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Research Article

KinModRe: A Repository of Whole Cell Kinetic Models

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Abstract

Whole-cell kinetic models represent cellular processes as mechanistic reaction networks governed by kinetic rate laws, enabling simulation of metabolic dynamics and system-level cellular behaviour. Despite their scientific value, executable implementations of such models remain relatively scarce and many published models are distributed only as static descriptions within manuscripts. To address this limitation, we present KinModRe (https://github.com/mauriceling/kinmodre), a repository of executable whole-cell kinetic models derived from modelling work using the AdvanceSyn Toolkit. The repository currently contains more than 130 models, including 31 *de novo* / *ab initio* kinetic reconstructions with the rest converted from genome-scale metabolic networks. Model sizes range from small pathway-level systems to large knowledge-base reconstructions containing tens of thousands of metabolites. Each model includes reaction definitions, kinetic rate laws, parameter sets and runnable simulation scripts. By publishing executable kinetic models as reusable computational artefacts, KinModRe provides a resource for research, methodological development and education in mechanistic systems modelling.

Keywords: Whole-Cell Kinetic Models; Systems Biology Modelling; Genome-Scale Metabolic Networks; Model Repositories; Enzyme Kinetics; Computational Systems Biology; Synthetic and Systems Biology

Introduction

Whole-cell kinetic models describe cellular processes as networks of biochemical reactions governed by kinetic rate laws. By explicitly representing molecular interactions, enzyme activities and metabolite dynamics, such models enable mechanistic exploration of metabolic regulation, pathway dynamics and system-level cellular behaviour. In contrast to constraint-based metabolic modelling approaches, which typically represent steady-state flux distributions, kinetic models allow simulation of time-dependent biological dynamics and perturbation responses. Large-scale modelling studies have demonstrated the potential of whole-cell simulations to integrate diverse biological processes and generate quantitative predictions of cellular behaviour [1].

Despite these advances, constructing whole-cell kinetic models remains challenging. Detailed reaction networks must be specified, kinetic rate laws must be defined and parameter values must be assembled from heterogeneous experimental sources. As a result, many kinetic models remain available only as textual descriptions or mathematical formulations in publications, while executable implementations are rarely distributed in reusable form. Public repositories such as the BioModels Database provide curated collections of published computational models, often distributed in standardized formats such as SBML but executable implementations of large collections of kinetic models derived from modelling workflows remain relatively uncommon.

The AdvanceSyn Toolkit was previously developed to support the construction and simulation of whole-cell kinetic models by providing a programmable environment for defining reaction systems and kinetic rate laws [2]. Over time, numerous models were developed using this toolkit for methodological exploration and computational experimentation. As the number of models increased, maintaining them within the same repository as the modelling framework became impractical. To improve modularity and accessibility, these models were separated into a dedicated repository, KinModRe (Kinetic Model Repository), to provide a curated collection of executable whole-cell kinetic models that can be reused for research, methodological development and education in computational systems biology.

Repository Overview

KinModRe is designed as a repository of executable kinetic models derived from modelling work performed using the AdvanceSyn Toolkit [2]. By separating model implementations from the modelling framework, the repository preserves models as reusable computational artefacts while allowing the modelling framework to evolve independently. Each model in the repository includes:

- reaction network definitions describing biochemical transformations
- kinetic rate laws specifying reaction dynamics
- annotated parameter sets
- example simulation scripts demonstrating model execution

Models are organised according to their origin and structure, with accompanying metadata documenting model characteristics such as metabolite counts, reaction counts, parameter provenance, and recommended simulation commands. Although the models were originally constructed using the AdvanceSyn Toolkit [2], the repository is intentionally framework-agnostic at the model level. Users may run the provided scripts directly or adapt the models to alternative simulation environments or analysis workflows.

Model Collection

KinModRe currently contains 31 *de novo* / *ab initio* kinetic reconstructions and 102 models converted from genome-scale metabolic models found in BiGG database [3]. These models span a wide range of scales, from small pathway-level systems to extensive reaction networks representing integrated biochemical knowledge bases.

The smallest model in the repository is derived from the widely used *Escherichia coli* core metabolic reconstruction (*e_coli_core*) and contains 72 metabolites participating in 95 reactions [4]. At the other extreme, the largest model represents an ab initio kinetic reconstruction from the entire KEGG knowledge base (UniKin2), comprising 30669 metabolites and 9420 enzymes participating in 9420 reactions [5-7]. Excluding the UniKin2 reconstruction, the set of 30 *de novo* / *ab initio* kinetic models constructed using the AdvanceSyn Toolkit exhibits substantial scale [2,7]. On average, these models contain 893.3 metabolites, 502.5 enzymes and 1108.9 reactions, demonstrating that the repository includes large reaction systems approaching whole-cell scale. Across the repository, models span more than two orders of magnitude in network size, providing a diverse set of reaction systems for computational experimentation and methodological development.

Example Simulation

Each model in KinModRe includes at least one example simulation demonstrating model execution. A typical workflow consists of:

1. Cloning the model directory from the repository
2. Executing a simulation script that integrates the system of ordinary differential equations describing the reaction network
3. Analysing time-series outputs representing metabolite concentrations or reaction fluxes

For example, a representative *de novo* / *ab initio* model provides a single-command time-course simulation that integrates system dynamics and generates time-series outputs of metabolite concentrations. These simulations confirm that the models stored in the repository are fully executable computational models, rather than static mathematical descriptions. As the models are implemented as programmatic reaction systems, users can readily modify parameters, alter kinetic rate laws or extend reaction networks to explore alternative biological hypotheses.

Intended Uses and Impact

KinModRe serves multiple roles within the computational biology and systems modelling communities: (a) Research reuse. Researchers may reuse existing kinetic models as starting points for new studies, comparative analyses or model extensions. (b) Methodological development. The repository provides reference reaction systems suitable for benchmarking modelling algorithms, parameter estimation methods and simulation techniques. (c) Education and training. Executable kinetic models provide practical examples for teaching mechanistic modelling and dynamic simulation of biological systems. Hence, by publishing executable models as reusable computational artefacts, KinModRe improves reproducibility, transparency and accessibility in whole-cell kinetic modelling.

Conclusion and Future Work

KinModRe provides a curated repository of executable whole-cell kinetic models derived from modelling work using the AdvanceSyn Toolkit. The repository currently contains more than 130 models, including both *de novo* / *ab initio* kinetic reconstructions and models converted from genome-scale metabolic networks.

By separating model implementations from the modelling framework, KinModRe improves modularity and preserves models as reusable scientific resources. The repository offers readily executable kinetic models that support computational studies of cellular dynamics, methodological research and teaching of mechanistic modelling approaches.

KinModRe is intended to continue expanding through further model development and community contributions, forming a growing library of executable whole-cell kinetic models.

Supplementary Materials

The KinModRe repository is publicly accessible at https://github.com/mauriceling/kinmodre

Conflict of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship and/or publication of this article.

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Data Availability Statement

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

Ethical Statement

The project did not meet the definition of human subject research under the preview of the IRB according to federal regulations and therefore was exempt.

Informed Consent Statement

Not applicable.

Authors' Contributions

All authors contributed equally to this paper.

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