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Non-Intrusive Polynomial Chaos Expansion Applied to Full-Order Stochastic CFD

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Contents

I. Introduction to Uncertainty Quantification (UQ)

Importance of CFD & Deterministic Approach Challenges

- CFD : a critical piece of every engineering projects.
  - Cost & Time efficient.
  - Extensive conditions & designs testing.
  - Pre-experimental decision support.

- Deterministic approach limits.
  - 1 solution for 1 given set of input.
  - Lot of uncertainties in dynamic systems.

Need for **Uncertainty Quantification** !

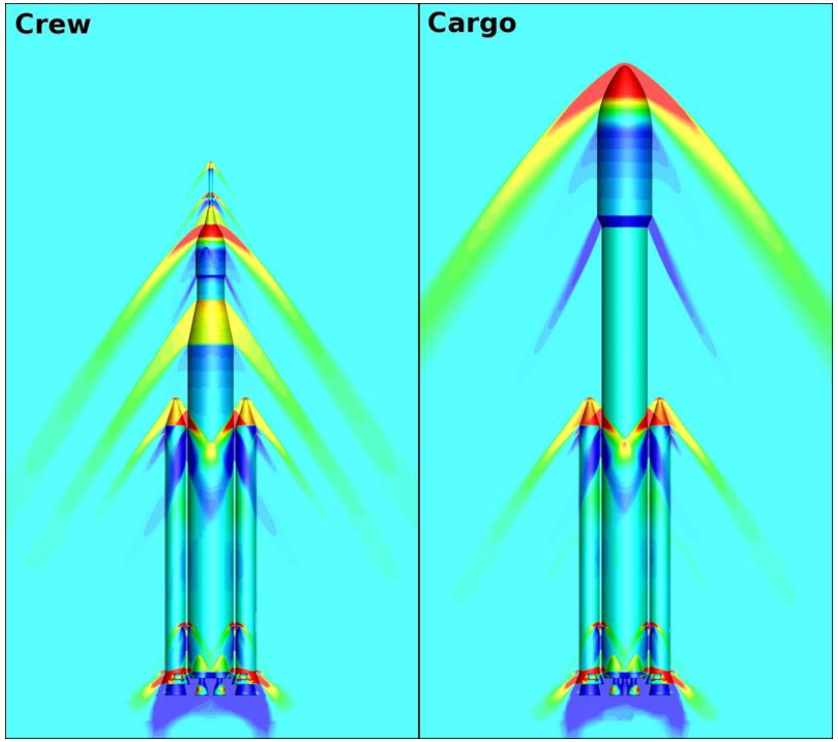


Image Credit : NASA

Uncertainty Quantification

- UQ Goals :
    - Assess reliability of predictions.
    - Manage variability.
    - Assist in decision-making.

- Uncertainty Types :
    - **Aleatoric** : Inherent randomness.
    - Epistemic : Knowledge gaps.

- Key Methods :
    - Deterministic : Error propagation using sensitivity derivatives,...
    - **Probabilistic** ones : Monte Carlo, PCE,...

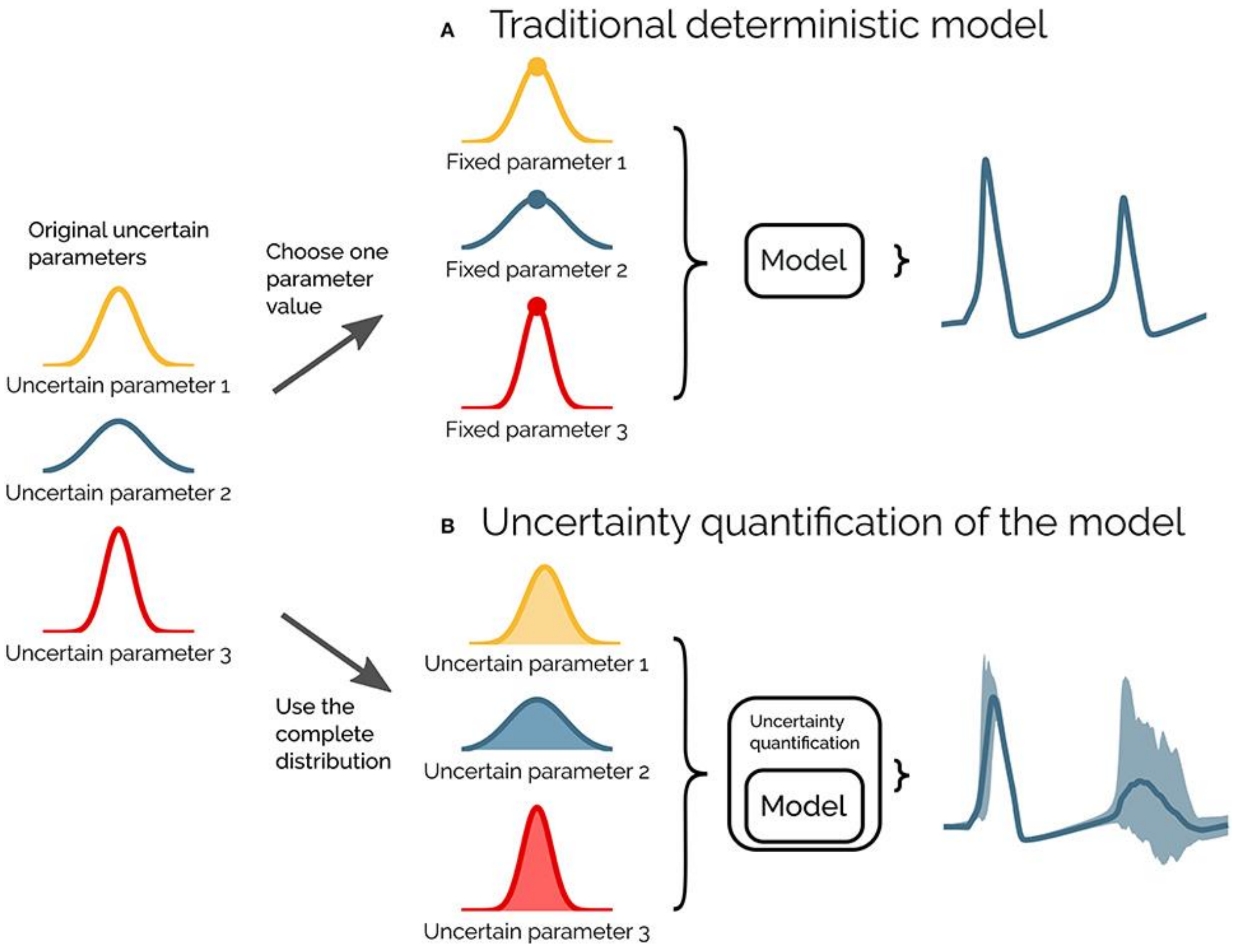


Image Credit : https://www.frontiersin.org/articles/10.3389/fninf.2018.00049/full

Monte Carlo Method and the Push for Alternatives

- Monte Carlo Basics :
  - Intuitive and easy implementation.
  - Statistical analysis : calculate mean, variance, determines confidence intervals.

- Limitations :
  - High sample requirement.
  - Prohibitive computation cost.

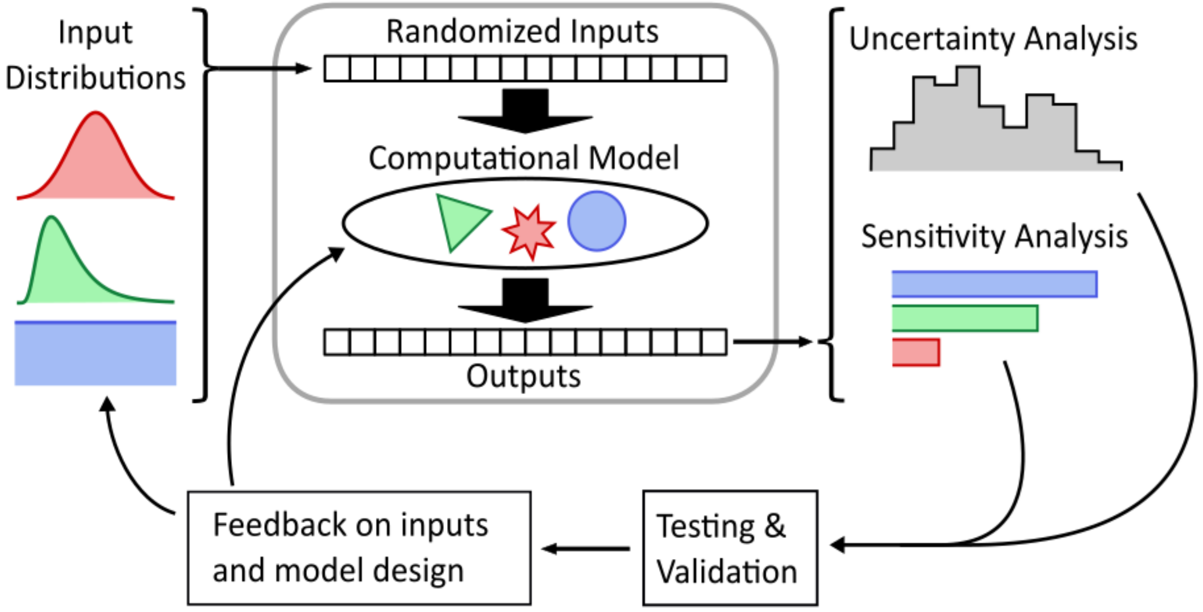


Image Credit : Scott Shambaugh

Need for alternatives : PCE and NIPCE as promising and efficient UQ solutions.

II. Theory of NIPCE

Fundamentals

- Polynomial Chaos Expansion (PCE) is a polynomial surrogate model

$$\Theta(\vec{x},\vec{\xi}\,) \approx \sum_{i=0}^{P} \theta_i(\vec{x})\psi_i(\vec{\xi}\,)$$

- It is also a linear combination in an orthogonal polynomial basis, weighted by deterministic coefficients

Θ : Stochastic output

$\vec{\xi} = \left(\vec{\xi}_1, \vec{\xi}_2, \cdots, \vec{\xi}_n\right)$: n-dimensional random variable vector

$\vec{x}$: Position vector

θ_i : deterministic components

ψ_i : polynomial basis functions

Fundamentals

- Total number of elements of approximation:

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

- Optimal polynomial basis depends on Probability Density Function (PDF) of $\vec{\xi}$ components, because orthogonality depends on the weight function

For two functions $f(\vec{\xi})$ and $g(\vec{\xi})$ the inner product is defined as:

$$\left\langle f(\vec{\xi}), g(\vec{\xi}) \right\rangle = \int_{\Omega} f(\vec{\xi}) g(\vec{\xi}) w(\vec{\xi}) d\vec{\xi}$$

Distribution	PDF	Polynomial family	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$	Hermite $H_n(x)$	$e^{-\frac{x^2}{2}}$	$[-\infty, +\infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1, 1]$
Beta	$\frac{(1-x)^\alpha (1+x)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^\alpha (1+x)^\beta$	$[-1, 1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0, +\infty]$
Gamma	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^\alpha(x)$	$x^\alpha e^{-x}$	$[0, +\infty]$

