

Preface

The Sixth International Conference on Automatic Differentiation (AD2012) held July 23–27, 2012, in Fort Collins, Colorado (USA), continued this quadrennial conference series. While the fundamental idea of differentiating numerical programs is easy to explain, the practical implementation of this idea for many nontrivial numerical computations is not. Our community has long been aware of the discrepancy between the aspiration of an *automatic* process suggested by the name automatic differentiation and the reality of its practical use, which often requires substantial effort from the user. New algorithms and methods implemented in differentiation tools improve their usability and reduce the need for user intervention. On the other hand, the demands to compute derivatives for numerical models on parallel hardware, using a wide variety of libraries and having components implemented in different programming languages, pose new challenges, particularly for the efficiency of the derivative computation. These challenges, as well as new applications, have been driving research for the past four years and will continue to do so. Despite retaining automatic differentiation in the conference name, the editors purposely switched to *algorithmic differentiation* (AD) in the proceedings title. Thus, the conference proceedings follow somewhat belatedly the more appropriate naming chosen by Andreas Griewank for the first edition of his seminal monograph covering our subject area. This name better reflects the reality of AD usage and the research results presented in the papers collected here.

The 31 contributed papers cover the application of AD to many areas of science and engineering as well as aspects of AD theory and its implementation in tools. For all papers the referees, selected from the program committee and the wider AD community, as well as the editors have emphasized accessibility of the presented ideas also to non-AD experts.

In the AD tools arena new implementations are introduced covering, for example, Java and graphical modeling environments, or join the set of existing tools for Fortran. New developments in AD algorithms target: efficient derivatives for matrix-operation, detection and exploitation of sparsity, partial separability, the treatment of nonsmooth functions, and other high-level mathematical aspects of the numerical computations to be differentiated.

Applications stem from the Earth sciences, nuclear engineering, fluid dynamics, and chemistry, to name just a few. In many cases the applications in a given area of science or engineering share characteristics that require specific approaches to enable AD capabilities or provide an opportunity for efficiency gains in the derivative computation. The description of these characteristics and of the techniques for successfully using AD should make the proceedings a valuable source of information for users of AD tools.

The image on the book cover shows the high-harmonic emission spectrum of a semiconductor quantum dot for different excitation conditions. To favor specific frequencies one has to find an appropriate input pulse within a large parameter space. This was accomplished by combining a gradient-based optimization algorithm with AD. The data plots were provided by Matthias Reichelt.

Algorithmic differentiation draws on many aspects of applied mathematics and computer science and ultimately is useful only when users in the science and engineering communities become aware of its capabilities. Furthering collaborations outside the core AD community, the AD2012 program committee invited leading experts from diverse disciplines as keynote speakers. We are grateful to Lorenz Biegler (Carnegie Mellon University, USA), Luca Capriotti (Credit Suisse, USA), Don Estep (Colorado State University, USA), Andreas Griewank (Humboldt University, Germany), Mary Hall (University of Utah, USA), Barbara Kaltenbacher (University of Klagenfurt, Austria), Markus Püschel (ETH Zurich, Switzerland), and Bert Speelpenning (MathPartners, USA) for accepting the invitations.

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