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Adjoint based optimisation of reactive compressible flows

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ABSTRACT

We derive adjoint equations for the reactive compressible Navier–Stokes equations. Therein the reaction rate is modelled by an Arrhenius approach. The adjoint equations are validated by means of a comparison between the adjoint solution and a finite difference expression. An adjoint based optimisation framework for reactive compressible flows is presented. Formulations for different target functions are shown. One- and two-dimensional laminar flame configurations are presented. We find, that the adjoint approach works well despite the strong non-linearity of the reaction terms.

1. Introduction

Adjoint equations have attracted great attention during the last years in the field of numerical fluid dynamics, as they directly provide the optimal change of a flow configuration for obtaining a desired goal. An example is the classical aerodynamic design goal of the optimal shape of a body in a flow to get a high lift/drag ratio [1]. Also for active flow control [2], sensitivity analysis [3] and model reduction problems [4,5] they have become a vital tool. Thus, a large variety of methods will be available if the adjoint approach can also be applied to reactive flows.

In particular the adjoint equations provide a locally optimal improvement step, which is a great advantage over a try and error approach. The improvement step is in principle restricted to be small, because the adjoint formalism involves the linearisation of the fully non-linear flow equations [6]. Due to this the adjoint equations have to be re-evaluated after every improvement step. Thus the confidence range of the linearisation is crucial. For non-reactive flows this seems to be a small issue in practice.

Reactive flows are described by the transport of species and reaction rates, which reduce reactants and increase products (exhausts) and heat. The reaction rate itself strongly depends on the temperature. It is often described by an Arrhenius approach, which involves an exponential temperature dependence.

In principle the adjoint equations for reactive flows can be derived in the same manner as for non-reactive flows. However, as one has to linearise the equations, one has to linearise an exponential and stiff temperature dependence. One might expect, that the confidence range of the linearisation is much smaller due to the exponential term and becomes such a strong restriction as to render the adjoint approach useless. This might explain why the adjoint approach is rarely applied to compressible reactive flows. To the authors knowledge the closest to the present work is [7,8].

We derive instationary reactive adjoint equations analytically in order to be able to trace all resulting terms. The focus is the analysis of the exponential term. Other terms are simplified to keep the resulting equations as simple as possible in this study. Therefore we neglect the friction. The heat capacities, the species and heat transport are assumed to be constant. Inclusion of this terms is not difficult in principle and was done for non-reactive flows before. The analytical adjoint approach instead of the automated differencing is known to introduce a mild discrepancy between the simulation and its adjoint on the discrete level [9]. But for the sake of clarity it seems to be the appropriate choice here.

We find that the adjoint framework works well for the analysed laminar reactive flows. The stiff non-linear reaction rate does not pose a big problem in contrast to our first expectations.

The current work differs in essential points from [7,8]. The authors make use of an automated tool to create discrete adjoint equations, and focus on uncertainty quantification of stationary flows. Most importantly in our view, they use a turbulent flamelet approach, which reduces the stiffness of the equations. Our final aim are unsteady simulations with strong pressure fluctuations and a corresponding adjoint based optimisation framework. We therefore prefer to include the chemical mechanism instead of a flamelet approach.

The paper is structured as follows: Section 2 describes the governing equations and the applied simplifications. In Section 3,

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the corresponding adjoint equations are derived and an adjoint based framework is presented. In Section 4, test cases and a detailed analysis of the adjoint compressible reactive Navier–Stokes equations are presented. In Appendix A, the full expansion of the adjoint equations for one- and two-dimensional reactive flow configurations can be found.

2. Governing equations

2.1. Reactive compressible Navier–Stokes equations

The reactive compressible Navier–Stokes equations are given by

$$\partial_t \varrho + \partial_\alpha(\varrho u_\alpha) = 0 \tag{1a}$$

$$\partial_t \varrho u_\beta + \partial_{x_\alpha}\left(\varrho u_\alpha u_\beta + p\delta_{\alpha\beta}\right) = \partial_{x_\alpha}\tau_{\alpha\beta} \tag{1b}$$

$$\partial_t \varrho e_s + \partial_{x_\alpha}(u_\alpha \varrho e_s + p u_\alpha) - u_\alpha \partial_{x_\alpha} p + \sum_{k=1}^{N} \Delta h^o_{f,k}\dot{\omega}_k = \tau_{\alpha\beta}\partial_{x_\alpha}u_\alpha + \partial_{x_\alpha}(\lambda \partial_{x_\alpha} T) \tag{1c}$$

$$\partial_t \varrho Y_k + \partial_{x_\alpha}\varrho u_\alpha Y_k - \dot{\omega}_k = \partial_{x_\alpha}\left(\varrho D_k \frac{W_k}{W}\partial_{x_\alpha} X_k\right). \tag{1d}$$

Therein ϱ denotes the density, u_α the velocity in direction α, p the pressure, e_s the energy (sensible), W the mean molecular weight, Y_k the mass fraction of species k of N and X_k the mole fraction. We applied Fick's law for diffusion. λ and D_k are the heat and species diffusion coefficients. The viscous stress tensor is defined by $\tau_{\alpha\beta} = \mu(\partial_{x_\alpha}u_\beta + \partial_{x_\beta}u_\alpha) + (\mu_d - 2/3\mu)\delta_{\alpha\beta}\partial_{x_\gamma}u_\gamma$, where μ is the shear viscosity and μ_d the bulk viscosity. $\Delta h^o_{f,k}$ corresponds to the mass formation enthalpy and $\dot{\omega}_k$ to the reaction rate, which is modelled by an Arrhenius approach

$$\dot{\omega}_k = W_k \nu_k A e^{\left(\frac{-T_a}{T}\right)} \prod_{l=1}^{N} [X_l]^{\nu'_l}. \tag{2}$$

W_k denotes the molecular weight and ν_k the molar stoichiometric coefficients of species k, A the pre-exponential factor, T the temperature, T_a the activation temperature and $[X_l]$ the molar concentration of species l. Reverse rates are neglected since a forward dominant reaction will be considered. The nomenclature is based on [10]. The heat release $\dot{\omega}_T$ is given by $-\sum_{k=1}^{N}\Delta h^o_{f,k}\dot{\omega}_k$. The equation system is closed with the ideal gas law. The summation convention applies.

