

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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Bibliography

- [AB74] R.S. Anderssen and P. Bloomfield, *Numerical differentiation proceedings for non-exact data*, Numer. Math. **22** (1974), 157–182.
- [AB04] N. Arora and L.T. Biegler, *A trust region SQP algorithm for equality constrained parameter estimation with simple parameter bounds*, Comput. Optim. Appl. **28**, (2004), 51–86.
- [Alk98] B. Alkire, *Parallel computation of Hessian matrices under Microsoft Windows NT*, SIAM News **31**, December 1998, 8–9.
- [AC92] J.S. Arora and J.B. Cardoso, *Variational principle for shape design sensitivity analysis*, AIAA **30** (1992), 538–547.
- [AC⁺92] B.M. Averick, R.G. Carter, J.J. Moré, and G.-L. Xue, *The MINPACK-2 Test Problem Collection*, Preprint MCS-P153-0692, ANL/MCS-TM-150, Rev. 1, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, 1992.
- [ACP01] P. Aubert, N. Di Césaré, and O. Pironneau, *Automatic differentiation in C++ using expression templates and application to a flow control system*, Comput. Vis. Sci. **3** (2001) 197–208.
- [AH83] G. Alefeld and J. Herzberger, *Introduction to Interval Computations*, Academic Press, New York, 1983.
- [AHU74] A.V. Aho, J. Hopcroft, and J.D. Ullman, *The Design and Analysis of Computer Algorithms*, Addison-Wesley, Reading, MA, 1974.
- [Bau74] F.L. Bauer, *Computational graphs and rounding error*, SIAM J. Numer. Anal. **11** (1974), 87–96.
- [BBC94] M.C. Bartholemew-Biggs, L. Bartholemew-Biggs, and B. Christianson, *Optimization and automatic differentiation in Ada: Some practical experience*, Optim. Methods Softw. **4** (1994), 47–73.
- [BB⁺95] A.W. Bojanczyk, R.P. Brent, and F.R. de Hoog, *Stability analysis of a general Toeplitz system solver*, Numer. Algorithms **10** (1995), 225–244.

- [BB⁺96] M. Berz, C.H. Bischof, G. Corliss, and A. Griewank (eds.), *Computational Differentiation—Techniques, Applications, and Tools*, SIAM, Philadelphia, 1996.
- [BB⁺97] C.H. Bischof, A. Bouaricha, P.M. Khademi, and J.J. Moré, *Computing gradients in large-scale optimization using automatic differentiation*, INFORMS J. Comput. **9** (1997), 185–194.
- [BB⁺99] I. Bauer, H.G. Bock, S. Körkel, and J.P. Schlöder, *Numerical methods for initial value problems and derivative generation for DAE models with application to optimum experimental design of chemical processes*, in Proc. of Scientific Computing in Chemical Engineering II, Hamburg, Springer, Berlin, 1999, pp. 338–345.
- [BB⁺08] C.H. Bischof, H.M. Bücker, P. Hovland, U. Naumann, J. Utke, (eds.), *Advances in Automatic Differentiation*, Lect. Notes Comput. Sci. Eng. **64**, Springer, Berlin, 2008.
- [BCG93] C.H. Bischof, G. Corliss, and A. Griewank, *Structured second- and higher-order derivatives through univariate Taylor series*, Optim. Methods Softw. **2** (1993), 211–232.
- [BCL01] A. Ben-Haj-Yedder, E. Cances, and C. Le Bris, *Optimal laser control of chemical reactions using automatic differentiation*, in [CF⁺01], pp. 205–211.
- [BC⁺92] C.H. Bischof, G.F. Corliss, L. Green, A. Griewank, K. Haigler, and P. Newman, *Automatic differentiation of advanced CFD codes for multidisciplinary design*, J. Comput. Syst. in Engrg. **3** (1992), 625–638.
- [BC⁺96] C.H. Bischof, A. Carle, P.M. Khademi, and A. Mauer, *The ADIFOR 2.0 system for the automatic differentiation of Fortran 77 programs*, IEEE Comput. Sci. Engrg. **3** (1996).
- [BC⁺06] M. Bücker, G. Corliss, P. Hovland, U. Naumann, and B. Norris (eds.), *Automatic Differentiation: Applications, Theory, and Implementations*, Lect. Notes Comput. Sci. Eng. **50**, Springer, New York, 2006.
- [BCP96] K.E. Brenan, S.L. Campbell, and L.R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, Classics Appl. Math. **14**, SIAM, Philadelphia, 1996.
- [BD95] C.H. Bischof and F. Dilley, *A compilation of automatic differentiation tools*, SIGNUM Newsletter **30** (1995), no. 3, 2–20.
- [BD⁺02] L.S. Blackford, J. Demmel, J. Dongarra, I. Duff, S. Hammarling, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petitet, R. Pozo, K. Remington, and R.C. Whaley, *An updated set of basic linear algebra subprograms (BLAS)*, ACM Trans. Math. Softw. **28** (2002), no. 2, 135–151.

- [BDL08] J. Bolte, A. Daniilidis, and A.S. Lewis, *Tame mappings are semismooth*, to appear in Math. Program. (2008).
- [Bel07] B.M. Bell, *A Package for C++ Algorithmic Differentiation*, <http://www.coin-or.org/CppAD/>, 2007.
- [Ben73] Ch. Bennett, *Logical reversibility of computation*, IBM J. Research and Development **17** (1973), 525–532.
- [Ber90a] M. Berz, *Arbitrary order description of arbitrary particle optical systems*, Nuclear Instruments and Methods **A298** (1990), 26–40.
- [Ber90b] M. Berz, *The DA Precompiler DAFOR*, Tech. Report, Lawrence Berkeley National Laboratory, Berkeley, CA, 1990.
- [Ber91b] M. Berz, *Forward algorithms for high orders and many variables with application to beam physics*, in [GC91], pp. 147–156.
- [Ber95] M. Berz, *COSY INFINITY Version 7 Reference Manual*, Tech. Report MSUCL-977, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI, 1995.
- [Ber96] M. Berz, *Calculus and numerics on Levi-Civita fields*, in [BB⁺96], pp. 19–35.
- [Ber98] M. Berggren, *Numerical solution of a flow control problem: Vorticity reduction by dynamic boundary action*, SIAM J. Sci. Comput. **19** (1998), 829–860.
- [Bes98] A. Best, *Vergleich von Minimierungsverfahren in der Umformsimulation unter Verwendung des Automatischen Differenzierens*, diploma thesis, Technische Universität Dresden, Germany, 1998.
- [Bey84] W.J. Beyn, *Defining equations for singular solutions and numerical applications*, in Numerical Methods for Bifurcation Problems, T. Küpper, H.D. Mittelman, and H. Weber, eds., Internat. Ser. Numer. Math., Birkhäuser, Boston, 1984, pp. 42–56.
- [BGL96] M. Berggren, R. Glowinski, and J.L. Lions, *A computational approach to controllability issues for flow-related models. I: Pointwise control of the viscous Burgers equation*, Int. J. Comput. Fluid Dyn. **7** (1996), 237–252.
- [BGP06] R.A. Bartlett, D.M. Gay, and E.T. Phipps: *Automatic differentiation of C++ codes for large-scale scientific computing*, in Proceedings of ICCS 2006, V. Alexandrov et al., eds., Lecture Notes in Comput. Sci. **3994**, Springer, Berlin, 2006, pp. 525–532.
- [BH96] C.H. Bischof and M.R. Haghghat, *Hierarchical approaches to automatic differentiation*, in [BB⁺96], pp. 83–94.

