

Workshop Agenda 1st Day

Introduction (Chair, Tom Schlager)

8:30 Welcome by: BNL Director Praveen Chaudhari...

Session 1: System Development Status (Chair, Michael McGuigan)

- 8:45 QCDOC System Overview and Status – Bob Mawhinney Columbia University
Riken BNL Research Center
- 9:15 QCDOC Operation System developments, applications and performance
Peter Boyle - University of Edinburgh
- 9:45 SciDAC software on QCDOC - Chulwoo Jung - BNL

10:10 coffee break

- 10:25 The SciDAC API for Lattice Field Theory – Richard C. Brower - BU
- 10:50 BlueGene/L Architecture Hardware – Al Gara - IBM
- 11:30 BlueGene/L Software Overview, Operation System, compilers performance
tools, Job scheduling, etc – Manish Gupta – IBM
- 12:10 Lunch Break (Tour of QCDOC area, for those interested)

Session 2: Application experiences w/ BlueGene/L + QCDOC (Chair, Ed Jedlicka)

- 1:00
 - Protein Folding – Blue Matter - Robert Germain - IBM
 - Molecular Dynamics Simulation of a Biotoxin on QCDOC
Yuefan Deng – SUNY-SB
 - Linpack performance on BlueGene – James Sexton - IBM

2:30 coffee break

- 2:45
 - Climate Modeling: HOMME - Richard Loft, Henry Tufo - IBM
 - QCD on BlueGene/L – Dong Chan, Pavlos Vranas - IBM
 - QCD on QCDOC – Peter Boyle University of Edinburgh
 - AB Initio Molecular Dynamics: CPMD – Alessandro Curioni - IBM
- 4:00
 - Astrophysics: FLASH – Katherine Riley – ANL
 - Using BG/L for Calculations of Beam - Beam Interactions in RHIC.
N. Malitsky and N. L. D'Imperio – BNL
 - ParaDiS: A dislocation dynamics code on BlueGene/L - Kim Yates –
LLNL

5:30 Social Hour (Berkner Hall)

6:30 Dinner (Berkner Hall)

Speaker David Keyes “Supercomputing in China”

Workshop Agenda 2nd Day

Session 3: Applications (cont.) (Chair, Jim Davenport)

- 8:30 BlueGene/L discussion:
 - Determining BlueGene/L application fit – Andrew Siegel ANL
 - BlueGene/L Optimization Tips – Bob Walkup IBM
 - MPI implementation and trade offs Gheorghe Almasi IBM

11:00 coffee break

- 11:15 BlueGene/L Apps Gyan Bhanot IBM
 - “Optimizing Mapping of Apps on the BlueGene/L Torus to minimize communication time”, Gyan Bhanot – IBM
 - FFT on BlueGene/L Franz Franchetti – CMU, Stefan Kral & Juergen Lorenz Vienna University of Technology.

12:45 – 1:30 Lunch Break

- 1:30 **Performance & BlueGene/L Consortium**
 - Performance Monitoring & Tuning, MASS, MASSV, ESSL DavidKlepacki & Bob Walkup – IBM
 - BlueGene/L Consortium Activities: - Ed Jedlicka -ANL Organization, Working groups Web documentation

Adjourn