Implementation and efficiency analysis of RI-MP2 static polarizability

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Abstract: In this work, we show the implementation of Møller-Plesset second order perturbation (MP2) static polarizability, with approximation of resolution-of-identity (RI, also known as density-fitting). Technically, this task is second derivative to RI-MP2 energy w.r.t. perturbation of external dipole electric field, which involves intense tensor derivatives with constraints. We try to optimize floating point operations (FLOPs) and perform efficiency analysis. We expect this work will be incorporated with doubly hybrid density functional approximations to produce accurate static polarizability with affordable computational cost.