Performance and Scalability of Parallel Computing in Biosimulation/modeling Platforms for Pharmacometric Solutions

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Purpose: The continued growth of PK/PD modeling in pharmaceutical industry is creating a challenge for all PK/PD software industry. The performance and scalability of software and hardware is always a constraint [1,2]. To improve performance of computationally intensive algorithms by parallel computing and to take full advantage of available computing resources, a few platforms (Figure 1) were explored for remote execution of Phoenix® NLME™ 7.0 jobs.

Methods: Parallel computing platforms investigated include Linux Grid servers (TORQUE and SGE), Window’s MPI Cluster, and Amazon Elastic Compute Cloud. Phoenix® NLME™ engine is farmed to these parallel computing platforms to evaluate scientific validation, performance and scalability. Multiple job submission to these computing nodes validated the scalability issues. Examples include some long-running jobs such as bootstrap analysis and covariate search. The parallel computing platforms include: 1) Windows single core, 2) Windows 4 core MPI, 3) 24 core Windows MPI cluster, 4) 32 core Linux Grid, 5) 48 node Amazon cloud.

Results: The execution time recorded for scenarios running on the above platform include: bootstrap analysis using 100, 250, 1000 and 5000 replicates and covariate search including 8, 64, 256 scenarios. The ratio of the execution time between multiple cores and single run was calculated for the analysis on the trend of increasing nodes with different platform setups.

Conclusion: Performance improves proportional to the number of compute nodes employed, with execution times reduced from a few hours to a few minutes. Multiple runs show that: 1) The Linux grid (Torque or SGE) gets best performance. 2) Windows MPI cluster suffers from latency and bandwidth problems. 3) Smaller runs such as 8 covariate search or 100 replicate bootstrap jobs do not gain from increasing the number of nodes. 4) Amazon Cloud has best scalability capability for multiple jobs in contrary to other platform setups.

References:
1. Sanduja, Cloud computing NONMEM., CPT-PSP, 2015,4 537-546

Figure 1: Parallel computing framework