



Dassault +SUPAERO meeting

Prof. J. Morlier

Institut Supérieur de l'Aéronautique et de l'Espace



Facilities

INSTITUT CLÉMENT ADER
Université Toulouse Midi-Pyrénées / UMR CNRS 5312
3 rue Camille Aigle
31400 Toulouse, France

Structures

- L'Institut Clément Ader
- Groupe MS2M
- Groupe MSC
- Groupe MICS
- Groupe SUHO
- Axes transverses
- Antennes

Actualités

Bienvenue sur le site de l'**Institut Clément Ader (ICA, CNRS UMR 5312)**. L'ICA est un laboratoire de recherche qui s'attache à l'étude des **structures**, des **systèmes** et des **procédés mécaniques**. Nos secteurs d'activités s'inscrivent dans ceux des industries mécaniques avec une attention particulière accordée aux projets des domaines de l'**aéronautique**, de l'**espace**, du **transport** et de l'**énergie**. Nos travaux portent généralement sur la **modélisation du comportement**, l'**instrumentation** et l'**étude de la durabilité** des structures ou produits considérés. Une part importante de nos recherches porte sur les **matiériaux composites**, lesquels prennent aujourd'hui une place importante dans les structures.

Calendrier des événements scientifiques

Consulter le calendrier de l'ICA > tous les événements

Master Recherche @ ICA

Master SHMS

Master DET

Info pratiques

Page d'accueil

Offres d'emploi

Contact et Accès

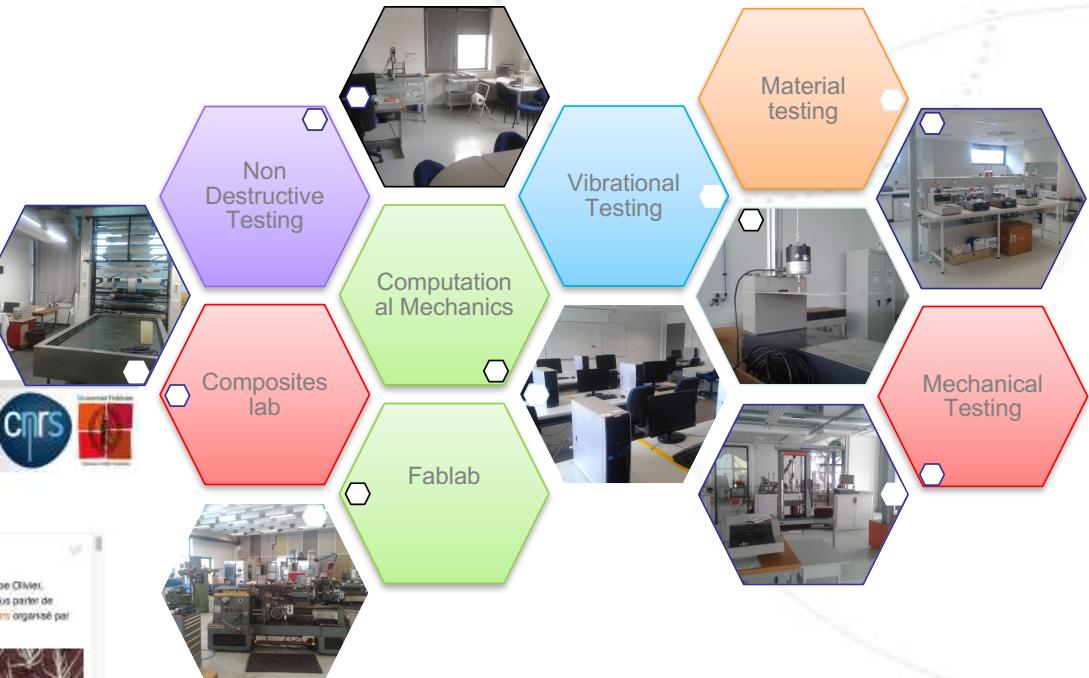
ICA France
ICA, France

Le 16 juil. vendredi écouter Philippe Oliver, Directeur de l'ICA France, nous parler de l'avenir du futur au #ForondaCm organisé par ICNIRBM.

QUE RESTE-T-IL À DÉCOUVRIR ?

