Implementation of discrete adjoint method for parameter sensitivity analysis in chemically reacting flows

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In this research, a framework based on the discrete adjoint method is presented for evaluating the sensitivities of a set of parameters related to chemically reacting flows. The presented formulation is implemented to laminar, incompressible regimes with constant density. The discrete adjoint formulation demands the solution of two sets of equations, namely the flow (primal) equations and the adjoint (dual) equations. The flow equations consisting of a coupled system of three models, namely fluid flow, thermal energy transfer and species mass transfer, are discretized using the stabilized finite element formulation while an implicit scheme is implemented to solve the discretized equations. The adjoint equations including a coupled linear system of equations employ the transpose of the exact Jacobian matrices, incompletely calculated for the implicit solution of the flow equations. The coupled systems of equations deduced from both the flow and the adjoint equations are solved in a staggered manner while a highly-parallel preconditioned scheme for fractional solvers with high scalability properties is employed. Some two-dimensional examples corresponding to the sensitivity analysis of a set of parameters are delivered here for the uncoupled as well as the coupled problems. The comparison of the calculated sensitivities with the ones obtained from the finite difference proves the accuracy and robustness of the proposed method.

I. Introduction

Typically, chemically reacting flows are simulated using computational fluid dynamics (CFD) where a mathematical model consisting of a system of coupled partial differential equations (PDEs) is solved numerically using a discretization scheme such as finite difference, finite volume or finite element method. These simulations rely on a set of tunable parameters involved in the calculation of the reaction rate coefficients. The effect of these parameters on engineering quantities is of importance for design optimization and uncertainty quantification. In order to assess this effect numerically, a sensitivity analysis procedure is mostly performed where the sensitivities (gradients) of a given desirable objective functional to these parameters are calculated.

A common approach for calculating the sensitivities is finite difference scheme. Although the implementation of the finite difference is straightforward for an available CFD code, the computational cost related to this method grows massively if the number of design variables, \( N_d \), increases. An efficient approach for reducing the computational cost of the gradient calculation is the adjoint method where the gradients of a single objective functional with respect to a set of design variables can be calculated through the solution

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of the adjoint equations, independently from $N_{d}$, with a cost approximately equal to a single flow solution. The main idea of the adjoint method is based on the control theory originally developed by Pironneau \(^3\) for the fluid mechanics. Afterwards, this method has widely used for error estimation, sensitivity analysis and uncertainty quantification in most of the engineering fields. These applications include aerodynamics mesh adaptation \(^4, 5\), aerodynamic shape optimization \(^6-9\), flow control over aerodynamic bodies \(^10\), aerodynamic design under uncertainty \(^11\), aerodynamic risk assessment \(^12\) electromagnetic shape optimization \(^13\), acoustic shape optimization \(^14\), acoustic noise reduction \(^15\). Also, the adjoint method is studied in the field of chemically reacting flows for sensitivity analysis of air pollution models \(^16, 17\), sensitivity analysis of laminar flames \(^18\) and uncertainty quantification of hypersonic flows \(^19, 20\). Although the adjoint method is well-established in aerodynamic, acoustic and electromagnetic fields, the implementation of this method for chemically reacting flows requires more studies.

In order to solve the adjoint equations two different procedures, namely the continuous formulation and the discrete formulation, have been developed by researchers. In the continuous formulation the continuous form of the governing flow equations is first differentiated and then discretized, whereas the discrete formulation directly differentiates the discretized form of the governing equations. Although the continuous adjoint formulation has the advantage of less memory requirements, the implementation of the discrete formulation has been increased recently due to the simplicity of implementation and the unique capability of providing the exact discrete sensitivities. This simplicity comes from the fact that the transpose of the global Jacobian matrix, already calculated for the implicit solution of the flow equation, is utilized directly for the solution of the linear system of equations which arise from the discrete adjoint formulation. In the case that the approximate Jacobian is utilized for the solution of the flow equations, the exact Jacobian can be evaluated with minor additional calculations. On the other hand, the treatment of the boundary conditions is quite straightforward in the case of the discrete formulation. A comprehensive comparison of the continuous and discrete adjoint formulations is presented in \(^21\).

The main goal of this research is to develop a framework for evaluating the sensitivities of an objective functional with respect to a set of parameters related to the chemically reacting flows (namely Arrhenius preexponential parameters) using discrete adjoint formulation. In order to reach this end, the chemically reacting flows are modeled by a CFD solver where a coupling of three models, namely fluid flow, thermal energy transfer and species mass transfer, is considered for a viscous incompressible flow in a constant-density steady state regime. The solution of the flow equations is based on the stabilized finite element formulation \(^1\) where an implicit scheme is utilized. The obtained coupled system of equations is solved in a staggered manner where each module is resolved separately. Having calculated the exact Jacobian matrix of each model, the discrete adjoint method is implemented to the original CFD code for evaluating the gradients. A block Jacobi method is considered for the solution of the coupled adjoint system of equations maintaining the solution procedure staggered. The main novelty of this work is the implementation of the discrete adjoint method to a coupled system of equations involving chemical reactions using a stabilized finite element discretization.

The layout of this paper is the following: In Section 2 the governing equations of the chemically reacting flows are described. Section 3 delivers the system of flow equations including the implemented stabilized finite element formulation a well as the solution procedure of the flow equations. The derivation of the discrete adjoint system along with its solution strategy are presented in Section 4. The numerical results corresponding to the proposed strategy for different disciplines are shown in Section 5. Finally, conclusions and general remarks are summarized in Section 6.

