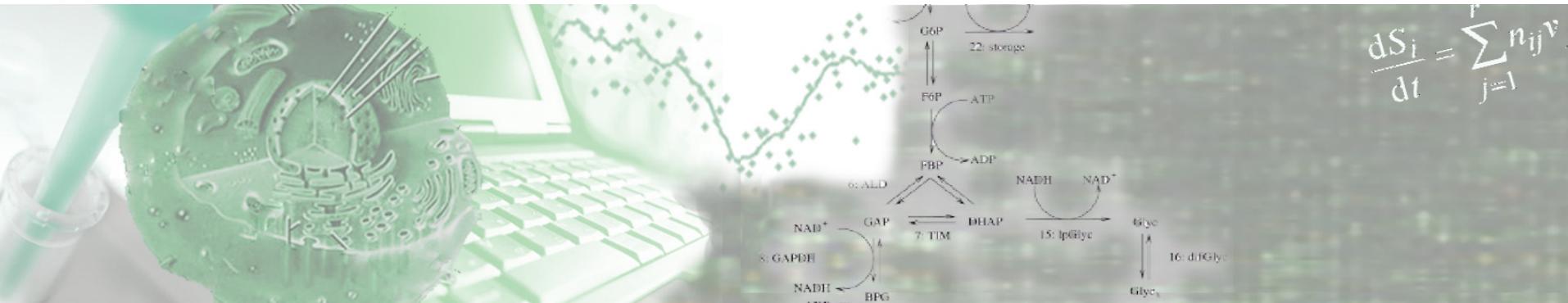


$$\frac{dS_i}{dt} = \sum_{j=1}^r n_{ij} v_j$$



Wintersemester 2016

Fachkurs – Introduction

Katja Tummler, Edda Klipp

Humboldt-Universität zu Berlin
Institut für Biologie
Theoretische Biophysik



Content

Language?

Script

Time table

Papers to chose

Time Table

Dienstag, 21. 11. '17

10.00-11.30	Introduction	Katja
12.30-14.00		
14.15-15.45	Python Intro I	Jens, Maria
16.00-17.30		

Dienstag, 28. 11. '17

10.00-11.30	Project work	-
12.30-14.00	Project work	-
14.15-15.45	Project work	-
16.00-17.30	Project work	-

Mittwoch, 22. 11. '17

10.00-11.30	Python II	Jorin, Jens
12.30-14.00	Presentation techniques	Judith
14.15-15.45	Python II	Jorin, Jens
16.00-17.30		

Mittwoch, 29. 11. '17

10.00-11.30	Project Work	-
12.30-14.00	Project Work	-
14.15-15.45	Project Work	-
16.00-17.30	Project Work	-

Donnerstag, 23. 11. '17

10.00-11.30	How to write a paper	Edda
12.30-14.00		
14.15-15.45	Tellurium	Tom, Katja
16.00-17.30		

Donnerstag, 30. 11. '17

10.00-11.30	Project Work	-
12.30-14.00	Project Work	-
14.15-15.45	Project Work	-
16.00-17.30	Project Work	-

Freitag, 24. 11. '17

10.00-11.30	Tellurium	Björn, Tom
12.30-14.00		
14.15-15.45	Python packages	Josch, Katja
16.00-17.30		

Freitag, 1. 12. '17

10.00-11.30		
12.30-14.00	Project Presentations	
14.15-15.45		all
16.00-17.30		



Own Contribution

Talk - Presentation of a publication and own simulations

1. Read and understand paper
2. Create the presented model, using Python (tellurium)
3. Reproduce the simulations shown in the publication
4. Analysis and modification of the model
 - Which analyses are made by the authors?
 - Does the model change with parameter changes?
 - Own ideas for model analysis or model improvement?
5. Analysis of model presentation
 - is it possible to reproduce the model from the information given in the paper?
6. Preparation of presentation
 - Summary of the paper
 - Presentation of own results



Own contribution

Talk - Presentation of a publication and own simulations

Form groups of 2 students (in case biophysicists/non-biophysicists)

Time is foreseen in time table

Every paper is connected to a mentor. Contact them!!!



Structure of presentation

Front page – presenters, publication (Title, authors)

Summary of the publication

Summary of open questions and problems

Presentation of own simulations including
problems/implementation

Summary and conclusions

Acknowledgement (to mentor, in case fellow students)

Olufemi Bolaji



Modeling the Cell Cycle: Why Do Certain Circuits Oscillate?

