Reliability Engineering and System Safety 138 (2015) 210–218

Contents lists available at ScienceDirect

Reliability Engineering and System Safety

journal homepage: www.elsevier.com/locate/ress

Scientific computer simulation review

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ARTICLE INFO

Article history:
Received 17 July 2014
Received in revised form
4 December 2014
Accepted 14 January 2015
Available online 28 January 2015

Keywords:
Scientific computer simulation review
Maturity assessment
Measurement of simulation trustworthiness
Requirements for simulation trustworthiness
Code review
Maturity framework

ABSTRACT

Before the results of a scientific computer simulation are used for any purpose, it should be determined if those results can be trusted. Answering that question of trust is the domain of scientific computer simulation review. There is limited literature that focuses on simulation review, and most is specific to the review of a particular type of simulation. This work is intended to provide a foundation for a common understanding of simulation review. This is accomplished through three contributions. First, scientific computer simulation review is formally defined. This definition identifies the scope of simulation review and provides the boundaries of the review process. Second, maturity assessment theory is developed. This development clarifies the concepts of maturity criteria, maturity assessment sets, and maturity assessment frameworks, which are essential for performing simulation review. Finally, simulation review is described as the application of a maturity assessment framework. This is illustrated through evaluating a simulation review performed by the U.S. Nuclear Regulatory Commission. In making these contributions, this work provides a means for a more objective assessment of a simulation's trustworthiness and takes the next step in establishing scientific computer simulation review as its own field.

1. Introduction

The objective of every scientific computer simulation is the same: to accurately predict some behavior of the physical universe. However, this alone does not make a simulation useful. A simulation does not become useful until its results are influential in some way. Typically, that influence is either in (a) a decision-making process (i.e., influencing a decision being made) or (b) knowledge of the physical universe (i.e., influencing a scientist's understanding). However, before the results of a simulation should influence a decision or increase knowledge, an assessor must determine if the results can be trusted for the simulation's intended purpose. That purpose could be something as trivial as answering a homework question to something as crucial as assuring the safe operation of a nuclear power plant. Determining if the results of a simulation should be trusted for its intended purpose is the focus of scientific computer simulation review.

This paper is based on the work by Kaizer [1] and has three objectives: First, to define and develop the concept of scientific computer simulation review; second, to develop a theoretical foundation for concepts known as maturity assessment frameworks; and third, to demonstrate how scientific computer simulation review is the application of such a framework. Section 1 of this paper will provide the definitions needed to understand scientific computer simulation review, how it differs from other terms commonly used in the Modeling and Simulation (M&S) community, and its history. Section 2 of this paper will develop the concept of a maturity assessment framework and provide a list of characteristics that are needed for its adaptation and improvement. Section 3 of this paper will explain how all scientific computer simulation review can be understood as the application of a maturity assessment framework. At the conclusion of Section 3, a scientific computer simulation review performed at the U. S. Nuclear Regulatory Commission (NRC) will be analyzed and explained in terms of such a framework. By meeting these objectives, it is hoped that practitioners of simulation review will better understand scientific computer simulation review, will better understand the role of maturity assessment frameworks in scientific computer simulation review, and will be able to perform better reviews in the future.

1.1. What is a scientific computer simulation

Like many communities, the terms of the M&S community take on different shades of meaning depending upon who is speaking to whom. Different authors can have distinctly different definitions for even the most basic terms like *computer model* or *simulation*. To avoid potential confusion, this paper has chosen to define all such terms. An attempt was made to choose definitions

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http://dx.doi.org/10.1016/j.ress.2015.01.020

that would have broad agreement among the M&S community, but at the very least the definitions will be apt for communicating the ideas of this paper. To lay the foundations for these definitions, it is appropriate that the first word defined should be *model* and the next *simulation*.

There is a rather large variability in the definition of word *model*. Some M&S texts, such as Maki and Thompson [2], do not define the word *model*, but instead give examples of different kinds of models (physical, theoretical, logical, and mathematical). Other texts first define a *system* and then state that a model is a representation of a system [3–5]. These texts have definitions similar to the definition put forward by the AIAA [6] where a model is defined as "a representation of a physical system or process intended to enhance our ability to understand, predict, or control its behavior". While the AIAA's definition is practical, it can be argued that requiring all models to be representations of only physical systems or process and also requiring models to have a specific purpose (i.e., enhancing our ability to understand, predict, or control its behavior) is unnecessarily restrictive. In their definition, the U.S Department of Defense (DoD) [7] removed these restrictions as they defined a model as "a physical, mathematical, or otherwise logical representation of a system, entity, phenomenon, or process". Similar to AIAA's definition, the DoD's definition is also practical, but by restricting the representations to only those models that are physical, mathematical, or logical, this definition neglects the theoretical models defined by Maki and Thompson [2].