- [BIP88] J. Burns, K. Ito, and G. Prost, *On nonconvergence of adjoint semi-groups for control systems with delays*, SIAM J. Control Optim. **26** (1988), 1442–1454.
- [BJ⁺96] C.H. Bischof, W.T. Jones, J. Samareh-Abolhassani, and A. Mauer, *Experiences with the application of the ADIC automatic differentiation tool to the CSCMDO 3-D volume grid generation code*, AIAA Paper 96-0716, Jan. 1996.
- [BK⁺59] L.M. Beda, L.N. Korolev, N.V. Sukkikh, and T.S. Frolova, *Programs for Automatic Differentiation for the Machine BESM*, Tech. Report, Institute for Precise Mechanics and Computation Techniques, Academy of Science, Moscow, 1959.
- [BK78] R.P. Brent and H.T. Kung, *Fast algorithms for manipulating formal power series*, Assoc. Comput. Mach. **25** (1978), 581–595.
- [BK⁺97] C.H. Bischof, P.M. Khademi, A. Bouaricha, and A. Carle, *Efficient computation of gradients and Jacobians by dynamic exploitation of sparsity in automatic differentiation*, Optim. Methods Softw. **7** (1997), 1–39.
- [BL⁺01] H.M. Bücker and B. Lang and D. an Mey and C.H. Bischof, *Bringing together automatic differentiation and OpenMP*, in ICS '01: Proceedings of the 15th international conference on Supercomputing, ACM, New York, 2001, 246–251.
- [BP97] Å. Björck and V. Pereyra, *Solution of Vandermonde systems of equations*, Math. Comp. **24** (1997), 893–903.
- [BPS06] S. Basu, R. Pollack, and M.-F. Roy, *Algorithms in Real Algebraic Geometry*, Springer, New York, 2006.
- [BR01] R. Becker and R. Rannacher, *An optimal control approach to a-posteriori error estimation in finite element methods*, Acta Numerica **10** (2001), pp. 1–102.
- [BRM97] C.H. Bischof, L. Roh, and A. Mauer, *ADIC: An Extensible Automatic Differentiation Tool for ANSI-C*, Tech. Report ANL/MCS-P626-1196, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, 1997.
- [Bro98] S.A. Brown, *Models for Automatic Differentiation: A Conceptual Framework for Exploiting Program Transformation*, Ph.D. thesis, University of Hertfordshire, Hertfordshire, UK, 1998.
- [BRW04] H.M. Bücker, A. Rasch, and A. Wolf, *A class of OpenMP applications involving nested parallelism*, in SAC '04: Proceedings of the 2004 ACM Symposium on Applied Computing, 2004, pp. 220–224.

- [BS83] W. Baur and V. Strassen, *The complexity of partial derivatives*, Theoret. Comput. Sci. **22** (1983), 317–330.
- [BS92] D. Bestle and J. Seybold, *Sensitivity analysis of constraint multibody systems*, Arch. Appl. Mech. **62** (1992), 181–190.
- [BS96] C. Bendsten and O. Stauning, *FADBAD, a Flexible C++ Package for Automatic Differentiation Using the Forward and Backward Methods*, Tech. Report IMM-REP-1996-17, Department of Mathematical Modelling, Technical University of Denmark, Lyngby, Denmark, 1996.
- [Cac81a] D.G. Cacuci, *Sensitivity theory for nonlinear systems. I. Nonlinear functional analysis approach*, Math. Phys. **22** (1981), 2794–2802.
- [Cac81b] D.G. Cacuci, *Sensitivity theory for nonlinear systems. II. Extensions of additional classes of responses*, Math. Phys. **22** (1981), 2803–2812.
- [Cam89] S.L. Campbell, *A computational method for general higher index nonlinear singular systems of differential equations*, IMACS Trans. Sci. Comp. **1.2** (1989), 555–560.
- [CC86] T.F. Coleman and J.-Y. Cai, *The cyclic coloring problem and estimation of sparse Hessian matrices*, SIAM J. Algebraic Discrete Methods **7** (1986), 221–235.
- [CC94] Y.F. Chang and G.F. Corliss, *ATOMFT: Solving ODEs and DAEs using Taylor series*, Comput. Math. Appl. **28** (1994), 209–233.
- [CDB96] B. Christianson, L.C.W. Dixon, and S. Brown, *Sharing storage using dirty vectors*, in [BB⁺96], pp. 107–115.
- [CD⁺06] W. Castings, D. Dartus, M. Honnorat, F.-X. Le Dimet, Y. Loukili, and J. Monnier, *Automatic differentiation: A tool for variational data assimilation and adjoint sensitivity analysis for flood modeling*, in [BC⁺06], pp. 250–262.
- [Cés99] N. Di Césaré, *Outils pour l’optimisation de forme et le contrôle optimal, application à la mécanique des fluides*, Ph.D. thesis, de l’Université Paris 6, France, 2000.
- [CF96] A. Carle and M. Fagan, *Improving derivative performance for CFD by using simplified recurrences*, in [BB⁺96], pp. 343–351.
- [CF⁺01] G. Corliss, C. Faure, A. Griewank, L. Hascoët, and U. Naumann (eds.), *Automatic Differentiation: From Simulation to Optimization*, Computer and Information Science, Springer, New York, 2001.
- [CG97] W.G. Choe and J. Guckenheimer, *Computing periodic orbits with high accuracy*, Comput. Methods Appl. Mech. Engrg., **170** (1999), 331–341.

- [CGT92] A.R. Conn, N.I.M. Gould, and P.L. Toint, *LANCELOT, a Fortran package for large-scale nonlinear optimization (release A)*, Comput. Math. **17**, Springer, Berlin, 1992.
- [Cha90] R.W. Chaney, *Piecewise C^k -functions in nonsmooth analysis*, Nonlinear Anal. **15** (1990), 649–660.
- [Che06] B. Cheng, *A duality between forward and adjoint MPI communication routines*, in Computational Methods in Science and Technology, Polish Academy of Sciences, 2006, pp. 23–24.
- [Chr92] B. Christianson, *Reverse accumulation and accurate rounding error estimates for Taylor series coefficients*, Optim. Methods Softw. **1** (1992), 81–94.
- [Chr94] B. Christianson, *Reverse accumulation and attractive fixed points*, Optim. Methods Softw. **3** (1994), 311–326.
- [Chr01] B. Christianson, *A self-stabilizing Pantoja-like indirect algorithm for optimal control*, Optim. Methods Softw. **16** (2001), 131–149.
- [Cla83] F.H. Clarke, *Optimization and Nonsmooth Analysis*, Classics Appl. Math. **5**, SIAM, Philadelphia, 1990.
- [CM83] T.F. Coleman and J.J. Moré, *Estimation of sparse Jacobian matrices and graph coloring problems*, SIAM J. Numer. Anal. **20** (1983), 187–209.
- [CMM97] J. Czyzyk, M.P. Mesner, and J.J. Moré, *The Network-Enabled Optimization Server*, Preprint ANL/MCS-P615-1096, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, 1997.
- [Coe01] G.C. Cohen, *Higher-Order Numerical Methods for Transient Wave Equations*, Springer, New York, 2001.
- [Con78] J.H. Conway, *Elementary Numerical Analysis*, North-Holland, Amsterdam, 1978.
- [Cos00] M. Coste, *An Introduction to O -minimal Geometry*, Dip. Mat. Univ. Pisa, Dottorato di Ricerca in Matematica, Istituti Editoriale e Poligrafici Internazionali, Pisa, 2000.
- [Cou81] P. Cousot, *Semantic foundations of program analysis*, in Program Flow Analysis: Theory and Applications, S.S. Muchnick and N.D. Jones, eds., Prentice-Hall, Englewood Cliffs, NJ, 1981, pp. 303–342.
- [CPR74] A.R. Curtis, M.J.D. Powell, and J.K. Reid, *On the estimation of sparse Jacobian matrices*, J. Inst. Math. Appl. **13** (1974), 117–119.

