



DATA ASSIMILATION FOR IMPERFECT MODELS

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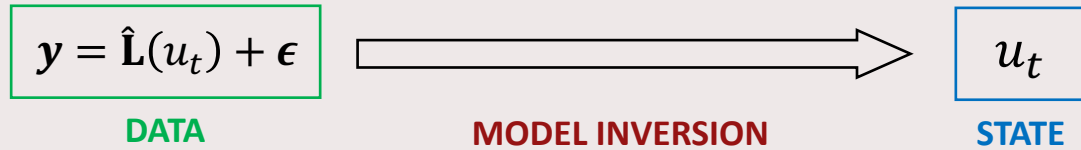
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RWTH Aachen

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INTRODUCTION

STATE ESTIMATION: AN INVERSE PROBLEM



STATE ESTIMATION: EMPLOYING IMPLICIT MODEL



SPACE BASE METHODS (β_i)

- GEIM, PBDW[2]
- (Kriging)
- ...

[2] Maday, Y., Patera, A.T., Penn, J.D., Yano, M. : A parameterized background data weak approach to variational data assimilation: formulation, analysis, and application to acoustics (2014).

STATE ESTIMATION: EMPLOYING IMPLICIT MODEL



SPACE BASE METHODS (β_i)

- GEIM, PBDW[2]
- (Kriging)
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Requires proper approximation space and is usually more prone to noise effects because of the large number of coefficients to be estimated.

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STATE ESTIMATION: EMPLOYING EXPLICIT MODEL



MODEL BASED METHODS (μ_t)

- 3D-VAR[1]
- Kalman Filters
- ...

[1] Aretz-Nellesen, N., Grepl, M.A., Veroy, K. : 3D-VAR for Parametrized Partial Differential Equations: A Certified Reduced Basis Approach (2019).

STATE ESTIMATION: EMPLOYING EXPLICIT MODEL



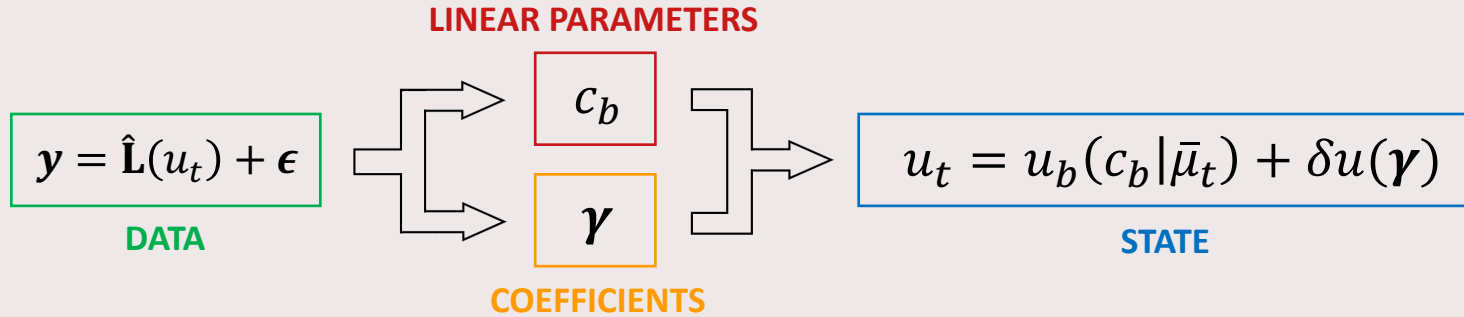
MODEL BASED METHODS (μ_t)

- 3D-VAR[1]
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Expensive whenever the model is nonlinear and in all the cases when the parameters are not linear control variables.

[1] Aretz-Nellesen, N., Grepl, M.A., Veroy, K. : 3D-VAR for Parametrized Partial Differential Equations: A Certified Reduced Basis Approach (2019).

