AD-based perturbation methods for uncertainties and errors

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Abstract: The progress of automatic differentiation (AD) and its impact on perturbation methods is the object of this paper. AD studies show an important activity for developing methods addressing the management of modern CFD kernels, taking into account the language evolution and intensive parallel computing. The evaluation of a posteriori error analysis and of resulting correctors will be addressed. Recent works in the AD-based construction of second-derivatives for building reduced-order models based on a Taylor formula will be presented on the test case of a steady compressible flow around an aircraft.

Keywords: automatic differentiation; AD; second-order derivatives; uncertainty; error correction; design; CFD; systems modelling; simulation.

Reference to this paper should be made as follows: Martinelli, M., Dervieux, A., Hascoët, L., Pascual, V. and Belme, A. (2010) 'AD-based perturbation methods for uncertainties and errors', *Int. J. Engineering Systems Modelling and Simulation*, Vol. 2, Nos. 1/2, pp.65–74.

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Valérie Pascual as a student at Ecole Normale Supérieure de Jeunes Filles in Paris, she received her PhD in Computer Science from Paris XI University in 1983. She joined INRIA in 1984 as a Permanent Researcher. She developed programming environments and structured editors for Lisp and Java languages and worked on interactive structured editing tools using program transformations. In 1999 she joined the new TROPICS team. Her current area of research includes analysis and transformation of programs applied to automatic differentiation. She participates in the development of the TAPENADE automatic differentiation tool.

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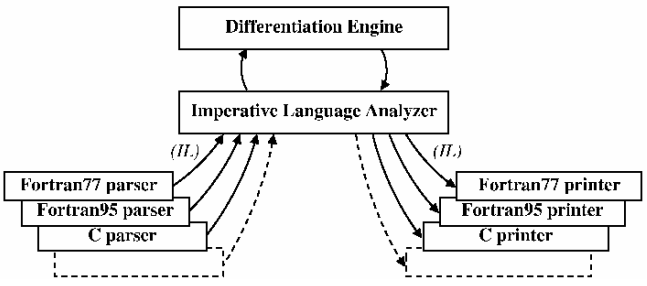
1 Introduction

While high fidelity models are mainly used for deterministic design, which assumes a perfect knowledge of the environmental and operational parameters, uncertainty can arise in many aspects of the entire design-production-operational process: from the assumptions done in the mathematical model describing the underlying physical process to the manufacturing tolerances and to the operational parameters and conditions that could be affected by unpredictable factors (e.g., atmospheric conditions). Exact and approximate techniques for propagating these uncertainties require additional computational effort but are progressively well-established. The proposed study takes place in NODESIM-CFD FP6 project (Martinelli and Hascoët, 2008; NODESIM-CFD, 2008). The automatic differentiation (AD) tool TAPENADE (Hascoët and Pascual, 2004) is discussed in Section 2. It has been developed for a large range of applications where the code-to-code direct and reverse differentiation is needed. Direct and reverse ADs are used for addressing numerical error reduction since they help building correctors (Section 3). In Section 4, uncertainty propagation is addressed by a perturbation technique using the first terms of Taylor series of the high-fidelity model (method of moments). Previous investigation of these methods can be found in Ghate and Giles (2006, 2007). We present as example the response surface of a wing.

2 AD improvements

Our AD tool TAPENADE has been extended to deal with Fortran95 and with ANSI C (Pascual and Hascoët, 2005; Pascual and Hascoët, 2008). Figure 1 shows the architecture of TAPENADE. It is implemented mostly in Java (115,000 lines) except for the separate front-ends which can be written in their own languages. Front- and back-ends communicate with the kernel via an intermediate abstract language ('IL') that makes the union of the constructs of individual imperative languages. Notice also the clear separation between the general-purpose program analysis and the differentiation engine itself.

Figure 1 Overall architecture of TAPENADE



Thanks to the language-independent internal representation of programs, this still makes a single and only tool and every development benefits to differentiation of each input language. One of these developments concerned the pointer analysis. The reverse mode now accepts most uses of pointers and allocation. Another development concerned declarations. The differentiated program respects the order of declarations, uses the include files and keeps the comments from the original program. Generated codes are more readable and often smaller. We also investigated extensions to TAPENADE to successive differentiations, in particular to efficiently handle tangent differentiation of the stack primitives present in the reverse differentiated codes. We implemented user directives for the reverse differentiation of a frequent class of parallel loops (directive `II-LOOP`) and for optimal checkpointing in reverse differentiation (Naumann et al., 2008; Hascoët et al., 2008; Tber et al., 2007). TAPENADE lets the user specify finely which procedure calls must be checkpointed or not with the directive `NOCHECKPOINT`.

3 Numerical errors reduction

3.1 Error estimates and correctors

Let us recall first how linearised – direct or adjoint – states can be useful for improving numerical accuracy issues.

