## Parametric Problems, Uncertainty Quantification, and Model Reduction

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## Overview

1. Parameter dependent problems
2. Associated linear process
3. Factorisations/ Reparametrisations
4. Model reduction and sparse representation
5. Examples and conclusion

## Parameter dependent entities

Assume $r(p)$ to be the parameter dependent input, the properties, or the output of some system dependent on a parameter $p \in \mathcal{P}$.

$$
\text { Special case: } \mathcal{P} \text { is a probability space. }
$$

Here $p$ can be a number, function, field, or similar, e.g. a random variable (RV), a stochastic process, a random field.

The parameter space $\mathcal{P}$ may be high-dimensional.
How to re-parametrise problem?
How to approximate $p \rightarrow r(p)$ to keep computation and memory low?
Computation of $r(p)$ involves approximation.
Allow comparable error to have sparse representation.

## Deterministic model, discretisation, solution

Consider operator equation, physical system modelled by $A$ :

$$
\begin{array}{rl}
A(u)=f & u \in \mathcal{U}, f \in \mathcal{F}, \\
\Leftrightarrow \forall v \in \mathcal{U}: & \langle A(u), v\rangle=\langle f, v\rangle,
\end{array}
$$

$\mathcal{U}$ - space of states, $\mathcal{F}$ - dual space of actions / forcings.
Solution is usually by first discretisation

$$
\boldsymbol{A}(\boldsymbol{u})=\boldsymbol{f} \quad \boldsymbol{u} \in \mathcal{U}_{N} \subset \mathcal{U}, \boldsymbol{f} \in \mathcal{F}_{N} \subset \mathcal{F}
$$ and then (iterative) numerical solution process

$$
\boldsymbol{u}_{k+1}=\boldsymbol{\Phi}\left(\boldsymbol{u}_{k}\right), \quad \lim _{k \rightarrow \infty} \boldsymbol{u}_{k}=\boldsymbol{u}
$$

$\boldsymbol{\Phi}$ evaluates (pre-conditioned) residua $\boldsymbol{f}-\boldsymbol{A}\left(\boldsymbol{u}_{k}\right)$.

## Model with uncertainties

With uncertainties modelled by appropriate probab. space $(\Omega, \mathbb{P}, \mathfrak{A})$ :

$$
A[\omega](u(\omega))=f(\omega) \quad \text { a.s. in } \omega \in \Omega,
$$

State $u(\omega)$ is $\mathcal{U}$-valued random variable ( RV ), solution is in a tensor space $\mathcal{W}=\mathcal{U} \otimes \mathcal{S}$.

Variational statement: $\forall v \in \mathcal{W}: \quad \mathbb{E}(\langle A[\cdot](u(\cdot)), v\rangle)=\mathbb{E}(\langle f(\cdot), v\rangle)$.
Similarly after semi-discretisation in $\mathcal{U}$ :

$$
\boldsymbol{A}[\omega](\boldsymbol{u}(\omega))=\boldsymbol{f}(\omega) \quad \text { a.s. in } \omega \in \Omega
$$

assume $\left\{\boldsymbol{v}_{j}\right\}_{j=1}^{N}$ a basis in $\mathcal{U}_{N}$, then the approx. solution in $\mathcal{U}_{N} \otimes \mathcal{S}$

$$
\boldsymbol{u}(\omega)=\sum_{j=1}^{N} u^{j}(\omega) \boldsymbol{v}_{j}
$$

## Uncertainty in modelling of concrete



Viaduct de Millau

$16 \times 32$ specimen

## Scales in concrete



Concrete

mortar

## Heterogeneous on many scales


close-up

fracture process zone

## Multi-scale coupling strategy

Strategy key ideas: Sub-domain wrapped in interface layer, interface layer coarse interpolation, localised Lagrange multipliers: independent dual compatibility.


