Poster presentation

CaliBayes: Integration of GRID based simulation and data resources for Bayesian calibration of biological models

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Complex, quantitative biological models are gaining increasing significance for research hypothesis formulation in biological and medical science. These models are typically described using a set of reactions and parameters such as kinetic rate constants. Measuring these parameters directly from experiments is laborious, or even under certain physiological conditions, impossible. Therefore current research focuses on computational and statistical methods to infer parameter values from experimental high throughput data.

The process of determining parameter values based on a comparison of experimental data with output from a model is known as calibration. Bayesian methods provide a framework for dealing with all sources of uncertainty in the calibration process. These methods use considerably fewer evaluations of the model than some global optimisation techniques (such as simulated annealing and genetic algorithms), and are therefore ideal for large, complex models that are time-consuming to run.

The primary aim of the CaliBayes www.calibayes.ncl.ac.uk project is to capitalise on the development of GRID-based modelling and simulation resources such as BASIS www.basis.ncl.ac.uk by building a computational GRID facility designed for inferring parameters of simulation models. The goal is to find a combination of parameters that give the best match to available experimental data, together with some idea of the uncertainty in these parameter values. The calibration algorithm carefully selects parameter combinations at which the simulator will be run.

The inference engine is implemented in the statistical computing language R with optimised routines written in C and C++, and communicates with the BASIS simulator using SSOAP. The inference engine manipulates models specified in the Systems Biology Markup Language (SBML), submits the SBML model description to BASIS and retrieves the simulation results using standard web-service (WS) protocols.

The Bayesian calibration method is demonstrated by analysing a gene regulatory model of the cell cycle in frog eggs.