

# Loose Ends, Remarks, Footnotes, ...

Christoph Flamm

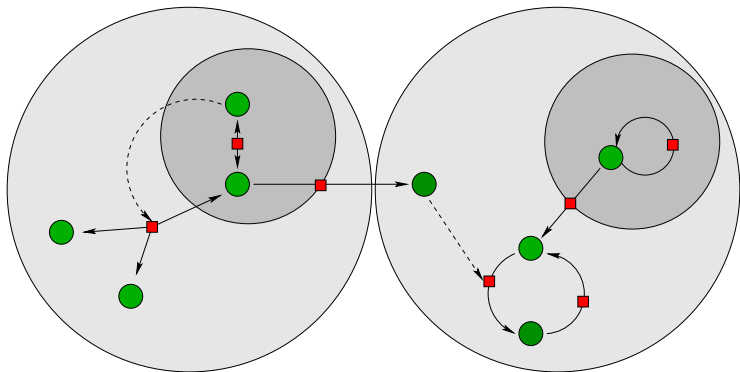
Institute for Theoretical Chemistry  
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<http://www.tbi.univie.ac.at/~xtof/>

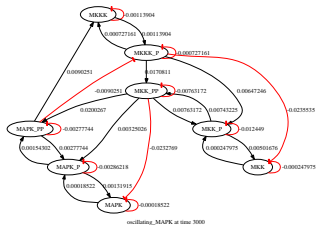
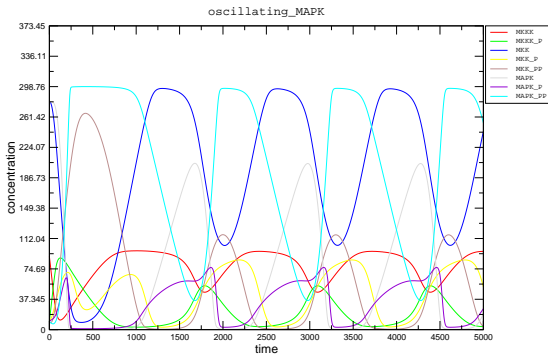
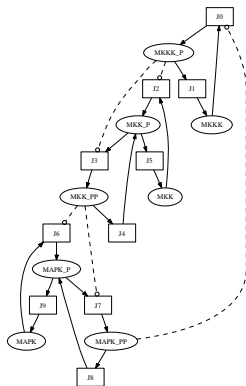
25th February 2005

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# SBML the *lingua franca* for Computational Models



# The SBML\_odeSolver



oscillating\_MAPK at time 3000

# Inverse Problem Primer

Definition due to Hadamard, 1915: Given mapping  
 $A : X \rightarrow Y$ , equation

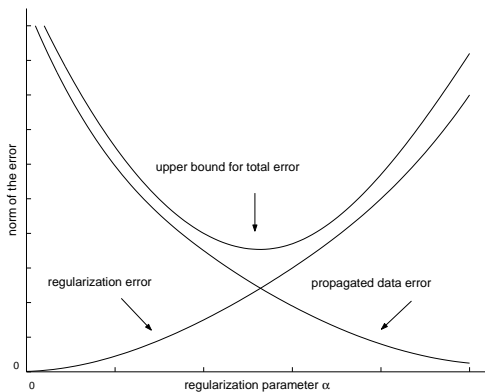
$$Ax = y$$

is **well-posed** provided

- ▶ (Existence) For each  $y \in Y$ ,  $\exists x \in X$  such that  $Ax = y$
- ▶ (Uniqueness)  $Ax_1 = Ax_2 \implies x_1 = x_2$ .
- ▶ (Stability)  $A^{-1}$  is continuous.

Equation is **ill-posed** if one of the above conditions is violated.

# Regularization a way to overcome Instabilities



Replace the **ill-posed** problem by a family of neighboring **well-posed** problems.

