Online Monitoring and Manipulation for Computational Steering of Massive Parallel Fluid Dynamics Simulations

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Quality and efficiency of numerical algorithms in computational fluid dynamic (CFD) systems have increased dramatically in the last forty years. For this reason, CFD became the most powerful tool in many application domains, one of them being aircraft design. Additionally, computer architectures performance is increasing dramatically. Nowadays, it is common for many research facilities to operate and maintain their own teraflop cluster system and petaflop cluster systems are available at large computation centers. Exascale systems are targeted to be available in the year 2018. Therefore, numerical analysis of aerodynamic flow fields provides highly accurate result data with enormous and still increasing extent.

One of the problems of existing CFD solutions is the sequential manner of their traditional work-flow. The main steps of the work-flow are the definition of the flow effects to be examined, mesh generation and mesh partitioning, the actual calculation on a cluster system and a subsequent analysis in a post-processing and visualization step. The main flaw is that parameters chosen wrong in the first place can only be recognized after the whole work-flow finished. A correction of those parameters leads to re-execution of at least some parts of the work-flow. Finally, this entire process needs to be iterated until the result meets the required standards, a time-consuming situation to be avoided on supercomputer systems where computational time is not available exclusively and comes with high costs for usage and storage.

Computational Steering is assumed to provide more flexible work-flows capable of reducing required simulation time and iteration counts. Therefore, adequate online monitoring techniques are required providing to sufficiently judge the state of an ongoing simulation. Computational steering itself is the process of changing a simulation state at runtime. The benefit for CFD applications is that simulation parameters can be tweaked during a simulation run without the need to start the work-flow all over again.

This thesis addresses the problems of sequential CFD work-flows by introducing online monitoring and computational steering concepts into existing CFD systems. The focus is on application-dependent visualization methods needed to provide sufficient information about ongoing simulations and their quality. A software infrastructure needs to be developed supporting coupling strategies to numerical algorithms. Data transfer schemes are required to transfer data between distributed computing and visualization clusters as well as bringing changes back into running parallel simulations.