# Gradient-enhanced least-square Polynomial Chaos expansions in uncertainty quantification and robust optimization

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AIAA AVIATION Forum and Exposition, 2-6 August 2021



This project has received funding from the European Union's Horizon 2020
research and innovation programme under grand agreement N. 769025 (MADELEINE)

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# Polynomial Chaos Expansion – General Introduction


$$f(\mathbf{x}) \approx \sum_{j=1}^{n} k_j \psi_j(\mathbf{x})$$

| | |
|---|---|
| $f$ | quantity of interest (qoi) |
| $\mathbf{x}$ | vector of uncertain variables with given probability density functions (pdfs) |
| $\psi_j$ | orthogonal (or orhonormal) polynomials |

**KNOWN**

| | |
|---|---|
| $k_j$ | coefficients of the expansion |

**TO BE ESTIMATED**

# Polynomial Chaos Expansion – Estimation of Coefficients

How can we calculate the coefficients of the expansion?

1) QUADRATURE

2) REGRESSION

$$\boxed{\tilde{\mathbf{k}} = \underset{\mathbf{k}}{\operatorname{argmin}} \|\boldsymbol{A}\mathbf{k} - \mathbf{b}\|_2 .}$$

where

$$\boldsymbol{A}_{\mathcal{F}}(i, \boldsymbol{j}) = \omega_i \boldsymbol{\psi}(\boldsymbol{x}_i), \qquad \boldsymbol{j} \in \mathcal{J}, \;\; i = 1, \ldots, r,$$

$$\mathbf{b}_{\mathcal{F}}(i) = \omega_i f(\boldsymbol{x}_i), \qquad i = 1, \ldots, r,$$

$\boldsymbol{A}$ and $\mathbf{b}$ are obtained from $\boldsymbol{A}_{\mathcal{F}}$ and $\mathbf{b}_{\mathcal{F}}$ with some appropriate methodology.

# Polynomial Chaos Expansion – Gradient Enhancement

What if we have gradient information (i.e. coming from an adjoint solver)?

APPROACH 1: (STACKED) We can increment our least square approximation using the derivative information

$$\boxed{\tilde{\mathbf{k}} = \underset{\mathbf{k}}{\operatorname{argmin}} \left\| \begin{pmatrix} \boldsymbol{A} \\ \boldsymbol{C} \end{pmatrix} \mathbf{k} - \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \end{pmatrix} \right\|_2 ,}$$

$$\boldsymbol{C}_{\mathcal{F}}^{(k)}(i,\boldsymbol{j}) = \frac{\partial \psi(\boldsymbol{x_i})}{\partial x^{(k)}}, \qquad \boldsymbol{j} \in \mathcal{J}, \quad i = 1, \ldots, r, \qquad \boldsymbol{C}_{\mathcal{F}} = \begin{pmatrix} \boldsymbol{C}_{\mathcal{F}}^{(1)} \\ \vdots \\ \boldsymbol{C}_{\mathcal{F}}^{(d)} \end{pmatrix} \quad \text{and} \quad \mathbf{d}_{\mathcal{F}} = \begin{pmatrix} \mathbf{d}_{\mathcal{F}}^{(1)} \\ \vdots \\ \mathbf{d}_{\mathcal{F}}^{(d)} \end{pmatrix},$$

$$\mathbf{d}_{\mathcal{F}}^{(k)}(i) = \frac{\partial f(\boldsymbol{x}_i)}{\partial x^{(k)}}, \qquad i = 1, \ldots, r,$$

Similarly to $\mathbf{A}$ and $\mathbf{b}$, $\mathbf{C}$ and $\mathbf{d}$ can be determined from $\boldsymbol{C}_{\mathcal{F}}$ and $\mathbf{d}_{\mathcal{F}}$ by subsampling the quadrature points, following a given heuristic.

# Polynomial Chaos Expansion – Gradient Enhancement

What if we have gradient information (i.e. coming from an adjoint solver)?

