東北大学 流体科学研究所
Institute of Fluid Science, Tohoku University

不確定性定量化のための効果的手法の確立に向けた基礎研究

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第6回EFD/CFD融合ワークショップ，2014年1月30日

Outline

- ✓ *Fundamentals of Uncertainty Quantification*
- ✓ *Research Topics*
  - ● *Polynomial Chaos Expansion with Order Adjustment*
    - ✳ *Prof. Shigeru Obayashi (Tohoku Univ.)*
    - ✳ *Mr. Akihiro Inoue (Tohoku Univ.)*
    - ✳ *JAXA/NSRG*
  - ● *Dynamic Adaptive Sampling based on Kriging Surrogate Model*
    - ✳ *Dr. Soshi Kawai (JAXA/ISAS)*
    - ✳ *Prof. Juan J. Alonso (Stanford Univ.)*
- ✓ *Summary & Future Work*

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CFD Challenges

Vision 2030 "Where we believe CFD should go"

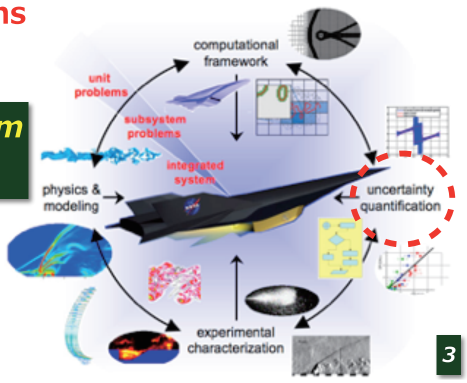
[Andersen 2012]

- Accurate prediction of boundary layer transition
- Improved RANS model for efficient complex flow analysis
- Accurate prediction recovery, dynamic distortion, and swirl patterns at the Aerodynamic Interface Plane (AIP) for propulsion integration
- Accurate prediction of shock-boundary layer in presence of corner flows
- An advanced turbulence model within a single framework for accurate unsteady flow phenomena
- Efficient and robust mesh adaptation for complex configurations
- **Error estimation and uncertainty predictions**
- Multidisciplinary analysis (aeroelasticity, etc.)

Predictive Science Academic Alliance Program (PSSAP)

[pssap.stanford.edu]

Predictive Simulations of Multi-Physics Flow Phenomena, with Application to Integrated Hypersonic Systems



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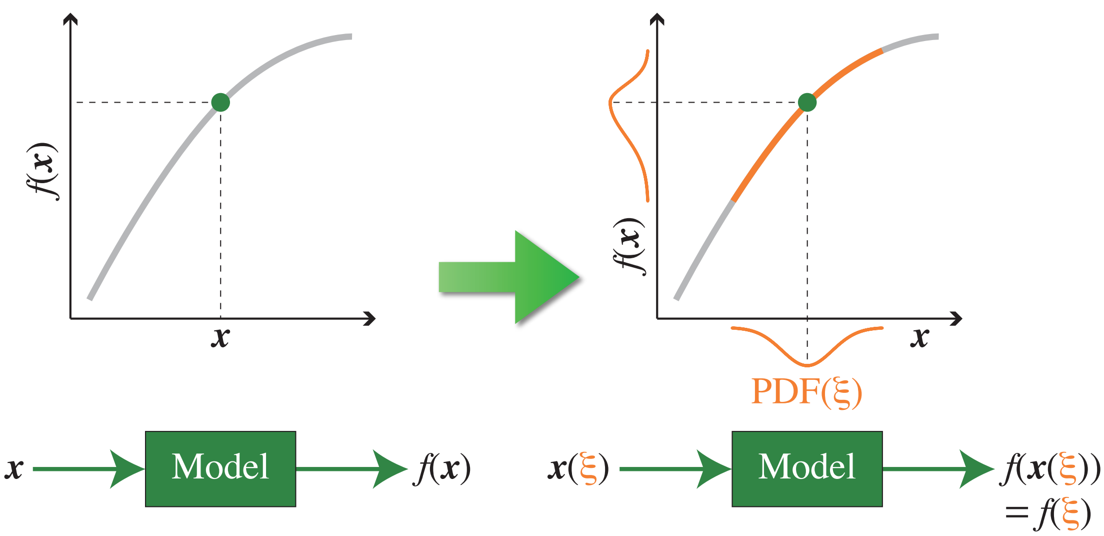
Uncertainty Quantification (UQ)

Science of quantitative characterization and reduction of uncertainties in applications

[wikipedia.org]



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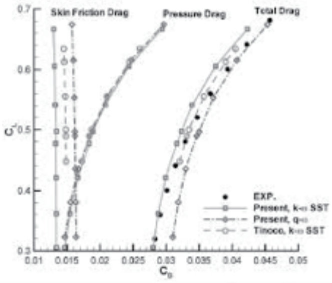
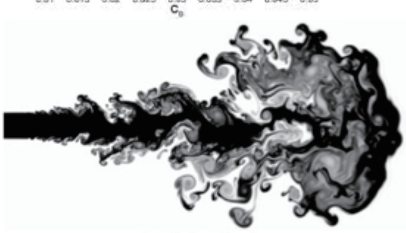
Contributions of UQ

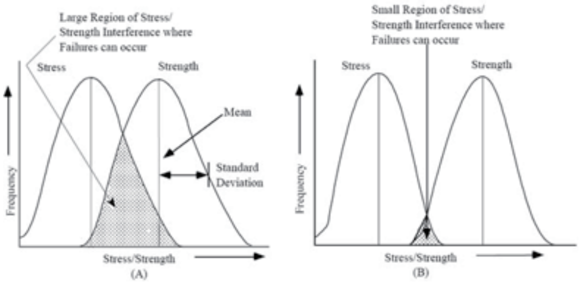
✓ Simulation
- Assist verification and validation
- Make perfect models



✓ Physics
- Understand complex phenomena
- Find exact principles



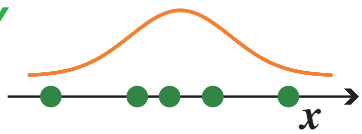
✓ Design
- Evaluate robustness
- Ensure reliability



Types of Uncertainty

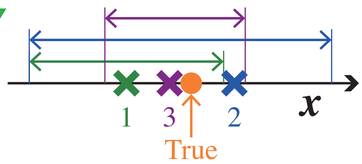
✓ *Aleatory (Irreducible) Uncertainty*
- Inherent variation associated with the system under consideration
- Defined in a probabilistic framework

→ Material properties, operating conditions, manufacturing tolerances, …



✓ *Epistemic (Reducible) Uncertainty*
- Lack of knowledge or information in any phase or activity of the modeling process
- Involves a single but unknown true value

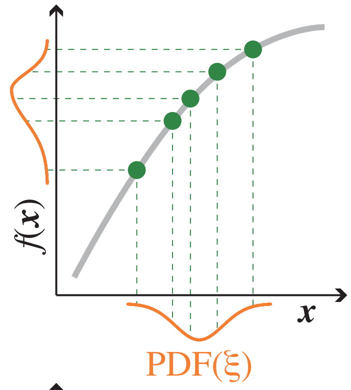
→ Turbulence models, chemical process models, …



Types of Uncertainty Propagation

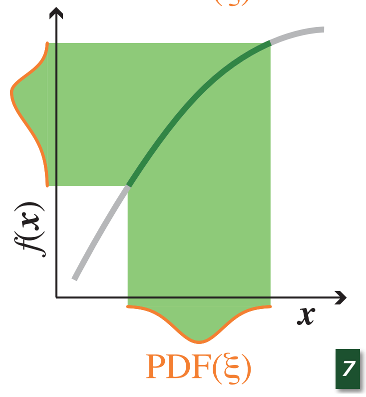
✓ Non-Intrusive Methods

- Only require (multiple) solutions of the original (deterministic) model
- Treat the model as a black box
- Less efficient to compute



✓ Intrusive Methods

- Require the formulation and solution of a stochastic version of the original model
- Need to know the mathematical structure of the model
- More efficient to compute



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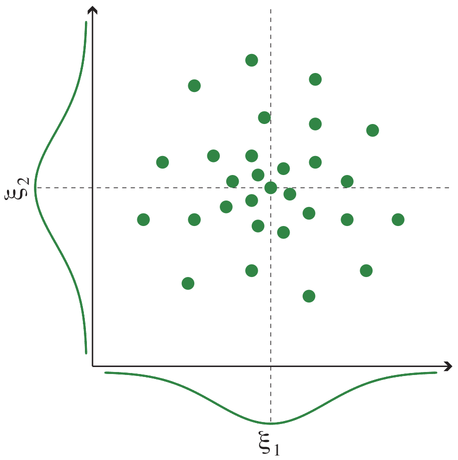
Sampling Methods

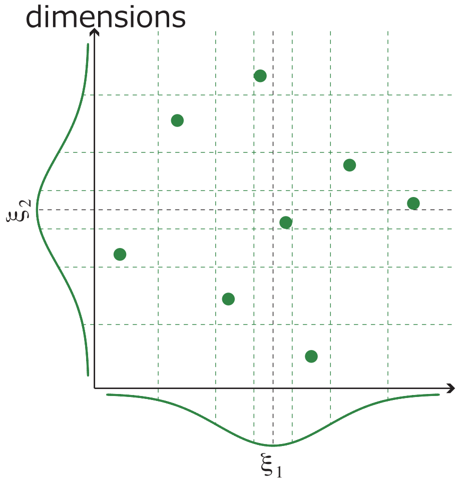
✓ Monte Carlo (MC)

Samples all points randomly



✓ Latin Hypercube Sampling (LHS) [Mckay *et al.* 1979]

- Samples a point in each equi-probability partition randomly
- Does not allow overlapping partitions to be sampled for all dimensions



