Part III
 Reactive Flows

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The three contributions in the section “Reactive Flows” continue the successful work of the last year. Two projects are based on the OpenFOAM and the third one on the in-house code TASCOM3D. They increase the efficiency of the codes by implementing some parts of the Cantera-code (chemical reaction) directly into the OpenFOAM software, they apply the code to more complex applications and they improve the LES modeling, respectively.

In the first contribution by T. Zirwes, F. Zhang, J. Denev, P. Habisreuther, H. Bockhorn about “Automated code generation for maximizing performance of detailed chemistry calculations in DNS of turbulent combustion” a DNS-code for turbulent flames is considered. In the last year this group presented a code with a reaction mechanism with 18 species and 69 fundamental reactions, containing the optically active OH radical. The main goal was the investigation of the correlation between heat release rate and the luminescent species in turbulent flames. The implementation was based on the open source software OpenFOAM for the CFD part and Cantera for the chemical reaction. Now in this year they could get additional performance gains by extracting relevant classes from Cantera and implementing them directly into an OpenFOAM library, so that Cantera is not an external dependency anymore and its methods are called by the OpenFOAM solver directly. This led to further performance improvements. In this way, highly specialized code leads to a decrease of total simulation time by up to 40%, and the performance improvement increases with the complexity of the reaction mechanism. The optimization concept is applied to a realistic combustion case simulated on two high performance clusters with different network architectures,
Hazel Hen and ForHLR II, showing good parallel performance on up to 28,800 CPU cores.

The authors of the second contribution about “A resolved simulation study on the interactions between droplets and turbulent flames using OpenFOAM” are B. Wang, H. Chu, A. Kronenburg, and O.T. Stein. In the last year this group used the OpenFOAM software package for DNS. The results were compared to benchmark data obtained from a dedicated high order DNS solver, to study the effects of the lower order discretization provided by OpenFOAM. The results are provided in a concise manner and the computations performed with OpenFOAM were in good agreement with the benchmark of the more specialized code. Now in this year the group applied the code to a more complex setting and present a direct numerical simulations (DNS) of turbulent reacting flows around evaporating single fuel droplets and droplet arrays. Statistical analysis of interactions between the droplets and the turbulent flames are used to develop sub-grid scale models for mixture fraction based on approaches such as flamelet or conditional moment closure (CMC) methods. The specific challenges are posed by the effects of the evaporating spray on the composition field in inter-droplet space and by the presence of combustion. They suggest an optimal setup for fully resolved spray DNS that ensures a good balance between computational cost and solution accuracy. Furthermore, adequate scalability of OpenFOAM for the different setups is reported.

The subject of the third contribution about “Towards affordable LES of rocket combustion engines” by R. Keller, M. Grader, P. Gerlinger, and M. Aigner” is still the compressible, implicit combustion code TASCOM3D as in the year before. At that time the code was validated by nonreactive and reactive benchmark tests at high pressures. The simulation results matched experimental observations very well in a qualitative and quantitative manner. In this year the authors present new simulations with affordable LES based on different DES-models. They compare and evaluate the results on two simple test cases. The version “iDDES” shows promising results to be used in future rocket combustion engine simulations.