16-18 JUILLET 2018 TOULOUSE

> tous les articles



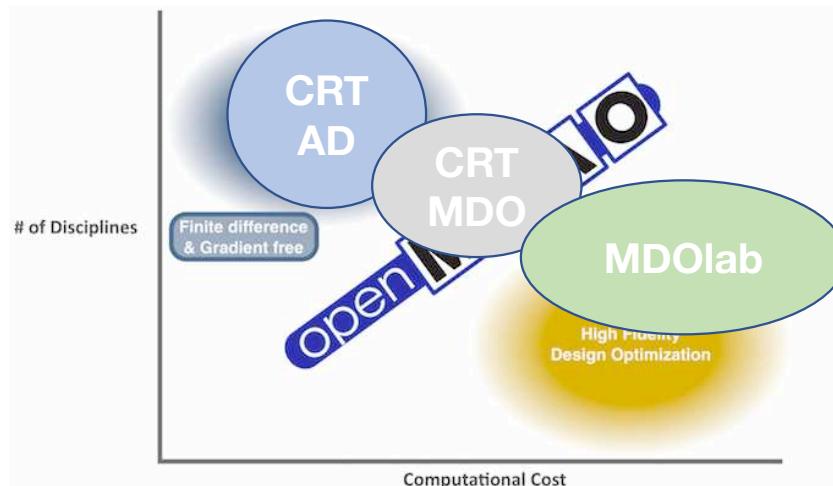
Currently I'm working on the fields:

- MDO, Topology optimization, surrogate modeling, machine learning applied to aircraft,

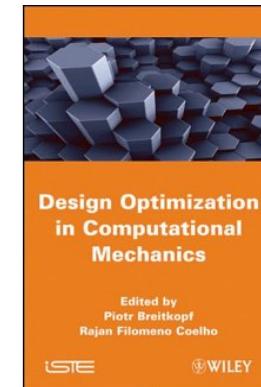
But in the past

- SHM, composites structures, system identification, Neural networks applied to aircraft

Common Research Team (ONERA-SUPAERO) : New in 2015



MDO Workshop@DLR



Started in 2007 with
Manuel Samuelides &
Nathalie Bartoli

Our Goals

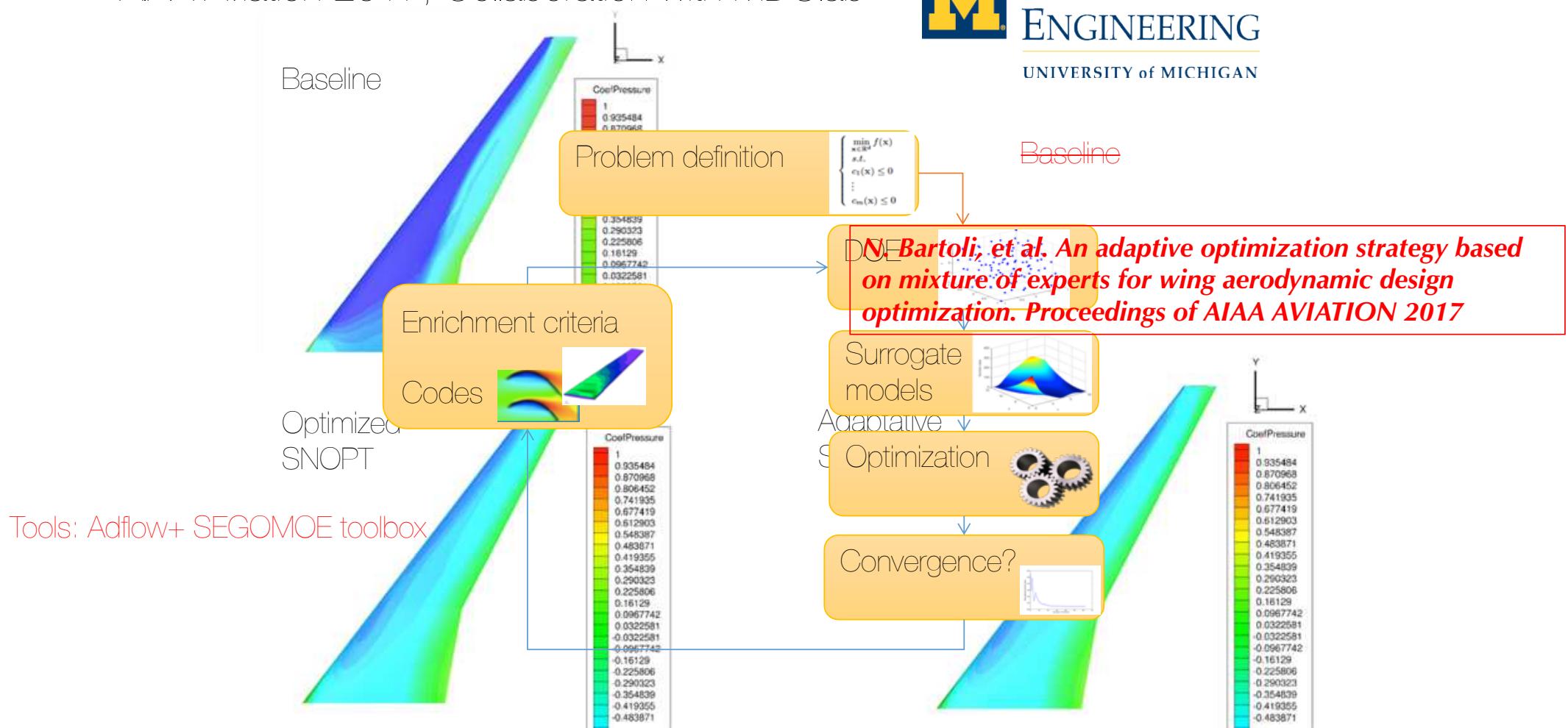
- Reduce in a « smart way » the computation time of optimization for coupled simulations
- Global Optimization using surrogate modeling → fixed budget (enriching process)
- Specialized surrogates for HD (engineering) problems and UQ
- Taking into account different levels of fidelity

