CellVis – Modeling, Simulating, and Analyzing Cellular Processes
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Motivation
- Investigation of cellular transport processes
- Current state of model design in Systems Biology:
  - Validate model and refine
  - Run simulation
  - Validate model and refine
- CellVis developed at VISUS supports
  - Model design, simulation, and analysis
  - User control at every stage to allow Computational Steering

Visualization on the Atomic Scale
- Add information on atomic structures from PDB
- Deeper immersion into the data
- Useful for education or artistic renderings

Visualization of signal transduction processes in the crowded environment of the cell.

References

Analysis
- Strong focus on visualization at the present time
- GPU-based techniques for interactive visualization
- Visualizations can be used to
  - Validate simulation results
  - Gain new insight by exploration
  - Illustrate biological processes
- Classical approaches like tables and 2D plots are included

Simulation
- Spatial particle-based Monte Carlo simulation
- Simulation with CUDA on the GPU
- Speed-up factor of 2 to 10 possible compared to CPU
- Chemical interactions according to
  - Mass-action kinetics
  - Michaelis-Menten kinetics
- Reaction dynamics

Ongoing Work
- Statistical analysis of simulation results
- Moments of the signal distribution
- Mean time before a signal arrives at the nucleus
- Average of distances covered by molecules
- Histories of individual molecules
- Comparative visualization between simulation runs

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Visualizations can be combined freely. Additional views like tables or plots are available to study the data set in detail.

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