Optimal Sensor Placement for the Quantification of Model Uncertainty

A functional analysis perspective

Professor Karen Veroy-Grepl
SFB 1294 Data Assimiliation Colloquium – 08 May 2020

European Research Council
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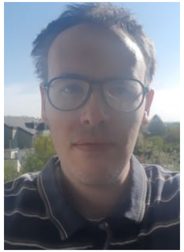
EINDHOVEN
UNIVERSITY OF
TECHNOLOGY

Team


Nicole Aretz-Nellesen
PhD Student (RWTH)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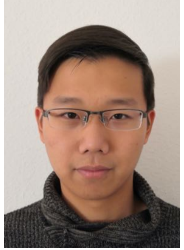
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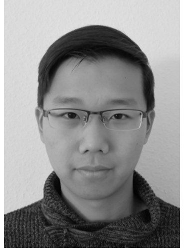

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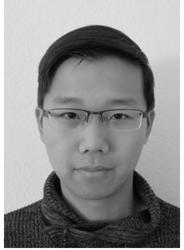

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Acknowledgments

Collaborators

Mathematics (RWTH Aachen)

Prof. Martin Grepl

Dr. Mark Kärcher (now at NavVis)

Geophysics (RWTH Aachen)

Prof. Florian Wellmann

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Oden Institute (UT Austin)

Dr. Peng Chen

Prof. Tan Bui-Thanh

Funding

erc
European Research Council
Established by the European Commission

DFG Deutsche Forschungsgemeinschaft

The Plan

1	**Model**	Parametrized PDEs
2	**Model + Data**	Data Assimilation
3	**Data**	Stability-based Optimal Experimental Design via Projection-based Model Order Reduction
4	**Connections**	Bayesian Setting

1 - MODEL

PARAMETRIZED PDEs

Parametrized PDEs

Model

Find $\boldsymbol{u}$ in $\boldsymbol{V}$ such that

$$a(u, v) = f(v) \qquad\qquad \forall\, v \in \boldsymbol{V}$$

Parametrized PDEs

Model

Find $\boldsymbol{u}$ in $\boldsymbol{V}$ such that

$$\boldsymbol{a(u,v) = f(v)} \qquad \forall\ \boldsymbol{v} \in \boldsymbol{V}$$

$$\mathbf{Au = f}$$

Parametrized PDEs

Model

Find $\boldsymbol{u}$ in $\boldsymbol{V}$ such that

$$\boldsymbol{a(u,v) = f(v)} \qquad \forall\ \boldsymbol{v} \in \boldsymbol{V}$$

where the space $\boldsymbol{V}$ is equipped with

inner product $\quad (\cdot,\cdot)_{\boldsymbol{V}}$

norm $\quad \|\cdot\|_{\boldsymbol{V}} = (\cdot,\cdot)_{\boldsymbol{V}}^{\frac{1}{2}}$

Parametrized PDEs

Parametrized Model

Find $\boldsymbol{u}(\boldsymbol{\theta})$ in $\boldsymbol{V}$ such that

$$\boldsymbol{a}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{v}; \boldsymbol{\theta}) = \boldsymbol{f}(\boldsymbol{v}) \qquad \forall\ \boldsymbol{v} \in \boldsymbol{V}$$

where the space $\boldsymbol{V}$ is equipped with

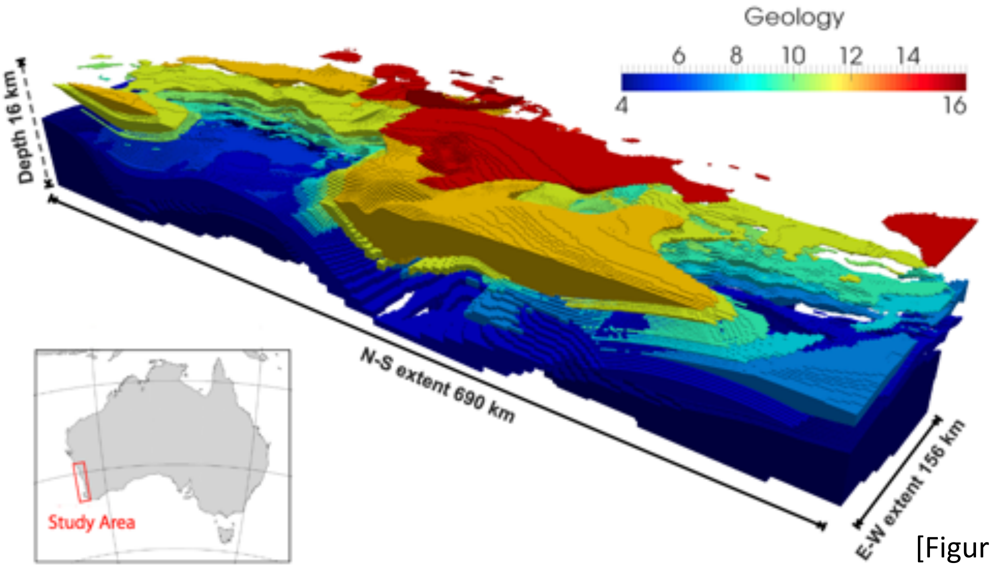
inner product $(\cdot,\cdot)_{\boldsymbol{V}}$

norm $\|\cdot\|_{\boldsymbol{V}} = (\cdot,\cdot)_{\boldsymbol{V}}^{\frac{1}{2}}$

and the **hyper-parameter**, $\boldsymbol{\theta} \in \mathcal{D}$, represents variabilities or uncertainties.

Parametrized PDEs

Example



Perth Basin

- Model: heat conduction
- Hyper-parameters: conductivities

[Figure courtesy of F. Wellmann (RWTH Aachen)]

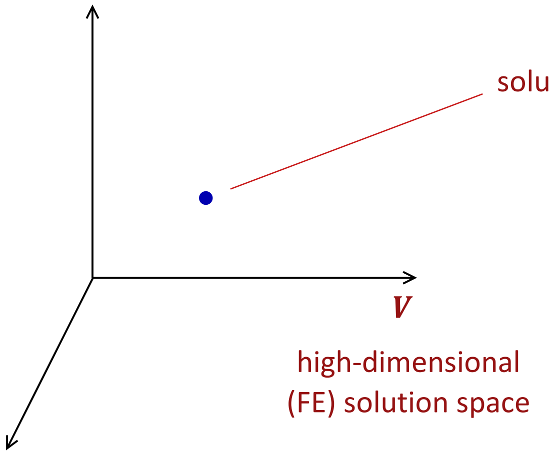
Wellmann and Reid, “Basin-scale Geothermal Model Calibration: Experience from the Perth Basin, Australia”, Energy Procedia, 59:382-389, 2014.

Parametrized PDEs

Parametrized Model

Find $\boldsymbol{u}(\boldsymbol{\theta})$ in $\boldsymbol{V}$ such that

$$a(u(\theta), v; \theta) = f(v) \qquad \forall\, v \in V$$



solution $\boldsymbol{u}(\boldsymbol{\theta})$ for some $\boldsymbol{\theta}$ in $\boldsymbol{\mathcal{D}}$

$\boldsymbol{V}$

high-dimensional
(FE) solution space

Parametrized PDEs

Parametrized Model

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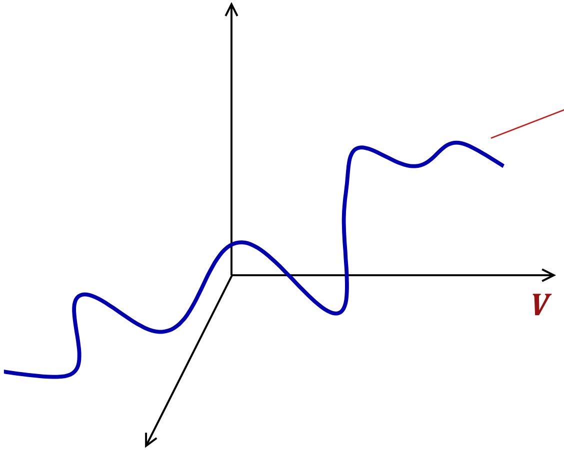


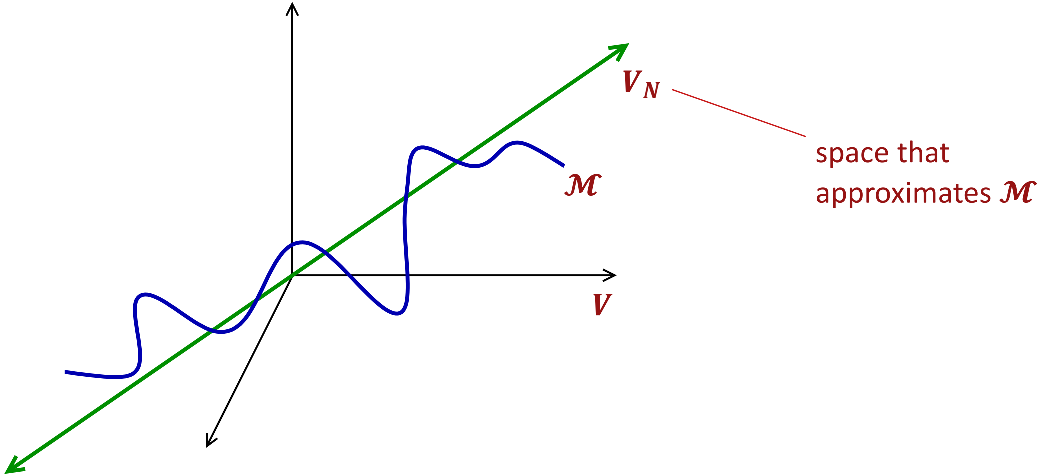
solution manifold
$\mathcal{M} := \{\boldsymbol{u}(\boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathcal{D}\}$

Parametrized PDEs

Parametrized Model

For $\boldsymbol{\theta} \in \boldsymbol{\mathcal{D}}$, find $\boldsymbol{u}(\boldsymbol{\theta})$ in $\boldsymbol{V}$ such that

$$a(u(\theta), v; \theta) = f(v) \qquad \forall\, v \in \boldsymbol{V}$$



space that approximates $\mathcal{M}$

Parametrized PDEs

Parametrized Model

Find $\boldsymbol{u}(\boldsymbol{\theta})$ in $\boldsymbol{V}$ such that

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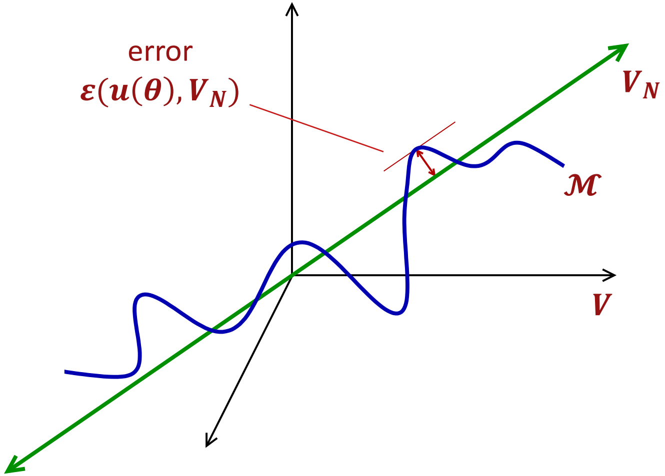

For each $\boldsymbol{\theta} \boldsymbol{\epsilon} \boldsymbol{\mathcal{D}}$, the error is

$$\boldsymbol{\varepsilon}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{V}_N) \coloneqq \inf_{\boldsymbol{v} \in \boldsymbol{V}_N} \|\boldsymbol{u}(\boldsymbol{\theta}) - \boldsymbol{v}\|$$

(see, e.g., [COHEN & DEVORE, ’15])

Parametrized PDEs

Parametrized Model

Find $\boldsymbol{u}(\boldsymbol{\theta})$ in $\boldsymbol{V}$ such that

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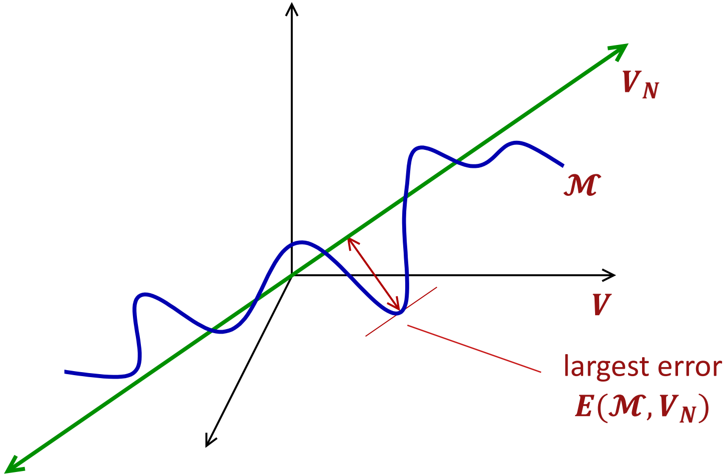

largest error $E(\mathcal{M}, V_N)$

For each $\boldsymbol{\theta} \in \boldsymbol{\mathcal{D}}$, the error is

$$\boldsymbol{\varepsilon}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{V_N}) := \inf_{\boldsymbol{v} \in \boldsymbol{V_N}} \|\boldsymbol{u}(\boldsymbol{\theta}) - \boldsymbol{v}\|$$

