MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

LQResNet: Using DNNs for Learning of Dynamical Systems

Peter Benner

Joint work with Pawan Goyal (and others. . .)

Workshop on Control of Dynamical Systems
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BiG max MAX PLANCK RESEARCH NETWORK on big-data-driven materials science

hrzz Hrvatska zaklada za znanost

ConDyS

Outline

Joint Work With . . .

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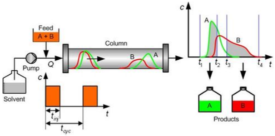

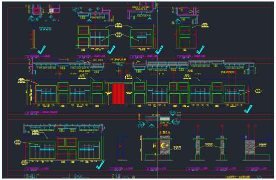

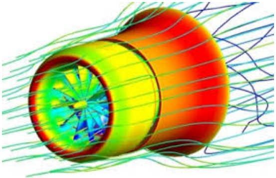

Dynamic models are important

- to analyze transient behavior under operating conditions;
- for controller design;
- design studies w.r.t. (material/geometry) parameter variations;
- long-time horizon reliability prediction.

Problem set-up

- Construct a mathematical model

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t))$$

describing the dynamics of the process.

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Learning Dynamics from Data

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- Construct a mathematical model

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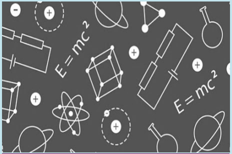
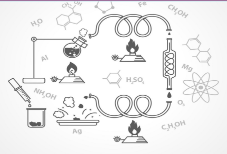
  describing the dynamics of the process.
- Neural network-based approaches: e.g., recurrent neural networks and long short time memory networks.
- Leverage all prior information about the process for efficient learning.

Key sources of information



Physical laws

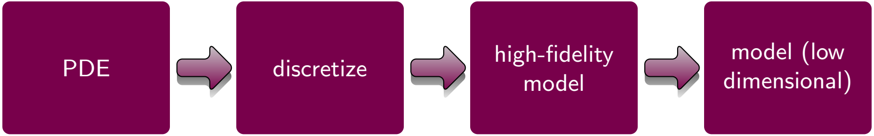
Domain knowledge



Collected data

Learning Dynamics from Data

- Engineering processes are supported by domain knowledge and first principles
  $\rightsquigarrow$ a PDE model can be obtained that adequately explains the dynamics



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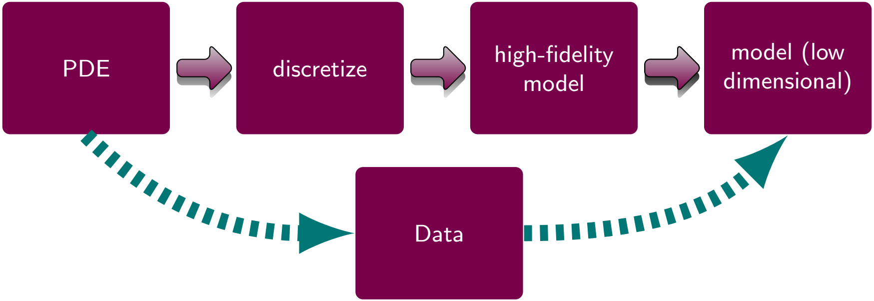

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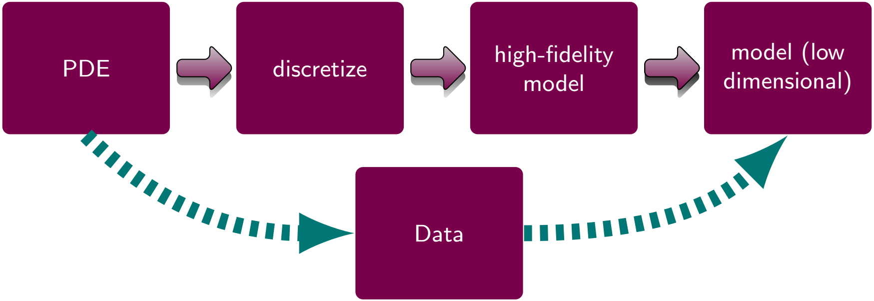