- [CS⁺01] D. Casanova, R.S. Sharp, M. Final, B. Christianson, and P. Symonds, *Application of automatic differentiation to race car performance optimisation*, in [CF⁺01], pp. 113–120.
- [CV96] T.F. Coleman and A. Verma, *Structure and efficient Jacobian calculation*, in [BB⁺96], pp. 149–159.
- [CW⁺80] D.G. Cacuci, C.F. Weber, E.M. Oblow, and J.H. Marable, *Sensitivity theory for general systems of nonlinear equations*, Nuclear Sci. Engrg. **88** (1980), 88–110.
- [dB56] F. de Bruno, *Note sur une nouvelle formule de calcul différentiel*, Quart. J. Math. **1** (1856), 359–360.
- [DB89] J.C. Dunn and D.P. Bertsekas, *Efficient dynamic programming implementations of Newton's method for unconstrained optimal control problems*, J. Optim. Theory Appl. **63** (1989), 23–38.
- [DD⁺90] J.J. Dongarra, J.J. Du Croz, I.S. Duff, and S.J. Hammarling, *A set of level 3 basic linear algebra subprograms*, ACM Trans. Math. Software **16** (1990), 1–17.
- [DER89] I.S. Duff, A.M. Erisman, and J.K. Reid, *Direct Methods for Sparse Matrices*, Monogr. Numer. Anal., Oxford University Press, New York, 1989.
- [Deu94] A. Deutsch, *Interprocedural may-alias analysis for pointers: Beyond k-limiting*, ACM SIGPLAN Notices, **29** (1994), no. 6, 230–241.
- [Dix91] L.C.W. Dixon, *Use of automatic differentiation for calculating Hessians and Newton steps*, in [GC91], pp. 114–125.
- [DLS95] M. Dobmann, M. Liepelt, and K. Schittkowski, *Algorithm 746 POCOMP: A Fortran code for automatic differentiation*, ACM Trans. Math. Software **21** (1995), 233–266.
- [DM48] P.S. Dwyer and M.S. Macphail, *Symbolic Matrix Derivatives*, Ann. Math. Statist. **19** (1948), 517–534.
- [DPS89] P.H. Davis, J.D. Pryce, and B.R. Stephens, *Recent Developments in Automatic Differentiation*, Appl. Comput. Math. Group Report ACM-89-1, The Royal Military College of Science, Cranfield, UK, January 1989.
- [DR69] S.W. Director and R.A. Rohrer, *Automated network design—the frequency-domain case*, IEEE Trans. Circuit Theory **CT-16** (1969), 330–337, reprinted by permission.
- [DS96] J.E. Dennis, Jr., and R.B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Classics Appl. Math. **16**, SIAM, Philadelphia, 1996.

- [Dwy67] P.S. Dwyer, *Some applications of matrix derivatives in multivariate analysis*, J. Amer. Statist. Assoc. **62** (1967), 607–625.
- [EB99] P. Eberhard and C.H. Bischof, *Automatic differentiation of numerical integration algorithms*, J. Math. Comp. **68** (1999), 717–731.
- [Fat74] R.J. Fateman, *Polynomial multiplication, powers and asymptotic analysis: Some comments*, SIAM J. Comput. **3** (1974), 196–213.
- [Fau92] C. Faure, *Quelques aspects de la simplification en calcul formel*, Ph.D. thesis, Université de Nice, Sophia Antipolis, France, 1992.
- [FB96] W.F. Feehery and P.I. Barton, *A differentiation-based approach to dynamic simulation and optimization with high-index differential-algebraic equations*, in [BB⁺96], pp. 239–252.
- [FDF00] C. Faure, P. Dutto and S. Fidanova, *Odyssée and parallelism: Extension and validation*, in Proceedings of the 3rd European Conference on Numerical Mathematics and Advanced Applications, Jyväskylä, Finland, July 26–30, 1999, World Scientific, pp. 478–485.
- [FF99] H. Fischer and H. Flanders, *A minimal code list*, Theoret. Comput. Sci. **215** (1999), 345–348.
- [Fis91] H. Fischer, *Special problems in automatic differentiation*, in [GC91], pp. 43–50.
- [FN01] C. Faure and U. Naumann, *Minimizing the Tape Size*, in [CF⁺01], pp. 279–284.
- [Fos95] I. Foster, *Designing and Building Parallel Programs: Concepts and Tools for Parallel Software Engineering*, Addison-Wesley Longman Publishing Co., Inc., Boston, MA, 1995.
- [Fra78] L.E. Fraenkel, *Formulae for high derivatives of composite functions*, J. Math. Proc. Camb. Philos. Soc. **83** (1978), 159–165.
- [Gar91] O. García, *A system for the differentiation of Fortran code and an application to parameter estimation in forest growth models*, in [GC91], pp. 273–286.
- [Gay96] D.M. Gay, *More AD of nonlinear AMPL models: Computing Hessian information and exploiting partial separability*, in [BB⁺96], pp. 173–184.
- [GB⁺93] A. Griewank, C. Bischof, G. Corliss, A. Carle, and K. Williamson, *Derivative convergence of iterative equation solvers*, Optim. Methods Softw. **2** (1993), 321–355.

