Hybrid Physics-AI for efficient bias-aware state estimation

IAIFI Summer Workshop

Thursday, August 15,

Stiven Briand God MASSALA(ENS Paris-Saclay, NTU) , Ludovic Chamoin(ENS Paris-Saclay), Massimo Ciamarra(NTU Singapore)

Challenges & Objectives

Decision-making for critical urban systems

- Real-life engineering application
  - Complex (Non Linear, Multi-scale/Physics, Large) system
  - Uncertain environnement
  - Numerical complexity
  - Heterogeneous, noisy(+Expensive) data
  - Biased Model of system behaviour
- Objectives
  - Numerical Approaches for on-the-fly, real-time, data assimilation
  - Performance in term of robustness & Accuracy (Safe decision-making)
- Strategy
  - Use of simplified a priori physics-based models & ROM (Not costly High Fidelity models)
  - Effective correction of model ignorance (data-based enrichment) —> Hybrid twins
  - Biais-aware (Naturally hybrid) data assimilation technics
    - Coarse initial model + rich data —> Parameterized Background Data Weak (PBDW)

DesCartes

Basic Formulation

PBDW Framework [Maday & al 2015]

- Non Intrusive / Reduced-basis / Variational approach
- Key Idea : Approximation of the true state employing projection by data

$$u_{N,M} = z_{N,M} + \eta_{N,M}$$

Physics-based estimation : Computed from ROM

Data-based correction : Informed by experimental observations

Basic Formulation

PBDW Framework [Maday & al 2015]

- Non Intrusive / Reduced-basis / Variational approach
- Key Idea : Approximation of the true state employing projection by data

$$u_{N,M} = z_{N,M} + \eta_{N,M}$$

Physics-based estimation : Computed from ROM

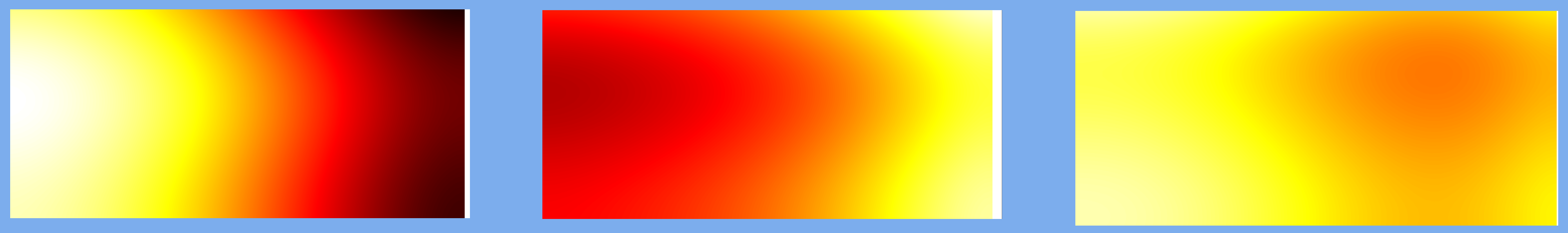
Data-based correction : Informed by experimental observations

- Parametrized best-knowledge model(PDE)

$$-(1+\epsilon\mu i)\Delta u(x) - \mu^2 u(x) = \mu q(x)$$

- Parametric domain : $\mu \in \mathscr{D}$

$\longrightarrow$ Manifold of solutions $\mathscr{M}^{\mathrm{bk}} = \{u(\mu) \mid \mu \in \mathscr{D}\}$



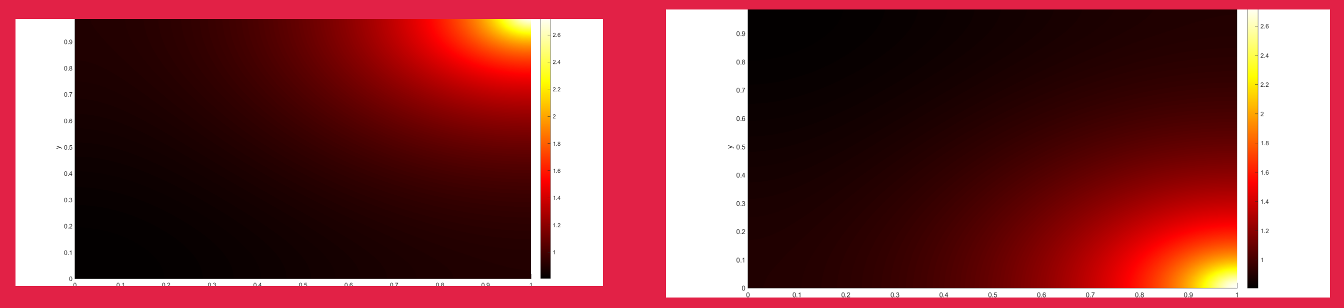
$\longrightarrow$ $\mathrm{Compression}_N\left(\mathscr{M}^{\mathrm{bk}}\right) \to \mathscr{Z}_N := \mathrm{span}\{\zeta_n\}_{n=1}^{N}$

