A reduced basis approach for efficient non-intrusive polynomial chaos in CFD

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Outline

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- Conclusion

UMRIDA(EU-FP7 project)

Uncertainty Management for Robust Industrial Design in Aeronautics

- The objective of UMRIDA is to upgrade the TRL of UQ in aeronautics to level 5-6
- Within UMRIDA different methodologies to deal with UQ will be investigated by research groups from:
  - *6 European airframe and engine industries*
  - *13 major aeronautical research establishments and academia*

@VUB:

UQ methods for efficient handling of large number of uncertainties

- Reduced basis approach using polynomial chaos method
- In Doostan et al. (2007) such an approach was used within the context of intrusive Polynomial Chaos
- Here the methodology is extended to non-intrusive PC and is applied to 2D and 3D industrial applications

Motivation

- Uncertainty in physical properties, input data and model parameters result in uncertainties in the system output.

- For the design refinement and optimization, it is necessary to include all uncertainty information in the output results using UQ schemes.

- Many complex CFD calculations (e.g. Turbomachinery) require 3D fine computational mesh, small time-step and high-dimensional space for stochastic analysis.

- These dramatically increases the computational cost that can be partially reduced using efficient UQ schemes.

Motivation

- Classical uncertainty quantication schemes (e.g., Monte Carlo, polynomial chaos) suffer from the *curse of dimensionality*.

- To overcome *curse of dimensionality* several schemes have been proposed. Examples are:
  - Efficient sampling methods(e.g. Sparse sampling)
  - Sensitivity analysis (e.g. Sobol indicies)
  - Surrogate modeling (e.g. Kriging)
  - Model Reduction (e.g. GSD)
  - Multilevel Monte Carlo
- In practice a single technique may not be sufficient, and combination of techniques need to be employed.

- In this study we focus on the "POD-based Model Reduction" approach.

UQ using intrusive polynomial chaos

- All uncertainties were introduced in the governing equation.
- System of equations was solved
- Needed to rewrite code
- Not possible for complex 3D applications

1D advection equation is given by

$$\frac{du}{dt} + a\frac{du}{dx} = 0;$$

$$P + 1 = \frac{(p+n)!}{p!n!}$$

p=order of PC
n=#uncertainties

We assume uncertainty in u at boundary.
After expansion i.e.

$$u(x,\zeta) = \sum_{i=0}^{P} u_i(x)\psi_i(\zeta)$$

substitution in the original equation

$$\sum_i \frac{du_i}{dt}\psi_i + a\sum_i \frac{du_i}{dx}\psi_i = 0;$$

Multiplying with ψ_k and performing the scalar products, one obtains

$$\frac{du_k}{dt} + a\frac{du_k}{dx} = 0; \qquad k=0,1,2,3\ldots P$$

Non-intrusive UQ using polynomial chaos

- Uncertain input parameters: IC, BC, geometry, modeling parameters
- PC expansion: $$u(x,\zeta)=\sum_{i=0}^{P} u_i(x)\psi_i(\zeta)$$

$P+1=(p+n_s)!/p!n_s!$
p=order of PC
n_s=# uncertainties

Input parameters:

$a_1=a_{10}+a_{11}*\zeta_1$
$a_2=a_{20}+a_{21}*\zeta_2$
……
$a_{ns}=a_{n0}+a_{n1}*\zeta ns$

→ Computational model →

Output solution

$$u(x,\zeta)=\sum_{i=0}^{P} u_i(x)\psi_i(\zeta)$$

- Statistical solution

$$Mean = u_0$$
$$Variance = \sum_{i=1}^{P} u_i(x)^2 < \psi_i^2 >$$

Non-intrusive UQ using polynomial chaos (contd)

- PC terms can be calculated via

1. Numerical quadrature

PC approximation of the solution: $u(x,\zeta) = \sum_{i=0}^{P} u_i(x)\psi_i(\zeta)$

This integral can be solved using numerical quadrature method

Inner product: $u_i(x)\langle \psi_i^2 \rangle = \langle u(x,\zeta).\psi_i(\zeta) \rangle = \int u(x,\zeta).\psi_i(\zeta) f(\zeta) d\zeta$

$$\Rightarrow u_i(x) = \frac{1}{\langle \psi_i^2 \rangle} \sum_{j=1}^{S} u^j(x)\psi_i(\zeta_j) w_j$$

Where:
- f :*is PDF of* ζ
- ζ_j :*are quadrature points*
- w_j : *are weights of quadrature points*
- $u_j(x)$: *are sample solution*

S=(p+1)^ns deterministic samples
p=2,ns=5 ➔243 samples
p=2,ns=10 ➔59049 samples
p=3,ns=10 ➔ 1048576 samples

 # deterministic samples increases exponentially with increasing pc order and n_s

Non-intrusive UQ using polynomial chaos (contd)

2. Regression method

- PC approximation of the solution $\sum_{i=0}^{P} u_i(x)\psi_i(\zeta) = u(x,\zeta)$

$$u_0(x)\psi_0(\zeta) + u_1(x)\psi_1(\zeta) + \ldots\ldots\ldots + u_P(x)\psi_P(\zeta) = u(x,\zeta)$$

$$\underbrace{\begin{pmatrix} \psi_0(\zeta^0) & \cdots & \psi_i(\zeta^0) & \cdots & \psi_P(\zeta^0) \\ \vdots & \vdots & \cdots & \vdots & \\ \psi_0(\zeta^s) & \cdots & \psi_i(\zeta^s) & \cdots & \psi_P(\zeta^s) \\ \vdots & \vdots & \cdots & \vdots & \\ \psi_0(\zeta^P) & \cdots & \psi_i(\zeta^P) & \cdots & \psi_P(\zeta^P) \end{pmatrix}}_{\Psi(\zeta^s)} \underbrace{\begin{pmatrix} u_0(x) \\ \vdots \\ u_i(x) \\ \vdots \\ u_P(x) \end{pmatrix}}_{\text{PC coefficients}} = \underbrace{\begin{pmatrix} u(x;\zeta^0) \\ \vdots \\ u(x;\zeta^s) \\ \vdots \\ u(x;\zeta^P) \end{pmatrix}}_{\text{Solution samples}}$$

Oversampling

S=2(P+1) deterministic samples
p=2,ns=5 ➔42 samples
p=2,ns=10 ➔132 samples
p=3,ns=10 ➔ 572 samples

- Matrix can be solved by over sampling for PC coefficients $u_i(x)$

 # deterministic samples increases exponentially with increasing pc order and n_s

Reduced basis approach:

- The POD-based model reduction is a method that provides an optimal basis (or modes) to represent the dynamic of a system.

