# Multiresolution Coupled-Cluster

Jakob S. Kottmann, September 14, 2018.

Multiresolution analysis is a wavelet based framework to represent arbitrary functions to a given numerical precision on adaptive grids. In quantum chemistry a multiresolution representation allows to compute properties with controlled numerical error and without the usage of pre-optimized basis-sets. The corresponding quantum chemical models are reformulated into integral equations which define the functions to solve on the adaptive mesh. This leads to a decreased computational scaling due to the absence of virtual orbitals but also to a large prefactor. In my talk I will introduce the key ideas of multiresolution analysis and illustrate how to reformulate the coupled-cluster model without virtual orbitals on real-space grids.

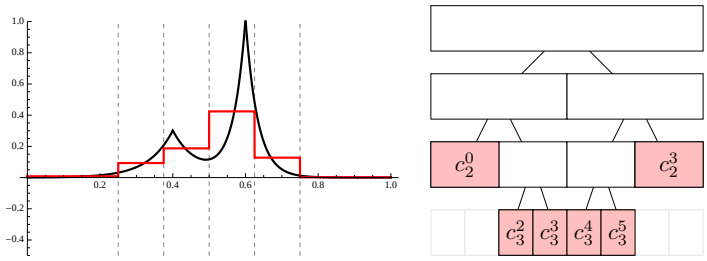


Figure 1: Left: Illustration of the multiresolution representation of a one dimensional function using only piecewise constant functions. Right: The tree-structure holding the coefficients.

## References

[1] J. S. Kottmann and F. A. Bischoff, J. Chem. Theory Comput. **13** (2017) (12), pp. 5945–5955, 10.1021/acs.jctc.7b00694

[2] J. S. Kottmann and F. A. Bischoff, J. Chem. Theory Comput. **13** (2017) (12), pp. 5956–5965, 10.1021/acs.jctc.7b00695

[3] R. J. Harrison, G. I. Fann, T. Yanai, Z. Gan and G. Beylkin, J. Chem. Phys. **121** (2004) (23), pp. 11587–11598, 10.1063/1.1791051