The Hebrew University of Jerusalem האוניברסיטה העברית בירושלים

Efficient Simulation of Complex Reaction Networks

by:

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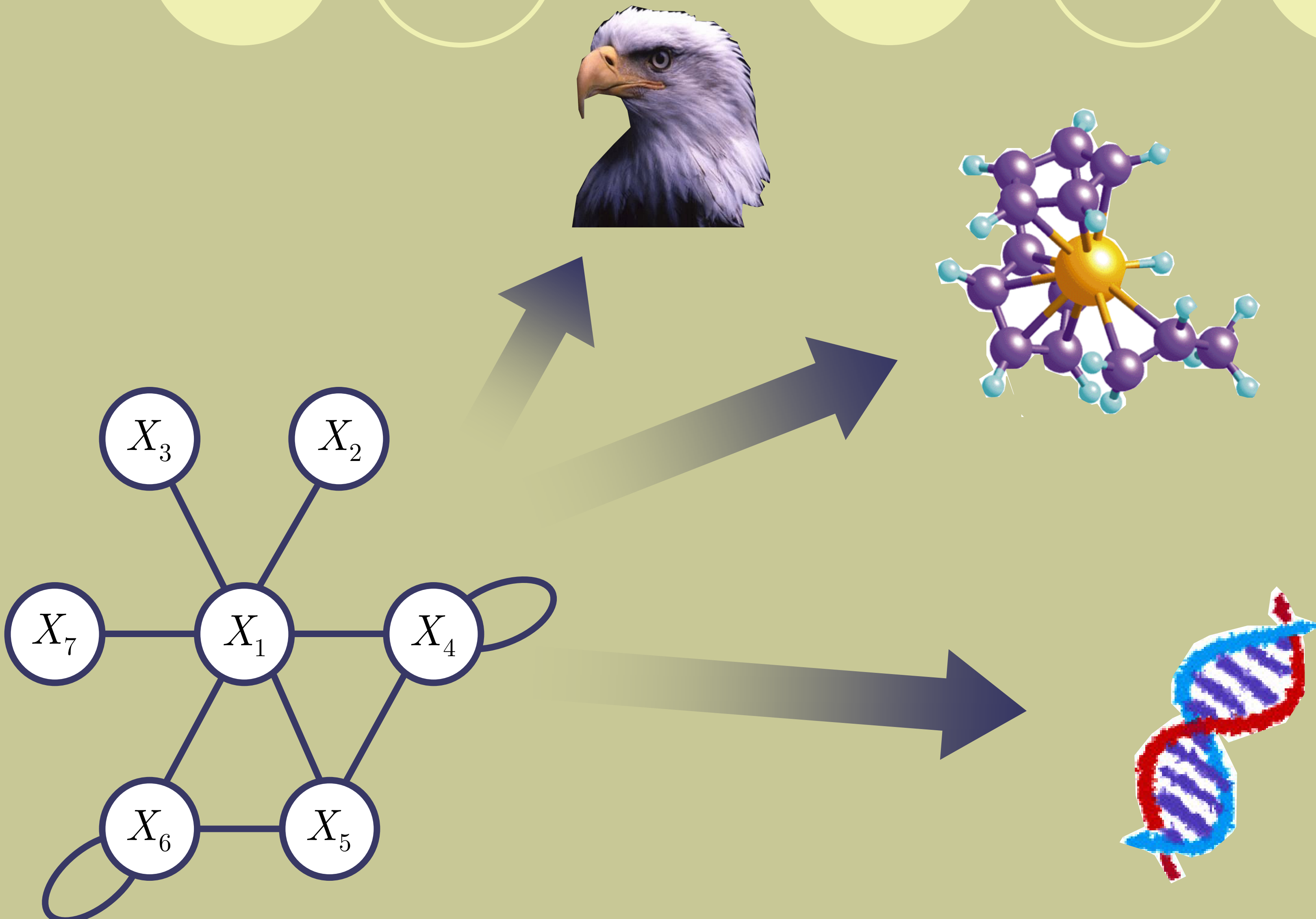
ECCS - DRESDEN 2007