Numerical error involves the deviation between the solution $W = W(x, y, z)$ of mathematical model, i.e., of the non-linear PDE symbolised by:

$$\Psi(W) = 0, \tag{1}$$

and the output data produced by the computations, i.e., the more or less perfect numerical solution of the discrete system:

$$\mathbf{\Psi}_h(\mathbf{W}_h) = 0 \in \mathbb{R}^N. \tag{2}$$

The discrete unknown $\mathbf{W}_h$ is the N-dimensional array of degrees of freedom:

$$\mathbf{W}_h \in \mathbb{R}^N, \mathbf{W}_h = [(\mathbf{W}_h)_i].$$

The output data produced by the computation do not involve a function W_h but, instead the array $\mathbf{W}_h$ which needs to be transformed via an interpolation: let $V \in L^2(\Omega)$ a space of rather smooth function. In practice, $V \subset \mathcal{C}^0(\bar{\Omega})$. Let R_h be a linear interpolation operator transforming an array of N degrees of freedom into a continuous function:

$$R_h : \mathbb{R}^N \to V \ \mathbf{v}_h \mapsto R_h \mathbf{v}_h. \tag{3}$$

Let:

$$W_h(x, y, z) = (R_h \mathbf{W}_h)(x, y, z).$$

Similarly, we need an operator from continuous functions to arrays. Let T_h be an operator transforming a continuous function into an array of N degrees of freedom:

$$T_h : V \to \mathbb{R}^N \quad v \mapsto T_h v. \tag{4}$$

It is useful to take the adjoint of R_h :

$$T_h = R_h^*. \tag{5}$$

The deviation between the PDE solution and the numerical one can be defined as $W - W_h$. It consists mainly of approximation errors, of algorithmic errors arising typically because iterative algorithms are not iterated infinitely, and of round-off errors due to the fact that the programme is run in floating point arithmetic. We discuss here mainly of approximation errors, although the other ones may be also addressed in part by the method studied here. Another way to post-process a computation is to use it for evaluating a 'scalar' functional:

Let j a smooth linear functional applying W into the scalar number:

$$j(u) = (g, W)_{L^2(\Omega)}$$

where g is a given $L^2(\Omega)$ function. This allows to define:

$$\mathrm{g}_h = T_h g$$

$$g_h = R_h \mathrm{g}_h = R_h T_h g \tag{6}$$

The continuous adjoint writes:

$$(\frac{\partial \Psi}{\partial W})^* p = g.$$

The discrete adjoint equation is then defined by:

$$\left[\frac{\partial \Psi_h}{\partial W_h}\right]^T \mathrm{p}_h = T_h g. \tag{7}$$

And we can then consider:

$$p_h = R_h \mathrm{p}_h.$$

A fundamental assumption of the present analysis is that this discrete adjoint is a good enough approximation of continuous adjoint p for allowing to replace p by p_h the calculations which follow. In order to evaluate the approximation error, two kinds of estimates can be applied:

- *A posteriori* estimate:

$$\Psi(W) - \Psi(W_h) = -\Psi(W_h) \tag{8}$$

where $\Psi(W_h)$ is the continuous residual applied to discrete solution. Then:

$$W - W_h \approx -\left[\frac{\partial \Psi}{\partial W}\right]^{-1} \Psi(W_h). \tag{9}$$

- *A priori* estimate:

$$\Psi_h(T_h W) - \Psi_h(W_h) = -\Psi_h(T_h W) \tag{10}$$

where $\Psi_h(T_h W)$ is the discrete residual applied to discretised continuous solution. Then:

$$T_h W - \mathbf{W}_h \approx -\left[\frac{\partial \Psi_h}{\partial W_h}\right]^{-1} \Psi_h(T_h W). \tag{11}$$

We observe that these estimates involve unavailable continuous functions. In the *a posteriori* estimate, the solution of the continuous linearised system can be approximated thanks to the discrete Jacobian. For the *a priori* estimate, we can also solve this issue in some particular case (see Loseille, 2008), by replacing $\Psi_h(T_h W)$ by an expression $T_h \Theta h(W_h)$ depending only of W_h. Corresponding to these estimates, we have the following 'field correctors':

$$\delta W_h = -R_h \left[\frac{\partial \Psi_h}{\partial W_h}\right]^{-1} T_h \Psi(W_h) \tag{12}$$

$$\delta R_h \mathbf{W}_h = -R_h \left[\frac{\partial \Psi_h}{\partial W_h}\right]^{-1} T_h \Theta h(W_h) \tag{13}$$

and the following 'direct-linearised goal-oriented correctors':

$$\delta_1 j = -\left(g, R_h \left[\frac{\partial \Psi_h}{\partial W_h}\right]^{-1} T_h \Psi(W_h)\right)_{L^2(\Omega)} \tag{14}$$

$$\delta_2 j = -\left(g, R_h \left[\frac{\partial \Psi_h}{\partial W_h}\right]^{-1} T_h \Theta_h(W_h)\right)_{L^2(\Omega)} \tag{15}$$

Also follows the 'adjoint-based goal-oriented correctors':

$$\delta_1 j = -(p_h, T_h \Psi(W_h))_{L^2(\Omega)} \tag{16}$$

$$\delta_2 j = -(p_h, T_h \Theta_h(W_h))_{L^2(\Omega)} \tag{17}$$

We recognize here the superconvergent corrector of Pierce and Giles (1998). We observe that, thanks to the choice of T_h as the adjoint operator of R_h, the linearised-based and adjoint-based formulation are perfectly equivalent. At the contrary, the effort to compute them is very different, particularly in the case of unsteady PDE, since the adjoint system has to be solved reverse in time while using the state solution at all time levels (Hascoët and Dauvergne, 2008). This remark leads to the following recommendations:

- use the direct linearised formulation in any case, you only need a corrector for the field as well as a corrector for one or several output functionals
- the adjoint formulation is compulsory when you wish to derive a goal-oriented optimal mesh.

The second recommendation is motivated by the fact that an optimal mesh will be derived from minimisation of the error term in which we need to put in evidence the dependance of error with respect to mesh. Since the adjoint is an approximation of a continuous function, it does not much depend of mesh. At the contrary, the continuous residual $T_h \Psi(W_h)$ or the truncation error $T_h \Theta_h(W_h)$ are

proportional to a power of the mesh size. In Loseille (2008), the truncation error is expressed in terms of second derivatives of solution field and allows the derivation of an optimal mesh.