Macro-Micro Cube


One Micro-Cube with Random Inclusions

## Computation


micro inclusions strain

fractured bonds

## Direct integration / sampling solution

Builds on fact that ultimately a quantity of interest $\mathbb{E}(\Psi(u))$ is wanted.

$$
\mathbb{E}(\Psi(u))=\int_{\Omega} \Psi(\omega, u(\omega)) \mathbb{P}(\mathrm{d} \omega) \approx \sum_{z=1}^{Z} \mathrm{w}_{z} \Psi\left(\omega_{z}, u\left(\omega_{z}\right)\right)
$$

Pick (e.g. Monte Carlo) $\left\{\omega_{z}\right\}_{z=1}^{Z}$ points, $\forall \omega_{z}$ do solution process

$$
\begin{gathered}
\boldsymbol{u}_{k+1}\left(\omega_{z}\right)=\boldsymbol{\Phi}\left[\omega_{z}\right]\left(\boldsymbol{u}_{k}\left(\omega_{z}\right)\right), \\
\text { giving } \boldsymbol{u}\left(\omega_{z}\right)=\sum_{j} u^{j}\left(\omega_{z}\right) \boldsymbol{v}_{j}=\sum_{j} u_{z}^{j} \boldsymbol{v}_{j} .
\end{gathered}
$$

Effectively choosing $\mathcal{S}_{Z} \subset \mathcal{S}$, solution is in $\mathcal{W}_{N, Z}:=\mathcal{U}_{N} \otimes \mathcal{S}_{Z}$. (Usually $\boldsymbol{u}\left(\omega_{z}\right)$ discarded after use in integration.)

Random state represented by solution samples $\left[\boldsymbol{u}\left(\omega_{0}\right), \ldots, \boldsymbol{u}\left(\omega_{Z}\right)\right]$, or the tensor $\mathbf{u}_{Z}^{N}:=\left\{u_{z}^{j}\right\}_{z=1, \ldots, Z}^{j=1, \ldots, N}$.

## Solution by emulation / functional approximation

Emulation - replace expensive simulation by inexpensive approximation ( alias response surfaces, proxy / surrogate models, etc.)

Choose subspace $\mathcal{S}_{B} \subset \mathcal{S}$ with basis $\left\{X_{\beta}\right\}_{\beta=1}^{B}$, make ansatz for each $u_{j}(\omega) \approx \sum_{\beta} u_{j}^{\beta} X_{\beta}(\omega)$, giving

$$
\boldsymbol{u}(\omega)=\sum_{j, \beta} u_{j}^{\beta} X_{\beta}(\omega) \boldsymbol{v}_{j}=\sum_{j, \beta} u_{j}^{\beta} X_{\beta}(\omega) \otimes \boldsymbol{v}_{j} .
$$

Solution is in tensor product $\mathcal{W}_{N, B}:=\mathcal{U}_{N} \otimes \mathcal{S}_{B} \subset \mathcal{U} \otimes \mathcal{S}=\mathcal{W}$.
Random state $\boldsymbol{u}(\omega)$ represented by tensor $\mathbf{u}_{N}^{B}:=\left\{u_{j}^{\beta}\right\}_{j=1, \ldots, N}^{\beta=1, \ldots, B}$, computed by sampling (pre-conditioned) residua $\boldsymbol{f}(\omega)-\boldsymbol{A}[\omega]\left(\boldsymbol{u}_{k}(\omega)\right)$.

## Model problem with uncertainties



Aquifer


2D model domain $\mathcal{G}$

Simple stationary model of groundwater flow with uncertain data

$$
-\nabla \cdot(\kappa(x, \omega) \nabla u(x, \omega))=f(x, \omega) \quad x \in \mathcal{G} \subset \mathbb{R}^{d} \quad \& \text { b.c. }
$$

Probabilistic modelling of uncertainty.
Parameter $\omega \in \Omega$ (realisations of $\kappa$ and $f$ ) is in a probability space.

