Dynamische Strukturbildung und Systemrisiko in biologischen Systeme

Peter Schuster

Institut für Theoretische Chemie, Universität Wien, Austria
and
The Santa Fe Institute, Santa Fe, New Mexico, USA

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Web-Page für weitere Informationen:

http://www.tbi.univie.ac.at/~pks

Peter Schuster. 2015. Ebola – Challenge and Revival of Theoretical Epidemiology. *Complexity* **20**(5):7-12

Peter Schuster. 2016. Major Transitions in Evolution and Technology. *Complexity* **21**(4):7-13

Peter Schuster. 2016. Some Mechanistic Requirements for Major Transitions. *Phil.Trans.R.Soc.B* **371**(1701):e20150439

Peter Schuster. 2016. Increase in Complexity and Information through Molecular Evolution. *Entropy* **18**(11):e397

Autocatalysis is rare in chemistry but obligatory in biology.

Biological organisms store information in encoded form and have a record of their history.

Particle numers are large in chemistry and small in biology.

Stochastic phenomena have relatively little importance in chemistry but dominate biology.

What distiguishes biology from chemistry?

Sources of risk relevant uncertainties in predictions:

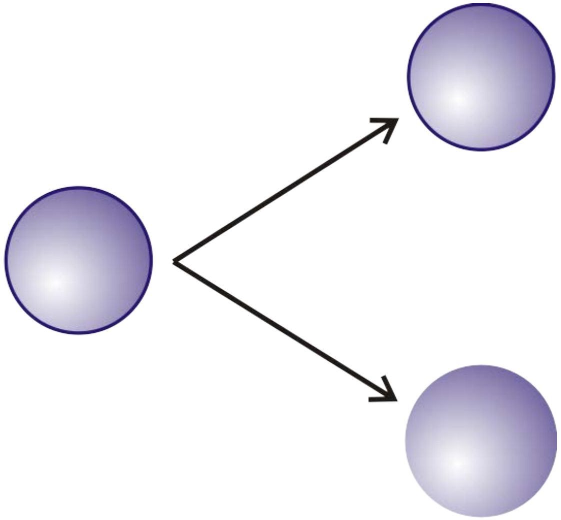
(i) exponential growth,

(ii) complex internal dynamics,

(iii) multiple quasistationary states,

(iv) reintroduction of extiguished species.

