EE382N (20): Computer Architecture - Parallelism and Locality

Lecture 13 – Parallelism in Software IV

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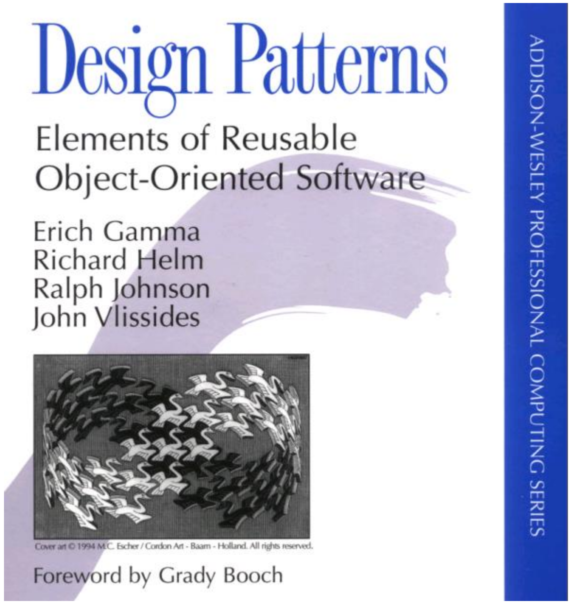
Credits

- 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

Patterns in Object-Oriented Programming

- Design Patterns: Elements of Reusable Object-Oriented Software (1995)
  - Gang of Four (GOF): Gamma, Helm, Johnson, Vlissides
  - Catalogue of patterns
  - Creation, structural, behavioral



Patterns for Parallelizing Programs

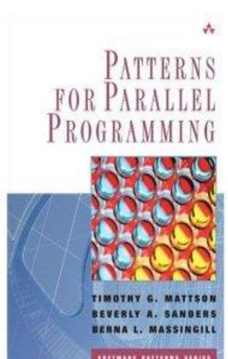
4 Design Spaces

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



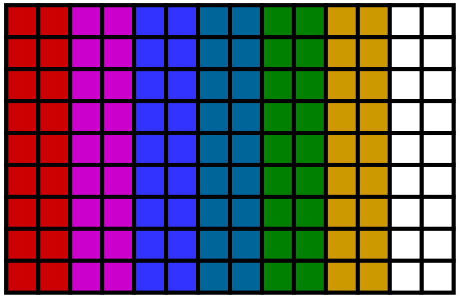
Patterns for Parallel Programming. Mattson, Sanders, and Massingill (2005).