3.2 An example

To end this discussion, we give a numerical example of corrector evaluation built on a finite-element approximation. We can write Euler equations under the form:

$$\begin{aligned} &W \in V = H^1(\Omega)^5, \quad \forall \phi \in V, \\ &\int_\Omega \mathcal{F}(W)\nabla\phi d\Omega - \int_{\partial\Omega} \phi\hat{\mathcal{F}}(W).n\, d\Gamma = 0 \end{aligned} \tag{18}$$

where $\hat{\mathcal{F}}(W)$ accounts for the different boundary conditions. Let us introduce a discretisation of the previous EDP. Let τ_h a tetrahedrisation of Ω with N vertices. It will rely on a discrete space of functions:

$$V_h = \{\phi_h \in H^1(\Omega)^5, \forall T \in \tau_h, \phi_h | T \in \mathcal{P}^1\}$$

the canonical basis of which is denoted:

$$V_h = span[N_i], N_i(x_j) = \delta_{ij} \forall i, j, \text{ vertices of } \tau_h,$$

and on the interpolation operator:

$$\prod_h : \mathcal{V} \to V_h, \prod_h \phi(x_i) = \phi(x_i), \forall i, \text{ vertex of } \tau_h.$$

Comparing with the previous abstract theory, we get:

$$\begin{aligned} &R_h : \mathbb{R}^{5N} \to V_h, \quad \mathbf{f}_h \mapsto R_h\mathbf{f}_h = \Sigma_i[\mathbf{f}_h]_i N_i, \\ &T_h : \mathcal{V} \to \mathbb{R}^{5N}, \quad \phi \mapsto T_h\phi = [\phi(x_i)]. \end{aligned}$$

The discretisation is set into the discrete space, but also it differs from the continuous statement in two features, a discrete flux $\mathcal{F}_h$ instead of $\mathcal{F}$:

$$\mathcal{F}_h : \mathcal{V} \to V'$$

and an extra term of artificial diffusion D_h:

$$\begin{aligned} &W_h \in V_h, \ \forall \phi_h \in V_h, (\Psi_h(W_h), \phi_h)_{V' \times V} = 0, \\ &\text{with} \\ &(\Psi_h(W_h), \phi_h)_{V' \times V} = \int_\Omega \phi_h \bar{\mathcal{F}}_h(W_h).n \ d\Gamma \\ &+ \int_\Omega \phi_h D_k(W_h) d\Omega. \end{aligned} \tag{19}$$

The discrete fluxes are chosen as follows:

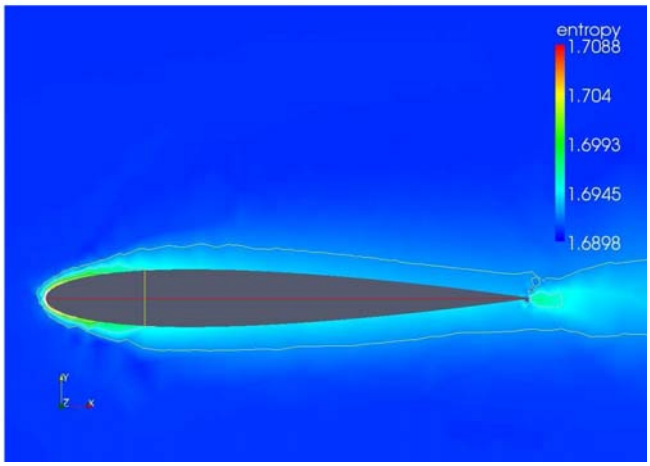
$$\begin{aligned} &\mathcal{F}_h(W) = \mathcal{F}_h(\prod_h W) = \prod_h \mathcal{F}(\prod_h W). \\ &\bar{\mathcal{F}}_h(W) = \bar{\mathcal{F}}_h(\prod_h W) = \prod_h \bar{\mathcal{F}}(\prod_h W). \end{aligned} \tag{20}$$

After some calculations and simplifications, the main error term appears as follows:

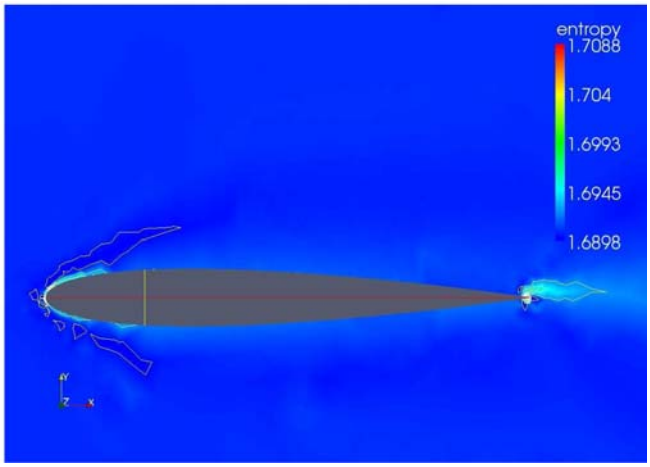
$$\begin{aligned} &(\frac{\partial\Psi_h}{\partial W_h}\delta W_h, \phi_h) = -\int_\Omega \nabla\phi_h(\mathcal{F}(W) - \prod_h \mathcal{F}(W)) d\Omega \\ &+ \int_\Gamma \phi_h(\hat{\mathcal{F}}^{out}(W) - \prod_h \hat{\mathcal{F}}^{out}(W)).n \ d\Omega \end{aligned} \tag{21}$$

with $\bar{\mathcal{F}}(W).n = \mathcal{F}(W).n - \hat{\mathcal{F}}(W).n$. A Gauss quadrature is applied for the evaluation of the right hand side. We have applied this to a steady subsonic flow and give some preliminary results. Figure 2 compares the entropy generation in the flow computed directly and the same flow corrected by formula (21). Entropy level is one order of magnitude smaller.