Fundamentals

- With the inner product defined, we can project the PCE on the k-th basis

$$\left\langle \Theta(\vec{x},\vec{\xi}\,), \psi_k(\vec{\xi}\,) \right\rangle = \sum_{i=0}^{P} \left\langle \theta_i(\vec{x})\psi_i(\vec{\xi}\,), \psi_k(\vec{\xi}\,) \right\rangle$$

- Due to orthogonality of the basis:

$$\theta_k(\vec{x}) = \frac{\left\langle \Theta(\vec{x},\vec{\xi}\,), \psi_k(\vec{\xi}\,) \right\rangle}{\left\langle \psi_k(\vec{\xi}\,), \psi_k(\vec{\xi}\,) \right\rangle}$$

Point-collocation method

- NIPCE: Non-Intrusive Polynomial Chaos Expansion
- Many methods are available for a non-intrusive approach, but the selected one is point-collocation
- Take N+1 different input scenarios.

$$\begin{bmatrix} \psi_0(\vec{\xi_0}) & \psi_1(\vec{\xi_0}) & \psi_2(\vec{\xi_0}) & \cdots & \psi_P(\vec{\xi_0}) \\ \psi_0(\vec{\xi_1}) & \psi_1(\vec{\xi_1}) & \psi_2(\vec{\xi_1}) & \cdots & \psi_P(\vec{\xi_1}) \\ \psi_0(\vec{\xi_2}) & \psi_1(\vec{\xi_2}) & \psi_2(\vec{\xi_2}) & \cdots & \psi_P(\vec{\xi_2}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \psi_0(\vec{\xi_N}) & \psi_1(\vec{\xi_N}) & \psi_2(\vec{\xi_N}) & \cdots & \psi_P(\vec{\xi_N}) \end{bmatrix} \begin{Bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{Bmatrix} = \begin{Bmatrix} \Theta_0 \\ \Theta_1 \\ \Theta_2 \\ \vdots \\ \Theta_N \end{Bmatrix}$$

- if N=P, then we have a square linear system, thus there is a unique solution

Point-collocation method

- Common practice: take more samples than needed
- Oversampling ratio:

$$N_p = \frac{\text{number of samples}}{P+1}$$

- Solve oversampled system by using regression: least squares minimization
- Stochastic post-processing:

$$\mu_\Theta = \int \left(\sum_{i=0}^{P} \theta_i \psi_i(\vec{\xi}) \right) w(\vec{\xi})\, \mathrm{d}\vec{\xi} = \theta_0$$

$$\sigma_\Theta^2 = \int \left(\sum_{i=0}^{P} \theta_i \psi_i(\vec{\xi}) \right)^2 w(\vec{\xi})\, \mathrm{d}\vec{\xi} = \sum_{i=1}^{P} \theta_i^2$$

Methodology

- Full Order Model (FOM) used: OpenFOAM
- 2 test cases studied:
  - Lid-driven cavity problem
  - Dynamical characterization of NACA0012 airfoil
- 1st test case: demonstrate the use of the NIPCE method with the chaospy
- 2nd test case: parametric study
- We will validate the PCE results by comparing with the FOM and literature

OpenFOAM®

III. Case study : Lid-driven cavity problem

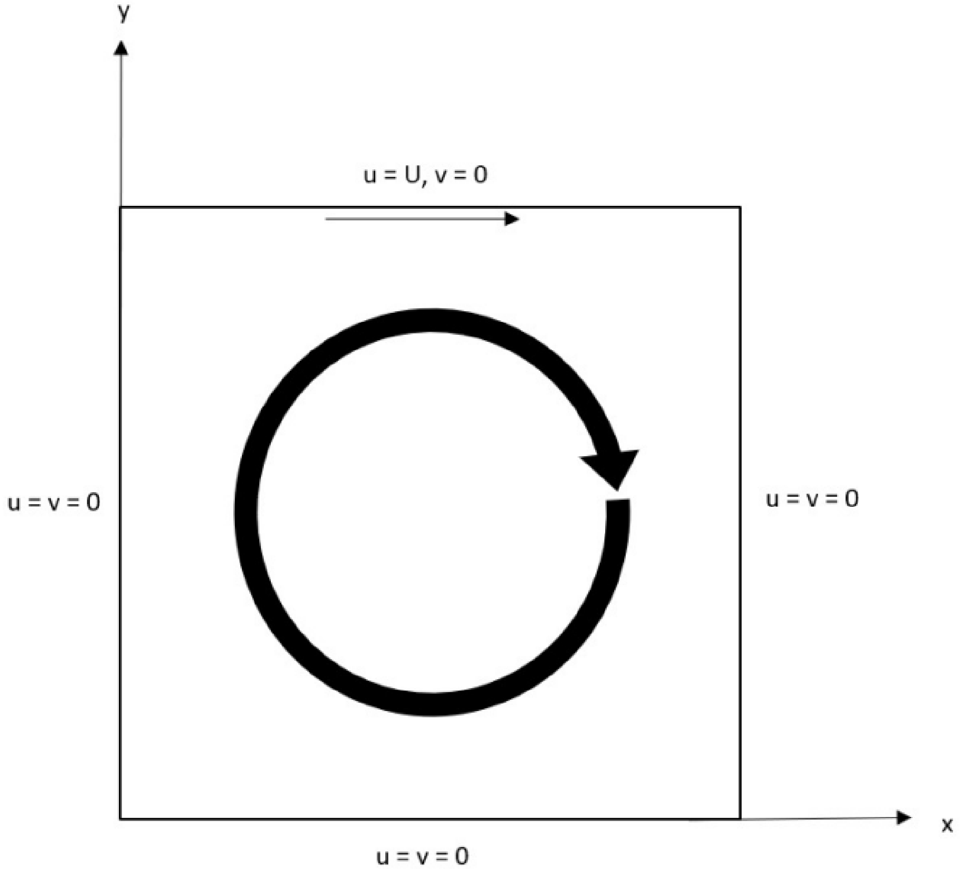
Formulation of the problem

- Domain: square with side length L
- Physics behind the problem:

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial \vec{u}}{\partial t} = -(\vec{u} \cdot \nabla)\vec{u} - \nabla p + \frac{1}{R_e}\Delta \vec{u}$$

- Reynolds number is the only parameter influencing the simulation
- Literature to compare: Ghia et al.
- Boundary conditions:
    - pressure: $\nabla p = 0$
    - velocity: $\begin{cases} u = U \text{ and } v = 0, \text{ if } y = L \\ u = v = 0, \text{ otherwise} \end{cases}$

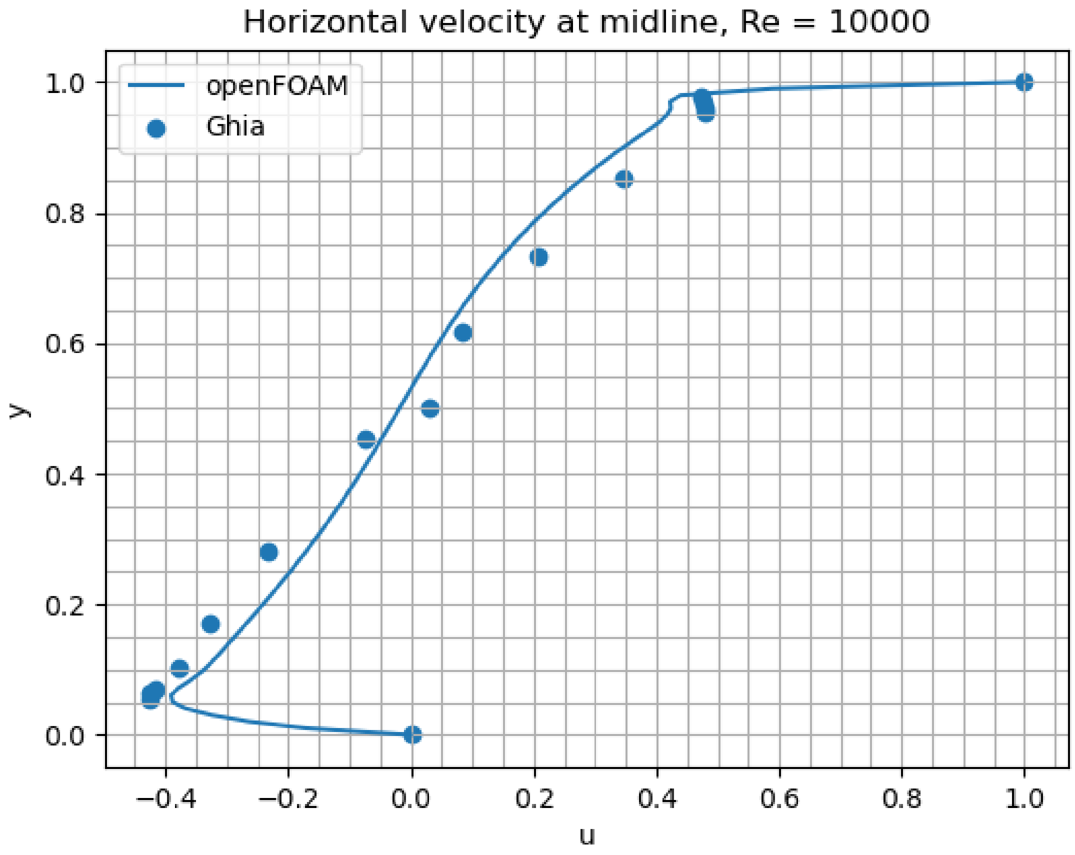


Ghia, UKNG, Kirti N Ghia, and CT Shin: *High-re solutions for incompressible flow using the navier-stokes equations and a multigrid method.* Journal of computational physics, 48(3):387–411, 1982.

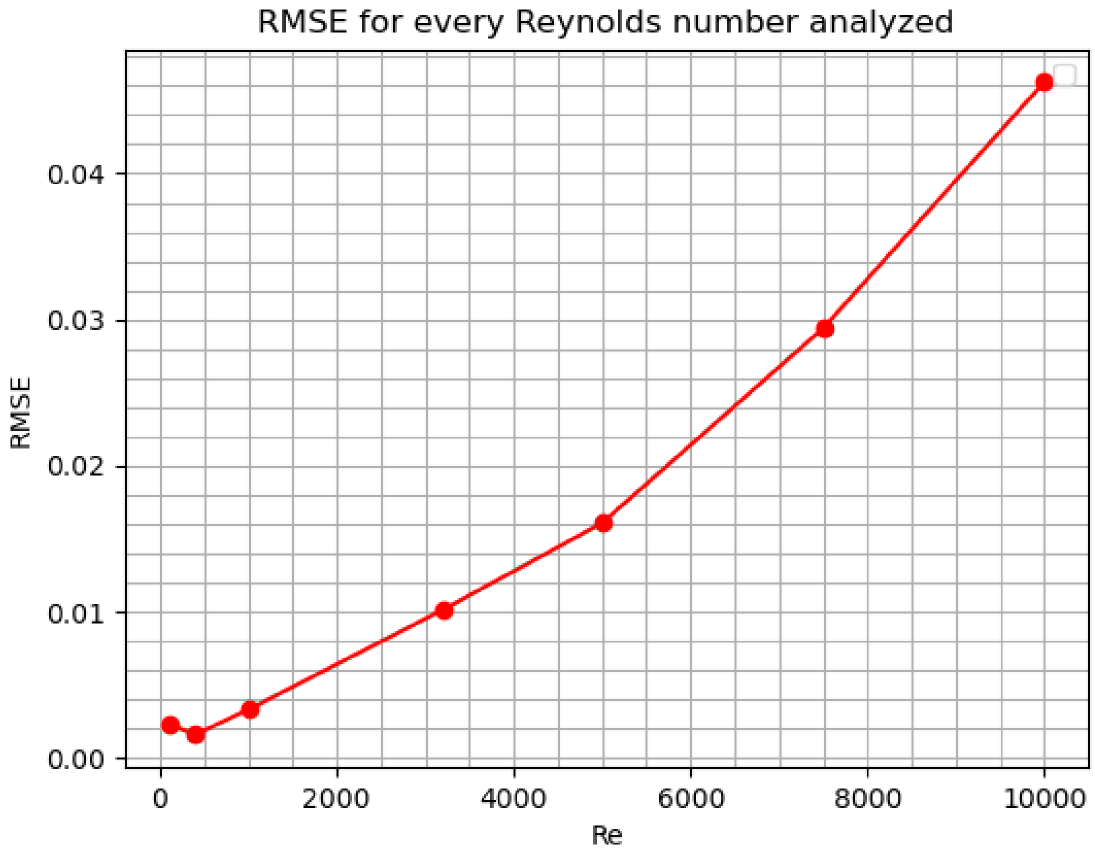
OpenFOAM implementation

- First step: determine where the solver used is reliable
- OpenFOAM solver selected is icoFoam
  - solves the incompressible laminar Navier-Stokes equations using the PISO (Pressure-Implicit with Splitting of Operators) algorithm
  - Transient code
- Secondly: Determine the minimum final step and number of cells to achieve convergence
- Finally: Reynolds number will be the only parameter influencing results, thus we can use the PCE method and assess its validity