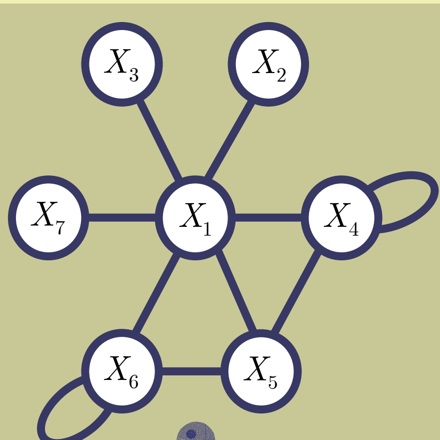
Reaction Networks



Simulation Methodologies

The Rate Equations:

$$\frac{dN_i}{dt} = f_i - w_i N_i - \sum_j a_{ij} N_i N_j$$

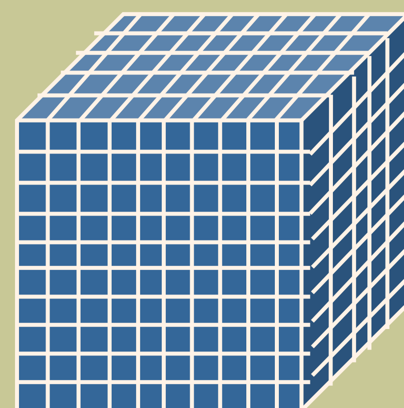


Highly efficient

Does not account for stochasticity

The Master Equation:

$$\dot{P}(N_1, \cdots, N_J) = \cdots$$



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

Always valid

Infeasible for complex networks

The Moment Equations

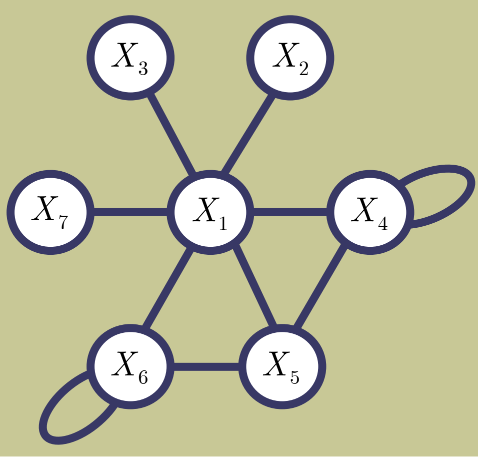
The population size and the production rate are given by the moments:

$$\frac{d\langle N_i^q\rangle}{dt} = \sum_{N=0}^{\infty} N_i^q \dot{P}(N_1, \cdots, N_J)$$

Node: $\langle N_i \rangle$

Edge: $\langle N_i N_j \rangle$

Loop: $\langle N_i^2 \rangle$



For example:

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

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

B. Barzel and O. Biham, *Astrophys. J. Lett.*, **115** 20941 (2007)

B. Barzel and O. Biham, *J. Chem. Phys.* In press (2007)

The Moment Equations

The truncation scheme:

$$\left\langle N_i^3 \right\rangle = 3\left\langle N_i^2 \right\rangle - 2\left\langle N_i \right\rangle$$

$$\left\langle N_i^2 N_j \right\rangle = \left\langle N_i N_j \right\rangle$$

$$\left\langle N_i N_j N_k \right\rangle = 0$$

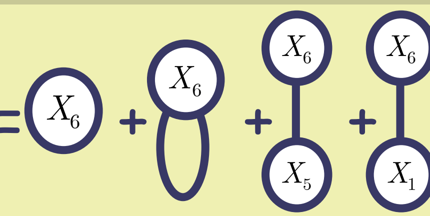
The “miracle”:

The truncation is based on a low population assumption.

But the equations are valid far beyond that…

Automation of the equations:

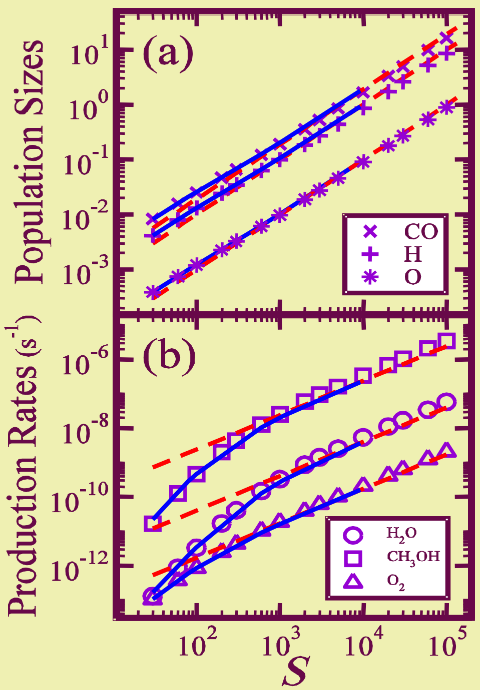
$$\frac{d\left\langle N_6 \right\rangle}{dt} =$$



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

Summary & Results

The results:



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

- 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

THANK YOU FOR LISTENING