## Realisation of $\kappa(x, \omega)$ - $\beta$-distributed



## Stochastic PDE and variational form

Solution $u(x, \omega)$ is sought in tensor product space

$$
\mathcal{W}:=\mathcal{U} \otimes \mathcal{S}=\stackrel{\circ}{H}^{1}(\mathcal{G}) \otimes L_{2}(\Omega)
$$

Variational formulation: find $u \in \mathcal{W}$ such that $\forall v \in \mathcal{W}$ :

$$
\begin{aligned}
& \mathrm{a}(v, u):=\mathbb{E}\left(\int_{\mathcal{G}} \nabla v(x, \omega) \cdot \kappa(x, \omega) \cdot u(x, \omega) \mathrm{d} x\right) \\
&=\mathbb{E}\left(\int_{\mathcal{G}} v(x, \omega) f(x, \omega) \mathrm{d} x\right)=:\langle\langle v, f\rangle\rangle .
\end{aligned}
$$

Lax-Milgram lemma $\rightarrow$ well-posedness.
Galerkin discretisation on $\mathcal{W}_{B, N}=\mathcal{U}_{N} \otimes \mathcal{S}_{B} \subset \mathcal{U} \otimes \mathcal{S}=\mathcal{W}$ leads to

$$
\mathbf{A} \mathbf{u}=\left(\sum_{m=1}^{M} \xi_{m} \boldsymbol{A}_{m} \otimes \boldsymbol{\Delta}^{(m)}\right) \mathbf{u}=\mathbf{f}
$$

Céa's lemma $\rightarrow$ Galerkin converges.

## Example solution



$\operatorname{Pr}\{u(x)>8\}$

## Parametric problems

For each $p$ in a parameter set $\mathcal{P}$, let $r(p)$ be a 'solution' to some problem in a Hilbert space $\mathcal{V}$ (for simplicity).

$$
\text { With } r: \mathcal{P} \rightarrow \mathcal{V} \text {, denote } \mathcal{U}=\overline{\operatorname{span}} r(\mathcal{P})=\overline{\operatorname{span}} \operatorname{im} r .
$$

What we are after: other representations of $r$ or $\mathcal{U}=\overline{\operatorname{span}} \operatorname{im} r$.
To each function $r: \mathcal{P} \rightarrow \mathcal{U}$ corresponds a linear map $R: \mathcal{U} \rightarrow \tilde{\mathcal{R}}$ :

$$
R: \mathcal{U} \ni u \mapsto\langle r(\cdot) \mid u\rangle_{\mathcal{V}} \in \tilde{\mathcal{R}}=\operatorname{im} R \subset \mathbb{R}^{\mathcal{P}} .
$$

By construction $R$ is injective. Use this to make $\tilde{\mathcal{R}}$ a pre-Hilbert space:

$$
\forall \phi, \psi \in \tilde{\mathcal{R}}:\langle\phi \mid \psi\rangle_{\mathcal{R}}:=\left\langle R^{-1} \phi \mid R^{-1} \psi\right\rangle_{\mathcal{U}} .
$$

$R^{-1}$ is unitary on completion $\mathcal{R}$.

## RKHS and classification

$\mathcal{R}$ is a reproducing kernel Hilbert space -RKHS— with kernel

$$
\varkappa\left(p_{1}, p_{2}\right)=\left\langle r\left(p_{1}\right) \mid r\left(p_{2}\right)\right\rangle_{\mathcal{U}} \in \mathbb{R}^{\mathcal{P} \times \mathcal{P}}
$$

Reproducing property:

$$
\forall \phi \in \mathcal{R}:\langle\varkappa(p, \cdot) \mid \phi(\cdot)\rangle_{\mathcal{R}}=\phi(p) .
$$

In other settings (classification, machine learning, SVM), when different subsets of $\mathcal{P}$ have to be classified, the space $\mathcal{U}$ and the map $r: \mathcal{P} \rightarrow \mathcal{U}$ is not given, but can be freely chosen.

It is then called the feature map.
The whole procedure is called the kernel trick.

