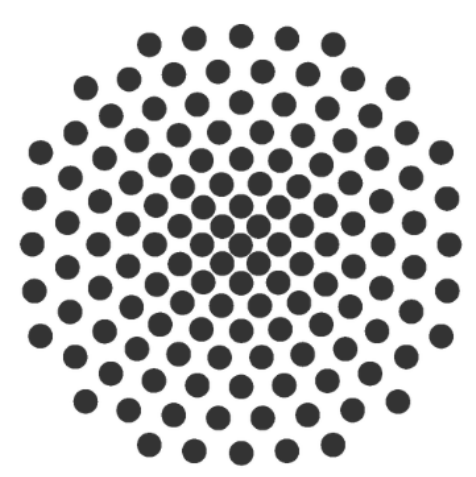




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Exploring Thermodiffusive Instabilities in Hydrogen Combustion on Supercomputers

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Motivation

Background: With the shift to hydrogen-rich fuel mixtures or even pure hydrogen, flames become more prone to form thermodiffusive instabilities. Understanding the formation of these instabilities is an important task for designing combustion devices capable of burning hydrogen-rich fuels.

Challenges: Accurate prediction of these instabilities requires full spatial and temporal resolution of the flame and flow as well as detailed molecular transport models that not only include Fickian diffusion, but also Soret diffusion (transport of chemical species due to temperature gradients). This makes simulations costly and requires the use of modern supercomputers.

Solution: In this work, we adopt two strategies to speed up the reacting flow simulations with little to no loss of accuracy: first, a new Soret diffusion model was implemented that is more efficient but provides similar accuracy compared to benchmark implementations [1]. Second, we added a new code interface that allows different parts of the code be compiled with different compilers and optimization flags to balance performance and usability of the code.

Computational Setup

Generic flame-in-a-box cases of hydrogen flames were conducted with the in-house code EBI-DNS [2]. The code uses the finite volume method to solve the

