Generation of a Database with Detailed Numerical Simulation of Mixed-Mode Combustion

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\section*{Introduction}
- Combustion provides over 80 \% of the world’s primary energy
- A better understanding of mixed-mode combustion is necessary in order to make future combustion systems more efficient
- A very detailed numerical simulation is validated for a mixed-mode combustion flame, which presents a challenging task for current combustion codes

\section*{Code Development and Code Coupling}
- The code \cite{1} is implemented in the CFD package OpenFOAM
- It is coupled to the open-source kinetics library Cantera in order to provide detailed gas properties from gas kinetic theory
- The code employs detailed gas properties and complex chemistry and can use unstructured grids
- Code Development is a cooperation between the Steinbuch Centre for Computing (SCC) and the Engler-Bunte-Institute (EBI).

\section*{Objective}
- Detailed numerical simulation of realistic turbulent flames
- Creation of a comprehensive numerical database for a well-documented mixed-mode flame

\section*{Code Optimization}
- The simulation can only be performed on massively parallel clusters
- In a recent work \cite{2}, load balancing issues have been fixed with EXTRAE/Paraver and ScoreP/Scalasca/Vampir (EoCoE workshop)
- Below: Green/Blue: Computing time; Red: Communication time

\section*{Example: Turbulent “Sydney” Flame}
- Simulation of the partially premixed “Sydney flame” on a mesh with 150mil. cells. 10 TB Data, which will be made public in a database.

\section*{Lagrangian Particle Tracking}
- Particle tracking is used to obtain temporal data at specific locations
- With this technique, time signals of flow and flame properties can be investigated \cite{3}
- Efficient distribution of the particles is still a challenge in HPC

\section*{High Performance Computing}
- The code was run on ForHLR II at SCC on up to 10,000 CPU cores and on Hazel Hen at HLRS on up to 28,800 CPU cores
- Scaling results show that the code can be efficiently used for high number of chemical species

\section*{References}
\begin{itemize}
  \item \cite{1} F. Zhang, H. Bonart, T. Zirwes et al., Springer, 2015.
  \item \cite{2} T. Zirwes, F. Zhang, J.A. Denev et al., Springer, 2017
  \item \cite{3} F. Zhang, T. Zirwes et al., Combustion and Flame, 2017
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