The error on $\boldsymbol{\mathcal{M}}$ is then

$$\boldsymbol{E}(\boldsymbol{\mathcal{M}}, \boldsymbol{V_N}) := \sup_{\boldsymbol{\theta} \in \boldsymbol{\mathcal{D}}} \boldsymbol{\varepsilon}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{V_N})$$

(see, e.g., [COHEN & DEVORE, '15])

Parametrized PDEs

Parametrized Model

Find $\boldsymbol{u(\theta)}$ in $\boldsymbol{V}$ such that

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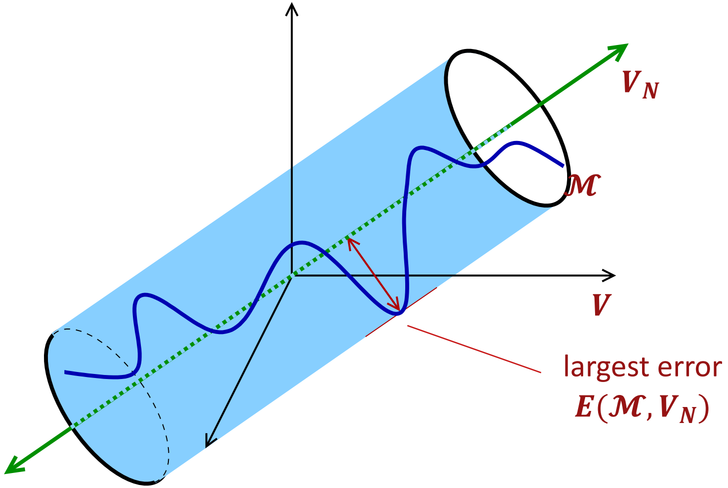

largest error
$E(\mathcal{M}, V_N)$

For each $\boldsymbol{\theta} \,\epsilon\, \boldsymbol{\mathcal{D}}$, the error is

$$\varepsilon(u(\theta), V_N) \;:=\; \inf_{v\, \in V_N} \|u(\theta) - v\|$$

The error on $\boldsymbol{\mathcal{M}}$ is then

$$E(\mathcal{M}, V_N) \;:=\; \sup_{\theta\, \in\, \mathcal{D}} \;\varepsilon(u(\theta), V_N)$$

(see, e.g., [COHEN & DEVORE, ’15])

2 - MODEL + DATA

DATA ASSIMILATION

pPDEs and Least Squares

Method of Least Squares

Given observations $\boldsymbol{d} = \boldsymbol{L}(\boldsymbol{u}_{\mathbf{t}}) + \boldsymbol{\delta} \in \mathbb{R}^{\boldsymbol{M}}$, find the state $\boldsymbol{u}^* \in \boldsymbol{\mathcal{M}}$ such that

true state
"$\boldsymbol{u}$-true"

$$\boldsymbol{u}^* = \arg\min_{\boldsymbol{u} \in \boldsymbol{\mathcal{M}}} \|\boldsymbol{L}(\boldsymbol{u}) - \boldsymbol{d}\|_{\boldsymbol{Z}}^{\mathbf{2}}$$

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Remarks

- Let $\boldsymbol{L}(\boldsymbol{u}) = [\, \boldsymbol{l}_{\boldsymbol{1}}(\boldsymbol{u}), \boldsymbol{l}_{\boldsymbol{2}}(\boldsymbol{u}), \dots, \boldsymbol{l}_{\boldsymbol{i}}(\boldsymbol{u}), \dots \boldsymbol{l}_{\boldsymbol{M}}(\boldsymbol{u}) \,]^{\boldsymbol{T}}$ represent $\boldsymbol{M}$ measurements
- How do we choose the norm, $\|\boldsymbol{v}\|_{\boldsymbol{Z}}^{\boldsymbol{2}} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{Z}\,\boldsymbol{v}$?
- Standard choice is $\boldsymbol{Z} = \boldsymbol{C}^{-\boldsymbol{1}}$, where $\boldsymbol{C}$ is the observation error covariance matrix
- Here, we choose $\boldsymbol{Z}$ such that we measure the **observable distance** between $\boldsymbol{u}$ and $\boldsymbol{u}_{\mathrm{t}}$

pPDEs and Least Squares

Given the measurement functionals $\boldsymbol{l_i}$, let $\boldsymbol{T_M} \subset \boldsymbol{V}$ be the measurement space of observable states:

$$\boldsymbol{T_M := \text{span}\,\{\ \underbrace{\tau_i}_{\text{orthonormal basis}}\ ,\ \ i = 1, \ldots, M\ \} = \text{span}\,\{\ \underbrace{\rho_i}_{\text{Riesz representers of the measurement functionals}}\ ,\ \ i = 1, \ldots, M\ \}}$$

where

$$\boldsymbol{l_i(v) = (\rho_i, v)_V \qquad \forall v \in V}$$

[BENNETT, ’85]
[MADAY, PATERA, PENN & YANO, ’14]
[MOORE, ARANGO, EDWARDS, ’17]

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orthonormal basis

Riesz representers
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[MADAY, PATERA, PENN & YANO, ’14]
[MOORE, ARANGO, EDWARDS, ’17]

By letting

$$\boldsymbol{Z_{ij}^{-1} = (\rho_j, \rho_i)_V}$$

it can be shown that

$$\boldsymbol{\|L(u) - d\|_Z^2 = \|\Pi_{T_M}(u - u_t)\|_V^2}$$

pPDEs and Least Squares

Method of Least Squares

Given (perfect) observations

$$\boldsymbol{d} = \boldsymbol{L}(\boldsymbol{u}_{\mathbf{t}}) \in \mathbb{R}^{\boldsymbol{M}}$$

find $\boldsymbol{u}^*\in\boldsymbol{\mathcal{M}}$ such that

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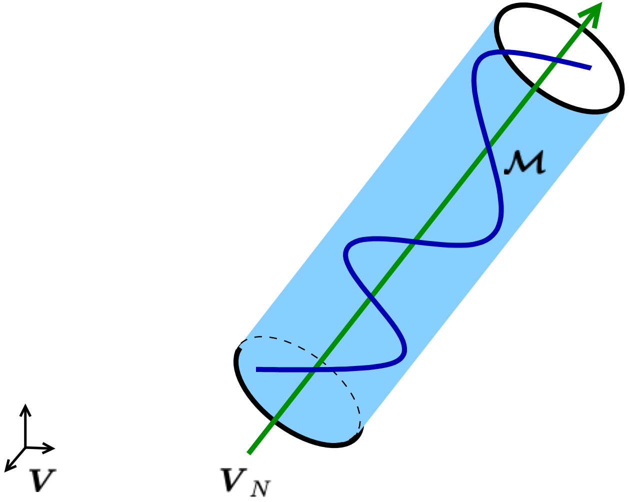

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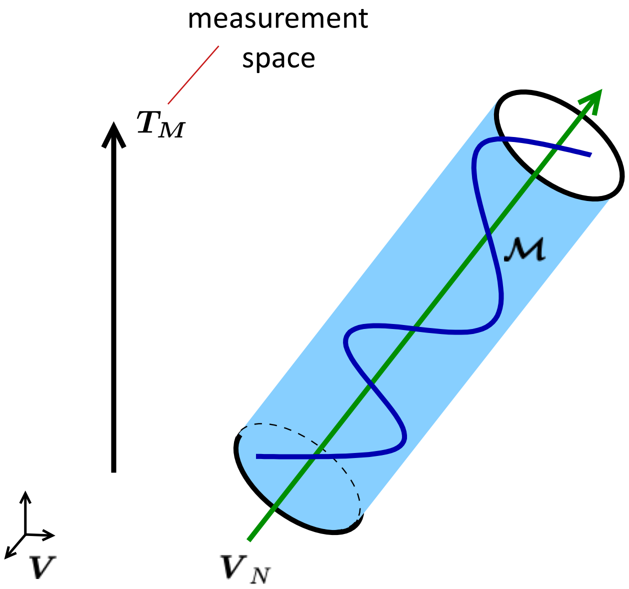

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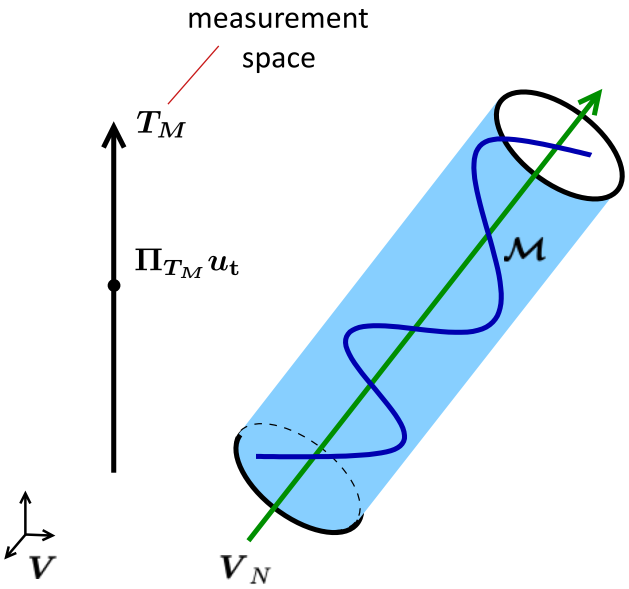

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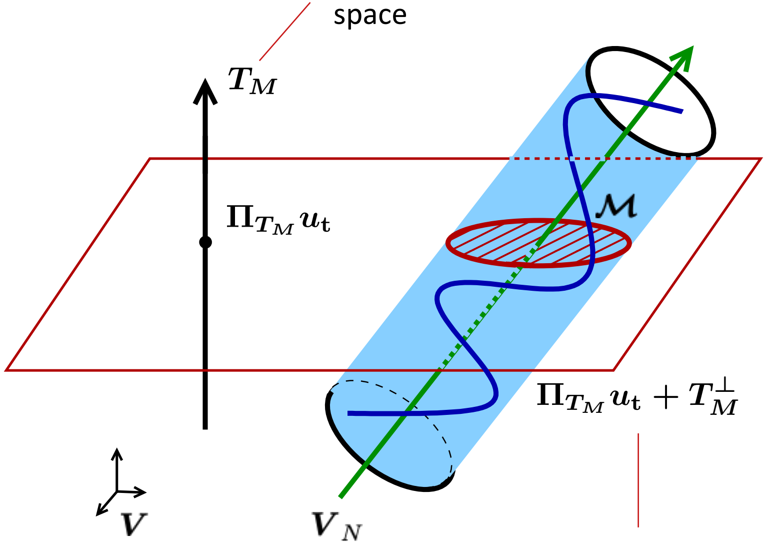

measurement space

space of all states that agree with the data

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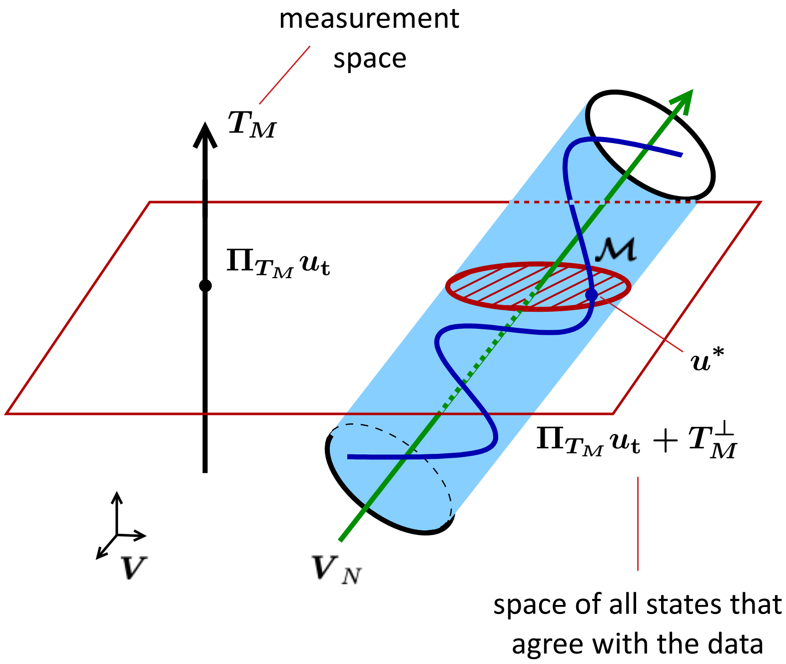

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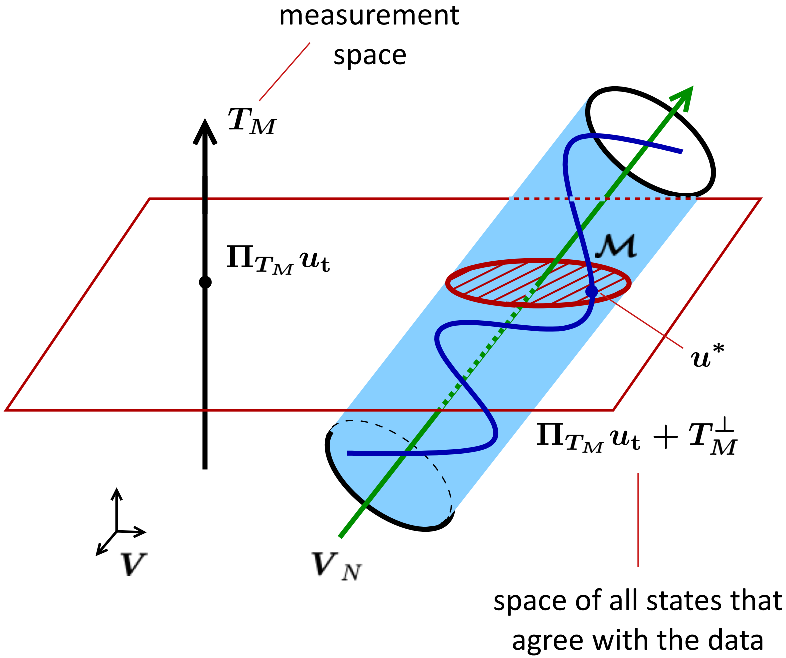
Remark:

