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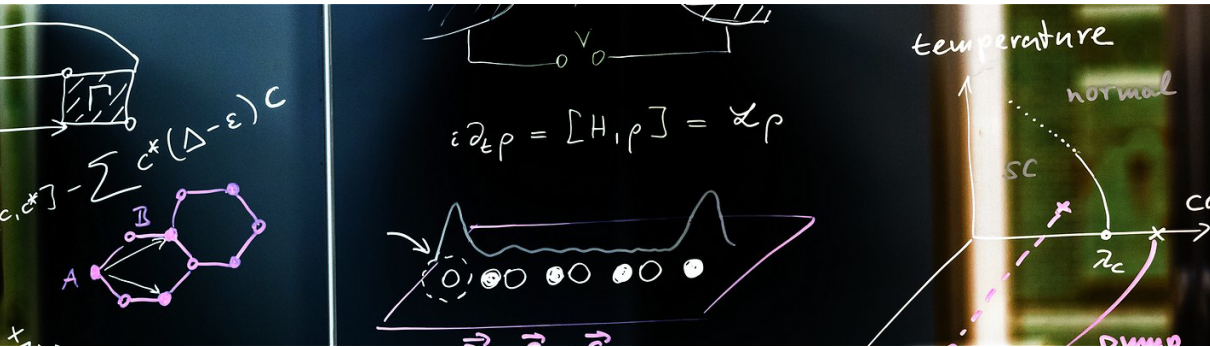
FAKULTÄT
FÜR MATHEMATIK, INFORMATIK
UND NATURWISSENSCHAFTEN



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: `Nk`
- Number of processors for the whole job = `Np` $\implies$ number of processors in one pool = $\frac{\texttt{Np}}{\texttt{Nk}}$

Plane-wave (PW) Parallelization

- Calculations for the group of k points in one pool are automatically parallelized
- This means: wave function coefficients in real and reciprocal space are distributed among processors
- Includes parallelization of fourier transforms: planes of the real grid or columns of G-vectors respectively are distributed among processors
- Also called R & G space parallelization

Linear Algebra Parallelization

- Parallelization level running alongside PW parallelization
- Distributes matrix diagonalization and orthonomalization of wave functions
- Relevant parameter: `Nd`
- Groups of `Nd` processors in every pool