- Hilbert space (Norm + Inner product)
- Observation functional :

$$\ell_m(v) = \frac{1}{\sqrt{2\pi r_m^2}} \int_{\mathscr{R}_m} v(x) e^{\frac{(x-x_m^c)^2}{2r_m^2}} dx$$

- Riesz reprensenters : $q_m := R_{\mathscr{U}}\left(\ell_m^{\mathrm{obs}}\right)$

$$(u, q_m) = \ell_m(u)$$



$\longrightarrow$ $\mathscr{U}_M := \mathrm{span}\{q_m\}_{m=1}^{M}$

Basic Formulation

PBDW Framework

- Non Intrusive / Reduced-basis / Variational approach

$$u_{N,M} = z_{N,M} + \eta_{N,M}$$

$$\sum_{n=1}^{N} \zeta_n \cdot \mathbf{z}_n \qquad \sum_{m=1}^{M} q_m \cdot \eta_m$$

- Implementation (Online) : $$\left(z^{\xi}_{N,M}, \eta^{\xi}_{N,M}\right) = \underset{\substack{z \in \mathcal{Z}_N \\ \eta \in \mathcal{U}_M}}{\arg\inf} \left(\xi \|\eta\|^2 + \frac{1}{M} \sum_{m=1}^{M} \left\| \, l_m(z+\eta) - y_m \, \right\|_2^2\right)$$

- Saddle-point problem $$\begin{bmatrix} \xi M \mathbb{I}_M + \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\eta_\theta}^\star \\ \mathbf{z}^\star \end{bmatrix} = \begin{bmatrix} \boldsymbol{y} \\ \mathbf{0} \end{bmatrix} \qquad \mathbb{A}_{i,j} = (q_i, q_j), \mathbb{B}_{i,j} = (\xi_i, q_j)$$