APPROACH 2:
NULL-SPACE

We can approach the task of determining the coefficient of the expansion as an equality constrained optimization problem:

$$\tilde{\mathbf{k}} = \underset{\mathbf{k}}{\operatorname{argmin}} \quad \|\boldsymbol{C}\mathbf{k} - \mathbf{d}\|_2 \,.$$
$$\text{subject to} \quad \boldsymbol{A}\mathbf{k} = \mathbf{b}.$$

With this approach, we assume that the qoi information (coming from the direct solver) is more reliable than the gradient information (coming from the adjoint solver) as this often contains a larger degree of noise. The above mathematical problem can be solved using the null-space method from Bjork ("Numerical methods in matrix computations", Springer 2015)

# Verification – Simple test case

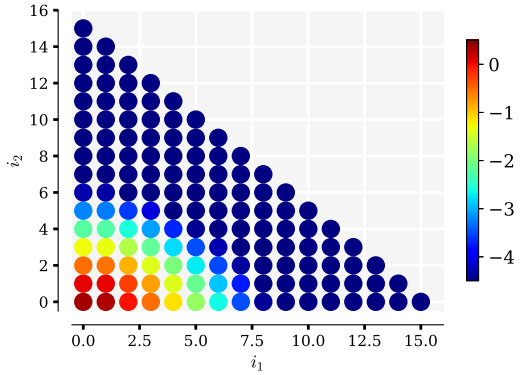
$$f(x_1, x_2) = exp(2x_1 + x_2)$$

$$\nabla f = \begin{pmatrix} 2exp(2x_1 + x_2) + \kappa \\ exp(2x_1 + x_2) + \kappa \end{pmatrix}.$$

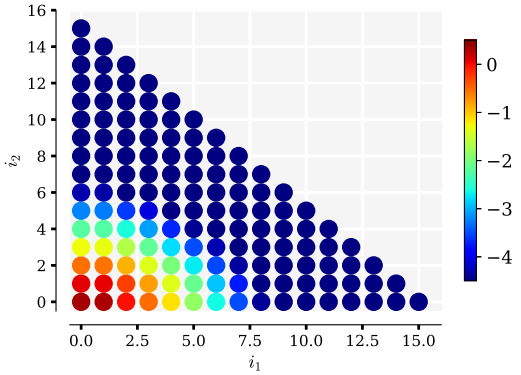
$x_1 = \mathcal{U}[-1:1]$, $x_2 = \mathcal{U}[-1:1]$, $\kappa$ is random (white) noise of different levels. We use a 15th order Polynomial Chaos expansion.

$\kappa = 0$

STACKED




NULL-SPACE



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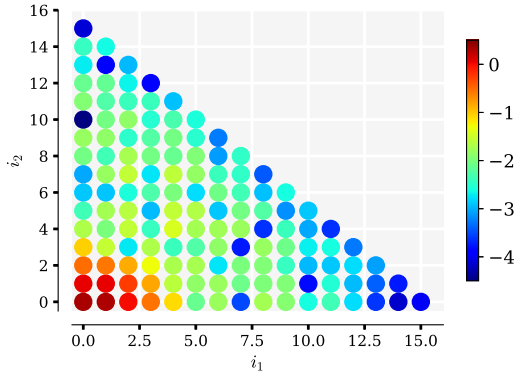
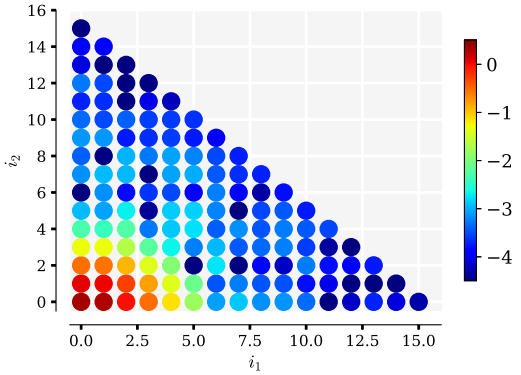
$\kappa = \mathcal{N}(0, 0.01)$

