Calibration-Based ALE Model Order Reduction for Hyperbolic Problems with Self-Similar Traveling Discontinuities

Davide Torlo, Monica Nonino

Dipartimento di Matematica "Guido Castelnuovo" – Università di Roma Sapienza
davidetorlo.it

Torino - 30th January 2025

SAPIENZA
UNIVERSITÀ DI ROMA

Summary of Classical Model Order Reduction

Context: Parametric PDE

$$\partial_t u(x,t;\boldsymbol{\mu}) + \mathcal{L}(u(x,t;\boldsymbol{\mu});\boldsymbol{\mu}) = 0 \qquad + \text{BC} \qquad + \text{IC} \qquad u \in \mathbb{R}^{\mathcal{N}}$$

Linear Subspace Ansatz

- Suppose that $u(\boldsymbol{\mu}) \approx \sum_{i=1}^{N_{RB}} \hat{u}_i(\boldsymbol{\mu})\psi_i$
- $N_{RB} \ll \mathcal{N}$

MOR

- Reduced Space $\mathbb{V}_{N_{RB}} := \langle \psi_i \rangle_{i=1}^{N_{RB}}$
- Galerkin projection for $j = 1, \dots, N_{RB}$
  $(\psi_j, \psi_i)\hat{u}_i(\boldsymbol{\mu}) + (\psi_j, \psi_i)\hat{\mathcal{L}}_i(u;\boldsymbol{\mu}) = 0$

Summary of Classical Model Order Reduction

Context: Parametric PDE

$$\partial_t u(x,t;\boldsymbol{\mu}) + \mathcal{L}(u(x,t;\boldsymbol{\mu});\boldsymbol{\mu}) = 0 \qquad + \text{BC} \qquad + \text{IC} \qquad u \in \mathbb{R}^{\mathcal{N}}$$

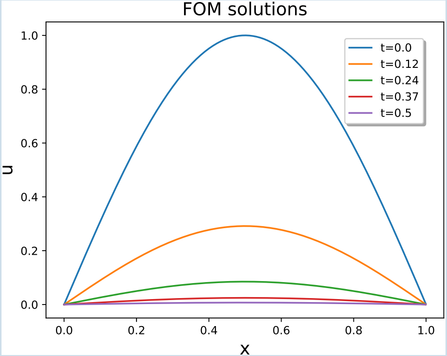
Linear Subspace Ansatz

- Suppose that $u(\boldsymbol{\mu}) \approx \sum_{i=1}^{N_{RB}} \hat{u}_i(\boldsymbol{\mu})\psi_i$
- $N_{RB} \ll \mathcal{N}$

MOR

- Reduced Space $\mathbb{V}_{N_{RB}} := \langle \psi_i \rangle_{i=1}^{N_{RB}}$
- Galerkin projection for $j = 1, \dots, N_{RB}$
  $(\psi_j, \psi_i)\hat{u}_i(\boldsymbol{\mu}) + (\psi_j, \psi_i)\hat{\mathcal{L}}_i(u;\boldsymbol{\mu}) = 0$

Example: Diffusion problem $\partial_t u = \partial_{xx} u$



Summary of Classical Model Order Reduction

Context: Parametric PDE

$$\partial_t u(x,t;\boldsymbol{\mu}) + \mathcal{L}(u(x,t;\boldsymbol{\mu});\boldsymbol{\mu}) = 0 \qquad + \text{BC} \qquad + \text{IC} \qquad u \in \mathbb{R}^{\mathcal{N}}$$

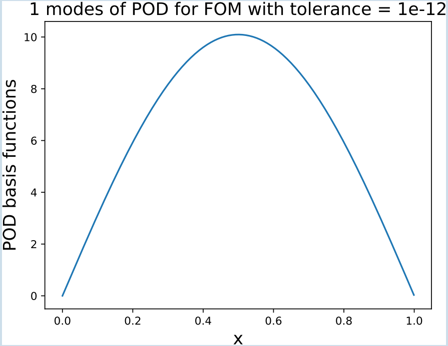
Linear Subspace Ansatz

- Suppose that $u(\boldsymbol{\mu}) \approx \sum_{i=1}^{N_{RB}} \hat{u}_i(\boldsymbol{\mu})\psi_i$
- $N_{RB} \ll \mathcal{N}$

MOR

- Reduced Space $\mathbb{V}_{N_{RB}} := \langle \psi_i \rangle_{i=1}^{N_{RB}}$
- Galerkin projection for $j = 1, \dots, N_{RB}$
  $(\psi_j, \psi_i)\hat{u}_i(\boldsymbol{\mu}) + (\psi_j, \psi_i)\hat{\mathcal{L}}_i(u;\boldsymbol{\mu}) = 0$

Example: Diffusion problem $\partial_t u = \partial_{xx} u$



Summary of Classical Model Order Reduction

Proper orthogonal decomposition (POD)

INPUT: Collection of functions $\{f_j\}_{j=1}^N$
OUTPUT: Reduced basis spaces

$$RB = \underset{U|dim(U)=N_{POD}}{\arg\min} \sum_{j=1}^{N} ||f_j - \mathcal{P}_U(f_j)||_2$$

- Based on SVD
- Prescribed tolerance to stop the algorithm
- Global optimizer of the problem

Greedy algorithm

INPUT: Collection of functions $\{f_j\}_{j=1}^N$
OUTPUT: Reduced basis space RB

- There is an error estimator (normally cheap) $\varepsilon_{RB}(f) \sim ||f - \mathcal{P}_{RB}(f)||$
- Iteratively choose the worst represented function $f^{worst} = \arg\max_f \varepsilon_{RB}(f)$
- Add f^{worst} to the RB space
- Stop up to a certain tolerance

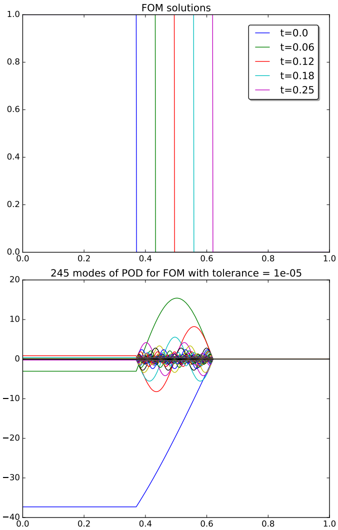
Issues with advection dominated

Issues

- As many basis functions as positions of the shock
- Slow decay of Kolmogorov N–width

$$d_N(\mathcal{S},\mathbb{V}) := \inf_{\mathbb{V}_N\subset\mathbb{V}} \sup_{f\in\mathcal{S}} \inf_{g\in\mathbb{V}_N} ||f-g|| \approx O(N^{-\frac{1}{2}})$$

- Large RB space
- few parameters problem (highly non linear dependence on parameters in linear ROM)
- Reduced linear space ansatz is WRONG!



2D Example

Double Mach Reflection, time = parameter

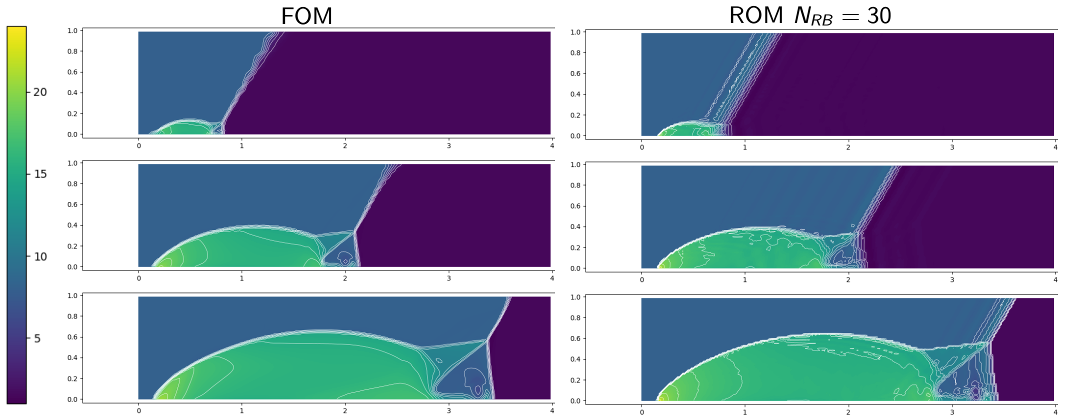


Table of contents

Goal parametric hyperbolic systems, Euler equations of gas dynamics

$$\begin{cases} \partial_t \rho + \nabla_{\boldsymbol{x}} \cdot \boldsymbol{m} = 0 & \text{in } \mathcal{P} \times \Omega, \\ \partial_t \boldsymbol{m} + \nabla_{\boldsymbol{x}} \cdot \left(\frac{\boldsymbol{m} \otimes \boldsymbol{m}}{\rho} + p\, I \right) = 0 & \text{in } \mathcal{P} \times \Omega, \\ \partial_t E + \nabla_{\boldsymbol{x}} \cdot \left(\frac{\boldsymbol{m}}{\rho}(E+p) \right) = 0 & \text{in } \mathcal{P} \times \Omega, \end{cases} \qquad p = (\gamma - 1)(E - \tfrac{1}{2}|\boldsymbol{m}|^2/\rho),$$

Properties

- $\rho, \boldsymbol{m}, E$ non linear dependence on $\boldsymbol{\mu}$!
- $\boldsymbol{\mu}$ can influence boundaries, flux, initial conditions

Motivation and solvers

- Why: many physical applications to fluid equations
- Classical solvers: FV, FEM, FD, RD (Slow for high–resolution).
- Many query task (UQ, optimization, etc.)

MOR algorithms

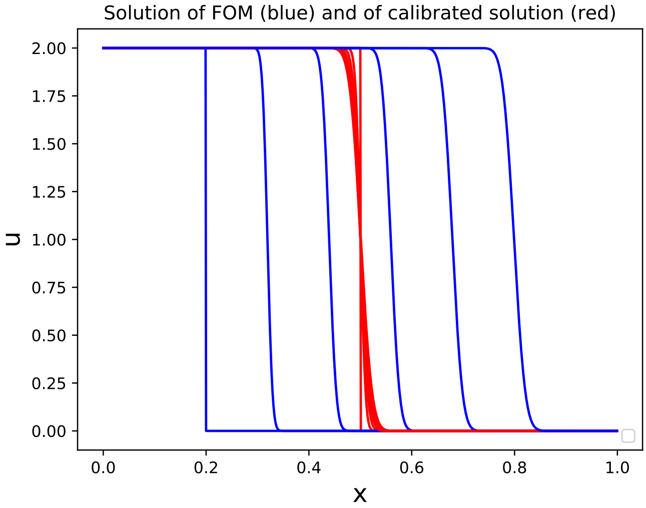
Offline:

- POD
- Greedy
- EIM

Online:

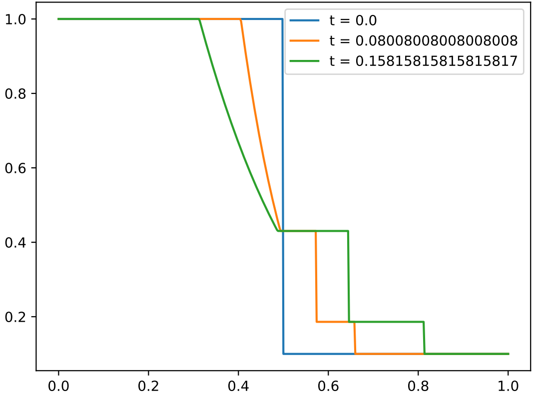
- Galerkin projection
- Neural Networks
- Other Regression

Examples



Solution of FOM (blue) and of calibrated solution (red)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
u
0.0
0.2
0.4
0.6
0.8
1.0
x

Examples


t = 0.0
t = 0.08008008008008008
t = 0.15815815815815817
1.0
0.8
0.6
0.4
0.2
0.0
0.2
0.4
0.6
0.8
1.0

Possible solutions and research directions

Some possibilities to incorporate the advection into RB framework

- Freezing **Ohlberger, M. and Rave, S.**
- Shifted POD **Reiss, J., Schulze, P., Sesterhenn, J., Mehrmann, V., Demo, N., Burela, S., Krah, P.**
- Lagrangian basis method **Mojgani, R. and Balajewicz, M.**
- Advection modes by optimal mass transport **Iollo, A., Lombardi, D., Mula, O., Taddei, T.**
- Calibration (also 2D non–periodic boundaries) **Cagniart, N., Stamm, B. and Maday, Y.**, **Crisovan, R. and Abgrall, R.**
- Online adaptive bases and samplings **Peherstorfer, B.**
- Gradient-preserving DEIM **Pagliantini, C.**
- Transport Reversal **Rim, D., Moe, S. and LeVeque R. J.**
- Registration method **Taddei, T., Ohlberger, M., Kleikamp, H.**
- Optimization based implicit feature tracking **Zahr, M., Mirhoseini, M.A.**
- Preprocessing reduced basis **Karatzas, E., Nonino, M., Ballarin, F., Rozza, G. and Maday, Y.**
- Manifold learning via Neural Network, convolutional autoencoders **Carlberg, K. and Lee, K.; Lye, K., Mishra S. and Ray, D.; Fresca, S., Dedè, L. and Manzoni, A., Venkat, S., Smith, R.C., Kelley, C.T.**
- Dynamic Modes **Lu, H. and Tartakovsky, D. M.**
- Dynamical Low Rank **Kazashi, Y., Nobile, F., Trigo Trindade, T., Vidličková, E., Ceruti, G., Kusch, J., Einkemmer, L., Frank, M.**
- Graph Neural Network **Pichi, F., Moya, B., Hesthaven, J.**
- Sinkhorn Loss and Wasserstein Kernel **Khamlich, M., Pichi, Rozza, G.**

Possible solutions and research directions

Some possibilities to incorporate the advection into RB framework

- Freezing **Ohlberger, M. and Rave, S.**
- Shifted POD **Reiss, J., Schulze, P., Sesterhenn, J., Mehrmann, V., Demo, N., Burela, S., Krah, P.**
- Lagrangian basis method **Mojgani, R. and Balajewicz, M.**
- Advection modes by optimal mass transport **Iollo, A., Lombardi, D., Mula, O., Taddei, T.**
- Calibration (also 2D non–periodic boundaries) **Cagniart, N., Stamm, B. and Maday, Y.**, **Crisovan, R. and Abgrall, R.**
- Online adaptive bases and samplings **Peherstorfer, B.**
- Gradient-preserving DEIM **Pagliantini, C.**
- Transport Reversal **Rim, D., Moe, S. and LeVeque R. J.**
- Registration method **Taddei, T., Ohlberger, M., Kleikamp, H.**
- Optimization based implicit feature tracking **Zahr, M., Mirhoseini, M.A.**
- Preprocessing reduced basis **Karatzas, E., Nonino, M., Ballarin, F., Rozza, G. and Maday, Y.**
- Manifold learning via Neural Network, convolutional autoencoders **Carlberg, K. and Lee, K.; Lye, K., Mishra S. and Ray, D.; Fresca, S., Dedè, L. and Manzoni, A., Venkat, S., Smith, R.C., Kelley, C.T.**
- Dynamic Modes **Lu, H. and Tartakovsky, D. M.**
- Dynamical Low Rank **Kazashi, Y., Nobile, F., Trigo Trindade, T., Vidličková, E., Ceruti, G., Kusch, J., Einkemmer, L., Frank, M.**
- Graph Neural Network **Pichi, F., Moya, B., Hesthaven, J.**
- Sinkhorn Loss and Wasserstein Kernel **Khamlich, M., Pichi, Rozza, G.**

Possible solutions and research directions

Some possibilities to incorporate the advection into RB framework

- Freezing **Ohlberger, M. and Rave, S.**
- Shifted POD **Reiss, J., Schulze, P., Sesterhenn, J., Mehrmann, V., Demo, N., Burela, S., Krah, P.**
- Lagrangian basis method **Mojgani, R. and Balajewicz, M.**
- Advection modes by optimal mass transport **Iollo, A., Lombardi, D., Mula, O., Taddei, T.**
- Calibration (also 2D non–periodic boundaries) **Cagniart, N., Stamm, B. and Maday, Y.**, **Crisovan, R. and Abgrall, R.**
- Online adaptive bases and samplings **Peherstorfer, B.**
- Gradient-preserving DEIM **Pagliantini, C.**
- Transport Reversal **Rim, D., Moe, S. and LeVeque R. J.**
- Registration method **Taddei, T., Ohlberger, M., Kleikamp, H.**
- Optimization based implicit feature tracking **Zahr, M., Mirhoseini, M.A.**
- Preprocessing reduced basis **Karatzas, E., Nonino, M., Ballarin, F., Rozza, G. and Maday, Y.**
- Manifold learning via Neural Network, convolutional autoencoders **Carlberg, K. and Lee, K.; Lye, K., Mishra S. and Ray, D.; Fresca, S., Dedè, L. and Manzoni, A., Venkat, S., Smith, R.C., Kelley, C.T.**
- Dynamic Modes **Lu, H. and Tartakovsky, D. M.**
- Dynamical Low Rank **Kazashi, Y., Nobile, F., Trigo Trindade, T., Vidličková, E., Ceruti, G., Kusch, J., Einkemmer, L., Frank, M.**
- Graph Neural Network **Pichi, F., Moya, B., Hesthaven, J.**
- Sinkhorn Loss and Wasserstein Kernel **Khamlich, M., Pichi, Rozza, G.**

Possible solutions and research directions

Some possibilities to incorporate the advection into RB framework

- Freezing **Ohlberger, M. and Rave, S.**
- Shifted POD **Reiss, J., Schulze, P., Sesterhenn, J., Mehrmann, V., Demo, N., Burela, S., Krah, P.**
- Lagrangian basis method **Mojgani, R. and Balajewicz, M.**
- Advection modes by optimal mass transport **Iollo, A., Lombardi, D., Mula, O., Taddei, T.**
- Calibration (also 2D non–periodic boundaries) **Cagniart, N., Stamm, B. and Maday, Y.**, **Crisovan, R. and Abgrall, R.**
- Online adaptive bases and samplings **Peherstorfer, B.**
- Gradient-preserving DEIM **Pagliantini, C.**
- Transport Reversal **Rim, D., Moe, S. and LeVeque R. J.**
- Registration method **Taddei, T., Ohlberger, M., Kleikamp, H.**
- Optimization based implicit feature tracking **Zahr, M., Mirhoseini, M.A.**
- Preprocessing reduced basis **Karatzas, E., Nonino, M., Ballarin, F., Rozza, G. and Maday, Y.**
- Manifold learning via Neural Network, convolutional autoencoders **Carlberg, K. and Lee, K.; Lye, K., Mishra S. and Ray, D.; Fresca, S., Dedè, L. and Manzoni, A., Venkat, S., Smith, R.C., Kelley, C.T.**
- Dynamic Modes **Lu, H. and Tartakovsky, D. M.**
- Dynamical Low Rank **Kazashi, Y., Nobile, F., Trigo Trindade, T., Vidličková, E., Ceruti, G., Kusch, J., Einkemmer, L., Frank, M.**
- Graph Neural Network **Pichi, F., Moya, B., Hesthaven, J.**
- Sinkhorn Loss and Wasserstein Kernel **Khamlich, M., Pichi, Rozza, G.**

Transfomation of the domain

Geometry map T

$$T : \mathcal{P} \times \mathcal{R} \to \Omega$$

- $\exists\, T^{-1} : \mathcal{P} \times \Omega \to \mathcal{R}$ such that
  - $T^{-1}[\mu](T[\mu](\hat{x})) = \hat{x}$ for $\hat{x} \in \mathcal{R}$
  - $T[\mu](T^{-1}[\mu](x)) = x$ for $x \in \Omega$
- $u_{\mathcal{N}}(T[\boldsymbol{\mu}], \hat{x}), \boldsymbol{\mu}) \approx \bar{v}(\hat{x}), \quad \forall \boldsymbol{\mu} \in \mathcal{P}, \hat{x} \in \mathcal{R}$

ALE formulation

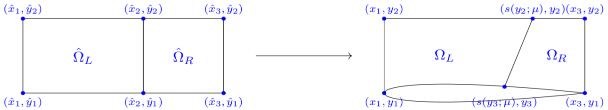
$$\partial_t u(x, \boldsymbol{\mu}, t) + \nabla F(u(x, \boldsymbol{\mu}, t); \boldsymbol{\mu}) = 0 \Longrightarrow \frac{\partial}{\partial t} v(\hat{x}, \boldsymbol{\mu}, t) + \frac{d\hat{x}}{dx} \frac{d}{d\hat{x}} F(v, \mu) - \frac{d\hat{x}}{dx} \frac{dv}{d\hat{x}} \frac{\partial T}{\partial t} = 0$$

$$v(\hat{x}, \boldsymbol{\mu}, t) := u(T[\boldsymbol{\mu}](\hat{x}), \boldsymbol{\mu}, t)$$

Transformation map for MOR

Examples: θ is the point of maximum height or of steepest solution, or some random points.