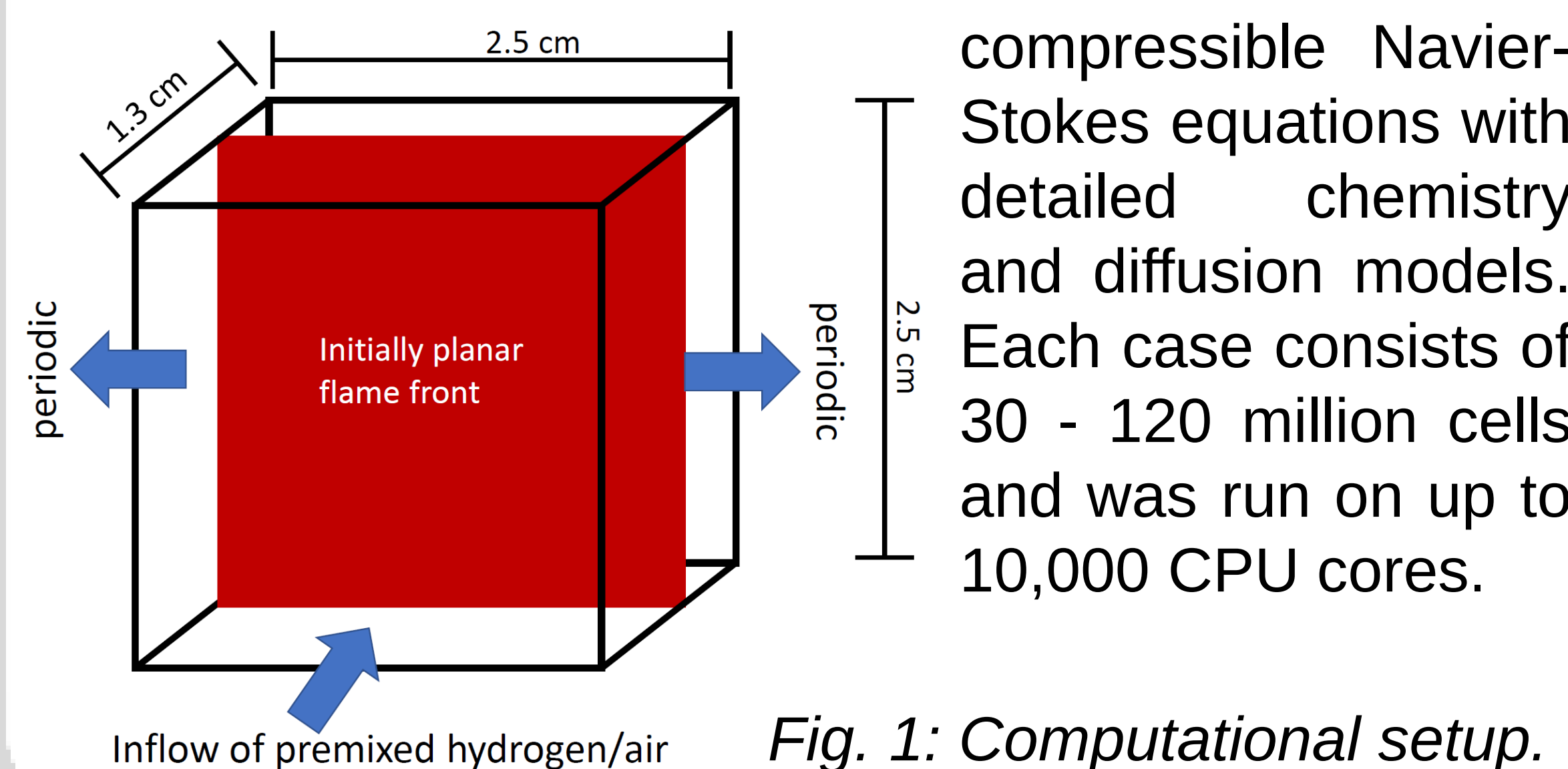


Fig. 1: Computational setup.

compressible Navier-Stokes equations with detailed chemistry and diffusion models. Each case consists of 30 - 120 million cells and was run on up to 10,000 CPU cores.

Results

Instability morphology: Figure 2 shows temperature iso-contours after cellular instabilities have developed on the flame [3]. The local curvature is strongly correlated with heat release from chemical reactions (left) and the displacement speed (right).

