Low Rank Solutions of Time Dependent Stochastic PDEs

Alessio Spantini

**Advisors**: Lionel Mathelin Youssef Marzouk

1,3 Department of Aeronautics and Astronautics
MIT

2 CNRS

ACDL Qualifying Exam
01/29/2013
Outline

1. Motivation
2. General Formulation and Methodology
3. Numerical Example
4. Conclusions
**Definition**

We say that \( u(x, \xi) \in \mathcal{V}_x \otimes S_\xi \) is **low rank** if it admits a low order \( r \)-term separable expansion.

\[
u(x, \xi) \approx \sum_{j \leq r} \sigma_j w_j(x) \lambda_j(\xi) \quad w \in \mathcal{V}_x, \lambda \in S_\xi
\]
Why Do We Care about Low Rank Fields?

Advantages of Low Rank Fields

1. Efficient **storage** (truncate the field)
2. Efficient **integration** in the context of stochastic PDEs

- Galerkin Proper Orthogonal Decomposition (**POD**) [Lumley 1996]
- Proper Generalized Decomposition (**PGD**) [Nouy 2007–12]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \nu(\xi) \frac{\partial u}{\partial x} = 0 \]

\[ \nu(\xi) = 1 + 0.3u(\xi) \]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail

Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \mathcal{V}(\xi) \frac{\partial u}{\partial x} = 0 \]

\[ \mathcal{V}(\xi) = 1 + 0.3 U(\xi) \]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail

Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \nu(\xi) \frac{\partial u}{\partial x} = 0 \]

\[ \nu(\xi) = 1 + 0.3 U(\xi) \]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail

Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[
\frac{\partial u}{\partial t} + \mathcal{V}(\xi) \frac{\partial u}{\partial x} = 0
\]

\[
\mathcal{V}(\xi) = 1 + 0.3 \mathcal{U}(\xi)
\]

Time: 0.6 s

Progressive **increase** of the rank

\[
u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi)
\]

Any discretization of the parameter space will eventually fail

**Long time integration issues** [Karniadakis 2005]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \mathcal{V}(\xi) \frac{\partial u}{\partial x} = 0 \]

\[ \mathcal{V}(\xi) = 1 + 0.3 \mathcal{U}(\xi) \]

1. Progressive increase of the rank 
   \[ u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \]

2. Any discretization of the parameter space will eventually fail
   Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[
\frac{\partial u}{\partial t} + \mathcal{V}(\xi) \frac{\partial u}{\partial x} = 0
\]

\[
\mathcal{V}(\xi) = 1 + 0.3 U(\xi)
\]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail
   Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \nu(\xi) \frac{\partial u}{\partial x} = 0 \]
\[ \nu(\xi) = 1 + 0.3 U(\xi) \]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail Long time integration issues [Karniadakis 2005]
Stochastic Advection Equation

\[ \frac{\partial u}{\partial t} + \nu(\xi) \frac{\partial u}{\partial x} = 0 \]
\[ \nu(\xi) = 1 + 0.3U(\xi) \]

1. Progressive increase of the rank \( u^n(x, \xi) = \sum_{i=1}^{r(n)} w_i(x) \lambda_i(\xi) \)

2. Any discretization of the parameter space will eventually fail

Long time integration issues [Karniadakis 2005]
The Necessity of Our Approach

Claim

Being able to enforce a low rank structure in time allows one to:

1. Exploit efficient solvers for low rank fields (PGD, POD) avoiding systems of prohibitive size
2. Efficiently store the field
3. Address long time integration issues
4. Extend the range of applicability of model reduction techniques (i.e., PGD) for time dependent stochastic PDEs
The Goal

Proposed Approach

Precondition the original problem using local time stretching to decrease the rank of the solution field.
Previous Work on Time Stretching

O.P. Le Maître, L. Mathelin, O. M. Knio, M. Y. Hussaini
*Asynchronous time integration for polynomial chaos expansion of uncertain periodic dynamics* (2009)
- Dynamical systems with limit cycles: no concept of low rank solutions

A. Alexanderian, O.P. Le Maître, H.N. Najm, O.M. Knio
*Multiscale stochastic preconditioners in non-intrusive spectral projection* (2011)
- Dynamical systems: no concept of low rank solutions
- A-posteriori time stretching based on historical data
Outline

1. Motivation
2. General Formulation and Methodology
3. Numerical Example
4. Conclusions
A Model Problem

We consider problems of the form: find \( u(x, t, \xi) \in \mathcal{V}_{xt} \otimes S_{\xi} \) s.t.

\[
\begin{aligned}
\frac{\partial u}{\partial t} + \mathcal{F}(u; \xi) &= 0 \quad t \in [0, T] \\
\text{b.c.} \\
u(x, 0, \xi) &= u_0(x, \xi)
\end{aligned}
\]

Remarks

- \( \mathcal{F} \) is a differential operator, possibly \textit{nonlinear}.
- A second order PDE in time can be rewritten as a system of first order PDEs (i.e., \textit{wave equation})
Time Stretching