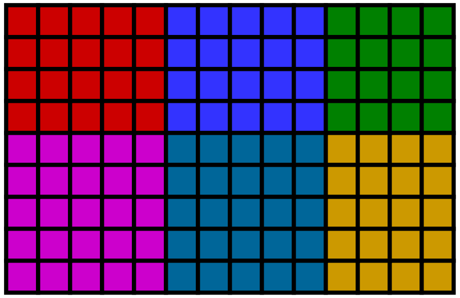
Guidelines for Task Decomposition

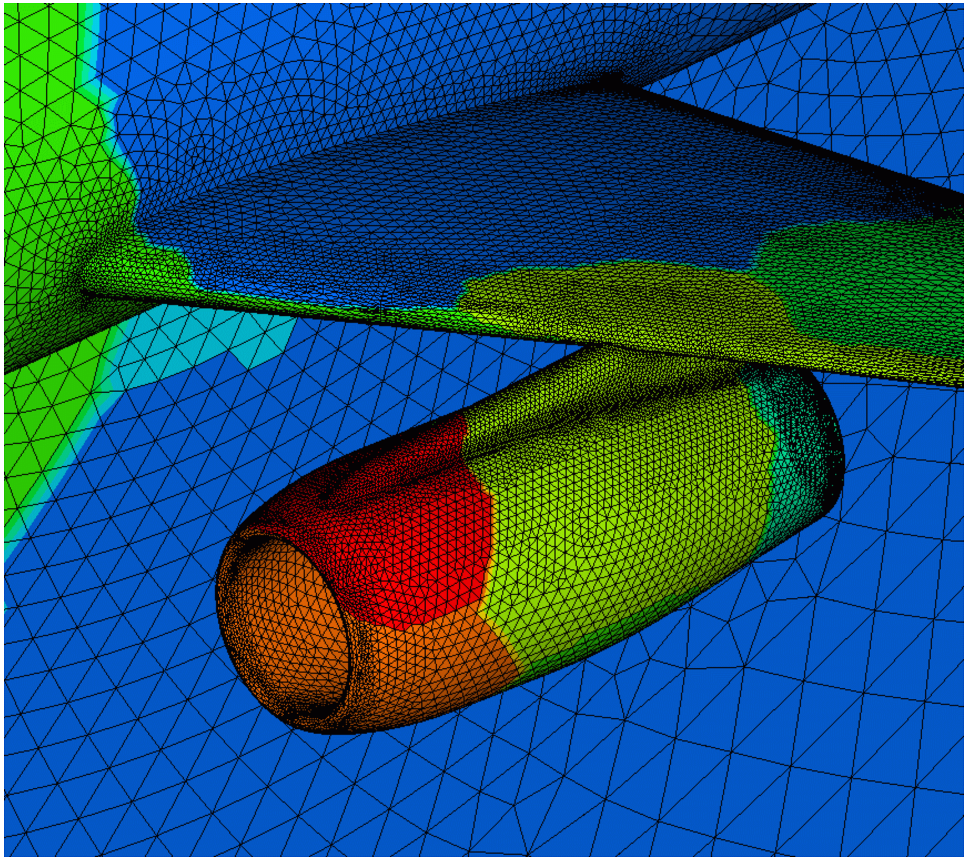
- Flexibility
  - Program design should afford flexibility in the number and size of tasks generated
    - Tasks should not tied to a specific architecture
    - Fixed tasks vs. Parameterized tasks
- Efficiency
  - Tasks should have enough work to amortize the cost of creating and managing them
  - Tasks 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

Common Data Decompositions

- Geometric data structures
  - Decomposition of arrays along rows, columns, blocks
  - Decomposition of meshes into domains







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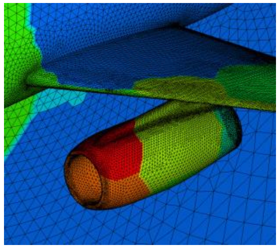
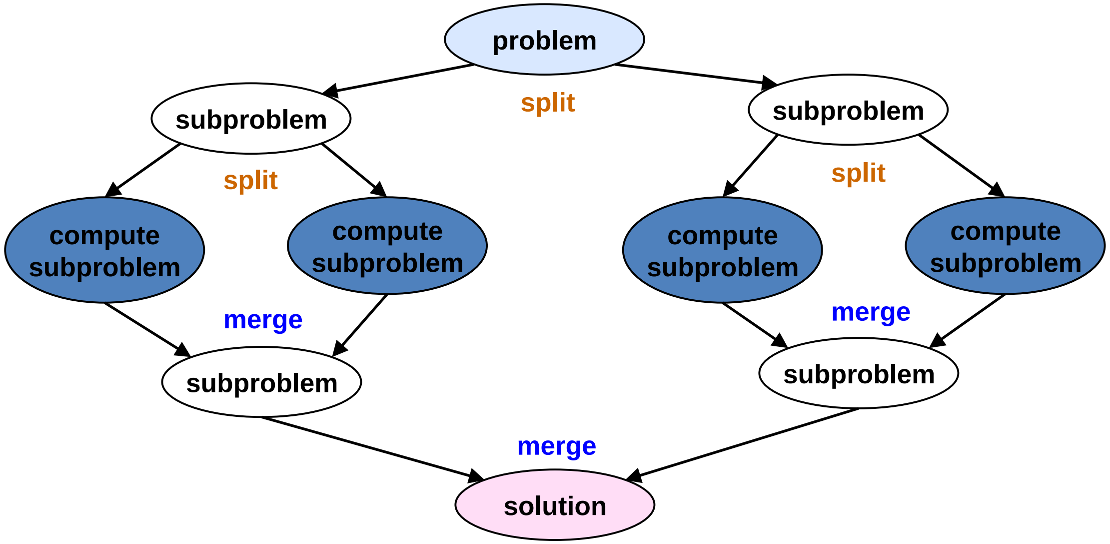


