

# JSC Guest Student Colloquium

30. 9. & 1. 10. 2013 – building 16.4, Rotunda



Blue Gene Q supercomputer

## Monday, 30. 9. 2013

9.30 Welcome & Session I

**Dominik Gräser, Wuppertal**

*Domain decomposition for simulating the route choice of pedestrians*

**Qian Zhang, Aachen**

*Self-consistent atomic orbital computation and visualization*

**Erik Järleberg, Stockholm**

*Communication-avoiding strategies for massively parallel N-body simulations*

11.35 Lunch 

13.00 Session II

**Nicola Cadenelli, Brescia**

*Enable basic MPI-3 support for the Score-P performance measurement system*

**Patrick Steinbrecher, Bielefeld**

*How to deal with very small matrices in spacetime*

14.20 Coffee Break 

14.40 Session III

**Benjamin Schott, Leipzig**

*Physical annealing in the microcanonical ensemble*

**Maciej Golik, Kraków**

*Standalone client for the UFTP data transfer tool*

**Jannis Ehrlich, Bremen**

*Completely and highly efficient parallel implementation of the Lowe-Andersen thermostat*

## Tuesday, 1. 10. 2013

9.30 Opening Remarks & Session IV

**Martin Perdacher, Wien**

*Benchmarking performance and scalability of the package PRIMME for sequences of dense correlated eigenproblems*

**Hadeer El Habashy, Cairo**

*MD simulations to study the irregular stiffness behavior of poly(N-isopropylacrylamide)*

**Henrik Larsson, Kiel**

*Molecular orbital generation sequences*

11.35 Lunch 

13.00 Session V

**Markus Werner, Bonn**

*Performance and energy efficiency characterization of an embedded GPU platform*

**Alexander Aschikhin, Hamburg**

*Hybridization and tuning of a PIC code on JUQUEEN*

14.20 Coffee Break 

14.40 Keynote Talk

**Costas Bekas & Alessandro Curioni**

IBM Zurich Research Laboratory

*The road to Exascale: How algorithmic re-engineering can help break the power and performance brick walls*

16.00 Concluding Remarks