Vietnam Journal of Mathematics (2018) 46: 717–721
https://doi.org/10.1007/s10013-018-0319-6

Preface: IWR Special Issue on Scientific Computing

Dedicated to Hans Georg Bock on the Occasion of His 70th Birthday

Willi Jäger[1] · Hoang Xuan Phu[2] · Sebastian Sager[3] · Johannes P. Schlöder[1]

Published online: 18 October 2018

Abstract
This is the second issue of the annual series of Vietnam Journal of Mathematics, which is named IWR Special Issue on Scientific Computing and is led by the Interdisciplinary Center for Scientific Computing (IWR) of Heidelberg University. This issue is dedicated to Prof. Hans Georg Bock, Director and former Managing Director of IWR, on the occasion of his 70th birthday, which he celebrated on May 9, 2018. It includes 16 papers written by authors having close ties to Hans Georg Bock. Their contributions cover various areas of Mathematics and its applications, reflecting Hans Georg Bock's influence in Mathematical Modeling, Simulation, and Optimization and practical applications of Mathematics, an emerging key methodology for science, economy, and technology in the third millenium.

1 A Driver of Innovations in Mathematical Modeling, Simulation, and Optimization

Hans Georg Bock was born on May 9, 1948, in Bottrop, Germany (Fig. 1). After his Diploma in Mathematics at University of Cologne (advisor: Roland Z. Bulirsch), he joined

✉ Hoang Xuan Phu
hxphu@math.ac.vn

Willi Jäger
wjaeger@iwr.uni-heidelberg.de

Sebastian Sager
sager@ovgu.de

Johannes P. Schlöder
schloeder@iwr.uni-heidelberg.de

[1] Interdisciplinary Center for Scientific Computing, Heidelberg University, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany

[2] Institute of Mathematics, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet Road, Cau Giay District, Hanoi, Vietnam

[3] Institute of Mathematical Optimization, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Fig. 1 Prof. Dr. Dr. h.c. mult. Hans Georg Bock

the collaborative research center *Approximation and Optimization* at University of Bonn, where he founded the research group *Simulation and Optimization*. After his PhD in Applied Mathematics at University of Bonn (1986, advisors: Roland Z. Bulirsch, Jens Frehse), he served as Visiting Professor at Heidelberg University from 1987–1988; after that, he was appointed Full Professor at Augsburg University and, since 1991, he has been Full Professor at the IWR, Heidelberg University.

Hans Georg Bock is a passionate mathematician. He has been defining new trends in scientific computing, developing state-of-the-art methods in particular for optimization with differential equations, and solving challenging application problems in science and technology as well as in the humanities. He has been educating, influencing, and promoting a large number of young scientists by serving as a role model and establishing new concepts in PhD training. In interdisciplinary research, he has been analyzing and modeling challenging problems, often with a direct economic impact. In many cases, groundbreaking new mathematics was developed, in most cases via efficient algorithms, associated theory, and unprecedented numerical results. Hans Georg Bock received many honors and awards, among them honorary doctorates from the Vietnam Academy of Science and Technology and the Russian Academy of Sciences. Since 2008, he is elected member of the Heidelberg Academy of Sciences and Humanities. In 2011, he received an ERC Advanced Grant (with Sebastian Engell). The Heidelberg Club International accepted him as member in 2018.

2 Hans Georg Bock's Contributions to Modern Mathematics

Motivated by challenges of practical (often industrial) problems, Hans Georg Bock has been developing many predictive dynamic models, often in the form of ordinary differential equations (ODE), differential-algebraic equations (DAE), or partial differential equations (PDE). He has been developing mathematical methods and efficient algorithms for simulation, sensitivity analysis, design optimization, optimal feedback control, and real-time optimization under uncertainties. He and his coworkers achieved many breakthroughs in this area. Well-known are his optimization boundary-value-problem methods (e.g., *multiple shooting*) for parameter estimation and optimal control (covering path constraints as well as integer valued control functions). His new *first-discretize, then-optimize* (*direct multiple*

shooting, *simultaneous*, *all-at-once*, *one-shot*) methods for nonlinear optimal control, optimum experimental design for parameter estimation in nonlinear dynamic process models, and real-time estimation and optimizing control of dynamic systems (also with integer valued controls) have been at the forefront of mathematical research since the 1980s. The underlying principle of lifting into a higher-dimensional space comes with a bunch of advantages, allowing better initialization, parallelization, and a reduction of nonlinearity and an improvement of stability.

