Data-driven Modeling and Control of Complex Dynamical Systems

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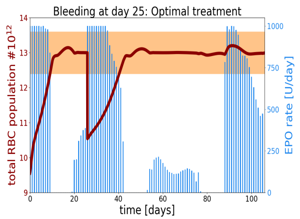
Our Motivation for the Research

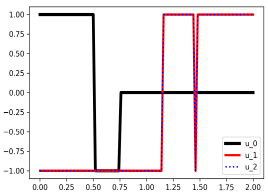
Parametrized Dynamical System: for parameter $\mu \in \mathcal{M}_{\text{ad}}$ and input $u \in \mathcal{U}_{\text{ad}}$

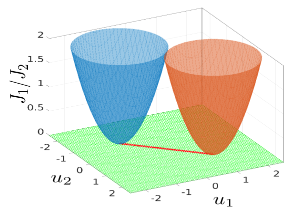
$$\dot{y}(t) = f(t, y(t), u(t); \mu) \text{ for } t > 0, \quad y(0) = y_\circ, \quad z(t) = h(t, y(t)) \text{ for } t > 0$$

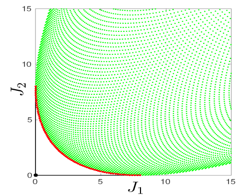
Optimal Design and Control:

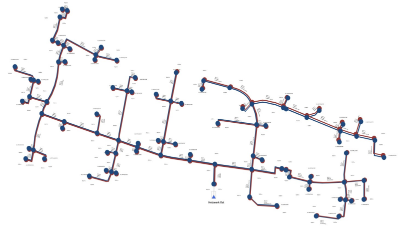
- optimal feedback (MPC, tailored open-loop optimization methods)
- optimal experimental design (bilevel optimization, inverse problems)
- multiobjective aspects (optimal compromises, set-oriented methods)
- network optimization (complex couplings, different types of dynamical systems)







