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

Š. Papáček, V. Lynnyk, B. Rehák

JU v Č. Budějovicích/ÚTIA - AV ČR, v.v.i.,
Konference COMSOL Multiphysics, ČR 2021

Vinařství U Kapličky, Zaječí, 28.5.

Remembering COMSOL conference 2017 & one old (not yet resolved) problem: *How to model the sh 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

Outline

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

Introduction-Motivation

- Do you solve a **PARAMETER ESTIMATION PROBLEM**)?
  (or in other words) Do you perform MODEL CALIBRATION?

Introduction-Motivation

- Do you solve a **PARAMETER ESTIMATION PROBLEM**)? (or in other words) Do you perform MODEL CALIBRATION?
- Do you **DESIGN EXPERIMENTS**?

Introduction-Motivation

- Do you solve a **PARAMETER ESTIMATION PROBLEM**)? (or in other words) Do you perform MODEL CALIBRATION?
- Do you **DESIGN EXPERIMENTS**?
- Do you measure responses to *Constant* & *Harmonic* input signals?

Introduction-Motivation

- Do you solve a **PARAMETER ESTIMATION PROBLEM**)? (or in other words) Do you perform MODEL CALIBRATION?
- Do you **DESIGN EXPERIMENTS**?
- Do you measure responses to *Constant* & *Harmonic* input signals?
- If the (quasi) steady state is expected... how to disregard transients (mainly for the *harmonic forcing*)?

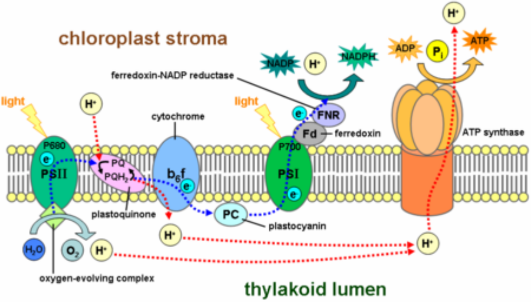
Introduction-Motivation

- Do you solve a **PARAMETER ESTIMATION PROBLEM**)? (or in other words) Do you perform MODEL CALIBRATION?
- Do you **DESIGN EXPERIMENTS**?
- Do you measure responses to *Constant* & *Harmonic* input signals?
- If the (quasi) steady state is expected... how to disregard transients (mainly for the *harmonic forcing*)?
- *Exo-system* and **COMSOL Multipysics (Equation-Based Modeling)** can help !!!

Outline

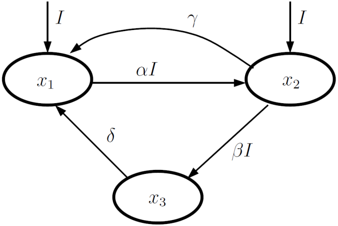
1. Introduction-Motivation
2. PSF Model Calibration – Problem Formulation
3. COMSOL Model - Equation-Based Modeling
4. Postprocessing – Conclusion

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



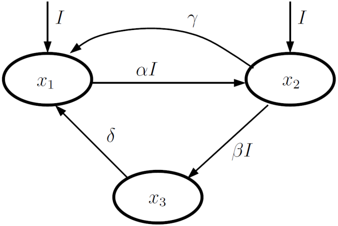
Microalgae photosynthesis in real (micro)scale: Photosynthetic protein complexes (PSII and PSI); Light and dark reactions: water splitting, CO_2 xation, etc. vs. 3-state PSF model (please, see the next slides :)

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



Stavovy vektor $x = (x_1; x_2; x_3)^T$: molarn frakce bunek ve stavu klidu (x_1), aktivace (x_2), resp. inhibice (x_3), tj. plat $x_1 + x_2 + x_3 = 1$.
Substratem{vstupem (r zenym) je **irradiance**{ozarenost $I(t)$.
4 parametry PSF modelu jsou "*transition rates*" ; (in [s ^{1}=irrad: unit]), ; [s ^{1}]. Plat , . Tzn. existence aspon dvou casovych skal (pro *svetelne a temnotn reakce* a proces *fotoinhibice*).

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



Stavovy vektor $x = (x_1; x_2; x_3)^T$: molarn frakce bunek ve stavu klidu (x_1), aktivace (x_2), resp. inhibice (x_3), tj. plat $x_1 + x_2 + x_3 = 1$. Substratem{vstupem (r zenym) je **irradiance**{ozarenost $I(t)$.
4 parametry PSF modelu jsou "*transition rates*" ; (in [$s\ ^1$=irrad: unit]), ; [$s\ ^1$]. Plat , . Tzn. existence aspon dvou casovych skal (pro *svetelne a temnotn reakce* a proces *fotoinhibice*).