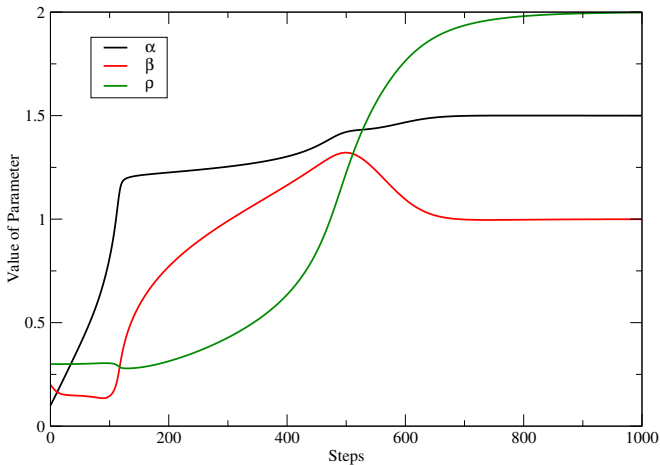
In other words:

Find an **approximation** (Tikhonov, Landweber Regularization) to the true solution, that depends on the actual data in a **stable** way.

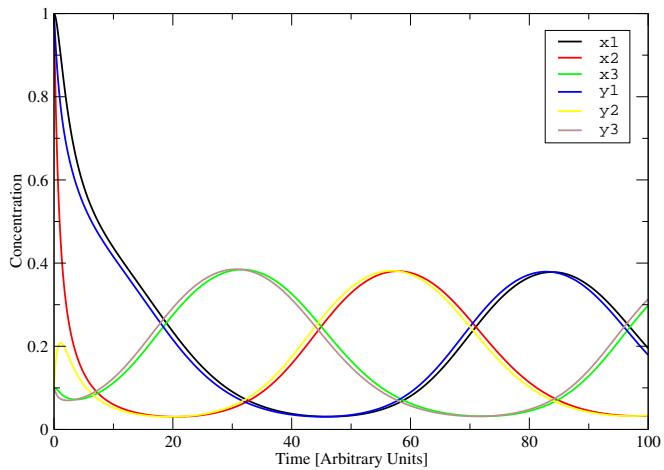
# Parameter Optimization

$$\dot{x}_i = \beta \cdot (y_i - x_i)$$

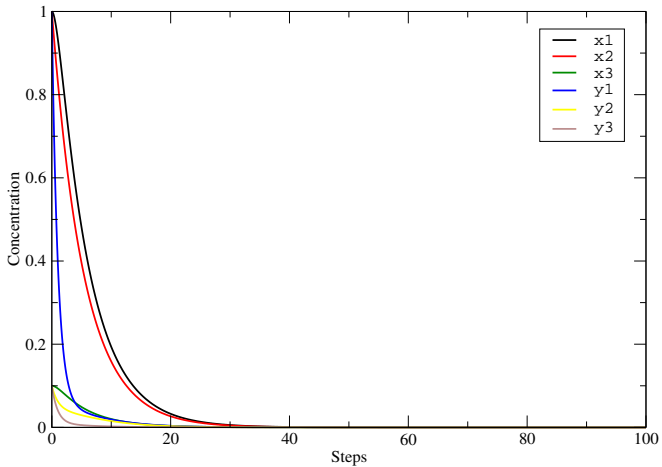
$$\dot{y}_i = \alpha \cdot \frac{x_i}{1 + x_i + \rho \cdot x_{i-1}} - y_i$$



