Towards clean propulsion with synthetic fuels: Hierarchical, cluster-modularized simulations with node-level optimization and deep learning

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Development of new clean propulsion technology with synthetic fuels, such as oxymethylene ethers (OMEx), is difficult as the parameter space of possible realizations is large and cannot be investigated cost efficiently by experimental methods as, for example, geometry optimizations require manufacturing. The only way to overcome this issue is by combining experimental and simulation techniques. However, also simulation techniques struggle with the wide range of involved scales, and a direct approach would exceed the currently available computing capacities. Therefore, this work presents a hierarchical simulation approach employing direct numerical simulations (DNSs) as high-order models as well as large-eddy simulations (LESs) as reduced-order models. For this, different Tier-0/1 and Tier-2 machines of the German supercomputing landscape are utilized.

The models of different order differ decisively in terms of the resulting communication patterns. While the used high-order models mainly rely on all-to-all communication, the reduced-order models mostly require local communication. Consequently, the DNSs were performed on JUQUEEN, Jülich Supercomputing Centre (JSC), with its 5D torus network as it allows good performance for all-to-all communication. The LESs were done on Hazel Hen at High-Performance Computing Center, Stuttgart (HLRS) in order to benefit from the higher amount of memory per core compared to JUQUEEN, which allows more efficient data usage in the computational fluid dynamic (CFD) simulations without considerable penalty for the less performant network due to mainly local communication. As the data of the DNSs are required as boundary conditions (BCs) for the LESs, coupling is needed. In this work, a convolutional neural network (CNN) was trained with the DNS data in order to reduce the required data transfer from terabytes (TBs) to gigabytes (GBs). This training was done using modularized computing on JUQUEEN/JURECA at JSC with on-the-fly data streaming. In this way, JURECA's GPUs were efficiently used and classical I/O avoided. Pre- and postprocessing was done on CLAIX16 at the IT Center, RWTH Aachen University. Its nodes with up to 1 TB memory were optimal for data modifications and visualization. The optimal cluster choices enabled very good scaling and node performance. Overall, the combination of hierarchical simulations, modularized computing and deep learning allowed an iterative technology development cycle, as feedback to the experiment at Argonne National Laboratories (ANL) was possible on time (edge2cloud). Optimizations with respect to nozzle geometry, injection conditions and fuel properties were realized.

Besides presenting physical results and the hierarchical, modularized computing approach, this work focusses on scaling and single node performance of the used CIAO code. Multiple improvements are shown and discussed. Scaling plots and performance measurements in terms of FLOPS are presented.

Additional notes:

- This project used computing time via GCS (GCS-MRES) and via JARA-HPC (JARA0188, JHPC55, JHPC18)
- The optimizations on Hazel Hen were awarded by the Golden Spike Award 2018 by the High-Performance Computing Center, Stuttgart