N. Bartoli et al, Improvement of efficient global optimization with mixture of experts: methodology developments and preliminary results in aircraft wing design, Proceedings of AIAA 2016

- Methods applied to AD Aircraft Design,: Put the aircraft structure / aeroelasticity in the loop at the early stage of MDO process
- compatible with



AIAA Aviation 2017, Collaboration with MDOlab



Outlines

1. Overview of Machine learning techniques
2. Aeroelasticity- Similarity
3. Discrete Continuous Optimization in CSM

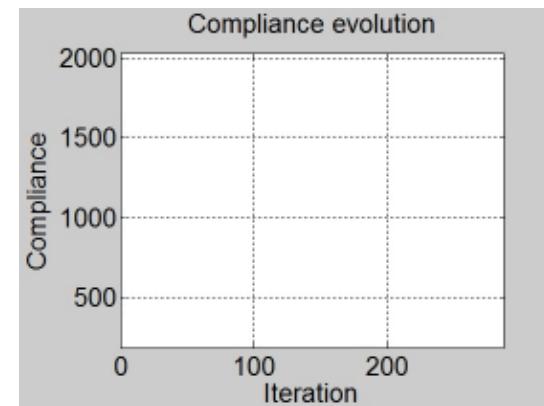
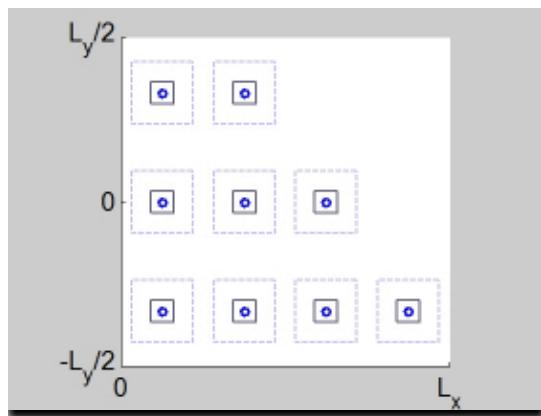
Outlines

