

# Numerical analysis for density functional theory

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The quantification of precision of DFT computation has been a major subject of interest in recent years. This is complicated by the large number of approximations and numerical parameters needed for a given computation. This has also been a source of inquiry in the applied mathematics community, where a number of approaches (a priori and a posteriori error analysis, uncertainty quantification) enable the computation of error bars, inside a given model (e.g. Born-Oppenheimer DFT with PBE and a given pseudopotential). I will describe recent work aimed at making this a reality for DFT computations, focusing in particular on the understanding of errors in Brillouin zone sampling, and the computation of a posteriori error estimators for the discretization error of plane-wave DFT.