Plenary Speech

Physical Sciences

Estimation of parameters in mathematical and statistical models and validation and verification of scientific simulations

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Mathematical and statistical models that describe real world phenomena consist of many parameters from which, some of the parameters cannot easily be identified. If there is a doubt in how those parameters can be estimated then there is an uncertainty of the validity of such models. Sometimes the loss that from an investment which uses such models would be very high if the parameters were not identified with sufficient accuracy. Therefore the estimation of parameters accurately is very important in mathematical and statistical modeling. It is well known that deciding the choice of values from the parameter space is a difficult task. There are many techniques for choosing values for those parameters. Within the first part of this talk, the usefulness of one of the freely available piece of software called PEST for estimating such parameters will be discussed. PEST software need to be provided with the details of the parameters, executable computer program that simulates the solution of the mathematical model that describe real world problem considered, and the relevant data. PEST program does not change the model or the data but it uses the model and data for estimating suitable parameters for the given model.

When the computer programs that simulate mathematical models are considered, it is again very important to validate and verify the numerical techniques and the associated computer codes used for simulations. Second part of this talk concentrates on the validation and the verification of numerical simulations using the Method of Manufactured Solutions (MMS) which has been discussed in scientific literature. MMS considers the use of exact solutions to construct mathematical models that are similar to the mathematical models that has no exact solutions in order to test the numerical method and its implementation within the computer codes in order to verify and validate the numerical simulations.

In conclusion, it is noted the importance of the identification of accurate parameters for the mathematical/statistical models and the verification and validation of computer simulations of those models in order to have realistic solutions or simulations for real world problems.

Keywords: Parameter estimation, Mathematical and statistical models, Numerical simulations, Method of manufactured solutions