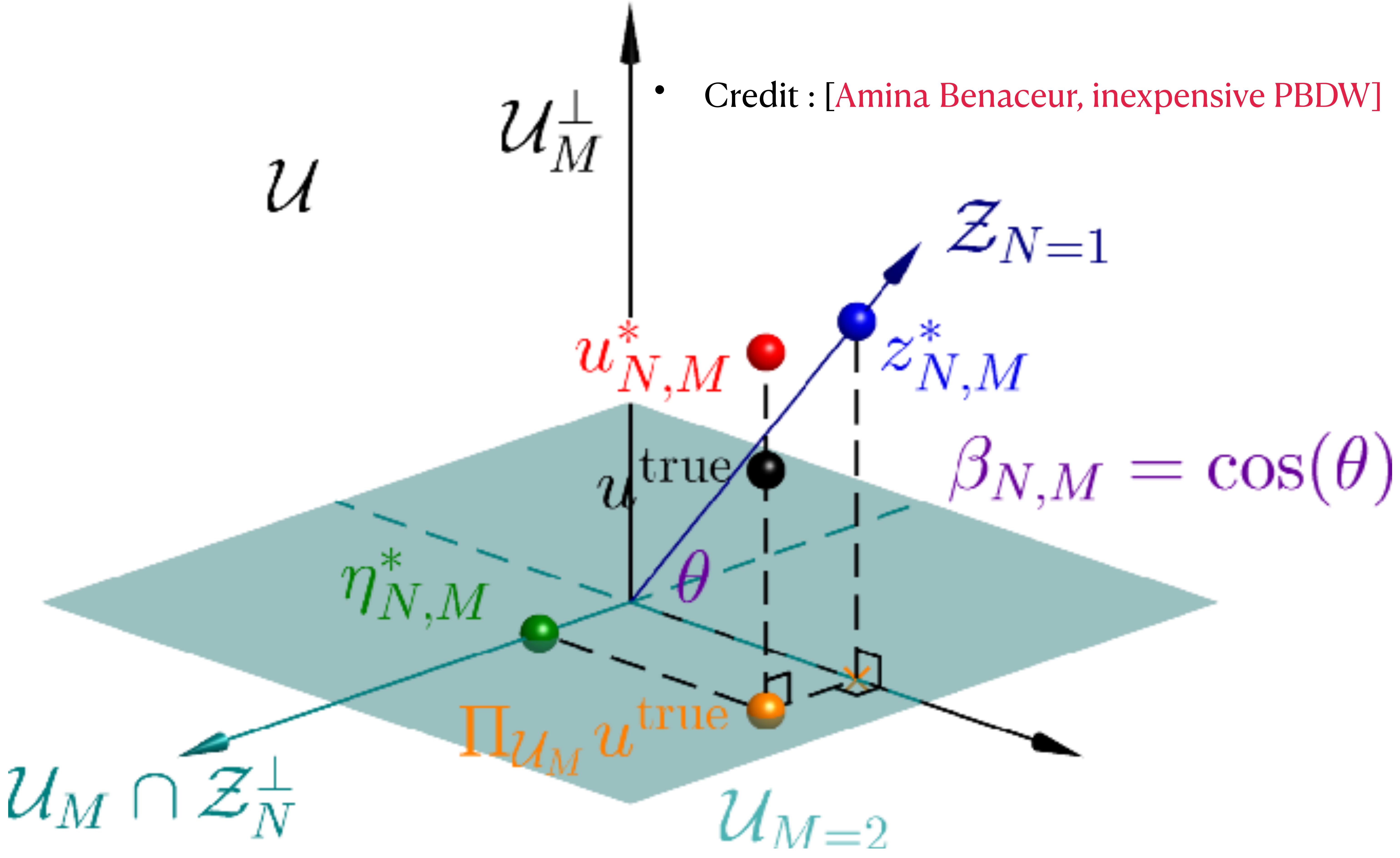
Properties

- Full error convergence analysis [Gong et al.]
- Orthogonality between what is known and learnt
- Optimal data management(Right data, right place)
  - balancing Stability-Approximation (S-Greedy)
    - Max stability

$$\beta_{N,M} = \inf_{z\in\mathcal{Z}_N} \sup_{q\in\mathcal{U}_M} \frac{((z,q))}{\|z\|\,\|q\|}.$$

    - Min approximation error

$$\inf_{\eta\in\mathcal{U}_M\cap\mathcal{Z}_N^\perp} \left\| \Pi_{\mathcal{Z}_N^\perp} u^{\text{true}} - \eta \right\|$$



- Credit : [Amina Benaceur, inexpensive PBDW]

PBDW + Neural Operator

Bias-Operator : Learn Deviation constrained in $\mathcal{U}_M \cap \mathcal{Z}_N^\perp$

