A Short Summary of MsC Research Period

Enes Savli

Thesis : Posteriori MOR Strategies for Seismic Applications in Geophysics

March 8, 2019

Overview

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Personal Information

I am a open-minded and curious Mechanical Engineer who;

- was born in Istanbul at 1989,
- is a life-long student, good learner and self motivated person,
- likes seas and literature also is a cine guru,

- Got the BsC Degree in 2011 in Mechanical Engineering (3.02/4)
- Final Poject : Exergy/Energy Analysis of an Active Co-generation System in ERDEMIR
- Technical interests are computational mechanics, numerical analysis...

Master Program

- Called Modeling for Science and Engineering given by Applied Mathematics division of UAB
- Interdisciplinary program is based on two pillars;
  - Modeling of Systems
  - Numerical simulation or Resolution of Systems

- Taken classes like Optimization, Dynamical Systems Modeling, Parallel Programming, Applied Modeling and Simulation
- Various small/mid scale projects on science/computer science and engineering.

Barcelona Supercomputer Center

- BSC is the national super-computing centre in Spain which specialise in HPC and manage MareNostrum, one of the most powerful supercomputers in Europe.
- With a total staff of more than 500 researchers and professionals focuses on four main fields: Computer, Life, Earth Sciences and Applications in Engineering and 24 sub-areas.

Necessity of ROM & Previous Works

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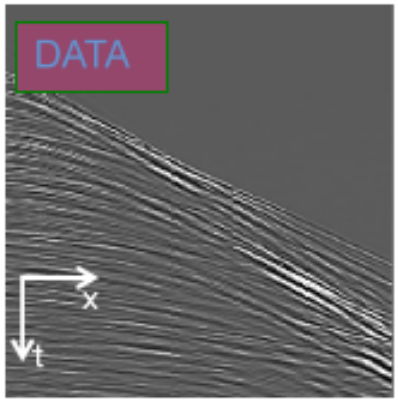

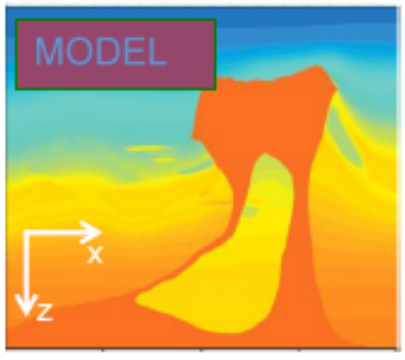

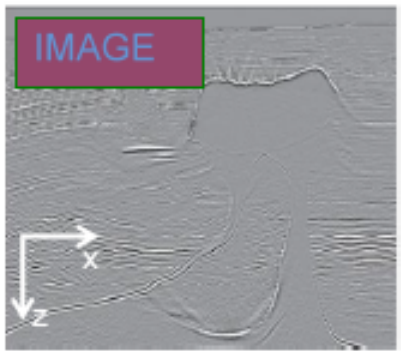

- Seismic applications requires repetitive expensive solutions
  - Seismic Imaging
  - Reverse Time Migration
  - Inversion Techniques
- In Geosciences Applications Group of BSC, ROM techniques have been already conducting for some years.
- Group was specialized in a-priori methods mainly PDG (Proper Generalized Decompositions) [1] [2]

Thesis plan & Objectives

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In broad manner objectives were;

- Exploring on various posteriori methods which are much more easy to implement than PDG
- Seeking for possibility to adaptation to the high fidelity solver of BSC

- At first sight due to dealing with huge data, POD-SVD methods have been chosen
- For latter, Pereyra's strategies has been planned for implementation and comparison.[4, 5, 3]

In particular objectives were;

- Building the surrogate models of large parameterized wave propagation models by using ROM.
- Analyze the snapshot method (SVD) advantages and drawbacks and discuss the cost of offline stage.
- Get over the burden by implementations of cheaper QR representations [5]
- Test different parameterizations.(frequency,positions)

