

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

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## 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

## Code Development and Code Coupling

- The code [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)

OpenFOAM (Fluid Flow)

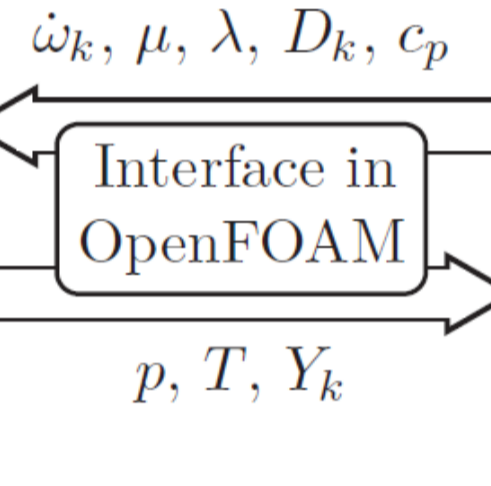
Solution of governing equations:

- total mass
- momentum
- energy
- species masses
- equation of state

Cantera (Chemistry, serial)

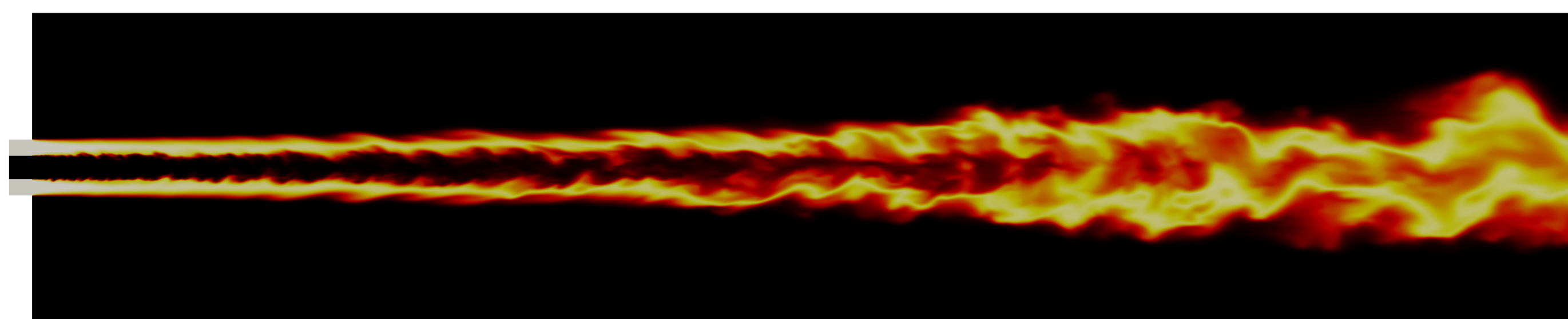
Evaluation of thermo-chemical properties:

- reaction rates  $\dot{\omega}_k$
- molecular viscosity  $\mu$
- thermal conductivity  $\lambda$
- diffusion coefficients  $D_k$
- heat capacity  $c_p$