James E. Ferrell, Jr.,^{1,2,*} Tony Yu-Chen Tsai,^{1,2} and Qiong Yang¹

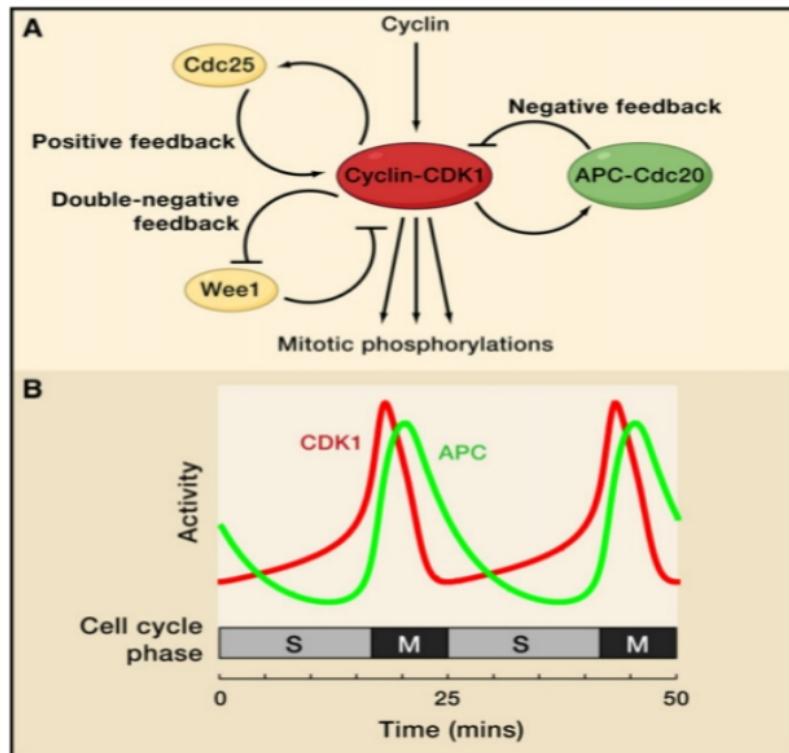


Figure: Simplified Depiction of the Embryonic Cell Cycle,
Highlighting the Main Regulatory Loops

Tasks:

- Read and understand the paper.
- Reproduce the one-, Two, and Three ODEs model. Discuss their stability analyses.
- Can you make the one-ODE model oscillate? Make a simulation.
- Reproduce the Two-delay differential equation model.
- Make a presentation.

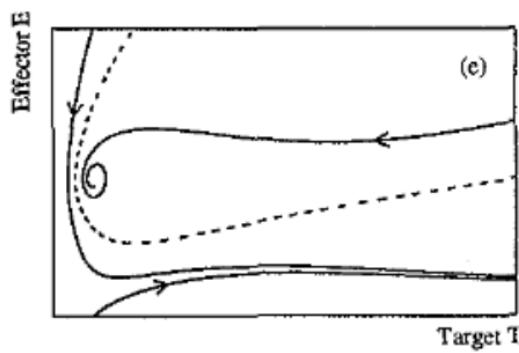
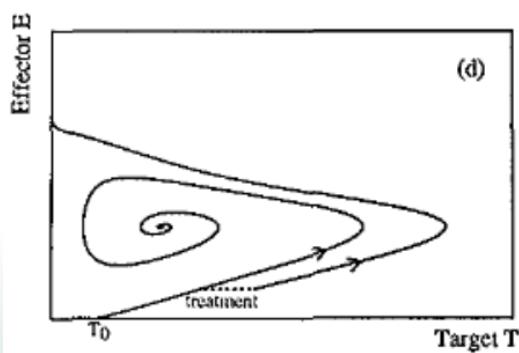
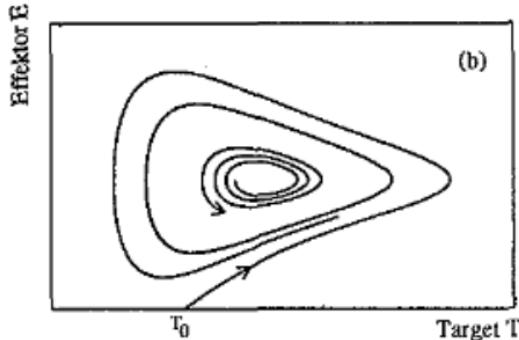
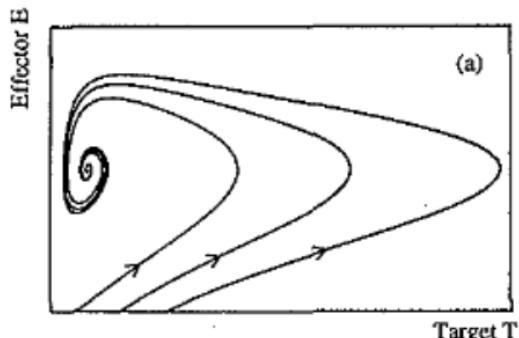
Olufemi Bolaji (Rm. 505)
olufemi.bolaji@hu-berlin.de



A basic mathematical model of the immune response

H. Mayer, K. S. Zaenker and U. an der Heiden

Ultimate goal: understand the beautiful richness of behaviour in a seemingly simple nonlinear dynamical system!