### II. Governing Equations

In order to simulate the behavior of chemically reacting flows, a number of models consisting of fluid flow, thermal energy transfer and species mass transfer must be utilized. The fluid flow model is simulated by the incompressible constant-density Navier-Stokes equations whereas the thermal energy balance equation and species mass balance equations are considered to simulate the energy transfer mode and the species mass transfer model, respectively. The governing PDEs corresponding to each model can be expressed in residual form as following

**Navier-Stokes**
\[ r_{mi} := \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \] (1)

\[ r_c := \frac{\partial u_i}{\partial x_i} = 0 \] (2)

**Thermal energy**

\[ r_t := \rho C_p \left[ \frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} \right] + \rho \left( \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} \right) \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \lambda_t \frac{\partial T}{\partial x_i} \right) + \sum_{k=1}^{N} h_k w_k = 0 \] (3)

**Species mass**

\[ r_{sk} := \rho \left[ \frac{\partial Y_k}{\partial t} + u_i \frac{\partial Y_k}{\partial x_i} \right] - \frac{\partial}{\partial x_i} (\rho Y_k V_{k,i}) - w_k = 0 \] (4)

where \( i, j = 1, n_d \) with \( n_d \) as the number of space dimensions and \( k = 1, n_s \) by defining \( n_s \) as the number of species. In the above equations, \( r_{mi}, r_c, r_t \) and \( r_{sk} \) denote the residual vectors related to the momentum, continuity, thermal energy balance and species mass balance equations, respectively. Equations 1, 2, 3 and 4 contain a set of unknown variables including \( u, p, T \) and \( Y \) which represent the velocity vector, the pressure, the temperature and the vector of mass fractions, respectively. The variables \( \rho, C_p, \lambda_t \) and \( w \) are the density, the specific heat of the mixture, the thermal diffusion coefficient of the mixture and the reaction rate vector, respectively. Also, the variables \( C_{p,k} \) and \( h_k \) are the specific heat and the enthalpy for the species \( k \) which are obtained from experimental data.

By defining \( D_k \) as the species diffusion coefficient for the species \( k \), the species diffusion velocity \( V_{k,i} \) is determined using Fick’s law

\[ Y_k V_{k,i} = -D_k \frac{\partial Y_k}{\partial x_i} \] (5)

Also, the viscous stress tensor \( \tau \) for a Newtonian fluid with the viscosity coefficient \( \mu \) is defined as

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \] (6)

where \( \mu \) is calculated from Sutherland’s law.

In order to simplify the equations, the Lewis number is assumed to be one and the properties \( D_k, C_p, \lambda_t \) are assumed to be constant. Although these assumptions are slightly inconsistent and they are not able to predict truly the behavior of the chemically reacting flows but they considerably facilitate demonstration of the capabilities related to the presented sensitivity analysis method. It is to be noted that these assumptions are used before by other researchers for the simulation of the combustion\(^{22}\) as well as the sensitivity analysis of the laminar flames\(^{18}\).

### A. Reaction Rates

Let us consider a general chemical system of \( n_s \) species reacting through \( M \) reactions as

\[ \sum_{k=1}^{n_s} \alpha_{k,r} A_k \leftrightarrow \sum_{k=1}^{n_s} \beta_{k,r} A_k \quad \text{for} \quad r = 1, M \] (7)

where \( A_k \) represents the molar concentrations of species \( k \) (reactants or products), \( \alpha_{k,r} \) is the stoichiometric coefficient of species \( k \) in the reactants of reaction \( r \) and \( \beta_{k,r} \) is the stoichiometric coefficient of species \( k \) in the products of reaction \( r \).

Based on the principle of the mass conservation, the source term \( w_k \) is given for a general set of reactions by the following equation

\[ w_k = M_k \sum_{r=1}^{M} (\beta_{k,r} - \alpha_{k,r})(R_{f,r} - R_{b,r}) \] (8)
with \( M_k \) as the molecular mass of species \( k \). Also, \( R_{f,r} \) and \( R_{b,r} \) represent the forward and backward reaction rates in reaction \( r \), respectively, which are defined as

\[
R_{f,r} = k_{f,r} \prod_{k=1}^{N} \left( \frac{\rho Y_k}{M_k} \right)^{\alpha_{k,r}} 
\]

\[
R_{b,r} = k_{b,r} \prod_{k=1}^{N} \left( \frac{\rho Y_k}{M_k} \right)^{\beta_{k,r}} 
\]

where \( k_{f,r} \) and \( k_{b,r} \) are the forward and backward rate of reaction \( r \), respectively, These coefficients are usually modeled using the empirical Arrhenius law as

\[
k_{f,r} = A_{f,r} T^{\eta_{f,r}} e^{-\frac{E_{f,r}}{RT}} 
\]

\[
k_{b,r} = A_{b,r} T^{\eta_{b,r}} e^{-\frac{E_{b,r}}{RT}} 
\]

where \( A_{f,r} \) and \( A_{b,r} \) are the preexponential constants related to the forward and backward reaction \( r \), \( \eta_{f,r} \) and \( \eta_{b,r} \) represent the temperature exponent of the forward and backward reaction \( r \), respectively, \( E_{f,r} \) and \( E_{b,r} \) are the activation energies for the forward and backward reaction \( r \), respectively, and \( R \) is the perfect gas constant.

In the current work, the constants \( \eta_{f,r} \) and \( \eta_{b,r} \) are assumed to be zero.

**III. System of Flow Equations**

The derivation of the equations related to the flow problem as well as the solution approach of these equations are presented in this section.

**A. Stabilized FEM Formulation**

The continuous governing Equations 1, 2, 3 and 4 are discretized using a stabilized finite element method (FEM) based on the Galerkin Least-Square (GLS) approach originally developed by Tezduyar\(^1\) for incompressible flows. This approximation method allows the use of elements that have equal-order shape functions for the velocity and the pressure without producing spurious pressure solutions in the incompressible flow regime. Also, this formulation is able to handle the problems with highly convected flows.

