Using network topology to optimize molecular production in an artificial chemistry model

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Outline

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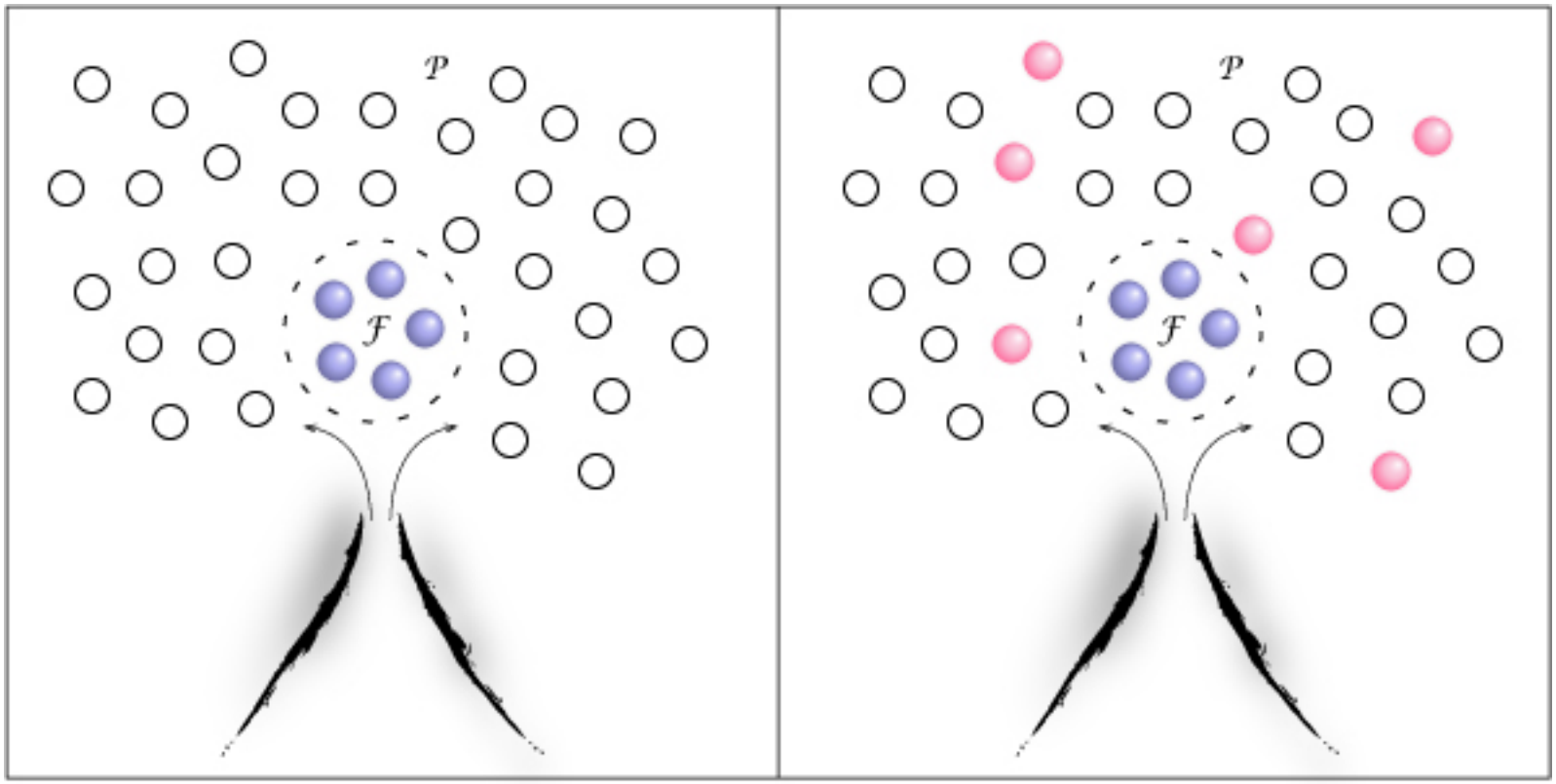
- Did it require all of the components that we seen in life to be built at the same time or were they induced incrementally?
- How did the organization in life emerge?
- Origin of metabolic networks: From the large set of possible organic reactions, only a few participate in life.

Pre-biotic organization



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Notations

- Consider a set $\mathcal{F} = \{m_1, m_2, m_3, \ldots, m_f\}$ of f moieties (small compounds) present abundantly and homogenously in a pre-biotic niche: Input or 'Food' set.

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$$A + B \underset{}{\overset{C}{\rightleftharpoons}} D$$

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- A, B, C, ... can represent any member of set $\mathcal{F}$ or the product set, $\mathcal{P}$.

The model

- $\mathrm{A} = (m_1)^{a_1}(m_2)^{a_2}(m_3)^{a_3}\ldots(m_f)^{a_f}$ where $0 \leq a_i \leq n$, $\sum_i a_i = n$, $i = 1, 2, 3, \ldots f$. n is the maximum number of moieties a molecule can have.

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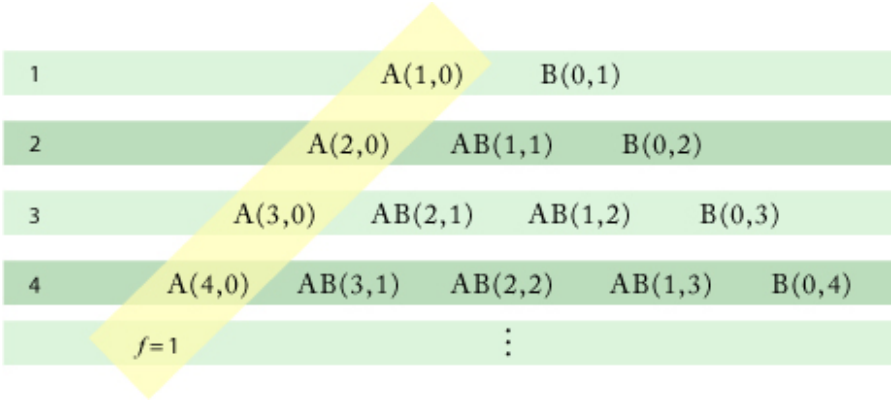

Reaction system

For $f = 1$ reaction system will look as following:

$$\begin{aligned}
\mathrm{A}(1) + \mathrm{A}(1) &\rightleftharpoons \mathrm{A}(2) \\
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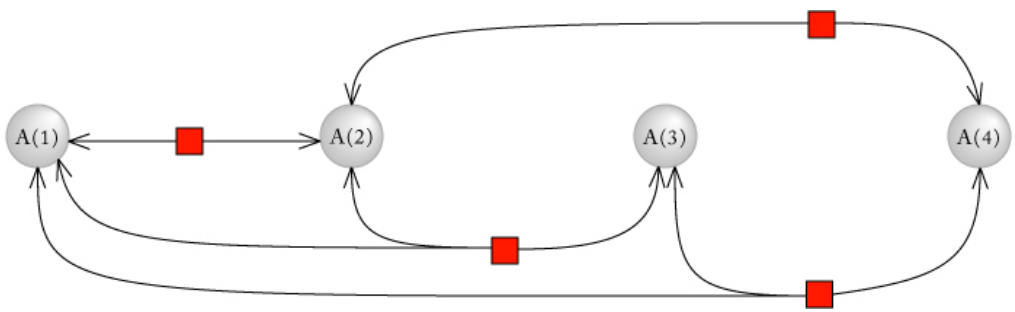

Dynamical equation

Using rate action kinetics one can write a differential equation for the the change in concentration of each molecule:

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& + \sum_{n>2} k_r x_{\mathrm{A}(n)} \\
& - \phi x_{\mathrm{A}(2)}
\end{aligned}
$$

Dynamical system

For all the molecules, one can write following coupled non-linear differential equations:

$$\begin{aligned}\dot{x}_{\mathrm{A}} &= \frac{1}{2}\sum_{(\mathrm{B},\mathrm{C})\in l_{\mathrm{A}}} \kappa^{F}_{\mathrm{B},\mathrm{C}} x_{\mathrm{B}} x_{\mathrm{C}} + \sum_{\mathrm{B},(a_i+b_i\leq n_i)} \kappa^{R}_{\mathrm{A},\mathrm{B}} x_{\mathrm{A}B} \\ &\quad - \sum_{\mathrm{B},(a_i+b_i\leq n_i)} \kappa^{F}_{\mathrm{A},\mathrm{B}} x_{\mathrm{A}} x_{\mathrm{B}} - \frac{1}{2}\sum_{(\mathrm{B},\mathrm{C})\in l_{\mathrm{A}}} \kappa^{R}_{\mathrm{B},\mathrm{C}} x_{\mathrm{A}} - \phi_{\mathrm{A}} x_{\mathrm{A}}\end{aligned}$$

here, $x_{\mathrm{A}} = [\mathrm{A}]$, $l_{\mathrm{A}} = \{(\mathrm{B},\mathrm{C}) : \mathrm{BC} = \mathrm{A}\}$, ϕ is the decay constant, and, κ^{F} and κ^{R} are the rate constant matrices (symmetric), given by,

$$\kappa^{F} = \begin{pmatrix} 2k_f & k_f & k_f & \dots \\ k_f & 2k_f & k_f & \\ k_f & k_f & 2k_f & \\ \vdots & & & \ddots \end{pmatrix}; \kappa^{R} = \begin{pmatrix} 2k_r & k_r & k_r & \dots \\ k_r & 2k_r & k_r & \\ k_r & k_r & 2k_r & \\ \vdots & & & \ddots \end{pmatrix}$$

Dynamical system

- k_f and k_r are the spontaneous forward and backward rate constants, respectively. When we consider catalyzed reactions, $k_{f/r}$ can be replaced by $k'_{f/r}$.

$$k'_{f/r} = k_{f/r}(1 + \beta \; x \; [Catalyst])$$

β is Catalytic Efficiency of the catalyst.

