**GronOR - GNOME at warp speed**

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**Abstract**

Non-orthogonal configuration interaction is an attractive method for applications that benefit from the conceptually intuitive description of individually optimized electronic states. Based on the GNOME software developed at the University of Groningen in the late seventies for the calculation of single non-orthogonal matrix elements, GronOR is a computational framework for the evaluation of the Hamiltonian matrix for assemblies of molecules described by non-orthogonal anti-symmetrized product wave functions from multi-configuration constituent molecular wave functions. This presentation chronicles the development of the highly efficient implementation of GronOR for massively parallel GPU-accelerated architectures, demonstrating near-perfect scalability on Summit, the worldâ€™s largest and fastest supercomputer. GronOR is a collaboration of the University of Groningen and the Oak Ridge National Laboratory.