- Translation: $T(\theta,\hat{x}) = \hat{x} + \theta - 0.5$
- Dilatation: $T(\theta,\hat{x}) = \frac{\hat{x}\theta}{(2\theta-1)\hat{x}+1-\theta}$
- Piece-wise Cubic Hermite Interpolator Polynomial
- Higher degree polynomials
- Gordon-Hall



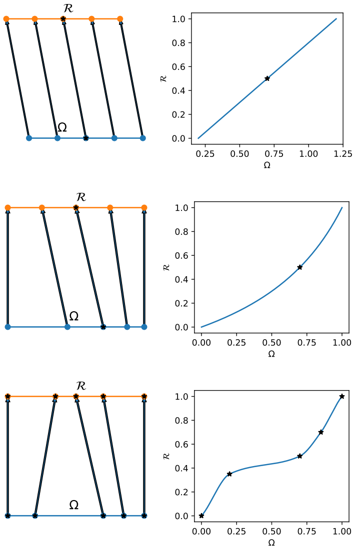
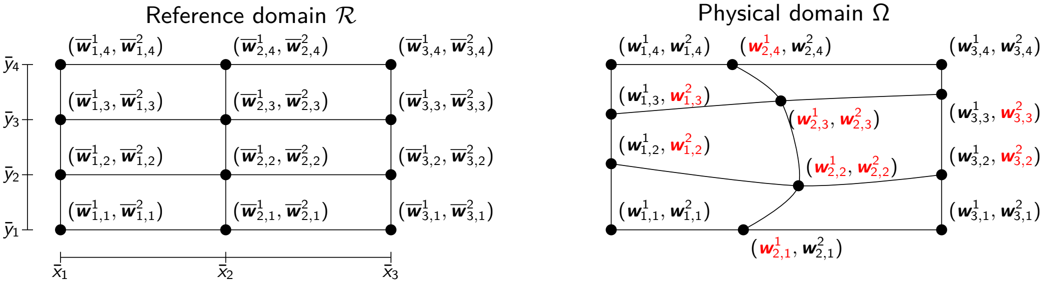


Table of contents

Control points and free coordinates



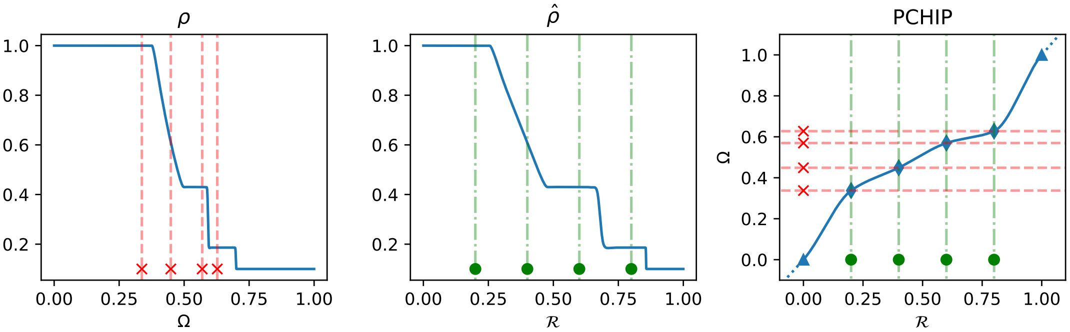
Quantities

- Control points $\boldsymbol{w}$
- Free coordinates $\boldsymbol{w}$

Goals

- Find map $T[\boldsymbol{w}(\boldsymbol{\mu})] : \mathcal{R} \to \Omega(\boldsymbol{\mu})$
- $T[\boldsymbol{w}(\boldsymbol{\mu})](\overline{\boldsymbol{w}}_{i,j}) = \boldsymbol{w}_{i,j}$
- Regular in space $T[\boldsymbol{w}(\boldsymbol{\mu})] \in \mathcal{C}^1(\mathcal{R}, \Omega(\boldsymbol{\mu}))$
- Invertible and regular $T^{-1}[\boldsymbol{w}(\boldsymbol{\mu})] \in \mathcal{C}^1(\Omega(\boldsymbol{\mu}), \mathcal{R})$
- Regular in parameters $T \in \mathcal{C}^1(W, \mathcal{C}^1(\mathcal{R}, \Omega(\boldsymbol{\mu})))$

Piece-wise Cubic Hermite Polynomials (PCHIP)



Properties in 1D

- Polynomials
- Monotone
- Easy to differentiate (for ALE formulation)

Piece-wise Cubic Hermite Polynomials (PCHIP)

$$T[\boldsymbol{w}(\boldsymbol{\mu})](\hat{x},\hat{y}) := \left(T^x[\boldsymbol{w}(\boldsymbol{\mu})](\hat{x},\hat{y}),\, T^y[\boldsymbol{w}(\boldsymbol{\mu})](\hat{x},\hat{y})\right),$$

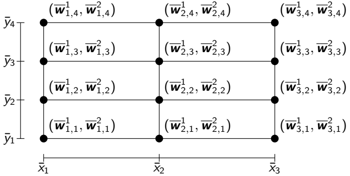
$$T^x[\boldsymbol{w}(\boldsymbol{\mu})](\hat{x},\hat{y}) := \sum_{\ell=1}^{M_2} \gamma^y_\ell(\hat{y}) P^x_\ell(\hat{x}),$$

$$T^y[\boldsymbol{w}(\boldsymbol{\mu})](\hat{x},\hat{y}) := \sum_{k=1}^{M_1} \gamma^x_k(\hat{x}) P^y_k(\hat{y}).$$

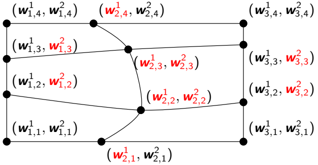
2D Extension

- P^x_ℓ is a PCHIP interpolating $\{\overline{\boldsymbol{w}}^1_{\alpha_1,\ell}, \boldsymbol{w}^1_{\alpha_1,\ell}(\boldsymbol{\mu})\}_{\alpha_1=1}^{M_1}$;
- P^y_k is a PCHIP interpolating $\{\overline{\boldsymbol{w}}^2_{k,\alpha_2}, \boldsymbol{w}^2_{k,\alpha_2}(\boldsymbol{\mu})\}_{\alpha_2=1}^{M_2}$;
- $\gamma^y_\ell(\cdot)$ is a PCHIP interpolating $\{\overline{\boldsymbol{w}}^2_{\alpha_1,\alpha_2}, \delta_{\alpha_2,\ell}\}_{\alpha_2=1}^{M_2}$;
- $\gamma^x_k(\cdot)$ is a PCHIP interpolating $\{\overline{\boldsymbol{w}}^1_{\alpha_1,\alpha_2}, \delta_{\alpha_1,k}\}_{\alpha_1=1}^{M_1}$;
- Convex combinations;
- $T^x[\boldsymbol{w}^{\text{opt}}(\boldsymbol{\mu})](\hat{x}, \hat{y} = \overline{\boldsymbol{w}}^2_{\alpha_1,\alpha_2}) = P^x_{\alpha_2}(\hat{x})$;
- $T^y[\boldsymbol{w}^{\text{opt}}(\boldsymbol{\mu})](\hat{x} = \overline{\boldsymbol{w}}^1_{\alpha_1,\alpha_2}, \hat{y}) = P^y_{\alpha_1}(\hat{y})$.

Reference domain



Physical Domain



Piece-wise Cubic Hermite Polynomials (PCHIP)

Constraints on control points!

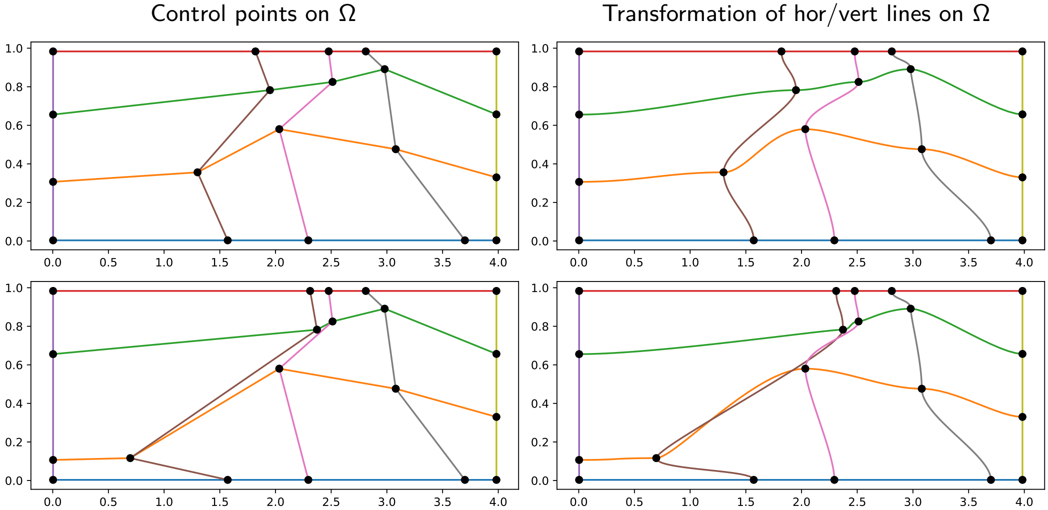


Table of contents

What do we need to apply the transformation?

What do we have?

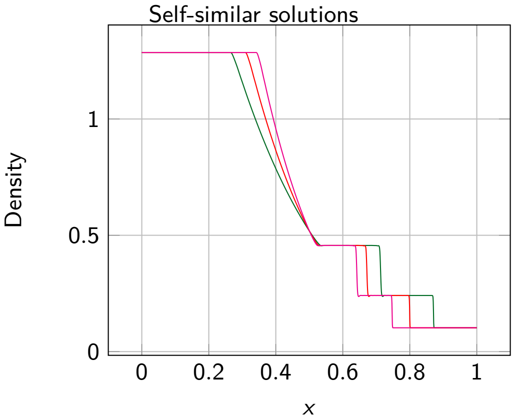
- Simulations for different parameters/times

What do we need?

- Control points $\boldsymbol{w}(\boldsymbol{\mu})$ for each parameter/time

Goal?

- Optimize the registration of the solution
- If possible $u(T[\boldsymbol{\mu}](\hat{\mathbf{x}}), \boldsymbol{\mu}) \approx \bar{u}(\hat{\mathbf{x}})$ with $\hat{\mathbf{x}} \in \mathcal{R}$
- If not possible, new manifold should be easily reproducible
- $\hat{\mathcal{M}} := \{u(T[\boldsymbol{\mu}](\cdot), \boldsymbol{\mu}) \forall \boldsymbol{\mu}\} : \exists N_{RB} \ll \mathcal{N}$ s.t. $u(T[\boldsymbol{\mu}](\hat{\mathbf{x}}), \boldsymbol{\mu}) \approx \sum_{i=1}^{N_{RB}} \hat{u}_i(\boldsymbol{\mu})\psi_i(\hat{\mathbf{x}})$



What do we need to apply the transformation?

What do we have?

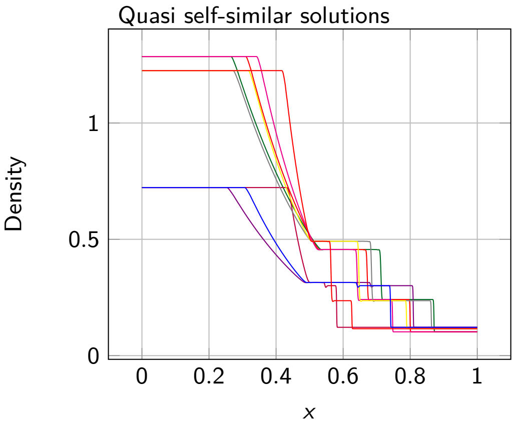
- Simulations for different parameters/times

What do we need?

- Control points $\boldsymbol{w}(\boldsymbol{\mu})$ for each parameter/time

Goal?

- Optimize the registration of the solution
- If possible $u(T[\boldsymbol{\mu}](\hat{\mathbf{x}}),\boldsymbol{\mu}) \approx \bar{u}(\hat{\mathbf{x}})$ with $\hat{\mathbf{x}} \in \mathcal{R}$
- If not possible, new manifold should be easily reproducible
- $\hat{\mathcal{M}} := \{u(T[\boldsymbol{\mu}](\cdot),\boldsymbol{\mu})\,\forall \boldsymbol{\mu}\} : \exists N_{RB} \ll \mathcal{N}$ s.t. $u(T[\boldsymbol{\mu}](\hat{\mathbf{x}}),\boldsymbol{\mu}) \approx \sum_{i=1}^{N_{RB}} \hat{u}_i(\boldsymbol{\mu})\psi_i(\hat{\mathbf{x}})$



Optimization for self-similar solutions

Minimization functional

$$\forall \boldsymbol{\mu} \in \Xi_{\text{train}} \qquad \min_{\mathbf{w}(\boldsymbol{\mu})\in\mathbb{R}^Q} \| u(T[\mathbf{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu}) - \bar{u}\|_{L^2(\mathcal{R})} + \frac{\delta}{2}\|\partial_{\boldsymbol{\mu}} \mathbf{w}(\boldsymbol{\mu})\|^2_{\ell^2(\mathcal{P})} +$$
$$\frac{\alpha}{2} \max_{\mathbf{x}\in\Omega} \left(\max\left\{ \|\nabla T[\mathbf{w}(\boldsymbol{\mu})](\hat{\mathbf{x}})\|, \left\|\nabla T^{-1}[\mathbf{w}(\boldsymbol{\mu})](\mathbf{x})\right\| \right\}\right),$$

constrained to $\det(\nabla T[\mathbf{w}(\boldsymbol{\mu})](\hat{x})) > 0 \quad \forall \hat{x} \in \mathcal{R}, \quad \mathbf{w}(\boldsymbol{\mu})$ does not switch order, $\quad \mathbf{w}(\boldsymbol{\mu}) \in \mathcal{R}$.

Details

- Ξ_{train} is a training set of parameters
- Abuse of notation $T[\mathbf{w}(\boldsymbol{\mu})] = T[\boldsymbol{\mu}]$
- $\bar{u}$? Typically one representative parameter
- $\|\partial_{\boldsymbol{\mu}} \mathbf{w}(\boldsymbol{\mu})\|^2_{\ell^2(\mathcal{P})}$ how to compute?
  Approximation with previous parameters

Algorithm

- Choose $\bar{u}$
- For all $\boldsymbol{\mu} \in \Xi_{\text{train}}$ solve minimization with
  - Sequential Least SQuares Programming (SLSQP) scipy.optimize.minimize
  - Initial guess the closes parameter already computed control points

Optimization for quasi self-similar solutions

Desiderata minimization functional

$$
\begin{aligned}
\min_{\mathbf{w}(\Xi_{\text{train}})\in\mathbb{R}^{Q\times N_{\text{train}}}} \sum_{\boldsymbol{\mu}\in\Xi_{\text{train}}} & \left\| u(T[\mathbf{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu}) - \Pi_{V_{\text{POD}}} u(T[\mathbf{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu}) \right\|_{L^2(\mathcal{R})} + \frac{\delta}{2}\left\|\partial_{\boldsymbol{\mu}}\mathbf{w}(\boldsymbol{\mu})\right\|^2_{\ell^2(\mathcal{P})} + \\
& \frac{\alpha}{2}\max_{\mathbf{x}\in\Omega}\left(\max\left\{\left\|\nabla T[\mathbf{w}(\boldsymbol{\mu})](\hat{\mathbf{x}})\right\|, \left\|\nabla T^{-1}[\mathbf{w}(\boldsymbol{\mu})](\mathbf{x})\right\|\right\}\right), \\
\text{with } & V_{\text{POD}} := \text{POD}\left(\{u(T[\mathbf{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\Xi_{\text{train}}}\right) \\
\text{constrained to } & \det(\nabla T[\mathbf{w}(\boldsymbol{\mu})](\hat{x})) > 0 \quad \forall \hat{x}\in\mathcal{R}, \quad \mathbf{w}(\boldsymbol{\mu}) \text{ does not switch order}, \quad \mathbf{w}(\boldsymbol{\mu})\in\mathcal{R}.
\end{aligned}
$$

Changes

- Minimization on all parameters all together
- No reference solution
- Projection onto reduced space generated by the calibrated solutions

Too expensive

- Dimension of minimization problem is too large
- The functional depends on a POD to be solved at each iterative step

Optimization for quasi self-similar solutions

Compromise minimization functional (few parameters)

$$\min_{\boldsymbol{w}(\Xi_{\text{few}})\in\mathbb{R}^{\mathbb{Q}\times\mathbb{N}_{\text{few}}}} \sum_{\boldsymbol{\mu}\in\Xi_{\text{few}}} \|u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu}) - \Pi_{V_{\text{POD}}} u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu})\|_{L^2(\mathcal{R})} + \frac{\delta}{2}\|\partial_{\boldsymbol{\mu}}\boldsymbol{w}(\boldsymbol{\mu})\|^2_{\ell^2(\mathcal{P})} +$$
$$\frac{\alpha}{2}\max_{\boldsymbol{x}\in\Omega}\left(\max\left\{\|\nabla T[\boldsymbol{w}(\boldsymbol{\mu})](\hat{\boldsymbol{x}})\|,\left\|\nabla T^{-1}[\boldsymbol{w}(\boldsymbol{\mu})](\boldsymbol{x})\right\|\right\}\right),$$
$$\text{with } V_{\text{POD}} := \text{POD}\left(\{u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\Xi_{\text{few}}}\right)$$

Compromise minimization functional (all parameters)

$$\forall\boldsymbol{\mu}\in\Xi_{\text{train}}\quad \min_{\boldsymbol{w}(\boldsymbol{\mu})\in\mathbb{R}^{Q}} \|u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu}) - \Pi_{V_{\text{POD}}} u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu})\|_{L^2(\mathcal{R})} + \frac{\delta}{2}\|\partial_{\boldsymbol{\mu}}\boldsymbol{w}(\boldsymbol{\mu})\|^2_{\ell^2(\mathcal{P})} +$$
$$\frac{\alpha}{2}\max_{\boldsymbol{x}\in\Omega}\left(\max\left\{\|\nabla T[\boldsymbol{w}(\boldsymbol{\mu})](\hat{\boldsymbol{x}})\|,\left\|\nabla T^{-1}[\boldsymbol{w}(\boldsymbol{\mu})](\boldsymbol{x})\right\|\right\}\right),$$
$$\text{with } V_{\text{POD}} := \text{POD}\left(\{u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot);\boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\Xi_{\text{few}}}\right)$$

Table of contents

Summary

What we did?

- Compute FOM for various $\boldsymbol{\mu} \in \Xi_{\text{train}}$
- Find $\boldsymbol{w}(\boldsymbol{\mu})$ for each $\boldsymbol{\mu}$ with optimization

What we have?

- For all $\boldsymbol{\mu} \in \Xi_{\text{train}}$ we know how to calibrate
- Now, $\{u(T[\boldsymbol{w}(\boldsymbol{\mu})](\cdot), \boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\Xi_{\text{train}}}$ is decently reducible!!

What is missing for the online phase?

- Knowing $\boldsymbol{w}(\boldsymbol{\mu})$ for a new parameter $\boldsymbol{\mu}$
- Reduction of calibrated solutions

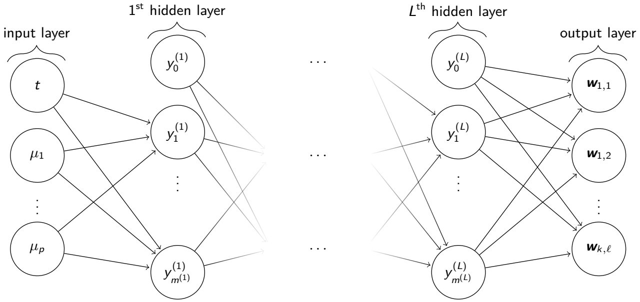
Learning $\boldsymbol{w}$

Artificial Neural Network

- Use calibrated $\boldsymbol{w}$ to get an estimator $\widehat{\boldsymbol{w}}(\boldsymbol{\mu})$
- ANN with 4 hidden layers, 16 neurons each, tanh activation

Properties

- Minimization constraints cannot be fulfilled
- Enforcing $\boldsymbol{w}_{i,j} < \boldsymbol{w}_{i+1,j}$, learning positive quantities $\boldsymbol{w}_{i+1,j} - \boldsymbol{w}_{i,j}$ with (positive) Softplus final activation function



POD-NN

Offline phase

- $\mathrm{POD}\left(\{u(T[\boldsymbol{\mu}](\cdot);\boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\Xi_{\text{train}}}\right) =: \mathbb{V}_{N_{RB}}$
- Projection onto $\mathbb{V}_{N_{RB}}$

$$(\psi_j,\psi_i)\hat{u}_i(\boldsymbol{\mu}) = (\psi_j, u(T[\boldsymbol{\mu}](\cdot);\boldsymbol{\mu})) \qquad i=1,\dots,N_{RB}, \qquad \boldsymbol{\mu}\in\Xi_{\text{train}}$$

- Learn the map $\boldsymbol{\mu}\to\hat{u}_i(\boldsymbol{\mu})$ for all $i=1,\dots,N_{RB}$.