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- As the members of the set $\mathcal{F}$ are replenished continually, any amount drawn or produced does not affect their concentrations. It is thus assumed that the concentrations of members of set $\mathcal{F}$ do not change over time.

Equation in dimensionless variables

Consider a concentration scale ω and a time scale τ.
Re-writing equation in terms of these dimensionless variables gives:

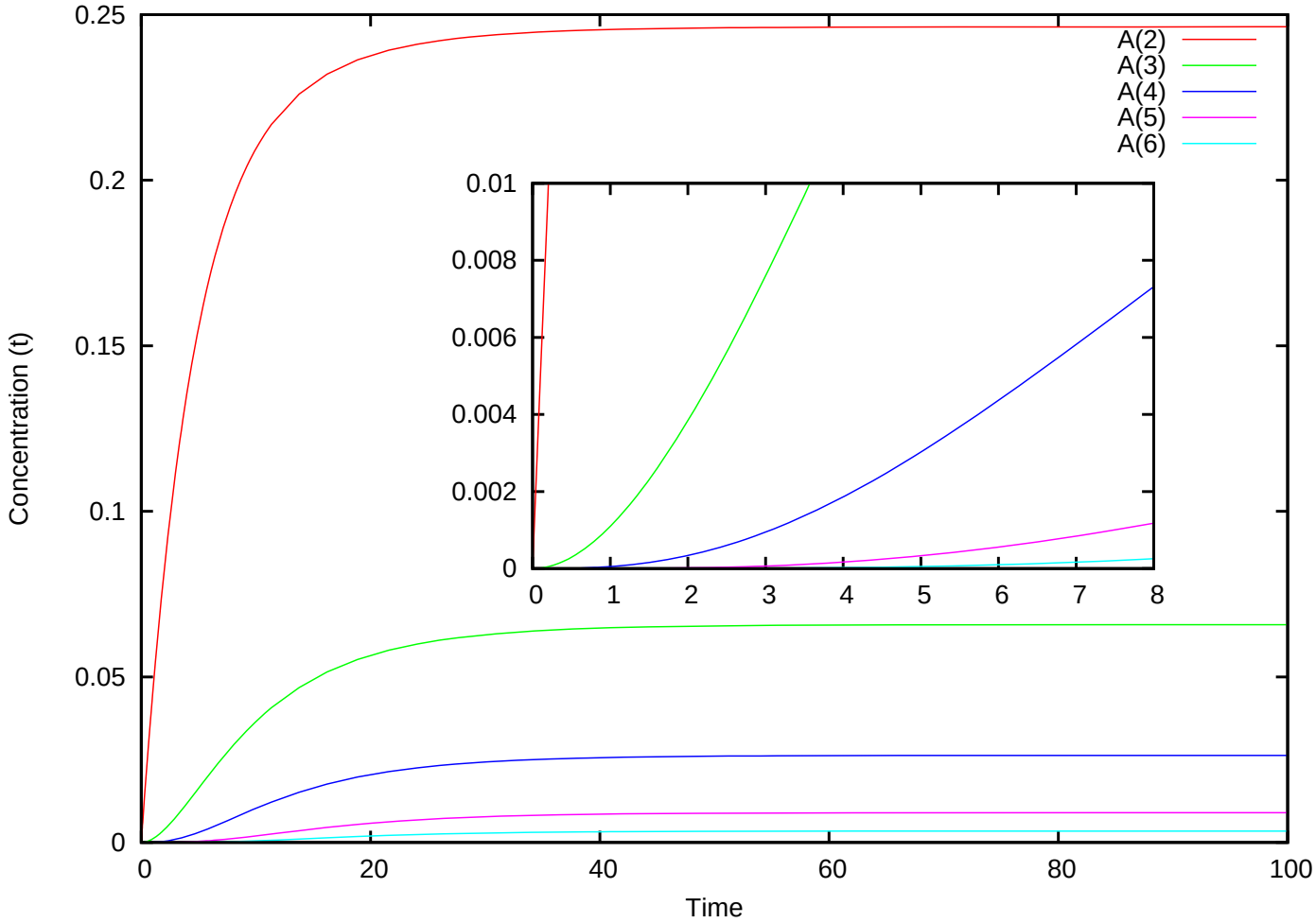
$$\begin{aligned}\dot{x}'_{\mathrm{A}} &= \frac{1}{2}\sum_{(\mathrm{B},\mathrm{C})\in I_{\mathrm{A}}} \kappa'^{F}_{\mathrm{B},\mathrm{C}} x'_{\mathrm{B}} x'_{\mathrm{C}} + \sum_{\mathrm{B},(a_i+b_i\leq n_i)} \kappa'^{R}_{\mathrm{A},\mathrm{B}} x'_{\mathrm{A}B} \\ &\quad - \sum_{\mathrm{B},(a_i+b_i\leq n_i)} \kappa'^{F}_{\mathrm{A},\mathrm{B}} x'_{\mathrm{A}} x'_{\mathrm{B}} - \frac{1}{2}\sum_{(\mathrm{B},\mathrm{C})\in I_{\mathrm{A}}} \kappa'^{R}_{\mathrm{B},\mathrm{C}} x'_{\mathrm{A}} - \phi'_{\mathrm{A}} x'_{\mathrm{A}}\end{aligned}$$

here,

$$\begin{aligned} x'_{\mathrm{A}} &= \frac{x_{\mathrm{A}}}{\omega} \\ \dot{x}'_{\mathrm{A}} &= \frac{\dot{x}_{\mathrm{A}}\tau}{\omega} \\ \kappa'^{F} &= \kappa^{F}\omega\tau \\ \kappa'^{R} &= \kappa^{R}\tau \\ \phi' &= \phi\tau \\ \beta' &= \beta\omega \end{aligned}$$

