The Future of CFD Simulations (from a numerical & computational perspective) - Faster and more reliable predictions are needed to compete with AI

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The main aim of this talk is to discuss how modern High Performance Computing (HPC) techniques regarding massively parallel hardware with millions of cores together with very fast, but lower precision accelerator hardware can be applied to numerical simulations of PDEs so that a much higher computational, numerical and hence energy efficiency can be obtained. Here, as prototypical extreme-scale PDE-based applications, we concentrate on nonstationary flow simulations with hundreds of millions or even billions of spatial unknowns in long-time computations with many thousands up to millions of time steps. For the expected huge computational resources in the coming exascale era, such type of spatially discretized problems which typically are treated sequentially in time, that means one time after the other, are too small to exploit adequately the huge number of compute nodes, resp., cores so that further parallelism, for instance w.r.t. time, might get necessary.

In this context, we discuss how "parallel-in-space & parallel/simultaneous-in-time" Newton-Krylov Multigrid approaches can be designed which allow a much higher degree of parallelism. Moreover, to exploit current accelerator hardware in lower precision (for instance, GPUs from NVIDIA built for AI applications), we discuss the concept of "pre-handling" (in contrast to "preconditioning") of the corresponding ill-conditioned systems of equations, for instance arising from Poisson-like problems. Here, we assume a transformation into an equivalent linear system with similar sparsity but with much lower condition numbers so that the use of lower precision hardware might get feasible. In our talk, we provide for both aspects numerical results as "proof-of-concept" and discuss the challenges, particularly for incompressible flow problems.