We shall:

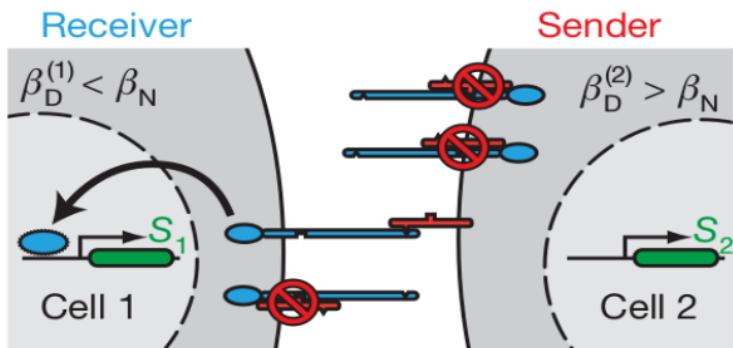
- detailly read the paper
- learn the basic techniques in analysis of nonlinear dynamical systems
- perform time simulations &
- phase-space simulations
- discuss implications of results

Jorin Diemer



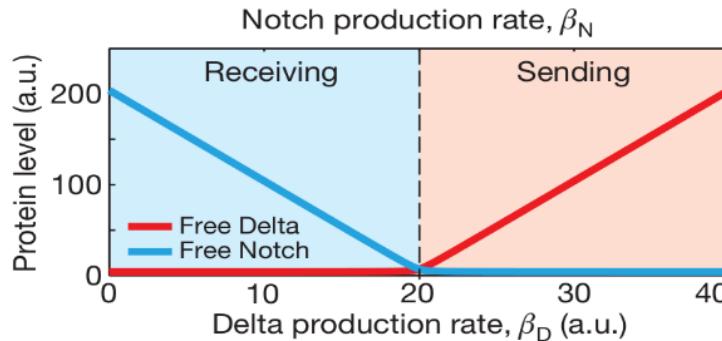
Cis-interactions between Notch and Delta generate mutually exclusive signalling states

David Sprinzak¹, Amit Lakhpal¹, Lauren LeBon¹, Leah A. Santat¹, Michelle E. Fontes¹, Graham A. Anderson², Jordi Garcia-Ojalvo³ & Michael B. Elowitz¹



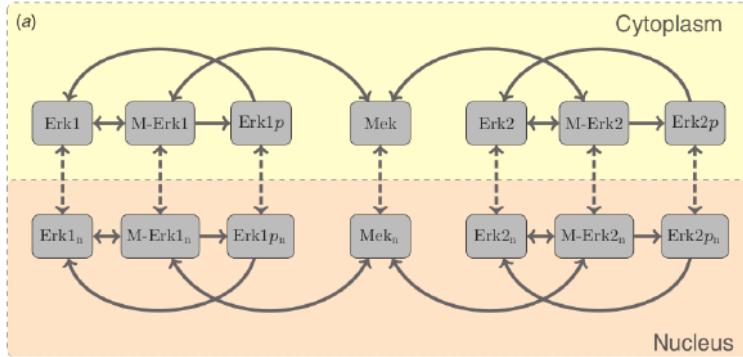
- Communication of cells during developement
- Find out how cells find their destiny !!!
- 3 equations, 6 parameters, but a lot to learn

- understand the paper
- implement model
- Timecourses; reproduce figure in Box 1
- Present and evaluate the paper



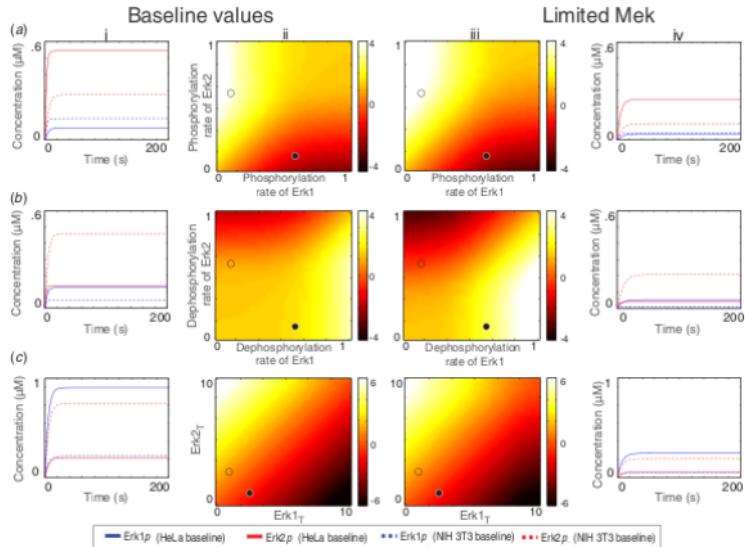
Maria Dost

Mathematical modeling reveals the functional implications of the different nuclear shuttling rates of Erk1 and Erk2