Let us assume a problem domain \( \Omega \) with a boundary \( \Gamma \). By defining \( w \) as the standard weighting function vector, the resulting stabilized finite element equations corresponding to the Equations 1, 2, 3 and 4 are given by

**Navier-Stokes**

\[
R_{m,j} = \int_{\Omega} w \tau_{m,j} d\Omega + \sum_{e} \int_{\Omega_e} \rho \tau_{m,ij} \left[ \frac{\partial w}{\partial t} + u_i \frac{\partial w}{\partial x_j} \right] \tau_{m,j} d\Omega_e 
\]

\[
R_{c} = \int_{\Omega} w \tau_{c} d\Omega + \sum_{e} \int_{\Omega_e} \rho \tau_{m,ij} \frac{\partial w}{\partial x_i} \tau_{m,j} d\Omega_e 
\]

**Thermal energy**

\[
R_{t} = \int_{\Omega} w \tau_{t} d\Omega + \sum_{e} \int_{\Omega_e} \rho \tau_{t,ij} \left[ \frac{\partial w}{\partial t} + u_i \frac{\partial w}{\partial x_j} \right] \tau_{m,j} d\Omega_e 
\]

**Species mass**

\[
R_{s,k} = \int_{\Omega} w \tau_{s,k} d\Omega + \sum_{e} \int_{\Omega_e} \rho \tau_{s,k} \left[ \frac{\partial w}{\partial t} + u_i \frac{\partial w}{\partial x_i} \right] \tau_{s,k} d\Omega_e 
\]

where \( n_e \) represents the number of the elements. In the above equations, \( R_{m,j} \), \( R_{c} \), \( R_{t} \) and \( R_{s,k} \) denote the approximated residual vectors of the momentum, the continuity, the thermal energy balance and the species
mass balance equations, respectively, related to the stabilized finite element strategy. The stabilization parameters \( \tau_m \), \( \tau_t \) and \( \tau_s \) are given in the references \(^1\),\(^2\),\(^3\),\(^4\).

Based on the FEM, the unknown variables \( u \), \( p \), \( T \) and \( Y \) are approximated within each element by \( \bar{u} \), \( \bar{p} \), \( \bar{T} \) and \( \bar{Y} \), respectively, with the following expansions

\[
\begin{align*}
\mathbf{u} \simeq \bar{\mathbf{u}} &= \sum_{J=1}^{n} N_J \bar{u}_J \\
p \simeq \bar{p} &= \sum_{J=1}^{n} N_J \bar{p}_J \\
T \simeq \bar{T} &= \sum_{J=1}^{n} N_J \bar{T}_J \\
Y \simeq \bar{Y} &= \sum_{J=1}^{n} N_J \bar{Y}_J
\end{align*}
\]

where \( N_J \) is the continuous linear shape functions of the \( J^{th} \) node and \( n = 3 \) for linear triangles.

The Galerkin form of the discretized equations is obtained by making the weighting functions equal to the shape functions (\( \mathbf{w} = \mathbf{N} \)). The final formulation of the stabilized finite element method is obtained by substituting Equations 17, 18, 19 and 20 into Equations 13, 14, 15 and 16. In the following, the solution strategy of the flow equations is discussed.

**B. Flow Solution**

The solution of the flow equation can be summarized to a system of coupled equations with the following form

\[
\mathbf{R}(\mathbf{U}) = \begin{bmatrix}
\mathbf{R}_m \\
\mathbf{R}_c \\
\mathbf{R}_t \\
\mathbf{R}_s
\end{bmatrix} = 0 \quad \text{with} \quad \mathbf{U} = \begin{bmatrix}
\mathbf{u} \\
\mathbf{p} \\
\mathbf{T} \\
\mathbf{Y}
\end{bmatrix}
\]

where \( \mathbf{U} \) represents the unknown vector and \( \mathbf{R} \) is the residual vector.

The coupled system of flow equations presented in Equations (13), (14), (15) and (16) is solved in a staggered manner where each model, namely Navier-Stokes, thermal energy and species mass, is considered separately introducing an iteration loop over the models. The linearization of each model gives rise to the following equations

\[
\begin{bmatrix}
\frac{\partial \mathbf{R}_m}{\partial \mathbf{u}} & \frac{\partial \mathbf{R}_m}{\partial \mathbf{p}} \\
\frac{\partial \mathbf{R}_c}{\partial \mathbf{u}} & \frac{\partial \mathbf{R}_c}{\partial \mathbf{p}}
\end{bmatrix}^n \begin{bmatrix}
\mathbf{u} \\
\mathbf{p}
\end{bmatrix}^{n+1} = \begin{bmatrix}
\mathbf{b}_u \\
\mathbf{b}_p
\end{bmatrix}^n
\]

\[\begin{bmatrix}
\frac{\partial \mathbf{R}_t}{\partial \mathbf{T}} \\
\frac{\partial \mathbf{R}_s}{\partial \mathbf{Y}}
\end{bmatrix}^n \begin{bmatrix}
\mathbf{T} \\
\mathbf{Y}
\end{bmatrix}^{n+1} = \begin{bmatrix}
\mathbf{b}_t \\
\mathbf{b}_s
\end{bmatrix}^n
\]

where \( \mathbf{b}_u, \mathbf{b}_p, \mathbf{b}_t \) and \( \mathbf{b}_s \) represent the RHS terms coming from the FEM approximation and \( n \) denotes the iteration number.

The solution of each model and the iteration loop are performed in ALYA, a house-developed code in Barcelona Supercomputing Center.

