# Summary

Computational fluid dynamics (CFD) becomes increasingly important in the design process of modern systems involving reacting flows. Design and optimisation of, for instance, industrial combustion devices, is intensely guided by numerical simulations nowadays. The complexity of the processes occurring in such systems demands for accurate models and advanced numerical methods. Direct numerical simulation (DNS) and large-eddy simulation (LES) are very powerful high-fidelity CFD tools that have the potential to meet these demands. Unfortunately, these tools can only predict quantitative results if the underlying algorithms are capable of dealing with time-accurate simulations of reacting flows.

Many algorithms used by researchers, although performing well for constant density (non-reacting) flows, give rise to instabilities in the solution when adopted in variable density flows, where density can strongly vary from cell to cell. These algorithms are part of the class denoted here as *continuity-constraint pressure-correction schemes*. Other algorithms perform better with respect to stability, but predict solutions that are far from physically possible: the predicted states do not correspond to the realistic equation of state. These algorithms are denoted here as *analytical compatibility-constraint pressure-correction schemes*. Because of these shortcomings, I develop an algorithm that (i) is stable and robust, (ii) conserves mass and scalars, such as energy and fuel elements mass, (iii) predicts states that match exactly with the equation of state, (iv) can be efficiently implemented and (v) allows time-accurate solutions. Using this type of algorithm should provide a consistent code, that can serve as a basis for quantitative predictions and further model development in LES, without fearing unexpected instabilities. The algorithm's applicability contains low-Mach number flows of general fluids, described by an unlimited amount of scalar transport equations and an arbitrary equation of state. Its primary area of application, however, is in these cases where a non-linear equation of state exists. Turbulent non-premixed flames are a key example for this area of interest.

The developed algorithm is situated in the class of pressure-correction algorithms. In this segregated approach, the equations are solved sequentially. At the end of every timestep, a global correction step is needed to account for the pressure influence. The pressure follows from an elliptic equation, derived from a constraint on the velocity field. I construct the constraint from a combination of the discrete equations of continuity and scalars, imposing that the newly predicted state should be compatible, in agreement

with the equation of state. This leads to the *discrete compatibility-constraint pressure-correction algorithm*. It is different from the standard pressure-correction schemes, where the constraint is formulated either solely based on the continuity equation (continuity-constraint pressure-correction scheme) or from an analytical combination of the material derivative of the equation of state and the continuity and scalar equations (analytical compatibility-constraint pressure-correction scheme).

Specifically when the equation of state expresses a non-linear relationship between the state variables, the developed algorithm reveals its superior qualities. The extreme case of a reacting flow where chemistry is assumed infinitely fast (the Burke-Schumann chemistry model) imposes a highly non-linear, non-differentiable relationship between density and fuel elements mass. In this case, all standard algorithms fail, whereas the newly developed algorithm predicts a correct result. This is clearly shown in a set of one-dimensional test cases, involving convection and diffusion of sharp initial scalar gradients. In these test-cases, three fluid types are investigated: a single-fluid ideal gas at different temperatures, a two-fluid non-reacting flow and a two-fluid combusting flow. The continuity-constraint pressure-correction scheme reveals instabilities in the solutions in nearly all cases and can therefore not be adopted in variable density flows with sharp density gradients. The analytical compatibility-constraint pressure-correction scheme yields stable results, but predicts states that deviate strongly from the equation of state in case of a non-linear equation of state (combusting flow) and is therefore inaccurate. The discrete compatibility-constraint pressure-correction scheme does yield stable and accurate results in all cases.

The algorithm still proves reliable in more-dimensional configurations, albeit that the issue of odd-even decoupling needs to be resolved first. Indeed: if a collocated grid arrangement is used, a spurious mode for the pressure can appear. I construct a velocity-interpolation formula for variable density flows, that can be applied in combination with the developed algorithm, to suppress the spurious mode and still guarantee a solution, even in enclosed systems.

The resulting collocated algorithm is validated on two-dimensional test cases, including a thermally driven cavity with large horizontal temperature differences. For a broad range of Rayleigh numbers, good solutions are obtained, even on relatively coarse meshes. Moreover, the spurious pressure mode is suppressed. In a second test case, the stability and convergence of the method are demonstrated by means of a reacting and a non-reacting mixing layer. I conclude from this test case that, especially in combusting flows, the continuity-constraint pressure-correction algorithm cannot be stabilised, unless measures are taken that corrupt time-accuracy. The analytical compatibility-constraint pressure-correction algorithm is stable, but predicts a converged solution that differs noticeably from the exact result. The reason for this stems from the uncontrollable drift from the non-linear equation of state. On the other hand, the here presented algorithm yields a stable result and predicts states that exactly match the equation of state. The benefits of higher robustness and greater accuracy are acquired with only a minimal additional computational effort, as compared to the other algorithms, yielding an algorithm that is not only stable and accurate, but also efficient.

In conclusion, I show in this work that, because of the non-linearity of e.g. the combustion process, standard algorithms are bound to fail and novel algorithms, based on discrete compatibility-constraint formulations are to be adopted, yielding stable and more accurate time-dependent solutions.