- Investigates Erk and Mek transport from cytosol to nucleus
- Analysis activity levels of Erk based on experimental data and modelling

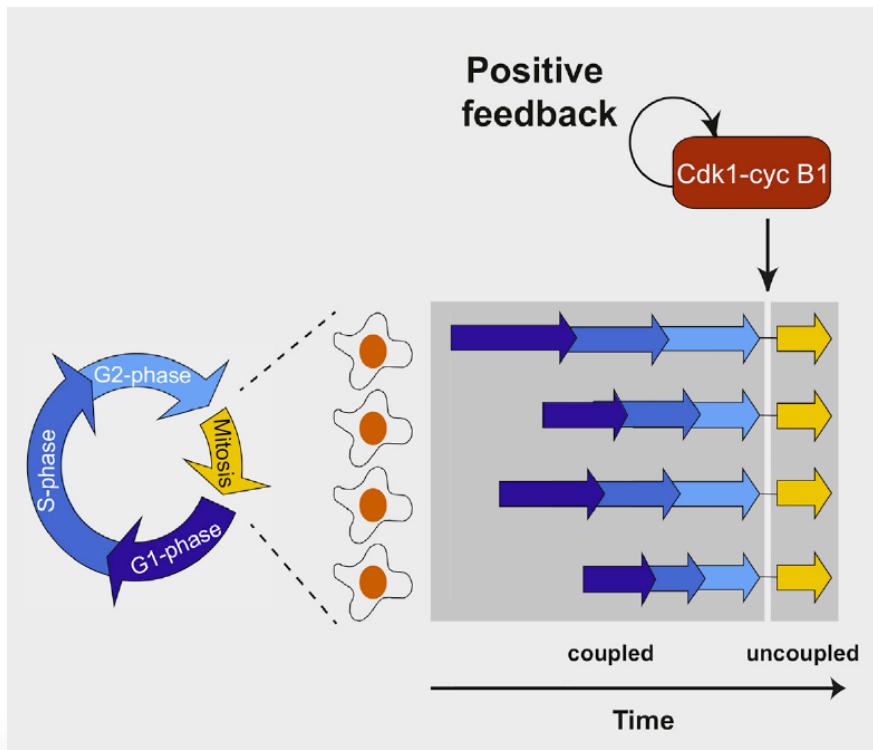
- Reconstruct the model in python
- Try to recreate the timecourses in the simulation



Severin Ehret

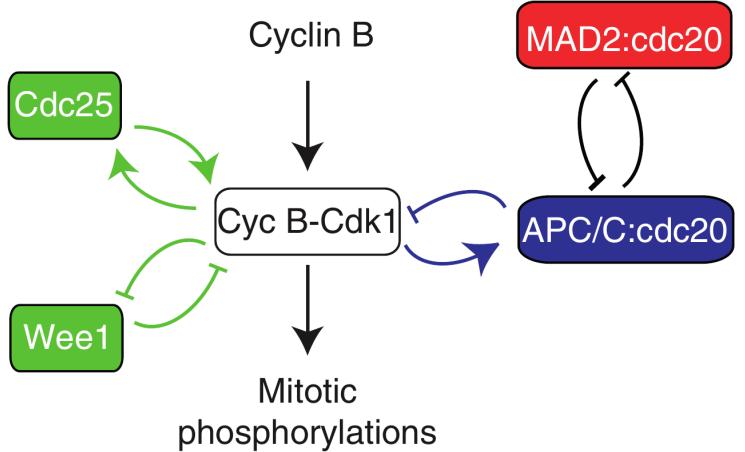
Molecular Cell

Positive Feedback Keeps Duration of Mitosis Temporally Insulated from Upstream Cell-Cycle Events