Definition

Let \( \tau (t, \xi) \) be a time transformation such that \( \tau (0, \xi) = 0 \) a.s. and let:

\[
u (x, t, \xi) = y (x, \tau (t, \xi), \xi)\]

\[
[\theta (t, \xi)]^{-1} \equiv \frac{\partial \tau (t, \xi)}{\partial t}
\]

Preconditioned Equations

\[
\begin{align*}
\frac{\partial u}{\partial t} + \mathcal{F} (u; \xi) &= 0 \\
b.c.
\end{align*}
\]

\[
\begin{align*}
u (x, 0, \xi) &= u_0 (x, \xi) \\
b.c.
\end{align*}
\]

\[
\begin{align*}
\frac{\partial y}{\partial t} + \theta (t, \xi) \mathcal{F} (y; \xi) &= 0 \\
b.c.
\end{align*}
\]

\[
\begin{align*}
y (x, 0, \xi) &= u_0 (x, \xi)
\end{align*}
\]

\( \theta (t, \xi) \) is the preconditioner to be determined!
How to Integrate the Preconditioned Equations?

Idea

Write \( y^{n+1} (x, \xi) \) as a low rank perturbation of a reference \( y^{n+1}_{ref} (x) \)

\[
Z (x, \xi) \triangleq y^{n+1} (x, \xi; \theta) - y^{n+1}_{ref} (x)
\]
How to Integrate the Preconditioned Equations?

**Idea**

Write $y_{n+1}^{(x, \xi)}$ as a low rank perturbation of a reference $y_{ref}^{n+1}(x)$

$$z(x, \xi) \triangleq y_{n+1}^{n+1}(x, \xi; \theta) - y_{ref}^{n+1}(x)$$
How to Get the Preconditioner?

Notice that:

\[ z(x, \xi; \theta) = \sum_k \sqrt{\gamma_k} w_k(x) \lambda_k(\xi) \]

where \( \{\gamma_k\} \) are the eigenvalues of \( \mathbb{E}[z(x, \xi; \theta) \otimes z(x, \xi; \theta)] \)

**Original Minimization Problem**

\[ \theta^n(\xi) = \arg\min_{\theta > 0} \text{rank}\left[\mathbb{E}[z(\theta) \otimes z(\theta)]\right] \]

- **Nonconvex and nondifferentiable** [Boyd 2004]

**Best Convex Relaxation** [Parrilo 2010]

\[ \theta^n(\xi) = \arg\min_{\theta > 0} \text{trace}\left[\mathbb{E}[z(\theta) \otimes z(\theta)]\right] \]
Rank Minimization

**Equivalent Minimization Problem**

\[
\theta^n (\xi) = \arg\min_{\theta > 0} \| z (x, \xi; \theta) \|_{\mathcal{N}_x \otimes S_\xi}^2
\]

where \( z (x, \xi; \theta) = y^{n+1} (x, \xi; \theta) - y_{ref}^{n+1} (x) \)

- At this stage we can use a coarse, low order, time explicit, and even unstable discretizations for \( y^{n+1} (x, \xi; \theta) \)
- **Quadratic** over the parameter space \( S \) (even if PDE is nonlinear)
- No SVD required

**Some Intuition**

\[
\min \text{ rank } [X] \simeq \min_{\text{rank}[X_0]=1} \| X - X_0 \|_F^2
\]
Low Rank Methods

- The **complexity** of the time integration step depends on the **rank** of the solution

**Newly devised integration method**

*Randomized* Proper Generalized Decomposition

---

flowchart: Yes/No

- **Low rank?**
  - Yes: \( \theta^n(\xi) = \theta^{n+1}(\xi) \)\n  - No: \( \mathcal{U}(y^n, y_{ref}^{n+1}) \)

\[ y_{ref}^{n+1}(x) \]

\[ \theta^n(\xi) \]

\[ y^n(x, \xi) \]

\[ \theta^{n+1}(\xi) \]

\[ y^{n+1}(x, \xi) \]
How to Go Back?

Recover the Original Field

We can easily sample the original field $u(x, t, \xi)$ at $\xi_k$ by evaluating:

$$u(x, t, \xi_k) = y(x, \tau(t, \xi_k), \xi_k)$$

an inexpensive low rank functional exploitable in the context of inverse problems, design, and optimization.
Outline

1. Motivation

2. General Formulation and Methodology

3. Numerical Example

4. Conclusions
Numerical Example: Stochastic Inviscid Burgers’

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial \left( \frac{1}{2} u^2 \right)}{\partial x} &= 0 \\
u_0 (x, \xi_1, \xi_2, \xi_3)
\end{align*}
\]

