Code Performance and Scaling

Kent Milfield from the STAMPEDE support team made some test to assess the memory requirements per job. Test jobs with 20 nodes and 200 and 320 tasks ran without any problems. Kent reported that after the first six minutes the Lustre activity begins, and builds up to 1.4GB/s with 3,400 Requests/per second. The 2D classification jobs use 0.4-0.9 GB/task and the IO uses about 17GB in the cache. The OS uses about 3.5GB; so for the test jobs the usage was 31GB. Since then we have used -N 20 and -n 200 for our other jobs without problems and switched to the tacc_affinity numa control.

Relion 1.2 has been used also in GORDON (San Diego Super Computing Center), Some examples of the typical usage are as follows:

52904 particles 360x360 (26 GB) 12 cycles **Number of processors** 256 **WallTime** 1442.8 **Charge SU** 6156.0

52904 particles 360x360 (26 GB) 38 cycles **Number of processors** 512 **WallTime** 1516.0 **Charge SU** 12937.0

22551 particles 360x360 50 cycles **Number of processors** 512 **WallTime** 920.7 **Charge SU** 7857.0