

Transformace bilineární soustavy ODR s
harmonickým buzením na soustavu PDR
*(Efficient Solution of a Parameter Estimation
Problem using Equation-Based Modeling in
COMSOL)*

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Remembering COMSOL conference 2017 & one old (not yet resolved) problem: *How to model the fish swimming while optimizing the design of aquaculture technology?*

And now for something completely different (let see one even older problem)...

Outline

- 1 Introduction-Motivation
- 2 PSF Model Calibration – Problem Formulation
- 3 COMSOL Model - Equation-Based Modeling
- 4 Postprocessing – Conclusion

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- If the (quasi) steady state is expected... how to disregard transients (mainly for the *harmonic forcing*)?

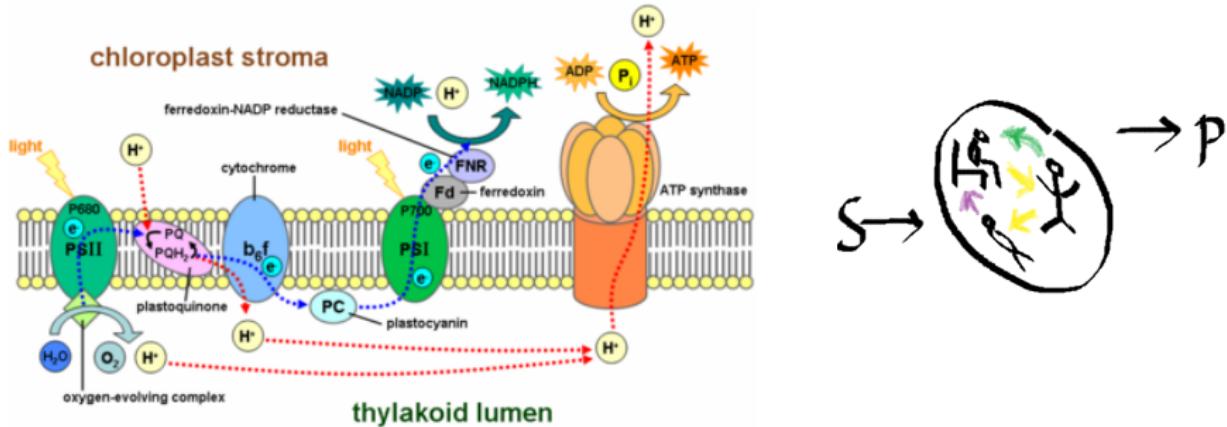
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- *Exo-system* and **COMSOL Multipysics (Equation-Based Modeling)** can help !!!

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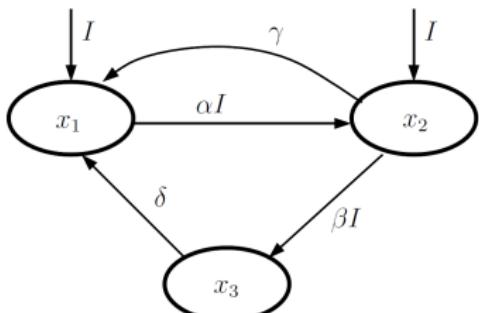
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Real (micro) scale model of microalgae photosynthesis vs. phenomenological model of photosynthetic factory (PSF)



Microalgae photosynthesis in real (micro)scale: Photosynthetic protein complexes (PSII and PSI); Light and dark reactions: water splitting, CO_2 fixation, etc.
vs. 3-state PSF model (please, see the next slides :)

Model calibration for 3-state 5-parameter mechanistic model of photosynthetic factory

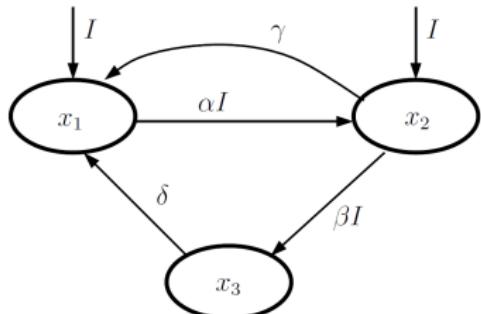


Stavový vektor $x = (x_1, x_2, x_3)^T$: molární frakce buněk ve stavu klidu (x_1), aktivace (x_2), resp. inhibice (x_3), tj. platí $x_1 + x_2 + x_3 = 1$.