We parametrize the update η with a Deeponets $\eta_\theta(v)(x_m)$

$$u_{N,M} = z_{N,M} + \eta_\theta$$

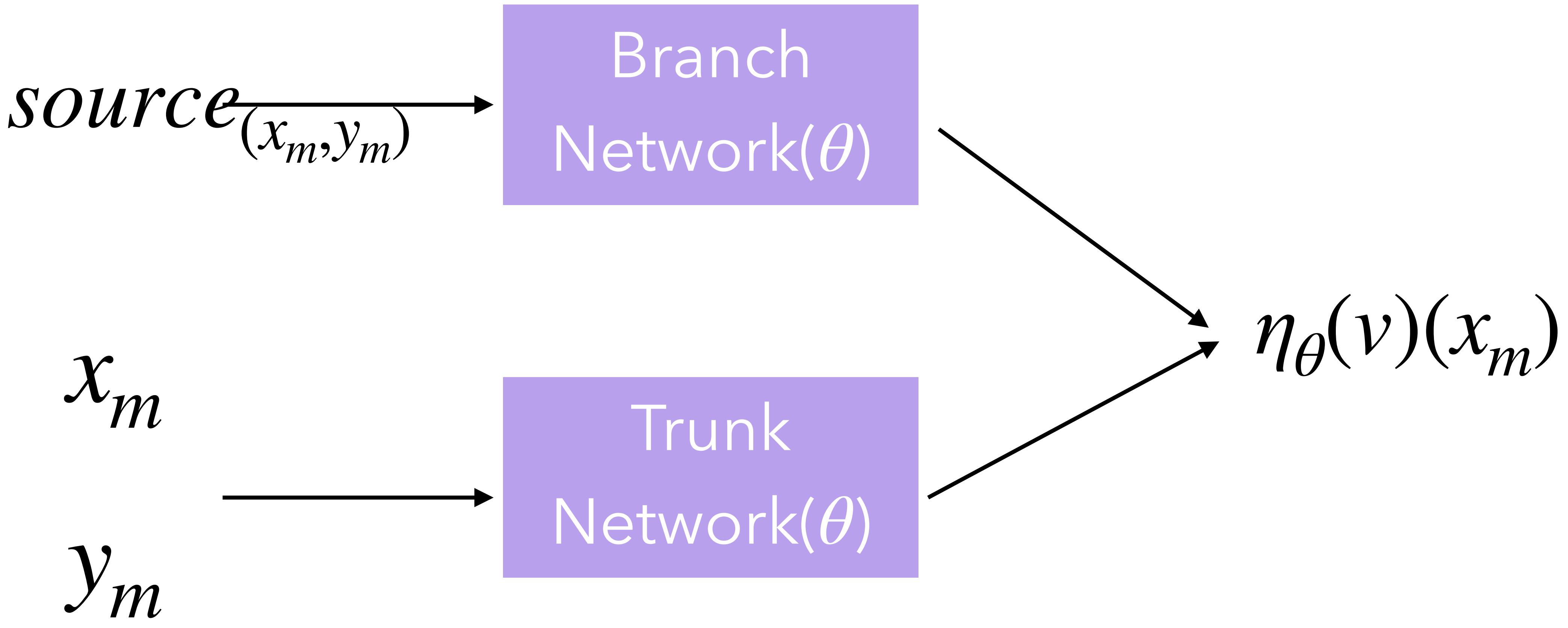
$$\mathcal{Z}_N \qquad \mathcal{U}_M \cap \mathcal{Z}_N^\perp$$

$$\eta_\theta = \sum_{m=1}^{M} q_m \cdot \eta_\theta(v)(x_m)$$

Goal : Enforce $\eta_\theta \in \mathcal{Z}_N^\perp$

$$\in \mathcal{U}_M := \mathrm{span}\{q_m\}_{m=1}^{M}$$

Weak-Constrain



$\in \mathscr{Z}_N^{\perp}$

$$L(\theta) = \frac{\omega_1}{N_\eta} \sum_{i=1}^{N_\eta} \left[\eta\left(y_i; \theta\right) - \eta^*\left(y_i\right)\right]^2 + \omega_2 \sum_{j=1}^{N_{modes}} \left| \left(\eta_j\left(y; \theta\right), B_j\right) \right|$$

Orthogonality with anticipated modes

$$\eta_\theta = \sum_{m=1}^{M} q_m \cdot \eta_\theta(v)(x_m)$$

Strong-Constrain

Branch Network(θ)