- computational expense



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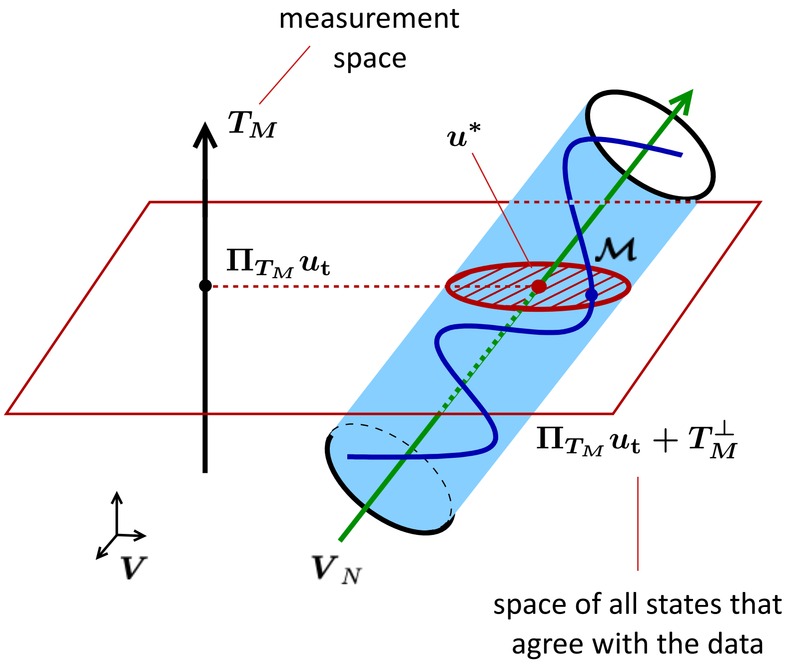


Remark:

- computational expense
- replace $\mathcal{M}$ by low-dimensional V_N

$\Longrightarrow$ <u>P</u>arametrized <u>B</u>ackground <u>D</u>ata <u>W</u>eak Method

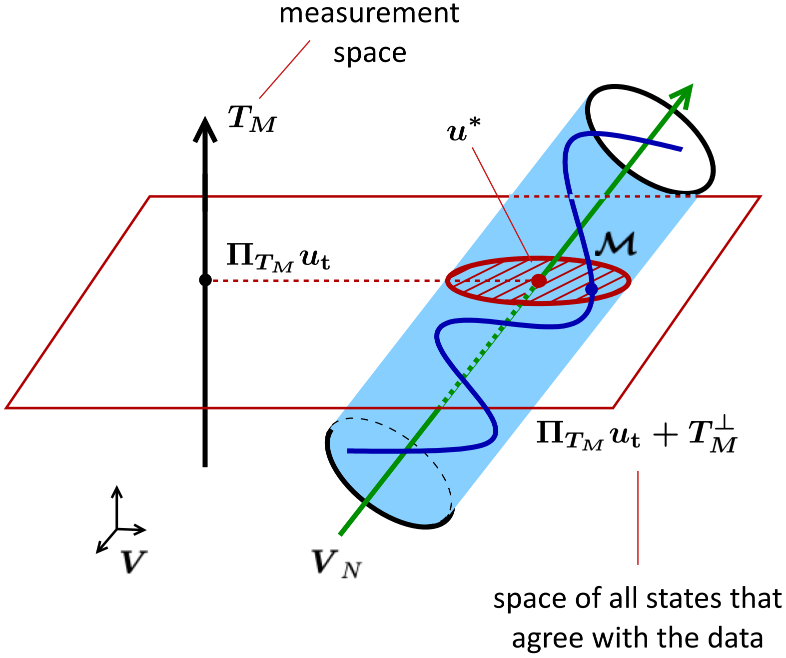
pPDEs and Least Squares

Parametrized Background Data Weak Formulation

Find z_N^* given by

$$\arg \inf_{z \in V_N} \|\Pi_{T_M}(z - u_t)\|^2$$

[MADAY, PATERA, PENN & YANO, ’14]



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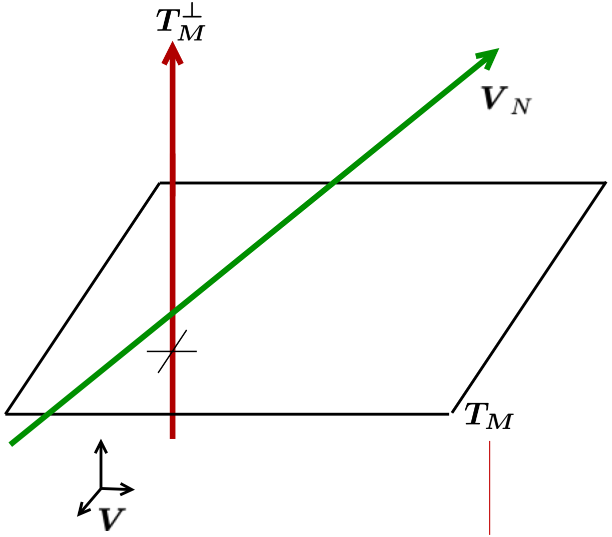

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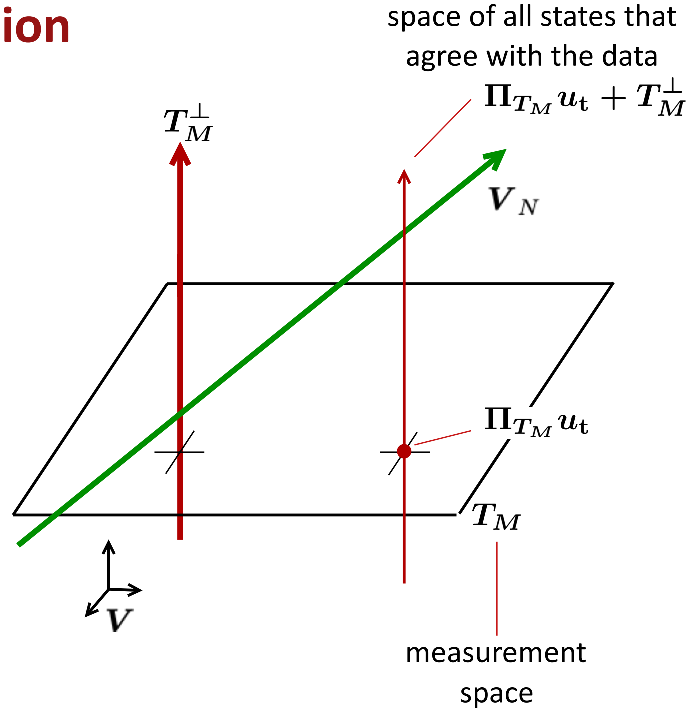

pPDEs and Least Squares

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misfit

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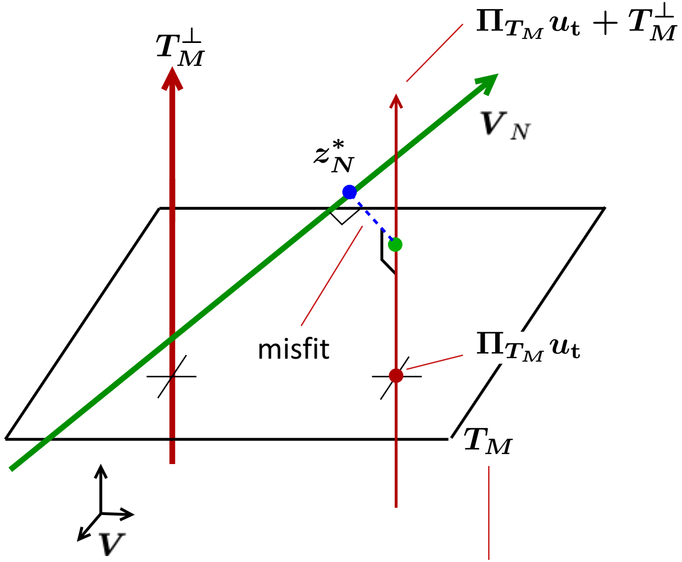

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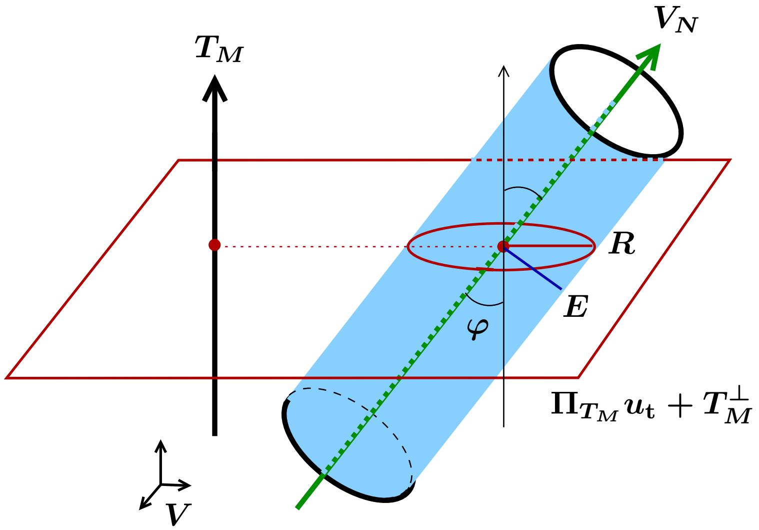

Angle φ between V_N and T_M plays an important role:

$$R = \frac{E}{\cos \varphi}$$

pPDEs and Least Squares

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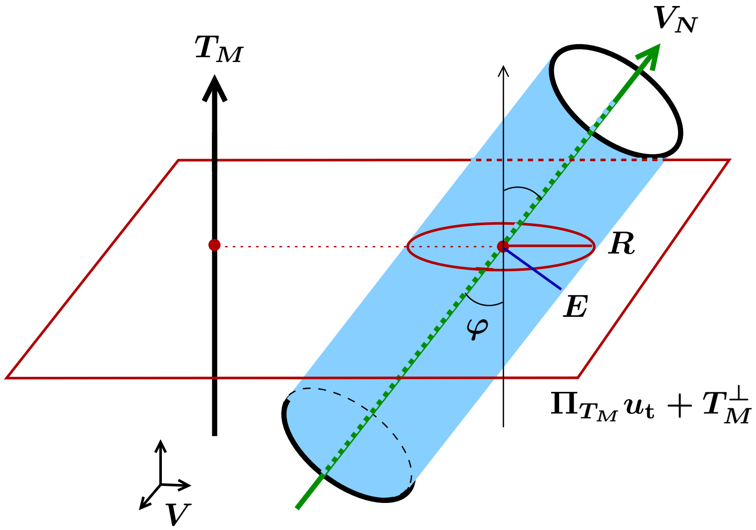


Angle φ between V_N and T_M plays an important role:

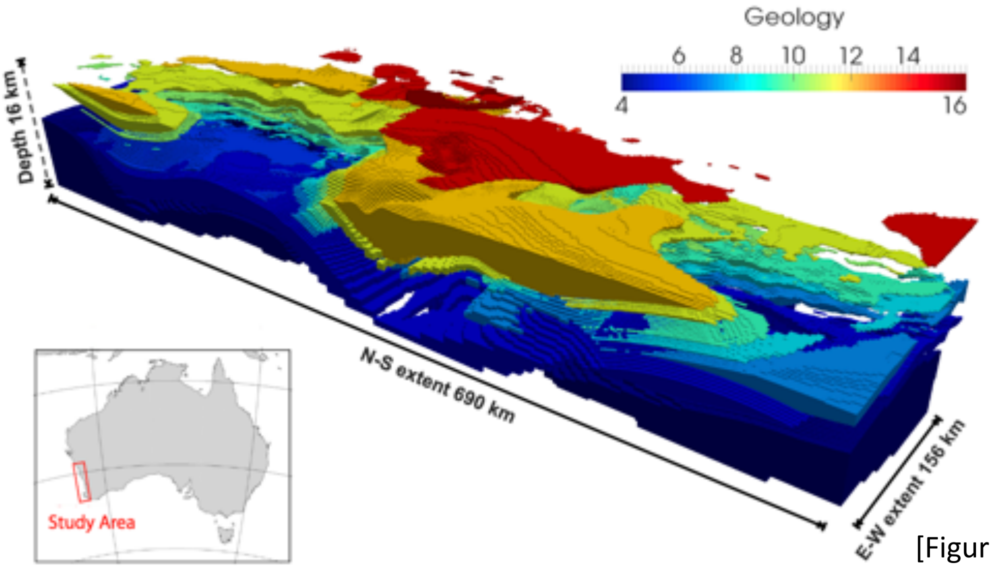
$$R = \frac{E}{\cos\varphi}$$

where

$$\cos\varphi = \inf_{v \in V_N} \sup_{\tau \in T_M} \frac{(v, \tau)_V}{\|v\|_V \, \|\tau\|_V}$$

Our Context

Geophysics Example



Perth Basin

- Model: heat diffusion
- Hyper-parameters: conductivities

[Figure courtesy of F. Wellmann (RWTH Aachen)]

Wellmann and Reid, “Basin-scale Geothermal Model Calibration: Experience from the Perth Basin, Australia”, Energy Procedia, 59:382-389, 2014.