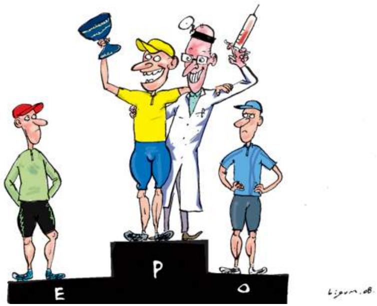


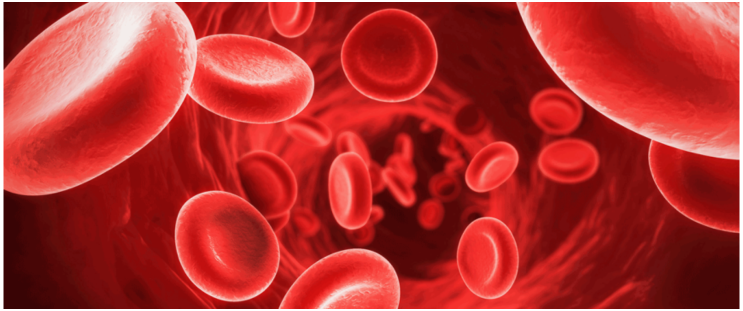


Our Foci: PDEs, model-order reduction (MOR), fast optimization algorithms

Outline of the Talk

1 Optimal EPO Dosing in Hemodialysis





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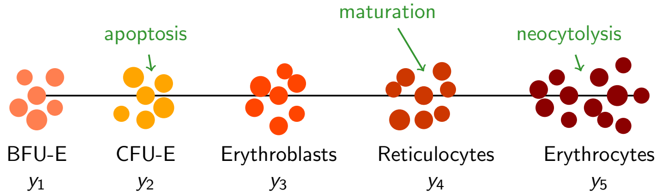
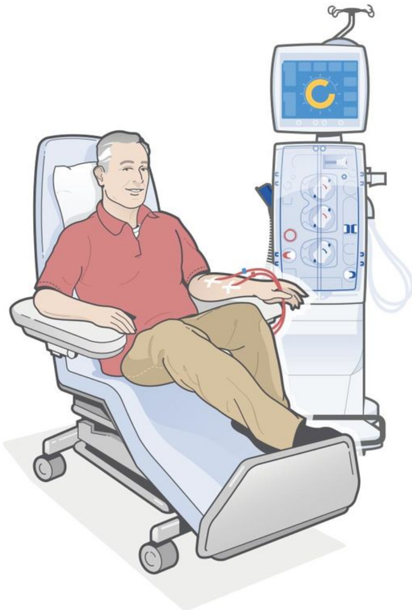
References:

[1] Beermann: *Reduced-order methods for a parametrized model for erythropoiesis involving structured population equations with one structural variable*, 2015
[2] Fuertinger: *A model of erythropoiesis*, 2012
[3] Fuertinger/Kappel/Thijssen/Levin/Kotanko: *A model of erythropoiesis in adults with sufficient iron availability*, 2013
[4] Grüne/Pannek: *Nonlinear Model Predictive Control: Theory and Algorithms*, 2016
[5] Rogg/Fuertinger/V./Kappel/Kotanko: *Optimal EPO dosing in hemodialysis patients using a non-linear model predictive control approach*, 2019

Hormone EPO (Erythropoietin):
- produced in kidneys
- drives production of new red blood cells (erythrocytes)
- low EPO levels cause neocytolysis (active reduction of erythrocytes)





Chronic Kidney Disease:
- insufficient production and release of EPO
- chronic anemia (chronic lack of blood)
- exogenous EPO administration during hemodialysis treatments

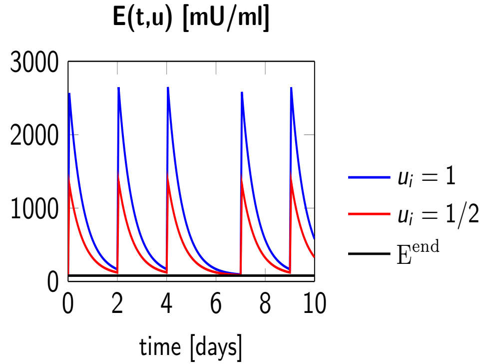
Question: What are the „optimal“ EPO doses?

Control Input [5]:

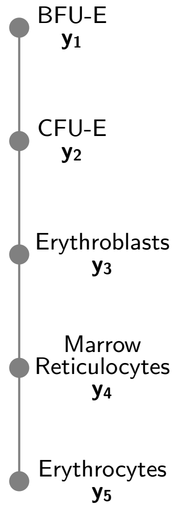
- administration time points (3 times per week): $t_1^*, t_2^*, t_3^*, \ldots, t_m^* \in [t_\circ, t_\mathsf{f}]$
- find EPO dose in $[0, E_{\mathsf{max}}]$ for every t_i^*
- vector $u = (u_1, \ldots, u_m) \in \mathbb{R}^m$, $\mathcal{U}_{\mathsf{ad}} = \{u \in \mathbb{R}^m \mid 0 \le u_i \le 1 \text{ for } 1 \le i \le m\}$

EPO Concentration in the Blood:

- $E(t,u) = E^{\mathsf{ex}}(t,u) + E^{\mathsf{end}}$ with remaining endogeneous E^{end}
- $E^{\mathsf{ex}}(t,u) = \frac{1}{c_{\mathsf{tbv}}} \sum_{i=1}^{m} u_i \chi_i(t)$ with $\chi_i(t) = E_{\mathsf{max}} e^{-\lambda(t-t_i^*)} \chi_{[t_i^*,\infty)}(t)$ and total blood volume $c_{\mathsf{tbv}} > 0$



State Vector: $y = (y_1, \ldots, y_5)$ with population densities $y_i(t,x)$ and maturity $x \in [a_i, b_i]$



