Banff Workshop on Modeling and Simulation

Zhangxin John Chen (University of Calgary), Dong Liang (York University), Yanping Lin (University of Alberta)

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1 Overview of the Field of Modeling and Simulation

Computational Science has been called a third branch of science, along with theory and experiment. In truth, it is part of theory and part of experiment, but it is different from either. Many theoretical problems can only be solved using a high performance computer. Modeling and simulation, the major component of computational science, is much more than simply elaborating pure theory. In the last two decades there have been rapid developments of computer power and sophisticated computational techniques. These advances have permitted the application of high performance computing to modeling and simulation with unprecedented accuracy and scope. These sophisticated processes are now being applied to a wide range of important engineering and science problems that require a thorough understanding of the underlining principles of physics, chemistry, mathematical modeling, numerical solution techniques, and computing infrastructure. The effect is to create a more comprehensive understanding of emerging issues. These developments have profound implications in mathematics, science, engineering, and industry. Modeling and simulation is a critical tool for analyzing many different types of important phenomena such as flow and transport, weather prediction, wave propagation, novel material design, computational chemistry, and genome sequencing and analysis.

2 Recent Developments and Open Problems of Modeling and Simulation

Our living environment, economic development, natural resource management, and national security are all influenced by our understanding of complex physical and chemical processes occurring in and around the earth. Groundwater contamination, oil and gas reservoir production, discovering new oil reserves, ocean hydrodynamics, CO2 storage and sequestration, and air quality control are all vital to our economic and social well being. Modeling and simulation research is driven by the rapid changes worldwide in each of these capacities.

Energy and environmental modeling and simulation require the observation of natural scientists, the technical expertise of engineers, the modeling and numerical skills of mathematicians, and the modern techniques of computer scientists. The engineering and science problems in these areas tend to culminate in coupled systems of nonlinear, time-dependent partial differential equations (PDEs). Numerical solutions of these PDEs are very challenging due to the multiple temporal and spatial scales presented, the nonlinear effects, and the large scale and unusually long duration simulations required [1, 2, 3].

3 Workshop Presentation Highlights

The workshop themes include: (A) Mathematics of Multiphase Fluid Flow and Transport; (B) High-Quality Discretization of Flow and Transport; (C) Computational Modeling of Multiscale Phenomena; (D) Parallel Computing; (E) Nonlinear Effects on Propagation Properties of Numerical Models.

20 presentations in this workshop have dealt with these topics. Speakers have been carefully selected to ensure that a range of modeling and simulation techniques can be explored. This diversity is necessary in order to address various phenomena arising from emerging issues in the energy and environment sectors. Many of our speakers are world class, such as Todd Arbogast, Jim Douglas, Jr., Ismael Herrera, and Kirk Jordan. Four female participants and five young graduate students attended the workshop. A feature of this workshop is the opportunity provided for interactions between the participants. Workshop organizers have facilitated round-table sessions in which questions and answers have been shared, and lively discussions have been encouraged. Invited participants are from diverse interdisciplinary background and top in their field. Such a combination of ideas and perspectives has been beneficial to all attendees. The workshop presentations, discussion in the round-table sessions, and possible future collaborations amongst participants have created the opportunity for significant progress in the field of energy and environment modeling and simulation.

4 Scientific Progress Made in Modeling and Simulation

The objective of this workshop is to bring together the worlds top active researchers (and their more junior counterparts) who study energy and environmental modeling and simulation to discuss past, recent, and prospective advances in this area. The speakers have summarized important advances from the past two decades and have discussed the current understandings, the state-of-the-art techniques, and the current major challenges. Each session of this workshop has provided a vehicle for participants to learn novel techniques and new advances in this area of work. The content has been academic in nature while addressing the many significant applications for industry.

The ultimate goal of the workshop is to expose workshop participants (in particular, junior researchers) to the latest developments in the field of modeling and simulation, while emphasizing the impact of this field on science, engineering, and industry.

The study of the diverse topics presented in the workshop through laboratory experiments, mathematical theory, and computational techniques requires interdisciplinary collaboration between engineers, mathematicians, computational scientists, and researchers working in industry, government laboratories, and academy. The collaborative work of researchers in this workshop will create meaningful progress in predicting, understanding, and optimizing many complex phenomena. The rational for this two-day BIRS workshop is to hold lectures that pull together the major ideas and recent research results, chart future directions, and address newly emerging issues for energy and environment modeling and simulation. It is anticipated that the participants have left the workshop knowing the future research directions and the needed potential applications.

5 Outcome of the Workshop

The Banff International Research Station is a beautiful location for learning and building relationships. Its common areas have supported our goals to have researchers engaged in discussion throughout the workshop event. We have brought researchers from around the world to share their perspectives, test ideas, and create new connections both intellectually and socially while exploring the latest developments in modeling and simulation. This workshop has promoted, enhanced, and stimulated cross-continental research interactions and collaborations in mathematical sciences and will shape changes in the research work completed with modeling and simulation.

References

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