(POD)-Neural Network

- Same architecture as for learning $\boldsymbol{w}$
- 4 hidden layers
- 16 neurons each
- tanh as activation function

Table of contents

Sod shock tube test case: no parameters only time dependence

Euler Equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{EOS: } E = \frac{p}{\rho(\gamma-1)} + \frac{u^2}{2} \end{cases}$$

Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$

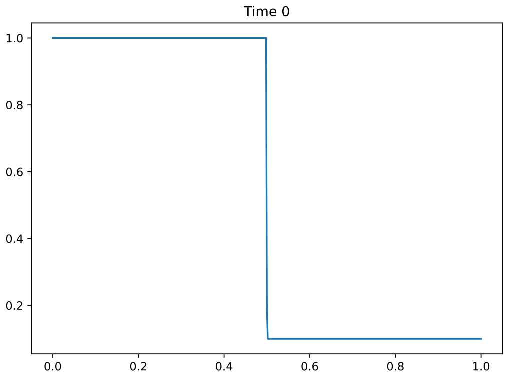
Sod shock tube test case: no parameters only time dependence

Euler Equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{ EOS: } E = \frac{p}{\rho(\gamma-1)} + \frac{u^2}{2} \end{cases}$$

Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$



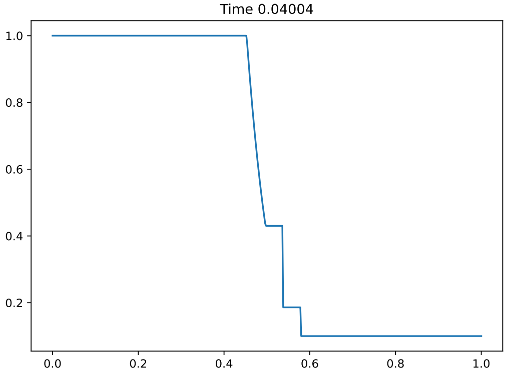
Sod shock tube test case: no parameters only time dependence

Euler Equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{EOS: } E = \frac{p}{\rho(\gamma - 1)} + \frac{u^2}{2} \end{cases}$$

Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$



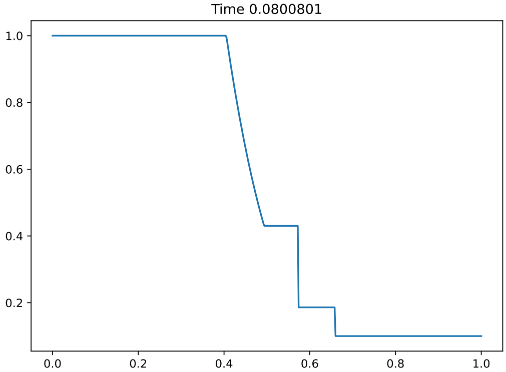
Sod shock tube test case: no parameters only time dependence

Euler Equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{ EOS: } E = \frac{p}{\rho(\gamma-1)} + \frac{u^2}{2} \end{cases}$$

Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$



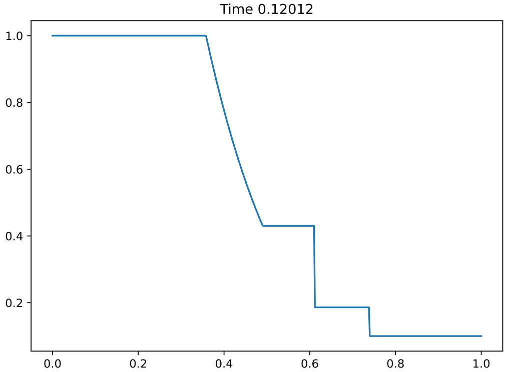
Sod shock tube test case: no parameters only time dependence

Euler Equations

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{EOS: } E = \frac{p}{\rho(\gamma-1)} + \frac{u^2}{2} \end{cases}$$

Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$



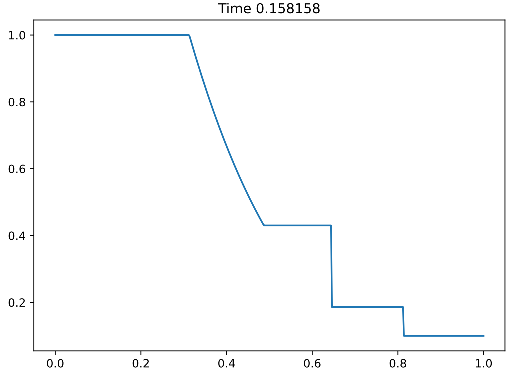
Sod shock tube test case: no parameters only time dependence

Euler Equations

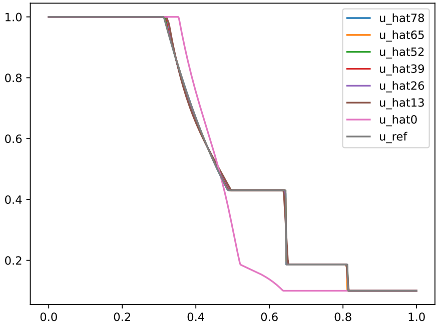
$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x(u(\rho E + p)) = 0 \\ + \text{EOS: } E = \frac{p}{\rho(\gamma - 1)} + \frac{u^2}{2} \end{cases}$$

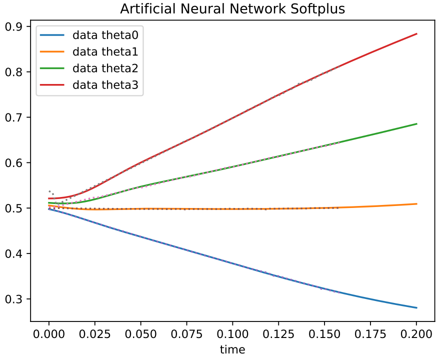
Riemann Problem: Sod Shock tube

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 1 \end{pmatrix}^T & \text{if } x < 0.5 \\ \begin{pmatrix} 0.1 & 0 & 0.125 \end{pmatrix}^T & \text{if } x > 0.5 \end{cases}$$



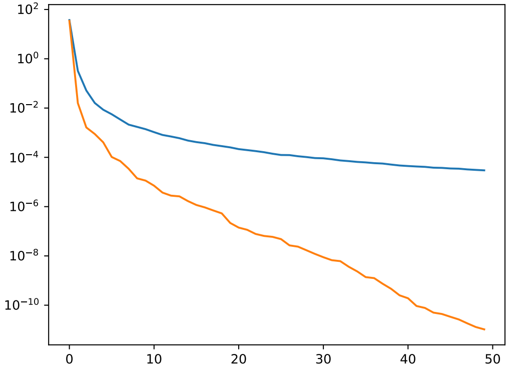
Transformations and calibration



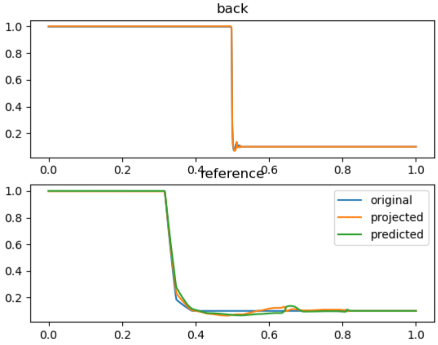


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

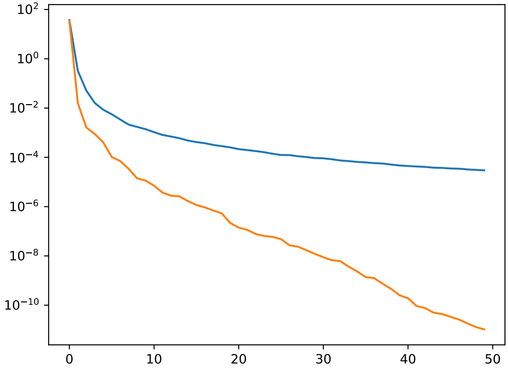


Multilayer Perceptron Regression for θ

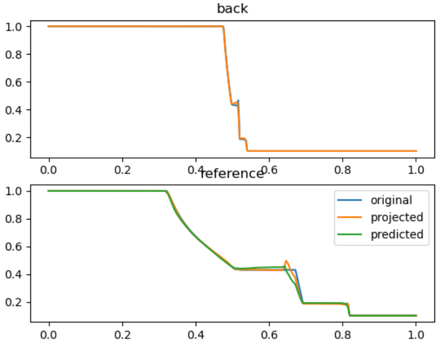


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

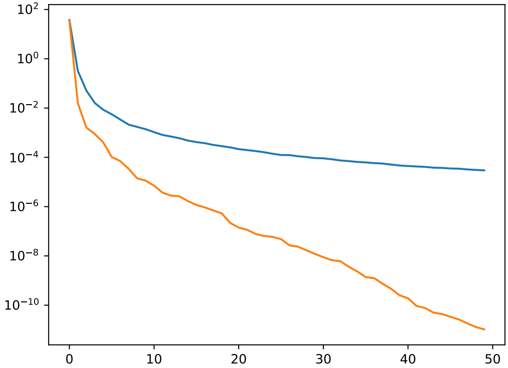


Multilayer Perceptron Regression for θ

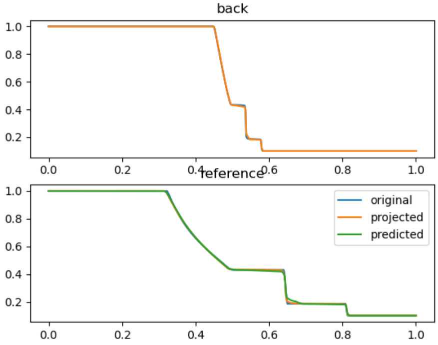


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

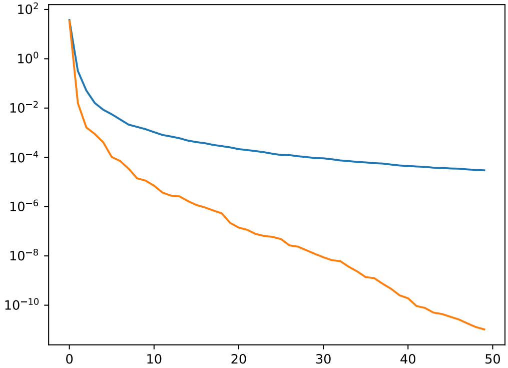


Multilayer Perceptron Regression for θ

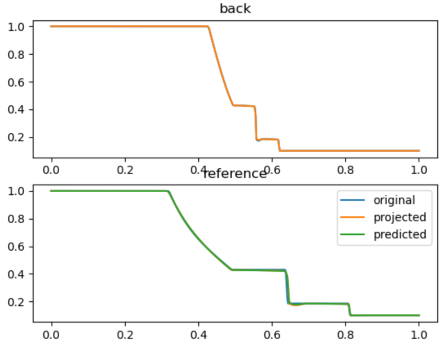


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

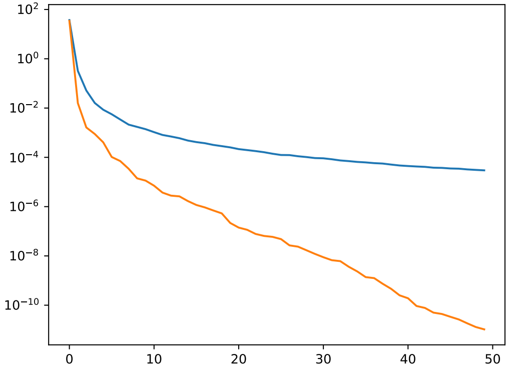


Multilayer Perceptron Regression for θ

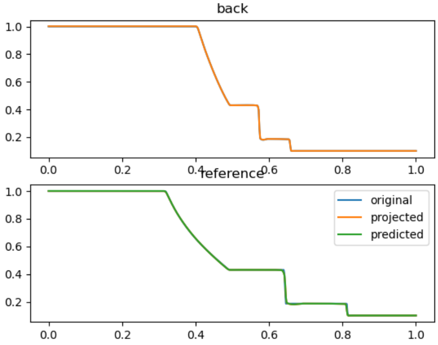


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

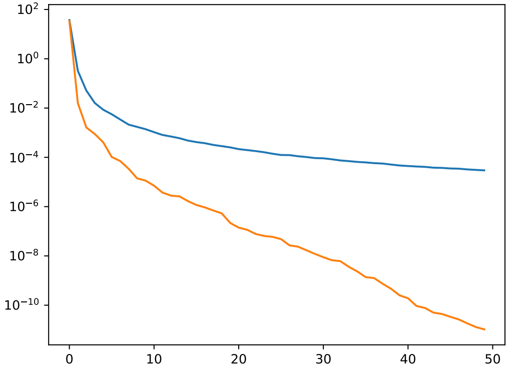


Multilayer Perceptron Regression for θ

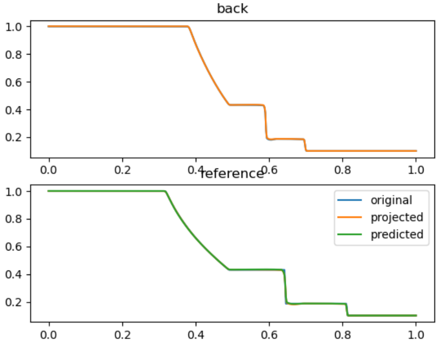


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

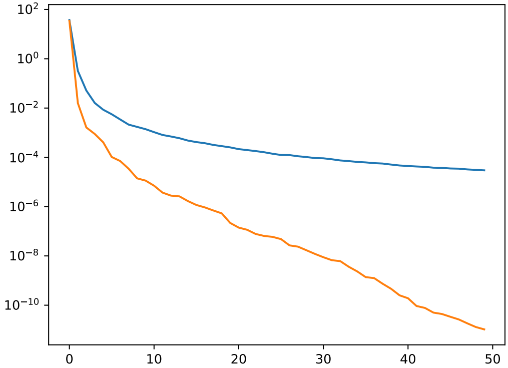


Multilayer Perceptron Regression for θ

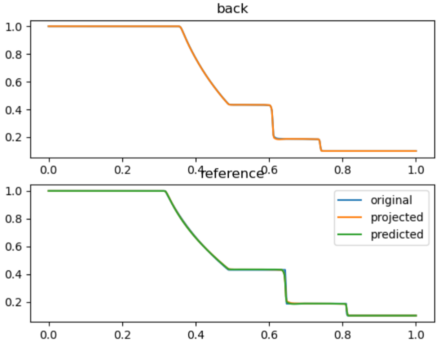


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

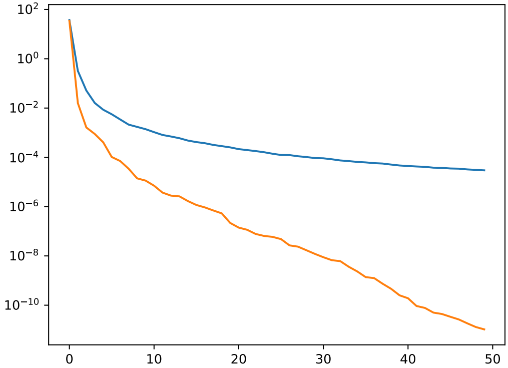


Multilayer Perceptron Regression for θ

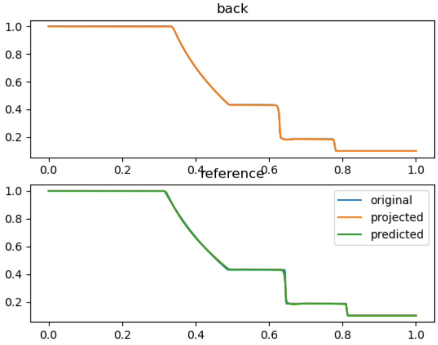


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

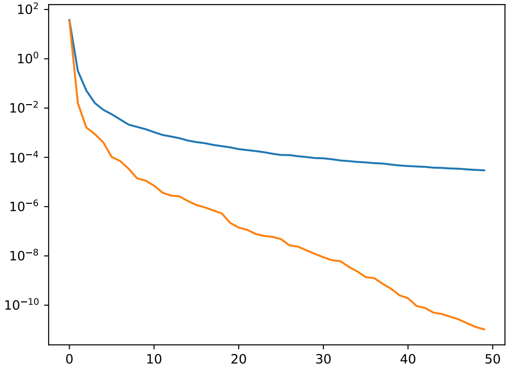


Multilayer Perceptron Regression for θ

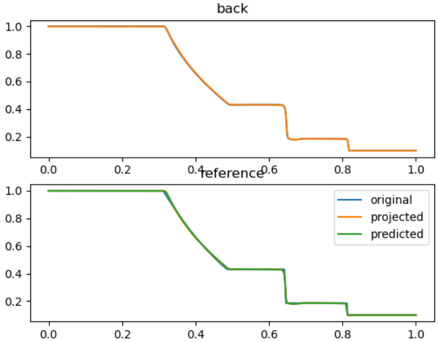


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

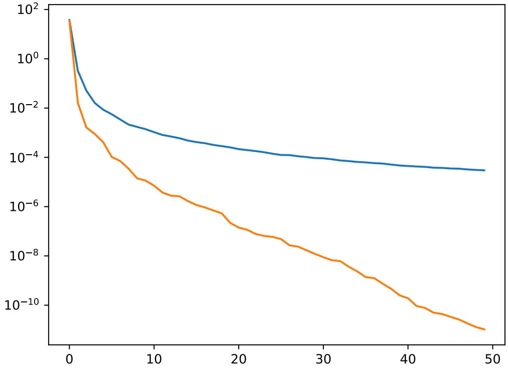


Multilayer Perceptron Regression for θ

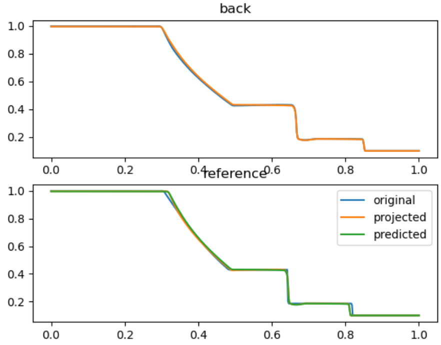


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)

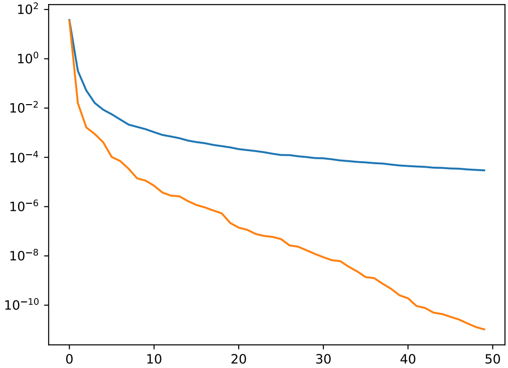


Multilayer Perceptron Regression for θ

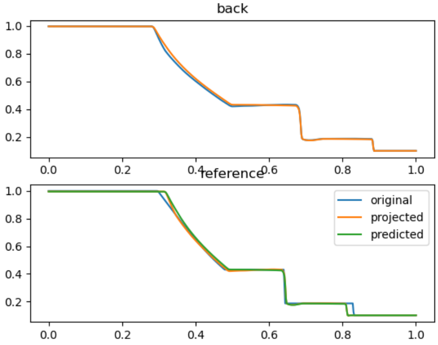


Results: online with POD-NN

Singular values decay for original problem (blue) and transformed problem (orange)