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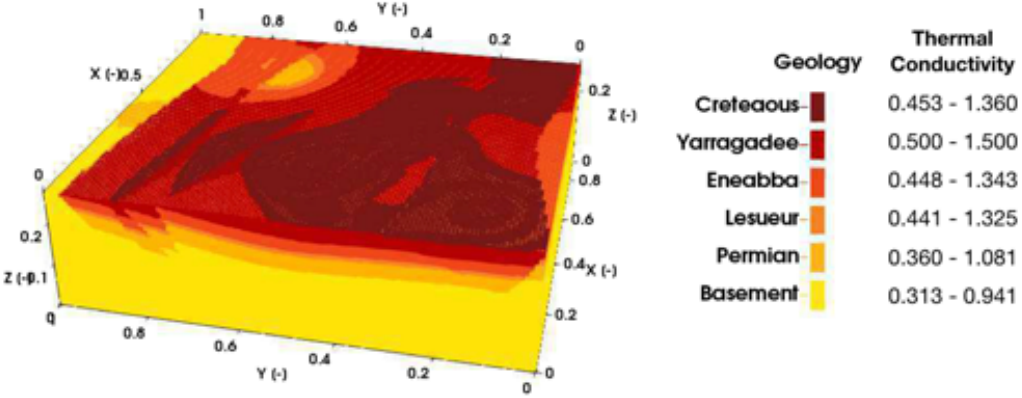

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Degen, V. & Wellmann. 2019. *Certified Reduced Basis Method in Geosciences Addressing the Challenge of High Dimensional Problems*. EarthArXiv.

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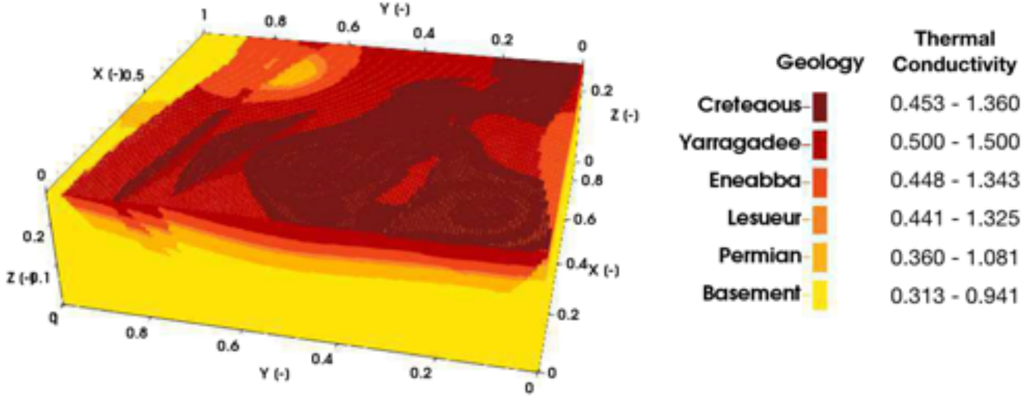

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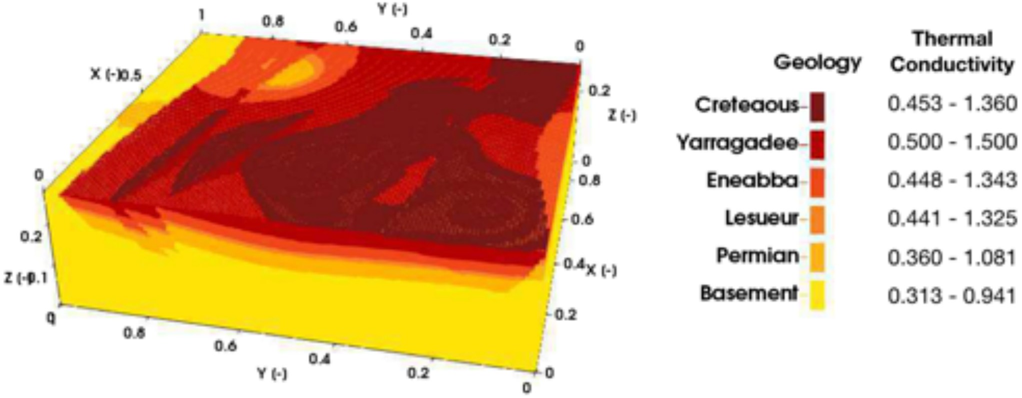

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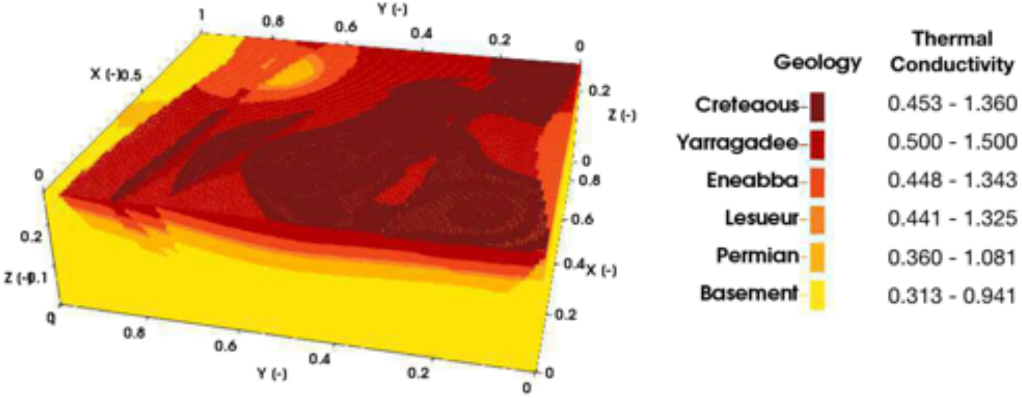
Remarks

- Importance of model and (hyper-)parameters for prediction

Degen, V. & Wellmann. 2019. *Certified Reduced Basis Method in Geosciences Addressing the Challenge of High Dimensional Problems*. EarthArXiv.

Our Context

Geophysics Example



Perth Basin

- Model: heat diffusion
- Hyper-parameters: conductivities
- Parameters: boundary condition

Remarks

- Importance of model and (hyper-)parameters for prediction
- Well-posedness + number of measurements

Degen, V. & Wellmann. 2019. *Certified Reduced Basis Method in Geosciences Addressing the Challenge of High Dimensional Problems*. EarthArXiv.

Variational Data Assimilation

Find $(\boldsymbol{p}^*(\boldsymbol{\theta}), \boldsymbol{u}^*(\boldsymbol{\theta})) \in \boldsymbol{\mathcal{C}} \times \boldsymbol{V}$ that solves

parameter
(model correction)

regularization parameter

$$\min_{\boldsymbol{p} \in \boldsymbol{\mathcal{C}}} \frac{1}{2} \| \boldsymbol{p} \|_{\boldsymbol{\mathcal{C}}}^2 + \frac{\boldsymbol{\lambda}}{2} \| \boldsymbol{\Pi}_{\boldsymbol{T_M}} (\boldsymbol{u_t} - \boldsymbol{u}) \|_{\boldsymbol{V}}^2$$

observable misfit

s.t. $$\boldsymbol{a}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{v}; \boldsymbol{\theta}) = \boldsymbol{f}_{\mathbf{bk}}(\boldsymbol{v}) + \boldsymbol{f}_{\mathbf{co}}(\boldsymbol{p}(\boldsymbol{\theta}), \boldsymbol{v}), \quad \forall \, \boldsymbol{v} \in \boldsymbol{V}$$

pPDE constraint

best knowledge

model correction

[ARETZ-NELLESEN, GREPL, V., ’19]

- Enforces model as a constraint
- Permits and learns corrections to the model through parameter $\boldsymbol{p}$
- Regularizes by balancing trust in the model vs trust in the data

Variational Data Assimilation

Find $(p^*(\theta),\, u^*(\theta)) \in \mathcal{C} \times V$ that solves

parameter
(model correction)

regularization parameter

$$\min_{p\,\in \mathcal{C}} \; \frac{1}{2} \| \, p \, \|^2_{\mathcal{C}} + \frac{\lambda}{2} \| \, \Pi_{T_M}(u_t - u) \, \|^2_V$$

observable misfit

s.t. $$a(u(\theta), v; \theta) \; = \; f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p(\theta), v), \quad \forall \, v \in V$$

pPDE constraint

best knowledge

model correction

[ARETZ-NELLESEN, GREPL, V., ’19]

- Variational data assimilation (3D-/4D-VAR) has a long history in weather forecasting
  [LORENC, ’81], [LE DIMET, ’81], [COURTIER, ’85], [LE DIMET & TALAGRAND, ’86], …
  …, [LAW, STUART & ZYGALAKIS , ’15], [REICH & COTTER, ’15], …
- Differs from PBDW in regularization term (*) and in PDE-constraint

Variational Data Assimilation

Find $(p^*(\theta),\, u^*(\theta)) \in \mathcal{C} \times V$ that solves

parameter
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regularization parameter

$$\min_{p\,\in\mathcal{C}} \ \frac{1}{2}\|\, p \,\|_{\mathcal{C}}^2 + \frac{\lambda}{2}\|\, \Pi_{T_M}(u_t - u)\,\|_V^2$$

observable misfit

s.t. $$a(u(\theta), v; \theta) \ = \ f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p(\theta), v), \quad \forall\, v \in V$$

pPDE constraint

best knowledge

model correction

[ARETZ-NELLESEN, GREPL, V., ’19]

- Variational data assimilation (3D-/4D-VAR) has a long history in weather forecasting

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…, [LAW, STUART & ZYGALAKIS , ’15], [REICH & COTTER, ’15], …

- Differs from PBDW in regularization term (*) and in PDE-constraint
- Computationally expensive

3 - DATA

STABILITY-BASED OED via MODEL ORDER REDUCTION

Joint work with N. Aretz-Nellesen & M. Grepl

Variational Data Assimilation

Find $(p^*(\theta),\, u^*(\theta)) \in \mathcal{C} \times V$ that solves

$$\min_{p\,\in\mathcal{C}} \; \frac{1}{2}\|\, p\,\|_{\mathcal{C}}^2 + \frac{\lambda}{2}\|\, \Pi_{T_M}(u_{\mathrm{t}} - u)\,\|_V^2$$

s.t. $$a(u(\theta), v; \theta) \;=\; f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p(\theta), v), \quad \forall\, v \in V$$ pPDE constraint

[ARETZ-NELLESEN, GREPL, V., ’19]

Lagrangian

$$\mathcal{L}(u, \varphi, p; \theta) = \underbrace{\frac{1}{2}\,\|\, p\,\|_{\mathcal{C}}^2 \,+\, \frac{\lambda}{2}\,\|\, \Pi_{T_M}(u - u_{\mathrm{t}})\,\|_V^2}_{\text{cost function}} \,+\, \underbrace{a(u, \varphi) \,-\, f_{\mathrm{bk}}(\varphi) \,-\, f_{\mathrm{co}}(p, \varphi)}_{\text{constraint}}$$

Variational Data Assimilation

Lagrangian

$$\mathcal{L}(u,\varphi,p;\theta) = \frac{1}{2}\,\|\,p\,\|_{\mathcal{C}}^{2} + \frac{\lambda}{2}\,\|\,\Pi_{T_M}(u-u_{\mathrm{t}})\,\|_{V}^{2} + a(u,\varphi) - f_{\mathrm{bk}}(\varphi) - f_{\mathrm{co}}(p,\varphi)$$

Optimality Conditions

$$\begin{array}{rcll}
f(\chi,\varphi^{*}) - (p^{*},\chi)_{\mathcal{C}} & = & 0 & \mathcal{L}_{p} \\
\lambda\,(\zeta,\Pi_{T_M}(u_{\mathrm{true}} - u^{*}))_{V} - a(\zeta,\varphi^{*}) & = & 0 & \mathcal{L}_{u} \\
f_{\mathrm{bk}}(\xi) + f_{\mathrm{co}}(p^{*},\xi) - a(u^{*},\xi) & = & 0 & \mathcal{L}_{\varphi}
\end{array}$$

$$\forall\,\chi \in \mathcal{C},\;\; \zeta \in V,\;\; \xi \in V$$

Stability Analysis

One can show that

$$\begin{aligned} \|(p_\theta^*, u_\theta^*)\|_{\mathcal{C}\times V} &\leq C_\theta^1(\lambda)\|\Pi_{T_M} u_{\mathrm{t}}\|_V + C_\theta^2(\lambda)\|f_{\mathrm{bk}}\|_{V'} \\ \|\varphi_\theta^*\|_V &\leq C_\theta^3(\lambda)\|\Pi_{T_M} u_{\mathrm{t}}\|_V + C_\theta^4(\lambda)\|f_{\mathrm{bk}}\|_{V'} \end{aligned}$$

