Particle Based Domain Decomposition

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Particle Methods

- Molecular Dynamics (MD)
- Direct Simulation Monte Carlo (DSMC)
- Event Driven / Hard Sphere MD (ED)
- Smoothed Particle Hydrodynamics (SPH)
- Lattice Gas Automata (LGA)
- Boltzmann Lattice Gas Automata (BLGA)
- Contact Dynamics
- .... and many more

Differences to Grid based algorithms

- Equation of motion:

$$\frac{\partial^2}{\partial t^2} x_i = F(x_1, \ldots, x_N)$$

- One possibility: treat with standard methods for ordinary differential equation
- BUT: the Grid is moving every timesteps:
  - Grid/particle distribution should be cheap
  - possible load imbalance problems
  - physics may help to find efficient algorithm

General questions of the physical approach

- Type of interaction
  - pair interaction (superposition of forces)
  - multi-particle interaction
- Range of interaction
  - long range (gravitation) (Hierarchical methods, fast multipole methods)
  - short range
- Distribution of particles in space
  - homogeneous/inhomogeneous
  - bounded/unbounded
  - regular/irregular shape of domain
- Necessary number of particles

Case study: short range Molecular Dynamics

- N particles interact with each other

$$m_i \frac{\partial}{\partial t} v_i = F_i = \sum_{j=1}^{N} F_{ij} = \sum_{j=1}^{N} F(r_i, r_j)$$

- Due to the short range interaction the Force Matrix F is a sparse Matrix

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x				x					x					
2		x	x		x	x	x								
3		x	x	x			x	x							
4			x	x				x	x						
5	x	x			x	x				x	x	x			
6		x			x	x	x					x	x		
7		x	x			x	x	x					x	x	x
8			x	x			x	x	x						x
9				x				x	x						x
10	x				x					x	x				
11					x					x	x	x	x		
12					x	x					x	x	x		
13						x	x				x	x	x	x	
14							x						x	x	x
15							x	x	x					x	x

Approach 1: Particle Decomposition

- Every processor gets N/P particles
- Every processor calculates the forces on its particles and keeps track of their position
- To calculate the forces, every processor needs to know all other particle positions (all-to-all communication)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x				x					x					
2		x	x		x	x	x								
3		x	x	x			x	x							
4			x	x				x	x						
5	x	x			x	x				x	x	x			
6		x			x	x	x					x	x		
7		x	x			x	x	x					x	x	x
8			x	x			x	x	x						x
9				x				x	x						x
10	x				x					x	x				
11					x					x	x	x	x		
12					x	x					x	x	x		
13						x	x				x	x	x	x	
14							x						x	x	x
15							x	x	x					x	x

Approach 1: Particle Decomposition

+ No load imbalance if workload linear to particle number
+ Also works for long range interaction

- Lot of communication
- Huge memory demand on every processor

Approach 2: Force Decomposition

- Every Processor calculates a part of the Force Matrix
- Only Knowledge of 2*N/sqrt(P) particles needed

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x				x					x					
2		x	x		x	x	x								
3		x	x	x			x	x							
4			x	x				x	x						
5	x	x			x	x				x	x	x			
6		x			x	x	x					x	x		
7		x	x			x	x	x					x	x	x
8			x	x			x	x	x						x
9				x				x	x						x
10	x				x					x	x				
11					x					x	x	x	x		
12					x	x					x	x	x		
13						x	x				x	x	x	x	
14							x						x	x	x
15							x	x	x					x	x

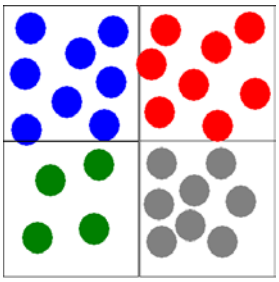
Advantages and Disadvantages of Approach 2

+ Only Knowledge of 2*N/sqrt(P) particles needed, less memory consumption
+ Good load balance if interaction between particles is “random”

- Does not scale with N/P

Approach 3: Domain Decomposition

- Every Processor is responsible for a domain in real space
- It calculates the force on the particles in this domain
- Only N/P particle positions are stored



Approach 3: Domain Decomposition

- Force Matrix in case of Domain Decomposition:

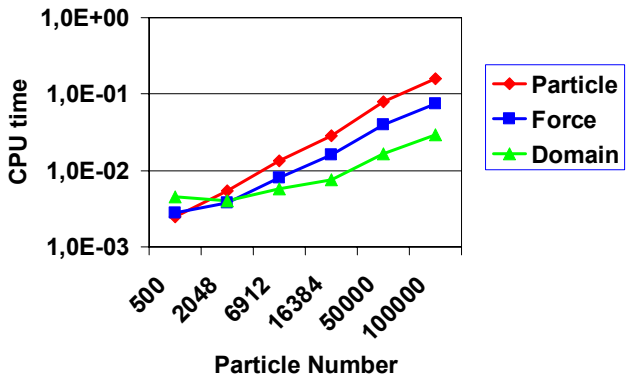
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	x	x		x	x					x					
2	x	x	x		x	x									
3		x	x	x											
4	x		x	x											
5	x	x			x	x				x	x	x			
6		x			x	x	x			x		x	x		
7						x	x	x							x
8							x	x	x						x
9							x	x	x						x
10	x				x	x				x	x				
11					x					x	x	x	x		
12					x	x					x	x	x		
13						x					x	x	x	x	
14												x	x	x	x
15							x	x	x					x	x

