# Analytical gradients of Random Phase Approximation correlation energies in Range-Separated-Hybrid context : theory and implementation

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In view of the recent revival of interest in the Random Phase Approximation (RPA) in a range-separated hybrid (RSH) context as a method to calculate ground-state correlation energies of electronic systems, in particular systems where long-range electron-electron interaction play an important role, we propose a method to obtain the gradient of RSH-RPA energies.

Taking advantage of the Lagrangian formalism and using several versions of the Riccati equations associated to the RPA problem (which are in some cases equivalent to the rCCD expressions), we obtain a compact matrix formulation for the energy gradient. The resulting algebra is implemented in the Molpro program suite, exploiting analogies with the analytical gradient of the Møller–Plesset (MP2) energy.

Simple test cases and examples of geometry optimization of intermolecular complexes are shown.