Interpretable and flexible non-intrusive reduced-order models using reproducing kernel Hilbert spaces

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Projection-based intrusive model reduction

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{f}\big(\mathbf{q}(t)\big) \qquad \mathbf{q}(t) \in \mathbb{R}^{n_q}$$ LARGE

$\mathbf{q}(t) \approx \mathbf{g}\big(\tilde{\mathbf{q}}(t)\big)$ approximation

$\mathbf{g} : \mathbb{R}^r \to \mathbb{R}^{n_q}$ decompression

$\mathbf{h} : \mathbb{R}^{n_q} \to \mathbb{R}^r$ compression

$\mathbf{g} \circ \mathbf{h} : \mathbb{R}^{n_q} \to \mathbb{R}^{n_q}$ projection

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathbf{q}}(t) = \mathbf{h}'(\mathbf{g}(\tilde{\mathbf{q}}(t)))\mathbf{f}(\mathbf{g}(\tilde{\mathbf{q}}(t))) \qquad \tilde{\mathbf{q}}(t) \in \mathbb{R}^{r}$$ small

Requirements

1) **Data** to choose the projection map
2) **Direct access** to original system dynamics

Projection-based intrusive model reduction

$$\boxed{\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{I}}$$

POD Basis

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{f}\big(\mathbf{q}(t)\big) = \mathbf{A}\mathbf{q}(t) + \mathbf{H}[\mathbf{q}(t) \otimes \mathbf{q}(t)] \qquad \mathbf{q}(t) \in \mathbb{R}^{n_q}$$

LARGE

$$\mathbf{q}(t) \approx \mathbf{g}(\tilde{\mathbf{q}}(t)) = \mathbf{V}\tilde{\mathbf{q}}(t) \qquad \mathbf{h}(\mathbf{q}(t)) = \mathbf{V}^\mathsf{T}\mathbf{q}(t) \qquad (\mathbf{g} \circ \mathbf{h})(\mathbf{q}(t)) = \mathbf{V}\mathbf{V}^\mathsf{T}\mathbf{q}(t)$$

approximation decompression compression projection

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathbf{q}}(t) &= \mathbf{V}^\mathsf{T}\mathbf{f}\big(\mathbf{V}\tilde{\mathbf{q}}(t)\big) = \mathbf{V}^\mathsf{T}\mathbf{A}\mathbf{V}\tilde{\mathbf{q}}(t) + \mathbf{V}^\mathsf{T}\mathbf{H}(\mathbf{V} \otimes \mathbf{V})[\tilde{\mathbf{q}}(t) \otimes \tilde{\mathbf{q}}(t)] \\ &= \tilde{\mathbf{A}}\tilde{\mathbf{q}}(t) + \tilde{\mathbf{H}}[\tilde{\mathbf{q}}(t) \otimes \tilde{\mathbf{q}}(t)]\end{aligned} \qquad \tilde{\mathbf{q}}(t) \in \mathbb{R}^{r}$$

small

projection preserves polynomial structure

<u>Requirements</u>

1) **Data** to choose the matrix $\mathbf{V}$
2) **Direct access** to matrices $\mathbf{A},\ \mathbf{H}$

Regression-based non-intrusive model reduction

no direct access

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{f}\big(\mathbf{q}(t)\big)$$

$$\mathbf{q}(t) \approx \mathbf{g}\big(\hat{\mathbf{q}}(t)\big)$$
approximation

$$\mathbf{g} : \mathbb{R}^r \to \mathbb{R}^{n_q}$$
decompression

$$\mathbf{h} : \mathbb{R}^{n_q} \to \mathbb{R}^r$$
compression

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) = \hat{\mathbf{f}}\big(\hat{\mathbf{q}}(t)\big)$$

regression

$$\hat{\mathbf{f}} = \operatorname*{arg\,min}_{\mathbf{s}\in S} \left\{ \sum_{j=1}^{n_t} \left\| \dot{\hat{\mathbf{q}}}_j - \mathbf{s}\big(\hat{\mathbf{q}}_j\big) \right\|_2^2 + \mathcal{R}(\mathbf{s}) \right\}$$

Function space

$$\hat{\mathbf{q}}_j = \mathbf{h}(\mathbf{q}(t_j))$$
state data

$$\dot{\hat{\mathbf{q}}}_j = \frac{\hat{\mathbf{q}}_j - \hat{\mathbf{q}}_{j-1}}{t_j - t_{j-1}} \approx \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h}(\mathbf{q}(t))\Big|_{t=t_j}$$
time derivative data

Requirements

1) **Data** to choose the projection **and** drive the regression
2) **Structure specification** for the reduced-order model

