Macroscopic and molecular aspects of water properties at petaflops supercomputers. We employ the Fragment Molecular Orbital (FMO) method to calculate accurate quantum chemical properties on a large scale. This method is used to perform ab initio QM calculations on a variety of molecules, including large water clusters, to explore the interplay between microscopic and macroscopic properties. The FMO method is a density functional theory (DFT) approach that combines the fragmented molecular geometry optimization and electronic structure calculation in a single step, allowing for efficient treatment of large systems. We demonstrate the scalability of the FMO method by calculating the energies of water clusters using the FMO method on the 16,384-core nodes of the Emerald system at NERSC.

**Implementation of scripting for weakly coupled ensembles**

In GAMES, we implement two types of ensemble calculations (DC) to achieve better scalability and efficiency for the performance of large-scale runs. Two weakly coupled DCs, requiring little or no communication between batches of jobs, are implemented to analyze properties that are not efficiently calculated by the strong DC. We employ a two-level weak DC for the analysis of properties that require large system sizes. In this method, FMO calculations are performed at the weak DC level, and the weak DC results are used to initialize the strong DC calculations. This approach allows for efficient parallelization and scalability of the calculations.

**Conclusion**

We have developed a coupled ensemble calculation, consisting of a weakly coupled DC and a strongly coupled DC, to explore the properties of water at petaflops supercomputers. This approach allows for efficient simulation of large water clusters, enabling the exploration of the interplay between microscopic and macroscopic properties. The FMO method is a scalable and efficient approach for these calculations, demonstrating its potential for future high-performance computing environments.