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Parallelization of a multigrid method for PDEs with open boundary conditions

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The solution of PDEs with so-called open boundary conditions plays an important role in different areas, e.g. in the simulation of molecules or in aerospace engineering. An example is the Poisson equation

$$-\Delta u(x) = f(x)$$
, for all $x \in \mathbb{R}^3$, where $u(x) \stackrel{\|x\|_2 \to \infty}{\longrightarrow} 0$,

as it is needed in molecular dynamics simulation. In [2] we extended the method developed by Washio and Oosterlee in [3]. In contrast to the original method the modification guarantees that the number of levels depends on the grid size of the finest level, only. The optimality of the method w.r.t. the number of unknowns was proven in [1].

For large-scale simulations, as they are carried out e.g. in the chemical industry, a highly scalable method is needed. The parallelization of the method is not straightforward, as either an imbalance of the work occurs on some levels, or a sophisticated communication scheme is required.

In the talk the multigrid method is described, the two parallelization approaches are outlined and a comparison of the two is presented.

Bibliography

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