Features of ViennaCL in PETSc

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Typical solver packages for the large-scale solution of linear and nonlinear systems of equations provide insufficient support for heterogeneous hardware, in particular graphics processing units (GPUs). Unfortunately, this implies that scientists have to write their own GPU code if they intend to use GPUs on supercomputers. This, however, would hamper their productivity and reduce the overall scientific output. Therefore, better GPU support in solver packages would greatly increase productivity on these heterogeneous machines.

This VSC School project[1] aims to build the necessary software infrastructure to better support heterogeneous supercomputers. To do so, we enhanced the GPU capabilities in the software library ViennaCL[2] [1]. Since ViennaCL only targets shared-memory nodes, its functionality is not directly available for distributed memory nodes. On the other hand, certain features such as ViennaCL's algebraic multigrid preconditioners [2] are made available in the popular large-scale solver library PETSc[3] through a plugin-mechanism. We report on the enhancements in ViennaCL and the new GPU capabilities available in PETSc through ViennaCL. With these new functionalities, it is now possible to simultaneously use all computing hardware available in a heterogeneous supercomputer, rather than using only the CPUs or the GPUs (but not both).

Case Study: MatMatMult. One example for a native optimization in PETSc is the case of matrix-matrix optimizations (routine `MatMatMult`), for which we ported ViennaCL's highly optimized routines [3]. We present benchmark results for squaring system matrices based on commonly used finite-difference stencils in two and three dimensions. As depicted in Fig. 1, up to twofold performance gains are obtained on INTEL Ivy-Bridge CPUs (cf. VSC-3).

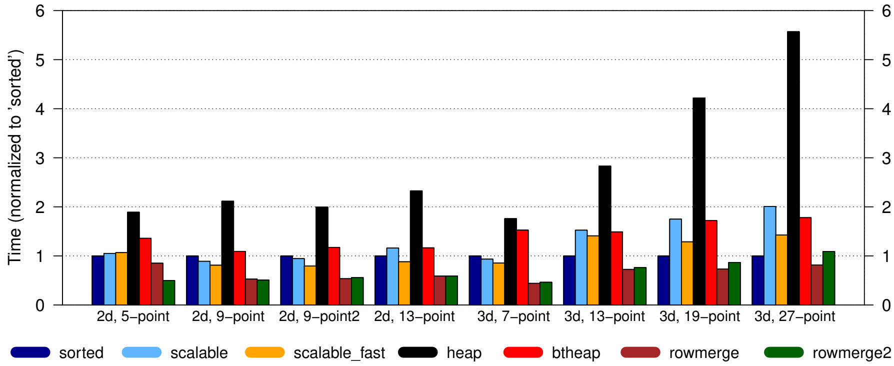

Fig. 1: Comparison of execution times for different sequential matrix-matrix multiplication implementations in PETSc. Our new routines 'rowmerge' and 'rowmerge2' offer up to twofold performance gains over PETSc's routines (default: 'sorted').

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References

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[2] Rudolf, F., Morhammer, A., Rupp, K., Weinbub, J., AHPC 2017, 40 (2017).

[3] Morhammer, A., Rupp, K., Rudolf, F., Weinbub, J., AHPC 2016, 23 (2016).

[1] https://github.com/viennacl/vsc-school/
[2] http://viennacl.sourceforge.net/
[3] http://mcs.anl.gov/petsc/