Autocatalysis, exponential growth, and prediction

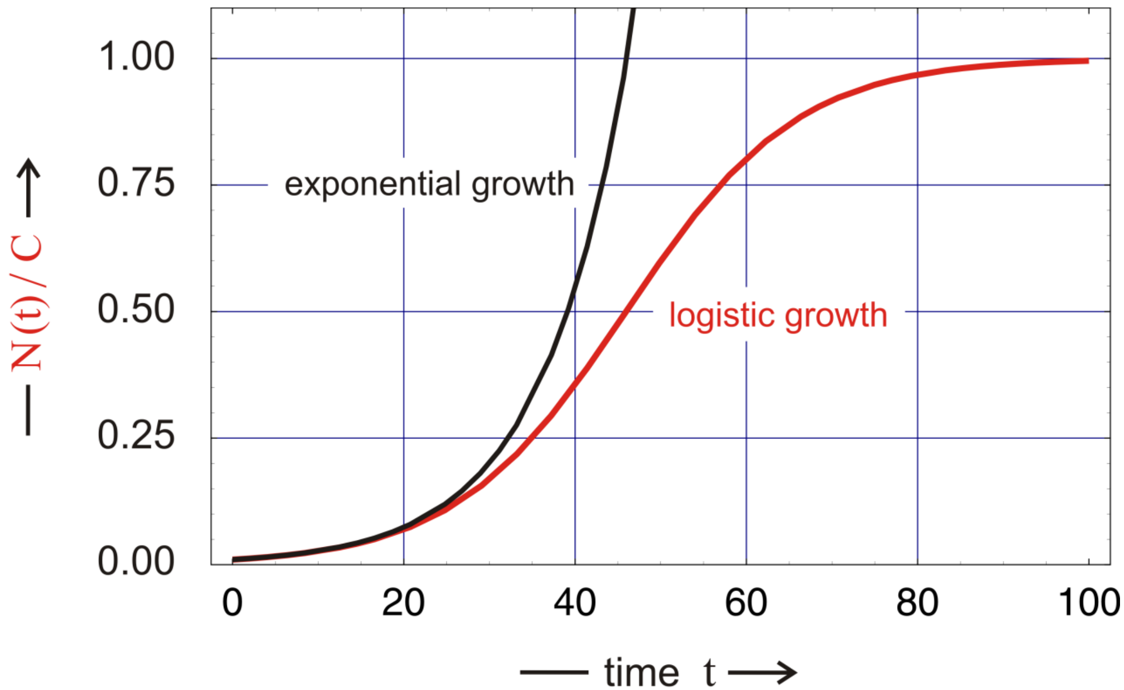


(A) + X = 2 X

$$\frac{dN}{dt} = f\,x \quad \Rightarrow \quad N(t) = N(0)\,e^{f\,t}$$

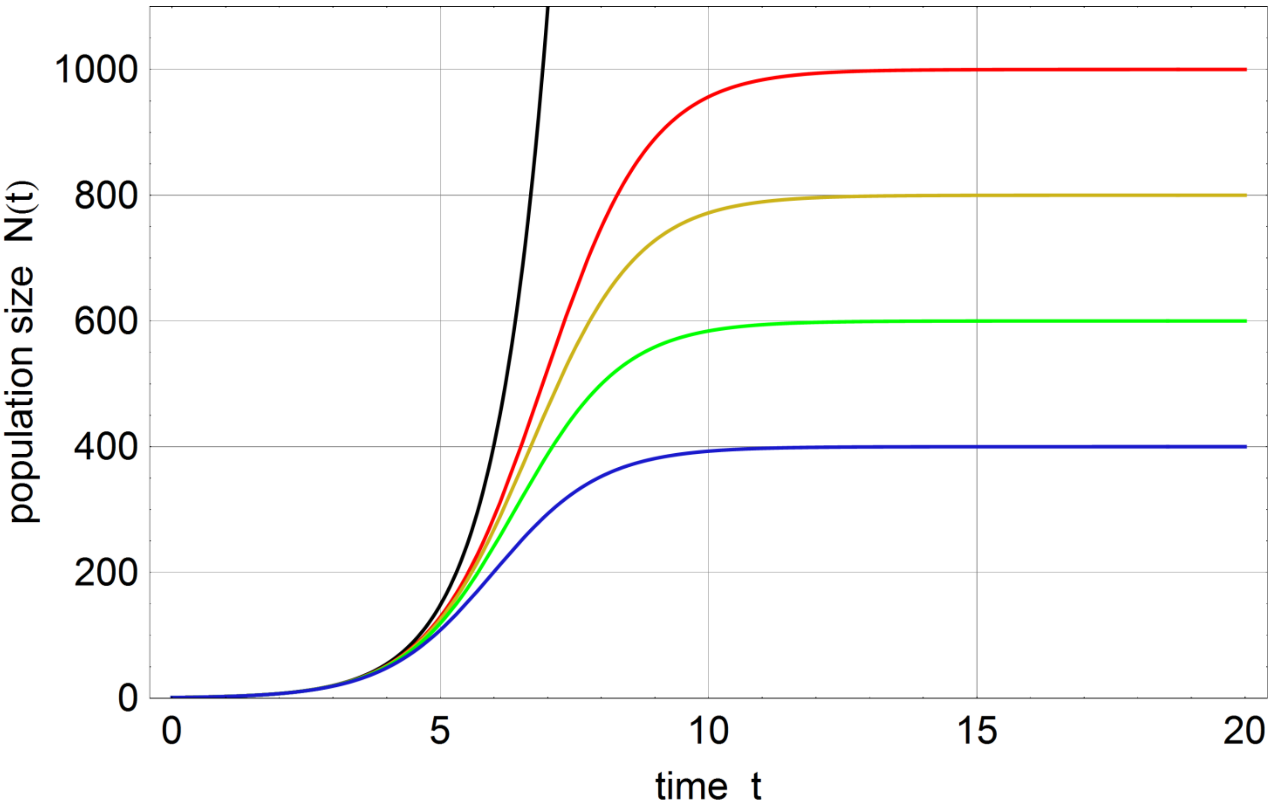
exponential growth

Pierre-François Verhulst,
1804 - 1849



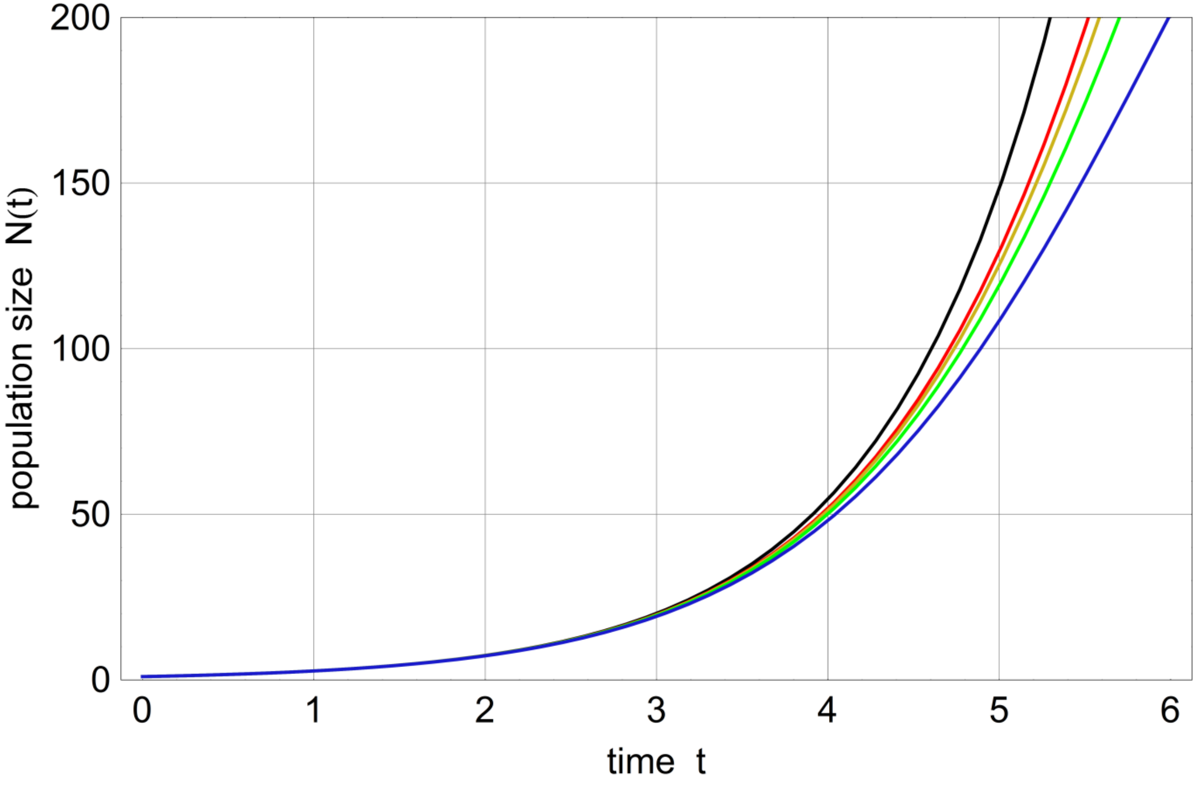
$$\frac{dN}{dt} = f\,N\left(1 - \frac{N}{C}\right) \quad \Rightarrow \quad N(t) = N(0)\,\frac{C}{N(0) + \big(C - N(0)\big)e^{-f\,t}}$$

The logistic equation has been conceived in 1838.



Logistic growth with different carrying capacity:

C = ∞ , 1000, 800, 600, 400

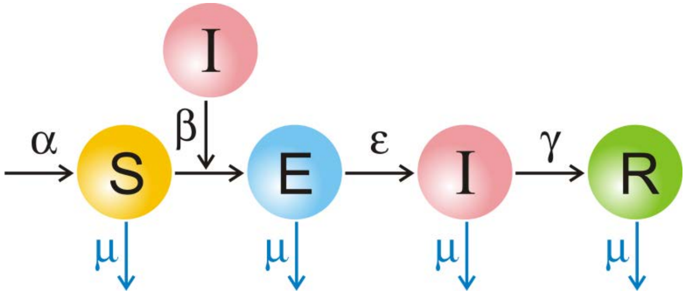


Enlargment of the logistic curves:

C = ∞ , 1000, 800, 600, 400

A.A. King, M.D. de Cellès, F.M.G. Magpantay, P. Rohani. Avoidable errors in the modelling of outbreaks of emerging pathogens, with special reference to Ebola. Proc.Roy.Soc.B 282:e20150347

Complex dynamics and prediction



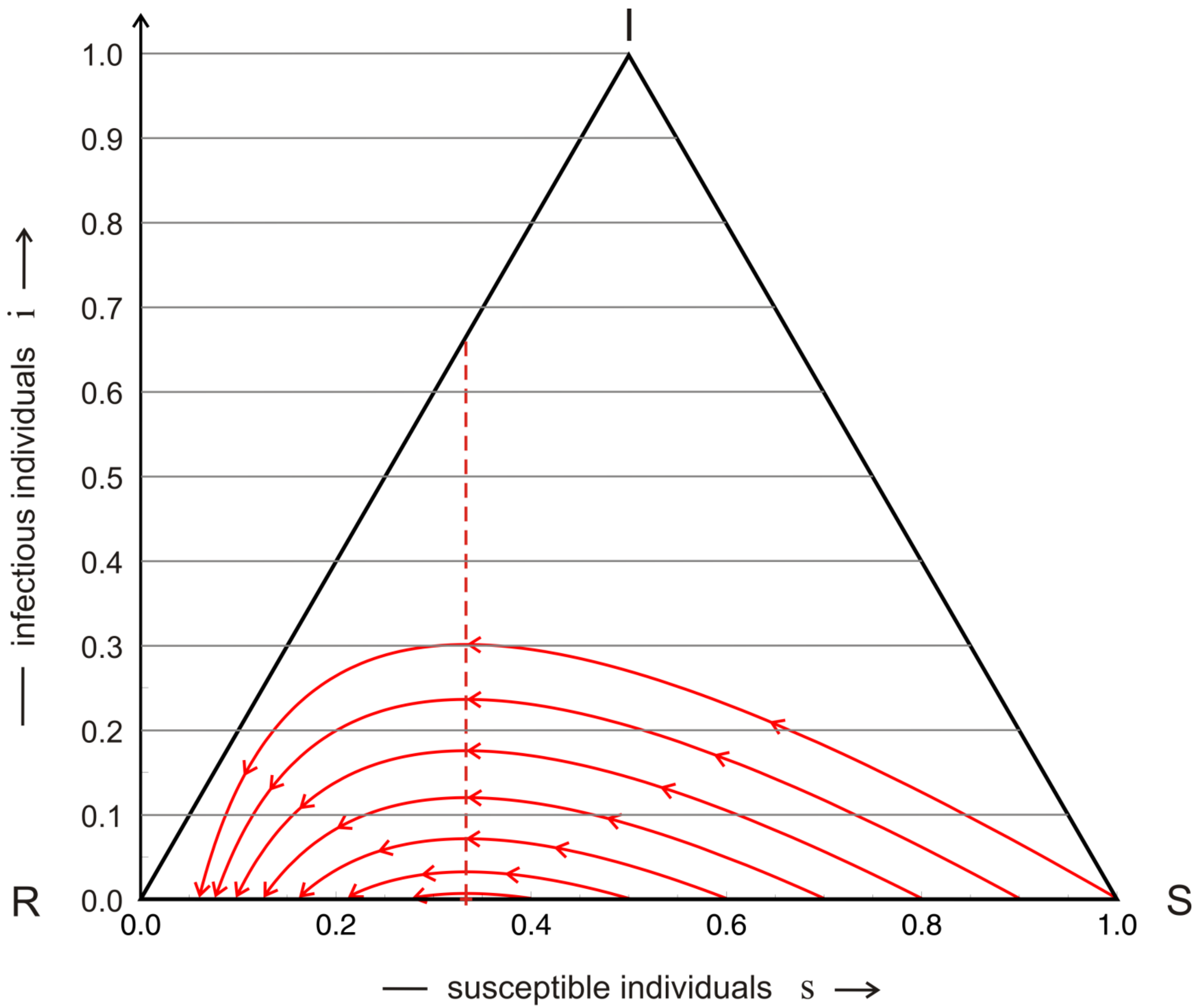
$$\frac{dS}{dt} = \alpha - \beta S I - \mu S$$