- Several model reduction techniques have been proposed for uncertainty quantitation. Two informative examples are:

  - Generalize Spectral Decomposition (GSD) Nouy (2007)
  - An intrusive model reduction technique for chaos representation of a SPDE Doostan et al. (2007)

- The model reduction used here is a POD-based model reduction scheme, similar to the one proposed by Doostan et al. (2007), but in non-intrusive framework.

Reduced basis approach:

Basic idea: Restrict the number of PC expansions coefficients that have to be calculated.

- Ideal expansion:
  Karhunen-Loeve = POD

$$u(x,\zeta)-\langle u(x)\rangle=\sum_{i=1}^{m}u^{i}(x)z_{i}(\zeta)$$

- POD eigenvalues decay very fast.
- First few eigenvalues contain all the information

m=very small (# of dominating eigenvalues of POD) ⇨ few u^i to calculate

POD requires covariance R(x,y) of u which is unknown!

$$R(x,y)=\int_{\xi}(u(x,\zeta)-\langle u(x)\rangle)(u(y,\zeta)-\langle u(y)\rangle)PDF.d\zeta$$

Reduced basis approach (contd)

- Calculate PC coefficients ($u_i(x)$) on a coarse mesh
- Calculate covariance matrix R(x,y)

$$R(x_i, x_j) = \sum_{k=1}^{P} u_k(x_i) u_k(x_j) < \psi_k^2 >$$

- Karhunen-Loeve expansion (POD)

➔ Few $u_i(x)$ to calculate on a fine grid

➔ Solution on fine grid can be written as:

$$u(x;\zeta) = \sum_{i=0}^{m} \hat{u}_i(x) z_i(\zeta)$$

➔ Statistics: $< u(x;\zeta) >= \hat{u}_0 \quad \sigma^2 = \sum_{i=1}^{m} (\hat{u}_i)^2 < z_i, z_i >$

➔ 2(m+1) samples are needed in fine grid, where m<<P

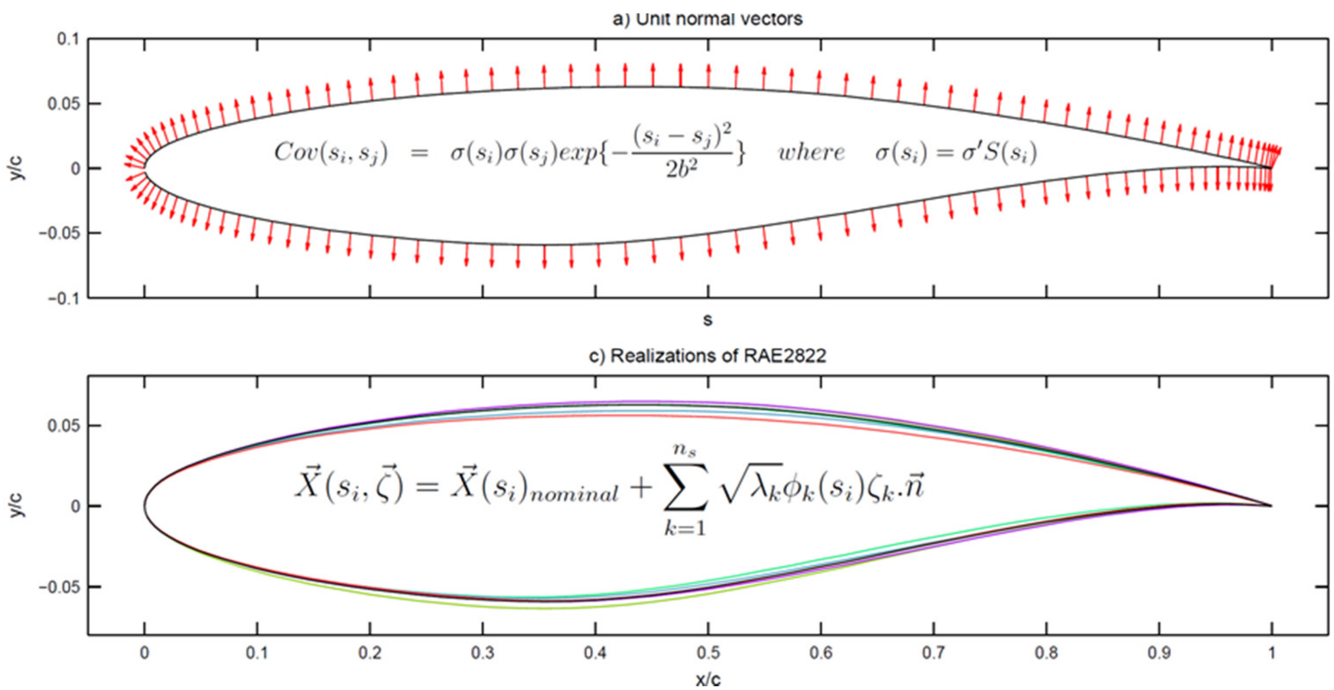
Idea is to extract the optimal orthogonal basis via cheap calculations on a coarse mesh and then use them for the fine scale analysis.