STATE ESTIMATION: EMPLOYING IMPERFECT EXPLICIT MODEL



u_b : IMPERFECT MODEL SOLUTION

c_b : IMPERFECT MODEL LINEAR PARAMETER

PRACTICAL MOTIVATION FOR IMPERFECT MODEL (COMPLEXITY)

Plenty of problems admit decent linear approximation solutions:

Heat & Mass Transfer

- Radiative HT [$\sim T^4$]
- Nonlinear H&MT [$k(T), D(T, c)$]

Neutron Kinetics

- Neutron Transport
- H&MT Coupling [$\chi(E, T, c)$]

Electrodynamics

- HT Coupling [$\mu(T), \varepsilon(T)$]
- Charge carriers diffusion [$\varepsilon(E, c)$]

Solid Mechanics

- Finite strain [$\dots + \nabla \mathbf{u}^T \cdot \nabla \mathbf{u}$]
- Non-Hookean Solids [$\sigma(\varepsilon)$]

EPISTEMIC MOTIVATION FOR IMPERFECT MODEL (UNCERTAINTY)

Physical Coefficients

Geometrical Parameters

Boundary Conditions

...



Even for linear problems, the direct estimation of these quantities from experimental data results in non-linear-quadratic and non-convex optimization problems.

We can incorporate complexity and uncertainty into a Bias Space to account for all the missing information of the Approximated Model

THE METHOD

3D-VAR : PERFECT MODEL FORMULATION

$$\mathbf{y} = \hat{\mathbf{L}}(u_t) + \boldsymbol{\epsilon}$$

DATA

where

$$\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \boldsymbol{\Sigma})$$

NOISE

and

$$\mathcal{A}_\mu(u_t, \psi) = \mathcal{S}_\mu(c_t, \psi) \quad \forall \psi \in \mathcal{U}$$

PERFECT MODEL

3D-VAR : BIASED MODEL FORMULATION

$$\mathbf{y} = \hat{\mathbf{L}}(u_t) + \boldsymbol{\epsilon}$$
DATA

where
$$\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \boldsymbol{\Sigma})$$
NOISE and
$$A_{\bar{\mu}}(u_b, \psi) = S_{\bar{\mu}}(c_b, \psi) \quad \forall \psi \in \mathcal{U}$$
APPROXIMATED LINEAR MODEL

with
$$u_t - u_b = \delta u$$
MODEL BIAS

3D-VAR : BIASED MODEL FORMULATION

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DATA
NOISE
APPROXIMATED LINEAR MODEL

with

$$\boxed{u_t - u_b = \delta u}$$

MODEL BIAS

We can approximate the inverse problem :

$$(u^*, \delta u^*, c^*) = \underset{(u, \delta u, c) \in \mathcal{U} \times \mathcal{B} \times \mathcal{C}}{\operatorname{argmin}} \frac{1}{2} \|\mathcal{L}(u) - \mathbf{y}\|_{\boldsymbol{\Sigma}^{-1}}^2 + \boxed{\dots}$$

s. t. $A_{\bar{\mu}}(u, \psi) - A_{\bar{\mu}}(\delta u, \psi) = S_{\bar{\mu}}(c, \psi) \quad \forall \psi \in \mathcal{U}$

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$$\text{s. t.} \quad A_{\bar{\mu}}(u, \psi) - A_{\bar{\mu}}(\delta u, \psi) = S_{\bar{\mu}}(c, \psi) \quad \forall \psi \in \mathcal{U}$$

δu accounts for the model bias and for the error in μ . It's assumed to be a **small** correction.

ASYMPTOTIC BEHAVIOURS

Case of $\lambda \rightarrow 0$ (δu^* , δc^* free)



Reconstructed state is to least square approximation in the space $\text{span}\{\mathcal{B}, \mathcal{V}_{\bar{\mu}}\}$. **It may be exact.**

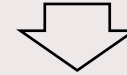
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Case of : $\lambda \rightarrow \infty$: ($\delta u^* = 0$)



Reconstruction reduced 3D-VAR, based on a bias model. **Less coefficients to be estimated.**

3D-VAR : BIASED MODEL FORMULATION

$$\boxed{\mathbf{y} = \hat{\mathbf{L}}(u_t) + \boldsymbol{\epsilon}} \quad \text{where} \quad \boxed{\boldsymbol{\epsilon} \sim \mathbf{N}(\mathbf{0}, \boldsymbol{\Sigma})} \quad \text{and} \quad \boxed{A_{\bar{\mu}}(u_b, \psi) = S_{\bar{\mu}}(c_b, \psi) \quad \forall \psi \in \mathcal{U}}$$

DATA **NOISE** **APPROXIMATED LINEAR MODEL**

with $\boxed{u_t - u_b = \delta u}$

MODEL BIAS

We can approximate the inverse problem :

$$(u^*, \delta u^*, c^*) = \underset{(u, \delta u, c) \in \mathcal{U} \times \mathcal{B} \times \mathcal{C}}{\operatorname{argmin}} \frac{1}{2} \|\mathcal{L}(u) - \mathbf{y}\|_{\boldsymbol{\Sigma}^{-1}}^2 + \frac{\lambda}{2} \|\delta u\|_{\mathcal{U}}^2$$

s. t. $A_{\bar{\mu}}(u, \psi) - A_{\bar{\mu}}(\delta u, \psi) = S_{\bar{\mu}}(c, \psi) \quad \forall \psi \in \mathcal{U}$

HOW TO SOLVE?

