EE382N (20): Computer Architecture - Parallelism and Locality
Spring 2015

Lecture 15 – Parallelism in Software III

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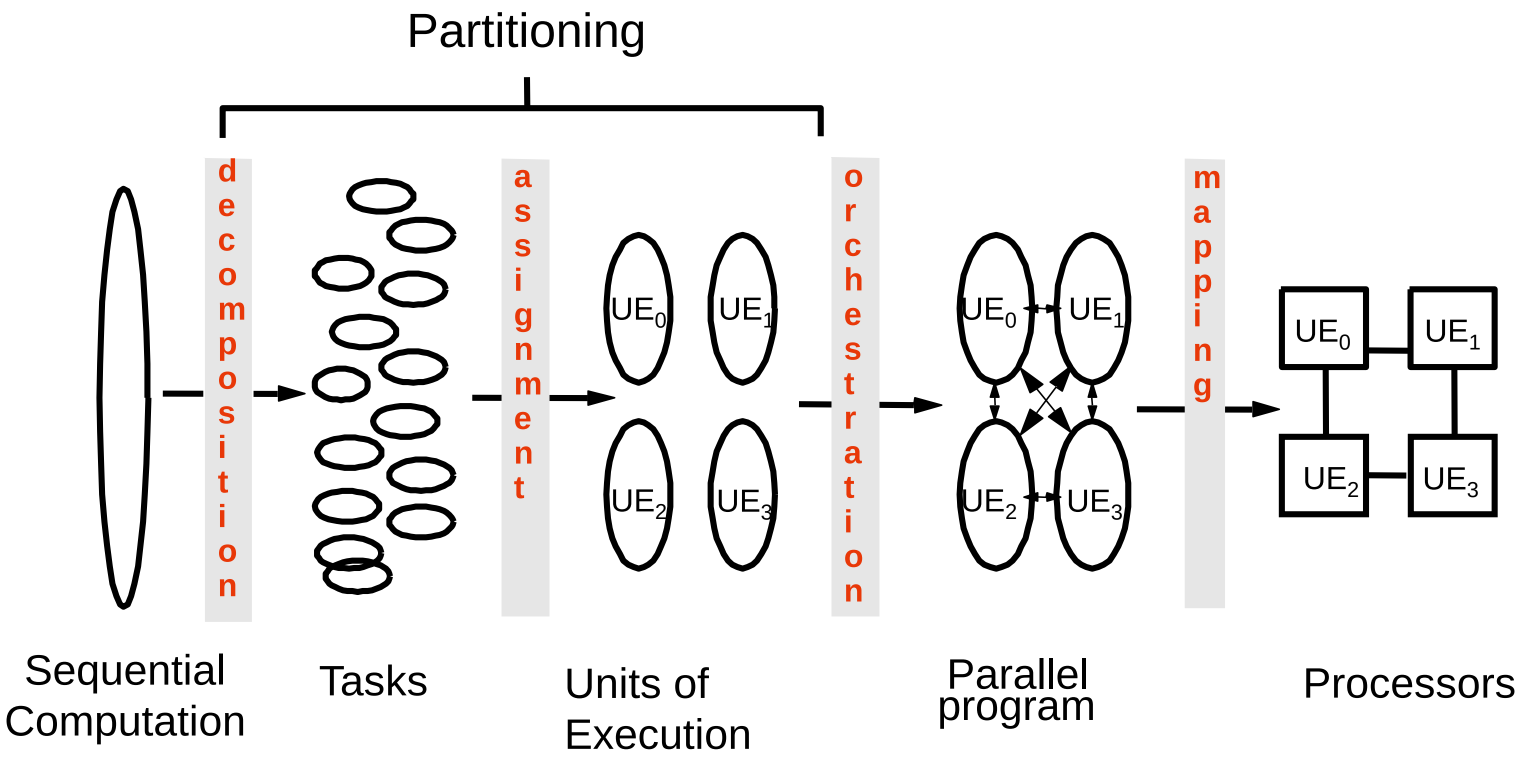
Credits

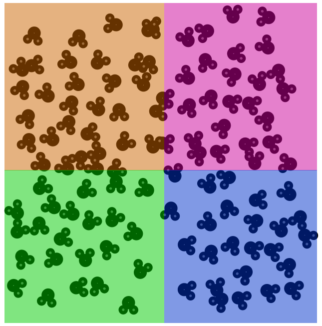
- Most of the slides courtesy Dr. Rodric Rabbah (IBM)
  - Taken from 6.189 IAP taught at MIT in 2007
- Parallel Scan slides courtesy David Kirk (NVIDIA) and Wen-Mei Hwu (UIUC)
  - Taken from EE493-AI taught at UIUC in Sprig 2007