STACKED




NULL-SPACE

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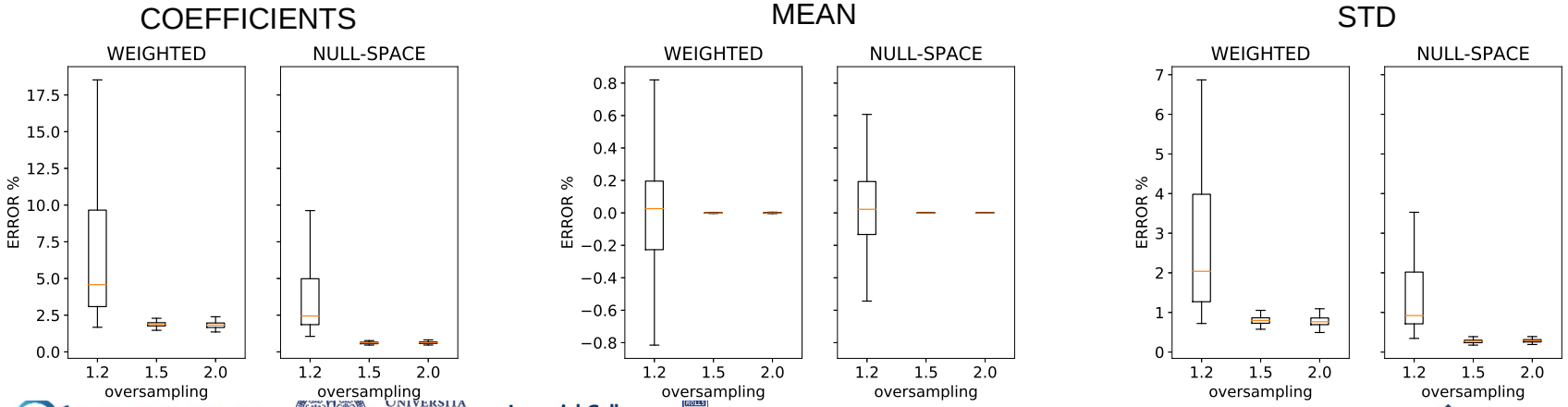




MADELEINE

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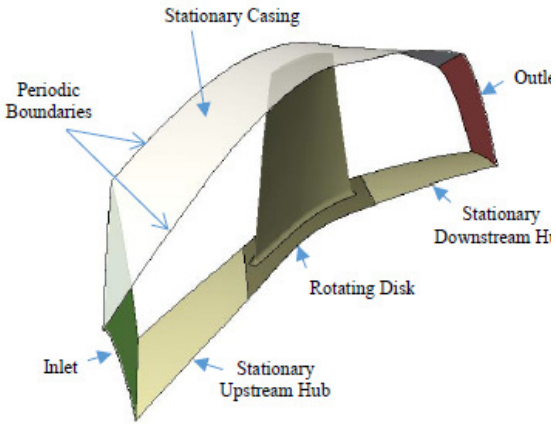
AIAA SHAPING THE FUTURE OF AEROSPACE

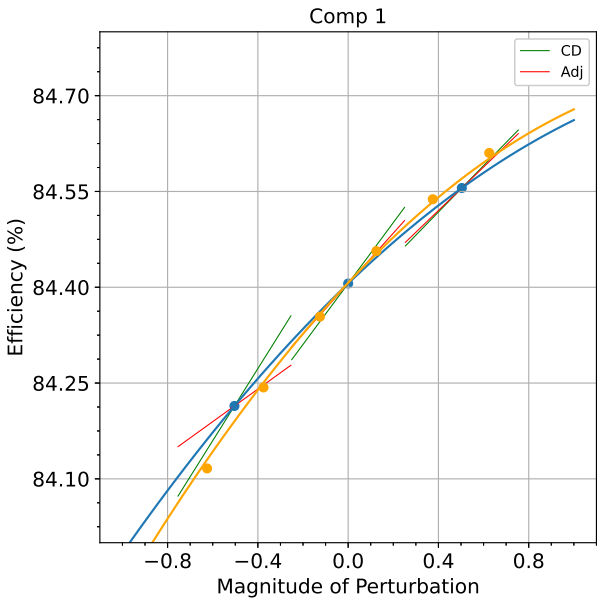
# Verification – Real Case (Rotor37)




- qoi: adiabatic efficiency
- 5 uncertain variables (tangential stacking)

4 METHODS
- SGNI (sparse grid numerical integration) 2nd order
- SGNI-G (SGNI, with gradient) 1st o.
- LSA-G (least-square approx. with gradient, stacked) 2nd o.
- LSA-G-NS (least-square approx with gradient, null-space) 2nd o.