SOLUTION THROUGH LAGRANGIAN OPTIMIZATION

$$\mathcal{L}(u, \delta u, \delta c, p) = \frac{1}{2} \|\hat{\mathbf{L}}(u) - \mathbf{y}\|_{\Sigma^{-1}}^2 + \frac{\lambda}{2} \|\delta u\|_u^2 + \frac{\gamma}{2} \|\delta c\|_c^2 + A_{\bar{\mu}}(u - \delta u, p) - S_{\bar{\mu}}(\bar{c} + \delta c, p)$$

SOLUTION THROUGH LAGRANGIAN OPTIMIZATION

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A first order optimality condition can be easily derived:

$$\left\{ \begin{array}{lll} \hat{\mathbf{L}}(\psi)^T \Sigma^{-1} \hat{\mathbf{L}}(u) + A_{\bar{\mu}}(\psi, p) & = \hat{\mathbf{L}}(\psi)^T \Sigma^{-1} \mathbf{y} & \forall \psi \in \mathcal{U} \\ \lambda(\varphi, \delta u)_{\mathcal{U}} - A_{\bar{\mu}}(\varphi, p) & = 0 & \forall \varphi \in \mathcal{B} \\ \gamma(\eta, \delta u)_{\mathcal{C}} - S_{\bar{\mu}}(\eta, p) & = 0 & \forall \eta \in \mathcal{C} \end{array} \right\} \text{ Adjoint Equations}$$

$$\left\{ \begin{array}{ll} A_{\bar{\mu}}(u, \phi) - A_{\bar{\mu}}(\delta u, \phi) - S_{\bar{\mu}}(\delta c, \phi) = S_{\bar{\mu}}(\bar{c}, \phi) & \forall \phi \in \mathcal{U} \end{array} \right\} \text{ Approximated Model}$$

DISCRETIZATION

We need 3 functional spaces to set up the problem:

$$\mathcal{U} \longrightarrow \mathcal{U} \approx \mathcal{U}_h \text{ or } \mathcal{U}_R = \text{MOR}\{\mathcal{V}\}$$

$$\mathcal{B} \longrightarrow \mathcal{B} = \text{MOR}\{\mathcal{M} \cup \mathcal{V}\}$$

$$\mathcal{C} \longrightarrow \mathcal{C} = \mathcal{C}_R \text{ is assumed sufficiently low dimensional}$$

SPACES CONSTRUCTION AND DISCRETIZATION

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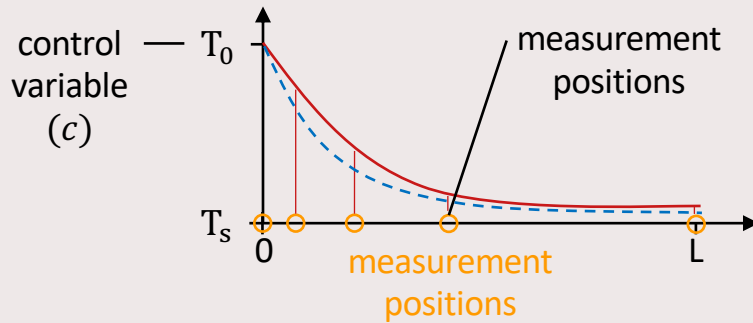
NB : If we choose for \mathcal{B} the space spanned by the Rietz representations of the elements of the linear functional $\hat{\mathbf{L}}$, the method coincides with the APBDW [3]

