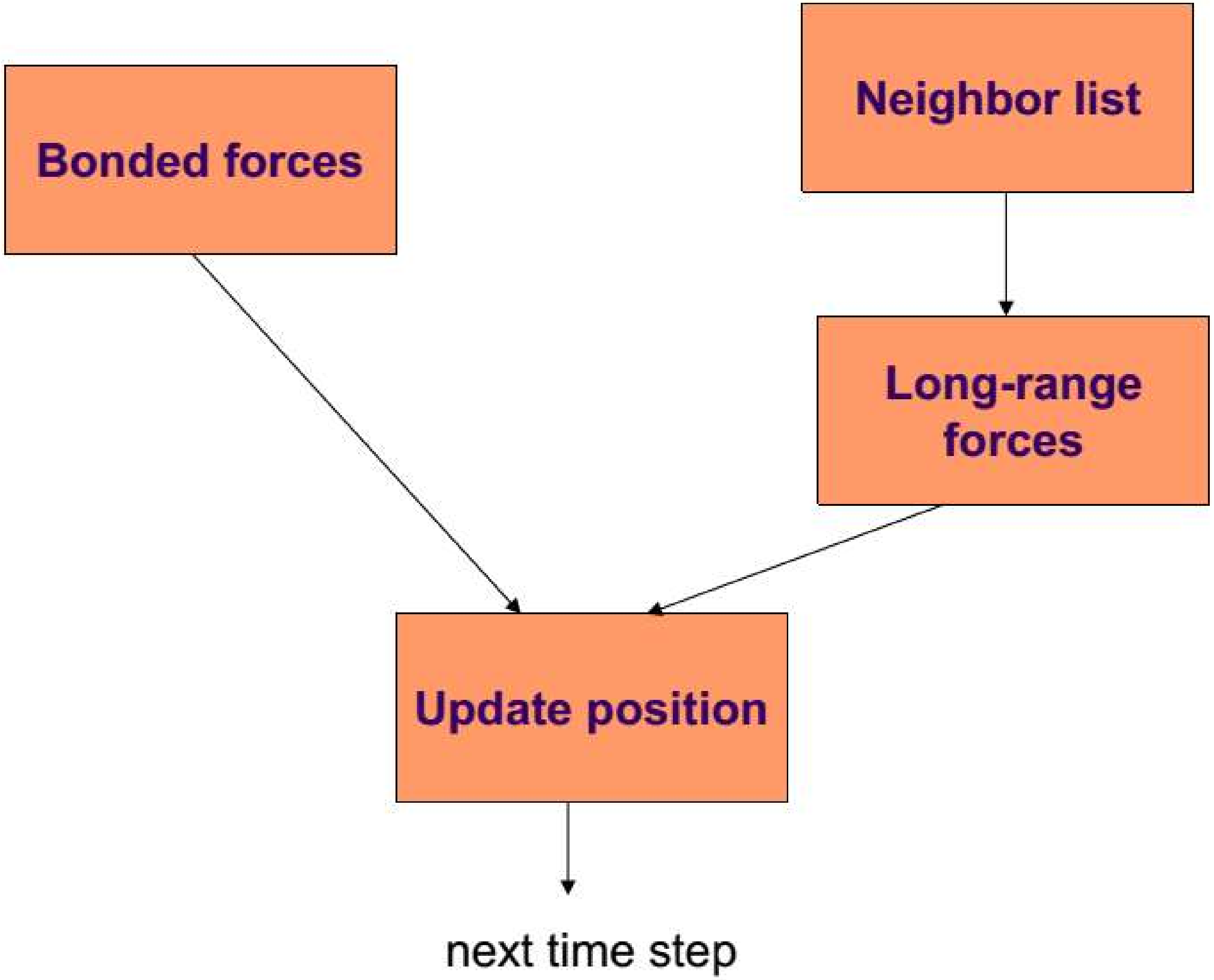


Decomposition Patterns

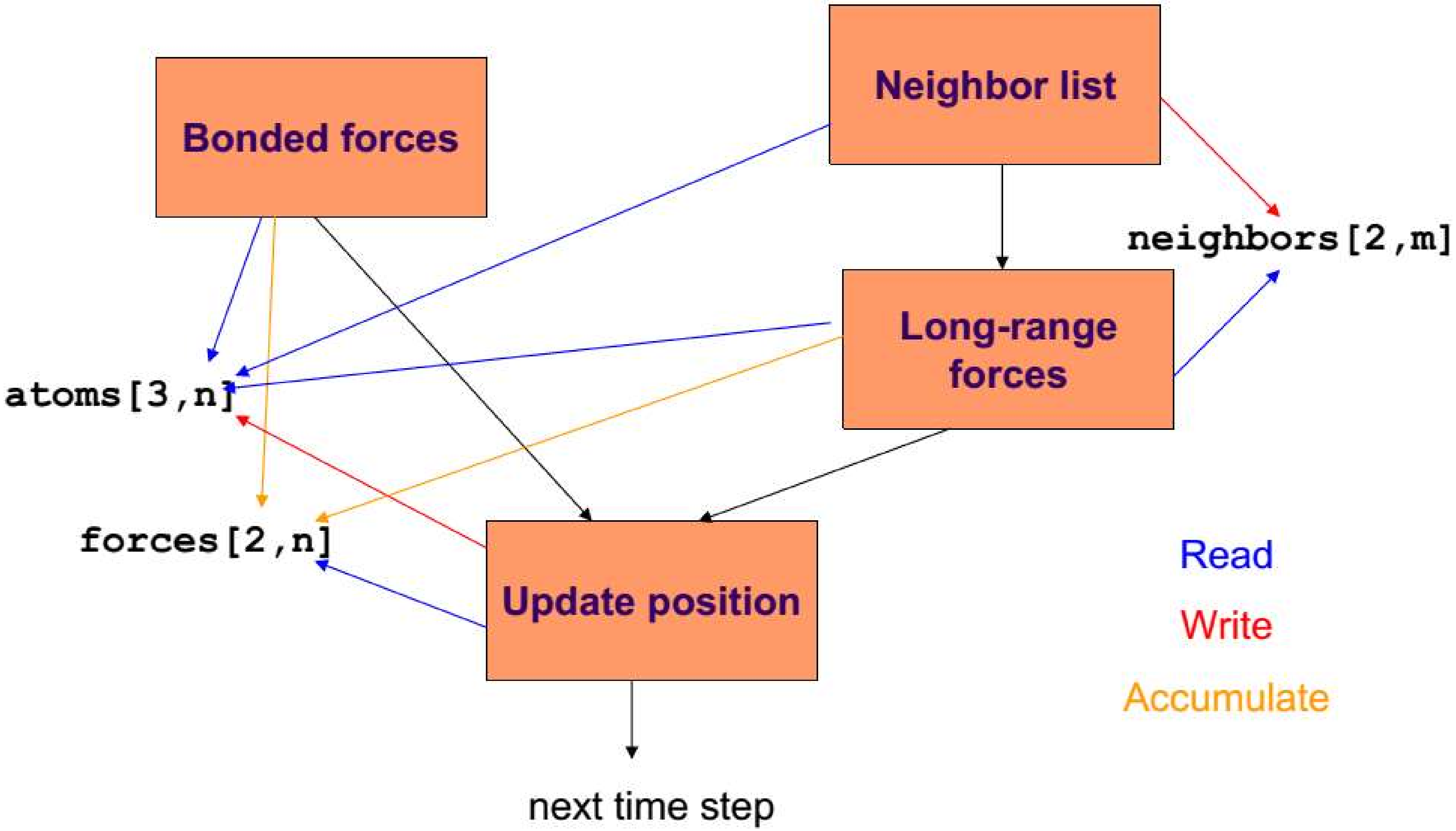
- Main computation is a loop over atoms
- Suggests task decomposition
  - Task corresponds to a loop iteration
    - Update a single atom
  - Additional tasks
    - Calculate bonded forces
    - Calculate long range forces
    - Find neighbors
    - Update position
- There is data shared between the tasks

```
for time = 1 to steps and
  for each atom
      Compute bonded forces
      Compute neighbors
      Compute long-range forces
      Update position
end loop
```