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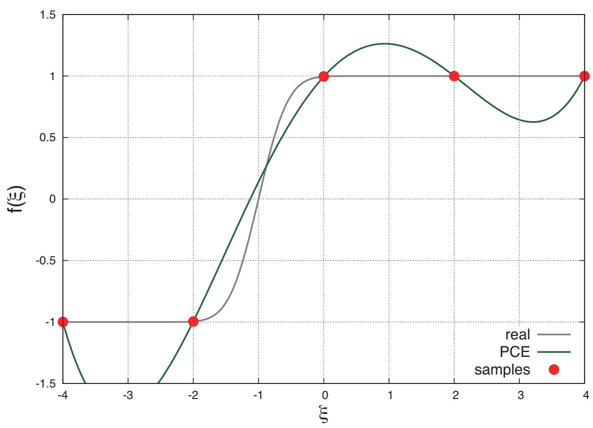
Approximation Methods

$$f(\xi) \simeq \sum_{i=1}^{P} \alpha_i \phi_i(\xi)$$



✓ ***Polynomial Chaos Expansion (PCE)*** **[Xiu & Karniadakis 2002]**

- Approximates as a linear combination of orthogonal polynomials
- Estimates coefficients for known orthogonal polynomials

✓ ***Stochastic Collocation (SC)*** **[Xiu & Hesthaven 2005]**

- Approximates as a linear combination of interpolation polynomials
- Forms interpolation functions for known coefficients

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Polynomial Chaos Expansion (PCE)

$$f(\xi) \simeq \sum_{i=1}^{P} \alpha_i \phi_i(\xi)$$

where $P = \dfrac{(n+p)!}{n!p!}$

n: **# dimensions in ξ**

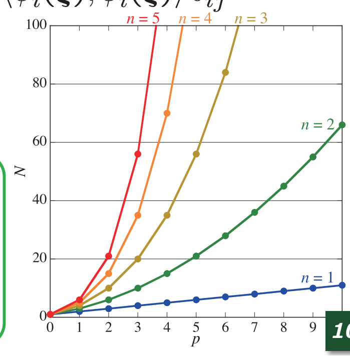
p: **Polynomial order**

Input uncertainty PDF(ξ)	Polynomial $\phi_i(\xi)$
Uniform	Legendre
Normal	Hermite
Gamma	Laguerre
Beta	Jacobi

$$\left\langle \phi_i(\xi), \phi_j(\xi) \right\rangle = \int_{-\infty}^{\infty} \phi_i(\xi)\phi_j(\xi)\mathrm{PDF}(\xi)\mathrm{d}\xi = \left\langle \phi_i(\xi), \phi_i(\xi) \right\rangle \delta_{ij}$$

$\alpha_1, \alpha_2, \cdots, \alpha_P$ obtained from N ($\geq P$) samples

$$f(\xi^{(j)}) = \sum_{i=1}^{P} \alpha_i \phi_i(\xi^{(j)}) \quad (j = 1, 2, \cdots, N)$$



$$\mu_f = \mathrm{E}[f(\xi)] \simeq \alpha_1$$

$$\sigma_f{}^2 = \mathrm{Var}[f(\xi)] \simeq \sum_{i=2}^{P} \alpha_i{}^2 \left\langle \phi_i(\xi), \phi_i(\xi) \right\rangle$$

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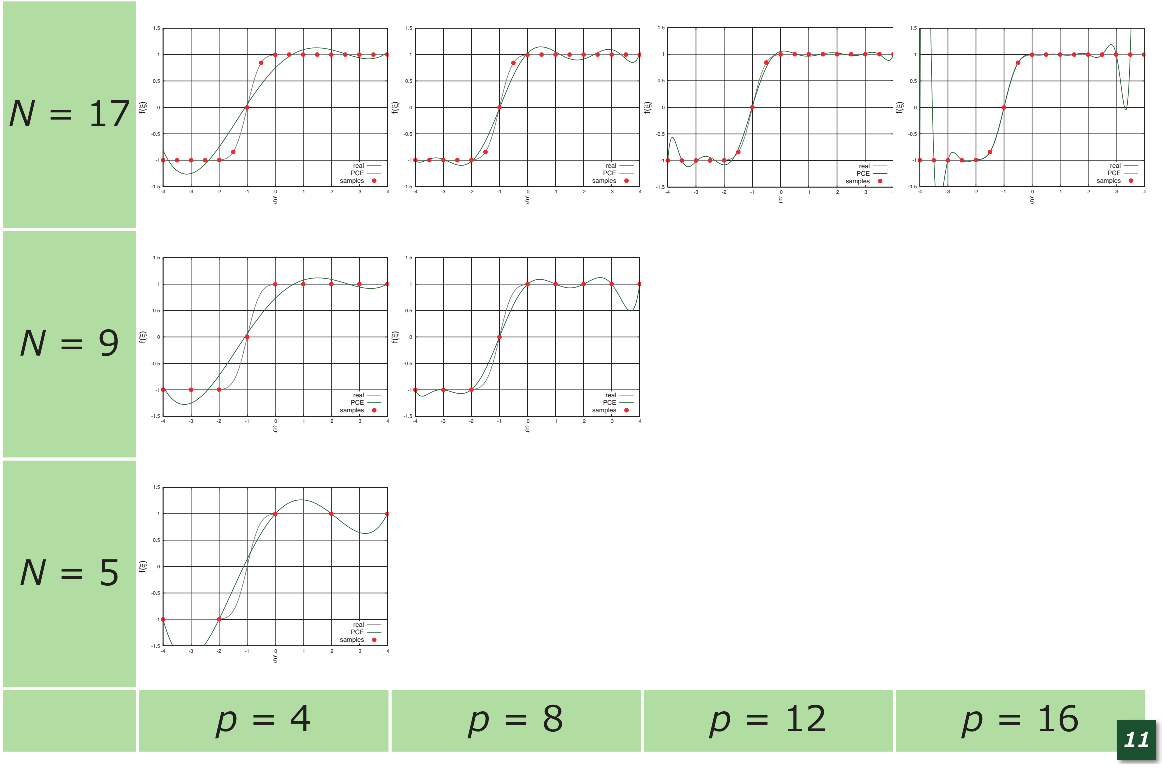
PCE Examples



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Outline

✓ Fundamentals of Uncertainty Quantification

✓ Research Topics

- Polynomial Chaos Expansion with Order Adjustment
  - ✳Prof. Shigeru Obayashi (Tohoku Univ.)
  - ✳Mr. Akihiro Inoue (Tohoku Univ.)
  - ✳JAXA/NSRG
- Dynamic Adaptive Sampling based on Kriging Surrogate Model
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✓ Summary & Future Work

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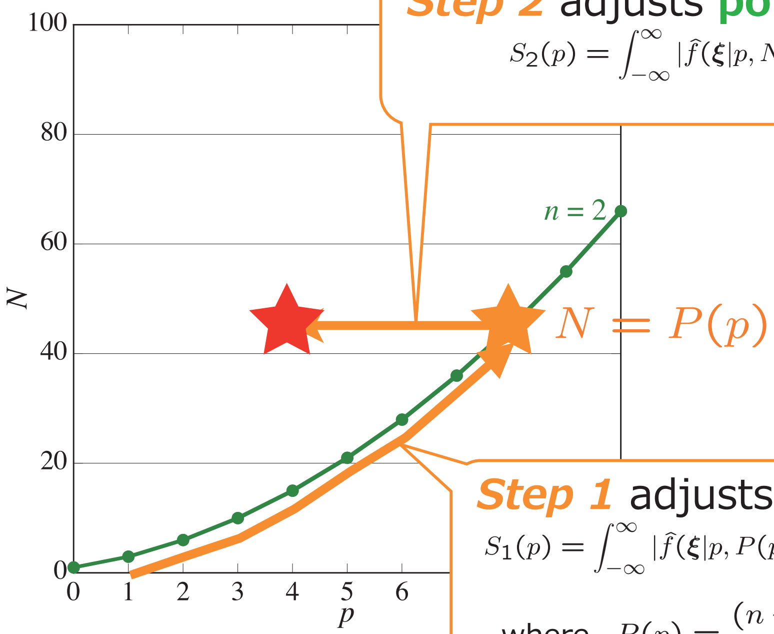
Order Adjustment in PCE



Step 2 adjusts **polynomial order**

$$S_2(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, N) - \hat{f}(\boldsymbol{\xi}|p-1, N)| \times \mathrm{PDF}(\boldsymbol{\xi})d\boldsymbol{\xi}$$

Step 1 adjusts **# samples**

$$S_1(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, P(p)) - \hat{f}(\boldsymbol{\xi}|p-1, P(p-1))| \times \mathrm{PDF}(\boldsymbol{\xi})d\boldsymbol{\xi}$$

where $P(p) = \dfrac{(n+p)!}{n!p!}$

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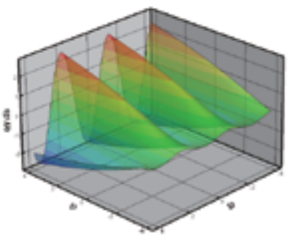
Numerical Tests (2D Func.)