A PRACTICAL EXAMPLE

PRACTICAL EXAMPLE - 1D RADIATIVE HEAT TRANSFER

Exact Model

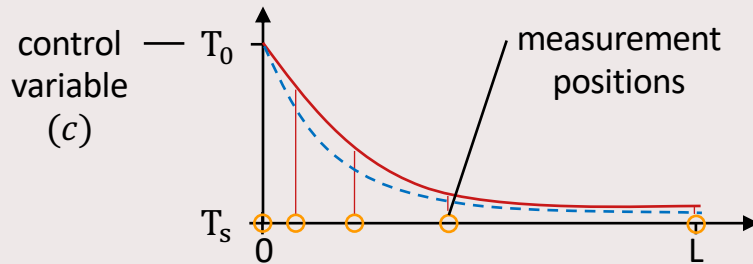
$$-kA \frac{d^2T}{dx^2} = -P\varepsilon\sigma(T^4 - T_s^4) + \text{b. c.}$$



PRACTICAL EXAMPLE - 1D RADIATIVE HEAT TRANSFER

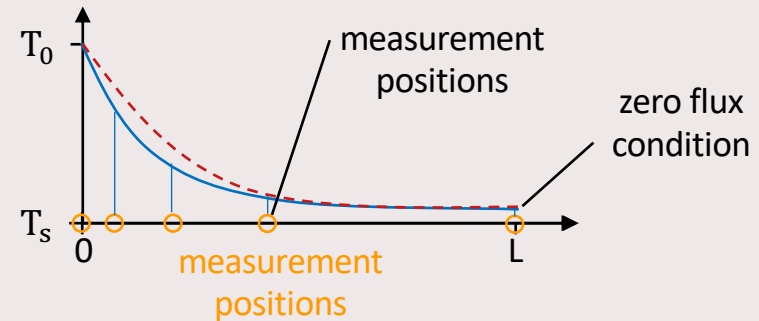
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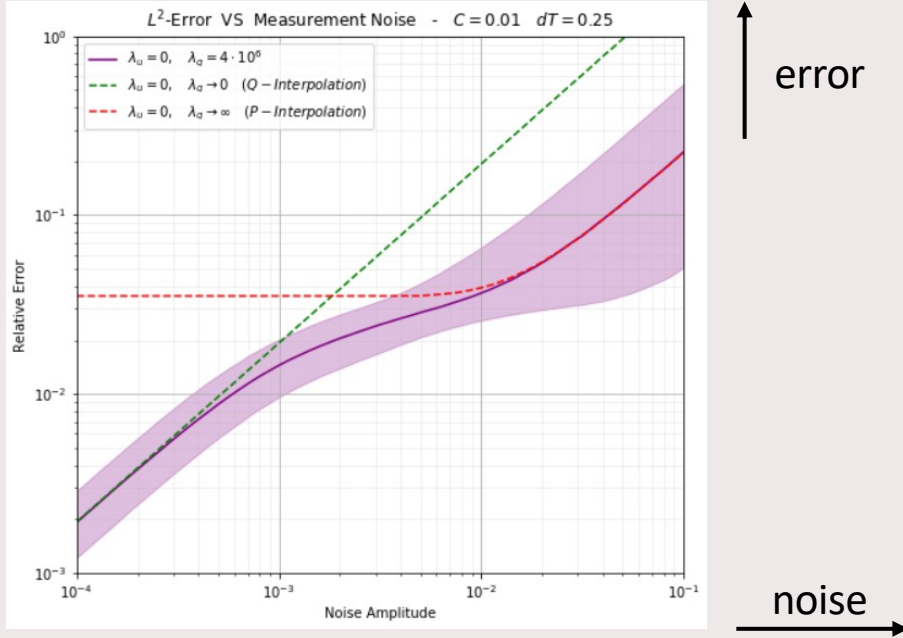


Biased Model

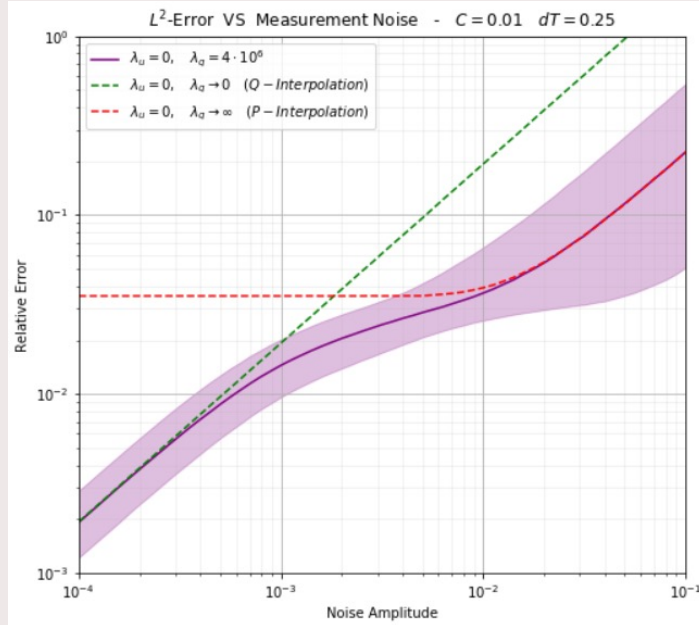
$$-kA \frac{d^2T}{dx^2} = -4P\epsilon\sigma T_s^3(T - T_s) + \text{b. c.}$$