Example of typical noisy gradients:



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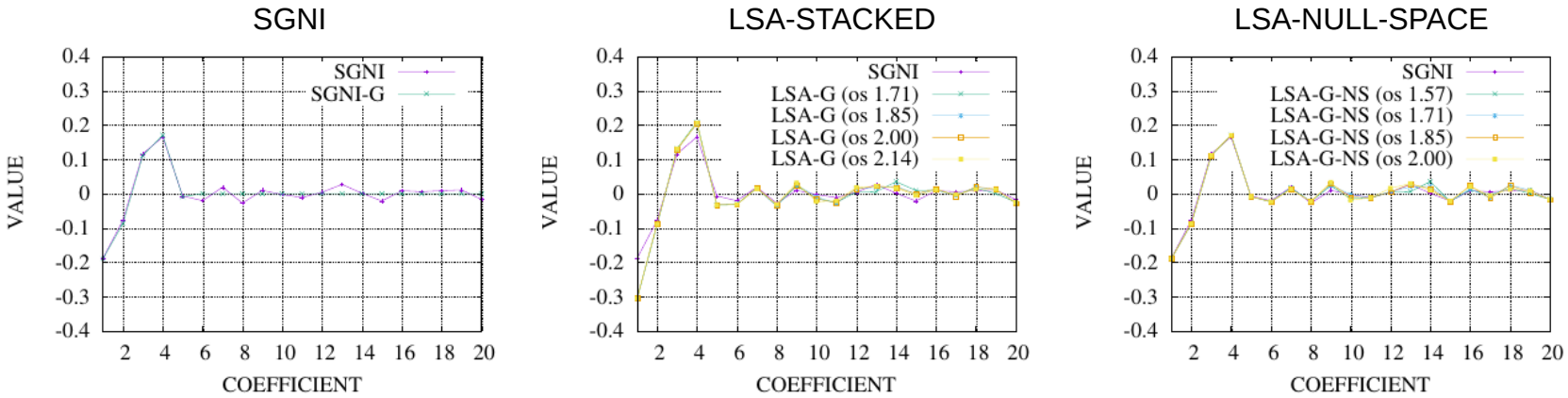


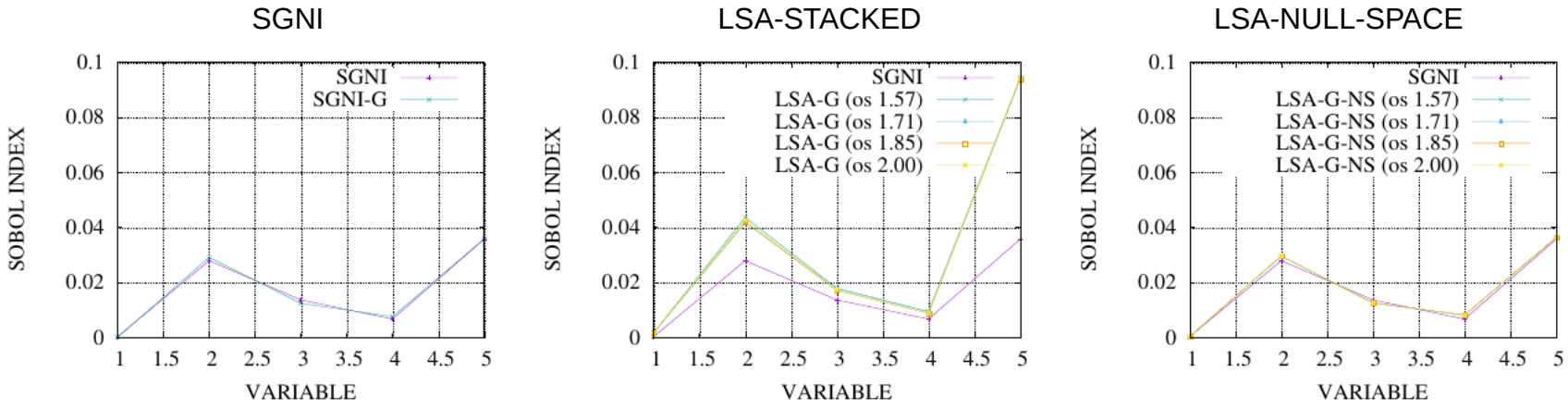

(a) 2nd-order SGNI withtout gradients vs 1st-order SGNI-G with gradients

(b) 2nd-order SGNI withtout gradients vs 2nd-order LSA-G with gradients

(c) 2nd-order SGNI withtout gradients vs 2nd-order LSA-G-NS with gradients

**Fig. 9 Polynomial Chaos expansion coefficients comparison using different methodologies. LSA approaches are tested with different levels of oversampling (o-s)**