Solution in coarse grid ➔ Covariance ➔ POD ➔ Final solution in fine grid

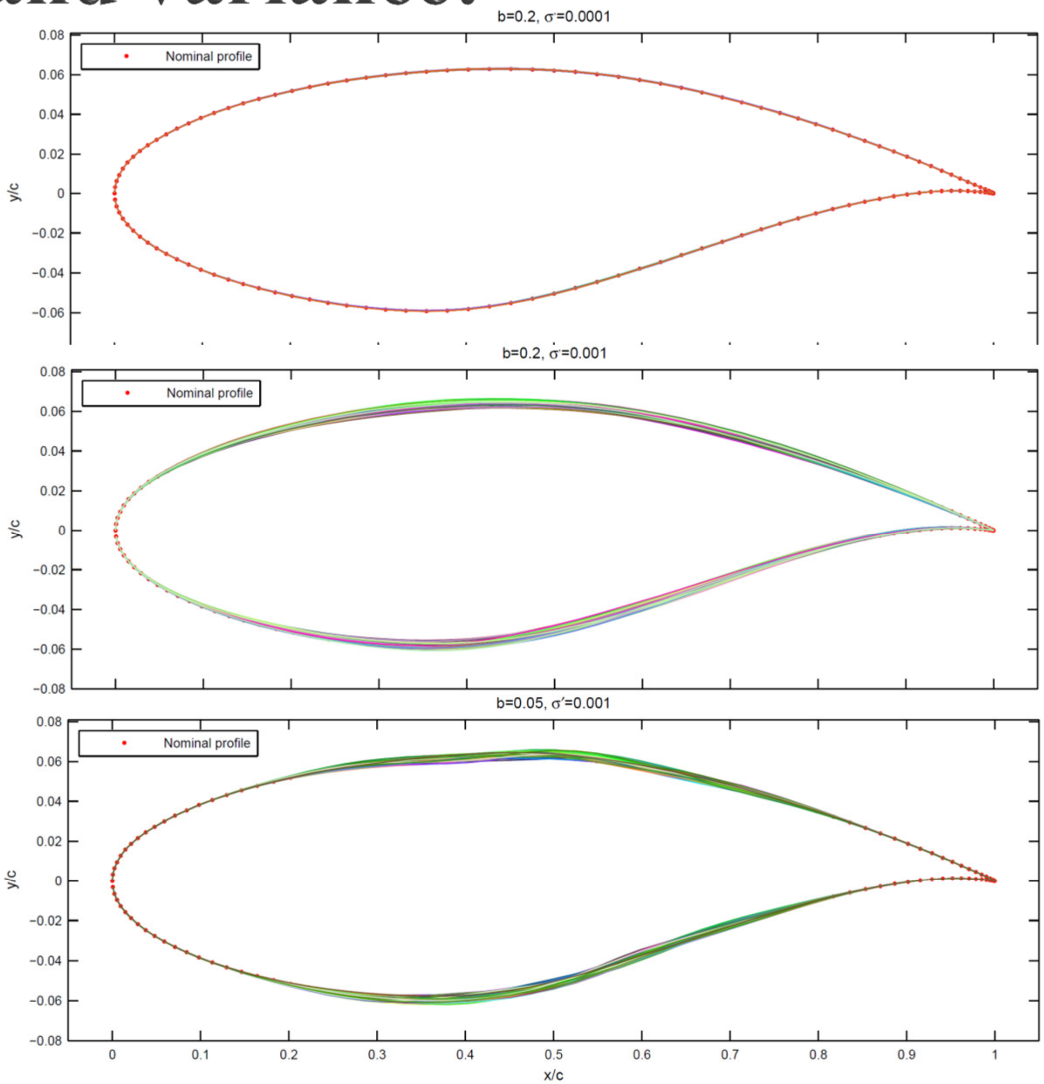
Test case1:
RAE2822 Airfoil, Geometrical uncertainty

Covariance function

Geometry realization using KL expansion



Airfoil geometry realizations with correlation length and variance:



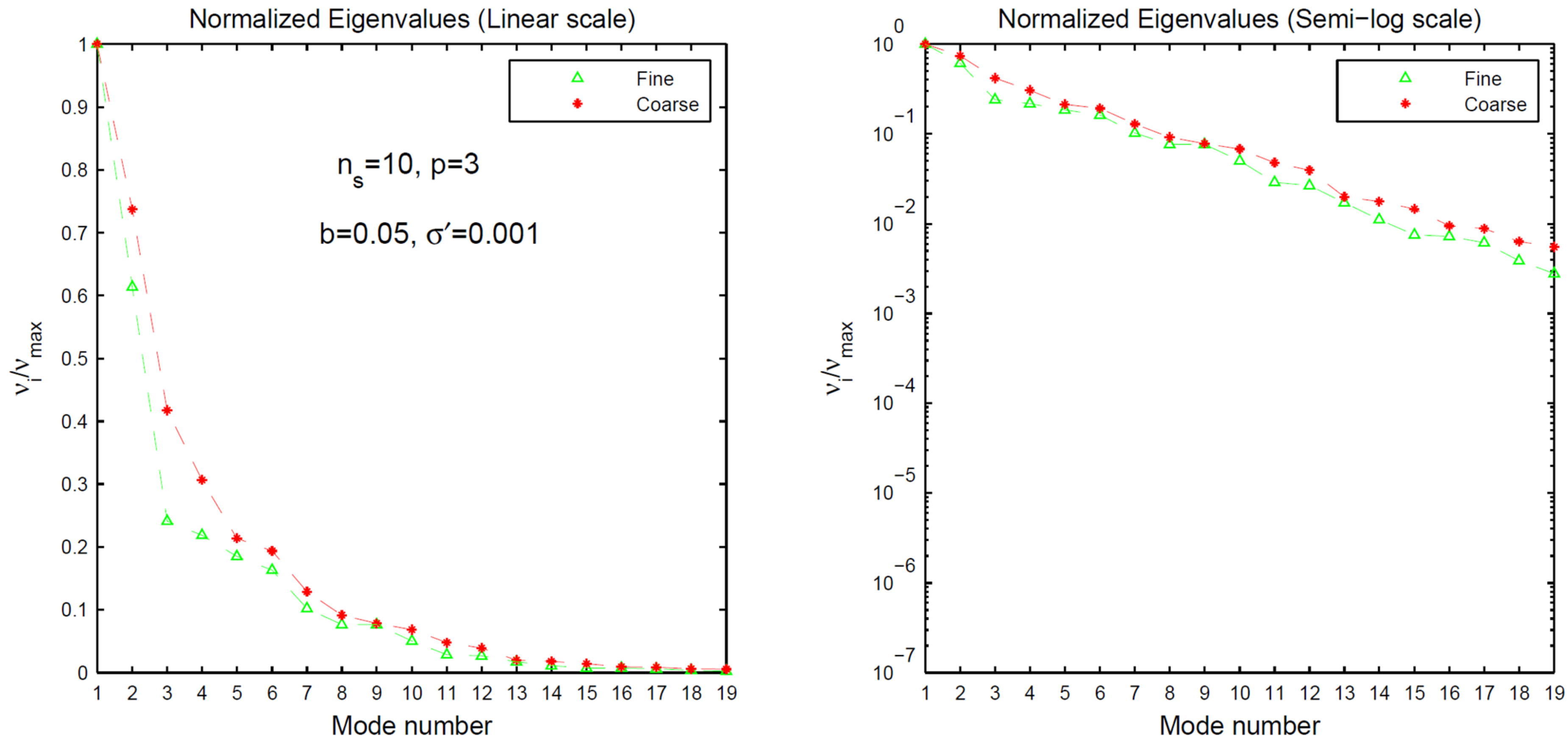
b=0.2
σ=0.0001

b=0.2
σ=0.001

b=0.05
σ=0.0001

Computational parameters for RAE2822 geometrical uncertainty

- AoA=2.79°
- Mach #= 0.734
- Re # = 6.5x10^6
- Uncertain profile with10 terms in KL expansion and σ'=0.001 & b=0.05
- Polynomial order: 3
- Coarse grid: 3.0x10^3
- Fine grid: 4.4x10^4
- Covariance: ρ, ρu, ρv and ρE
- Turbulence model: Spallart Allmaras
- Convective terms: 2nd-order upwind