Authors

Ana Rita Araujo, Lendert Gelens,
Rahuman S.M. Sheriff,
Silvia D.M. Santos



Björn Goldenbogen

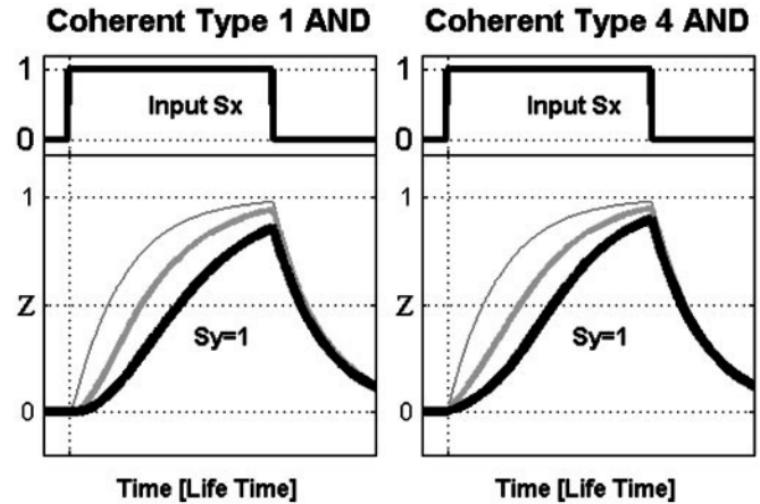
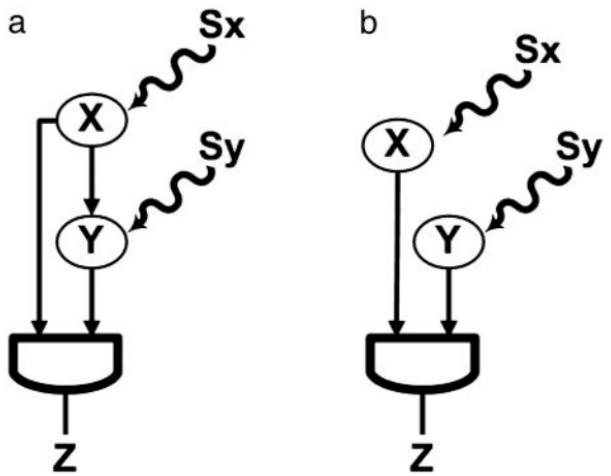


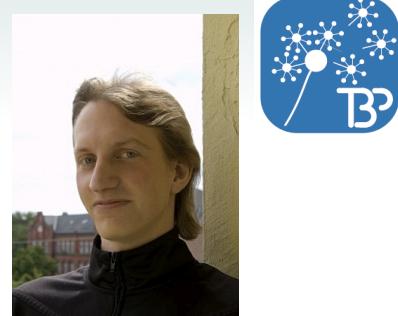
Structure and function of the feed-forward loop network motif

S. Mangan and U. Alon[†]

Departments of Molecular Cell Biology and Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

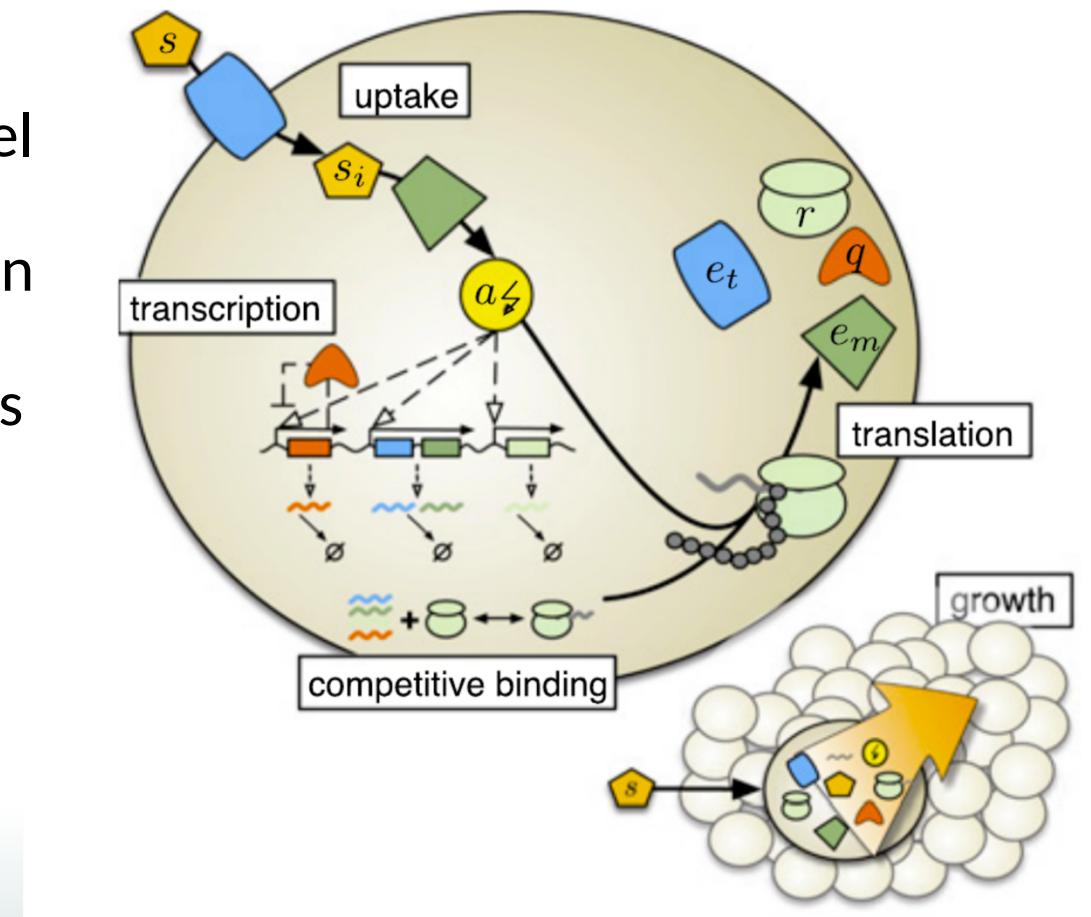
Edited by Arnold J. Levine, Institute for Advanced Study, Princeton, NJ, and approved August 25, 2003 (received for review June 22, 2003)