Outline

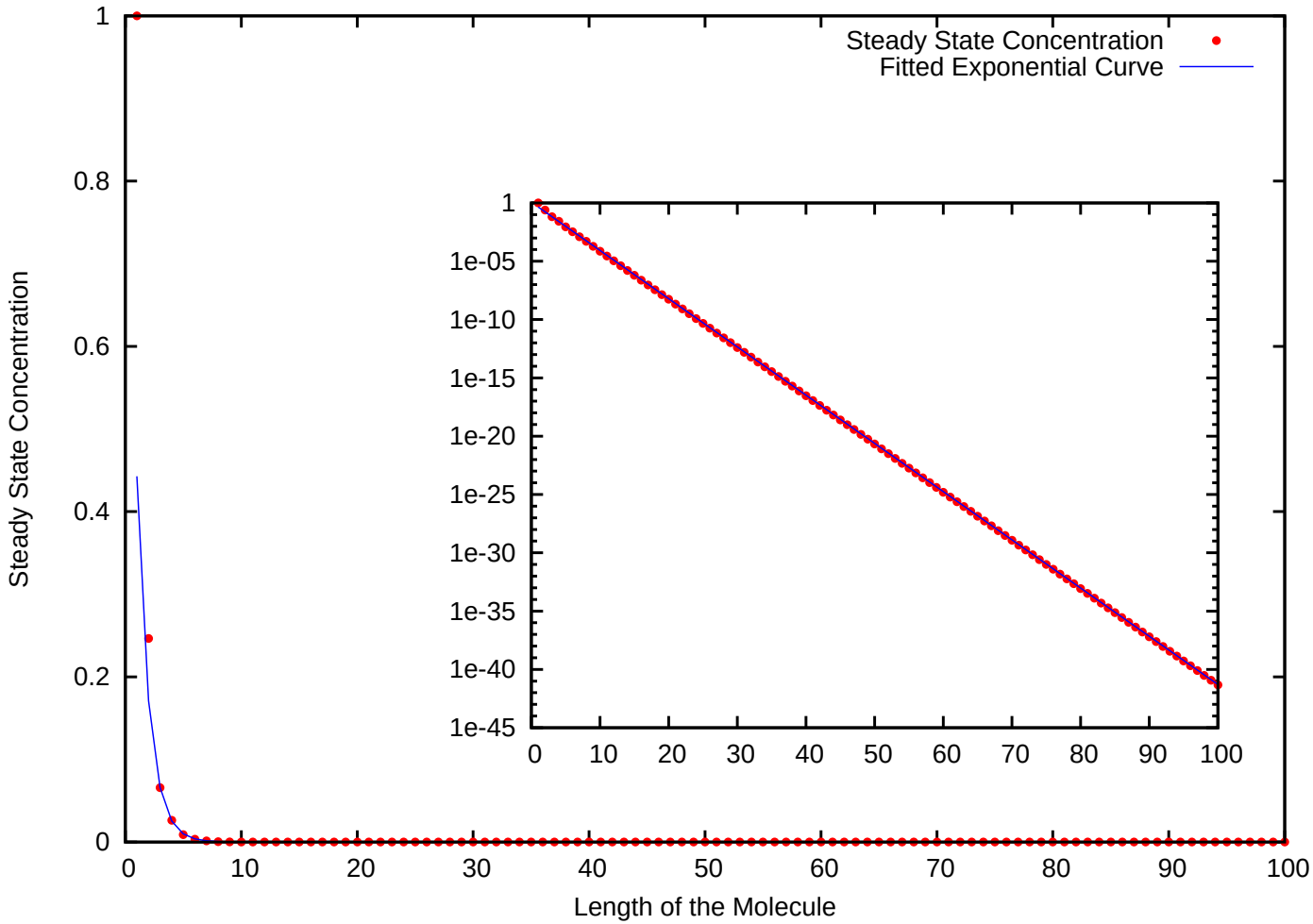
Time evolution of concentrations



$f = 1, n_1 = 100, \phi = 0.1, k_f = k_r = 0.05, x_{A(1)} = 1$

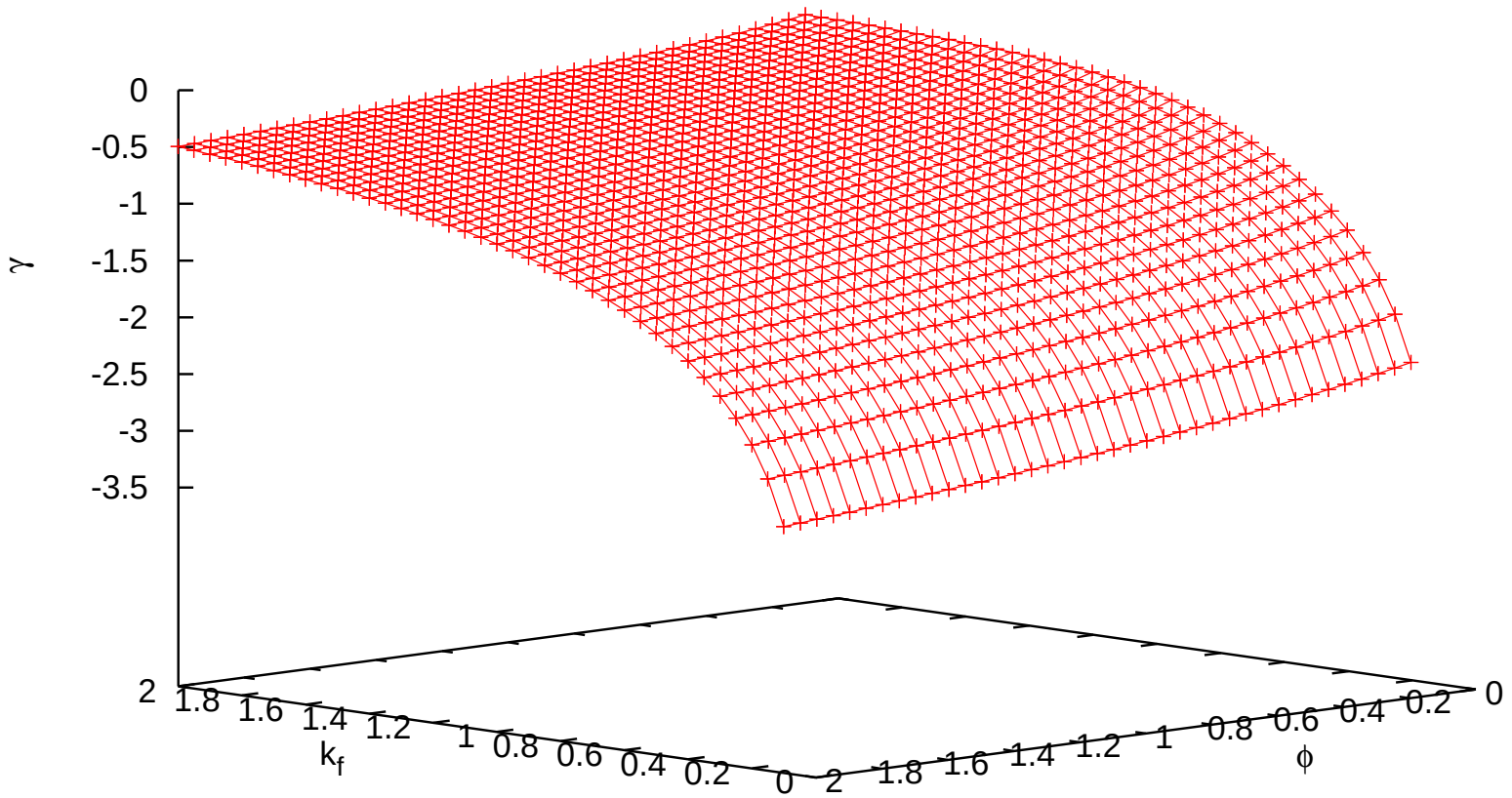
Time evolution of concentrations when there are only spontaneous reactions in the system.

Steady state concentration v/s Length



An exponential decay in concentrations is observed when there are no catalysed reactions in the network: $x_{\mathrm{A}(i)} \propto exp(\gamma \times i); \gamma = -0.952127$

Phase space portrait



γ versus k_f and ϕ,

keeping $k_r = 1$ and $x_{A(1)} = 1$

Dynamics with catalysed reactions in the network

- Random catalysis: We selected a fraction ρ of reactions from the network and assigned a catalyst to each one of them drawn randomly from the set $\mathcal{P}$.
- Doing so yields no significant effect on the concentrations. Steady state concentrations follow exponential decay with (approximately) the same γ as when there are no catalysed reactions.

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Dynamics with catalysed reactions in the network

Let us consider the following set of catalysed reactions in the network in addition to the spontaneous chemistry.

$$\mathrm{A}(1) + \mathrm{A}(1) \overset{A(2)}{\rightleftharpoons} \mathrm{A}(2)$$

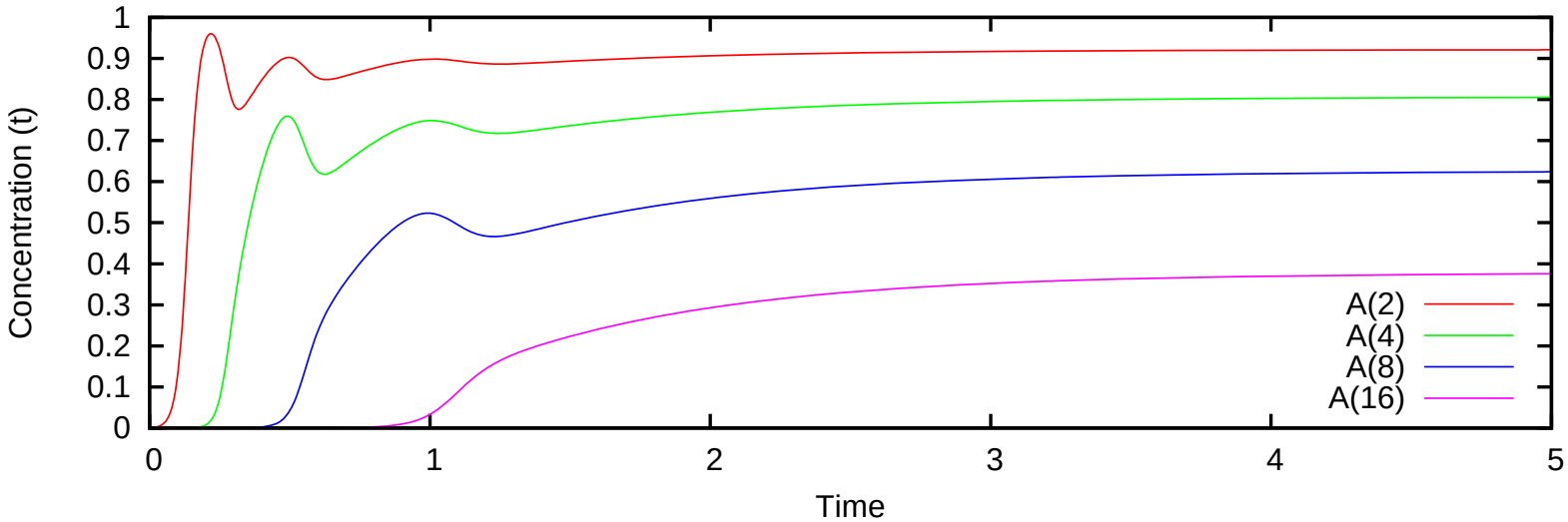
$$\mathrm{A}(2) + \mathrm{A}(2) \overset{A(4)}{\rightleftharpoons} \mathrm{A}(4)$$

$$\mathrm{A}(4) + \mathrm{A}(4) \overset{A(8)}{\rightleftharpoons} \mathrm{A}(8)$$

$$\mathrm{A}(8) + \mathrm{A}(8) \overset{A(16)}{\rightleftharpoons} \mathrm{A}(16)$$

