Scientific Computing in Chemical Engineering II

Keil · Mackens · Voß · Werther (Eds.)

Scientific Computing in Chemical Engineering II

Simulation, Image Processing, Optimization, and Control

With 144 Figures and 42 Tables

Springer

Editors:

Prof. Dr. Frerich Keil
Technical University of Hamburg-Harburg
Chair of Chemical Reaction Engineering
Eißendorfer Straße 38
D-21071 Hamburg / Germany

Prof. Dr. Wolfgang Mackens
Technical University of Hamburg-Harburg
Section of Mathematics
Schwarzenbergstraße 95
D-21073 Hamburg / Germany

Prof. Dr. Heinrich Voß
Technical University of Hamburg-Harburg
Section of Mathematics
Schwarzenbergstraße 95
D-21073 Hamburg / Germany

Prof. Dr.-Ing. Joachim Werther
Technical University of Hamburg-Harburg
Chemical Engineering I
Denickestraße 15
D-21071 Hamburg / Germany

ISBN 3-540-65851-3 Springer-Verlag Berlin Heidelberg New York

Cataloging-in-Publication Data applied for

Die Deutsche Bibliothek - CIP-Einheitsaufnahme
Scientific computing in chemical engineering / F. Keil ... (ed.). - Berlin ; Heidelberg ; New York ; Barcelona ; Hong Kong ; London ; Milan ; Paris ; Singapore ; Tokyo : Springer, 1999
2. Simulation, image processing, optimization, and control : with tables. - 1999
ISBN 3-540-65851-3

Typesetting: Camera-ready by authors
Cover-design: E. Kirchner, Heidelberg
SPIN:10728414 02 / 3020 - 5 4 3 2 1 0 - Printed on acid-free paper

Preface

The present proceedings assemble the contributions to the second workshop on "Scientific Computing in Chemical Engineering". The two volumed edition covers the wide spectrum of computational activities in chemical process engineering encompassing tasks from process development, process design and optimization to process operations and control. The increasing performance of computers and the rapid advancement of numerical techniques encourages the employment of more sophisticated models. Quantum chemical approaches, molecular dynamics and Monte Carlo methods penetrate engineering design of catalysts and the calculation of phase transfer phenomena. Computational fluid dynamics of multi-phase flow is now a standard tool in chemical plant design. Numerical simulations replace time consuming and, therefore, expensive experiments to an ever increasing extent. The present workshop reflects these developments.

The large number of contributions made it necessary to split the proceedings into two volumes. We grouped the contributions into ten sections with the headings *Simulation of Reactive Flows, Reaction Engineering, Reaction Diffusion Problems, Molecular Properties, Computer Aided Process Design, Combustion and Flame, Image Processing, Optimization, Control* and *Neural Networks*. The present volume deals with the last six of them including the invited presentations related to these topics. The companion volume deals with the leading four.

The workshop was organized by the Collaborative Research Center (Sonderforschungsbereich) 238 of the Deutsche Forschungsgemeinschaft "In-situ measuring techniques and dynamic modelling of multiphase flow systems" at the Technical University of Hamburg-Harburg in cooperation with the German Society for Chemical Apparatus, Chemical Engineering and Biotechnology e.V. (DECHEMA), the special interest groups "Scientific Computing" and "Industrial Mathematics" of the Deutsche Mathematiker Vereinigung (DMV), the joint special interest group "Numerical Software" of the DMV, the Gesellschaft für Angewandte Mathematik und Mechanik (GAMM), and the Gesellschaft für Informatik (GI), as well as the GAMM special interest group "Scientific Computing".

We thank all the people from these societies and groups who helped to realize both these proceedings and the workshop. We are grateful to our large number of referees for their careful inspection of the contributed papers and their valuable comments which increased the quality of the proceedings considerably.

Last but not least it is a pleasure for us to thank Dipl.-Phys. Ing. Vera Lochmann and Margitta Janssen for their untiring efforts in collecting all contributions and adapting them to the Springer LaTeX conventions.

