SC13 Short lecture @ AICS

November 2013

Name	Dr. Truong Vinh Truong Duy (Japan Advanced Institute of Science and Technology, Field 2)
Title of your Presentation	Massive Parallelization of a Linear Scaling DFT Code OpenMX
Abstract	OpenMX is an open-source first-principles calculation code based on density functional theory for explaining and predicting materials' properties. In this work, we massively parallelize OpenMX by developing a domain decomposition method for atoms and grids. In the atom decomposition, we develop a modified recursive bisection method based on the moment of inertia tensor for reordering the atoms from 3D to 1D along a principal axis so that the atoms that are close in real space are also close on the axis to ensure data locality. The atoms are then divided into sub-domains depending on their projections onto the principal axis in a balanced way among the processes. In the grid decomposition, we define four data structures to make data locality consistent with that of the clustered atoms, and propose a 2D decomposition method for solving the Poisson equation using 3D FFT with communication volume minimized. Benchmark results show that the parallel efficiency at 131,072 cores is 67.7% compared to the baseline of 16,384 cores with 131,072 atoms of the diamond structure on the K computer.