Figure 2 Entropy spurious generation for, (a) direct computation of a steady flow (b) for a corrected one (see online version for colours)



(a)



(b)

4 Uncertainty propagation

In optimisation problems, uncertainty propagation analysis may concern the study of the 'cost functional'

$$j : \gamma \mapsto j(\gamma) := J(\gamma, W) \in \mathbb{R} \tag{22}$$

where all varying parameters are represented by the 'uncertain (i.e., not-deterministic) control variables; $\gamma \in \mathbb{R}^n$, and where the state variables $W = W(\gamma) \in \mathbb{R}^N$ are solution of the (non-linear) 'state equation'

$$\Psi(\gamma, W) = 0. \tag{23}$$

It is important to note that the state equation (23) contains the governing PDE of the mathematical model of the physical system of interest (for example, the stationary part of the Euler or Navier-Stokes equations) and it can be viewed as an 'equality constraint' for the functional (22). The basic probabilistic approaches for analysing the propagation of uncertainties are Monte-Carlo methods. A full non-linear Monte-Carlo method gives us complete and exact information about uncertainty propagation in the form of its PDF, but with a prohibitively expensive cost in terms of CPU time. In NODESIM-CFD, several other 'probabilistic' approaches for analysing the propagation of uncertainties are considered such as Latine Hypercubes and Polynomial Chaos. We contribute on perturbative methods based on the Taylor expansion (Martinelli, 2007).

4.1 Perturbation methods

To reduce the computational cost, we may think to use only some (derivate) quantities characterising the distribution of the input variables instead of an entire sample drawn from a population with a given PDF. Therefore, the idea behind the method of moments is based on the Taylor series expansion of the original non-linear functional (22) around the 'mean value' of the input control ($\mu_\gamma = E[\gamma]$), and then computing some statistical moments of the output (usually mean and variance). In this way, we are assuming that the input control γ can be decomposed as sum of a fully deterministic quantity μ_γ with a stochastic perturbation $\delta\gamma_u$ with the property $E[\delta\gamma_u] = 0$. With these definitions, the Taylor series expansion of the functional $j(\gamma)$ around the mean value μ_γ is:

$$j(\gamma) = j(\mu_\gamma + \delta\gamma_u) = j(\mu_\gamma) + G\delta\gamma_u + \frac{1}{2}\delta\gamma_u^* H \delta\gamma_u + O(\|\delta\gamma_u\|^3) \tag{24}$$

where $G = \left.\frac{\partial j}{\partial \gamma_u}\right|_{\mu_\gamma}$ is the gradient of the functional respect to the uncertain variables and $H = \left.\frac{\partial^2 j}{\partial {\gamma_u}^2}\right|_{\mu_\gamma}$ is the Hessian matrix, both evaluated at the mean of the input variables μ_γ.

By considering various orders of the Taylor expansion (24) and taking the first and the second statistical moment, we can approximate the mean μ_j and the variance σ_j^2 of the functional $j(\gamma)$ in terms of its derivatives evaluated at μ_γ and in terms of statistical moments of the control γ.

First order moment methods:

$$\begin{cases} \mu_j = j(\mu_\gamma) + O\left(E[\delta\gamma_u^2]\right) \\ \sigma_j^2 = E\left[(G\delta\gamma_u)^2\right] + O\left(E[\delta\gamma_u^3]\right) \end{cases} \tag{25}$$

Second order moment methods:

$$\begin{aligned} &\mu_j = j(\mu_\gamma) + \frac{1}{2}E\left[\delta\gamma_u^* H \delta\gamma_u\right] \\ &+O\left(E[\delta\gamma_u^3]\right) \\ &\sigma_j^2 \\ &= E\left[(G\delta\gamma_u)^2\right] + E\left[(G\delta\gamma_u)(\delta\gamma_u^* H\delta\gamma_u)\right] \\ &-\frac{1}{4}E\left[\delta\gamma_u^* H\delta\gamma_u\right]^2 + \frac{1}{4}E\left[(\delta\gamma_u^* H\delta\gamma_u)^2\right] \\ &+O\left(\delta\gamma_u^4\right) \end{aligned}$$

With this method, it is clear that we are using only some partial information about the input uncertainties, in fact, we are using only some statistical moments of the control variable instead of full information available with its PDF, and we will not have anymore the PDF of the propagated uncertainty, but only its approximate mean and variance. Another important point is that the method of moments is applicable only for small uncertainties, due to the local nature of Taylor expansion approximation.

Two things should be noted here: the first one is that for the method of moments 'we need the derivatives' of the functional respect to the control variables affected by uncertainties: in particular, we need the gradient for the first order method, and gradient and Hessian for the second order method. Due to the fact that $j(\gamma) = j(\gamma, W)$, where $W = W(\gamma)$ is the solution of the state equation (23), we have for the derivative:

$$\frac{\partial j}{\partial \gamma_u} = \frac{\partial J}{\partial \gamma_u} + \frac{\partial J}{\partial W}\frac{\partial W}{\partial \gamma_u}$$