$$\frac{dE}{dt} = \beta S I - \varepsilon E - \mu E$$

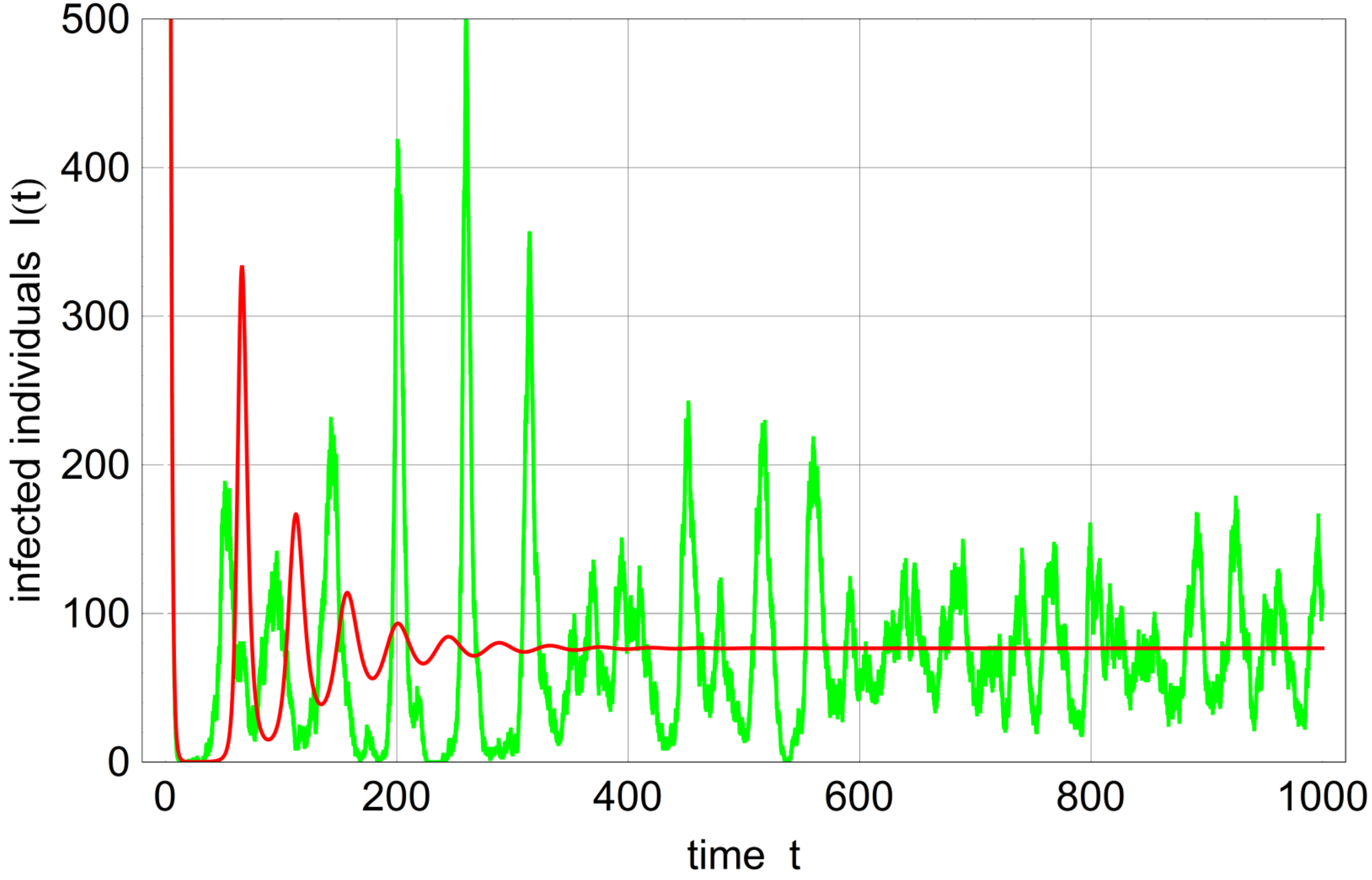
$$\frac{dI}{dt} = \varepsilon E - \gamma I - \mu I$$

$$\frac{dR}{dt} = \gamma I - \mu R$$

The SEIR model of theoretical epidemiology



I
R
S
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
0.2
0.4
0.6
0.8
1.0
— infectious individuals i ⟶
— susceptible individuals s ⟶

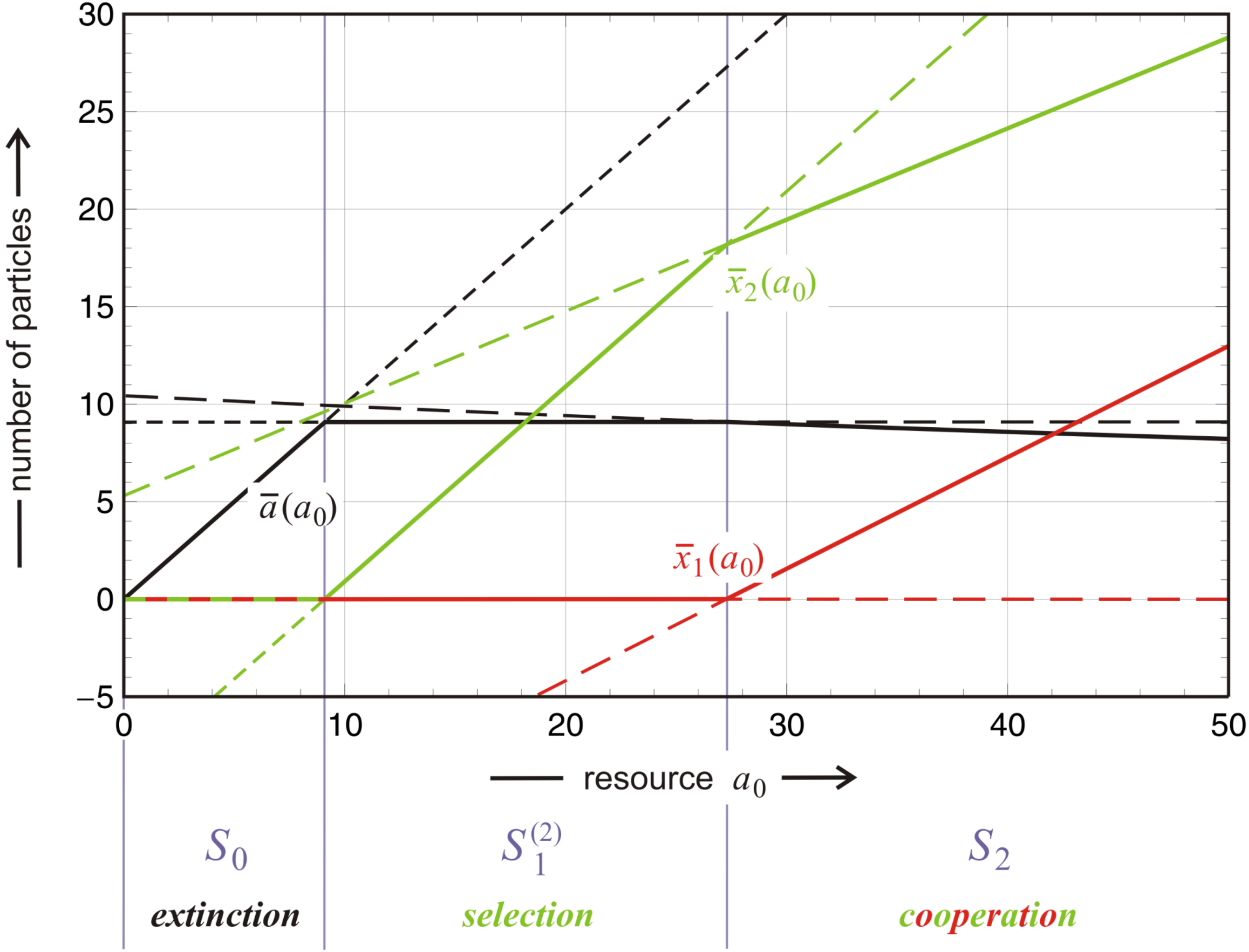


The SEIR model: ODE integration and stochastic simulation

Stochastic phenomena at small particle numbers

$$
\begin{aligned}
\star &\xrightarrow{a_0 \cdot r} A \\
A + X_1 &\xrightarrow{k_1} 2\,X_1 \\
A + X_2 &\xrightarrow{k_2} 2\,X_2 \\
A + X_1 + X_2 &\xrightarrow{l_1} 2\,X_1 + X_2 \\
A + X_2 + X_1 &\xrightarrow{l_2} 2\,X_2 + X_1 \\
A &\xrightarrow{r} \varnothing \\
X_1 &\xrightarrow{r} \varnothing \\
X_2 &\xrightarrow{r} \varnothing
\end{aligned}
$$

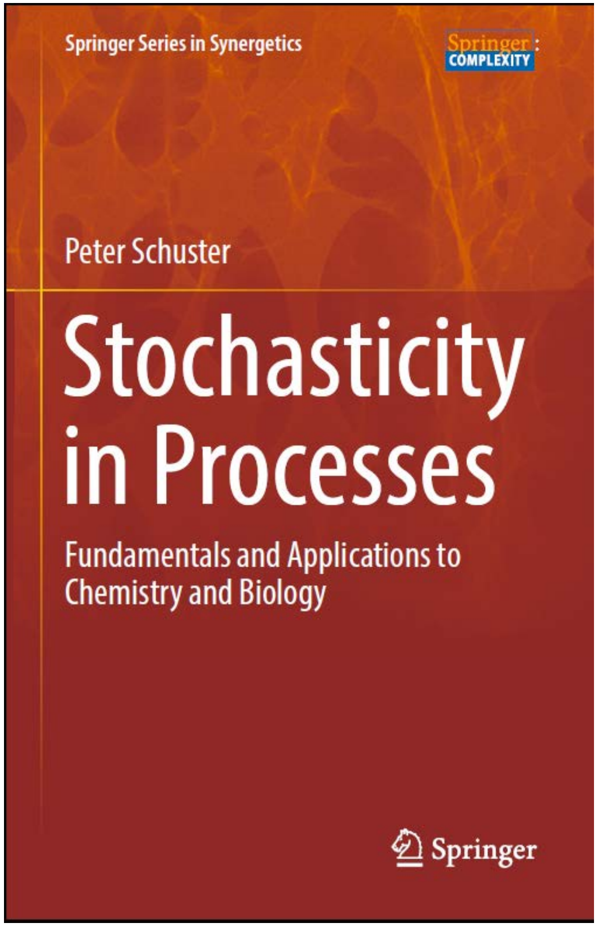
Reproduction and catalyzed reproduction of two species



