Universität Rostock

Traditio et Innovatio

Simulation Galleries: Combining Experiment Design and Visual Analytics

Tom Warnke, Lars Roesicke, Hans-Jörg Schulz, Adelinde M. Uhrmacher

Overview

The complexity and size of simulation models is steadily increasing. As a consequence, input and output of simulations increase in complexity as well. This is particularly true for spatial, multi-level models where different structures might be of interest. Therefore, new methods are required that support the experimentation process with these models.

We propose a novel method to interactively and iteratively explore the parameter space of simulation models. We expect it to provide valuable support to domain experts when calibrating and validating complex simulation models.

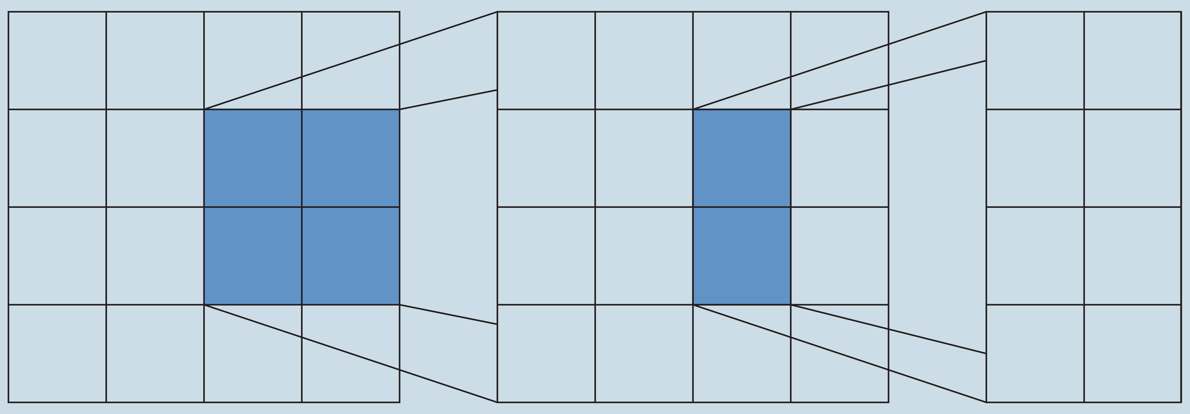
Case Study: Actin Filament Branching

The extracellular surroundings of osteoblasts (cells involved in bone synthesis) significantly influence their intracellular processes. For example, osteoblasts growing on surfaces with regular micro-geometry show an adapted cytoskeleton. The cytoskeleton is built through polymerization, branching, and severing of actin filaments, resulting in complex spatial patterns, which can be observed with microscopes. Simulation models of the cytoskeleton buildup in osteoblasts can be calibrated and validated by comparing their output to those patterns. This is done by knowledgeable domain experts.

The SImulation Galleries Loop

(Re-)Sampling the Parameter Space

Based on initial conditions or the selections of the user, parameter combinations from a specific area of the model parameter space are sampled for experimentation. By repeating the process, the parameter subspace under investigation is pruned and refined.



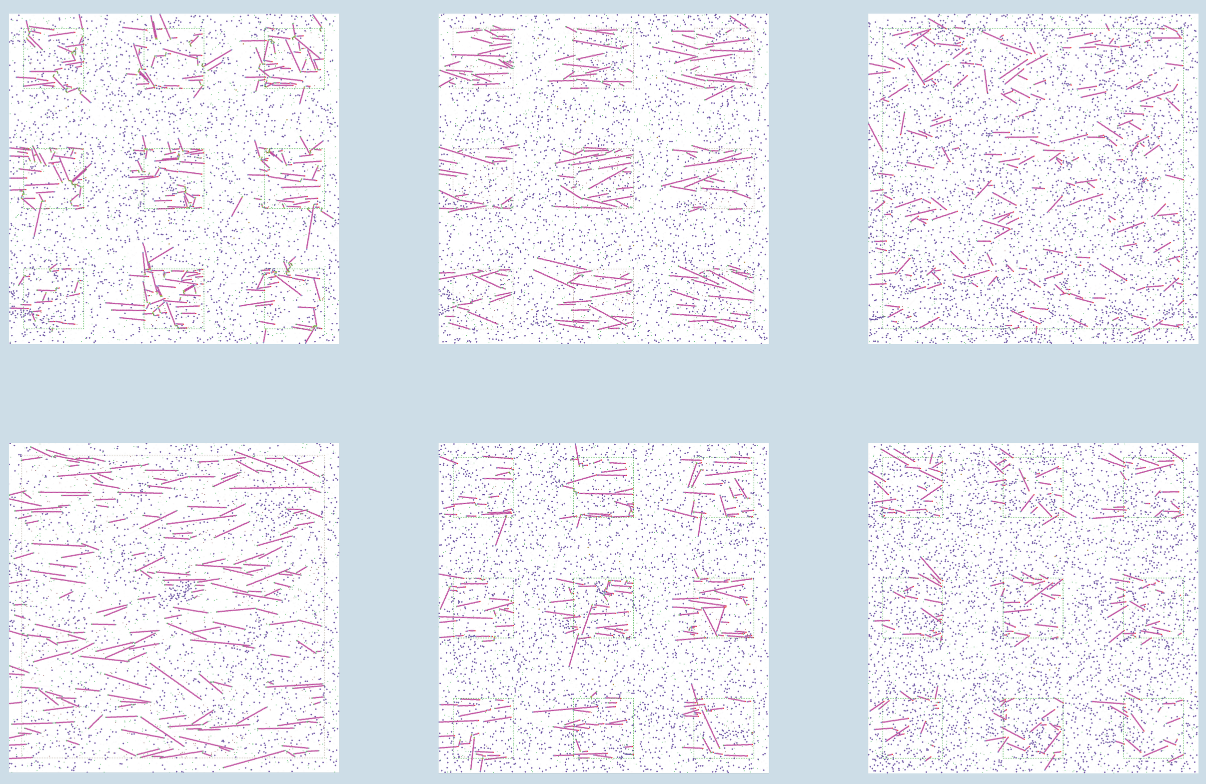
Executing Simulation Runs

Simulation Experiment Specification on a Scala Layer (SESSL) enables readable and executable experiment specifications