4 Common Steps to Creating a Parallel Program

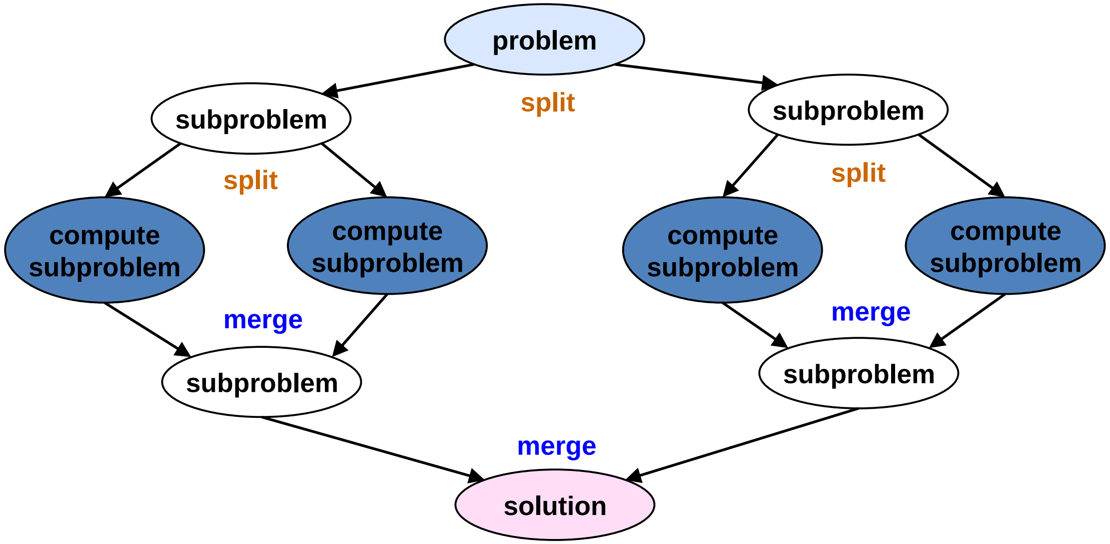


Data Decomposition Examples

- Molecular dynamics
  - Geometric decomposition



- Merge sort
  - Recursive decomposition



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

T_1

`a = x + y`

T_2

`b = x + z`

$R_1 = \{ x, y \}$
$W_1 = \{ a \}$

$R_2 = \{ x, z \}$
$W_2 = \{ b \}$

$$R_1 \bigcap W_2 = \phi$$

$$R_2 \bigcap W_1 = \phi$$

$$W_1 \bigcap W_2 = \phi$$

Patterns for Parallelizing Programs

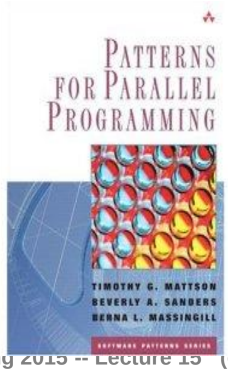
4 Design Spaces

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



Patterns for Parallel Programming. Mattson, Sanders, and Massingill (2005).

Algorithm Structure Design Space

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

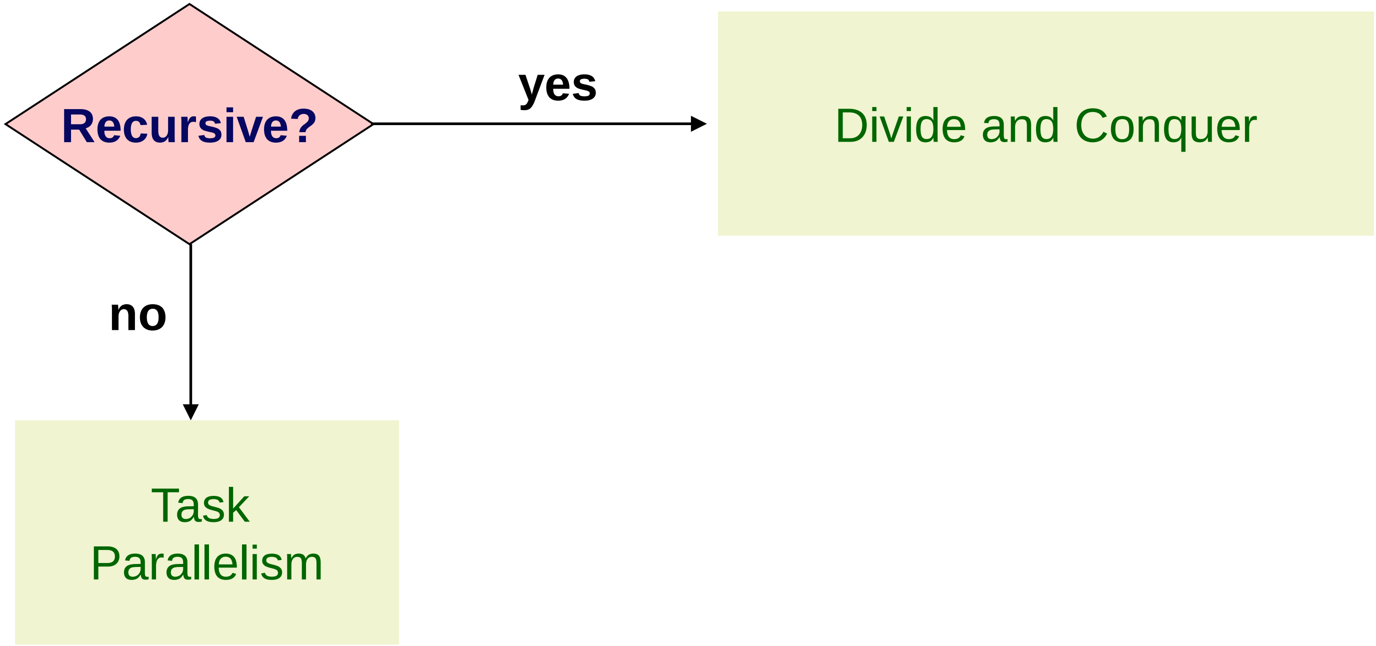
- Important considerations
  - Magnitude of number of execution units platform will support
  - Cost of sharing information among execution units
  - Avoid tendency to over constrain the implementation
    - Work well on the intended platform
    - Flexible enough to easily adapt to different architectures

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?