Overview of Reduced Order Modeling

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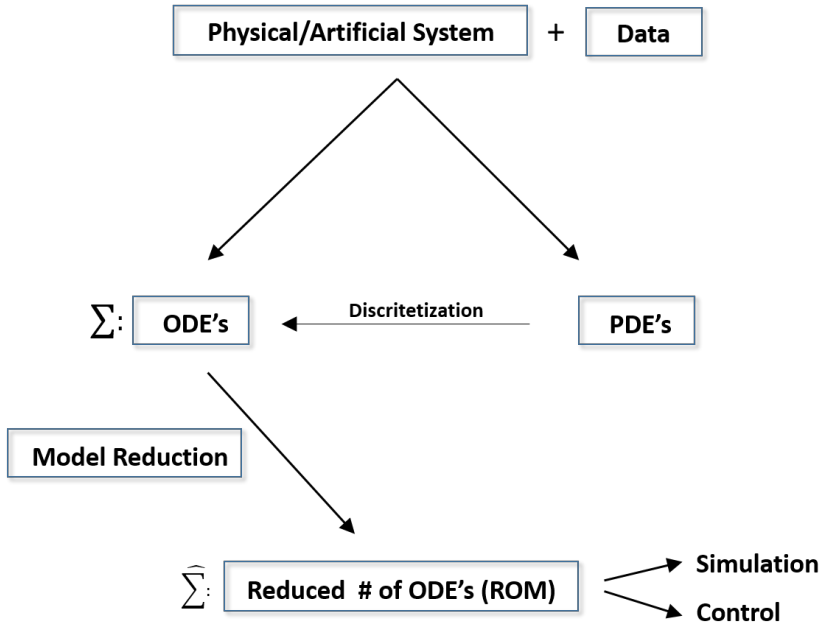

- Approximates the high order model in low order one by preserving stucture.
- In general, projection on to the reduced basis
- Expensive step is computation of reduced basis a.k.a "Offline Stage"

Why POD?

- Data dependent, non-intrusive implementation, guarantees the optimality
- More stable, compatibility to larger data-sets (PCA relation)

Workflow of POD Snapshot Method

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State Space System

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t),$$
$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t)$$

High Fidelity Simulations

$$\mathbf{Y} := [\mathbf{y}(t_1), \mathbf{y}(t_2), ..., \mathbf{y}(t_m)] \in \mathbb{R}^{N\times m}$$

Singular Value Decomposition

$$Y = U\begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} V^T =: U\Sigma V^T \qquad \mathbf{U} \in \mathbb{R}^{N\times m}$$

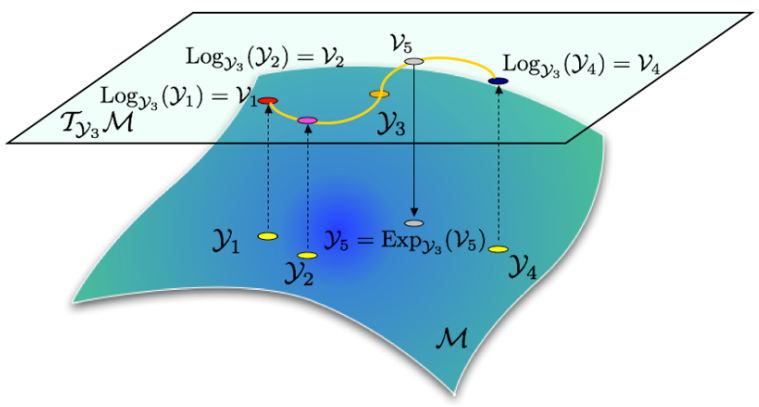
Truncation/Get Optimal Basis

$$\mathbf{y}(x,t) \approx \mathbf{U}_k\mathbf{a}(t).$$

A

B

C



Ar

B′

Cr

Reduced State Space System

$$\frac{d}{dt}\mathbf{a}(t) = \mathbf{U}_k^T\mathbf{A}\mathbf{U}_k\mathbf{a}(t) + \mathbf{U}_k^T\mathbf{B}\mathbf{u}(t)$$
$$\mathbf{y}(t) = \mathbf{C}\mathbf{U}_k\mathbf{a}(t)$$