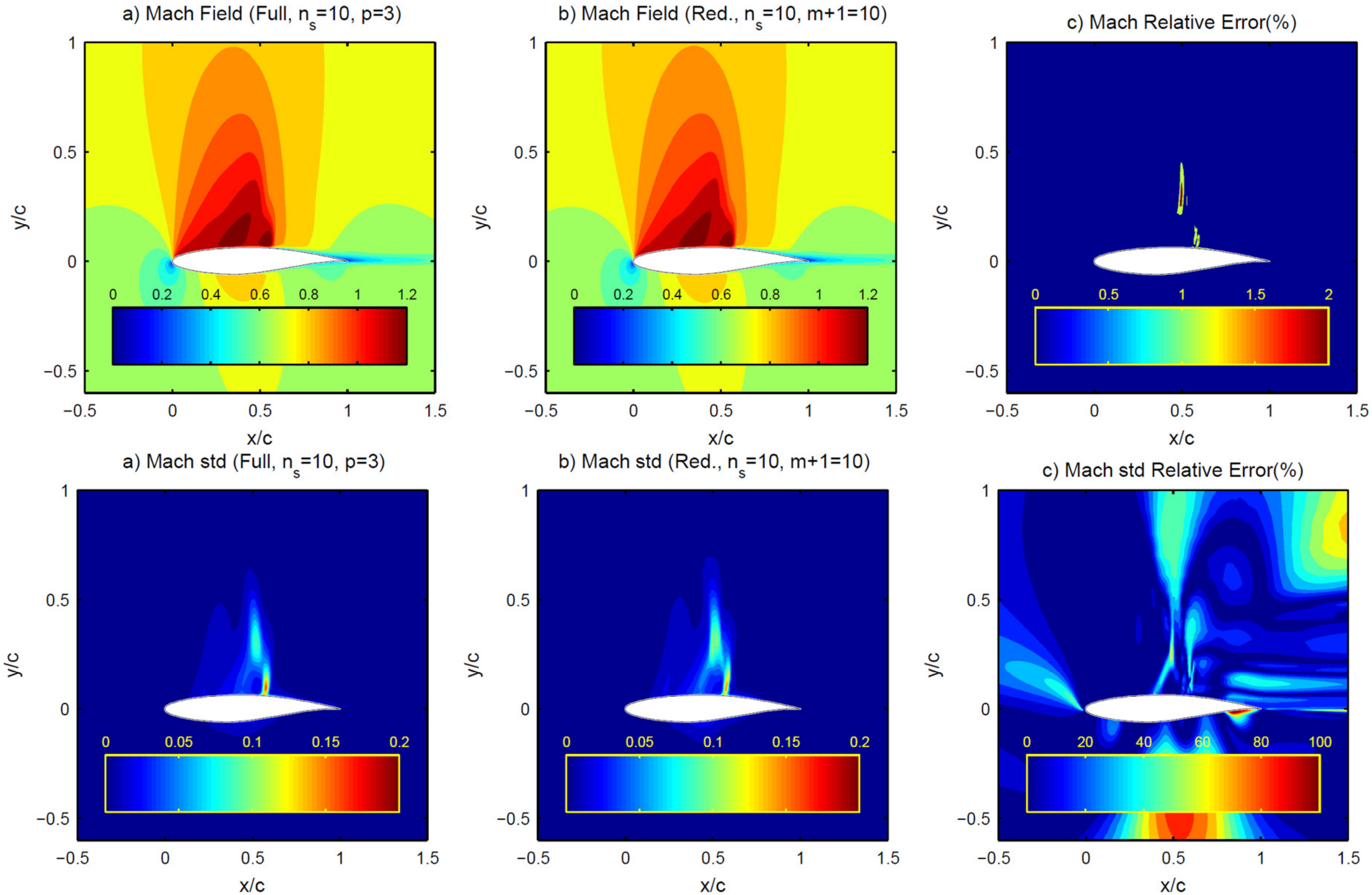


Normalized Eigenvalues (Linear scale)
Fine
Coarse
n_s=10, p=3
b=0.05, σ′=0.001
ν_i/ν_max
Mode number
Normalized Eigenvalues (Semi−log scale)
Fine
Coarse
ν_i/ν_max
Mode number

