Abstract Submitted for the OSS17 Meeting of The American Physical Society

GPU-Accelerated Lanczos Diagonalization¹ JUAN MANFREDI, Michigan State Univ — Nuclear structure calculations involve the diagonalization of a symmetric Hamiltonian matrix. The Lanczos algorithm is typically used to calculate a tridiagonal matrix (which is then easily diagonalizable) similar to the original Hamiltonian. Graphics processing units (GPUs) are particularly well suited for the sparse matrix-vector multiplications involved in Lanczos diagonalization. Although modern GPUs have limited onboard memory, future generations could be valuable for performing cutting-edge structure calculations. In this work, the Lanczos algorithm is implemented and evaluated on a GPU with a variety of sparse matrix-vector multiplication algorithms.

¹National Nuclear Security Administration Stewardship Science Graduate Fellowship

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Date submitted: 07 Apr 2017

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