Universität Rostock

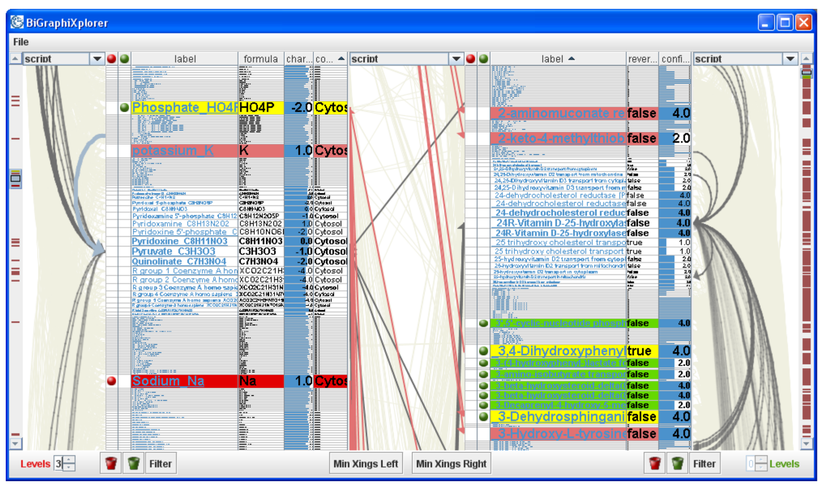
Traditio et Innovatio

Visual Analytics for Stochastic Simulation in Cell Biology

Hans-Jörg Schulz, Steffen Hadlak, Adelinde M. Uhrmacher, Heidrun Schumann

Visual Analytics is a data analysis paradigm that combines visual and computational methods. Rarely though, Visual Analytics goes beyond the mere dataset and also incorporates the data generating processes that have led to the data in the first place. In many cases, this is hardly possible, as these processes cannot be captured to be analyzed themselves. Simulation is an exception to this, as the data generating process runs *in silico* and can thus be logged and stored alongside the simulation result. We take advantage of this property and employ Visual Analytics for stochastic simulation in cell biological applications. We present Visual Analytics solutions for all stages of this particular data generating process – the model, the experiment, the simulation runs, and a combination of all three.

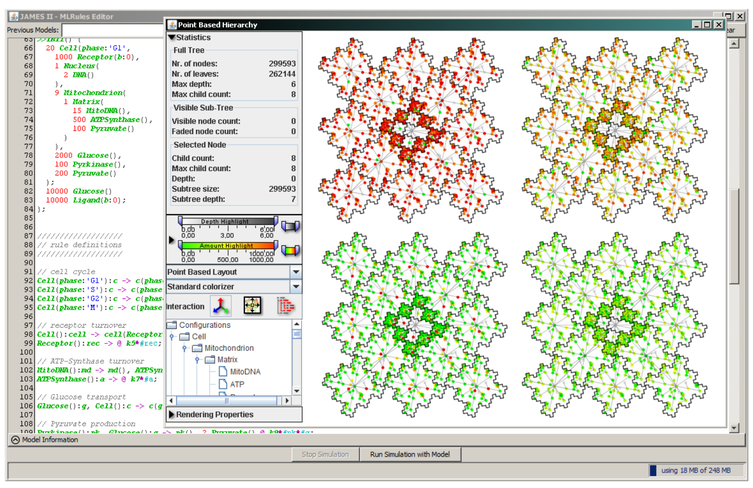
VISUAL ANALYTICS FOR MODELS



The **BiGraphiXplorer** visualizes biological models, such as the reactome of a cell as a bipartite graph with compounds on the left, reactions on the right, and links between them if a compound partakes in a reaction. It facilitates interactive model traversal via a script-based selection mechanism to aid the analysis of the model topology.