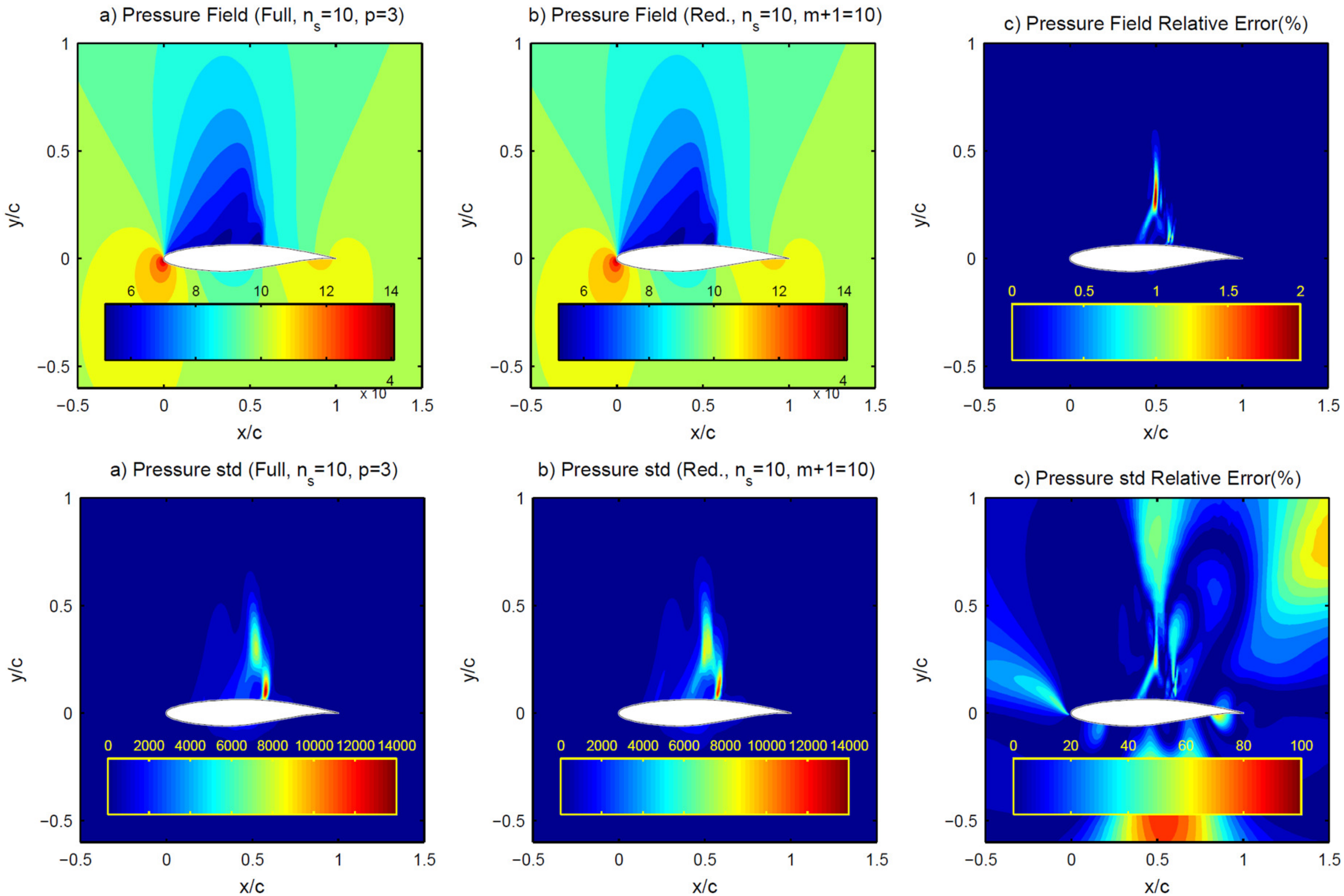
Results (ϵ =0.9): Mach field

$$\frac{\sum_{i=1}^{m} \lambda_i}{\sum_i \lambda_i} \leq \epsilon$$

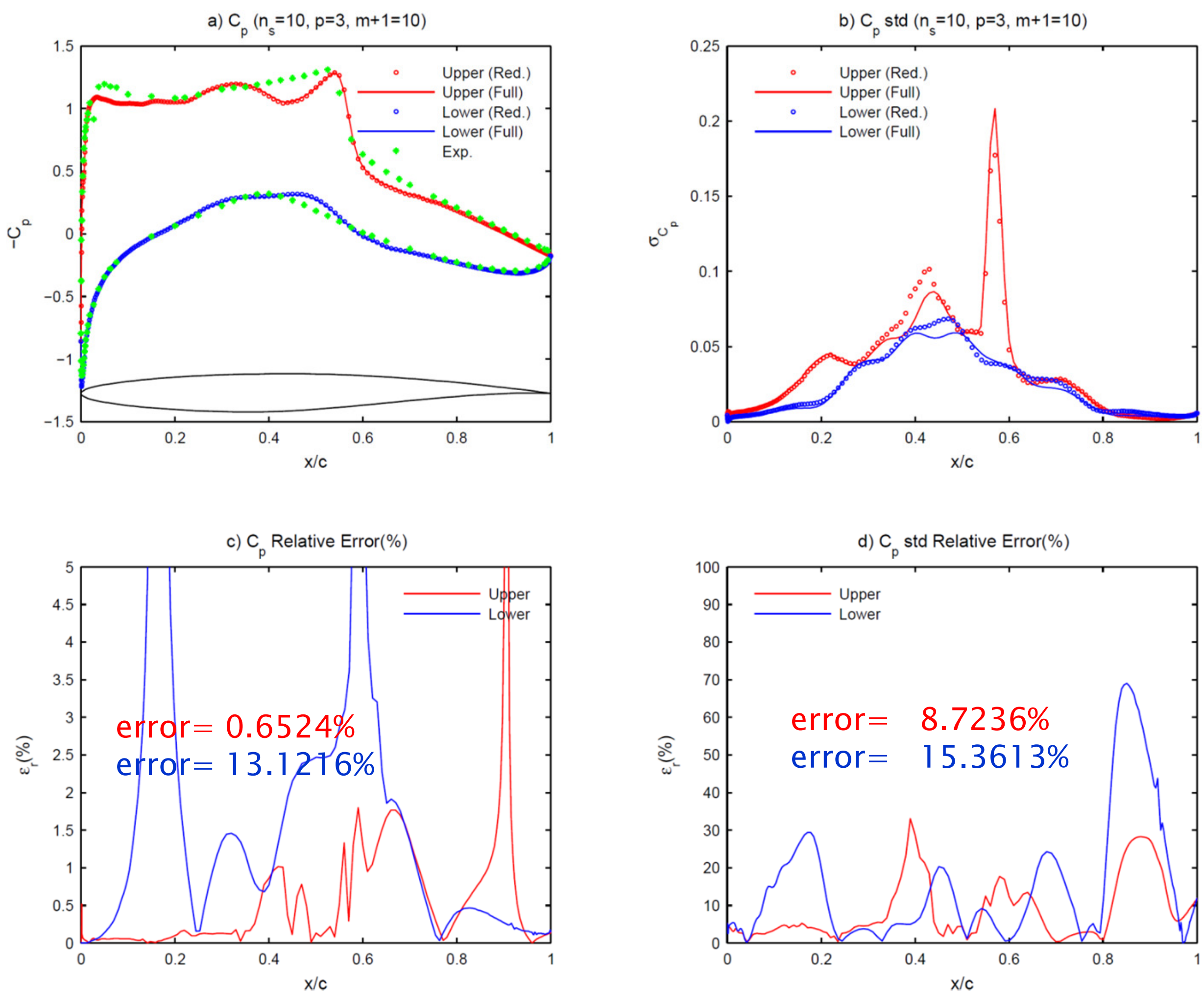
ϵ : measure of dominating eigenvalues



Results (ϵ =0.9): Pressure field