Regression-based non-intrusive model reduction

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{f}\big(\mathbf{q}(t)\big) = \mathbf{A}\mathbf{q}(t) + \mathbf{H}[\mathbf{q}(t) \otimes \mathbf{q}(t)]$$

$$\mathbf{q}(t) \approx \mathbf{g}(\hat{\mathbf{q}}(t)) = \mathbf{V}\hat{\mathbf{q}}(t)$$

approximation

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) = \hat{\mathbf{f}}\big(\hat{\mathbf{q}}(t)\big) = \hat{\mathbf{A}}\hat{\mathbf{q}}(t) + \hat{\mathbf{H}}[\hat{\mathbf{q}}(t) \otimes \hat{\mathbf{q}}(t)]$$

Function space: $S(\hat{\mathbf{A}}, \hat{\mathbf{H}}) = \left\{\hat{\mathbf{q}} \mapsto \hat{\mathbf{A}}\hat{\mathbf{q}} + \hat{\mathbf{H}}[\hat{\mathbf{q}} \otimes \hat{\mathbf{q}}]\right\}$

$$\hat{\mathbf{A}}, \hat{\mathbf{H}} = \operatorname*{arg\,min}_{\hat{\mathbf{A}},\hat{\mathbf{H}}} \left\{ \sum_{j=1}^{n_t} \left\| \dot{\hat{\mathbf{q}}}_j - \left(\hat{\mathbf{A}}\hat{\mathbf{q}}_j + \hat{\mathbf{H}}[\hat{\mathbf{q}}_j \otimes \hat{\mathbf{q}}_j]\right) \right\|_2^2 + \lambda_1^2 \left\|\hat{\mathbf{A}}\right\|_F^2 + \lambda_2^2 \left\|\hat{\mathbf{H}}\right\|_F^2 \right\}$$

operator inference regression

Regression-based non-intrusive model reduction

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{f}\big(\mathbf{q}(t)\big)$$

$$\mathbf{q}(t) \approx \mathbf{g}(\hat{\mathbf{q}}(t))$$

approximation

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) = \hat{\mathbf{f}}\big(\hat{\mathbf{q}}(t)\big) = \boldsymbol{\Omega}^{\mathsf{T}} K\big(\hat{\mathbf{Q}}, \hat{\mathbf{q}}(t)\big)$$

Reproducing kernel Hilbert space (RKHS): $S = \mathcal{H}_K^r = \mathcal{H}_K \times \mathcal{H}_K \times \cdots \times \mathcal{H}_K$

$$\hat{\mathbf{f}} = \operatorname*{arg\,min}_{\mathbf{s}\in\mathcal{H}_K^r} \left\{ \sum_{j=1}^{n_t} \left\| \dot{\hat{\mathbf{q}}}_j - \mathbf{s}\big(\hat{\mathbf{q}}_j\big) \right\|_2^2 + \lambda \left\|\mathbf{s}\right\|_{H_K^r}^2 \right\}$$

regularized kernel interpolation

Non-intrusive model reduction: comparison

	Interpretable ROM structure mirrors FOM	**Flexible** approximate arbitrary structure	**Error Estimates** certified ROM solutions
Neural networks	No	Yes	No*
Operator inference	Yes	No	No*
Kernel ROMs	Yes	Yes	Yes*

Regularized kernel interpolation

Kernel function

- $K : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}$
- $K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}', \mathbf{x})$
- if $\mathbf{X} = [\, \mathbf{x}_1 \quad \cdots \quad \mathbf{x}_m \,]$, then $K(\mathbf{X}, \mathbf{X}) = [K(\mathbf{x}_i, \mathbf{x}_j)]$ positive semi-definite

Reproducing kernel Hilbert space (RKHS)

$$\mathcal{H}_K = \overline{\operatorname{span}\{K(\mathbf{x}, \cdot\,) \,:\, \mathbf{x} \in \mathbb{R}^{n_x}\}}$$

Representer Theorem

$$\underbrace{\mathbf{X} = [\, \mathbf{x}_1 \quad \cdots \quad \mathbf{x}_m \,]}_{\text{input data}} \in \mathbb{R}^{n_x \times m}, \qquad \underbrace{\mathbf{Y} = [\, \mathbf{y}_1 \quad \cdots \quad \mathbf{y}_m \,]}_{\text{output data}} \in \mathbb{R}^{n_y \times m}, \qquad \underbrace{\mathbf{x}_j \mapsto \mathbf{y}_j}_{\text{data pairs}}$$

$$\underbrace{\min_{\mathbf{s} \in \mathcal{H}_K^{n_y}} \left\{ \sum_{j=1}^{m} \|\mathbf{y}_j - \mathbf{s}(\mathbf{x}_j)\|_2^2 + \gamma \|\mathbf{s}\|_{\mathcal{H}_K^{n_y}}^2 \right\}}_{\text{regularized kernel interpolation}} \longrightarrow \boxed{\begin{gathered} \mathbf{s}(\mathbf{x}) = \mathbf{\Omega}^{\mathsf{T}} K(\mathbf{X}, \mathbf{x}) \\ \text{where} \\ (K(\mathbf{X}, \mathbf{X}) + \gamma \mathbf{I})\mathbf{\Omega} = \mathbf{Y}^{\mathsf{T}} \end{gathered}}$$