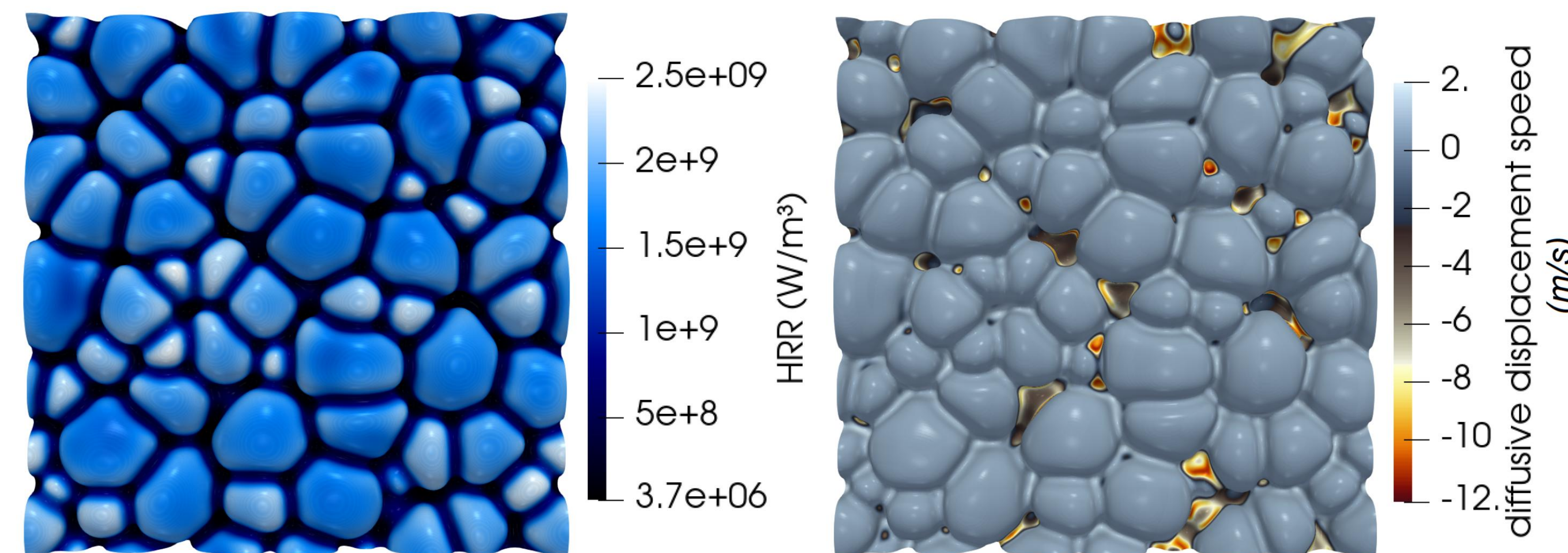


Fig. 2: Temperature iso-contour colored by heat release (left) and disp. speed (right).

Impact of Soret diffusion: One important characteristic is the local extinction at negatively curved flame segments, which form deep cusps reaching into the burnt gas (see Fig. 3). The growth of these instabilities is determined by the thermodiffusive properties of the flame. Figure 4 compares the increase in flame surface area (left) and the efficiency factor I (right) with/without Soret diffusion depending as function of the perturbation wave length λ .