Results (ϵ =0.9): Pressure coefficient

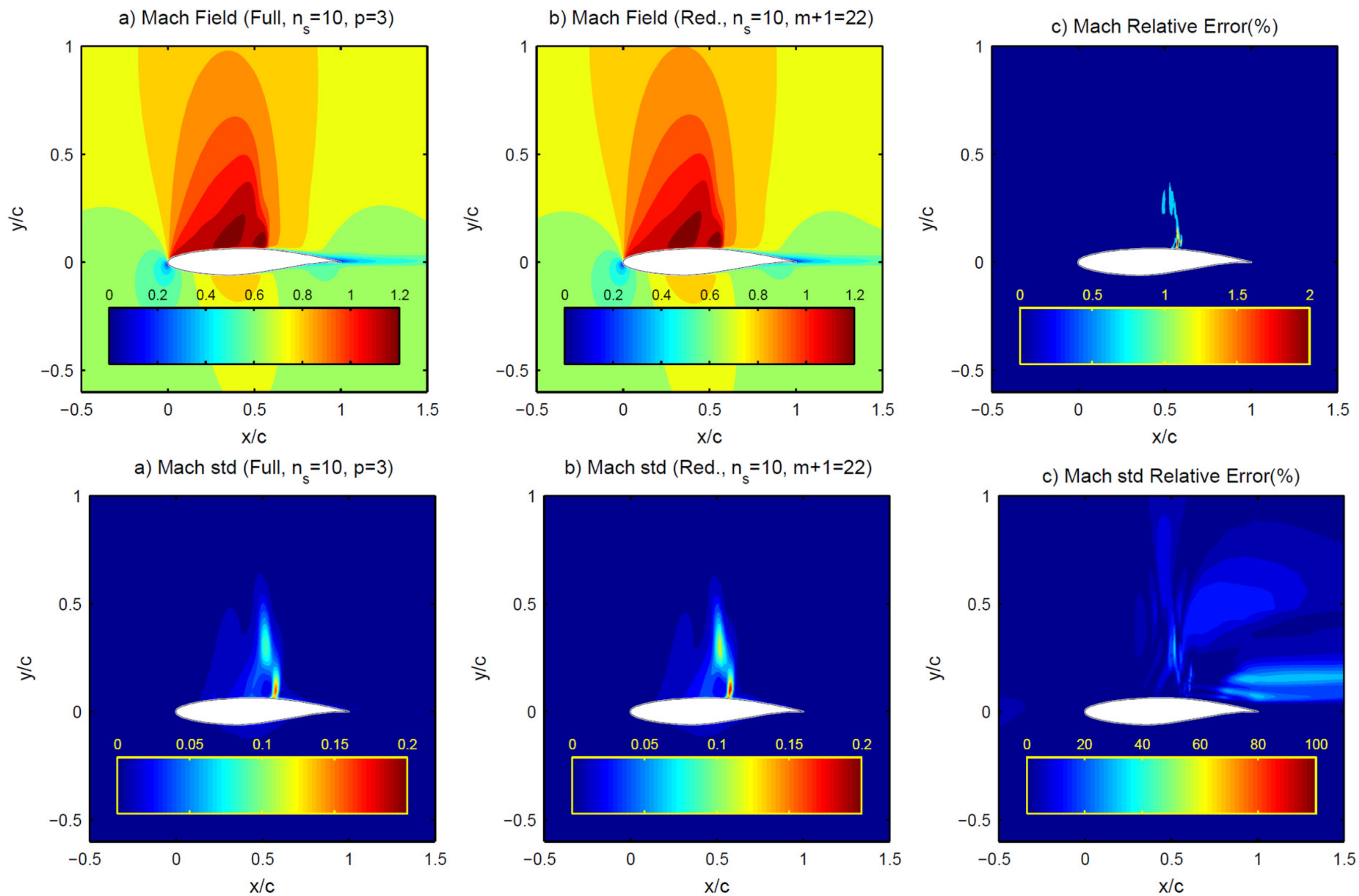


Coarse grid: 3.0×10^3
Fine grid: 4.4×10^4
➔ grid ratio ~= 14

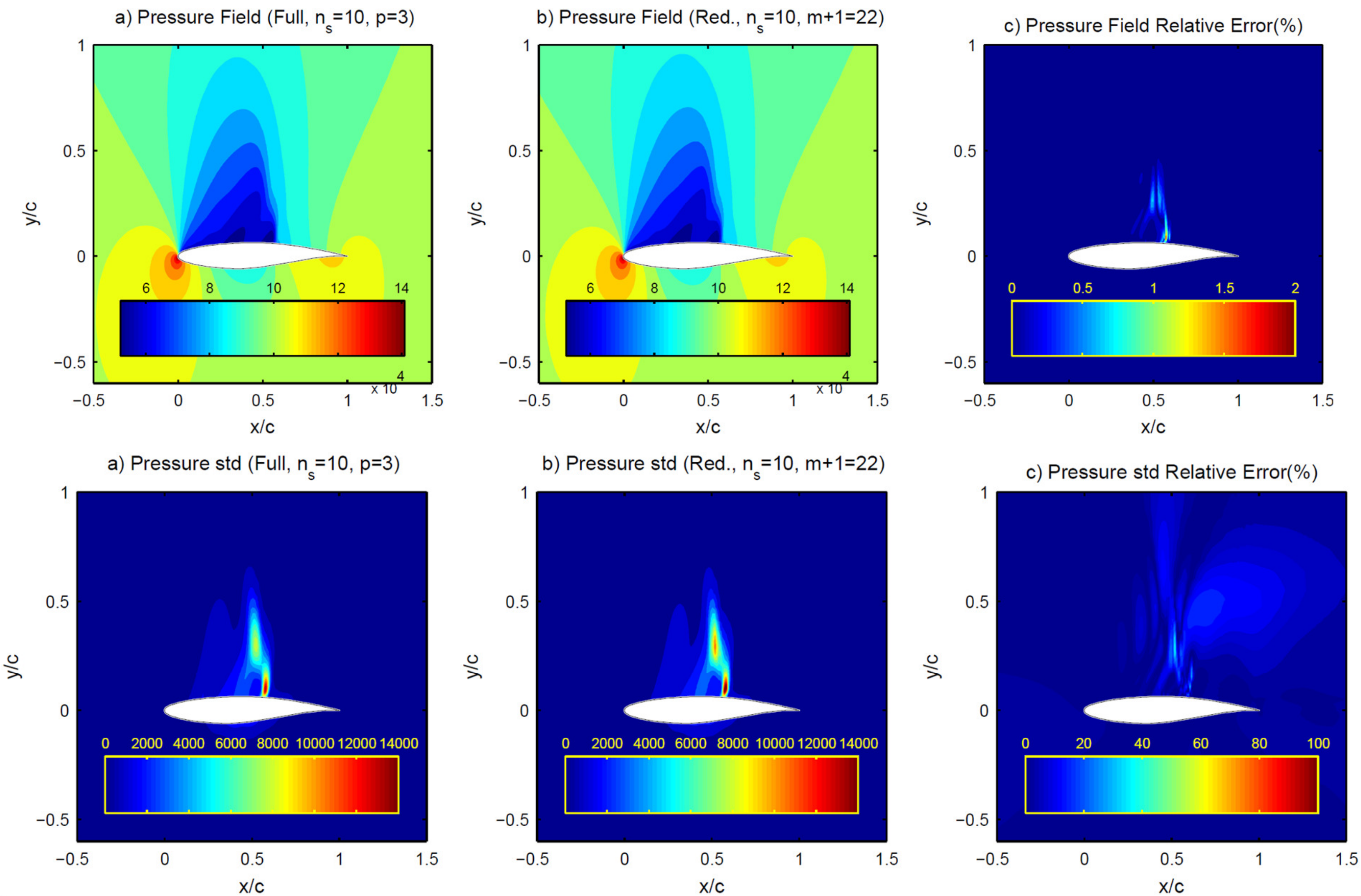
CPU time:
Classical PC:
572 samples in fine mesh
= 572 t

