MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

A Deep Learning Approach to Operator Inference

Physics-Informed Learning for Nonlinear Dynamical Systems

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Joint work with Pawan Goyal

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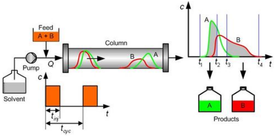

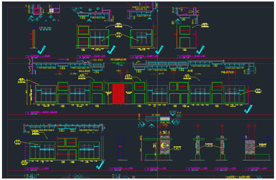

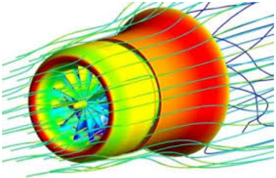

Dynamic models are important

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

Our Objective

Problem set-up

- Construct a mathematical model

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

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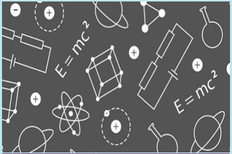
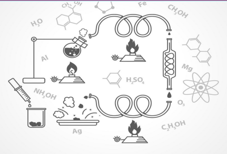
  describing the dynamics of the process.
- Neural network-based approaches: e.g., recurrent neural networks and long short time memory networks.
- Leverage all prior information about the process for efficient learning.

Key sources of information



Physical laws

Domain knowledge



Collected data

Learning Complex Engineering Process Models

- Engineering processes are supported by domain knowledge and first principles

  $\rightsquigarrow$ a PDE model can be obtained that adequately explains the dynamics

PDE $\Rightarrow$ discretize $\Rightarrow$ high-fidelity model $\Rightarrow$ model (low dimensional)

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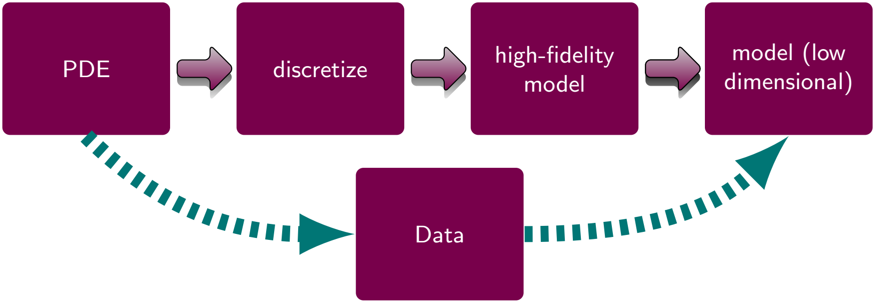

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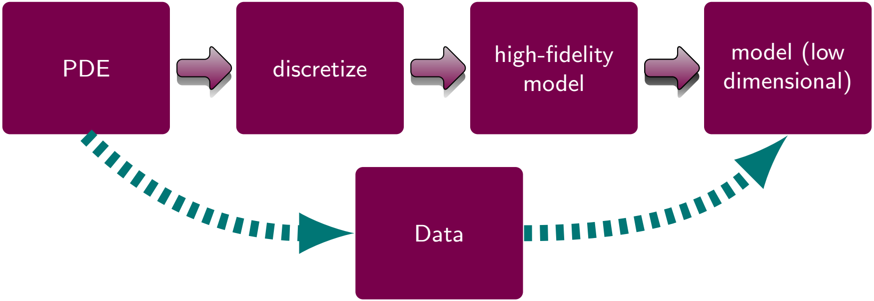

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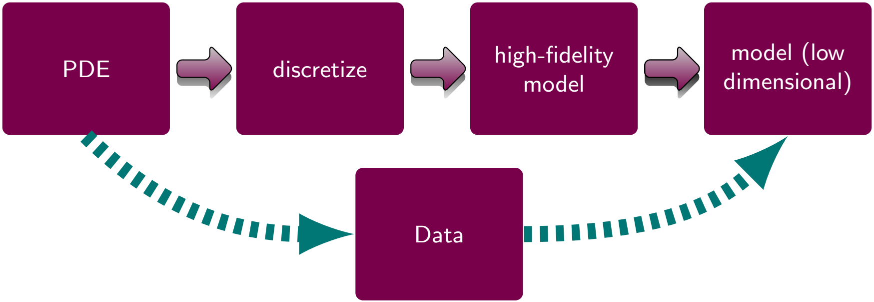

- Data collection: obtained using a legacy code, or commercial software, or experiments.
- Ideal goal: obtain the same reduced-order model (ROM) as obtained by intrusive model order reduction using data, so that error bounds and convergence analysis for ROMs can be directly employed!

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 form $\frac{\partial x}{\partial t} = \mathcal{A}(x) + \mathcal{H}(x)$ 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 [Peherstorfer/Willcox '16]

A ROM of the form

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

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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Remarks:

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[Peherstorfer '20]

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Remarks:

- Notice that we do not require at any step the full-order discretized model.
- 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]

Operator Inference for General Nonlinear Systems

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.

