Evalulation of parallel efficiency for NONMEM, using multi-core processors and Intel Xeon Phi Co-processors

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Objectives: The long computation time spent at model estimation has been a burden to pharmacometricians. So, there is a need to develop methods to reduce the computation time by optimizing the performance of software and/or hardware system. The aim of this study was to identify the parallel-run efficiency of NONMEM (Ver. 7.3) when using the multi-core x86_64 architecture CPU and Intel MIC architecture (Xeonphi) co-processor.

Methods: Two PK models and five different-sized datasets with 500 ~ 3000 subjects were made up for this study. All estimation steps were run on a Linux operating system. The Message Passing Interface (MPI) method was used for all of the tests used in this study. First, three types of X86_64 architecture processors (4, 8 and 24-core CPU) were used as host environments to explore the influence of adding -maxlim option on the running speed of parallel-optioned NONMEM (-parafile). Second, The performance of Xeon-phi (60-core co-processor) with or without SIMD vectorization installed at the 8-core CPU system was also tested in comparison with the performance of the 8-core system before installing Xeon-phi. The SIMD vectorization to accelerate the co-processor performance was done by modifying the Fortran source codes and compile options of NONMEM. The speedup ratio and parallel efficiency were employed as parameters of the computation speed.

Results: The maxlim option accelerated the computing speed of the three host environment systems by about 1.9 times when the subject number of the dataset were more than 1000. The co-processor with SIMD vectorization accelerated the computing speed of the 8-core CPU system by about 30~40%.

Conclusions: We found that the -maxlim option was helpful to speed up NONMEM running of large data (> 1000 subjects) under multi-core desktop computer environments. Additionally, next generation co-processors that support the advanced vector extensions (AVX) is expected to further improve the speed