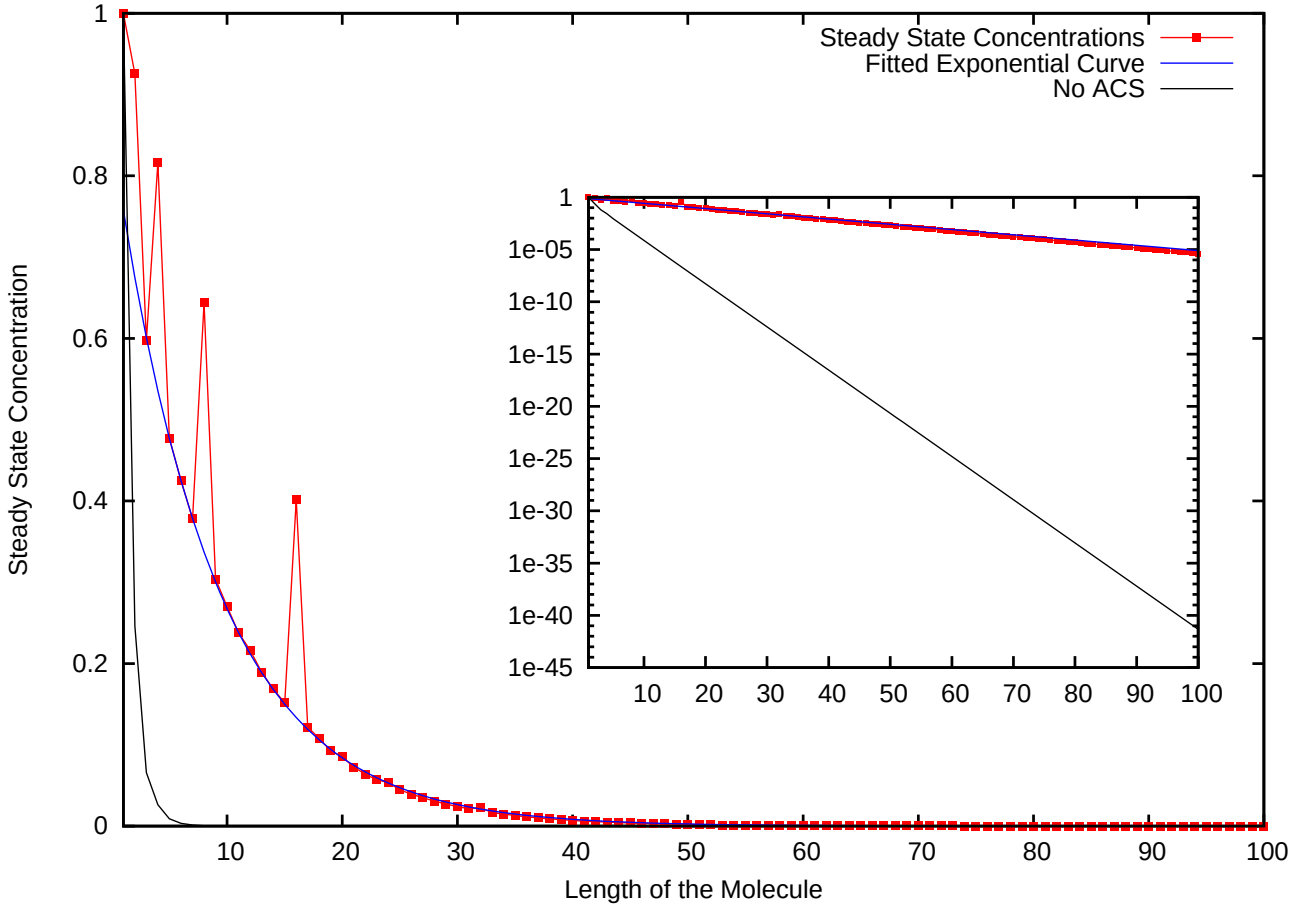
Set 1

Time evolution of concentrations



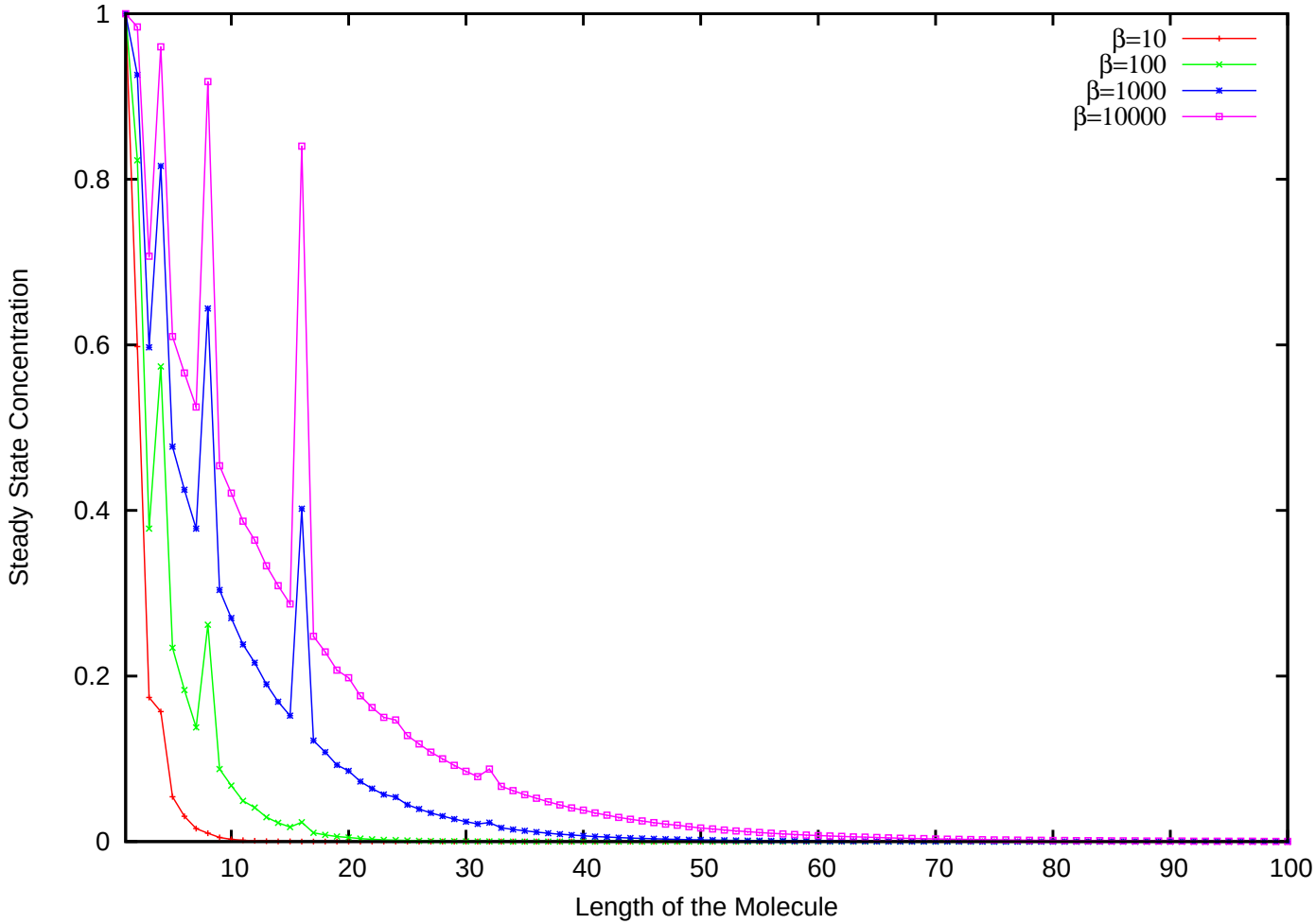
$f = 1, n_1 = 100, \phi = 0.1, k_f = k_r = 0.05, x_{A(1)} = 1, \beta = 1000$

Steady-state concentrations



The molecules produced in Set 1 outperform other species. Blue curve is the fitted exponential calculated by ignoring input molecule and the members produced in Set 1. $\gamma_{background} = -0.115635$

Effect of β on concentrations



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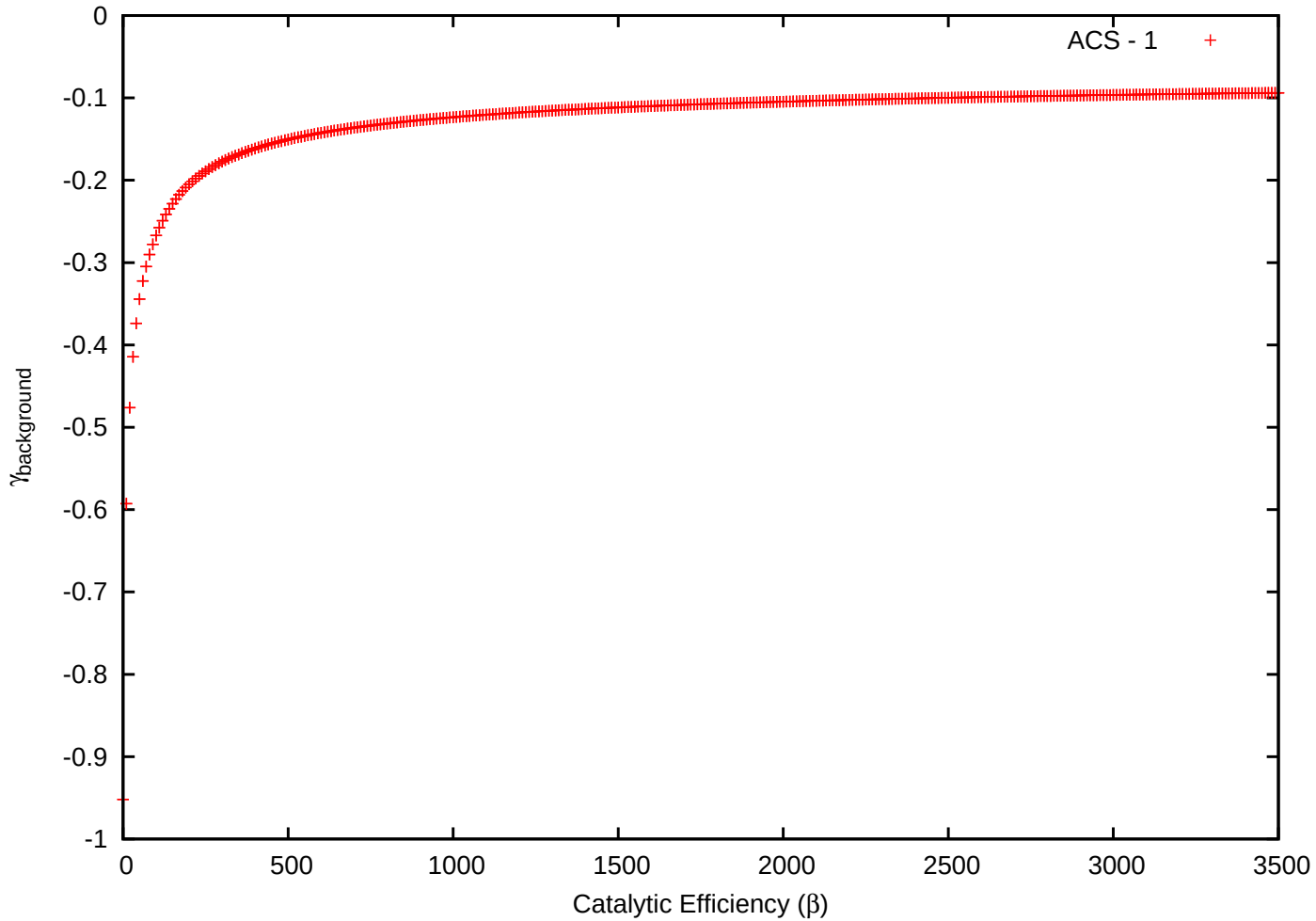