- Recursive data structures
  - Example: decomposition of trees into sub-trees



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

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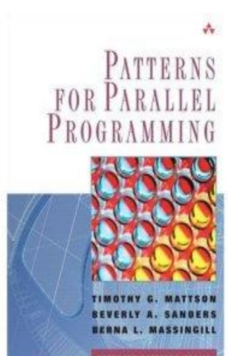

Patterns for Parallel Programming. Mattson, Sanders, and Massingill (2005).

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

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

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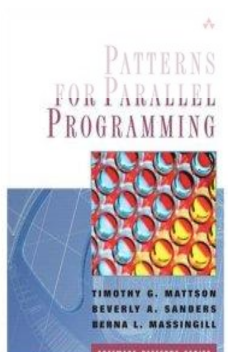

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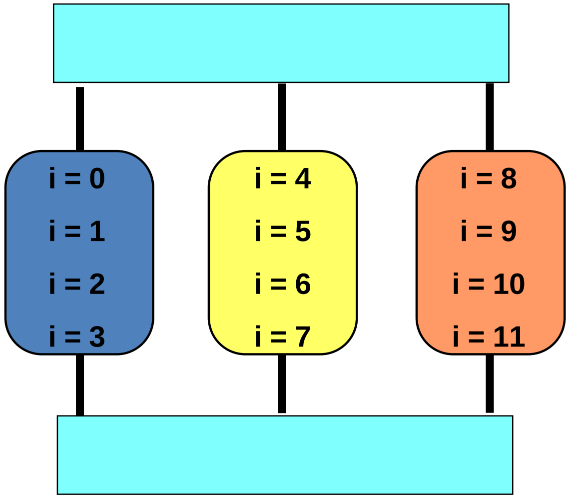
Code Supporting Structures

