ILDM Reduced Chemistry Tailored For Large Scale Reaction Mechanisms in Complex Reactive Flow Applications

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1. Introduction

Detailed chemical reaction mechanism are required in the modeling of complex technical combustion processes. These reaction mechanisms can be formally described as systems of ordinary differential equations (ODE) in a mean-field kinetic approach. However, the direct application of large scale mechanisms in CFD simulations is often prohibited by both size and stiffness of the associated ordinary differential equation system.

Model reduction facilitates the implementation of detailed mechanisms even under these circumstances. The central idea of almost all model reduction approaches for reaction mechanisms stems from the fact that many processes in chemical reaction systems take place on largely different timescales [3]. The model reduction task is then to identify and eliminate the fast processes in an appropriate way and purely describe the "long-term" dynamics of the system.

In contrast to former reduction methods like quasi-steady-state assumptions (QSSA) and partial equilibrium assumptions, the Intrinsic Low-Dimensional Manifold (ILDM) method (introduced by Maas and Pope [4]) *automatically* reduces the reaction mechanisms.

The basic idea of the ILDM method is to determine the "fast" and "slow" variables by a decomposition of the eigenspace of the Jacobian. With this we can represent most chemical variables as a function of a small subset of parameters (given in the vector \mathbf{z}) by solving

$$F(\boldsymbol{\psi}) = \begin{pmatrix} \mathbf{Q}_{\text{fast}}^T(\boldsymbol{\psi}) S(\boldsymbol{\psi}) \\ P(\boldsymbol{\psi}, \mathbf{z}) \end{pmatrix} = \mathbf{0} \in \mathbb{R}^n$$
(1)

iteratively with a good initial guess ψ_0 . Here Q_{fast} is the part of the Schur-decomposition that projects a vector from the state space to the fast eigenspace, $S(\psi)$ is the right-hand side of the ODE system and $P(\psi, \mathbf{z})$ is the parametrisation fixing the parameters \mathbf{z} .

The state vector $\boldsymbol{\psi}$ consists of temperature, pressure, mixture fraction and the mass fractions of the chemical species.

Equation (1) is solved for different parameters \mathbf{z} and the resulting compositions $\boldsymbol{\psi}$ are saved in tables.

While the general concept of ILDM-reduced chemistry is mathematically simple, issues to be addressed remain in efficient computation, tabulation, data storage and the interaction between the CFD code and the ILDM-reduced chemistry.

2. Improvements of ILDM computation and usage

In [1, 2], two major improvements for the coupling of CFD codes with ILDM-reduced chemistry have been presented.

A key species implementation allows to use an ILDM reduced mechanism like a conventionally reduced mechanism. The CFD code is supplied with a minor subset of chemical species that fulfills mass and enthalphy conservations approximately.

Secondly, the *in-situ tabulation* allows for smaller ILDM tables adapted to the CFD code user specific demands. ILDM points are only computed if they are requested by the CFD code user or if they are required to compute the requested ILDM point.

We present further developments aiding the efficient computation and use of ILDM reduced mechanisms in CFD simulations of complex technical combustion systems.

2.1. Parallelisation of ILDM table calculations

For the calculation of full ILDM tables (i.e. for given spectra of temperature, mixture fraction and the reaction progress variables), the parallel computation of ILDM points leads to significantly lower computation time.

In the parallelisation approach used, a *master* processor manages lists of points that have to be calculated as well as the file in-/output, while the *slave* processors are responsible for the actual computations of ILDM points according to (1).

2.2. AVL trees

Particularly for the in-situ tabulation of ILDM points, the usage of AVL trees is advisable, as the structure of an in situ ILDM table is constantly changing. This requires frequent insertion of ILDM points in the table. On the other hand fast searching is required for an efficient use of the ILDM data in a CFD code.

For AVL-balanced binary trees, the cost for search, deletion and insertion are kept low. Hence AVL trees are able to provide an efficient data storage within the ILDM code and fast data access within the CFD code.

2.3. Adaptive coordinate stepsize

The successful computation of an ILDM point highly relies on a good initial value for the solution of equation (1). Usually the data from neighbouring ILDM points are successfully used as initial values. In very stiff regions however, these points might be too far from the desired new ILDM point.

An overall decrease of the stepsize is not advisable, as this would lead to significantly bigger ILDM tables, that might become too hard to handle.

Hence we implemented an automatic step size refinement in our algorithm. We start the calculations with a coarse step-size that is reduced where the solution of (1) fails with a

given initial value. This assures that the stepsize can be adapted to the stiffness of the ODE system.

2.4. Dimension switching

A difficulty in using ILDM reduced chemistry lies in the fact that in different regions of the state space, different dimensions of the ILDM are necessary. Close to the equilibrium point one or two progress variables are enough to satisfactorily describe the chemistry, but further away, three progress variables are required.

However, using a 3-D ILDM tables close to the equilibrium point leads to very small stepsizes (or erroneous results, if too big stepsizes are used) as the system has too many degrees of freedom. Hence it is desirable to use 2-D ILDM tables close to the equilibrium point and 3-D ILDM tables where necessary.

We present a way of modelling the reaction rate of a third progress variable from a twodimensional ILDM. Therefore the reaction rate of this third progress variable is split up in a part parallel to the ILDM and the relaxation rate to the 2-D ILDM.

With this, the CFD code user can simultaneously use a 2-D and a 3-D ILDM table and hence for all (3-D) ILDM parameters use the data that describes the chemistry in more detail.

3. Results

3.1. Computational time

The efficiency of the parallelisation was tested in terms of the time needed for the computation of a complete 2-D ILDM table. This time could be reduced to about 46%, 32% and 20% for 3,4 or 6 processors respectively.

3.2. Consistency

To assure the consistency of reduced models even for large and stiff mechanisms, a dimension adjustment for the domain close to the equilibrium point and an adaptive coordinate stepsize for stiff regions have been introduced.

For the dimension adjustment, an error criterion which determines the required minimal dimension of an ILDM for sufficiently accurate representation of the full mechanism is desirable. A related concept is presented in [5]. Similar approaches may turn out useful also for the discussed ILDM implementation.

3.3. Application in computation of 1-D laminar flames

Even though a 1-D laminar flame might still be computable without reduced chemistry, the application of ILDM to this simple test case might give some ideas of the capabilities of ILDM reduced chemistry.

The improvements mentioned above are tested for 1-D laminar flames and compared with results achieved using detailed chemistry and ILDM reduced chemistry without these improvements.

Especially the results for using 3-D ILDM, 2-D ILDM and the dimension switching between both are of interest.

References

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