Driven by practical requirements, in particular calculation of solutions in real-time, Hans Georg Bock and his coworkers have been developing various approaches to exploit structures. This comprehends the efficient and error-controlled evaluation of differential equations and their sensitivities (*automatic differentiation*, *internal numerical differentiation*), the solution of linear equation systems (*condensing*), improving global convergence (*Newton-type continuation methods*, *restricted monotonicity test*), analyzing and improving local convergence (*Generalized Gauß–Newton algorithm*, *Bock's local contraction theorem*, *high-rank updates*), adapting real-time algorithms (*initial value embedding*, *real-time iterations*, *multi-level iterations*), decomposing integrality (*outer convexification*, *combinatorial integral approximation*), and efficient implementation in software packages like *DAESOL*, *MUSCOD*, *PARFIT*, *qpOASES*, or *VPLAN*.

With these and further building blocks, his mathematical innovations and contributions have been impacting in particular the areas (mixed-integer) nonlinear optimization, (mixed-integer) nonlinear optimal control, (mixed-integer) nonlinear model predictive control, (real-time) state and parameter estimation, optimum experimental design for parameter estimation and model discrimination, (robust) optimization under uncertainty, parametric optimization, inverse simulation and inverse optimal control, and bi-level optimization.

3 Contributions to Visibility of Mathematics

Hans Georg Bock has been making decisive contributions to establish scientific computing as the third pillar of science, complementary to theory and experiment. As stated above, his mathematical research has often been driven by applications, e.g., in aerospace, mechanical and biomechanical engineering, vehicle dynamics, chemical and process engineering, psychology, systems biology, medicine, or the cultural heritage. His results can be found not only in genuine mathematical journals but also in journals of other disciplines. His oeuvre comprises more than 200 scientific papers and several co-edited books. They document the unique character of Hans Georg Bock's research: analysis and solution of challenging, highly complex problems by developing efficient numerical methods and using these methods to simulate and optimize processes.

He has been establishing and shaping research alliances sponsored by the *Deutsche Forschungsgemeinschaft* (DFG), the *German Federal Ministry of Education and Research* (BMBF) and the European Union, among others. As chairman and founder of the strategic alliance KoMSO, the *Committee for Mathematical Modeling, Simulation and Optimization*, he has been increasing the visibility of mathematics as an engine for innovation in today's and tomorrow's society in addition to exploring possibilities to entrench state-of-the-art mathematics as a new field of technology in industry and academia.

Many workshops and conferences, prominently among them the conference series *High Performance Scientific Computing* in Hanoi, were organized with substantial support of Hans Georg Bock and increased the visibility of scientific computing. For several international journals, he has been working as editor or co-editor and is an internationally

sought-after referee in many appointments of academic staff and for funding agencies. At Heidelberg University, Hans Georg Bock serves as a consultant of the *Rektor*. He has been identifying research areas that may benefit from close interactions with scientific computing, e.g., psychology (complex problem solving) or archaeology (virtual temple reconstructions).

4 Educating Scientific Computing and Promoting Young Scientists

Hans Georg Bock is a motivating teacher. He has been involving undergraduate students already into exciting research projects and covering state-of-the-art research in his lectures on various topics in numerics and optimization. Under his supervision, countless diploma and master's theses were written. He was the main advisor in more than 45 PhD projects and the second advisor in a similar number. Sixteen of his former PhD candidates are now professors at higher education institutions, among them six are full professors at German universities (Moritz Diehl, Christian Kirches, Katja Mombaur, Sebastian Sager, Volker Schulz, and Marc Steinbach) and a significant number of them are now leading scientists in industry. Figure 2 shows a scientific genealogical wine grape.

