

Industrial and Biomedical CFD Workflows Enhanced with In Situ Knowledge Capture and Computational Steering

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Abstract

Over the past decade, the convergence of accessible HPC and high-fidelity simulation has created a bottleneck in analysis workflows: writing, managing and reading very large files. There has been much research performed on mechanisms to access information directly from the memory of the running solver code, known variously as ‘in situ’ or ‘co-processing’. Several software solutions have been developed to implement these mechanisms, such as Paraview/Catalyst, VisIt/Libsim and SENSEI. These tools are developed with visualization as the primary goal, and are highly dependent upon VTK (kitware, USA). This paper describes a new approach to enhancing CFD workflows that provides services for visualization, data science, job monitoring, provenance capture and logging along with computational steering of the solver code. The software, called Kombyne™ accomplishes these functions with a very low code footprint, few to no external dependencies (VTK is not required) and direct support for ‘in transit’ operation where the workload and memory requirements are delegated to a separate process, working in tandem with the solver code.

This paper documents three recent examples of Kombyne™ applied to industrial-scale CFD analyses. In the first case, high-fidelity frequency analysis of a cylinder in supersonic crossflow was needed to calibrate data science workflows with experiment. The unique requirement here is obtaining a block of sample points at *every solver timestep*, to ensure that no temporal aliasing artifacts were present in the data used for the FFT analysis. The NASA Overflow2 solver was instrumented with Kombyne™ and its data science pipelines used to directly create matrices for Matlab. The analysis demonstrated that the primary acoustic signal in the test was caused by the oscillation of the separation location on the cylinder.

The second application is a biomedical workflow intended to demonstrate the feasibility of using quick-turnaround CFD to advise surgeons on the condition of a patient’s aneurysms. Here, unsteady simulation via OpenFOAM is used with geometry obtained through a patient’s scans. The time to write and read large files would be prohibitive to the goal of automatic overnight turnaround. OpenFOAM was instrumented with Kombyne™ and pipelines were activated to create extracts of surface geometries colored by biomedical markers of use to the surgeons. These extracts could then be easily visualized in the user’s choice of visualization tools.

Solver steering has been a topic of discussion and research for many years. The third example uses "Computational Steering" where the Rolls-Royce production flow solver Hydra was instrumented with

the Kombyne™ software to enable on-the-fly changes of the computational setup for the production of compressor maps for gas turbine engines. These maps show the relationship between efficiency, pressure ratio and corrected mass flow for a given corrected shaft speed. In typical CFD workflows, several sets of operating conditions, each capturing several points per curve are computed by means of multiple simulation runs with manual assembly of data points into the plot which constitute the map. For this application, the exit flow boundary condition is changed while the solver is running, treating the CFD simulation like a virtual experiment where operating conditions can be changed while the "virtual engine" is running. The benefits of this approach are rapid turnaround time, more confidence in producing the compressor maps and convenient production of visualization extracts for verification and reporting.