Stability Analysis

One can show that

$$\begin{aligned} \|(p_\theta^*, u_\theta^*)\|_{\mathcal{C}\times V} &\leq C_\theta^1(\lambda)\|\Pi_{T_M} u_{\mathrm{t}}\|_V + C_\theta^2(\lambda)\|f_{\mathrm{bk}}\|_{V'} \\ \|\varphi_\theta^*\|_V &\leq C_\theta^3(\lambda)\|\Pi_{T_M} u_{\mathrm{t}}\|_V + C_\theta^4(\lambda)\|f_{\mathrm{bk}}\|_{V'} \end{aligned}$$

where the positive stability constants are “better behaved” for

$$\eta(\theta) := \inf_{(p,u)\in\mathcal{H}^0(\theta)} \frac{\|u\|_V}{\|p\|_{\mathcal{C}}} \geq 0, \qquad \beta_{T_M}(\theta) := \inf_{v\in V_\theta} \sup_{\tau\in T_M} \frac{(v,\tau)_V}{\|v\|_V\|\tau\|_V} \geq 0$$

as large as possible. Here,

$$\begin{aligned} \mathcal{H}^0(\theta) &:= \{\ (p,u) \in \mathcal{C}\times V : a_\theta(u,\psi) = f_{\mathrm{co}}(p,\psi) \quad \forall\psi\in V\ \}, \\ V_\theta &:= \{\ v\in V : \exists\ p \in \mathcal{C} \text{ s.t. } a_\theta(v,\psi) = f_{\mathrm{co}}(p,\psi) \quad \forall\psi\in V\ \}. \end{aligned}$$

Stability Analysis

Find $(\boldsymbol{p}^*(\boldsymbol{\theta}),\, \boldsymbol{u}^*(\boldsymbol{\theta})) \in \boldsymbol{\mathcal{C}} \times \boldsymbol{V}$ that solves

$$\min_{p \in \mathcal{C}} \frac{1}{2} \| p \|_{\mathcal{C}}^2 + \frac{\lambda}{2} \| \Pi_{T_M} (u_{\mathrm{t}} - u) \|_V^2$$

s.t. $$a(u(\theta), v; \theta) \quad = \quad f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p(\theta), v), \quad \forall\, v \in V$$ pPDE constraint

[ARETZ-NELLESEN, GREPL, V., ’19]

Stability Analysis

Find $\boldsymbol{\theta}^* \in \boldsymbol{\mathcal{D}}$ and $(\boldsymbol{p}^*(\boldsymbol{\theta}^*), \boldsymbol{u}^*(\boldsymbol{\theta}^*)) \in \boldsymbol{\mathcal{C}} \times \boldsymbol{V}$ that solves

$$\left(\min_{\boldsymbol{\theta} \in \boldsymbol{\mathcal{D}}}\right) \min_{\boldsymbol{p} \in \boldsymbol{\mathcal{C}}} \ \frac{\mathbf{1}}{\mathbf{2}} \| \boldsymbol{p} \|^{\mathbf{2}}_{\boldsymbol{\mathcal{C}}} + \frac{\boldsymbol{\lambda}}{\mathbf{2}} \| \boldsymbol{\Pi}_{\boldsymbol{T_M}} (\boldsymbol{u}_{\mathbf{t}} - \boldsymbol{u}) \|^{\mathbf{2}}_{\boldsymbol{V}}$$

s.t. $$\boldsymbol{a}(\boldsymbol{u}(\boldsymbol{\theta}), \boldsymbol{v}; \boldsymbol{\theta}) \quad = \quad \boldsymbol{f}_{\mathbf{bk}}(\boldsymbol{v}) + \boldsymbol{f}_{\mathbf{co}}(\boldsymbol{p}(\boldsymbol{\theta}), \boldsymbol{v}), \quad \forall\ \boldsymbol{v} \in \boldsymbol{V}$$

pPDE constraint

[ARETZ-NELLESEN, GREPL, V., ’19]

Stability Analysis

Find $(\boldsymbol{p}^*(\boldsymbol{\theta}), \boldsymbol{u}^*(\boldsymbol{\theta})) \in \boldsymbol{\mathcal{C}} \times \boldsymbol{V}$ that solves

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[ARETZ-NELLESEN, GREPL, V., ’19]

Stability Analysis

Find $(p_N^*(\theta),\, u_N^*(\theta)) \in \mathcal{C} \times V_N$ that solves

$$\min_{p_N \in \mathcal{C}} \; \frac{1}{2} \| \, p_N \, \|_{\mathcal{C}}^2 + \frac{\lambda}{2} \| \, \Pi_{T_M} (u_t - u_N) \, \|_V^2$$

s.t. $$a(u_N(\theta), v; \theta) \;=\; f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p_N, v), \quad \forall \, v \in V_N$$

[ARETZ-NELLESEN, GREPL, V., ’19]

Stability Analysis

Find $(p_N^*(\theta), u_N^*(\theta)) \in \mathcal{C} \times V_N$ that solves

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s.t. $$a(u_N(\theta), v; \theta) = f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(p_N, v), \quad \forall\, v \in V_N$$

[ARETZ-NELLESEN, GREPL, V., ’19]

Assume that

$$\|u - u_N\|_V \leq \varepsilon_\theta \|u\|_V \qquad \text{where} \quad 0 \leq \varepsilon_\theta \ll 1$$

Then

$$\beta_T(\theta) \geq (1 - \varepsilon_\theta)\, \beta_{T,N}(\theta) - \varepsilon_\theta$$

Stability Analysis

Find $(\boldsymbol{p}_N^*(\theta), \boldsymbol{u}_N^*(\theta)) \in \mathcal{C} \times V_N$ that solves

$$\min_{p_N \in \mathcal{C}} \frac{1}{2} \| p_N \|_{\mathcal{C}}^2 + \frac{\lambda}{2} \| \Pi_{T_M}(u_t - u_N) \|_V^2$$

s.t. $$a(u_N(\theta), v; \theta) = f_{\mathrm{bk}}(v) + f_{\mathrm{co}}(v; p_N), \quad \forall\, v \in V_N$$

[ARETZ-NELLESEN, GREPL, V., ’19]

- Order reduction for PDE (governing the model dynamics) or for optimization space

e.g., [Robert, Durbiano, Blayo, Verron, Blum, Le Dimet, ’05], [Chen, Navon, Fang, ’09], [Dimitriu, Apreutesei, Stefanescu, ’10], [Stefanescu, Sandu, Navon, ’15], [Nadal, Chinesta, Diez, Fuenmayor & Denia, ’15] …

- Order reduction for entire control problem (also $\mathcal{C}_N$)

connection bet. 3D-/4DVAR and control —— ([Le Dimet & Talagrand ‘86])

model order reduction for 4DVAR —— **[Kärcher, Boyaval, Grepl & V., ’18]**

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$
\begin{array}{rclll}
(\boldsymbol{p}_\theta^*, \boldsymbol{\chi})_{\boldsymbol{\mathcal{C}}} - f_{\mathrm{co}}(\boldsymbol{\chi}, \boldsymbol{\varphi}_\theta^*) & = & \mathbf{0} & \forall\, \boldsymbol{\chi} \in \boldsymbol{\mathcal{C}} & \text{control} \\
a_\theta(\boldsymbol{\zeta}, \boldsymbol{\varphi}_\theta^*) - \boldsymbol{\lambda}(\boldsymbol{\zeta}, \boldsymbol{d}_\theta^*)_{\boldsymbol{V}} & = & \mathbf{0} & \forall\, \boldsymbol{\zeta} \in \boldsymbol{V} & \text{adjoint} \\
a_\theta(\boldsymbol{u}_\theta^*, \boldsymbol{\xi}) - f_{\mathrm{co}}(\boldsymbol{p}_\theta^*, \boldsymbol{\xi}) & = & f_{\mathrm{bk}}(\boldsymbol{\xi}) & \forall\, \boldsymbol{\xi} \in \boldsymbol{V} & \text{state} \\
(\boldsymbol{u}_\theta^* + \boldsymbol{d}_\theta^*, \boldsymbol{\tau})_{\boldsymbol{V}} & = & (\boldsymbol{u}_{\mathrm{t}}, \boldsymbol{\tau})_{\boldsymbol{V}} & \forall\, \boldsymbol{\tau} \in \boldsymbol{T}_M & \text{misfit}
\end{array}
$$

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$
\begin{aligned}
(p_\theta^*, \chi)_{\mathcal{C}} - f_{\mathrm{co}}(\chi, \varphi_\theta^*) &= 0 && \boxed{\forall\, \chi \in \mathcal{C} \qquad \text{control}} \\
a_\theta(\zeta, \varphi_\theta^*) - \lambda(\zeta, d_\theta^*)_V &= 0 && \forall\, \zeta \in V \qquad \text{adjoint} \\
a_\theta(u_\theta^*, \xi) - f_{\mathrm{co}}(p_\theta^*, \xi) &= f_{\mathrm{bk}}(\xi) && \forall\, \xi \in V \qquad \text{state} \\
(u_\theta^* + d_\theta^*, \tau)_V &= (u_{\mathrm{t}}, \tau)_V && \forall\, \tau \in T_M \qquad \text{misfit}
\end{aligned}
$$

$\mathcal{C}$

Assume that the (control) space of
model corrections is low dimensional

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$(p^*_\theta, \chi)_{\mathcal{C}} - f_{\mathrm{co}}(\chi, \varphi^*_\theta) = 0 \qquad \forall\, \chi \in \mathcal{C} \qquad \text{control}$$

$$a_\theta(\zeta, \varphi^*_\theta) - \lambda(\zeta, d^*_\theta)_V = 0 \qquad \forall\, \zeta \in V \qquad \text{adjoint}$$

$$\boxed{a_\theta(u^*_\theta, \xi) - f_{\mathrm{co}}(p^*_\theta, \xi) = f_{\mathrm{bk}}(\xi) \qquad \forall\, \xi \in V \qquad \text{state}}$$

$$(u^*_\theta + d^*_\theta, \tau)_V = (u_{\mathrm{t}}, \tau)_V \qquad \forall\, \tau \in T_M \qquad \text{misfit}$$

$$\mathcal{C} \longrightarrow V_{u,N}$$

Construct an RB space for the state
Note that T_M is not yet required!

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$\begin{array}{rcllr}
(p^*_\theta, \chi)_{\mathcal{C}} - f_{\mathrm{co}}(\chi, \varphi^*_\theta) & = & 0 & \forall\, \chi \in \mathcal{C} & \text{control} \\
a_\theta(\zeta, \varphi^*_\theta) - \lambda(\zeta, d^*_\theta)_V & = & 0 & \forall\, \zeta \in V & \text{adjoint} \\
a_\theta(u^*_\theta, \xi) - f_{\mathrm{co}}(p^*_\theta, \xi) & = & f_{\mathrm{bk}}(\xi) & \forall\, \xi \in V & \text{state}
\end{array}$$

$$\boxed{(u^*_\theta + d^*_\theta, \tau)_V = (u_{\mathrm{t}}, \tau)_V \qquad \forall\, \tau \in T_M \qquad \text{misfit}}$$

$$\begin{tikzcd} \mathcal{C} \arrow[r] & V_{u,N} \arrow[r] & T_M \end{tikzcd}$$

Select optimal measurements via
greedy algorithm in the hyper-parameter domain +
orthogonal matching pursuit [BINEV et al., ’18]

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$(p_\theta^*, \chi)_{\mathcal{C}} - f_{\mathrm{co}}(\chi, \varphi_\theta^*) = 0 \qquad \forall\, \chi \in \mathcal{C} \qquad \text{control}$$

$$\boxed{a_\theta(\zeta, \varphi_\theta^*) - \lambda(\zeta, d_\theta^*)_V = 0 \qquad \forall\, \zeta \in V \qquad \text{adjoint}}$$

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$$(u_\theta^* + d_\theta^*, \tau)_V = (u_{\mathrm{t}}, \tau)_V \qquad \forall\, \tau \in T_M \qquad \text{misfit}$$

$$\begin{tikzcd} \mathcal{C} \arrow[r] & V_{u,N} \arrow[r] & T_M \arrow[r] & V_{\varphi,N} \end{tikzcd}$$

Construct an RB space for the adjoint

Computational Procedure

Projection-based Model Order Reduction

Recall optimality conditions

$$(p_\theta^*, \chi)_{\mathcal{C}} - f_{\mathrm{co}}(\chi, \varphi_\theta^*) = 0 \qquad \forall\, \chi \in \mathcal{C} \qquad \text{control}$$

$$\boxed{a_\theta(\zeta, \varphi_\theta^*) - \lambda(\zeta, d_\theta^*)_V = 0 \qquad \forall\, \zeta \in V \qquad \text{adjoint}}$$

$$a_\theta(u_\theta^*, \xi) - f_{\mathrm{co}}(p_\theta^*, \xi) = f_{\mathrm{bk}}(\xi) \qquad \forall\, \xi \in V \qquad \text{state}$$

$$(u_\theta^* + d_\theta^*, \tau)_V = (u_{\mathrm{t}}, \tau)_V \qquad \forall\, \tau \in T_M \qquad \text{misfit}$$

$$\mathcal{C} \longrightarrow V_{u,N} \longrightarrow T_M \longrightarrow V_{\varphi,N} \longrightarrow V_N = V_{u,N} + V_{\varphi,N}$$

