Optimization of Communication-bound Applications

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How to Become Faster

Where we come from:

- **Molecular Dynamics Simulations** (MDS) on HPC Clusters in Jülich
- project FMHub (FMSolvr $\rightarrow$ Laura Morgenstern)

Computation:

- use faster/more processors
- improve methods
- improve resource awareness
- adaptive algorithms

struggle with communication overhead

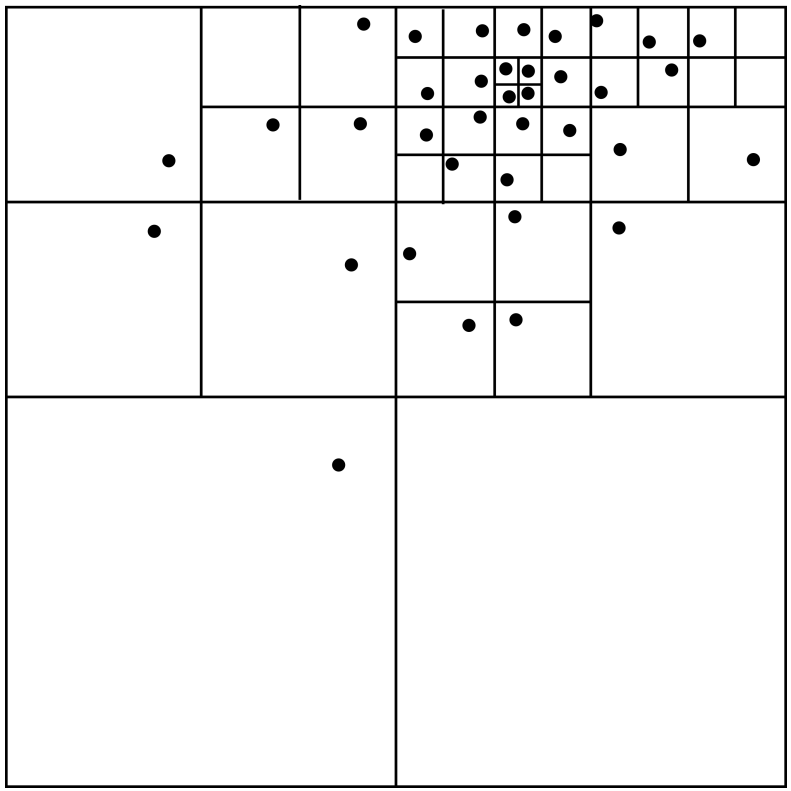
Communication:

- apply efficient communication schemes
- analyze the impact of message load
- adaptive algorithms