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

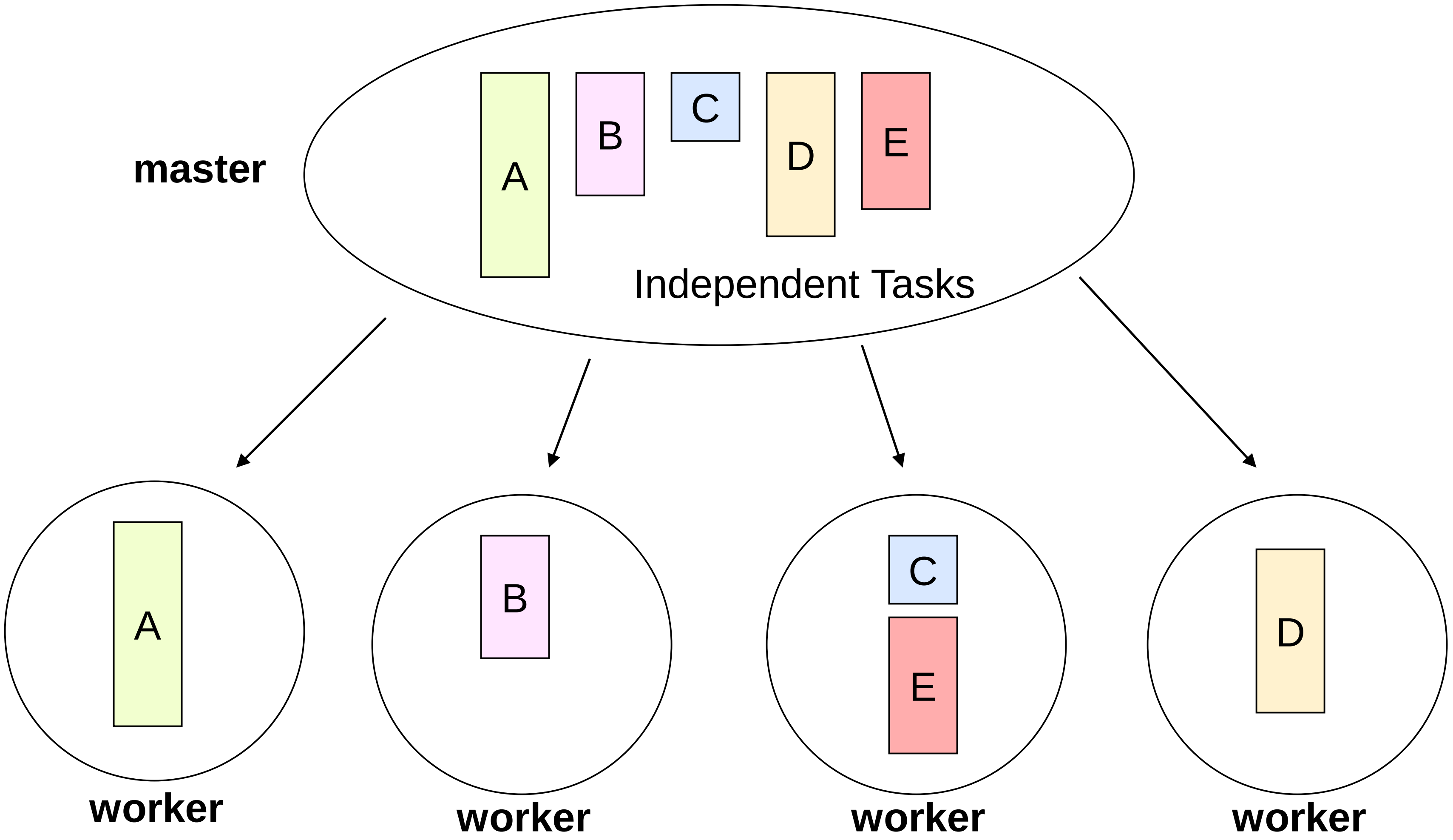
Loop Parallelism Pattern

- 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

Task Dataflow

- Dependence graph of tasks
- Usually, inputs and outputs explicitly defined (to form the dataflow)

Transactions

- Mutual exclusion is useful but costly
- Transactions assume tasks are parallel and check for conflicts of exclusion
- On conflict – re-execute conflicts (and serialize)
- Software and hardware approaches

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
  - Hardware transactions

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
  - Transactions

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

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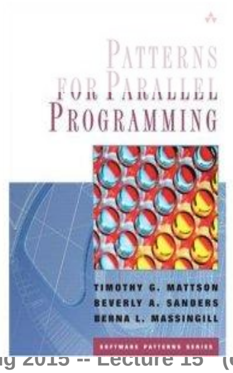

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ILP, DLP, and TLP in SW and HW

- 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						
DLP						
TLP						

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

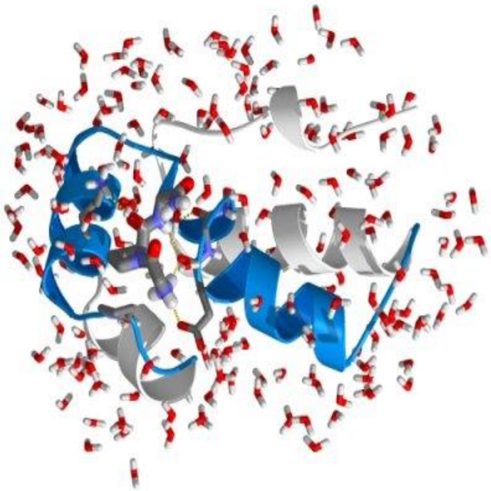
	SPMD	Loop Parallelism	Master/ Worker	Fork/Join
ILP	pipeline	unroll	inline	inline
DLP	natural or local-conditional	natural	local-conditional	after enough divisions + local-conditional
TLP	natural	natural	natural	natural

