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Petascale resources and CP2K: enabling sampling, large scale models or correlation beyond DFT

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Already with modest computer resources, GGA DFT simulations of models containing a few hundred atoms can contribute greatly to chemistry, physics and materials science. With the advent of petascale resources, new length, time and accuracy scales can be explored. Recently, we have made progress in all three directions:

1. A novel Tree Monte Carlo (TMC) algorithm introduces a further level of parallelism and allows for generating long Markov chains. Sampling 100'000s of configurations with DFT, the dielectric constant and order-disorder transition in water ice Ih/XI has been studied.[1]
2. The removal of all non-linear scaling steps from GGA DFT calculations and the development of a massively parallel GPU-accelerated sparse matrix library make structural relaxation and MD possible for systems containing 10'000s of atoms.[2]
3. A well parallelized implementation of a novel algorithm to compute four center integrals over molecular states (RI-GPW), allows for many-body perturbation theory (MP2, RPA) calculations on a few hundred atoms. Sampling liquid water at the MP2 level yields a very satisfying model of liquid water, without empirical parameters.[3,4]

References:

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- [3] Mauro Del Ben, Mandes Schönherr, Jürg Hutter, and Joost VandeVondele JPCL 4, 3753 (2013)
- [4] Mauro Del Ben, Jürg Hutter, and Joost VandeVondele, JCTC 9, 2654 (2013)