Real-time Equation-of-Motion Coupled-Cluster Cumulant Green's Function Method: Heterogeneous Parallel Implementation Based on the Tensor Algebra for Many-body Methods Infrastructure

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We will present the details of the implementation of the real-time equation-of-motion coupled-cluster cumulant Green's function method [J. Chem. Phys. 152, 174113 (2020)] within the Tensor Algebra for Many-body Methods (TAMM) infrastructure. TAMM is a massively parallel heterogeneous tensor library designed for utilizing soon-to-be-available exascale computing resources. The two-body electron repulsion matrix elements are Cholesky-decomposed, and we imposed the spin-explicit forms of the various operators when evaluating the tensor contractions. Unlike our previous real algebra Tensor Contraction Engine implementation, this new implementation supports fully complex algebra.
We observe high scalability for large systems (700-1400 basis functions) up to 500 GPU nodes. Further, numerical results focusing on photoemission spectra of large chemical systems will be presented.