Multilayer Perceptron Regression for θ



Sod: Validation of calibration strategy

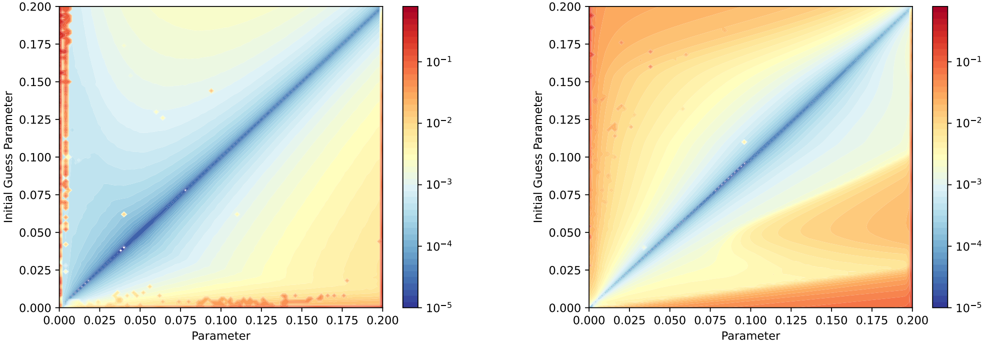


Figure: Calibration error for Sod 1D at different times (parameter $\boldsymbol{\mu}$) using different initial guess times (parameter $\bar{\boldsymbol{\mu}}$), for the FV solutions. Left: $\overline{\rho} = \rho(\bar{\boldsymbol{\mu}})$, $\boldsymbol{w}^{(0)}(\boldsymbol{\mu}) = \boldsymbol{w}^{ex}(\bar{\boldsymbol{\mu}})$, error measure $||\boldsymbol{\theta}^{opt}(\boldsymbol{\mu}) - \boldsymbol{\theta}^{ex}(\boldsymbol{\mu})||_1$. Right: $\overline{\rho} = \rho(\bar{\boldsymbol{\mu}})$ and $\bar{\boldsymbol{w}} = \boldsymbol{w}^{(0)}(\boldsymbol{\mu}) = \{0.2, 0.4, 0.6, 0.8\}$ for all $\boldsymbol{\mu}$, error measure $||\hat{\rho}(\boldsymbol{\mu}, \boldsymbol{w}(\boldsymbol{\theta}^{opt}(\boldsymbol{\mu}))) - \Pi_{\overline{\rho}}\hat{\rho}(\boldsymbol{\mu}, \boldsymbol{w}(\boldsymbol{\theta}^{opt}(\boldsymbol{\mu})))||_2^2$

Sod: Validation of calibration strategy

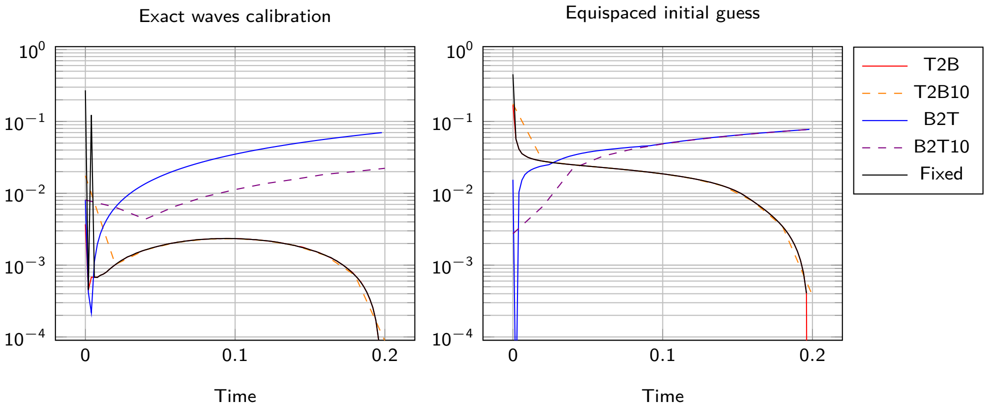
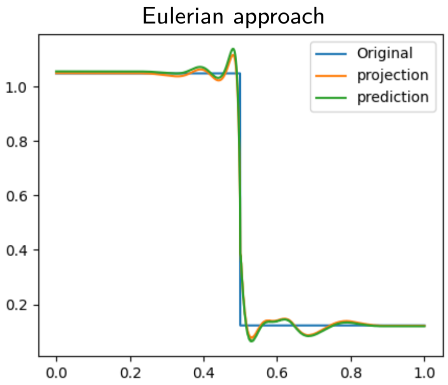


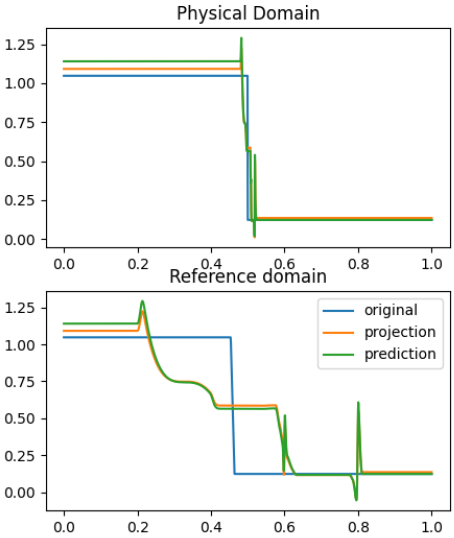
Figure: Calibration error for Sod 1D at different times (parameters) using different calibration strategies, for the FV solutions. Left: exact waves calibration as initial guess and right for equispaced initial guess calibration points. Error measure: $||\boldsymbol{\theta}^{opt}(\boldsymbol{\mu}) - \boldsymbol{\theta}^{ex}(\boldsymbol{\mu})||_1$ (left) and $||\hat{\rho}(\boldsymbol{\mu}, \boldsymbol{w}(\boldsymbol{\theta}^{opt}(\boldsymbol{\mu}))) - \Pi_{\overline{\rho}}\hat{\rho}(\boldsymbol{\mu}, \boldsymbol{w}(\boldsymbol{\theta}^{opt}(\boldsymbol{\mu})))||_2^2$ (right)

Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

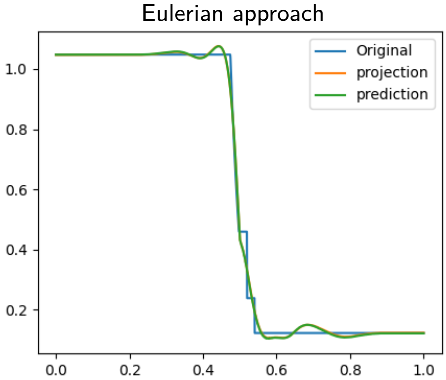


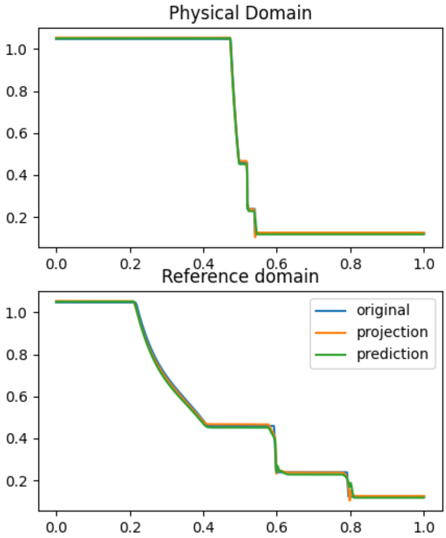


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

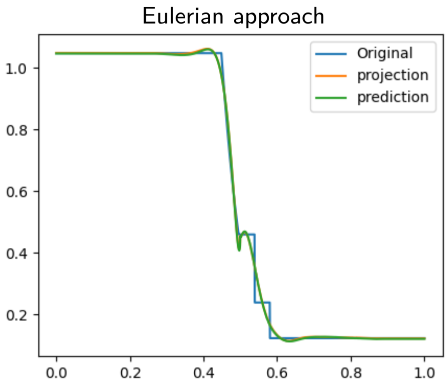


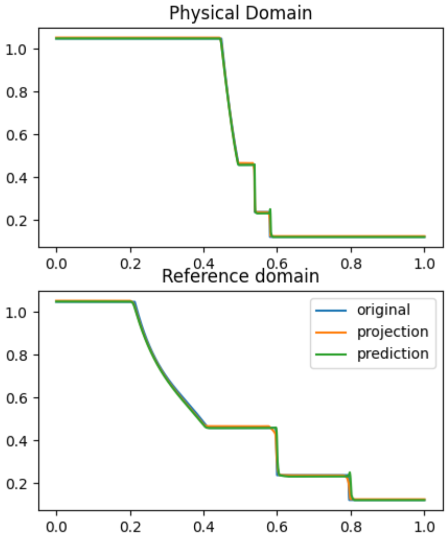


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

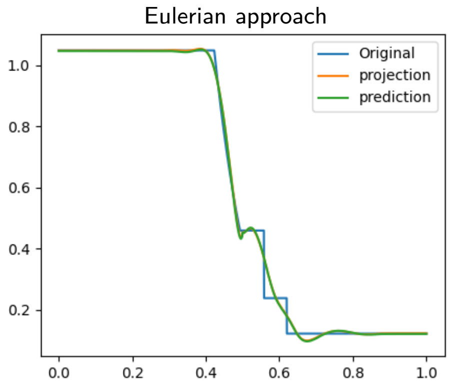


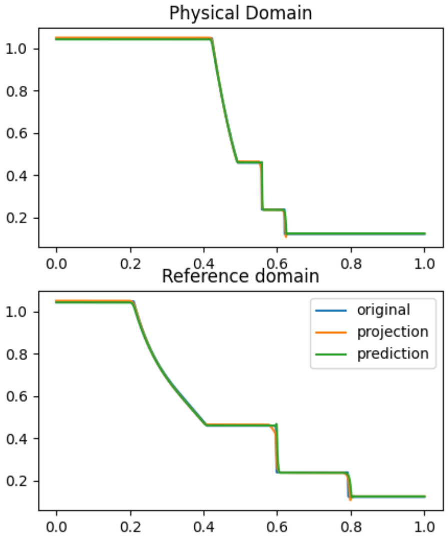


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

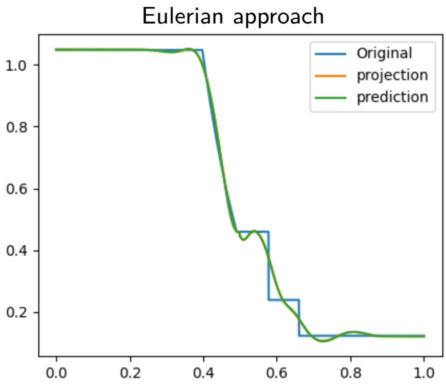


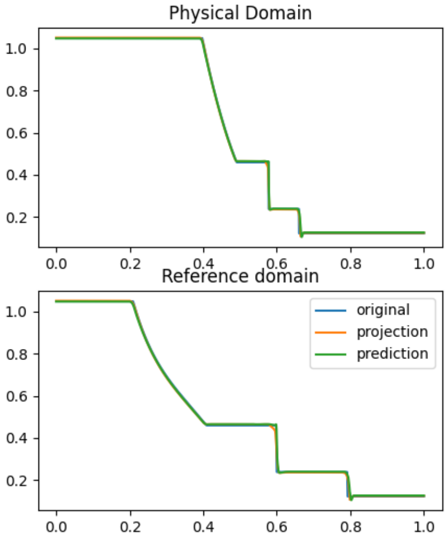


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

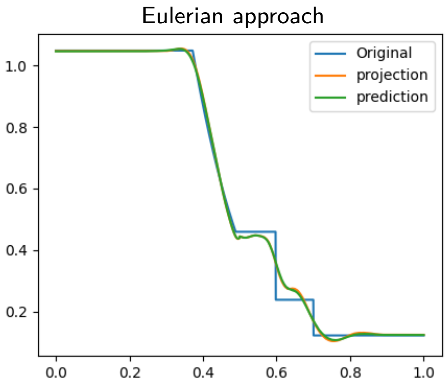


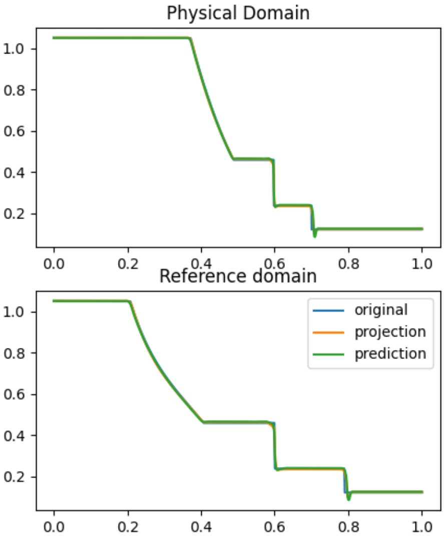


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

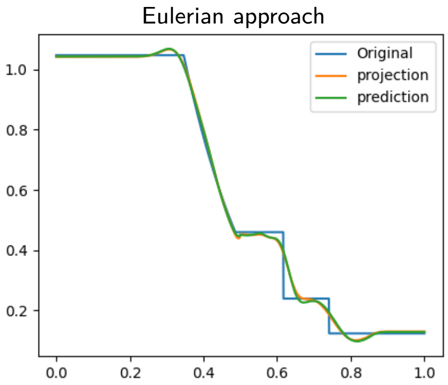


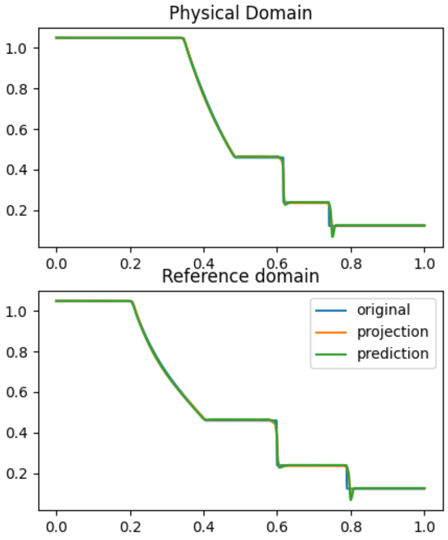


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

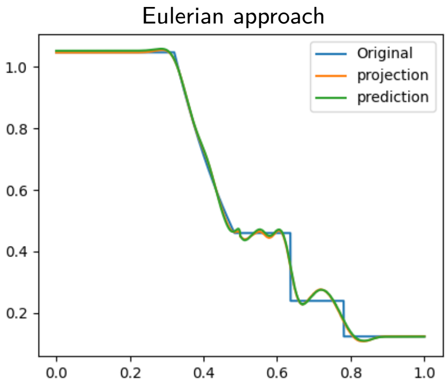


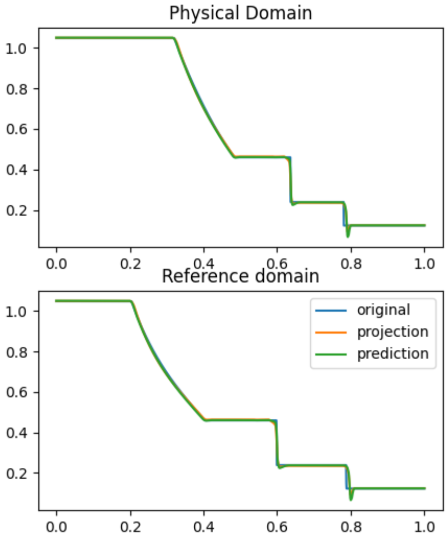


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

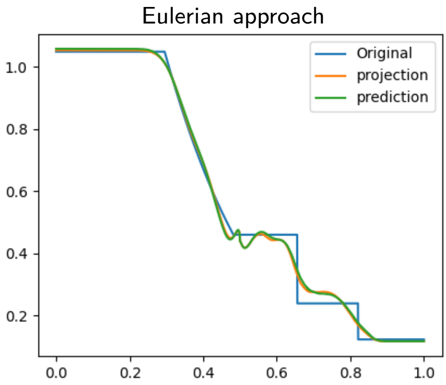


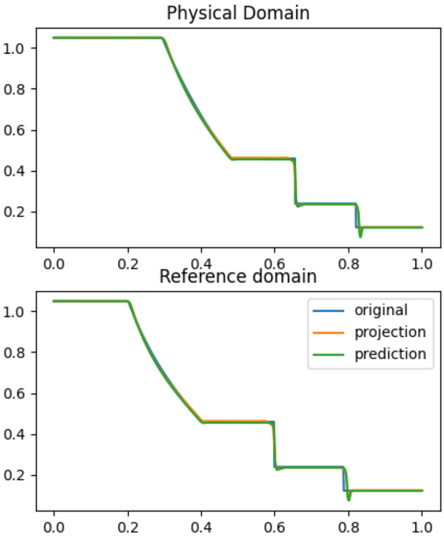


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

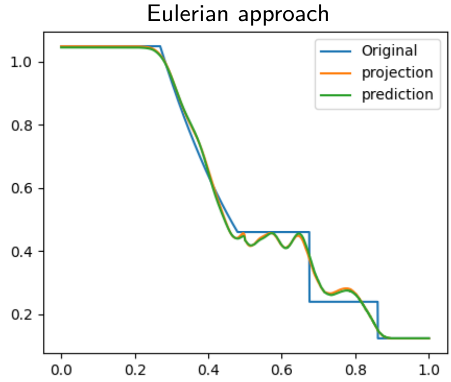


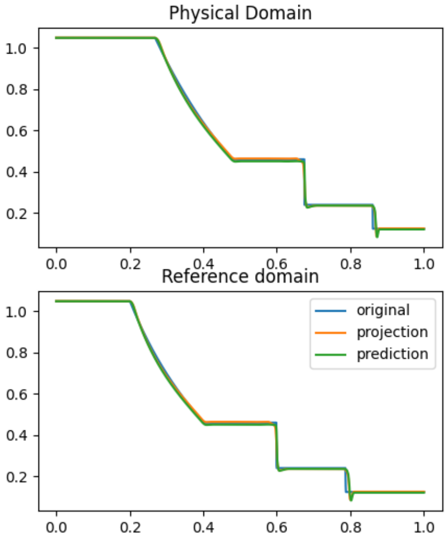


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$

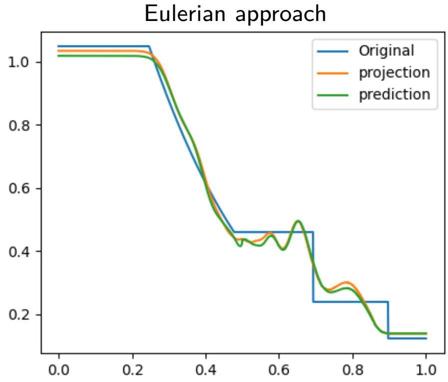


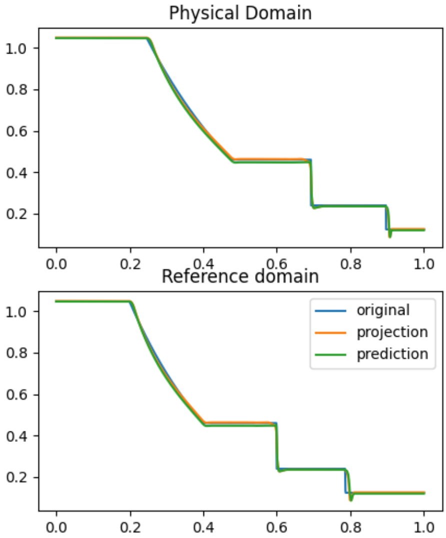


Parameter dependent Sod: Eulerian vs ALE

Parameters

- $\rho_L \in [0.7, 1.3]$, $\rho_R = [0.1, 0.15]$
- $p_L \in [0.7, 1.3]$, $p_R = [0.05, 0.15]$





Parametric Sod: POD eigenvalue decay

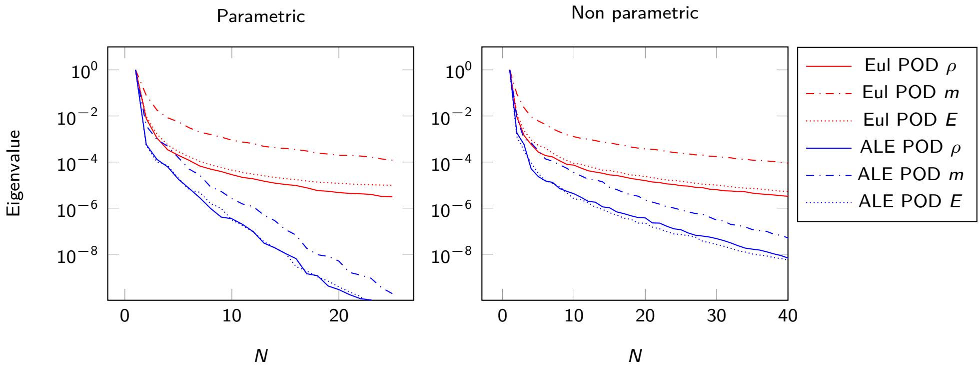


Figure: Sod 1D: Eigenvalue decay of the PODs (normalized to have $\lambda_1 = 1$) non parametric (left) and parametric (right)