Approximatited Solution

$$\tilde{\mathbf{y}} = \mathbf{U}_k\mathbf{a}(t)$$

Some Results on Validation Phase

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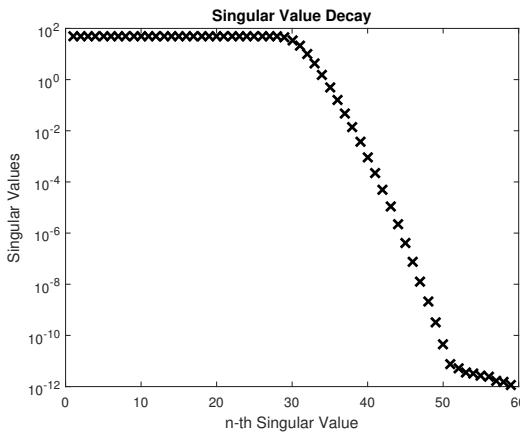
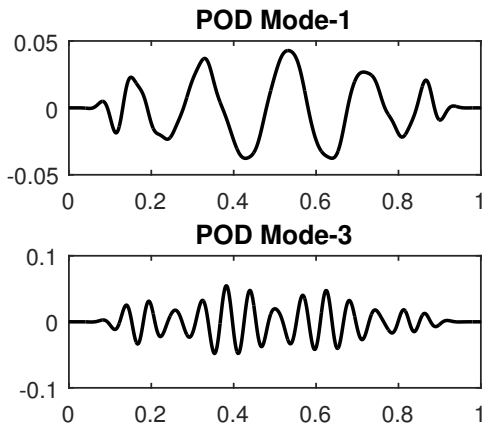
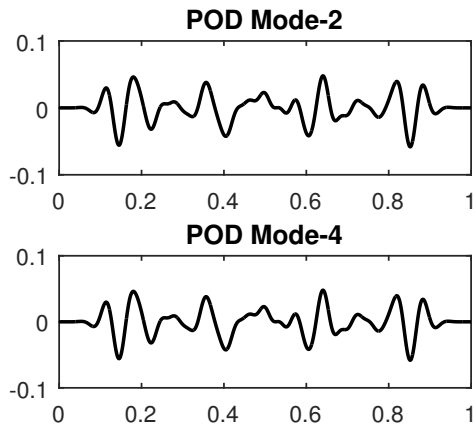
First trials have been done in;

- 1D Frequency Domain FE model with frequency parameterization.
- 2D Time domain high order FD schemes with source and time parameterization.







Some Results on Validation Phase

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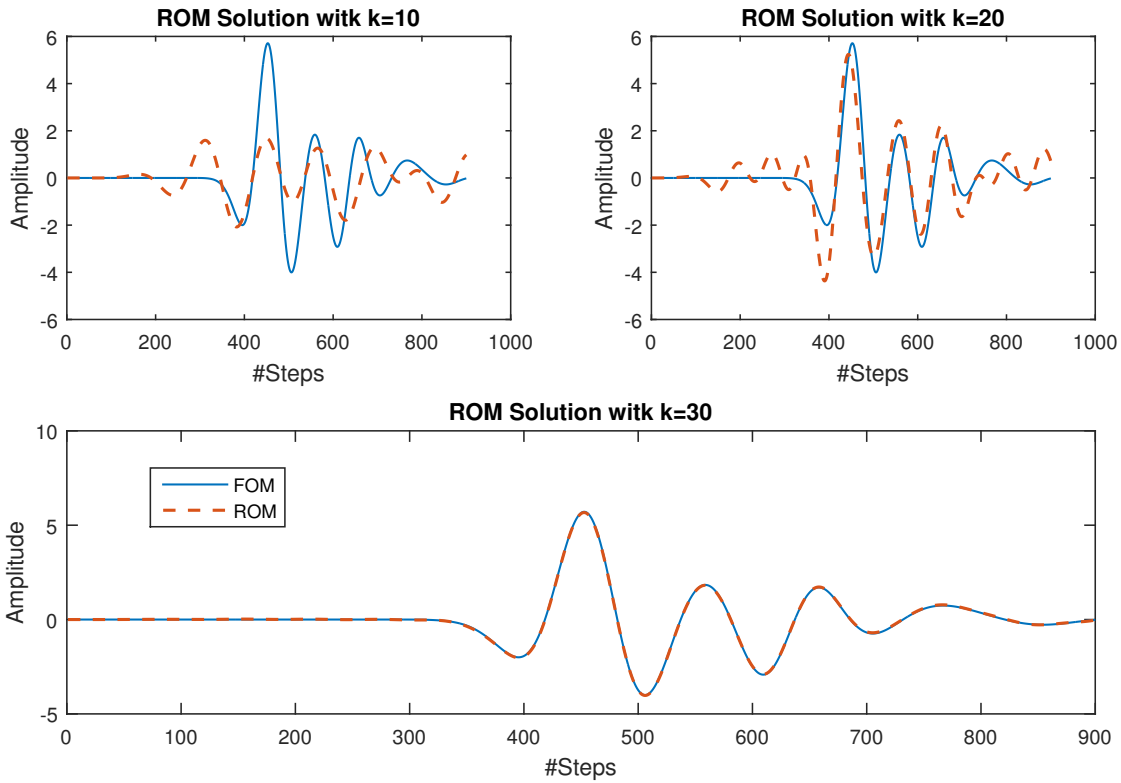
- All the steps have been examined and shown in deeper aspects in both models.
- POD method in Acoustic Wave Propagation models have been explored and validated.
- It is shown that SVD is not a feasible option for large scale seismic applications for high memory requirement and complexity $\mathcal{O}(min(mn^2, m^2n)$.