Numerical Experiment

Thermal Block

- **State space**

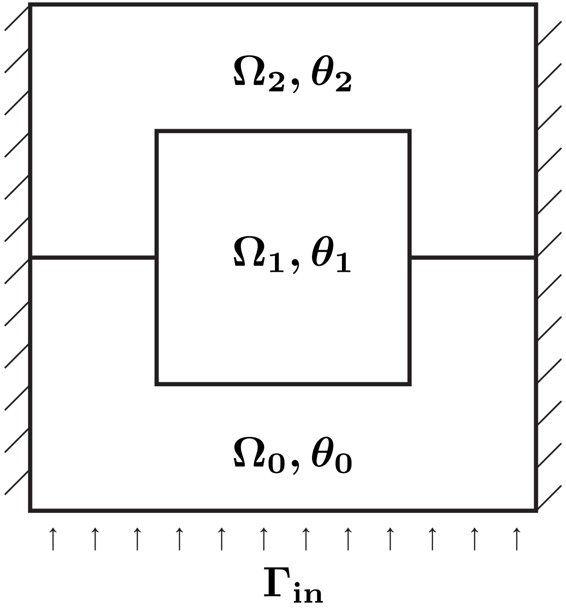
  $\boldsymbol{V}$ is an FE-discretization of

$$\mathcal{V} = \{v \in H^1(\Omega) \,:\, v|_{\Gamma_D} = 0\}$$

- **Hyper-parameter**

$$a_\theta(u, v) := \sum_{i=0}^{2} \theta_i \int_{\Omega_i} \nabla u \cdot \nabla w \, dx$$

where $\theta_0 = 1, \theta = (\theta_1, \theta_2) \in [0.1, 10]^2$



Numerical Experiment

Thermal Block

- **"Best-knowledge" boundary condition**

  Constant heat flux

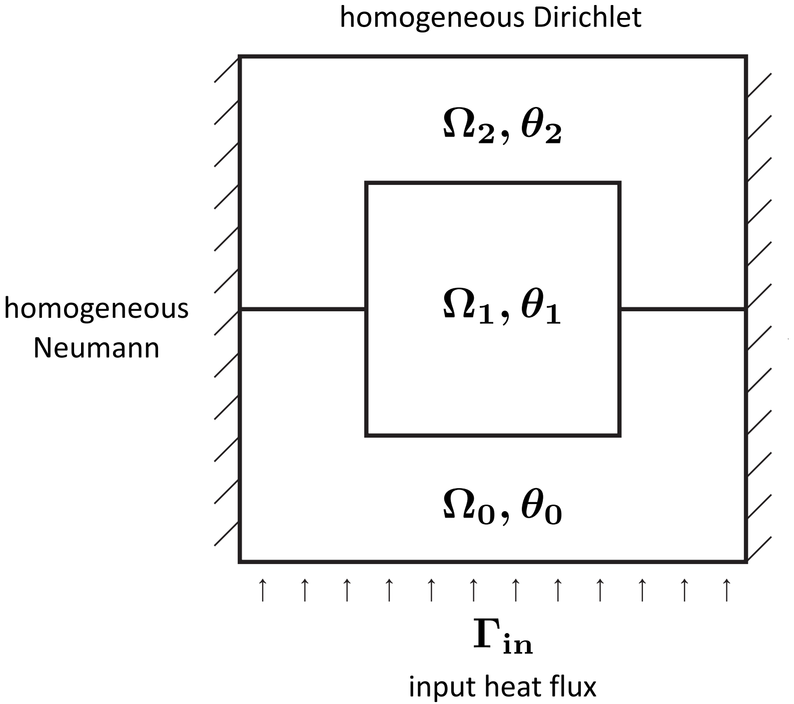
$$f_{\mathrm{bk}}(v) = \int_{\Gamma_{\mathrm{in}}} 1 \cdot v \, d\Gamma$$

- **Correction**

$$f_{\mathrm{co}}(p, v) = \int_{\Gamma_{\mathrm{in}}} p \, v \, d\Gamma, \quad p \in \mathcal{C} := L^2(\Gamma_{\mathrm{in}})$$

- **Low-dimensional approximation**

$$\mathcal{C}_N = \mathbb{P}_3 \quad \text{(polynomial space)}$$



Numerical Experiment

Thermal Block

- **“Unknown” true quantities**

Conductivity $\theta_{\mathrm{t}} = (7.0, 0.3) \in \mathcal{D}$

Input flux $p_{\mathrm{t}}(x) = 1.5 + 0.3\sin(2\pi x)$

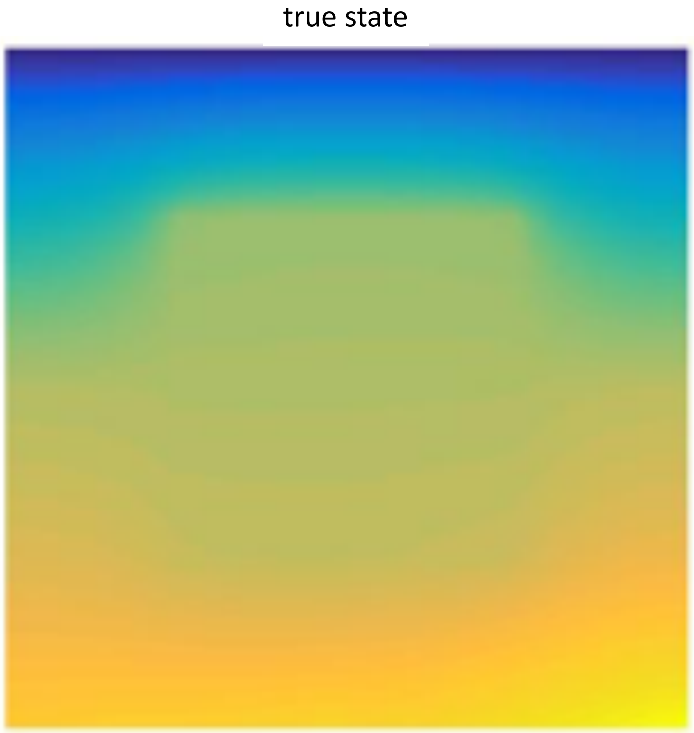
$x \in \Gamma_{\mathrm{in}}$

State $u_{\mathrm{t}} = u_{\theta_{\mathrm{t}}}(p_{\mathrm{t}})$

- **Measurements**

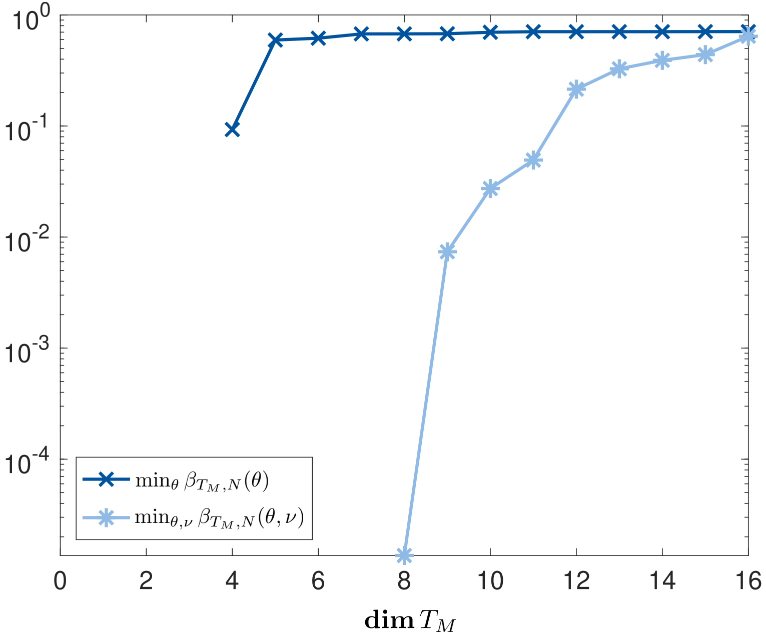
T_M is to be chosen from a library

$\mathcal{L}$ of a 49x49 grid of Gaussian functionals

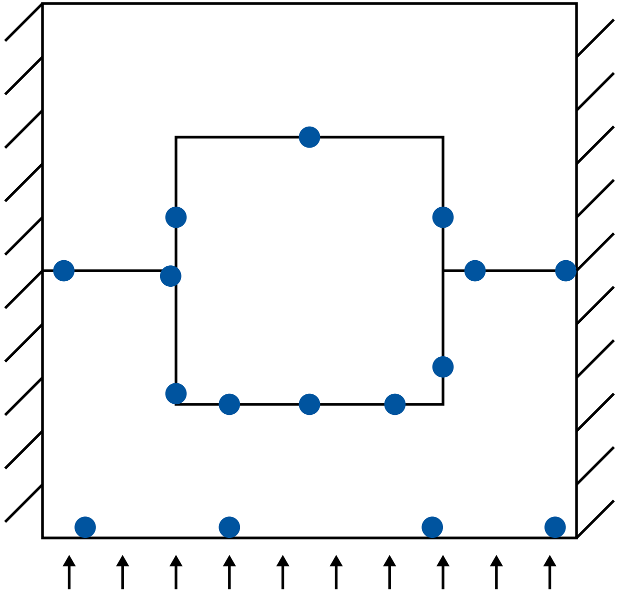


Numerical Experiment

Selection of the measurement space



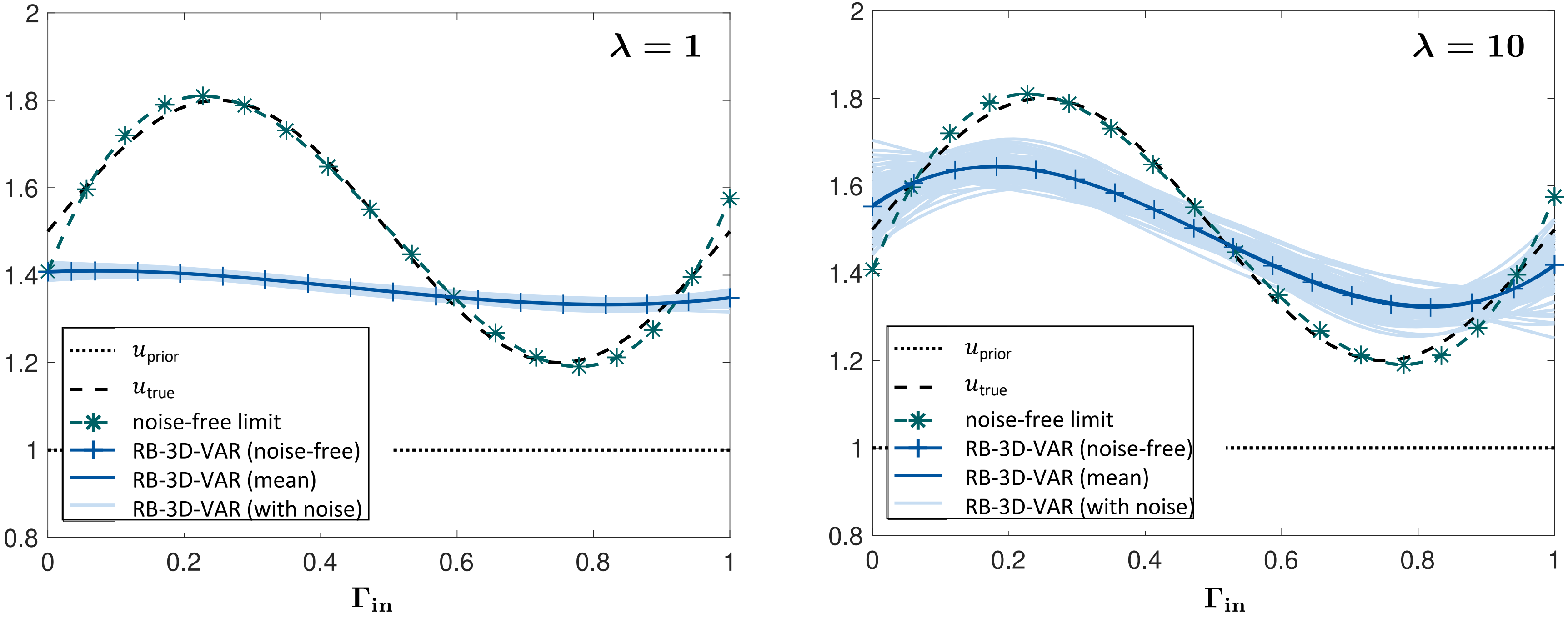
inf-sup constants during sensor selection



