

# Exploring the Use of Rewriting Systems in Coupled-Cluster Theory

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I will discuss my recent experience with an interesting and challenging aspect of theoretical chemistry: the connection to mathematics and computer science. A well-known example of this connection is group theory's presence in molecular symmetry. Currently I am exploring a similar connections between the algorithmic generation of residual terms and rewriting systems from computer science.

During the investigation of a new bosonic coupled-cluster method for vibrational problems, it became necessary to generate the summation terms for calculating first derivatives. For simple linear equations (see below) deriving the terms by hand is a reasonable proposition, with only 20 or so terms for the two equations. Moving to the quadratic equations (figure2) the number of terms grows to 60 per equation, each with different prefactors and index combinations; while it is still possible to do this by hand, it is tedious, and the likelihood of mistakes increases significantly. Finally, the motivation for automatic generation of these terms becomes clear when considering the prospect of deriving cubic equations (figure3) or higher dimensions by hand.

I developed a program that generates the summation terms automatically, and renders them in two forms: Latex code to produce the printed, viewable summation; and Python code to calculate the same equations. Initially this effort was driven by the need to solve a practical problem in an efficient manner, but subsequently I became interested in the similarity of my work with existing work in rewriting systems. My current goal is to create a formal definition of the program for generating these terms based on work done in the rewriting field. Rather than relying on a one-off implementation as I have constructed, my hope is that the use of already established rewriting programs such as Maude or ELAN will be more robust and hopefully applicable by other researchers. It may be that such a formal connection would also have uses in other theoretical chemistry methods.

$$\begin{aligned} \hat{\Omega} = \hat{t}^j \hat{t}^j \\ LHS = i \left( \frac{dt^i}{dt} + \frac{dt^i}{dt} t_j + t^i \frac{dt^j}{dt} + t^j \varepsilon + t^i t_j \varepsilon \right) \\ RHS = (f h^i + h^i t^i + f \frac{1}{2!} h_{ij} t^i t^j - \frac{1}{2!} h_{ij} t^i t^j - h^i t^i + f h^i t^i + f h^i t^i) \\ + (h^i t^i + f \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{2!} h^i t^i t^j - \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + h^i t^i t^j + h^i t^i t^j) \\ + (\frac{1}{2!} h_0 + \frac{1}{3!} h^i t^i + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{3!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (f h_0 - \frac{1}{2!} h^i t^i + f \frac{1}{2!} h_{ij} t^i t^j - \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (f h^i - \frac{1}{2!} h^i t^i + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (h_0 + \frac{1}{2!} h^i t^i + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \end{aligned}$$
  

$$\begin{aligned} \hat{\Omega} = \hat{t}^j \hat{t}^j \hat{k} \\ LHS = i \left( \frac{dt^i k}{dt} + \frac{dt^i}{dt} t_j k + t^i \frac{dt^j k}{dt} + \frac{dt^i}{dt} t_k + t^j \frac{dt^i}{dt} + \frac{dt^i}{dt} t_j t_k + t^i \frac{dt^j}{dt} t_k + t^i t_j \frac{dt^k}{dt} + t^j k \varepsilon + t^i t_j k \varepsilon + t^j t_k \varepsilon + t^i t_j t_k \varepsilon \right) \\ RHS = (h_0 t_{ij} + f \frac{1}{2!} h_{ij} t_{ij} + h^i t_{ij}^i + f h^i t_{ij}^i + f h^i t_{ij}^i + f \frac{1}{2!} h^i t_{ij}^i + \frac{1}{2!} h_{ij} t_{ij}^i) \\ + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{2!} h_{ij} t^i t^j + h^i t_{ij}^i t^j + h^i t_{ij}^i t^j + h^i t_{ij}^i t^j + h^i t_{ij}^i t^j \\ + (\frac{1}{3!} h_0 + \frac{1}{4!} h^i t^i + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{4!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (\frac{1}{2!} h_0 + \frac{1}{3!} h^i t^i + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{3!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (f \frac{1}{2!} h^i + \frac{1}{3!} h^i t^i + \frac{1}{2!} h^i t^i t^j + \frac{1}{3!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (\frac{1}{2!} h_0 + \frac{1}{3!} h^i t^i + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{3!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (\frac{1}{2!} h_{ij} + \frac{1}{3!} h^i t^i + f \frac{1}{2!} h_{ij} t_{ij}^i + \frac{1}{2!} h_{ij} t_{ij}^i + \frac{1}{2!} h_{ij} t_{ij}^i + \frac{1}{2!} h_{ij} t_{ij}^i) \\ + (f h^i + \frac{1}{2!} h^i t^i + \frac{1}{2!} h^i t^i t^j + f \frac{1}{2!} h_{ij} t_{ij}^i + \frac{1}{2!} h^i t_{ij}^i + \frac{1}{2!} h^i t_{ij}^i) \\ + (\frac{1}{2!} h_0 + \frac{1}{3!} h^i t^i + \frac{1}{2!} h_{ij} t^i t^j + \frac{1}{3!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (f h^i + \frac{1}{2!} h^i t^i + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \\ + (\frac{1}{2!} h_{ij} + \frac{1}{3!} h^i t^i + \frac{1}{2!} h_{ij} t_{ij}^i + \frac{1}{3!} h^i t_{ij}^i + \frac{1}{2!} h^i t_{ij}^i + \frac{1}{2!} h^i t_{ij}^i) \\ + (h_0 + \frac{1}{2!} h^i t^i + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j + \frac{1}{2!} h^i t^i t^j) \end{aligned}$$