Since we know the solution $W(\gamma)$ by its numerical values as result of a program (implementing an appropriate method, e.g., fixed point method), it is interesting to use of AD tools (like TAPENADE) in order to obtain the needed derivatives (Martinelli et al., 2007). The same remarks apply to the computation of the Hessian matrix. In particular, we note that the derivatives are computed at the mean value of the control μ_γ, so they are fully deterministic and can be picked out from the expectations in the equations (25) or (26). In other words, we can write

$$\begin{aligned} E &= \left[(G\delta\gamma_u)^2\right] = \sum_{i,k} G_i G_k E\left[\delta\gamma_u^{(i)}\delta\gamma_u^{(k)}\right] = \sum_{i,k} G_i G_k C_{ik} \\ E &= \left[\delta\gamma_u^* H\delta\gamma_u\right] = \sum_{i,k} H_{ik} E\left[\delta\gamma_u^{(i)}\delta\gamma_u^{(k)}\right] = \sum_{i,k} G_i G_k C_{ik} \\ E &= \left[(G\delta\gamma_u)(\delta\gamma_u^* H\delta\gamma_u)\right] = \sum_{i,k,l} G_l H_{ik} E\left[\delta\gamma_u^{(i)}\delta\gamma_u^{(k)}\delta\gamma_u^{(l)}\right] \\ E &= \left[(\delta\gamma_u^* H\delta\gamma_u)^2\right] = \sum_{i,k,l,m} H_{ik} H_{lm} E\left[\delta\gamma_u^{(i)}\delta\gamma_u^{(k)}\delta\gamma_u^{(l)}\delta\gamma_u^{(m)}\right] \end{aligned} \tag{26}$$

where $G_i = \left.\frac{\partial j}{\partial \gamma_u^{(i)}}\right|_{\mu_\gamma}$ are the elements of the gradient, $H_{ik} = \left.\frac{\partial^2 j}{\partial \gamma_u^{(i)} \partial \gamma_u^{(k)}}\right|_{\mu_\gamma}$ are the elements of the Hessian matrix and $C_{ik} = E[\delta\gamma_u^{(i)} \delta\gamma_u^{(k)}] = \mathrm{cov}(\gamma_u^{(i)} \gamma_u^{(k)})$ are the elements of the 'covariance matrix'. Every expectation term $E[\ldots]$ in the equation (26) is defined by the statistical model of the uncertainties and could be computed in a pre-processing phase.

For example, for the important case where the uncertainties are random and normally distributed, we have:

$$E\left[\delta\gamma_u^{(i)} \delta\gamma_u^{(k)} \delta\gamma_u^{(l)}\right] = 0$$
$$E\left[\delta\gamma_u^{(i)} \delta\gamma_u^{(k)} \delta\gamma_u^{(l)} \delta\gamma_u^{(m)}\right] = C_{ik}C_{lm} + C_{il}C_{km} + C_{im}C_{kl}$$

and if these (normal) uncertainties are independent, then hold the relation $C_{ik} = \sigma_i^2 \delta_{ij}$ where $\sigma_i^2 = E\left[\delta\gamma_u^{(i)} \delta\gamma_u^{(i)}\right]$ and the equations (26) become

$$\begin{aligned} E &= \left[(G\delta\gamma_u)^2\right] = \sum_i G_i^2 \sigma_i^2 \\ E &= \left[\delta\gamma_u^* H \delta\gamma_u\right] = \sum_i H_{ii} \sigma_i^2 \\ E &= \left[(G\delta\gamma_u)(\delta\gamma_u^* H \delta\gamma_u)\right] = 0 \\ E &= \left[(\delta\gamma_u^* H \delta\gamma_u)^2\right] = \sum_{i,k} (H_{ii}H_{kk} + 2H_{ik}^2) \sigma_i^2 \sigma_k^2 \end{aligned} \tag{27}$$

Since we have the term $E = \left[(\delta\gamma_u^* H \delta\gamma_u)^2\right] / 4$, the error is still of the order of $E = \left[\delta\gamma_u^4\right]$. Computing the other terms of same order require the knowledge of order of derivatives higher than the second. From the previous discussion, it is clear that in order to apply the method of moments we need to solve only one (expensive) non-linear system with derivatives (at the mean μ_γ) and then apply the (inexpensive) equations (25) or (26) where, for the fully non-linear Monte-Carlo approach of the previous section, we need to solve $N \gg 1$ non-linear systems (23).

4.2 First and second-order derivatives of a functional

We are interested by obtaining the first and second derivatives of a functional j depending of $\gamma \in \mathbb{R}^N$, and expressed in terms of a state $W \in \mathbb{R}^N$ as follows:

$$\begin{cases} \psi(\gamma) = \Psi(\gamma, W(\gamma)) = 0 \\ j(\gamma) = J(\gamma, W(\gamma)) \end{cases} \tag{28}$$

Our problem can be viewed from two different points of view: the first one is consider the solution algorithm for state equation as part of j itself, i.e., considering j as a function of the control variables γ only. The second one is consider the system made by two different routines: one of them is the routine that solves the non-linear system $\Psi(\gamma, W(\gamma)) = 0$ (and contains the evaluation the residual $\Psi(\gamma, W)$), and the other is the routine $J(\gamma, W)$ that computes the value of the functional from the state variables W and (eventually) the control variables γ.

The first approach leads to a straightforward algorithm for first order derivatives, in fact, we just need to differentiate the entire routine j with tangent or reverse mode. In this context, the routine j contains the iterative solver method for the state equation, and the differentiated routines will also contain this loop in differentiated form. If we need n_{iter} loop iterations in order to obtain the non-linear solution, and we assume for each iteration a unitary cost, we can analyse the cost for the gradient of the functional.

Using tangent mode, the cost for the entire gradient will be $n(n_{\text{iter}}\alpha_T)$ where n is the number of components of the gradient and $1 < \alpha_T < 4$ is the overhead associated with the differentiated code respect to the original one. For this strategy, the memory requirements will be of the same order of the undifferentiated code.