chosen sensor locations

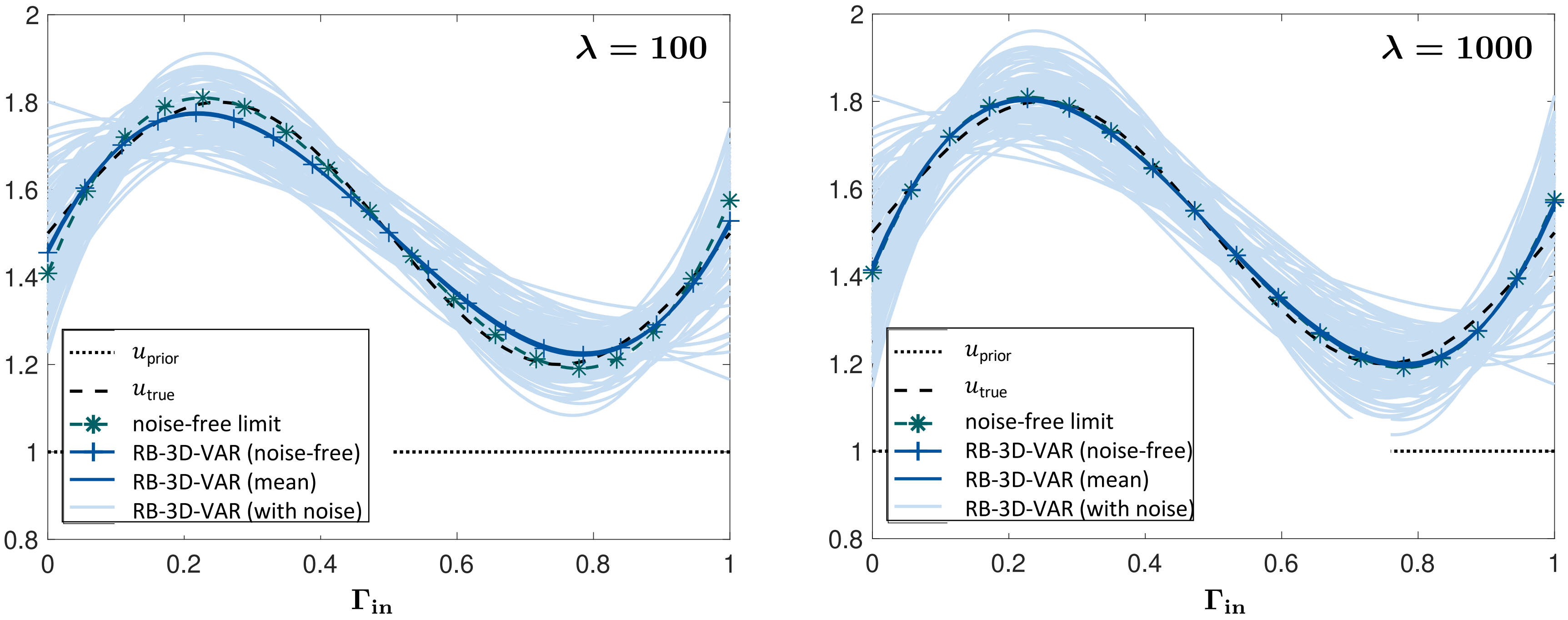
Numerical Experiment

3D-VAR Correction



Numerical Experiment

3D-VAR Correction



Numerical Experiment

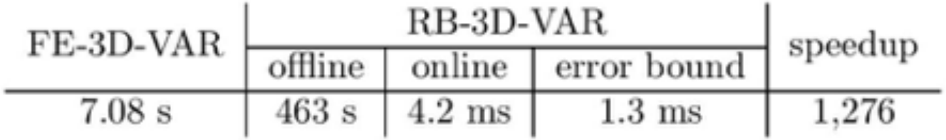
Construction of RB Spaces

$$\mathcal{C}_N \longrightarrow \boldsymbol{V}_{\boldsymbol{u},\boldsymbol{N}} \longrightarrow \boldsymbol{T}_{\boldsymbol{M}} \longrightarrow \boldsymbol{V}_{\boldsymbol{\varphi},\boldsymbol{N}} \longrightarrow \boldsymbol{V}_{\boldsymbol{N}} = \boldsymbol{V}_{\boldsymbol{u},\boldsymbol{N}} + \boldsymbol{V}_{\boldsymbol{\varphi},\boldsymbol{N}}$$

Space Dimensions

	$\boldsymbol{\mathcal{C}_N}$	$\boldsymbol{V}_{\boldsymbol{u},\boldsymbol{N}}$	$\boldsymbol{V}_{\boldsymbol{\varphi},\boldsymbol{N}}$	$\boldsymbol{V}_{\boldsymbol{N}}$	$\boldsymbol{T}_{\boldsymbol{M}}$
dim	4	64	95	159	16

Computational Time



FE-3D-VAR	RB-3D-VAR			speedup
	offline	online	error bound	
7.08 s	463 s	4.2 ms	1.3 ms	1,276

4 - CONNECTIONS

BAYESIAN SETTING

Joint work with N. Aretz-Nellesen & P. Cheng,
Thanks also to M. Grepl, D. Degen & F. Wellmann

Bayesian Inversion

Measurement Data and Noise

We model the measurement data $\boldsymbol{d}$ to be of the form

$$\boldsymbol{d} = \boldsymbol{L}\boldsymbol{u}_{\boldsymbol{\theta}}(\boldsymbol{p}) + \boldsymbol{\delta} = \boldsymbol{G}_{\boldsymbol{\theta},\boldsymbol{L}}(\boldsymbol{p}) + \boldsymbol{\delta}$$

with

Observation operator	$\boldsymbol{L} = (\boldsymbol{l}_1, \ldots, \boldsymbol{l}_M)^T : \boldsymbol{V} \to \mathbb{R}^M$
Gaussian additive noise	$\boldsymbol{\delta} \sim \mathcal{N}(0, \boldsymbol{\sigma}^2 \boldsymbol{\Sigma}_L)$
Noise covariance matrix	$\boldsymbol{\Sigma}_L \in \mathbb{R}^M \times \mathbb{R}^M$
Parameter-to-observable map	$\boldsymbol{G}_{\boldsymbol{\theta},\boldsymbol{L}} : \mathbb{R}^P \to \mathbb{R}^M,$ with $\boldsymbol{G}_{\boldsymbol{\theta},\boldsymbol{L}}(\boldsymbol{p}) := \boldsymbol{L}\boldsymbol{u}_{\boldsymbol{\theta}}(\boldsymbol{p})$

Bayesian Inversion

Measurement Data and Noise

We model the measurement data $\boldsymbol{d}$ to be of the form

$$d = Lu_\theta(p) + \delta = G_{\theta,L}(p) + \delta$$

with

linear in parameter

Observation operator	$L = (l_1, \ldots, l_M)^T : V \to \mathbb{R}^M$
Gaussian additive noise	$\delta \sim \mathcal{N}(0, \sigma^2 \Sigma_L)$
Noise covariance matrix	$\Sigma_L \in \mathbb{R}^M \times \mathbb{R}^M$
Parameter-to-observable map	$G_{\theta,L} : \mathbb{R}^P \to \mathbb{R}^M,$ with $G_{\theta,L}(p) := Lu_\theta(p)$

Bayesian Inversion

Hyper-parametrized Bayesian Inverse Model

Given the prior probability density π_0 , the posterior density is

$$\pi_{\text{post}}(\,\cdot\,|d) \propto \pi_0(\,\cdot\,)\,\pi_{\text{like}}(d|\,\cdot\,)$$

Bayesian Inversion

Hyper-parametrized Bayesian Inverse Model

Given the prior probability density π_0 , the posterior density is

$$\pi_{\text{post}}(\cdot\,|d) \propto \pi_0(\cdot)\,\pi_{\text{like}}(d|\cdot)$$

With additive Gaussian noise, the posterior density is then

$$\pi_{\text{post}}(\cdot\,|d) \propto \exp\left(-\frac{1}{2\sigma^2}||G_{\theta,L}(p) - d||^2_{\Sigma_L^{-1}} - \frac{1}{2}||p||^2_{\mathcal{C}}\right)$$

Bayesian Inversion

Hyper-parametrized Bayesian Inverse Model

Given the prior probability density π_0 , the posterior density is

$$\pi_{\text{post}}(\,\cdot\,|d) \propto \pi_0(\,\cdot\,)\,\pi_{\text{like}}(d|\,\cdot\,)$$

With additive Gaussian noise, the posterior density is then

$$\pi_{\text{post}}(\,\cdot\,|d) \propto \exp\left(-\frac{1}{2\sigma^2}\|G_{\theta,L}(p) - d\|^2_{\Sigma_L^{-1}} - \frac{1}{2}\|p\|^2_{\mathcal{C}}\right)$$

Since $G_{\theta,L}$ is linear, the posterior is Gaussian, with

$$m^{\theta,L}_{\text{post}}(d) = \Sigma^{\theta,L}_{\text{post}}\left(G^*_{\theta,L}\,\Sigma_L^{-1}d\right) \qquad \text{mean}$$

$$\Sigma^{\theta,L}_{\text{post}} = \left(\frac{1}{\sigma^2}G^*_{\theta,L}\Sigma_L^{-1}G_{\theta,L} + \Sigma_0^{-1}\right)^{-1} \qquad \text{covariance matrix}$$

Sensor Selection Strategy

Objective

Given sensor library $\mathcal{L} = \{l_i\}_{i=1}^{K}$ of K sensors

choose observation operator $L = (\,l_{k_1}, \ldots, l_{k_M}),\; 1 \leq k_i \leq K$

so that L is uniformly “good” for all hyper-parameters $\theta \in \mathcal{D}$

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(Bayesian) Optimal Experimental Design

OED

… [UCINSKI, '04], [PATAN, '04], [ATKINSON, DONEV & TOBIAS, '07]
[RANIERI, CHEBIRA & VETTERLI, '14], [HERZOG, RIEDEL & UCINSKI, '17] …

OED in the Bayesian setting

… [BERGER & PERICCHI, '01], [RYAN, DROVANDI, McGREE & PETTITT, '16]
[AGGARWAL, DEMKOWICZ, MARZOUK, '14], **[ALEXANDERIAN, GLOOR & GHATTAS, '16]**
[ALEXANDERIAN, PETRA, STADLER, & GHATTAS, '16], [WALSH, WILDEY, JAKEMAN, '17] …

OED + MOR

… [ALONSO, FROUZAKIS, KEVREKIDIS, '04], [BINEV, COHEN, MULA & NICHOLS, '18]
[BENNER, HERZOG, LANG, RIEDEL & SAAK, '19], [MADAY, PATERA, PENN & YANO, '14/'15]
[MADAY & TADDEI '19], [HAMMOND, CHAKIR, BOURQUIN & MADAY '19] …

Sensor Selection Strategy

(Some) Bayesian OED Criteria

For given $\boldsymbol{L},\boldsymbol{\theta}$, let $\boldsymbol{\alpha_i}$ be the eigenvalues of $\boldsymbol{\Sigma}_{\textbf{post}}^{\boldsymbol{\theta},\boldsymbol{L}}$ with orthonormal eigenvectors, $\boldsymbol{s_i}$, $\boldsymbol{i = 1, \dots, P}$

- **A-Optimality** minimizes the mean axis of the uncertainty ellipsoid

$$\min \operatorname{trace}(\boldsymbol{\Sigma}_{\textbf{post}}^{\boldsymbol{\theta},\boldsymbol{L}}) = \sum_{i=1}^{P} \boldsymbol{\alpha_i}$$

- **D-Optimality** minimizes the volume of the uncertainty ellipsoid

$$\min \det(\boldsymbol{\Sigma}_{\textbf{post}}^{\boldsymbol{\theta},\boldsymbol{L}}) = \prod_{i=1}^{P} \boldsymbol{\alpha_i}$$

Sensor Selection Strategy

Eigenvalue Upper Bound

For $i = 1, \dots, M$, we can show that $\alpha_i \leq \left(\frac{1}{\sigma^2} \beta_{L,\theta}^2 \eta_{X_\theta^\perp,\theta}^2 \| \Pi_{X_\theta^\perp} s_i \|_{\mathbb{R}^M}^2 + \gamma_{\Sigma_0^{-1}}^2 \right)^{-1}$

with **norm equivalence constant** $\gamma_{\Sigma_0^{-1}} := \inf_{p \in \mathbb{R}^M} \frac{\|p\|_{\Sigma_0^{-1}}}{\|p\|_{\mathbb{R}^M}}$

parameter subspace $X_\theta^\perp := \{p \in \mathbb{R}^M : u_\theta(p) = 0\}^\perp$

variability coefficient $\eta_{X_\theta^\perp,\theta}^2 := \inf_{p \in X_\theta^\perp} \frac{\|u_\theta(p)\|_V}{\|p\|_C} \geq 0$

observability coefficient $\beta_{L,\theta} := \inf_{p \in X_\theta^\perp} \frac{\|L u_\theta(p)\|_{\Sigma_L^{-1}}}{\|u_\theta(p)\|_V}$

Sensor Selection Strategy

Eigenvalue Upper Bound

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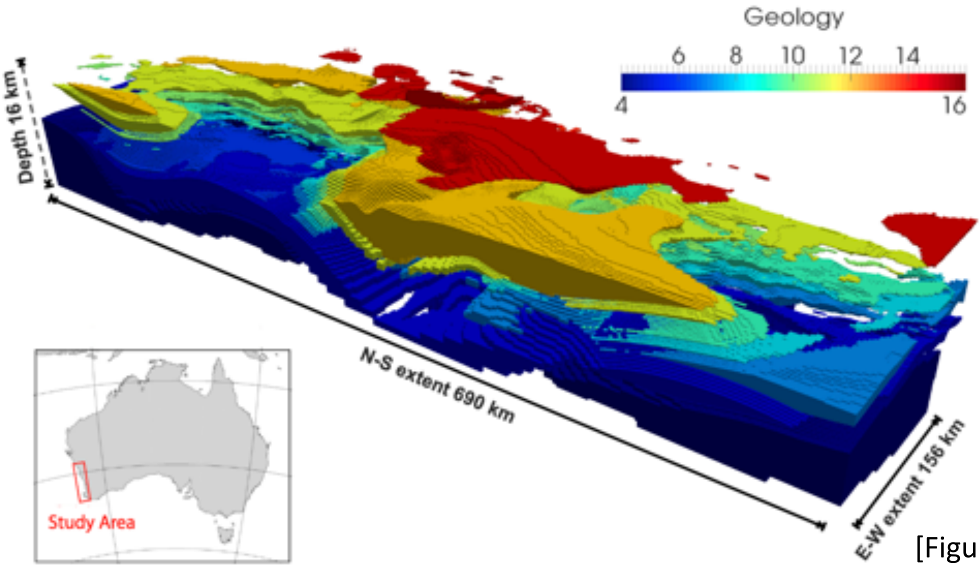
- non-decreasing for all θ with expanding L
- greedy-OMP algorithm
- model order reduction

Our Context

Geophysics Example



Perth Basin

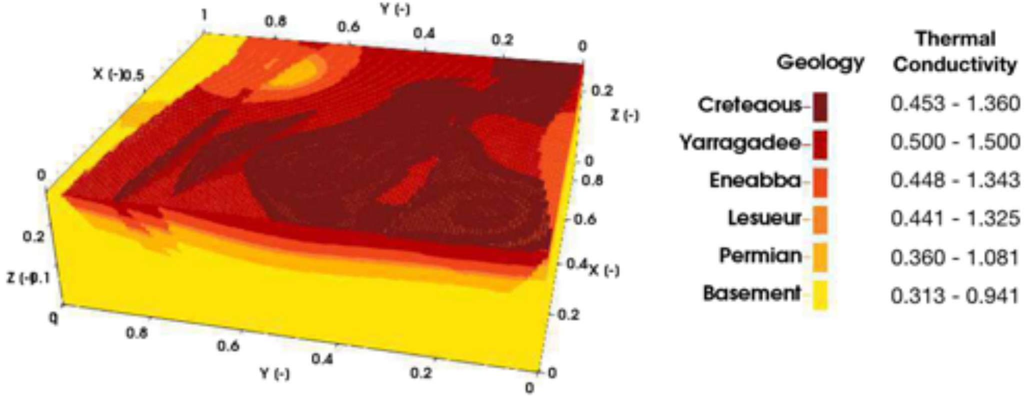
- Model: heat diffusion
- Hyper-parameters: conductivities
- Parameters: boundary condition

[Figure courtesy of F. Wellmann (RWTH Aachen)]

Wellmann and Reid, “Basin-scale Geothermal Model Calibration: Experience from the Perth Basin, Australia”, Energy Procedia, 59:382-389, 2014.