Adaptive QR Decomposition Method - I

- A novel algorithm proposed by Victor Pereyra (2011) claimed as a replacement of SVD
- It is progressive because it advances with the high fidelity simulation
- It is adaptive because selects the y_i snapshot according to angle between existing basis and snapshot y_i.
- Storing snapshot matrix is not required and evaluation of $\mathbf{Q}$ is just a backward accumulation. $\Rightarrow$ cheaper!
- Projection with $\tilde{\mathbf{p}} = \mathbf{Q}\mathbf{a}(t)$ instead of $\tilde{\mathbf{p}} = \mathbf{U}\mathbf{a}(t)$

Adaptive QR Decomposition Method - I

Algorithm 1: Adaptive QR Algorithm

Input: $\mathbf{X} \in \mathbb{R}^m$ Solution at t timestep, $V \in \mathbb{R}^{mxk}$ Computed Householder vectors, Threshold δ;
Output: Q orthogonal basis;
At the k*th* step;
for *i = 1,..,k* **do**
    Householder Transition until $\mathbf{X}_{1:k}$;
    $X = \mathbf{X} - 2 * V(:,i) * (V(:,i)' * \mathbf{X})$

Calculate the $\alpha = -sign(\mathbf{X}_{k:end}(1)) * \|\mathbf{X}_{k:end}\|_2$ (Diagonal term of R);
Compute the threshold $\mu = \|\alpha|/\|\mathbf{X}\|_2$;
if $\mu > \delta$ **then**
    Compute the new snaphot's HH vector and save it;
    $v = (\mathbf{X}_{k:end} - \alpha * e)./\|\mathbf{X}\|_2, \quad$ where $e^T = (1, 0, ..0)$;
    $v \rightarrow V$;
    $k+ = 1$;
else
    Try next snapshot;

Compute the Orthogonal Basis $Q \in \mathbb{R}^{mxn}$ $(n << m)$ by backward accumulation of $V \in \mathbb{R}^{mxn}$
Householder Vectors **for** *j = n,n-1,...,2* **do**
    $\mathbf{Q} = \mathbf{Q} - 2 * V(:,j) * (V(:,j)' * \mathbf{Q})$

Combining Domain & QR Decompositions

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- QR-I has limitations too and some manipulations to system might be done to make QR applicable.
- Proposed application is "skeletonization" by reducing the size of the "saved" entitites $N \Rightarrow N_r$ with arbitrary $\mathbf{C} \in \mathbb{R}^{Nr \times N}$. This reduction provides new snapshots $\tilde{\mathbf{Y}} = \mathbf{CY}$.
- Then we can't use direct orthogonal parts as $\mathbf{Q}^{Y} \neq \mathbf{Q}^{\tilde{Y}}$.
- Idea comes from "Oblique Projections". Using $\tilde{\mathbf{y}} = \tilde{\mathbf{Y}}\mathbf{a}(\mathbf{t})$ instead $\tilde{\mathbf{y}} = \mathbf{Q}\mathbf{a}(\mathbf{t})$ and interpolate back!