PRACTICAL EXAMPLE - NOISE VS RELATIVE ERROR

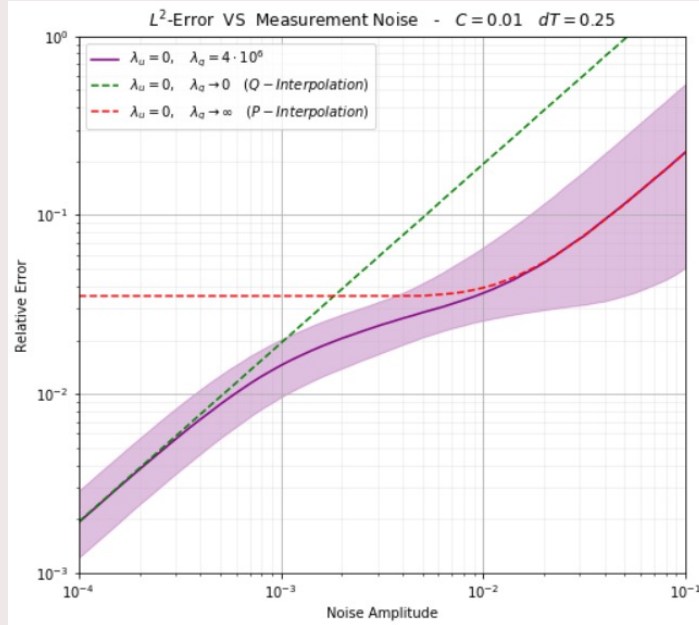


PRACTICAL EXAMPLE - NOISE VS RELATIVE ERROR



For $\lambda \rightarrow 0$, the method reduces to a least square estimation in the Bias Space (\mathcal{B}). It's optimal in noise free conditions.

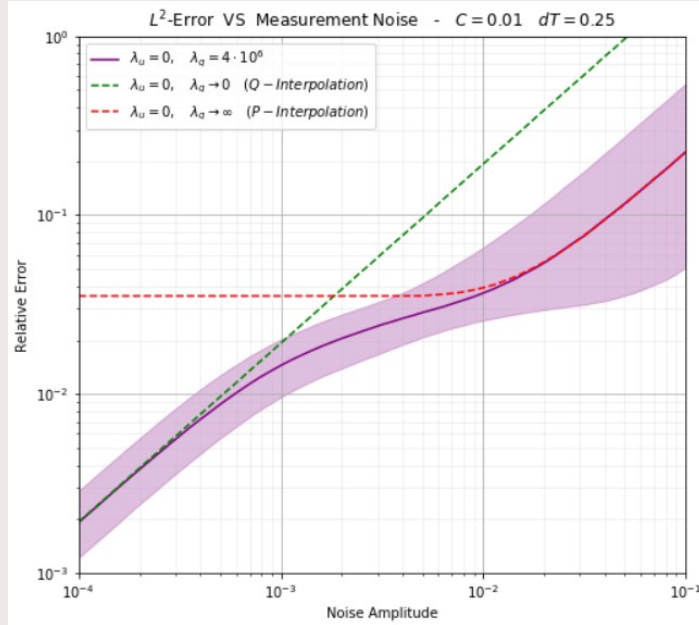
PRACTICAL EXAMPLE - NOISE VS RELATIVE ERROR



For $\lambda \rightarrow 0$, the method reduces to a least square estimation in the Bias Space (\mathcal{B}). It's optimal in noise free conditions.

For $\lambda \rightarrow \infty$, the method reduces to the 3D-VAR employing the Biased Model. In noise free conditions the error coincide with the Bias energy.