**IV. System of Adjoint Equations**

The derivation of the equations related to the sensitivity calculation as well as the solution procedure of these equations are discussed in this section.
A. Discrete Adjoint Formulation

In order to calculate the sensitivities of a scalar-valued objective functional $F$ to a set of design variables $D$, the discrete formulation of the adjoint method is implemented here. A general formulation of the functional for a stationary problem can be expressed as

$$F = F(D, U(D))$$  \hspace{1cm} (25)

where $U$ is the steady state solution of the flow equations satisfying

$$R(D, U(D)) = 0$$  \hspace{1cm} (26)

with $R(D, U(D))$ as the global residual related the coupled system. In fact the above equation can be interpreted as a physical constraint. As shown in Equations (25) and (26), both the functional $F$ and the residual vector $R$ are the functions of design variables $D$ as well as the flow variables $U$.

The procedure of calculating the sensitivities $dF/dD$ consists of differentiating the functional and then applying the chain role which gives rise to the following expression

$$\frac{dF}{dD} = \frac{\partial F}{\partial D} + \frac{\partial F}{\partial U} \frac{\partial U}{\partial D} \hspace{1cm} (27)$$

In order to determine the term $\frac{\partial U}{\partial D}$, Equation (26) can be differentiated with respect to the design variables $D$ via the chain rule as

$$\frac{dR}{dD} = \frac{\partial R}{\partial D} + \frac{\partial R}{\partial U} \frac{\partial U}{\partial D} = 0 \hspace{1cm} (28)$$

Hence, the term $\frac{\partial U}{\partial D}$ can be formulated as

$$\frac{\partial U}{\partial D} = -\left[ \frac{\partial R}{\partial U} \right]^{-1} \frac{\partial R}{\partial D} \hspace{1cm} (29)$$

The final expression for the sensitivities $\frac{dF}{dD}$ can be deduced by substituting Equation (29) into Equation (27) as

$$\frac{dF}{dD} = \frac{\partial F}{\partial D} - \frac{\partial R}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1} \frac{\partial R}{\partial D} \hspace{1cm} (30)$$

By transposing both sides of Equation 30, the formulation of the discrete adjoint problem is obtained as

$$\frac{dF^T}{dD} = \frac{\partial F^T}{\partial D} - \frac{\partial R^T}{\partial D} \left[ \frac{\partial R}{\partial U} \right]^{-T} \frac{\partial F^T}{\partial U} \hspace{1cm} (31)$$

where $[.]^{-T}$ represents the inverse of the transposed matrix.

Equation (31) demonstrates that the procedure of the sensitivity evaluation involves the calculation of four terms $\frac{\partial F}{\partial D}$, $\frac{\partial F}{\partial U}$, $\frac{\partial R}{\partial D}$, $\frac{\partial R}{\partial U}$ which are calculated using a hand-coded linearization in this work. The most costly part of the sensitivity evaluation is related to the calculation and inversion of the full Jacobian matrix $\frac{\partial R}{\partial U}$ whereas the calculation of the remaining terms demand much less computational cost.

Due to the fact that a direct inversion of the full Jacobian matrix can be very expensive, the discrete adjoint equation is introduced as

$$\Lambda = -\left[ \frac{\partial R}{\partial U} \right]^{-T} \frac{\partial F^T}{\partial U} \hspace{1cm} \text{or} \hspace{1cm} \left[ \frac{\partial R}{\partial U} \right]^{T} \Lambda = -\frac{\partial F^T}{\partial U} \hspace{1cm} (32)$$

where $\Lambda$ is defined as the vector of the adjoint variables. Once $\Lambda$ is calculated using Equation (32), the final formulation for the sensitivity evaluation can be expressed as

$$\frac{dF^T}{dD} = \frac{\partial F^T}{\partial D} + \frac{\partial R^T}{\partial D} \Lambda \hspace{1cm} (33)$$

where the sensitivities are evaluated via matrix-vector products independently from the number of design variables.

In the following, the solution approach of the discrete adjoint equation, Equation (32), is discussed.
B. Adjoint Solution

As the full Jacobian matrix \( \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \) is needed for the solution of Equation (32), a full linearization of the residual vector \( \mathbf{R} \) with respect to the unknown vector \( \mathbf{U} \), including self-model (diagonal) as well as inter-model (off-diagonal) terms must be considered as

\[
\begin{bmatrix}
\frac{\partial \mathbf{R}}{\partial u}^T \\
\frac{\partial \mathbf{R}}{\partial p}^T \\
\frac{\partial \mathbf{R}}{\partial Y}^T
\end{bmatrix}^T =
\begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T & \frac{\partial R_u}{\partial Y}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T & \frac{\partial R_p}{\partial Y}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T & \frac{\partial R_Y}{\partial Y}^T
\end{bmatrix}
\]

(34)

It is to be noted that the full Jacobian matrix \( \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \) implemented for the solution of the adjoint equation is a completed form of the ones presented in Equations (22), (23) and (24) utilized for the solution of the flow equations. Due to the fact that transposing the assembled full Jacobian matrix is a costly process, the transpose operation is performed in the elemental level and the elemental matrices, already transposed, are sent to the assembly step.