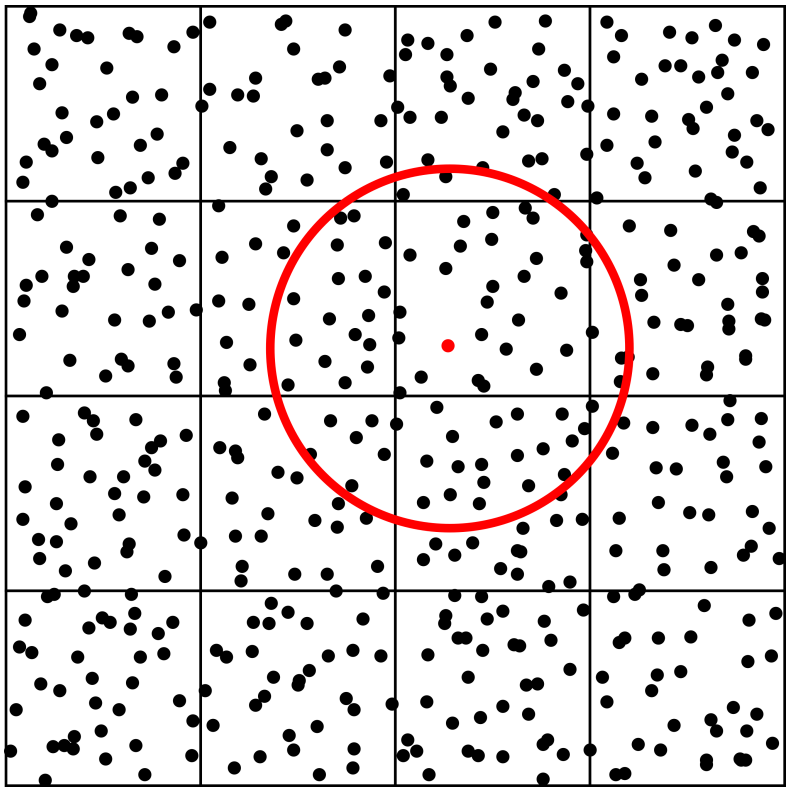
Structure

Particle Simulation

Spatial Decomposition and Range Limit

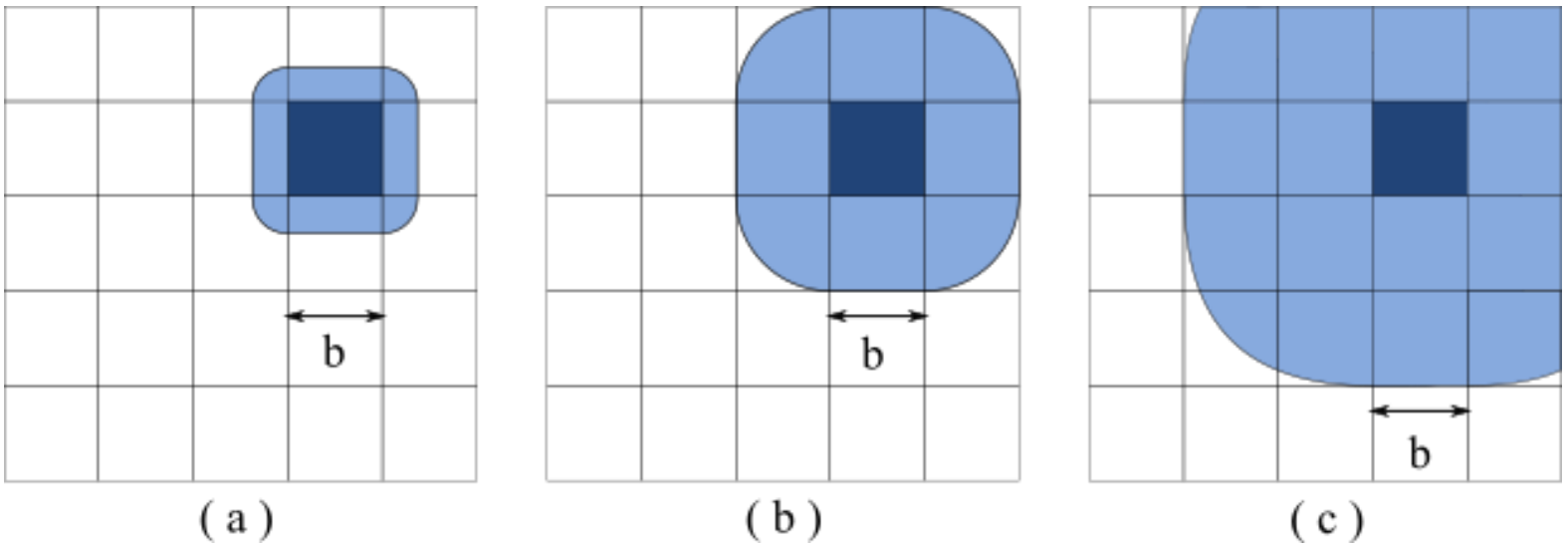


Sparse particle system



Dense particle system

Cut-off Radius R_{cut}