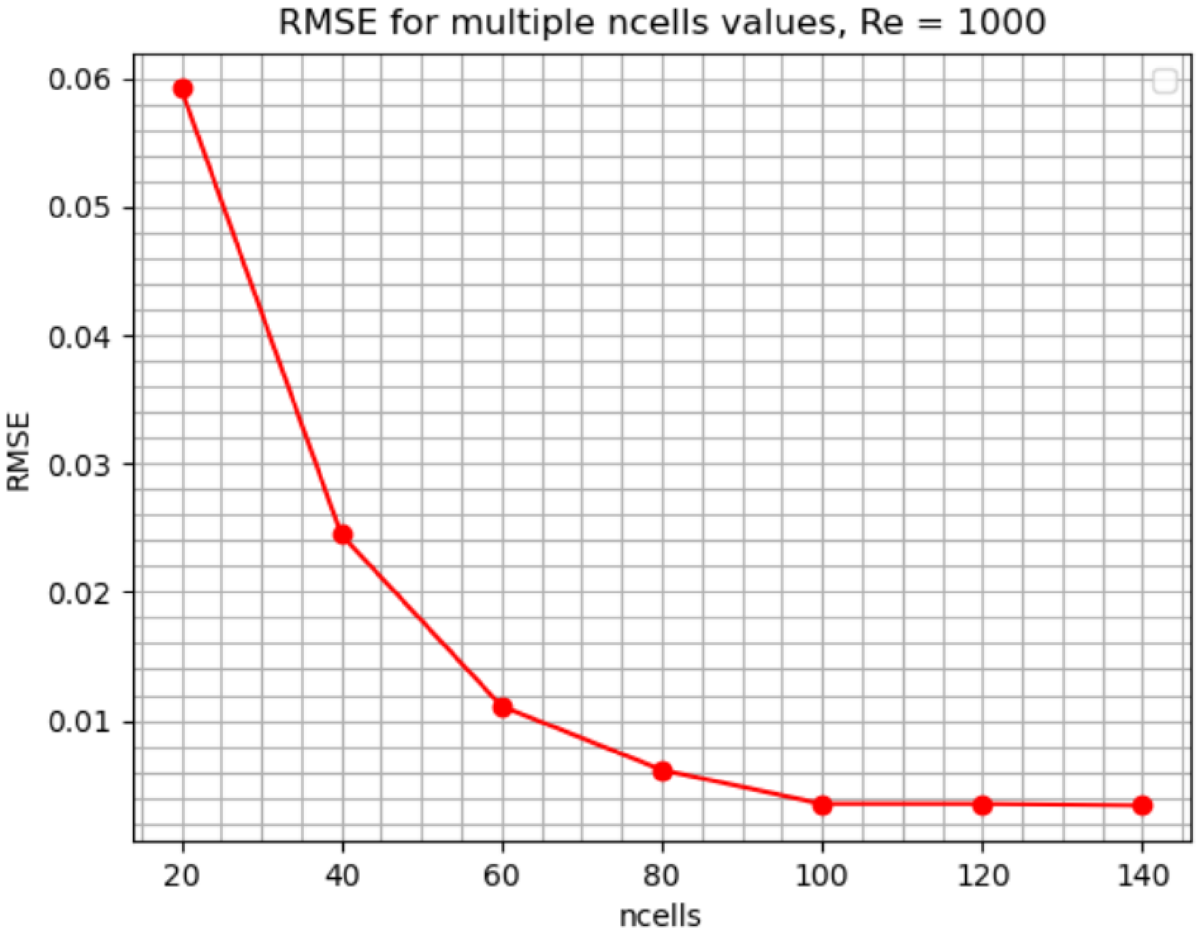
First step of analysis: Determine where the solver is reliable



First step of analysis: Determine where the solver is reliable



Second step of analysis: Convergence study



Final step of analysis: Implementing NIPCE

- Vary the Reynolds number as follows:

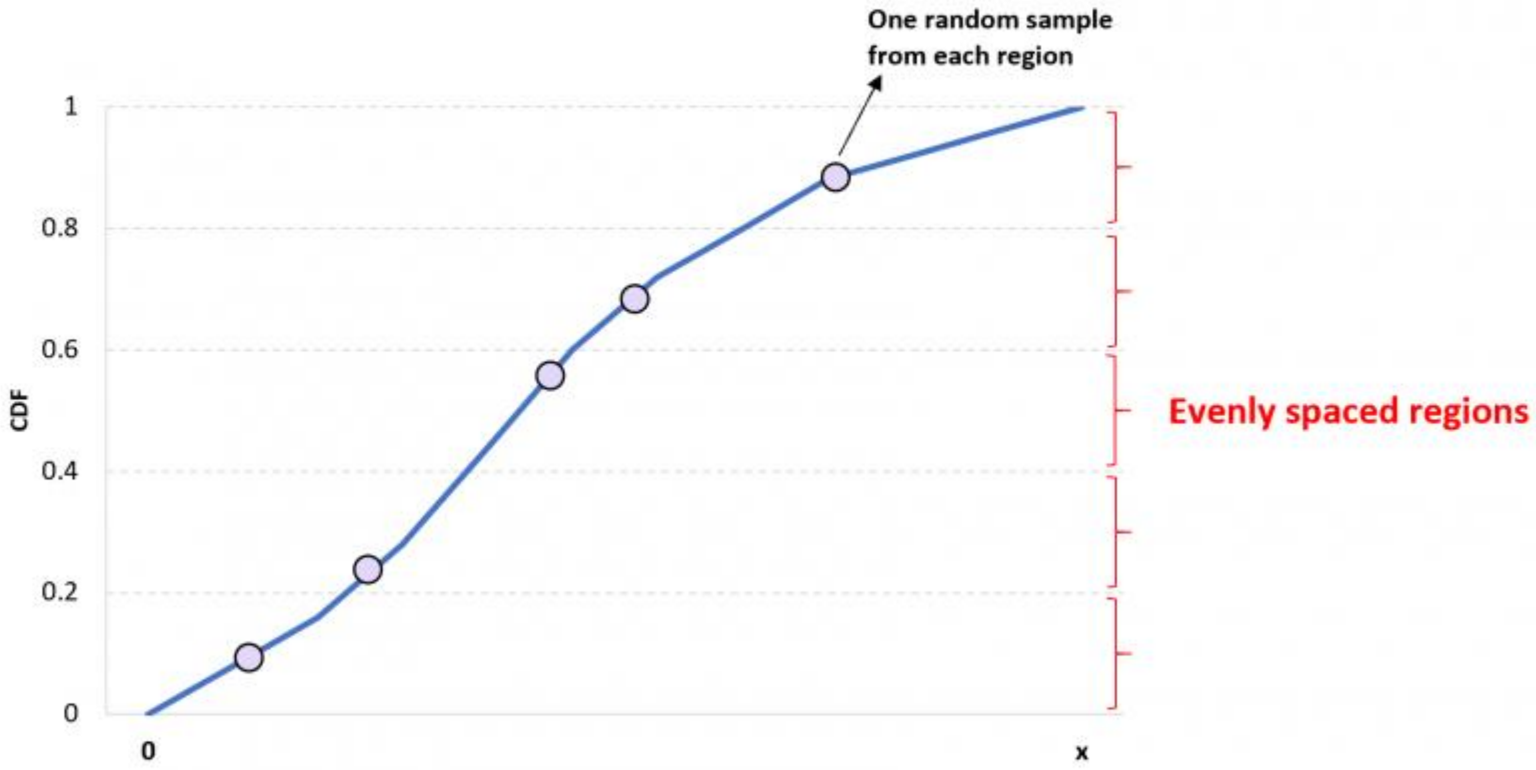
$$R_e \sim \mathcal{N}(R_{e,avg}, R_{e,std}) \longrightarrow R_e \sim \mathcal{N}(1000, 100)$$

- Necessity to build a PCE surrogate for each y coordinate of OpenFOAM results
- Simulations for polynomial chaos order and oversampling ratio following:

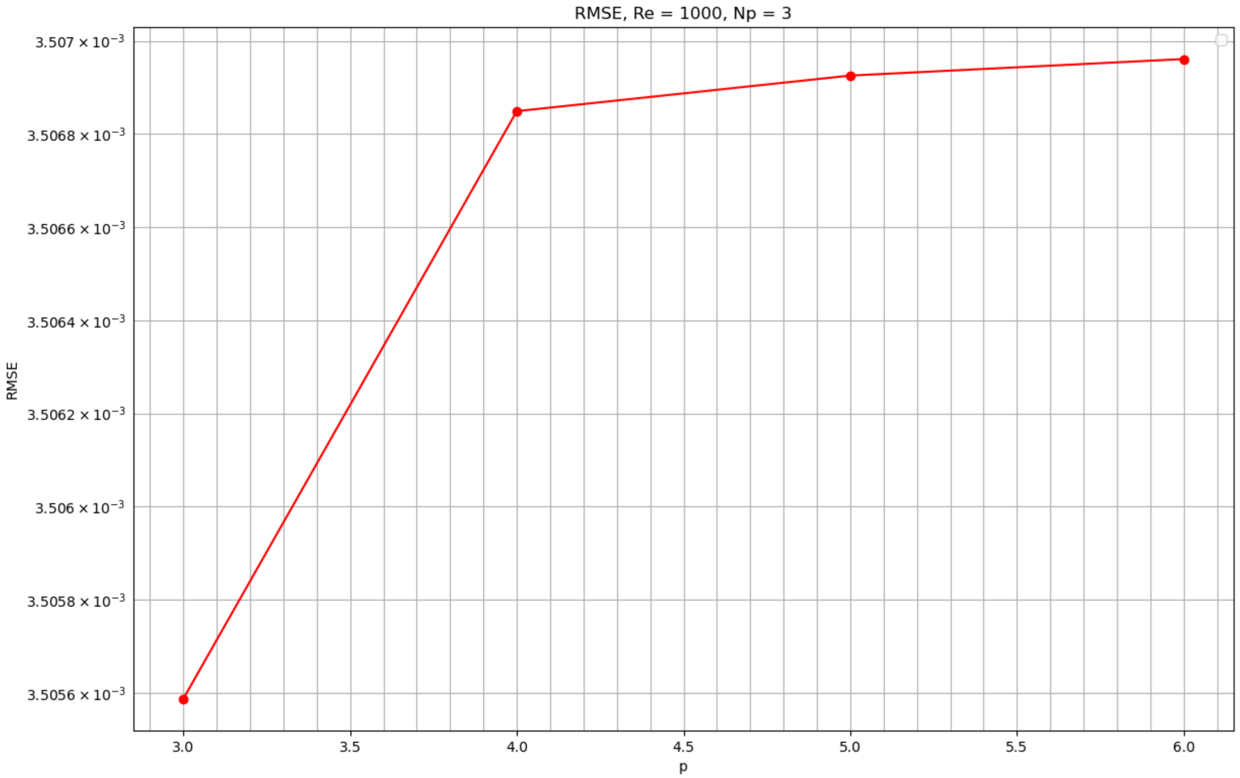
$$p \in [\![3, 6]\!] \text{ and } N_p \in [\![1, 3]\!]$$