Substrátem-vstupem (řízeným) je **irradiance**-ozářenost $I(t)$.

4 parametry PSF modelu jsou "transition rates" α, β (in $[s^{-1}/\text{irrad. unit}]$), $\gamma, \delta [s^{-1}]$. Platí $\alpha \gg \beta$, $\gamma \gg \delta$. Tzn. existence aspoň dvou časových škál (pro světelné a temnotní reakce a proces fotoinhibice).

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Propojení fenomenologických stavů s reálným světem (**měřitelnou spec. růstovou rychlosť** μ) je následující (5. parametr κ):

$$\mu = \frac{\kappa\gamma}{T} \int_0^T x_2(t) dt . \quad (1)$$

Hodnota součinu $\kappa\gamma \approx 10^{-4}$ $[s^{-1}]$, což představuje škálový skok (ze vteřin na hodiny, tj. 3. časová škála)!

PSF: Bilineární systém s jedním (skalárním) vstupem

$$\dot{x} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & \gamma & \delta \\ 0 & -\gamma & 0 \\ 0 & 0 & -\delta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + I(t) \begin{bmatrix} -\alpha & 0 & 0 \\ \alpha & -\beta & 0 \\ 0 & \beta & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad (2)$$

- IVP: "přirozené" počáteční podmínky (po inkubaci ve tmě) jsou:
 $x(t_0) = [1, 0, 0]^T$.
- BVP: okrajové podmínky (periodic BC) jsou: $x(0) = x(T)$.
- Pro konstantní vstup I má matice soustavy $[\mathcal{A} + I(t)\mathcal{B}]$ 2 záporná reálná vlast. čísla. Třetí vl. číslo je 0 a k němu vl. vektor je x_{ss} .

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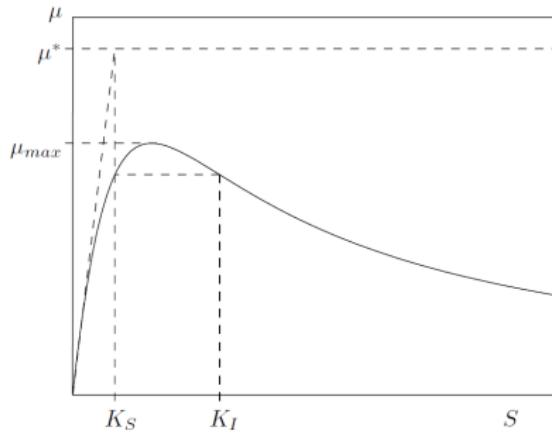
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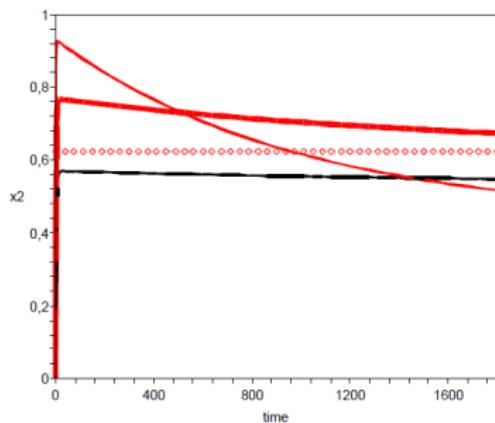
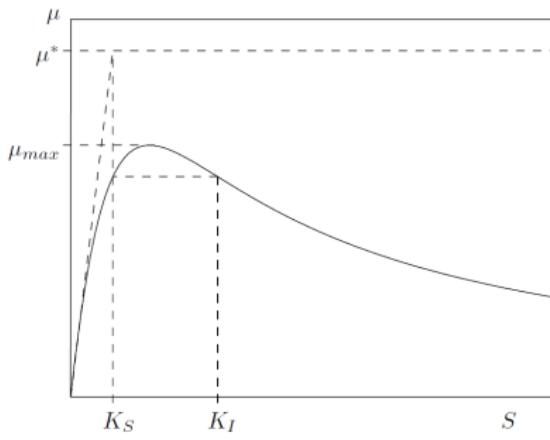
 Š. Papáček, S. Čelikovský, D. Štys and J. Ruiz-León. Bilinear system as a modelling framework for analysis of microalgal growth. *Kybernetika*, 43(1):1–20, 2007.