Mechanistic Links Between Cellular Trade-offs, Gene Expression, and Growth

- Minimal whole-cell model
- Driving force of regulation
- Switch between nutrients



Paula Martinell

FEBS Letters 499 (2001) 230–234



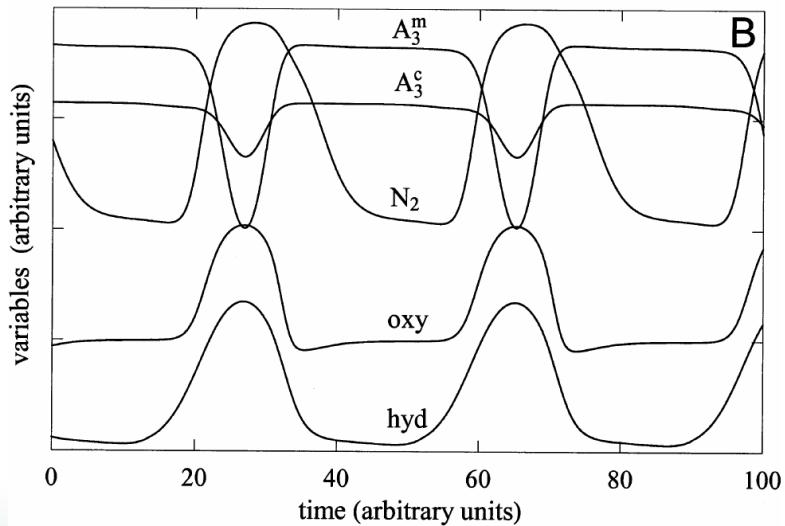
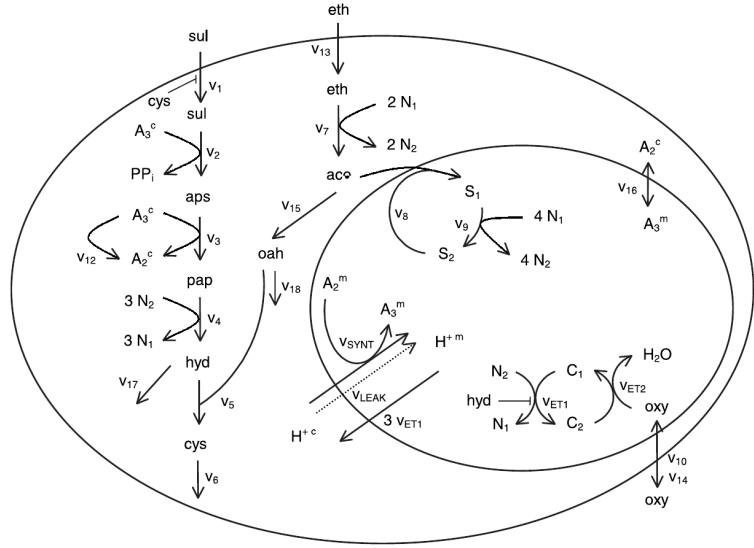
Mathematical analysis of a mechanism for autonomous metabolic oscillations in continuous culture of *Saccharomyces cerevisiae*

Jana Wolf^{a,*}, Ho-Yong Sohn^{b,1}, Reinhart Heinrich^a, Hiroshi Kuriyama^{b,2}

^aHumboldt University, Institute of Biology, Theoretical Biophysics, Invalidenstr. 42, 10115 Berlin, Germany

^bBiochemical Engineering Laboratory, National Institute of Bioscience and Human Technology, 1-1 Higashi, Tsukuba, Ibaraki 305-8566, Japan