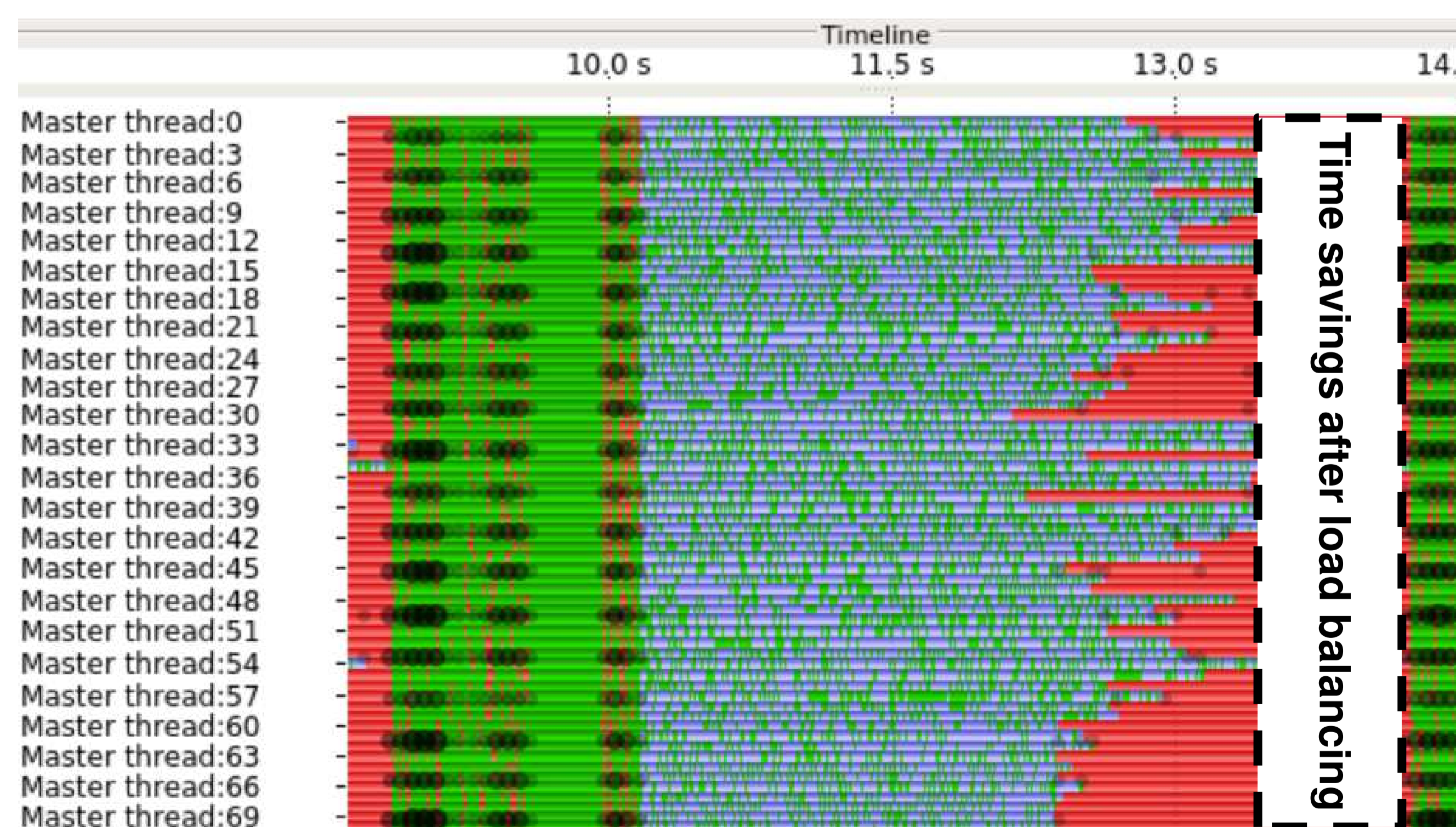
## Objective

- Detailed numerical simulation of realistic turbulent flames
- Creation of a comprehensive numerical database for a well-documented mixed-mode flame



