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## Bayesian Calibration Tool

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### ABSTRACT

Fitting a model to data is common practice in many fields of science. The models may contain unknown parameters and often, the goal is to obtain good estimates of them. A variety of methods have been developed for this purpose. They often differ in complexity, efficiency and accuracy and some may have very limited applications. Bayesian inference methods have recently become popular for the purpose of calibrating model's parameters. The way they treat unknown quantities is completely different from any classical methods. Even though the unknown quantity is a constant, it is treated as a random variable and the desired outcome is its probability distribution. Good estimates and confidence intervals can then be easily produced from probability distributions. Another important feature of Bayesian inference is the ability to include prior knowledge in the calculations. However, Bayesian inference has to be done computationally as it involves solving multidimensional integrals. The Bayesian Calibration tool is an easy-to-use, well documented tool to efficiently carry out the calculations of the calibration process. The tool is open-source and uses fast Markov Chain Monte Carlo (MCMC) algorithms. The tool is run on nanoHUB, making it easily accessible without installing any software, etc. Given data and a model, the tool performs MCMC simulation of the model and returns the Bayesian posterior probability distributions of the model's unknown parameters.

### KEYWORDS

Bayesian calibration, uncertainty quantification, online simulation, nanoHUB, MCMC, curve fitting