Bio-molecular Simulations on Future Computing Architectures

Oak Ridge, Tennessee

Location: JICS Auditorium, Building 5100, Oak Ridge National Laboratory

Day 1: September 16th

8:00 – 8:30 am **Meet and Greet (Breakfast provided)**

Session I: Emerging Architecture Trends for Scientific Computing

Chair: Pratul Agarwal, Oak Ridge National Laboratory

8:30 – 8:40 am **Arthur Barney Maccabe**
Welcome

8:40 – 9:20 am **Al Geist, Oak Ridge National Laboratory**
"The Co-Design Challenges of going from Petascale to Exascale"

9:20 – 9:50 am **Duncan Poole, NVIDIA**
"GPU architecture and applications supporting life science development"

9:50 – 10:00 am **Coffee Break**

10:00 – 10:30 am **Eric Stahlberg, Wittenberg University**
"Confidence in Computing –Interfaces, Portability, Reliability and Performance"

10:30 – 11:00 am **Gilad Shainer, Mellanox Technologies**
"The Development of Mellanox-NVIDIA GPUDirect over InfiniBand – a New Model for GPU to GPU Communications"

11:00 – 11:30 am **Robert Hinde, University of Tennessee, Knoxville**
"GPU-accelerated quantum Monte Carlo simulations"

11:30 – 12:15 pm **Round Table Discussion A**

12:15 – 1:00 pm **Lunch (Provided)**

Session II: Exploiting GPUs and FPGAs for Biomolecular Simulations

Chair: Qiang Cui, University of Wisconsin

1:00 – 1:40 pm **John Stone, University of Illinois at Urbana-Champaign**
"High Performance Molecular Simulation, Visualization, and Analysis on GPUs"

1:40 – 2:10 pm **Gianni De Fabritiis, Universitat Pompeu Fabra, Spain**
"High-throughput molecular dynamics simulations using ACEMD on GPUs"

2:10 – 2:40 pm **Joshua Anderson, University of Michigan**
"Simulating nano-materials, polymers, and complex fluids on GPUs with HOOMD-blue"

2:40 – 3:00 pm **Coffee Break**

3:00 – 3:30 pm **Martin Herbordt, Boston University**
"FPGA Acceleration of Molecular Dynamics and Docking"

3:30 – 4:00 pm **Scott LeGrand, NVIDIA**
TENTATIVE: "Adapting AMBER particle mesh Ewald and generalized Born molecular dynamics to GPUs"

4:00 – 5:00 pm **Round Table Discussion B**

Day 2: September 17th

7:45 – 8:00 am **Meet and Greet (Breakfast provided)**

Session III: Challenges and Solutions for Biomolecular Simulations on Future Architectures

Chair: Paul Crozier, Sandia National Laboratories

8:00 – 8:40 am **John Levesque, Cray Inc.**
"Future Exascale architectures and the challenges they impose on the application developers"

8:40 – 9:10 am **Dave Norton, High Performance Fortran Associates**
"Programming GPUs with PGI's Compilers and Tools"

9:10 – 9:40 am **Erik Lindahl, Stockholm University, Sweden**
"How can molecular simulation reach the exascale? Challenges in performance and parallelism"

9:40 – 10:00 am **Coffee Break**

10:00 – 10:30 am **Laxmikant (Sanjay) Kale, University of Illinois at Urbana-Champaign**
"Strong scaling issues for classical molecular dynamics"

10:30 – 11:00 am **Pratul Agarwal, Oak Ridge National Laboratory**
"Optimal biomolecular simulations on future computing architectures"

11:00 – 12:00 pm **Round Table Discussion C**

12:00 – 1:00 pm **Lunch (Provided)**

Session IV: Novel methods and better simulations

Chair: Kennie Merz, University of Florida

1:00 – 1:40 pm **Kennie Merz, University of Florida**
"Quantum Chemical Insights into the Computation of Absolute Interaction Energies"

1:40 – 2:10 pm **Imran Haque, Vijay Pande's Lab., Stanford University**
"Hybrid Vigor: Using Heterogeneous HPC to Accelerate Chemical Informatics"

2:10 – 2:40 pm **David Hardy, University of Illinois at Urbana-Champaign**
"Simulating Biomolecules on GPUs with the Multilevel Summation Method"

2:40 – 3:00 pm **Coffee Break**

3:00 – 3:30 pm **Jaydeep Bardhan, Rush University Medical Center**
"Simultaneous Evolution of Physical Models and Computing Architectures: An Engineering Perspective"

3:30 – 4:00 pm **Chakra Chennubhotla, University of Pittsburgh**
"Automatic discovery of energetically coherent sub-states and rare events in a protein's conformational landscape"

4:00 – 4:30 pm **Round Table Discussion D & Wrap-up**

NOTES:

- Shuttle service for pick-up and drop-off will be provided from Oak-Ridge hotels (Double-tree & Staybridge Suites) to the location.
- Please remember to bring suitable government issued identification to enter Oak Ridge National Laboratory. If you are NOT a US citizen, please bring your passport (and Green-card, if applicable).