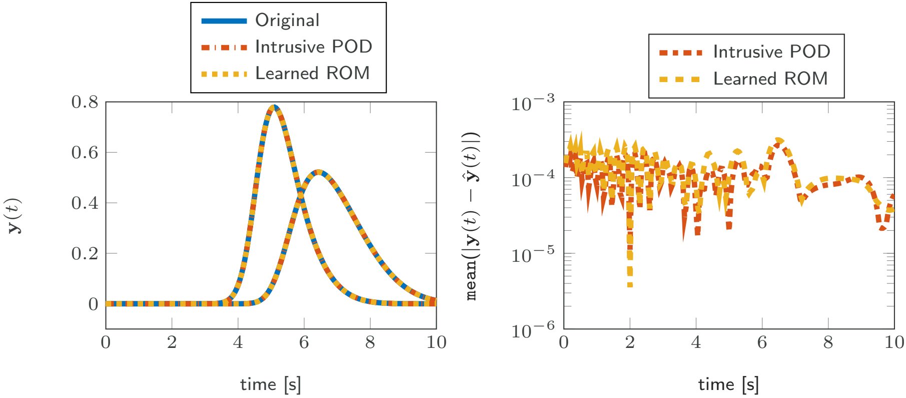
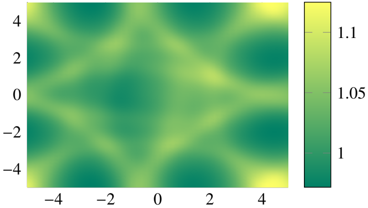
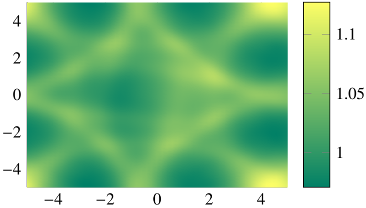


Figure: Batch chromatography example: A comparison of the POD intrusive model with the learned model of order $r = 4 \times 22$, where $n = 1600$ and $\mathrm{Pe} = 2000$.

- Learning low-dimensional parametric models with application to shallow water equations. [Yildiz et al. '20]

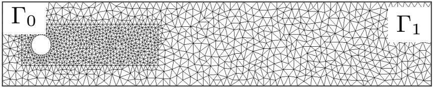


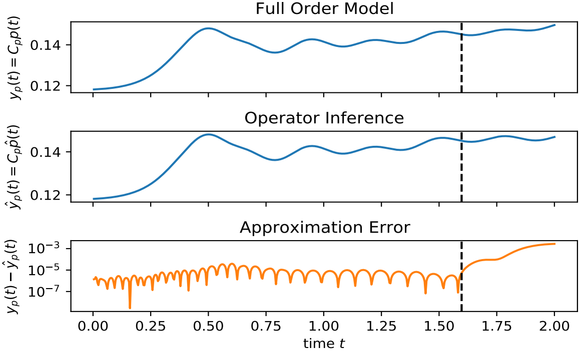
(a) True solution (in testing)



(b) Learned model using OpInf (in testing)

- Learning low-dimensional parametric models with application to shallow water equations. [Yildiz et al. '20]
- 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.,

  $\mathbf{f}(\mathbf{v}) := \mathbf{A}\mathbf{v}(t) + \mathbf{H}\left(\mathbf{v} \otimes \mathbf{v}\right).$
- 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

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

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

Fisher's equation

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

Operator Inference for General Nonlinear Systems

For simplicity, consider the form:

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

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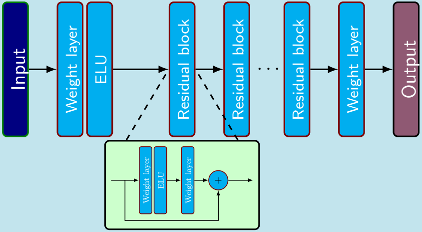
Residual networks

[He/Ren/Sun '16]

- Have shown their power in computer vision applications.



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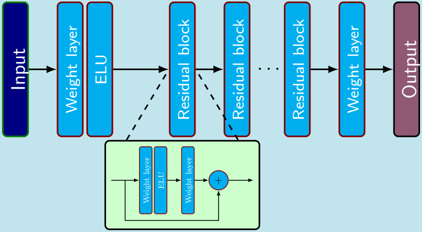

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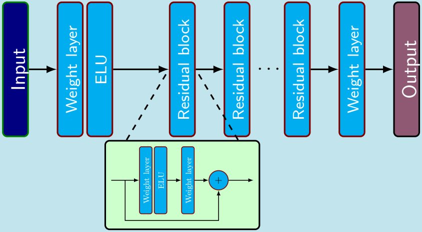
- There is an established connection to dynamical systems.
- Residual type connections hint to adaptive refinement of solution or features.