Understand Control Dependences



Understand Data Dependences



Evaluate Design

- What is the target architecture?
  - Shared memory, distributed memory, message passing, …
- Does data sharing have enough special properties (read only, accumulate, temporal constraints) that we can deal with dependences efficiently?
- If design seems OK, move to next design space

Dependence Analysis

- Given two tasks how to determine if they can safely run in parallel?

Bernstein's Condition

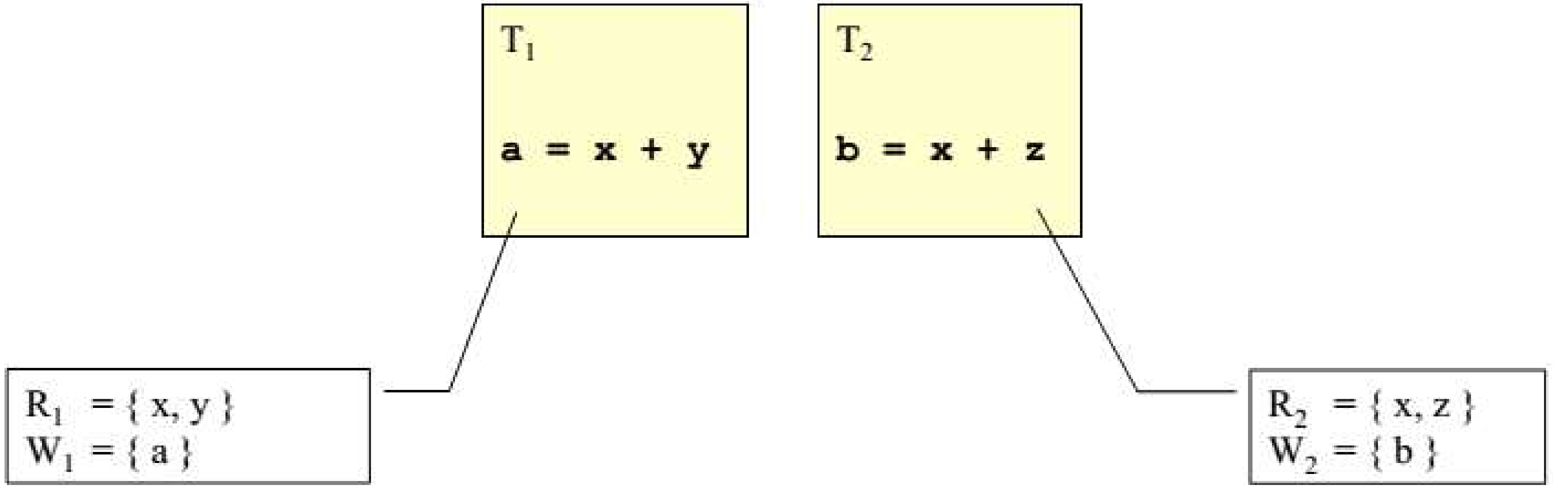
✓ R_i: set of memory locations read (input) by task T_i

✓ W_j: set of memory locations written (output) by task T_j

✓ Two tasks T_1 and T_2 are parallel if

- input to T_1 is not part of output from T_2
- input to T_2 is not part of output from T_1
- outputs from T_1 and T_2 do not overlap

Example



$$R_1 \bigcap W_2 = \phi$$

$$R_2 \bigcap W_1 = \phi$$

$$W_1 \bigcap W_2 = \phi$$

Algorithm Structure Design Space

- Given a collection of concurrent tasks, what's the next step?
- Map tasks to units of execution (e.g., threads)