Import area (light blue) of the dark blue target box with different R_{cut}

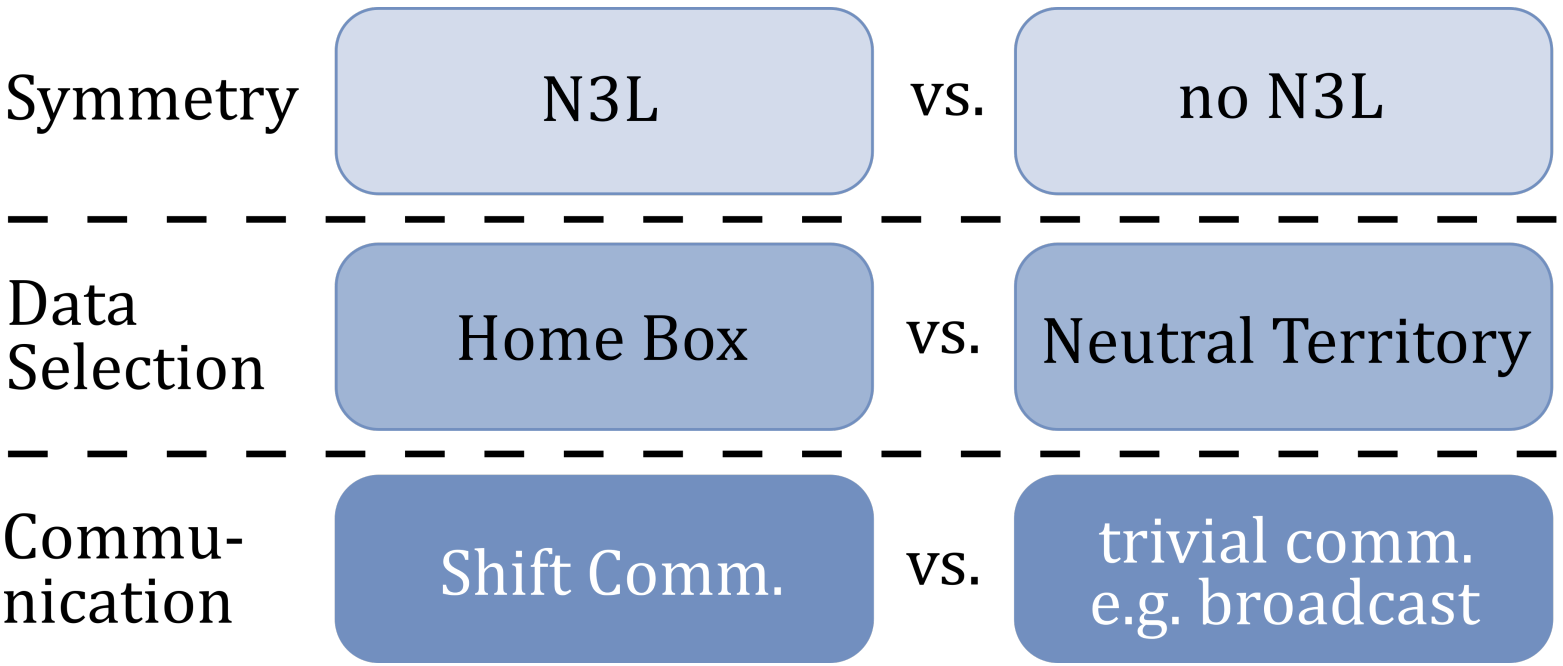
(a) $R_{\text{cut}} < b$

(b) $R_{\text{cut}} = b$

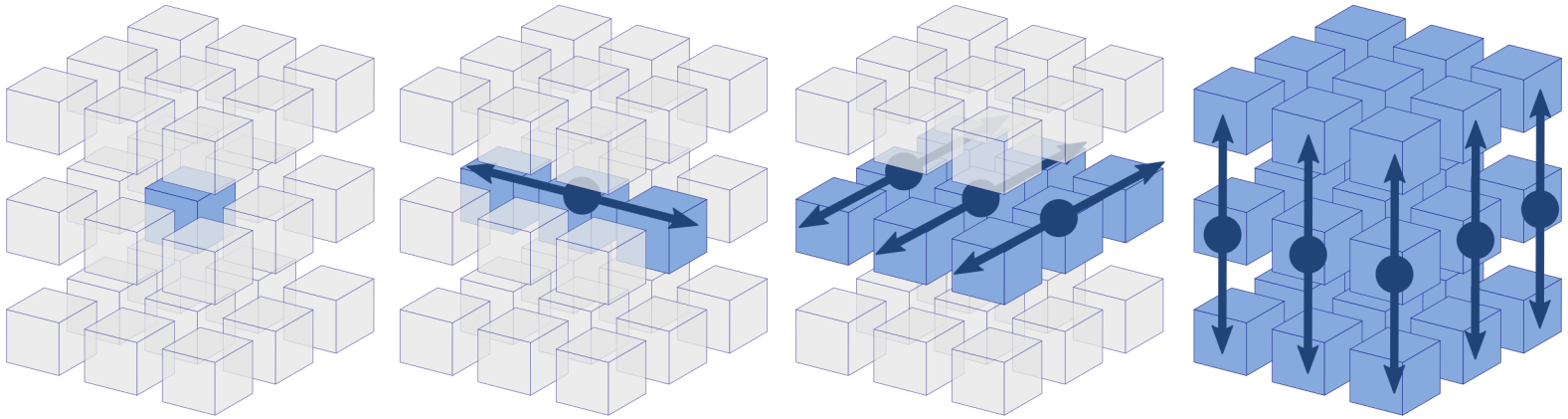
(c) $R_{\text{cut}} > b$

Communication

Categorization [Werner et al., 2022]