\# \sigma / \sigma_{\text{max}} > 10^{-6}

Rank over Time

Initial Rank

\begin{figure}
\centering
\includegraphics[width=\textwidth]{image}
\caption{Graph showing rank over time for Stochastic Inviscid Burgers’ equation.}
\end{figure}
Flow of Complexity

\[ u^n(x, \xi_1, \xi_2, \xi_3) \xrightarrow{\text{PDE}} \theta^n(\xi_1, \xi_2, \xi_3) \]
Outline

1. Motivation
2. General Formulation and Methodology
3. Numerical Example
4. Conclusions
Main Contributions

1. Introduced a **new method** for reducing the **rank** of a SPDE solution field
2. Addressed **long time integration** issues for SPDE
3. Introduced a new low rank method: **Randomized PGD**
Current Limitations

- The preconditioner presented has no dynamic (Tikhonov regularization and low order schemes)
- **Heuristic** for rank minimization. For other SVD based heuristics see:
  1. [Boyd 2003–04] \( \min \left\{ \log \left( \prod_{i} \gamma_i \right) \right\} \)
  2. [Venturi 2011] \( \min \left\{ 1 - \gamma_1 / \sum_{i \geq 1} \gamma_i \right\} \) (complementary energy)
- Time **interpolation** required to recover the original field
Ongoing and Future Work

- **Space dependent time stretching:**
  \[ \tau(t, \xi) \rightarrow \tau(x, t, \xi) \]

- **Space stretching** for stationary problems:
  \[ x \rightarrow \hat{X}(x, \xi) \]

- Different separated formats:
  \[ w(x, t) \lambda(\xi, t) \rightarrow w(x, t) \lambda(\xi) \]

- Implications in **data compression**
### Main Contributions
- Introduced a **new method** for reducing the **rank** of a SPDE solution
- Addressed **long time integration** issues for SPDE
- Introduced a new low rank method: **Randomized PGD**

### Ongoing and Future Work
- **Space dependent time stretching**: \( \tau(t, \xi) \rightarrow \tau(x, t, \xi) \)
- **Space stretching** for stationary problems: \( x \rightarrow \hat{X}(x, \xi) \)
- Different **separated** formats: \( w(x, t) \lambda(\xi, t) \rightarrow w(x, t) \lambda(\xi) \)
- Implications in **data compression**
References I

O.P. Le Maître, L. Mathelin, O. M. Knio, M. Y. Hussaini
Asynchronous time integration for polynomial chaos expansion of uncertain periodic dynamics

A. Alexanderian, O.P. Le Maître, H.N. Najm, M. Iskandarani and O.M. Knio
Multiscale stochastic preconditioners in non-intrusive spectral projection,

X. Wan, G. E. Karniadakis
Long-term behavior of polynomial chaos in stochastic flow simulations
Daniele Venturi
A fully symmetric nonlinear bi-orthogonal decomposition theory for random fields.

M. Fazel, H. Hindi, S. Boyd
*Rank minimization and applications in system theory*

B. Recht, M. Fazel, and P. A. Parrilo.,
Guaranteed Minimum-Rank Solutions of Linear Matrix Equations via Nuclear Norm Minimization.
*SIAM Rev. 52, 3 (August 2010), 471-501.*
Outline

5 Proper Generalized Decomposition (PGD)

6 Galerkin Proper Orthogonal Decomposition (POD)

7 Advective Singular Value Decomposition (A-SVD)

8 Nonintrusive Methods
Proper Generalized Decomposition

- **Strong form**: find \( u(p) \) s.t.

\[
A(p)u(p) = b(p)
\]

- **Weak form**: find \( u(p) \in \mathbb{R}^n \otimes S_m \) s.t.

\[
E \left[ v^T A(p) u(p) \right] = E \left[ v^T b(p) \right] \quad \forall v \in \mathbb{R}^n \otimes S_m
\]

**Approximation format**

\[
u(p) \approx \sum_{\alpha=1}^{r} u_\alpha \lambda_\alpha(p) = W\Lambda
\]

\[
\left\{ \begin{array}{l}
W = [u_1|...|u_r] \\
\Lambda = \left\{ \begin{array}{c}
\lambda_1(p) \\
\vdots \\
\lambda_r(p)
\end{array} \right\}^T
\end{array} \right.
\]
PGD: Decoupled Problems

**Stochastic Problem**
Assume $\mathbf{W} \in \mathbb{R}^{n \times r}$ is known, then find $\mathbf{u}(p) \in \text{span}\{\mathbf{W}\} \otimes S_m$ through map $f$

$$\mathbb{R}^{n \times r} \ni \mathbf{W} \mapsto \Lambda = f(\mathbf{W}) \in \mathbb{R}^r \otimes S_m$$

**Deterministic Problem**
Assume $\Lambda \in \mathbb{R}^r \otimes S_m$ is known, then find $\mathbf{u}(p) \in \mathbb{R}^n \otimes \text{span}\{\Lambda\}$ through map $F$

$$\mathbb{R}^r \otimes S_m \ni \Lambda \mapsto \mathbf{W} = F(\Lambda) \in \mathbb{R}^{n \times r}$$