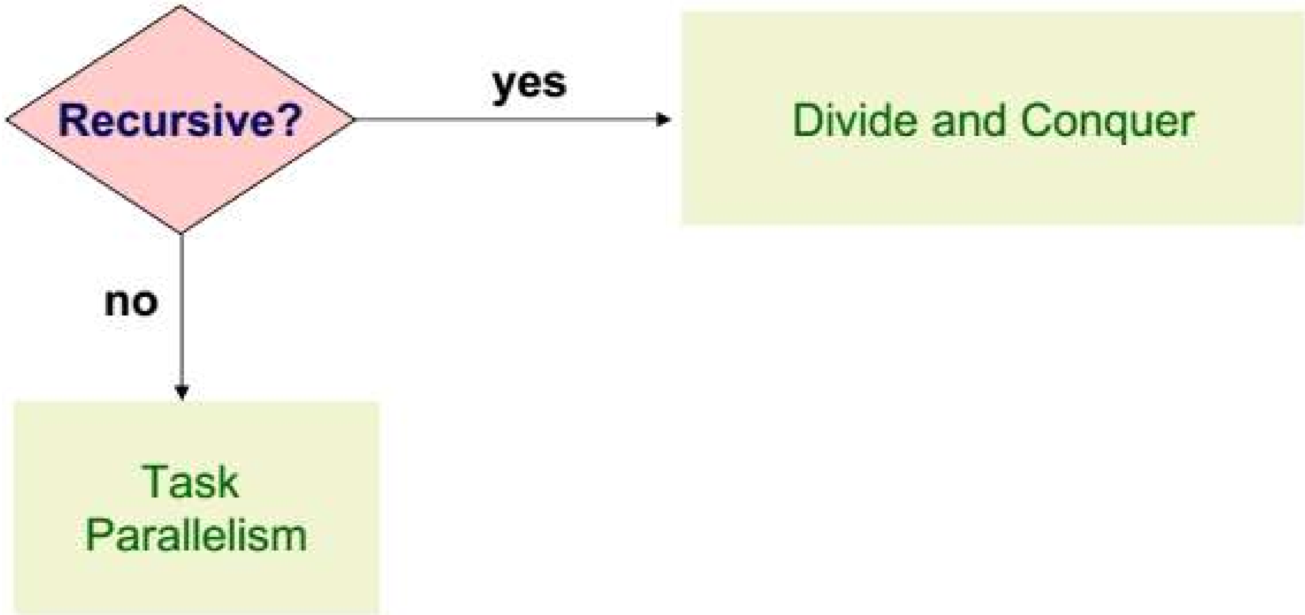
- Important considerations
  - Magnitude of number of execution units platform will support
  - Cost of sharing information among execution units
  - Avoid tendency to over constrain the implementation
    - Work well on the intended platform
    - Flexible enough to easily adapt to different architectures

Major Organizing Principle

- How to determine the algorithm structure that represents the mapping of tasks to units of execution?

- Concurrency usually implies major organizing principle
  - Organize by tasks
  - Organize by data decomposition
  - Organize by flow of data

Organize by Tasks?