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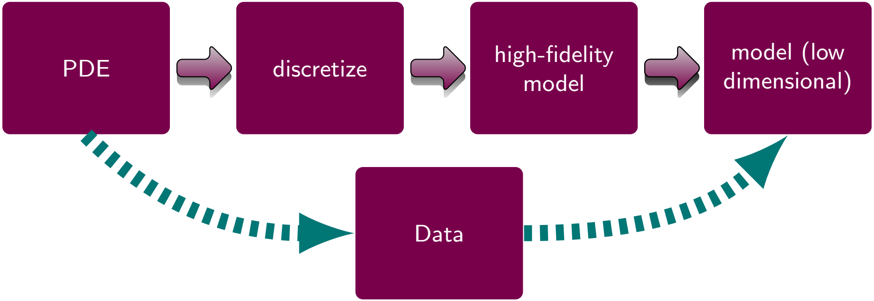

- Data collection: obtained using a legacy code, or commercial software, or experiments.
- Ideal goal: obtain the same reduced-order model (ROM) as obtained by intrusive model order reduction using data, so that error bounds and convergence analysis for ROMs can be directly employed!

Operator inference framework [Peherstorfer/Willcox '16]

- Operator inference leverages the known physical structure at the PDE level.
- Assume a quadratic high-fidelity model resulting from an underlying PDE $\frac{\partial x}{\partial t} = \mathcal{A}(x) + \mathcal{H}(x)$ with linear and quadratic terms:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{H}(\mathbf{x}(t) \otimes \mathbf{x}(t))$$

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- Data preparation (in reduced dimension)

  1. Build temporal snapshot matrix $\mathbf{X} := \begin{bmatrix} | & | & & | \\ \mathbf{x}_0 & \mathbf{x}_1 & \cdots & \mathbf{x}_k \\ | & | & & | \end{bmatrix}$.

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3. Reduced state vectors

$$\hat{\mathbf{X}} := V^T\mathbf{X} = \begin{bmatrix} | & | & & | \\ \hat{\mathbf{x}}_0 & \hat{\mathbf{x}}_1 & \cdots & \hat{\mathbf{x}}_k \\ | & | & & | \end{bmatrix}, \qquad \hat{\mathbf{X}}^{\otimes} := \begin{bmatrix} | & | & & | \\ \hat{\mathbf{x}}_0^{\otimes} & \hat{\mathbf{x}}_1^{\otimes} & \cdots & \hat{\mathbf{x}}_k^{\otimes} \\ | & | & & | \end{bmatrix}.$$

with $\hat{\mathbf{x}}_i = \mathbf{V}^\top \mathbf{x}_i$ and $\hat{\mathbf{x}}_i^{\otimes} = \hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i$

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4. Approximate time-derivative data $\dot{\hat{\mathbf{X}}} := \begin{bmatrix} | & | & & | \\ \dot{\hat{\mathbf{x}}}_0 & \dot{\hat{\mathbf{x}}}_1 & \cdots & \dot{\hat{\mathbf{x}}}_k \\ | & | & & | \end{bmatrix}$.

Operator inference framework

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A ROM of the form

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can be obtained using projected data by solving the optimization problem

$$\min_{\hat{\mathbf{A}},\hat{\mathbf{H}}} \left\| \dot{\hat{\mathbf{X}}} - \hat{\mathbf{A}}\hat{\mathbf{X}} - \hat{\mathbf{H}}\hat{\mathbf{X}}^{\otimes} \right\|.$$

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[Peherstorfer '20]

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- Operator inference recovers intrusive POD reduced model if data are Markovian.
  [Peherstorfer '20]
- Typically, the least-squares problem is ill-conditioned, hence need regularization.
  [McQuarrie et al. '21, B./Goyal/Heiland/Pontes '21]

Nonlinear systems [B./Goyal/Kramer/Peherstorfer/Willcox '20]

- Consider a nonlinear system of the form

$$\frac{\partial s}{\partial t} = \mathcal{A}(s) + \mathcal{H}(s) + \mathcal{F}(t, s),$$

where the analytic form of $\mathcal{F}(t, s)$ is known.