Advantages and Disadvantages of Approach 3

+ Scales with N/P
+ Little memory consumption, all information is distributed across CPUs

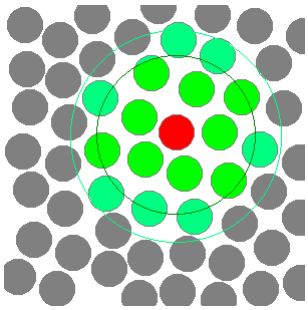
- Possible load imbalance if particles distribution is not homogeneous in space
- Algorithm is more complicated to implement

Comparison of Different Approaches



Molecular Dynamics with Verlet Neighbor Lists

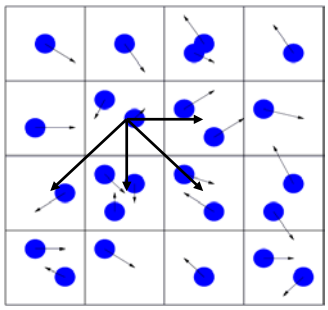
- Basic idea: limit the calculation of forces to particles within interaction range



- Problem: creation of verlet neighbor lists is still of order N*N

Molecular Dynamics with Linked Cell Algorithm

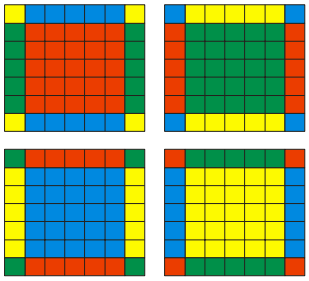
- Calculation of forces with linked cell algorithm
  - cells with length >= cut-of-length of interaction
  - interaction limited to cell and its direct neighbors
  - use of actio=reactio
  - results in O(N) algorithm



Parallel Molecular Dynamics

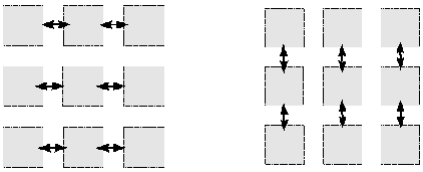
• Grid of linked cell algorithm is useful for parallel algorithm

• The information about particles in cells at processor boundaries needs to be communicated



Details of Communication: General Pattern

- Solution 1: Direct Communication
  Send all data directly to the neighbors
  (27 in three Dimension, 9 in two)
- Solution 2: Plimpton scheme:



Advantage: only 6 communications (4 for two dimension)
Disadvantage: second stage can only start after first has finished

Details of Communication: actio=reactio across CPUs

- Approach 1: calculate once, communicate results to all CPUs where this particle is in ghost cells.
- Approach 2: don't use actio=reactio across CPU boundaries. Calculate forces with ghost particles twice (or several times in corners).

Which approach is better depends on your communication and computation speed. In other words: how many data your particle contains and how expensive your force calculation is.

The general rule is, that communication is more expensive than computation.

Details of Communication: Problem of buffer space

- Problem: the exact amount of data is unknown at the receiver

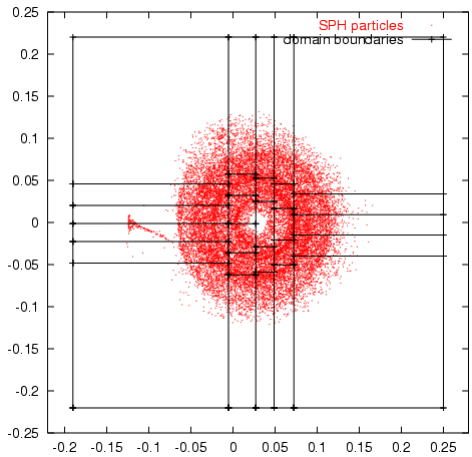
```
MPI_Send(buffer,count,my_type,dest,tag,comm);
MPI_Recv(buffer,max_count,my_type,...);
```

- Solutions:
  - `max_count` might be known
  - use `MPI_Probe` to determine size of pending message
  - send two messages, the first announces the amount of data
  - use `MPI_Pack` and use the first item to distinguish whether the message is a request to increase buffer at the receiver. Manage receiver buffer size also at the sender.

Load Balancing

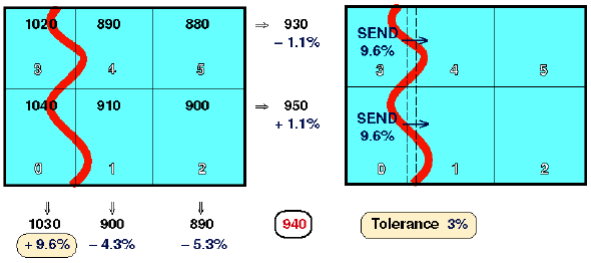
•For inhomogeneous density you will need static or dynamic load balancing.

• General load balancing will change your topology between processors.



Simple Load Balancing

- Keep Topology unchanged
- Results in good load balancing for quasi-one-dimensional density gradients.
- You have to check your physics, whether this holds



Summary

- Which approach is the best depends on your specific problem
- Some basic principles and problems are general
  - unknown particle numbers in communication
  - general scaling, but crossover will depend on interaction
  - load balancing problems
- Even a simple algorithm gets complicated when it comes to the details