2.2. Model assumptions

To keep the derivation of the adjoint equations as transparent as possible, we make some simplifications to the governing equations. By reducing the number of terms and dependencies also the adjoint equations are simplified. We assume, that the main difficulty is the exponential term, so we will focus on this. The neglected terms can be added and should not pose any difficulty, as these terms are accounted for in non-reactive adjoint analysis.

In laminar flames, which are treated in this study, the viscous friction can be neglected in comparison to the heat- and species diffusion. Therefore the corresponding terms are neglected in the considered set of equations.

By assuming that the specific heat capacity is $c_v \neq c_v(T)$ the energy equation Eq. (1c) can be rewritten in terms of pressure.

$$e_s = \int_{T_0}^{T} c_v \mathrm{d}T - \frac{RT_0}{W} = c_v(T - T_0) - \frac{RT_0}{W} = c_v\frac{pW}{\varrho R} - c_p T_0 = \frac{p}{\varrho}\frac{1}{\gamma - 1} - c_p T_0 \tag{3}$$

The constant term $c_p T_0$ can be eliminated by conservation of mass. The energy equation becomes:

$$\partial_t \frac{p}{\gamma - 1} + \partial_{x_\alpha}\left(\frac{\gamma u_\alpha p}{\gamma - 1}\right) - u_\alpha \partial_{x_\alpha} p + \sum_{k=1}^{N}\Delta h^o_{f,k}\dot{\omega}_k = \partial_{x_\alpha}(\lambda \partial_{x_\alpha} T). \tag{4}$$

For further simplification constant heat and species diffusion coefficients $\lambda = \lambda_0 T^n_{\mathrm{ref}} = \hat{\lambda}$ and $\varrho D_k = D_{0,k} T^n_{\mathrm{ref}} = \hat{D}_k$ are assumed.

In addition, only premixed flames with one step chemistry are considered. Therefore only one species is modelled. The mean molecular weight is simply given by $W = W_k$. The species transport equation becomes:

$$\partial_t \varrho Y + \partial_{x_\alpha}\varrho u_\alpha Y - \dot{\omega} = \partial_{x_\alpha}(\varrho D \partial_{x_\alpha} Y). \tag{5}$$

While only premixed flames are analysed in this work the derivation of the adjoint equations is done for multi species $k \geqslant 1$.

2.2.1. Resulting computational model

Overall the set of governing differential equations Eqs. (1a)–(1d) can be rewritten with f as source term as

$$\partial_t \begin{pmatrix} \varrho \\ \varrho u_\beta \\ \frac{p}{\gamma-1} \\ \varrho Y_k \end{pmatrix} + \partial_{x_\alpha}\begin{pmatrix} \varrho u_\alpha \\ \varrho u_\alpha u_\beta + p\delta_{\alpha\beta} \\ \frac{\gamma u_\alpha p}{\gamma-1} \\ \varrho u_\alpha Y_k \end{pmatrix} - u_\alpha \partial_{x_\alpha}\begin{pmatrix} 0 \\ 0 \\ p \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \sum_{k=1}^{N}\Delta h^o_{f,k}\dot{\omega}_k \\ -\dot{\omega}_k \end{pmatrix} = \partial^2_{x_\alpha}\begin{pmatrix} 0 \\ 0 \\ \hat{\lambda} T \\ \hat{D}_k Y_k \end{pmatrix} + f, \tag{6}$$

which corresponds to

$$\partial_t a + \partial_{x_\alpha} b^\alpha + C^\alpha \partial_{x_\alpha} c + d = \partial^2_{x_\alpha} e + f. \tag{7}$$

The matrix C^α is given by $C^\alpha_{ij} = -u_\alpha \delta_{i,2+\alpha}\delta_{j,2+\alpha}$, with the Kronecker delta $\delta_{i,j}$.

2.3. Numerical implementation

The discretisation in space is realised by finite difference schemes of high order (4th and 6th). Lower-order schemes would be equally applicable. The time discretisation is realised with an explicit Runge–Kutta scheme of fourth order. Due to the fact that both the direct and adjoint equations will have a similar structure, the corresponding computations are discretised in the same manner. Uniform grids are used.

For stability reasons the momentum equation Eq. (1b) is implemented in skew symmetric form [11]

$$\frac{1}{2}(\partial_t \varrho \cdot + \varrho \partial_t \cdot)u_\alpha + \frac{1}{2}(\partial_{x_\beta} u_\beta \varrho \cdot + u_\beta \varrho \partial_{x_\beta}\cdot)u_\alpha + \partial_{x_\alpha} p = 0. \tag{8}$$

More standard schemes would be applicable too. Further stabilisation of the computations, mainly for the adjoint equations, is achieved by using implicit filtering [12].

3. Adjoint equations

3.1. General considerations

To guide the reader through the following derivation, the necessary steps are first sketched on an abstract level. Therefore a matrix–vector notation is used. The vector space is the full solution in space and time. The derivation closely follows [6].

While the Navier–Stokes equations describe physical phenomena of flows, the corresponding adjoint equations are implied by