- We can learn a ROM of the form

$$\dot{\hat{\mathbf{s}}}(t) = \hat{\mathbf{A}}\hat{\mathbf{s}} + \hat{\mathbf{H}}\left(\hat{\mathbf{s}} \otimes \hat{\mathbf{s}}\right) + \hat{\mathbf{f}}(t, \hat{\mathbf{s}})$$

directly from data!

- Simulation of reduced nonlinear system can be further accelerated using hyper-reduction.

- The dynamics of a batch chromatography column can be described by the coupled PDE system of advection-diffusion type:

$$\frac{\partial c_i}{\partial t} + \frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t} + \frac{\partial c_i}{\partial x} - \frac{1}{\mathrm{Pe}}\frac{\partial^2 c_i}{\partial x^2} = 0,$$
$$\frac{\partial q_i}{\partial t} = \kappa_i \left(q_i^{Eq} - q_i \right).$$

- It is a coupled PDE; thus, the coupling structure is desired to be preserved in learned ROM
- This is achieved by block diagonal projection, thereby not mixing separate physical quantities.

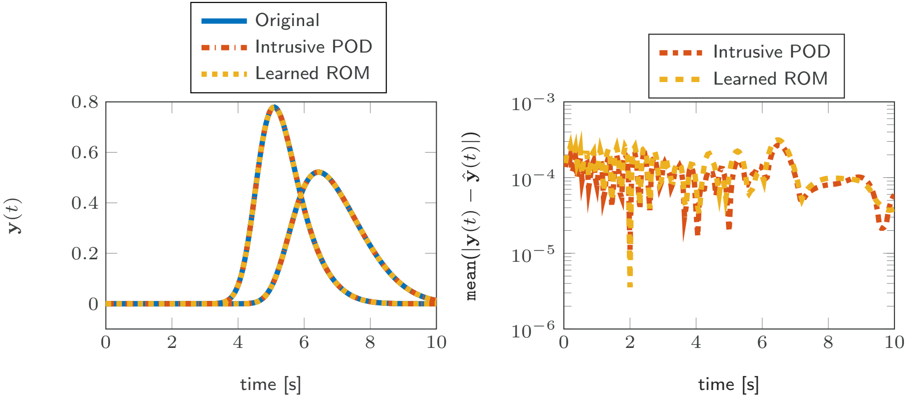

Figure: Batch chromatography example: A comparison of the POD intrusive model with the learned model of order $r = 4 \times 22$, where $n = 1600$ and $\mathrm{Pe} = 2000$.

Parameterized Shallow Water Equations

- Parameterized shallow water equations are given by [Yildiz et al '20]

$$\frac{\partial}{\partial t}\tilde{u} = -h_x + \sin\theta\ \tilde{v} - \tilde{u}\tilde{u}_x - \tilde{v}\tilde{u}_y + \delta\cos\theta(h\tilde{u})_x - \frac{3}{8}\left(\delta\cos\theta\right)^2\left(h^2\right)_x,$$
$$\frac{\partial}{\partial t}\tilde{v} = -h_y + \sin\theta\ \tilde{u} + \frac{1}{2}\delta\sin\theta\cos\theta\ h - \tilde{u}\tilde{v}_x - \tilde{v}\tilde{v}_y$$
$$+\delta\cos\theta\left((h\tilde{u})_y + \frac{1}{2}h\left(\tilde{v}_x - \tilde{u}_y\right)\right) - \frac{3}{8}\left(\delta\cos\theta\right)^2\left(h^2\right)_y,$$
$$\frac{\partial}{\partial t}h = -(h\tilde{u})_x - (h\tilde{v})_y + \frac{1}{2}\delta\cos\theta(h^2)_x.$$

- Parameterized by the latitude θ.
- $\tilde{\mathbf{u}} =: (\tilde{u}; \tilde{v})$ is the canonical velocity.
- h is the height field.
- We collect the training data for 5 different parameter realizations θ in $\left[\frac{\pi}{6}, \frac{\pi}{3}\right]$.
- Infer a reduced parametric model directly from data of order $r = 75$.

