PARALLEL RI-MP2 ENERGIES AND GRADIENTS: IMPLEMENTATION AND APPLICATIONS

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The so-called “resolution of the identity” integral approximation applied to second-order many-body perturbation theory (RI-MP2) is a method well-suited to the treatment of large chemical systems at a much lower computational cost than conventional MP2 calculations. In addition, features of the RI-MP2 method make it more efficient to implement on parallel computers than the conventional MP2 approach, an important advantage in pushing the limits of large-scale correlated calculations.

I will describe the RI-MP2 method itself and the implementation of both energies and gradients, emphasizing the important differences from the conventional MP2 as well as the parallelism. I will discuss fitting basis sets, introduced by the RI approximation, and present results from several RI-MP2 applications, including energy calculations on systems of more than 2400 AO basis functions, which run an estimated 30 times faster than the equivalent conventional MP2 calculation.