- [GC91] A. Griewank and G.F. Corliss (eds.), *Automatic Differentiation of Algorithms: Theory, Implementation, and Application*, SIAM, Philadelphia, 1991.
- [GC⁺97] A. Griewank, G.F. Corliss, P. Henneberger, G. Kirlinger, F.A. Potra, and H.J. Stetter, *High-order stiff ODE solvers via automatic differentiation and rational prediction*, in *Numerical Analysis and Its Applications*, Lecture Notes in Comput. Sci. **1196**, Springer, Berlin, 1997, pp. 114–125.
- [Gil07] M.B. Giles, *Monte Carlo Evaluation of Sensitivities in Computational Finance*. Report NA-07/12, Oxford University Computing Laboratory, 2007.
- [Gei95] U. Geitner, *Automatische Berechnung von dünnbesetzten Jacobimatrizen nach dem Ansatz von Newsam-Ramsdell*, diploma thesis, Technische Universität Dresden, Germany, 1995.
- [Ges95] Gesellschaft für Anlagen- und Reaktorsicherheit mbH, Garching, *ATHLET Programmers Manual, ATHLET Users Manual*, 1995.
- [GF02] A. Griewank and C. Faure, *Reduced functions, gradients and Hessians from fixed point iterations for state equations*, Numer. Algorithms **30** (2002), 113–139.
- [GGJ90] J. Guddat, F. Guerra, and H.Th. Jongen, *Parametric Optimization: Singularities, Pathfollowing and Jumps*, Teubner, Stuttgart, John Wiley, Chichester, 1990.
- [Gil92] J.Ch. Gilbert, *Automatic differentiation and iterative processes*, Optim. Methods Softw. **1** (1992), 13–21.
- [GJ79] M.R. Garey and D.S. Johnson, *Computers and Intractability. A Guide to the Theory of NP-completeness*, W.H. Freeman and Company, 1979.
- [GJU96] A. Griewank, D. Juedes, and J. Utke, *ADOL—C, a Package for the Automatic Differentiation of Algorithms Written in C/C++*, ACM Trans. Math. Software **22** (1996), 131–167; <http://www.math.tu-dresden.de/~adol-c/>.
- [GK98] R. Giering and T. Kaminski, *Recipes for adjoint code construction*, ACM Trans. Math. Software **24** (1998), 437–474.
- [GK⁺06] R. Giering and T. Kaminski, R. Todling, R. Errico, R. Gelaro, and N. Winslow, *Tangent linear and adjoint versions of NASA/GMAO's Fortran 90 global weather forecast model*, in [BC⁺06], pp. 275–284.
- [GK05] A. Griewank and D. Kressner, *Time-lag in Derivative Convergence for Fixed Point Iterations*, Revue ARIMA, Numéro Spécial CARI'04, pp. 87–102, 2005.

- [GLC85] S. Gomez, A.V. Levy, and A. Calderon, *A global zero residual least squares method*, in Numerical Analysis, Proceedings, Guanajuato, Mexico, 1984, Lecture Notes in Math. 1230, J.P. Hennart, ed., Springer, New York, 1985, pp. 1–10.
- [GM96] J. Guckenheimer and M. Myers, *Computing Hopf bifurcations II: Three examples from neurophysiology*, SIAM J. Sci. Comput. **17** (1996), 1275–1301.
- [GM97] P. Guillaume and M. Masmoudi, *Solution to the time-harmonic Maxwell's equations in a waveguide: Use of higher-order derivatives for solving the discrete problem*, SIAM J. Numer. Anal. **34** (1997), 1306–1330.
- [GMP05] A.H. Gebremedhin, F. Manne, and A. Pothen, *What color is your Jacobian? Graph coloring for computing derivatives*, SIAM Rev. **47** (2005), no. 4, 629–705.
- [GMS97] J. Guckenheimer, M. Myers, and B. Sturmfels, *Computing Hopf bifurcations I*, SIAM J. Numer. Anal. **34** (1997), 1–21.
- [GN93] J.Ch. Gilbert and J. Nocedal, *Automatic differentiation and the step computation in the limited memory BFGS method*, Appl. Math. Lett. **6** (1993), 47–50.
- [GOT03] N. Gould, D. Orban and Ph.L. Toint, *CUTEr, a constrained and unconstrained testing environment*, revisited, ACM Trans. Math. Software, **29** (2003), 373–394.
- [GP01] M.B. Giles and N.A. Pierce, *An introduction to the adjoint approach to design*, Flow, Turbulence and Combustion **65** (2001), 393–415.
- [GP+96] J. Grimm, L. Potter, and N. Rostaing-Schmidt, *Optimal time and minimum space-time product for reversing a certain class of programs*, in [BB+96], pp. 95–106.
- [GP+06] A.H. Gebremedhin, A. Pothen, A. Tarafdar, and A. Walther, *Efficient Computation of Sparse Hessians Using Coloring and Automatic Differentiation*, to appear in INFORMS J. Comput. (2006).
- [GR87] A. Griewank and P. Rabier, *Critical points of mixed fluids and their numerical treatment*, in Bifurcation: Analysis, Algorithms, Applications, T. Küpper, R. Reydel, and H. Troger, eds., Birkhäuser, Boston, 1987, pp. 90–97.
- [GR89] A. Griewank and G.W. Reddien, *Computation of cusp singularities for operator equations and their discretizations*, J. Comput. Appl. Math. **26** (1989), 133–153.

- [GR91] A. Griewank and S. Reese, *On the calculation of Jacobian matrices by the Markowitz rule*, in [GC91], pp. 126–135.
- [Gri80] A. Griewank, *Starlike domains of convergence for Newton's method at singularities*, Numer. Math. **35** (1980), 95–111.
- [Gri89] A. Griewank, *On automatic differentiation*, in Mathematical Programming: Recent Developments and Applications, M. Iri and K. Tanabe, eds., Kluwer, Dordrecht, The Netherlands, 1989, pp. 83–108.
- [Gri90] A. Griewank, *Direct calculation of Newton steps without accumulating Jacobians*, in Large-Scale Numerical Optimization, T.F. Coleman and Y. Li, eds., SIAM, Philadelphia, 1990, pp. 115–137.
- [Gri91] A. Griewank, *Achieving logarithmic growth of temporal and spatial complexity in reverse automatic differentiation*, Optim. Methods Softw. **1** (1992), 35–54.
- [Gri93] A. Griewank, *Some bounds on the complexity of gradients, Jacobians, and Hessians*, in Complexity in Nonlinear Optimization, P.M. Pardalos, ed., World Scientific, River Edge, NJ, 1993, pp. 128–161.
- [Gri94] A. Griewank, *Tutorial on Computational Differentiation and Optimization*, University of Michigan, Ann Arbor, MI, 1994.
- [Gri95] A. Griewank, *ODE solving via automatic differentiation and rational prediction*, in Numerical Analysis 1995, Pitman Res. Notes Math. Ser. **344**, D.F. Griffiths and G.A. Watson, eds., Addison-Wesley Longman, Reading, MA, 1995.
- [Gri03] A. Griewank, *A mathematical view of automatic differentiation*, Acta Numerica **12** (2003), 321–398.
- [Gru97] D. Gruntz, *Automatic differentiation and bisection*, MapleTech **4** (1997), 22–27.
- [GS02] M.B. Giles and E. Süli, *Adjoint methods for PDEs: A-posteriori error analysis and postprocessing by duality*, Acta Numerica **11** (2002), 145–236.
- [GT⁺07] A.H. Gebremedhin, A. Tarafdar, F. Manne, and A. Pothén, *New acyclic and star coloring algorithms with application to computing Hessians*, SIAM J. Sci. Comput. **29** (2007), 1042–1072.
- [GT82] A. Griewank and Ph.L. Toint, *On the unconstrained optimization of partially separable objective functions*, in Nonlinear Optimization 1981, M.J.D. Powell, ed., Academic Press, London, 1982, pp. 301–312.