 B. Rehák, S. Čelikovský, Š. Papáček. Model for Photosynthesis and Photoinhibition: Parameter Identification Based on the Harmonic Irradiation O₂ Response Measurement *IEEE Transactions on Automatic Control*, 53(1): 101–108, 2008.

PSF model (2) vede (pro $I \equiv S = const.$) na kinetiku inhibice substrátem (SIK-Haldane: Obr. vlevo)



PSF model (2) vede (pro $I \equiv S = const.$) na kinetiku inhibice substrátem (SIK-Haldane: Obr. vlevo)



Obr. vpravo simuluje odezvu $x_2(t)$ (pro $x_2(0) = 0$) na skokovou změnu I_i , viz 2 škály.

Resumé pro kalibraci PSF modelu: 3 z 5 parametrů popisují steady state a 2 popisují dynamiku, (i) pomalou $\sim photoinhibition$, (ii) rychlou (lze kalibrovat pomocí tzv. *L-D cycles* indukovaných harmonickým signálem $I(t) = K(1 - \cos(\omega t))$, viz další sekce).

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1st attempt: The Global ODEs and DAEs (ge) interface under the Mathematics branch (*How to set up the BVP?*)

The screenshot shows the COMSOL Multiphysics interface. The left panel, titled 'Model Builder', displays a hierarchical tree of model components. The 'Global ODEs and DAEs (ge)' node is selected, highlighted with a blue background. The right panel, titled 'Properties' and 'Global Equations', shows the configuration for the selected node. The 'Label' field is set to 'Global Equations 1'. Under the 'Global Equations' section, a table lists two equations: $f(u, u_t, u_{tt}, t) = 0$, $u(t_0) = u_0$, and $u_t(t_0) = u_{t0}$. The table includes columns for 'Name', 'Equation', and 'Initial value (u_0)'. The first equation is $f(u, u_t, u_{tt}, t)$ with initial value 0. The second equation is $x t + (1+q5)*(q2+K*(1-\cos(w*t)))^*x$ with initial value 0. The third equation is $y t + q5/((1+q5)*q2)^*y - q5*K*(1-\cos(w*t))$ with initial value 0. At the bottom of the properties panel, there is a text input field for defining the function $f(u, u_t, u_{tt}, t)$.

Model Builder

- COMSOL-ODE-PSF-omega.mph (root)
 - Global Definitions
 - Parameters 1
 - Materials
 - Component 1 (comp 1)
 - Definitions
 - Geometry 1
 - Materials
 - Global ODEs and DAEs (ge)
 - Global Equations 1
 - Mesh 1
 - Study 1
 - Results
 - Datasets
 - Derived Values
 - Tables
 - 1D Plot Group 1
 - Export
 - Reports
 - Report 1

