Biosystem modeling methods at multiple scales

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Experience in biological modeling at the cellular and developmental scales has led to a systematic approach to creating and exploiting these heterogeneous and complex models. A model specification phase uses quasi-equilibrium and/or steady-state statistical mechanics of molecular complexes such as those applicable to gene regulation and metabolism at the molecular scale, and an algebra of time-evolution operators at coarser scales to marry stochastic rewrite rules (acting on parameter-carrying objects) with continuous-time differential equations and thereby to computably express multiscale dynamics. Current frontiers in model specification include formalizing such modeling languages for the dynamical geometries and topologies of biological objects, and integrating developmental with evolutionary models. Stochastic and hybrid simulation algorithms with varying speed and accuracy tradeoffs may be derived from the resulting time-evolution operators. In addition to simulation, some kind of analysis is needed. A computer algebra environment aids model analysis in some cases; other analyses require approximate model reduction. A recent approach to nonlinear model reduction approximates the time-evolution of probability distributions over states using a generalization of graphical models with dynamically varying parameters.