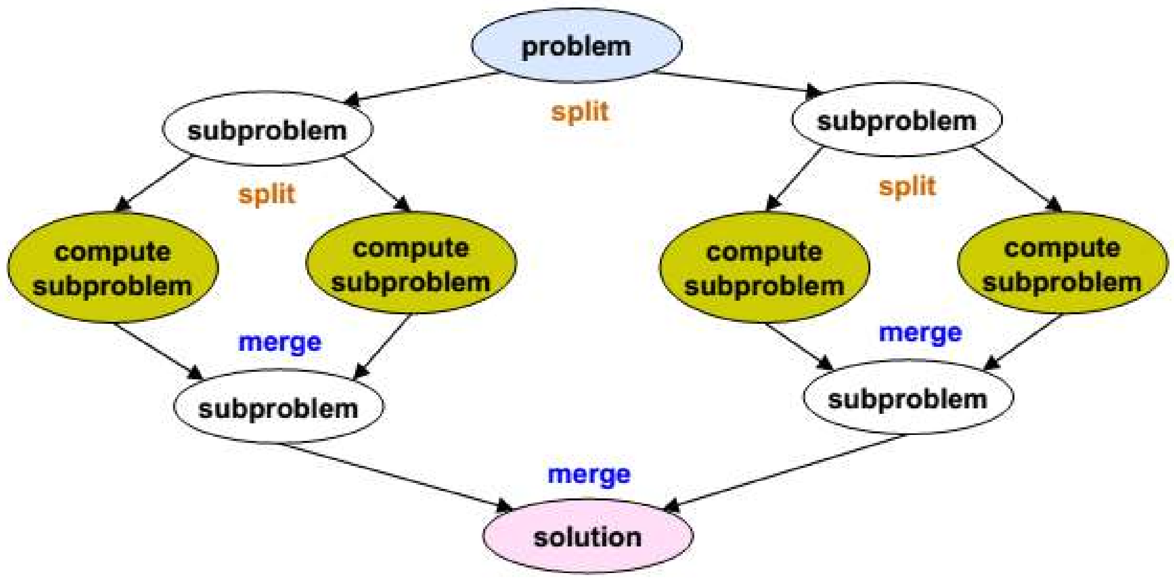


Task Parallelism

- Ray tracing
  - Computation for each ray is a separate and independent
- Molecular dynamics
  - Non-bonded force calculations, some dependencies
- Common factors
  - Tasks are associated with iterations of a loop
  - Tasks largely known at the start of the computation
  - All tasks may not need to complete to arrive at a solution

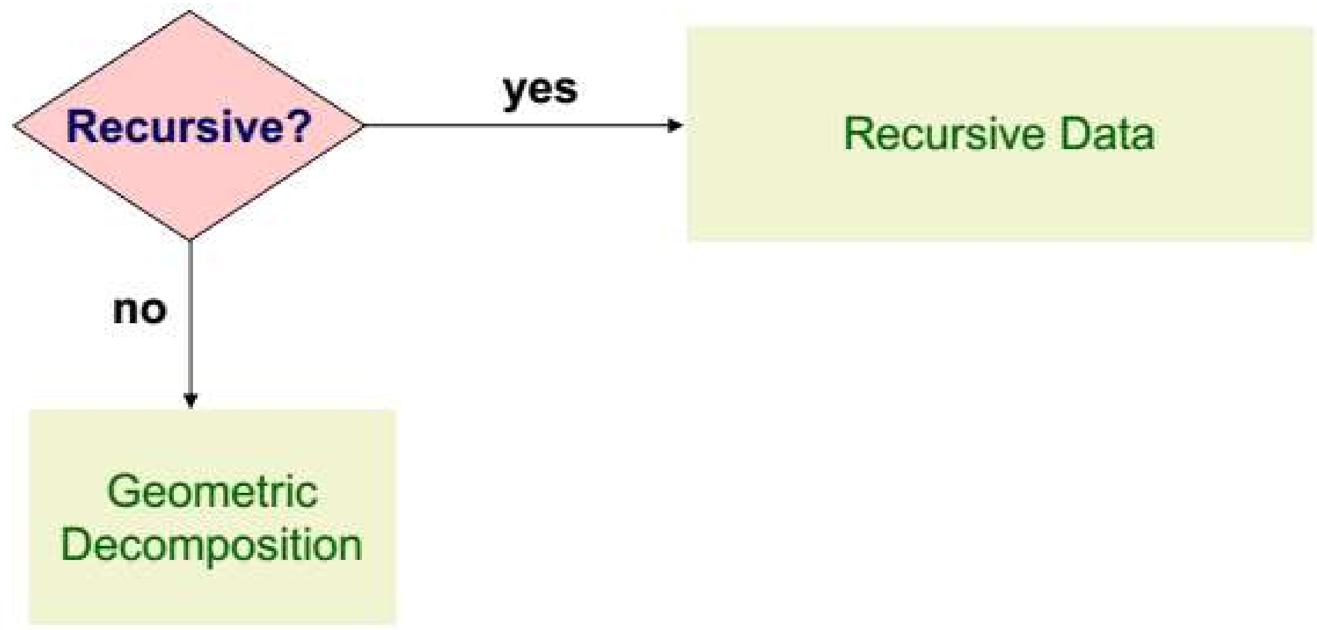
Divide and Conquer

- For recursive programs: divide and conquer
  - Subproblems may not be uniform
  - May require dynamic load balancing



Organize by Data?