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)

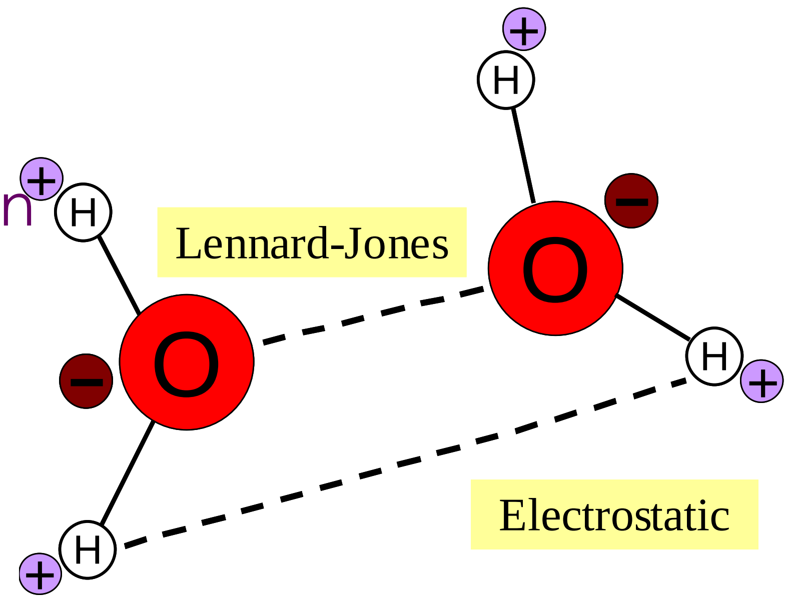


Gromacs Components

- 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

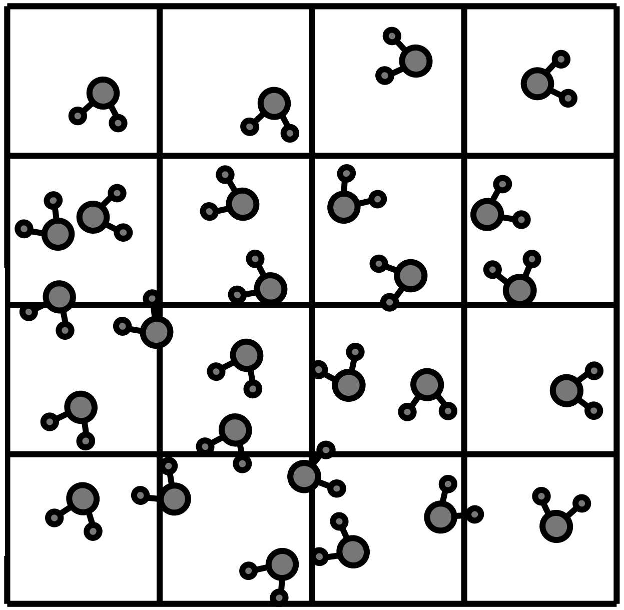


$$V_{nb} = \sum_{i,j} \left[\frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}} + \left(\frac{C_{12}}{r_{ij}^{12}} - \frac{C_6}{r_{ij}^{6}} \right) \right]$$

