Uncertainty Quantification for Simulation-Based Predictions

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Assessing the performance, safety, and reliability of the nuclear weapon stockpile is complicated by the Comprehensive Test Ban Treaty that forbids underground nuclear testing. Hence, assessing the current nuclear stockpile relies on the use of detailed, physics-based computer codes. These simulation models can be refined by utilizing information from historical nuclear tests, as well as from ongoing experimental campaigns, to predict weapon behavior. For more information see Refs. [1,2].

Currently substantial statistical research is focused on the development of methodology for utilizing detailed simulation codes to carry out inference for physical systems. Issues such as calibration of simulator input parameters, generation of predictions, and characterization of prediction uncertainty are of particular interest. Simulation of well-understood physical processes is typically based on fundamental physical principles. In such problems, the actual amount of observed field data from this process can often be very limited. It is the simulator code that contains the structure of the actual process being modeled. Because of this, useful inference is possible even with only minimal amounts of observed data on the actual physical system. Figure 1 describes a simple application where a mathematical model enhances our ability to predict how long it will take an object to reach the ground when dropped from a tower.

The statistical methodology we have developed in support of nuclear weapon certification requires a limited amount of field data, which may be from experiments or observations on the physical system, along with an ensemble of computer-model simulations. Gaussian processes are used to model the simulator output at untried input settings. This model for the simulator is then embedded in a larger statistical framework so that parameter estimation (i.e., calibration) and prediction can be carried out.

Although originally developed for weapons-related applications, the statistical methodologies we have developed have potential use in any investigation where a computer model is available to model a given system. To date we have applied these methodologies to a wide range of application areas: engineering, particle physics, manufacturing, climate and cosmology (see Fig. 2).

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[1] D. Higdon, et al., *SIAM J. Sci. Comput.* **26**, 448–466 (2004).
[2] B. Williams, et al., *Bayesian Anal.* **1**, 765–792 (2006).
[3] K. Heitmann, et al., *Astrophys. J. Lett.* **646**, L1, (2006).

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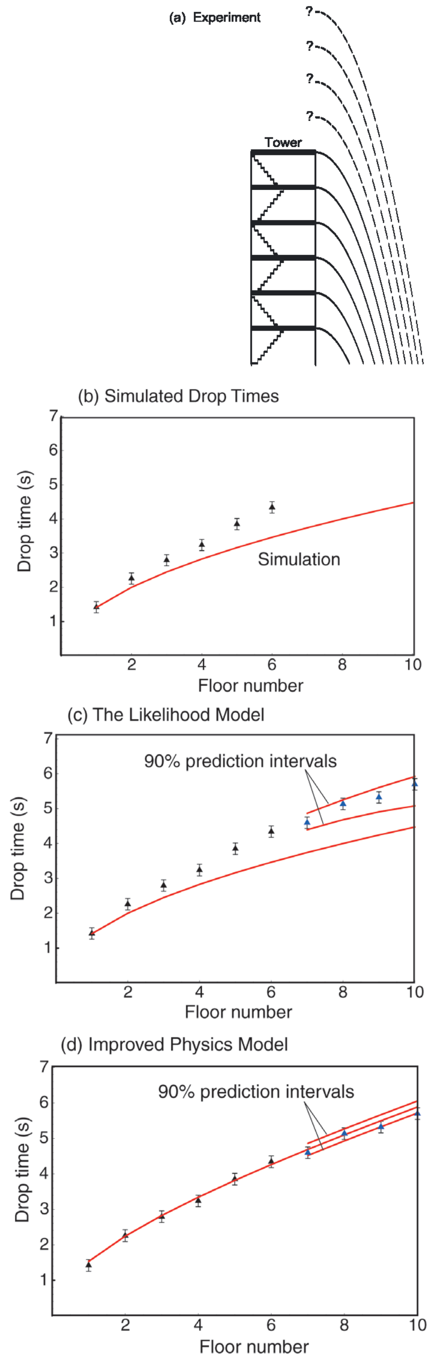

Fig. 1.
Dropping an Object from a Tower
(a) The time it takes an object to drop from each of six floors of a tower is recorded. There is an uncertainty in the measured drop times of about ±0.2 s. Predictions for times are desired for drops from floors 7–10, but they do not yet exist.

(b) A mathematical model is developed to predict the drop times as a function of drop height. The simulated drop times (red line) are systematically too low when compared with the experimental data (triangles). The error bars around the observed drop times show the observation uncertainty.

(c) This systematic deviation between the mathematical model and the experimental data is accounted for in the likelihood model. A fitted correction term adjusts the model-based predictions to better match the data. The resulting 90% prediction intervals for floors 7–10 are shown in this figure. Note that the prediction intervals become wider as the drop level moves away from the floors with experimental data. The cyan triangles corresponding to floors 7–10 show experimental observations taken later only for validation of the predictions.

(d) An improved simulation model was constructed that accounts for air resistance. A parameter controlling the strength of the resistance must be estimated from the data, resulting in some prediction uncertainty (90% prediction intervals are shown for floors 7–10). The improved model captures more of the physics, giving reduced prediction uncertainty.

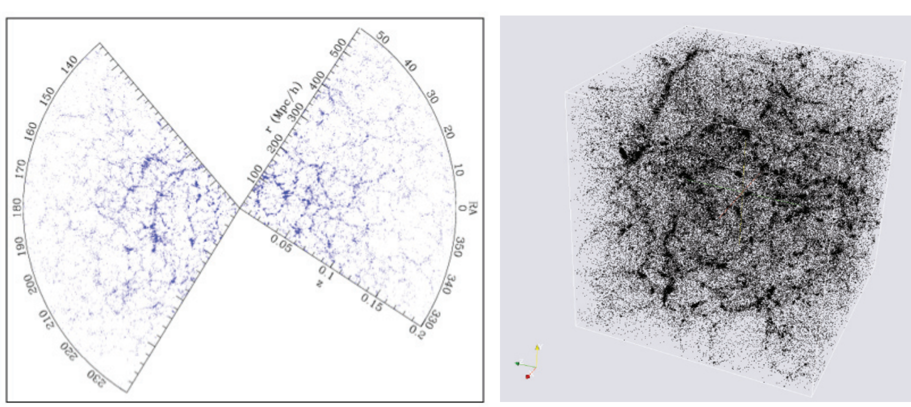

Fig. 2.
Methodology originally developed for nuclear weapon certification has been applied to investigations in cosmology. Here observations from the Sloan Digital Sky Survey (left) and large-scale gravity simulations (right) are used to constrain cosmological parameters that describe the evolution of the universe. See Ref. [3] for details.

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