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

$$\mu = \frac{\kappa\gamma}{T} \int_0^T x_2(t)\mathrm{d}t \ . \qquad (1)$$

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

PSF: Bilineární systém s jedním (skalárním) vstupem

$$\underline{x} = \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \underline{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & & \\ 0 & & 0 \\ 0 & 0 & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + I(t) \begin{bmatrix} & 0 & 0 \\ & & 0 \\ 0 & & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad (2)$$

- IVP: "prirozene" pocatecn podm nky (po inkubaci ve tme) jsou: $x(t_0) = [1; 0; 0]^T:$
- BVP: okrajove podm nky (periodic BC) jsou: $x(0) = x(T):$
- Pro konstantn vstup I ma matice soustavy $\left[A + I(t)B\right]$ 2 zaporna realna vlast. c sla. Tret vl. c slo je 0 a k nemu vl. vektor je x_{ss}.

PSF: Bilineární systém s jedním (skalárním) vstupem

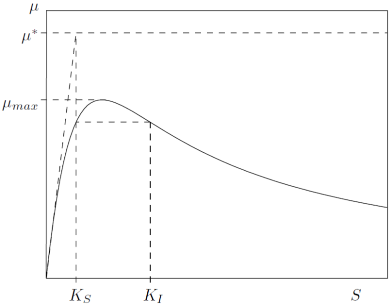
$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 & & \\ 0 & & 0 \\ 0 & 0 & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + I(t) \begin{bmatrix} & 0 & 0 \\ & & 0 \\ 0 & & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad (2)$$

- IVP: "prirozene" pocatecn podm nky (po inkubaci ve tme) jsou: $x(t_0) = [1; 0; 0]^T$:
- BVP: okrajove podm nky (periodic BC) jsou: $x(0) = x(T)$:
- Pro konstantn vstup I ma matice soustavy $[A + I(t)B]$ 2 zaporna realna vlast. c sla. Tret vl. c slo je 0 a k nemu vl. vektor je x_{ss}.

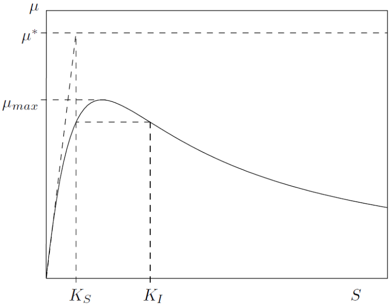
Š. Papáček, S. Celikovsky, D. Stys and J. Ruiz-Leon. Bilinear system as a modelling framework for analysis of microalgal growth. *Kybernetika*, 43(1):1{20, 2007.

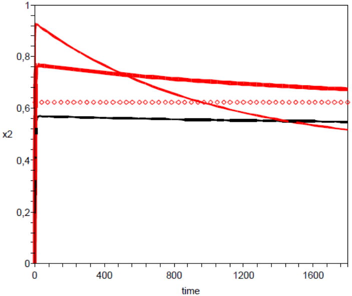
B. Rehak, S. Celikovsky, S. Papacek. Model for Photosynthesis and Photoinhibition: Parameter Identi cation Based on the Harmonic Irradiation 0_2 Response Measurement *IEEE Transactions on Automatic Control*, 53(1): 101{108, 2008.

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



PSF model (2) vede (pro $I \quad S = const.$) 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.

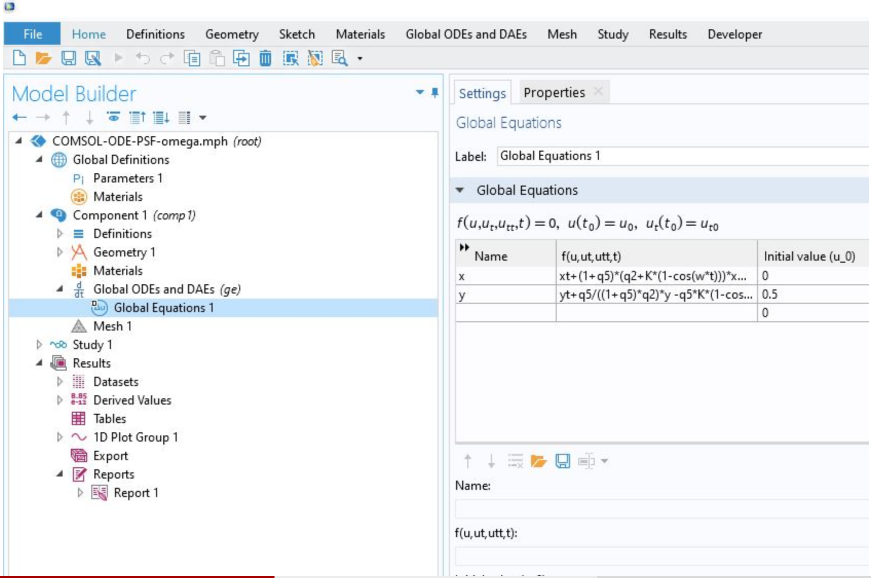
Resumé pro kalibraci PSF modelu: 3 z 5 parametrů popisují **steady state** a 2 popisují **dynamiku**, (i) pomalou *photoinhibition*, (ii) rychlou (lze kalibrovat pomoci tzv. *L-D cycles* indukovaných harmonickým signálem $I(t) = K(1 \quad cos(\omega\ t))$, viz další sekce).

