Stochastic Simulation of Cellular Reaction Networks

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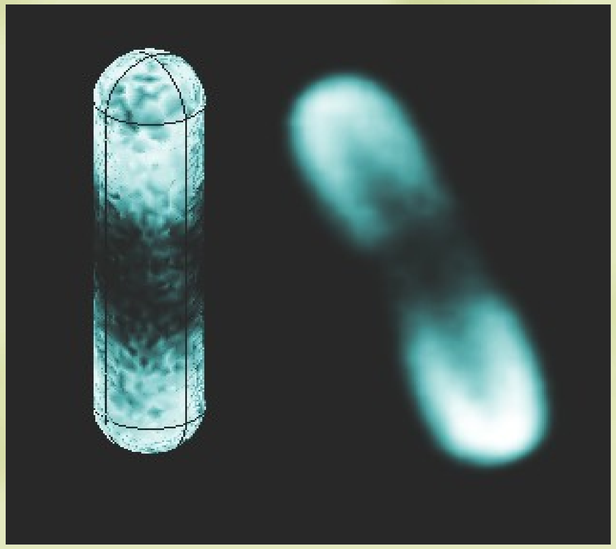
Stochastic modeling
Proteins in living cells appear in small numbers. Reactions between them are stochastic events. To describe such a system the model has to be stochastic.

The probability for the system state is given by a Master equation. Solving it is intractable due to its vast dimensionality. Instead we compute single realizations of the system.

Discretized diffusion
Probabilistic interpretation put extra constraints on the diffusion matrix. The expected time until a diffusion event must be non-negative. This is not fulfilled for many traditional discretization techniques.

We compared two different discretizations, a previously used FEM and a FVM implemented by us.

Inconsistency
FEM produces negative probabilities, which have to be zeroed out. The discretization is then not



Concentration of the MinD protein on the membrane of an *E. coli* bacterium, in silico and in vivo*.

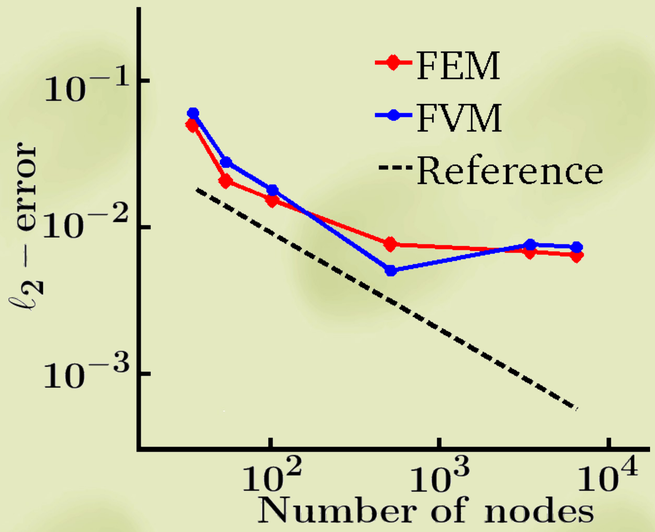
consistent with the diffusion equation. The used FVM has an intrinsic inconsistency.

Discretization models
We found that the FEM and FVM approaches have stunningly similar accuracy. Both had worrysome discretization errors, but still reproduced the qualitative behaviour of the studied systems.

It is uncertain how much effect these errors have in realistic problems.

Location of cell division
A much studied example is the Min system of E. coli. The Min proteins inhibit cell division. By oscillating from end to end of the bacterium they direct the division to the middle of the bacterium.

On the left we show the result of a stochastic simulation next to an image of a real bacterium.



Error curves for the two diffusion discretizations. Note how they do not converge.

* Image by Giovanni Meacci and Karsten Kruse.