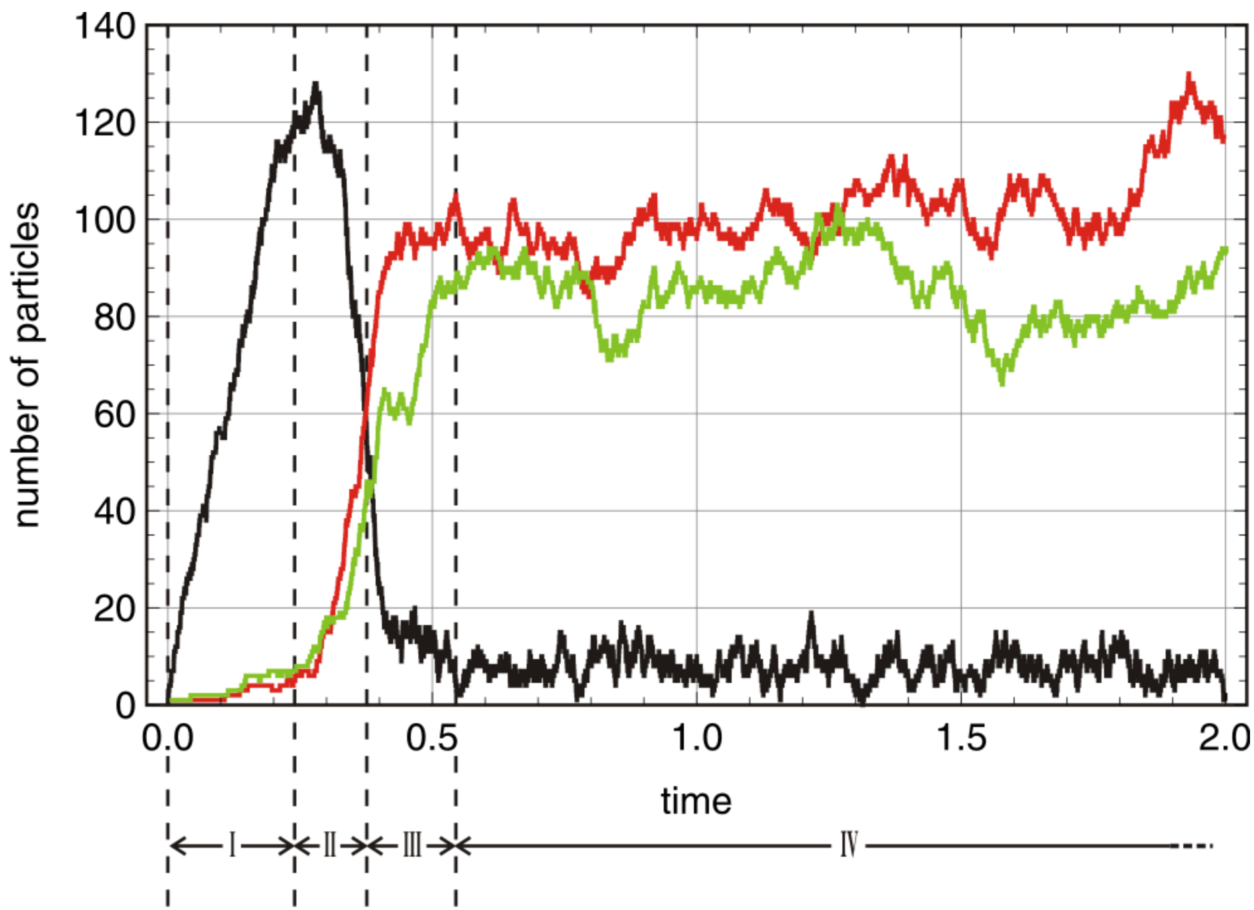
30
25
20
15
10
5
0
−5
0
10
20
30
40
50
number of particles
resource a_0
$\bar{a}(a_0)$
$\bar{x}_2(a_0)$
$\bar{x}_1(a_0)$
S_0
$S_1^{(2)}$
S_2
extinction
selection
cooperation

Stochastic modeling of chemical and biological systems

Stochastic simulation: D.T. Gillespie, Annu.Rev.Phys.Chem. 58:35-55, 2007



Peter Schuster. Stochasticity in Processes. Fundamentals and Applications in Chemistry and Biology. Springer-Verlag, Berlin 2016

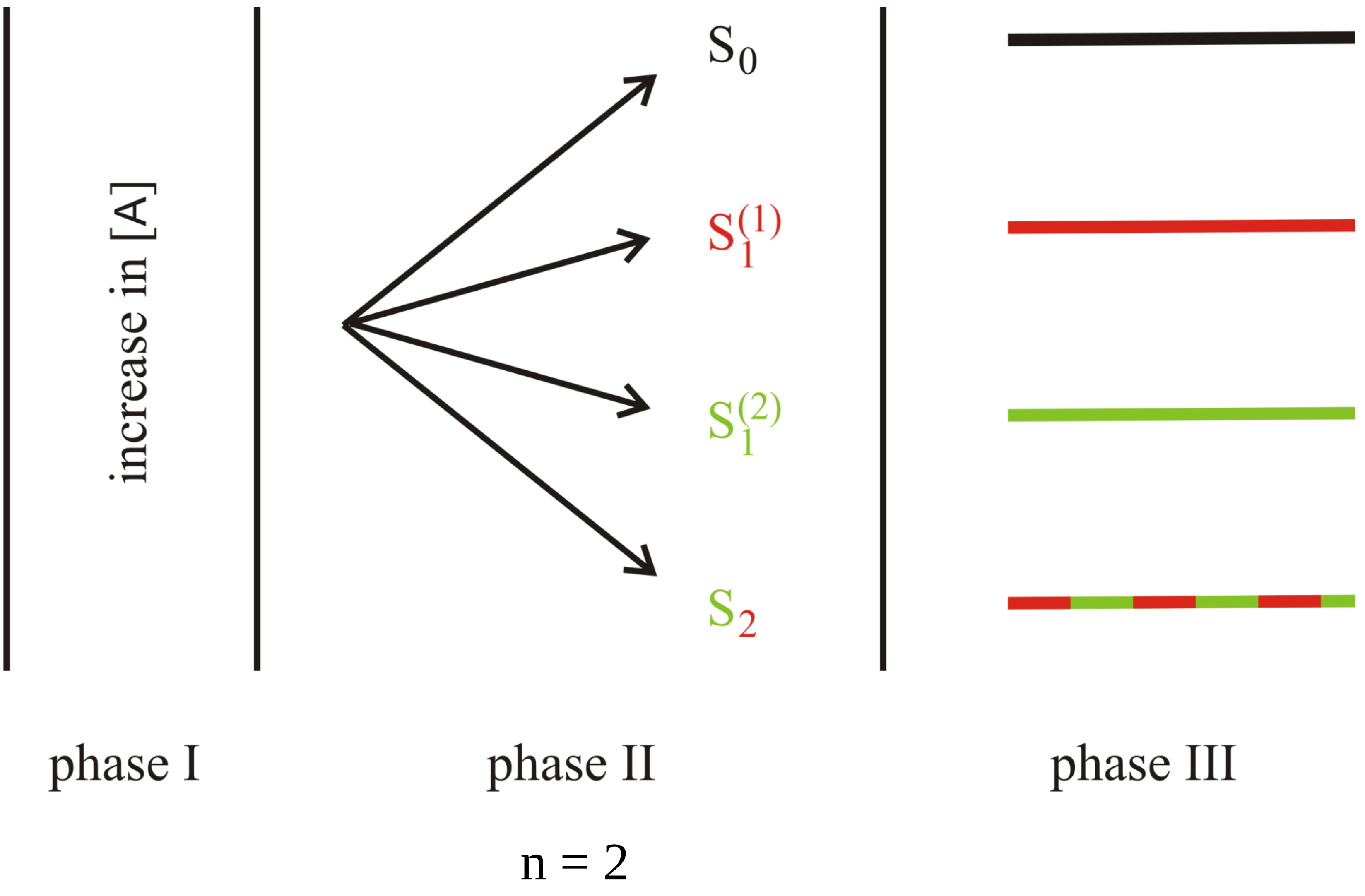


phase I: raise of [**A**]