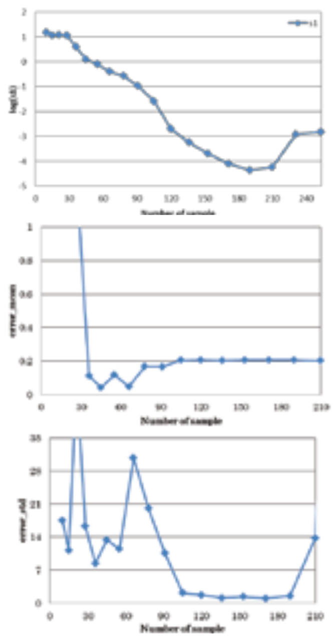


$$f(x_1, x_2) = \ln\left(1 + {x_1}^2\right)\sin(5x_2)$$

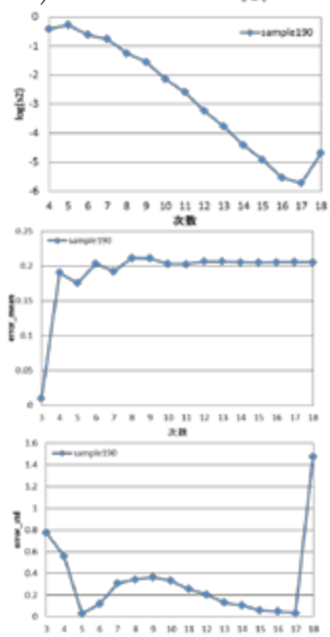
$$x_k = 2 + 0.4\xi_k \quad (k = 1, 2)$$

$$\mathrm{PDF}(\xi_1, \xi_2) = \prod_{k=1}^{2} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{{\xi_k}^2}{2}\right)$$

✓ **Step 1**



✓ **Step 2**



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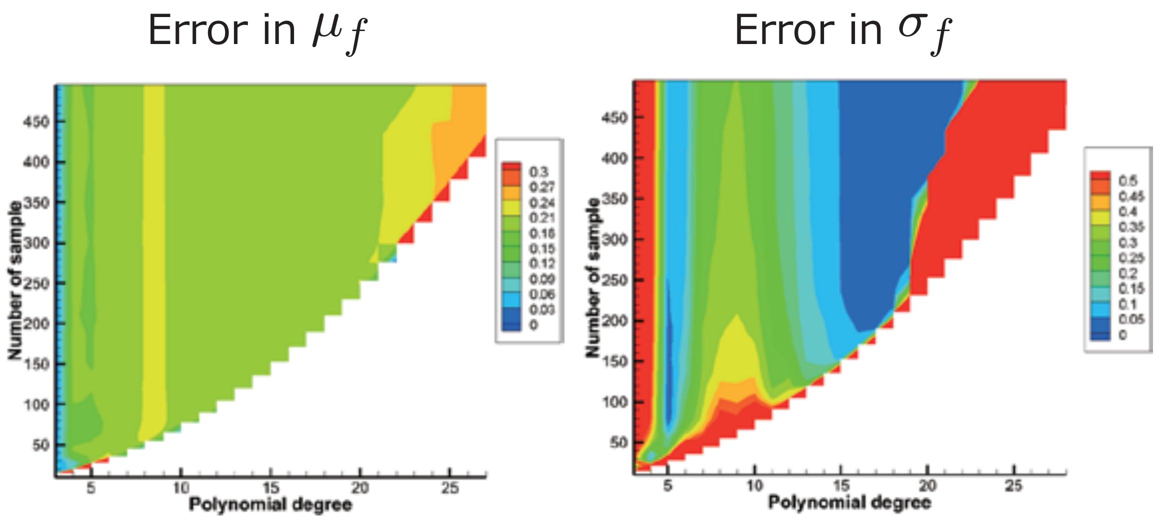
Numerical Tests (2D Func.)



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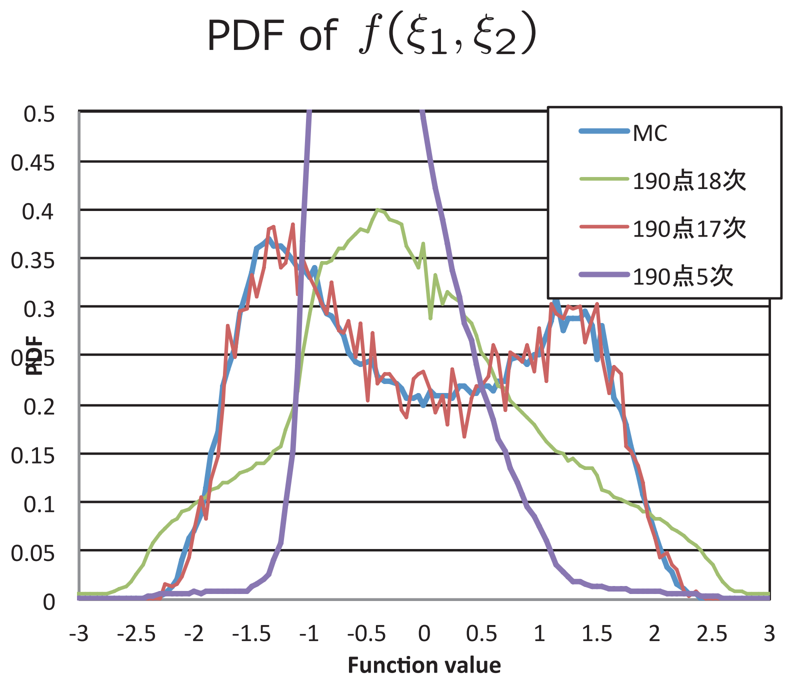
Numerical Tests (2D Func.)



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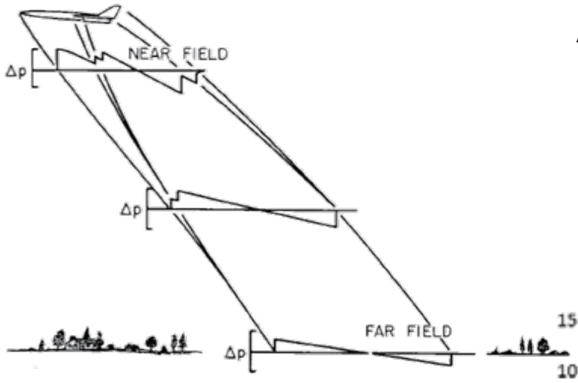
Application (Sonic Boom)

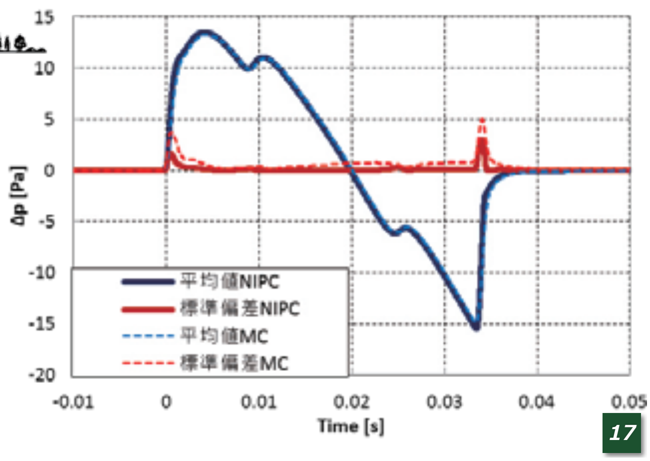


[Carlson 1967]

Augmented Burgers equation
[Cleveland and Blackstock 1996]

with atmospheric uncertainties

- Temperature
- Humidity
- Wind (speed & direction)



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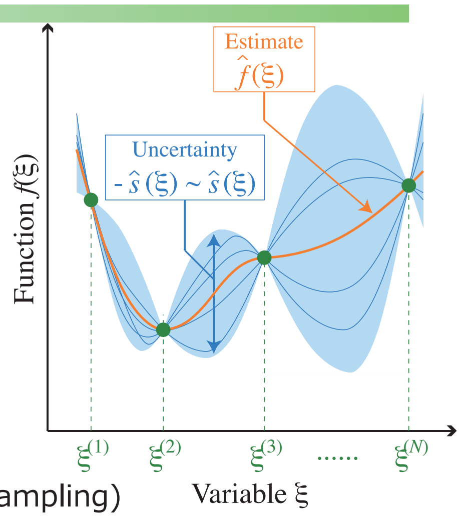
Kriging-Based Methods

✔ *Kriging Surrogate Model*

[Sacks *et al.* 1989]

- Based on the Bayesian statistics
- Adapts well to non-linear functions
- Estimates not only the function values but also their fit uncertainties



[Yamazaki 2013]

Inferior to a classical PCE (without adaptive sampling)

[Dwight and Han 2009]

Adaptive sampling based the fit uncertainty in the Kriging predictor and the PDF of input parameter uncertainties

[Bilionis and Zabaras 2012]

Adaptive refinement based on the fit uncertainty predicted by the Gaussian process regression

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Kriging Surrogate Model

Deterministic $f(\xi)$

Realization

Stochastic $F(\xi) = \mu + Z(\xi)$

where

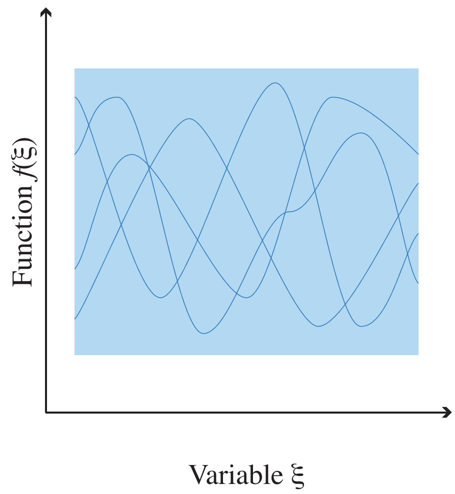
$$\mathrm{E}[Z(\xi)] = 0$$

$$\mathrm{Cov}[Z(\xi), Z(\xi')] = \sigma^2 k(\xi, \xi')$$

Correlation function (kernel)

- Depends on $|\boldsymbol{h}| = |\xi - \xi'|$
- With a set of constants $\ominus$ ***(hyperparameters)***

Prior distribution



Determined by the ***maximum likelihood estimation***

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Kriging Surrogate Model (cont.)