Received 5 April 2001; revised 24 May 2001; accepted 26 May 2001

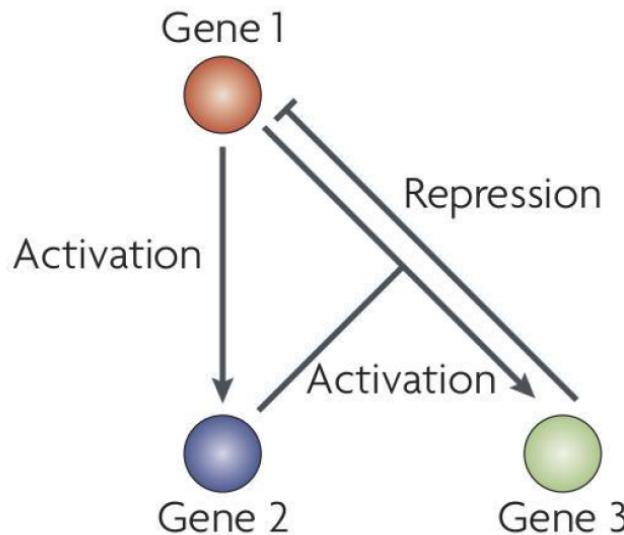


Roman Rainer

Modelling and analysis of gene regulatory networks



By Guy Karlebach and Ron Shamir



- Read the paper
- Implement the ODEs
- Evaluate the paper
- Presentation in english

Roman Rainer (505)

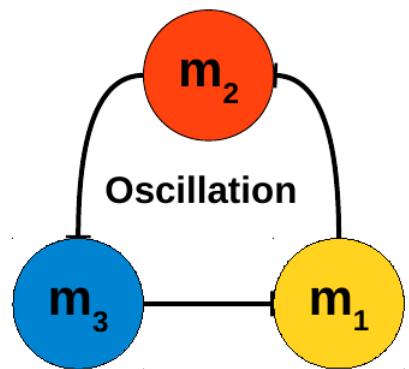
Juia Katharina Schlichting

Construction of a genetic toggle switch in Escherichia coli

T. S. Gardner , C. R. Cantor & J. J. Collins

Supervisor: Julia Katharina Schlichting, Room 505

$$\begin{aligned}\frac{dU}{dt} &= \frac{\alpha_1}{1+V^\beta} - U \\ \frac{dV}{dt} &= \frac{\alpha_2}{1+U^\gamma} - V\end{aligned}$$



Tasks:

- (1) Choose a paper
- (2) implement the system
- (3) reproduce characteristic model features



$$\begin{aligned}\frac{dm_i}{dt} &= -m_i + \frac{\alpha}{1+p_j^n} + \alpha_0 \\ \frac{dp_i}{dt} &= -\beta(p_i - m_i)\end{aligned}$$

Supervisor: Julia Katharina Schlichting, Room 505

M. B. Elowitz & S. Leibler

A synthetic oscillatory network of transcriptional regulators

Lost in Transition: Start-Up of Glycolysis Yields Subpopulations of Nongrowing Cells

Johan H. van Heerden,^{1,2,3} Meike T. Wortel,^{1,2,3} Frank J. Bruggeman,^{1,3} Joseph J. Heijnen,^{2,4} Yves J. M. Bollen,^{3,5} Robert Planqué,⁶ Josephus Hulshof,⁶ Tom G. O'Toole,⁷ S. Aljoscha Wahl,^{2,4} Bas Teusink^{1,2,3*}

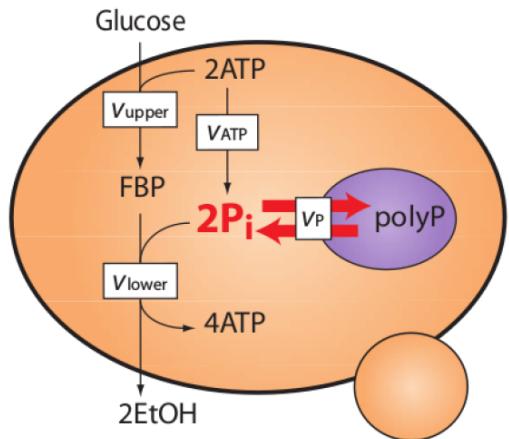
Aufgaben:

- Paper lesen & verstehen
- Implementation & Simulation Minimalmodell
- Paper bewerten
- Zusatzaufgaben



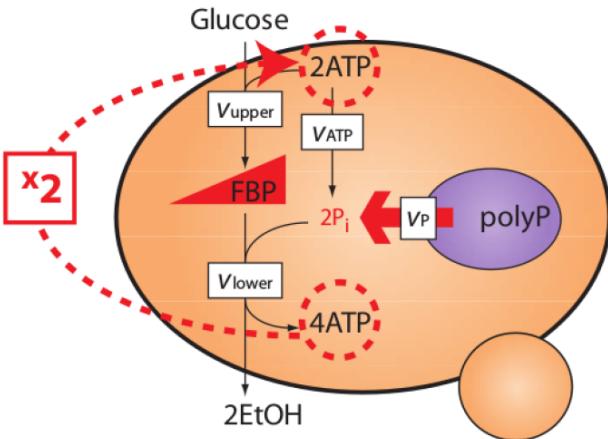
A

Steady state



B

Imbalanced state



Friedemann Uschner

Supervisor: Friedemann Uschner (Raum 502)

