



Preface

High performance computing for advanced modeling and simulation of materials



The First International Workshop on High Performance Computing for Advanced Modeling and Simulation of Materials (HPCMS2015) was held in Austin, Texas, USA, Nov. 18, 2015. HPCMS 2015 was organized by Computer Network Information Center (Chinese Academy of Sciences), University of Michigan, Universidad Complutense de Madrid, University of Science and Technology Beijing, Pittsburgh Supercomputing Center, China Institute of Atomic Energy, and Ames Laboratory.

Supercomputers are rapidly evolving as advances in architecture and semiconductor technology. High performance computing has been applied to accelerate material advanced modeling and engineering. The current trend will provide challenges in parallelism because of increased processing units, accelerators, complex hierarchical memory systems, interconnection networks, storage and uncertainties in programming models. The interdisciplinary collaboration is becoming more and more important in high performance computation. Realistic material simulation needs to combine material modeling methods, mathematical models and parallel algorithms for exploiting supercomputers effectively.

HPCMS 2015 focused on novel mathematical modeling, parallel algorithms, high performance computing tools and experiences in large-scale material science and engineering applications and supercomputers. The program aimed at bringing different researchers including domain experts, applied mathematicians and computer scientists together to discuss the interdisciplinary research of modeling methods and parallel algorithm design for the simulation of materials performance on current and future supercomputers.

HPCMS 2015 covered the following topics:

- Use of hardware accelerators (MIC, GPUs and FPGA) and heterogeneous hardware in computational material science.

- Numerical methods and parallel algorithms for the advanced modeling and simulation of materials.
- Mathematical modeling and high performance computing tools in large-scale material simulation.
- Big data of materials science.
- Large-scale material modeling based on the new features of message passing programming model.

The review process of the special issue is the same with the regular issue.

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