**Fixed Point Iteration**
Let $\mathbf{T} = F \circ f$, then $\mathbf{W}$ is a valid solution iff:

$$\mathbf{T}(\mathbf{W}) = (\mathbf{W})$$
Algorithm: Subspace Iteration (SI-PGD)

SI-PGD

1. Initialize $W^{(0)} \in S_{n,r}$
2. for $k = 1$ to $k_{max}$ do
   3. Compute $W^{(k)} = T(W^{(k-1)})$
   4. Orthonormalize $W^{(k)}$ (e.g. by QR factorization)
3. endfor
4. Set $W = W^{(k)}$ and compute $\Lambda = f(W)$
Algorithm: Arnoldi Iteration ($A^{r+s}$-PGD)

A-PGD

1. Initialize $u_1 \in \mathbb{R}^n$ and set $u_1 = \frac{u_1}{||u_1||}$
2. for $i = 1$ to $r + s$ do
3.     Compute $u = T(u_i)$
4.     for $j = 1$ to $i$ do
5.         $u = u - \left( u_j^T u \right) u_j$ (modified Gram Schmidt)
6.     endfor
7.     $u_{i+1} = \frac{u}{||u||}$
8. endfor
9. Set $W = (u_1, u_2, ..., u_i)$ and compute $\Lambda = f(W)$
10. (select best $r$-subspace)
Algorithm: Power Iteration (P-PGD)

P-PGD

1. Set $\tilde{b} = b$
2. for $i = 1$ to $r$ do
3.   Initialize $\lambda_i \in S_m$ and $R_i^{(0)} = 0$
4.   for $k = 1$ to $k_{max}$ do
5.     $u_i = F(\lambda_i)$
6.     $u_i = \frac{u_i}{||u_i||}$
7.     $\lambda_i = f(u_i)$
8.   end for
9.   $\tilde{b} = \tilde{b} - A\lambda_i u_i$ (operator deflation)
10. endfor
11. Set $W = [u_1, u_2, ..., u_r]$ and $\Lambda = [\lambda_1, \lambda_2, ..., \lambda_r]^T$
Algorithm: Power Iteration with Updating (PU-PGD)

PU-PGD

1. Set $\tilde{b} = b$
2. for $i = 1$ to $r$ do
3. Initialize $\lambda_i \in S_m$ and $R_i^{(0)} = 0$
4. do step (4) → (13) of P-PGD algorithm
5. Orthonormalize $[u_1, ..., u_i]$
6. $[\lambda_1, ..., \lambda_i] = f ([u_1, ..., u_i])$
7. $\tilde{b} = b - A [u_1, ..., u_i] [\lambda_1, ..., \lambda_i]^T$ (operator deflation)
8. endfor
9. Set $W = [u_1, u_2, ..., u_r]$ and $\Lambda = [\lambda_1, \lambda_2, ..., \lambda_r]^T$
New Algorithm: Randomized iteration (R-PGD)

**R-PGD**

1. Initialize $[\omega_1, ..., \omega_{r+p}] \ni \Omega \in \mathbb{R}^{m \times (r+s)}$ Gaussian Random Matrix
2. for $i = 1$ to $r + s$ do (in PARALLEL)
3. Compute $u_i = F(\omega_i)$
4. endfor
5. Compute $[u_1, ..., u_{r+s}] = QR$ (QR factorization)
6. Compute $\Lambda = f(Q)$
7. Compute $\Lambda = U_\Lambda S_\Lambda V^*_\Lambda$ (SVD factorization)
8. Truncate to the best $r$-term (e.g. $\tilde{U}_\Lambda \leftarrow U_\Lambda$)
9. Set $W = Q\tilde{U}_\Lambda$ and $\Lambda = \tilde{S}_\Lambda \tilde{V}^*_\Lambda$
Comparison with existing algorithms

<table>
<thead>
<tr>
<th></th>
<th>Full Galerkin</th>
<th>SI-PGD</th>
<th>A-PGD</th>
<th>PU-PGD</th>
<th>R-PGD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Complexity</td>
<td>$m^3 n^3$</td>
<td>$r^3 m^3 + r^3 n^3$</td>
<td>$r^3 m^3 + rn^3$</td>
<td>$r^4 m^3 + rn^3$</td>
<td>$r^3 m^3 + rn^3$</td>
</tr>
</tbody>
</table>

Table: Asymptotic Complexity of the PGD algorithms

The new Randomized-PGD algorithm is:
- Parallelizable
- Cheap (Lowest complexity)
- Accurate
Test Problem: Stochastic Heat Equation

\[ \int_{\Omega} \kappa \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx + \int_{\partial_2 \Omega} g v \, ds \]

\[ \kappa(x, p) = \kappa_{\text{mean}} + \sum_{i=1}^{3} p_i \kappa_i(x) \]

\[ p_i \sim \mathcal{U}(-1, 1) \]