Properties

Global Equations

Label: Global Equations 1

Global Equations

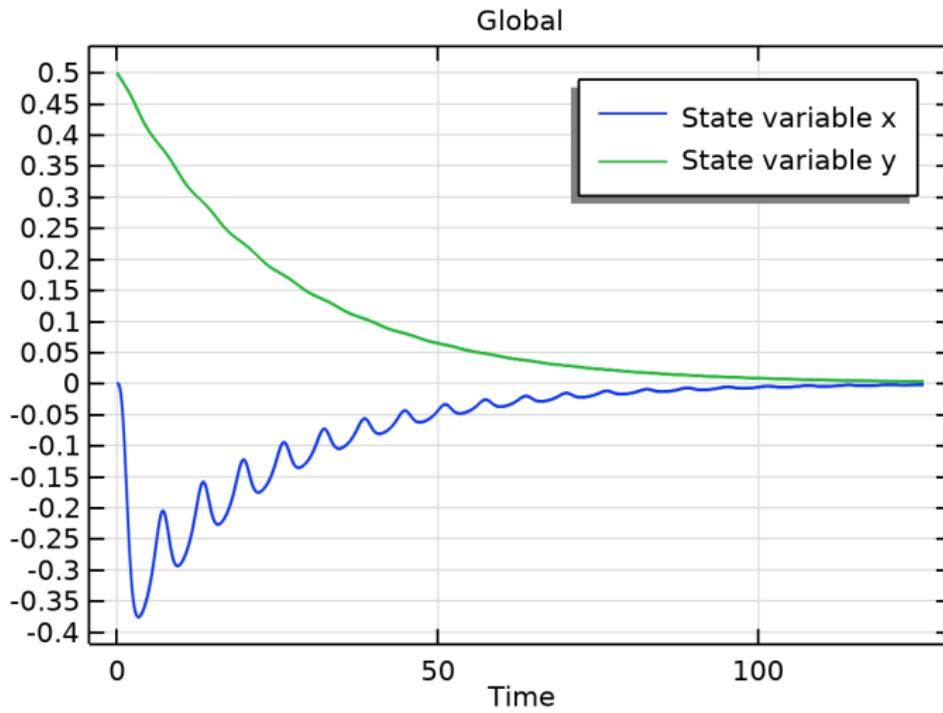
Name	Equation	Initial value (u_0)
x	$x t + (1+q5)*(q2+K*(1-\cos(w*t)))^*x$	0
y	$y t + q5/((1+q5)*q2)^*y - q5*K*(1-\cos(w*t))$	0.5

Name:

f(u, u_t, u_{tt}, t):

Initial value problem gives the transient behavior...

(dependent variables transformation was used → both steady state values are 0)



How to get the periodic solution for the periodic input ?

Introducing an Exo-system as the harmonic input signal generator → ODEs are transformed to a **stationary PDE system (4)** with 2 independent and 2 dependent variables x_2, x_3 .

Let us define the harmonic input as follows:

$$u(t) = K(1 - \cos(\omega t)) = K(1 - w_2), \text{ where } w(t) = [\sin(\omega t), \cos(\omega t)]^T.$$

Thus, the input signal is generated by an external autonomous system, so-called **EXOSYSTEM**.

Moreover, it holds

$$\dot{w}(t) = \begin{bmatrix} \dot{w}_1 \\ \dot{w}_2 \end{bmatrix} = \omega \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \omega S w, \quad (3)$$

and further

$$\dot{x} = \nabla x(w(t)) \dot{w}(t) = \omega \nabla x(w) S w = [\mathcal{A} + u(w) \mathcal{B}] x(w), \quad (4)$$

where $\nabla x := [\nabla x_1, \nabla x_2, \nabla x_3]^T$, and $\nabla x_i = [\frac{\partial x_i}{\partial w_1}, \frac{\partial x_i}{\partial w_2}]$.

2nd (successful) attempt: General Form PDE interface under the Mathematics branch (2D - stationary)

Model Builder

- PSF2d-Exo-PDE_v1.mph (root)
 - Global Definitions
 - Parameters 1
 - Materials
 - Component 1 (comp 1)
 - Definitions
 - Geometry 1
 - Materials
 - General Form PDE (g)
 - General Form PDE 1
 - Zero Flux 1
 - Initial Values 1
 - Mesh 1
- Study 1
- Results

Settings Properties

General Form PDE

Label: General Form PDE 1

Domain Selection

Selection: All domains

Override and Contribution

Show equation assuming:
Study 1, Stationary

$$e_x \frac{\partial^2 \mathbf{u}}{\partial t^2} + d_x \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \Gamma = f$$

