GBmolDD Performance Assessment Summary

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The GBmolDD audit identified two main areas for improvement, one is to introduce Hybrid MPI + OpenMP parallelization to improve the scalability and reduce communication which is currently MPI only. The other is to implement parallel I/O. Changes made based on these suggestions will allow for more science to be done using this application.

Duplicate force calculations are used to avoid expensive communication between MPI processes. This got worse on larger core counts, using a hybrid MPI + OpenMP parallelisation would reduce the amount of duplicate force calculations. The audit also identified that the I/O was spending a large amount of time in meta-data phase as each MPI process was writing to its own file, and the reading of molecule data was serialised. The recommendation was made to use a parallel file format such as parallel NetCDF or parallel HDF5.

GBmolDD is a Fortran and MPI molecular dynamics code for the simulation of coarse-grained molecular systems composed of isotropic and/or anisotropic particles. It uses the standard Lennard-Jones potential function to approximate the interaction between molecules using the Lorentz-Berthelot combining rule.

A full technical report can be found at ***https://pop-coe.eu/sites/default/files/pop_files/pop-ar-gbmoldd.pdf***

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