$\mathscr{Z}_N^{\perp} := \mathrm{span}\{\phi_i\}$

$\eta_\theta(v)(\phi_i)$

$$\phi_i = \phi_i - \sum_{j=1}^{i-1} \Pi_{\zeta_j} \phi_i$$

$$\downarrow$$

$$\langle \eta_\theta(v)(\phi), \zeta_n \rangle = 0$$

$$\downarrow$$

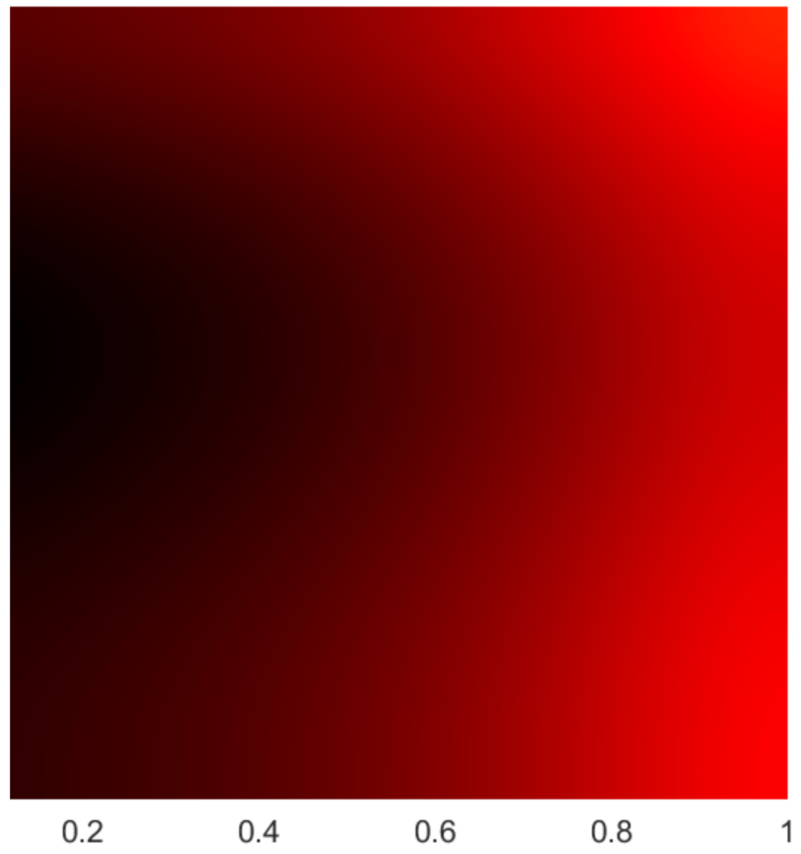
$$\eta_\theta(v)(\phi) \in \mathscr{Z}_N^{\perp}$$

$$L(\theta) = \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} \left[\sum_{j=1}^{M} \hat{\eta}_j \left(y_i; \theta\right) \cdot \phi_j - \eta^* \left(y_i\right) \right]^2$$