## ‘Correlation’

If there is another inner product $\langle\cdot \mid \cdot\rangle_{\mathcal{Q}}$ on a subspace $\mathcal{Q} \subset \mathbb{R}^{\mathcal{P}}$, (e.g. if $(\mathcal{P}, \mu)$ is a measure space define $\mathcal{Q}:=L_{2}(\mathcal{P}, \mu)$ ),
a linear map $C$ may be defined in $\mathcal{U}$ by

$$
\forall u, v \in \mathcal{U} ;\langle C u, v\rangle_{\mathcal{U}^{\prime} \times \mathcal{U}}=\langle R u \mid R v\rangle_{\mathcal{Q}} .
$$

$C$ is the 'correlation' operator (adjoint in $\mathcal{Q}=L_{2}(\mathcal{P})$ ):

$$
C:=R^{*} R=\int_{\mathcal{P}} r(p) \otimes r(p) \mu(\mathrm{d} p)
$$

is self-adjoint and positive semi-definite $\rightarrow$ has spectrum $\sigma(C) \subseteq \mathbb{R}_{+}$.
Spectral decomposition with projectors $E_{\lambda}$

$$
C u=\int_{0}^{\infty} \lambda \mathrm{d} E_{\lambda} u=\sum_{\lambda_{j} \in \sigma_{p}(C) \subset \mathbb{R}_{+}} \lambda_{j}\left\langle v_{j} \mid u\right\rangle_{\mathcal{U}} v_{j}+\int_{\mathbb{R}_{+} \backslash \sigma_{p}(C)} \lambda \mathrm{d} E_{\lambda} u
$$

## Spectral decomposition

Often $C$ has a pure point spectrum (e.g. $C$ compact) $\Rightarrow$ last integral vanishes, i.e. $\sigma(C)=\sigma_{p}(C)$ :

$$
C u=\sum_{j} \lambda_{j} \sum_{k}^{\text {mult. } \lambda_{j}}\left\langle v_{j}^{k} \mid u\right\rangle_{\mathcal{U}} v_{j}^{k}=\sum_{\lambda_{j} \in \sigma_{p}(C)} \lambda_{j} \sum_{k}^{\text {mult. } \lambda_{j}}\left(v_{j}^{k} \otimes v_{j}^{k}\right) u .
$$

If $\sigma(C) \neq \sigma_{p}(C)$ : generalised eigenvectors $v_{\lambda}$ and Gelfand triplets (rigged Hilbert spaces) for the continuous spectrum:

$$
\int_{\mathbb{R}_{+} \backslash \sigma_{p}(C)} \lambda \mathrm{d} E_{\lambda} u=\sum_{k}^{\text {mult. }} \int_{\mathbb{R}_{+}} \lambda\left(v_{\lambda}^{k} \otimes v_{\lambda}^{k}\right) u \varrho_{k}(\mathrm{~d} \lambda) .
$$

Representation as sum / integral of rank-1 operators.
Numerical approximation will give a sum. Assumed from now on.

## Singular value decomposition

$C$ unitarily equivalent to multiplication operator $M_{k}$, with $k \geq 0$ :

$$
\begin{aligned}
C=V M_{k} V^{*}= & \left(V M_{k}^{1 / 2}\right)\left(V M_{k}^{1 / 2}\right)^{*}, \text { with } M_{k}^{1 / 2}=M_{\sqrt{k}} \\
& \left(M_{k} f(\zeta):=k(\zeta) f(\zeta)\right)
\end{aligned}
$$

This connects to the singular value decomposition (SVD)

$$
\text { of } R=S M_{k}^{1 / 2} V^{*}, \text { with a (here) unitary } S
$$

$$
\text { With } \sqrt{\lambda_{m}} s_{m}:=R v_{m} \in \mathcal{R} \text { : }
$$

$$
(R u)(p)=\langle r(p) \mid u\rangle_{\mathcal{U}}=\sum_{m} \sqrt{\lambda_{m}}\left\langle v_{m} \mid u\right\rangle_{\mathcal{U}} s_{m}(p)
$$

$$
R=\sum_{m} \sqrt{\lambda_{m}}\left(v_{m} \otimes s_{m}\right) .
$$

Model reduction possible by truncating the sum.