N samples $f(\boldsymbol{\xi}^{(i)}) = F(\boldsymbol{\xi}^{(i)})$ $(i = 1, 2, \cdots, N)$

Likelihood function

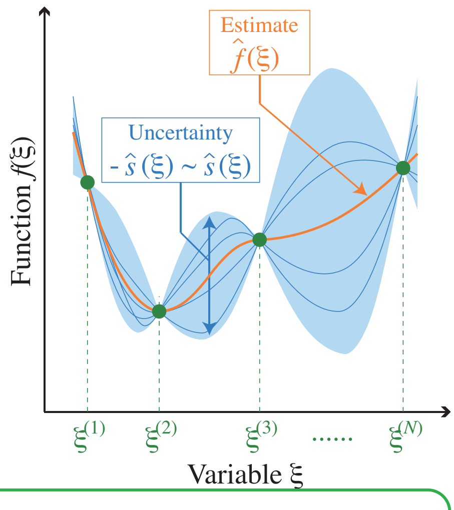
$$Ln(\mu, \sigma^2, \Theta) = -\frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln\sigma^2 - \frac{1}{2}\ln|\boldsymbol{R}| - \frac{(\boldsymbol{f} - \boldsymbol{1}\mu)^\top \boldsymbol{R}^{-1}(\boldsymbol{f} - \boldsymbol{1}\mu)}{2\sigma^2}$$

Maximization

$$\hat{\mu} = \frac{\boldsymbol{1}^\top \boldsymbol{R}^{-1}\boldsymbol{f}}{\boldsymbol{1}^\top \boldsymbol{R}^{-1}\boldsymbol{1}}$$

$$\hat{\sigma}^2 = \frac{(\boldsymbol{f} - \boldsymbol{1}\hat{\mu})^\top \boldsymbol{R}^{-1}(\boldsymbol{f} - \boldsymbol{1}\hat{\mu})}{N}$$

Posterior distribution



Best linear unbiased predictor

$$\hat{f}(\boldsymbol{\xi}) = \hat{\mu} + \boldsymbol{r}^\top(\boldsymbol{\xi})\boldsymbol{R}^{-1}(\boldsymbol{f} - \boldsymbol{1}\hat{\mu})$$

$$\hat{s}^2(\boldsymbol{\xi}) = \hat{\sigma}^2\left[1 - \boldsymbol{r}^\top(\boldsymbol{\xi})\boldsymbol{R}^{-1}\boldsymbol{r}(\boldsymbol{\xi}) + \frac{\left(1 - \boldsymbol{1}^\top \boldsymbol{R}^{-1}\boldsymbol{r}(\boldsymbol{\xi})\right)^2}{\boldsymbol{1}^\top \boldsymbol{R}^{-1}\boldsymbol{1}}\right]$$

where

$R_{ij} = k(\boldsymbol{\xi}^{(i)}, \boldsymbol{\xi}^{(j)})$

$r_i(\boldsymbol{\xi}) = k(\boldsymbol{\xi}, \boldsymbol{\xi}^{(i)})$

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Dynamic Adaptive Sampling

✓ **Criterion 1** **[Dwight and Han 2009]**

$$\mathrm{Crit}(\boldsymbol{\xi}) = \hat{s}(\boldsymbol{\xi}) \times \mathrm{PDF}(\boldsymbol{\xi})$$

✓ **Criterion 2**

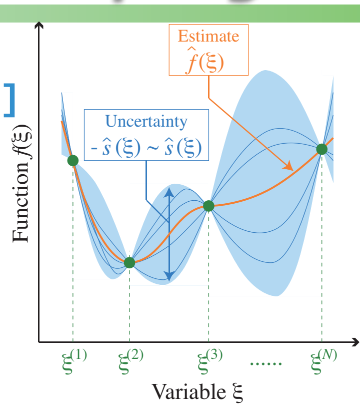
$$\mathrm{Crit}(\boldsymbol{\xi}) = \left|\frac{\partial \hat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right| \times \mathrm{PDF}(\boldsymbol{\xi})$$

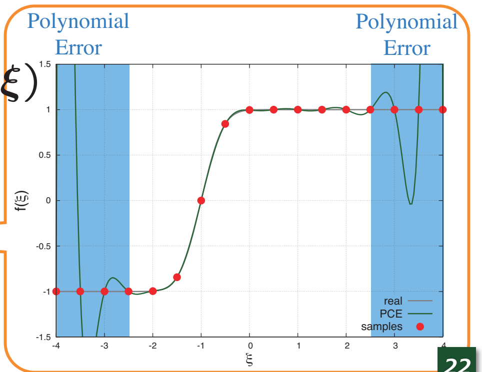
✓ **Criterion 3**

$$\mathrm{Crit}(\boldsymbol{\xi}) = \left|\frac{\partial \hat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right| \times \hat{s}(\boldsymbol{\xi}) \times \mathrm{PDF}(\boldsymbol{\xi})$$

$= 0$

in smooth regions





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Dynamic Adaptive Sampling (cont.)

✓ *Criterion 4* **(proposed)**

$$\mathrm{Crit}(\xi) = \left(\left| \frac{\partial \hat{f}(\xi)}{\partial \xi} \right| \times \Delta\xi + D_{\hat{f}}(\xi) \right) \times \hat{s}(\xi) \times \mathrm{PDF}(\xi)$$

$$\Delta\xi = \min_{i=1,2,\cdots,N} |\xi - \xi^{(i)}|$$

$$D_{\hat{f}}(\xi) = |\hat{f}(\xi) - \hat{f}_{\mathrm{pre}}(\xi)|$$

Current (N samps.) Previous (N-1 samps.)

Summary of Sampling Criteria

✓ *Criterion 1* **[Dwight and Han 2009]**
considers only **fit uncertainty**

✓ *Criterion 2*
considers only **gradient**

✓ *Criterion 3*
considers both **fit uncertainty** & **gradient**

✓ *Criterion 4* **(proposed)**
adds an extra **error-estimate term** in criterion 3

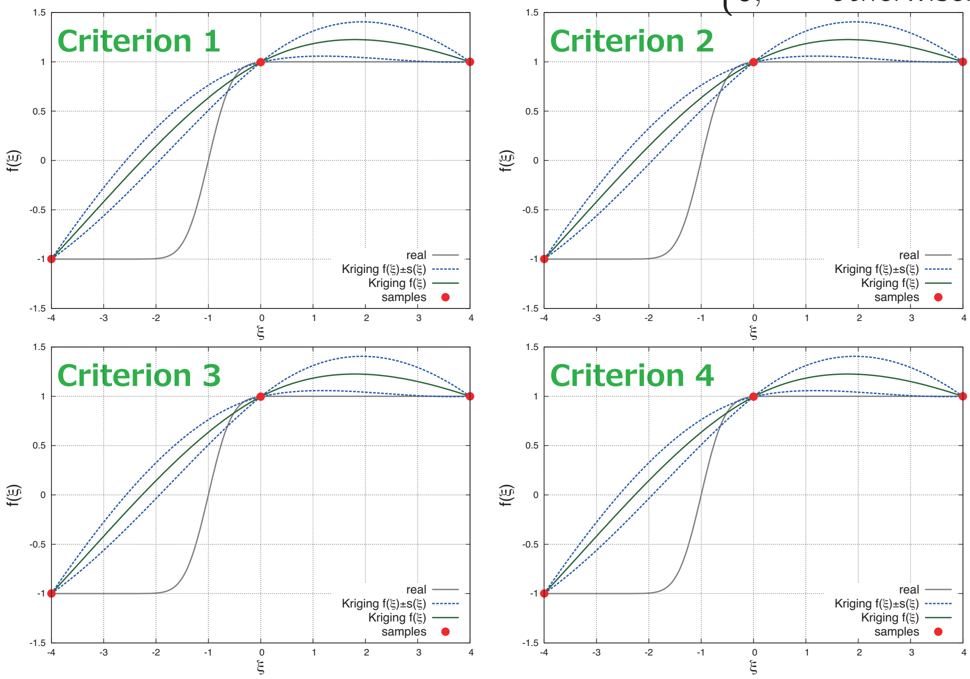
Numerical Tests (1D Funcs.)

3 samples

(evenly distributed)

$$f(\xi) = \mathrm{erf}\left[2(\xi+1)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \leq \xi \leq 4, \\ 0, & \text{otherwise.} \end{cases}$$



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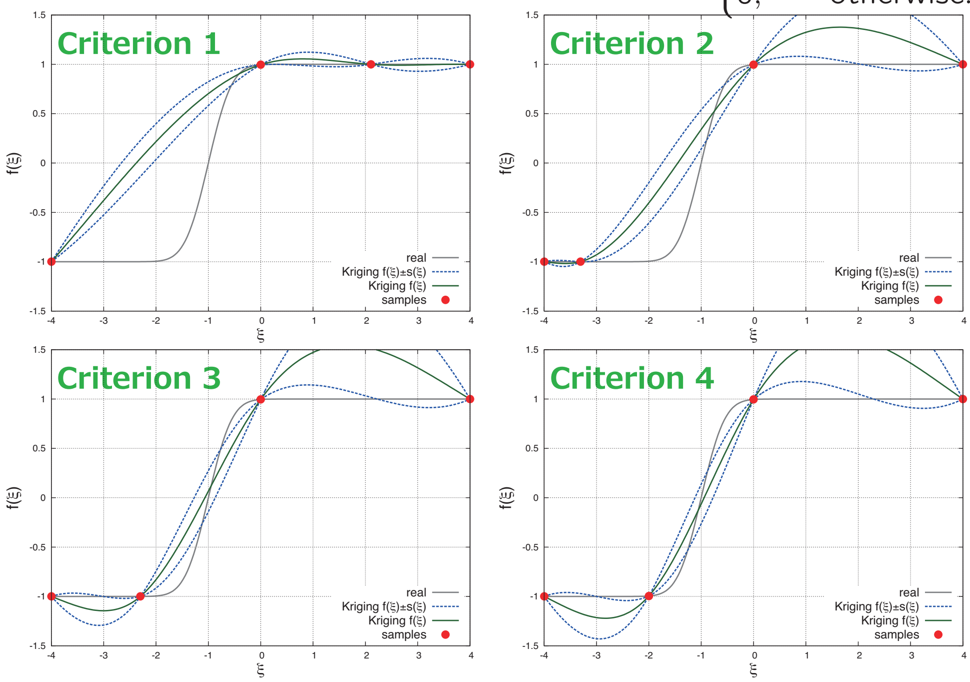
Numerical Tests (1D Funcs.)