- [GUW00] A. Griewank, J. Utke, and A. Walther, *Evaluating higher derivative tensors by forward propagation of univariate Taylor series*, Math. Comp. **69** (2000), 1117–1130.
- [GW00] A. Griewank and A. Walther, *Revolve: An implementation of checkpointing for the reverse or adjoint mode of computational differentiation*, ACM Trans. Math. Softw. **26** (2000), 19–45.
- [GW04] A. Griewank and A. Walther, *On the efficient generation of Taylor expansions for DAE solutions by automatic differentiation*, Proceedings of PARA'04, in J. Dongarra et al., eds., Lecture Notes in Comput. Sci. **3732**, Springer, New York, 2006, 1089–1098.
- [GV96] G.H. Golub and C.F. Van Loan, *Matrix Computations*, third ed., Johns Hopkins University Press, Baltimore, 1996.
- [Han79] E.R. Hansen, *Global optimization using interval analysis—the one-dimensional case*, J. Optim. Theory Appl. **29** (1979), 331–334.
- [HB98] P.D. Hovland and C.H. Bischof, *Automatic differentiation of message-passing parallel programs*, in Proceedings of the First Merged International Parallel Processing Symposium and Symposium on Parallel and Distributed Processing, IEEE Computer Society Press, 1998, pp. 98–104.
- [HBG71] G.D. Hachtel, R.K. Bryton, and F.G. Gustavson, *The sparse tableau approach to network analysis and design*, IEEE Trans. Circuit Theory **CT-18** (1971), 111–113.
- [Her93] K. Herley, *Presentation at: Theory Institute on Combinatorial Challenges in Computational Differentiation*, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, 1993.
- [HKP84] H.J. Hoover, M.M. Klawe, and N.J. Pippenger, *Bounding fan-out in logical networks*, Assoc. Comput. Mach. **31** (1984), 13–18.
- [HNP05] L. Hascoët, U. Naumann, and V. Pascual, *“To be recorded” analysis in reverse-mode automatic differentiation*, Future Generation Comp. Sys. **21** (2005), 1401–1417.
- [HNW96] E. Hairer, S.P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems*, second revised ed., Computational Mechanics **14**, Springer, Berlin, 1996.
- [Hor92] J.E. Horwedel, *Reverse Automatic Differentiation of Modular Fortran Programs*, Tech. Report ORNL/TM-12050, Oak Ridge National Laboratory, Oak Ridge, TN, 1992.
- [Hos97] A.K.M. Hossain, *On the Computation of Sparse Jacobian Matrices and Newton Steps*, Ph.D. thesis, Department of Informatics, University of Bergen, Norway, 1997.

- [Hov97] P. Hovland, *Automatic Differentiation of Parallel Programs*, Ph.D. thesis, Department of Computer Science, University of Illinois, Urbana, 1997.
- [HP04] L. Hascoët, and V. Pascual, *TAPENADE 2.1 User's Guide*, Technical report, INRIA 300, INRIA, 2004.
- [HR99] R. Henrion and W. Römisch, *Metric regularity and quantitative stability in stochastic programs with probabilistic constraints*, Math. Program. **84** (1999), 55–88.
- [HS02] S. Hossain and T. Steihaug, *Sparsity issues in the computation of Jacobian matrices*, in Proceedings of the International Symposium on Symbolic and Algebraic Computing, T. Mora, ed., ACM, New York, 2002, pp. 123–130.
- [HW96] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, second revised ed., Computational Mechanics **14**, Springer, Berlin, 1996.
- [HW06] V. Heuveline and A. Walther, *Online checkpointing for parallel adjoint computation in PDEs: Application to goal oriented adaptivity and flow control*, in Proceedings of Euro-Par 2006, W. Nagel et al., eds., Lecture Notes in Comput. Sci. **4128**, Springer, Berlin, 2006, pp. 689–699.
- [Iri91] M. Iri, *History of automatic differentiation and rounding error estimation*, in [GC91], pp. 1–16.
- [ITH88] M. Iri, T. Tsuchiya, and M. Hoshi, *Automatic computation of partial derivatives and rounding error estimates with applications to large-scale systems of nonlinear equations*, Comput. Appl. Math. **24** (1988), 365–392.
- [JM88] R.H.F. Jackson and G.P. McCormic, *Second order sensitivity analysis in factorable programming: Theory and applications*, Math. Programming **41** (1988), 1–28.
- [JMF06] K-W. Joe, D.L. McShan, and B.A. Fraass, *Implementation of automatic differentiation tools for multicriteria IMRT optimization*, in [BC⁺06], pp. 225–234.
- [KB03] M. Knauer and C. Büskens, *Real-time trajectory planning of the industrial robot IRB 6400*, PAMM **3** (2003), 515–516.
- [Ked80] G. Kedem, *Automatic differentiation of computer programs*, ACM Trans. Math. Software **6** (1980), 150–165.
- [Keh96] K. Kehler, *Partielle Separabilität und ihre Anwendung bei Berechnung dünnbesetzter Jacobimatrizen*, diploma thesis, Technische Universität Dresden, Germany, 1996.

- [KHL06] J.G. Kim, E.C. Hunke, and W.H. Lipscomb, *A sensitivity-enhanced simulation approach for community climate system model*, in Proceedings of ICCS 2006, V. Alexandrov et al., eds., Lecture Notes in Comput. Sci. **3994**, Springer, Berlin, 2006, pp. 533–540.
- [Kiw86] K.C. Kiwiel, *A method for solving certain quadratic programming problems arising in nonsmooth optimization*, IMA J. Numer. Anal. **6** (1986), 137–152.
- [KK⁺86] H. Kagiwada, R. Kalaba, N. Rasakhoo, and K. Spingarn, *Numerical Derivatives and Nonlinear Analysis*, Math. Concepts Methods Sci. Engrg. **31**, Plenum Press, New York, London, 1986.
- [KL91] D. Kalman and R. Lindell, *Automatic differentiation in astrodynamical modeling*, in [GC91], pp. 228–243.
- [KM81] U.W. Kulisch and W.L. Miranker, *Computer Arithmetic in Theory and Practice*, Academic Press, New York, 1981.
- [KN⁺84] K.V. Kim, Yu.E. Nesterov, V.A. Skokov, and B.V. Cherkasski, *Efektivnyi algoritm vychisleniya proizvodnykh i ekstremal'nye zadachi*, Ekonomika i Matematicheskie Metody **20** (1984), 309–318.
- [Knu73] D.E. Knuth, *The Art of Computer Programming 1*, Fundamental Algorithms, third ed., Addison-Wesley, Reading, MA, 1997.
- [Knu98] D.E. Knuth, *The Art of Computer Programming 3*, Sorting and Searching, second ed., Addison-Wesley, Reading, MA, 1998.
- [Koz98] K. Kozłowski, *Modeling and Identification in Robotics*, in Advances in Industrial Control, Springer, London, 1998.
- [KRS94] J. Knoop, O. Rüthing, and B. Steffen, *Optimal code motion: Theory and practice*, ACM Trans. Program. Languages Syst. **16** (1994), 1117–1155.
- [KS90] E. Kaltofen and M.F. Singer, *Size Efficient Parallel Algebraic Circuits for Partial Derivatives*, Tech. Report 90-32, Rensselaer Polytechnic Institute, Troy, NY, 1990.
- [KT51] H.W. Kuhn and A.W. Tucker, *Nonlinear programming*, in Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability, J. Newman, ed., University of California Press, Berkeley, 1951, pp. 481–492.
- [Kub98] K. Kubota, *A Fortran 77 preprocessor for reverse mode automatic differentiation with recursive checkpointing*, Optim. Methods Softw. **10** (1998), 319–335.
- [Kub96] K. Kubota, *PADRE2—Fortran precompiler for automatic differentiation and estimates of rounding error*, in [BB⁺96], pp. 367–374.