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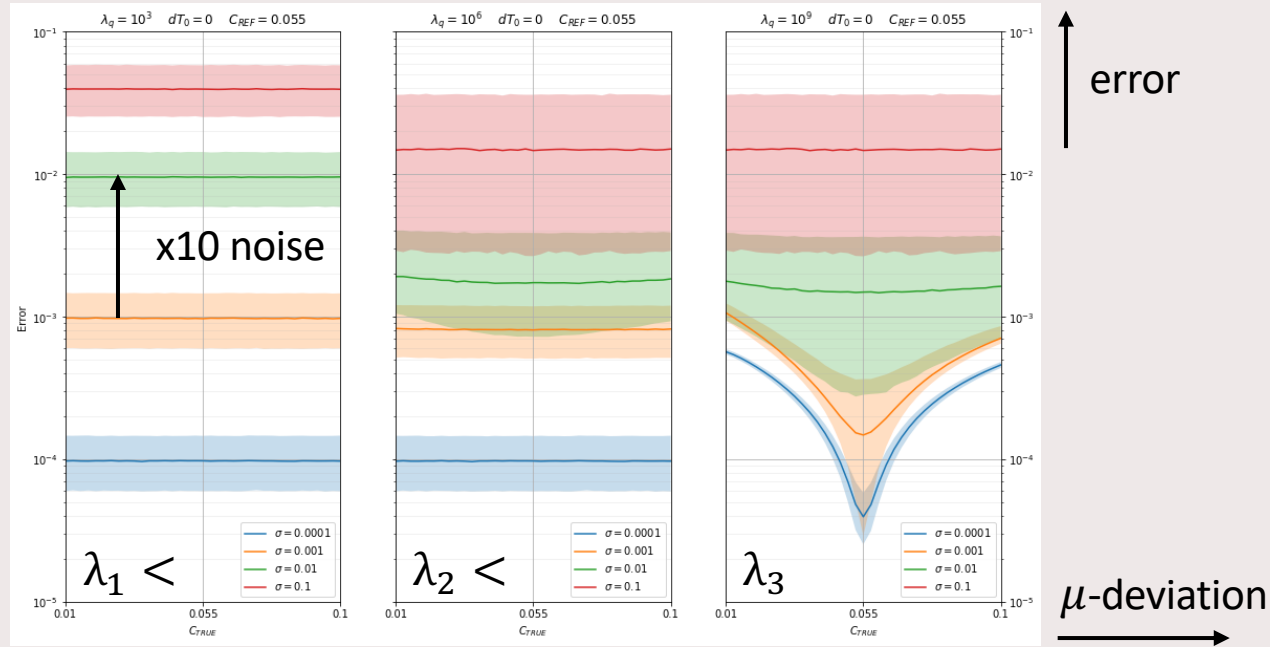


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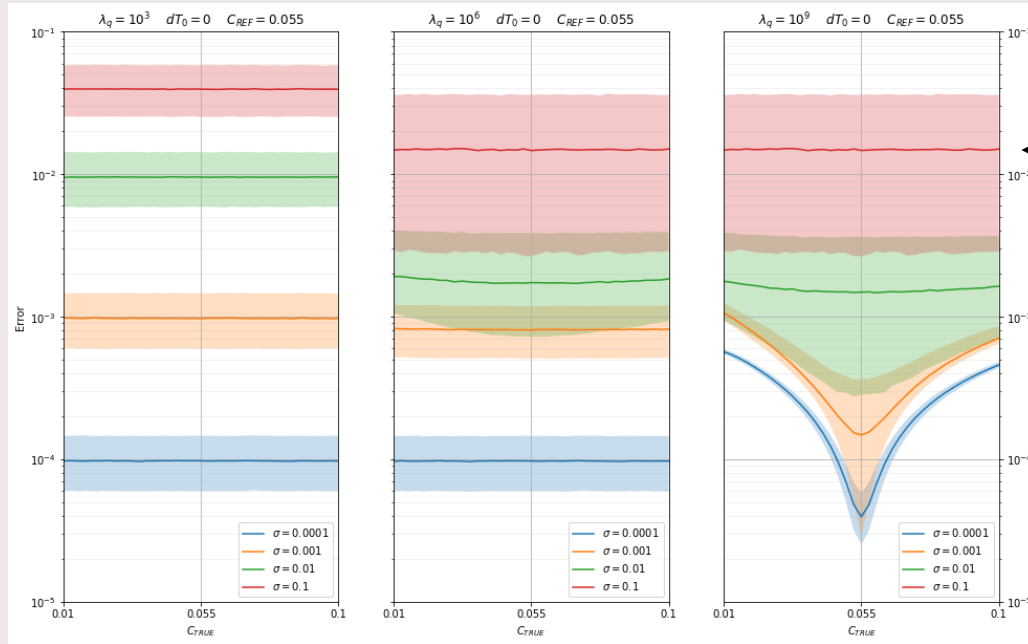
For $\lambda \rightarrow \infty$, the method reduces to the 3D-VAR employing the Biased Model. In noise free conditions the error coincide with the Bias energy.