Final step of analysis: Implementing NIPCE

- Sampling method used: Latin Hypercube Sampling (LHS)



Final step of analysis: Implementing NIPCE



IV. Case study : NACA0012 Airfoil

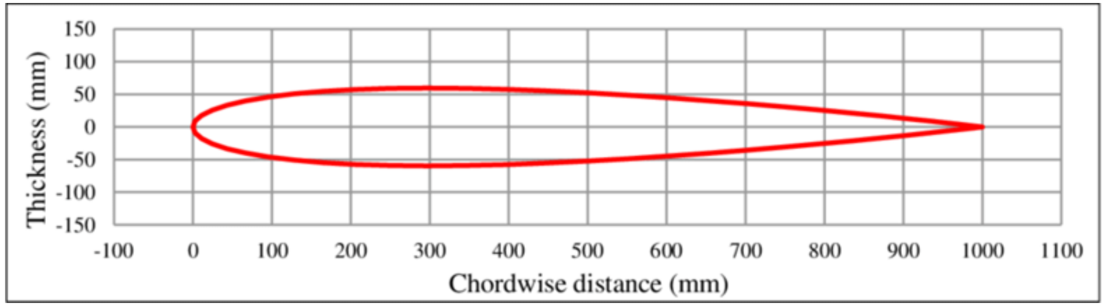
Case Presentation

- NACA0012 profile : Standard aerodynamic test model.

- Focus on two critical parameters :
  - Angle of Attack.
  - Upstream Mach Number.

- Simulation Goals :
  - Compute Cl (Lift Coefficient)
  - Compute Cd (Drag Coefficient)

$$C_L = \frac{L}{\frac{1}{2}\rho V^2 S} \qquad C_D = \frac{D}{\frac{1}{2}\rho V^2 S}$$



NACA0012 Profile

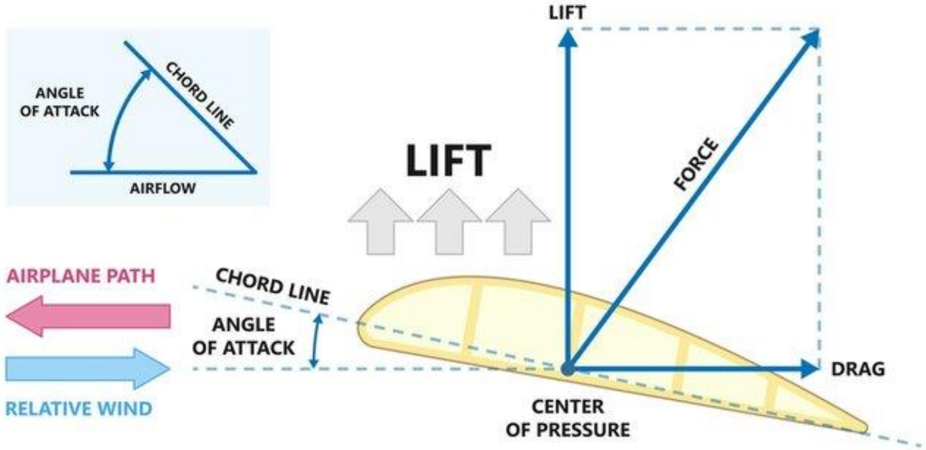


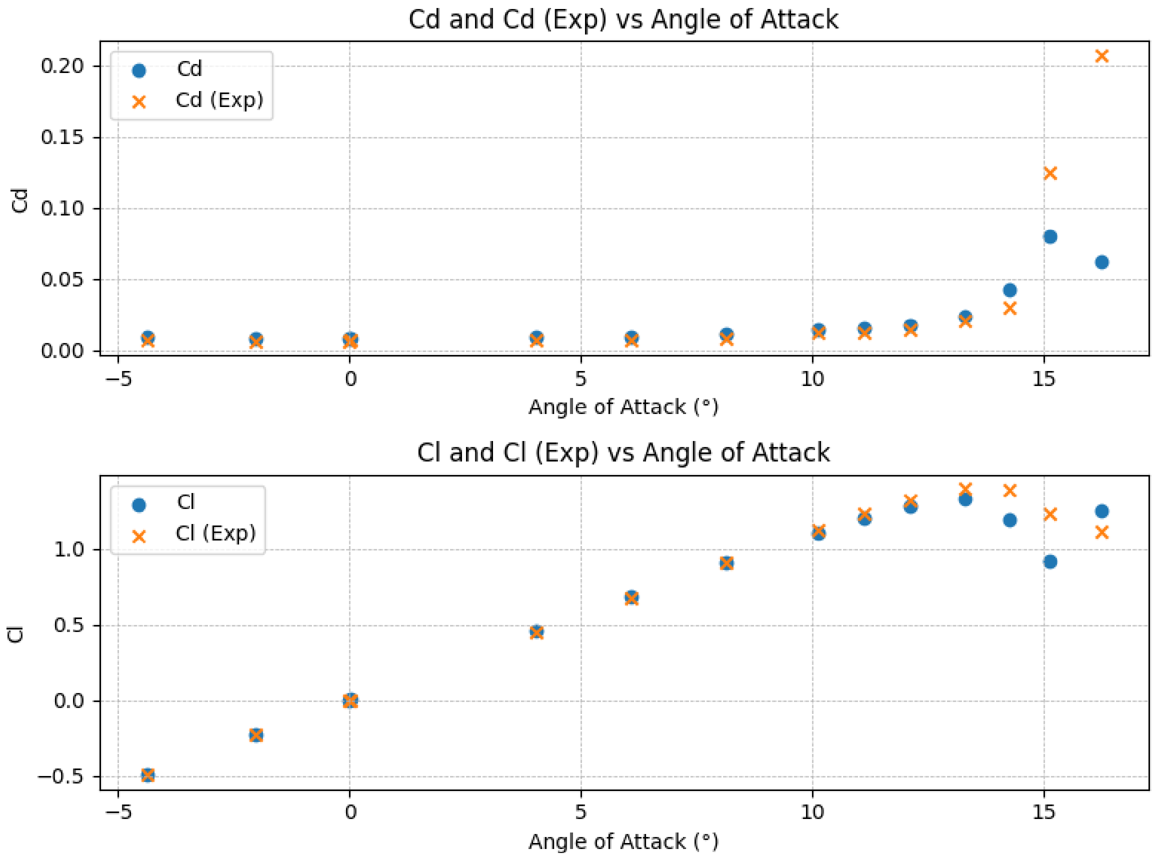
Image Credit : Adobe Stock

Numerical Implementation on OpenFOAM

- Adapted from an existing OpenFOAM case (cf. Appendices for key simulation parameters).

- Convergence issues encountered:
  - High Mach Number instabilities (~0.7)
  - Stall phenomena at high Angles of Attack (~13°)

- Streamlining with Python and validation against NASA Data.



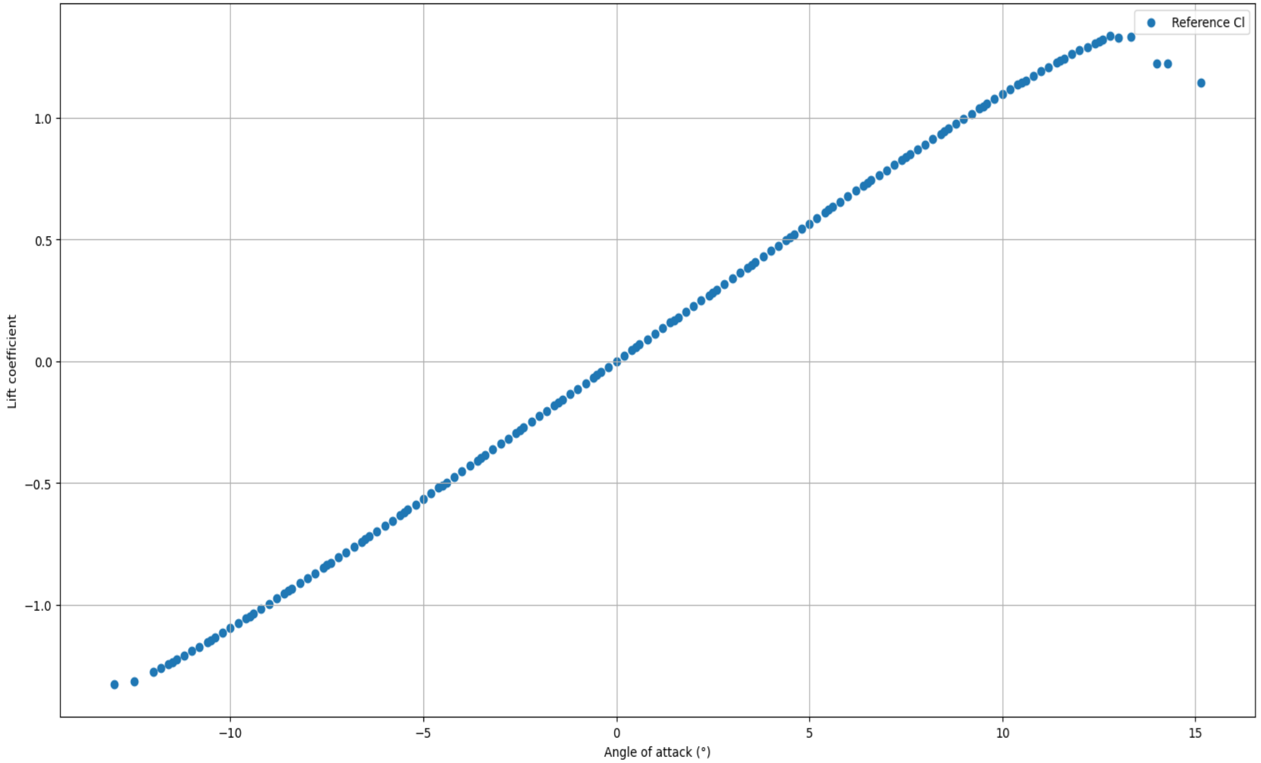
Cl as the only output for UQ. AOA range limited to [-12°,12°] for reliable analysis.