- [KW06] A. Kowarz and A. Walther, *Optimal checkpointing for time-stepping procedures*, in Proceedings of ICCS 2006, V. Alexandrov et al., eds., Lecture Notes in Comput. Sci. **3994**, Springer, Berlin, 2006, pp. 541–549.
- [KW00] W. Klein and A. Walther, *Application of techniques of computational differentiation to a cooling system*, Optim. Methods Softw. **13** (2000), 65–78.
- [Lin76] S. Linnainmaa, *Taylor expansion of the accumulated rounding error*, BIT **16** (1976), 146–160.
- [LU08] A. Lyons and J. Utke, *On the practical exploitation of scarcity*, in C. Bischof et al., eds., Advances in Automatic Differentiation, to appear in Lecture Notes in Comput. Sci. Eng., Springer (2008).
- [Lun84] V.Yu. Lunin, *Ispol'zovanie algoritma bystrogo differentsirovaniya v zadache utochneniya znachenij faz strukturnykh faktorov*, Tech. Report UDK 548.73, Naychnyj Tsenter Biologicheskikh Nauk, AN SSSR, Pushchino, 1984.
- [Mar57] H.M. Markowitz, *The elimination form of the inverse and its application*, Management Sci. **3** (1957), 257–269.
- [Mar96] K. Marti, *Differentiation formulas for probability functions: The transformation method*, Math. Programming **75** (1996), 201–220.
- [Mat86] Yu.V. Matiyasevich, *Real numbers and computers*, Cybernet. Comput. Mach. **2** (1986), 104–133.
- [MG⁺99] J. Marotzke, R. Giering, K.Q. Zhang, D. Stammer, C. Hill, and T. Lee, *Construction of the adjoint MIT ocean general circulation model and application to Atlantic heat transport sensitivity*, J. Geophys. Res. **104** (1999), no. C12, p. 29.
- [Mic82] M. Michelson, *The isothermal flash problem, part I. Stability*, Fluid Phase Equilibria **9** (1982), 1–19.
- [Mic91] L. Michelotti, *WXYZPTLK: A C++ hacker's implementation of automatic differentiation*, in [GC91], pp. 218–227.
- [Min06] A. Miné, *Field-sensitive value analysis of embedded C programs with union types and pointer arithmetics*, in LCTES '06: Proceedings of the 2006 ACM SIGPLAN/SIGBED Conference on Language, Compilers, and Tool Support for Embedded Systems, ACM, New York, 2006, pp. 54–63.
- [MIT] MITgcm, *The MIT General Circulation Model*, <http://mitgcm.org>.

- [MN93] Mi.B. Monagan and W.M. Neuenschwander, *GRADIENT: Algorithmic differentiation in Maple*, in Proceedings of ISSAC '93, ACM Press, New York, 1993, pp. 68–76.
- [Mog00] T.A. Mogensen, *Glossary for Partial Evaluation and Related Topics*, Higher-Order Symbolic Comput. **13** (2000), no. 4.
- [Moo66] R.E. Moore, *Interval Analysis*, Prentice–Hall, Englewood Cliffs, NJ, 1966.
- [Moo79] R.E. Moore, *Methods and Applications of Interval Analysis*, SIAM, Philadelphia, 1979.
- [Moo88] R.E. Moore, *Reliability in Computing: The Role of Interval Methods in Scientific Computations*, Academic Press, New York, 1988.
- [Mor85] J. Morgenstern, *How to compute fast a function and all its derivatives, a variation on the theorem of Baur-Strassen*, SIGACT News **16** (1985), 60–62.
- [Mor06] B.S. Mordukhovich, *Variational Analysis and Generalized Differentiation. I: Basic Theory*, Grundlehren Math. Wiss. **330**, Springer, Berlin, 2006.
- [MPI] MPI, *The Message Passing Interface Standard*, <http://www.mcs.anl.gov/mpi>.
- [MR96] M. Monagan and R.R. Rodoni, *Automatic differentiation: An implementation of the forward and reverse mode in Maple*, in [BB⁺96], pp. 353–362.
- [MRK93] G.L. Miller, V. Ramachandran, and E. Kaltofen, *Efficient parallel evaluation of straight-line code and arithmetic circuits*, Computing **17** (1993), 687–695.
- [MS93] S.E. Mattsson and G. Söderlind, *Index reduction in differential-algebraic equations using dummy derivatives*, SIAM J. Sci. Comput. **14** (1993), 677–692.
- [Mun90] F.S. Munger, *Applications of Defnir Algebra to Ordinary Differential Equations*, Aftermath, Golden, CO, 1990.
- [Mur93] J.D. Murray, *Mathematical Biology*, second ed., Biomathematics, Springer, Berlin, 1993.
- [Nau99] U. Naumann, *Efficient Calculation of Jacobian Matrices by Optimized Application of the Chain Rule to Computational Graphs*, Ph.D. thesis, Technische Universität Dresden, Germany, 1999.

- [Nau04] U. Naumann, *Optimal accumulation of Jacobian matrices by elimination methods on the dual computational graph*, Math. Program. **99** (2004), 399–421.
- [Nau06] U. Naumann, *Optimal Jacobian accumulation is NP-complete*, Math. Program. **112** (2008), 427–441.
- [NAW98] J.C. Newman, K.W. Anderson, and D.L. Whitfield, *Multidisciplinary Sensibility Derivatives Using Complex Variables*, Tech. Report MSSU-COE-ERC-98-08, Mississippi State University, Mississippi State, MS, 1998.
- [Ned99] N.S. Nedialkov, *Computing Rigorous Bounds on the Solution of an Initial Value Problem for an Ordinary Differential Equation*, Ph.D. thesis, University of Toronto, Toronto, ON, 1999.
- [Nei92] R.D. Neidinger, *An efficient method for the numerical evaluation of partial derivatives of arbitrary order*, ACM Trans. Math. Softw. **18** (1992), 159–173.
- [NH⁺92] P.A. Newman, G.J.W. Hou, H.E. Jones, A.C. Taylor, and V.M. Kori, *Observations on Computational Methodologies for Use in Large-Scale, Gradient-Based, Multidisciplinary Design Incorporating Advanced CFD Codes*, Techn. Mem. 104206, NASA Langley Research Center, 1992, AVSCOM Technical Report 92-B-007.
- [NP05] N.S. Nedialkov and J.D. Pryce, *Solving differential-algebraic equations by Taylor series. I: Computing Taylor coefficients*, BIT **45** (2005), 561–591.
- [NR83] G.N. Newsam and J.D. Ramsdell, *Estimation of sparse Jacobian matrices*, SIAM J. Algebraic Discrete Methods **4** (1983), 404–418.
- [NS96] S.G. Nash and A. Sofer, *Linear and nonlinear programming*, McGraw–Hill Series in Industrial Engineering and Management Science, McGraw–Hill, New York, 1996.
- [NU⁺04] U. Naumann, J. Utke, A. Lyons, and M. Fagan, *Control Flow Reversal for Adjoint Code Generation*, in Proceedings of SCAM 2004 IEEE Computer Society, 2004, pp. 55–64.
- [Oba93] N. Obayashi, *A numerical method for calculating the higher order derivatives used multi-based number*, Bull. Coll. Lib. Arts **29** (1993), 119–133.
- [Obl83] E.M. Oblow, *An Automated Procedure for Sensitivity Analysis Using Computer Calculus*, Tech. Report ORNL/TM-8776, Oak Ridge National Laboratory, Oak Ridge, TN, 1983.

