Lecture Notes in Computer Science 1947

Tor Sørevik Fredrik Manne Randi Moe
Assefaw Hadish Gebremedhin (Eds.)

Applied Parallel Computing

New Paradigms for HPC in Industry and Academia

5th International Workshop, PARA 2000
Bergen, Norway, June 2000
Proceedings

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Preface

The papers in this volume were presented at PARA 2000, the Fifth International Workshop on Applied Parallel Computing. PARA 2000 was held in Bergen, Norway, June 18-21, 2000. The workshop was organized by Parallab and the Department of Informatics at the University of Bergen. The general theme for PARA 2000 was *New paradigms for HPC in industry and academia* focusing on:

- High-performance computing applications in academia and industry,
- The use of Java in high-performance computing,
- Grid and Meta computing,
- Directions in high-performance computing and networking,
- Education in Computational Science.

The workshop included 9 invited presentations and 39 contributed presentations. The PARA 2000 meeting began with a one-day tutorial on OpenMP programming led by Timothy Mattson. This was followed by a three-day workshop.

The first three PARA workshops were held at the Technical University of Denmark (DTU), Lyngby (1994, 1995, and 1996). Following PARA'96, an international steering committee for the PARA meetings was appointed and the committee decided that a workshop should take place every second year in one of the Nordic countries. The 1998 workshop was held at Umeå University, Sweden. One important aim of these workshops is to strengthen the ties between HPC centers, academia, and industry in the Nordic countries as well as worldwide. The University of Bergen organized the 2000 workshop and the next workshop in the year 2002 will take place at the Helsinki University of Technology, Espoo, Finland.

October 2000

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Organization

PARA 2000 was organized by the Department of Informatics at the University of Bergen and by Parallab.

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Speaker Information

Industrial Applications: Challenges in Modeling and Computing

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Abstract. Complex industrial applications can be examined using modeling and computing even when theoretical and experimental approaches fail. Modeling and computing are rapidly developing tools for engineering and science, but applying these tools in practice is a challenge. This article focuses on industrial multi-physics and multi-scale problems in the production of silicon crystals and the design of paper machines.

Keywords: Modeling, computing, multi-physics, multi-scale, industry, parallel computing, numerical methods, paper machines, silicon crystals.

1 Introduction

Scientific and engineering problems can be examined using modeling and computing [5,17], but this approach poses several challenges. We focus on industrial multi-physics applications, such as the growth of silicon crystals [16] and the modeling of paper machines [12,6].

The growth of silicon crystals, shown in Fig. 1, contains coupled physical phenomena: electromagnetism, fluid dynamics, heat transfer, and structural mechanics. Thorough modeling of this application requires multi-scale modeling spanning several length and time scales [3,16].

Modeling of paper machines is a different kind of challenge. The headbox of a paper machine, presented in Fig. 2, contains flows in a complex geometry. These flows are three-dimensional, turbulent and multi-phase. A comprehensive mathematical model leads to demanding computational tasks.

Computation of a multi-physics problem is a challenge. Coupled problems lead to systems of nonlinear equations, which have to be solved iteratively. Solving these coupled systems can be a huge computational effort. We'll present some ideas on numerical solution strategies in multi-physics problems. In addition, we'll discuss how to combine computational fluid dynamics and optimization.

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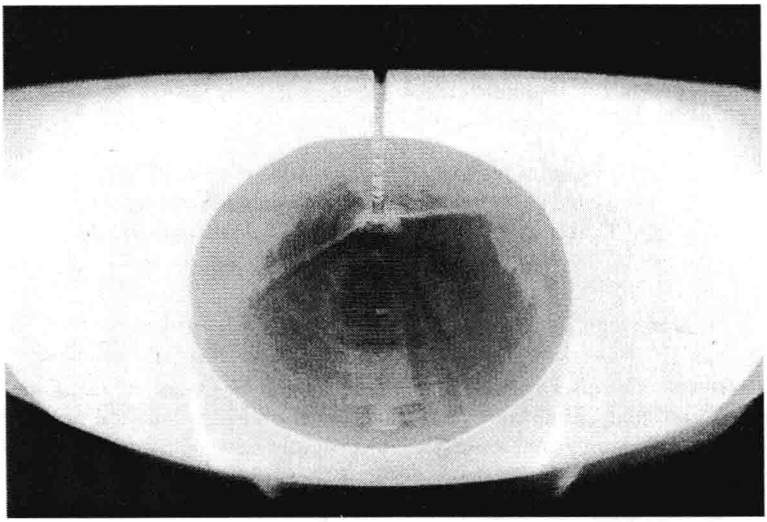

Fig. 1. Growth of a silicon crystal.