Model Equations [1, 2, 3]:

$$y_t(t,x) + \overbrace{\nu(E(t,\boldsymbol{u}))}^{\text{maturation velocity}} y_x(t,x) = \Big(\overbrace{\beta}^{\text{proliferation}} - \overbrace{\alpha(E(t,\boldsymbol{u}),x)}^{\text{apoptosis}} \Big) y(t,x), \quad y(t_\circ,x) = y_\circ(x)$$

Boundary Conditions:

$$y_1(t,a_1) = S_0, \qquad y_2(t,a_2) = y_1(t,b_1), \qquad y_3(t,a_3) = y_2(t,b_2)$$

$$y_4(t,a_4) = \frac{y_3(t,b_3)}{\nu(E(t,\boldsymbol{u}))}, \qquad y_5(t,a_5) = \nu\big(E(t,\boldsymbol{u})\big)\, y_4(t,b_4)$$

Patient-Depending Coefficient Functions:

$$\alpha_2(E) = \frac{\mu_1}{1+\exp\big(\mu_2 E - \mu_3\big)}, \quad \alpha_5(E,x) = \alpha_5^0 + \chi_{[x_{\text{min}},x_{\text{max}}]}(x)\cdot\widetilde{\alpha}_5(E), \quad \nu(E) = \frac{\mu_4-\mu_5}{1+\exp\big(-\mu_6 E+\mu_7\big)} + \mu_5$$

Control Input: $E(t,u) = \frac{1}{c_{\text{tbv}}}\sum_{i=1}^{m} u_i\chi_i(t) + E^{\text{end}}$ with $\chi_i(t) = E_{\text{max}} e^{-\lambda(t-t_i^*)}\chi_{[t_i^*,\infty)}(t)$

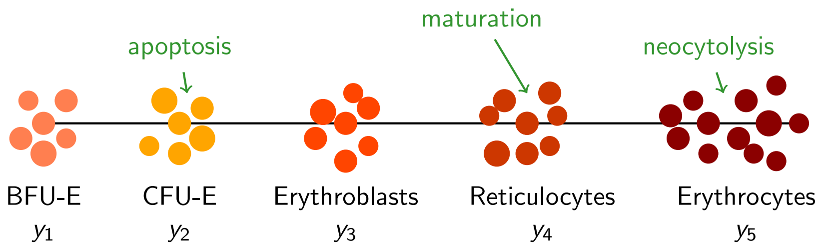
Desired Total Population: hemoglobin target range of 10-11 g/dl

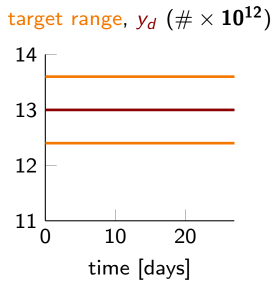
Total Erythrocytes Population: $\int_{a_5}^{b_5} y_5(t,x)\,\mathrm{d}x$

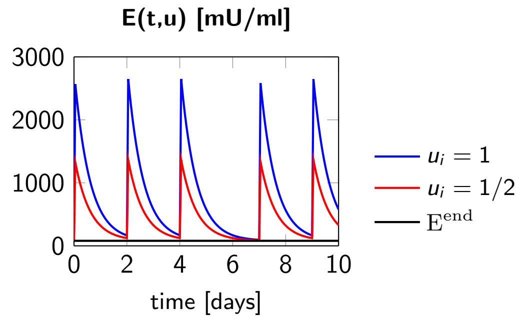
Cost Functional [5]:

$$J(y,u) = \frac{\sigma_\Omega}{2}\int_{t_\circ}^{t_f}\Big|\int_{a_5}^{b_5} y_5(t,x)\,\mathrm{d}x - y_d\Big|^2\mathrm{d}t + \frac{\sigma_f}{2}\Big|\int_{a_5}^{b_5} y_5(t_f,x)\,\mathrm{d}x - y_d\Big|^2 + \frac{1}{2}\sum_{i=1}^{m}\gamma_i\,|u_i|^2$$

with weights $\sigma_\Omega, \sigma_f, \gamma_i > 0$







Goal: closed-loop/feedback control taking into account changes in parameters and data