In addition to this large number of young scientists whom he shaped directly by his supervision, he had an indirect impact on even more PhD students. He rendered outstanding services to the development of structured, internationally linked, and interdisciplinary doctoral programs by innovations like the mentoring system in his positions as spokesperson of several research training groups of the DFG since 1992 and as director of the *Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences* which he significantly designed and shaped. PhD students from different countries from all over the world have been pursuing interdisciplinary doctoral projects with advisors from at least two disciplines.

Fig. 2 Academic descendants of Hans Georg Bock. Children with full name, grandchildren with initials. Illustration by Moritz Diehl

5 Outline of This Special Issue

We selected 16 peer-reviewed contributions for this special issue, which shed light on various aspects which are closely related to Hans Georg Bock's scientific work. All authors have been interacting with Hans Georg Bock—either as students, collaborators, competitors, friends, or even all of the aforementioned.

This special issue comprises papers on invariance, approximability, and discretization errors of numerical schemes, "Invariance Preserving Discretization Methods of Dynamical Systems" by *Zoltán Horváth, Yunfei Song, and Tamás Terlaky*; "The Grand Four: Affine Invariant Globalizations of Newton's Method" by *Peter Deuflhard*; "Model and Discretization Error Adaptivity within Stationary Gas Transport Optimization" by *Volker Mehrmann, Martin Schmidt, and Jeroen J. Stolwijk*; and "On the Numerical Approximability of Stable Dynamical Systems" by *Rolf Rannacher*.

Several aspects of optimal control with underlying systems of ordinary or partial differential equations systems are treated in "Computational Approaches for Mixed Integer Optimal Control Problems with Indicator Constraints" by *Michael N. Jung, Christian Kirches, Sebastian Sager, and Susanne Sass*; "An Optimization Framework for the Computation of Time-Periodic Solutions of Partial Differential Equations" by *Thomas Richter and Winnifried Wollner*; "New Results for the Handling of Additional Equality Constraints in One-Shot Optimization" by *Andrea Walther, Lisa Kusch, and Nicolas R. Gauger*; "Regulator Problems on Unbounded Domains: Stationarity–Optimal Control–Asymptotic Controllability" by *Sabine Pickenhain and Angie Burtchen*; "L^2–Tracking of Gaussian Distributions via Model Predictive Control for the Fokker–Planck Equation" by *Arthur Fleig, Lars Grüne*; and "On the Scalability of Classical One-Level Domain-Decomposition Methods" by *F. Chaouqui, G. Ciaramella, M. J. Gander, and T. Vanzan*.

Also, challenging types of optimization problems are addressed in this issue in "Minimal Surface Convex Hulls of Spheres" by *Josef Kallrath and Markus Frey* and "Shape Optimization for Interface Identification with Obstacle Problems" by *Björn Führ, Volker Schulz, and Kathrin Welker*.

The papers "Numerical Analysis in Visual Computing: What we can Learn from each Other" by *Uri M. Ascher and Hui Huang* and "A Survey on Surrogate Approaches to Nonnegative Matrix Factorization" by *Pascal Fernsel and Peter Maass* give insight into current efficient mathematical approaches in image processing, another important area of scientific computing.

Finally, new and exciting structure exploiting optimization algorithms for optimal control are presented in "Recent Advances in Quadratic Programming Algorithms for Nonlinear Model Predictive Control" by *Dimitris Kouzoupis, Gianluca Frison, Andrea Zanelli, and Moritz Diehl* and "Structure Exploitation in an Interior-Point Method for Fully Discretized State Constrained Optimal Control Problems" by *Andreas Huber, Matthias Gerdts, and Enrico Bertolazzi*.

We are happy to have compiled such a diversity of exciting and challenging topics in scientific computing, with manifold connections to the work of Hans Georg Bock. We would like to express our sincere thanks to all of the authors for their state-of-the-art contributions, as well as to the reviewers for their valuable and indispensable support.

Dear Georg, thank you for being the person you are—tutor and mentor, colleague, driver of innovations, critic, role model, fun-to-have-around guy, musician, friend, and excellent mathematician. All the best to you! We hope you enjoy this special issue.

Willi, *Phu*, *Sebastian*, and *Johannes*