Outline

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

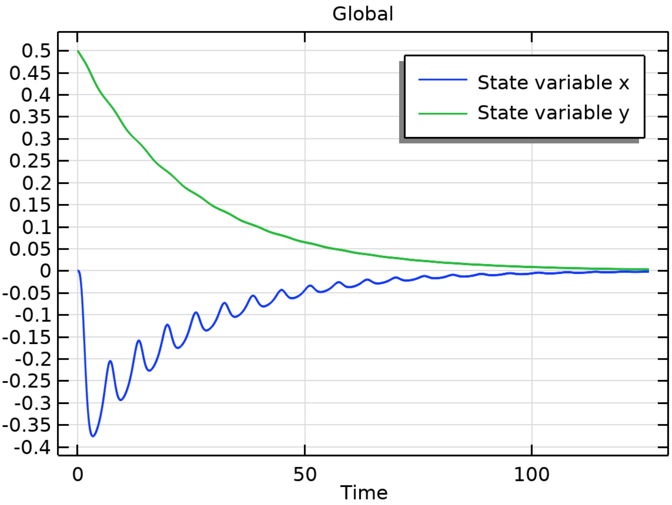
1^{st} attempt: The Global ODEs and DAEs (ge) interface

under the **Mathematics** branch *(How to set up the BVP?)*



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 $\rightarrow$ 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:
$u(t) = K(1 - \cos(\omega t)) = K(1 - w_2)$, 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

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

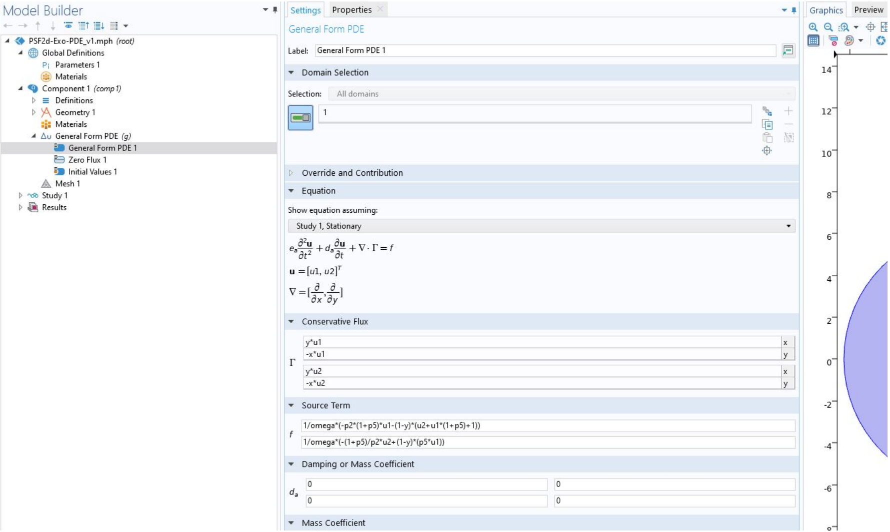
and further

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

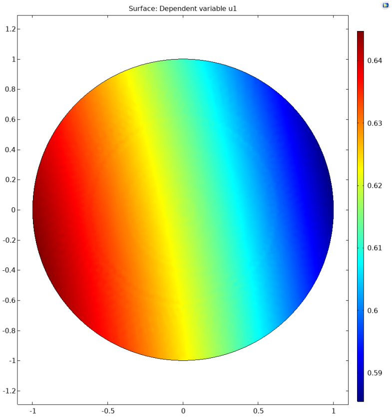
where $\nabla x := [\nabla x_1, \nabla x_2, \nabla x_3]^T$, and $\nabla x_i = [\frac{\partial x_i}{\partial w_1}, \frac{\partial x_i}{\partial w_2}]$.

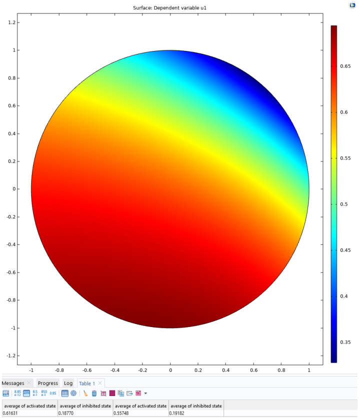
2^{nd} (successful) attempt: General Form PDE interface

under the **Mathematics** branch *(2D - stationary)*



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...

Outline

1 Introduction-Motivation

2 PSF Model Calibration – Problem Formulation

3 COMSOL Model - Equation-Based Modeling

4 Postprocessing – Conclusion

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