Replacing Equation (34) into Equation (32), the adjoint system of equations gets the following structure

\[
\begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T & \frac{\partial R_u}{\partial Y}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T & \frac{\partial R_p}{\partial Y}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T & \frac{\partial R_Y}{\partial Y}^T
\end{bmatrix}
\begin{bmatrix}
\Lambda_u \\
\Lambda_p \\
\Lambda_T \\
\Lambda_Y
\end{bmatrix} =
\begin{bmatrix}
\frac{dF}{du}^T \\
\frac{dF}{dp}^T \\
\frac{dF}{dT}^T \\
\frac{dF}{dY}^T
\end{bmatrix}
\]

(35)

where \( \Lambda_u, \Lambda_p, \Lambda_T \) and \( \Lambda_Y \) are the adjoint variables corresponding the velocity, the pressure, the temperature and the species concentrations, respectively. It is to be noted that the full Jacobian matrix \( \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \) is calculated using the converged steady-state flow solution. As seen in Equation (35), the discrete adjoint method gives rise to a linear system of equations. The same as the flow equations, the adjoint equations are solved in a staggered manner where each model is considered separately using the block Jacobi iterative scheme. This yields to a set of coupled equations with the form of

\[
\begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T
\end{bmatrix}
\begin{bmatrix}
\Lambda_u \\
\Lambda_p \\
\Lambda_T \\
\Lambda_Y
\end{bmatrix}^{n+1} =
\begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T
\end{bmatrix}
\begin{bmatrix}
\Lambda_u^n \\
\Lambda_p^n \\
\Lambda_T^n \\
\Lambda_Y^n
\end{bmatrix} -
\begin{bmatrix}
\frac{dF}{du}^T \\
\frac{dF}{dp}^T \\
\frac{dF}{dT}^T \\
\frac{dF}{dY}^T
\end{bmatrix}
\]

(36)

\[
\frac{\partial R_i}{\partial T} \Lambda_T^{n+1} = \frac{\partial R_i}{\partial T} \Lambda_T^n - \begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T
\end{bmatrix}
\begin{bmatrix}
\Lambda_u^n \\
\Lambda_p^n \\
\Lambda_T^n \\
\Lambda_Y^n
\end{bmatrix} -
\begin{bmatrix}
\frac{dF}{du}^T \\
\frac{dF}{dp}^T \\
\frac{dF}{dT}^T \\
\frac{dF}{dY}^T
\end{bmatrix}
\]

(37)

\[
\frac{\partial R_i}{\partial Y} \Lambda_Y^{n+1} = -\frac{\partial R_i}{\partial Y} \Lambda_T^n - \begin{bmatrix}
\frac{\partial R_u}{\partial u}^T & \frac{\partial R_u}{\partial p}^T \\
\frac{\partial R_p}{\partial u}^T & \frac{\partial R_p}{\partial p}^T \\
\frac{\partial R_Y}{\partial u}^T & \frac{\partial R_Y}{\partial p}^T
\end{bmatrix}
\begin{bmatrix}
\Lambda_u^n \\
\Lambda_p^n \\
\Lambda_T^n \\
\Lambda_Y^n
\end{bmatrix} -
\begin{bmatrix}
\frac{dF}{du}^T \\
\frac{dF}{dp}^T \\
\frac{dF}{dT}^T \\
\frac{dF}{dY}^T
\end{bmatrix}
\]

(38)

where \( n \) denotes the iteration number.

Similar to the flow solution, the adjoint solution of each model and the iteration loop are performed in ALYA.
V. Numerical Results

A set of examples are introduced in this section to examine the performance of the presented sensitivity analysis scheme in chemically reacting flows. The idea is to compare the sensitivities calculated by the proposed method with the ones obtained from the finite difference scheme. In order to make a fair comparison, the converged flow solution to machine zero is considered for the computation of the finite difference sensitivities. It is to be mentioned that the validation of ALYA code for the solution of the flow (primal) problem has been demonstrated in previous works and this is not shown here.

In the first example, the sensitivity validation case involving the Navier-Stokes equations is presented. The coupling of the Navier-Stokes and thermal energy equations in sensitivity analysis is investigated in the second example whereas the sensitivities related to the fully coupled system are validated in the third example. Having validated the proposed sensitivity analysis approach in these three examples, the implementation of this method to a two-dimensional model of a real-world plug flow reactor is studied in the fourth example.

A. Laminar Flow in Cavity

This example is a classical benchmark to study incompressible flows containing a viscous flow with a constant viscosity in a square cavity of unit size, where its upper edge slides in the tangent direction. A prescribed velocity of magnitude 1.0 in the tangent direction and 0.0 in the normal direction is considered on the upper edge while the no-slip boundary condition is applied on the rest of the cavity edges. The pressure is assumed zero at one node located in a lower corner of the cavity. The domain is divided using a uniform mesh of 20 \times 20 (400) triangles with 441 nodes.

The viscosity is assumed as the design variable whereas the functional \( F \) is defined as the summation of the velocity magnitudes in all over the domain. In order to verify the capability of the proposed sensitivity analysis method in different flow conditions, three values 1.0, 0.1 and 0.01 are assumed for \( \mu \).

The obtained solutions of the flow problem with \( \mu = 0.1 \), including the \( x \) component of the velocity and the pressure, are presented in Figure 1 while the convergence graph of the residuals related to the continuity and the momentum equations are demonstrated in Figure 2 showing that the flow solution is converged to machine zero.

![Figure 1: Laminar flow in cavity. Obtained flow solution: (a) \( x \) component of velocity and (b) pressure.](image-url)
Figure 2: Laminar flow in cavity. Convergence of the residuals related to continuity and momentum equations.

The obtained solutions for the $x$ component of adjoint velocity and the adjoint pressure are depicted in Figure 3 demonstrating that the discrete adjoint method along with the presented stabilized FEM gives rise to smooth solutions. The convergence of the residuals related to the adjoint continuity and the adjoint momentum equations is shown in Figure 4 proving that the system of the adjoint equations is fully converged.

Figure 3: Laminar flow in cavity. Obtained adjoint solution: (a) $x$ component of adjoint velocity and (b) adjoint pressure.
The calculated sensitivities using the adjoint method and finite difference method (with perturbation of order $10^{-8}$) as well as the relative error $\epsilon$ between these two sets of values are presented in Table 1 for different values of $\mu$. It can be understood that the presented adjoint method is able to accurately evaluate the sensitivities in different flow conditions.