# Verification – Real Case (Rotor37)



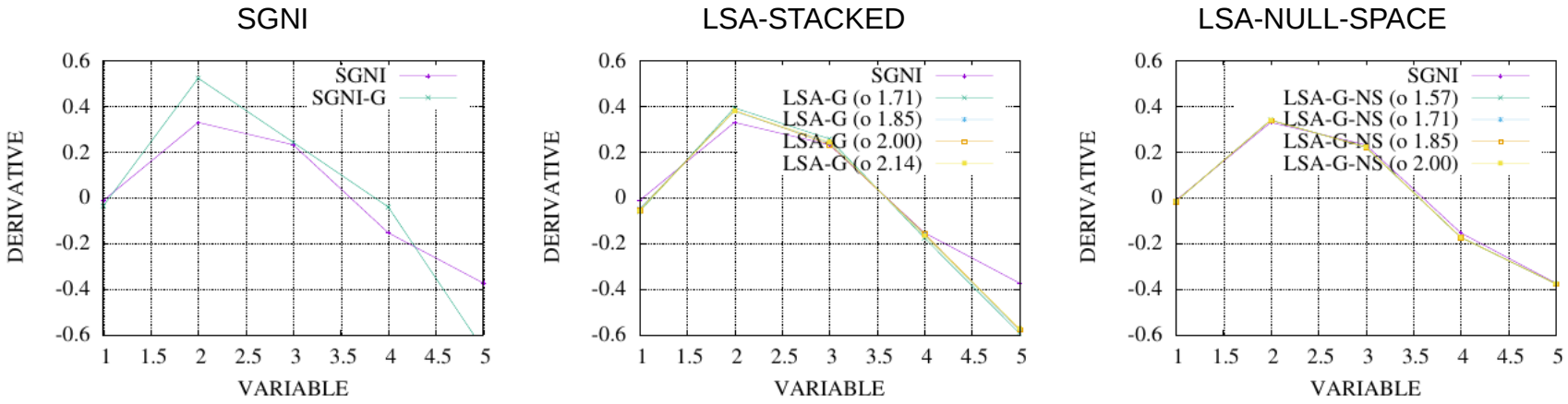

(a) 2nd-order SGNI withtout gradients vs 1st-order SGNI with gradients

(b) 2nd-order SGNI withtout gradients vs 2nd-order LSA with gradients

(c) 2nd-order SGNI withtout gradients vs 2nd-order LSA-NS with gradients

**Fig. 10 Sobol indices comparison using different methodologies. LSA approaches uare tested with different levels of oversampling (o-s)**

