Optimization of Communication-bound Applications

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Introduction

With the current development of increasing node numbers in High Performance Computing (HPC) and the problem that HPC applications become communication-bound, there is a need for optimized communication. We specialize in the field of Molecular Dynamics Simulations (MDS) and in specific on short-range particle interactions. One of three approaches in MDS is to distribute the simulation space over the computation nodes; this is called spatial decomposition. Since we focus on range-limited interaction, this leaves us to optimize "range-limited" communication between nodes, so communication between nodes that hold adjoining regions of the simulation space.

Conducting a Systematic Literature Review (SLR) [4] we found two promising communication algorithms, the Shift [3] (see Fig.1) and the Team Shift [2]. In order to compare these two methods formally, we aim to define a formal model of both.

Results

So far, we followed an approach with timed-transitions Petri nets and the (max,+) algebra [1]. It allows to observe the time behavior of one of the nodes and how it is influenced by its neighbors' timing. From here we want to see if there is a way to fold the Petri nets and use time-afflicted tokens. This would allow a global view on the timing of the whole network.

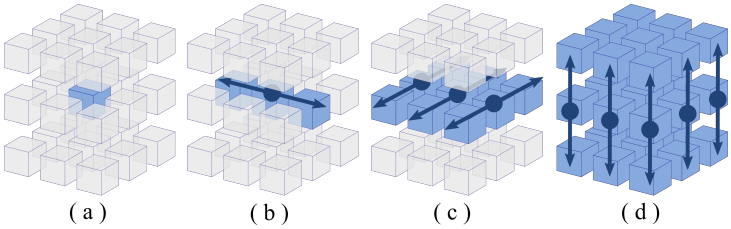

Figure 1: Shift communication [3]: The data of the blue box is first distributed along the x-dimension, then by help of its neighbors along the y-dimension and last along the z-dimension.

References

[1] François Baccelli, Guy Cohen, Geert Jan Olsder, and Jean-Pierre Quadrat. *Synchronization and Linearity, An Algebra for Discrete Event Systems*. 1992.

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[3] Steve Plimpton. Fast parallel algorithms for short-range molecular dynamics. *Journal of Computational Physics*, 117(1):1–19, 1995.

[4] Theresa Werner, Ivo Kabadshow, and Matthias Werner. Systematic literature review of data exchange strategies for range-limited particle interactions. In *Proceedings of the 12th International Conference on Simulation and Modeling Methodologies, Technologies and Applications*, pages 218–225, 2022.