Table 1: Laminar flow in cavity. Comparison between the sensitivities obtained from finite difference and adjoint method for different values of $\mu$.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>Finite difference</th>
<th>Adjoint</th>
<th>$\epsilon$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>$2.20608058E-4$</td>
<td>$2.20608028E-4$</td>
<td>$1.35987779E-5$</td>
</tr>
<tr>
<td>0.1</td>
<td>11.4698695</td>
<td>11.4698752</td>
<td>5.02708424E-5</td>
</tr>
<tr>
<td>0.01</td>
<td>41.71500913</td>
<td>41.7149396</td>
<td>1.66678635E-4</td>
</tr>
</tbody>
</table>

B. Laminar Flow in Channel

This example involves the coupling of the Navier-Stokes equations with the thermal energy equations. The problem contains the flow of an incompressible viscous flow in a rectangular domain of size 1.0 m in the vertical direction and 5.0 m in the horizontal direction where a variable viscosity calculated from Sutherland’s law is considered. The temperature is fixed to 300 K on the left edge (inlet) where on the top and the bottom edges it is assumed to be 500 K. The velocity vector on the inlet is assumed to have only a constant normal component $u_{inl}$ while the no-slip condition is applied to the velocity vector on the top and the bottom edges. No condition is applied on the temperature and the velocity on the right edge (outlet). Also, the pressure is fixed to a constant value at one node in the lower edge of the domain. The initial values of the velocity and the temperature for the nodes inside the domain are set to their corresponding inlet values. Constant values 1200 J/(kg K) and 0.04 W/(m K) are assumed for the specific heat coefficient $C_p$ and the thermal diffusion coefficient $\lambda_t$, respectively. The domain is discretized using a uniform mesh of $20 \times 40$ (800) rectangles, corresponding to 861 nodes.

The functional as the previous example is considered here whereas the specific heat coefficient $C_p$ and the thermal diffusion coefficient $\lambda_t$ are assumed as the design variables. In order to demonstrate the importance of linearization accuracy on the solution of the adjoint equations, two different cases are considered for this example. In the first case, an approximate linearization is considered where the partial derivatives of the stabilization parameters $\tau_m$ and $\tau_t$ respect to the velocity and temperature values are not included while an exact linearization is assumed for the second case. To check the robustness of the presented sensitivity analysis method in different flow conditions, three values 0.1 m/s, 1.0 m/s and 10.0 m/s are assumed for
Figure 5 shows the results obtained for the $x$ component of the velocity and the temperature (by assuming $u_{inl} = 10.0$) whereas the convergence graph of the residuals related to the momentum, continuity and temperature equations is presented in Figure 6.

![Figure 5](image1)

(a)

![Figure 6](image2)

(b)

Figure 5: Laminar flow in channel. Obtained flow solution: (a) $x$ component of velocity and (b) temperature.

Figure 6: Laminar flow in channel. Convergence of the residuals related to the continuity, momentum and temperature equations.

By considering an exact linearization, the obtained solution for the $x$ component of the adjoint velocity and the adjoint temperature are depicted in Figure 7 where it can be seen that the presented stabilized FEM can provide smooth solution for the adjoint equations. By observing the convergence graph of the residuals corresponding to the adjoint equations in Figure 8, we understand that the solution of the adjoint equations is converged completely.

![Figure 7](image3)

![Figure 8](image4)

Figure 7: Laminar flow in channel. Obtained solution for the $x$ component of the adjoint velocity and the adjoint temperature.

Figure 8: Convergence graph of the residuals corresponding to the adjoint equations.
Figure 7: Laminar flow in channel. Obtained adjoint solution: (a) $x$ component of velocity and (b) temperature.

Figure 8: Laminar flow in channel. Convergence of the residuals related to the adjoint continuity, adjoint momentum and adjoint temperature equations.

Tables 2 and 3 demonstrate the comparison of the sensitivities derived from the adjoint scheme with the ones obtained from the finite difference method for design variables $C_p$ and $\lambda_t$, respectively, in different flow conditions where the adjoint sensitivities are calculated using the exact linearization as well as the approximate one. Also, the relative errors $\epsilon_{\text{exact}}$ and $\epsilon_{\text{approx}}$ related to the exact and the approximate linearizations, respectively, are presented in these tables. Good agreement with the finite difference results is observed for both design variables $C_p$ and $\lambda_t$ using the exact linearization whereas this agreement is lost when the approximate linearization is used, especially for the case with the higher velocities where the stabilization parameters get involved more.
Table 2: Laminar flow in channel. Sensitivity values calculated by finite difference and adjoint methods (approximate and exact approaches) along with corresponding relative errors for design variable \( C_p \) in different flow conditions.

<table>
<thead>
<tr>
<th>( u_{inl} )</th>
<th>Finite difference</th>
<th>Approximate adjoint</th>
<th>Exact adjoint</th>
<th>( \epsilon_{approx}(%) )</th>
<th>( \epsilon_{exact}(%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2.35791422E-7</td>
<td>2.36978414E-7</td>
<td>2.35769135E-7</td>
<td>5.0340E-1</td>
<td>9.4517E-3</td>
</tr>
<tr>
<td>1.0</td>
<td>2.88568078E-5</td>
<td>2.96565822E-5</td>
<td>2.88568663E-5</td>
<td>2.7715</td>
<td>2.0272E-4</td>
</tr>
<tr>
<td>10.0</td>
<td>9.55304525E-2</td>
<td>7.6882549E-2</td>
<td>9.55306844E-2</td>
<td>1.9520E+1</td>
<td>2.4274E-4</td>
</tr>
</tbody>
</table>

Table 3: Laminar flow in channel. Sensitivity values calculated by finite difference and adjoint methods (approximate and exact approaches) along with corresponding relative errors for design variable \( \lambda_i \) in different flow conditions.