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Algorithm 1: Nonlinear model predictive control [4, 5]

1: Get initial time $t_\circ \in [0,T]$ and initial condition $y_\circ$;

2: Choose prediction horizon $\Delta T = N\Delta t$ and set $t_\mathsf{f} = t_\circ + \Delta T$;

3: Minimize the cost (by projected BFGS method with Armijo line search)

$$J(y,u) = \frac{\sigma_\Omega}{2}\int_{t_\circ}^{t_\mathsf{f}} \Big| \int_{a_5}^{b_5} y_5(t,x)\,\mathrm{d}x - y_d \Big|^2 \mathrm{d}t + \frac{\sigma_\mathsf{f}}{2}\Big| \int_{a_5}^{b_5} y_5(t_\mathsf{f},x)\,\mathrm{d}x - y_d \Big|^2 + \frac{1}{2}\sum_{i=1}^{m} \gamma_i\,|u_i|^2$$

subject to PDE constraints and bilateral control constraints;

4: Apply only the first component of the resulting optimal control;

5: Set new initial time $t_\circ = t_\circ + \Delta t$ and repeat iteratively

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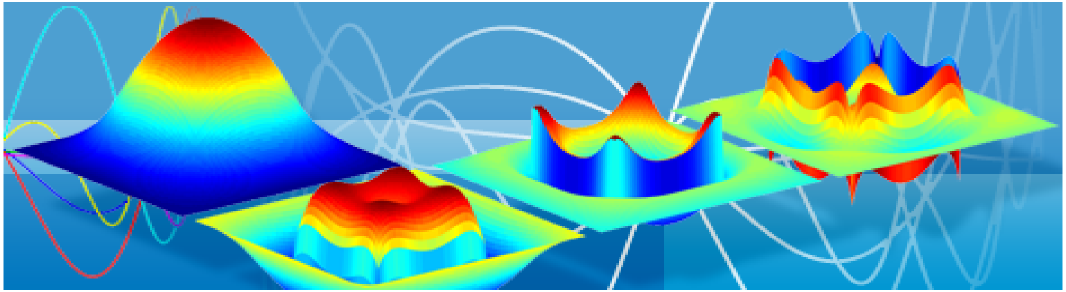
Problem: nonconvexity due to the nonlinearities

Idea: linearize the model to get a convex linear-quadratic open-loop problem

2 Extended Dynamic Mode Decomposition (EDMD) for MPC



References:

[6] Alfatlawi/Srivastava: *An incremental approach to online dynamic mode decomposition for time-varying systems with applications*, 2019

[7] Benner/Himpe/Mitchell: *On reduced input-output dynamic mode decomposition*, 2018

[8] Casper/Fuertinger/Kotanko/Mechelli/Rohleff/V.: *Data-driven modeling and control of complex dynamical systems arising in renal anemia therapy*, 2021

[9] Grüne/Pannek: *Nonlinear Model Predictive Control: Theory and Algorithms*, 2017

[10] Korda/Mezić: *Linear predictors for nonlinear dynamical systems: Koopman operator meets model predictive control*, 2018

[11] Kutz/Brunton/Brunton/Proctor: *Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems*, 2016

[12] Rohleff: *An incremental approach to dynamic mode decomposition for time-varying systems with applications to a model for erythropoiesis*, 2020

