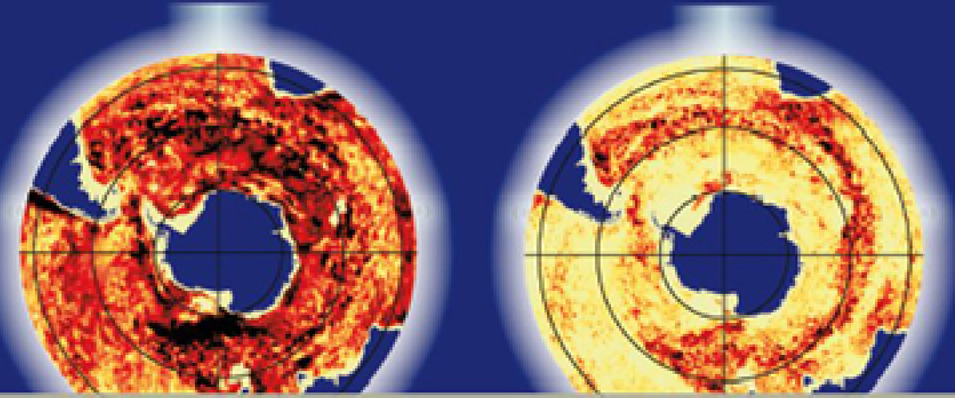

LECTURE NOTES IN COMPUTATIONAL SCIENCE AND ENGINEERING 64

Christian H. Bischof · H. Martin Bücker
Paul Hovland · Uwe Naumann · Jean Utke Editors

Advances in Automatic Differentiation

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in Computational Science
and Engineering

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Advances in Automatic Differentiation

With 111 Figures and 37 Tables

Springer

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Preface

The Fifth International Conference on Automatic Differentiation held from August 11 to 15, 2008 in Bonn, Germany, is the most recent one in a series that began in Breckenridge, USA, in 1991 and continued in Santa Fe, USA, in 1996, Nice, France, in 2000 and Chicago, USA, in 2004. The 31 papers included in these proceedings reflect the state of the art in automatic differentiation (AD) with respect to theory, applications, and tool development. Overall, 53 authors from institutions in 9 countries contributed, demonstrating the worldwide acceptance of AD technology in computational science.

Recently it was shown that the problem underlying AD is indeed NP-hard, formally proving the inherently challenging nature of this technology. So, most likely, no deterministic "silver bullet" polynomial algorithm can be devised that delivers optimum performance for general codes. In this context, the exploitation of domain-specific structural information is a driving issue in advancing practical AD tool and algorithm development. This trend is prominently reflected in many of the publications in this volume, not only in a better understanding of the interplay of AD and certain mathematical paradigms, but in particular in the use of hierarchical AD approaches that judiciously employ general AD techniques in application-specific algorithmic harnesses. In this context, the understanding of structures such as sparsity of derivatives, or generalizations of this concept like scarcity, plays a critical role, in particular for higher derivative computations.

On the tool side, understanding of program structure is the key to improving performance of AD tools. In this context, domain-specific languages, which by design encompass high-level information about a particular application context, play an increasingly larger role, and offer both challenges and opportunities for efficient AD augmentation. This is not to say that tool development for general purpose languages is a solved issue. Advanced code analysis still leads to improvements in AD-generated code, and the set of tools capable of both forward- and reverse mode AD for C and C++ continues to expand. General purpose AD tool development remains to be of critical importance for unlocking the great wealth of AD usage scenarios, as the user interface and code performance of such tools shape computational practitioners' view of AD technology.

Overall, the realization that simulation science is a key requirement to fundamental insight in science and industrial competitiveness continues to grow. Hence, issues such as nonlinear parameter fitting, data assimilation, or sensitivity analysis of computer programs are becoming de rigueur for computational practitioners to adapt their models to experimental data. Beyond the "vanilla" nonlinear least squares formulation one needs also to question in this context which parameters can at all be reliably identified by the data available in a particular application context, a question that again requires the computation of derivatives if one employs methods based on, for example, Fisher information matrix. Beyond that, experimental design then tries to construct experimental setups that, for a given computer model, deliver experimental data that have the highest yield with respect to model fitting or even model discrimination. It is worth noting that all these activities that are critical in reliably correlating computer model predictions with real experiments rely on the computation of first- and second-order derivatives of the underlying computer models and offer a rich set of opportunities for AD.

These activities are also examples of endeavors that encompass mathematical modeling, numerical techniques as well as applied computer science in a specific application context. Fortunately, computational science curricula that produce researchers mentally predisposed to this kind of interdisciplinary research continue to grow, and, from a computer science perspective, it is encouraging to see that, albeit slowly, simulation practitioners realize that there is more to computer science than "programming," a task that many code developers feel they really do not need any more help in, except perhaps in parallel programming.

Parallel programming is rising to the forefront of software developers' attention due to the fact that shortly multicore processors, which, in essence, provide the programming ease of shared-memory multiprocessors at commodity prices, will put 32-way parallel computing (or even more) on desk- and laptops everywhere. Going a step further, in the near future any substantial software system will, with great probability, need to be both parallel and distributed. Unfortunately, many computer science departments consider these issues solved, at least in theory, and do not require their students to develop practical algorithmic and software skills in that direction. In the meantime, the resulting lag in exploiting technical capabilities offers a great chance for AD, as the associativity of the chain rule of differential calculus underlying AD as well as the additional operations inserted in the AD-generated code provide opportunities for making use of available computational resources in a fashion that is transparent to the user. The resulting ease of use of parallel computers could be a very attractive feature for many users.

Lastly, we would like to thank the members of the program committee for their work in the paper review process, and the members of the Institute for Scientific Computing, in particular Oliver Fortmeier and Cristian Wente, for their help in organizing this event. The misfit and velocity maps of the Southern Ocean on the cover were provided by Matthew Mazloff and Patrick Heimbach from Massachusetts Institute of Technology and are a result of an ocean state estimation project using automatic differentiation. We are also indebted to Mike Giles from Oxford University, Wolfgang Marquardt from RWTH Aachen University, Arnold Neumeier from the

University of Vienna, Alex Pothen from Old Dominion University, and Eelco Visser from the Technical University in Delft for accepting our invitation to present us inspirations on AD possibilities in their fields of expertise. We also acknowledge the support of our sponsors, the Aachen Institute for Advanced Study in Computational Engineering Science (AICES), the Bonn-Aachen International Center for Information Technology (B-IT), and the Society for Industrial and Applied Mathematics (SIAM).

Aachen and Chicago,
April 2008

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