Figure: Computational domain
Error convergence

**Figure**: Relative error in the $L_2$ norm

**Figure**: Relative error in the $A$-norm
Eigen-modes convergence

Figure: Leading Eigen-modes SVD

Figure: Leading Eigen-modes R-PGD
A. Nouy
A generalized spectral decomposition technique to solve a class of linear stochastic partial differential equations

A. Nouy
*Generalized spectral decomposition method for solving stochastic finite element equations : invariant subspace problem and dedicated algorithms.*

A. Nouy and O.P. Le Maître
Generalized spectral decomposition for stochastic nonlinear problems
Outline

5  Proper Generalized Decomposition (PGD)

6  Galerkin Proper Orthogonal Decomposition (POD)

7  Advective Singular Value Decomposition (A-SVD)

8  Nonintrusive Methods
Consider the parametric linear problem: find $u(\xi) \in \mathbb{R}^{N_x} \otimes S(\Xi, dp(\xi))$

\[
A(\xi)u(\xi) = f(\xi) \quad \text{with} \quad A(\xi) : \Xi \mapsto \mathbb{R}^{N_x \times N_x} \quad f(\xi) : \Xi \mapsto \mathbb{R}^{N_x}
\]

where $\mathbb{R}^{N_x}$ is endowed with the discrete inner product $\langle , \rangle_w$

Pod Basis

We want to find a orthonormal POD basis $w_1, \ldots, w_\ell$ in $\mathbb{R}^{N_x}$ for $u(\xi)$:

\[
\hat{w}_1, ..., \hat{w}_\ell = \arg\max_{\tilde{w}_1, ..., \tilde{w}_\ell \in \mathbb{R}^{N_x}} \sum_{j=1}^{\ell} \int_{\Xi} | \langle u(\xi), \tilde{w}_j \rangle |^2 dp(\xi)
\]

Depending on how we discretize the integral $\int_{\Xi} dp(\xi)$ we obtain different formulations (e.g., Quadratures, Monte Carlo, ...)

MIT
Galerkin POD: Method of Snapshots

Discrete POD Problem

Let \( \{ \alpha_k \}_{k=1}^{N_x} \) and \( \{ \xi_k \}_{k=1}^{N_x} \) be discrete weights and nodes so that:

\[
\mathbf{w}_1, \ldots, \mathbf{w}_\ell \approx \arg\max_{\tilde{\mathbf{w}}_1, \ldots, \tilde{\mathbf{w}}_\ell} \sum_{k=1}^{N_x} \sum_{j=1}^{\ell} \alpha_k | \langle \mathbf{u}_k, \tilde{\mathbf{w}}_j \rangle |^2
\]

where \( \mathbf{u}_k = \mathbf{u}(\xi_k) \) is a snapshot obtained solving \( A(\xi_k) \mathbf{u}_k = \mathbf{f}(\xi_k) \)

Method of Snapshots [Sirovich 1987]

Let \( \mathbf{D} = \text{diag} \{ \alpha_1 \ldots \alpha_{N_x} \} \), \( \mathbf{U} = \begin{bmatrix} \mathbf{u}_1 & \ldots & \mathbf{u}_{N_x} \end{bmatrix} \) and

\[
\mathbf{U} = \mathbf{W}^{1/2} \mathbf{U} \mathbf{D}^{1/2} \in \mathbb{R}^{N_x \times N_x}. \text{ Then } \mathbf{w}_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{U} \mathbf{D}^{1/2} \mathbf{v}_i \text{ where } \mathbf{v}_i \text{ s.t.}
\]

\[
\mathbf{U}^T \mathbf{U} \mathbf{v}_i = \lambda_i \mathbf{v}_i \quad i = 1, \ldots, \ell
\]
Once we have a POD basis $w_1, \ldots, w_\ell$ of rank $\ell$ in $\mathbb{R}^{N_x}$ for $u(\xi) \in \mathbb{R}^{N_x} \otimes S$ we solve the reduced order model.

### Reduced Order Model

Find $u^\ell(\xi) \in \mathbb{R}^\ell \otimes S$ s.t.

$$A_{r,\ell}(\xi) u^\ell(\xi) = f_{r,\ell}(\xi)$$

with

$$\begin{bmatrix} \langle A_r(\xi) w_i, A \xi w_j \rangle \end{bmatrix}_{ij} = \langle w_i, f(\xi) \rangle_W$$

with associated error estimate [Volkwein 2007]:

$$\int_\Xi \|u(\xi) - u^\ell(\xi)\|_W^2 dp(\xi) \leq C(\text{shape } \Xi) \sum_{j=\ell+1}^\infty \lambda_j$$
Galerkin POD: References

D. P. Holmes, J. L. Lumley, G. Berkooz
Turbulence, Coherent Structures, Dynamical Systems and Symmetry
Cambridge University Press, New York, 1996

L. Sirovich
Turbulence and the dynamics of coherent structures, part 1: coherent structures.

M. Kahlbacher and S. Volkwein
Galerkin proper orthogonal decomposition methods for parameter dependent elliptic systems.
Outline

