EXACT DIAGONALIZATION OF LARGE SCALE EIGENVALUE PROBLEMS USING GPU COMPUTING

R.KAUSHIK RAGAVAN [1,2]
Dr. BHUPENDER THAKUR [2]
Dr. DAVID KOPPELMAN [1]

1. Electrical & Computer Engineering Department, Louisiana State University 2. Center for Computation & Technology, Louisiana State University

Abstract:

Computations on large spare matrices are one of the most useful, yet, time-consuming parts of many scientific applications like Density Matrix Renormalization Group (DMRG) and Exact Diagonalization of lattice systems. The goal of our research is to solve large scale eigenvalue problems of interest in lattice and chemical systems using a heterogeneous computing model. Exact Diagonalization for large sparse matrices is often carried out using iterative solvers such as Lanczos Algorithm to achieve the desired scaling on most super-computing clusters. In this paper we have implemented the Lanczos Algorithm for a single node CPU/GPU system which will yield the full Tri-diagonal matrix for a given sparse matrix. The eigenvalues can be readily obtained from the Tri-diagonal matrix using QR or QL factorization. The advantage of using Lanczos over other algorithms is that the full matrix is never required as an input and only an action on a vector is required, leaving the implementation of SpMV to the user. We have done preliminary tests for sparse matrices of the order 25k, 50k, 125k and 2.5M and obtained a 35 X speedup compared to a single CPU for a SpMV and an overall speedup of 3X for the Lanczos Algorithm. The sparse matrices employ the ELLPACK form of compression for the SpMV.

Keywords: Density Matrix Renormalization Group (DMRG), Lanczos Algorithm, Spare Matrix-Vector Multiplication (SpMV), Graphics Processing Unit (GPU) and ELLPACK format.