NIPCE Implementation : AOA uncertainty analysis

- Study Parameters:
  - Mach Number set at 0.3
  - AOA : Normal Distribution, mean 0°, STD 5°

- NIPCE Python Implementation:
  - Inputs : FOM, AOA distribution, Expansion order, Sample size, Sampling method, Fitting Method
  - Point Collocation Technique to compute the PCE

- Parametric study:
  - Creation of a reference database to assess the surrogate models accuracy
  - L2 relative error as accuracy metric



Reference values for the Lift Coefficient

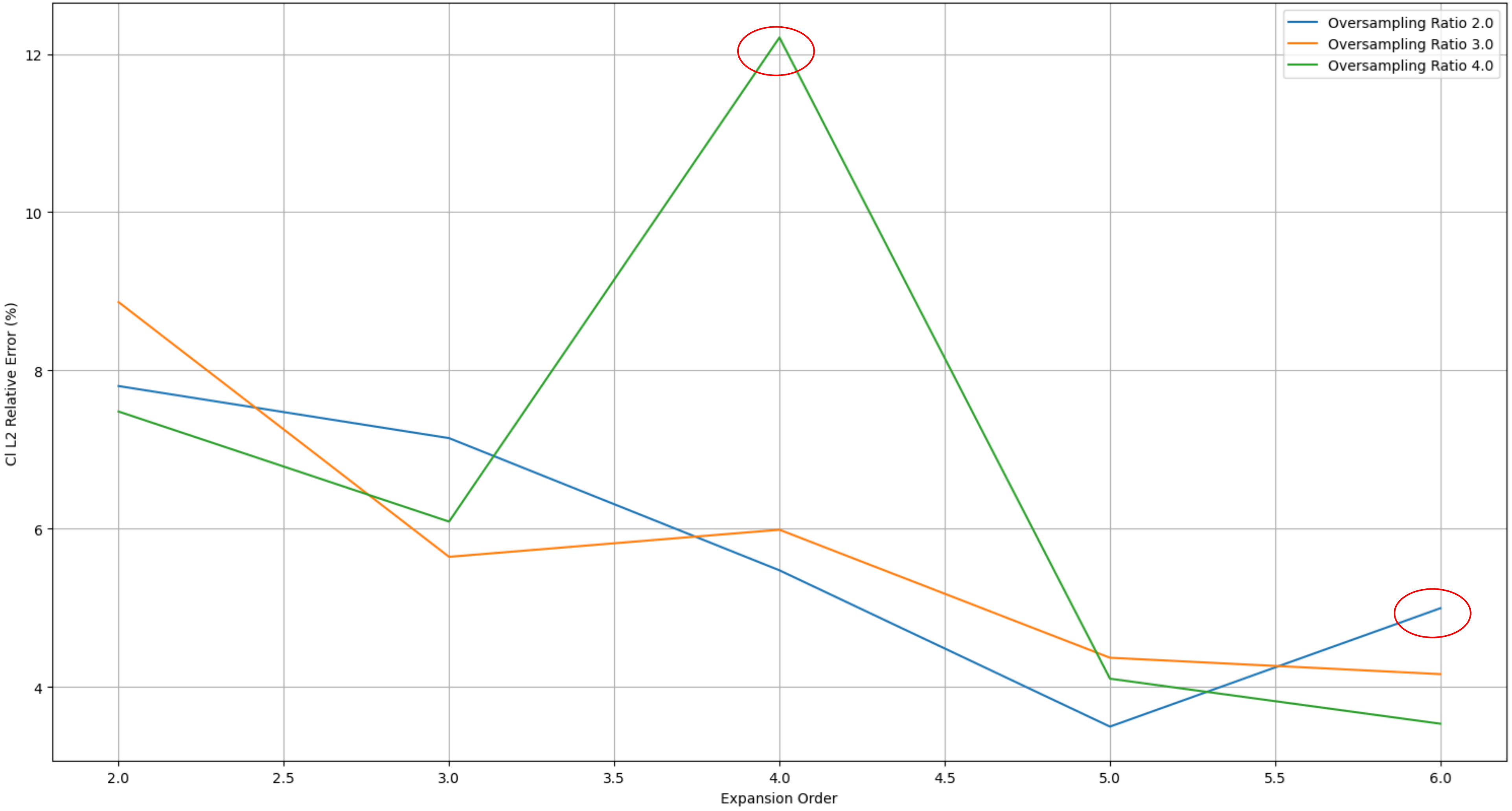
$$\epsilon = 100 \times \frac{\sqrt{\sum_{t=1}^{n}(C_{l_t}^{\mathrm{FOM}} - C_{l_t}^{\mathrm{PCE}})^2}}{\sqrt{\sum_{t=1}^{n}(C_{l_t}^{\mathrm{FOM}})^2}}\%$$

Impact of Sampling Technique : LHS vs Random

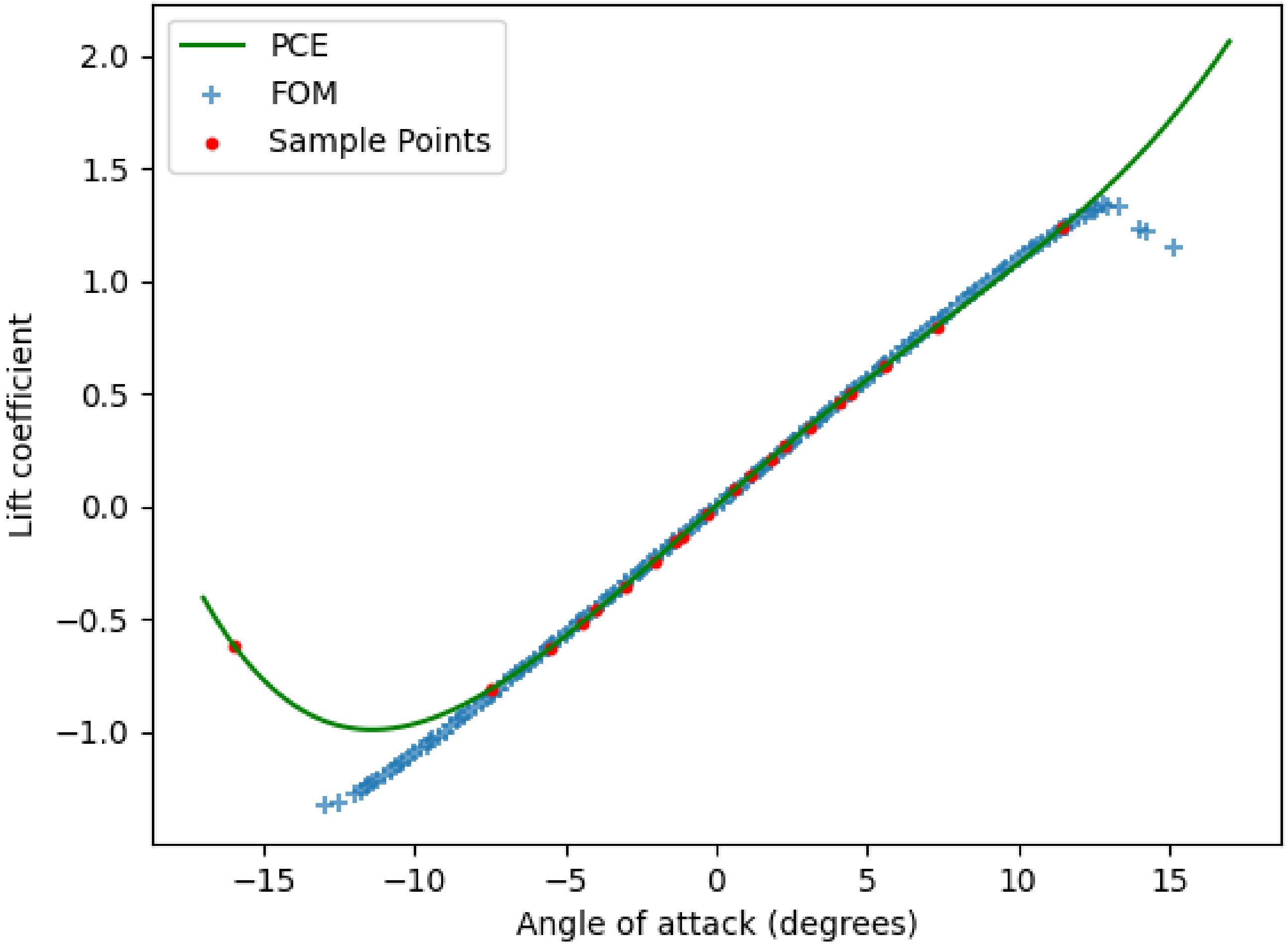
Expansion order	Number of Samples	Sampling method	Cl L2 relative error (%)
3	6	Random	8.7
3	6	LHS	6.1
3	9	Random	6.2
3	9	LHS	6.1
4	8	Random	7.5
4	8	LHS	7.3
4	12	Random	7.5
4	12	LHS	5.6
5	10	Random	3.4
5	10	LHS	7.3
2	4	Random	8.9
2	4	LHS	8.1
5	15	Random	3.34
5	15	LHS	2.7

LHS outperforms the Random sampling in most cases.

