Abstract

This Ph.D. thesis deals with the development, programming and application of Computational Fluid Dynamics (CFD) methods for the numerical prediction of flow fields and the optimization of aerodynamic shapes using deterministic methods and the exact hessian matrix of the cost function and the constraints. Emphasis is put on the suitable formulation of the above on hybrid grids. The thesis is structured in two basic parts. The first part covers the solution of the state problem and consists of the mathematical formulation of the flow equations for turbulent compressible flows, the discretization of the aforementioned equations on hybrid grids and the iterative schemes used for their solution. The second part presents the mathematical formulation of the discrete adjoint problem for the computation of the first- and second-order sensitivities, as well as the necessary tools which use the computed adjoint field in the context of inverse design/optimization and the a posteriori error analysis for computing functionals with arbitrary accuracy.

In the field of CFD, the thesis' contribution is a complete methodology for solving turbulent flows on 2D and 3D hybrid grids. The methodology comprises the grid data structure and the formulation of appropriate discretization schemes. The method is validated through an adequate set of 2D and 3D case studies of internal and external aerodynamics. Proposed numerical schemes, the interpolation of nodal values to the finite volume edges and their contribution to the numerical fluxes must be reported. In addition, a hybrid grid refinement strategy was also developed; this can be used either as a traditional grid adaptation or in conjunction with discrete adjoint methods for reducing the error in the computation of quantities such as the lift, the drag or the total pressure losses of turbomachinery cascades.

In the field of optimization, a novel method for computing first- and second-order sensitivities using the discrete adjoint method is proposed. The method covers functionals used in inverse design and total pressure losses minimization problems and utilizes their so-computed sensitivities in designing optimal geometries subject to geometric and flow constraints using deterministic optimization methods. The developed software comprises only hand-differentiated routines, in order to achieve maximized efficiency and memory savings, in contrast to other works which almost exclusively depend on automatic differentiation. A
Newton method was implemented, which uses the exactly computed Hessian matrix to rapidly locate the optimum in inverse design and total pressure losses optimization problems. Furthermore, the hybridization of the Newton method with quasi-Newton methods was also explored, to further increase the efficiency of the optimization algorithm.

In addition to the aforementioned Newton methods, the a posteriori error analysis method for hybrid grids was also developed, which combines the discrete adjoint method and the refinement technique developed in this thesis, to accurately predict quantities with practical interest, such as the lift, the total pressure losses or the entropy generation in the flow field.