Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.
http://www.simfit.org.uk

Simulation is used to predict the outcome of experiments where a deterministic mathematical model has been formulated, so that the effect of varying parameters and independent variables can be investigated. Once a profile for exact data has been generated it can be perturbed to resemble various types of uncertainty, for instance that resulting from stochastic processes or experimental error.

SIMFIT provides the following procedures.

- Program **random**

  This allows the creation of random matrices or vectors from specified distributions and also provides facilities for scrambling a vector, generating random Latin squares for use in experimental design, and testing the Uniform(0,1) generator. As computers cannot calculate genuine random numbers, they first accumulate pseudo-random numbers from a Uniform(0,1) distribution using techniques that have a large cycle and minimal autocorrelation. Alternative distributions can then be simulated from such Uniform(0,1) numbers, and the ability to test the generator is provided so users can appreciate sample sizes required (often hundreds) before the histograms generated resemble the simulated distributions.

- Program **makdat**

  This program allows the creation of exact data sets in just two cases.

  1. The model is available from one of the SIMFIT library of models
  2. The model is supplied from a user-defined script

  Users simply supply the model parameters and the range, size, and number of data points to be simulated. The simulated data sets are then written to coordinate files.

- Program **deqsol**

  This is used if the deterministic model is set of nonlinear differential equations.

- Program **adderr**

  This accepts an exact data set then adds random noise to simulate uncertainty or experimental error as summarized below.

  Model $\longrightarrow$ **makdat** $\longrightarrow$ [Exact data] $\longrightarrow$ **adderr** $\longrightarrow$ [Simulated data]

- Program **makcsa**

  This creates random histograms, for example, to simulate flow cytometry investigation of cell surface antigens.

Simulation should be used where a model has been fitted to some data and best-fit parameters have been estimated, because then the model can be simulated in order to get some idea of how to interpret the goodness of fit statistics, and also what reliance to place on the point estimates for the parameter values. This is because the procedures used to fit nonlinear models are iterative, and the objective function solution point will depend on the starting estimates and may not be unique. Further, the statistical techniques used to calculate parameter standard error estimates and make decisions about goodness of fit are only approximations, and usually only close to the assumed distributions with very large numbers of observations.