PARALLEL COMPUTING APPLICATION

The scientific or engineering problem being considered is block Jacobi method for the symmetric Eigen value problem.

In certain applications where simulations based on quantum mechanics, it is requires to solve a medium sized (size = 10,000) symmetric Eigen value problem millions of times.

The solution of the symmetric eigenvalue problem is based on tridiagonalization. The input matrix is transformed to a symmetric tridiagonal matrix by orthogonal transformations, then the eigenvalues
And eigenvectors of the tridiagonal matrix are computed, and the eigenvectors of the original matrix are computed by back-transformation.

The block Jacobi algorithm is simple and consists of only two types of computations, solution of a small Eigen problem and matrix multiplication. It has high parallelism in it; when the block size is L, each processor can perform O (L^3) floating-point operations.

The block Jacobi program is written in C and parallelized using MPI.
Libraries: LAPACK
Supercomputer: University of Tokyo's T2K supercomputer.

The block size is L= 125 and the matrix size N is set to 2LP^1/2 where P is the number of processor cores used. The values of p used are 4, 16,64,256,1024.

References:

1)http://www.iam.fmph.uniba.sk/algoritmy2012/(PERFORMANCE OF THE BLOCK JACOBI METHOD FOR THE SYMMETRIC EIGENVALUE PROBLEM ON A MODERN MASSIVELY PARALLEL COMPUTER).