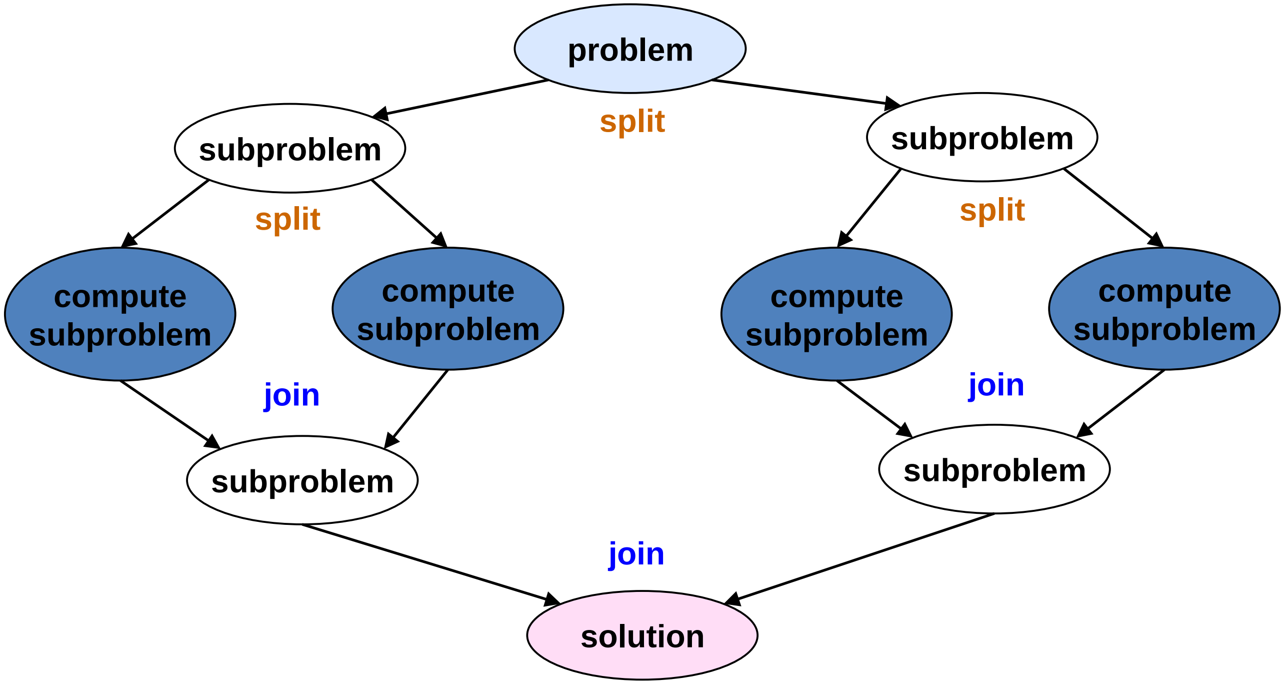


Task Parallelism

- 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

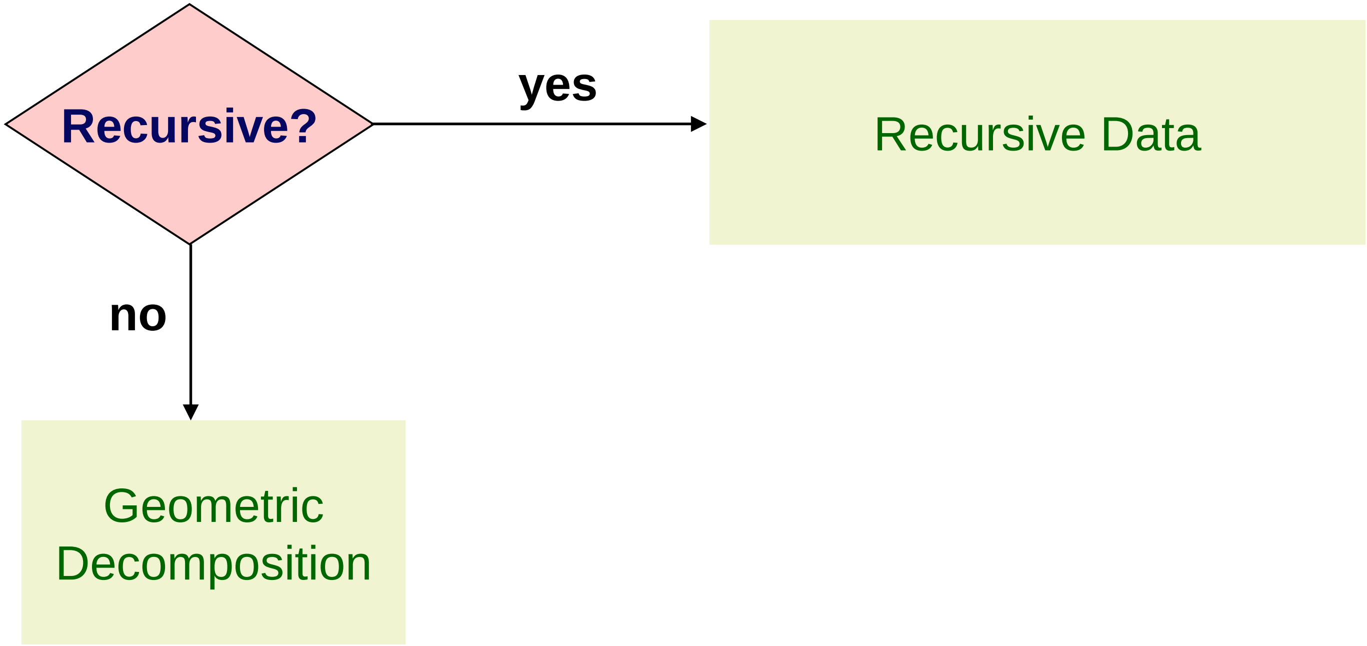
Divide and Conquer

- 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



Recursive?