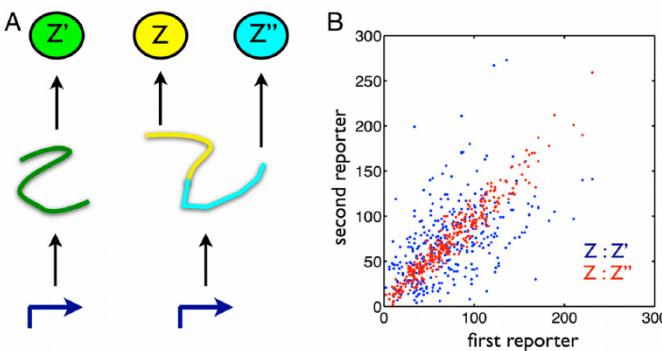
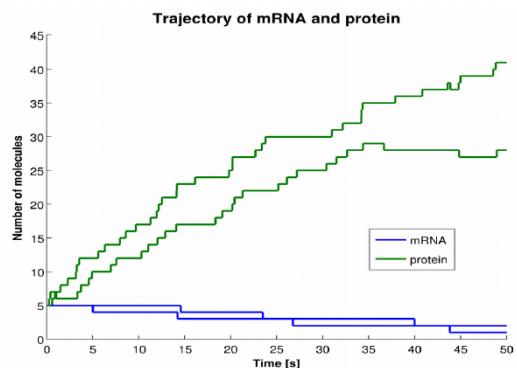
HUMBOLDT-UNIVERSITÄT ZU BERLIN



Identifying sources of variation and the flow of information in biochemical networks

Clive G. Bowsher^{a,1} and Peter S. Swain^{b,1}

- Investigates a general way to decompose variation in experiment & modeling
 - Sound mathematical interpretation
 - Complete proof of statements
- Applications to various data-sets (gene expression, signal transduction, components of variation, etc.) and different interesting ideas
- Used framework: Stochastics (Conditional probability theory), others depending on detail



$$V[Z(t)] = \overbrace{E\{V[Z(t)|(M, Y_e)^\mathcal{H}]\}}^{\text{translational}} + \overbrace{E\{V[E[Z(t)|(M, Y_e)^\mathcal{H}]|Y_e^\mathcal{H}]\}}^{\text{transcriptional}} + \overbrace{V\{E[Z(t)|Y_e^\mathcal{H}]\}}^{\text{from extrinsic effects}}. \quad [3]$$

Objectives:

- Studying and understanding the paper - detail will be determined together with the students
- Realization of the Gillespie SSA
- Simulation of a model of gene expression & its application as done in the paper
- Presentation in English

Judith Wodke

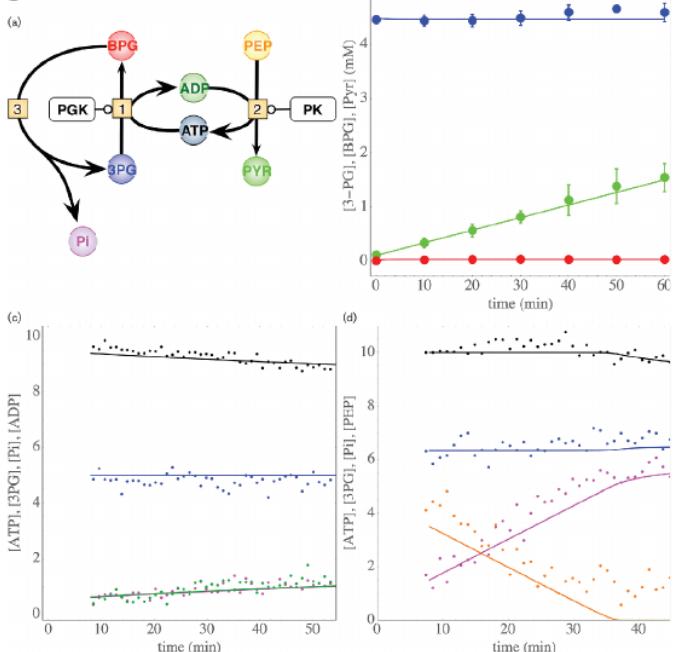


Phosphoglycerate kinase acts as a futile cycle at high temperature

T. Kouril, J.J. Eicher, B. Siebers, J.L. Snoep

- comparison of gluconeogenic conversion at 30°C (*S. cerevisiae*) and 70°C (*S. solfataricus*)
- intermediates with high chemical potential are unstable (BGP) → futile cycle of phosphoglycerate kinase (PGK)
- requirement of special adaptation strategies for life at high temperature

fig3 - kouril6.xml



TODO:

- read & understand the paper
- re-implement the models (kouril4.xml, kouril5.xml, kouril6.xml, kouril7.xml)
- reproduce figures 1-4
- evaluate the paper
- make nice presentation



Betreuung: Judith Wodke,
Raum 503