It exists an optimal λ , which optimally bridges the two behaviors. The transition occurs when noise and bias are comparable.

PRACTICAL EXAMPLE - MODEL BIAS AND NOISE EFFECTS

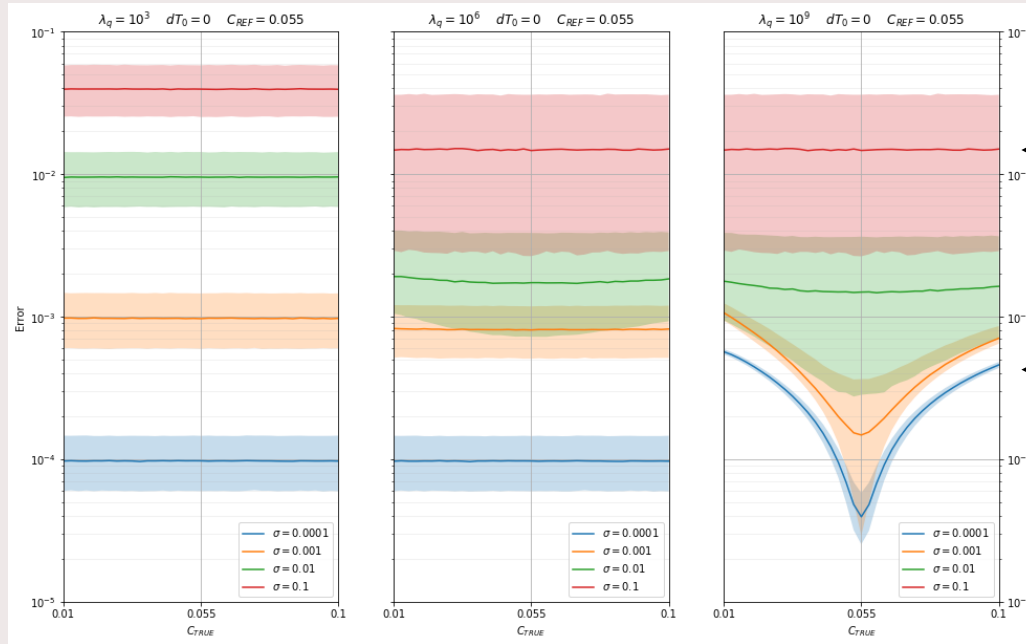


PRACTICAL EXAMPLE - MODEL BIAS AND NOISE EFFECTS



A larger λ mitigates error in presence of large noise. The smaller number of coefficients estimated is dominant.

PRACTICAL EXAMPLE - MODEL BIAS AND NOISE EFFECTS



A larger λ mitigates error in presence of large noise. The smaller number of coefficients estimated is dominant.

In weak noise conditions, a large λ may correspond to poorer reconstructions. That's because the bias effects are not mitigated.

CONCLUSIONS

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- We've developed a new method bridging two approaches to state estimation
- We've proven the well-posedness of the method and tested over a toy problem
- We observed that a prior knowledge on the magnitude of the bias is still required

FUTURE DEVELOPMENTS

- We're developing bounds for the variance of the reconstruction error
- We're studying more complex problems in more than 1D
- We're thinking to extend the method to time dependent problems

RELATED LITERATURE

- [1] Maday, Y., Patera, A.T., Penn, J.D., Yano, M. : A parameterized background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics (2014)
- [2] Aretz-Nellesen, N., Grepl, M.A., Veroy, K. : 3D-VAR for Parametrized Partial Differential Equations: A Certified Reduced Basis Approach (2019)
- [3] Maday, Y., Taddei, T. : Adaptive PBDW Approach to State Estimation: Noisy Observations; UserDefined Update Spaces (2019)
- [4] Binev, P., Cohen, A., Mula, O., Nichols, J. : Greedy algorithms for optimal measurements selection in state estimation using reduced models (2018)

THANK YOU FOR YOUR ATTENTION!

TIME FOR QUESTIONS!