yes

Recursive Data

no

Geometric Decomposition

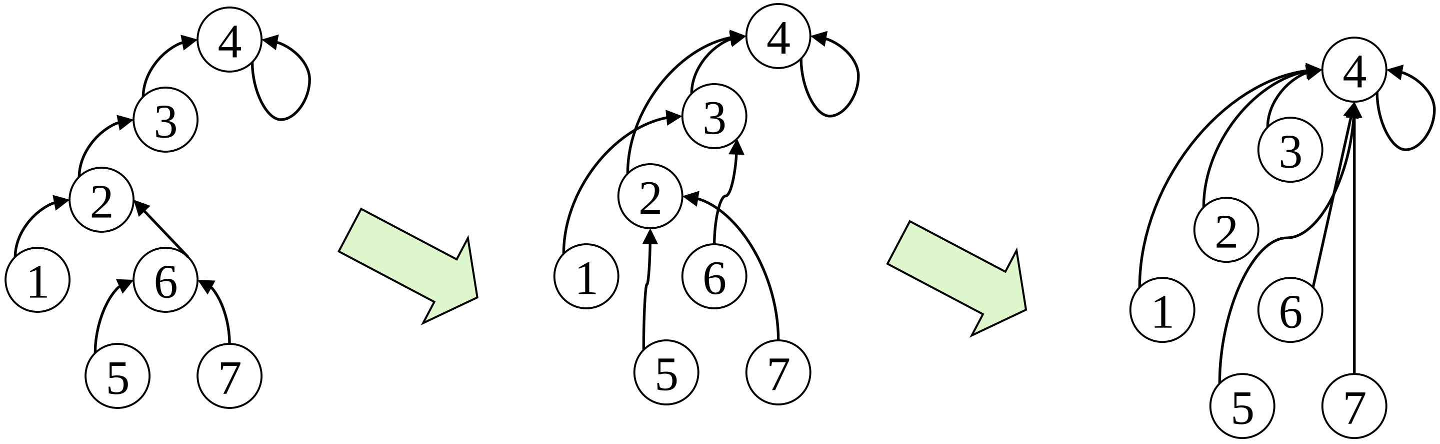
Recursive Data

- 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)



Step 1

Step 2

Step 3

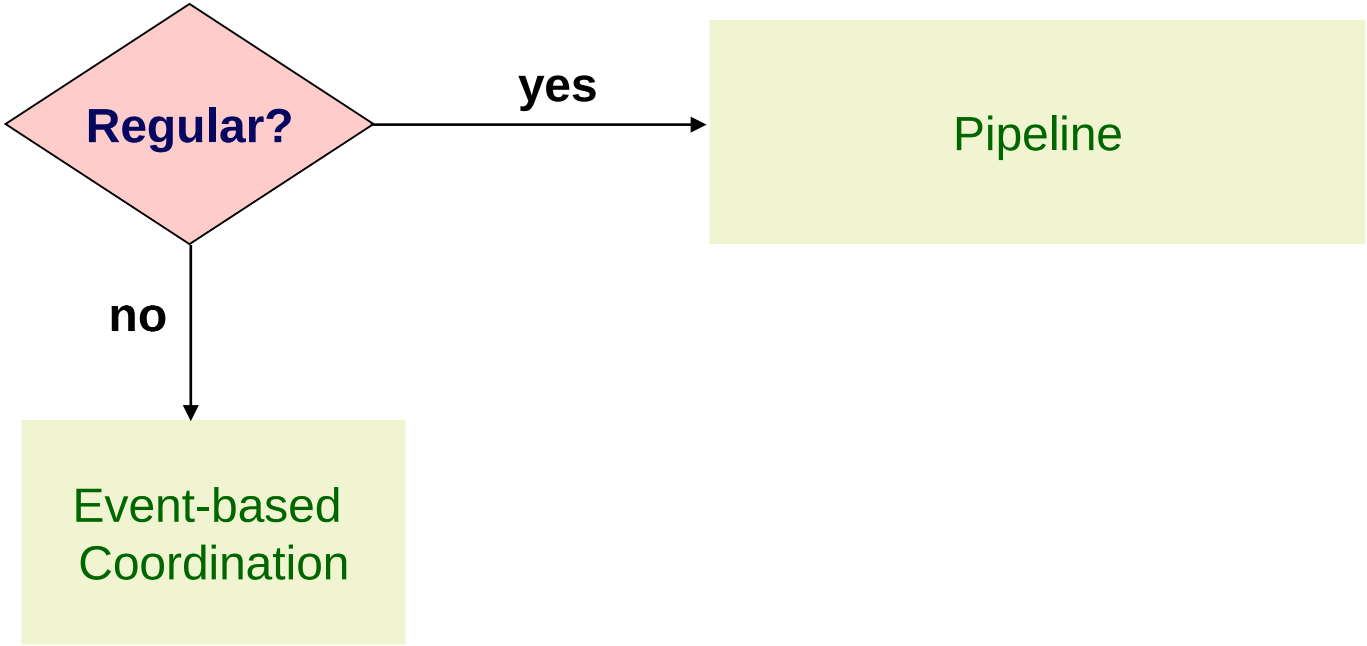
Work vs. Concurrency Tradeoff

- 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 a danger for applications that use this pattern
  - Dynamic scheduling has overhead and may be inefficient
    - Granularity a major concern
- Another option is various "static" dataflow models
  - E.g., synchronous dataflow

Patterns for Parallelizing Programs

4 Design Spaces

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Software Construction

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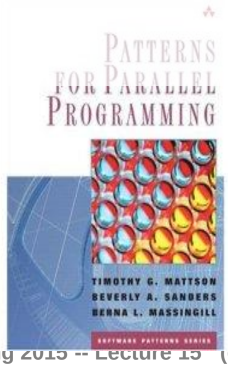
  - Code and data structuring patterns
- Implementation Mechanisms
  - Low level mechanisms used to write parallel programs



Patterns for Parallel Programming. Mattson, Sanders, and Massingill (2005).