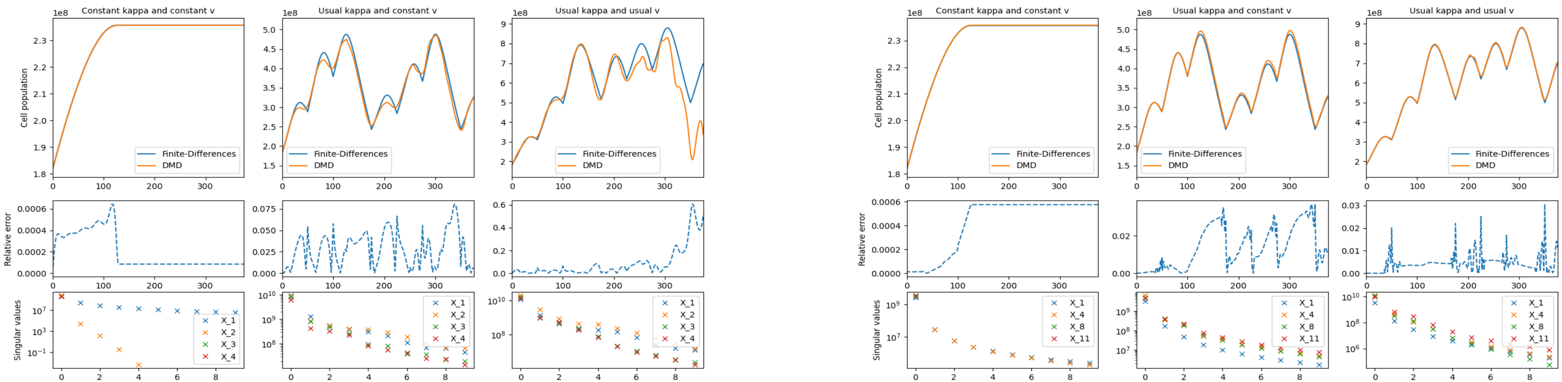
[13] Zhang/Rowley/Deem/Cattafesta: *Online dynamic mode decomposition for time-varying systems*, 2017

Idea of DMDc [7, 11]: $y_{k+1} = F(t_k, y_k, u_k) \overset{\text{DMDc}}{\approx} Ay_k + Bu_k$ for $k \geq 0$ and $y_0 = y_\circ$

Computation: for $Y_0 = [y_0 \,|\, \ldots \,|\, y_{m-1}]$, $Y_1 = [y_1 \,|\, \ldots \,|\, y_m]$, $U = [u_0 \,|\, \ldots \,|\, u_{m-1}]$ solve

$$[A, B] = \underset{\tilde{A},\tilde{B}}{\arg\min} \|Y_1 - \tilde{A}Y_0 - \tilde{B}U\|_F \;\to\; [A \,|\, B] = Y_1 \begin{bmatrix} Y_0 \\ U \end{bmatrix}^\dagger$$ & eigendecomposition of A for MOR

Approximation for time-varying systems: computation of time-varying DMDc [6, 12, 13]



Extended Dynamic Mode Decomposition (EDMD) [10, 11]

Discrete Dynamical System: $y_0 = y_\circ$, $y_{k+1} = F(t_k, y_k, u_k)$ and $z_k = h(t_k, y_k)$ for $k \geq 0$

Lifting/observable functions: $\psi = (\psi_1, \ldots, \psi_{n_\psi}) : \mathbb{R}^n \to \mathbb{R}^{n_\psi}$ with $n_\psi < n$

Computation: for $\hat{Y}_0 = [\psi(y_0) \,|\, \ldots \,|\, \psi(y_{m-1})]$, $\hat{Y}_1 = [\psi(y_1) \,|\, \ldots \,|\, \psi(y_m)]$, $U = [u_0 \,|\, \ldots \,|\, u_{m-1}]$ solve

$$[\hat{A}, \hat{B}] = \operatorname*{arg\,min}_{\tilde{A}, \tilde{B}} \|\hat{Y}_1 - \tilde{A}\hat{Y}_0 - \tilde{B}U\|_F, \quad \hat{C} = \operatorname*{arg\,min}_{\tilde{C}} \|\hat{Y}_0 - \tilde{C}Y_0\|_F$$