Original System;

$\mathbf{y_{tt}} = \mathbf{Ay} + \mathbf{Bu(t)}$ *introducing* $\mathbf{y} = \mathbf{Ya(t)}$;

$\mathbf{CYa_{tt}} = \mathbf{CAYa} + \mathbf{Cbu(t)}$

and we can subsitute $CY = QR$;

$\mathbf{QRa_{tt}} = \mathbf{CAYa} + \mathbf{Cbu(t)}$ *and finally*;

$\mathbf{a_{tt}} = \mathbf{R^{-1}Q^{t}CAYa} + \mathbf{R^{-1}Q^{t}Cbu(t)}$

and;

$\mathbf{y} = \mathbf{CYa}$.

- As seen, $\mathbf{R^{-1}}$ term occurs in reduced system.
- Well-conditioned $\mathbf{R^{-1}}$ is needed.
- Adaptive QR decomposition II is proposed focusing on condition number κ of $\mathbf{R}$ by using modified scheme of QR-I.
- Advancing in time is modified to avoid from systematic skipping.

Results

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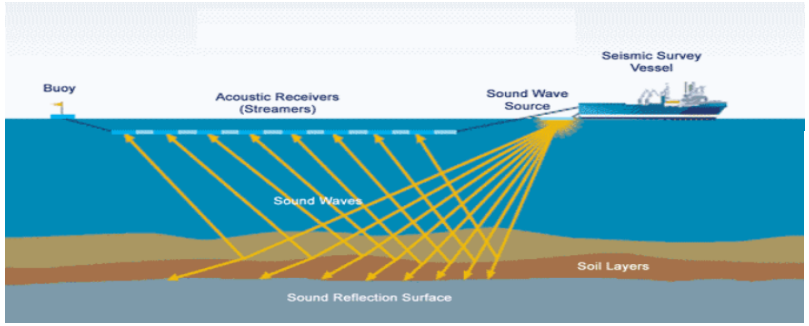
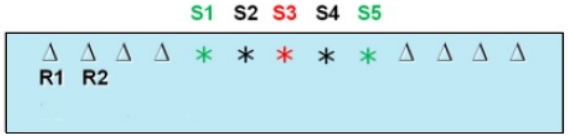
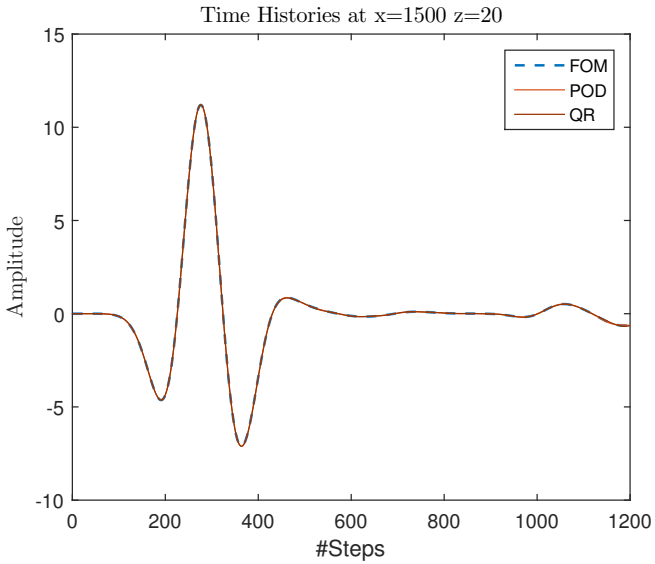
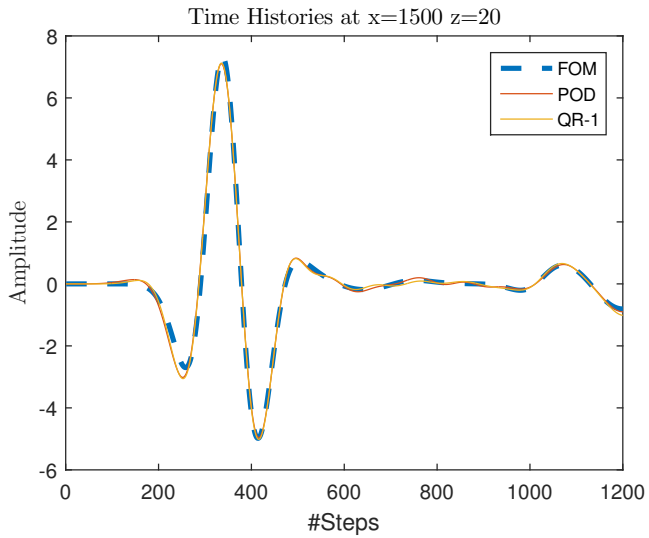




- Tests are done as figures above parameterization of source to be realistic with miscellaneous domain sizes.





