I Parallelization of DFPT calculations

I.1 Optimal parallelization parameters for DFPT calculations

I.1.1 k point parallelization

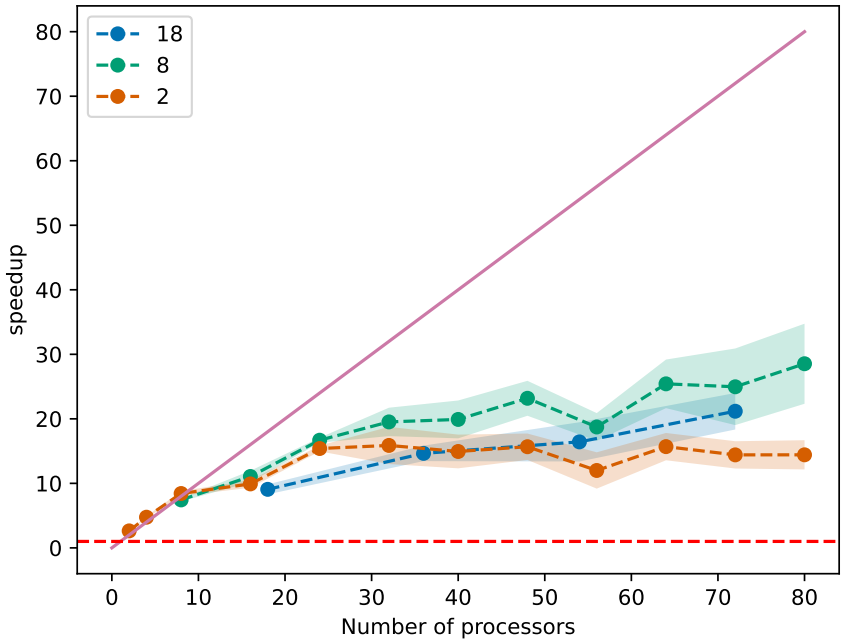

Figure I.1: *CAPTION*

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

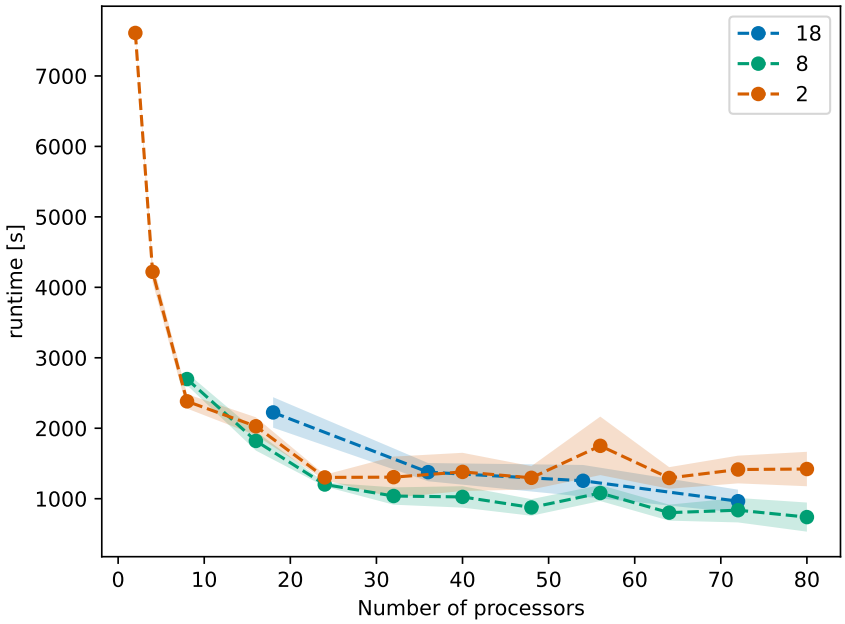

