Preface

Most problems in science involve many scales in time and space. An example is turbulent flow where the important large scale quantities of lift and drag of a wing depend on the behavior of the small vortices in the boundary layer. Another example is chemical reactions with concentrations of the species varying over seconds and hours while the time scale of the oscillations of the chemical bonds is of the order of femtoseconds. A third example from structural mechanics is the stress and strain in a solid beam which is well described by macroscopic equations but at the tip of a crack modeling details on a microscale are needed.

A common difficulty with the simulation of these problems and many others in physics, chemistry and biology is that an attempt to represent all scales will lead to an enormous computational problem with unacceptably long computation times and large memory requirements. On the other hand, if the discretization at a coarse level ignores the fine scale information then the solution will not be physically meaningful. The influence of the fine scales must be incorporated into the model.

This volume is the result of a Summer School on Multiscale Modeling and Simulation in Science held at Bosön, Lidingö outside Stockholm, Sweden, in June 2007. Sixty PhD students from applied mathematics, the sciences and engineering participated in the summer school.

The purpose of the summer school was to bring together leading scientists in computational physics, computational chemistry and computational biology and in scientific computing with PhD students in these fields to solve problems with multiple scales of research interest. By training the students to work in teams together with other students with a different background to solve real life problems they will be better prepared for their future work in academia, institutes, or industry. The importance of interdisciplinary science will certainly grow in the coming years.

There were lectures on computational multiscale techniques in the morning sessions of the first week. Most of these lectures are found in the first, tutorial part of this volume. The afternoons were devoted to the solution of mathematical and computational exercises in small groups. The exercises are interspersed in the articles in the first part. The speakers and the titles of their lectures were:

- Jørg Aarnes, Department of Applied Mathematics, SINTEF, Oslo: *Multiscale Methods for Subsurface Flow*
- Björn Engquist, Department of Numerical Analysis, KTH, Stockholm, and Department of Mathematics, University of Texas, Austin: *Introduction to Analytical and Numerical Multiscale Modeling*
- Heinz-Otto Kreiss, Department of Numerical Analysis, KTH, Stockholm: *Ordinary and Partial Differential Equations with Different Time Scales*
- Claude Le Bris, CERMICS, École Nationale des Ponts et Chaussées, Marne la Vallée: *Complex Fluids*
- Olof Runborg, Department of Numerical Analysis, KTH, Stockholm: *Introduction to Wavelets and Wavelet Based Homogenization*
- Richard Tsai, Department of Mathematics, University of Texas, Austin: *Heterogeneous Multiscale Method for ODEs*
- Lexing Ying, Department of Mathematics, University of Texas, Austin: *Fast Algorithms for Boundary Integral Equations*

In the second week, nine realistic problems from applications in astronomy, biology, chemistry, and physics were solved in collaborations between senior researchers and the PhD students. The problems were presented by experts in the applications in short lectures. Groups of students with different backgrounds worked together on the solutions with guidance from an expert. The week ended with oral presentations of the results and written papers. The student papers are found at the homepage of the summer school `www.ngssc.vr.se/S2M2S2`. The students received credit points at their home university for their participation as a part of the course work for the PhD degree. As a break from the problem solving sessions, there were three invited one hour talks on timely topics:

- Tom Abel, Department of Physics, Stanford University: *First Stars in the Universe*
- Lennart Bengtsson, Max Planck Institut für Meteorologie, Hamburg: *Climate Modeling*
- Yannis Kevrekidis, Department of Chemical Engineering, Princeton University: *Equation-free Computation for Complex and Multiscale Systems*

These are the nine different projects with the project leaders:

- **Climate Modeling**
  - Erland Källén, Heiner Körnich, Department of Meteorology, Stockholm University: *Climate Dynamics and Modelling* (two projects)
- **Solid State Physics**
  - Peter Zahn, Department of Physics, Martin-Luther-Universität, Halle-Wittenberg: *Complex Band Structures of Spintronics Materials*
  - Erik Koch, Eva Pavarini, Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich: *Orbital Ordering in Transition Metal Oxides*
- **Astrophysics**
  - Garrelt Mellema, Stockholm Observatory, Stockholm University: *Photo-Ionization Dynamics Simulation*

  - Axel Brandenburg, Nordita, Stockholm: *Turbulent dynamo simulation*
- **Quantum Chemistry**
  - Yngve Öhrn, Erik Deumens, Department of Chemistry and Physics, University of Florida, Gainesville: *Molecular Reaction Dynamics with Explicit Electron Dynamics*
- **Molecular Biology**
  - Håkan Hugosson, Hans Ågren, Department of Theoretical Chemistry, KTH, Stockholm: *Quantum Mechanics - Molecular Mechanics Modeling of an Enzyme Catalytic Reaction*
- **Flow in Porous Media**
  - James Lambers, Department of Energy Resources, Stanford University: *Coarse-scale Modelling of Flow in Gas-Injection Processes for Enhanced Oil Recovery*

The projects were chosen to contain a research problem that could be at least partly solved in a week by a group of students with guidance from a senior researcher. The problems had multiple scales where the finest scale cannot be ignored. Part two of this volume contains a short description of the projects mentioned above.

The summer school was organized by the Department of Numerical Analysis and Computer Science (NADA), KTH, Stockholm, the Department of Information Technology and the Centre for Dynamical Processes and Structure Formation (CDP) at Uppsala University with an organizing committee consisting of Timo Eirola, Helsinki, Björn Engquist, Stockholm, Bengt Gustafsson, Uppsala, Sverker Holmgren, Uppsala, Henrik Kalisch, Bergen, Per Lötstedt, Uppsala, Anna Önehag, Uppsala, Brynjulf Owren, Trondheim, Olof Runborg, Stockholm, Anna-Karin Tornberg, Stockholm.

Financial support was received from the Swedish National Graduate School in Scientific Computing (NGSSC), Swedish Foundation for Strategic Research (SSF), Centre for Dynamical Processes and Structure Formation (CDP), Nordita, NordForsk, Research Council of Norway, and Comsol. Computing resources were provided by Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX).

Stockholm, Uppsala,
September 2008

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http://www.springer.com/978-3-540-88856-7

Multiscale Modeling and Simulation in Science
Engquist, B.; Lötstedt, P.; Runborg, O. (Eds.)
2009, XIV, 320 p., Softcover
ISBN: 978-3-540-88856-7