Reduced approach:
572 samples in coarse grid
+20 samples in fine grid
=20t+572t/14
~ = 65t
➔ **~ 9 times efficient**

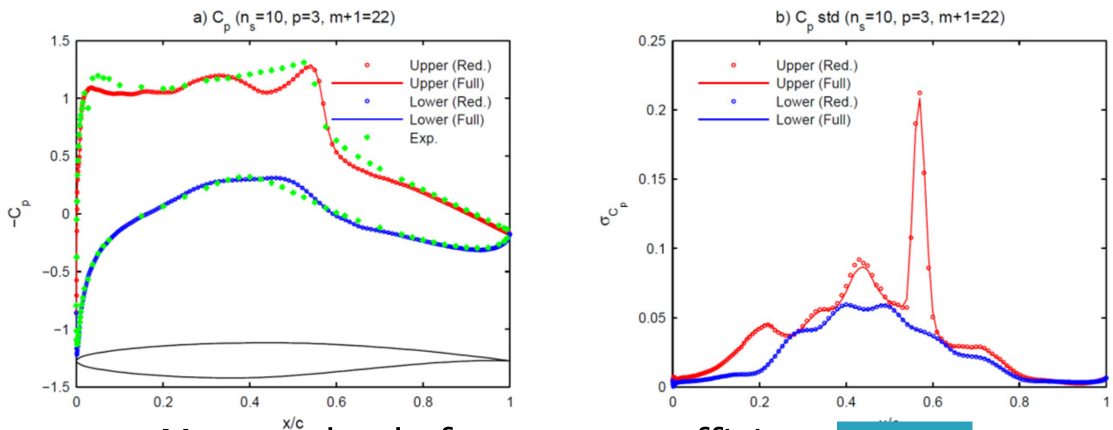
Results (ϵ =0.99):Mach field



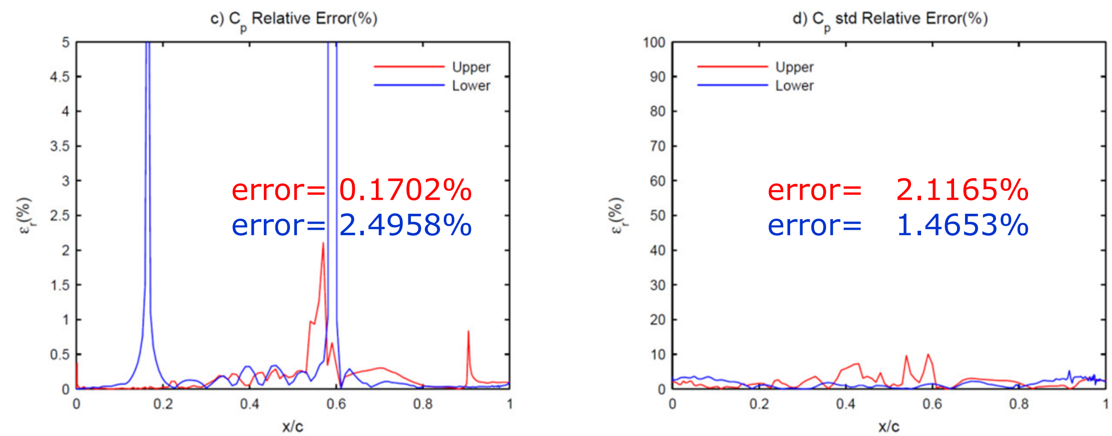
Results (ϵ =0.99): Pressure field



Results (ϵ =0.99): Pressure coefficient



Mean and std of pressure coefficient $\varepsilon = 0.99$



% difference in mean and std of pressure coefficient

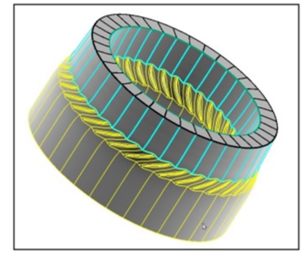
Coarse grid: 3.0×10^3
Fine grid: 4.4×10^4
➔ Grid ratio ~= 14

CPU time:
Classical PC:
572 samples in fine mesh
= 572 t

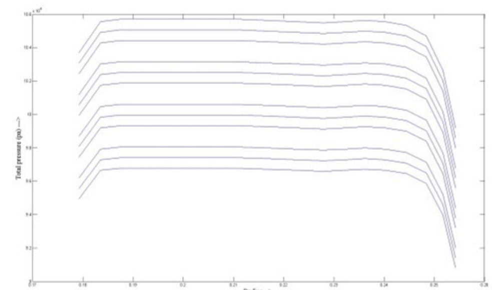
Reduced approach:
572 samples in coarse grid
+44 samples in fine grid
=44t+572t/14
~ = 85 t
➔ **~ 6-7 times efficient**

Become more efficient for higher order PC
(If more accurate statistics are needed)

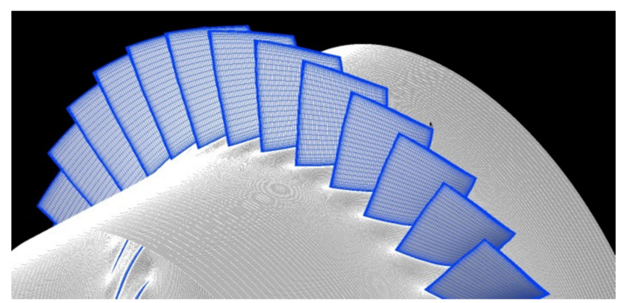
Test case: Transonic axial flow compressor (Rotor37)