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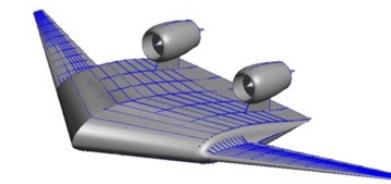
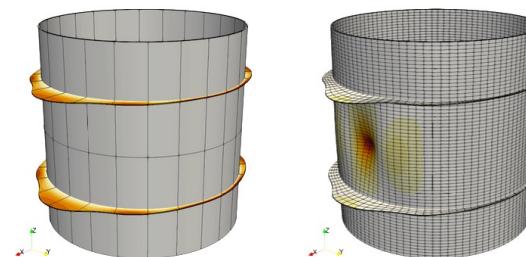
My Group

<http://www.institut-clement-ader.org/pageperso.php?id=jmorlier>

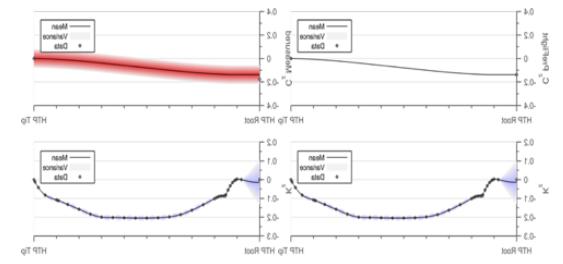
- 5 PhDs, 1 postdoc



MDO Workshop@DLR



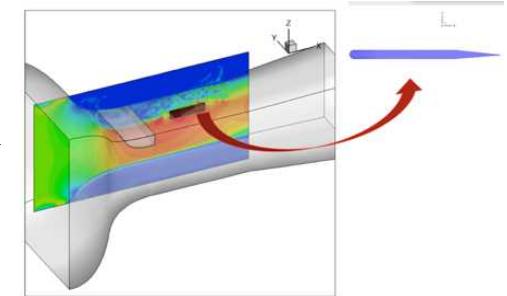
$$\begin{aligned} & \min_{(\boldsymbol{t}, \boldsymbol{A}) \in \mathbb{R}^{2N}, \boldsymbol{c} \in \Gamma^N} W(\boldsymbol{c}, \boldsymbol{t}, \boldsymbol{A}) \\ & \text{Subjected to: } \begin{aligned} & RF(\boldsymbol{c}, \boldsymbol{t}, \boldsymbol{A}, IL(\boldsymbol{c}, \boldsymbol{t}, \boldsymbol{A})) \geq 1 \\ & G(\boldsymbol{c}, \boldsymbol{t}, \boldsymbol{A}) \leq 0 \\ & \underline{t}(\boldsymbol{c}) \leq \boldsymbol{t} \leq \bar{\boldsymbol{t}}(\boldsymbol{c}) \\ & \underline{a}(\boldsymbol{c}) \leq \frac{\boldsymbol{A}}{bt} \leq \bar{a}(\boldsymbol{c}) \end{aligned} \end{aligned}$$



△ TSFC% solution, Volume fraction =0.39964 △ TSFC = 2.5276



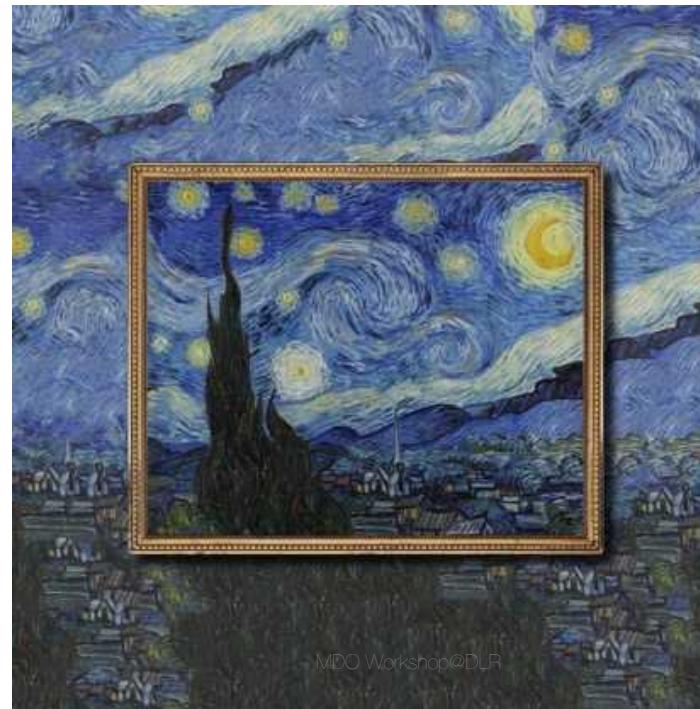
△ TSFC% solution, Volume fraction =0.49913 △ TSFC = 1.7554