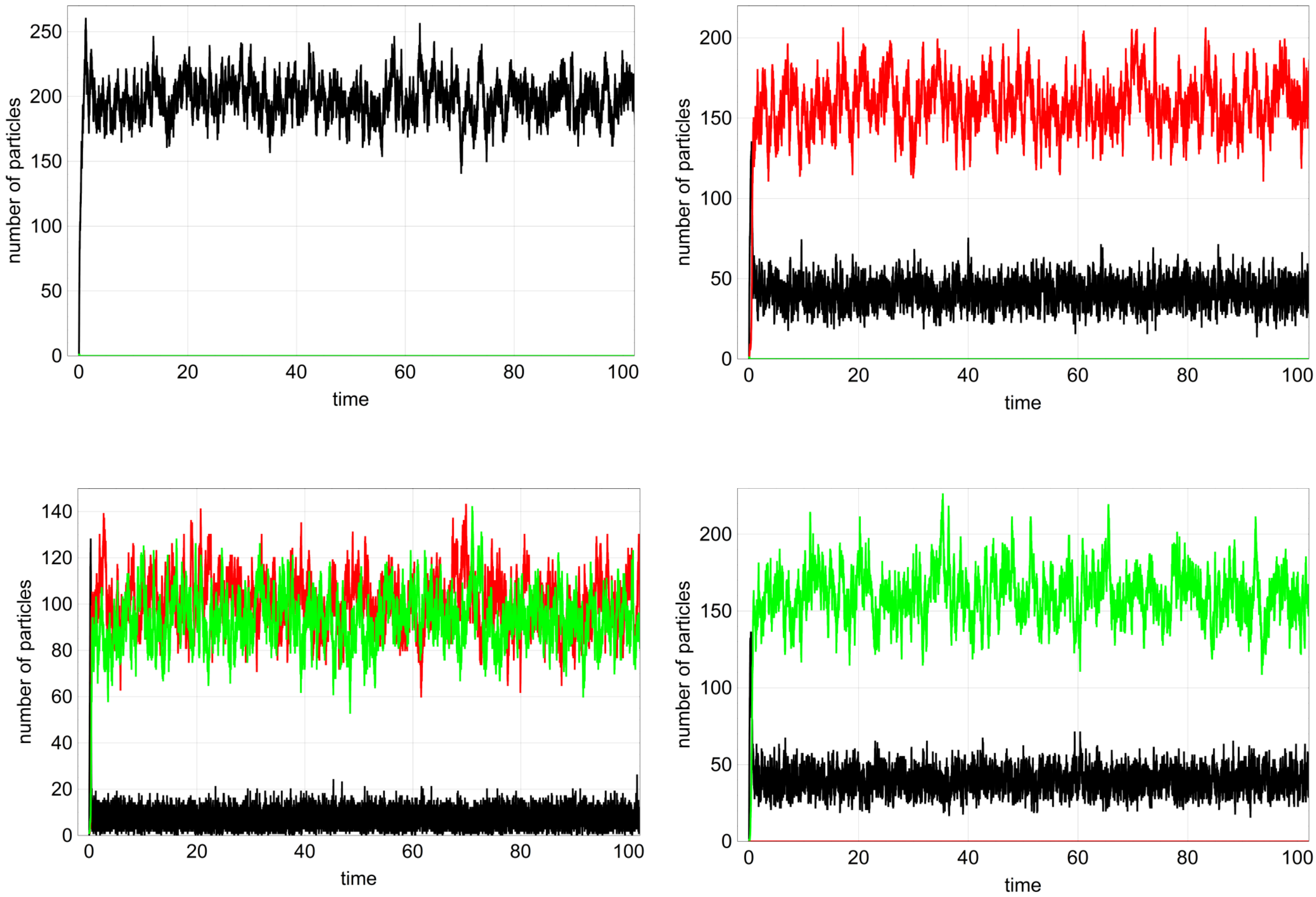
phase II: random choice of quasistationary state

phase III: convergence to the quasistationary state

phase IV: fluctuations around the quasistationary state



Random decision in the stochastic process



Competition and cooperation with $n = 2$

Initial values		Final states			
$X_1(0)$	$X_2(0)$	N_{S_0}	$N_{S_1^{(1)}}$	$N_{S_1^{(2)}}$	N_{S_2}
1	1	385.1 ± 23.6	1481.0 ± 36.8	1719.6 ± 37.8	6414.3 ± 53.8
2	2	14.9 ± 2.6	303.7 ± 16.0	354.5 ± 23.8	9326.8 ± 22.7
3	3	0	70.2 ± 10.0	106.2 ± 10.9	9823.4 ± 15.7
4	4	0	12.1 ± 2.6	28.0 ± 5.0	9959.9 ± 6.4

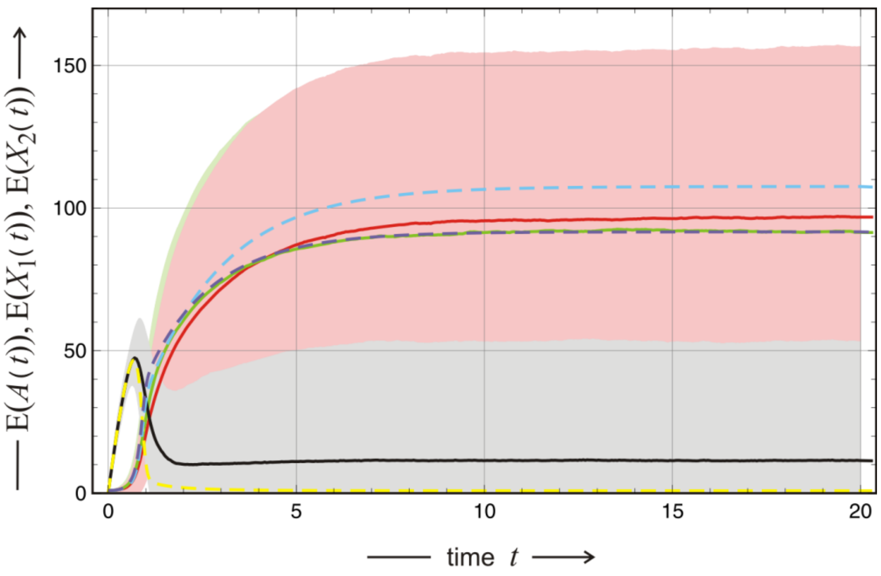
Choice of parameters: k_1 = 0.011 [$M^{-1}t^{-1}$]; k_2 = 0.009 [$M^{-1}t^{-1}$];

l_1 = 0.0050 [$M^{-2}t^{-1}$]; l_2 = 0.0045 [$M^{-2}t^{-1}$];

a_0 = 200; r = 0.5 [Vt^{-1}]; $a(0) = 0$

Competition and cooperation with $n = 2$

$a(0) = 0,\ x_1(0) = x_2(0) = 1$

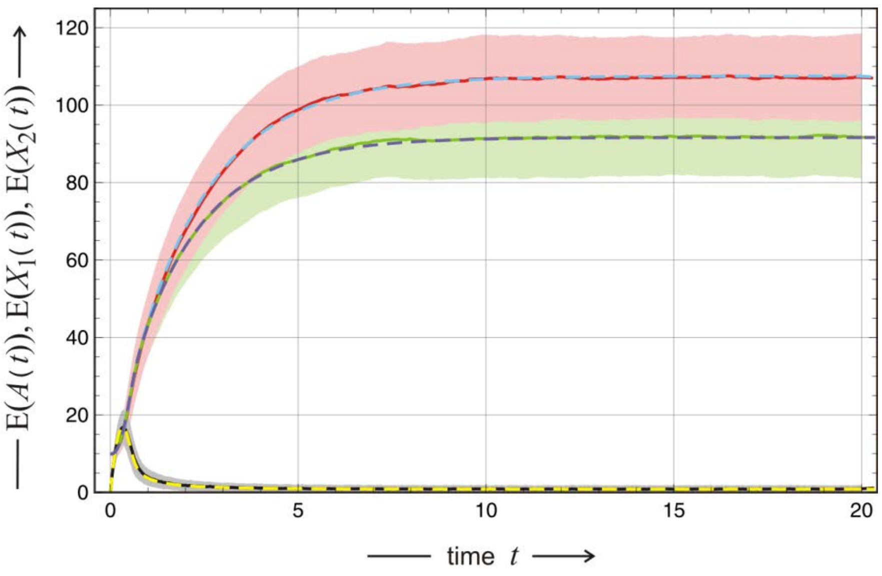


expectation values and 1σ-bands

choice of parameters: $a_0 = 200$, $r = 0.5$ [Vt^{-1}]

$k_1 = 0.09$ [$\mathrm{M}^{-1}\mathrm{t}^{-1}$], $k_2 = 0.11$ [$\mathrm{M}^{-1}\mathrm{t}^{-1}$],

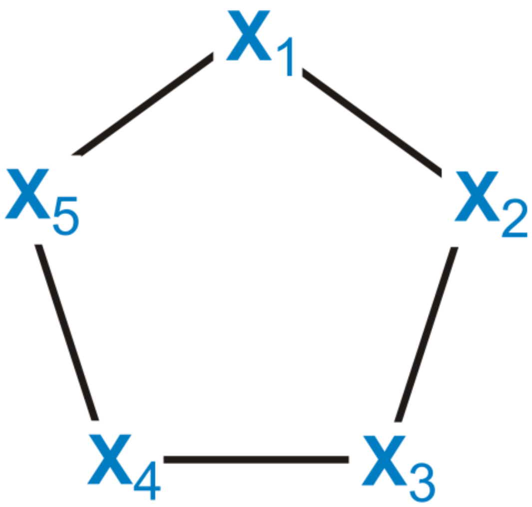
$l_1 = 0.0050$ [$\mathrm{M}^{-2}\mathrm{t}^{-1}$], $l_2 = 0.0045$ [$\mathrm{M}^{-2}\mathrm{t}^{-1}$]