Results

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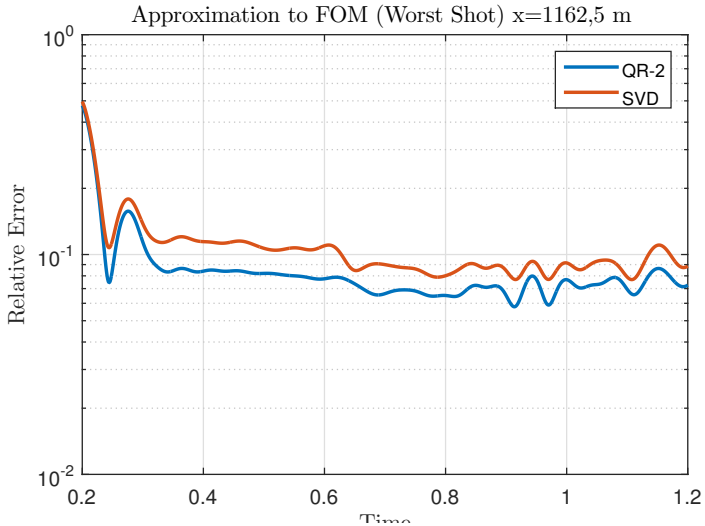
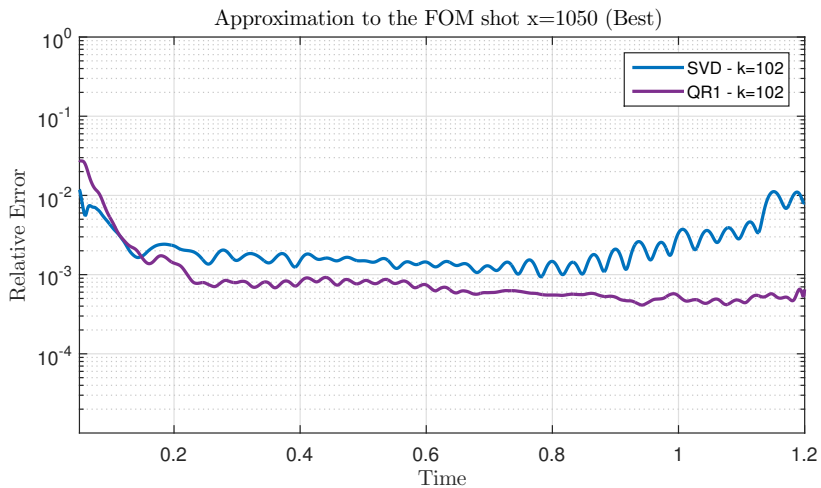
Criteria	Basis Selection
ϵ =0.9999	k=71
$\phi = 7$	k=102
Initial Criteria :10^8	k=164





A Classifier Example

As claimed that two of QR decomposition for replacement SVD, one synthetically example in homogeneous media is derived;

- Total solution matrix would be size 4410000 x 1300 for 2 shot

Table: Calculation Times

Algorithm	POD-SVD	QR-I	QR-II
Time(s)	N/A	9760	11080
# Basis	N/A	221	378

Conclusions & Some Notes

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- It is shown that a-posteriori methodology is a satisfactory phenomena and it is worthwhile to do further developments.
- All the methods gauged carefully and high compression ratios are obtained.
- It is shown that usage of POD method is an option for seismic applications.
- To get over the possible drawbacks (computational load of offline stage, memory), original and modified version of novel adaptive QR algorithm are introduced and implemented successfully.

- During this work, i have been contracted in BSC as Research Intern.
- In all works, in-house high fidelity models have been used as template.
- All related implementations are realized by me from the scratch.
- Matlab and Pyhton programming languages have been used.
- Apart this work, POD for non-linear models and some error estimation methods have been researched.
- Real life applications leaved as future works.

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Thank You!!