Application Of Parallelized Grid Search Method For Parameter Estimation Using PK-PD Models

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Pharmacokinetic (PK) and Pharmacodynamic (PD) modeling and simulation are well recognized tools in drug development.

Effective PK-PD modeling is expected to provide opportunities to accelerate the drug development process.

This research includes Parallelized Grid search method, Nelder-Mead method, Gauss-Newton method, Algebraic and Differential equation PK-PD Models.

Our PK-PD application is demonstrated to provide optimal solution in the case of multiple PK/PD models of varying complexity. We have employed known PK-PD models that fall into different classes such as a) single and multi-compartmental models b) algebraic and seven differential equations models c) Pharmacokinetic and Pharmacodynamics models and d) models with five to seven parameters. Here is an example of one such model:

The figure represents a multi-compartment model used in our case-study.

Here, A, B, C, Alpha, Beta, Gamma are the parameters.

The goal is to find such parameters for this model which best fits the data available.

Parallel implementation facilitates faster solutions to time-consuming Drug Discovery process in the Pharma domain.

HPC can provide much faster and scalable solutions for all combination of grid points and parameters.

The multiple models optimized and parallelized cover a wide range of modeling scenarios and in all the cases, significant improvement is observed on GPUs.