Goal oriented error estimators for Hartree Fock and Kohn Sham equations (DFT)

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Hartree Fock and DFT (density functional theory) is designed for computing the ground energy of a nonrelativistic N electron system, with various application in chemistry, solid physics and materialscience. Within the framework of *weighted dual residual methods* we present a posteriori error estimators measuring the error in the desired energy computation.

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