- Operations on a central data structure
  - Arrays and linear data structures
  - Recursive data structures



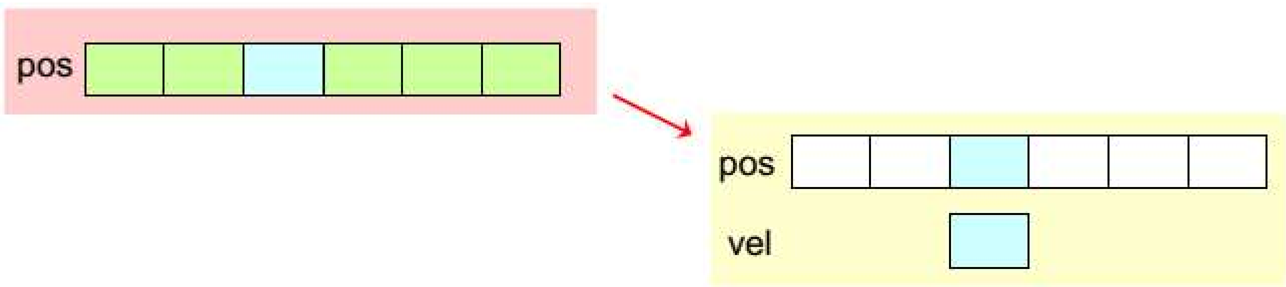
Geometric Decomposition

- Gravitational body simulator
  - Calculate force between pairs of objects and update accelerations

```
VEC3D acc[NUM_BODIES] = 0;

for (i = 0; i < NUM_BODIES - 1; i++) {
  for (j = i + 1; j < NUM_BODIES; j++) {
    // Displacement vector
    VEC3D d = pos[j] – pos[i];
    // Force
    t = 1 / sqr(length(d));
    // Components of force along displacement
    d = t * (d / length(d));

    acc[i] += d * mass[j];
    acc[j] += -d * mass[i];
  }
}
```



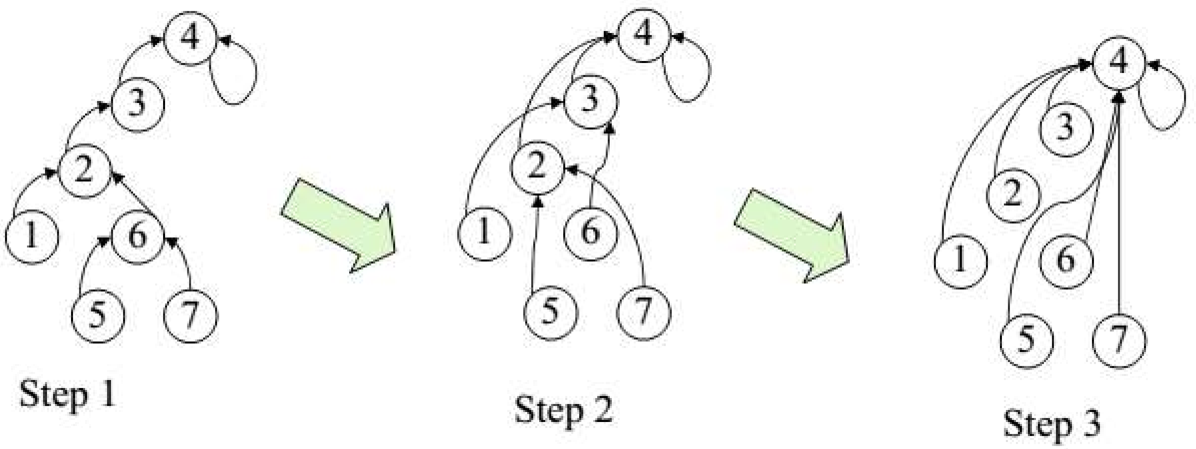
Recursive Data

- Computation on a list, tree, or graph
  - Often appears the only way to solve a problem is to sequentially move through the data structure

