Profiling of OpenMP Parallelization in Exact Diagonalization
SPENCER LEEPER, DAVID SMITH, CHRISTOPHER VARNEY, University of West Florida — Exact diagonalization is an essential tool for determining the ground and excited states of quantum systems. This is particularly important for models where other techniques break down, such as the quantum Monte Carlo sign problem on frustrated magnetic systems. As the size of the Hamiltonian matrix scales exponentially with the system size, utilizing symmetries inherent in either the model or geometry is essential for block-diagonalizing the matrix to minimize the memory requirements. Subsequent improvements can be obtained using OpenMP parallelization to efficiently utilize the computational resources. Here we analyze the impact of parallelization on different aspects of the Lanczos algorithm for a two-dimensional Heisenberg model.