A Global Network for Non-Collective Communication in Autonomous Systems

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Abstract
Large-scale simulation enables realistic 3D reproductions of micro-structure evolution in many problems of computational material science [1]. With an increasing number of processing units, global communications become a bottleneck and limit the scalability. Therefore, NAStJA[1] decomposes the simulated domain in small blocks and distributes those blocks over the processing units. Interacting processing units build a local neighborhood and act autonomously in this neighborhood. This limits the number of connections for each processing unit and therefore the local communication overhead, and leads to high scalability. Apart from the communication between local neighborhoods, a global information exchange is required. We explain the conditions and requirements for this exchange and present the benefits of a multidimensional Manhattan street network [8, 4, 5].

It is simple but sufficiently fast for a global information exchange, if the information is not time critical, i. e. the exchange has to be global only after several time steps. This global network satisfies the requirements for a global block management that connects the autonomous processes. Because of its super-linear scaling the approach is very useful for massively parallel simulations. The block distribution scales in a linear matter, and the communication overhead of the global block management can be neglected such that small blocks benefit from cache effects and result in a super-linear scaling, i. e. efficiency higher than unity. The global information exchange is based on a multi-hop exchange, where each message is sent to the direct neighbors and then spread to the whole network in a specified number of hops. Between these hops the computation goes on, so that the global exchange overlaps with the computation. The number of hops must be small enough to not influence the simulated physics.

NAStJA supports regular grids with a calculating stencil sweeping through the simulated domain. In computational material science many problems can be described using phase-field methods or cellular automata, both based on a regular grid. This is a grateful task for parallel programming. However, many of these problems require calculations only in small regions of the simulated domain. This is why NAStJA allocates and distributes only those blocks that contain such a computing region. As the computing regions move in the simulated domain

[1] Acronym for Neoteric Autonomous STencil code for Jolly Algorithm, a new developed code for arbitrary algorithms based on stencils or regular grids.

throughout the simulation, the corresponding blocks are created or deleted autonomously by the processes in the local neighborhood. The overhead for the local neighborhood communication is acceptable compared to the allocation of unneeded blocks. The current implementation of NAStJA is heavily under development, however, it is being already employed for a phase-field method specially for droplets [2], a phase-field crystal model [6, 3] and for the Potts model, a cellular automate for biological cells [7]. It can be simply extended with a wide range of algorithms that work on finite difference schema or other regular grid methods.

These techniques allow advancing to previously unfeasible, extremely large-scale simulation. Especially for phase-field simulations, the computing region is only a small part of the simulated domain. Here the calculation occurs only in the interface region between the phases. As an illustration, the morphology of a water droplet on a structured surface simulated with the phase-field method has a small computing region which is the interface region between the water and the surrounding gas. The simulated quantities are constant inside and outside of the droplet. In phase-field simulation the width of the interface is chosen as about 10 cells. Using a regular grid, the mandatory resolution of the finest structure defines the scale and thus the total number of cells in the simulation domain. For a 1 µl droplet and a structure size of 20 nm with a resolution of at least twice the interface width, this results in a simulation domain of $> 10^{12}$ cells. This is too large for a traditional phase-field code that allocates the whole simulated domain and results in an intractable computational task. The presented techniques from NAStJA address these issues and improve the feasibility of large-scale simulation. We show measurements and theoretical calculation for the Manhattan street network compared to a global collective communication. As an example application we present the phase-field method.

Keywords: large scale, autonomous systems, Manhattan street network, global communication, phase-field method

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