Supporting Information for "Nonlocal functionals inspired by the strongly interacting limit of DFT: exact constraints and implementation"

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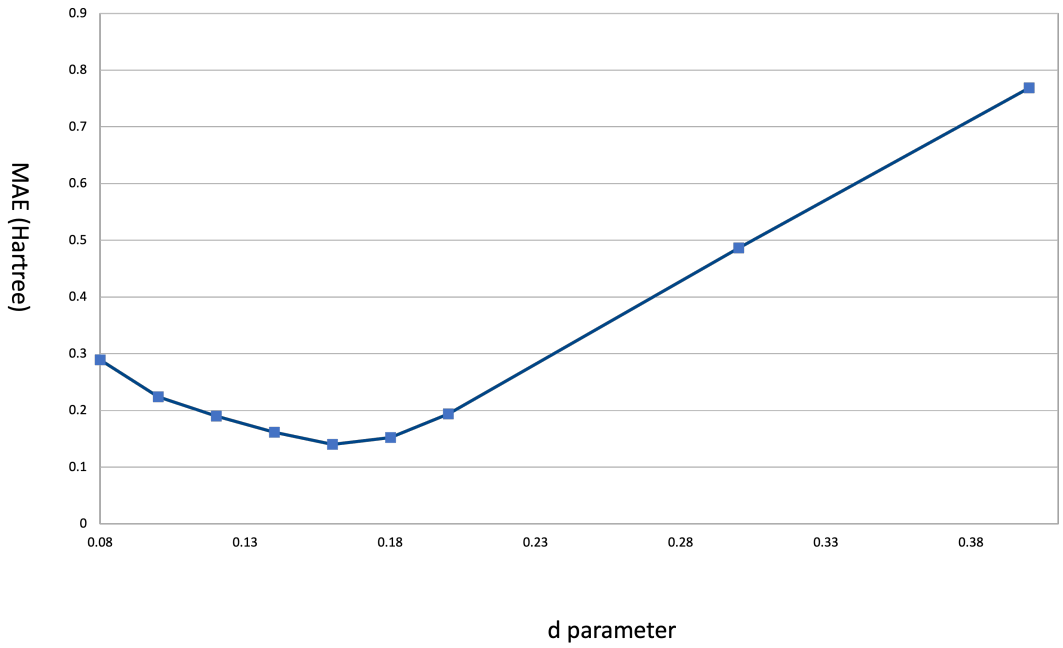

Figure S1: MAE of MRF's repulsion energies from Table 2 with the d parameter. The CCSD electron repulsion energies also of Table S2 are taken as a reference.

	CCSD basis	CCSD	d=0.8	d= 0.1	d=0.12	d=0.14	d=0.16	d=0.18	d=0.2	d=0.3	d=0.4	d=0.8
CH2F2	AVTZ	167.7566698	168.4513562	168.3049478	168.1665163	168.0349339	167.909516	167.7897011	167.675053	167.1674811	166.7480617	0.694686363
FMe	AVQZ	88.97299792	89.45138792	89.35869148	89.27072946	89.18680475	89.10647074	89.02935138	88.95517028	88.62157615	88.33815502	0.478389997
Methanol	AVTZ	80.64586625	81.04434112	80.95604763	80.87145548	80.78995106	80.71112812	80.63471122	80.56050122	80.2174965	79.91329727	0.39847487
Propyne	AVQZ	95.82463082	95.87585568	95.77532369	95.67926312	95.5866576	95.49685565	95.40943818	95.32409889	94.92266035	94.55434117	0.051224859
mol01a	AVQZ	30.98895768	31.24678302	31.20249964	31.15985267	31.11855214	31.07843102	31.03936063	31.00127358	30.82332294	30.66286905	0.257825344
mol02a	AVQZ	37.21828777	37.63707803	37.58805132	37.54108442	37.49595068	37.45245316	37.41045298	37.36986689	37.18510361	37.02582563	0.418790258
mol03a	AVQZ	137.7964411	138.2605503	138.1324068	138.0099612	137.8923541	137.7789979	137.6694771	137.563475	137.0787346	136.6567134	0.464109159
mol04a	AVQZ	130.1496729	130.6291043	130.5054178	130.3869585	130.2728415	130.1625057	130.0555458	129.9516691	129.4715444	129.0458302	0.479431369
mol16a	AVTZ	58.1145326	58.1880227	58.11881183	58.05262623	57.98876269	57.92680945	57.86645005	57.8075251	57.53014688	57.27553615	0.073290104
mol16b	AVQZ	49.5583119	49.57898366	49.51899092	49.46186223	49.40693116	49.35376769	49.30208778	49.25171695	49.01547706	48.7994985	0.020671759
mol19b	AVQZ	55.08991511	55.12944514	55.06625349	55.00594814	54.9478869	54.89170961	54.83717324	54.78409782	54.53677772	54.31376049	0.039530031
mol8	AVQZ	25.75383875	25.84682039	25.80688404	25.76857073	25.73147587	25.69541228	25.6602495	25.62586569	25.46361638	25.31442083	0.092981638

