# Diagrammatic Coupled Cluster Monte Carlo

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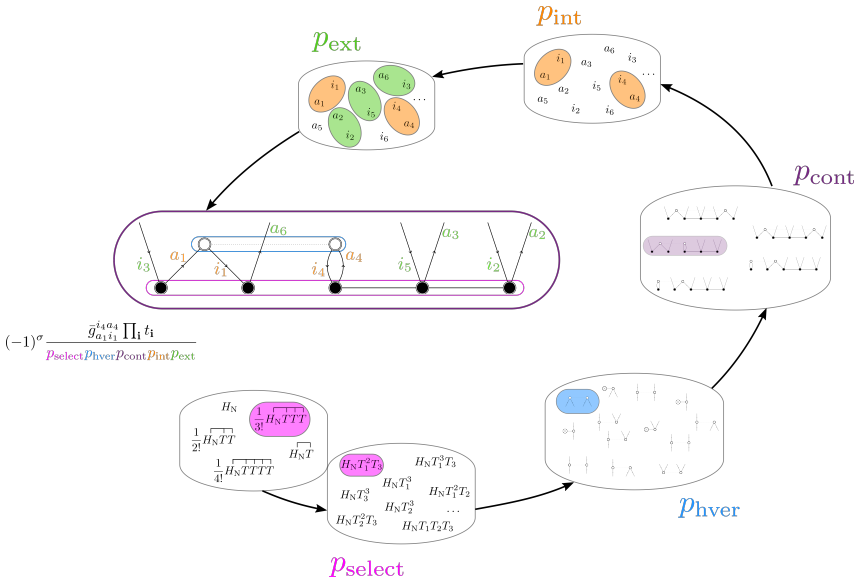
The coupled cluster model is arguably the most effective approximation for many-electron wavefunctions in weakly correlated systems. The model provides a systematically improvable hierarchy of approximations to the exact, full configuration interaction solution. Within a polynomial, rather than exponential, computational scaling, coupled cluster achieves size extensive and consistent results. This polynomial scaling remains however a challenge for its widespread application.
Monte Carlo sampling can circumvent the scaling wall, while remaining fully general with respect to truncation in the excitation hierarchy: an appealing feature when compared to other low-scaling, deterministic approaches.
We present the *diagrammatic coupled cluster Monte Carlo* (diagCCMC) algorithm that solves the linked equations of coupled cluster theory. We sample the connected expansion of the similarity-transformed Hamiltonian generating coupled cluster diagrams on the fly [1]. Results are thus rigorously size-extensive and consistent, even in the presence of stochastic noise. This affords a representation of noninteracting systems with a constant memory cost and reduced CPU cost. The algorithm can leverage locality without additional assumptions.




## References

1. C. J. C. Scott, R. Di Remigio, T. D. Crawford, A. J. W. Thom, *J. Phys. Chem. Lett.* **10** (2019), 925.