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

GROMACS Uses Non-Trivial Neighbor-List Algorithm

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



Efficient algorithm leads to variable rate input streams

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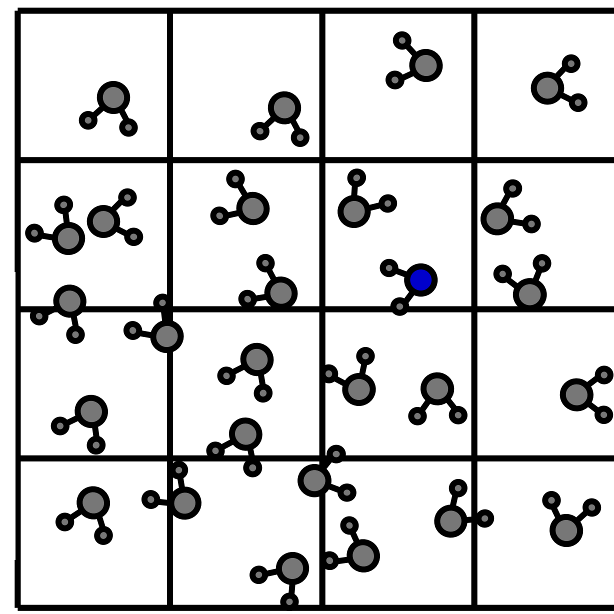
central molecules

neighbor molecules



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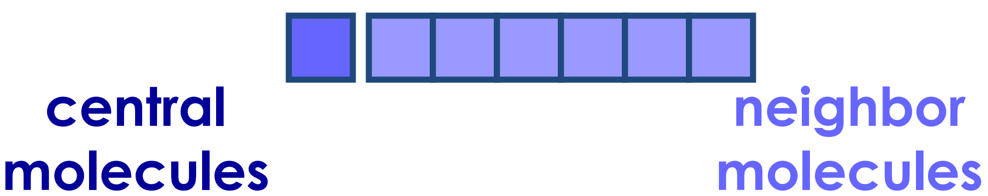