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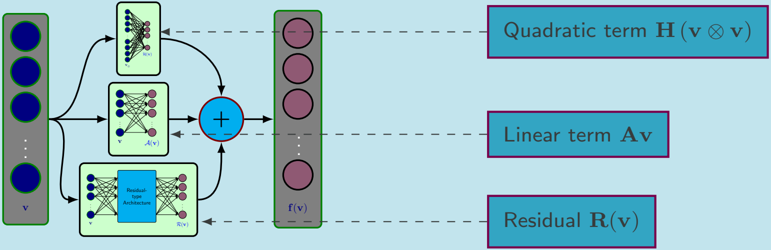
Linear-Quadratic Residual Networks (LQResNet) [Goyal/B. '21]



Advantages of the Architecture

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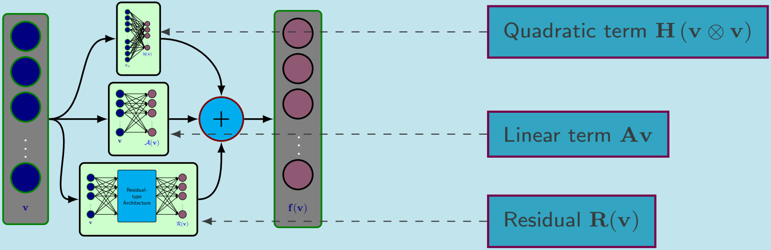
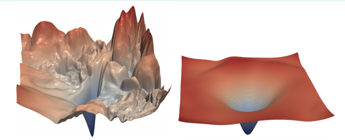


Remarks

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



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

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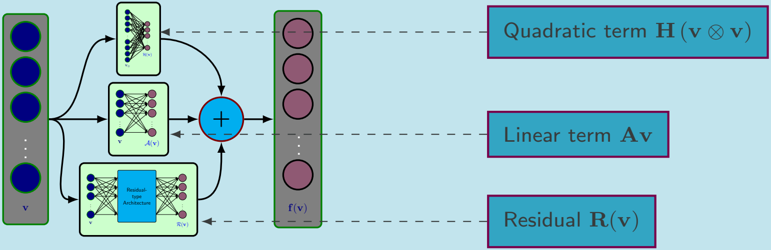

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- Layers can be added without restarting whole optimization as deep residual layers tend to refine the mapping.

Set-up

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

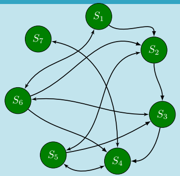

Figure: Interaction topology for 7 species.

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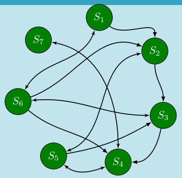

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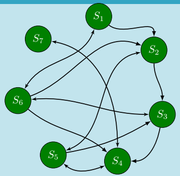

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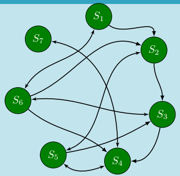

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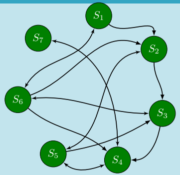
- Check the predictive capabilities under new condition.



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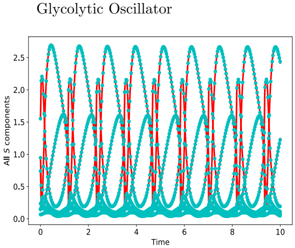

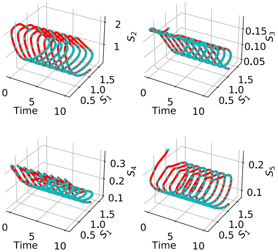

Tubular Reactor Model

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

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

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:

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

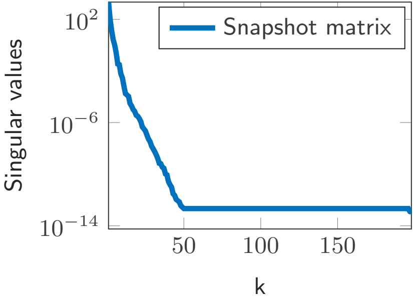

Figure: Decay of singular values of the snapshots.

- 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.

Tubular Reactor Model

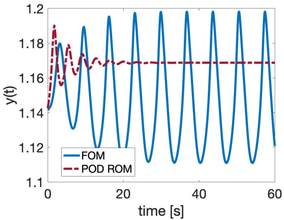

Figure: A comparison of the temperature oscillations at exit.

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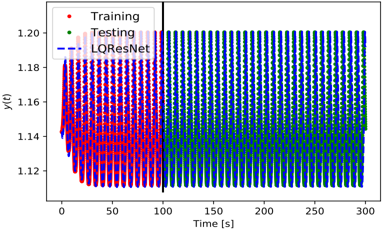
Tubular Reactor Model



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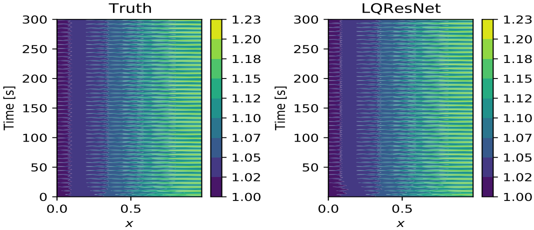

Figure: A comparison of the temperature oscillations in the whole domain.

- Rapid decay of singular values of training data $\rightsquigarrow$ possibility of lower order models.
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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]
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- Working with several applications in material science and chemical engineering.

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Thank you for your attention!!

CSC

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