Fast Parallel Algorithms for Short-range Molecular Dynamics [Plimpton, 1995]



Full-Shell Shift:

(a) start of data distribution of blue box

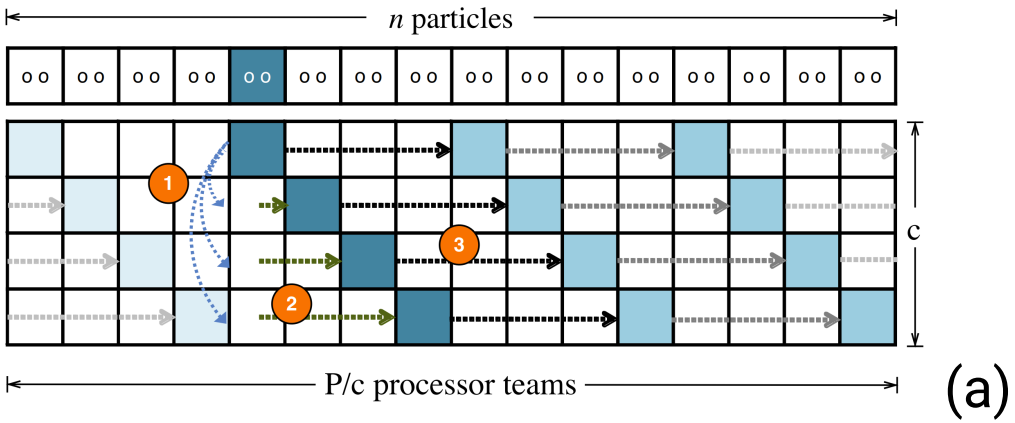
(b) data distributed along dimension 1

(c) accumulated row data distributed along dimension 2

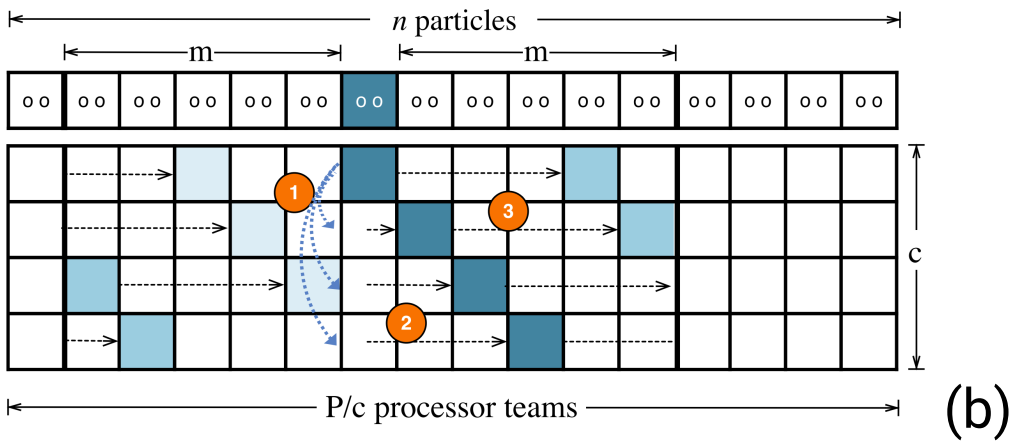
(d) accumulated plane data distributed along dimension 3

A Communication-Optimal N-Body Algorithm for Direct Interactions

[Driscoll et al., 2013]



(a)



(b)

