



Tjark Sievers – I. Institute of Theoretical Physics

Parallelization Levels in Quantum ESPRESSO



k-point Parallelization



Plane-wave Parallelization

wave-function coefficients



Linear Algebra Parallelization

distributes matrix diagonalization and matrix-matrix



Summary: Parallelization in pw.x

- ▶ plane wave: orbitals in plane wave basis set
- ► tasks: