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Multigrid solution of compact high-order finite differences for interface problems

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Compact high-order finite difference stencils are an interesting option for the discretizing elliptic equations on structured girds, since they can achieve high accuracy while maintaining the simplicity of a finite difference approach. In the world of ubiquitous parallelism, and in particular for massively parallel computing in distributed memory environments, they can profit from the simplicity of the data dependencies. This simplifies the communication structure and may improve the parallel efficiency by reducing message passing overhead.

Introduced in the 1960s by Lothar Collatz as "Hermitian methods" (in German "Mehrstellenverfahren") the method has been extended by Zhilin Li, Kazufumi Ito and others to the Immersed Interface Method and is thus applicable to cases with discontinuous coefficients.

One important application for these methods comes from problems in electrochemistry where the potential equation imposed by an ensemble of atoms has to be solved accurately and efficiently. Here not only the conservation of energy plays a major role, but the solution must be accurate enough so that also its derivatives, i.e. the forces, can be reconstructed accurately. Though frequency space methods based on the FFT are often used as solvers, multigrid methods are increasingly considered as interesting alternatives, since they are more flexible, have asymptotically better complexity, and may be enjoy better parallel efficiency.

In our contribution, we show how compact high-order finite difference stencils can be designed efficiently for elliptic problems with variable and jumping coefficients that arise from the field of electrochemistry. The application induces special constraints for the discretization, so that our problem is posed on a structured 3D rectilinear grid that has different step size in all dimensions. Techniques to choose the stencil coefficients optimally are developed. We demonstrate how the new high-order finite differences for variable and jumping coefficients can be integrated into the parallel, multigrid solver of the molec-

ular dynamics code "rsdft" that is used for ab initio simulations. Finally, we show numerical results for typical application benchmarks as well as a runtime performance evaluation.