# Desired Behavior

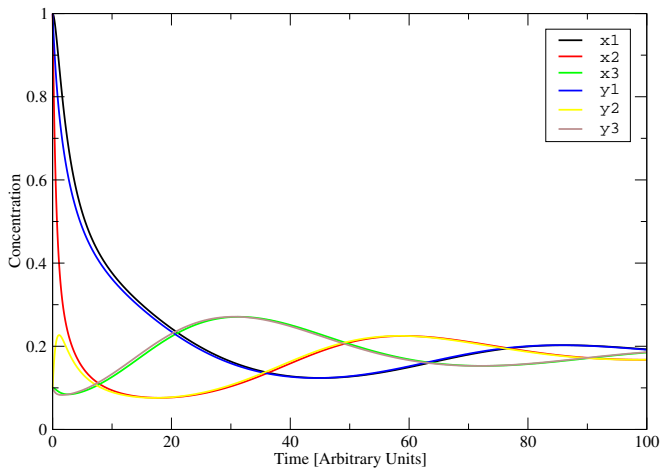


# Start Parameters =: (

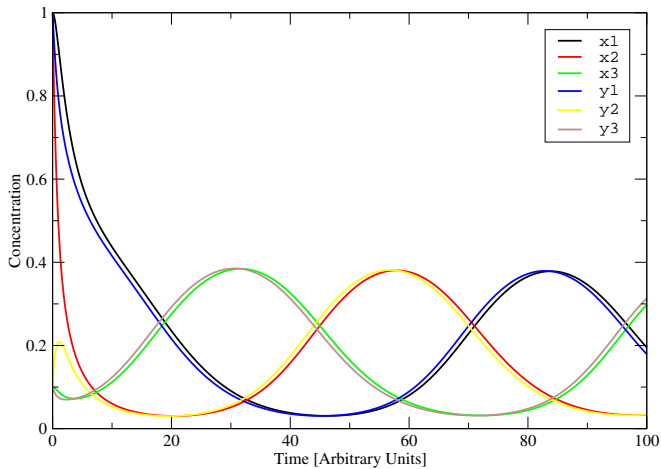




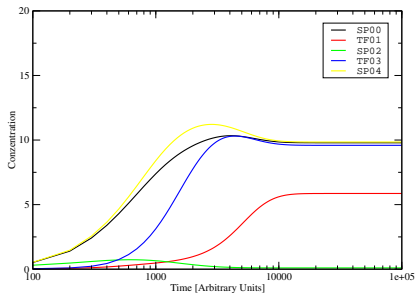
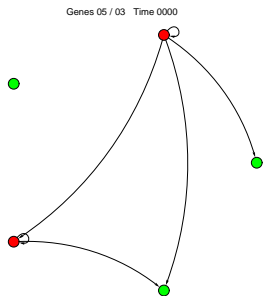
# Somewhere in the Middle =:o



EXIT\_SUCCESS = ;)

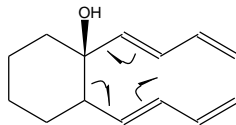
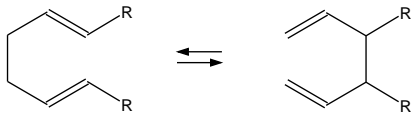


# The GRN's Dynamics as Phenotype

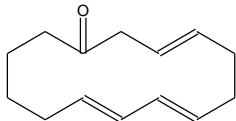
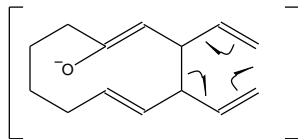
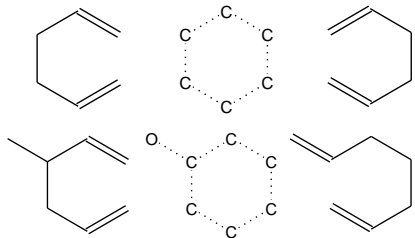


# GraphReWrite

## Cope Rearrangement



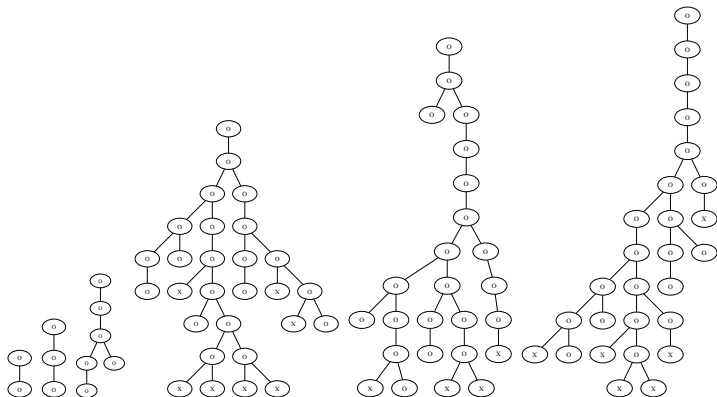
## Rewrite Rules



# L-System Mimicry

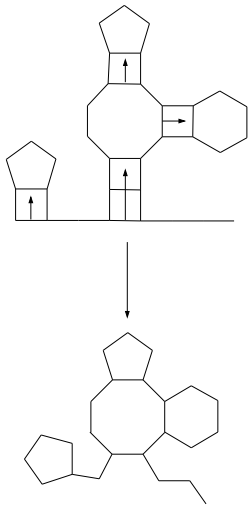
```
# Rule 1          # Rule 2          # Rule 3
#                #                #
# 1 2          1 3 2  # 1 2          1 /          # 1 2          1 3
# 0--X ==> 0--0--X  # 0--X ==> 0--0 3          # 0--X ==> 0--0
#                #                #
#                #                #
#                #                #
#                #                #
```

