

I represented the network with the stoichiometric matrix

$$V = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -2 & 0 & 1 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

where the rows correspond to the species

```
gene 1:    g1 = X(1)
gene 2:    g2 = X(2)
protein 1: p1 = X(3)
protein 2: p2 = X(4)
dimer 1:   d1 = X(5)
dimer 2:   d2 = X(6)
complex 1: c1 = X(7)
complex 2: c2 = X(8)
```

and the columns correspond to the reactions

```
g1 + d2 <-- k1/k2 --> c1
g2 + d1 <-- k3/k4 --> c2
p1 + p1 <-- k5/k6 --> d1
p2 + p2 <-- k7/k8 --> d2
g1      <-- k9 --> g1 + p1
g2      <-- k10 --> g2 + p2
c1      <-- k11 --> c1 + p1
c2      <-- k12 --> c2 + p2
```

The following is the Matlab script I used to simulate the network. I had little intuition for the kinetic rates and initial conditions, so I was unable to elicit the desired oscillatory behavior.

```
% Daniel S. Standage
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%
% Adapted from a script written by D.J. Higham, accessed at
% http://personal.strath.ac.uk/d.j.higham/chem/ssa_plot.m

clf

rand('state',100)

% Define stoichiometric matrix
V = [-1 0 0 0 0 0 0 0;
      0 -1 0 0 0 0 0 0;
      0 0 -2 0 1 0 1 0;
      0 0 0 -2 0 1 0 1;
      0 -1 1 0 0 0 0 0;
      -1 0 0 1 0 0 0 0;
      1 0 0 0 0 0 0 0;
      0 1 0 0 0 0 0 0];

% Parameters
nA = 6.023e23; % Avagadro's number
vol = 1e-15;   % volume of system
```

```

% Initial conditions for 8 biochemical species
X = zeros(8,1);
X(1) = 1e-6*nA*vol;    % gene 1
X(2) = 1e-6*nA*vol;    % gene 2
X(3) = 1e-7*nA*vol;    % protein 1
X(4) = 1e-7*nA*vol;    % protein 2
%X(5)    % dimer 1
%X(6)    % dimer 2
%X(7)    % complex 1
%X(8)    % complex 2

% Kinetic rates for 8 (12) reactions
c(1) = 1e-4; c(2) = 1e-10; % g1 + d2 <-- k1/k2 --> c1
c(3) = 1e-4; c(4) = 1e-10; % g2 + d1 <-- k3/k4 --> c2
c(5) = 1e-2; c(6) = 1e-6;  % p1 + p1 <-- k5/k6 --> d1
c(7) = 1e-2; c(8) = 1e-6;  % p2 + p2 <-- k7/k8 --> d2
c(9) = 1e-6;                % g1      <-- k9 --> g1 + p1
c(10) = 1e-6;               % g2      <-- k10 --> g2 + p2
c(11) = 1e-2;               % c1      <-- k11 --> c1 + p1
c(12) = 1e-2;               % c2      <-- k12 --> c2 + p2

% Algorithm
t = 0;
tfinal = 50;

count = 1;
tvals(1) = 0;
Xvals(:,1) = X;

while t < tfinal
    a(1) = -c(1)*X(1)*X(6) + c(2)*X(7);
    a(2) = -c(3)*X(2)*X(5) + c(4)*X(8);
    a(3) = 0.5*-c(5)*X(3)*X(3) + c(6)*X(5) + c(9)*X(1) + c(11)*X(7);
    a(4) = 0.5*-c(7)*X(4)*X(4) + c(8)*X(6) + c(10)*X(2) + c(12)*X(8);
    a(5) = -c(3)*X(2)*X(5) + c(4)*X(8) + 0.5*c(5)*X(3)*X(3) - c(6)*X(5);
    a(6) = -c(1)*X(1)*X(6) + c(2)*X(7) + 0.5*c(7)*X(4)*X(4) - c(8)*X(6);
    a(7) = c(1)*X(1)*X(6) - c(2)*X(7);
    a(8) = c(3)*X(2)*X(5) - c(4)*X(8);
    asum = sum(a);
    j = min(find(rand<cumsum(a/asum)) );
    tau = log(1/rand)/asum;
    X = X + V(:,j);

    count = count + 1;
    t = t + tau;
    tvals(count) = t;
    Xvals(:,count) = X;
end

%%%%%%%%%%%% Plots

L = length(tvals);
tnew = zeros(1,2*(L-1));
tnew(1:2:end-1) = tvals(2:end);
tnew(2:2:end) = tvals(2:end);
tnew = [tvals(1),tnew];

Svals = Xvals(1,:);

```

```
ynew = zeros(1,2*L-1);
ynew(1:2:end) = Svals;
ynew(2:2:end-1) = Svals(1:end-1);
plot(tnew,ynew,'go-')
hold on

Pvals = Xvals(4,:);
ynew = zeros(1,2*L-1);
ynew(1:2:end) = Pvals;
ynew(2:2:end-1) = Pvals(1:end-1);
plot(tnew,ynew,'r*-')

text(40,240,'Product','FontSize',16)
text(30,50,'Substrate','FontSize',16)

xlabel('Time','FontSize',14)
ylabel('Molecules','FontSize',14)

axis([0 55 0 310])

set(gca,'FontWeight','Bold','FontSize',12)
grid on
```