**Nonorthogonal Configuration Interaction with GronOR**

Tjerk P. Straatsma, Ria Broer, and Remco W. A. Havenith

Oak Ridge National Laboratory
straatsmatp@ornl.gov

**Abstract**

GronOR is our massively parallel application for non-orthogonal configuration interaction and developed to execute efficiently on GPU-accelerated large-scale computer systems. The application is based on a task-based implementation approach, which is an effective load-balancing enabling us to demonstrate linear scaling to 1024 nodes on Summit. Through directive-based OpenACC annotation of the computationally most intensive parts of the code, high accelerated performance has been demonstrated.