With reverse mode (Hascoët et al., 2005) we are able to obtain the entire gradient with a single evaluation of the differentiated routine, but the total cost (in terms of CPU time and memory) will depends on the strategy used by the AD tool to solve the problem of inverse order differentiation for the original routine. For the case of a store-all (SA) strategy, the CPU cost will be $(n_{\text{iter}}\alpha_R)$ with $1 < \alpha_R <$, i.e., α_R times the undifferentiated code, but the required memory will be n times greater. For a recompute-all (RA) strategy, the CPU cost will be $(n_{\text{iter}}^2\alpha_R)$, i.e., $(n_{\text{iter}}\alpha_R)$ the non-linear solution, but the memory will be the same of the undifferentiated routine. For real large programs, neither SA nor RA strategy can work, so we need a special storage/recomputation trade-off in order to be efficient using 'checkpoints'. Obviously, with checkpointing the CPU cost will be greater than the cost of SA strategy and can be shown that the cost for the differentiated code will be of the order of $s\sqrt[s]{n_{\text{iter}}}$ (where s is the number of snapshots available).

It is clear that for gradient computation with $n \gg 1$, the reverse mode is faster than tangent mode, but for a program containing an iterative algorithm, the reverse mode is not always applicable. The problem relies on the fact that the reverse mode computation is performed in the opposite way of the original code ('backward sweep') after a 'forward sweep' needed to store the variable needed in the successive phases.

For the previous arguments, we prefer differentiate not the entire program (solution of the state equation + functional evaluation), but the two main component in a separate way, using the fact that at the solution, the residuals will be zero (i.e., we do not differentiate the routine containing the main loop, but only the quantities involved after the last iteration). For this second approach,

we have to analyse the influence of state equation and the functional evaluation in more details. This is the purpose of the next sections.

4.2.1 First derivative

Using the chain rule, the gradient of the functional $j(\gamma) = J(\gamma, W(\gamma))$ is given by:

$$\frac{dj}{d\gamma} = \frac{\partial J}{\partial \gamma} + \frac{\partial J}{\partial W}\frac{dW}{d\gamma}$$

where the derivatives of the state variables $W(c)$ are obtained solving the linear system

$$\frac{d\psi}{d\gamma} = \frac{\partial \Psi}{\partial \gamma} + \frac{\partial \Psi}{\partial W}\frac{dW}{d\gamma} = 0.$$

Therefore, two strategies can be applied.

Direct differentiation

It consists in computing the Gateaux-derivatives with respect to each component direction $((e_i = (0,\ldots 0,1,0,\ldots,0)^T$, where 1 is at the i-esim component):

$$\frac{dj}{d\gamma_i} = \frac{dj}{d\gamma}e_i = \frac{\partial J}{\partial \gamma_i} + \frac{\partial J}{\partial W}\frac{dW}{d\gamma_i} \tag{29}$$

with:

$$\frac{\partial \Psi}{\partial W}\frac{dW}{d\gamma_i} = \frac{\partial \Psi}{\partial \gamma}e_i \tag{30}$$

This has to be applied to each component of γ, i.e., n times and the cost is n linearised N-dimensional systems to solve. If we choose to solve the single system (30) with an iterative matrix-free method, and the solution is obtained after n_{iter} step, the total cost will be of the order of $\alpha_T n_{\text{iter},T}$, i.e., $n_{\text{iter},T}$ evaluation of the matrix-by-vector operation $\left(\frac{\partial \Psi}{\partial W}\right)x$, where each evaluation costs α_T times the evaluation of the state residual $\Psi(\gamma, W)$ (and the cost of the state residual is taken as reference equal to 1). Therefore, the cost of the full gradient will be $n\alpha_T n_{\text{iter},T}$.

Inverse differentiation (reverse mode)

The complete gradient is given by the equation

$$\left(\frac{dj}{d\gamma}\right)^* = \left(\frac{\partial j}{\partial \gamma}\right)^* - \left(\frac{\partial \Psi}{\partial \gamma}\right)^* \Pi_0 \tag{31}$$

where Π_0 is the solution of the linear system

$$\left(\frac{\partial \Psi}{\partial W}\right)^* \Pi = \left(\frac{\partial j}{\partial W}\right)^* \tag{32}$$

This computation needs only one extra linearised N-dimensional system, the adjoint system (some methods for calculation of the adjoint solutions are described in). If we choose to solve the adjoint system (32) with an iterative matrix-free method, we can apply the same estimate done as in the case of the tangent mode differentiation, but this time the overhead associated with the evaluation of the matrix-by-vector operation $\left(\frac{\partial \Psi}{\partial W}\right)^* x$ respect to the state residual evaluation will be α_R and usually $\alpha_R > \alpha_T$, and the number of iteration $n_{\text{iter},R}$ for the convergence of the solution could be different from $n_{\text{iter},T}$ of the previous case (but the asymptotical rate of convergence will be the same of the original linear system $\left(\frac{\partial \Psi}{\partial W}\right)x = b$, see Pierce and Giles (1998) for more details. Therefore, the cost for the gradient will be $\alpha_R n_{\text{iter},R}$, and the reverse mode differentiation for the gradient computation is cheaper than the tangent mode if $n \gg 1$.

4.2.2 Second derivative

For second derivatives we have different possibilities.

Direct-direct option

This method was initially investigated along with various other algorithms, but the publication does not go into the implementation details for a generic fluid dynamic code. Here we present the mathematical background behind the idea and the efficient AD implementation of Ghate and Giles but with a different analysis of the computational cost.

