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Computational Developments for Coupled Cluster Theory With Triples and Three-Body Forces[1] JUSTIN LIETZ, MORTEN HJORTH-JENSEN, NSCL/MSU, GUSTAV JANSEN, ORNL — Solving the many-body Schrödinger equation for infinite matter systems is a great tool for producing observables about dense neutron matter. Quantities like the nuclear equation of state and single particle addition and removal energies can be calculated from a simulated periodic box of nuclear matter. Unfortunately, solving this problem exactly with a given basis set scales exponentially with the basis size, making the problem computationally infeasible. The coupled cluster (CC) approximation has had great success here as it scales polynomially with basis size, allowing for more physical calculations to be done. Recently however, higher order CC methods are being used to increase the precision of the solution, and three-body nuclear forces are often needed to gain reliably accurate observables. This increases the polynomial order of the CC approximation to the point that even modest basis sets demand extreme amounts of computational power and memory. Getting converged results for CC with full triples excitations and three-body forces becomes a computational challenge of efficient storage of large sparse tensors across many computational nodes and contracting these tensors using data structures that allow for scalable many-core tensor contraction via GPUs.

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