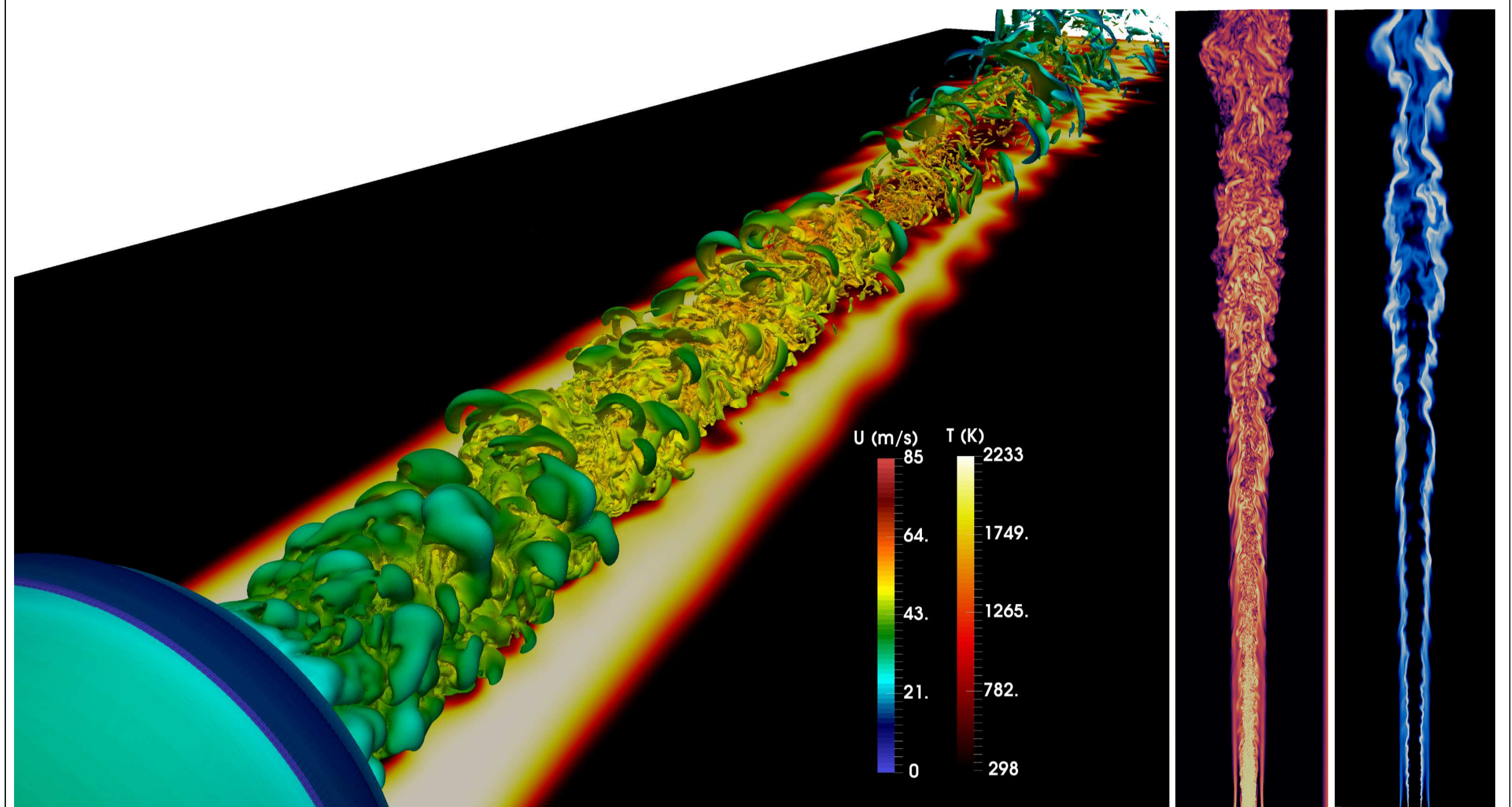
## Code Optimization

