Efficient SIMULATION OF COMPLEX REACTION NETWORKS

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Reaction Networks

Diagram showing various nodes labeled $X_1$, $X_2$, $X_3$, $X_4$, $X_5$, $X_6$, and $X_7$ connected in a network.
Simulation Methodologies

The Rate Equations:
\[
\frac{dN_i}{dt} = f_i - w_i N_i - \sum_j a_{ij} N_i N_j
\]

The Master Equation:
\[
\dot{P}(N_1, \ldots, N_J) = \ldots
\]

The number of variables grows exponentially with the number of reactive species

Highly efficient
Does not account for stochasticity

Always valid
Infeasible for complex networks
The Moment Equations

The population size and the production rate are given by
the moments:

\[
\frac{d \langle N^q_i \rangle}{dt} = \sum_{N=0}^{\infty} N^q_i \dot{P}(N_1, \ldots, N_J)
\]

Node: \( \langle N_i \rangle \)
Edge: \( \langle N_i N_j \rangle \)
Loop: \( \langle N^2_i \rangle \)

For example:

\[
\frac{d \langle N_6 \rangle}{dt} = f_6 - w_6 \langle N_6 \rangle - a_6 \left( \langle N_6^2 \rangle - \langle N_6 \rangle \right) - a_{1,6} \langle N_1 N_6 \rangle - a_{5,6} \langle N_5 N_6 \rangle
\]

\[
\frac{d \langle N^2_6 \rangle}{dt} = f_6 + (2f_6 + w_6 - 4a_6) \langle N_6 \rangle - (2w_6 - 8a_6) \langle N_6^2 \rangle - 4a_6 \langle N_6^3 \rangle - a_{1,6} \left( \langle N_1 N_6 \rangle - 2 \langle N_1 N_6^2 \rangle \right) - a_{5,6} \left( \langle N_5 N_6 \rangle - \langle N_5 N_6^2 \rangle \right)
\]

The Moment Equations

The truncation scheme:

\[
\langle N_i^3 \rangle = 3 \langle N_i^2 \rangle - 2 \langle N_i \rangle \\
\langle N_i^2 N_j \rangle = \langle N_i N_j \rangle \\
\langle N_i N_j N_k \rangle = 0
\]

The “miracle”:

The truncation is based on a low population assumption.

But the equations are valid far beyond that...

Automation of the equations:

\[
\frac{d\langle N_6 \rangle}{dt} = x_6 + x_6 + x_5 + x_6
\]

\[
\frac{d\langle N_6 \rangle}{dt} = f_6 - w_6 \langle N_6 \rangle - a_6 \left( \langle N_6^2 \rangle - \langle N_6 \rangle \right) - a_{1,6} \langle N_1 N_6 \rangle - a_{5,6} \langle N_5 N_6 \rangle
\]
Minimal number of equations for a stochastic simulation - 1 per species + 1 per reaction (nodes + edges)

Linear equations

Easy to automate

No need to adjust cutoffs

The results coincides with that of the master equation for any system size

Thank you for listening