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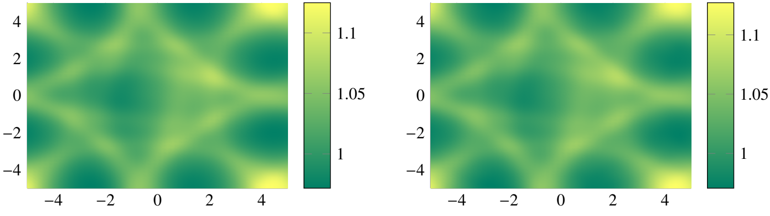
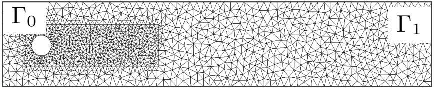
- Comparison of the height field for the parameter $\theta = \frac{5\pi}{24}$:

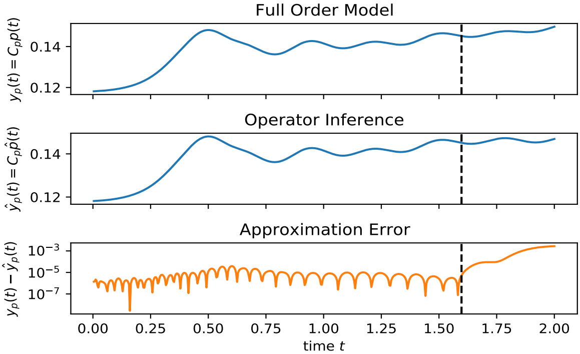


(a) FOM

(b) Learned parametric model

Tailored operator inference for incompressible Navier-Stokes equations, by heeding incompressibility condition. [B./Goyal/Heiland/Pontes '21]





Combining Operator Inference with Deep Learning

Operator Inference for General Nonlinear Systems

Problem formulation

$$\dot{\mathbf{v}}(t) = \mathbf{f}(\mathbf{v}(t)) + \mathbf{r}(\mathbf{v}(t))$$

- $\mathbf{f}(\mathbf{v}(t))$: known from physical laws or expert knowledge;
  - e.g., for chemical reaction models, we expect to have an Arrhenius-type term.
- $\mathbf{r}(\mathbf{v}(t))$: unknown terms
  - e.g., friction terms in robotics or vibration systems, effects of removed higher-frequency dynamics on the low-frequency response, etc.

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Observation

- Often, governing equations are **quadratic**, i.e.,

  $\mathbf{f}(\mathbf{v}) := \mathbf{A}\mathbf{v} + \mathbf{H}\left(\mathbf{v} \otimes \mathbf{v}\right).$
- If no additional information is given, we assume $\mathbf{f}$ to be quadratic.
- Moreover, possible to find artificial variables in which dynamics are quadratic.

  Philosophy: Lift & learn [Qian et al. '20]

Navier-Stokes equations

$$\rho\left(\frac{\partial u_r}{\partial t} + u_r\frac{\partial u_r}{\partial r} + u_z\frac{\partial u_r}{\partial z}\right) = -\frac{\partial p}{\partial r} + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_r}{\partial r}\right) + \frac{\partial^2 u_r}{\partial z^2} - \frac{u_r}{r^2}\right) + \rho g_r$$

$$\rho\left(\frac{\partial u_z}{\partial t} + u_r\frac{\partial u_z}{\partial r} + u_z\frac{\partial u_z}{\partial z}\right) = -\frac{\partial p}{\partial z} + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_z}{\partial r}\right) + \frac{\partial^2 u_z}{\partial z^2}\right) + \rho g_z$$

$$\frac{1}{r}\frac{\partial}{\partial r}(r u_r) + \dots$$

Fisher's equation

$$u_t = u(1-u) + u_{xx}$$

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Lifting

[Gu '09/'11, Benner/Breiten '15, Qian et al '20]