## Model reduction

For partly continuous spectrum we get

$$
r(p)=\sum_{k}^{\text {mult. }} \int_{\mathbb{R}_{+}} \sqrt{\lambda}\left\langle v_{\lambda}^{k}, u\right\rangle s_{\lambda}^{k}(p) \varrho_{k}(\mathrm{~d} \lambda)
$$

With approximation or only point spectrum

$$
r(p)=\sum_{m} \sqrt{\lambda_{m}} s_{m}(p) v_{m}, \quad r \in \mathcal{U} \otimes \mathcal{Q} .
$$

This is the Karhunen-Loève-expansion, due to the SVD. A sum of rank-1 operators / tensors.

Observe that $r$ is linear in the "coordinates" $s_{m}$, and also $\varsigma:=\sqrt{\lambda}$.
A representation of $r$, model reduction possible by truncation of sum.

## Kernel spectral decomposition

For $\phi, \psi \in L_{2}(\mathcal{P})$ we have also
$\left\langle R^{*} \phi \mid R^{*} \psi\right\rangle_{\mathcal{U}}=\iint_{\mathcal{P} \times \mathcal{P}} \phi\left(p_{1}\right) \varkappa\left(p_{1}, p_{2}\right) \psi\left(p_{2}\right) \mu\left(\mathrm{d} p_{1}\right) \mu\left(\mathrm{d} p_{2}\right)$.
To compute $R^{*}$, define an operator $\hat{C}=R R^{*}$ on $L_{2}(\mathcal{P})$ by
$(\hat{C} \phi)\left(p_{1}\right):=\int_{\mathcal{P}} \varkappa\left(p_{1}, p_{2}\right) \phi\left(p_{2}\right) \mu\left(\mathrm{d} p_{2}\right)=\left\langle\varkappa\left(p_{1}, \cdot\right) \mid \phi\right\rangle_{L_{2}(\mathcal{P})}$.
Eigenvalue problem for $\hat{C}$ gives (Mercer's theorem)

$$
\varkappa\left(p_{1}, p_{2}\right)=\sum_{m} \lambda_{m} s_{m}\left(p_{1}\right) s_{m}\left(p_{2}\right),
$$

$$
\begin{gathered}
\left\{s_{m}\right\} \text { is CONS in } L_{2}(\mathcal{P}),\left\{\sqrt{\lambda_{m}} s_{m}\right\} \text { is CONS in } \mathcal{R} . \\
R^{*} \phi=\sum_{m} \sqrt{\lambda_{m}} v_{m}\left\langle s_{m} \mid \phi\right\rangle_{L_{2}(\mathcal{P})}, \quad R^{-1} \phi=\sum_{m} \lambda_{m}^{-1 / 2} v_{m}\left\langle s_{m} \mid \phi\right\rangle_{L_{2}(\mathcal{P})} .
\end{gathered}
$$

## Factorisations

$R^{*}$ may serve as a representation. This is a factorisation of $C$. Let $C=B^{*} B$ be an arbitrary one. Some possible ones:

$$
C=R^{*} R=\left(V M_{k}^{1 / 2}\right)\left(V M_{k}^{1 / 2}\right)^{*}=C^{1 / 2} C^{1 / 2}=B^{*} B
$$

Each factorisation leads to a representation-all unitarily equivalent. When $C$ is a matrix, a favourite is Cholesky: $C=L L^{*}$ ).

Assume that $C=B^{*} B$ and $B: \mathcal{U} \rightarrow \mathcal{H}$, let $\left\{e_{k}\right\}$ be CONS in $\mathcal{H}$.

$$
\begin{aligned}
& \text { Unitary } Q: \ell_{2} \ni \boldsymbol{a}=\left(a_{1}, \ldots, a_{n}, \ldots\right) \mapsto \sum_{k} a_{k} e_{k} \in \mathcal{H} . \\
& \qquad \text { Let } \tilde{r}(\boldsymbol{a}):=B^{*} Q \boldsymbol{a}:=\tilde{R}^{*} \boldsymbol{a} \text {, i.e. } \tilde{R}^{*}: \ell_{2} \rightarrow \mathcal{U} . \text { Then } \\
& \qquad \tilde{R}^{*} \tilde{R}=\left(B^{*} Q\right)\left(Q^{*} B\right)=B^{*} B=C .
\end{aligned}
$$

## Integral decompositions

More decompositions and representations possible via $\hat{C}$.