$\mathbf{u} = [u_1, u_2]^T$

$\nabla = \left[\begin{array}{c} \frac{\partial}{\partial x} \quad \frac{\partial}{\partial y} \end{array} \right]$

Conservative Flux

Γ

$y^* u_1$	x
$-x^* u_1$	y
$y^* u_2$	x
$-x^* u_2$	y

Source Term

f

$$\frac{1}{\omega} \text{omegar}^*(-p2^*(1+p5)*u1 - (1-y)^*(u2^*+u1^*(1+p5)+1))$$

$$\frac{1}{\omega} \text{omegar}^*(-(1+p5)/p2^* u2^* + (1-y)^*(p5^* u1))$$

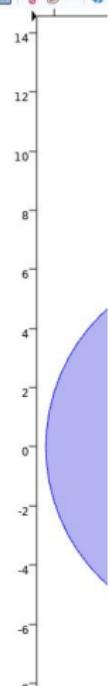
Damping or Mass Coefficient

d_s

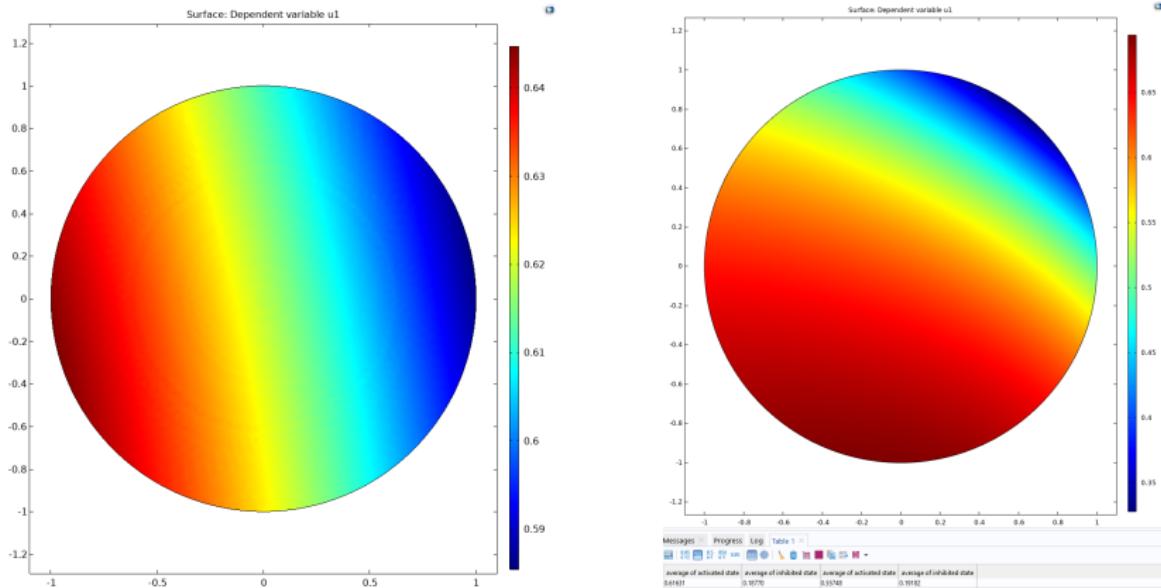
0	0	0
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Mass Coefficient

Graphics Preview



COMSOL generates simulated data (only the state x_2 is related to real world measurements)...



...and only the domain boundary is connected to the original problem...

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Postprocessing of COMSOL generated data and the PSF model parameter estimation

- COMSOL generates for different ω (according to our Experimental Design) and parameters (p_i) the average values of state x_2 , cf. Eq. (1).
- How to get this data? **Results-Derived Values-Line Average.**
- An optimization procedure (based on OLS method) then, find the optimal parameter values...
- ... special attention needs the "fast" parameter p_5 !

Conclusion – Questions?

Thanks for your kind attention!



*The ideal situation occurs
when the things that we
regard as beautiful are also
regarded by other people as
useful.*

– Donald Knuth