# Verification – Real Case (Rotor37)



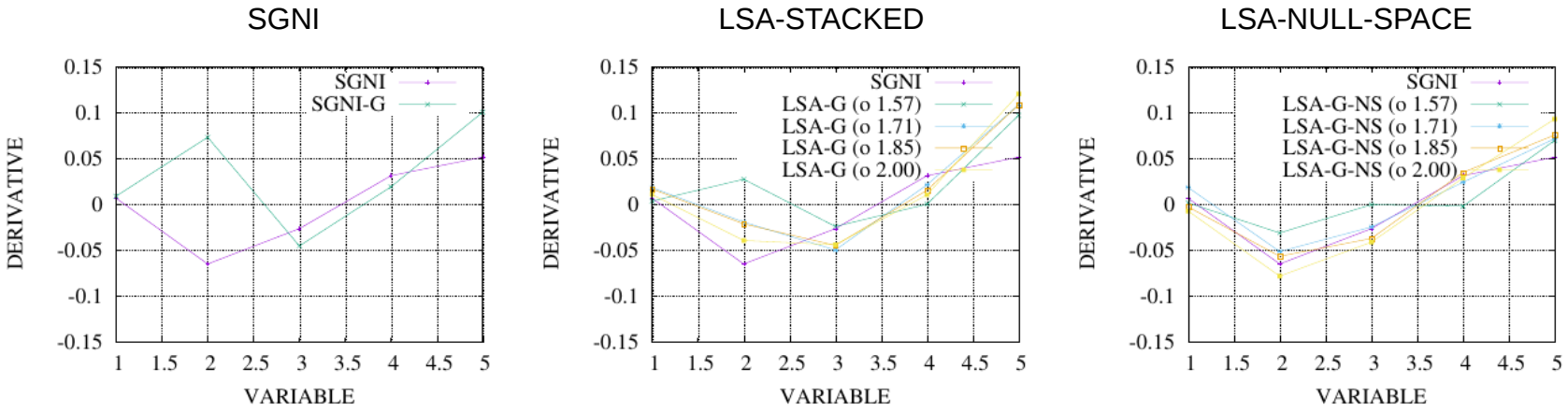

(a) 2nd-order SGNI withtout gradients vs 1st-order SGNI with gradients

(b) 2nd-order SGNI withtout gradients vs 2nd-order LSA with gradients

(c) 2nd-order SGNI withtout gradients vs 2nd-order LSA-NS with gradients

**Fig. 11 Gradient of the mean: comparison using different methodologies. LSA approaches uare tested with different levels of oversampling (o-s)**

# Verification – Real Case (Rotor37)



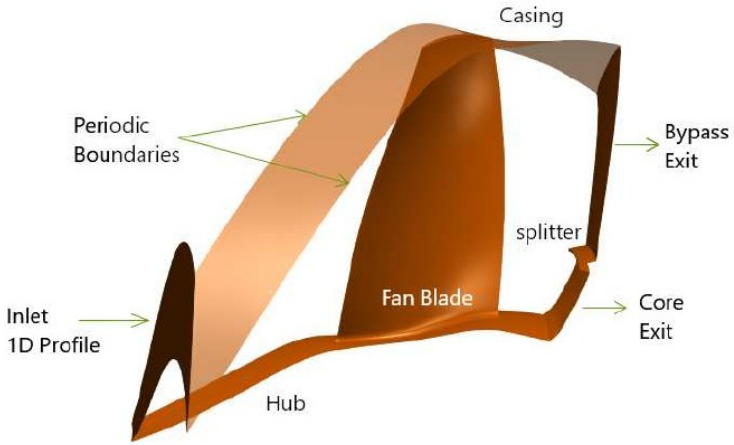

(a) 2nd-order SGNI withtout gradients vs 1st-order SGNI with gradients

(b) 2nd-order SGNI withtout gradients vs 2nd-order LSA with gradients

(c) 2nd-order SGNI withtout gradients vs 2nd-order LSA-NS with gradients

**Fig. 12 Gradient of the standard deviation: comparison using different methodologies. LSA approaches uare tested with different levels of oversampling (o-s)**

# Application – Robust Optimisation of Vital Fan




MEAN EFFICIENCY

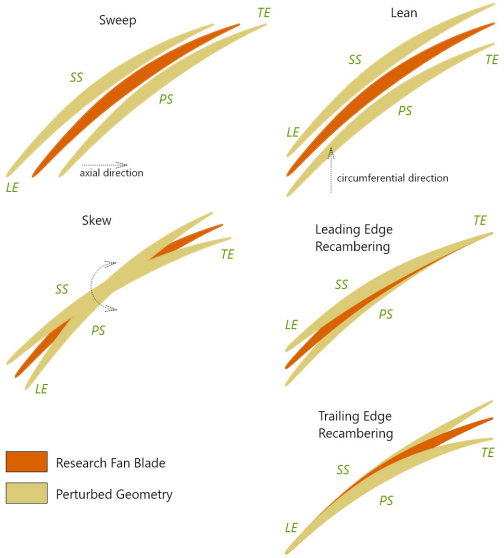
EFFICIENCY' STD

$$\underset{\mathbf{x}}{\text{minimize}} \quad \{-\mu(\eta(\mathbf{x},\omega)), \sigma(\eta(\mathbf{x},\omega))\}$$

