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Computer Architectures for Exascale Computational Fluid Dynamics

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In the exascale and upcoming post-Moore era, we are seeing a drastic increase in different heterogeneous computer architectures. In current supercomputers, we are seeing an explosion of GPUs from different vendors, novel multicore processors such as the A64FX, vector cards, and an increased interest in other, specialized, forms of computing such as field-programmable gate arrays (FPGA).

We have had the opportunity to explore several of these new computer architectures with our high-fidelity flow solver based on the spectral element method, Neko [1]. In this work, we will present the performance of Neko for a wide range of computer hardware ranging from classical Haswell Intel x86 processors, newer AMD CPUs, Nvidia and AMD GPUs, the NEC SX-Aurora Tsubasa, and whether it is feasible to run a large-scale CFD solver on FPGAs [2, 3].

We will discuss the key findings with regards to performance, ease of use, software development, and future trends for all of these different architectures and what their impact is for large-scale CFD simulations. As the characteristics of different computing units make them more or less well suited to algorithms and flow solvers, we will present what we have learned from Neko and the spectral element method, and what can be transferred to other solvers and discretizations. In the end, we discuss what we believe are the most important performance characteristics necessary for computer architectures to enable exascale and post-exascale fluid simulations.

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