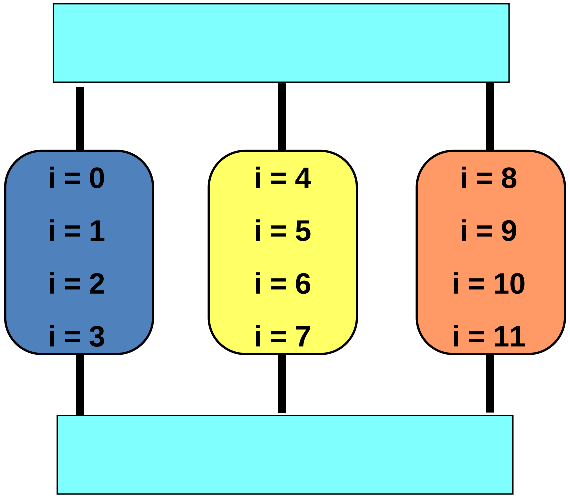
Code Supporting Structures

- Loop parallelism
- Master/Worker
- Fork/Join
- SPMD
- ***Map/Reduce***
- ***Task dataflow***

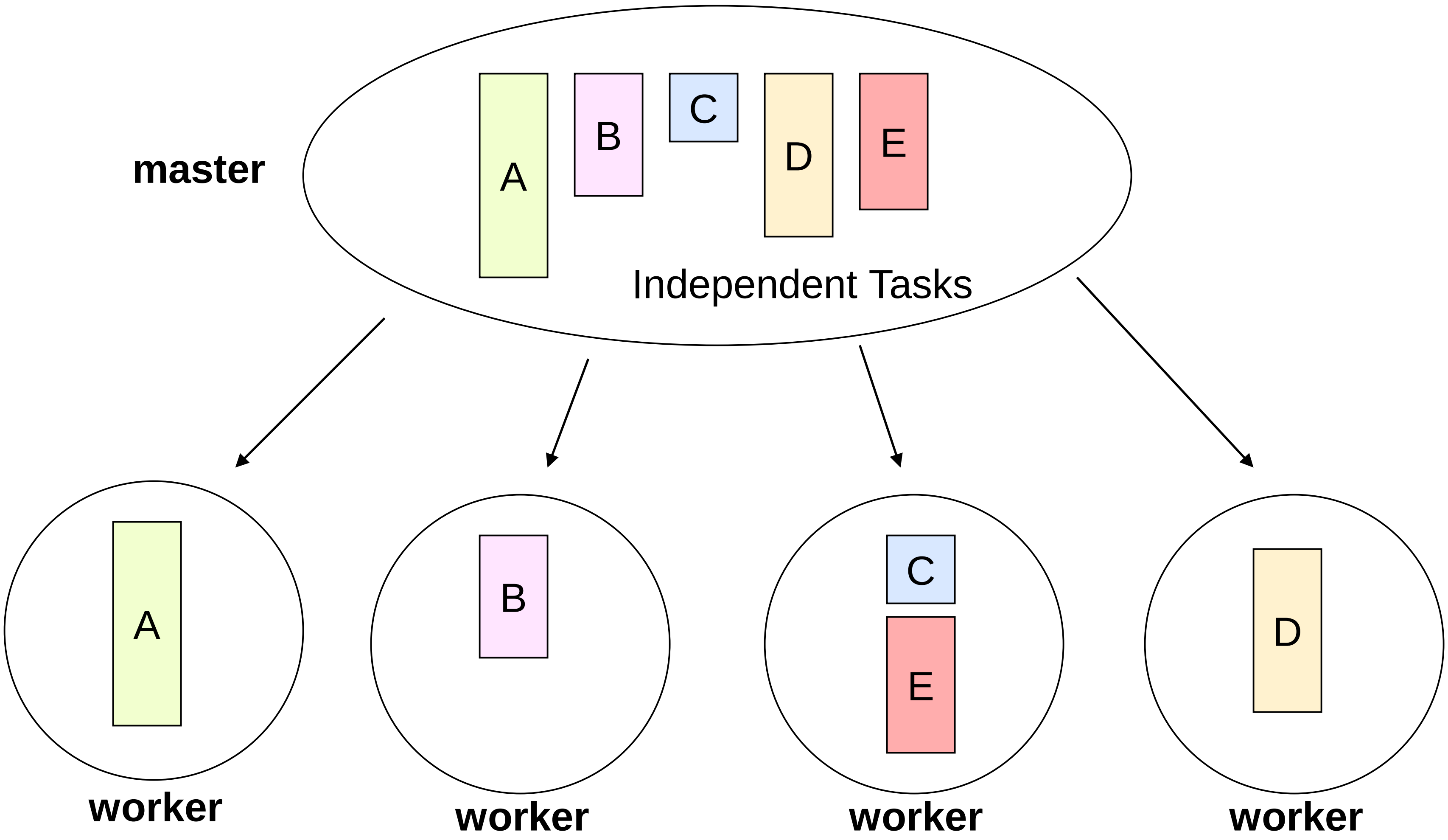
Loop Parallelism Pattern

- Many programs are expressed using iterative constructs
  - Programming models like OpenMP provide directives to automatically assign loop iteration to execution units
  - Especially good when code cannot be massively restructured

```
#pragma omp parallel for
for(i = 0; i < 12; i++)
      C[i] = A[i] + B[i];
```



Master/Worker Pattern



Master/Worker Pattern

- Particularly relevant for problems using task parallelism pattern where task have no dependencies
  - Embarrassingly parallel problems