$\mathbf{x} \in \chi \subseteq \mathbb{R}^m$ ⟶ DESIGN VARIABLES

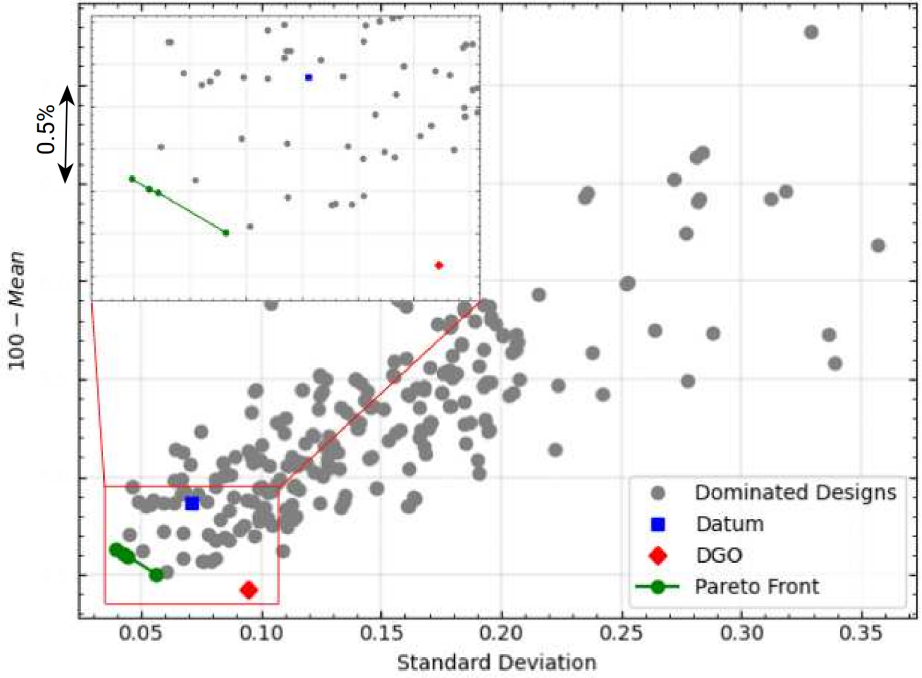
$\omega \in \Omega \subseteq \mathbb{R}^k$ ⟶ UNCERTAINTIES

$$\text{subject to} \quad 0.99\, PR_{datum} \leq PR(\mathbf{x}) \leq 1.05\, PR_{datum}$$