$a(0) = 0,\ x_1(0) = x_2(0) = 10$

Reintroduction of extinguished species through mutation

$$\mathbf{A} + \mathbf{X}_j + \mathbf{X}_{j+1} \xrightarrow{l_j} 2\,\mathbf{X}_j + \mathbf{X}_{j+1}\,;\; j = 1, \ldots, n;\; j \bmod n$$

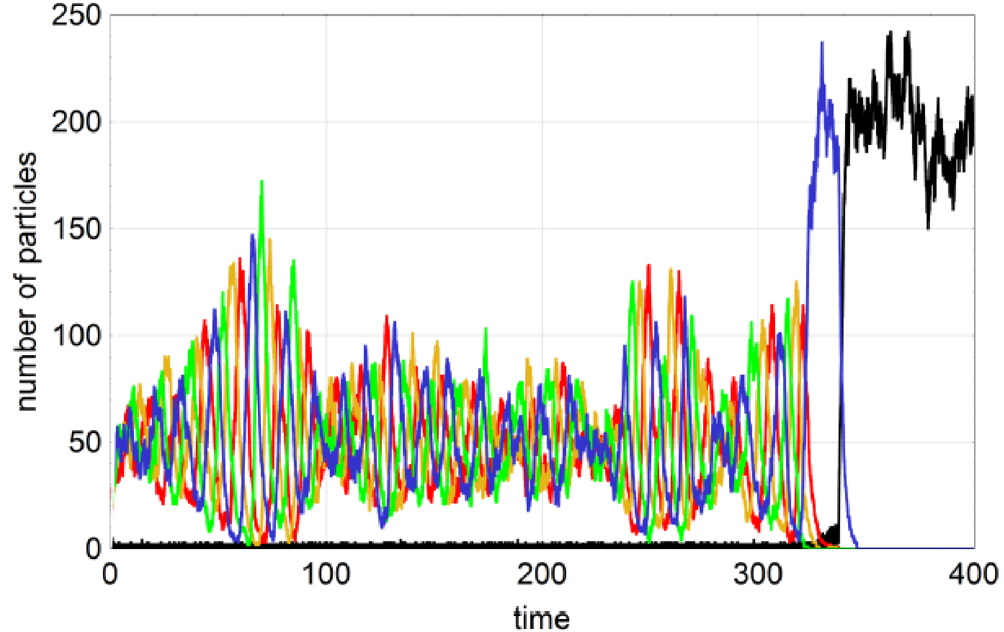


$$\mathbf{X}_n \Leftarrow \mathbf{X}_1 \Leftarrow \mathbf{X}_2 \Leftarrow \cdots \Leftarrow \mathbf{X}_{n-1} \Leftarrow \mathbf{X}_n$$

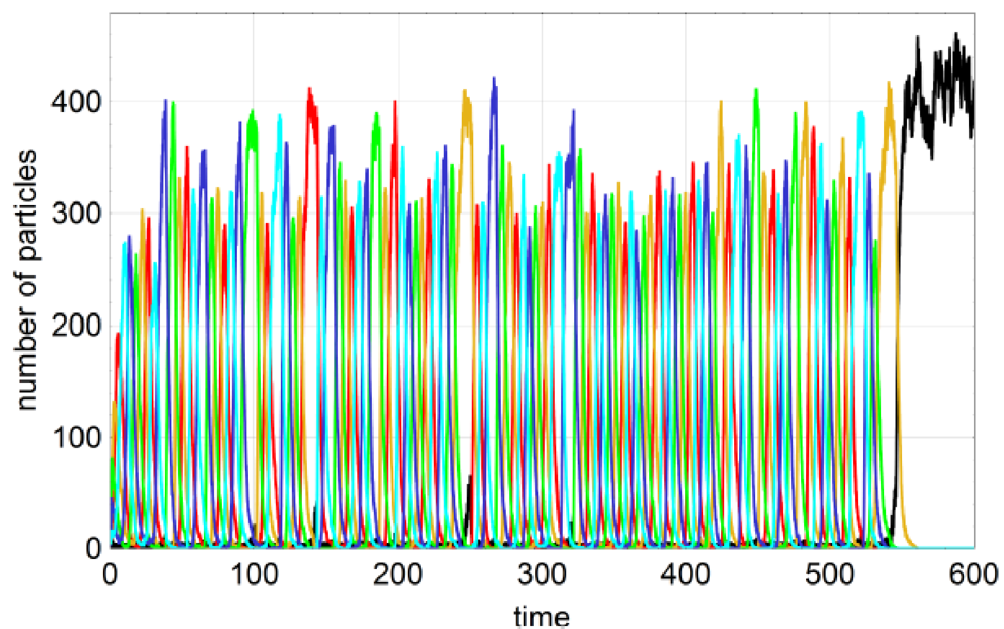
Catalytic hypercycles

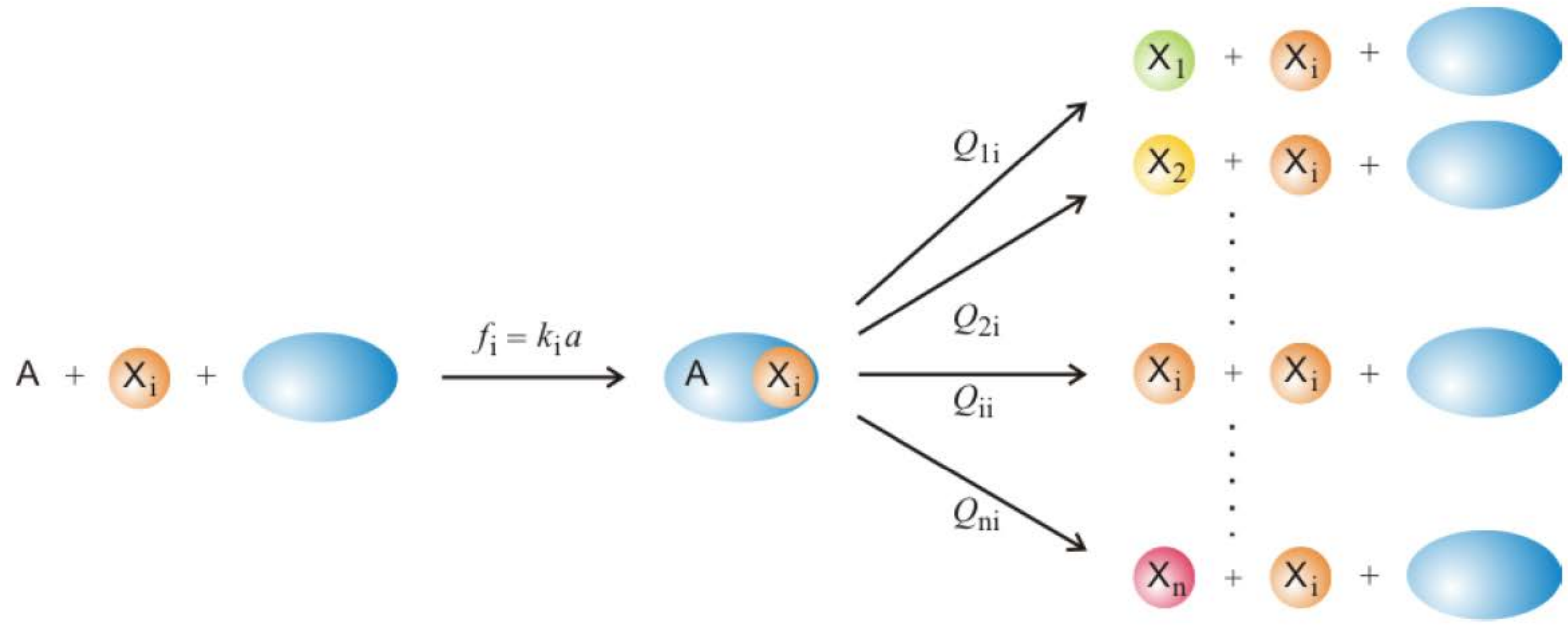
$$
\begin{aligned}
\star &\xrightarrow{a_0 \cdot r} \mathsf{A} \\
\mathsf{A} + \mathsf{X}_i + \mathsf{X}_{i+1} &\xrightarrow{l_i} 2\,\mathsf{X}_i + \mathsf{X}_{i+1}\,;\; i = 1, 2, \ldots, n;\; i \mod n \\
\mathsf{A} &\xrightarrow{r} \varnothing \\
\mathsf{X}_i &\xrightarrow{r} \varnothing
\end{aligned}
$$

