Morpheus: a user-friendly modeling environment for multiscale multicellular systems biology

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Introduction

Morpheus is a modeling environment for the simulation and integration of cell-based models with ordinary differential equations and reaction-diffusion systems (Starruß et al., Bioinformatics, 2014).

It allows rapid model development of multi-scale models in biological terms and mathematical expressions rather than programming code.

Its graphical user interface supports the entire workflow from model construction and simulation to visualization, archiving and batch processing.

Usability

✦ Modeling without programming
Morpheus separates modeling from programming by MorpheusML: a novel domain-specific SBML-like mark-up language for multicellular systems biology.

✦ Automated model integration
It automates model integration linking models of cellular, intra-cellular and extra-cellular dynamics.

✦ Graphical work-flow tools
The graphical interface provides tools for rapid model development, simulation, batch processing and archiving.

Graphical user interface

✦ Model editor
Rapid model development with add/remove, copy/paste, disable/enable model elements.

✦ Job scheduler
Scheduling of multi-threaded and parallel simulations, on both local and remote computing resources.

✦ Simulation archive
Browsable archive of simulation models with results, allows old models to be restored.

✦ High performance computing
Support for high performance computing with batch systems like LSF and SLURM. Syncing results back to local computer via sftp.

✦ Batch processing
Parameter exploration by creating sequences of simulations with different parameter sets.

Modeling and simulation

✦ Differential equations
Systems of ordinary, stochastic and delay differential equations can represent temporal dynamics such as gene regulation, metabolism or signaling and can be imported from SBML models available in repositories such as the BioModels database.

✦ Reaction-diffusion
Reaction-diffusion systems can be used to model e.g. the spatial distribution of morphogens and binding/unbinding to extracellular matrix components. The spatial domain may be imported from multi-stack images.

✦ Cell-based modeling
Cells can be represented as point-like objects or with explicit 2D or 3D cell shapes, e.g. imported from TIFF microscopy images. Interactions are specified between individual discrete cells. Cell motility and physical constraints may be added using the cellular Potts model (CPM) framework.

✦ Multiscale cellular models
To study feedbacks between various levels of biological organization, models can be constructed that couple cellular dynamics with intra- and/or extracellular dynamics.

MorpheusML

MorpheusML is a SBML-like language for multicellular systems biology. The markup language separates modeling from programming and enables users to describe computational models in biological and mathematical terminology rather than programming code.

Mathematical expressions (functions, differential equations and events) are specified in familiar infix notation.

MorpheusML enables model integration by automatically resolving dependencies between symbolic identifiers to determine e.g. the order in which model components must be updated.

Software

Morpheus is a self-contained application for Linux, Mac OSX and Windows that consists of two stand-alone programs: a C++-based simulator and a Qt-based graphical user interface.

It uses muparser to evaluate math expressions, eigen for matrix operations, openMP for parallel computing, libTIFF for import/export of 3D images, SQLite for archiving, and gnuplot as data visualization back-end.

Morpheus features a plug-in architecture that allows extensions to be written in C++. This transforms the current binary application into a flexible framework following the planned open-source release.

Key references