Auto-catalytic sets (ACS)

Definition

Consider a set $\mathcal{S} \subset \mathcal{P}$ of compounds such that for every member, s, of the set there exists a reaction that:

1. produces s
2. is catalyzed by a member of $\mathcal{S}$, and
3. has reactants drawn from $\mathcal{S} \cup \mathcal{F}$.

Such a set is an ACS.

Auto-catalytic sets (ACS)

$$\mathrm{A}(1) + \mathrm{A}(1) \underset{}{\overset{A(2)}{\rightleftharpoons}} \mathrm{A}(2)$$

$$\mathrm{A}(2) + \mathrm{A}(2) \underset{}{\overset{A(4)}{\rightleftharpoons}} \mathrm{A}(4)$$

$$\mathrm{A}(4) + \mathrm{A}(4) \underset{}{\overset{A(8)}{\rightleftharpoons}} \mathrm{A}(8)$$

$$\mathrm{A}(8) + \mathrm{A}(8) \underset{}{\overset{A(16)}{\rightleftharpoons}} \mathrm{A}(16)$$

Set 1

Here, $\mathcal{S} = \{\mathrm{A}(2), \mathrm{A}(4), \mathrm{A}(8), \mathrm{A}(16)\}$

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Set 1

Here, $\mathcal{S} = \{\mathrm{A}(2), \mathrm{A}(4), \mathrm{A}(8), \mathrm{A}(16)\}$

One may write several network topologies for a particular $\mathcal{S}$. Consider two such topologies for Set 1.

Different network topologies of Set 1

Set 1-1

$$\mathrm{A}(1) + \mathrm{A}(1) \underset{}{\overset{A(16)}{\rightleftharpoons}} \mathrm{A}(2)$$
$$\mathrm{A}(2) + \mathrm{A}(2) \underset{}{\overset{A(8)}{\rightleftharpoons}} \mathrm{A}(4)$$
$$\mathrm{A}(4) + \mathrm{A}(4) \underset{}{\overset{A(4)}{\rightleftharpoons}} \mathrm{A}(8)$$
$$\mathrm{A}(8) + \mathrm{A}(8) \underset{}{\overset{A(2)}{\rightleftharpoons}} \mathrm{A}(16)$$

Set 1-2

$$\mathrm{A}(1) + \mathrm{A}(1) \underset{}{\overset{A(16)}{\rightleftharpoons}} \mathrm{A}(2)$$
$$\mathrm{A}(2) + \mathrm{A}(2) \underset{}{\overset{A(16)}{\rightleftharpoons}} \mathrm{A}(4)$$
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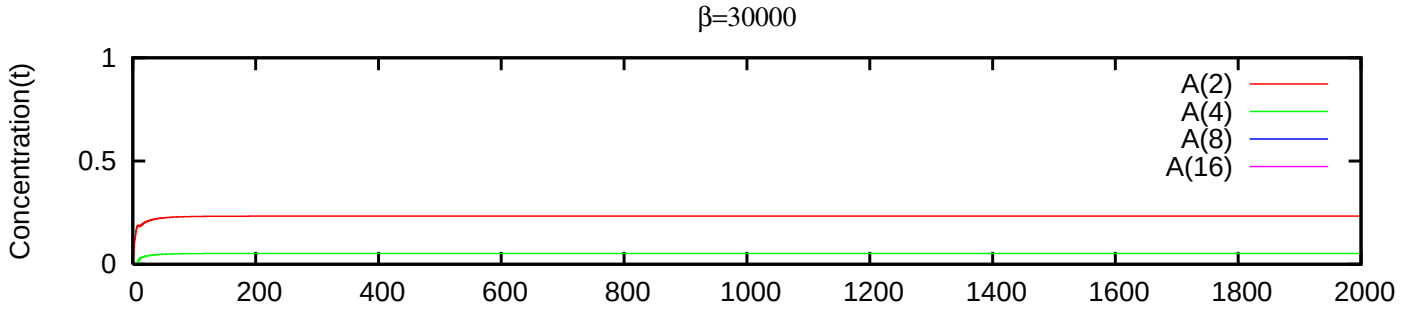
$$\mathcal{S} = \{\mathrm{A}(2), \mathrm{A}(4), \mathrm{A}(8), \mathrm{A}(16)\}$$

Time evolution of concentrations for different β (Set 1-1)



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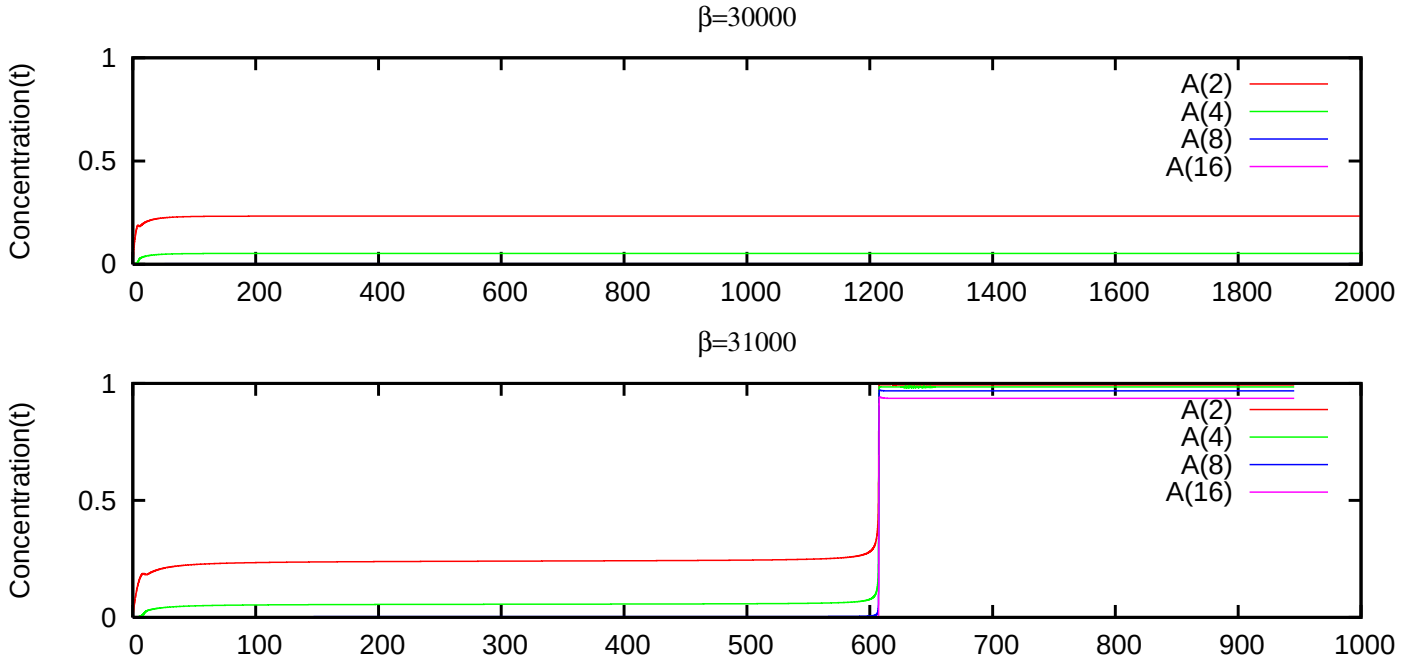

