

I Parallelization of DFPT calculations

Calculations with the PHonon package are significantly more time intensive than PWscf calculations, so good parallelization is of the essence to make these calculations manageable.

I.1 Optimal parallelization parameters for DFPT calculations

The PHonon package offers the same three parallelization levels as the PWscf package, namely plane wave, k point and linear algebra parallelization.

I.1.1 k point parallelization

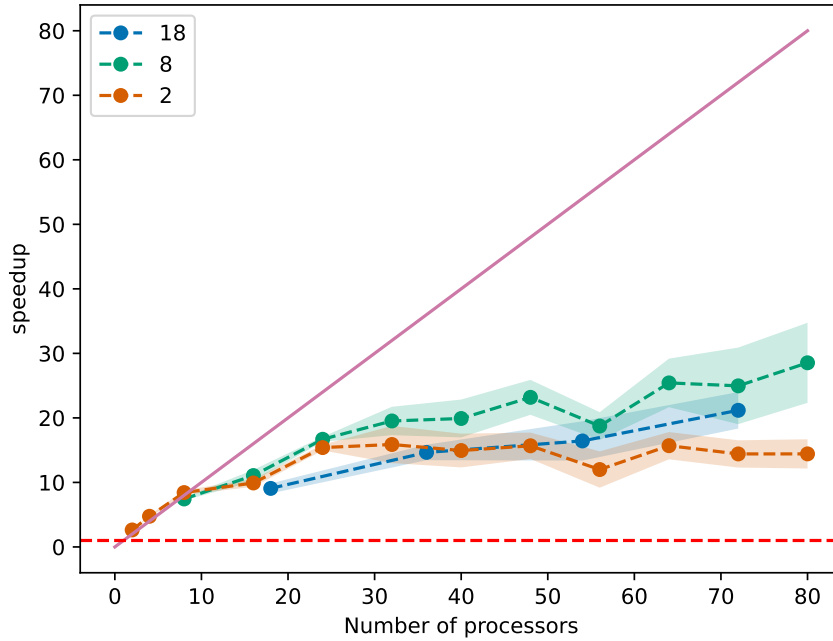


Figure I.1: *CAPTION*

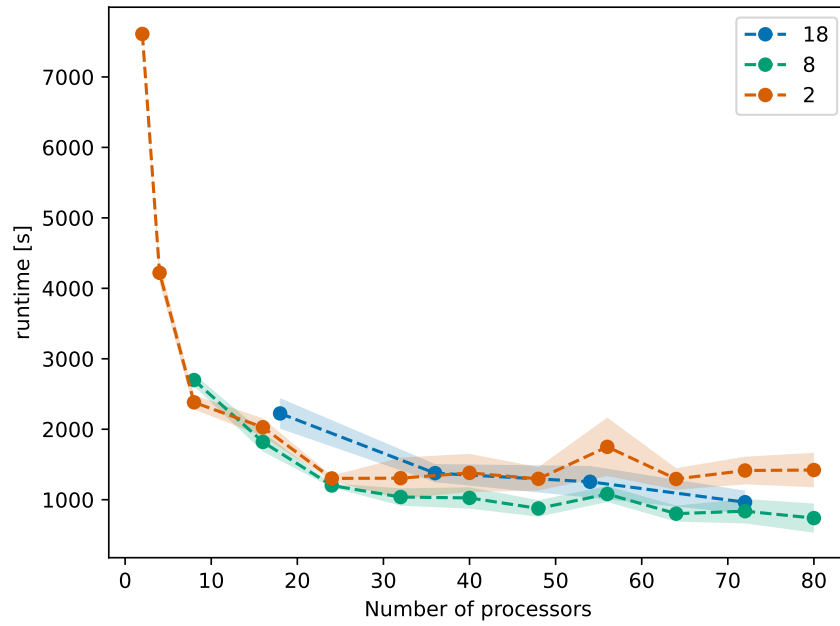


Figure I.2: *CAPTION*

I.1.2 Linear algebra parallelization

I.2 Image parallelization

Better introduction

When using image parallelization, QUANTUM ESPRESSO outputs a separate time report for every image, so one step is added to the analysis: The total runtime of a calculation is determined by the longest running image, so speedup will be calculated using that value, but another important measure to evaluate is variation of times between images.