Parametric Sod: POD basis

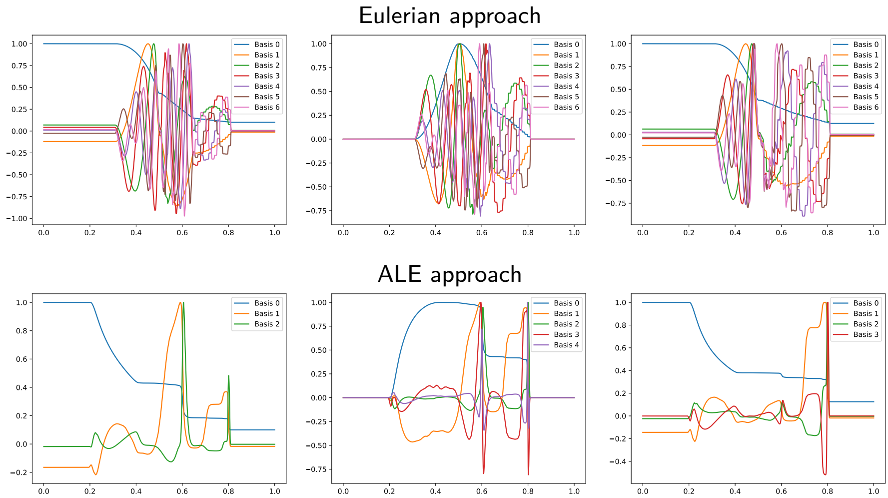
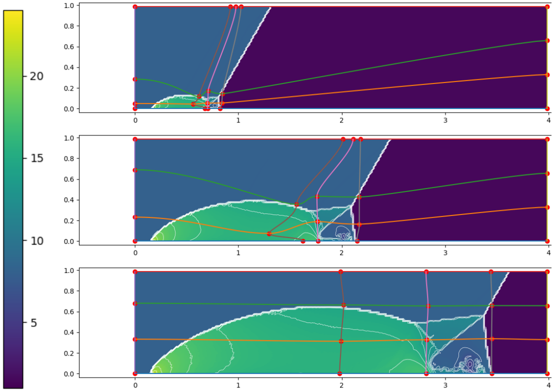


Figure: ρ (left), m (center) and E (right), with $\tau_{\text{POD}} = 10^{-4}$ and $N_{\text{POD}}^{\max} = 7$

Double Mach reflection 2D



Non parametric DMR

- Oblique shock hitting the bottom wall
- $\rho_L = 8$, $|\underline{u}_L| = 8.25$, $\arctan \underline{u} = \frac{\pi}{6}$, $p_L = 116.5$
- $\rho_R = 1.4$, $u_R = 0$, $v_R = 0$, $p_R = 1$

Parametric DMR

- Oblique shock hitting the bottom wall
- $\rho_L = 8$, $|\underline{u}_L| = 8.25$, $\arctan \underline{u} \in [0.1, 0.675]$, $p_L = 116.5$
- $\rho_R = 1.4$, $u_R = 0$, $v_R = 0$, $p_R = 1$

Double Mach reflection 2D

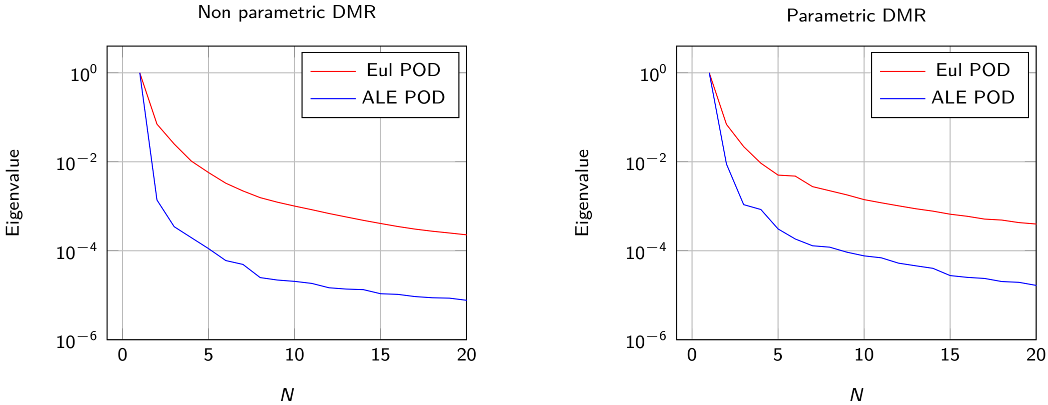


Figure: DMR: Eigenvalue decay of the PODs (normalized to have $\lambda_1 = 1$), non parametric on the left, parametric on the right

Double Mach reflection 2D (not parametric): calibration

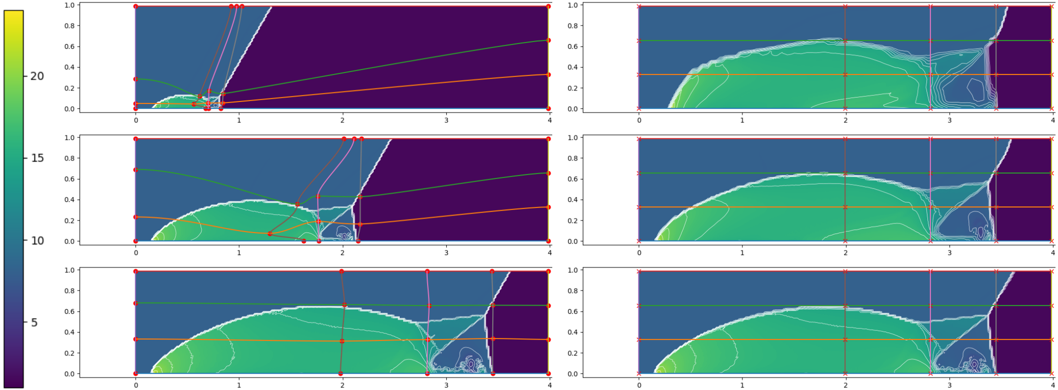


Figure: FOM solution for ρ for DMR non parametric at times 0.05 (top), 0.15 (center) and 0.25 (bottom) in the physical domain Ω (left) and, after calibration, in the reference configuration $\mathcal{R}$ (right). We mark on the plots the control points and the Cartesian grid that links them in the reference domain and its image through T on the physical one.

Double Mach reflection 2D (not parametric): error

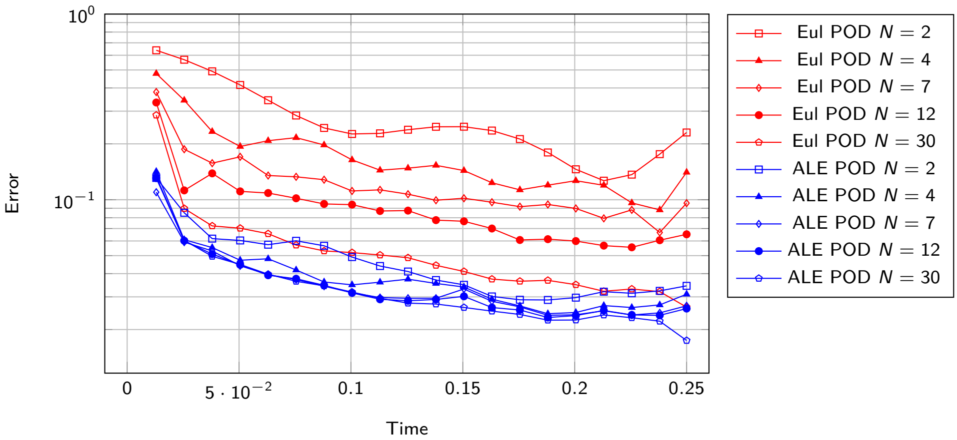


Figure: DMR non parametric: Error in time of reduced methods with different number N of modes

Double Mach reflection 2D (non parametric): simulations

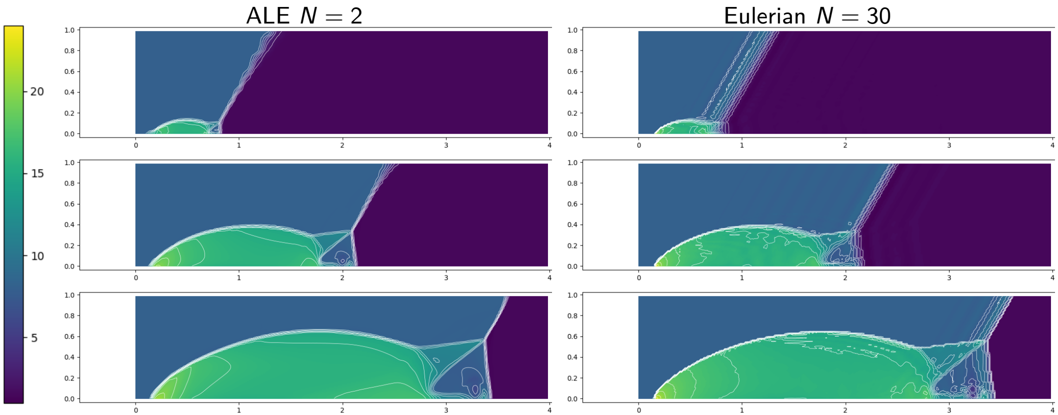


Figure: DMR non parametric: ROM solutions for ρ in Ω at times 0.05 (top), 0.15 (center) and 0.25 (bottom). Left column: ALE ROM solution with $N = 2$. Right column: Eulerian ROM solution with $N = 30$.

Double Mach reflection 2D (parametric): simulations

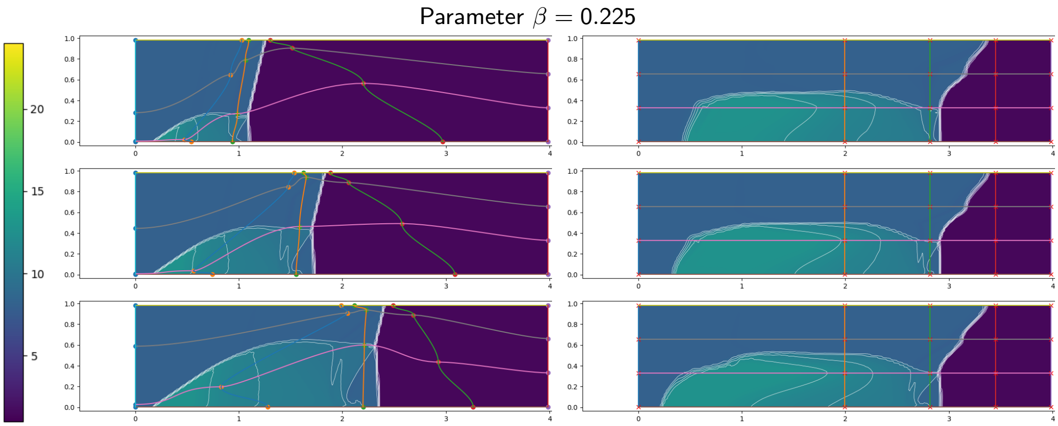


Figure: DMR parametric FOM solution for ρ at times $t = 0.096$, $t = 0.148$ and $t = 0.2$ (top to bottom) in the physical domain Ω (left) and, after calibration, in the reference configuration $\mathcal{R}$ (right).

Double Mach reflection 2D (parametric): simulations

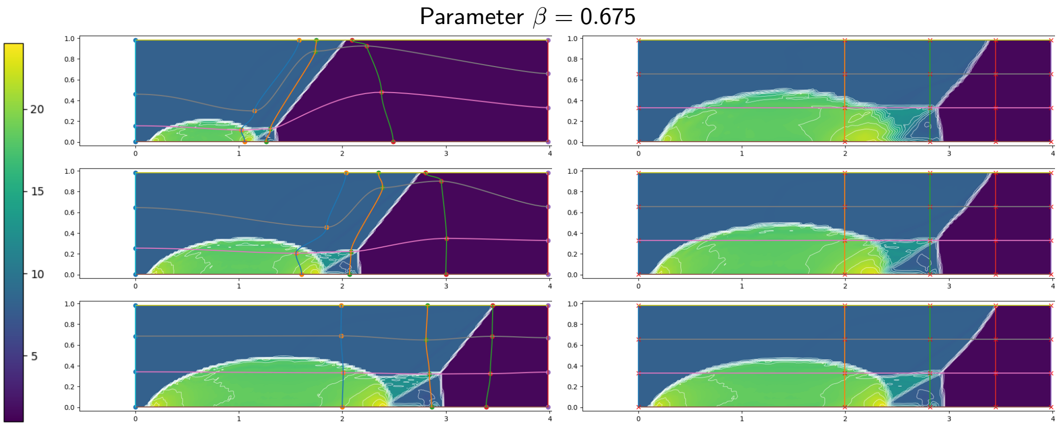


Figure: DMR parametric FOM solution for ρ at times $t = 0.096$, $t = 0.148$ and $t = 0.2$ (top to bottom) in the physical domain Ω (left) and, after calibration, in the reference configuration $\mathcal{R}$ (right).

Double Mach reflection 2D (parametric): error

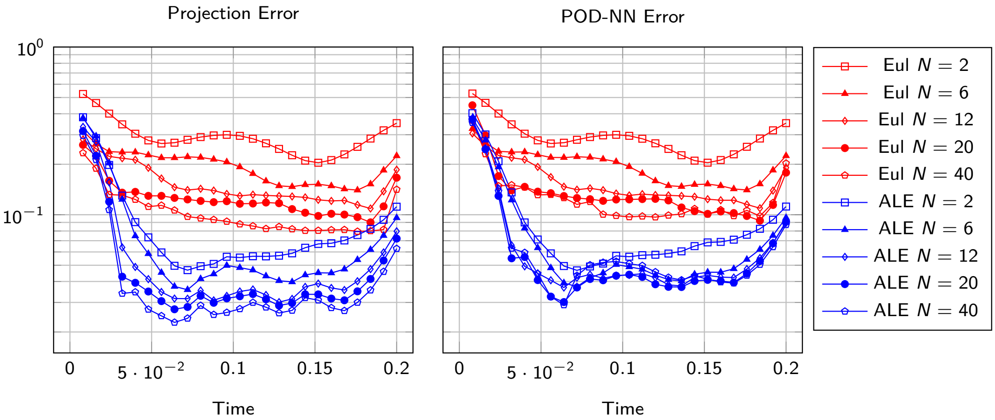


Figure: DMR parametric: Error in time of reduced methods with different number N of modes. Parameter in test set $\beta = 0.675$

Triple point (non parametric)

Problem setting

$\Omega = [0,7] \times [0,3]$

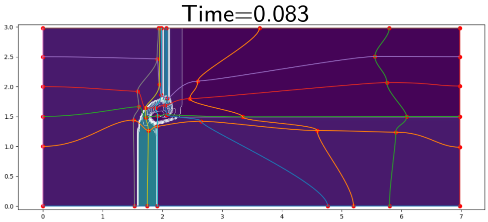
$W = [0,1] \times [0,3]$, $NE = [1,7] \times [1.5,3]$,

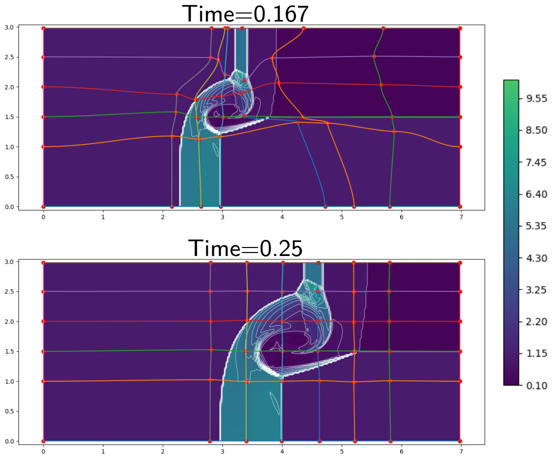
$SE = [1,7] \times [0,1.5]$,

$(\rho_W, u_W, v_W, p_W) = (1, 20, 0, 1)$, $\boldsymbol{x} \in W$,

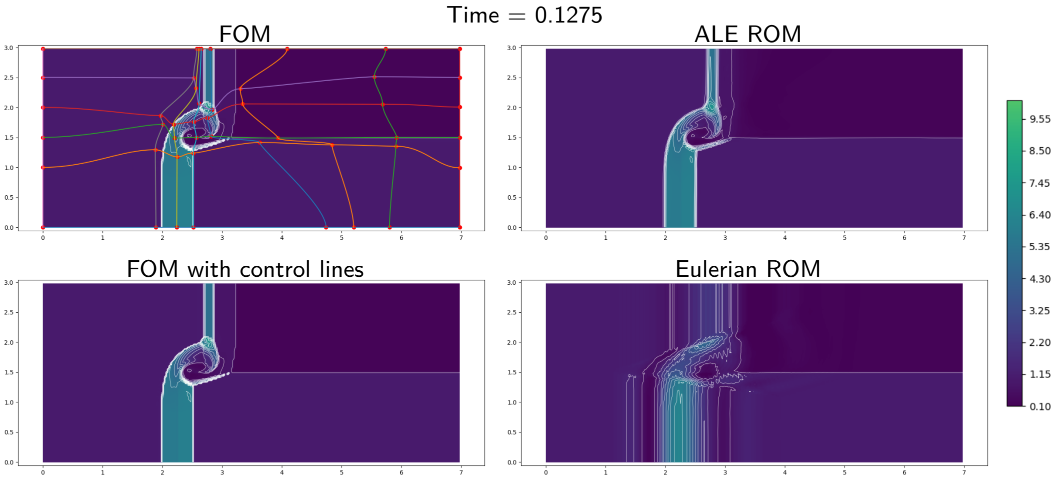
$(\rho_{NE}, u_{NE}, v_{NE}, p_{NE}) = (0.125, 0, 0, 0.1)$, $\boldsymbol{x} \in NE$,

$(\rho_{SE}, u_{SE}, v_{SE}, p_{SE}) = (1, 0, 0, 0.1)$, $\boldsymbol{x} \in SE$.





Triple Point Non-parametric: Simulations $N_{RB} = 7$



Triple Point Non-parametric: Simulations $N_{RB} = 7$

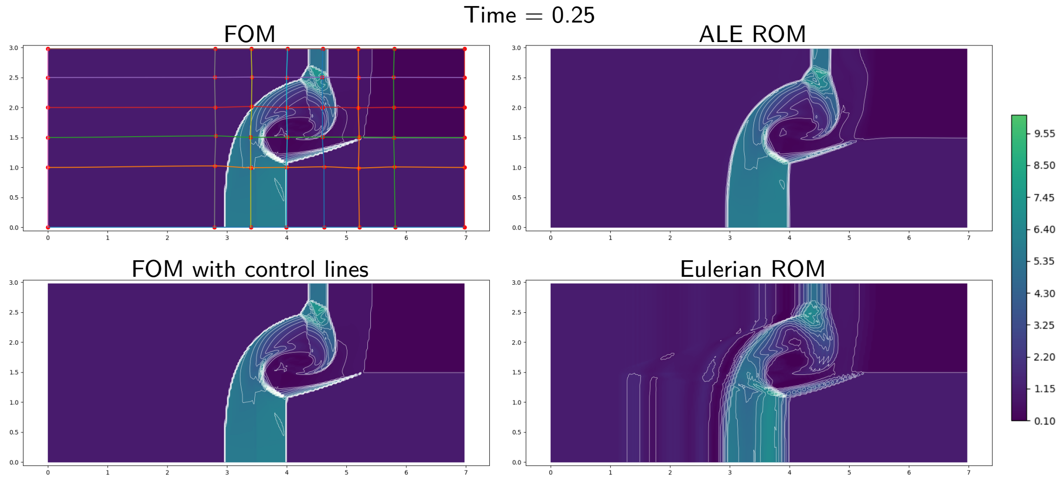


Table of contents

Extensions and limitations

Limitations

- Beginning of the simulation still tricky (singularity not handled)
- Chaotic simulations
- Extrapolatory regime
- Delicate optimization

Extensions

- ALE online solver
- Local ROM for different regimes
- Comparison with completely nonlinear ROMs

Extensions and limitations

Limitations

- Beginning of the simulation still tricky (singularity not handled)
- Chaotic simulations
- Extrapolatory regime
- Delicate optimization

Extensions

- ALE online solver
- Local ROM for different regimes
- Comparison with completely nonlinear ROMs

Thanks for the attention!