Table S2: Electron repulsion energies ($W_{\lambda=1}[\rho]$ of Eq. 3 + Hartree energy); from CCSD vs. those of MRF evaluated with Eq. 56 as a function of d parameter. Second column shows the basis set for CCSD. MRF has been evaluated at the HF/def2-SVP densities. Molecules are ordered in this Table as in Fig. 8 (for geometries see the zipped file).

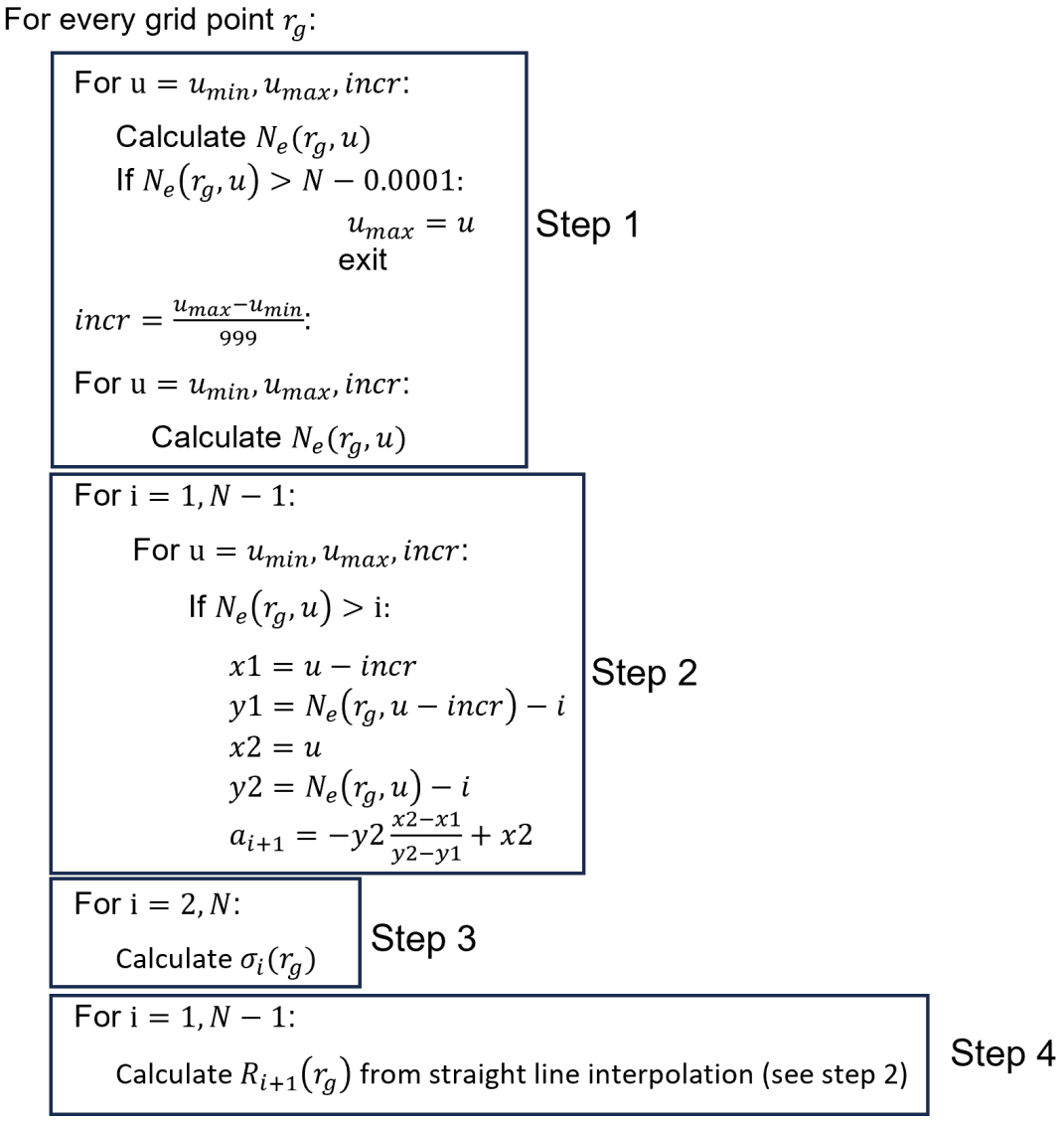

Figure S2: Pseudocode describing the implementation of MRF.