



Tjark Sievers – I. Institute of Theoretical Physics

Parallelization Levels in Quantum ESPRESSO

k-point Parallelization

- ▶ Highest level of parallelization I currently use
- ▶ Distributes k points to pools of processors
- ▶ Relevant parameter: N_k
- ▶ Number of processors for the whole job = $N_p \implies$ number of processors in one pool
 $= \frac{N_p}{N_k}$

Plane-wave (PW) Parallelization

- ▶ Calculations for the group of k points in one pool are automatically parallelized
- ▶ This means: Orbitals in plane wave basis set, charge density in real and reciprocal space are distributed among processors
- ▶ Also includes fourier transforms

Linear Algebra Parallelization

- ▶ Parallelization level running along PW parallelization
- ▶ Distributes matrix diagonalization and orthonormalization of wave functions
- ▶ Relevant parameter: N_d