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



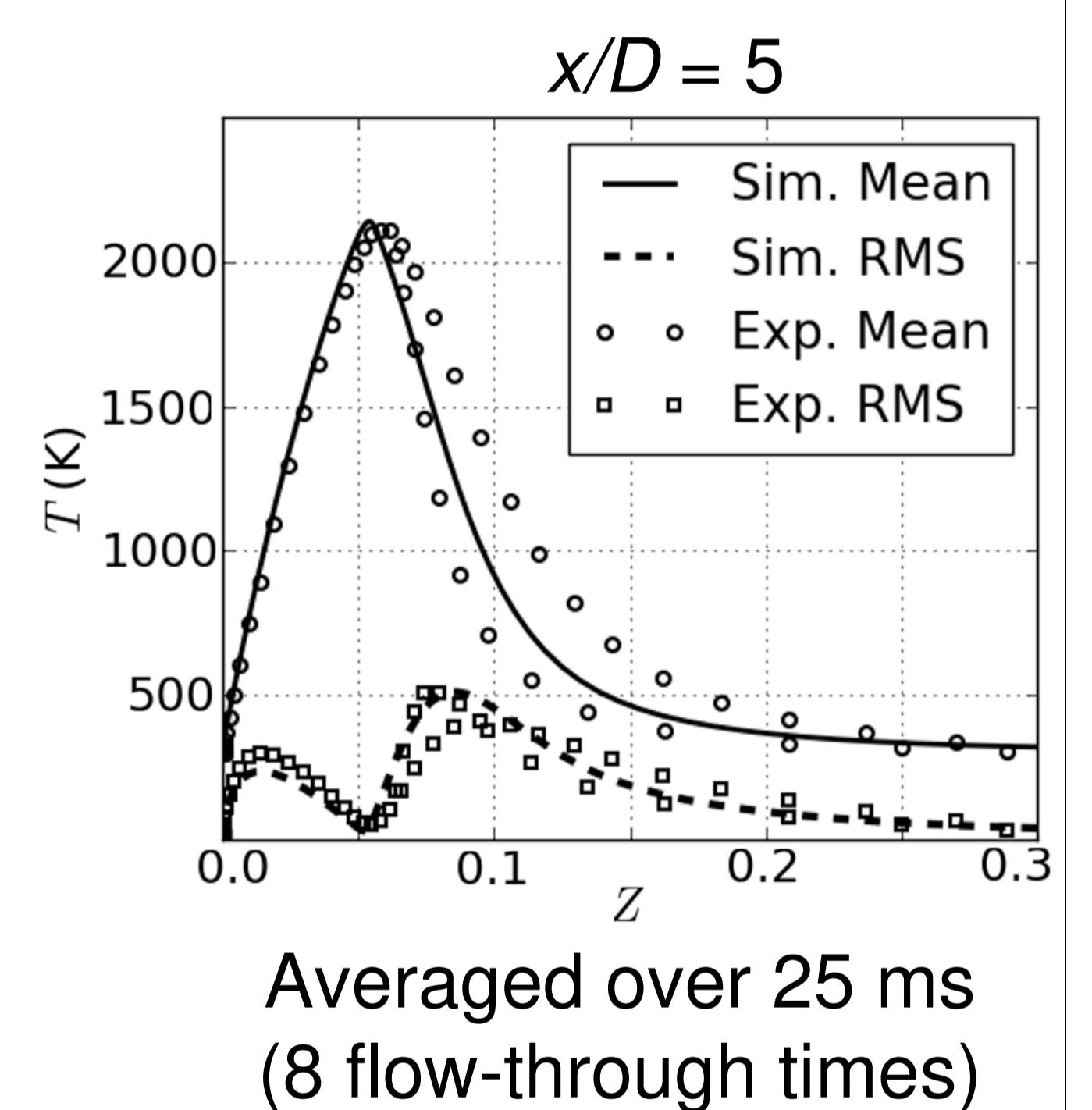