Graph Neural Network on vanishing viscosity solutions arxiv:2308.03378

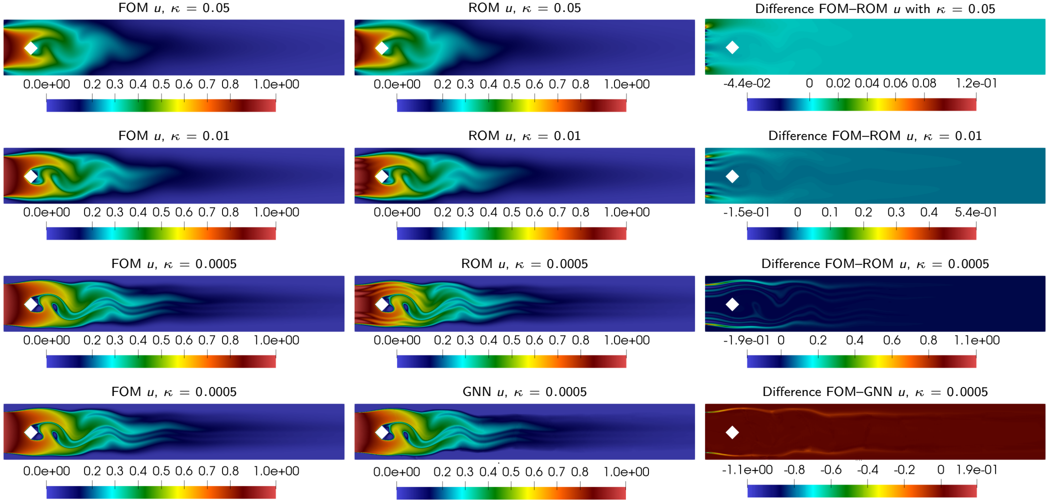


Figure: **VV.** Scalar concentration advected by incompressible flow for $i = 99$. Comparison of ROM approach at different viscosity levels $\kappa \in \{0.05, 0.01, 0.0005\}$ and GNN for $\kappa = 0.0005$.

Residual Distribution

- High order
- FE based
- Compact stencil
- Explicit
- Can recast some other FV, FE, FD, DG schemes [1]

[1] R. Abgrall. Computational Methods in Applied Mathematics, 2018

Residual Distribution

- High order
- FE based
- Compact stencil
- Explicit
- Can recast some other FV, FE, FD, DG schemes [1]

$$\partial_t U + \nabla \cdot F(U) = 0 \tag{1}$$

$$V_h = \{U \in L^2(\Omega_h, \mathbb{R}^D) \cap \mathcal{C}^0(\Omega_h),\ U|_K \in \mathbb{P}^k,\ \forall K \in \Omega_h\}. \tag{2}$$

$$U_h = \sum_{\sigma \in D_{\mathcal{N}}} U_\sigma \varphi_\sigma = \sum_{K \in \Omega_h} \sum_{\sigma \in K} U_\sigma \varphi_\sigma|_K \tag{3}$$

[1] R. Abgrall. Computational Methods in Applied Mathematics, 2018

Residual Distribution - Spatial Discretization

1. Define $\forall K \in \Omega_h$ a fluctuation term (total residual) $\phi^K = \int_K \nabla \cdot F(U) dx$
2. Define a nodal residual $\phi^K_\sigma \ \forall \sigma \in K$:

$$\phi^K = \sum_{\sigma \in K} \phi^K_\sigma, \quad \forall K \in \Omega_h. \tag{4}$$

3. The resulting scheme is

$$U^{n+1}_\sigma - U^n_\sigma + \Delta t \sum_{K|\sigma \in K} \phi^K_\sigma = 0, \quad \forall \sigma \in D_{\mathcal{N}}. \tag{5}$$

Residual Distribution

- High order
- Easy to code
- FE based
- Compact stencil
- No need of Riemann solver
- No need of conservative variables
- Can recast some other FV, FE schemes

Residual Distribution

- High order
- Easy to code
- FE based
- Compact stencil
- No need of Riemann solver
- No need of conservative variables
- Can recast some other FV, FE schemes

$$\partial_t U + \nabla \cdot A(U) = S(U) \tag{6}$$

$$V_h = \{U \in L^2(\Omega_h, \mathbb{R}^D) \cap \mathcal{C}^0(\Omega_h),\ U|_K \in \mathbb{P}^k,\ \forall K \in \Omega_h\}. \tag{7}$$

$$U_h = \sum_{\sigma \in D_{\mathcal{N}}} U_\sigma \varphi_\sigma = \sum_{K \in \Omega_h} \sum_{\sigma \in K} U_\sigma \varphi_\sigma|_K \tag{8}$$

Residual Distribution - Spatial Discretization

Focus on steady case.

1. Define $\forall K \in \Omega_h$ a fluctuation term (total residual) $\phi^K = \int_K \nabla \cdot A(U) - S(U) dx$
2. Define a nodal residual ϕ^K_σ $\forall \sigma \in K$:

$$\phi^K = \sum_{\sigma \in K} \phi^K_\sigma, \quad \forall K \in \Omega_h. \tag{9}$$

   Often done assigning $\phi^K_\sigma = \beta^K_\sigma \phi^K$, where must hold that

$$\sum_{\sigma \in K} \beta^K_\sigma = \mathrm{Id}. \tag{10}$$

3. The resulting scheme is

$$\sum_{K|\sigma \in K} \phi^K_\sigma = 0, \quad \forall \sigma \in D_{\mathcal{N}}. \tag{11}$$

   This will be called residual distribution scheme.

Residual distribution - Choice of the scheme

How to split total residuals into nodal residuals $\Rightarrow$ choice of the scheme.

$$\begin{aligned}
\phi_\sigma^{K,LxF}(U_h) &= \int_K \varphi_\sigma \left(\nabla \cdot A(U_h) - S(U_h)\right) dx + \alpha_K (U_\sigma - \overline{U}_h^K),\\
\overline{U}_h^K &= \int_K U_h, \quad \alpha_K = \max_{e \text{ edge } \in K} \left(\rho_S\left(\nabla A(U_h)\cdot \mathbf{n}_e\right)\right),\\
\beta_\sigma^K(U_h) &= \max\left(\frac{\Phi_\sigma^{K,LxF}}{\Phi^K}, 0\right)\left(\sum_{j\in K} \max\left(\frac{\Phi_j^{K,LxF}}{\Phi^K}, 0\right)\right)^{-1},\\
\phi_\sigma^{*,K} &= (1-\Theta)\beta_\sigma^K \phi_\sigma^K + \Theta \Phi_\sigma^{K,LxF}, \quad \Theta = \frac{|\Phi^K|}{\sum_{j\in K}\left|\Phi_j^{K,LxF}\right|},\\
\phi_\sigma^K &= \beta_\sigma^K \phi_\sigma^{*,K} + \sum_{e|\text{edge of } K} \theta h_e^2 \int_e [\nabla U_h]\cdot[\nabla \varphi_\sigma] d\Gamma.
\end{aligned} \tag{12}$$

Error estimator

Additional hypothesis:

- $Id + \Delta t \mathcal{L}$ is Liptschitz continuous with constant $C > 0$,
- There are N'_{EIM} extra functions and functionals that capture the evolution of the solutions. (experimentally not so strict),
- Initial conditions are exactly represented in the reduced basis RB.

Total error estimator:

- EIM error, estimated by other N'_{EIM} basis functions f and functional τ iterating the EIM procedure after the stop, cost $\mathcal{O}(N'_{EIM})$,
- RB error given by the Lipschitz constant times residual of the small system,
- additionally one can add the projection error of the initial condition when not in RB.

Empirical interpolation method (EIM)

INPUT: $\mathcal{L}^n(U^n, \boldsymbol{\mu}, t^n)$, for $\boldsymbol{\mu} \in \mathcal{P}_h$, $n \leq N_t$

OUTPUT: $EIM = (\tau_k, f_k)_{k=1}^{N_{EIM}}$ where functions $f_k \in \mathbb{R}^{\mathcal{N}}$ and $\tau_k \in (\mathbb{R}^{\mathcal{N}})'$ (Examples of τ_k are point evaluations)

- Greedy iterative procedure
- At each step chooses the worst approximated function via an error estimator $\mathcal{L}^{worst} = \arg\max_{\mathcal{L}} ||\mathcal{L} - \sum_{k=1}^{N_{EIM}} \tau_k(\mathcal{L}) f_k||$
- Maximise the functional τ on the function $\mathcal{L}^{worst}$ $\tau^{chosen} = \arg\max_{\tau} |\tau(\mathcal{L}^{worst})|$
- $EIM = EIM \cup (\tau^{chosen}, \mathcal{L}^{worst})$
- Stop when error is smaller than a tolerance

Proper orthogonal decomposition (POD)

INPUT: Collection of functions $\{f_j\}_{j=1}^N$

OUTPUT: Reduced basis spaces $RB = \underset{U | dim(U)=N_{POD}}{\arg\min} \sum_{j=1}^N ||f_j - \mathcal{P}_U(f_j)||_2$

- Based on SVD
- Prescribed tolerance to stop the algorithm
- Global optimizer of the problem

Greedy algorithm

INPUT: Collection of functions $\{f_j\}_{j=1}^N$

OUTPUT: Reduced basis space RB

- There is an error estimator (normally cheap) $\varepsilon_{RB}(f) \sim ||f - \mathcal{P}_{RB}(f)||$
- Iteratively choose the worst represented function $f^{worst} = \arg\max_f \varepsilon_{RB}(f)$
- Add f^{worst} to the RB space
- Stop up to a certain tolerance

MOR: Ingredients

- Discretized solution $u_{\mathcal{N}}(\cdot, t, \boldsymbol{\mu}) \in \mathbb{V}_{\mathcal{N}}$ for $t \in \mathbb{R}^+$, $\boldsymbol{\mu} \in \mathcal{P}$
- Solution manifold: $\mathcal{S} := \{u_{\mathcal{N}}(\cdot, t, \boldsymbol{\mu}) \in \mathbb{V}_{\mathcal{N}} : t \in \mathbb{R}^+, \boldsymbol{\mu} \in \mathcal{P}\}$
- Ansatz:

$$\mathcal{S} \approx \mathbb{V}_{N_{RB}} \subset \mathbb{V}_{\mathcal{N}}, \qquad N_{RB} \ll \mathcal{N} \tag{13}$$

- Example: diffusion equation $u_t + \mu u_{xx} = 0$ with $u_0 = \sin(x\pi)$

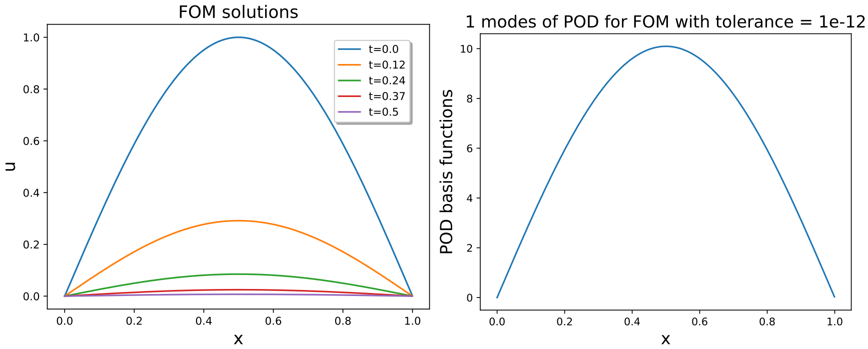


Figure: POD on a diffusion problem

MOR: Ingredients

Problem:

$$U^{n+1}(\boldsymbol{\mu}) - U^n(\boldsymbol{\mu}) + \mathcal{L}^n(U^n, \boldsymbol{\mu}) = 0, \quad U^n, U^{n+1} \in \mathbb{V}_{\mathcal{N}} \tag{14}$$

Objective:

$$\sum_{i=1}^{N_{RB}} \mathrm{u}_i^{n+1}(\boldsymbol{\mu})\psi_{RB}^i - \mathrm{u}_i^n(\boldsymbol{\mu})\psi_{RB}^i + \sum_{i=1}^{N_{RB}} \mathrm{L}^i(\mathrm{u}^n, \boldsymbol{\mu})\psi_{RB}^i = 0, \qquad \psi_{RB}^i \in \mathbb{V}_{\mathcal{N}}, \mathrm{u}^n, \mathrm{u}^{n+1} \in \mathbb{V}_{N_{RB}} \tag{15}$$

- EIM $\Rightarrow$ non–linear fluxes and scheme $\mathrm{L}^i(\mathrm{u}^n, \boldsymbol{\mu})$
- POD $\Rightarrow$ create the RB space and span the time evolution
- Greedy $\Rightarrow$ span the parameter space

Proper orthogonal decomposition (POD)

POD

INPUT:

- Collection of functions $\{f_j\}_{j=1}^N$

OUTPUT:

- Reduced basis spaces $\mathbb{V}_{N_{RB}} = \underset{U|dim(U)=N_{POD}}{\arg\min} \sum_{j=1}^N ||f_j - \mathcal{P}_U(f_j)||_2$

ALGORITHM:

- Based on SVD of matrix $\{f_j\}_{j=1}^N$
- We obtain (ordered) singular values and vectors
- Retain most energetic (largest singular value)
- Prescribed tolerance to stop the algorithm or maximum number of basis
- Related singular vectors gives $\mathbb{V}_{N_{RB}}$
- Global optimizer of the problem

Greedy algorithm

INPUT:

- Collection of functions $\{f_j\}_{j=1}^N$
- Cheap error estimator $\varepsilon_{RB}(f) \sim ||f - \mathcal{P}_{RB}(f)||$

OUTPUT:

- Reduced basis space $\mathbb{V}_{N_{RB}}$

ALGORITHM:

- Iteratively choose the worst represented function $f^{worst} = \arg\max_f \varepsilon_{RB}(f)$
- Add f^{worst} to the $\mathbb{V}_{N_{RB}}$ space
- Stop up to a certain tolerance
- Not globally optimal, but locally optimal at each iteration (Greedy)

Empirical interpolation method (EIM)

INPUT:

- $\mathcal{L}^n(U^n, \boldsymbol{\mu}, t^n)$, for $\boldsymbol{\mu} \in \mathcal{P}_h$, $n \leq N_t$

OUTPUT:

- $EIM = (\tau_k, f_k)_{k=1}^{N_{EIM}}$ where functions $f_k \in \mathbb{R}^{\mathcal{N}}$ and $\tau_k \in (\mathbb{R}^{\mathcal{N}})'$
  (τ_k, f_k) are often called magic points and functions, where τ_k are function evaluations

ALGORITHM:

- Greedy iterative procedure
- At each step chooses the worst approximated function via an error (estimator)
  $\mathcal{L}^{worst} = \arg\max_{\mathcal{L}} ||\mathcal{L} - \sum_{k=1}^{N_{EIM}} \tau_k(\mathcal{L}) f_k||$
- Maximise the functional τ on the function $\mathcal{L}^{worst}$ $\tau^{chosen} = \arg\max_{\tau} |\tau(\mathcal{L}^{worst})|$
- $EIM = EIM \cup (\tau^{chosen}, \mathcal{L}^{worst})$
- Stop when error is smaller than a tolerance

Offline Algorithm: PODEIM–Greedy [2]

PODEIM–Greedy

INITIALIZATION:

- EIM on $\mathcal{L}(U^n, \boldsymbol{\mu}_0, t^n)$ for $n \leq N_t$
- $\mathbb{V}_{N_{RB}} = POD(\{U^n(\boldsymbol{\mu}_0)\}_{n=0}^{N_t})$

ITERATION:

- Greedy algorithm spanning over the parameter space $\mathcal{P}_h$, with an error indicator $\varepsilon(\mathbf{U}(\boldsymbol{\mu}))$ where $\mathbf{U}(\boldsymbol{\mu}) \in \mathbb{R}^N \times \mathbb{R}^+$
- Choose worst parameter as $\boldsymbol{\mu}^* = \arg\max_{\boldsymbol{\mu} \in \mathcal{P}_h} \varepsilon(\mathbf{U}(\boldsymbol{\mu}))$
- Apply POD on time evolution of selected solution $POD_{add} = POD\left(\{U^n(\boldsymbol{\mu}^*)\}_{n=1}^{N_t}\right)$
- Update the $\mathbb{V}_{N_{RB}}$ with $\mathbb{V}_{N_{RB}} = POD\left(\mathbb{V}_{N_{RB}} \cup POD_{add}\right)$
- Update EIM basis function with $EIM_{space} = EIM_{space} \cup EIM(\{\mathcal{L}(U^n, \boldsymbol{\mu}^*, t^n)\}_{n=0}^{N_t})$

[2] B. Haasdonk and M. Ohlberger, in Hyperbolic problems: theory, numerics and applications, vol. 67, Amer. Math. Soc., 2009.

Online algorithm: PODEIM–Greedy

Reduced Order Model system

Solve the smaller system:

$$\sum_{i=1}^{N_{RB}} (\mathrm{u}_i^{n+1}(\boldsymbol{\mu}) - \mathrm{u}_i^{n}(\boldsymbol{\mu}))\psi_{RB}^i + \sum_{i=1}^{N_{RB}} \sum_{j=1}^{N_{EIM}} \tau_j(\mathcal{L}(U^n,\boldsymbol{\mu}))\Pi_{RB,i}(f_j)\psi_{RB}^i = 0$$

- $\Pi_{RB,i}(f_j)$ are the projection on $\mathbb{V}_{N_{RB}}$ of the EIM functions: offline
- $\tau_j(\mathcal{L}(U^n,\boldsymbol{\mu}))$ are inexpensive to compute, but depend on the method (for RD $\approx \mathcal{O}(d)$)
- MOR cost $\mathcal{O}(N_t N_{RB} N_{EIM})$ vs FOM cost $\mathcal{O}(N_t \mathcal{N})$
- Gain if $N_{RB}, N_{EIM} \ll \mathcal{N}$
- Error estimator

Learning of θ

Calibration map

- $\theta(\mu)$ tells us where a feature is (maximum point, steepest gradient)
- How to choose it? (second part)
- How to learn the map? (Offline we want to know the map in advance)
- Offline: optimization of θs on a training sample
- Generation of a regression map $\widehat{\theta}$

Piecewise linear regression for every timestep t^n

- If parameter domain is a grid $\Rightarrow$ Easy, fast
- Non–structured parameter domain $\Rightarrow$ Different algorithms, may be costly
- Precise if $|\mathcal{P}_h| \sim s^P$ with s big enough
- May not catch the nonlinear behavior and produce unreasonable results

Learning of θ

Calibration map

- $\theta(\mu)$ tells us where a feature is (maximum point, steepest gradient)
- How to choose it? (second part)
- How to learn the map? (Offline we want to know the map in advance)
- Offline: optimization of θs on a training sample
- Generation of a regression map $\widehat{\theta}$

Polynomial regression

- Hyperparameter p
- Risk of overfitting
- Can easily catch the nonlinear (polynomial) behavior
- Number of coefficients grows exponentially with p

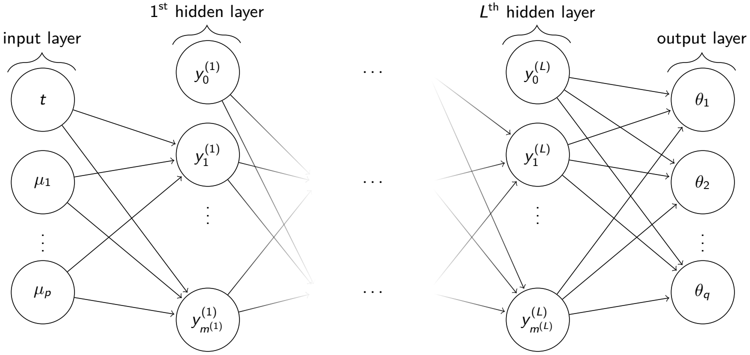
$$\theta(\boldsymbol{\mu}, t) \approx \sum_{|\alpha| \leq p} \beta_\alpha \boldsymbol{t}^{\gamma_0} \prod_{i=1}^{p} \mu_i^{\gamma_i}$$

Learning of θ

Neural networks

- Why? Naturally nonlinear, we may not have a structured dictionary
- Which one? Multi-layer-perceptron, N layers ($[4, 10]$), M_n nodes ($[6, 20]$)

Multilayer perceptron



Travelling wave, time evolution solution

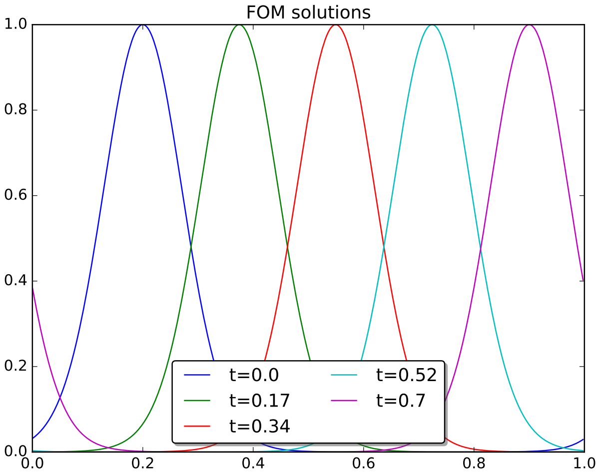


Figure: Solution of advection equation $\partial_t u + \partial_x u = 0$ with gaussian IC