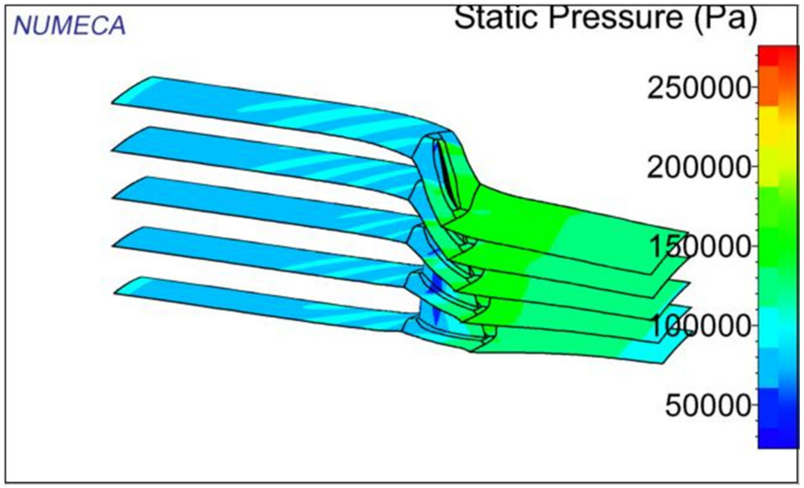
- Uncertain parameters (Boundary conditions):
    1. Total pressure profile at inlet: *uniform distribution, variance = 5% of mean*
    2. Static outlet pressure: *uniform distribution, variance =2% of mean*
- Rotational speed:17188 rpm
- Polynomial order: 2
- Coarse grid: 1.18×10^5
- Fine grid: 8.43×10^5
- Covariance: P
- Turbulence model: Spallart Allmaras
- Convective terms: 2nd-order upwind



Samples of total inlet pressure profile

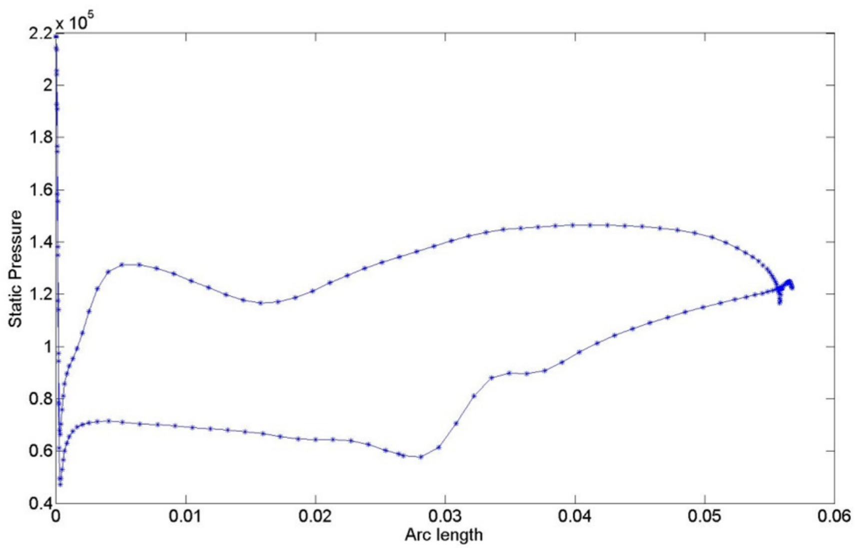


Test case2: Rotor37, Deterministic solution



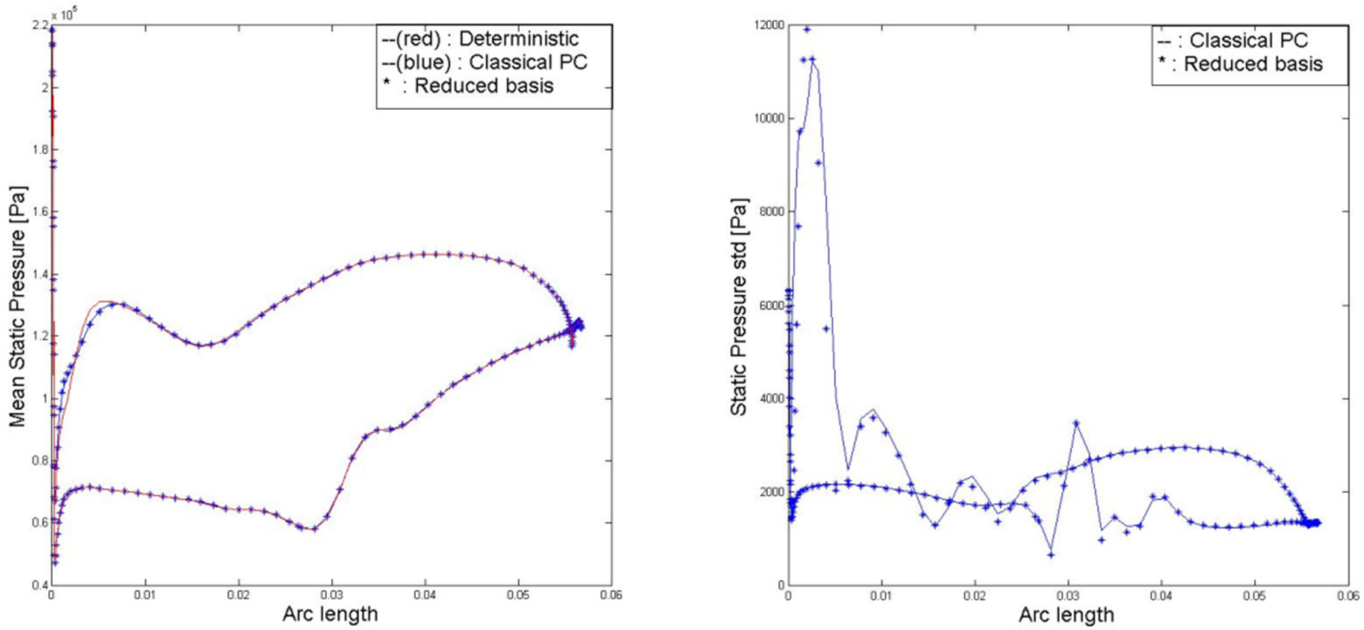
Pressure field on:

- *Hub*
- *25% span of blade*
- *Mid span of blade*
- *75% span of blade*
- *tip*



Pressure distribution around the blade at mid span

Results (ϵ =0.9): Rotor37, Non-deterministic



Mean and standard deviation of static pressure around the blade at mid span

CPU time Classical PC method : total 12 samples in fine grid ➔ CPU time =12t
Reduced approach : 6 samples in fine grid + 12 samples in coarse grid
➔CPU time = 6t +12t/8 = 7.5t (almost two times efficient !!!)

Become more efficient if one consider high dimensional stochastic problems!!!
(i.e., geometrical uncertainties)

Conclusion and future work

- The performance of a non-intrusive POD-based model reduction scheme for uncertainty quantification is evaluated for 2D and 3D cases using Fluent and NUMECA software.
- The reduced-order model is able to produce acceptable results for the statistical quantities.
- Memory requirement and CPU time for the reduced model is found to be much lower than classical methods.
- The performance of the model reduction scheme is more visible in very high dimensional stochastic problems.
- Additional computations for more complex cases involving large number of random variables will be performed.
- Higher order moments will be evaluated.

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Thank you!! ☺