Impact of Expansion Order

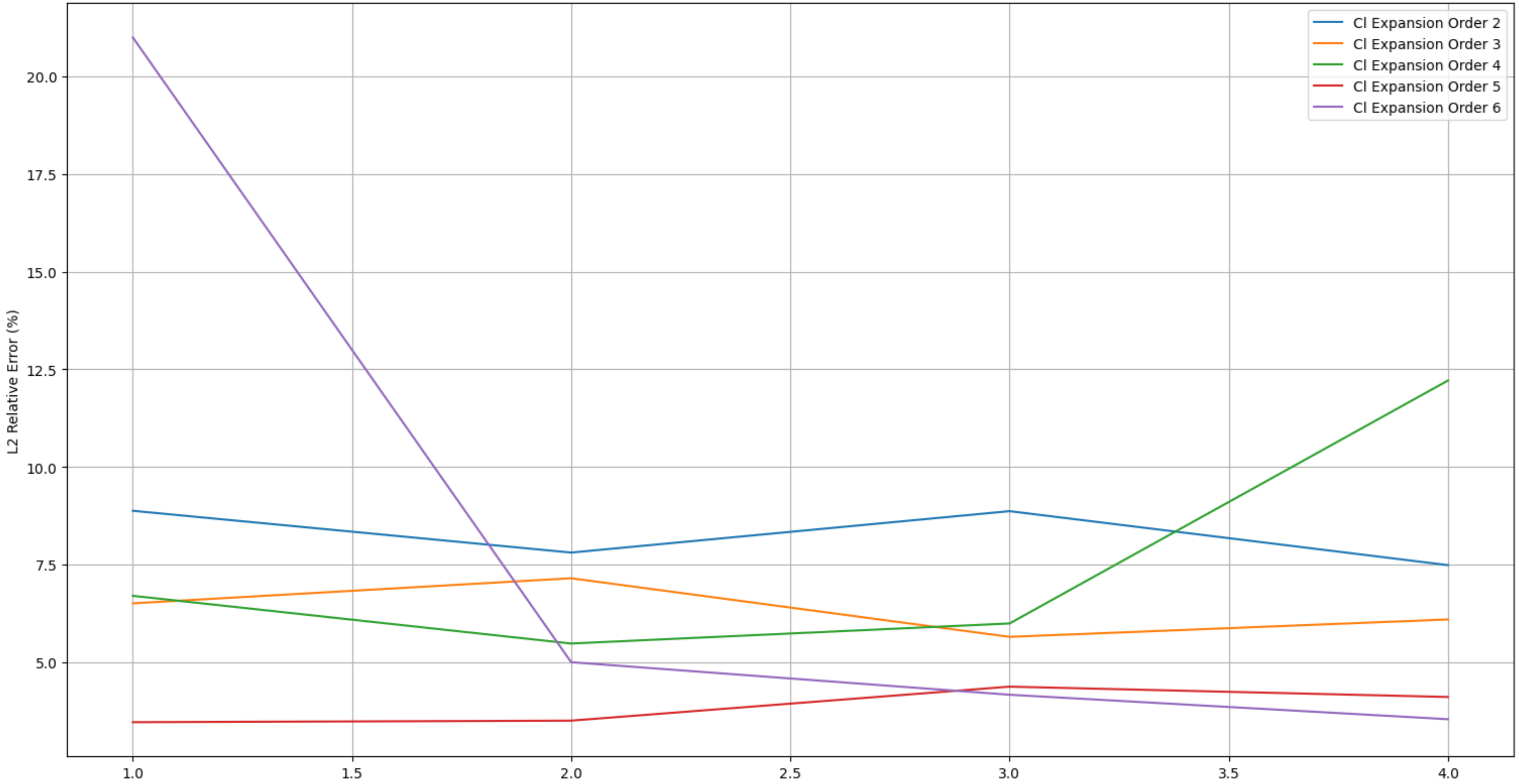


Impact of Expansion Order : Anomaly Explained

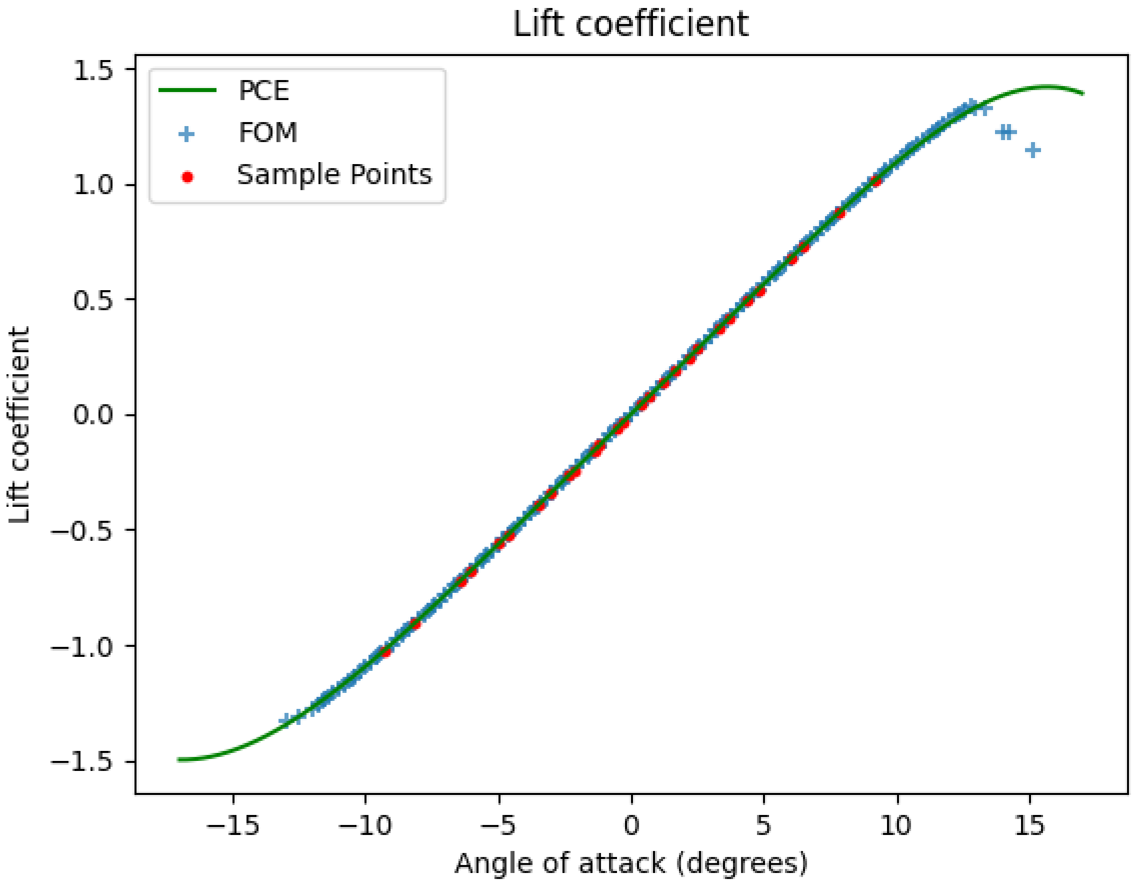


PCE obtained with an Expansion order of 4 and an oversampling ratio of 4

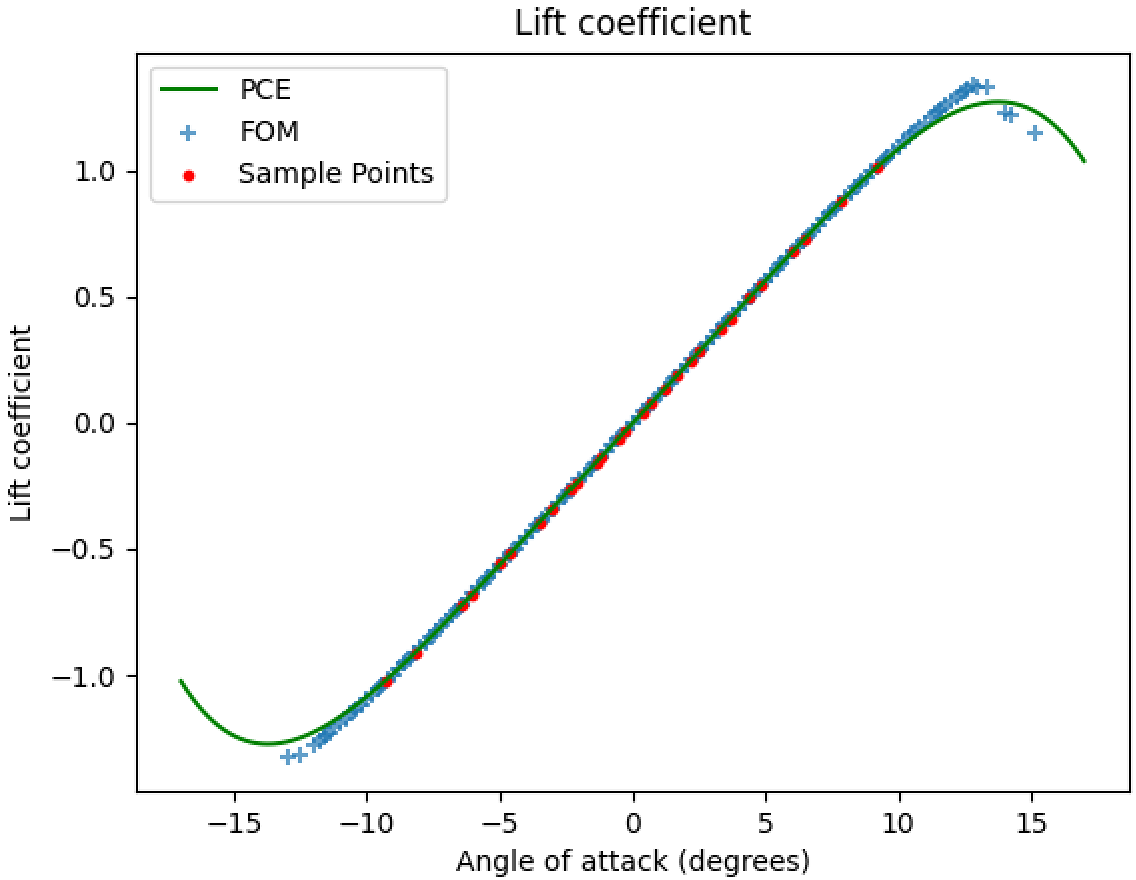
Impact of Oversampling Ratio



Impact of Fitting Method : Least Squares vs LASSO Regression



Best PCE obtained with Least Squares Regression
(Expansion order of 6 and oversampling ratio of 4)



Best PCE obtained with LASSO Regression, α =0.001
(Expansion order of 6 and oversampling ratio of 4)

Discussion

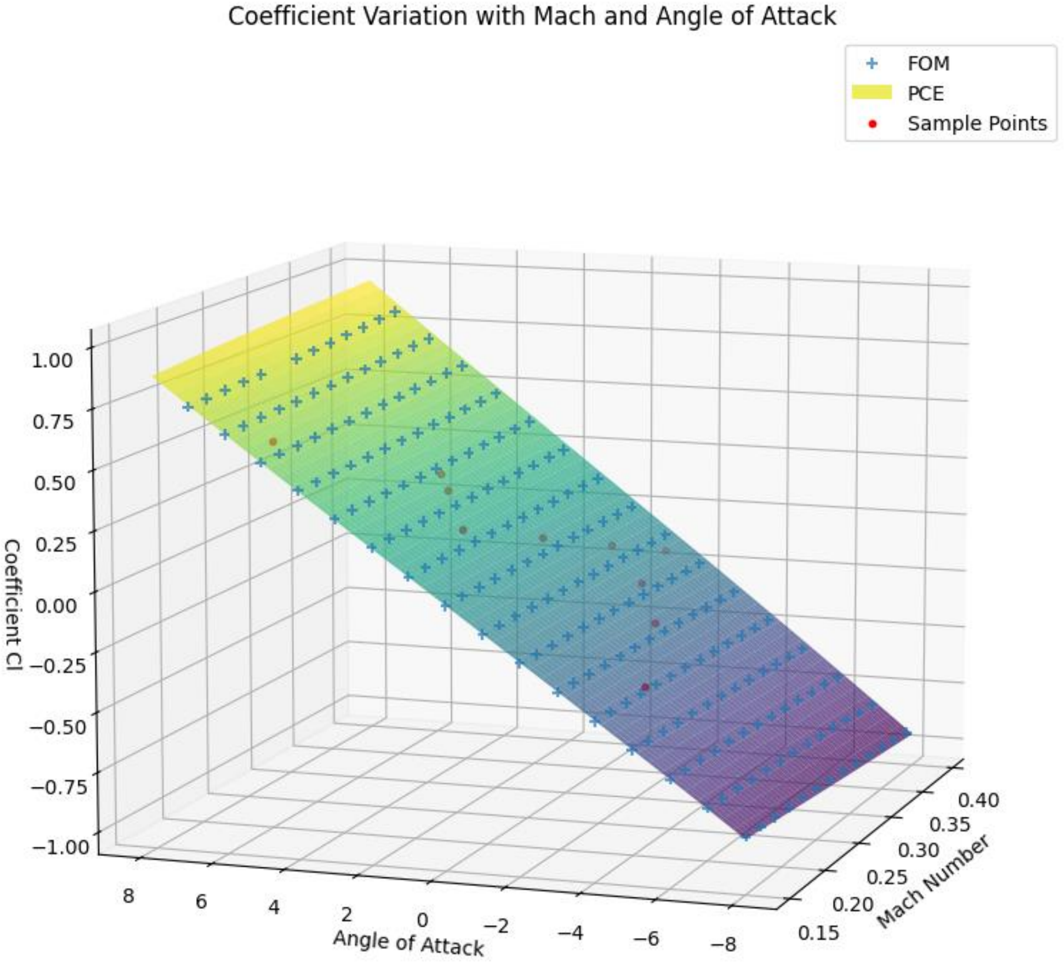
- NIPCE Efficacy:
  - Delivers accurate models with few FOM evaluations
  - Versatility in handling untrained data points.