Second order autocatalysis: hypercycles in the flow reactor n = 4

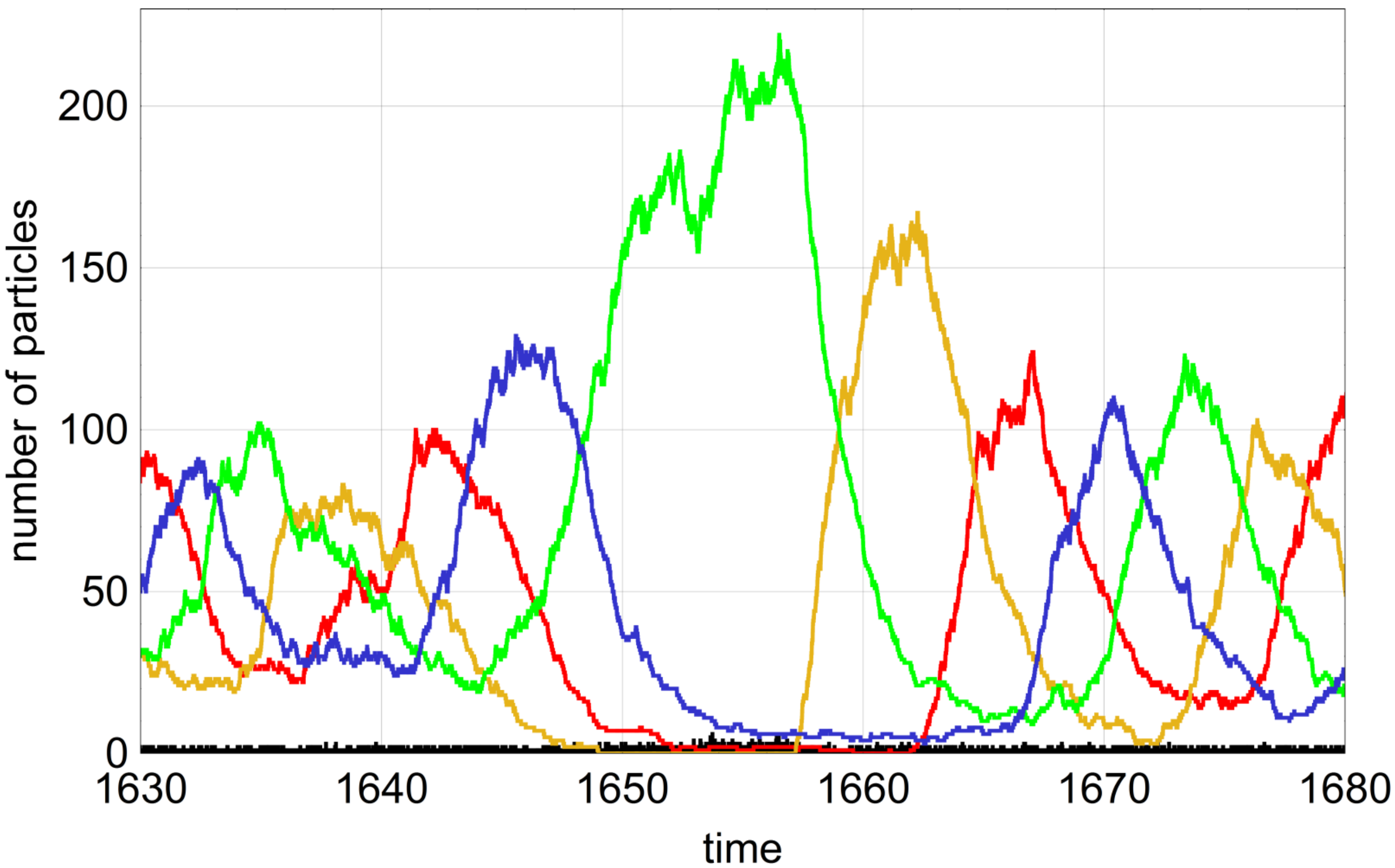

250
200
150
100
50
0
number of particles
0
100
200
300
400
time

n = 5

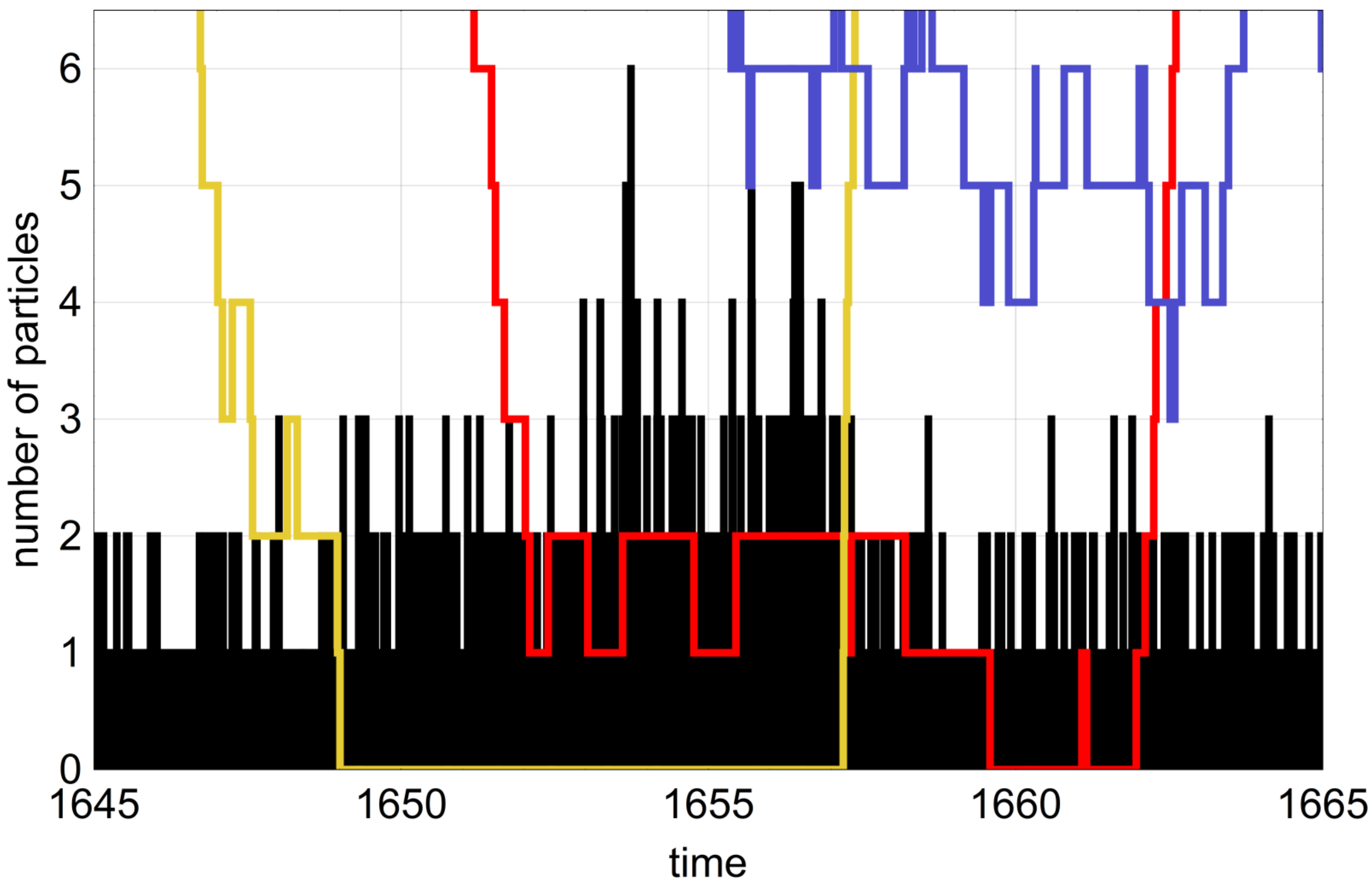

400
300
200
100
0
number of particles
0
100
200
300
400
500
600
time



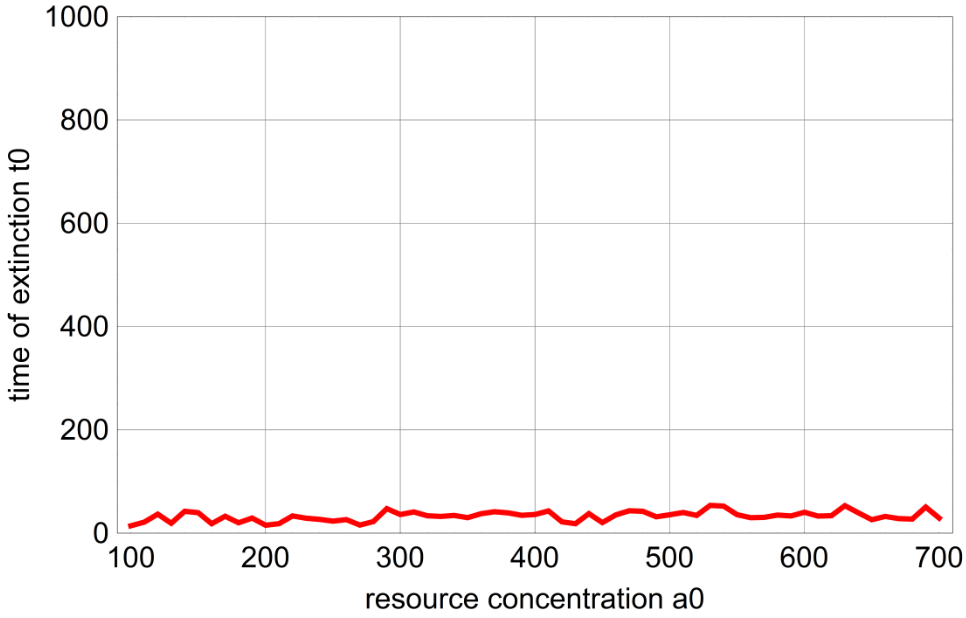
A molecular mechanism for mutation



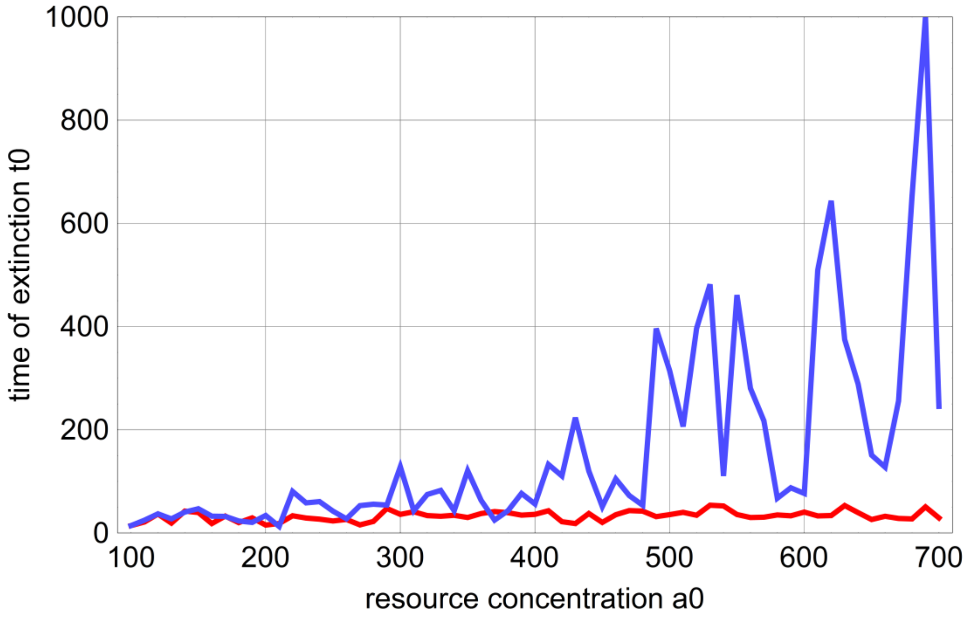
number of particles
200
150
100
50
0
1630
1640
1650
1660
1670
1680
time



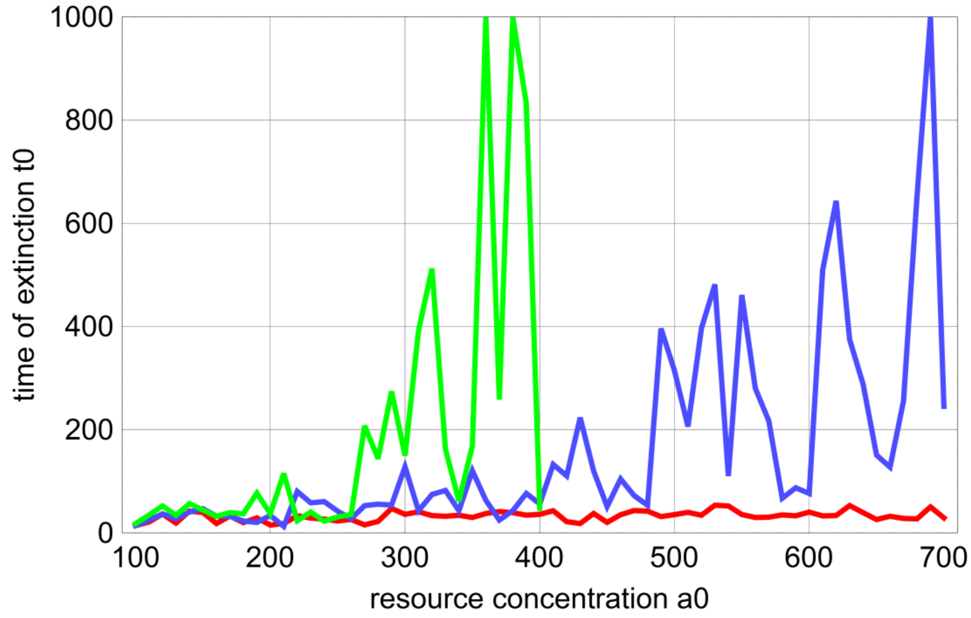
number of particles
0
1
2
3
4
5
6
1645
1650
1655
1660