While each of the above definitions has been used successfully in practice, they are not in agreement with each other. It could be argued that the difference is only semantics, but given the complex nature of this topic, a semantically clear definition is desired. Therefore, a definition for *model* was crafted such that any representation that would be considered a model by the literature [2–7] would also be considered a model by this definition. The proposed definition is a slight modification to that proposed by the DoD. A *Model* is a representation of a system, entity, phenomenon, or process.

There is also variability in the definition of the word *simulation*. Neelamkavil [3] defines a simulation as "the process of imitating important aspects of the behavior of the system". It is important to note that this definition is focusing on the purpose of a simulation. Juxtaposed to this definition are those of the DoD [7] "A method for implementing a model over time" and the AIAA [6] "The exercise or use of a model". These definitions are not focused on the purpose of the simulation, but the composition of the simulation itself. The proposed definition combines those of Neelamkavil [3], the AIAA [6], and the definition for "model" given above. A *Simulation* is the imitation of a behavior of a system, entity, phenomenon or process through the exercise or use of a model.

The important distinction between "model" and "simulation" is the difference between representation and imitation. A model *is* the representation. It continually exists as a representation, whether written down on paper, coded into a computer language, or as a figment of someone's imagination. A model can be changed, but does not change by its own accord. On the other hand, the simulation is the imitation of a behavior. The simulation is the exercise of the model with certain inputs. The simulation can be the calculation on the back of an envelope, the result of a computer run, or what someone believes will happen. These concepts are simple, but they form the necessary foundation for more complex concepts, such as that of a scientific computer simulation.

With the terms *model* and *simulation* defined, modifiers such as *scientific* and *computer* can now be discussed. The modifier *scientific* implies that the representation or imitation has to do with something in the physical universe and how that something behaves. Thus, a *Scientific Model* is a representation of a system, entity, phenomenon, or process in the physical universe (e.g., using a string tied at one end to represent a sound wave). Likewise, a *Scientific Simulation* is the imitation of a behavior of a system, entity, phenomenon or process in the physical universe through the exercise or use of a scientific model (e.g., moving the string to imitate a sound wave hitting a wall).

The modifier *computer* is more complicated. In general, computer models are a subset of mathematical models. Using concepts presented in Maki and Thompson [2], a *Mathematical Model* is a representation of a system, entity, phenomenon, or process using mathematical concepts, symbols, and relations. Likewise, a *Mathematical Simulation* is the imitation of a behavior of a system, entity, phenomenon or process using mathematical concepts, symbols, and relations through the exercise or use of a mathematical model.

Ideally, a mathematical model could be used directly, but this is rarely the case. Generally, the mathematical model must be made simpler in order for it to be used, because whatever is performing the computation (i.e., the computer) is limited in what mathematical processes it can perform. This re-making of the mathematical model is the basis for defining a computer model. A *Computer Model* is a representation of a system, entity, phenomenon, or process using limited mathematical concepts, symbols, and relations. It is important to note that this limitation is solely based on the computational device chosen. Likewise, a *Computer Simulation* is the imitation of a behavior of a system, entity, phenomenon or process using limited mathematical concepts, symbols, and relations through the exercise or use of a computer model.

Using these definitions, a *Scientific Computer Model* is a representation of a system, entity, phenomenon, or process in the physical universe using limited mathematical concepts, symbols, and relations. Likewise, a *Scientific Computer Simulation* is the imitation of a behavior of a system, entity, phenomenon or process in the physical universe using limited mathematical concepts, symbols, and relations through the exercise or use of a scientific computer model.

1.2. What is scientific computer simulation review

Scientific Computer Simulation Review is the process of analyzing the supporting evidence and determining (1) how trustworthy the results of a scientific computer simulation are, (2) how trustworthy the results need to be for an intended purpose, and based on this information, (3) if the specific simulation should be trusted for the intended purpose. In most cases, an assessor will perform an informal simulation review. That is, the assessor will not follow any documented procedures or guidelines; instead the assessor will review those areas of the simulation that he or she believes are the most important. For example, a student performing a simulation for homework will not submit the results to a professor until that student is satisfied that the results are adequate, at least enough to receive a personally satisfactory grade. In these cases of informal review, it is common to find that the analyst who performed the simulation and the assessor who determined the simulation is trustworthy and adequate are the same person.

While satisfactory for many situations, informal reviews are based on personal-value criteria of the assessor, and those criteria are entirely dependent on the assessor's knowledge level and experience. In certain situations, determining if the specific simulation should be trusted for the intended purpose is deemed too important a decision for one assessor to make alone, and a formal review process is needed. While making a review more formal certainly makes the review process more objective, it also makes the process more expensive and organizations must determine if the need justifies the expense.