Dynamic Load-Balancing of Thermodynamics and Chemistry in a Multi-Phase, Reacting CFD Solver

Victor Azizi[1], Gijs van den Oord[1], Mohamed Fathi Azarkhavarani[2], and Stefan Hickel[2]

[1]Netherlands eScience Center
[2]Aerodynamics Group, Faculty of Aerospace Engineering, TU Delft

November 8, 2021

High-fidelity computational fluid dynamics (CFD) simulations of chemically reacting, multi-phase turbulent flows are essential for the development and optimization of turbines, combustion engines, and chemical process plants. A realistic and detailed representation of such multi-physics fluid dynamics allows us to improve the design of these applications towards more efficient energy conversion and improved sustainability within the industrial production chains, transport and energy sectors.

However, the modeling of these phenomena remains computationally challenging. Large-scale parallel simulations of multi-phase and multi-species fluids tend to give rise to unbalanced workloads because the computation needed for, e.g., solving the stiff system of equations for chemical reactions is not evenly distributed over static mesh partitions. A prime example is the simulation of the ECN Spray-A benchmark[1], where cold fuel is injected at trans-critical conditions into a hot atmosphere, and computationally-demanding ignition cores appear within the spatially developing jet region. As the different parts of the physical model display drastically different computational load per mesh point, it may be beneficial to offload tasks to idle processors. Moreover, for transient setups like Spray-A, the load per mesh point for chemistry and thermodynamics can heavily vary in space and time. The re-partitioning can therefore not be pre-computed and dynamical load balancing (DLB) is required to eliminate processor idling and accelerate the computation.

We have implemented DLB in INCA, a multi-physics CFD solver that uses adaptive mesh refinement and incorporates chemical kinetics, vapour-liquid phase change and real-gas thermodynamics. We have developed a modular infrastructure within INCA to offload compute-intensive mesh points to other processors. The transfer of work over MPI has been implemented independently for the chemistry calculations and the evaluation of the caloric and kinematic equations of state, which dominate the computational profile for complex reacting flows like Spray-A. We use the computational load from previous time steps as a predictor for the expected work per mesh point. We have implemented several parallel re-partitioning strategies, from simple diffusive schemes to node-aware algorithms, and have benchmarked these methods within the context of Spray-A. We show that these strategies are fast enough to allow a re-partitioning every time step to mitigate the highly transient nature of the workload per mesh point. We also show that in this application of DLB, communication volumes are small and the quality of the balanced partitioning determines the total runtime.

As a result, we show we are able to substantially speed up the INCA code for reacting multi-phase flows by improving the processor utilization and parallel scaling of the application. This will enable users of INCA to increase the resolution and to achieve more accurate results.

References

[1] Jan Matheis and Stefan Hickel. “Multi-component vapor-liquid equilibrium model for LES of high-pressure fuel injection and application to ECN Spray A”. In: *International Journal of Multiphase Flow* 99 (2018), pp. 294–311.