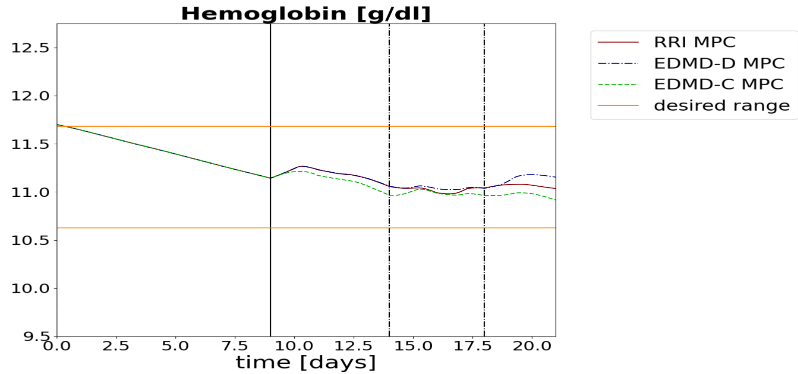
Surrogate model: $\hat{y}_0 = \psi(y_\circ)$, $\hat{y}_{k+1} = \hat{A}\hat{y}_k + \hat{B}u_k$ and $z_k \approx \hat{z}_k = \hat{C}\hat{y}_k$ for $k \geq 0$

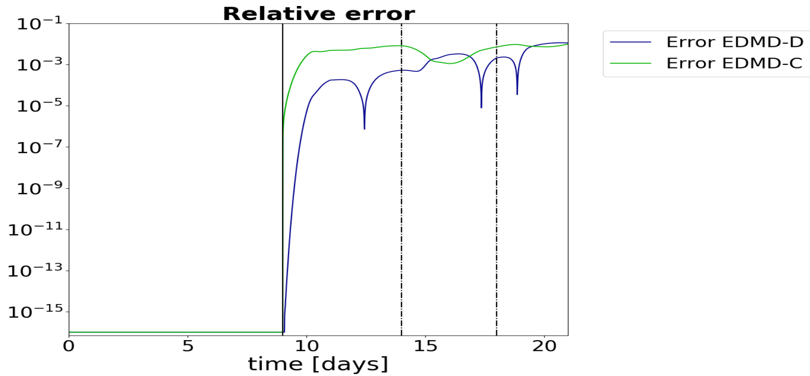
Objective: Recall that

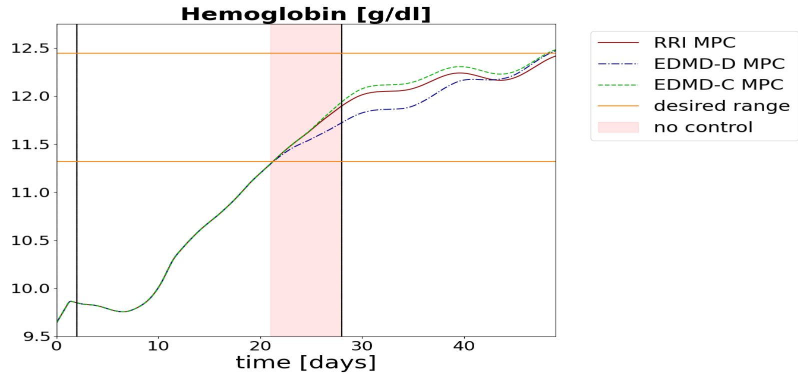
$$J(y,u) = \frac{\sigma_\Omega}{2} \int_{t_\circ}^{t_\mathrm{f}} \left| \int_{a_5}^{b_5} y_5(t,x)\,\mathrm{d}x - y_d \right|^2 \mathrm{d}t + \frac{\sigma_\mathrm{f}}{2} \left| \int_{a_5}^{b_5} y_5(t_\mathrm{f},x)\,\mathrm{d}x - y_d \right|^2 + \frac{1}{2}\sum_{i=1}^{m} \gamma_i |u_i|^2$$