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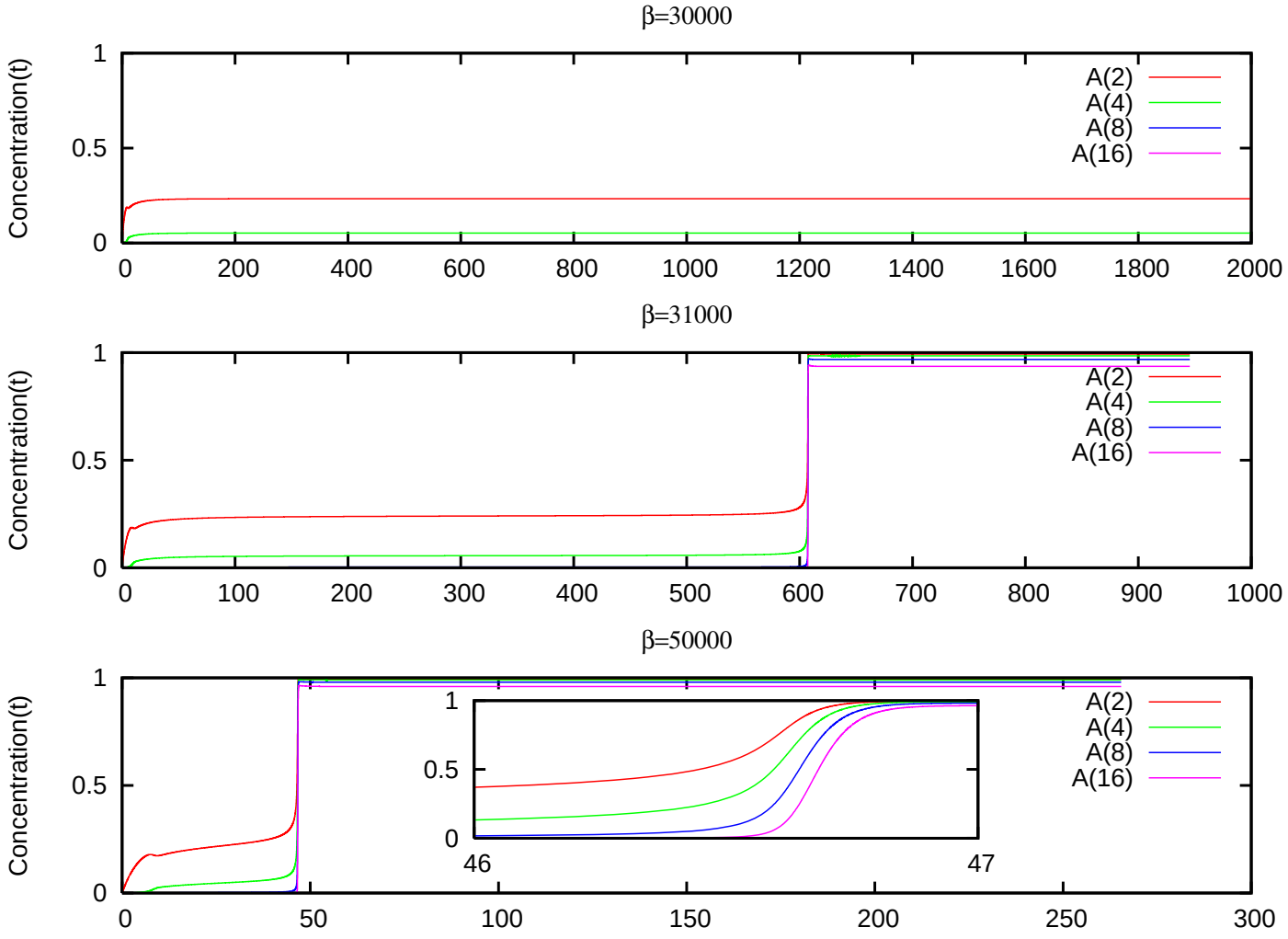
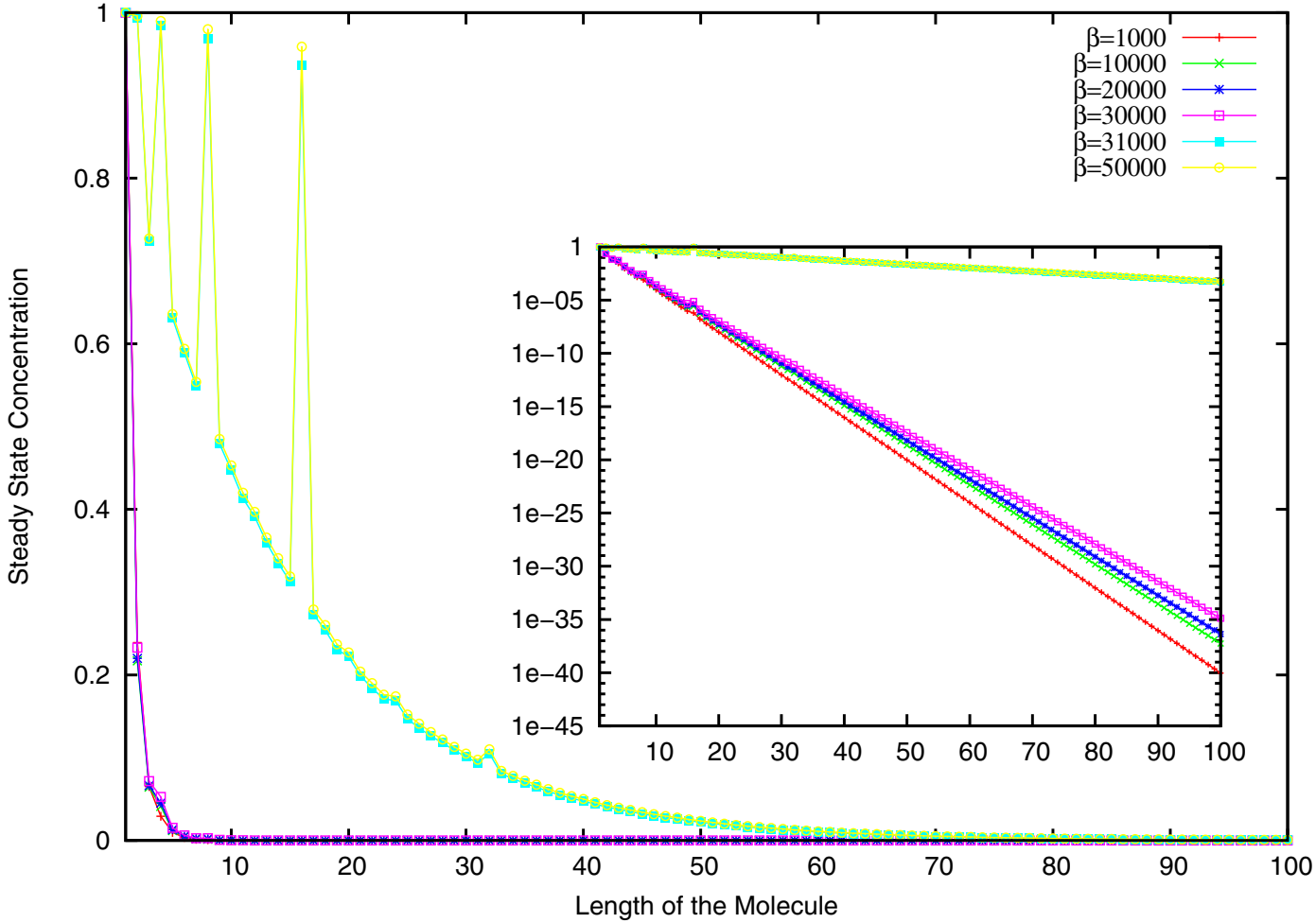
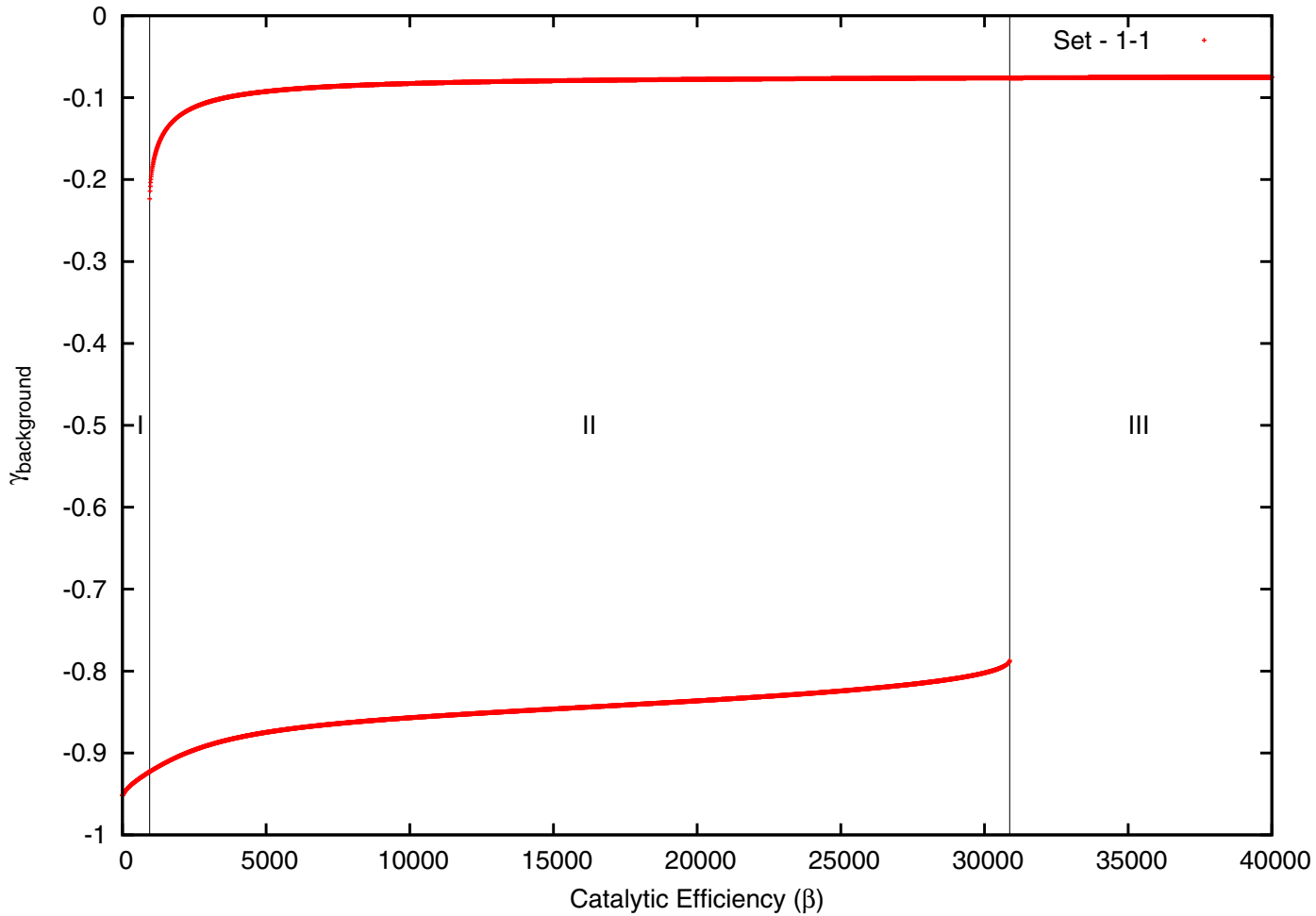


Set 1-1 only dominates above a threshold value.