5. Proper Generalized Decomposition (PGD)

6. Galerkin Proper Orthogonal Decomposition (POD)

7. Advective Singular Value Decomposition (A-SVD)

8. Nonintrusive Methods
Theorem: The Advective SVD

Given $U \in \mathbb{R}^{m \times n}$, let $U \approx u_0(x, \xi)$ be the initial condition of a stochastic linear transport problem with periodic boundary conditions and unitary advection speed. Compute the preconditioned problem until convergence of the preconditioner at time $T$. Choose $N \in \mathbb{N}$, $N > T$, $\min_{\xi} \tau(N, \xi) \geq T$ and store:

$$
\begin{align*}
&y(x, N, \xi) = \sum_{j \leq r} w_j(x) \lambda_j(\xi) \\
&\tau_N(\xi) = \tau(N, \xi)
\end{align*}
$$

Then:

$$
u_0(x, \xi_k) = \sum_{j \leq r} w_j(x - [t_k - N]) \lambda_j(\xi_k) \quad \text{with} \quad t_k = \tau_N(\xi_k)$$
A Full Rank Matrix

- Given $U \in \mathbb{R}^{m \times n}$, we are interested in computing its Singular Value Decomposition.

- You can think of $U$ as the solution field $u \in \mathcal{V}$ of a general parametric PDE or as the uncertain parameter (i.e. a permeability field) in a SPDE projected onto a finite dimensional space $\mathcal{V}$, where usually $\mathcal{V}$ is a tensor product space. Anyway, it does not really matter where the matrix $U$ comes from, it just need to have some, maybe hidden, structure. You want to think of cases in which $U$ is full rank (with slowly decaying spectrum) and no compact representation based on SVD is possible.

$$\Pi_{\mathcal{V}} : \mathcal{V} \rightarrow \mathbb{R}^{m \times n}$$

$$U = \Pi_{\mathcal{V}} (u)$$
A Generalization of the SVD

Definition

Let \( \phi : \mathcal{V} \rightarrow \mathcal{V}' \) be a bijection between vector spaces such that:

\[
\tilde{U} = \Pi_{\mathcal{V}'} (\phi [u]) \quad U = \Pi_{\mathcal{V}} (u)
\]

Thus:

\[
U = (\Pi_{\mathcal{V}} \circ \phi^{-1} \circ \Pi_{\mathcal{V}'}^{-1}) \tilde{U}
\]

Let:

\[
\tilde{U} = \sum_{i \leq r} w_i v_i'
\]

be a classical rank-one decomposition (SVD) for \( \tilde{U} \). We call \( \{w_i, v_i\} \) a \((\mathcal{V}\phi)\)-SVD of \( U \). It is clearly a generalization of the classical SVD which is obtained for \( \phi = \mathcal{I} \) identity operator.
Our idea is to find the map $\phi$ such that:

$$\phi = \arg\min_{\mathcal{F}: \mathcal{V} \rightarrow \mathcal{V}'} \{ \text{rank} \tilde{U} \}$$

- $\phi$ is a PDE and, with suitable choices of its functional form, the, possibly nonlinear, composition map $(\Pi_{\mathcal{V}} \circ \phi^{-1} \circ \Pi_{\mathcal{V}'}^{-1})$ can be described with very small dimensional parameters.

**Definition**

An **Advective-SVD** is a $(\mathcal{V}\phi)$-SVD where $\phi$ is a linear advection PDE parametrized by $\theta \in \mathcal{V}$ so that our minimization problem reduces to:

$$\tilde{\theta} = \arg\min_{\theta} \{ \mathcal{F} (\Pi_{\mathcal{V}}^{-1} U; \theta) \}$$
The Idea

Fact

The idea is to use a linear transport (advection) PDE $\phi$, to transport and condense part of the complexity associated to $U$ (full rank) into the parameter $\theta \in \mathcal{V}$. It is a redistribution of complexity.

Definition

$\mathcal{V}$ is a tensor product space, namely:

$$\mathcal{V} = \Omega_x \otimes \Omega_\xi$$

so that assume:

$$\Pi_{\mathcal{V}}^{-1} U = u (x, \xi) \in \Omega_x \otimes \Omega_\xi$$

and $\theta \in \Omega_\xi$. Notice that $\theta$ cannot belong to the full space $\Omega_x \otimes \Omega_\xi$, otherwise no gain in complexity will be made. By letting $\theta \in \Omega_\xi$, we make sure that any transfer of complexity to $\theta$ will result in an overall decrease of complexity of the system.
A Fake Transport Problem

Let:

\[ u(x, \xi) = u_0(x, \xi) \]

and consider the following transport problem, find \( u(x, t, \xi) \in \Omega_x \otimes \Omega_t \otimes \Omega_\xi \) such that:

\[
\begin{cases}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \\
\text{periodic b.c.} \\
u(x, 0, \xi) = u_0(x, \xi)
\end{cases}
\]

Fact

It is a 1D (in space) pde parametrized by \( \xi \), so we can set \( \Omega_x = [0, 1] \). In particular, it is a transport equation with unitary advection speed:

\[ v(\xi) = 1 \]

independent of the parameter.
**Fact**

The problem has periodic boundary conditions and the solution itself is periodic in time, that is:

\[ u(x, \tilde{t}, \xi) = u(x, \tilde{t} + N, \xi) \quad \forall N \in \mathbb{N} \]

with unitary period.