- There are however opportunities to reshape the operations in a way that exposes concurrency

Recursive Data Example: Find the Root

- Given a forest of rooted directed trees, for each node, find the root of the tree containing the node
  - Parallel approach: for each node, find its successor's successor, repeat until no changes
    - O(log n) vs. O(n)



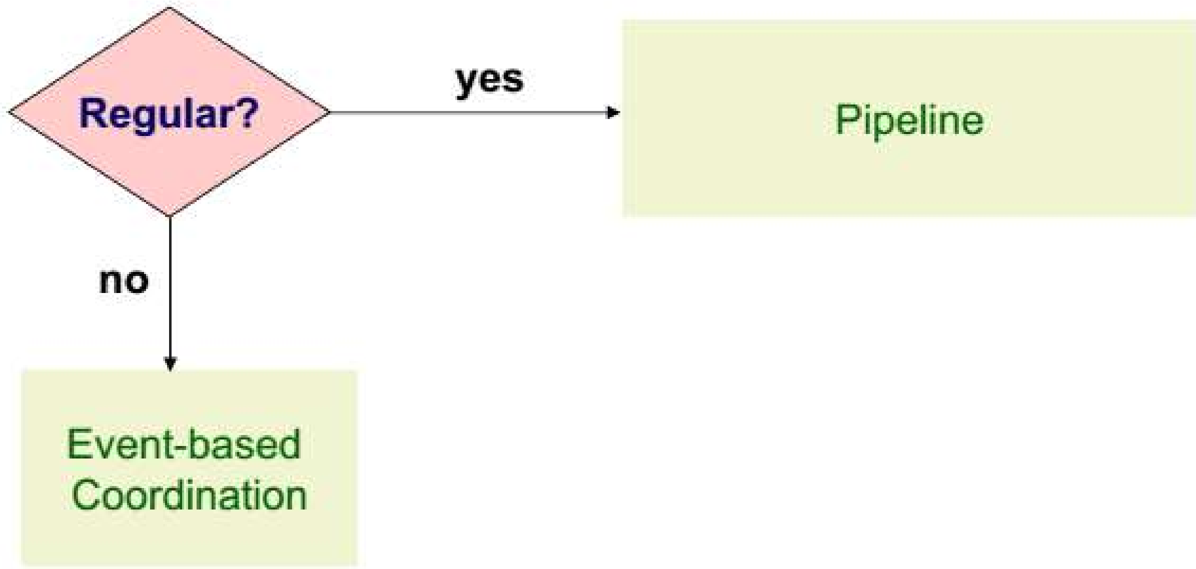
Work vs. Concurrency Tradeoff

- Parallel restructuring of find the root algorithm leads to O(n log n) work vs. O(n) with sequential approach

- Most strategies based on this pattern similarly trade off increase in total work for decrease in execution time due to concurrency

Organize by Flow of Data?

- In some application domains, the flow of data imposes ordering on the tasks
  - Regular, one-way, mostly stable data flow
  - Irregular, dynamic, or unpredictable data flow



Pipeline Throughput vs. Latency

- Amount of concurrency in a pipeline is limited by the number of stages
- Works best if the time to fill and drain the pipeline is small compared to overall running time
- Performance metric is usually the throughput
  - Rate at which data appear at the end of the pipeline per time unit (e.g., frames per second)
- Pipeline latency is important for real-time applications
  - Time interval from data input to pipeline, to data output

Event-Based Coordination

- In this pattern, interaction of tasks to process data can vary over unpredictable intervals
- Deadlocks are likely for applications that use this pattern