A Web-based Platform for Collaborative Development of Kinetic Models

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Motivation

Although many good tools for simulating and analysing kinetic models of biochemical processes are publicly available [1], good public-domain tools for assisting and thoroughly documenting collaborative model development are lacking. Such tools should effectively deal with the following four issues. First, model development often requires engaging multiple parties (experimental and computational) in an iterative testing/refinement process. Second, models always rely on some assumptions that are subject to discussion and eventual change. Third, *thorough documentation of assumptions, underlying rationale, and discussions eventually leading to improvement are critical for effective development. Abstracted from this contextual information, models are prone to misinterpretation and of little use to third parties.* Fourth, citability of contributions and credit tracking are important factors in productively engaging the community in a long-term effort.

We seek to develop a platform for model development that properly addresses these concerns.

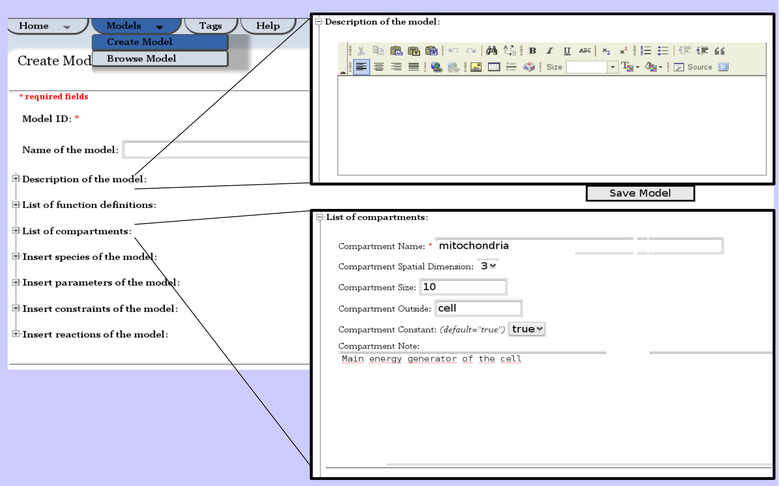
WikiModels functionality

User Authentication and Access Control

This platform is intended to adapt to contexts with different access policies. Further, citability and credit tracking make user identification indispensable. At present, that need is fulfilled by a simple login that gives access to all public resources in WikiModels. Future versions will include a configurable Role-Based Access-Control system.

Model creation

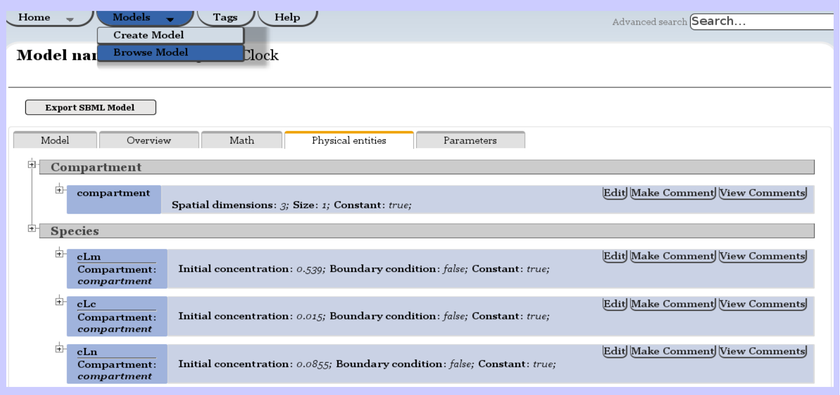
Once logged in, the collaborative activity begins. The first step is the creation of a new model around which the team will develop its ideas. Models can be either set up "from scratch" in WikiModels or imported as SBML [2] files.



Model Browsing

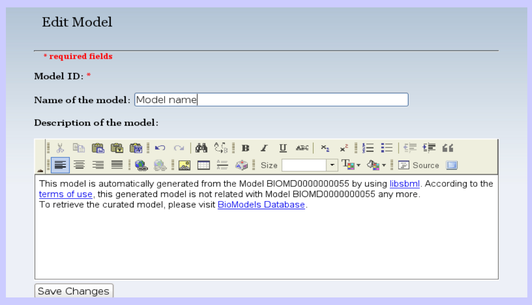
The information about a model can be browsed and visualised by users with the right permissions to do so. This information includes not only elements that define the model (*e. g.* compartments, chemical species, reactions, kinetics, parameters) but also comments documenting underlying assumptions, data sources, discussions, etc.

A unique immutable identifier (URL) is associated to each element allowing citation and linking within and outside WikiModels.



Model edition

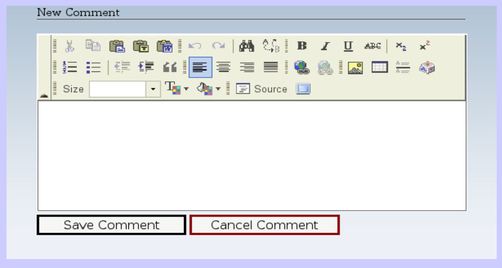
Users with the right permissions can add new elements or change any element of a model. Future versions of WikiModels will record the history of such changes.

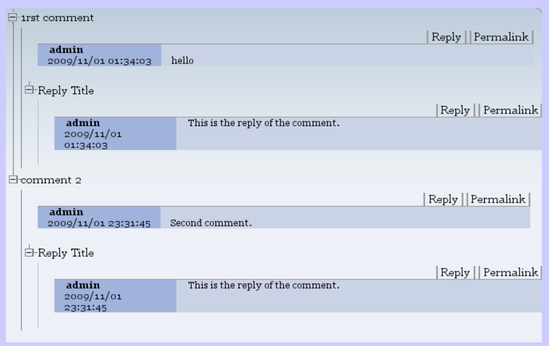


Make and view comments

Not every user of WikiModels has to be a modelling expert. Criticism from experimentalists that are knowledgeable of the biochemical processes and methodological issues involved is precious for developing reliable models.

In order to promote an open peer-review of the models, each model element can serve as root for a discussion list. Each such contribution is associated to a unique Identifier for citation and credit tracking purposes. Comments may include formatted text, tables, mathematical formulas, links, etc., which may be entered through a What You See Is What You Get (WYSIWYG) editor.





Architecture

The platform follows the principles of a REST[3] architecture, making it scalable.
The use of Semantic Web[4] technologies on the data management module makes it much easier and seamless to handle the information contained within the platform in completely innovative ways. This could include applying reasoners that find common elements or metabolic pathways among different models. It also raises the possibility to integrate with other Knowledge Bases that use the same approaches.
The clear separation between client applications and WikiModels Server, with a RESTful Web Service as interface, makes it relatively painless to develop clients in different platforms. Even by outside institutions or contributors.

Availability

A Beta version of WikiModels will be made accessible by February 2010.

Acknowledgements

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References

1. Alves, R., Antunes, F. & Salvador, A. Tools for kinetic modeling of biochemical networks. Nat Biotech 24, 667-672 (2006).

2. Hucka, M. et al. The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models. Bioinformatics 19, 524-531 (2003).

3. Fielding, R.T. & Taylor, R.N. Principled design of the modern Web architecture. ACM Trans. Internet Technol. 2, 115-150 (2002).

4. Lassila, O. & Hendler, J. Embracing "Web 3.0". Internet Computing, IEEE 11, 90-93 (2007).