$\Rightarrow$ applying of DMDc only for the y_5 variable

$\Rightarrow$ utilize 3 to seven Legendre polynomial evaluation of the snapshots for the ψ_i's







Patient	T	CPU times	Speed-up	Relative error
2	21 days	11.5 s	9.5	9.1×10^{-6}
3	21 days	5.3 s	10.3	9.0×10^{-10}
3	49 days	17.5 s	7.1	7.4×10^{-5}

See [5, 8]

3 Empirical Gramian-Based Approach

References:

[14] Condon/Ivanov: *Empirical balanced truncation of nonlinear systems*, 2004
[15] Garcia/Basilio: *Computation of reduced-order models of multivariable systems by balanced truncation*, 2002
[16] Himpe: *emgr – The empirical gramian framework*, 2018
[17] Himpe/Ohlberger: *A unified software framework for empirical gramians*, 2013
[18] Lall/Marsden/Glavaški: *Empirical model reduction of controlled nonlinear systems*, 2001
[19] Zhou/Doyle/Glover: *Robust and Optimal Control*, 1996

Linear Time Invariant (LTI) System:

$$\dot{y}(t) = Ay(t) + Bu(t) \text{ for } t > 0, \quad x(0) = y_\circ, \qquad z(t) = Cy(t) \text{ for } t > 0$$

Controllability Gramian [19]:

$$W_c = \int_0^\infty e^{At} B B^\top e^{A^\top t}\,\mathrm{d}t = \int_0^\infty \left(e^{At}B\right)\left(e^{At}B\right)^\top \mathrm{d}t$$

Observability Gramian [19]:

$$W_o = \int_0^\infty e^{A^\top t} C^\top C e^{At}\,\mathrm{d}t = \int_0^\infty \left(e^{A^\top t}C^\top\right)\left(e^{A^\top t}C^\top\right)^\top \mathrm{d}t$$

Linear Time Variant System:

$$\dot{y}(t) = A(t)y(t) + Bu(t) + g(t) \text{ for } t > 0, \quad x(0) = y_\circ, \qquad z(t) = Cy(t) \text{ for } t > 0$$

$\Rightarrow$ extension by empirical gramians which are based on simulations only

Linear Time Variant System:

$$\dot{y}(t) = A(t)y(t) + Bu(t) + g(t) \text{ for } t > 0, \quad x(0) = y_\circ, \qquad z(t) = Cy(t) \text{ for } t > 0 \tag{1}$$

Empirical Controllability Gramian [15, 16]:

$$\widehat{W}_c = \sum_{l=1}^{r} \sum_{m=1}^{s} \sum_{i=1}^{p} \frac{1}{rsc_m^2} \int_0^\infty Y^{ilm}(t)\,\mathrm{d}t \text{ with } Y^{ilm}(t) = \left(y^{ilm}(t) - \bar{y}^{ilm}\right)\left(y^{ilm}(t) - \bar{y}^{ilm}\right)^\top$$

where $y^{ilm}(t) \in \mathbb{R}^{n_y}$ solves (1) corresponding to the impulse input $u(t) = c_m T_l e_i \delta(t)$ with varying positive scalars c_m, orthogonal matrices T_l and unit vectors e_i

Empirical Observability Gramian [16, 17, 18]:

$$\widehat{W}_o = \sum_{l=1}^{r} \sum_{m=1}^{s} \frac{1}{rsc_m^2} \int_0^\infty T_l Z^{lm}(t) T_l^\top \,\mathrm{d}t \text{ with } Z_{ij}^{lm}(t) = \left(z^{ilm}(t) - \bar{z}^{ilm}\right)^\top \left(z^{jlm}(t) - \bar{z}^{jlm}\right)$$

where $z^{ilm}(t) \in \mathbb{R}^{n_z}$ is the output of (1) corresponding to the initial condition $y_\circ = c_m T_l e_i$.