- [OMP] OpenMP, *The OpenMP Specification for Parallel Programming*, <http://www.openmp.org>.
- [OR70] J.M. Ortega and W.C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables*, Academic Press, New York, 1970.
- [OVB71] G.M. Ostrovskii, Yu.M. Volin, and W.W. Borisov, *Über die Berechnung von Ableitungen*, Wiss. Z. Tech. Hochschule für Chemie **13** (1971), 382–384.
- [OW97] M. Overton and H. Wolkowicz (eds.), *Semidefinite Programming*, North-Holland, Amsterdam, 1997.
- [Pfe80] F.W. Pfeiffer, *Some Advances Related to Nonlinear Programming*, Tech. Report **28**, SIGMAP Bulletin, ACM, New York, 1980.
- [Pon82] J.W. Ponton, *The numerical evaluation of analytical derivatives*, Comput. Chem. Eng. **6** (1982), 331–333.
- [PR97] J.D. Pryce and J.K. Reid, *AD01: A Fortran 90 code for automatic differentiation*, Tech. Report RAL-TR-97, Rutherford-Appleton Laboratories, Chilton, UK, 1997.
- [Pry01] J. Pryce, *A simple structural analysis method for DAEs*, BIT **41** (2001), 364–394.
- [PT79] M.J.D. Powell and Ph.L. Toint, *On the estimation of sparse Hessian matrices*, SIAM J. Numer. Anal. **16** (1979), 1060–1074.
- [Ral81] L.B. Rall, *Automatic Differentiation: Techniques and Applications*, Lecture Notes in Comput. Sci. **120**, Springer, Berlin, 1981.
- [Ral84] L.B. Rall, *Differentiation in Pascal-SC: Type GRADIENT*, ACM Trans. Math. Softw. **10** (1984), 161–184.
- [RBB07] A. Rasch, H. M. Bücker, and C. H. Bischof, *Automatic computation of sensitivities for a parallel aerodynamic simulation*, in Proceedings of the International Conference on Parallel Computing (ParCo2007), Jülich, Germany, 2007.
- [RDG93] N. Rostaing, S. Dalmas, and A. Galligo, *Automatic differentiation in Odyssée*, Tellus **45A** (1993), 558–568.
- [RH92] L.C. Rich and D.R. Hill, *Automatic differentiation in MATLAB*, Appl. Numer. Math. **9** (1992), 33–43.
- [Rho97] A. Rhodin, *IMAS integrated modeling and analysis system for the solution of optimal control problems*, Comput. Phys. Comm. **107** (1997), 21–38.

- [RO91] L. Reichel and G. Opfer, *Chebyshev-Vandermonde systems*, Math. Comp. **57** (1991), 703–721.
- [RR99] K.J. Reinschke and K. Röbenack, *Analyse von Deskriptorsystemen mit Hilfe von Berechnungsgraphen*, Z. Angew. Math. Mech. **79** (1999), 13–16.
- [R-S93] N. Rostaing-Schmidt, *Différentiation automatique: Application à un problème d'optimisation en météorologie*, Ph.D. thesis, Université de Nice, Sophia Antipolis, France, 1993.
- [PS07] *PolySpace*, <http://www.mathworks.com/products/polyspace/>.
- [RT78] D.J. Rose and R.E. Tarjan, *Algorithmic aspects of vertex elimination on directed graphs*, SIAM J. Appl. Math. **34** (1978), 176–197.
- [Saa03] Y. Saad, *Iterative Methods for Sparse Linear Systems*, second ed., SIAM, Philadelphia, 2003.
- [Sch65] H. Schorr, *Analytic differentiation using a syntax-directed compiler*, Comput. J. **7** (1965), 290–298.
- [Sch94] S. Scholtes, *Introduction to Piecewise Differentiable Equations*, Preprint 53/1994, Institut für Statistik und Mathematische Wirtschaftstheorie, Universität Karlsruhe, 1994.
- [SH98] T. Steihaug and S. Hossain, *Computing a sparse Jacobian matrix by rows and columns*, Optim. Methods Softw. **10** (1998), 33–48.
- [SH03] R. Serban and A.C. Hindmarsh, *CVODES: An ODE Solver with Sensitivity Analysis Capabilities*, Tech. Report UCRL-JP-20039, Lawrence Livermore National Laboratory, Livermore, CA, 2003.
- [SH05] M. Hinze and J. Sternberg, *A-Revolve: An adaptive memory and run-time-reduced procedure for calculating adjoints; with an application to the instationary Navier-Stokes system*, Optim. Methods Softw. **20** (2005), 645–663.
- [Shi93] D. Shiriaev, *Fast Automatic Differentiation for Vector Processors and Reduction of the Spatial Complexity in a Source Translation Environment*, Ph.D. thesis, Institut für Angewandte Mathematik, Universität Karlsruhe, Germany, 1993.
- [SKH06] M.M. Strout, B. Kreaseck, and P.D. Hovland, *Data-flow analysis for MPI programs*, in Proceedings of ICCP '06, IEEE Computer Society, 2006, 175–184.
- [SMB97] T. Scott, M.B. Monagan, and J. Borwein (eds.), *MapleTech: Functionality, Applications, Education*, Vol. 4, Birkhäuser, Boston, 1997.