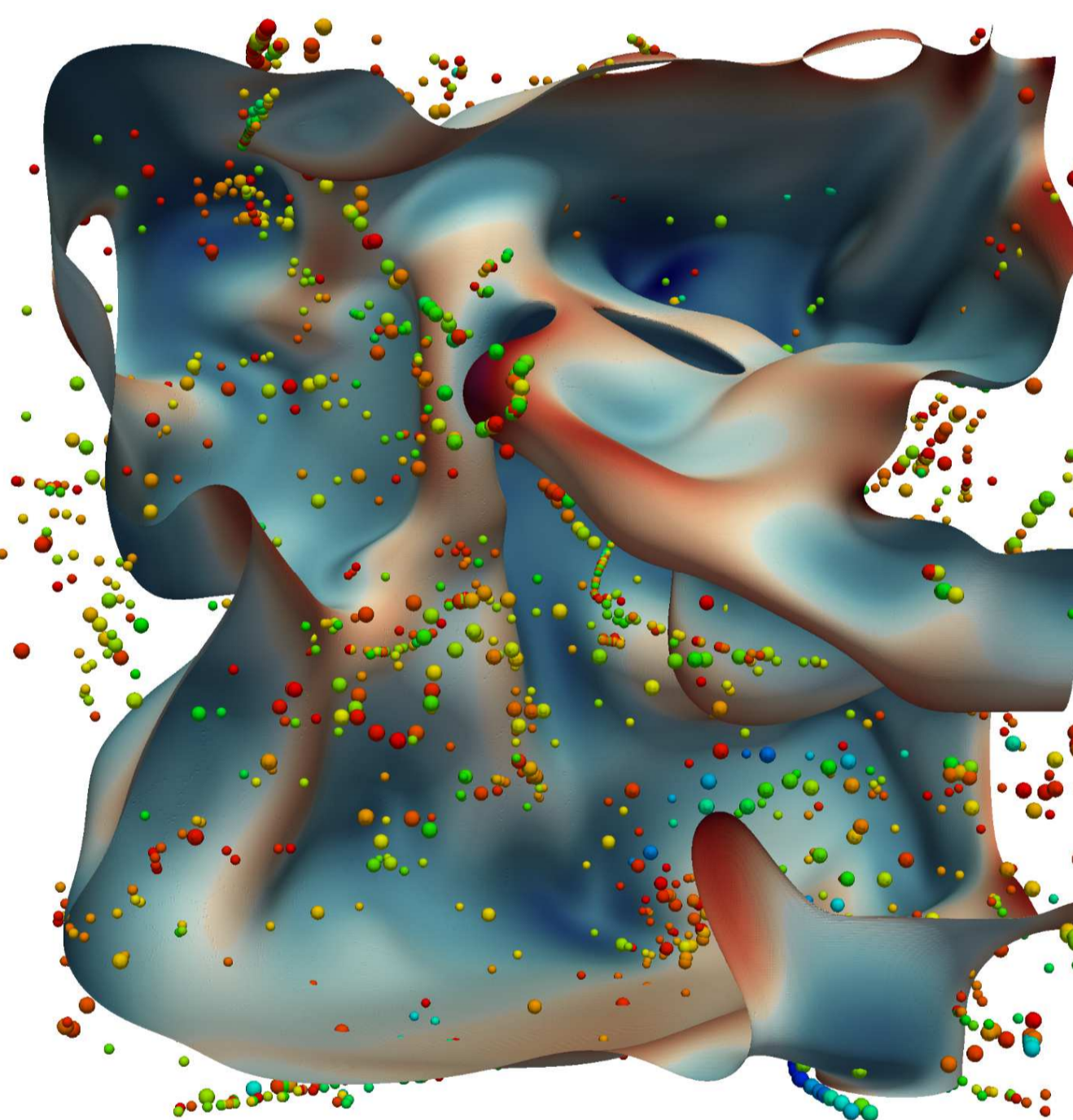
## Example: Turbulent "Sydney" Flame