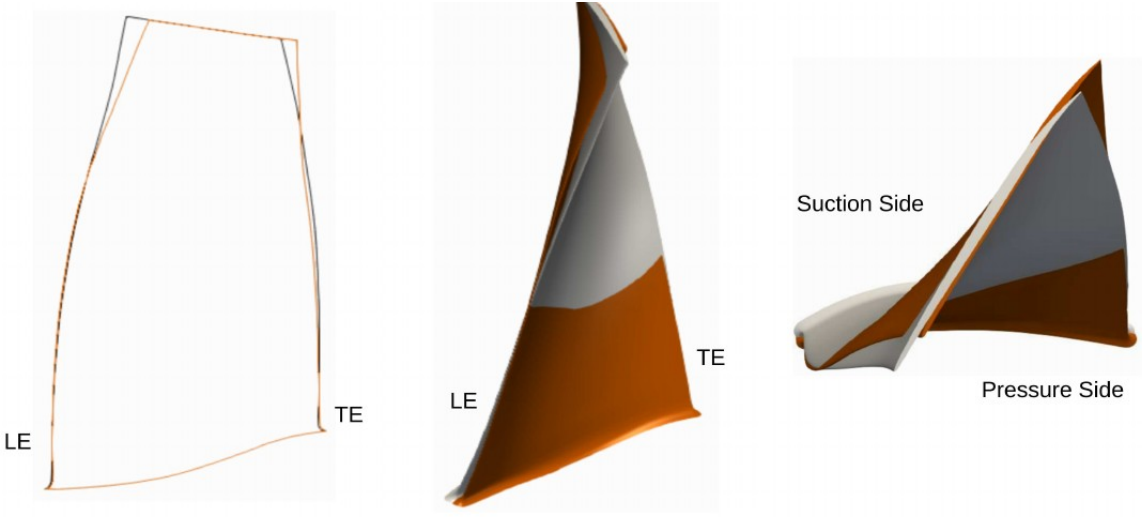

35 design variables
25 uncertainties

# Application – Robust Optimisation of Vital Fan



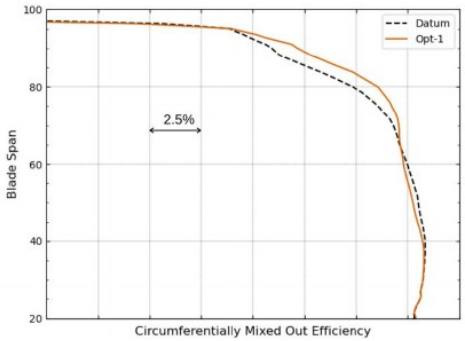

DGO = DETERMINISTIC GLOBAL OPTIMUM

# Application – Robust Optimisation of Vital Fan

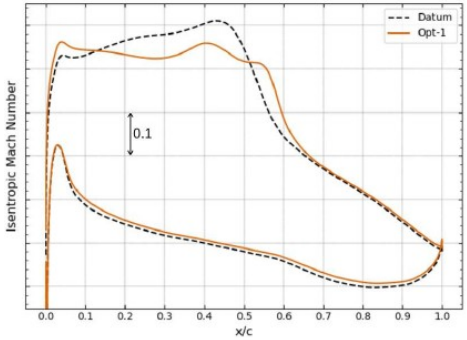



(a) Meridional View (b) Isometric View (c) View From the Top

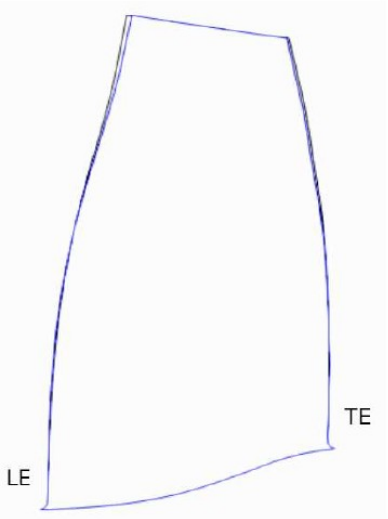
EFFICIENCY



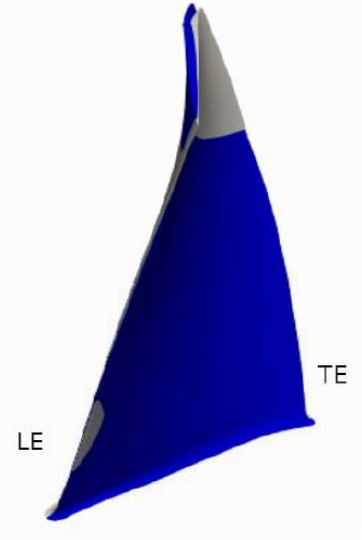

IS. MACH NUMBER 80% SPAN



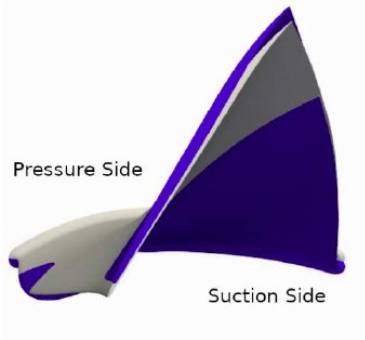
# Application – Robust Optimisation of Vital Fan




(a) Meridional View

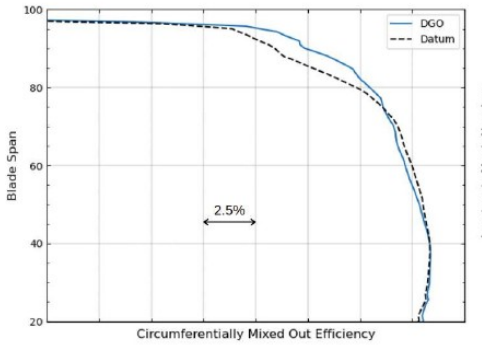


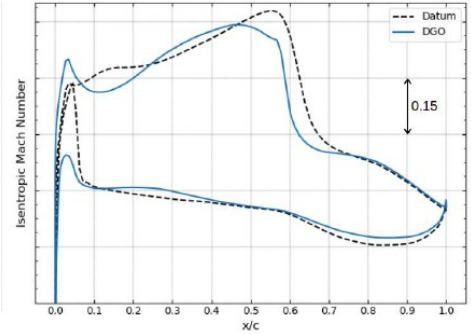

(b) Isometric View




(c) View From the Top

EFFICIENCY



# Conclusion

- We have presented an approach for constructing Polynomial Chaos approximations using gradient information
- The approach is more robust to noise in the gradients
- Its applicability has been demonstrated through test-cases of increasing complexity
- … and it has been applied to the robust optimisation of a a high-efficiency research fan blade

# Acknowledgments


- This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 769025 (MADELEINE)
- The authors would like to express their gratitude to Rolls-Royce plc. For their support and permission to publish the work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