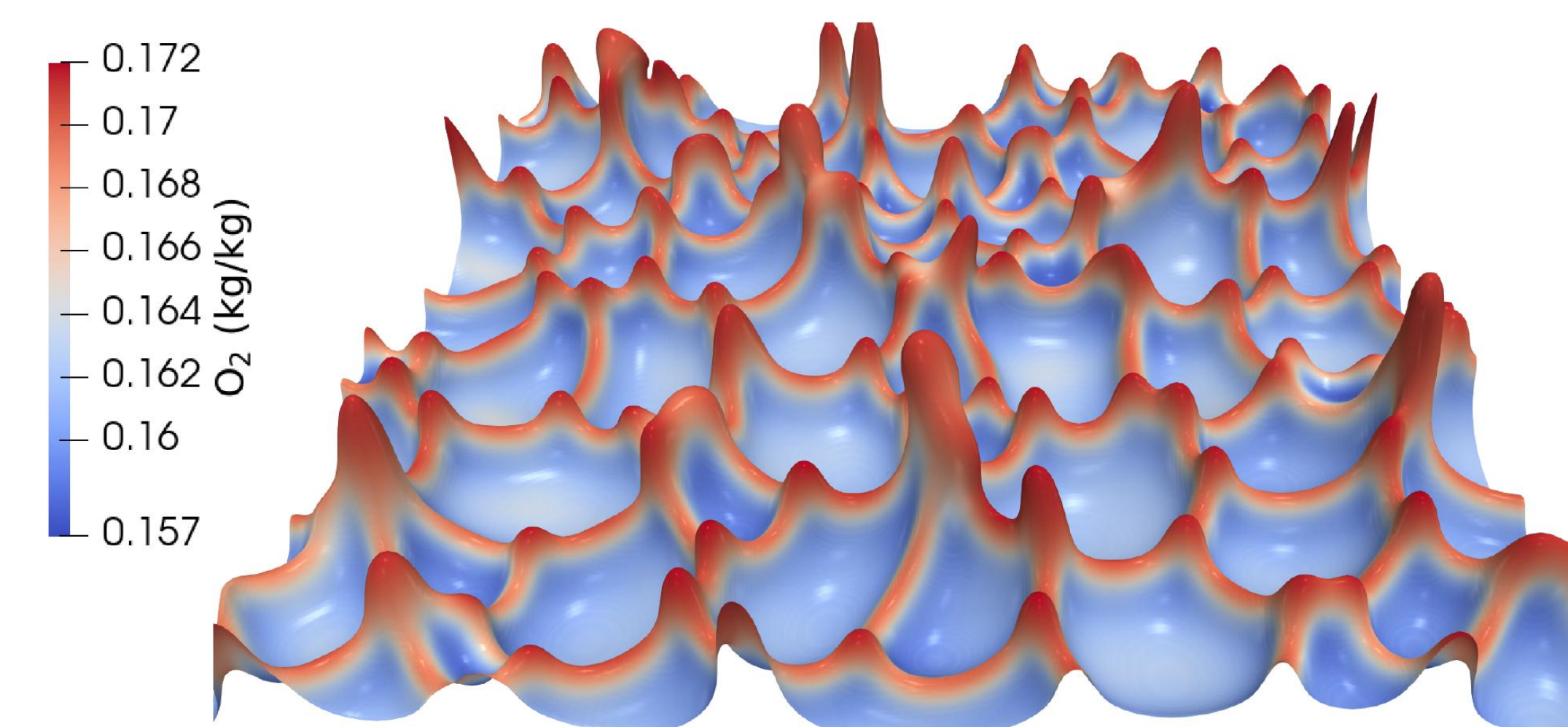


Fig. 3: Temperature iso-contour as seen from the burnt-gas side.