- [SO98] M. Snir and S. Otto, *MPI-The Complete Reference: The MPI Core*, MIT Press, Cambridge, MA, 1998.
- [Spe80] B. Speelpenning, *Compiling Fast Partial Derivatives of Functions Given by Algorithms*, Ph.D. thesis, University of Illinois at Urbana, Champaign, 1980.
- [SS77] R.W.H. Sargent and G.R. Sullivan, *The development of an efficient optimal control package*, in Proceedings of the 8th IFIP Conference on Optimization Technology 2, 1977.
- [SS⁺91] R. Seydel, F.W. Schneider, T. Kupper, and H. Troger (eds.), *Bifurcation and Chaos: Analysis, Algorithms, Applications*, Proceedings of the Conference at Würzburg, Birkhäuser, Basel, 1991.
- [Sta85] *IEEE Standard for Binary Floating-Point Arithmetic*, ANS, New York, 1985.
- [Sta97] O. Stauning, *Automatic Validation of Numerical Solutions*, Ph.D. thesis, Department of Mathematical Modelling, Technical University of Denmark, Lyngby, Denmark, October 1997, Technical Report IMM-PHD-1997-36.
- [Ste96] B. Steensgaard, *Points-to analysis in almost linear time*, in Symposium on Principles of Programming Languages, ACM Press, New York, 1996, pp. 32–41.
- [Str86] B. Stroustrup, *The C++ Programming Language*, Addison—Wesley, Reading, MA, 1986.
- [Stu80] F. Stummel, *Rounding error analysis of elementary numerical algorithm*, in Fundamentals of Numerical Computation, Comput. Suppl. **2**, Springer, Vienna, 1980, pp. 169–195.
- [SW85] D.F. Stubbs and N.W. Webre, *Data Structures with Abstract Data Types and Pascal*, Texts Monogr. Comput. Sci. Suppl. **2**, Brooks/Cole, Pacific Grove, CA, 1985.
- [Sym07] W.W. Symes, *Reverse time migration with optimal checkpointing*, Geophys. **72** (2007), SM213–SM221.
- [SZ92] H. Schramm and J. Zowe, *A version of the bundle idea for minimizing a nonsmooth function: Conceptual idea, convergence analysis, numerical results*, SIAM J. Optim. **2** (1992), 121–152.
- [Tad99] M. Tadjouddine, *La différentiation automatique*, Ph.D. thesis, Université de Nice, Sophia Antipolis, France, 1999.
- [Tal08] O. Talagrand, *Data Assimilation in Meteorology And Oceanography*, Academic Press Publ., 2008.

- [Tar83] R.E. Tarjan, *Data Structures and Network Algorithms*, CBMS-NSF Regional Conf. Ser. in Appl. Math. **44**, SIAM, Philadelphia, 1983.
- [Tha91] W.C. Thacker, *Automatic differentiation from an oceanographer's perspective*, in [GC91], pp. 191–201.
- [Tip95] F. Tip, *A survey of program slicing techniques*, J. Progr. Lang. **3** (1995), 121–189.
- [TKS92] S. Ta'asan, G. Kuruvila, and M.D. Salas, *Aerodynamic design and optimization in One Shot*, in Proceedings of the 30th AIAA Aerospace Sciences Meeting & Exhibit, AIAA 92-0025, 1992.
- [TR⁺02] E. Tijskens, D. Roose, H. Ramon, and J. De Baerdemaeker, *Automatic differentiation for solving nonlinear partial differential equations: An efficient operator overloading approach*, Numer. Algorithms **30** (2002), 259–301.
- [UH⁺08] J. Utke, L. Hascoët, C. Hill, P. Hovland, and U. Naumann, *Toward Adjoinable MPI*, Preprint ANL/MCS-P1472-1207, 2007, Argonne National Laboratory, Argonne, IL, 2008.
- [Utk96a] J. Utke, *Efficient Newton steps without Jacobians*, in [BB⁺96], pp. 253–264.
- [Utk96b] J. Utke, *Exploiting Macro- and Micro-structures for the Efficient Calculation of Newton Steps*, Ph.D. thesis, Technische Universität Dresden, Germany, 1996.
- [vdS93] J.L.A. van de Snepscheut, *What Computing Is All About*, Texts Monogr. Comput. Sci. Suppl. **2**, Springer, Berlin, 1993.
- [VD00] D.A. Venditti and D.L. Darmofal, *Adjoint error estimation and grid adaptation for functional outputs: Application to quasi-one-dimensional flow*, J. Comput. Phys. **164** (2000), 204–227.
- [Vel95] T.L. Veldhuizen, *Expression templates*, C++ Report **7** (1995), no. 5, pp. 26–31.
- [Ver99] A. Verma, *Structured Automatic Differentiation*, Ph.D. thesis, Cornell University, Ithaca, NY, 1999.
- [VO85] Yu.M. Volin and G.M. Ostrovskii, *Automatic computation of derivatives with the use of the multilevel differentiating technique—I: Algorithmic basis*, Comput. Math. Appl. **11** (1985), 1099–1114.
- [Wal99] A. Walther, *Program Reversal Schedules for Single- and Multi-Processor Machines*, Ph.D. thesis, Technische Universität Dresden, Germany, 1999.

- [Wan69] G. Wanner, *Integration gewöhnlicher Differentialgleichungen, Lie Reihen, Runge-Kutta-Methoden* **XI**, B.I-Hochschulschriften, no. 831/831a, Bibliogr. Inst., Mannheim-Zürich, Germany, 1969.
- [War75] D.D. Warner, *A Partial Derivative Generator*, Computing Science Technical Report, Bell Laboratories, 1975.
- [Wen64] R.E. Wengert, *A simple automatic derivative evaluation program*, Comm. ACM **7** (1964), 463–464.
- [Wer82] P.J. Werbos, *Application of advances in nonlinear sensitivity analysis*, in System Modeling and Optimization: Proceedings of the 19th IFIP Conference New York, R.F. Drenick and F. Kozin, eds., Lecture Notes in Control Inform. Sci. **38**, Springer, New York, 1982, pp. 762–770.
- [Wer88] P.J. Werbos, *Generalization of backpropagation with application to a recurrent gas market model*, Neural Networks **1** (1988), 339–356.
- [WG04] A. Walther and A. Griewank, *Advantages of binomial checkpointing for memory-reduced adjoint calculations*, in Numerical Mathematics and Advanced Applications: Proceedings of ENUMATH 2003, M. Feistauer et al., eds., Springer, Berlin, 2004, pp. 834–843.
- [WG99] A. Walther and A. Griewank, *Applying the checkpointing routine **treeverse** to discretizations of Burgers' equation*, in High Performance Scientific and Engineering Computing, H.-J. Bungartz, F. Durst, and C. Zenger, eds., Lect. Notes Comput. Sci. Eng. **8**, Springer, Berlin, 1999, pp. 13–24.
- [Wil65] G.J.H. Wilkinson, *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, UK, 1965.
- [WN⁺95] Z. Wang, I.M. Navon, X. Zou, and F.X. Le Dimet, *A truncated Newton optimization algorithm in meteorology applications with analytic Hessian/vector products*, Comput. Optim. Appl. **4** (1995), 241–262.
- [Wol82] P. Wolfe, *Checking the calculation of gradients*, ACM Trans. Math. Softw. **8** (1982), 337–343.
- [WO⁺87] B.A. Worley, E.M. Oblow, R.E. Pin, J.E. Maerker, J.E. Horwedel, R.Q. Wright, and J.L. Lucius, *Deterministic methods for sensitivity and uncertainty analysis in large-scale computer models*, in Proceedings of the Conference on Geostatistical, Sensitivity, and Uncertainty Methods for Ground-Water Flow and Radionuclide Transport Modelling, B.E. Buxton, ed., Battelle Press, 1987, pp. 135–154.
- [Wri08] P. Wriggers, *Nonlinear Finite Element Methods*, Springer, Berlin, Heidelberg, 2008.
- [Yos87] T. Yoshida, *Derivatives of probability functions and some applications*, Ann. Oper. Res. **11** (1987), 1112–1120.

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