<table>
<thead>
<tr>
<th>( u_{inl} )</th>
<th>Finite difference</th>
<th>Approximate adjoint</th>
<th>Exact adjoint</th>
<th>( \epsilon_{approx}(%) )</th>
<th>( \epsilon_{exact}(%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2.59458932E-6</td>
<td>2.63697811E-6</td>
<td>2.59458538E-6</td>
<td>1.6337</td>
<td>1.5185E-4</td>
</tr>
<tr>
<td>1.0</td>
<td>2.80444078E-4</td>
<td>2.94625889E-4</td>
<td>2.8044883E-4</td>
<td>5.0569</td>
<td>2.8726E-4</td>
</tr>
<tr>
<td>10.0</td>
<td>1.58041555E-3</td>
<td>1.90422429E-3</td>
<td>1.58041832E-3</td>
<td>2.0488E+1</td>
<td>1.7520E-4</td>
</tr>
</tbody>
</table>

C. Reacting Flow in Channel

In this example, the performance of the adjoint method is studied in a fully coupled system of equations where a laminar flow including chemical reactions of two species A and B with the form of

\[
A + B \leftrightarrow 2B
\]

passes through a channel. The considered domain is similar to the previous example with the same mesh characteristics. The imposed boundary conditions for the velocity, the pressure and the temperature are similar to the previous example (\( u_{inl} = 10.0 \)) whereas the concentrations of the species A and B are fixed to 0.1 and 0.9, respectively, at the inlet and they assumed free in the rest of the boundaries. The initial concentrations for the species A and B inside the domain are set to their corresponding inlet values. The preexponential constants \( A_f \) and \( A_b \) are assumed to be \( 1.0E+4 \) and \( 2.0E+3 \), respectively, while the values \( 2.5E + 4 \) and \( 2.0E + 4 \) are considered for the activation energies \( E_f \) and \( E_b \).

In this example, the design variables consist of the preexponential constants related to the forward and backward reaction, \( A_f \) and \( A_b \), whereas the objective functional \( F \) is defined as

\[
F = \sum_{k=1}^{n_s} \int_{\Omega} Y_k^2 d\Omega
\]

(40)

Because of the typical large order of preexponential constants \( A_{f,r} \) and \( A_{b,r} \), the gradient calculation using finite difference scheme needs some more considerations. For this reason, new design variables \( \epsilon_{f,r} \) and \( \epsilon_{b,r} \) are defined as

\[
\epsilon_{f,r} = \log_{10}(\frac{A_{f,r}}{A_{f,r}^0}) \quad \epsilon_{b,r} = \log_{10}(\frac{A_{b,r}}{A_{b,r}^0})
\]

(41)

where \( A_{f,r}^0 \) and \( A_{b,r}^0 \) are unperturbed preexponential constants and \( \epsilon_{f,r} \) and \( \epsilon_{b,r} \) represent the corresponding model parameters for the forward and backward rates. Using Equation (41), Equations (11) and (12) are modified as

\[
k_{f,r} = 10^{\epsilon_{f,r}} A_{f,r}^0 T^{\eta_{f,r}} e^{\frac{E_{f,r}}{RT}}
\]

(42)

\[
k_{b,r} = 10^{\epsilon_{b,r}} A_{b,r}^0 T^{\eta_{b,r}} e^{\frac{E_{b,r}}{RT}}
\]

(43)

The obtained solution for the concentrations of species A and B are shown in Figure 9 while the convergence graph of the residuals related to the mass species equations is presented in Figure 10.
Figure 9: Reacting flow in channel. Obtained solution for (a) concentration of species A and (b) concentration of species B.

Figure 10: Reacting flow in channel. Convergence of the residuals related to the mass species equations.

Figure 11 displays the obtained solution of the adjoint equations for some of the variables. It is observed that the nodes near the inlet has the most important effect on the defined functional. Figure 12 shows the convergence graph of the residuals of the adjoint equations related to the mass species.
Figure 11: Reacting flow in channel. Obtained solution for adjoint values corresponding to (a) concentration of species A and (b) concentration of species B.

Figure 12: Reacting flow in channel. Convergence of the residuals related to the adjoint mass species equations.

The sensitivity values obtained from the adjoint method as well as the ones deduced from the finite difference method along with the corresponding relative errors are presented in Table 4 for the design variables $\epsilon_f$ and $\epsilon_b$. It can be observed that the presented solution strategy for the adjoint method can provide accurate sensitivities.

Table 4: Reacting flow in channel. Sensitivity values calculated by finite difference and adjoint methods and corresponding relative errors for design variable $\epsilon_f$ and $\epsilon_b$.

<table>
<thead>
<tr>
<th></th>
<th>Finite difference</th>
<th>Adjoint</th>
<th>$\epsilon(%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$dF/d(\epsilon_f)$</td>
<td>$-3.42200967E-1$</td>
<td>$-3.42200973E-1$</td>
<td>$1.6667E-6$</td>
</tr>
<tr>
<td>$dF/d(\epsilon_b)$</td>
<td>$2.22932183E-1$</td>
<td>$2.22932299E-1$</td>
<td>$5.1768E-5$</td>
</tr>
</tbody>
</table>

