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Effective use of high performance computing resources in computational chemistry and materials science

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Effective use of high performance computing resources in computational chemistry and materials science

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ABSTRACT
When we say “Eskom” the first thing that comes to mind is loadshedding. It was suspended for a while, but before we knew it the constant power cuts were back, and this results in the loss of access to various nodes on the Lengau cluster. In addition, several nodes on the cluster are down due to their age. These factors together with the misuse of the resources by inexperienced users has resulted in individuals having to queue for elongated periods of time.
In this work focus will be placed on research conducted within the Computational Chemistry and Molecular Modelling (CCMM) Group at the University of Johannesburg and how to determine if simulations run with different software packages are making appropriate use of the resources being requested.
An upgrade of the current Centre for High Performance Computing (CHPC) cluster is eminent, but with more resources comes more misuse and it is hoped that this work will help shed light to HPC users and ensure that everyone makes use of the resources being provided fairly and responsibly.

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