



Performance benchmarking results for a parallel implementation of the discrete element method

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The Discrete Element Method (DEM[1]) has proven to be a valuable numerical method for simulating processes involving brittle failure and large deformations such as earthquakes[5], fault zone evolution[4] and granular media flow[3]. Whereas the DEM is computationally expensive compared to other numerical methods (e.g., FDM, FEM), it avoids on the other hand the need for complex algorithms such as mesh refinement and adaptation.

ESyS-Particle[2] is an Open Source implementation of the DEM designed to simulate geoscientific problems on parallel supercomputers, clusters and multi-core PCs. The C++ simulation engine implements spatial domain decomposition via the Message Passing Interface (MPI). A Python wrapper API provides flexibility in the design of numerical models, specification of modelling parameters and contact logic, and analysis of simulation data.

A previous study demonstrated weak scalability of ESyS-Particle for a linear elastic wave propagation benchmark problem [6]. Weak scalability is a measure of how efficiently a parallel implementation handles *increasing* total problem size: as the total problem size increases, more CPUs are assigned to maintain a constant problem size per CPU and, ideally, a constant computation time. For many applications amenable to simulation using the DEM, weak scalability is the primary concern. Brittle failure and granular media flow in particular, both display scaling (or emergent) dynamics. Experience has shown that to more accurately simulate such phenomena, a broader range of spatial scales must be included in the numerical model, thus increasing the overall problem size.

Another measure of parallel computation efficiency, strong scalability, indicates how efficiently a parallel implementation solves a problem of a *constant* total size compared with a serial implementation running the same problem. In addition to weak scalability, strong scalability would be desirable for DEM applications. This would reduce the overall computation time whilst permitting solution of increasingly large problems. In practise, parallel numerical algorithms rarely display both weak and strong scalability though. Investigations into the strong scalability of ESyS-Particle are ongoing, the results of which will be presented at the meeting.

References

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