- Simulation of the partially premixed "Sydney flame" on a mesh with 150mil. cells. 10 TB Data, which will be made public in a database.



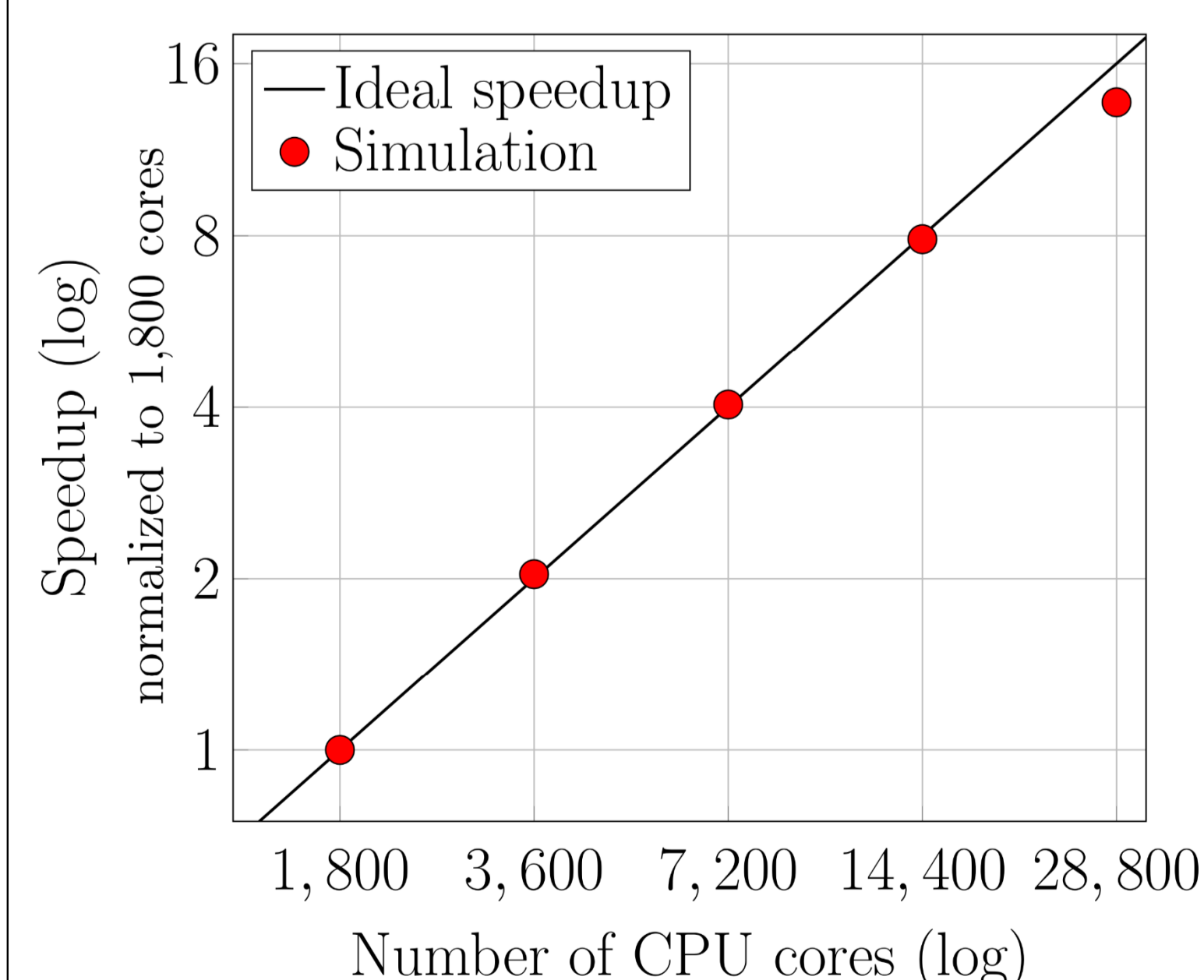
## Lagrangian Particle Tracking

- Particle tracking is used to obtain temporal data at specific locations
- With this technique, time signals of flow and flame properties can be investigated [3]
- Efficient distribution of the particles is still a challenge in HPC



## 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



## References

- [1] F. Zhang, H. Bonart, T. Zirwes et al., Springer, 2015.
- [2] T. Zirwes, F. Zhang, J.A. Denev et al., Springer, 2017
- [3] F. Zhang, T. Zirwes et al., Combustion and Flame, 2017

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