1138-68-392 **Russell F Thackston***, rthackston@georgiasouthern.edu, and **Ryan C Fortenberry**. *An efficient algorithm for the determination of force constants and displacements in numerical definitions of a large, general order Taylor series expansion.*

Taylor series expansions are commonly used in modeling complicated computational and quantum chemistry functions. However, brute force algorithms for generating the required force constant definitions and subsequent displacements are frequently used by researchers not formally trained in mathematics or computer science. These naive algorithms severely limit the number of variables that may be used in higher-order implementations. This research explores an algorithm based on a "lazy cartesian product" which intelligently generates the required force constant definitions and displacements with few extraneous computations. Large blocks of wasted computations – as found in brute force solutions – are bypassed with only non-zero rows of the cartesian product being calculated and produced, resulting in orders of magnitude gains in efficiency. This algorithm also provides researchers the ability to both parallelize and balance the workload across clusters of computational resources, opening the use of Taylor expansions to previously impossibly large molecules. A sample implementation using Python will be presented. (Received February 13, 2018)