Computational Challenges of Coupled Cluster Theory

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Coupled-cluster theory (CC) defines a set of quantum many-body methods that have proven extremely useful in predicting the structure, properties and reactivity of molecules. A limiting factor in their application in chemistry is the steep computational cost of these methods as well as the complexity of the equations that must be implemented. Significant progress in the application of CC has been made through the use of massively parallel implementations (e.g. NWChem) and automatic code generation (e.g. Tensor Contraction Engine). I will discuss these developments in detail and highlight multiple directions for future work, in particular, reduced-scaling algorithms (which introduce additional software and numerical complexity) and better programming models that reduce or otherwise optimize communication.