Starting from the derivative (29), we perform another differentiation respect to the variable γ_k obtaining

$$\frac{d^2 j}{d\gamma_i d\gamma_k} = D^2_{i,k}J + \frac{\partial j}{\partial W}\frac{d^2 W}{d\gamma_i d\gamma_k} \tag{33}$$

where

$$D^2_{i,k}J = \frac{\partial}{\partial \gamma}\left(\frac{\partial J}{\partial \gamma}e_i\right)e_k + \frac{\partial}{\partial W}\left(\frac{\partial J}{\partial \gamma}e_i\right)\frac{dW}{d\gamma_k} + \frac{\partial}{\partial W}\left(\frac{\partial J}{\partial \gamma}e_k\right)\frac{dW}{d\gamma_i} + \frac{\partial}{\partial W}\left(\frac{\partial J}{\partial W}\frac{dW}{d\gamma_i}\right)\frac{dW}{d\gamma_k}$$

Differentiating the equation (30) we get

$$D^2_{i,k}\Psi + \frac{\partial \Psi}{\partial W}\frac{d^2 W}{d\gamma_i d\gamma_k} = 0 \tag{34}$$

where

$$D^2_{i,k}\Psi = \frac{\partial}{\partial \gamma}\left(\frac{\partial \Psi}{\partial \gamma}e_i\right)e_k + \frac{\partial}{\partial W}\left(\frac{\partial \Psi}{\partial \gamma}e_i\right)\frac{dW}{d\gamma_k} + \frac{\partial}{\partial W}\left(\frac{\partial \Psi}{\partial \gamma}e_k\right)\frac{dW}{d\gamma_i} + \frac{\partial}{\partial W}\left(\frac{\partial \Psi}{\partial W}\frac{dW}{d\gamma_i}\right)\frac{dW}{d\gamma_k}$$

Substituting the second derivatives of the state respect to the control variables $\frac{d^2W}{d\gamma_i d\gamma_k}$ in equation (33) from equation (34) we get

$$\begin{aligned}\frac{d^2 j}{d\gamma_i d\gamma_k} &= D^2_{i,k}J - \frac{\partial J}{\partial W}\left(\frac{\partial \Psi}{\partial W}\right)^{-1} D^2_{i,k}\Psi \\ &= D^2_{i,k}J - \prod\nolimits_0^* D^2_{i,k}\Psi\end{aligned} \tag{35}$$

where $\prod_0$ is the solution of the adjoint system (32) evaluated at the point $(\gamma, W(\gamma))$ solution of the state equation $\Psi(\gamma, W) = 0$. The n derivatives $\frac{dW}{d\gamma_i}$ should be computed (and stored) using tangent mode differentiation of the non-linear solver algorithm, and each derivatives costs $n_{\text{iter}}\alpha_T$. If we need the full Hessian matrix, we have to evaluate the quantity (35) $n(n+1)/2$ times, i.e., we have to evaluate the terms $D^2_{i,k}\Psi$ and $D^2_{i,k}J$ for $i = 1,\ldots,n$ and $j = i,\ldots,n$ due to the symmetry of the Hessian, and each evaluation of ($D^2_{i,k}\Psi$ costs α_T^2 (the evaluation of $D^2_{i,k}J$) is negligible respect to $(D^2_{i,k}\Psi)$). Therefore, the full Hessian costs $n\alpha_T[n_{\text{iter},T} + (n+1)\alpha_T/2]$. With similar arguments, if we want only the diagonal part of the Hessian, the cost is $n\alpha_T[n_{\text{iter},T} + \alpha_T]$.

Inverse-direct

This consists in the direct derivation in any direction $e_i, i = 1, n$ of the (non-scalar) function:

$$\begin{aligned}\left(\frac{\partial j}{\partial \gamma}\right)^*(\gamma, W(\gamma)) &= \left(\frac{\partial J}{\partial \gamma}\right)^*(\gamma, W(\gamma)) \\ &\quad - \left(\frac{\partial \Psi}{\partial \gamma}\right)^* \prod(\gamma, W(\gamma))\end{aligned}$$

where $W(\gamma)$ and $\prod(\gamma, W(\gamma))$ are solutions of the above two state systems. With some algebra we obtain

$$\begin{aligned}\frac{\partial}{\partial \gamma_i}\left(\frac{\partial j}{\partial \gamma}\right)^* &= \left(\frac{\partial^2 j}{\partial^2}\gamma\right)e_i = \frac{\partial}{\partial \gamma}\left(\frac{\partial J}{\partial \gamma}\right)^* e_i \\ &\quad + \frac{\partial}{\partial W}\left(\frac{\partial j}{\partial \gamma}\right)^* \theta_i - \frac{\partial}{\partial \gamma}\left[\left(\frac{\partial \Psi}{\partial \gamma}\right)^* \prod_0\right] e_i \\ &\quad - \frac{\partial}{\partial W}\left[\left(\frac{\partial \Psi}{\partial \gamma}\right)^* \prod_0\right]\theta_i - \left(\frac{\partial \Psi}{\partial \gamma}\right)^* \lambda_i\end{aligned}$$

The derivation needs the solution of the adjoint systems

$$\left(\frac{\partial \Psi}{\partial W}\right)^* \prod_0 = \left(\frac{\partial j}{\partial W}\right)^* \tag{36}$$

and $2n$ perturbed *N*-dimensional linear systems (for the full Hessian):

$$\begin{cases} \dfrac{\partial \Psi}{\partial W}\theta_i = -\dfrac{\partial \Psi}{\partial \gamma}e_i \\ \left(\dfrac{\partial \Psi}{\partial W}\right)^* \lambda_i = \dfrac{\partial}{\partial \gamma}\left(\dfrac{\partial J}{\partial W}\right)^* e_i \\ + \dfrac{\partial}{\partial W}\left(\dfrac{\partial J}{\partial W}\right)^* \theta_i - \dfrac{\partial}{\partial \gamma}\left[\left(\dfrac{\partial \Psi}{\partial W}\right)^* \prod_0\right] e_i \\ - \dfrac{\partial}{\partial W}\left[\left(\dfrac{\partial \Psi}{\partial W}\right)^* \prod_0\right]\theta_i \end{cases}$$

where all the functions in the equations (36)–(37) are evaluated at the final state (in order to verify $\Psi(\gamma, W(\gamma)) = 0$).