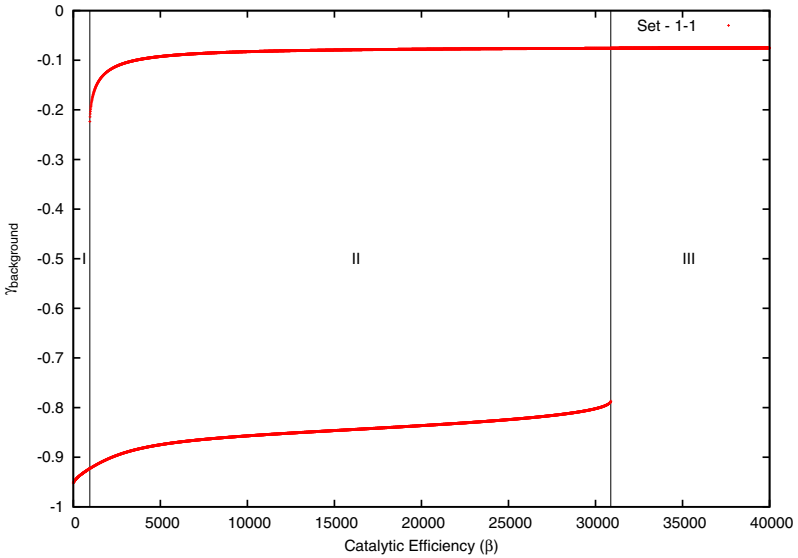
Steady state concentrations



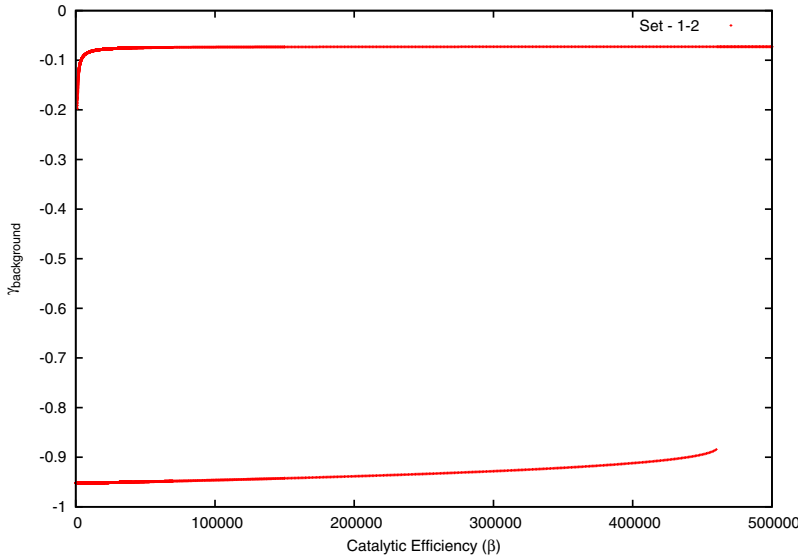
$\gamma_{background}$ v/s β



$\gamma_{background}$ v/s β

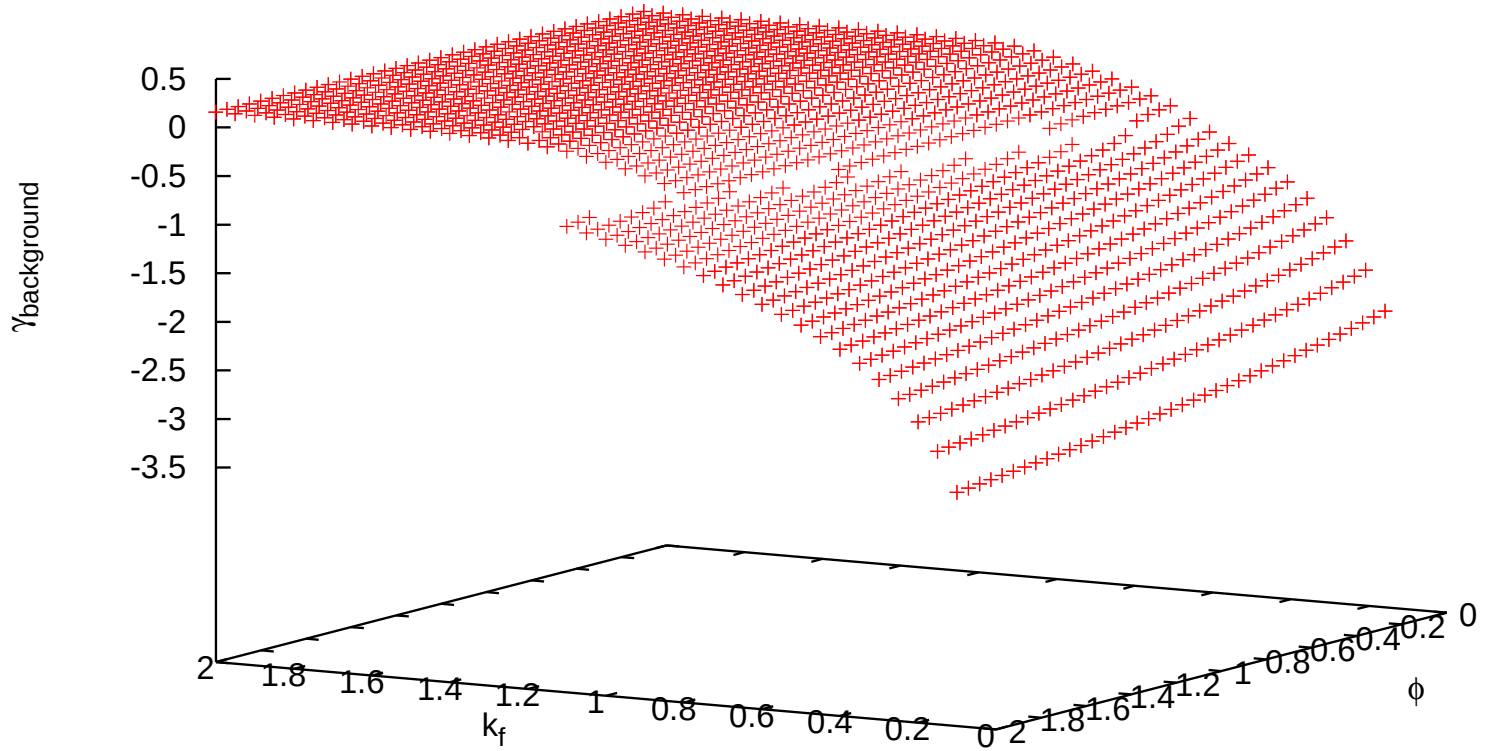


Set 1-1



Set 1-2

Phase portrait



$\gamma_{background}$ versus k_f and ϕ for a fixed β (=10,000), keeping $k_r = 1$ and $x_{A(1)} = 1$

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- When a large molecule is a catalyst for production of smaller molecules it can create a bottleneck. And hence require bigger β for domination of ACS.
- How does ACS domination depends on topology of catalysed network?

Network topology and ACS domination

- Define length of an ACS as the length of the largest molecule in the ACS. Consider the topology of catalytic network in which the largest molecule of the ACS acts as the catalyst for all the reactions that produce members of the ACS.

