Eighth IEEE International Workshop on High Performance Computational Biology (HiCOMB)

May 25, 2009 Rome, Italy

in conjunction with 23rd International Parallel and Distributed Processing Symposium

Message from the Workshop Chairs

Welcome to the Eighth International Workshop on High Performance Computational Biology (HiCOMB). The explosion of biological data and the compute-intensive nature of many biological applications, has caused computing to become an increasingly crucial resource for furthering biological knowledge, which, in turn, has led to the fast emergence of Computational Biology and Bioinformatics as important disciplines for academic research and industrial application. Moreover, it has become recognized that many biological applications require high-performance computing to handle the large runtime and memory requirements arising from the inherent complexity of biological problems, the large number and size of biological data sets, and the need to handle noisy, error-prone data. The goal of this workshop is to provide a forum for discussion of the latest research in developing high-performance computing solutions to problems arising from molecular biology.

The technical program was put together by Program Chair Michela Taufer and a distinguished program committee consisting of 19 members. The program includes 12 contributed papers and an invited keynote presentation by Charles L. Brooks III from the University of Michigan at Ann Arbor. We received eighteen submissions from around the world. Each submission was thoroughly reviewed by three program committee members. Based on the reviews, ten papers were selected for presentation at the workshop and inclusion in the workshop proceedings. Two additional papers were invited to provide additional coverage of topics from leading researchers in the community.

We are grateful to the program committee members for submitting timely and thoughtful reviews. We wish to thank all the authors who submitted manuscripts to this workshop, without which this highquality technical program would not have been possible. We plan to continue this workshop in the forthcoming years and look forward to your continuing support in this endeavor.

Michela Taufer, Srinivas Aluru, and David A. Bader

Workshop Organization

WORKSHOP CO-CHAIRS:

Srinivas Aluru, Iowa State University (USA) David A. Bader, Georgia Institute of Technology (USA)

PROGRAM CHAIR:

Michela Taufer, University of Delaware (USA)

PROGRAM COMMITTEE:

Dmitry A. Afonnikov, Novosibirsk State University and Institute of Cytology and Genetics SB RAS, Novosibirsk (Russia) Pratul K. Agarwal, Oak Ridge National Laboratory (USA) Nancy Amato, Texas A&M University (USA) Roger Armen, University of Michigan, Ann Arbor (USA) Georg Fuellen, Ernst-Moritz-Arndt-University Greifswald (Germany) Concettina Guerra, Georgia Tech (USA) and University of Padova (Italy) Ming-Ying Leung, University of Texas at El Paso (USA) Mark Miller, San Diego Supercomputer Center (USA) Aiichiro Nakano, University of South California (USA) Sandeep Patel, University of Delaware (USA) Geppino Pucci, University of Padova (Italy) Jacques Rougemont, EPFL (Switzerland) Alexandros Stamatakis, Ludwig-Maximilians-University Munich (Germany) Bertil Schmidt, Nanyang Technological University (Singapore) Heiko Schroder, RMIT University (Australia) John Stone, University of Illinois at Urbana-Champaign (USA) Wing-Kin Sung, National University of Singapore (Singapore) Jim Tisdall, DuPont (USA) Chau-Wen Tseng, University of Maryland, College Park (USA)

List of Accepted Papers

De Novo Modeling of GPCR Class A Structures (Invited Keynote). Charles L. Brooks III, University of Michigan, Ann Arbor

Parallel Reconstruction of Neighbor-Joining Trees for Large Multiple Sequence Alignments using CUDA. Yongchao Liu, Bertil Schmidt, and Douglas Maskell

Accelerating Error Correction in High-Throughput Short-Read DNA S4equencing Data with CUDA. Haixiang Shi, Bertil Schmidt, Weiguo Liu, and Wolfgang Mueller-Wittig

Parallel Monte Carlo Study on Caffeine-DNA Interaction in Aqueous Solution. Michael Kalugin and Alexandr Teplukhin

Dynamic Parallelization for RNA Structure Comparison. Eric Aubanel, Patricia Evans, and Eric Snow

HMMer Acceleration Using Systolic Array Based Reconfigurable Architecture. Yanteng Sun, Peng Li, Guochang Gu, Yuan Wen, Yuan Liu, and Dong Liu

A Resource-Efficient Computing Paradigm for Computational Protein Modeling Applications. Yaohang Li, Dougalas Wardell, and Vincent Freeh

Exploring FPGAs for Accelerating the Phylogenetic Likelihood Function. Nikolaos Alachiotis, Euripides Sotiriades, Apostolos Dollas, and Alexandros Stamatakis

Long Time-scale Simulations of in vivo Diffusion using GPU Hardware. Elijah Roberts, John Stone, Leonardo Sepulveda, Wen-Mei Hwu, and Zaida Luthey-Schulten

An Efficient Implementation Smith Waterman Algorithm on GPU using CUDA for Massively Parallel Scanning of Sequence Databases. Lukasz Ligowski and Witold Rudnicki

A Novel Framework for Modeling Ion Channels. May Siksik and Vikram Krishnamurthy

High-throughput Protein Structure Determination using Grid Computing. Jason W. Schmidberger, Blair Bethwaite, Colin Enticott, Mark A. Bate, Steve G. Androulakis, Noel Faux, Cyril F. Reboul, Jennifer M. N. Phan, James C. Whisstock, Wojtek J. Goscinski, Slavisa Garic, David Abramson, and Ashley M. Buckle

Folding@home: Lessons From Eight Years of Volunteer Distributed Computing. Adam L. Beberg, Guha Jayachandran, Siraj Khaliq, and Vijay S. Pande