- Considerations for critical perspective:
  - Use of L2 relative error and dataset construction could be seen as arbitrary
  - Some models might better predict specific phenomena despite overall larger error
  - Dependency on FOM robustness

Mach & Two Parameters Uncertainty Analysis

- Mach Number as sole parameter: the same study yielded similar outcomes (cf. Appendices)

- Two uncertain parameters:
  - Initial results are promising
  - Higher computational costs due to additional sample evaluations



PCE obtained for an expansion order of 3 and an oversampling ratio of 1

V. Conclusion and Outlook

Conclusion and Outlook

- Theoretical and practical exploration of the NIPCE for method for UQ in CFD simulations.
  - Effective integration using Chaospy
  - Parametric investigation

- Limitations
  - Dependent on the FOM's robustness
  - Computational capabilities

- Future directions:
  - Deeper dual-parameter uncertainty analysis
  - Robust FOM solver use
  - Transition to Object Oriented Programming
  - Potential comparison of NIPCE results with Monte Carlo simulations
  - Investigate other libraries
  - Machine Learning integration (Gaussian Process Modeling, ...)

Thank you all for the attention

Any questions ?

Appendix I : Numerical Implementation of NACA0012 Case on OpenFOAM

Parameter	Value
Pressure (p)	10^5 Pa
Temperature (T)	293 K
Gas Model	Air at room temperature (polytropic perfect gas)
Dynamic Viscosity (μ)	1.82×10^{-5}
Prandtl Number (Pr)	0.71
Turbulence Model	k-omega SST
Solver	rhoSimpleFoam

Fixed Parameter of the CFD simulation

First cell size ~0.2mm

```
aerofoil
{
    xLead   0;
    zLead   0;
    xTrail  1;
    zTrail  0;
    xUpper  0.3;
    zUpper  0.06;

    xLower  $xUpper;
    zLower  #neg $zUpper;
}
```

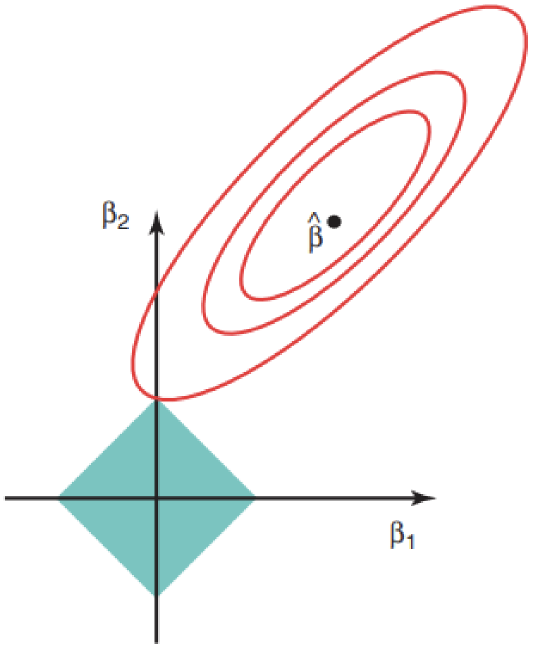
```
domain
{
    xMax  100;
    zMax  50;

    xMin #neg $xMax;
    zMin #neg $zMax;

    // Number of cells
    zCells  60; // aerofoil to far field
    xUCells 60; // upstream
    xMCells 25; // middle
    xDCells 50; // downstream

    // Mesh grading
    zGrading    30000;  // aerofoil to far field
    xUGrading   10;     // towards centre upstream
    leadGrading 0.005;  // towards leading edge
    xDGrading   400;    // downstream
}
```

Appendix II : LASSO Regression



Contours of the error and constraint functions for the lasso,The solid blue areas are the constraint regions, $|\beta 1| + |\beta 2| \le s$, while the red ellipses are the contours of the RSS

The sum of the squares of residuals :

$$\mathrm{RSS} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 .$$

The Lasso regression :

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \mathrm{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|.$$

Another formulation :

$$\underset{\beta}{\text{minimize}}\left\{\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2\right\} \quad \text{subject to} \quad \sum_{j=1}^{p}|\beta_j| \le s$$

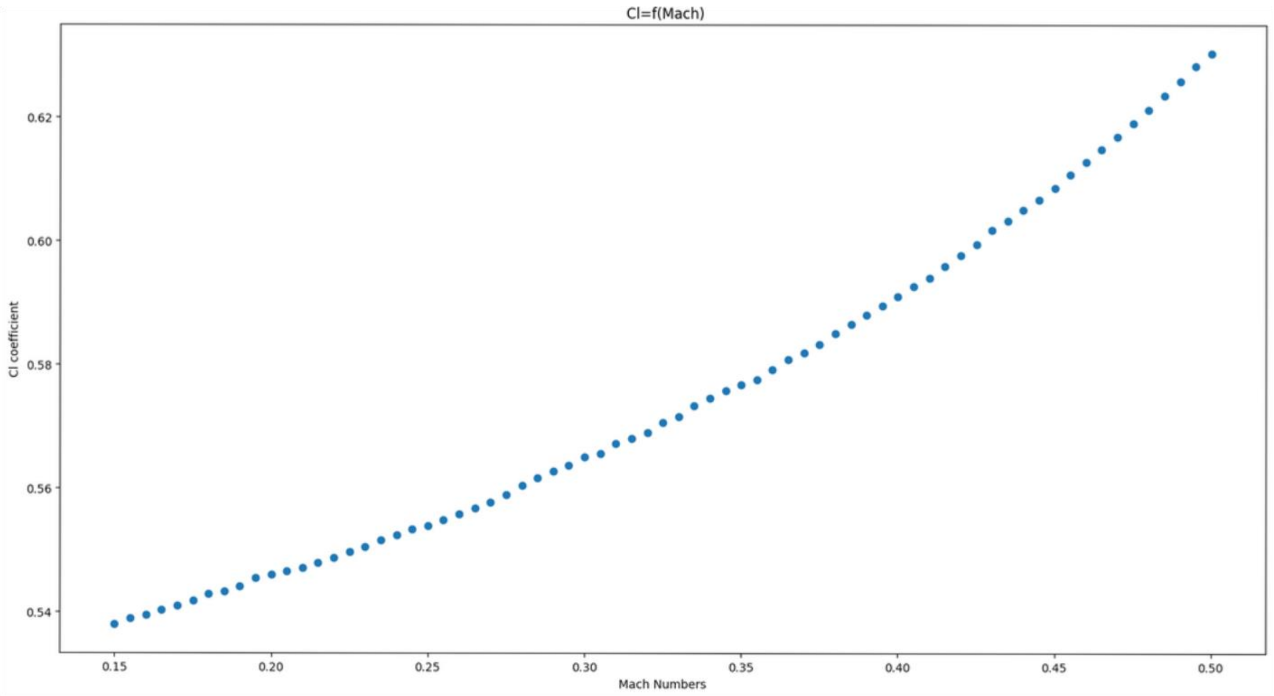
Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. An Introduction to Statistical Learning: with Applications in R. New York: Springer, 2013.

Appendix III : NIPCE Implementation : Mach Number uncertainty analysis

- Study Parameters:
  - AOA set at 5°
  - Mach : Normal Distribution, mean 0.325, STD 0.85

- NIPCE Python Implementation:
  - Inputs : FOM, AOA distribution, Expansion order, Sample size, Sampling method, Fitting Method
  - Point Collocation Technique to compute the PCE

- Parametric study:
  - Creation of a reference database to assess the surrogate models accuracy
  - L2 relative error as accuracy metric



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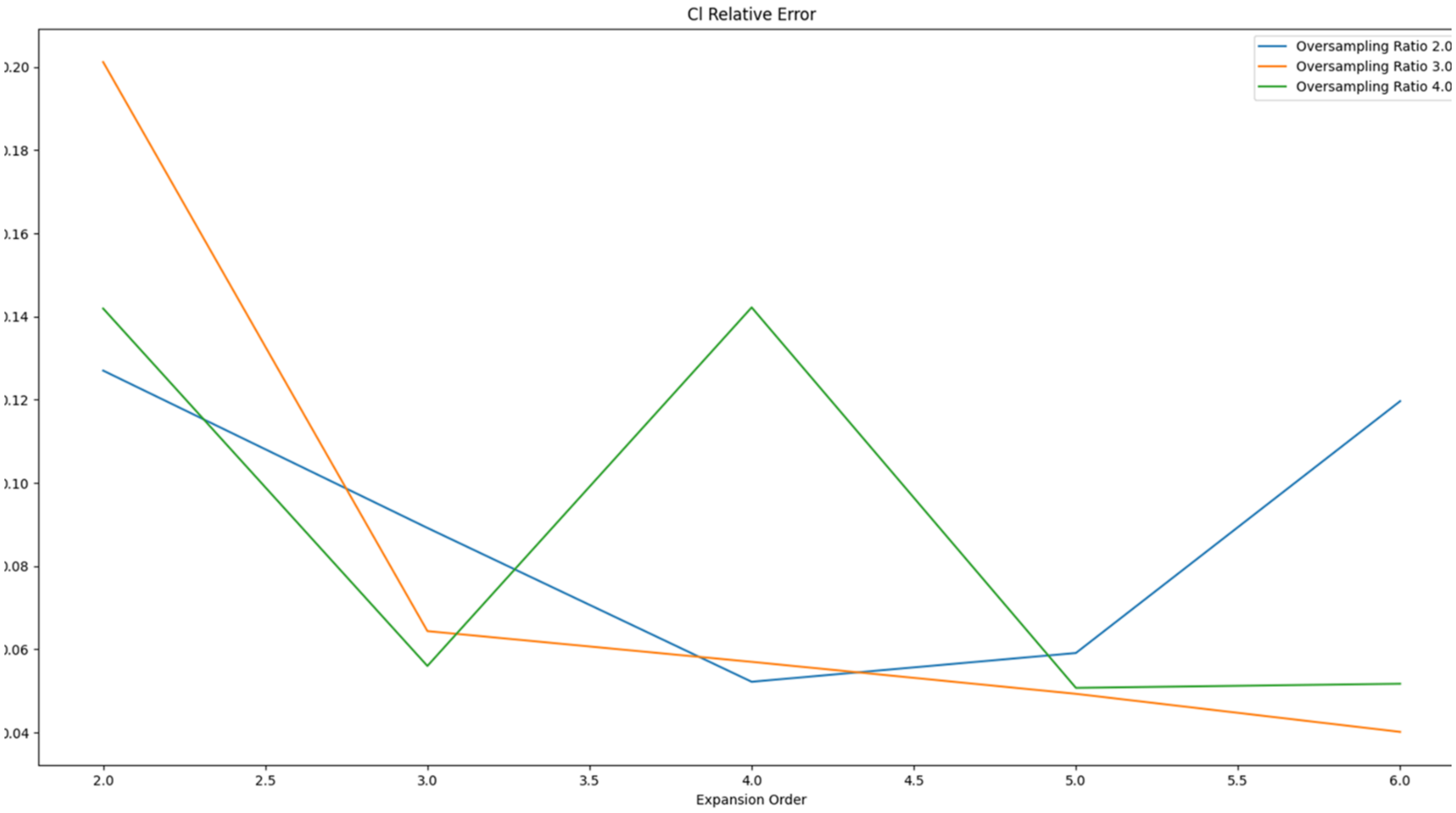
Appendix III : NIPCE Implementation : Mach Number uncertainty analysis