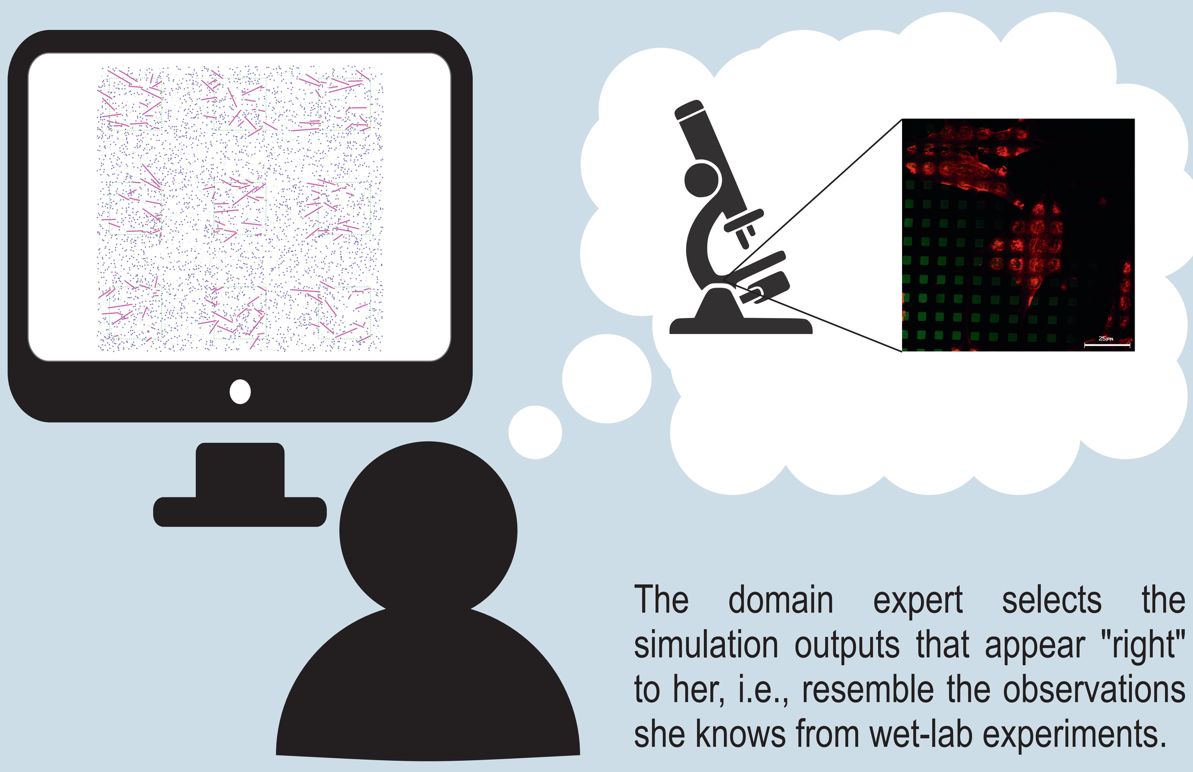
```
import sessl.mlrules._

new Experiment with Observation with ParallelExecution {
  model = "./actin-filaments.mlrj"
  simulator = HybridSimulator()
  parallelThreads = -1
  observeAt(range(0, 1, 100))
  observe("actin")
  stopCondition = AfterSimTime(100)
  replicationCondition = MeanConfidenceReached("actin")
}
```

Visualizing Simulation Results



Selecting Configurations



The domain expert selects the simulation outputs that appear "right" to her, i.e., resemble the observations she knows from wet-lab experiments.

Future Work

- Refine model of actin filament branching
- Implement continuous-spatial visualization methods for discrete-spatial simulations
- Ensure that simulations are fast enough for interactive tool
- Investigate different resampling strategies (LHC, Optimization, ML, ...)
- User study with domain experts from life sciences

References

A. T. Bittig et. al. 2014. Membrane Related Dynamics and the Formation of Actin in Cells Growing on Micro-Topographies: a Spatial Computational Model. BMC Systems Biology 8(1).

R. Ewald and A. M. Uhrmacher. 2014. SESSL: A Domain-Specific Language for Simulation Experiments. ACM TOMACS 24(2).

T. Helms et. al. 2017. Semantics and Efficient Simulation Algorithms of an Expressive Multilevel Modeling Language. ACM TOMACS 27(2).

J. Marks, et. al. 1997. Design Galleries: A General Approach to Setting Parameters for Computer Graphics and Animation. In Proceedings of the SIGGRAPH '97.

M. Sneddon et. al. 2011. Efficient Modeling, Simulation and Coarse-Graining of Biological Complexity with NFsim. Nature Methods 8(2).

Tom Warnke | tom.warnke@uni-rostock.de

Modeling and Simulation Group

University of Rostock

mosi.informatik.uni-rostock.de