The Editors

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Part I

Invited Presentations

Direct Multiple Shooting Methods for Control and Optimization of DAE in Chemical Engineering

Irene Bauer[1], H. Georg Bock[1], Daniel B. Leineweber[2], and Johannes P. Schlöder[1]

[1] Interdisciplinary Center for Scientific Computing(IWR), University of Heidelberg, Im Neuenheimer Feld 368, D-69120 Heidelberg, Germany
[2] Bayer AG, ZT-TE 2, D-51368 Leverkusen, Germany

Abstract. Optimization problems in chemical engineering often involve complex systems of nonlinear DAE as the model equations. The direct multiple shooting method has long been known as a fast off-line method for optimization problems in ODE and later in DAE.

Some known factors crucial for its fast performance are reviewed, such as structure exploiting quadratic programming, partitioned high rank updates and parallel solution approaches. New improvements are given, such as trust region globalisation for indefinite Hessian, use of boundary and algebraic consistency conditions and invariants for gradient and Hessian reduction techniques and extensions to real-time optimization .

Applications to the optimal control of a distillation column and a fed-batch fermentation process are discussed.

1 Introduction

Direct methods for optimization boundary value problems discretize the original infinite dimensional optimization problem as a finite nonlinear program. If the NLP problem is solved by an infeasible point method such as generalized Gauss-Newton or sequential quadratic programming (SQP), as in our approach, optimization and simulation proceed simultaneously in one loop. This simultaneous approach has proven much more efficient than the classical one, in which the simulation problem is solved iteratively in an inner loop.

One such boundary value problem approach is the *direct multiple shooting method* for optimal control problems introduced by Bock and Plitt [BP84,P81]. Here the discretization is deliberately chosen to lead to a large, but specially structured NLP problem. It can be solved very efficiently by a tailored SQP method , which takes advantage of the inherent problem structures in several ways, e.g., in the generation of gradients, the approximation of the block diagonal Hessian or the fast structure exploiting solution of the quadratic programming (QP) subproblems. The original approach was designed for ODE and could treat DAE of index one only by keeping consistency conditions feasible. Later it has been extended, e.g., to DAE of index

greater than one and infeasible point strategies for consistency conditions [BES88,L97a,SBS98,L99]. Multiple shooting has several distinguished advantages, which are crucial in the context of large-scale process optimization:

- Advanced adaptive DAE integrators are employed to calculate the function values and derivatives. Therefore, our technique can be conveniently combined with popular dynamic process simulators and modeling platforms.
- Since the integrations on different multiple shooting intervals are decoupled, the method is well suited for parallel computation.
- The approach allows a natural treatment of multistage problems, control and path constraints as well as multipoint boundary conditions.
- Multiple shooting has been shown to be considerably more stable and efficient than single shooting for the solution of optimization boundary value problems.

The efficiency of the approach, which has been observed in many practical applications, has several reasons. One important reason is the possibility to include information about the approximate behaviour of the state trajectory, which is often well known, into the initial guess for the iterative solution procedure. This damps the influence of poor initial guesses for the controls, which are usually much less known, and improves the convergence.

The original direct multiple shooting code MUSCOD, implemented by Plitt in 1981 [P81], since then has undergone several revisions. In this paper we present several features of our latest modular implementation MUSCOD2 (Leineweber [L97a,L97b,L99]), which lead to significant improvements of convergence, efficiency and range of applicability.

The paper is divided into six chapters:

- In chapter 2 we introduce a general class of optimal control problems that can be treated by the new MUSCOD2.
- In chapter 3, the reformulation of infinite dimensional control problems as finite dimensional NLP problems is described.
- In chapter 4, we sketch an SQP method specially tailored to the solution of such highly structured NLP problems.
- Chapter 5 treats applications to distillation columns and shows how the effort scales with the size of the problems.
- Chapter 6 treats extensions of direct multiple shooting to real-time control and gives an application to a fermentation process.

2 Multistage Optimal Control Problems

Many dynamic process optimization problems of practical relevance can be expressed as multistage optimal control problems in DAE . We consider the following class of M-stage optimal control problems, where the time horizon