# Grow your Phenotype

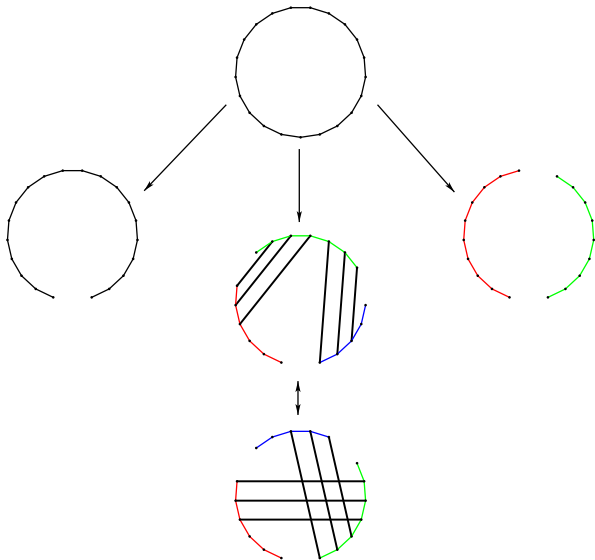


# A Codec for GRW Rules

C1CCC2CCCCC2C1	1	11
C1CCCCCCC1	8	10
CCC1CCCCC1CC	17	9
CCCCC1CCCCC1	29	8
CCCC1CCCCC1C	36	7
CC1CCCC1	45	6
CC1CCCCC1	73	5
C1CCCCC1	83	4
CC1CCCCC1C	97	3
CCC1CCCCC1	128	2
CCCCCCCCC	9483	1

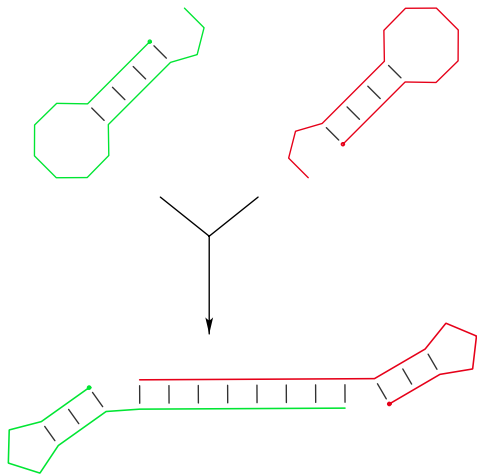


# The Genealogy of Folding Variants

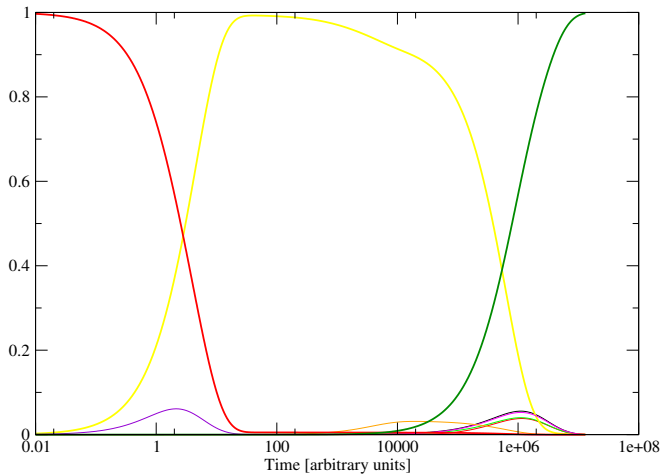




# The CoFold Problem



# CoFold Kinetics



THX to



Elvis Schuster (The King)

Peter Stadler

Ivo Hofacker

Rainer Machné (odeSolver)

Camille Stephan (CelloS)

Stefanie Widder (MiniCellSim)

Lukas Endler (MiniCellSim)

Stefan Müller (Param. Opti.)

Coming up the Cofold-Movie

... =;)