- Let \( \tilde{t} = 0 \) and notice that:

\[ u_0(x, \xi) = u(x, N, \xi) \quad \forall N \in \mathbb{N} \]
Preconditioning step

- The idea is to precondition the equation and make the field low rank. To this end, set:

\[ y(x, \tilde{\tau}(t, \xi), \xi) = u(x, t, \xi) \]

ans solve for \( y(x, t, \xi) \) and \( \theta(t, \xi) \):

\[
\begin{cases}
\frac{\partial y}{\partial t} + \theta(t, \xi) \frac{\partial u}{\partial x} = 0 \\
\frac{\partial \tilde{\tau}(t, \xi)}{\partial t} = \theta^{-1}(t, \xi)
\end{cases}
\]

periodic b.c.

\[
y(x, 0, \xi) = u_0(x, \xi)
\]

until the preconditioner \( \theta(t, \xi) \) becomes stationary in time for some periods of the system. Let \( \xi_{\text{ref}} \) be associated with the reference field:

\[ y_{\text{ref}}(x, t) = u(x, t, \xi_{\text{ref}}) \]
A Low Rank Solution

Fact

Since the original equation was not explicitly dependent on time (i.e. no forcing terms), the preconditioned equation is going to reach a stationary solution after, say, $T$ that we define formally as that time $T$ such that:

$$\theta(t, \xi) = \text{const} = 1 \quad \forall t \geq T, \forall \xi$$

and, by construction, the rank of $y(x, t, \xi)$ at each time step, cannot be higher than the original rank of $u_0(x, \xi)$. That is, in the worst case $\theta(t, \xi) = 1 \quad \forall t \geq 0, \forall \xi$.

- If the field had an hidden shifted structure we now have at time $k \geq T$:

$$y(x, k, \xi) = \sum_{j \leq r \ll m} w_j^k(x) \lambda_j^k(\xi)$$

that is, the field is low rank.
**Fact**

Pick $N \in \mathbb{N}$ such that $N > T$ and $\min_\xi \tilde{\tau}(N, \xi) \geq T$ where $T$ is the time at which the preconditioner became stationary ($\theta(t, \xi) = 1 \quad \forall t \geq T, \forall \xi$).

Notice that $T$ can be exactly determined by monitoring the convergence of $\theta(t, \xi)$ and $\tilde{\tau}(N, \xi)$. The **key** observation is the following:

$$u_0(x, \xi) = u(x, N, \xi) = y(x, \tau(N, \xi), \xi)$$

Notice that, by construction, $\tilde{\tau}(N, \xi_{ref}) = t_{ref} = N$ and let

$$y(x, \tilde{\tau}(N, \xi_{ref}), \xi) = y(x, N, \xi) = \sum_{j \leq r} w_j(x) \lambda_j(\xi)$$

and store $\{w_j(x), \lambda_j(\xi)\}_{j=1}^r$ at $t = N$. 
Assume we are interested in $u_0(x, \xi_k)$. Then:

$$u_0(x, \xi_k) = y(x, \tilde{\tau}(N, \xi_k), \xi_k) = y(x, t_k, \xi_k)$$

But we have $y(x, N, \xi) = \sum_{j \leq r} w_j(x) \lambda_j(\xi)$.

Collocate it at $\xi_k$:

$$y(x, N, \xi_k) = \sum_{j \leq r} w_j(x) \lambda_j(\xi_k) = y_N^k(x)$$
Fact

So, we just have to integrate in time, either backward or forward, to get $y(x, t_k, \xi_k)$ from:

$$\begin{cases}
\frac{\partial y(x,t)}{\partial t} + \theta(t, \xi_k) \frac{\partial y(x,t)}{\partial x} = 0 & t \in [N, t_k] \\
\text{periodic b.c.} \\
y(x, N, \xi_k) = y^k_N(x)
\end{cases}$$

Two important observation:

- For $t \in [N, t_k]$ we can assume the preconditioner constant and equal to:

$$\theta(t, \xi_k) = 1 \quad t \in [N, t_k]$$

and this is due to our choice of $N$. 
Thus, we are left with a transport equation with constant speed, namely:

\[ \frac{\partial y}{\partial t} + \frac{\partial y}{\partial x} = 0 \quad t \in [N, t_k] \]

periodic b.c.

\[ y(x, N) = y_N^k(x) \]

