Epilogue

Like the solution of systems of linear equations, the evaluation of derivatives for composite functions is a classical computational problem whose basic solution has been known for hundreds of years. Yet with every new class of mathematical models and perpetual changes in the characteristics of modern computing platforms, the old problem reappears in a new light, calling at least for adjustments if not innovations in the established solution methodology. In this book we have tried to provide a repository of concepts and algorithmic ideas that can be used to discuss and resolve the differentiation aspects of any nonlinear computational task. Many basic questions remain unresolved, many promising ideas untested, and many almost certain improvements unimplemented.

From a mathematical point of view the most important challenge seems to firmly connect AD with the theory of semi-algebraic and subanalytic functions. That would then allow in principle the rigorous foundation of generalized differentiation concepts and the provision of corresponding derivative objects. The practicality of that approach is not entirely clear since, for example, the composition of the sine function with the reciprocal must be excluded. Another very interesting question is whether direct and adjoint derivatives of iterates converge when these are not generated by an ultimately smooth and contractive fixed point iteration. This question concerns, for example, conjugate gradients and other Krylov subspace methods. It appears currently that in these important cases the piggyback approach discussed in sections 15.3–15.5 may not work at all. Then a separate iterative solver for the direct or adjoint sensitivity equation must be set up by the user or possibly a rather sophisticated AD tool.

So far, the application of AD in the context of PDE-constrained optimization problems is restricted to the discretize-then-optimize, or better discretize-then-differentiate, approach. Currently, the relation to the alternative differentiate-then-discretize, also known as discretize-then-optimize, forms an active research area. Of critical importance here is that gradients and Jacobians of continuous (differential) equations are defined in terms of appropriate inner- or other duality products. In contrast the algebraic differentiation of discretized equations always yields gradient representations with respect to the Euclidean inner product on the “design space” of independent variables. It may therefore need to be transformed to a more appropriate ellipsoidal norm by what is often called a smoothing step. These connections warrant further investigation and may lead to more flexible and convenient AD software in the future.

Another area of current interest is the quantification of sensitivities and moments in the presence of stochastic uncertainty, which typically involves the evaluation of second and higher order derivatives. These are also of great importance in numerical bifurcation and experimental design, where third or even fourth derivatives become indispensable. Moreover, as recently shown by Kubota [BB$^+$08], the evaluation of (sparse) permanents and some combinatorial graph problems can be recast as the task of evaluating mixed derivatives of high order. This observation provides another confirmation that some aspects of (algorithmic) differentiation are NP hard.

From a computer science point of view, the most pressing problem appears to be the identification, storage, and retrieval of those intermediate values or elemental partials that truly need to be passed from the recording sweep of a subroutine call to the corresponding returning sweep, which may take place much later. As the gap between processor speed and memory bandwidth continues to grow, all implementations of the basic reverse mode tend to become memory bound, whether they be based on source transformation or operator overloading. Therefore, to avoid disk storage of temporary data altogether, one may attempt to employ checkpointing and partial recomputation strategies of the kind developed in Chapter 12. Due to the associativity of the chain rule derivative computations typically allow for more concurrency than the underlying simulations. The promise and urgency to exploit this added parallelism grow as multicore processing become more and more prevalent. Therefore, appropriate strategies for the algorithmic differentiation of such codes turns into a significant aspect for the future acceptance of AD.

AD tool development has so far been carried out by small research groups with varying composition and fluent objectives. While a lot has been achieved in this way, it seems doubtful that sufficient progress toward a comprehensive AD system for all of Fortran 95 or C++ can be made in this “academic” fashion. Hence, wider collaboration to develop and maintain a compiler with “-ad” option as in the NAG Fortran compiler is a natural approach. Synergies of the required execution reversal technology can be expected with respect to parallelization and debugging. Operator overloading will continue to provide an extremely flexible and moderately efficient implementation of AD, and its efficiency may benefit from improved compiler optimization on user-defined types, possibly aided by the exploitation of expression templates on the statement level.

Concerning the general problem of evaluating derivatives, quite a few scientists and engineers have recently been convinced that it is simply an impossible task on their increasingly complex multilayered computer models. Consequently, some of them abandoned calculus-based simulation and optimization methods altogether in favor of “evolutionary computing approaches” that are based exclusively on function values and that often draw on rather colorful analogies with “real-life” processes. In contrast, we firmly believe that the techniques sketched in this book greatly enlarge the range of problems to which dreary old calculus methods can still be applied efficiently and even conveniently. In fact, they will be indispensable to the desired transition from system simulation to system optimization in scientific computing.

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