Regularized kernel interpolation

$$\mathbf{s}(\mathbf{x}) = \boldsymbol{\Omega}^\mathsf{T} K(\mathbf{X}, \mathbf{x})$$

where

$$\underbrace{\big(K(\mathbf{X}, \mathbf{X}) + \gamma\mathbf{I}\big)}_{m \times m}\boldsymbol{\Omega} = \mathbf{Y}^\mathsf{T}$$

$m \times m$ ($m =$ # of training points)

Kernel selection to design interpolant structure

General purpose: radial basis function (RBF) kernel

$$K(\mathbf{x}, \mathbf{x}') = \underbrace{\psi(\epsilon\|\mathbf{x} - \mathbf{x}'\|_2)}_{\text{RBF}}$$

$$\mathbf{s}(\mathbf{x}) = \boldsymbol{\Omega}^\mathsf{T}\boldsymbol{\psi}_\epsilon(\mathbf{x}) = \boldsymbol{\Omega}^\mathsf{T}\begin{bmatrix} \psi(\epsilon\|\mathbf{x}_1 - \mathbf{x}\|_2) \\ \vdots \\ \psi(\epsilon\|\mathbf{x}_m - \mathbf{x}\|_2) \end{bmatrix}$$

Known structure: feature map kernel

$$K(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\mathsf{T}\mathbf{G}\boldsymbol{\phi}(\mathbf{x}')$$

$$\underbrace{\boldsymbol{\phi} : \mathbb{R}^{n_x} \to \mathbb{R}^{n_\phi}}_{\text{feature map}}, \qquad \underbrace{\mathbf{G} \in \mathbb{R}^{n_\phi \times n_\phi}}_{\text{weight matrix}}$$

$$\mathbf{s}(\mathbf{x}) = \boldsymbol{\Omega}^\mathsf{T}\boldsymbol{\phi}(\mathbf{X})^\mathsf{T}\mathbf{G}\boldsymbol{\phi}(\mathbf{x}) = \mathbf{C}\boldsymbol{\phi}(\mathbf{x})$$

(precomputable)

Hybrid: feature map + RBF

$$K(\mathbf{x}, \mathbf{x}') = \underbrace{c_\phi\boldsymbol{\phi}(\mathbf{x})^\mathsf{T}\mathbf{G}\boldsymbol{\phi}(\mathbf{x}')}_{\text{feature map part}} + \underbrace{c_\psi\psi(\epsilon\|\mathbf{x} - \mathbf{x}'\|_2)}_{\text{RBF part}}$$

$$\mathbf{s}(\mathbf{x}) = \underbrace{\mathbf{C}\boldsymbol{\phi}(\mathbf{x})}_{\text{feature map}} + \underbrace{c_\psi\boldsymbol{\Omega}^\mathsf{T}\boldsymbol{\psi}_\epsilon(\mathbf{x})}_{\text{RBF}}$$

Regularized kernel interpolation for **Kernel ROMs**

$$\hat{\mathbf{Q}} = [\ \hat{\mathbf{q}}_1 \quad \cdots \quad \hat{\mathbf{q}}_{n_t}\ ] \in \mathbb{R}^{r \times n_t},$$
input data (states)

$$\dot{\hat{\mathbf{Q}}} = [\ \dot{\hat{\mathbf{q}}}_1 \quad \cdots \quad \dot{\hat{\mathbf{q}}}_{n_t}\ ] \in \mathbb{R}^{r \times n_t},$$
output data (ddts)

$$\hat{\mathbf{q}}_j \mapsto \dot{\hat{\mathbf{q}}}_j$$
data pairs

Quadratic feature map $\phi(\hat{\mathbf{q}}) = \begin{bmatrix} \hat{\mathbf{q}} \\ \hat{\mathbf{q}} \otimes \hat{\mathbf{q}} \end{bmatrix}$, Gaussian RBF $\psi(x) = \exp(-x^2)$

for example

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) &= \hat{\mathbf{C}}\phi(\hat{\mathbf{q}}(t)) + c_\psi \boldsymbol{\Omega}^{\mathsf{T}} \psi_\epsilon(\hat{\mathbf{q}}(t)) \\ &= \hat{\mathbf{A}}\hat{\mathbf{q}}(t) + \hat{\mathbf{H}}[\hat{\mathbf{q}}(t) \otimes \hat{\mathbf{q}}(t)] + c_\psi \boldsymbol{\Omega}^{\mathsf{T}} \begin{bmatrix} \psi(\epsilon \|\hat{\mathbf{q}}_1 - \hat{\mathbf{q}}(t)\|_2) \\ \vdots \\ \psi(\epsilon \|\hat{\mathbf{q}}_{n_t} - \hat{\mathbf{q}}(t)\|_2) \end{bmatrix}\end{aligned}$$