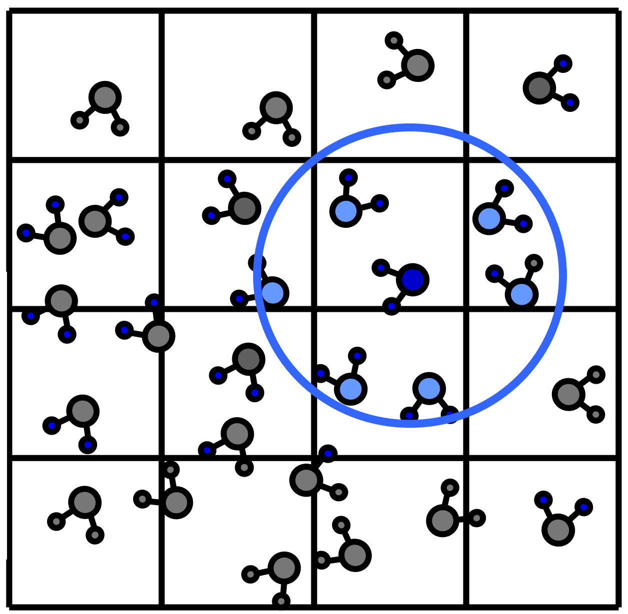

Efficient algorithm leads to variable rate input streams

GROMACS Uses Non-Trivial Neighbor-List Algorithm

- Full non-bonded force calculation is ***o(n²)***
- GROMACS approximates with a cutoff
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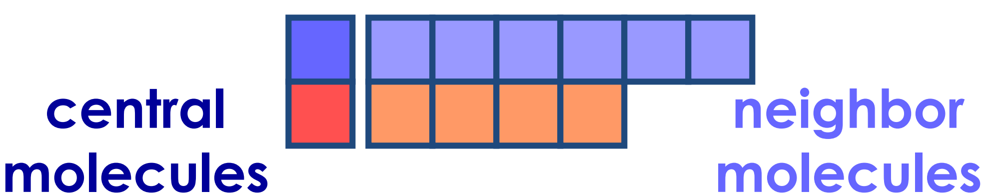
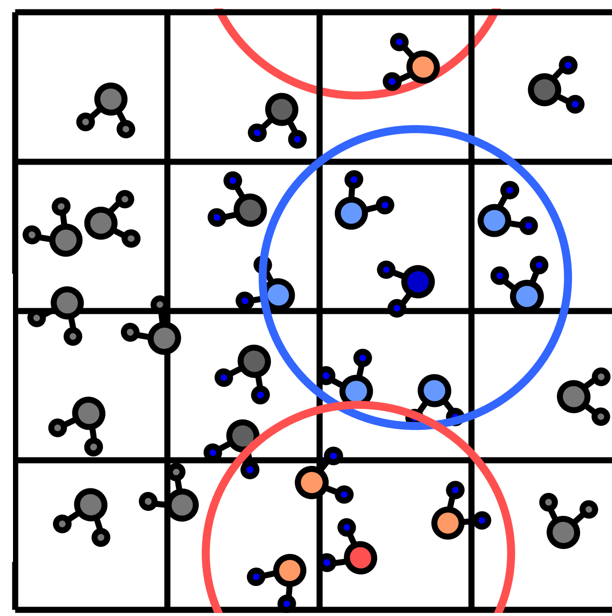
  - $O(nr_c^3)$

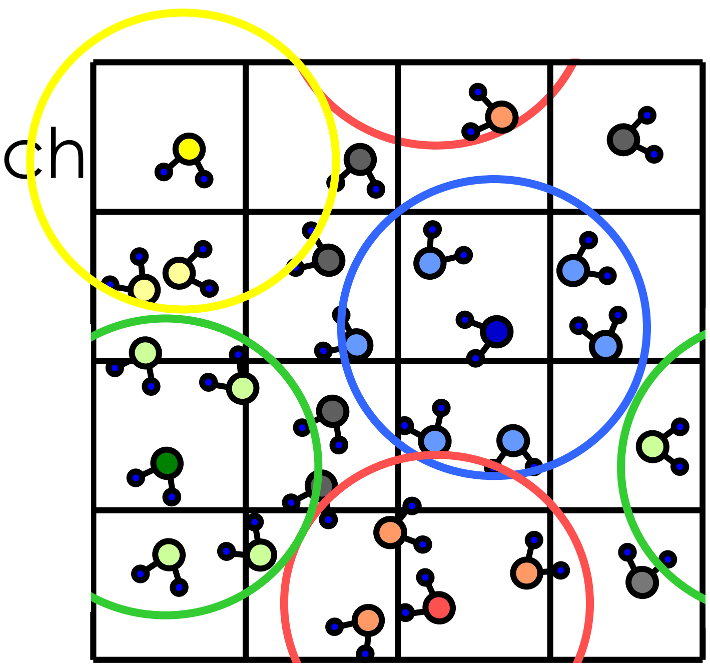


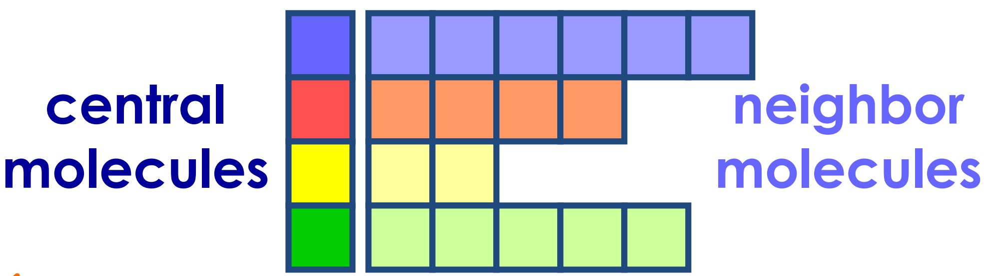


Efficient algorithm leads to variable rate input streams

GROMACS Uses Non-Trivial Neighbor-List Algorithm

- Full non-bonded force calculation is ***o(n²)***
- 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