Consider the nonlinear system:

$$\dot{\mathbf{x}} = -\mathbf{x} + e^{-\mathbf{x}}$$

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- Define $\mathbf{z}(t) = e^{-\mathbf{x}} \rightsquigarrow \dot{\mathbf{z}}(t) = -e^{-\mathbf{x}}\dot{\mathbf{x}} = -\mathbf{z}(t)\left(-\mathbf{x}(t) + \mathbf{z}(t)\right)$

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- The system becomes linear-quadratic in $(\mathbf{x}(t), \mathbf{z}(t))$, i.e.,

$$\begin{bmatrix} \dot{\mathbf{x}}(t) \\ \dot{\mathbf{z}}(t) \end{bmatrix} = \begin{bmatrix} -\mathbf{x}(t) + z(t) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \mathbf{z}(t)\left(\mathbf{x}(t) - \mathbf{z}(t)\right) \end{bmatrix}.$$

Linear-Quadratic Residual Networks

For simplicity, consider the form:

$$\dot{\mathbf{v}}(t) = f(\mathbf{v}(t)) = \mathbf{A}\mathbf{v}(t) + \mathbf{H}\left(\mathbf{v}(t) \otimes \mathbf{v}(t)\right) + \mathbf{r}(\mathbf{v}(t)),$$

where

- $\mathbf{r}(\mathbf{v}(t))$ can be interpreted as a residual that cannot be resolved by the quadratic-form or prior knowledge.

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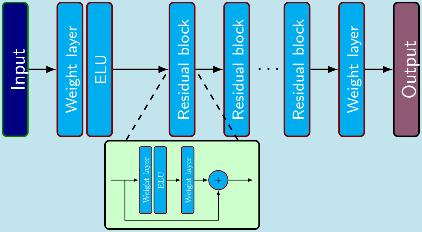
Residual networks

[He/Ren/Sun '16]

- Have shown their power in computer vision applications.



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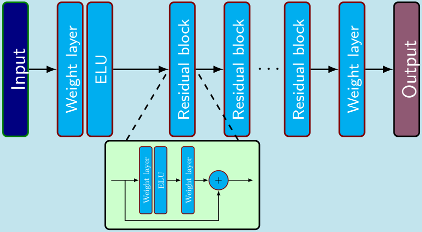
- There is an established connection to dynamical systems.



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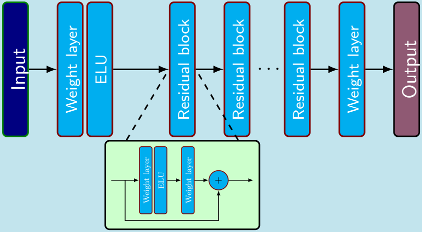
- There is an established connection to dynamical systems.
- Residual type connections hint to adaptive refinement of solution or features.



Linear-Quadratic Residual Networks

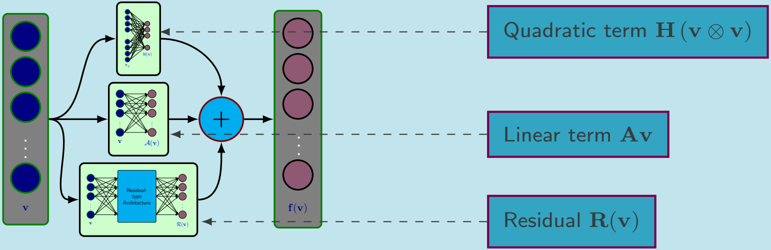
For simplicity, consider the form:

$$\dot{\mathbf{v}}(t) = f(\mathbf{v}(t)) = \mathbf{A}\mathbf{v}(t) + \mathbf{H}\left(\mathbf{v}(t) \otimes \mathbf{v}(t)\right) + \mathbf{r}(\mathbf{v}(t)),$$

where

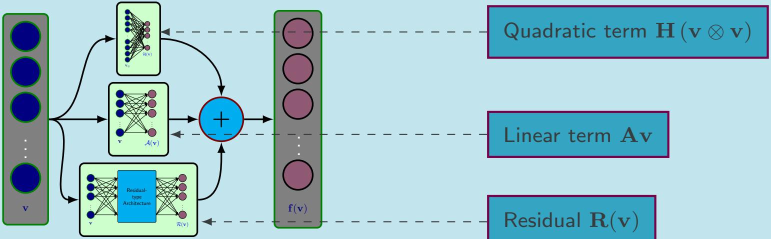
- $\mathbf{r}(\mathbf{v}(t))$ can be interpreted as a residual that cannot be resolved by the quadratic-form or prior knowledge.