Travelling wave, POD

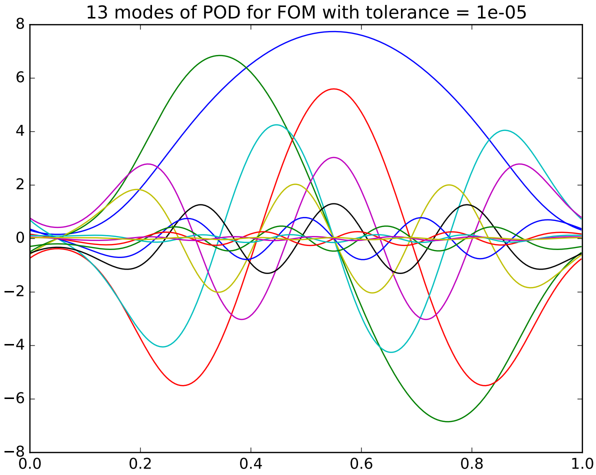


Figure: Solution of advection equation with wave IC

Travelling shock, time evolution solution, little diffusion

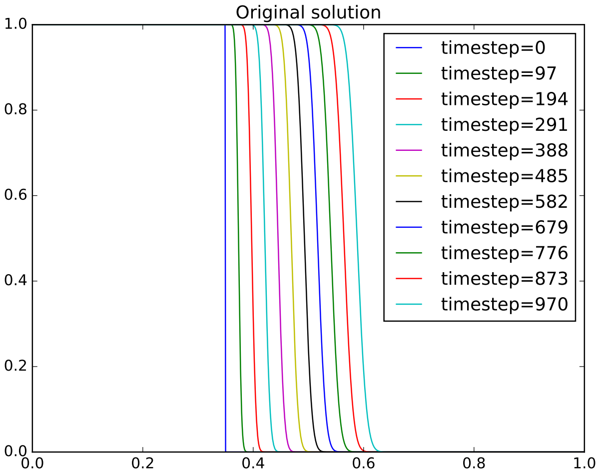


Figure: Solution of advection equation with shock IC

Travelling shock, POD, little diffusion

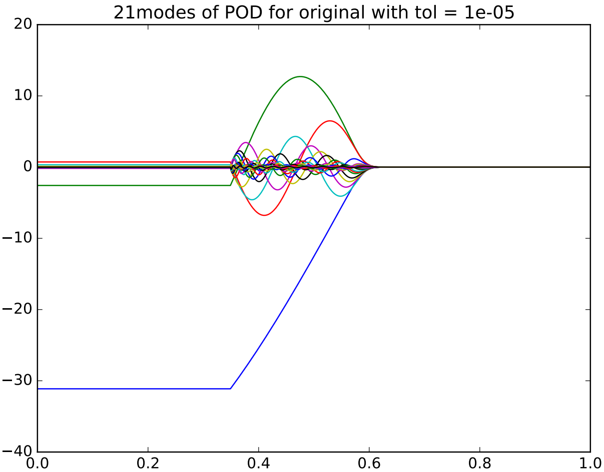


Figure: POD of time evolution of advection equation with shock IC

Travelling shock, time evolution solution, no diffusion

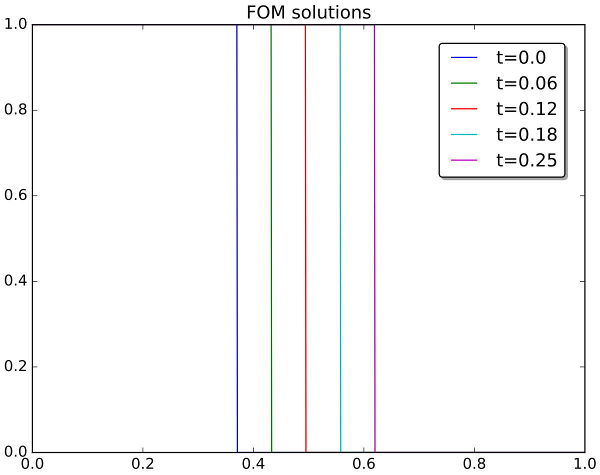


Figure: Solution of advection equation with shock IC

Travelling shock, POD, no diffusion

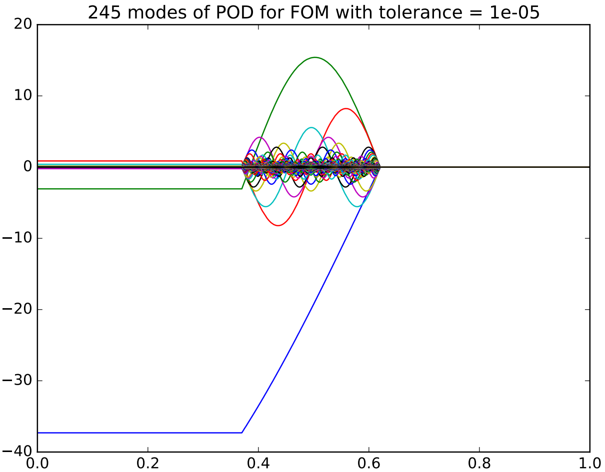


Figure: POD of time evolution of advection equation with shock IC

Common problems and properties

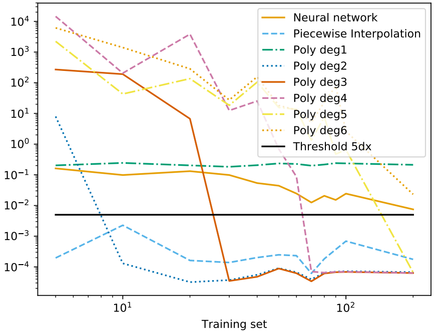
- As many basis functions as positions of the shock
- Slow decay of Kolmogorov N–width

$$d_N(\mathcal{S}, \mathbb{V}) := \inf_{\mathbb{V}_N \subset \mathbb{V}} \sup_{f \in \mathcal{S}} \inf_{g \in \mathbb{V}_N} ||f - g||$$

- Non linear dependency leads to big EIM and RB space
- 1/2 parameters problem (highly non linear dependence on parameters)

Advection: traveling wave

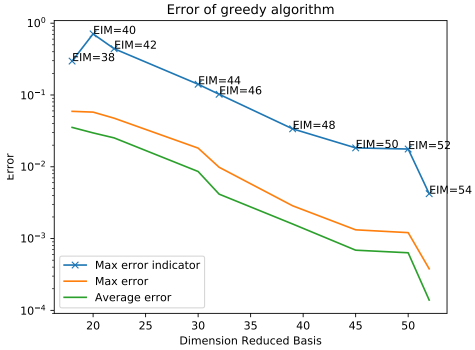
$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration	With calibration: Regressions
	

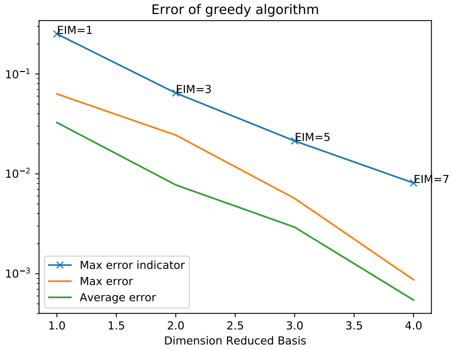
Advection: traveling wave

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration

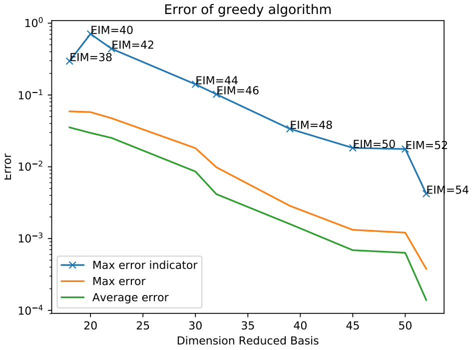
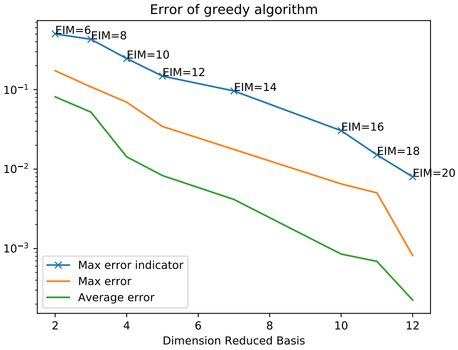


With calibration: Poly2



Advection: traveling wave

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration	With calibration: ANN
	

Advection: traveling wave

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration		With calibration: Poly2	
RB dim	52	RB dim	4
EIM dim	54	EIM dim	7
FOM time	191 s	FOM time	516 s
RB time	24 s	RB time	18 s
RB/FOM time	12%	RB/FOM time	3%

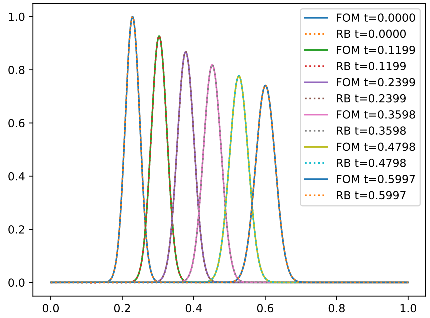
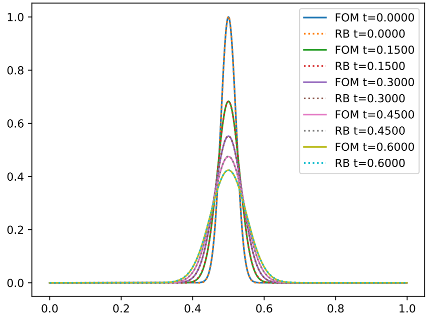
Advection: traveling wave

$$\begin{cases} u_t + \mu_0 u_x = 0,\ D = [0,1],\ T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration		With calibration: ANN	
RB dim	52	RB dim	12
EIM dim	54	EIM dim	20
FOM time	191 s	FOM time	516 s
RB time	24 s	RB time	38 s
RB/FOM time	12%	RB/FOM time	7%

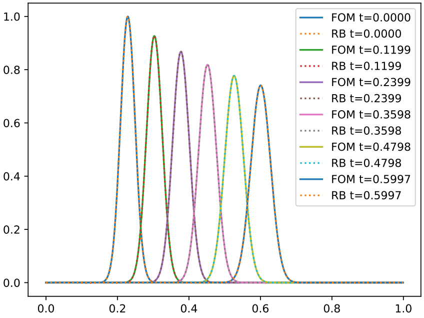
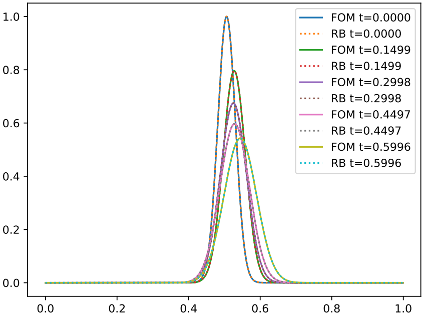
Advection: traveling wave

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration	With calibration: Poly2
	

Advection: traveling wave

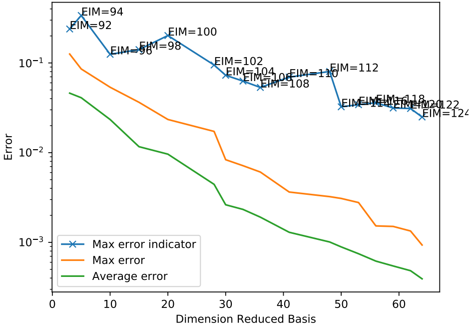
$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = e^{-\mu_1 (x-\mu_2)^2} \\ \mu_0 \sim \mathcal{U}([0,2]), \mu_1 \sim \mathcal{U}([500,1500]), \mu_2 \sim \mathcal{U}([0.1,0.3]) \end{cases}$$

Without calibration	With calibration: ANN
	

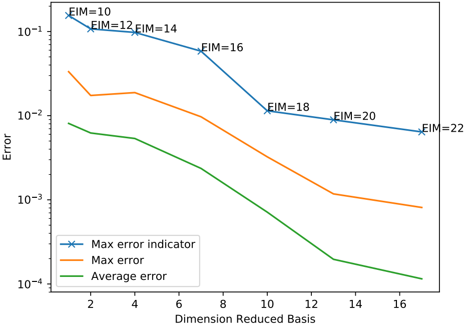
Advection: traveling shock

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 1.5, \text{ Dirichlet BC} \\ u_0(x, \boldsymbol{\mu}) = \begin{cases} \mu_1 & \text{if } x < 0.35 + 0.05\mu_2 \\ 0 & \text{else} \end{cases} \\ \mu_0 \sim \mathcal{U}([0,2]), \; \mu_1, \mu_2 \sim \mathcal{U}([-1,1]) \end{cases}$$

Without calibration



With calibration: Poly2



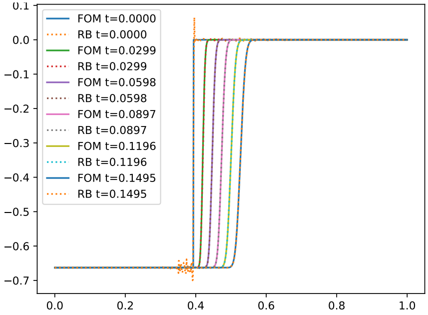
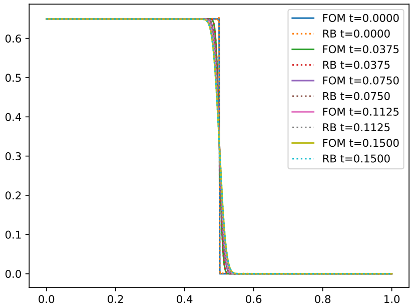
Advection: traveling shock

$$
\begin{cases}
u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 1.5, \text{ Dirichlet BC} \\
u_0(x, \boldsymbol{\mu}) = \begin{cases} \mu_1 & \text{if } x < 0.35 + 0.05\mu_2 \\ 0 & \text{else} \end{cases} \\
\mu_0 \sim \mathcal{U}([0,2]), \; \mu_1, \mu_2 \sim \mathcal{U}([-1,1])
\end{cases}
$$

Without calibration		With calibration: Poly2	
RB dim	64	RB dim	17
EIM dim	124	EIM dim	22
FOM time	49 s	FOM time	125 s
RB time	9 s	RB time	6 s
RB/FOM time	18%	RB/FOM time	5%

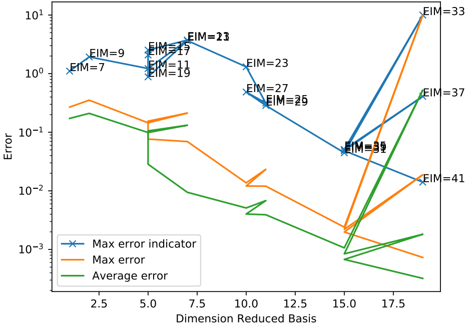
Advection: traveling shock

$$\begin{cases} u_t + \mu_0 u_x = 0, \; D = [0,1], \; T_{max} = 1.5, \text{ Dirichlet BC} \\ u_0(x, \boldsymbol{\mu}) = \begin{cases} \mu_1 & \text{if } x < 0.35 + 0.05\mu_2 \\ 0 & \text{else} \end{cases} \\ \mu_0 \sim \mathcal{U}([0,2]), \; \mu_1, \mu_2 \sim \mathcal{U}([-1,1]) \end{cases}$$

Without calibration	With calibration: Poly2
	

Burgers sine

$$
\begin{cases}
u_t + \mu_0(u^2/2)_x = 0,\ D = [0,\pi],\ T_{max} = 0.15, \text{ periodic BC}\\
u_0(x,\boldsymbol{\mu}) = |\sin(x+\mu_1)| + 0.1\\
\mu_0 \sim \mathcal{U}([0,2]),\ \mu_1 \sim \mathcal{U}([0,\pi])
\end{cases}
$$

Without calibration	With calibration: Poly3
	

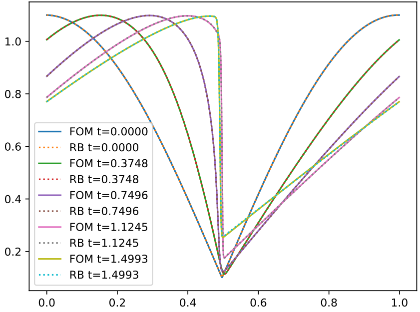
Burgers sine

$$\begin{cases} u_t + \mu_0(u^2/2)_x = 0, \; D = [0,\pi], \; T_{max} = 0.15, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = |\sin(x+\mu_1)| + 0.1 \\ \mu_0 \sim \mathcal{U}([0,2]), \; \mu_1 \sim \mathcal{U}([0,\pi]) \end{cases}$$

Without calibration		With calibration: Poly3	
RB dim	failed	RB dim	19
EIM dim	>600	EIM dim	41
FOM time	167 s	FOM time	444 s
RB time	∞	RB time	53 s
RB/FOM time	∞	RB/FOM time	11%

Burgers sine

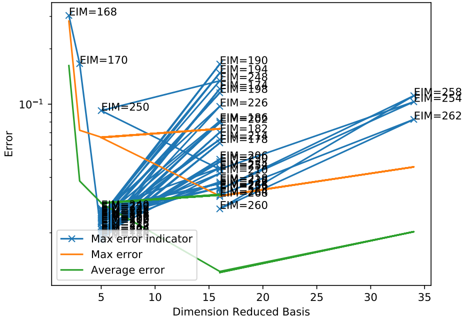
$$\begin{cases} u_t + \mu_0 (u^2/2)_x = 0, \ D = [0,\pi], \ T_{max} = 0.15, \text{ periodic BC} \\ u_0(x, \boldsymbol{\mu}) = |\sin(x+\mu_1)| + 0.1 \\ \mu_0 \sim \mathcal{U}([0,2]), \ \mu_1 \sim \mathcal{U}([0,\pi]) \end{cases}$$

Without calibration	With calibration: Poly3
	

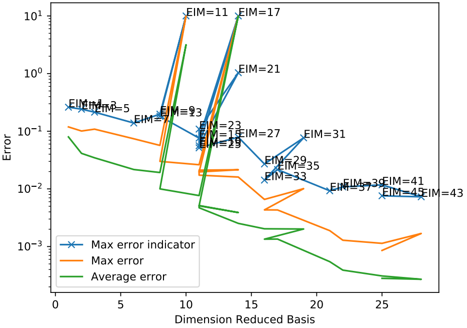
Buckley-Leverett equation

$$
\begin{cases}
\partial_t u + \partial_x \dfrac{u^2}{u^2 + \mu_0(1-u^2)} = 0, \; D = [0,1], \; T_{max} = 0.25, \; \text{periodic BC}\\
u_0(x,\boldsymbol{\mu}) = 0.5 + 0.2\mu_1 + 0.3\mu_1 \sin(2\pi(x-\mu_1-0.5))\\
\mu_0 \sim \mathcal{U}([0.001,2]), \; \mu_1 \sim \mathcal{U}([0.1,1])
\end{cases}
$$

Without calibration



With calibration: pwL



Buckley-Leverett equation

$$\begin{cases} \partial_t u + \partial_x \dfrac{u^2}{u^2+\mu_0(1-u^2)} = 0, \; D=[0,1], \; T_{max} = 0.25, \text{ periodic BC} \\ u_0(x,\boldsymbol{\mu}) = 0.5 + 0.2\mu_1 + 0.3\mu_1 \sin(2\pi(x-\mu_1-0.5)) \\ \mu_0 \sim \mathcal{U}([0.001, 2]), \; \mu_1 \sim \mathcal{U}([0.1,1]) \end{cases}$$

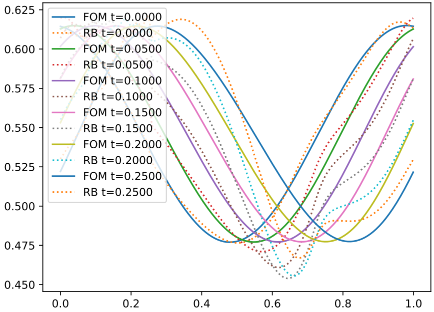
Without calibration[3]		With calibration: pwL	
RB dim	16	RB dim	25
EIM dim	270	EIM dim	45
FOM time	190 s	FOM time	462 s
RB time	69 s	RB time	79 s
RB/FOM time	36%	RB/FOM time	17%

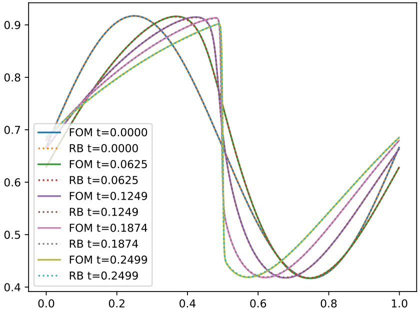
[3] It does not reach the requested tolerance 10^{-3}

Buckley-Leverett equation

$$
\begin{cases}
\partial_t u + \partial_x \dfrac{u^2}{u^2+\mu_0(1-u^2)} = 0, \; D=[0,1], \; T_{max} = 0.25, \text{ periodic BC}\\
u_0(x,\boldsymbol{\mu}) = 0.5 + 0.2\mu_1 + 0.3\mu_1 \sin(2\pi(x-\mu_1-0.5))\\
\mu_0 \sim \mathcal{U}([0.001,2]), \; \mu_1 \sim \mathcal{U}([0.1,1])
\end{cases}
$$

Without calibration	With calibration: pwL





Augmenting diffusion and ROMs

Problem: Advection diffusion.
Parameter: inlet channel width

Advection field data: given by Navier-Stokes simulation.
Discretization: DG

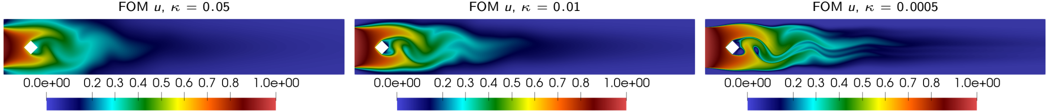


Figure: **VV.** Scalar concentration advected by incompressible flow for $i = 99$ at different viscosity levels $\kappa \in \{0.05, 0.01, 0.0005\}$

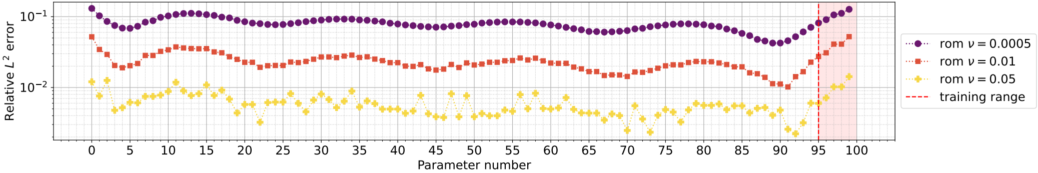


Figure: Relative errors of ROMs for different viscosities. Training correspond to the abscissae $0, 5, 10, \dots, 95$, the rest are test parameters. The dashed red background highlights the extrapolation range. The reduced dimensions of the ROMs are $\{N_{RB\Omega_i}\}_{i=1}^{K} = [5, 5, 5, 5]$ with $K = 4$ partitions.