Design based on **FOM structure** and the **approximation / projection**

Implementation details

Scaling: scale inputs, select weight matrix $\mathbf{G}$

$$K_{\boldsymbol{\nu}}(\mathbf{x}, \mathbf{x}') = K(\boldsymbol{\nu}(\mathbf{x}), \boldsymbol{\nu}(\mathbf{x}'))$$

$$\mathbf{G} = \begin{bmatrix} \frac{1}{\|\hat{\mathbf{Q}}\|_F}\mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \frac{1}{\|\hat{\mathbf{Q}}\|_F^2}\mathbf{I}_{r^2} \end{bmatrix}$$

Regularization: select λ

$$\hat{\mathbf{f}} = \operatorname*{arg\,min}_{\mathbf{s}\in\mathcal{H}_K^r} \left\{ \sum_{j=1}^{n_t} \left\| \dot{\hat{\mathbf{q}}}_j - \mathbf{s}(\hat{\mathbf{q}}_j) \right\|_2^2 + \lambda \|\mathbf{s}\|_{H_K^r}^2 \right\}$$

Kernel tuning: select ϵ and c_ψ

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{q}}(t) = \hat{\mathbf{A}}\hat{\mathbf{q}}(t) + \hat{\mathbf{H}}[\hat{\mathbf{q}}(t) \otimes \hat{\mathbf{q}}(t)] + c_\psi \boldsymbol{\Omega}^{\mathsf{T}} \begin{bmatrix} \psi(\epsilon\|\hat{\mathbf{q}}_1 - \hat{\mathbf{q}}(t)\|_2) \\ \vdots \\ \psi(\epsilon\|\hat{\mathbf{q}}_{n_t} - \hat{\mathbf{q}}(t)\|_2) \end{bmatrix}$$

A posteriori error bounds for Kernel ROMs

Theorem. If $\hat{\mathbf{f}}$ is an unregularized kernel interpolant of $\tilde{\mathbf{f}} + \boldsymbol{\delta} \in \mathcal{H}_K^r$ where $\|\boldsymbol{\delta}(\hat{\mathbf{q}}(s))\|_{\mathbf{M}} < \delta(s)$, then

$$\|\mathbf{q}(t) - \mathbf{g}(\hat{\mathbf{q}}(t))\|_{\mathbf{M}} \leq \int_0^t (\alpha_p(s) + \alpha_K(s)) e^{\int_s^t \beta(\tau) d\tau} ds + e^{\int_0^t \beta(\tau) d\tau} \|\mathbf{q}(t) - \mathbf{g}(\mathbf{h}(\mathbf{q}(0)))\|_{\mathbf{M}}$$