- Main challenge in determining when the entire problem is complete

Fork/Join Pattern

- Tasks are created dynamically
  - Tasks can create more tasks
- Manages tasks according to their relationship
- Parent task creates new tasks (fork) then waits until they complete (join) before continuing on with the computation

SPMD Pattern

- Single Program Multiple Data: create a single source-code image that runs on each processor
  - Initialize
  - Obtain a unique identifier
  - Run the same program each processor
    - Identifier and input data differentiate behavior
  - Distribute data
  - Finalize

SPMD Challenges

- Split data correctly
- Correctly combine the results
- Achieve an even distribution of the work
- For programs that need dynamic load balancing, an alternative pattern is more suitable

Map/Reduce Pattern

- Two phases in the program
- Map phase applies a single function to all data
  - Each result is a tuple of value and tag
- Reduce phase combines the results
  - The values of elements with the same tag are combined to a single value per tag -- ***reduction***
  - Semantics of combining function are associative
  - Can be done in parallel
  - Can be pipelined with map
- Google uses this for *all* their parallel programs

Communication and Synchronization Patterns

- Communication
  - Point-to-point
  - Broadcast
  - Reduction
  - Multicast
- Synchronization
  - Locks (mutual exclusion)
  - Monitors (events)
  - Barriers (wait for all)
    - Split-phase barriers (separate signal and wait)
      - Sometimes called "fuzzy barriers"
    - Named barriers allow waiting on subset

Quick recap

- Decomposition
  - High-level and fairly abstract
  - Consider machine scale for the most part
  - Task, Data, Pipeline
  - Find dependencies
- Algorithm structure
  - Still abstract, but a bit less so
  - Consider communication, sync, and bookkeeping
  - Task (collection/recursive)
  - Data (geometric/recursive)
  - Dataflow (pipeline/event-based-coordination)
- Supporting structures
  - Loop
  - Master/worker
  - Fork/join
  - SPMD
  - MapReduce

Algorithm Structure and Organization (from the Book)

	Task parallelism	Divide and conquer	Geometric decomposition	Recursive data	Pipeline	Event-based coordination
SPMD	****	***	****	**	***	**
Loop Parallelism	****	**	***			
Master/ Worker	****	**	*	*	****	*
Fork/ Join	**	****	**		****	****

- Patterns can be hierarchically composed so that a program uses more than one pattern

Algorithm Structure and Organization (my view)

	Task parallelism	Divide and conquer	Geometric decomposition	Recursive data	Pipeline	Event-based coordination
SPMD	****	**	****	**	****	*
Loop Parallelism	**** when no dependencies	*	****	*	**** SWP to hide comm.	
Master/ Worker	****	***	***	***	**	****
Fork/ Join	****	****	**	****		*

- Patterns can be hierarchically composed so that a program uses more than one pattern

Patterns for Parallelizing Programs

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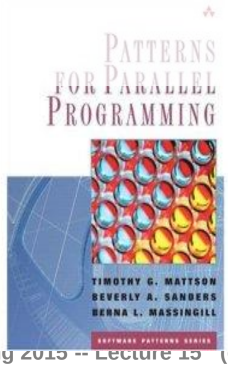

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ILP, DLP, and TLP in SW and HW

- ILP
  - OOO
  - Dataflow
  - VLIW
- DLP
  - SIMD
  - Vector
- TLP
  - Essentially multiple cores with multiple sequencers

- ILP
  - Within straight-line code
- DLP
  - Parallel loops
  - Tasks operating on disjoint data
    - No dependencies within parallelism phase
- TLP
  - All of DLP +
  - Producer-consumer chains

ILP, DLP, and TLP and Supporting Patterns

	Task parallelism	Divide and conquer	Geometric decomposition	Recursive data	Pipeline	Event-based coordination
ILP	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
DLP	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
TLP	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]

ILP, DLP, and TLP and Supporting Patterns

	Task parallelism	Divide and conquer	Geometric decomposition	Recursive data	Pipeline	Event-based coordination
ILP	inline / unroll	inline	unroll	inline	inline / unroll	inline
DLP	natural or local-conditions	after enough divisions	natural	after enough branches	difficult	local-conditions
TLP	natural	natural	natural	natural	natural	natural

ILP, DLP, and TLP and Implementation Patterns

	SPMD	Loop Parallelism	Mater/Worker	Fork/Join
ILP				
DLP				
TLP				

ILP, DLP, and TLP and Implementation Patterns

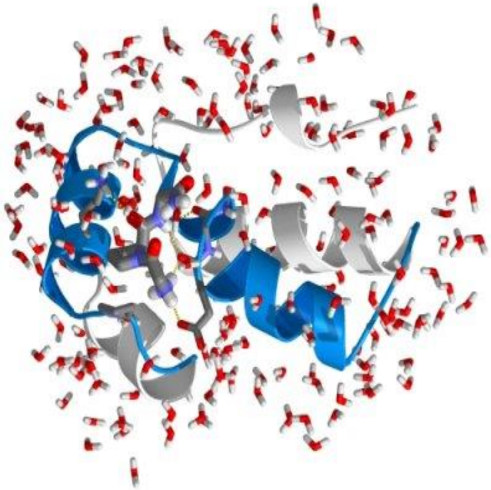
	SPMD	Loop Parallelism	Master/ Worker	Fork/Join
ILP	pipeline	unroll	inline	inline
DLP	natural or local-conditional	natural	local-conditional	after enough divisions + local-conditional
TLP	natural	natural	natural	natural

