**Mechanistic Models, Model Mechanisms, and Computational Models of Explanation for Biological Phenomena**

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In the highly interdisciplinary and diverse world of life sciences, uncertainties in semantics may prevent the appreciation of biological explanation, handicap the use of computational models, and hamper communications among scientists, engineers, and the public. The broad scientific community commonly, but sometimes loosely, relies on the term “mechanistic” to refer to the product of a process, often a model, of establishing a plausible causal explanation of a biological phenomenon. For researchers engaged in biological modeling, simulation, and computational biology, such loose definitions can compromise the clarity and credibility of a study. To help avoid such compromise moving forward, we first identify three distinguishable, widely employed models of explanation (of a phenomenon), which do not involve computation, by applying these descriptors: a *mechanistic explanation*, *description of a model of a mechanism*, and *description of a model mechanism*. Expanding, elaborating, and improving upon one of those explanations using mathematical and computational methods can produce any of a huge variety of computational models of explanation. We cluster them under four characterizations that are sufficiently different to merit semantic distinction. We suggest *mechanistic simulation*, *simulation of a model of a mechanism*, *simulation of a model mechanism*, and *computational model mechanism* as a working foundation for an ontology for simulation research in biology. We elaborate on differences, and provide examples. Understanding a biological phenomenon starts with measurements and continues with its *explanatory description*. In simulation research, that process most often leads into mathematical descriptions, transformation of those descriptions into equations and computer programs, culminating in *experimental* explorations of both model and simulation output. Different forms of biological problem solving and of explanation require different implementation and virtual experiment types. We evaluate how these different approaches fit into the broader spectrum of the biological sciences, and how these approaches impede or enhance clarity and model credibility.