= error from low-dimensional **state approximation**

+ error between **intrusive ROM** and kernel interpolant

+ error in **time derivative approximation**

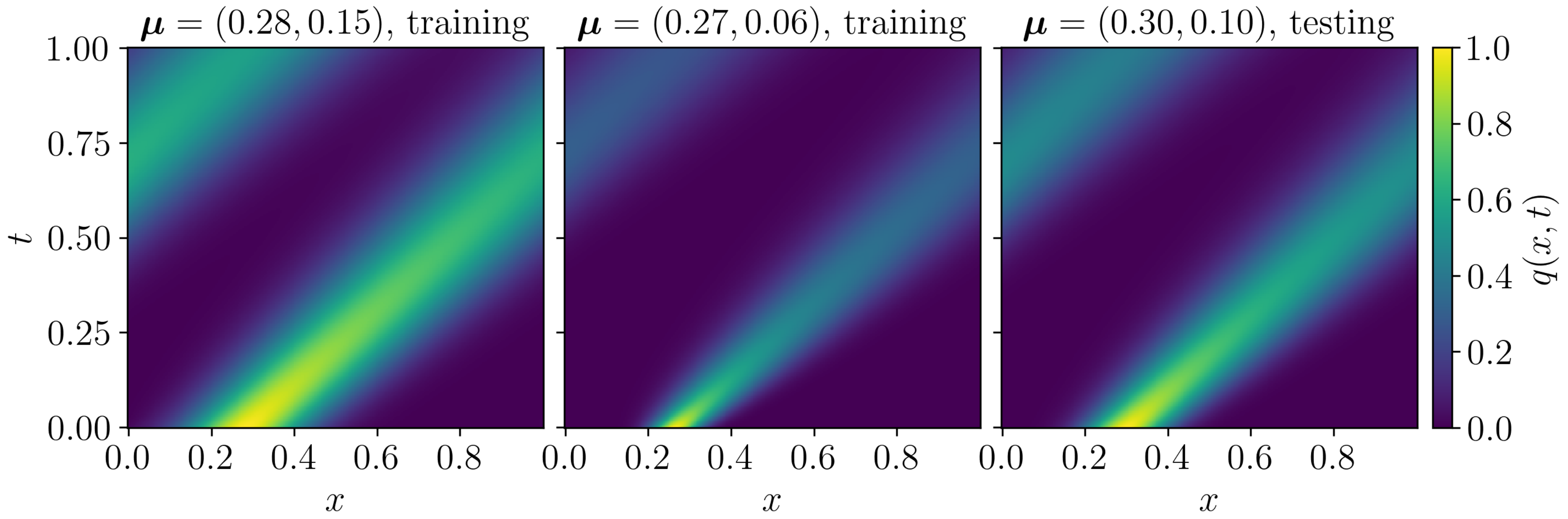
+ **initial condition** error

Error bound **computable** but requires **intrusive evaluations**

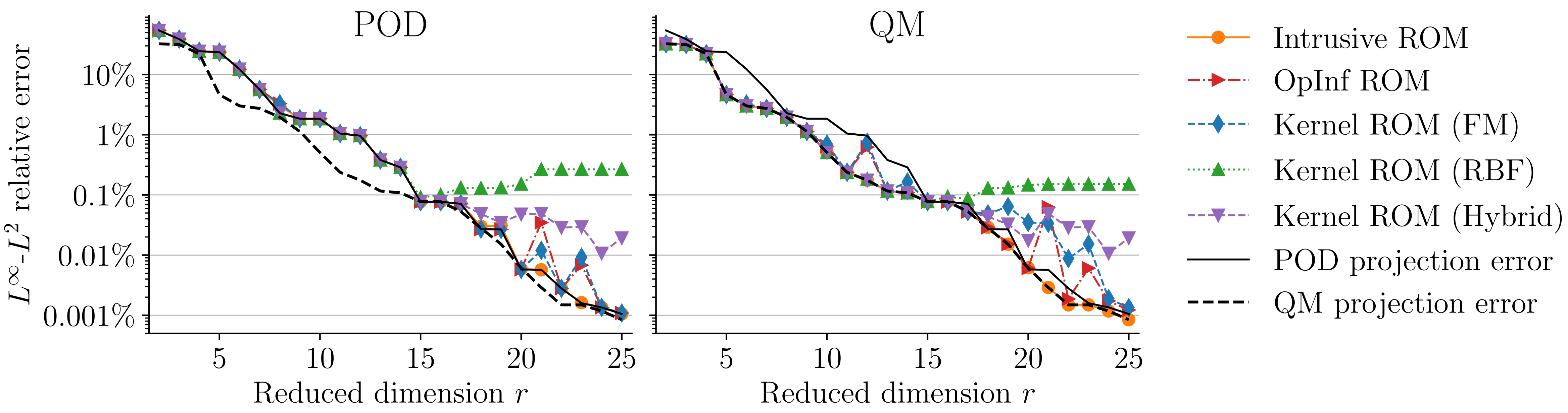
Linear example: Advection-diffusion

$$
\begin{aligned}
\frac{\partial}{\partial t}q(x,t) - \kappa\frac{\partial^2}{\partial x^2}q(x,t) + \beta\frac{\partial}{\partial x}q(x,t) &= 0, && x \in (0,1), \quad t \in (0,T), \\
q(0,t) = q(1,t), \quad \frac{\partial}{\partial x}q(0,t) &= \frac{\partial}{\partial x}q(1,t), && t \in (0,T), \\
q(x,0) = q_0(x;\boldsymbol{\mu}) &= e^{-(x-\mu_1)^2/\mu_2^2}, && x \in (0,1).
\end{aligned}
$$