The previous equation has an **analytic solution**, namely:

\[ y(x, t_k, \xi_k) = y_N^k(x - [t_k - N]) \]

and:

\[ u_0(x, \xi_k) = y_N^k(x - [t_k - N]) \]
Outline

5. Proper Generalized Decomposition (PGD)

6. Galerkin Proper Orthogonal Decomposition (POD)

7. Advective Singular Value Decomposition (A-SVD)

8. Nonintrusive Methods
Nonintrusive Spectral Methods: Overview [Nouy 2009]

Challenge

Approximate \( u(x, \xi) \in \mathcal{V} \otimes \mathcal{S}(\Xi, dP_\xi) \) s.t. \( \mathcal{L}(u(x, \xi); \xi) = f(x, \xi) \) with only \( \mathcal{V} \)-deterministic solvers

Classical nonintrusive spectral methods are:

1. \( L^2 \) projection
2. Regression
3. Stochastic Collocation

Pros and Cons

- **Uncoupled** deterministic problems
- Parallel Computations
- Large sample size
- Lack of rigorous **error estimators**
Nonintrusive Spectral Methods: $L^2$ projection

$L^2$ Projection

Fix a basis $\{H_\alpha(\xi)\}_{\alpha \in I} \subset \mathcal{S}$ and let $u(x, \xi) \approx \sum_{\alpha \in I} u_\alpha(x) H_\alpha(\xi)$ with:

$$\{u_\alpha(x)\}_{\alpha \in I} = \arg\min_{\tilde{u}_\alpha(x)} \left\| u - \sum_{\alpha \in I} \tilde{u}_\alpha H_\alpha \right\|^2_{S(\Xi, dP_\xi)}$$

If $\{H_\alpha(\xi)\}_{\alpha \in I}$ is orthonormal then:

$$u_\alpha(x) = \int_\Xi u(x, \xi) H_\alpha(\xi) dP_\xi(\xi) \approx \sum_{k=1}^{K} \omega_k u(x, \xi_k) H_\alpha(\xi_k) \quad \forall \alpha$$

for some weights $\{\omega_k\}$ and nodes $\{\xi_k\}$ (e.g., adaptive quadratures).
Nonintrusive Spectral Methods: Regression

Regression

Compute an $L^2$ projection with a **discrete inner product** over $S(\Xi, dP_\xi)$

$$\{u_\alpha(x)\}_{\alpha \in I} = \argmin_{\{\bar{u}_\alpha(x)\}_{\alpha \in I} \in V} \sum_{k=1}^{K} \omega_k \left\{ u(x, \xi_k) - \sum_{\alpha \in I} \bar{u}_\alpha H_\alpha(\xi_k) \right\}^2$$

equivalent to solve for $\left(U\right)_\alpha = u_\alpha(x)$ the **linear system**:

$$HU = Z$$

with

$$\begin{cases} 
(H)_{\alpha\beta} = \sum_{k=1}^{K} \omega_k H_\alpha(\xi_k) H_\beta(\xi_k) \\
(Z)_\alpha = \sum_{k=1}^{K} \omega_k u(x, \xi_k) H_\alpha(\xi_k)
\end{cases}$$

- If $\{H_\alpha(\xi)\}_{\alpha \in I}$ is orthonormal w.r.t the discrete inner product then $H = I$ and $U = Z$ so that **Regression** $= L^2$ projection
Stochastic Collocation Method [Xiu 2005]

Let $\Xi_I = \{\xi_1, ..., \xi_M\}$ be a set of interpolation nodes and $\{L_\alpha(\xi)\}_{\alpha=1}^M$ be the associated Lagrange polynomials. If $u(x, \xi) \approx \sum_{\alpha=1}^M u_\alpha(x) L_\alpha(\xi)$, then:

$$R(x, \xi)_{|\xi=\xi_i} = \{f(x, \xi) - L(u(x, \xi); \xi)\}_{|\xi=\xi_i} = 0 \quad \forall \alpha = 1, ..., M$$

\[\Downarrow\]

$$u_\alpha(x) = \text{argsol} \{L(\tilde{u}(x); \xi_\alpha) = f(x, \xi_\alpha)\} \quad \forall \alpha = 1, ..., M$$

- For high dimensions: Smolyak tensorization of univariate interpolation basis associated to cubature nodal sets $\Xi_I$
Remark

High rank fields are typically associated with long time integration issues.

\[
\text{Re} (\xi) = 100 + 20 \mathcal{U} (\xi)
\]

\[
\text{Cd} (\xi, t) \sim f [\sin (\alpha \xi t)]
\]

- Random vortex shedding frequency. Again, any discretization of the parameter space will eventually fail [Karniadakis 2005].
References

A. Nouy
Recent Developments in Spectral Stochastic Methods for the Numerical Solution of Stochastic Partial Differential Equations

D. Xiu and J. S. Hesthaven.

G. Hendra, N. Oki and S. Wono
A Formula for Angles Between Subspaces of Inner Product Spaces
Research report collection, (2009) 7 (3)