Outline

- Molecular dynamics example
  - Problem description
  - Steps to solution
    - Build data structures; Compute forces; Integrate for new; positions; Check global solution; Repeat
  - Finding concurrency
    - Scans; data decomposition; reductions
  - Algorithm structure
  - Supporting structures

GROMACS

- Highly optimized molecular-dynamics package
  - Popular code
  - Specifically tuned for protein folding
  - Hand optimized loops for SSE3 (and other extensions)

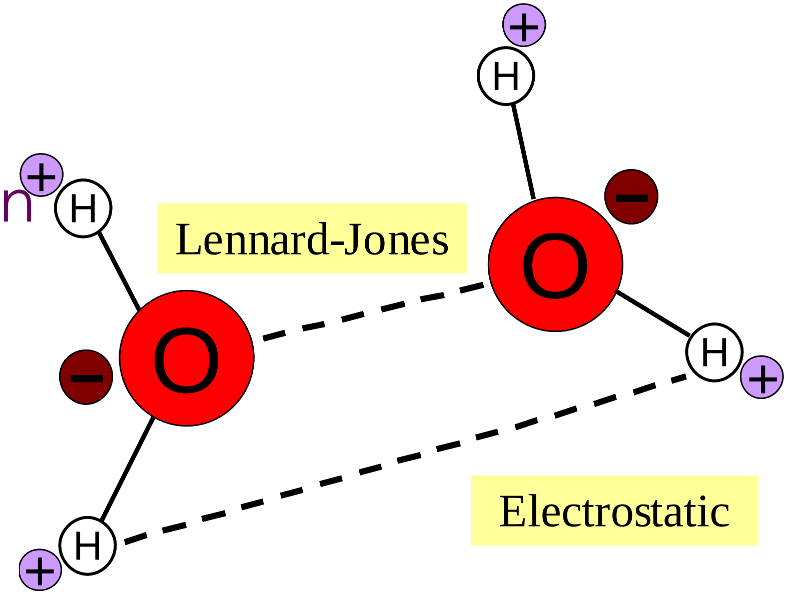


Gromacs Components

- Non-bonded forces
  - Water-water with cutoff
  - Protein-protein tabulated
  - Water-water tabulated
  - Protein-water tabulated
- Bonded forces
  - Angles
  - Dihedrals
- Boundary conditions
- Verlet integrator
- Constraints
  - SHAKE
  - SETTLE
- Other
  - Temperature–pressure coupling
  - Virial calculation

GROMACS Water-Water Force Calculation

- Non-bonded long-range interactions
  - Coulomb
  - Lennard-Jones
  - 234 operations per interaction

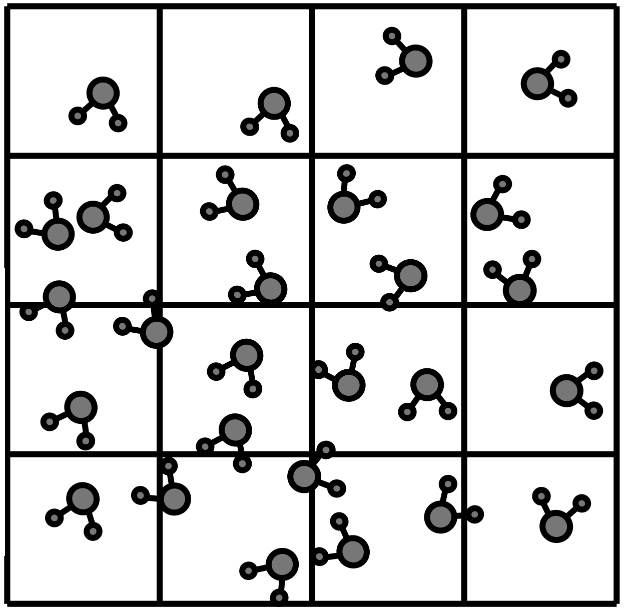


$$V_{nb} = \Sigma_{i,j} \left[\frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}} + \left(\frac{C_{12}}{r_{ij}^{12}} - \frac{C_6}{r_{ij}^{6}} \right) \right]$$

Water-water interaction ~75% of GROMACS run-time

GROMACS Uses Non-Trivial Neighbor-List Algorithm

- Full non-bonded force calculation is $o(n^2)$
- GROMACS approximates with a cutoff
  - Molecules located more than r_c apart do not interact
  - $O(nr_c^3)$



Efficient algorithm leads to variable rate input streams

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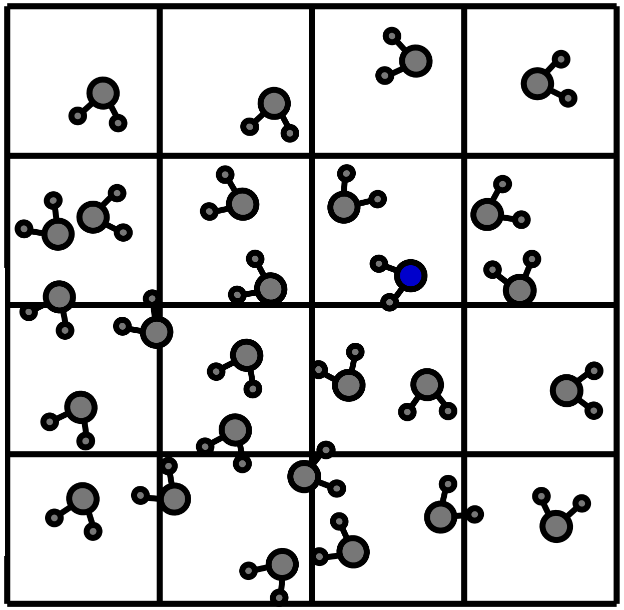