$$
\begin{gathered}
\text { Let } \varkappa\left(\omega_{1}, \omega_{2}\right)=\int_{Y} g\left(\omega_{1}, y\right) g\left(\omega_{2}, y\right) \nu(\mathrm{d} y) . \\
\text { Set } p(y)=R^{-1}(g(\cdot, y)) \text { to give } \\
R^{*} \phi=\int_{Y} p(y)\langle g(\cdot, y) \mid \phi\rangle_{L_{2}(\Omega)} \nu(\mathrm{d} y)=\int_{Y} p(y)(G \phi)(y) \nu(\mathrm{d} y) \\
\text { where }(G \phi)(y)=\int_{\Omega} g(\omega, y) \phi(\omega) \mu(\mathrm{d} \omega) \text { is an integral transform. } \\
\text { We can arrange } \mathcal{U}=\overline{\text { span }} \text { im } r=\overline{\text { span }} \text { im } p .
\end{gathered}
$$

Then $p(y)$ gives a representation over $Y$ : for $f \in L_{2}(Y, \nu)$

$$
\hat{R}^{*} f=\int_{Y} p(y) f(y) \nu(\mathrm{d} y)
$$

## Representations

We have seen several ways to represent the solution space by a-hopefully-simpler space.
These can all be used for model reduction, choosing a smaller subspace.

- The RKHS together with $R^{-1}$.
- The spectral decomposition over $\sigma(C)$ or via $V M_{k}^{1 / 2}$.
- The Karhunen-Loève expansion based on SVD via $R^{*}$.
- Other multiplicative decompositions, such as $C=B^{*} B$.
- The kernel decompositions and representation on $L_{2}(Y, \nu)$.

Choice depends on what is wanted / needed.

## Examples and interpretations

- If $\mathcal{V}$ is a space of centred $\mathrm{RVs}, r$ is a random field / stochastic process indexed by $\mathcal{P}$, kernel $\varkappa\left(p_{1}, p_{2}\right)$ is covariance function.
- If in this case $\mathcal{P}=\mathbb{R}^{d}$ and moreover $\varkappa\left(p_{1}, p_{2}\right)=c\left(p_{1}-p_{2}\right)$ (stationary process / homogeneous field), then diagonalisation $V$ is real Fourier transform, typically $\sigma_{p}(C)=\emptyset \Rightarrow$ need Gelfand triplets.
- If $\mu$ is a probability measure on $\mathcal{P}=\Omega(\mu(\Omega)=1)$, and $r$ is a centred $\mathcal{V}$-valued RV , then $C$ is the covariance.
- If $\mathcal{P}=\{1,2, \ldots, n\}$ and $\mathcal{R}=\mathbb{R}^{n}$, then $\varkappa$ is the Gram matrix of the vectors $r_{1}, \ldots, r_{n}$.
- If $\mathcal{P}=[0, T]$ and $r(t)$ is the response of a dynamical system, then $R^{*}$ leads to proper orthogonal decomposition (POD).


## Further factorisation

We have found representations in $\mathcal{U} \otimes \mathcal{S}$, where

$$
\mathcal{S}=\mathcal{R}, L_{2}(\mathcal{P}), L_{2}(\sigma(C)), \bigoplus_{k} L_{2}\left(\mathbb{R}, \mu_{k}\right), \ell_{2}, L_{2}(Y), \ldots
$$

Combinations may occur, so that $\mathcal{S}=\mathcal{S}_{I} \otimes \mathcal{S}_{I I} \otimes \mathcal{S}_{I I I} \otimes \ldots$
This was only a basic decomposition.
Often the problem allows $\mathcal{U}=\bigotimes_{k} \mathcal{U}_{k}$.
Or the parameters allow $\mathcal{S}=\bigotimes_{j} \mathcal{S}_{j}$.
In case of random fields / stochastic processes

$$
\mathcal{S}=L_{2}(\Omega) \cong \bigotimes_{j} L_{2}\left(\Omega_{j}\right) \cong L_{2}\left(\mathbb{R}^{\mathbb{N}}, \Gamma\right) \cong \bigotimes_{k=1}^{\infty} L_{2}\left(\mathbb{R}, \Gamma_{1}\right) \ldots
$$

