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Project Title: Electron-phonon coupling on a fine grid

Usage:
• Testbed

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Usage Description:
We will carry out the following work:

• Testing the performance of the existing code EPW. EPW code is part of the QE package and it can be compiled on ARM machines.

• Write a small program using Fortran and openmp/MPI that can read the output generated by EPW to efficiently calculate the Fourier transform of various physical quantities such as Hamiltonians, dynamical matrices and electron-phonon scattering matrices.

Computational Resources:
• Total node hours per year: 10,000

• Size (nodes) and duration (hours) for a typical batch job: One node for 72 hours.

• Disk space (home, project, scratch): home (40 GB), project (1 TB) and scratch (1 TB)

Personnel Resources:
None

Required software:
GCC, Python3.8, vim