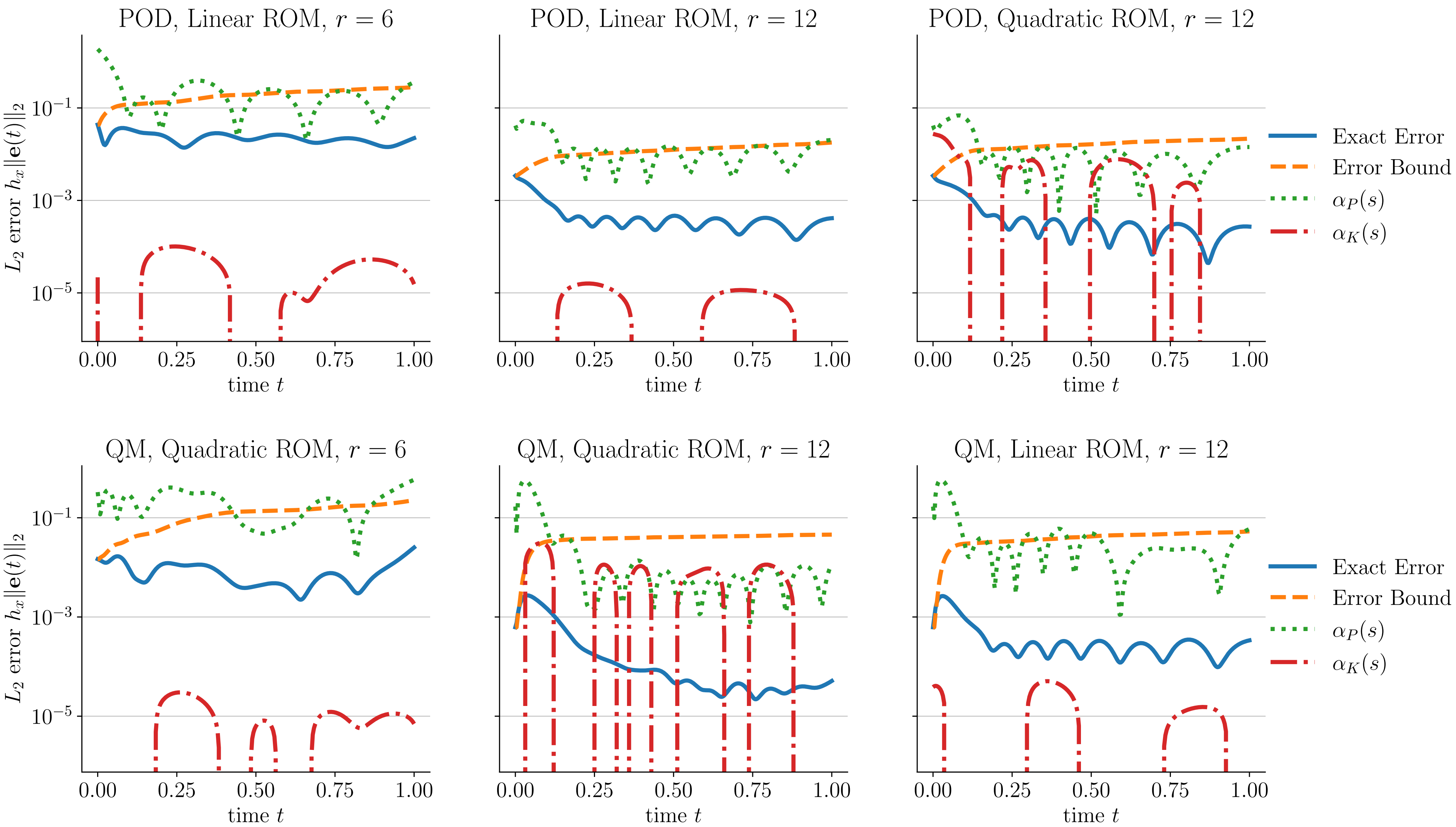
$$
\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{A}\mathbf{q}(t)
$$



Linear example: Advection-diffusion



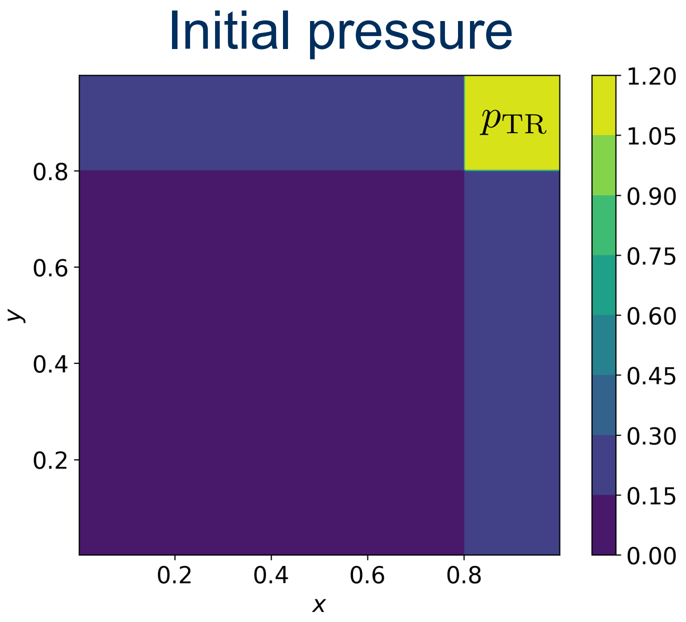
Linear example: Advection-diffusion



Challenging example: 2D Euler–Riemann problem

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u \\ \rho v \\ \rho E\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ \rho u v \\ (E+p)u\end{bmatrix} + \frac{\partial}{\partial y}\begin{bmatrix}\rho v \\ \rho u v \\ \rho v^2 + p \\ (E+p)v\end{bmatrix} = 0$$