I.3 Conclusion: Parameters for optimal scaling

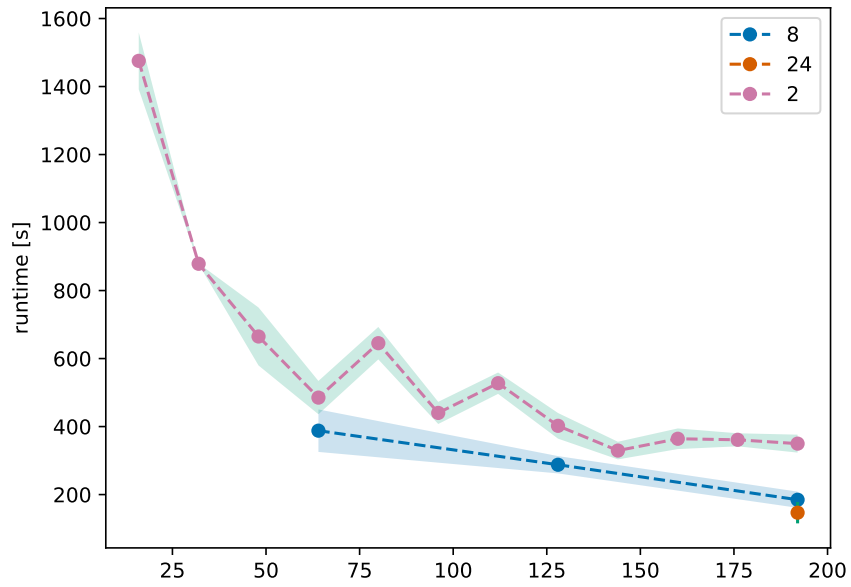


Figure I.3: CAPTION

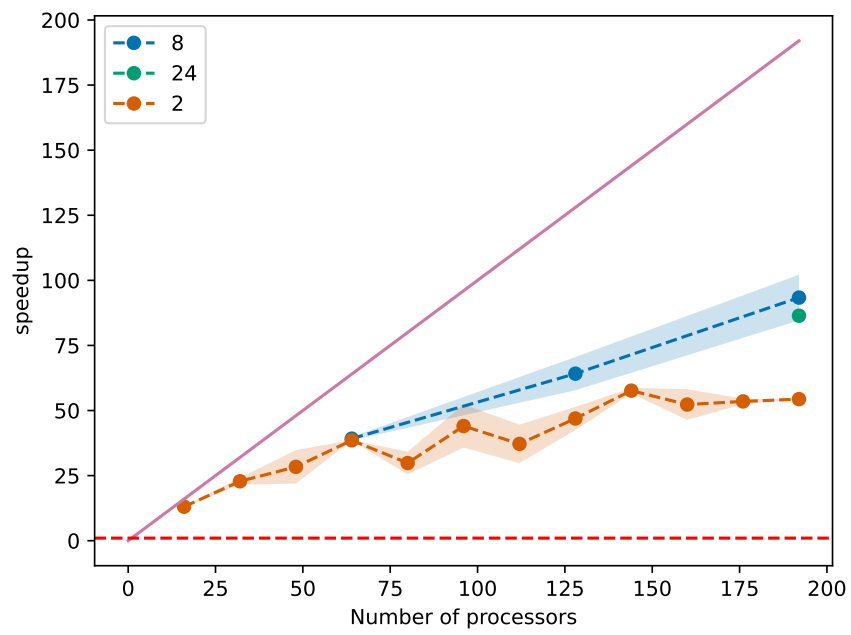


Figure I.4: CAPTION

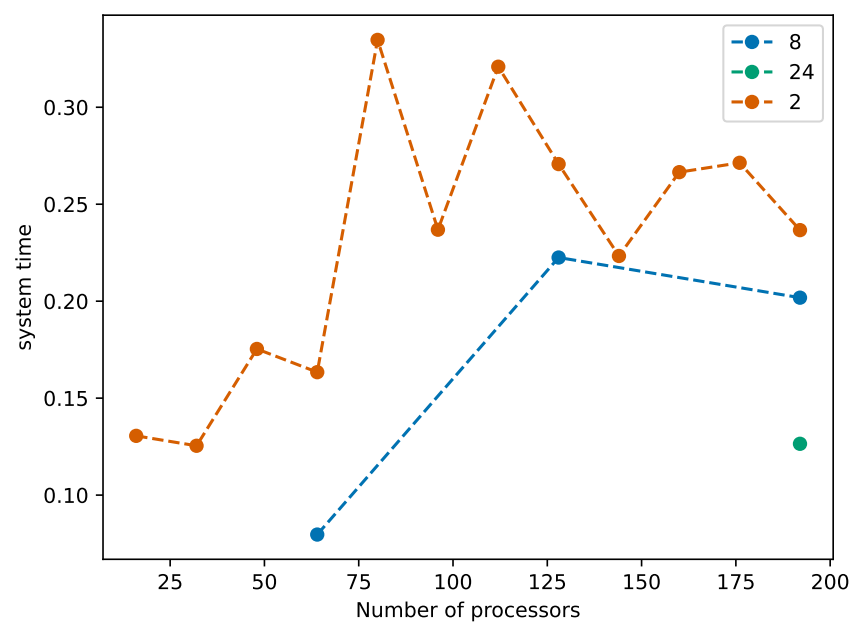


Figure I.5: CAPTION