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During the last years, a key research activity in PCOpt/NTUA has been the development of adjoint-based methods for the computation of first- and higher-order derivatives of objective functions used in aerodynamic optimization. The development is based on body-fitted in-house flow solvers (time-marching solvers for both compressible and incompressible flows, with the latter based on the pseudo-compressibility technique), OpenFOAM (pressure-based method for incompressible flows) and Cut- and Ghost-Cell solvers (compressible flows). On the in-house (U)RANS solver, both the continuous and discrete adjoint approaches have been developed, with emphasis laying on the former. The continuous adjoint approach has been exclusively used for OpenFOAM and the Cut- and Ghost-cell solvers. For constrained optimization problems, the adjoint method is used for both the objective and constraint functions.

Up to recently, regarding the mathematical formulation of continuous adjoint methods, two different approaches were available. The first one expresses the gradient in terms of only boundary/surface integrals (SI), is computationally cheap but, depending on the case, may compute inexact gradients on inadequately fine grids. This is especially pronounced in turbulent flow cases or cases with intense flow separation. The second one expresses the gradient in terms of both surface and field integrals (FI); it is accurate but computationally much more expensive, especially in case where many design variables are used. To bridge the gap between them, a new enhanced surface formulation (E-SI) assisted by the adjoint to a grid displacement model, which is accurate and cheap as it is free of volume integrals, has been recently proposed by PCOpt/NTUA.

Most research groups utilizing continuous adjoint make use of the so-called "frozen turbulence" assumption when computing sensitivity derivatives for turbulent flows, i.e. it is considered that turbulent quantities will remain unaffected by the changes in the optimized shape. PCOpt/NTUA was the first group to differentiate the turbulence model equations, demonstrating that, depending on the case, this omission can lead to even wrongly signed sensitivities. Since then, the most widely used turbulence models have been differentiated in low- and high-Re variants.

In the adjoint to the Cut- and Ghost-Cell methods developed by PCOpt/NTUA, the mathematical formulation takes into consideration the special treatment of the boundary conditions in the flow simulation, in order for the adjoint solver to become compatible with the primal one and lead to the accurate computation of sensitivity derivatives. The use of Cartesian meshes allows for large geometry deformations, leading to optimal solutions that cannot be easily achieved with body-fitted methods.

The challenge of developing and using adjoint-based methods for unsteady flows lays in the fact that the adjoint PDEs have to be integrated backwards in time and hence the flow solution has to be either fully stored (very high memory requirements) or re-computed from the initial time-step (very high CPU cost). PCOpt/NTUA contributes to the development of adjoint-based methods for unsteady flows by implementing and using suitable reduced-order models for the reconstruction of each flow field instance, leading to affordable gradient-based optimization loops, both memory- and CPU cost-wise.

Continuous adjoint methods for solving topology optimization problems for laminar and turbulent ducted flows of incompressible fluids, with or without heat transfer, have been developed by PCOpt/NTUA, utilizing both the porosity and level-set approaches. For turbulent flows, the adjoint approach is exact, i.e. includes the differentiation of the turbulence model. In addition, a back-to-CAD algorithm has been developed in order to convert the zero-level set solution of topology optimization to CAD compatible NURBS curves and surfaces.

In either the continuous or the discrete adjoint formulation, the adjoint methods have been extended to compute the (exact) Hessian of the objective function. It was concluded that the use of direct differentiation followed by the adjoint method (tangent-then-reverse in the terminology of AD methods) computes the Hessian with the lowest cost. This cost scales with the number of design variables; in small sized problems, the ability to compute the Hessian allows the use of the (exact) Newton method which, generally, outperforms steepest-descent or quasi-Newton methods. However, since the CPU cost of using the Newton method, with exact gradient and Hessian computations at each cycle, becomes prohibitively high in case of many design variables, PCOpt/NTUA proposed an efficient optimization scheme that computes the exact Hessian only once and then updates it in an approximated manner through the BFGS formula; the so called "exactly-initialized quasi-Newton method" outperforms (exact) Newton or quasi-Newton methods.

To avoid the Hessian computation (in large scale optimization problems, in particular), the truncated Newton algorithm can be used instead. The adjoint approach followed by the direct differentiation of both the flow and adjoint equations is proved to be the most efficient way to compute the product of the Hessian matrix with any vector required by the truncated Newton algorithm, in which the Newton equations are solved via the conjugate gradient or GMRES method. Considering that the cost of solving either the adjoint or the direct differentiation equations is approximately equal to that of solving the flow equations, the cost per Newton iteration scales linearly with the (small) number of conjugate gradient steps required, rather than the (much higher, in large scale problems) number of design variables (if the Hessian itself was computed).

The second-order second-moment (SOSM) approach, coupled with an adjoint-based algorithm, for the solution of robust design problem in aerodynamics, has been developed by PCOpt/NTUA. Since the objective function for the robust design problem comprises first- and second-order sensitivity derivatives of the baseline objective with respect to the uncertain parameters, the application of a gradient-based method, which requires the sensitivities of this function with respect to the design variables, calls for the computation of third-order mixed derivatives. To compute these derivatives with the minimum CPU cost, a combination of the direct differentiation and the adjoint variable method was proposed by PCOpt/NTUA, for the first time in the relevant literature.