4 samples

$$f(\xi) = \mathrm{erf}\left[2(\xi+1)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \leq \xi \leq 4, \\ 0, & \text{otherwise.} \end{cases}$$



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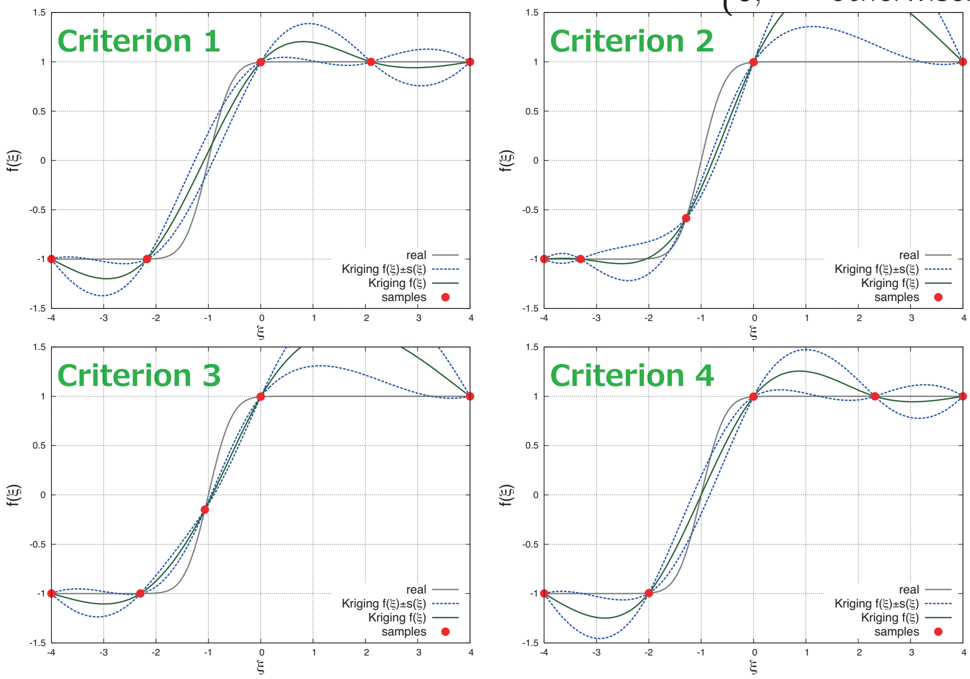
Numerical Tests (1D Funcs.)

5 samples

$$f(\xi) = \mathrm{erf}\left[2(\xi + 1)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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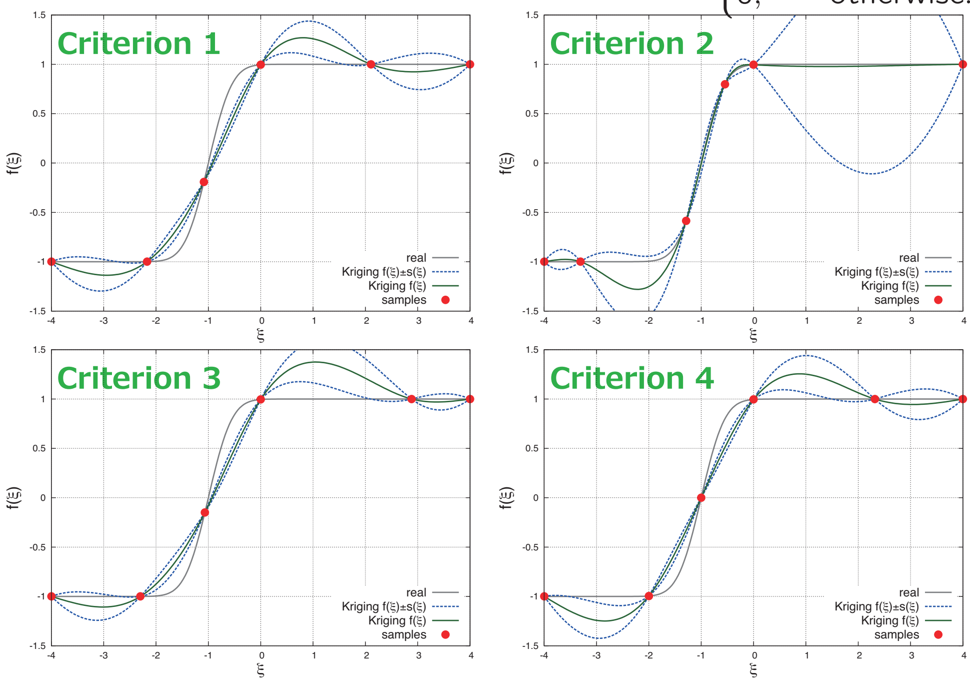
Numerical Tests (1D Funcs.)

6 samples

$$f(\xi) = \mathrm{erf}\left[2(\xi + 1)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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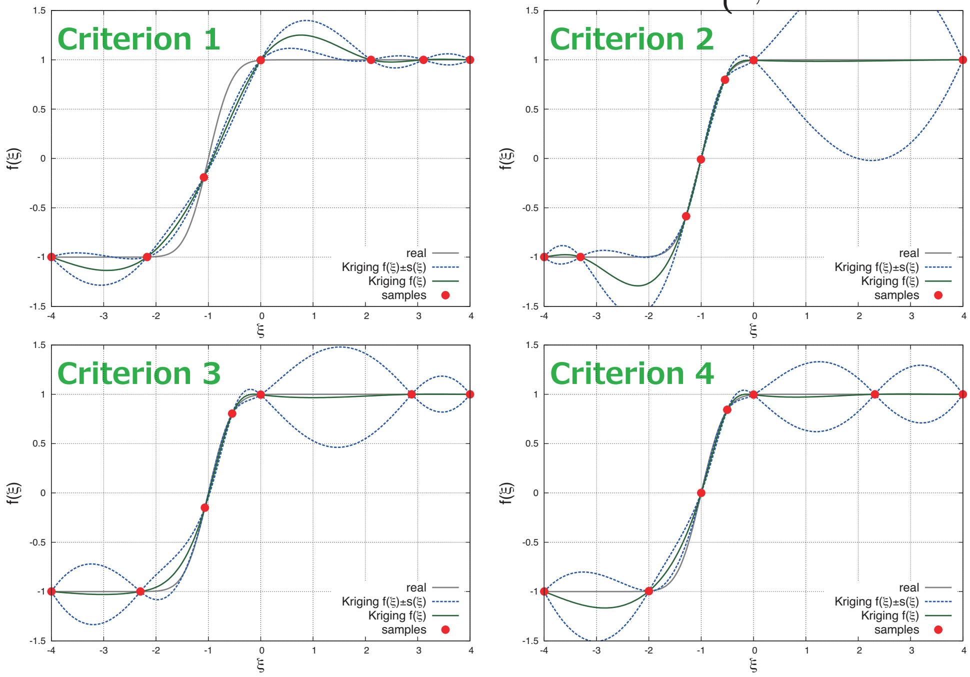
Numerical Tests (1D Funcs.)

7 samples

$$f(\xi) = \mathrm{erf}\,[2\,(\xi + 1)]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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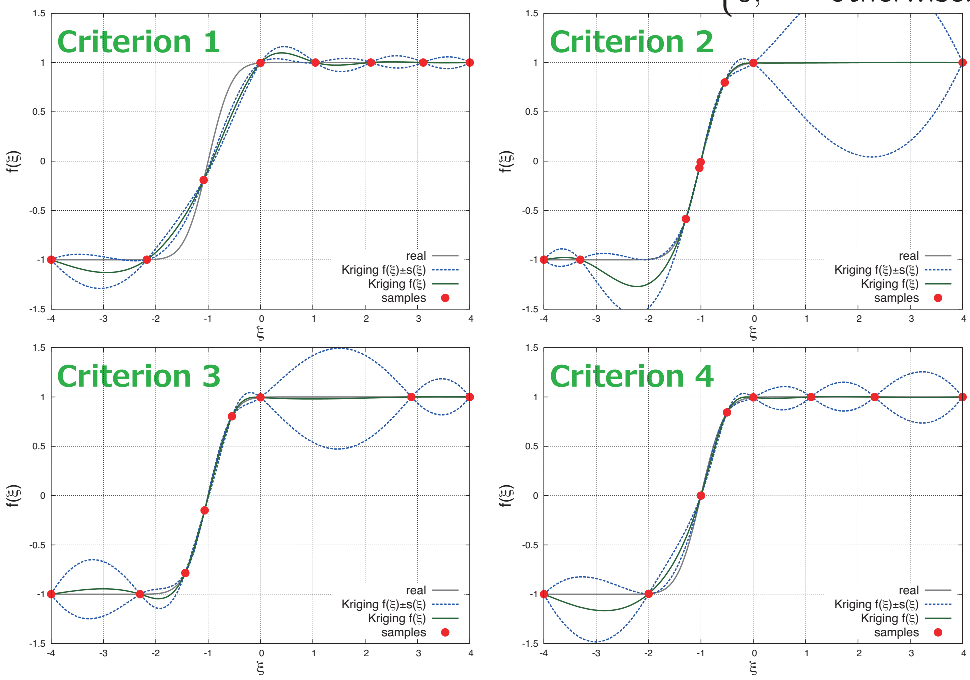
Numerical Tests (1D Funcs.)

8 samples

$$f(\xi) = \mathrm{erf}\,[2\,(\xi + 1)]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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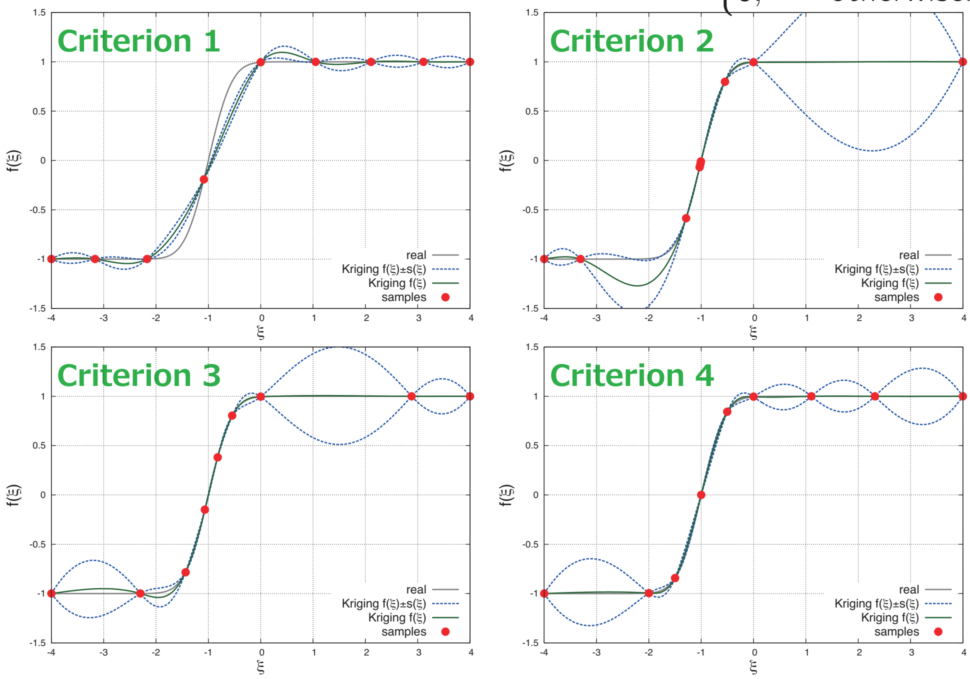
Numerical Tests (1D Funcs.)