HJ Schulz, M John, A Unger, H Schumann: Visual Analysis of Bipartite Biological Networks, Proc. VCBM'08, pp.135-142, 2008

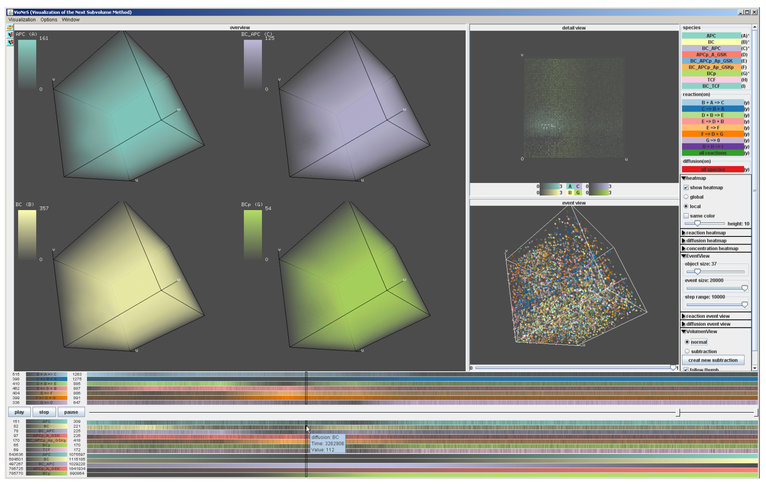
VISUAL ANALYTICS FOR CONFIGURATIONS



The **point-based layout** shows model configurations and allows the user to investigate the distribution of initial values. It is specifically designed to depict large, evenly structured hierarchical models, easing their comparison. Statistical methods to evaluate the configuration are integrated through the underlying JAMES II framework.

HJ Schulz, S Hadlak, H Schumann: Point-based Visualization for Large Hierarchies, IEEE TVCG 17(5), pp.598-611, 2011

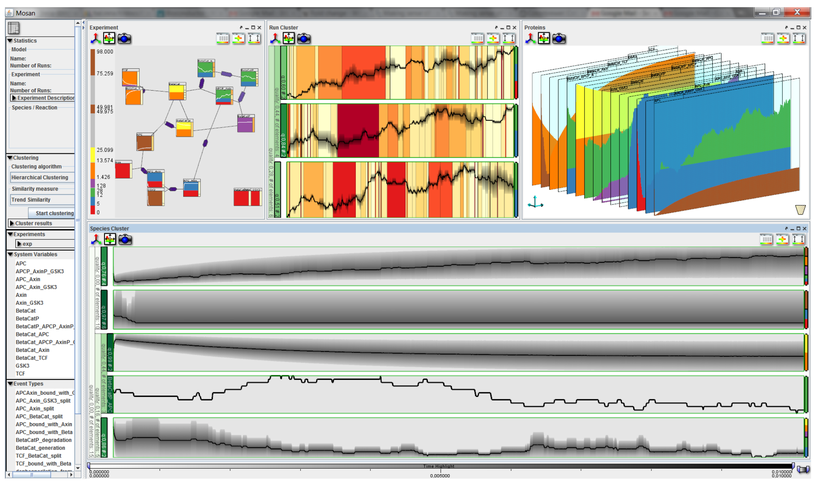
VISUAL ANALYTICS FOR SIMULATION RUNS



The **VioNeS toolkit** features a volumetric visualization of the spatial distribution of species concentrations (*states* – left) and occurring reactions (*events* – right) over simulation time. Showing both, states and events, supports the analysis of cause and effect, which is further assisted by computational means, such as steady state analysis.

A Unger, E Gutzeit, M Jeschke, H Schumann: Visual Support for the Analysis of the Next Sub-volume Method, Proc. IV'09, pp.10-17, 2009

INTEGRATED VISUAL ANYLTICS FOR SIMULATION



The **Mosan framework** incorporates linked views of the model, its configurations, and their simulation runs. Their integration enables users to explore the data generating process on all stages by moving fluently back and forth between them. The visual exploration is supported by analytical techniques, such as time series clustering.

A Unger, H Schumann: Visual Support for the Understanding of Simulation Processes, Proc. PacificVis'09, pp.57-64, 2009

Find more information in the paper: HJ Schulz, AM Uhrmacher, H Schumann: Visual Analytics for Stochastic Simulation in Cell Biology, Proc. i-Know/TAVA, 2011

INSTITUTE FOR COMPUTER SCIENCE
University of Rostock | 18051 Rostock, Germany

CHAIR FOR COMPUTER GRAPHICS
CHAIR FOR MODELING & SIMULATION
CHAIR FOR MULTIMEDIA COMMUNICATION