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central molecules

neighbor molecules

Efficient algorithm leads to variable rate input streams

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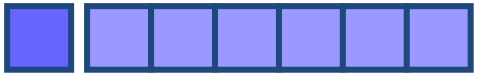
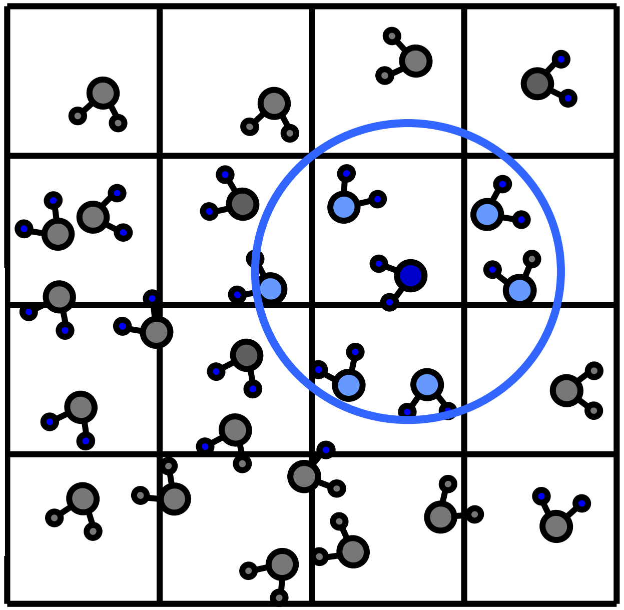


central molecules

neighbor molecules



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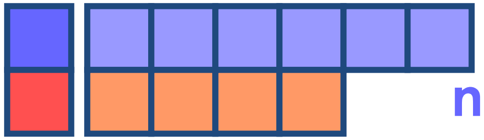

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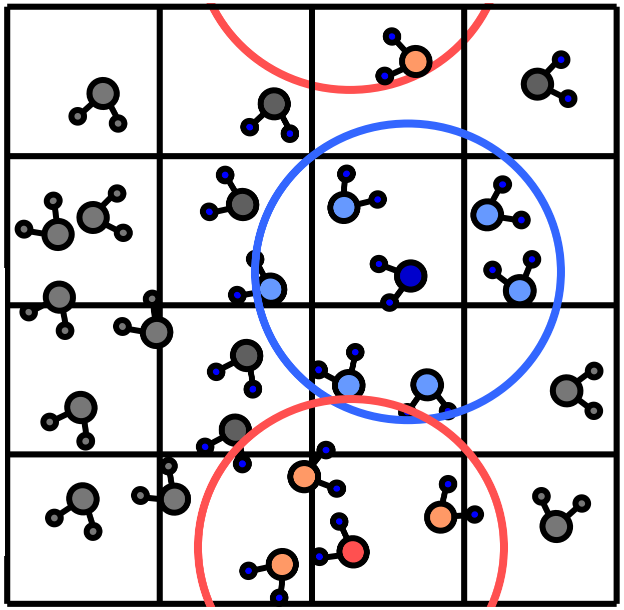

Efficient algorithm leads to variable rate input streams

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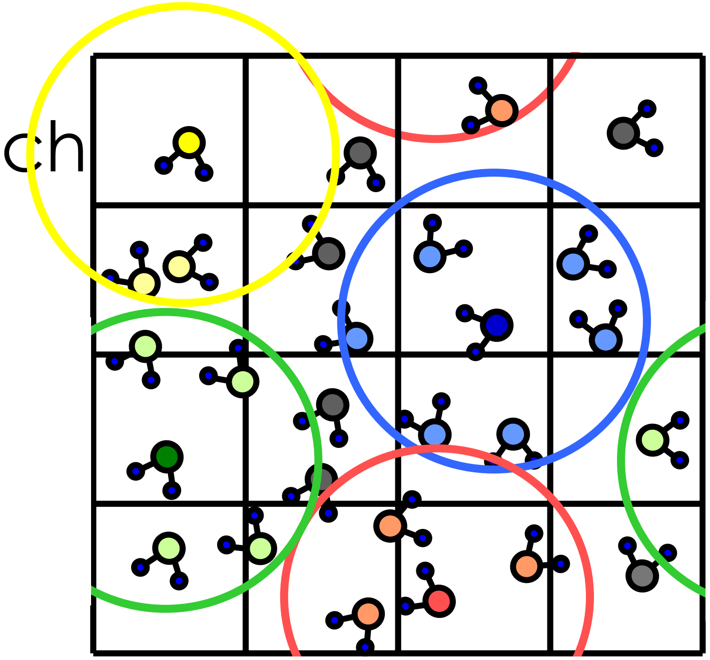
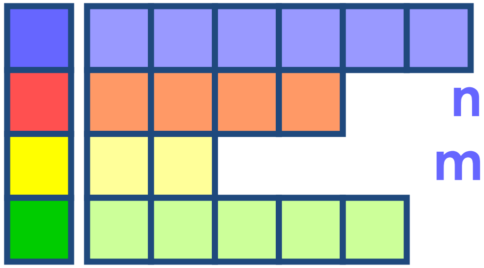
- Full non-bonded force calculation is $o(n^2)$
- GROMACS approximates with a cutoff
  - Molecules located more than r_c apart do not interact
  - $O(nr_c^3)$
- Separate neighbor-list for each molecule
  - Neighbor-lists have variable number of elements





Efficient algorithm leads to variable rate input streams

Other Examples

- More patterns
  - Reductions
  - Scans
    - Building a data structure
- More examples
  - Search
  - Sort
  - FFT as divide and conquer
  - Structured meshes and grids
  - Sparse algebra
  - Unstructured meshes and graphs
  - Trees
  - Collections
    - Particles
    - Rays