OpenFOAM & Combustion Simulation

Highly Accurate and Efficient Simulation of Combustion on Modern Supercomputers with OpenFOAM Coupled to Cantera

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Host: Yiqing Wang (Peking University)

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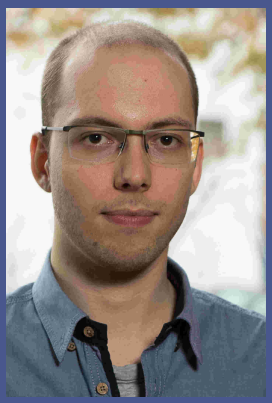
Abstract

The detailed simulation of combustion processes is an important aspect for gaining a better understanding of the underlying physics, which is required to improve future energy conversion systems. To achieve this, several prerequisites have to be met: on the one hand, the simulation has to employ a detailed description of both the chemical reaction rates as well as molecular diffusion processes; on the other hand, the simulation has to be computationally efficient since detailed simulation of turbulent flames require vast amounts of computational resources due to the large number of intermediate chemical species and the discrepancy between the fastest and slowest time scales. In this talk, several new additions to OpenFOAM's reacting flow solvers are presented. By coupling OpenFOAM with the open-source thermo-chemical library Cantera, transport coefficients for each chemical species derived from kinetic gas theory can be employed. To speed up the computation of chemical reaction rates, several improvements are discussed: the use of ODE integrators that are more efficient than the ones available in OpenFOAM can lead to significant time savings. Another approach is automated code generation, which helps to produce highly optimized source code that can be easily integrated into OpenFOAM. In total, these improvements can reduce simulation times of typical applications by about 70% without loss of accuracy. Applications of the new reacting flow solver, called EBIdnsFoam, ranging from laminar hot particle ignition to turbulent flames scaling up to 32000 CPU cores are presented. Lastly, even though OpenFOAM's finite volume approach is limited to an overall second order method, the use of higher order face interpolation schemes can help to significantly improve the numerical accuracy. This is demonstrated by several canonical test cases.

About the Speaker



Thorsten Zirwes received his PhD in chemical engineering from the Karlsruhe Institute of Technology. He has been using OpenFOAM for 10 years and is a contributor to OpenFOAM and co-author of Cantera. His research concerns the detailed simulation of combustion processes with a focus on high-performance computing. He developed several approaches that target performance optimization for large-scale applications of OpenFOAM and improve the accuracy of molecular transport models. His solvers and models are used by more than 25 research groups around the world as well as by industry. For his work, he received a best paper award at the ESI OpenFOAM conference and the Golden Spike Award from Germany's National High Performance Computing Centers. He teaches a biannual one-week OpenFOAM course in Germany and supports OpenFOAM users on the high-performance computing clusters at the Karlsruhe Institute of Technology. He is currently a visiting postdoctoral scholar at Stanford University as a DAAD PRIME fellow, working on pore-resolved simulations of porous media burners and ammonia combustion.