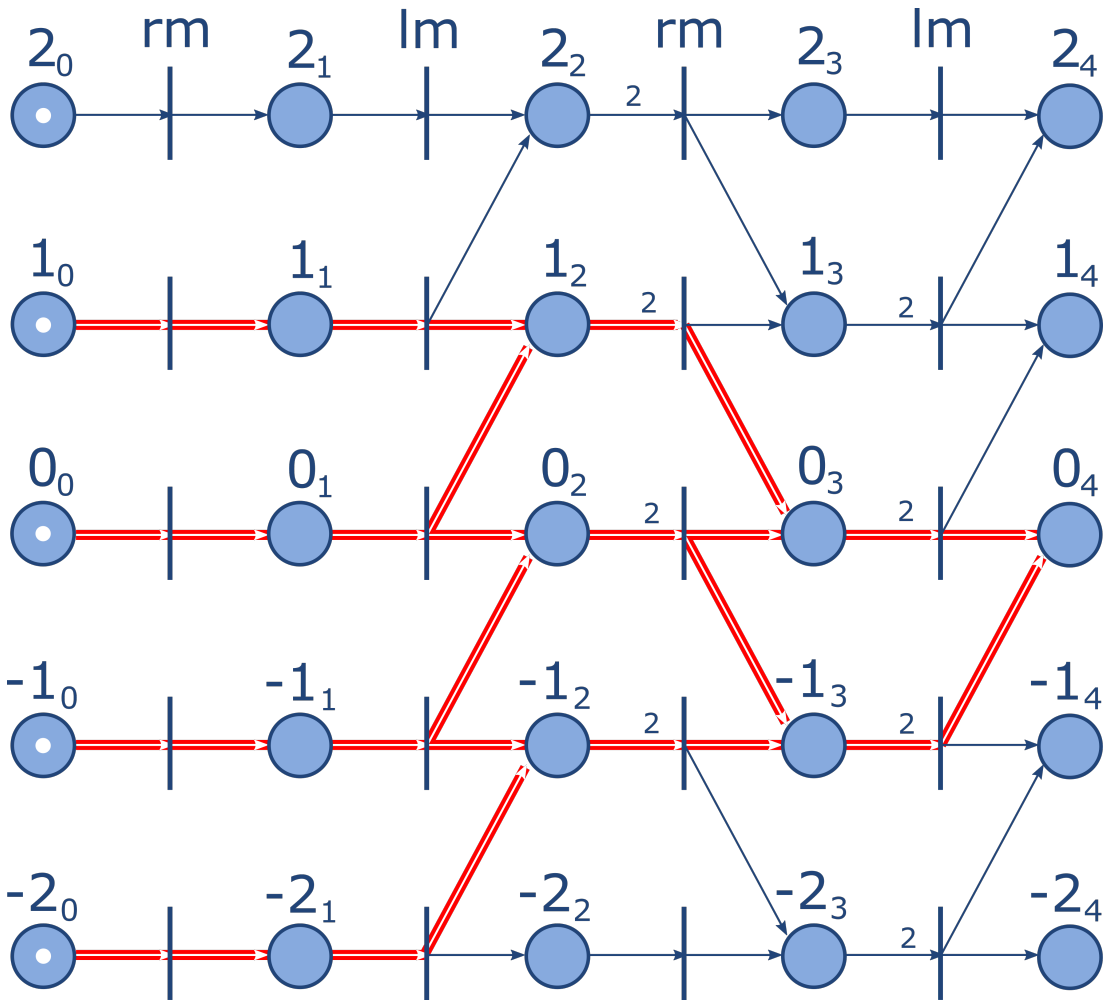
Team Shift:

(a) Team Shift for atom decomposition

(b) team Shift for spatial decomposition

Modeling

Petri Nets



local view on data/ time dependency of node 0 and its neighbors

global view requires a net where all nodes are connected or **folding**

(max,+) Algebra

(max,+)

$$a \oplus b = b \oplus a = \max\{a, b\}$$

$$a \otimes b = b \otimes a = a + b$$

(max,+) and Matrices

$$A \otimes B = \left[\sum_{k=1}^{m} a_{ik} \otimes b_{kj} \right]$$

(max,+) Matrices and Petri nets

- path from place x to place $y \rightarrow A_{xy} =$ transition time
- calculate longest path of length n: $A^* \cdot \vec{x} = \vec{v}$

  with $A^* = I \oplus A \oplus A^2 \oplus \ldots \oplus A^{n-1}$ where $A^k = \bigotimes_{i=1}^{k} A$

Summary

Current goals:

- finding efficient communication schemes for MDS ✓
- being able to formally compare them

We have:

- Shift and Team Shift
- **local model** of Shift and Team Shift with Petri nets and (max,+) algebra

We want:

- **global model** of Shift and Team Shift with Petri nets and (max,+) algebra
- **in the long run:** an (adaptive) communication module for the FMSolvr (especially for the P2P and M2L stages)

Thank You

Bibliography

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