EXPANSION ORDER	# SAMPLES	SAMPLING TECHNIQUE	Cd RELATIVE ERROR (%)	Cl RELATIVE ERROR (%)
3	6	Random	3,9	0,71
3	6	LHS	0,27	0,06
3	9	Random	1,5	0,34
3	9	LHS	0,38	0,1
4	8	Random	5,7	1
4	8	LHS	0,59	0,11
4	12	Random	4,1	0,75
4	12	LHS	0,309	0,056
5	10	Random	0,78	0,15
5	10	LHS	1,55	0,31
2	4	Random	1,04	0,33
2	4	LHS	0,31	0,12
5	15	Random	1,2	0,26
5	15	LHS	0,47	0,08

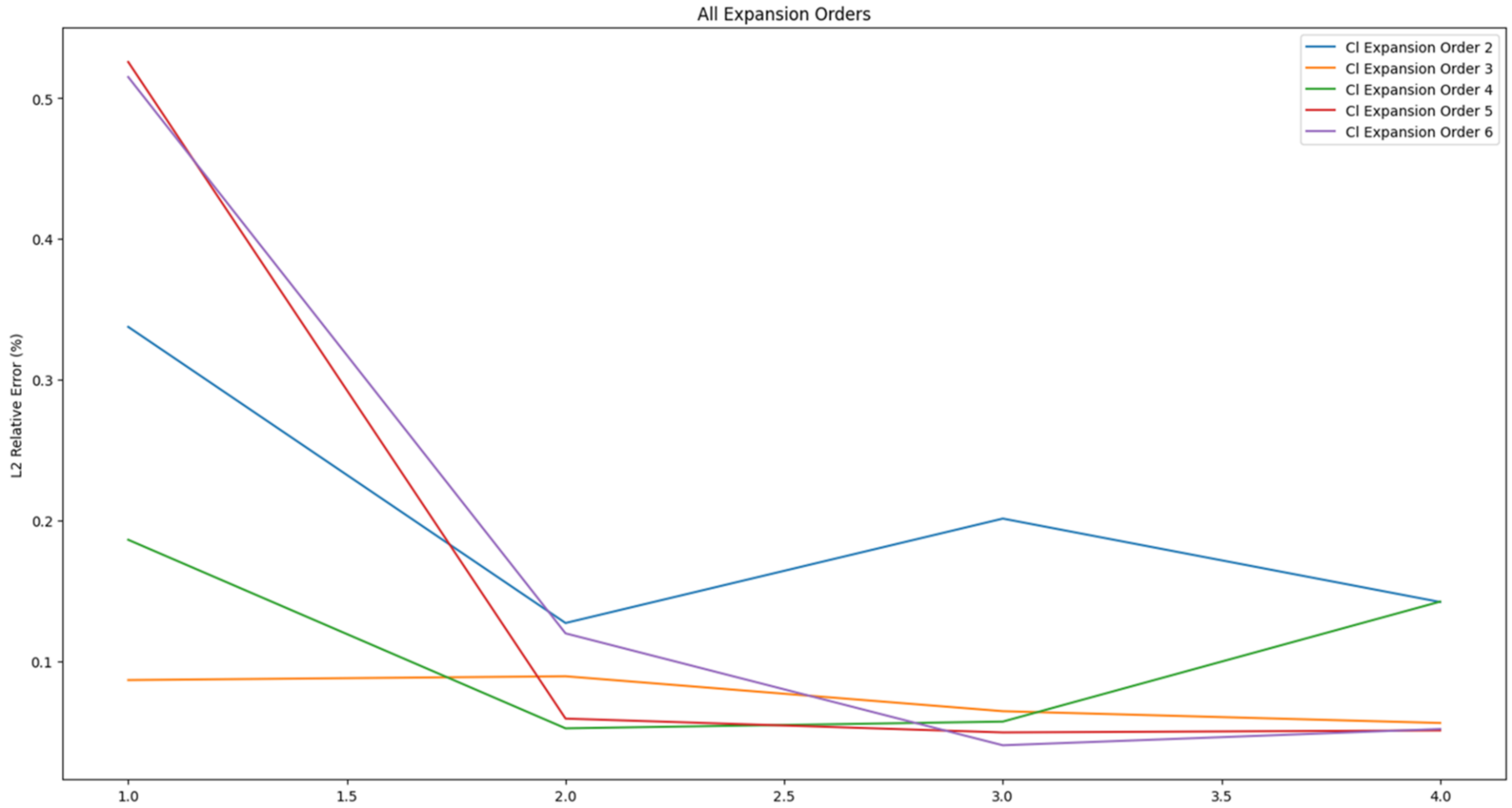
LHS vs Random Sampling

Appendix III : NIPCE Implementation : Mach Number uncertainty analysis



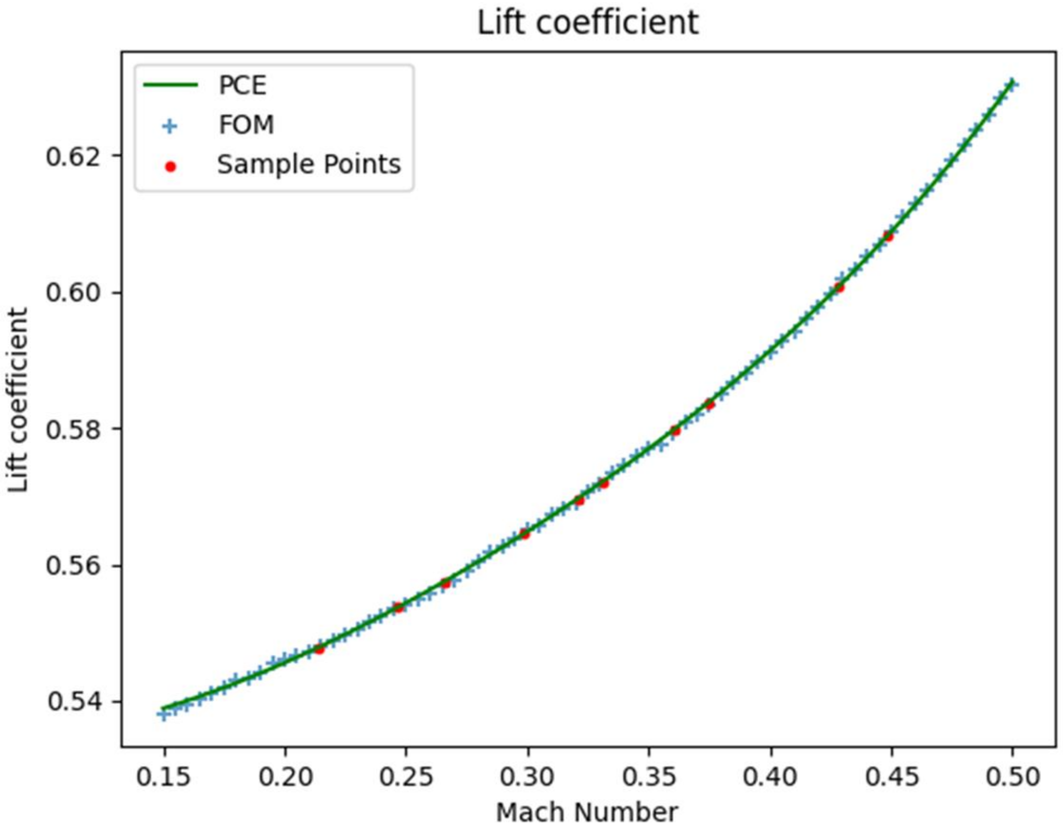
Impact of Expansion Order

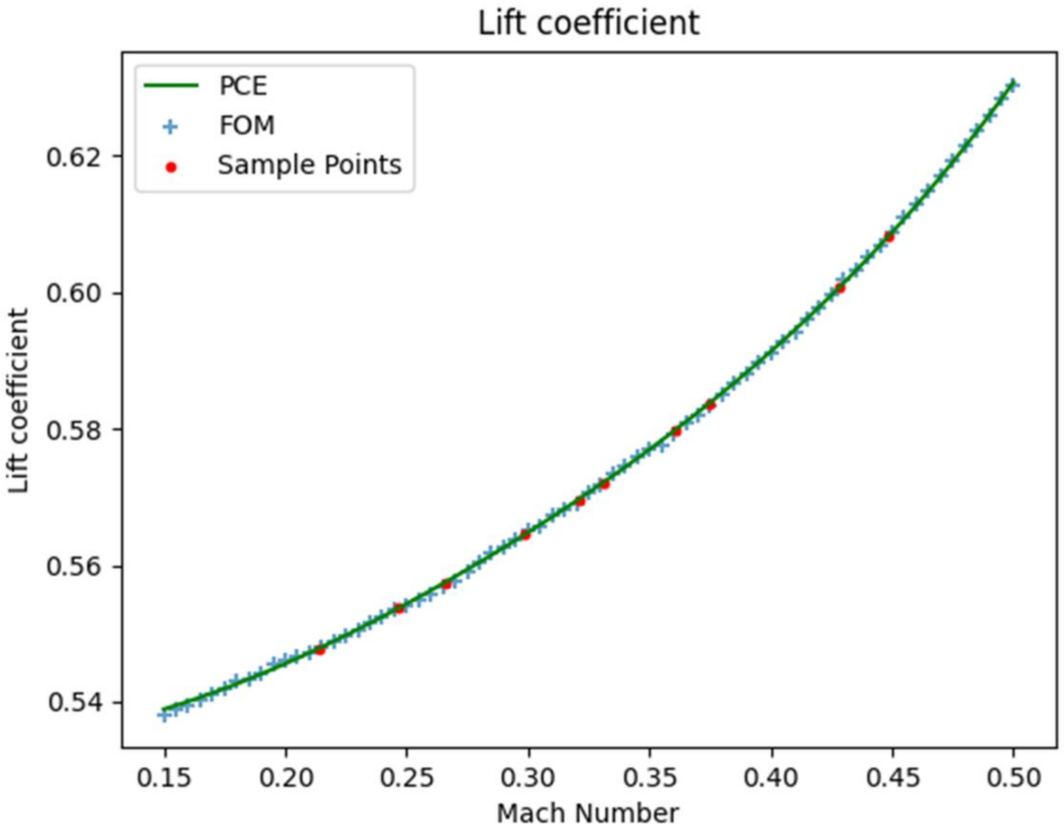
Appendix III : NIPCE Implementation : Mach Number uncertainty analysis



Impact of Oversampling Ratio

Appendix III : NIPCE Implementation : Mach Number uncertainty analysis





Expansion Order = 4
Oversampling Ratio = 2

Expansion Order = 4
Oversampling Ratio = 4