9 samples

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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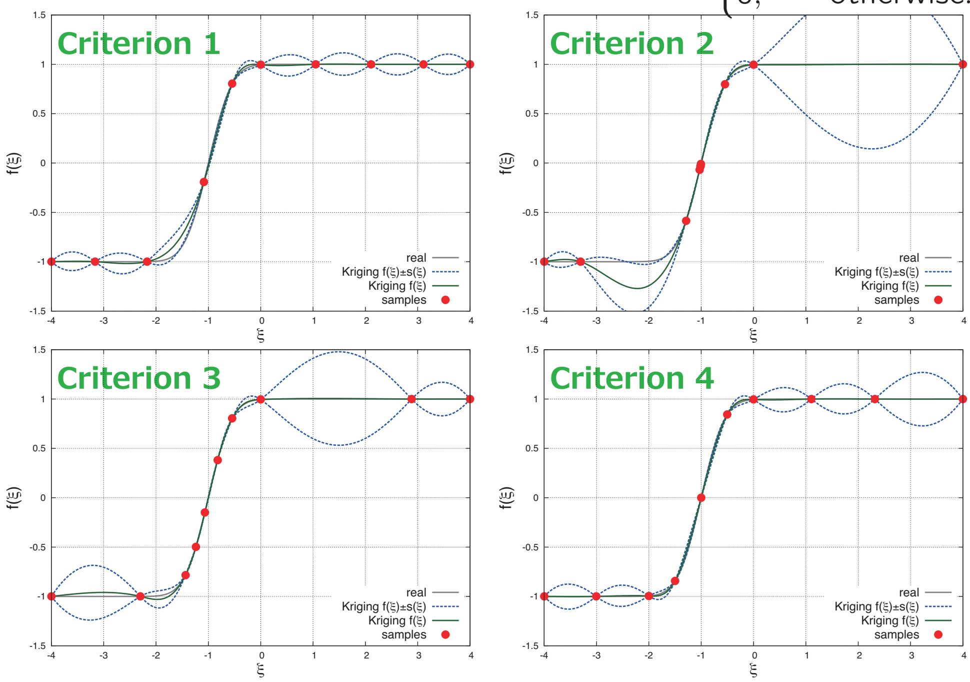
Numerical Tests (1D Funcs.)

10 samples

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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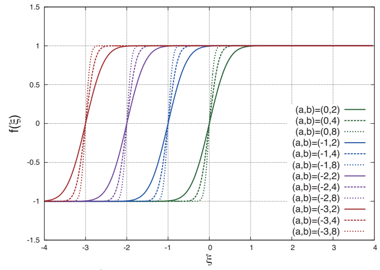
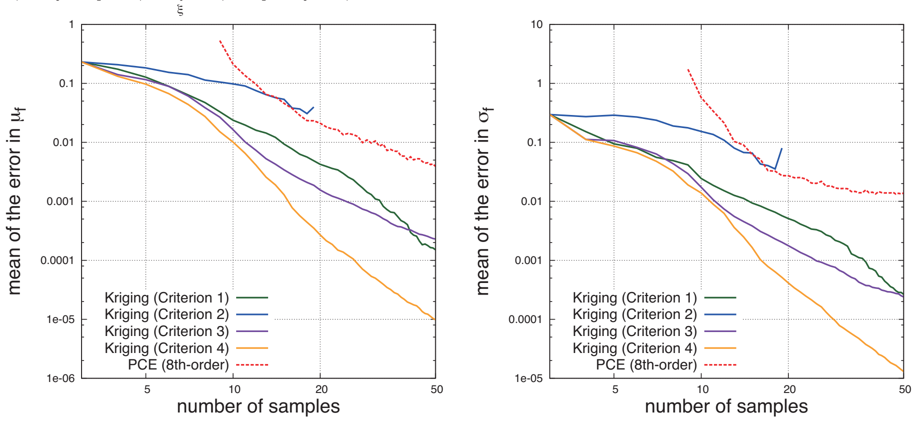
Numerical Tests (1D Funcs.)

Averaged on **30 trials from 3 initial samples (randomly generated)**
in **all cases (4 pos x 3 grad)**



$$f(\xi) = \mathrm{erf}\left[b\left(\xi - a\right)\right]$$

$$\mathrm{PDF}(\xi) = \begin{cases} 1/8, & \text{if } -4 \le \xi \le 4, \\ 0, & \text{otherwise.} \end{cases}$$



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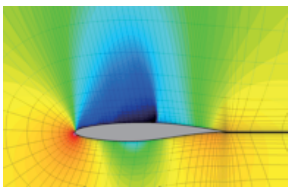
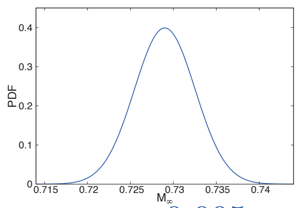
Application (Transonic Airfoil)

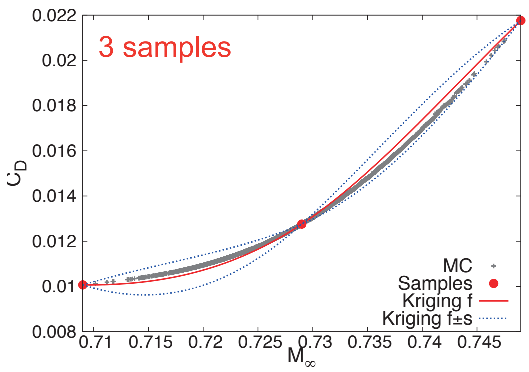


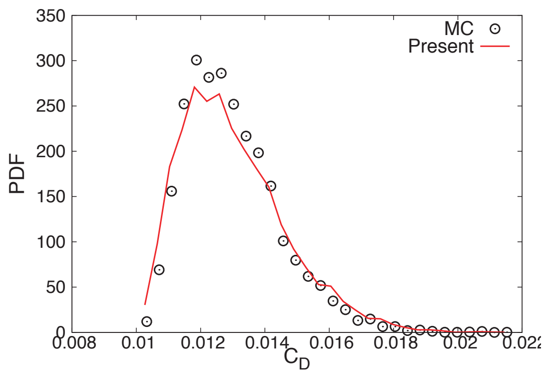
$M_\infty = 0.729$



$\sigma_M = 0.005$

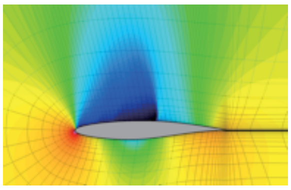
- 2D RANS (Baldwin-Lomax)
- $Re_c = 6.5 \times 10^6$
- $\alpha = 2.31$
- MC (10,000 pts.)





27

Application (Transonic Airfoil)



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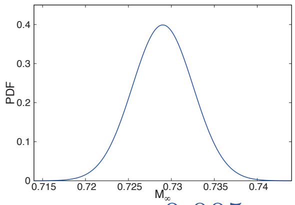

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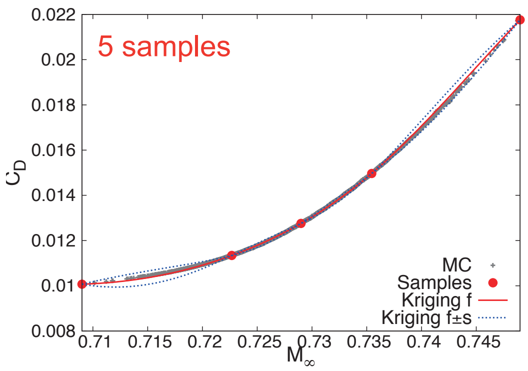

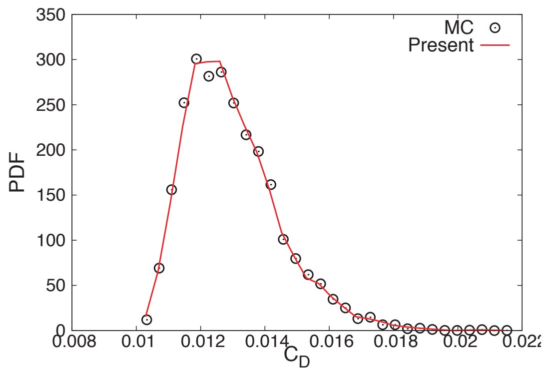

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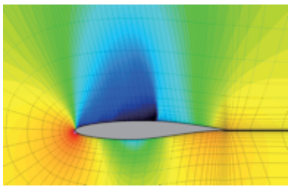
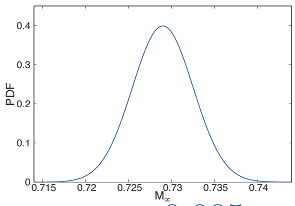
Application (Transonic Airfoil)



$M_\infty = 0.729$



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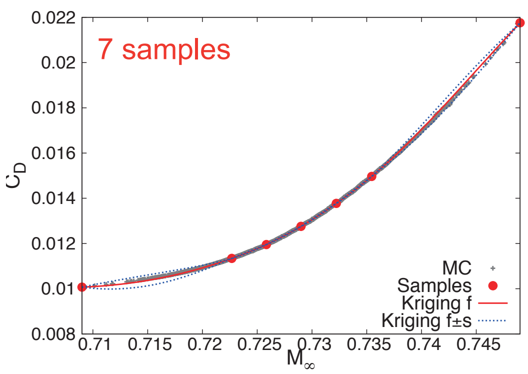