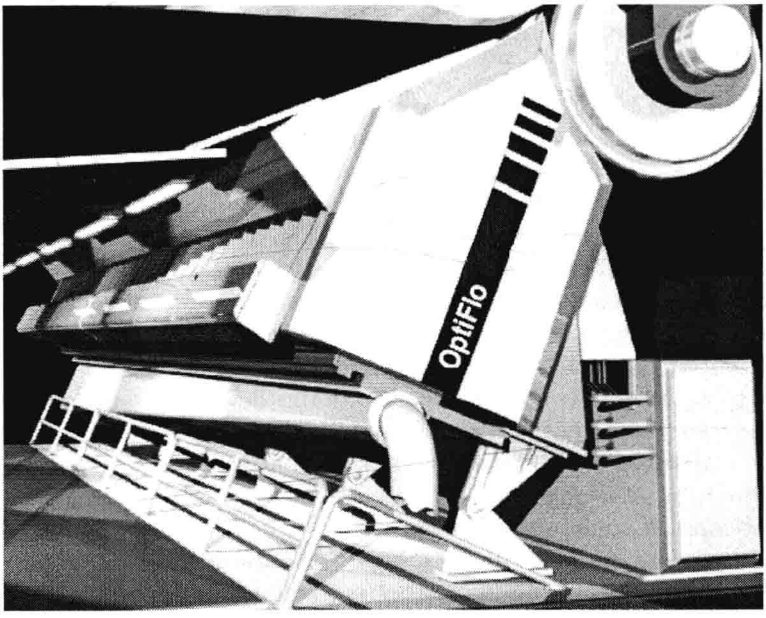

Fig. 2. The headbox of a paper machine.

2 Possibilities and Challenges in Industrial Applications

Industrial applications are difficult to model and compute: both the physical phenomena and the structures and geometries are typically very complex. These modeling tasks involve significant challenges for scientific computing, and high performance computing (HPC) is undoubtedly needed. Thus, HPC is an essential part of industrial research and development (R&D).

There are a multitude of modeling problems presented by the modern industry. Challenges are presented, for example, by phenomena in the human body or by the physics of miniaturized electronics components.

Microelectromechanical systems (MEMS) [20] pose a multi-physics problem, which contains electrostatistics, structural analysis, fluid dynamics and heat transfer in miniaturized geometries. In fact, modeling MEMS devices may require us to combine molecular dynamics and continuous models.

Multi-physics problems are solved increasingly often. As an example, the model may contain fluid-structure interactions. Other possibilities are free surface problems or phase-change problems. These problems are typically solved in 2D today, but in 3D in the future.

Another demanding task is the modeling the human body, which is of interest to the pharmaceutical industry. We may be interested in simulating the blood flow in 3D bifurcations, designing new drugs, or modeling how electromagnetic fields behave in living tissues.

The modeling of turbulence in fluid dynamics poses significant challenges. Today, the Reynolds stress model is applied routinely in industrial problems, and large eddy simulation (LES) is becoming feasible. However, direct numerical simulation (DNS) of the Navies-Stokes equations will be impossible for several years to come.

Another challenge are multi-phase problems. This is somewhat similar to turbulence modeling: there exist smaller and smaller phenomena arising from direct simulation, and it is less and less feasible to perform averaging. Furthermore, multi-scale problems present us with a combination of different scales (micro, meso and macro scales).

We may need to perform several simulations to solve a single problem. For example, one may be interested in finding the optimal geometry in a fluid dynamics application. This is an example of shape optimization in computational fluid dynamics (CFD). For each optimization run, one may have to solve a CFD problem tens, hundreds or thousands of times. Also, there are requirements for performing real-time interactive simulations, for example in a virtual reality environment, or a virtual learning system (Fig. 3).

3 The Three Methods of R&D

We can use three different approaches in industrial R&D: experimental, theoretical and computational (Fig. 4). All these approaches are essential and needed, and they are usually applied together to solve a problem.