Linear-Quadratic Residual Networks (LQResNet) [Goyal/B. '21]



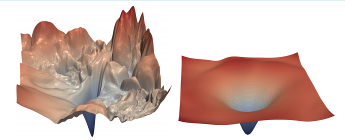
Advantages of the Architecture

Linear-Quadratic Residual Networks (LQResNet) [Goyal/B. '21]



Remarks

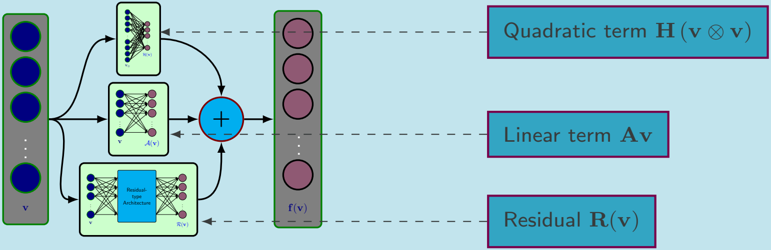
- Due to skip connections, loss landscape becomes less bumpy. [Li et al. '18]



(a) without skip connections (b) with skip connections

Advantages of the Architecture

Linear-Quadratic Residual Networks (LQResNet) [Goyal/B. '21]

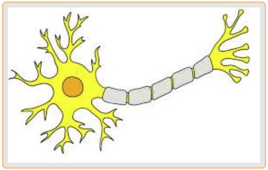


Remarks

- Due to skip connections, loss landscape becomes less bumpy. [Li et al. '18]
- Layers can be added without restarting whole optimization as deep residual layers tend to refine the mapping.

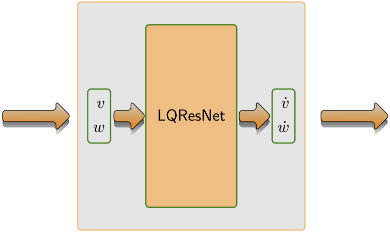
Set-up

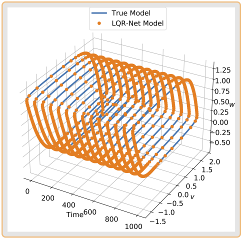
- The FitzHugh-Nagumo model is a coupled PDE-ODE model describing the spiking of a neuron.
- Assume to have time-series data for 10 different initial conditions.
- We build different networks for both variables.
- We check the predictive capabilities of the inferred model under new initial condition.



Governing equations

$$\dot{v}(t) = v - \frac{v^3}{3} - w + RI_{ext}$$
$$\dot{w}(t) = v + a - bw$$





Set-up

- Represents complex wide-range dynamical behavior in yeast glycolysis.

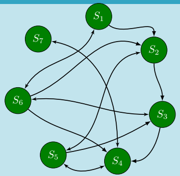
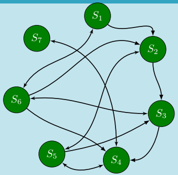


Figure: Interaction topology for 7 species.

Set-up

- Represents complex wide-range dynamical behavior in yeast glycolysis.
- There are 7 involved species.



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- Represents complex wide-range dynamical behavior in yeast glycolysis.
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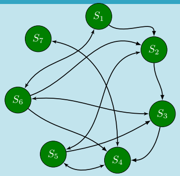
- Data for 30 different initial conditions.



