INTERACTIVE VISUAL EXPLORATION OF SIMULATOR ACCURACY:
A CASE STUDY FOR STOCHASTIC SIMULATION ALGORITHMS

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BACKGROUND / MOTIVATION

Stochastic (Spatial) Simulation (in Cell Biology)
BACKGROUND / MOTIVATION

Stochastic Simulation

SSAs:
- exact ones like Next Reaction Method: slow
- non-exact like tau-leaping: speed vs. accuracy
BACKGROUND / MOTIVATION

Stochastic Simulation

Accuracy depends on:
- parameters, simulation model, goal of study
BACKGROUND / MOTIVATION

Stochastic Simulation

Accuracy depends on:
• parameters, simulation model, goal of study
BACKGROUND / MOTIVATION

Stochastic Simulation

[Diagram showing a graph with a curve and a point labeled 'A']
BACKGROUND / MOTIVATION

Stochastic Simulation
BACKGROUND / MOTIVATION

Stochastic Simulation
BACKGROUND / MOTIVATION

Stochastic Simulation

Parameters
BACKGROUND / MOTIVATION

Non-exact Stochastic Simulation

Stochastic Simulator

Parameters

+ Accuracies along each trajectory
VISUALIZATION REQUIREMENTS

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Stochastic Simulator

Parameters

+ Accuracies along each trajectory
**VISUALIZATION REQUIREMENTS**

- show the data
- relate accuracies to data
- guide to desired accuracies
- feedback into parameter space

+ Accuracies along each trajectory
VISUALIZATION APPROACH

- show the data
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1 configuration
VISUALIZATION APPROACH

- show the data
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1 configuration
VISUALIZATION APPROACH

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1 configuration with α accuracies
VISUALIZATION APPROACH

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$n$ configurations with 1 accuracy
VISUALIZATION APPROACH

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$n$ configurations with 1 accuracy
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$n$ configurations with $a$ aggregated accuracies
VISUALIZATION APPROACH

• show the data
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• feedback into parameter space

a histograms of aggregated accuracies
VISUALIZATION APPROACH

- show the data
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$p$ parameters
VISUALIZATION APPROACH

- show the data
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- feedback into parameter space

\[ p \text{ parameters and } a \text{ aggregated accuracies} \]

\[ a_1, a_2, a_3, a_4 \]
VISUALIZATION DEMO
VISUALIZATION DEMO

Linear Chain System, 601 species, 50 s simulation time, 10,000 $S_0$, $S_{25}$, 500 time points, 1000 replications, 2200 different configurations
CONCLUSION

• Combined visualization of
  • simulation output
  • accuracies
  • parameters

• Independent of model and (non-exact) SSA

• Adaptable to different accuracy-measures and even beyond

  supports exploratory determination of parameters for further use
OUTLOOK

- Integration of metadata (e.g. execution time) and further species
- Comparison of different configurations
- Advanced sorting, statistics, clustering
THANK YOU!
QUESTIONS?