So $\mathcal{U} \otimes \mathcal{S} \cong\left(\otimes_{j} \mathcal{U}_{j}\right) \otimes\left(\otimes_{k} \mathcal{S}_{I, k}\right) \otimes\left(\otimes_{m} \mathcal{S}_{I I, m}\right) \otimes \ldots$

## Discretisation - model reduction

On continuous level discretisation is choice of subspace

$$
\mathcal{W}_{N, B}:=\mathcal{U}_{N} \otimes \mathcal{S}_{B} \subset \mathcal{U} \otimes \mathcal{S}=: \mathcal{W}
$$ and-important for computation-good basis in it.

On discrete level reduced models find sub-manifold $\mathcal{W}_{R} \subset \mathcal{W}_{N, B}$ with smaller dimensionality $\operatorname{dim} \mathcal{W}_{R}=R \ll N \times B=\operatorname{dim} \mathcal{W}_{N, B}$.

They can work on $\mathcal{S}_{B}$ or $\mathcal{U}_{N}$, or both.
Different approaches to choose reduced model:

- Before the solution process (e.g. modal projection).
- After the solution process (essentially data compression).
- During solution, computing solution and reduction simultaneously.


## Use in time-space sampling I

Example: UQ-computations of time-dependent shallow-water flow. 1:50 Scale model in Milano of Toce river (Italy)
(D. Liu)

## Use in time-space sampling II

Topography in model - uncertain elevation.


Also uncertain inflow and bed friction-Manning's coefficient.

## Use in time-space sampling III

Computation with QMC-sampling
Water level with 5 \% exceedance probability


## Use in emulation

Solution process to obtain co-efficients for stochastic problem

$$
\mathbf{u}_{k+1}=\boldsymbol{\Phi}\left(\mathbf{u}_{k}\right)
$$

may be written as tensorised mapping

$$
\begin{aligned}
& \mathbf{u}_{k+1}= \mathbf{u}_{k}-\boldsymbol{\Xi}\left(\mathbf{u}_{k}\right)=\mathbf{u}_{k}-\left(\sum_{m=1}^{M} \boldsymbol{Y}_{m} \otimes \boldsymbol{G}^{m}\right)\left(\mathbf{u}_{k}\right) . \\
& \text { With } \mathbf{u}_{0}=\sum_{j=1}^{R_{0}} \boldsymbol{y}_{0, j} \otimes \boldsymbol{g}^{0, j}, \text { this gives } \\
& \mathbf{u}_{1}= \sum_{j=1}^{R_{0}} \boldsymbol{y}_{0, j} \otimes \boldsymbol{g}^{0, j}-\sum_{m=1}^{M} \boldsymbol{Y}_{m}\left(\mathbf{u}_{0}\right) \otimes \boldsymbol{G}^{m}\left(\mathbf{u}_{0}\right) \\
& \text { Rank of } \mathbf{u}_{k+1} \text { grows by } M .
\end{aligned}
$$

Possible for pre-conditioned linear iteration, and modified-, full-, inexact- and quasi-Newton iteration.

## Truncated low-rank iteration

## Sparse representation entails

- reduce $\mathbf{u}_{N}^{B}:=\left[u_{j}^{\beta}\right]$ to important information $\mathbf{u} \approx \mathbf{u}_{N}^{B}$,
- never store all of $\mathbf{u}_{N}^{B}$, but only $\mathbf{u}$,
- operate efficiently on sparse representation $\mathbf{u}$.

