

# Lecture Notes in Computational Science and Engineering

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# High Performance Scientific and Engineering Computing

Proceedings of the  
International FORTWIHR Conference on HPSEC,  
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With 221 Figures, 44 in Colour,  
and 33 Tables



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## Editors

Hans-Joachim Bungartz  
Institut für Informatik  
Technische Universität München  
D-80290 München, Germany  
e-mail: bungartz@in.tum.de

Franz Durst  
Lehrstuhl für Strömungsmechanik  
Friedrich-Alexander-Universität Erlangen-Nürnberg  
Cauerstraße 4  
D-91058 Erlangen, Germany  
e-mail: durst@lstm.uni-erlangen.de

Christoph Zenger  
Institut für Informatik  
Technische Universität München  
D-80290 München, Germany  
e-mail: zenger@in.tum.de

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# Preface

Since the creation of the term “Scientific Computing” and of its German counterpart “Wissenschaftliches Rechnen” (whoever has to be blamed for that), scientists from outside the field have been confused about the somewhat strange distinction between scientific and non-scientific computations. And the insiders, i. e. those who are, at least, convinced of always computing in a very scientific way, are far from being happy with this summary of their daily work, even if further characterizations like “High Performance” or “Engineering” try to make things clearer – usually with very modest success, however. Moreover, to increase the unfortunate confusion of terms, who knows the differences between “Computational Science and Engineering”, as indicated in the title of the series these proceedings were given the honour to be published in, and “Scientific and Engineering Computing”, as chosen for the title of our book? Actually, though the protagonists of scientific computing persist in its independence as a scientific discipline (and rightly so, of course), the ideas behind the term diverge wildly. Consequently, the variety of answers one can get to the question “What is scientific computing?” is really impressive and ranges from the (serious) “nothing else but numerical analysis” up to the more mocking “consuming as much CPU-time as possible on the most powerful number crunchers accessible”.

Therefore, this volume can not and, certainly, does not intend to cover the whole field of numerical simulation of phenomena and processes from science and engineering on supercomputers (which is our understanding of scientific computing). What you have in your hands are just the proceedings of a three-day international conference held in Munich in March, 1998. In contrast to related events, this meeting with its nearly 200 participants was some kind of a hybrid: on the one hand, a standard conference bringing together mathematicians, computer scientists, physicists, chemists, and engineers from several countries, but, on the other hand, a forum for FORTWIHR, the Bavarian Consortium for High Performance Scientific Computing, to present the participating groups’ results at the end of its second term of funding, which may be an explanation for the impressive Bavarian presence in this book. This fact is also responsible for the topics dealt with, both at the conference and in this volume. The technical or engineering fields of fluid flow, optimal control, crystal growth, and semiconductor technology, to which 34 of the 38 contributions are related, have always been the focus of FORTWIHR’s interest, whereas other fields of applications or more principal questions from physics, chemistry, or biology do only make a fleeting appearance.

In the meantime, nearly seven years after its launching in April, 1992, FORTWIHR has entered its third period of life (and funding, of course). While the aims of this Bavarian research initiative – major progress in se-

lected areas of applications of high performance scientific computing (HPSC) by a strictly interdisciplinary approach and in close cooperation of university and industry, rapid transfer of all results to the industrial partners (especially small and medium-sized companies), education of qualified and experienced experts for industry, strengthening of HPSC in the degree programs of the participating universities – are still the same, its research program has seen a lot of changes. After a start with algorithmic, methodical, and more theoretical basics during the first term from 1992 to 1995, the second three-year term was dedicated to real application problems. Finally, there is the perhaps most challenging third and last part of ensuring the long-term acceptance and naturalness of HPSC in industrial practice, which is definitely work that is still in progress.

At that point, we feel the need to express our thanks to several persons and institutions having contributed in different ways to the conference and to these proceedings.

First, we like to thank our host, the Siemens AG, München, represented by Dr. Wolfgang Mayr-Knoch and Prof. Dr. Albert Gilg, for generously putting Siemens' perfect conference facilities in Neuperlach at our disposal. After BMW in 1993, now, for the second time, one of FORTWIHR's primary industrial partners hosted such a meeting, which is just another proof for the close cooperation of academic and industrial research groups within FORTWIHR.

Next, let us thank all of the FORTWIHR-crew of helping hands, especially Dr. Michael Breuer, Anton Frank, Christa Halfar, Christoph Kranz, Andreas Paul, and Dr. Stefan Zimmer, for all kinds of support before and during the conference.

Throughout the preparation and realization of this book, the cooperation with Dr. Martin Peters and Thanh-Ha Le Thi from Springer-Verlag was fruitful and pleasant and shall not be forgotten.

Moreover, before being too early too lavish with our gratitude, we have to mention Miriam Mehl. To her, we are especially indebted for her commitment concerning the compilation of this book. Certainly, everyone who has ever been in charge of collecting single contributions and of assembling them to something that is worth being called a book will have made the experience that layout guidelines for authors seem to be at least as challenging to circumvent as income tax laws.

Finally, and needless to say, neither the conference and these proceedings nor an important part of the results reported in many of the contributions would have been possible without the financial support of the Bavarian Research Foundation, the Bavarian Ministry for Science, Research, and Arts, and FORTWIHR's numerous industrial partners and sponsors.

München, January 1999

Hans-Joachim Bungartz  
Franz Durst  
Christoph Zenger

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