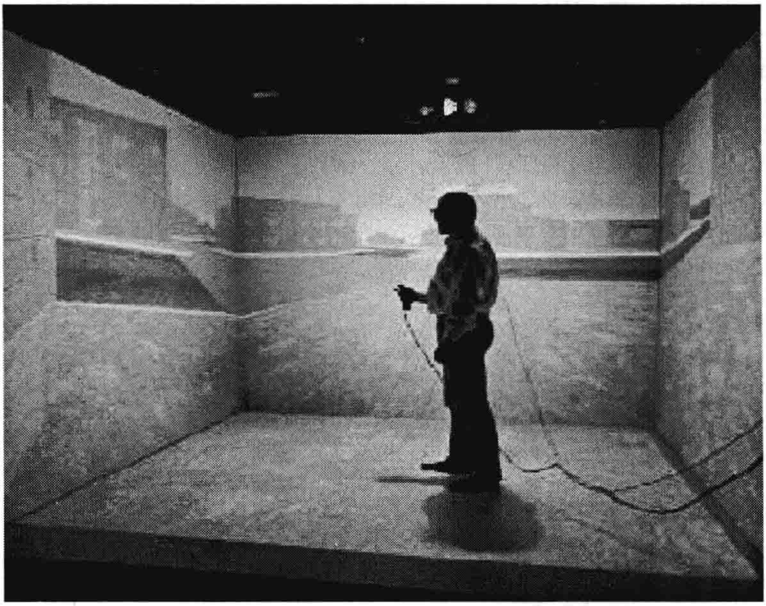

Fig. 3. Industrial R&D utilizes modern computer technology: interacting with a simulation in a virtual reality environment.

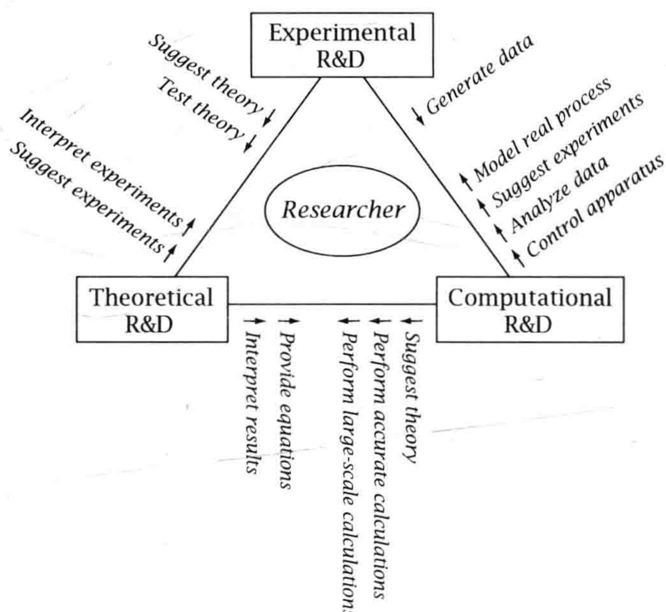

Fig. 4. The three methods of R&D.

The experimental approach is typically straightforward — basically, we measure what happens in the physical process we are interested in. Experiments are often reliable, at least to a known extent, which depends on the physical setup and the human interface of the experiment. Also, experiments are usually quantitative. However, experiments can be laborious or even impossible to carry out in complex cases. We mention the lack of commercial techniques to measure the turbulence of dense fiber-water suspensions. Experiments can also be very expensive and slow to carry out. For example, one may have to build a prototype to do the experiment.

The theoretical approach is efficient in simple cases. It is usually qualitative and suggestive — a good way to check the numerical or experimental results. However, the theoretical approach is insufficient in complex cases.

Computational modeling is repeatable, which is an asset: one does not need to build a new prototype to make a new experiment. However, there are a great many steps where mistakes can occur: mathematical modeling, selection of the numerical methods, and implementation of the methods. In addition, unanticipated hardware and software problems may occur during the computation.

4 The Challenges of Industrial HPC

Traditionally, industrial R&D has involved experiments and the internal know-how of a company. Nowadays R&D has shifted to a more innovative direction: combining the use of computation, experiments, and theory. Because all these approaches demand a different set of skills, this usually involves a collaboration of several experts.

The computational approach requires people who know how to solve mathematical models on a computer. Also, programming skills are required: real-life problems are not usually solvable using off-the-shelf software packages. Thus, R&D departments have to compete for talented people in other commercial sectors: www services, networking, etc.

The modeling and computing facilities of industrial companies are usually modest. Due to the fast development of this area, there is a continuing lack of know-how of numerical methods, programming, and computer technology (efficient workstations, clusters etc.). If one builds a computational research center from scratch, the costs easily exceed any budget. Therefore, industry is interested in co-operation with sites which have the required expertise, in addition to software and hardware resources. Usually this co-operation involves university laboratories.

However, also in the universities there is a lack of efficient training programs on HPC. At least in Finland, there may be just a single course on HPC topics, or none. Therefore, there is urgent need for teaching modeling and computing tools to the students at the university level. These courses should encourage students to use modeling techniques, numerical methods, commercial software packages, and programming languages.