$$p = (\gamma - 1)\big(\rho E - \tfrac{1}{2}\rho(u^2 + v^2)\big),$$



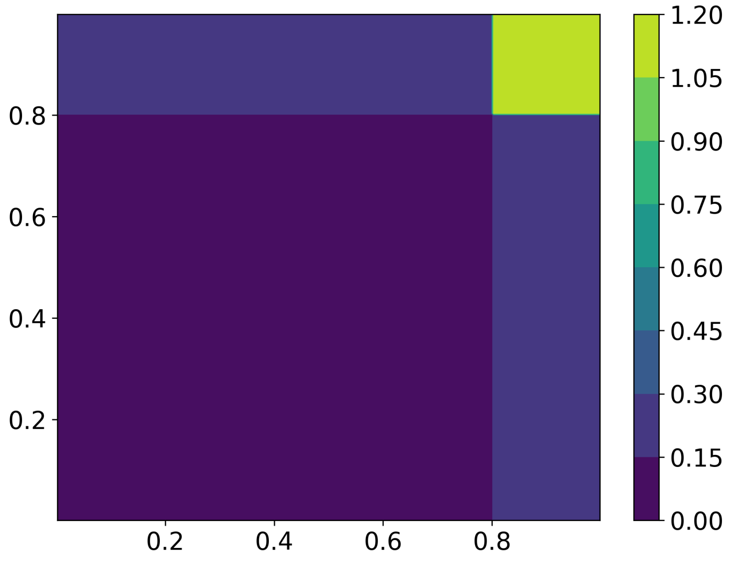
Experimental setup

- Parameterized by initial top-right pressure. Train: $p_{TR} \in \{0.5, 0.75, 1.0, 1.25, 1.5\}$, Test: $p_{TR} = 1.125$
- CCFV discretization, 256×256 uniform grid, SSP3 time stepping scheme, $\delta t = 10^{-3}$, $n_t = 800$
- Lift to specific volume form → quadratic model
  Kernel ROM with quadratic feature map

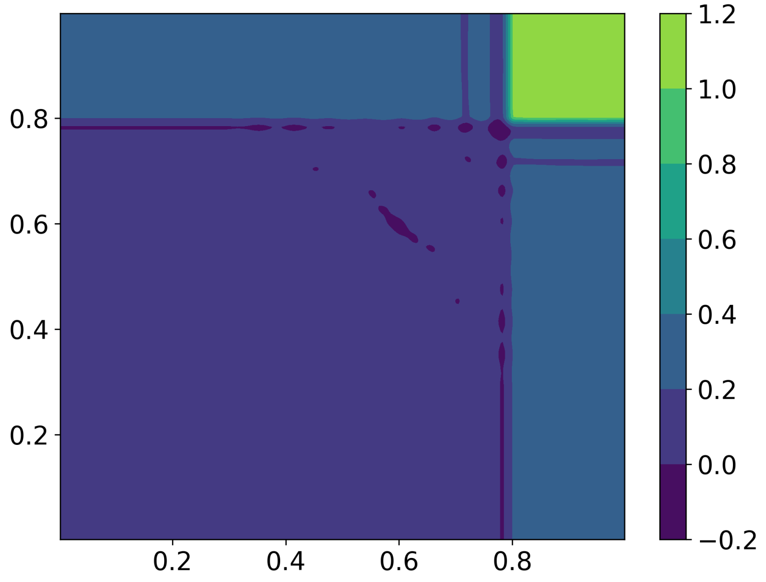
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{A}\mathbf{q}(t) + \mathbf{H}[\mathbf{q}(t)\otimes\mathbf{q}(t)], \quad \mathbf{q}(0) = \mathbf{q}_0(p_{\mathrm{TR}})$$