Network topology and ACS domination

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- For example, consider following topology of $\mathcal{S}$ (Set 1-2), wherein all the reactions are catalysed by the same catalyst (the largest molecule of the set):

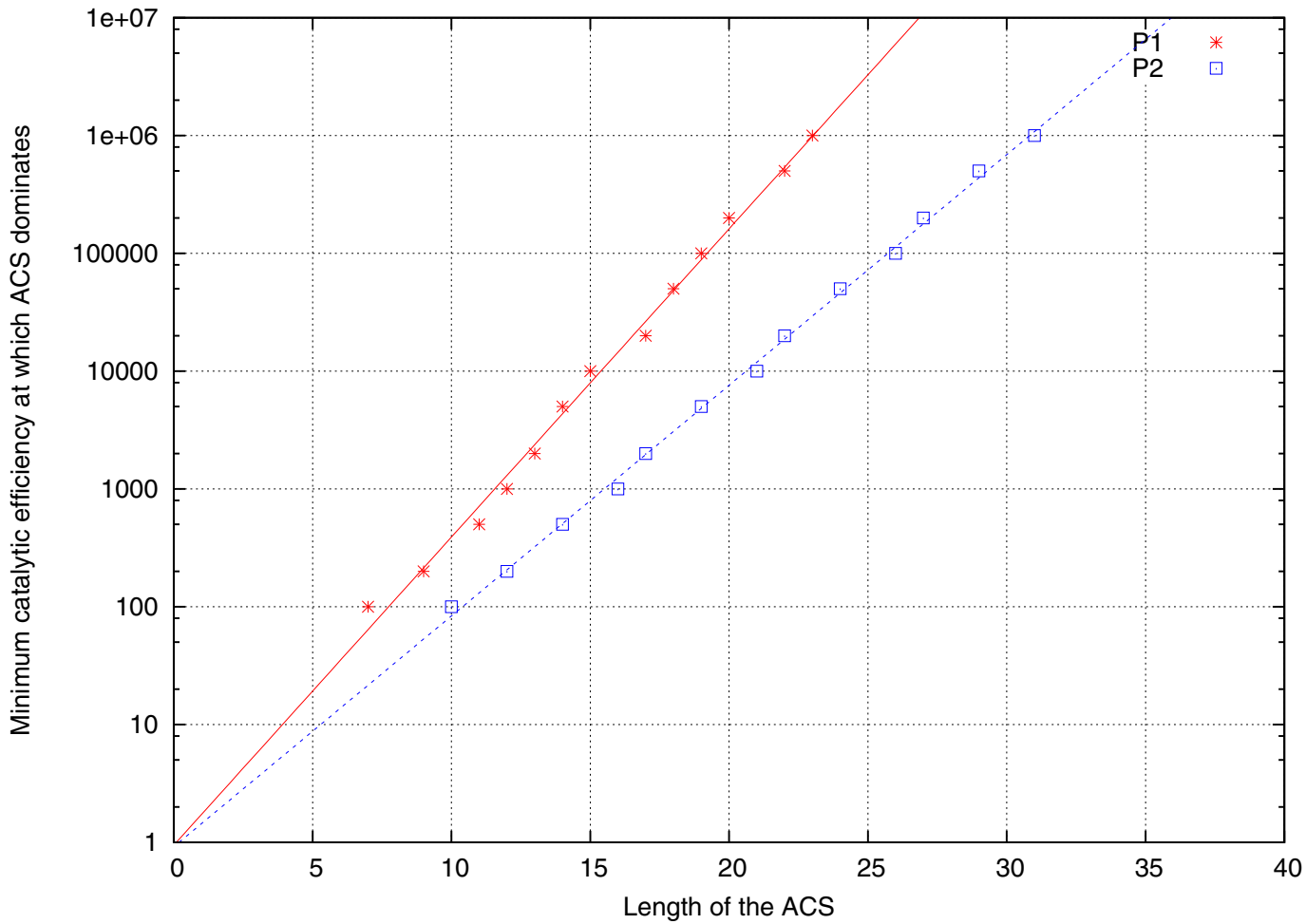
$$\mathrm{A}(1) + \mathrm{A}(1) \overset{A(16)}{\rightleftharpoons} \mathrm{A}(2)$$

$$\mathrm{A}(2) + \mathrm{A}(2) \overset{A(16)}{\rightleftharpoons} \mathrm{A}(4)$$

$$\mathrm{A}(4) + \mathrm{A}(4) \overset{A(16)}{\rightleftharpoons} \mathrm{A}(8)$$

$$\mathrm{A}(8) + \mathrm{A}(8) \overset{A(16)}{\rightleftharpoons} \mathrm{A}(16)$$

Length of ACS v/s Catalytic efficiency required for it to dominate



P1: $k_f = k_r = \phi = 0.05$, P2: $k_f = k_r = 0.1, \phi = 0.05$

Concentrating bigger ACSs

Set A

$$\mathrm{A}(1) + \mathrm{A}(1) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(2)$$

$$\mathrm{A}(2) + \mathrm{A}(2) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(4)$$

$$\mathrm{A}(4) + \mathrm{A}(4) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(8)$$

$$\mathrm{A}(8) + \mathrm{A}(8) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(16)$$

$$\mathrm{A}(16) + \mathrm{A}(16) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(32)$$

$$\mathrm{A}(32) + \mathrm{A}(32) \underset{}{\overset{A(64)}{\rightleftharpoons}} \mathrm{A}(64)$$

ACS is {A(2), A(4), A(8), A(16), A(32), A(64)}.

Concentrating bigger ACSs

Set A

$$\mathrm{A}(1) + \mathrm{A}(1) \xrightarrow{A(64)} \mathrm{A}(2)$$

$$\mathrm{A}(2) + \mathrm{A}(2) \xrightarrow{A(64)} \mathrm{A}(4)$$

$$\mathrm{A}(4) + \mathrm{A}(4) \xrightarrow{A(64)} \mathrm{A}(8)$$

$$\mathrm{A}(8) + \mathrm{A}(8) \xrightarrow{A(64)} \mathrm{A}(16)$$

$$\mathrm{A}(16) + \mathrm{A}(16) \xrightarrow{A(64)} \mathrm{A}(32)$$

$$\mathrm{A}(32) + \mathrm{A}(32) \xrightarrow{A(64)} \mathrm{A}(64)$$

ACS is {A(2), A(4), A(8), A(16), A(32), A(64)}.

Set B

$$\mathrm{A}(1) + \mathrm{A}(1) \xrightarrow{A(10)} \mathrm{A}(2)$$

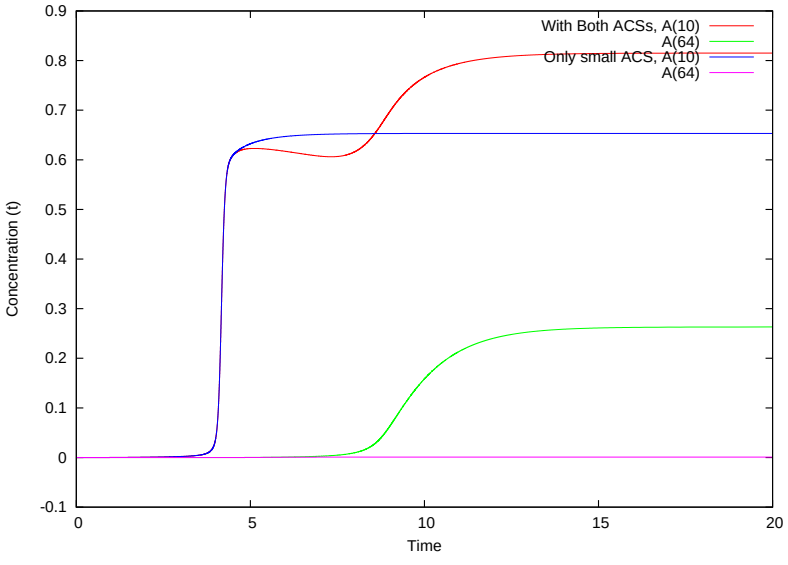
$$\mathrm{A}(1) + \mathrm{A}(2) \xrightarrow{A(10)} \mathrm{A}(3)$$

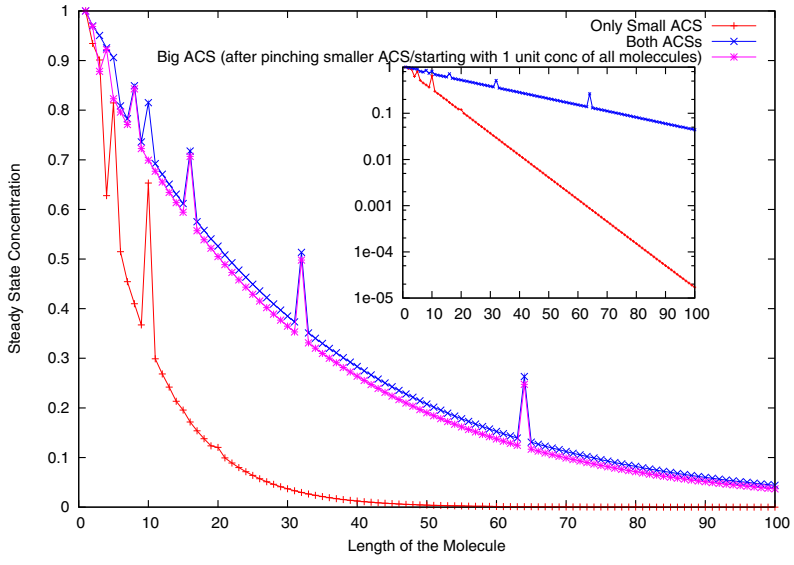
$$\mathrm{A}(2) + \mathrm{A}(3) \xrightarrow{A(10)} \mathrm{A}(5)$$

$$\mathrm{A}(5) + \mathrm{A}(5) \xrightarrow{A(10)} \mathrm{A}(10)$$

ACS is {A(2), A(3), A(5), A(10)}.

Big and small ACS





$$k_f = k_r = \phi = 1, \beta_{A10} = 800, \beta_{A64} = 50000$$

Outline

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Summary of results

- Molecular species produced in an autocatalytic networks can outperform other species.
- This behaviour is dependent on the strength/efficiency of the catalysts and the topology of the catalytic-reaction network.
- System can also exhibit bistability.
- A cascade of ACSs can be used to produce large molecules in sufficient numbers with reasonable catalytic efficiencies.
- Similar results are observed for two input species ($f = 2$).

Conclusions

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- Provides a mechanism via which long molecules could have been produced in sufficient numbers.
- Biochemistry is a very sparse subset of organic chemistry. This provides a mechanistic way via which a small subset of chemistry could have been chosen.

Thank you.