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FAKULTÄT
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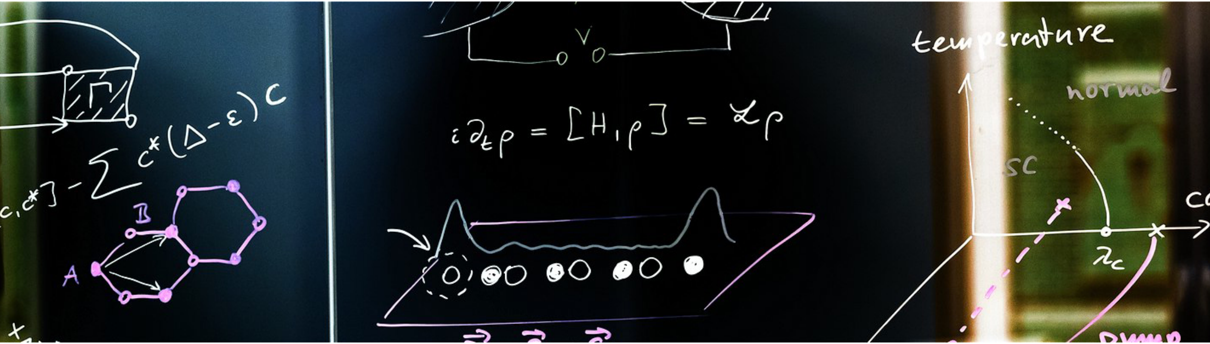
UND NATURWISSENSCHAFTEN



Tjark Sievers – I. Institute of Theoretical Physics 13th July 2022

Optimization of the Quantum Espresso Density Functional Theory Code for parallel execution on the PHYSnet-Cluster

Motivation

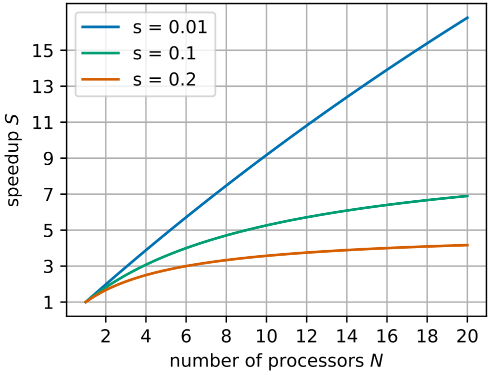
Speedup

How much faster can a problem be solved with N processors instead of one?

$$S := \frac{T_1}{T_N} \tag{1}$$

with serial runtime T_1, runtime on N cores T_N
ideal case: every processor needs the same time

$$T_N = \frac{T_1}{N} \implies S = \frac{T_1}{\frac{T_1}{N}} = N \tag{2}$$

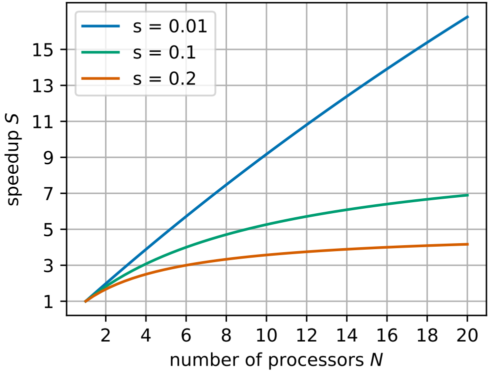


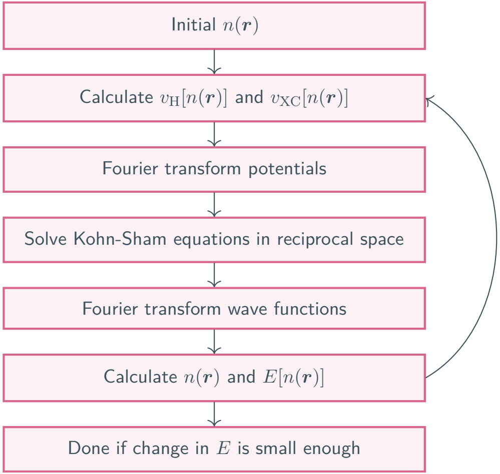
Amdahl's Law

In reality: several factors limiting parallelization

Simple model given by Amdahl's law:

- split serial time into a strictly serial part s and one which can be parallelized perfectly p
- normalize serial time $T_1 = s + p = 1$
- execution time on N processors: $T_N = s + \frac{p}{N}$
- speedup: $S = \frac{T_1}{T_N} = \frac{1}{s+\frac{p}{N}} = \frac{1}{s+\frac{1-s}{N}}$
- relevant features: limited by $1/s$, for smaller s: closer to linear speedup




Initial $n(\boldsymbol{r})$
Calculate $v_{\mathrm{H}}[n(\boldsymbol{r})]$ and $v_{\mathrm{XC}}[n(\boldsymbol{r})]$
Fourier transform potentials
Solve Kohn-Sham equations in reciprocal space
Fourier transform wave functions
Calculate $n(\boldsymbol{r})$ and $E[n(\boldsymbol{r})]$
Done if change in E is small enough

Factors limiting parallel execution