D. Two-Dimensional Plug Flow Reactor

As the last example demonstrated in this paper, the presented sensitivity analysis method is applied to a two-dimensional model of a real-world plug flow reactor. The simplified geometry of the reactor, considered
for the simulation, is shown in Figure 13 where the inlet and the outlet sections are labelled. The domain, which goes from 0.0 m to 3.0 m vertically and from 0.0 m to 21.0 m horizontally, is discretized by an unstructured mesh of 14584 nodes and 14221 triangles with an element size of approximately 0.04 m in all over the domain. The flow inside the reactor includes the injection of 7 species from the inlet while these species leave the domain from the outlet after passing the reactor containers where the chemical reactions happen. The considered reactions have the following forms

\[ S_1 + S_2 \rightarrow S_3 + S_4 \]  \hspace{1cm} (44)
\[ S_2 \rightarrow S_5 + S_6 \]  \hspace{1cm} (45)
\[ S_4 + S_6 \rightarrow S_7 \]  \hspace{1cm} (46)

The preexponential constants \( A_{f,r} \) and the activation energies \( E_{f,r} \) for the first, second and third reactions related to Equations 44, 45 and 46, respectively, are delivered in Table 5. At the inlet, the velocity vector is fixed to have the values of 30.0 and 0.0 m/s in the horizontal and vertical directions, respectively, and the temperature value is set to 363 K while the values presented in Table 6 are assumed for the concentrations. At the wall, all the domain edges except the inlet and the outlet, only slip condition is assigned to the velocity whereas all the variables are left free at the outlet.

The objective functional are defined the same as the previous example whereas the design variables consist of the preexponential constants of the forward reactions \( A_{f,r} \), the specific heat coefficient \( C_p \) and the thermal diffusion coefficient \( \lambda_t \). It is to be noted that the definition presented in Equation 41 is also applied in this example.

Table 5: Two-dimensional plug flow reactor. Assumed values for the preexponential constants \( A_{f,r} \) and the activation energies \( E_{f,r} \).

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( A_{f,r} )</th>
<th>( E_{f,r} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.9088E4</td>
<td>62732.7</td>
</tr>
<tr>
<td>2</td>
<td>4.4417E4</td>
<td>66915.9</td>
</tr>
<tr>
<td>3</td>
<td>5.8150E4</td>
<td>63987.4</td>
</tr>
</tbody>
</table>

Table 6: Two-dimensional plug flow reactor. Considered values for the species concentrations at the inlet.

<table>
<thead>
<tr>
<th></th>
<th>( Y_{S_1} )</th>
<th>( Y_{S_2} )</th>
<th>( Y_{S_3} )</th>
<th>( Y_{S_4} )</th>
<th>( Y_{S_5} )</th>
<th>( Y_{S_6} )</th>
<th>( Y_{S_7} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet value</td>
<td>0.673624</td>
<td>0.295737</td>
<td>0.01424</td>
<td>0.000072291</td>
<td>0.0157463</td>
<td>0.000312167</td>
<td>0.0002628777</td>
</tr>
</tbody>
</table>

The obtained solutions for some of the variables are displayed in Figure 14. It is to be mentioned that the source terms related to each mass species equation \( w_k \) are highly nonlinear in terms of the species concentrations \( Y_k \). This causes that the fully convergence of the species residuals to machine zero is not accessible here. Hence, the calculation of the sensitivities using the finite difference scheme can not be performed properly since the perturbation created by the finite difference method is polluted by the machine error. For this reason, the validation of the adjoint sensitivities with the finite difference ones is not considered.
here. Also, it is to be noted that the validation is not necessary where the presented adjoint-based sensitivity analysis method has been validated in previous examples.

Figure 14: Two-dimensional plug flow reactor. Obtained solution for (a) temperature, (b) concentration of species S1 and (c) concentration of species S2.

Figure 15 shows the obtained adjoint solution for some variables where it can be seen that each variable has its own importance zone with higher effect on the considered functional. The convergence of the adjoint residuals related to three first species equations is shown in Figure 16. The calculated sensitivities using the obtained adjoint variables are presented in Table 7.

Figure 15: Two-dimensional plug flow reactor. Obtained solution for adjoint values corresponding to (a) temperature, (b) concentration of species S1 and (c) concentration of species S2.
Adjoint Species S1
Adjoint Species S3
Adjoint Species S2

Figure 16: Two-dimensional plug flow reactor. Convergence of the residuals related to the adjoint mass species equations.

Table 7: Two-dimensional plug flow reactor. Calculated sensitivities respect to different design variables using adjoint method.

<table>
<thead>
<tr>
<th>$dF/d(\epsilon_{f,1})$</th>
<th>$dF/d(\epsilon_{f,2})$</th>
<th>$dF/d(\epsilon_{f,3})$</th>
<th>$dF/d(C_p)$</th>
<th>$dF/d(\lambda_t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2.18874862E-1$</td>
<td>$-3.42547931E-1$</td>
<td>$6.5150554E-2$</td>
<td>$2.5898754E-5$</td>
<td>$8.55700241E-7$</td>
</tr>
</tbody>
</table>

VI. Concluding Remarks

In this research, the discrete adjoint method was implemented for evaluating the sensitivities of a set of parameters to a prescribed functional in the context of the steady-state chemically reacting flows where the governing equations are discretized using a stabilized FEM. A staggered algorithm is presented for the solution of both flow and adjoint equations. The exact Jacobian matrix of the fully coupled system is calculated through a hand-coded linearization of the discretized residuals corresponding to each module. A set of numerical examples related to the uncoupled as well as the coupled systems were delivered to check the accuracy of the proposed sensitivity analysis scheme where the adjoint sensitivities were compared with ones obtained by the finite difference method. The presented results demonstrate that the discrete adjoint method can provide accurate sensitivities in different models. Finally, this scheme is implemented to a two-dimensional model of a real-world plug flow reactor. The present approach is to be utilized for sensitivity analysis of three-dimensional models with turbulence effects. The derived sensitivities will be used during an inverse problem in order to predict the preexponential constants of a system of multiple reactions.

References