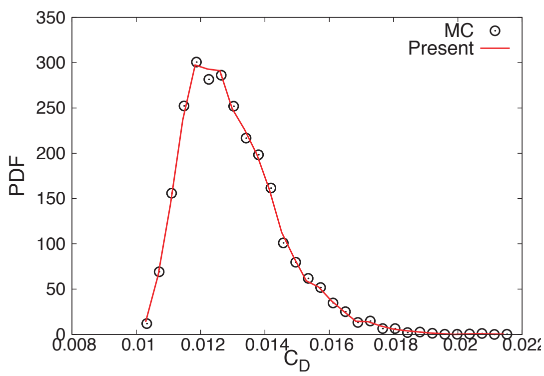

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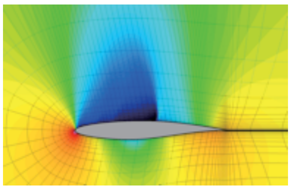
Application (Transonic Airfoil)



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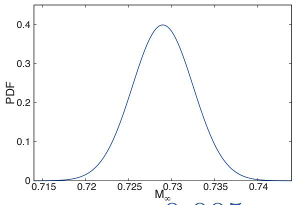

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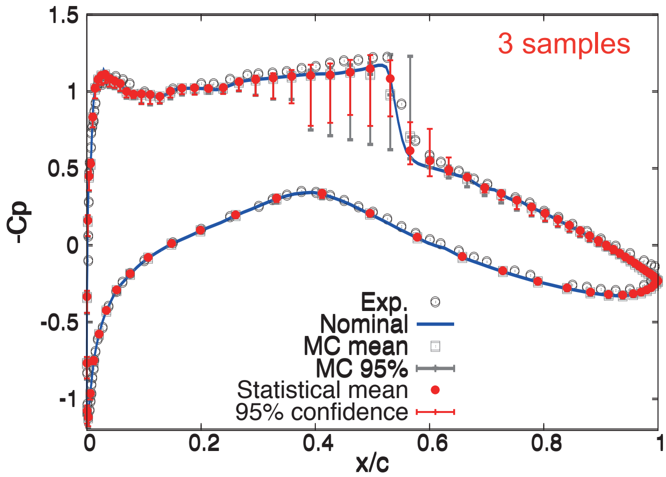

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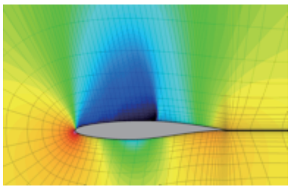
Application (Transonic Airfoil)



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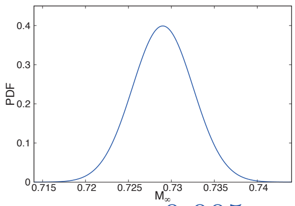

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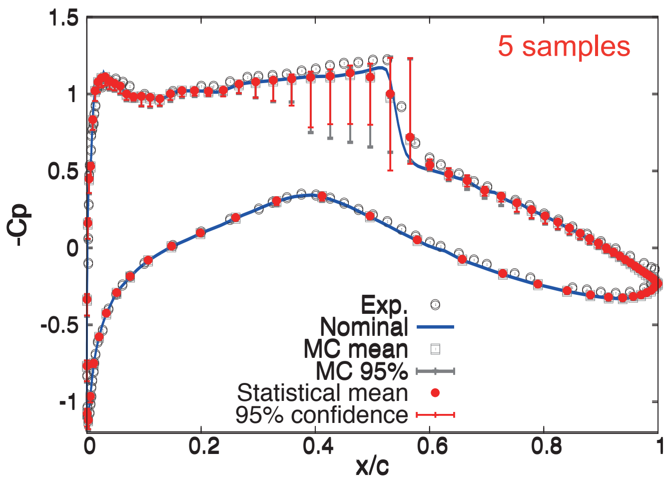

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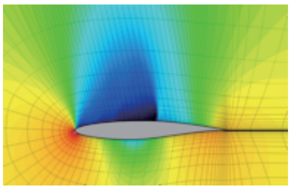
Application (Transonic Airfoil)



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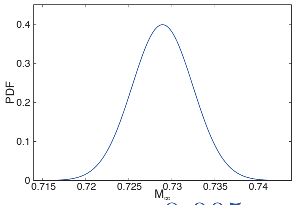

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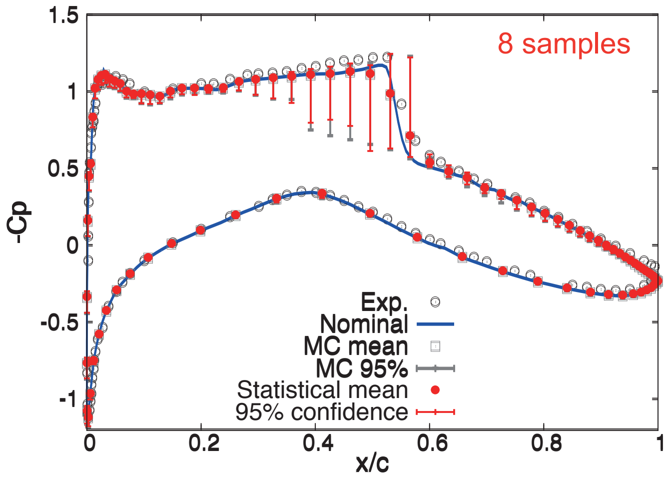

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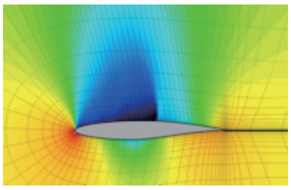
Application (Transonic Airfoil)



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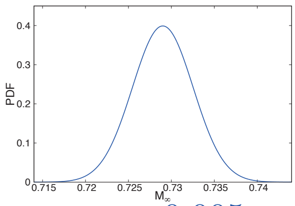

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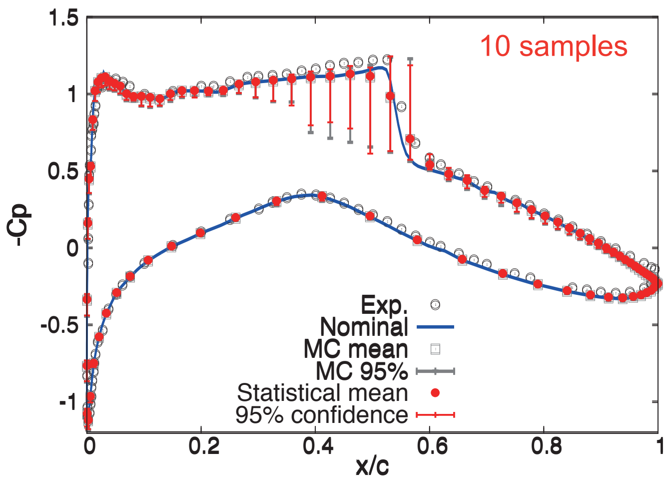