Challenging example: 2D Euler–Riemann problem

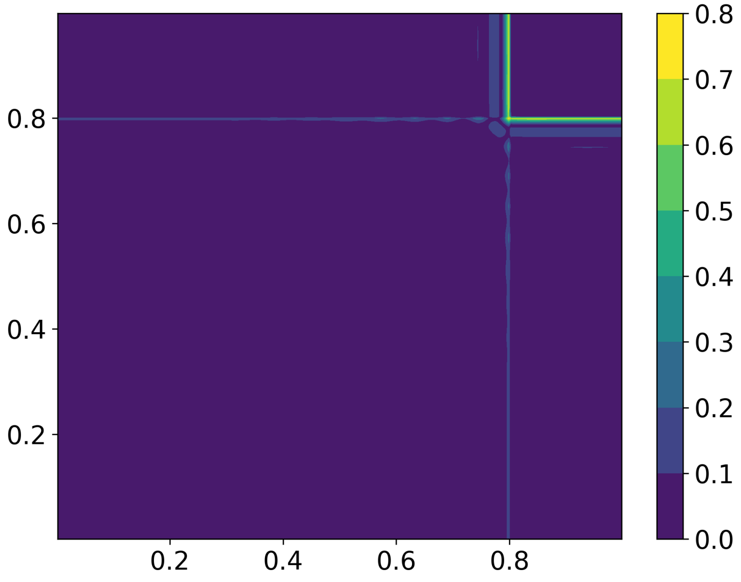
FOM pressure
$n_x = 262{,}144$



ROM pressure
$r = 20$



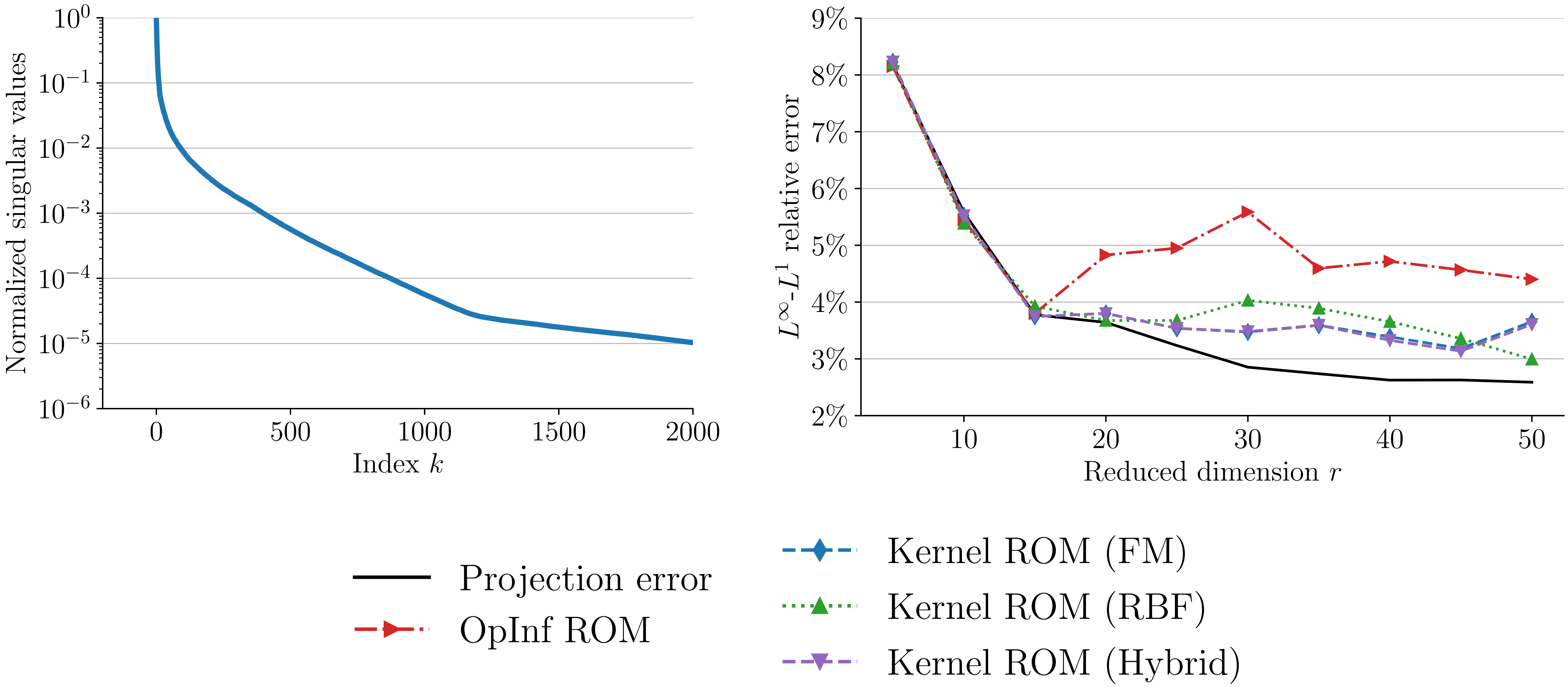
Pressure error
$r = 20$



Relative L_∞-L_1 error $= 3.65\%$

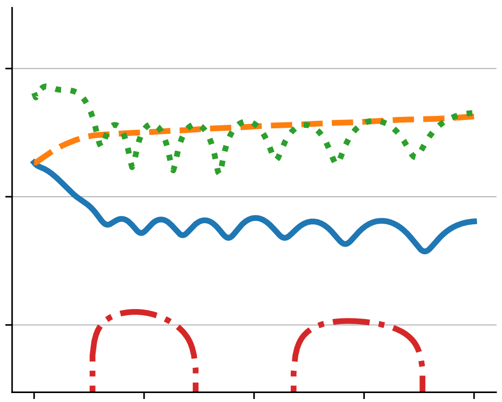
Relative speed up $= 344.8\times$

Challenging example: 2D Euler–Riemann problem



Summary

- **Non-intrusive** ROM construction using regularized kernel interpolation with RKHS
- Kernel ROMs are **flexible** but can be designed with **interpretable** structure
- RKHS theory gives *a posteriori* **error bounds** based on estimates from intrusive projection



arXiv

Future Work

- **Parametric** kernels for parametric problems
- Kernel tuning / selection, feature preservation
- Intelligent selection of **training** data
- Fully non-intrusive **error bounds**