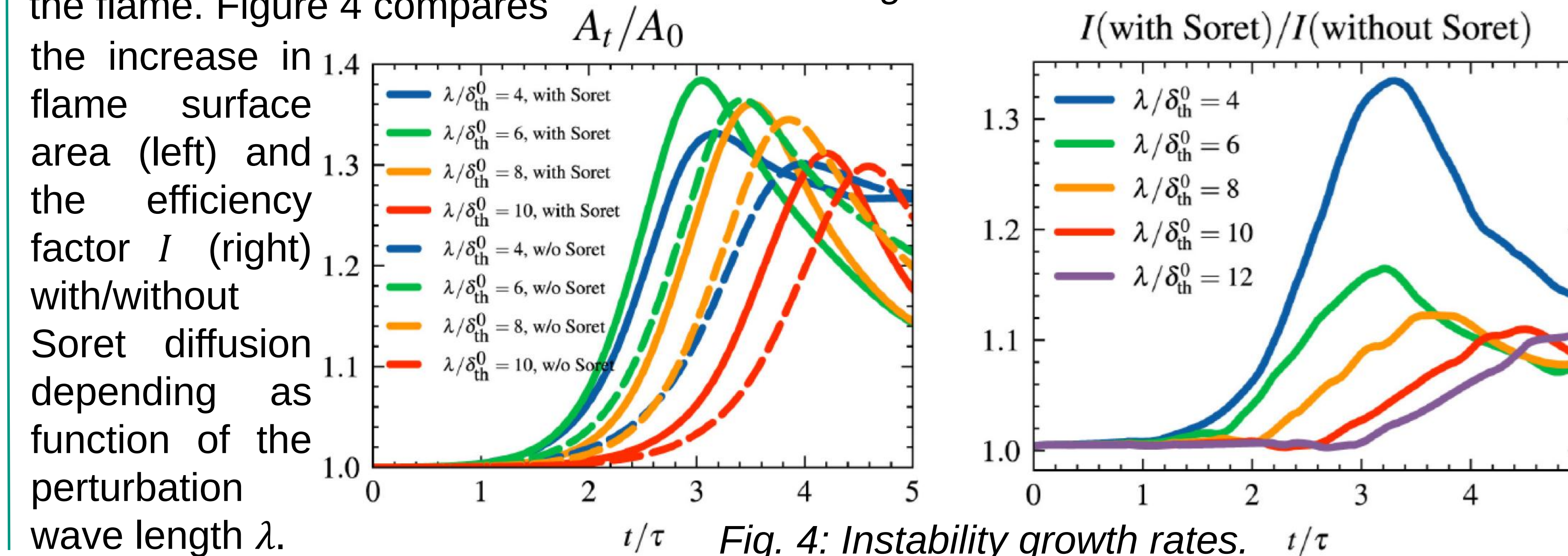
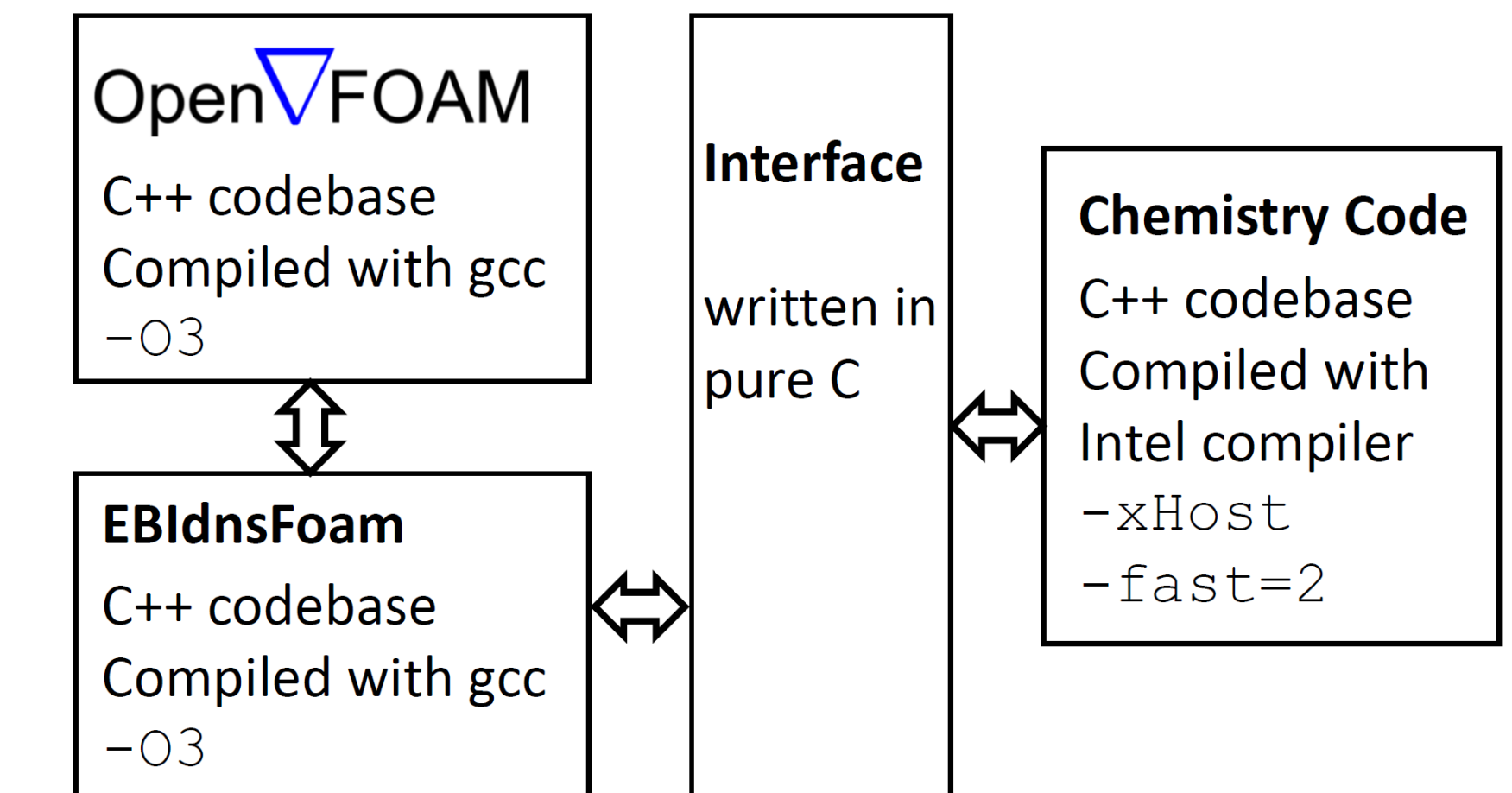
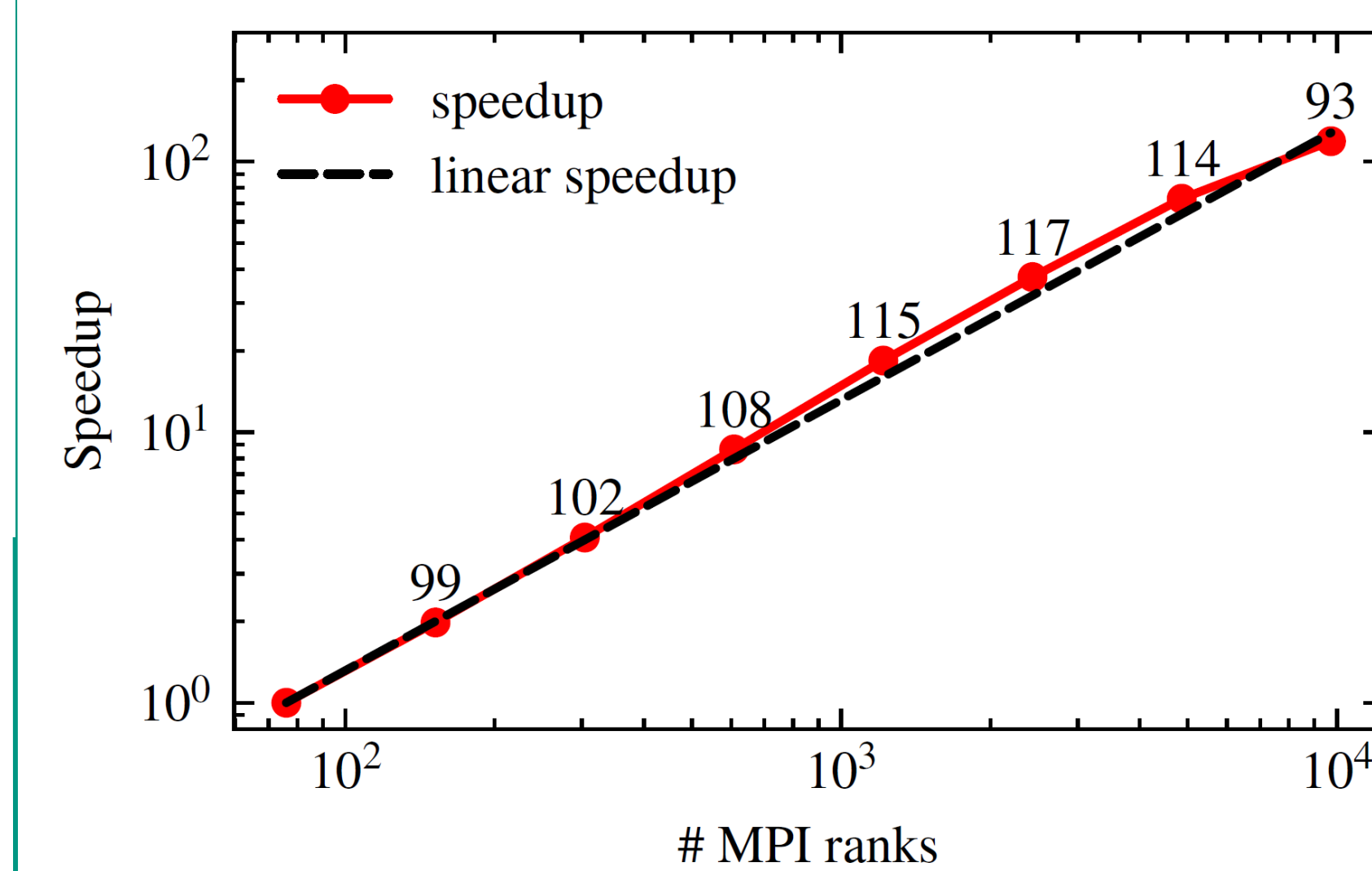


Fig. 4: Instability growth rates. t/τ

Performance

In order to maximize the efficiency of the simulation code on the supercomputer, we introduced a **new code interface** that separates different parts of the code. Particularly, this allows using the pre-installed cluster modules (in this case OpenFOAM), while compiling performance-critical parts (e.g. computation of chemical reaction rates) with different optimization flags and even different compilers (see Fig. 5). In our tests, the Intel compiler **generated up to 20% faster code** than gcc.

Fig. 5: New code interface separating pre-installed module code and performance-critical code.



The parallel scaling of the code is shown in Fig. 6. Linear scaling was observed up to 10,000 MPI ranks.

Fig. 6: Parallel scaling.

References

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