Machine learning for load estimation (Ankit Chiplunkar, AIRBUS FUND)

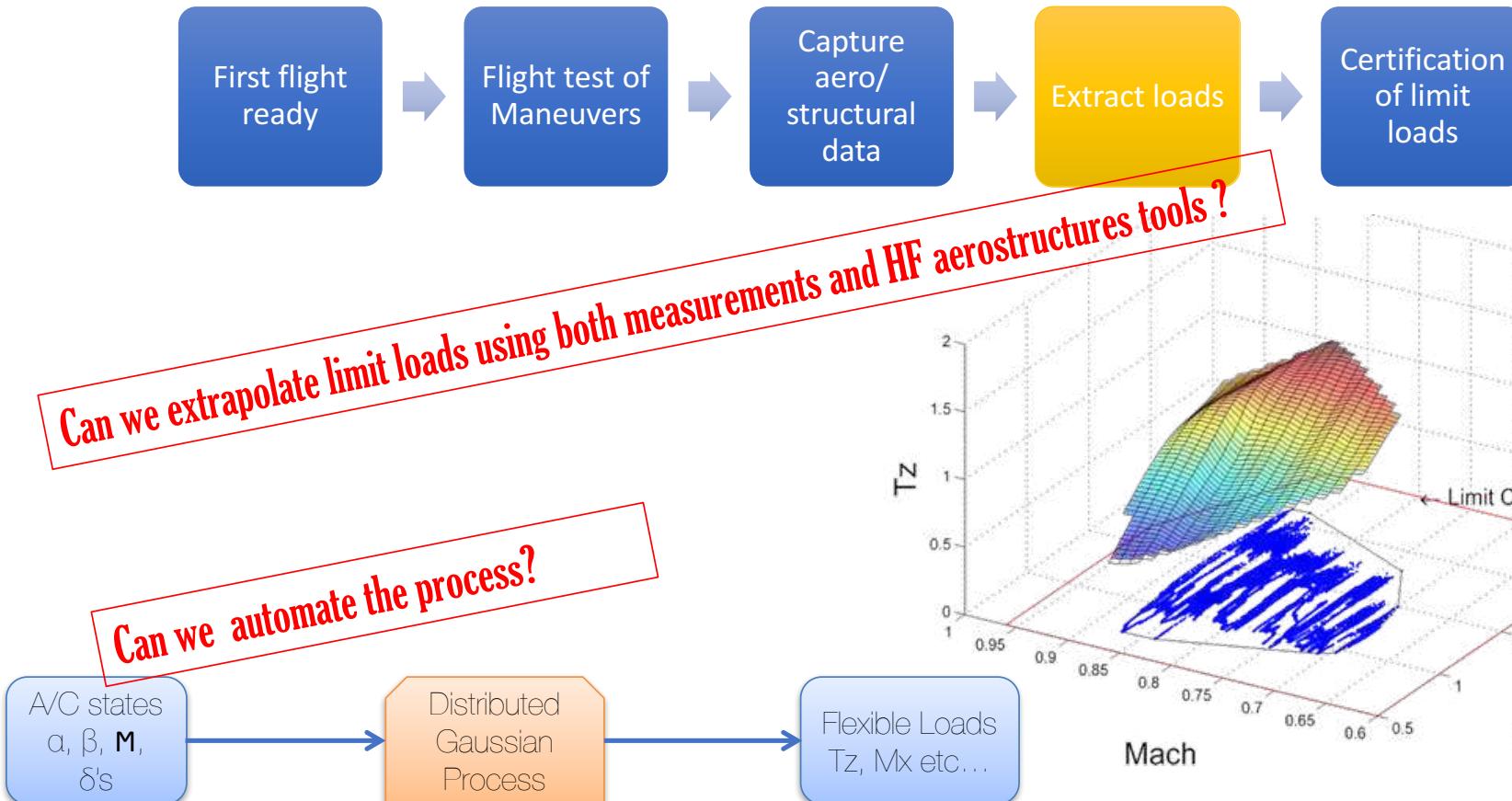
Kriging	Gaussian Processes
Developed by Daniel Krige – 1951; formalized by Georges Mathéron	Neural network with infinite neurons tend to Gaussian Process 1994
Evaluation: minimize error variance	Evaluation: Marginal Likelihood