If iteration and rank-truncation $\mathrm{T}_{\epsilon}$ are alternated, rank stays low. Here rank-truncation by updated SVD.

$$
\begin{gathered}
\hat{\mathbf{u}}_{k+1}=\sum_{j=1}^{R_{k}} \boldsymbol{y}_{k, j} \otimes \boldsymbol{g}^{k, j}-\sum_{m=1}^{M} \boldsymbol{Y}_{m}\left(\mathbf{u}_{k}\right) \otimes \boldsymbol{G}^{m}\left(\mathbf{u}_{k}\right), \\
\mathbf{u}_{k+1}=\mathbf{T}_{\epsilon}\left(\hat{\mathbf{u}}_{k+1}\right) \quad \text { with } \quad\left\|\mathbf{T}_{\epsilon}(\mathbf{v})-\mathbf{v}\right\| \leq \epsilon
\end{gathered}
$$

Truncated iteration converges until stagnation for linearly convergent process with contraction factor $\varrho$ to stagnation range $\epsilon /(1-\varrho)$.

## Computational complexity for linear case

Residuum is $\mathbf{f}-\mathbf{A} \mathbf{u}_{k}=\mathbf{f}-\left(\sum_{m=1}^{M} \xi_{m} \boldsymbol{A}_{m} \otimes \boldsymbol{\Delta}^{(m)}\right) \mathbf{u}_{k}$.
Computation on full $\mathbf{u}_{k}$ needs
$M \times B \boldsymbol{A}$-multiplications $+M \times N \boldsymbol{\Delta}$-multiplications.
Computation on low rank- $R$ tensor product $\mathbf{u}_{k}$ needs $M \times R \boldsymbol{A}$-multiplications $+M \times R \boldsymbol{\Delta}$-multiplications, which is much less.

Pre-conditioner $\mathbf{P}$ should be used as $\mathbf{P}=\sum_{p=1}^{P} \boldsymbol{\Lambda}^{(p)} \otimes \boldsymbol{P}_{p}$. Simplest example: mean value pre-conditioner $\mathbf{P}=\boldsymbol{I} \otimes \boldsymbol{P}_{0}$ with $\boldsymbol{P}_{0}$ pre-conditioner for $\mathbb{E}(\boldsymbol{A})$.

Similar savings as before, with $M$ replaced by $P$.

## Truncation accuracy

Accuracy of $k$-term tensor approximation.


## Iteration accuracy

## Convergence of truncated iteration.



## Number of iterations

Iteration count of truncated iteration.


## Dual weighted residuals

Given some functional of interest: $\boldsymbol{\psi}(\mathbf{u}) \approx \mathbb{E}(\Psi(\hat{u}))$
Error in functional $\epsilon=\boldsymbol{\psi}(\mathbf{u})-\boldsymbol{\psi}\left(\mathbf{u}_{R}\right) \approx\left\langle\delta \boldsymbol{\psi}, \mathbf{u}-\mathbf{u}_{R}\right\rangle$
For simplicity assume that $\mathbf{u}$ solves a linear system: $\mathbf{A u}=\mathbf{f}$, reduced solution has residual $\mathbf{r}=\mathbf{f}-\mathbf{A} \mathbf{u}_{R}$. Solve adjoint system $\mathbf{A}^{*} \mathbf{y}=\delta \boldsymbol{\psi}$ for sensitivity $\mathbf{y}$ :

$$
\langle\delta \boldsymbol{\psi}, \mathbf{u}\rangle=\left\langle\mathbf{A}^{*} \mathbf{y}, \mathbf{u}\right\rangle=\langle\mathbf{y}, \mathbf{A} \mathbf{u}\rangle=\langle\mathbf{y}, \mathbf{f}\rangle
$$

giving
$\epsilon \approx\left\langle\delta \boldsymbol{\psi}, \mathbf{u}-\mathbf{u}_{R}\right\rangle=\left\langle\mathbf{y}, \mathbf{A}\left(\mathbf{u}-\mathbf{u}_{R}\right)\right\rangle=\left\langle\mathbf{y}, \mathbf{f}-\mathbf{A} \mathbf{u}_{R}\right\rangle=\langle\mathbf{y}, \mathbf{r}\rangle$.
$\epsilon$ may be used for adaptive steering of model reduction process.

## Conclusion

- parametric models lead naturally to a number of factorisations
- For efficiency try and use sparse representation throughout: ansatz in low-rank tensor products, as well as storage of solution and residuum-and iterator in tensor products.
- Works in sampling and emulation /functional approximation.
- Works also for non-linear problems and solvers, time-dependent problems.