Figure I.2: *CAPTION*

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

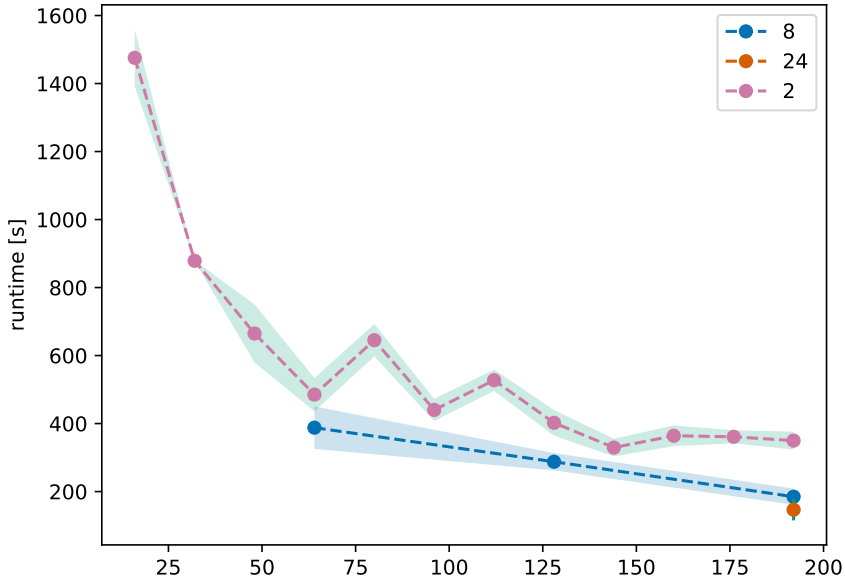

Figure I.3: *CAPTION*

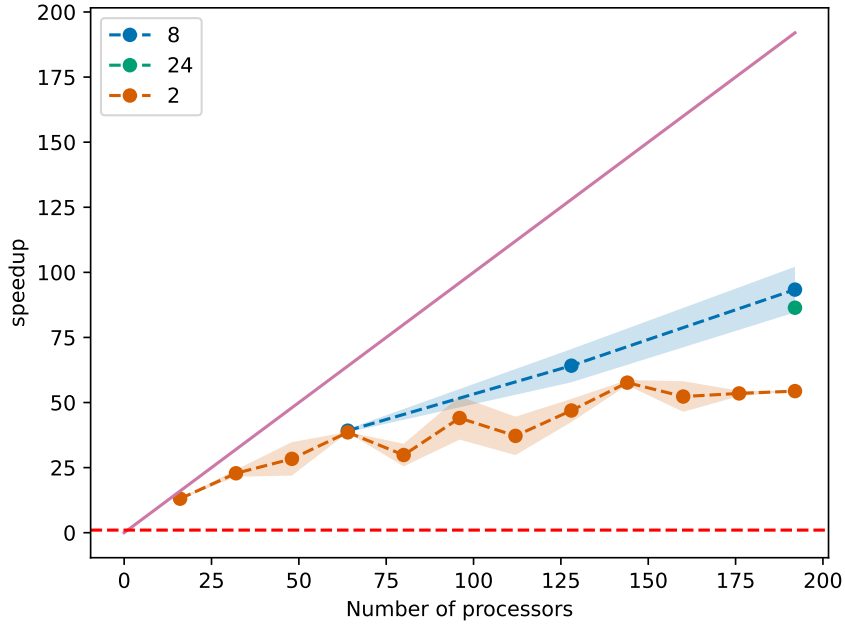

Figure I.4: *CAPTION*

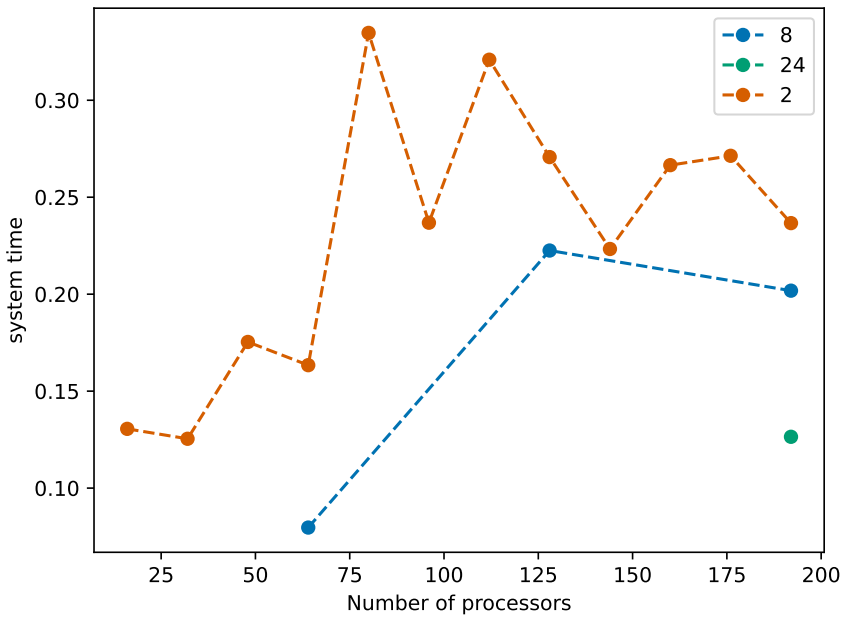

Figure I.5: *CAPTION*