Graph neural network architecture

Viscosity

- **Vanishing viscosity** guarantees the convergence towards physically relevant solution
- Viscosity can be **artificial** or physically modeled
- Higher viscosity can come from **coarser** grids
- **High viscosity** solutions do not suffer from slow decay of Kolomogorov n-width

Main idea

- Use classical ROM for high viscosity
- **Learn** with NN the vanishing viscosity limit

Architecture

Inputs

- **Local** data of reduced solutions from higher viscosity levels (cheap to compute) (solution, its gradient)
- Mesh connectivity (all)

Output

- "Vanishing" viscosity solution

Supervised learning

- Training data: ROMs for high viscosities, FOM for vanishing viscosity

Layers: arxiv:2308.03378

Training time: 1h

Results GNN

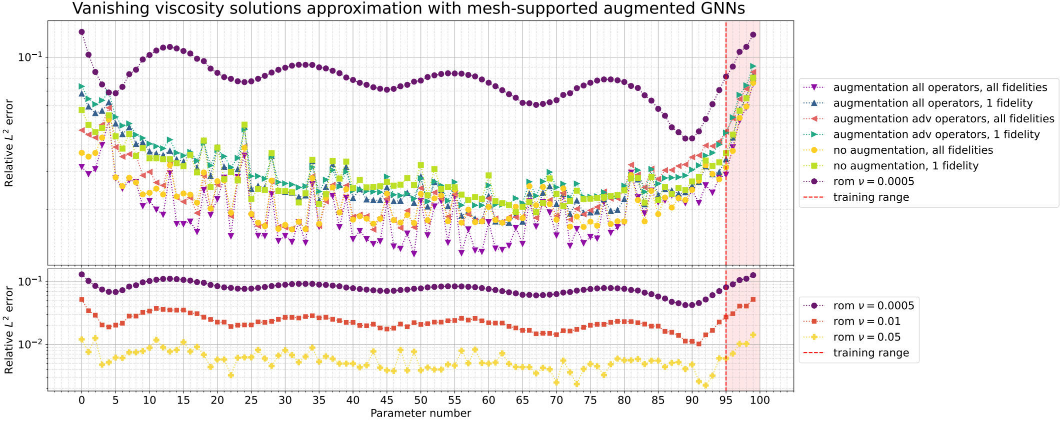


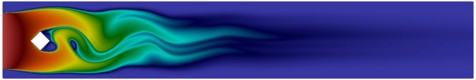
Figure: Relative errors for the scalar conservation advected by incompressible flow problem. **Top:** errors with different GNN approaches given by the three augmentation $\mathcal{O}_1$, $\mathcal{O}_2$ and $\mathcal{O}_3$ and by using either 1 viscosity level (1 fidelity) or 2 (all fidelities) and errors for DD-ROM with the same viscosity level $\nu = 0.0005$. **Bottom:** errors for ROM approaches at different viscosity levels. The reduced dimensions of the ROMs are $\{N_{RB\Omega_i}\}_{i=1}^{K} = [5, 5, 5, 5]$ with $K = 4$ partitions.

Results GNN

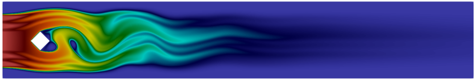
	FOM		ROM			
κ	N_h	time	$N_{RB\,i}$	time	speedup	mean L^2 error
0.05	43776	3.243 [s]	[5, 5, 5, 5]	59.912 [μs]	54129	0.00595
0.01	43776	3.236 [s]	[5, 5, 5, 5]	79.798 [μs]	40552	0.0235
0.0005	175104	9.668 [s]	[5, 5, 5, 5]	95.844 [μs]	100872	0.0796

κ	GNN training time	Single forward GNN online time	Average online time	GNN speedup	mean L^2 error
0.0005	$\leq$ 60 [min]	2.661 [s]	0.172 [s]	$\sim$ 56	0.0217

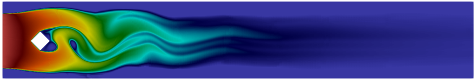
FOM u, $\kappa = 0.0005$



ROM u, $\kappa = 0.0005$



GNN u, $\kappa = 0.0005$



GNN architecture

Table: Mesh supported augmented GNN

Net	Weights $[f_{\text{inp}}, f_{\text{out}}]$	Aggregation	Activation
Input NNConv	$[3n_{\text{aug}}, 18]$	Avg_1	ReLU
SAGEconv	[18, 21]	Avg_2	ReLU
SAGEconv	[21, 24]	Avg_2	ReLU
SAGEconv	[24, 27]	Avg_2	ReLU
SAGEconv	[27, 30]	Avg_2	ReLU
Output NNConv	[30, 1]	Avg_1	-

NNConvFilters	First Layer $[2, l]$	Activation	Second Layer $[l, f_{\text{inp}} f_{\text{out}}]$
Input NNConv	[2, 12]	ReLU	$[12, 3n_{\text{aug}} \cdot 18]$
Output NNConv	[2, 8]	ReLU	[8, 30]

Arbitrary Lagrangian–Eulerian formulation

ALE formulation

$$\frac{\partial}{\partial t} v(y, \boldsymbol{\mu}, t) + \frac{dy}{dx}\frac{d}{dy} F(v, \mu) - \frac{dy}{dx}\frac{dv}{dy}\frac{\partial T}{\partial t} = 0$$

With ALE formulation we can apply the EIM procedure with points on the reference domain $\mathcal{R}$.

What does it imply?

- We must know $T(\theta(t, \boldsymbol{\mu}), y)$
  - Offline phase: detect some interesting points (maxima, steepest gradient) (second part)
  - Offline phase: optimize the transformation in some sense (T. Taddei, Ohlberger et al.) (second part)
  - Online phase: predict the value of the transformation. Regression (polynomials, ANN), projections (first part)
- Compute the Jacobian of the transformation $\frac{dy}{dx}$ and the new flux $\frac{dv}{dy}$ $\Rightarrow$ increasing computational costs also in online phase

Arbitrary Lagrangian–Eulerian formulation

ALE formulation

$$\frac{\partial}{\partial t} v(y, \boldsymbol{\mu}, t) + \frac{dy}{dx} \frac{d}{dy} F(v, \mu) - \frac{dy}{dx} \frac{dv}{dy} \frac{\partial T}{\partial t} = 0$$

With ALE formulation we can apply the EIM procedure with points on the reference domain $\mathcal{R}$.

What does it imply?

- We must know $T(\theta(t, \boldsymbol{\mu}), y)$
  - Offline phase: detect some interesting points (maxima, steepest gradient) (second part)
  - Offline phase: optimize the transformation in some sense (T. Taddei, Ohlberger et al.) (second part)
  - Online phase: predict the value of the transformation. Regression (polynomials, ANN), projections (first part)
- Compute the Jacobian of the transformation $\frac{dy}{dx}$ and the new flux $\frac{dv}{dy}$ $\Rightarrow$ increasing computational costs also in online phase

Review of the algorithm: PODEI-Greedy in ALE framework

INITIALIZATION of ALE-PODEI-Greedy:

- Compute some Eulerian FOMs
- Compute or optimize $\theta(\boldsymbol{\mu}_k, t^n)$ for some $\boldsymbol{\mu}_k \in \mathcal{P}$ and $n \leq N_t$
- Build the regression map $\hat{\theta} : \mathcal{P} \times \mathbb{R}^+ \to \mathbb{R}^q$

INITIALIZATION of PODEI-Greedy:

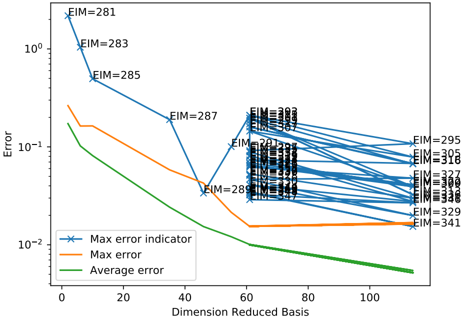
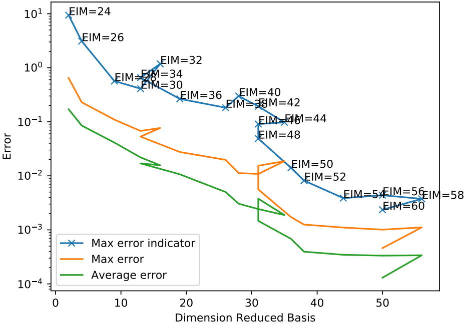
- EIM on ALE-RHS/fluxes of all times for a given parameter $\boldsymbol{\mu}_0$
- $RB = POD(\{v^n(\boldsymbol{\mu}_0)\}_{n=0}^{N_t})$

ITERATION:

- Greedy algorithm spanning over the parameter space $\mathcal{P}_h$, with an error indicator $\varepsilon(v(\boldsymbol{\mu}, t^n, \hat{\theta}(\boldsymbol{\mu}, t^n)))$
- Choose worst parameter as $\boldsymbol{\mu}^* = \arg\max_{\boldsymbol{\mu} \in \mathcal{P}_h} \varepsilon(\mathbf{v}(\boldsymbol{\mu}))$
- Apply POD on ALE time evolution of selected solution $POD_{add} = POD\left(\{v^n(\boldsymbol{\mu}^*)\}_{n=1}^{N_t}\right)$
- Update the RB with $RB = POD\,(RB \cup POD_{add})$
- Update EIM basis function with $EIM_{space} = EIM_{space} \cup EIM(\{RHS(\boldsymbol{\mu}^*, t^n, \hat{\theta}(\boldsymbol{\mu}^*, t^n))\}_{n=0}^{N_t})$

Burgers' equation

$$\begin{cases} u_t + \mu_0 (u^2/2)_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ Dirichlet BC} \\ u_0(x, \boldsymbol{\mu}) = \sin(2\pi(x + 0.1\mu_1)) e^{-(60+20\mu_2)(x-0.5)^2} (1 + 0.5\mu_3 x) \\ \mu_0 \sim \mathcal{U}([0,2]), \; \mu_1 \sim \mathcal{U}([0,1]), \; \mu_2, \mu_3 \sim \mathcal{U}([-1,1]) \end{cases}$$

Without calibration	With calibration: Poly3
	

Burgers' equation

$$\begin{cases} u_t + \mu_0 (u^2/2)_x = 0, \; D = [0,1], \; T_{max} = 0.6, \text{ Dirichlet BC} \\ u_0(x, \boldsymbol{\mu}) = \sin(2\pi(x + 0.1\mu_1)) e^{-(60+20\mu_2)(x-0.5)^2} (1 + 0.5\mu_3 x) \\ \mu_0 \sim \mathcal{U}([0,2]), \; \mu_1 \sim \mathcal{U}([0,1]), \; \mu_2, \mu_3 \sim \mathcal{U}([-1,1]) \end{cases}$$

Without calibration[3]

RB dim	153
EIM dim	335
FOM time	119 s
RB time	50 s
RB/FOM time	42%

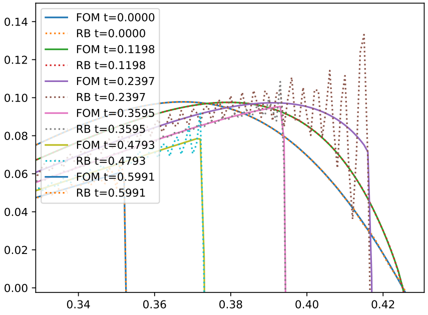
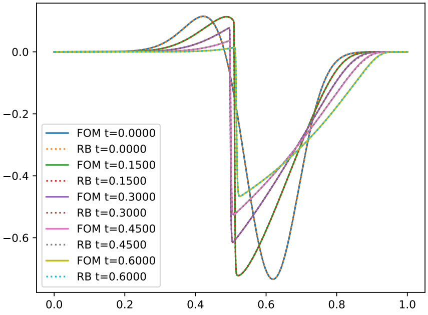
With calibration: Poly3

RB dim	50
EIM dim	60
FOM time	314 s
RB time	35 s
RB/FOM time	11%

[3] It does not reach the requested tolerance 10^{-3}

Burgers' equation

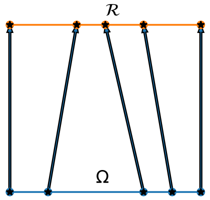
$$\begin{cases} u_t + \mu_0(u^2/2)_x = 0,\ D = [0,1],\ T_{max} = 0.6, \text{ Dirichlet BC} \\ u_0(x,\boldsymbol{\mu}) = \sin(2\pi(x+0.1\mu_1))e^{-(60+20\mu_2)(x-0.5)^2}(1+0.5\mu_3 x) \\ \mu_0 \sim \mathcal{U}([0,2]),\ \mu_1 \sim \mathcal{U}([0,1]),\ \mu_2,\mu_3 \sim \mathcal{U}([-1,1]) \end{cases}$$

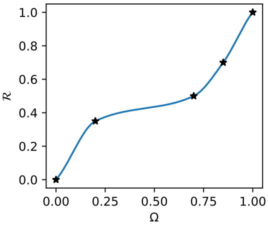
Without calibration	With calibration: Poly3
	

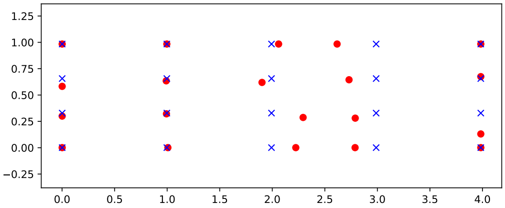
Multiple points to align

Piecewise Cubic Hermite Interpolating Polynomial PCHIP

- Interpolates some points (not optimizing on the whole mesh)
- Maintains monotonicity of the points (always invertible)
- Polynomials (easy to deal with)
- Easy generalization to Cartesian grids
- More complicated meshes ?







Optimal θs

Optimization

- Find θ that minimizes

$$||u(T(\theta,\cdot),t,\boldsymbol{\mu})-\bar{u}(\cdot)||_{\mathcal{R}}$$

- Penalization $|\partial_t\theta|$
- Penalization $\max_{y\in\mathcal{R}} \partial_y T(\theta,y)$ and $\max_{x\in\Omega} \partial_x T^{-1}(\theta,x)$
- Constraint on order $\theta_i < \theta_{i+1}$
- Initial guess, order of optimization
- Algorithm: Sequential Least Squares Programming

Optimal θs

What is $\bar{u}$?

- In some tests $u(t^{end}, \boldsymbol{\mu})$ is a good choice
- What if more parameters with different u values?

Optimization

- Find θ that minimizes

$$||u(T(\theta,\cdot),t,\boldsymbol{\mu}) - \bar{u}(\cdot)||_{\mathcal{R}}$$

- Penalization $|\partial_t \theta|$
- Penalization $\max_{y\in\mathcal{R}} \partial_y T(\theta, y)$ and $\max_{x\in\Omega} \partial_x T^{-1}(\theta, x)$
- Constraint on order $\theta_i < \theta_{i+1}$
- Initial guess, order of optimization
- Algorithm: Sequential Least Squares Programming

Optimal θs

Optimization

- Find θ that minimizes

$$||u(T(\theta,\cdot),t,\boldsymbol{\mu}) - \bar{u}(\cdot)||_{\mathcal{R}}$$

- Penalization $|\partial_t \theta|$
- Penalization $\max_{y\in\mathcal{R}} \partial_y T(\theta, y)$ and $\max_{x\in\Omega} \partial_x T^{-1}(\theta, x)$
- Constraint on order $\theta_i < \theta_{i+1}$
- Initial guess, order of optimization
- Algorithm: Sequential Least Squares Programming

What is $\bar{u}$?

- In some tests $u(t^{end}, \boldsymbol{\mu})$ is a good choice
- What if more parameters with different u values?

Generalization for more u values

- Find θ that minimizes

$$||u(T(\theta,\cdot),t,\boldsymbol{\mu}) - \mathcal{P}_{\mathbb{V}_{N_{RB}}}(u(T(\theta,\cdot),t,\boldsymbol{\mu}))||_{\mathcal{R}}$$

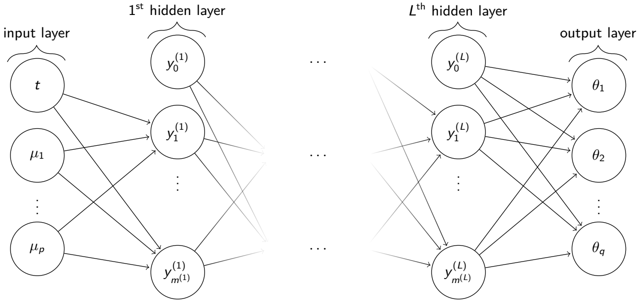
- What is $\mathbb{V}_{N_{RB}}$ at this point? Using few snapshots $\{u(\boldsymbol{\mu}_j, t^{end})\}_{j=1}^M$ for different parameters optimized
  - **Manually** (if possible multiple features detecting)
  - **Iteratively optimizing** $\theta(\boldsymbol{\mu}_j)$ using

$$\mathbb{V}_{N_{RB}} = POD(\{u(\boldsymbol{\mu}_j, t^{end}) \circ T(\theta(\boldsymbol{\mu}_j))\}_{j=1}^M)$$

Learning

Learning θ

- Use calibrated θ to get an estimator $\widehat{\theta}(t, \boldsymbol{\mu})$
- ANN with 4 hidden layers, 16 neurons each, tanh activation
- Enforcing $\theta_i < \theta_{i+1}$ with Softplus final activation function



Learning

Learning θ

- Use calibrated θ to get an estimator $\widehat{\theta}(t, \boldsymbol{\mu})$
- ANN with 4 hidden layers, 16 neurons each, tanh activation
- Enforcing $\theta_i < \theta_{i+1}$ with Softplus final activation function

Learning u_{RB} (POD-NN)

- Compute POD on $\{u \circ T(\widehat{\theta}, t^n, \boldsymbol{\mu}_j)\}_{j,n}$ extract $\mathbb{V}_{N_{RB}}$
- Project $\{u \circ T(\widehat{\theta}, t^n, \boldsymbol{\mu}_j)\}_{j,n}$ onto $\mathbb{V}_{N_{RB}}$ obtaining the reduced coefficients $u_{RB}(t^n, \boldsymbol{\mu}_j)$
- Learn the map $\widehat{u}_{RB}(t, \boldsymbol{\mu})$ with an ANN with 4 hidden layers, 16 neurons and tanh activation