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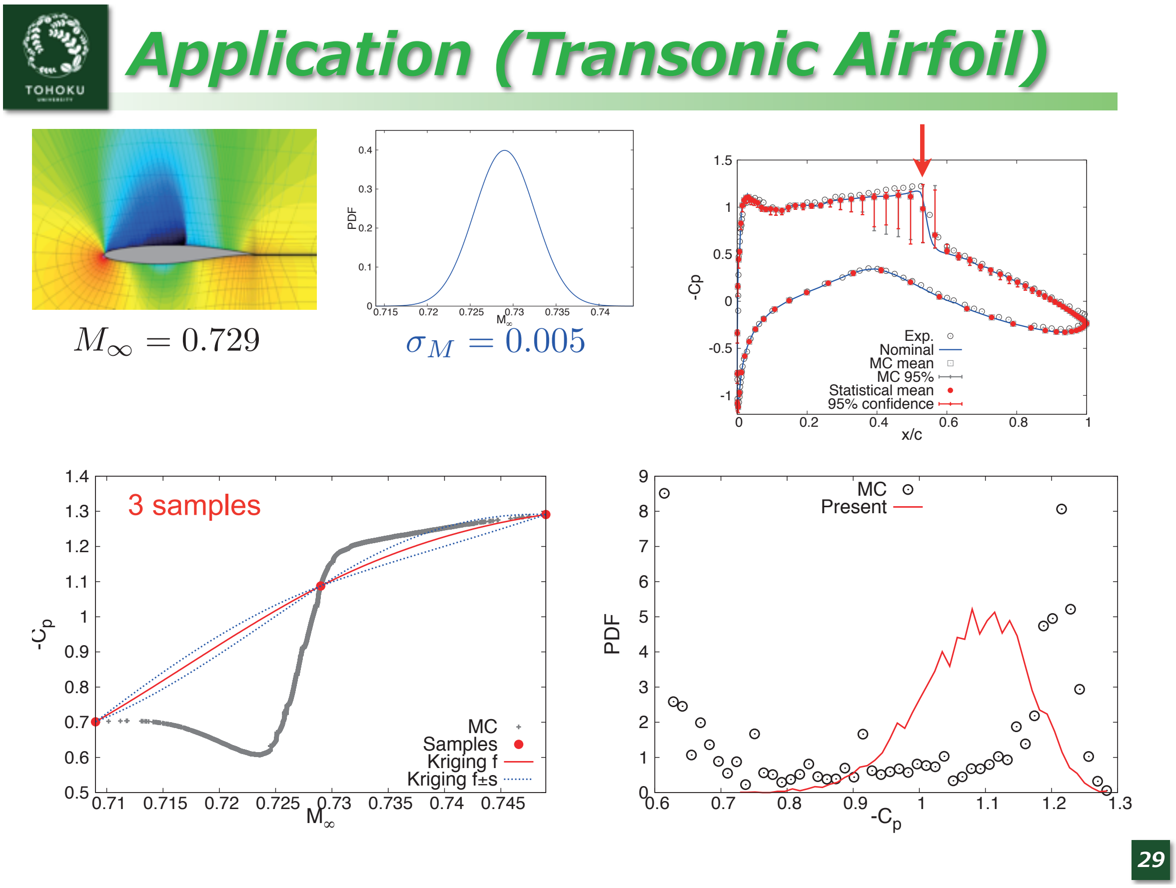
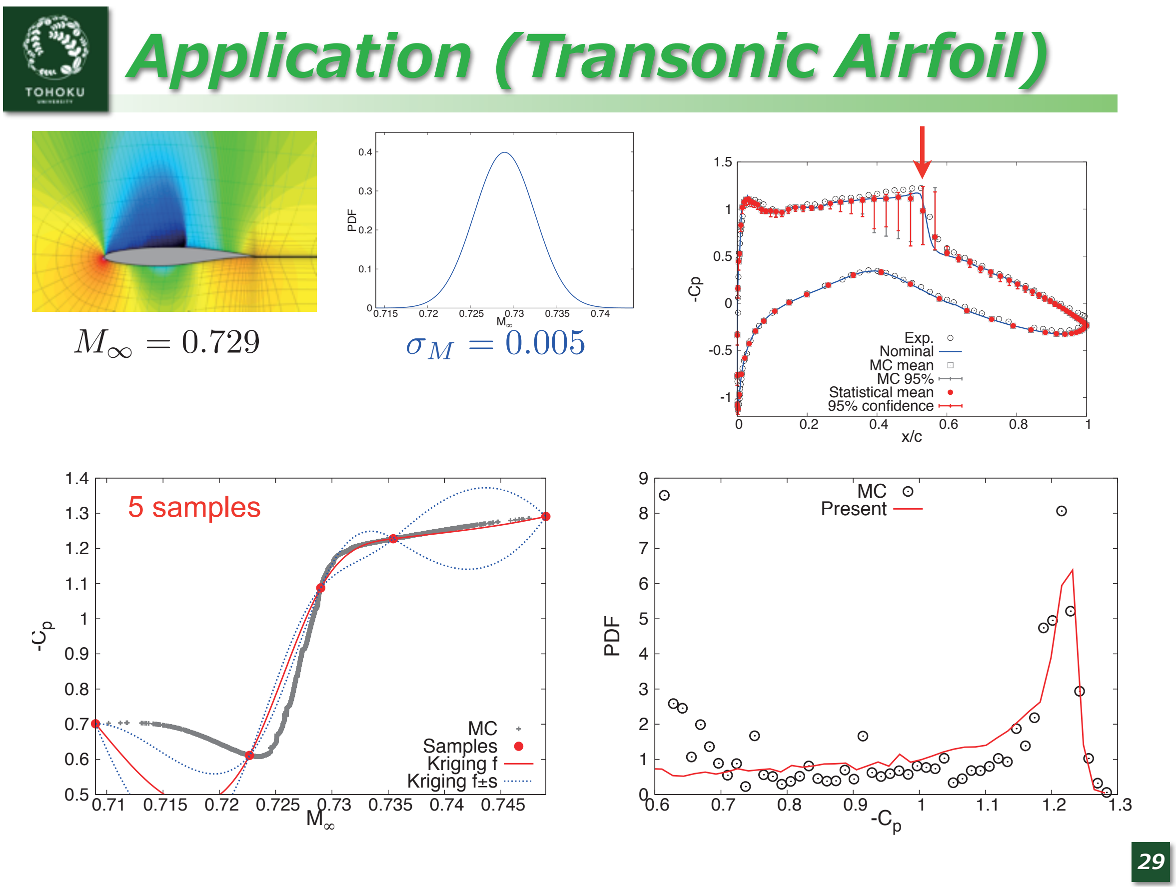
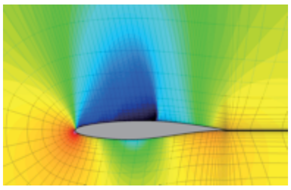

Application (Transonic Airfoil)
TOHOKU
M∞ = 0.729
PDF
σM = 0.005
-Cp
x/c
Exp.
Nominal
MC mean
MC 95%
Statistical mean
95% confidence
3 samples
-Cp
M∞
MC
Samples
Kriging f
Kriging f±s
PDF
-Cp
MC
Present
29


Application (Transonic Airfoil)
TOHOKU
M∞ = 0.729
PDF
σM = 0.005
-Cp
x/c
Exp.
Nominal
MC mean
MC 95%
Statistical mean
95% confidence
5 samples
-Cp
M∞
MC
Samples
Kriging f
Kriging f±s
PDF
-Cp
MC
Present
29

Application (Transonic Airfoil)



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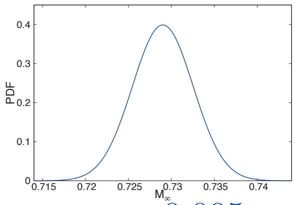

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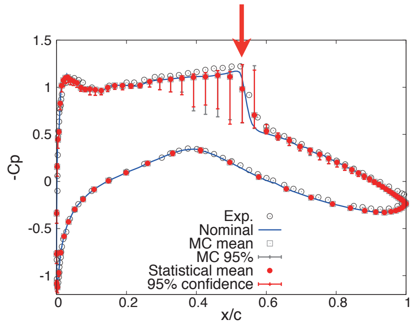

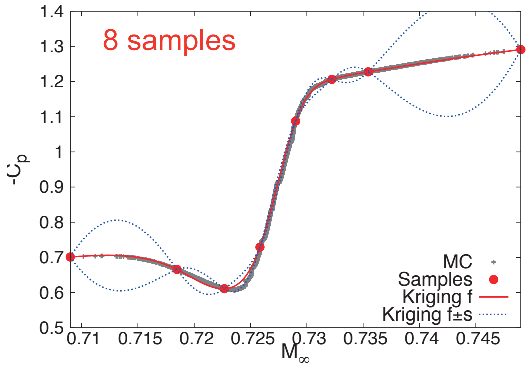

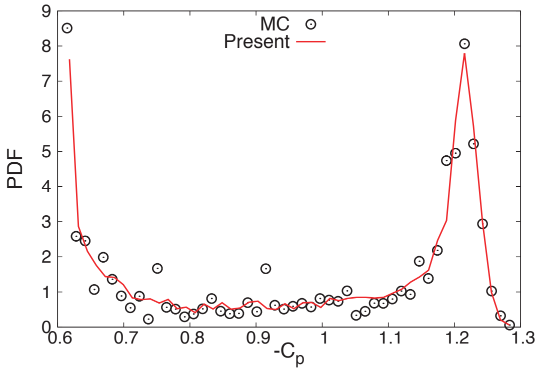

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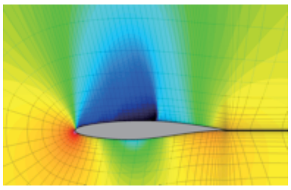

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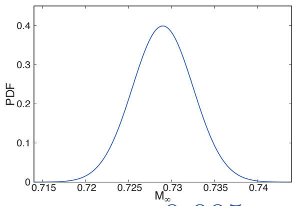

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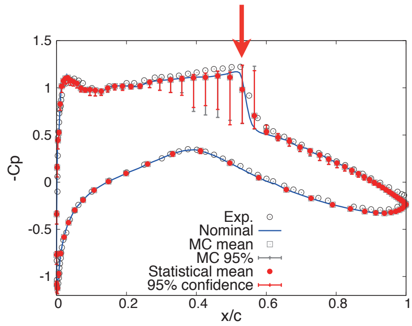

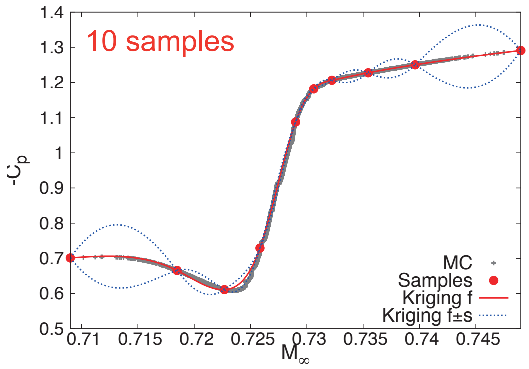

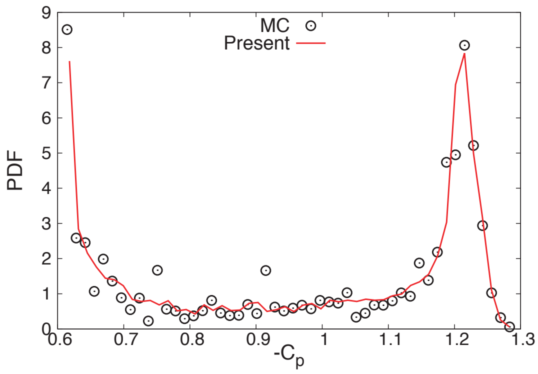

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Outline

- ✓ Fundamentals of Uncertainty Quantification
- ✓ Research Topics
  - ● Polynomial Chaos Expansion with Order Adjustment
    - ✳ Prof. Shigeru Obayashi (Tohoku Univ.)
    - ✳ Mr. Akihiro Inoue (Tohoku Univ.)
    - ✳ JAXA/NSRG
  - ● Dynamic Adaptive Sampling based on Kriging Surrogate Model
    - ✳ Dr. Soshi Kawai (JAXA/ISAS)
    - ✳ Prof. Juan J. Alonso (Stanford Univ.)
- ✓ **Summary & Future Work**

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Summary

✓ UQ is expected to contribute to the fields of simulation, physics, design, etc., but still has technical issues to be considered

✓ PCE can be well tuned through the order adjustment based on appropriate measures

✓ Kriging-based dynamic adaptive sampling can make UQ with discontinuity more effective

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Future Work

- ✓ Challenges for the curse of dimensionality
- ✓ Application to real-world simulation and design
- ✓ Contribution to EFC/CFD integration

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Acknowledgments

JSPS 独立行政法人 日本学術振興会 Japan Society for the Promotion of Science

- ✓ *Young Researcher Overseas Visits Program for Vitalizing Brain Circulation*
- ✓ *Grant-in-Aid for Young Scientists (B)*

JAXA 宇宙航空研究開発機構 Japan Aerospace Exploration Agency

- ✓ *International Top Young Fellowship Program*

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