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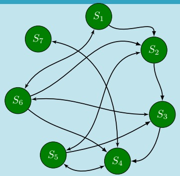

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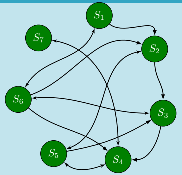

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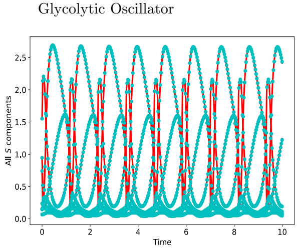

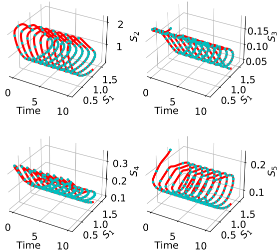

Tubular Reactor Model

- One dimensional model with a single reaction, describing dynamics of the species concentration $\psi(x,t)$ and temperature $\theta(x,t)$ via

$$\frac{\partial \psi}{\partial t} = \frac{1}{\mathrm{Pe}}\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial \psi}{\partial x} - \mathcal{D}\mathcal{F}(\psi,\theta;\gamma),$$
$$\frac{\partial \theta}{\partial t} = \frac{1}{\mathrm{Pe}}\frac{\partial^2 \theta}{\partial x^2} - \frac{\partial \theta}{\partial x} - \beta(\theta - \theta_{\text{ref}}) + \mathcal{B}\mathcal{D}\mathcal{F}(\psi,\theta;\gamma),$$

with spatial variable $x \in (0,1)$, time $t > 0$ and Arrhenius reaction term

$$\mathcal{F}(\psi,\theta;\gamma) = \psi \exp\left(\gamma - \frac{\gamma}{\theta}\right).$$

- The quantity of interest is the temperature oscillation at the reactor exit:

$$\mathbf{y}(t) = \theta(\mathbf{x} = 1, t).$$

Tubular Reactor Model

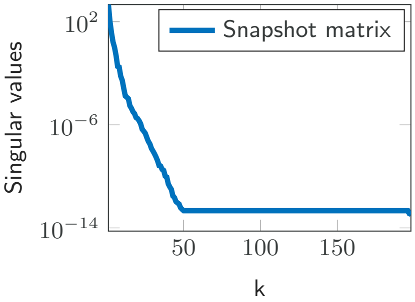

Figure: Decay of singular values of the snapshots.

- Rapid decay of singular values of training data $\rightsquigarrow$ possibility of lower order models.
- The dominant three POD modes capture more than 99.8% of the energy, yet the POD model is unstable.

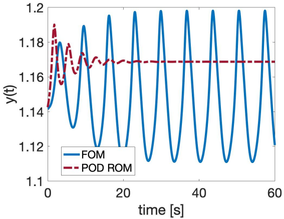

Figure: A comparison of the temperature oscillations at exit.

- Rapid decay of singular values of training data $\rightsquigarrow$ possibility of lower order models.
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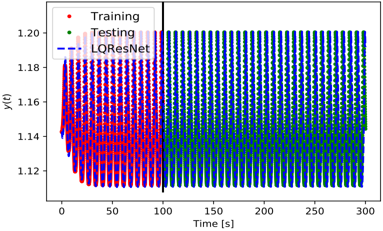

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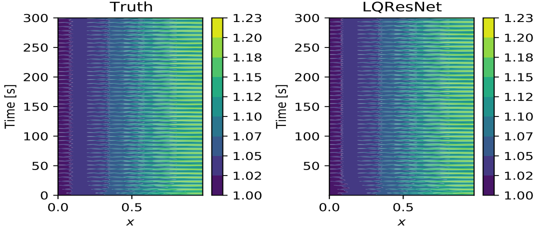

Figure: A comparison of the temperature oscillations in the whole domain.

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Contribution

- We have studied an approach to learn a mathematical model to describe nonlinear dynamics.
- Basis: operator inference and its extensions, utilizing prior PDE knowledge.
- New: model residual identified using architecture LQResNet, inspired by residual network.
- The design allows us to incorporate prior hypotheses about the process.

Outlook

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On-going work

- Very often, we can build a dictionary of good candidate basis functions, but probably do not want all of them in the dictionary. Therefore, we seek a parsimonious model
  - to pick few entries from the dictionary and learn residual by deep learning.
- Appropriate treatment of noise ... [Rudy/Kutz/Brunton '19]
- Missing/corrupted data in time series.
- Working with several applications in material science and chemical engineering.

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Thank you for your attention!!

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