

Heterogeneous Model Composability: Another Step Toward Scientifically Useful Multiscale Models

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We need increasingly credible formulations of dynamic system components and their interactions during simulations. To create such simulations we need to account for model heterogeneity and simulation scalability. A model-theoretic approach can serve a key role in describing interactions among models that have disparate knowledge representations and manipulation schemes. Specifically, our goal is to have interactions between submodels described in any two different modeling methods (or using different models of computation, MoC) to be specified according to a modeling theory and its execution protocol. Each submodel is capable of functioning standalone or originally designed to do so.

We will present a poly-formalism model composability methodology defined in terms of a Knowledge Interchange Broker (KIB) approach. It is intended to facilitate building and modularizing high-fidelity simulations. First, we describe and contrast this methodology to the mono-, super-, and meta-modeling methodologies independent of any particular domain of interest. We follow by describing a well-developed iteratively evaluated KIB application that addresses modeling interactions between human decision-making and landscape dynamics (yes, far removed from biology, but still interesting) for particular archeological uses. We exemplify heterogeneous model composition with three model types having particular uses: i) humans represented as discrete-event agent-based models, ii) landscape processes represented as time-stepped continuous models, and iii) human/landscape interactions represented by a KIB model.

Next, we describe a multiscale systems biology model (MSBM) being explored for simulating plausible causal cascades within a particular referent system. The MSBM includes a PDE determined chemotactic gradient, which is linked to a model of cell agents migrating in a 2D space. Stochastic cell behavior (migration) is driven by receptor-ligand binding and downstream processes, which are modeled as ODEs that are linked within and to those cell agents. Thus the model is descriptive of chemotactic cell behavior that can appear in a number of biological contexts.

Neither MSBM specifics nor the wet-lab referent are critical for this discussion. In fact, we argue that the linkage issues should be addressed early, ideally, prior to finalizing design of the initial hybrid MSBM and finalizing the validation/falsification protocol.

We identify and discuss issues and requirements governing KIB applicability for this class of MSBMs, and highlight basic technical similarities and differences between composing archeological submodels and composing MSBM submodels.

We conclude by summarizing benefits and limitations of KIB interaction models. Models to be composed remain independent (and capable of functioning standalone). Relationships that define composition, and thus the hybrid system's phenotype, are governed by independent KIBs. Executions of the composed and KIB models can be independent yet submodel executions can be concurrent. The KIB poly-formalism methodology simplifies model verification (grounding and correctness), face validation, and simulation validation (evaluating simulation experiments) modeling and simulation lifecycle activities.