Singular Value Decomposition for Balancing [14, 15]:

$$\widehat{W}_c^{1/2}\widehat{W}_o^{1/2} = U\Sigma V^\top = \left[U_1\,|\,U_2\right]\begin{bmatrix}\Sigma_1 & 0\\ 0 & \Sigma_2\end{bmatrix}\left[V_1\,|\,V_2\right]^\top = \begin{pmatrix}U_1\Sigma_1V_1^\top & 0\\ 0 & U_2\Sigma_2V_2^\top\end{pmatrix}$$

Reduced-Order Modeling: $y(t) \approx U_1 y^\ell(t)$

$$\begin{aligned}\dot{y}^\ell(t) &= \left[V_1^\top A(t)U_1\right]y^\ell(t) + \left[V_1^\top B\right]u(t) + g(t) \text{ for } t \in (0,T], \quad y^\ell(0) = V_1^\top y_\circ\\ z^\ell(t) &= \left[CU_1\right]y^\ell(t) \qquad\qquad\qquad\qquad\qquad\quad \text{ for } t \in [0,T]\end{aligned}$$

Quadratic Cost functional: $J(y,u) = \frac{1}{2}\int_0^T \|z(t) - z_Q(t)\|_2^2\,\mathrm{d}t + \frac{\sigma}{2}\int_0^T \|u(t)\|_2^2\,\mathrm{d}t$

First-Order Optimality System: $u(t) = B^\top p(t)/\sigma$, $q(t) = p(T-t)$

$$\dot{x}(t) = D(t)x(t) + \tilde{D}(t)x(T-t) + G(t) \text{ for } t \in (0,T), \quad x(0) = x_\circ \tag{2}$$

for $x = (y,q)$ and appropriate $D(t)$, $\tilde{D}(t)$ and $G(t)$
$\Rightarrow$ apply empirical gramian approach for (2) (instead of POD)

Dynamical System: heat equation with time varying convection

$$\begin{aligned} \frac{\partial y_u}{\partial t}(t,\boldsymbol{x}) - \lambda \Delta y_u(t,\boldsymbol{x}) + \alpha(t)(v(\boldsymbol{x}) \cdot \nabla y_u(t,\boldsymbol{x})) &= u(t,\boldsymbol{x}) + f(\boldsymbol{x}), & (t,\boldsymbol{x}) \in \Omega_T \\ \frac{\partial y_u}{\partial n}(t,\boldsymbol{s}) + \gamma y_u(t,\boldsymbol{s}) &= 0, & (t,\boldsymbol{s}) \in \Sigma_T \\ y_u(0,\boldsymbol{x}) &= y_\circ(\boldsymbol{x}), & \boldsymbol{x} \in \Omega \end{aligned}$$

First-Order Optimality System: localized distributed control

$$\dot{x}(t) = D(\alpha(t))x(t) + \tilde{D}x(T-t) + G(t) \text{ for } t \in (0,T), \quad x(0) = x_\circ \tag{3}$$

Input for (3): $\alpha(t) = c_m T_l e_i \hat{\alpha}(t)$

	gramian	POD
Relative error in u	$2.31 \cdot 10^{-4}$	$1.13 \cdot 10^{-1}$

	CPU time	speed-up
Full model	465.0 s	–
Gramian	43.1 s (+ 51.5 s)	10.8 (4.8)
POD	42.7 s (+225.8s)	10.9 (1.7)

Conclusions and Outlook

Conclusions:

- MPC for a nonlinear model describing EPO treatment
- speed-up by utilizing linearization based on EDMD
- empirical gramian approach for first-order optimality system

Outlook:

- properties of the EDMD approximation
- update strategies for EDMD
- comparison to other linearization techniques

More informations on our group: `https://www.mathematik.uni-konstanz.de/volkwein`

Thank you for your attention!