Our Context

Geophysics Example



Geology	Thermal Conductivity
Creteaous	0.453 - 1.360
Yarragadee	0.500 - 1.500
Eneabba	0.448 - 1.343
Lesueur	0.441 - 1.325
Permian	0.360 - 1.081
Basement	0.313 - 0.941

Perth Basin

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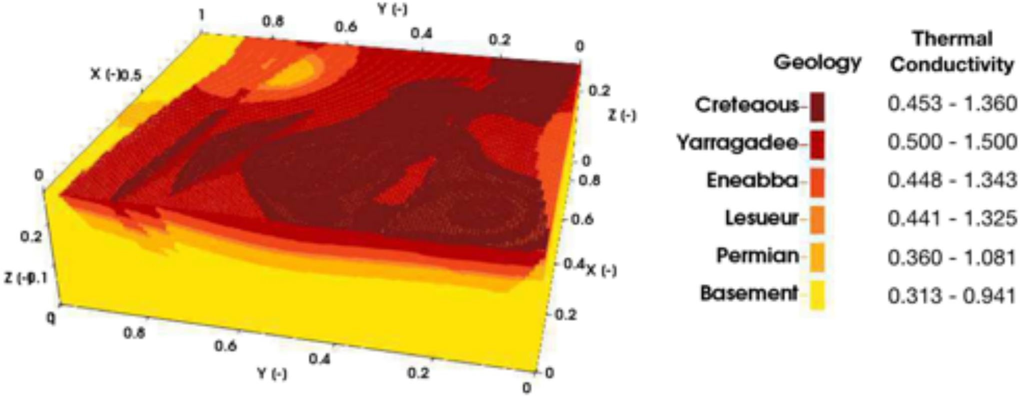
Work in collaboration with D. Degen & F. Wellmann

Our Context

Geophysics Example



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Sensor Library

- 47 x 47 grid of holes, 5 depths,
- total of 11,045 possible sensors
- only one measurement per hole

Noise covariance function

- provided by geophysicists, computed from measurements
- high correlation between different sensors

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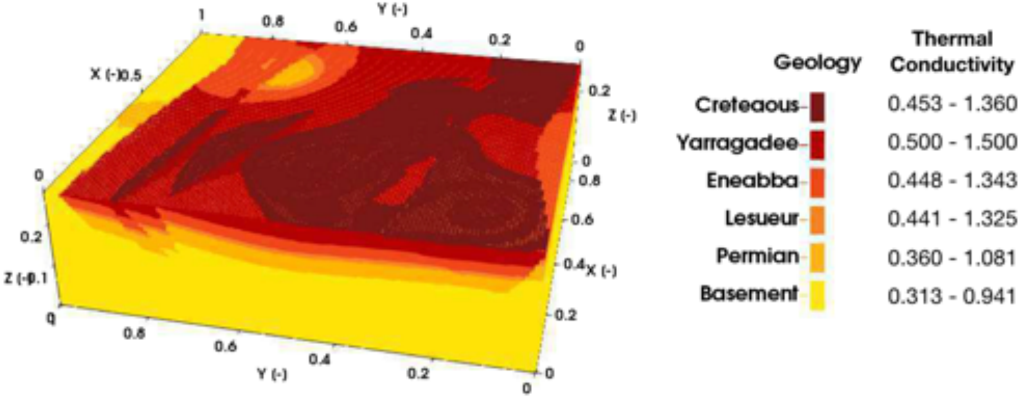
Our Context

Geophysics Example



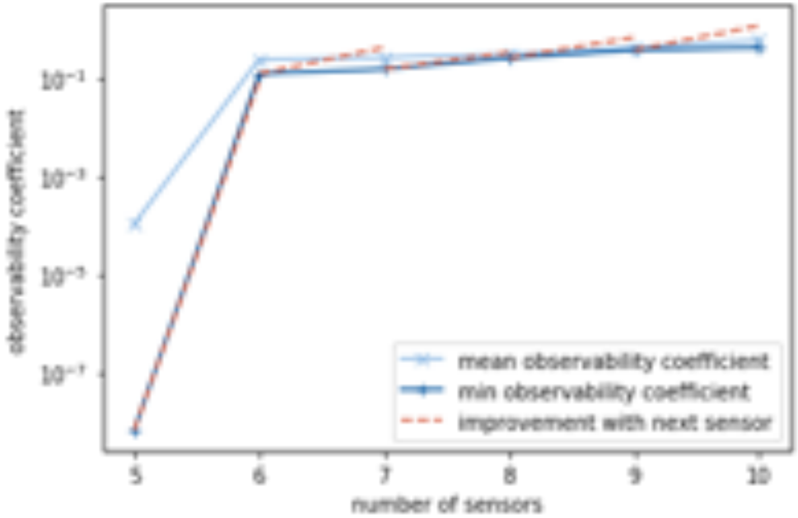
Sensor selection

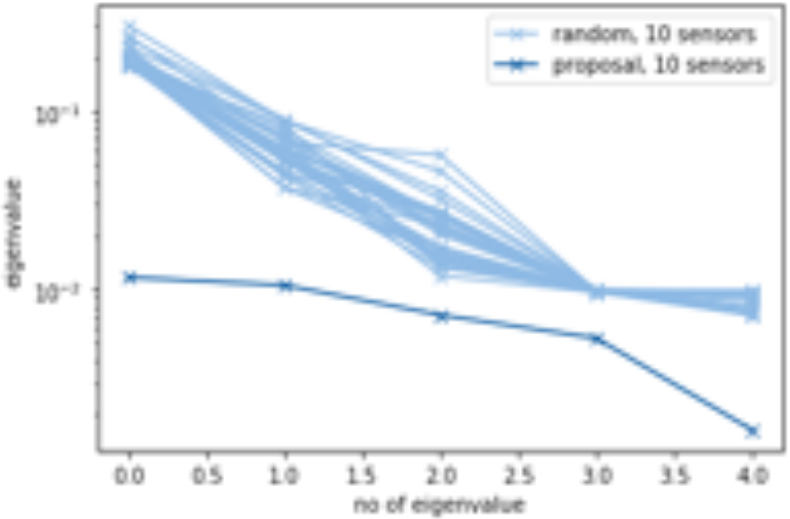
- 6 hyper-parameters, 5 parameters
- RB space of dimension 92
- offline time of 52 min
- relative target accuracy of 1% over random training set of 4E5 hyper-parameters
- choose 10 sensors from library
- min observability coefficient of 0.47

Work in collaboration with D. Degen & F. Wellmann

Numerical Results

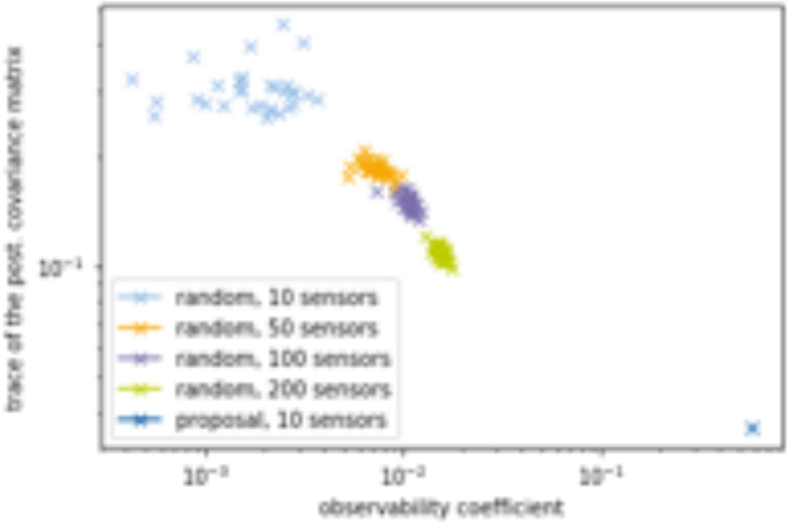
Observability coefficient and eigenvalues

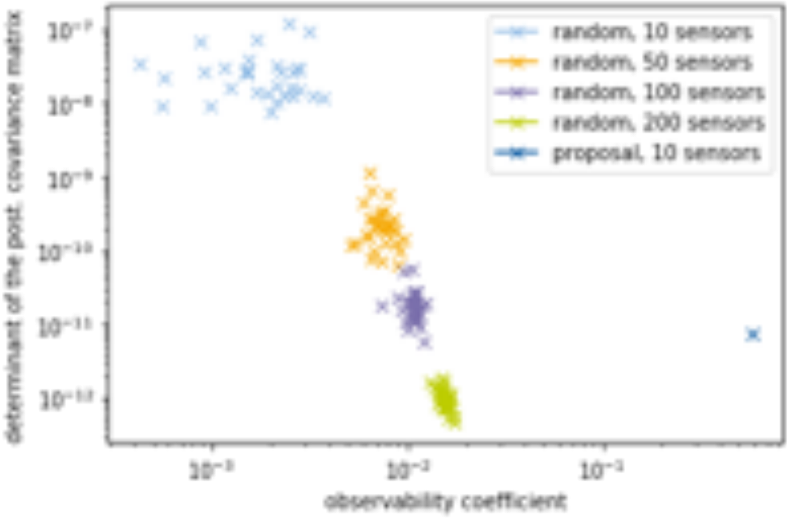




Numerical Results

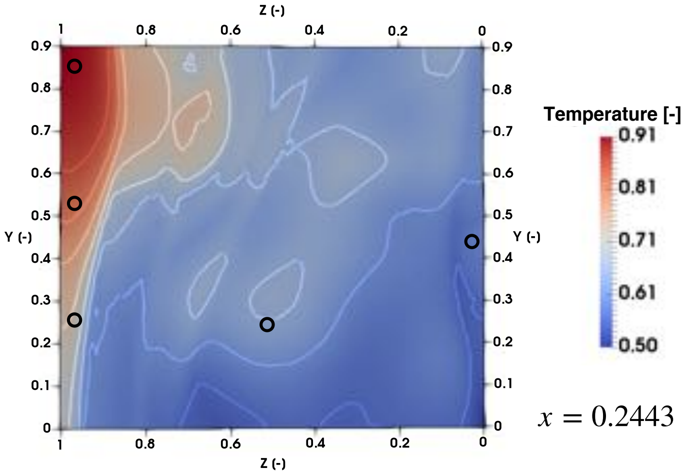
Bayesian A- and D-optimality Criteria





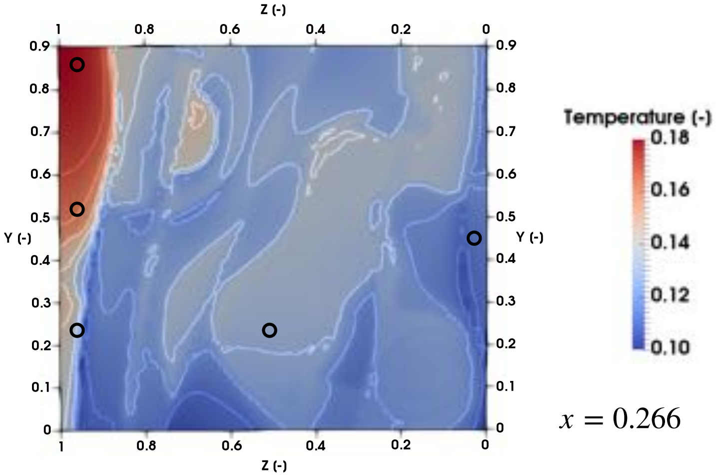
Numerical Results

Sensor Selection



$x = 0.2443$

Bottom-most layer with sensors



$x = 0.266$

Top-most layer with sensors

Final Remarks

Summary

- Considered physical systems governed by hyper-parametrized PDEs
- Built on variational data assimilation methods to estimate state, unknown parameters
- Through a stability analysis, developed framework for optimal sensor placement
- Used reduced order models to significantly reduce computational cost
- Extended and applied framework to Bayesian problem in geophysics
- Explored connections to A- and D-optimality

Outlook

- Extend to cases with nonlinear parameter-to-observable maps
- Extend to parabolic case, multi-scale problems, high-dimensional parameters, …