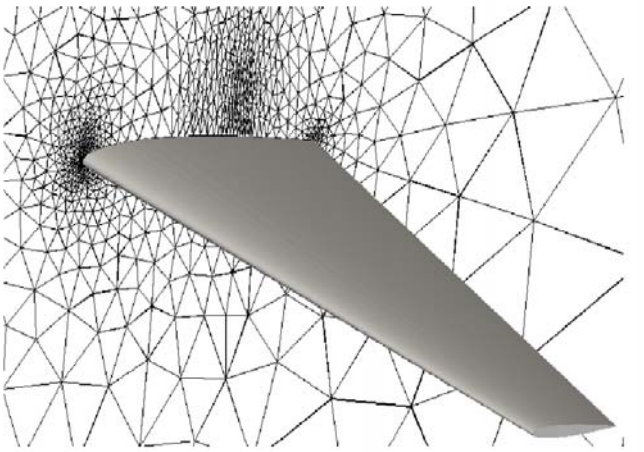
Inverse-inverse

If we are interested in a (scalar!) functional depending on the gradient, then it can be interesting to apply a second inverse differentiation. We do not focus on this direction at the moment.

5 Numerical experiments

The interest of this approach is briefly illustrated by the building of a response surface for the wing shape of a business aircraft (courtesy of Piaggio Aero Ind.), for a transonic regime (see the shape and the mesh in Figure 3). The nominal operational conditions are defined by the free-stream Mach number $M_\infty = 0.83$ and the incidence $\alpha = 2°$. We suppose that only these two quantities are subject to random fluctuations. For simplicity, we assume that their PDF are Gaussian with given mean and variance. The mean values correspond to the nominal values. The section of the initial wing shape corresponds to the NACA 0012 airfoil.

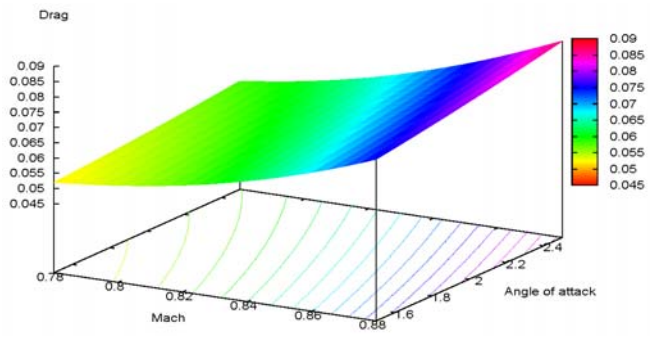
Figure 3 Wing shape and mesh in the symmetry



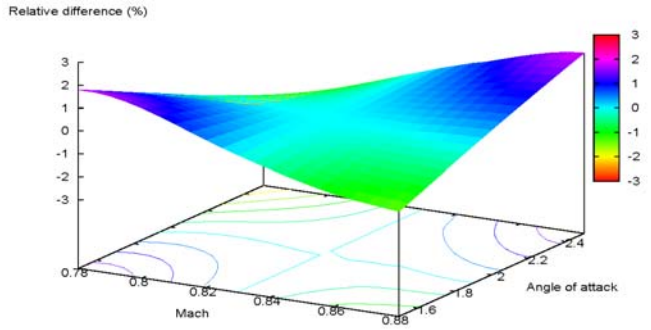
For the present work, due to the fact that we consider only two uncertain variables, we used a ToT approach for the Hessian evaluation. The accuracy of the second-order response surface obtained with the differentiated software is not different from the one obtained with other works, such

as those of Ghate and Giles (2007) (who, by the way, also used TAPENADE, but on another CFD software). We illustrate this accuracy in Figure 4. The direct evaluation required 21 × 21 non-linear simulations. The second-order approximation required only one non-linear state equation $\Psi = 0$ plus four linear systems using ToT. Relative error is less than 2% while using only first derivatives produce errors of 16%. Let us mention that this method compares also well with Kriging methods as was demonstrated in the comparison paper of Martinelli and Duvigneau (2008).

Figure 4 Drag coefficient vs. Mach number and angle of attack (first-order spatial accuracy) for the transonic wing, (a) non-linear simulations (b) percentage relative difference between the non-linear simulations and the second order Taylor approximation (see online version for colours)



(a)



(b)

Note: For the top plot we have solved 21 × 21 non-linear systems $\Psi = 0$.

6 Concluding remarks

AD methods and tools take place in a process which tends to make numerical simulation more secure by contributing to build the derived software necessary for addressing uncertainty and error. Thanks to AD, the derivation of this software is performed with more and more safety. This paper has displayed two main examples of this process. First, uncertain data are modelled by random variables and their impact on the simulation process is evaluated by a method of moments. The complexity of the proposed method is analysed for large number of uncertain variables. The two methods studied are already competitive for a small number of variables and even more for a large one.

Acknowledgments

These studies are supported in part by NODESIM-CFD, an FP-6 European project.

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