Application - Helmoltz Equation

Bias from source & boundary conditions

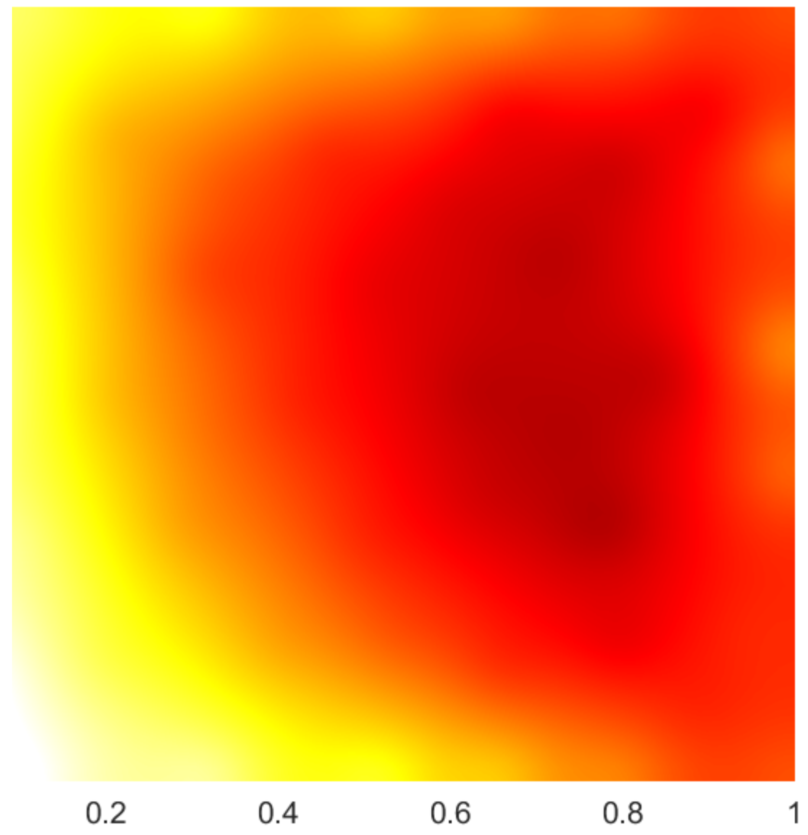
Physics based estimation



$z_{2,50}$

+

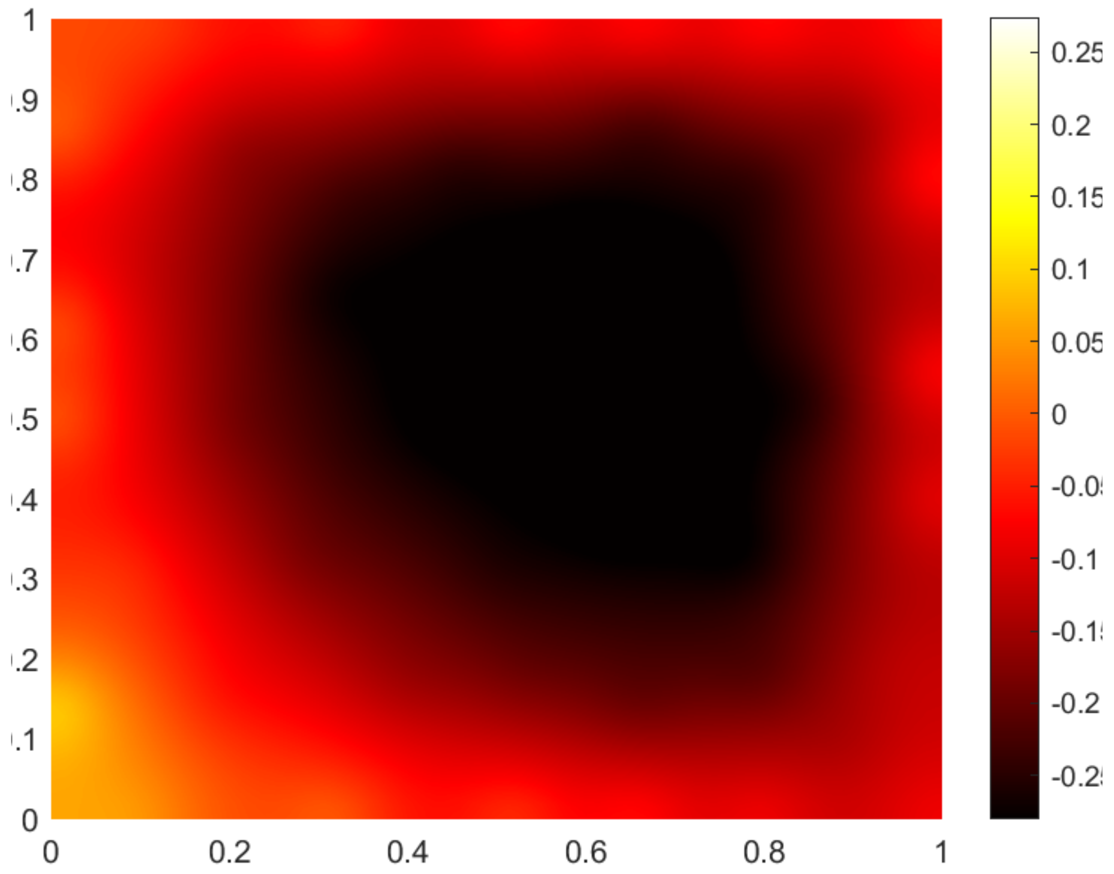
Predicted correction



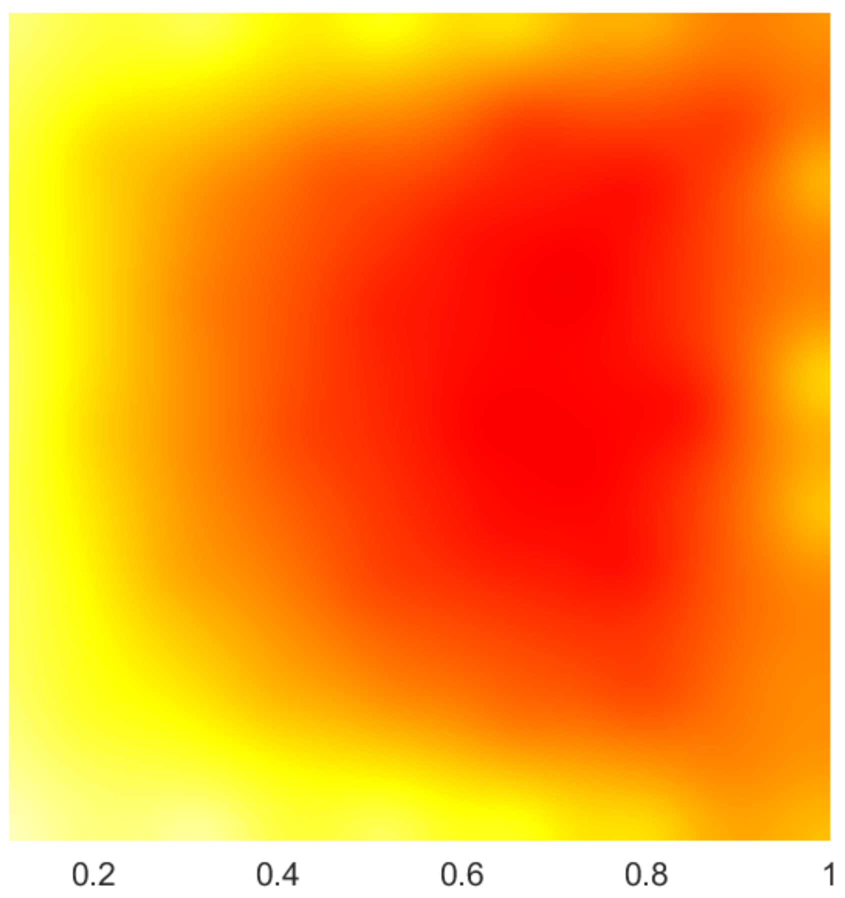
η_θ

=

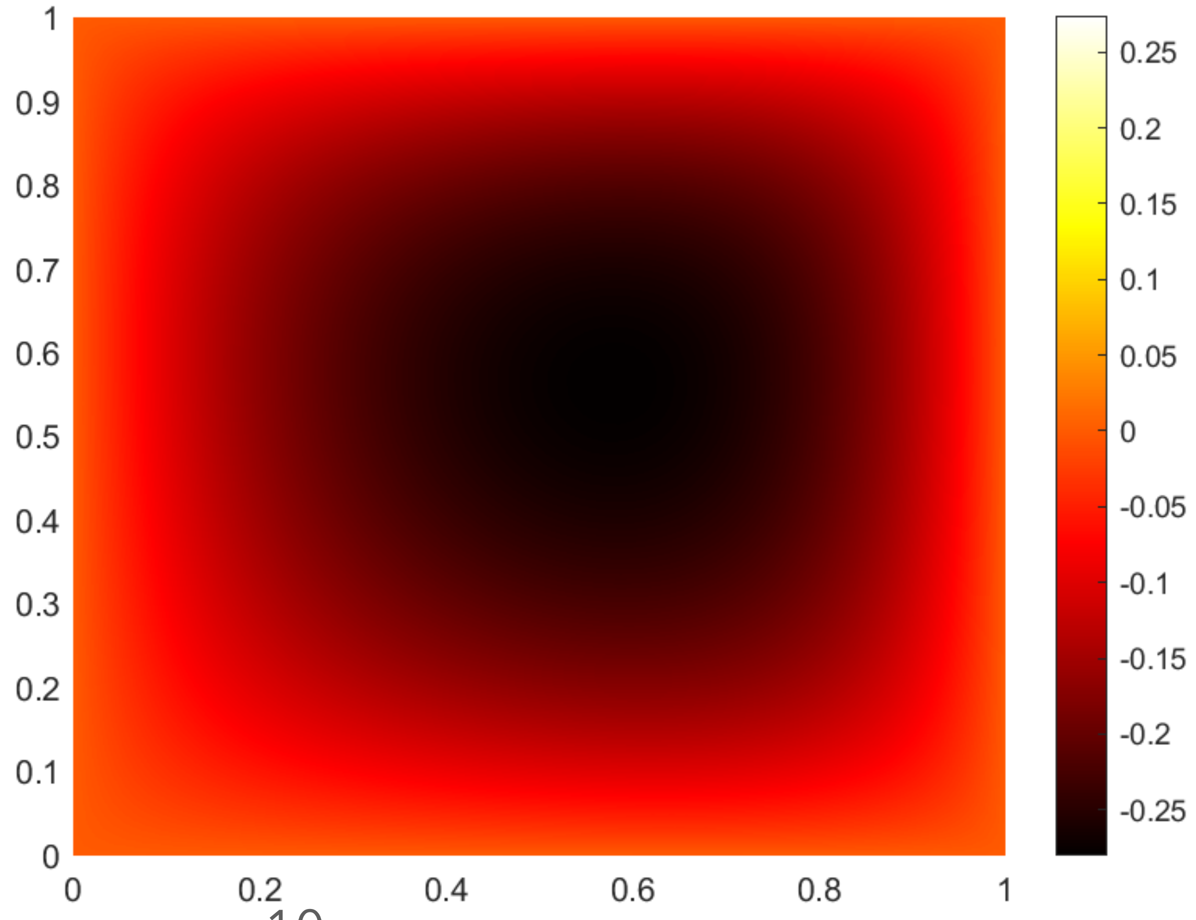
Corrected solution



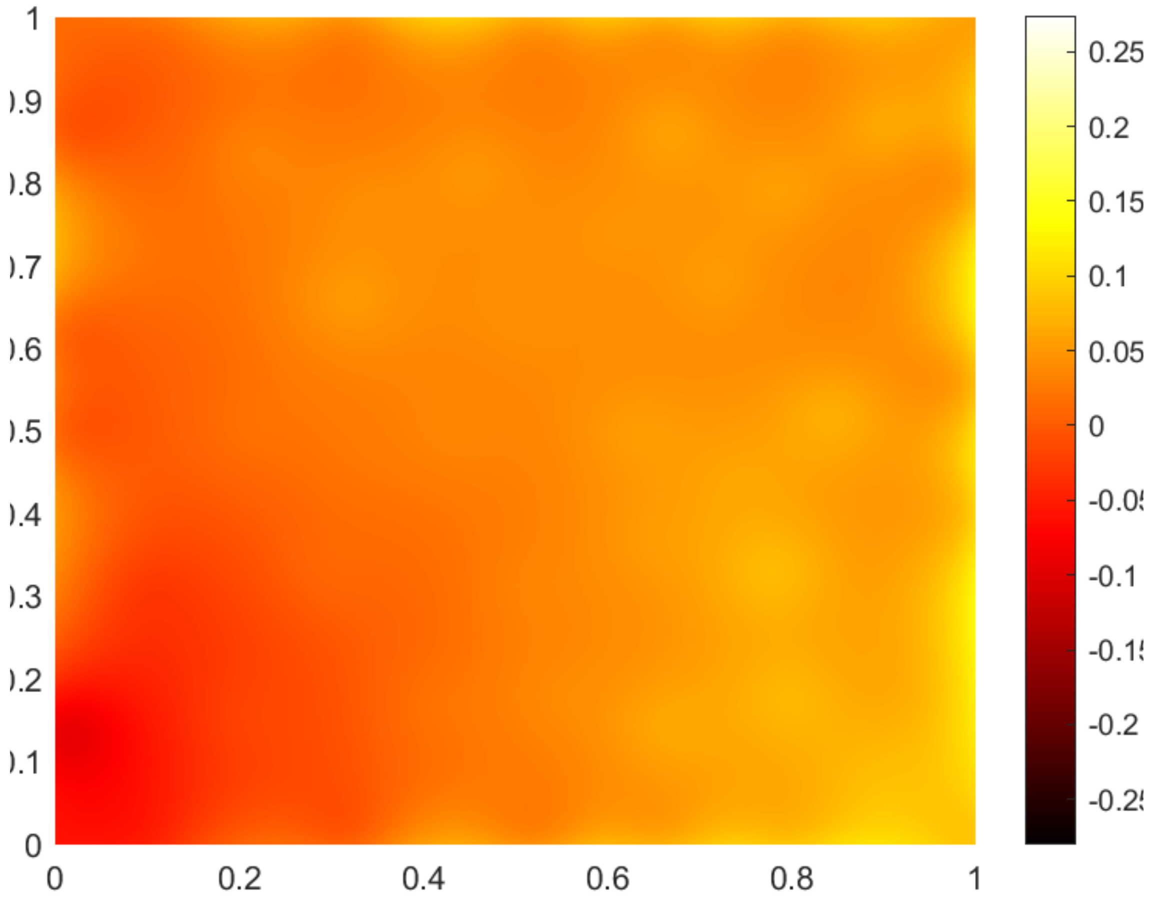
Proposed Hybrid-AI



Bias Original PBDW



u^{true}



Relative L2 eror

Few References

- Y. Maday, A.T. Patera, J.D. Penn, M. Yano, A parametrized background data weak approach to variational data assimilation: formulation, analysis, and application to acoustics, Int. J. Num. Meth. Eng., 102(5):933-965 (2015).
- Y. Maday, T. Taddei, Adaptive PBDW approach to state estimation: noisy observations, user-defined update paces, SIAM J. Scientific Computing, 41(4): 669-693 (2019)
- S. MASSALA, L. Chamoin, M. Ciamarra Hybrid twin using PBDW and Deeponets for the effective state estimation and prediction on complex systems (2024)
- W. Haïk, Y. Maday, L. C., A real-time variational data assimilation method with data-driven enrichment for time-dependent problems, Comput. Mech. Appl. Mech. Eng., 405:115868 (2023)