1665
time



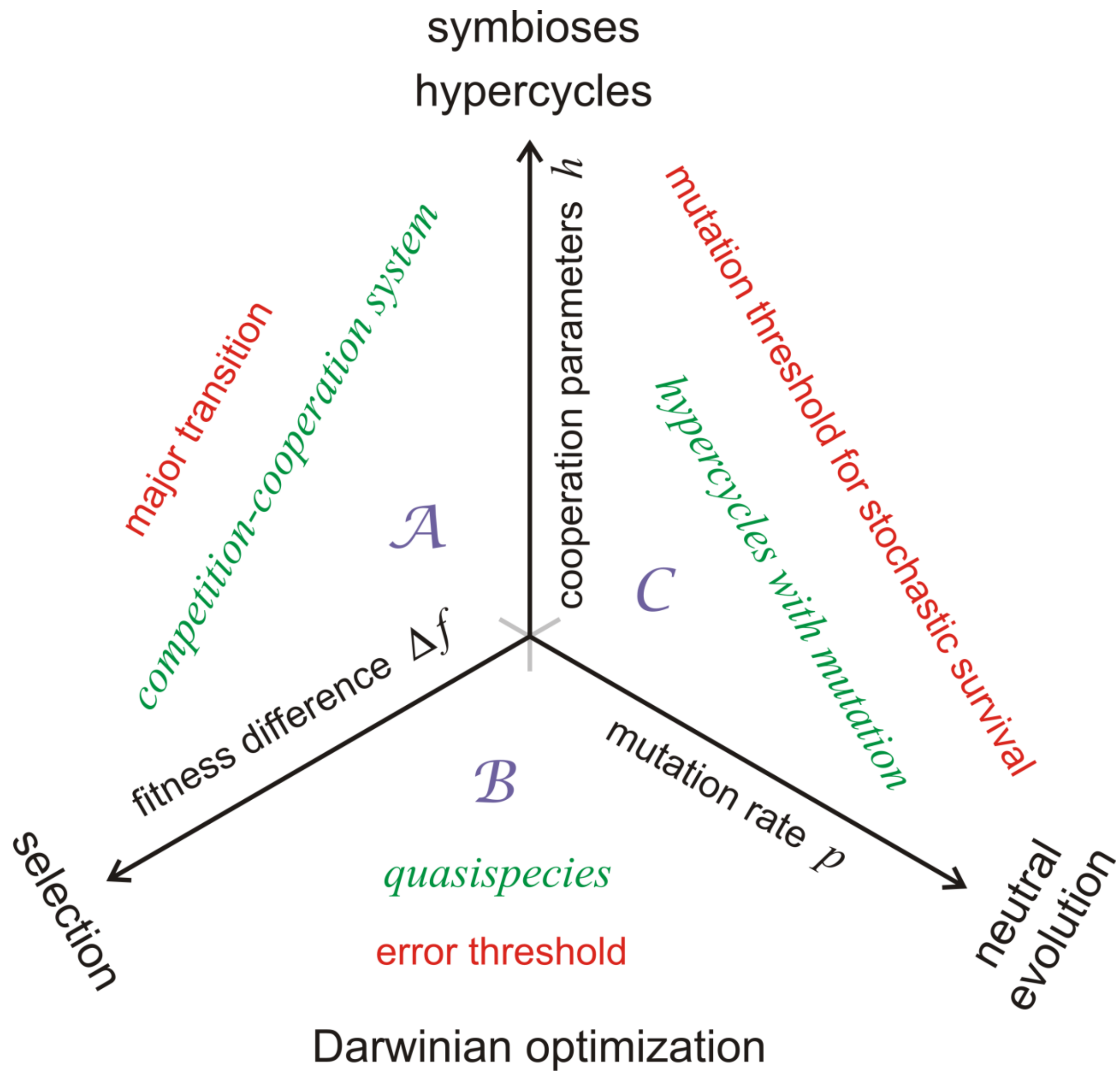
mutation rate: p = 0.0000



mutation rate: p = 0.0010



mutation rate: p = 0.0020


symbioses
hypercycles
cooperation parameters h
major transition
competition-cooperation system
mutation threshold for stochastic survival
hypercycles with mutation
$\mathcal{A}$
$\mathcal{C}$
fitness difference Δf
$\mathcal{B}$
mutation rate p
selection
neutral evolution
quasispecies
error threshold
Darwinian optimization

Danke für die Aufmerksamkeit!

Web-Page für weitere Informationen:

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