Fachbereich Computerwissenschaften

EINLADUNG
zum Gastvortrag am

Dienstag, 20. März 2012, 17:00 Uhr, T02
Institutsgebäude Jakob-Haringer-Str. 2, Itzling

von

Dr. Yusaku Yamamoto
Kobe University, Japan

zum Thema:

„The "K" Supercomputer and Large-Scale Scientific Computing in Kobe"

Abstract

This talk consists of two parts. In the first part, I will talk about the status of the "K" computer, which is the world's fastest supercomputer (as of November 2011) currently being installed in Kobe, Japan. The K computer is a distributed-memory parallel computer developed by Fujitsu under the contract with RIKEN, one of the leading national laboratories in Japan. It consists of 80,000 nodes, or 640,000 cores, connected by a 6-dimensional torus network and has a peak performance of more than 10 petaflops. Several projects to exploit the power of the K computer for ultra-large scale simulations are under way. Among them, I will briefly explain some projects related to Kobe University, such as the geo-dynamo simulation, molecular orbital calculation of proteins, and multi-scale electromagnetic particle simulation. The second part concerns development of an eigenvalue solver for the K computer. Eigenvalue problems with dense symmetric coefficient matrices arise in molecular orbital calculations and some kind of first-principles molecular dynamics. Often, the matrix size is not so large (10,000 to 40,000), but the problem needs to be solved very fast (in less than 10 seconds) using tens of thousands of processors. For this purpose, the conventional tri-diagonaliation based algorithm used in ScaLAPACK is not suitable because the communication cost dominates and the parallel efficiency becomes quite low. For this type of problem, an algorithm based on the block Jacobi method seems promising due to its large-grain parallelism. We report the performance of our preliminary block Jacobi solver on University of Tokyo's supercomputer with 1024 cores and discuss performance bottlenecks and possible improvements.

Univ.-Prof. Dr. Marian Vajtersic (Host)