AIRBUS



MDO Workshop@DLR

Loads identification (CIFRE AIRBUS)



Gaussian Process Regression

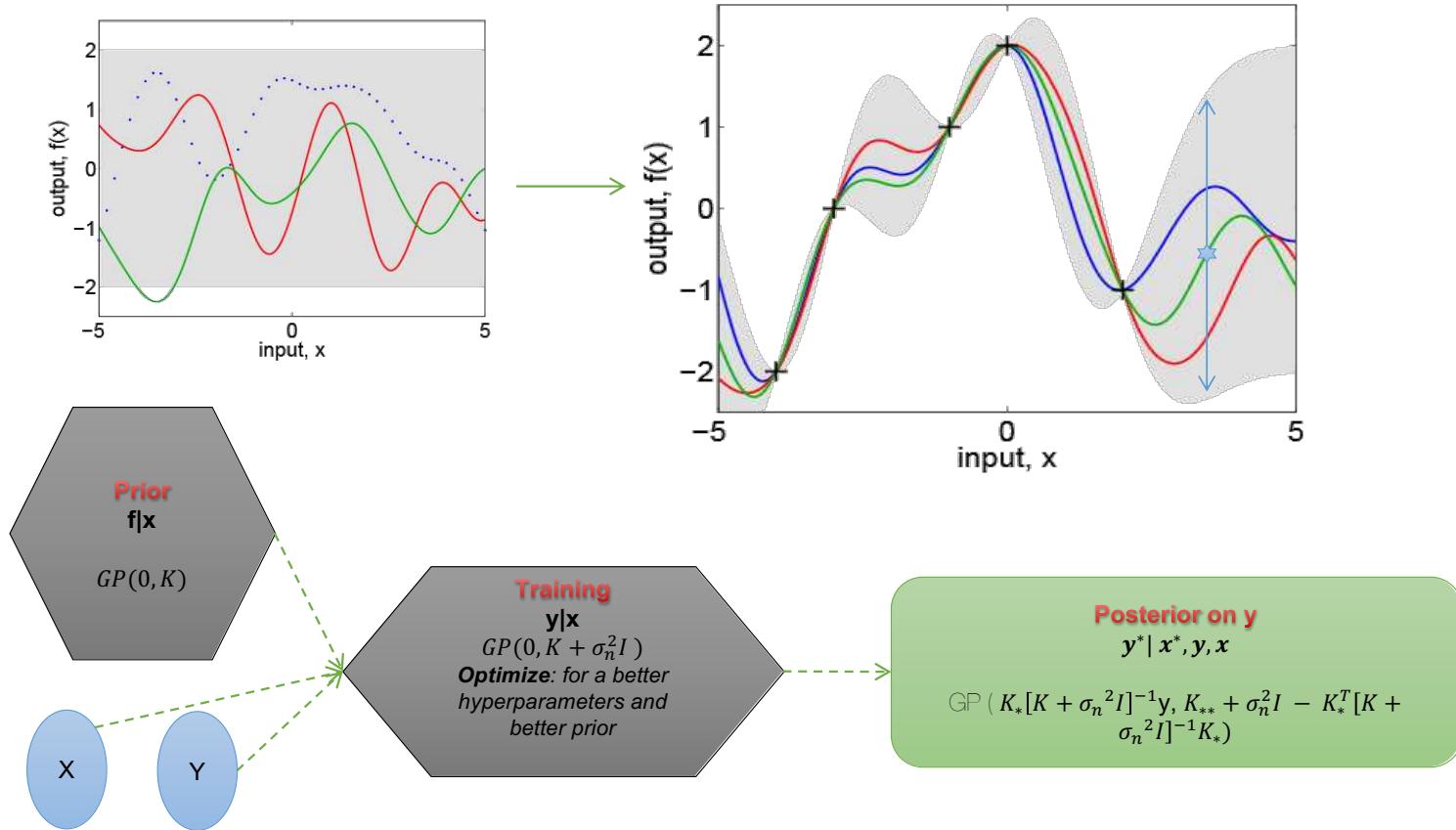
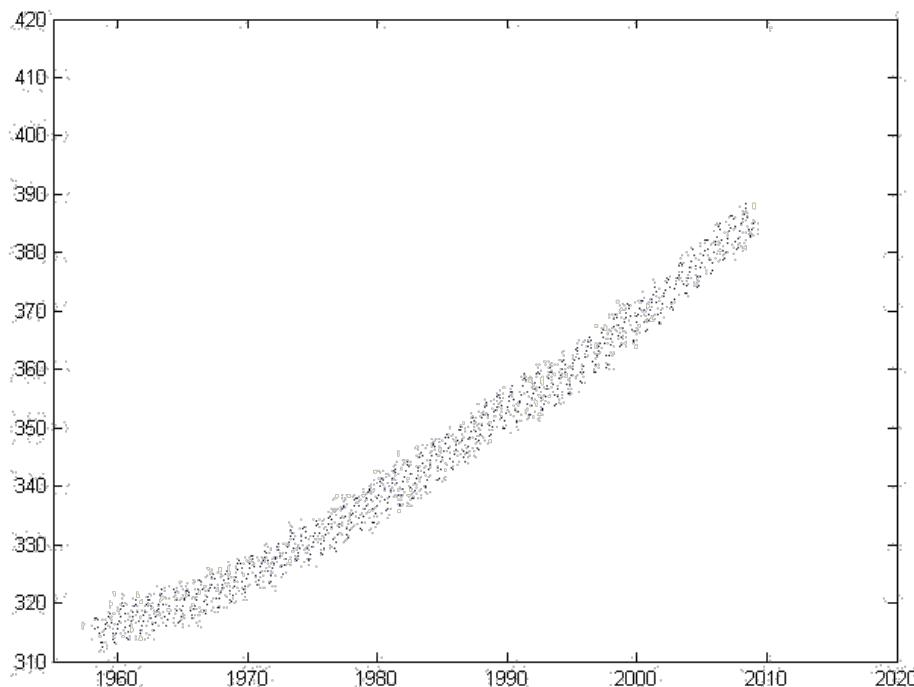


Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

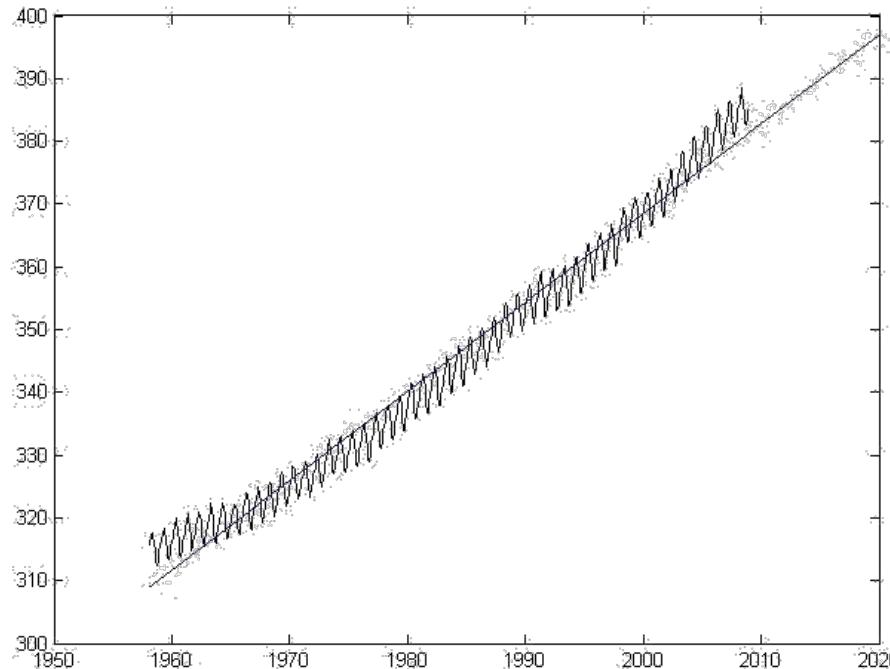
A SIMPLE Example



Month-wise data of CO₂ concentration in atmosphere at Hawaii

Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Example – Linear Regression



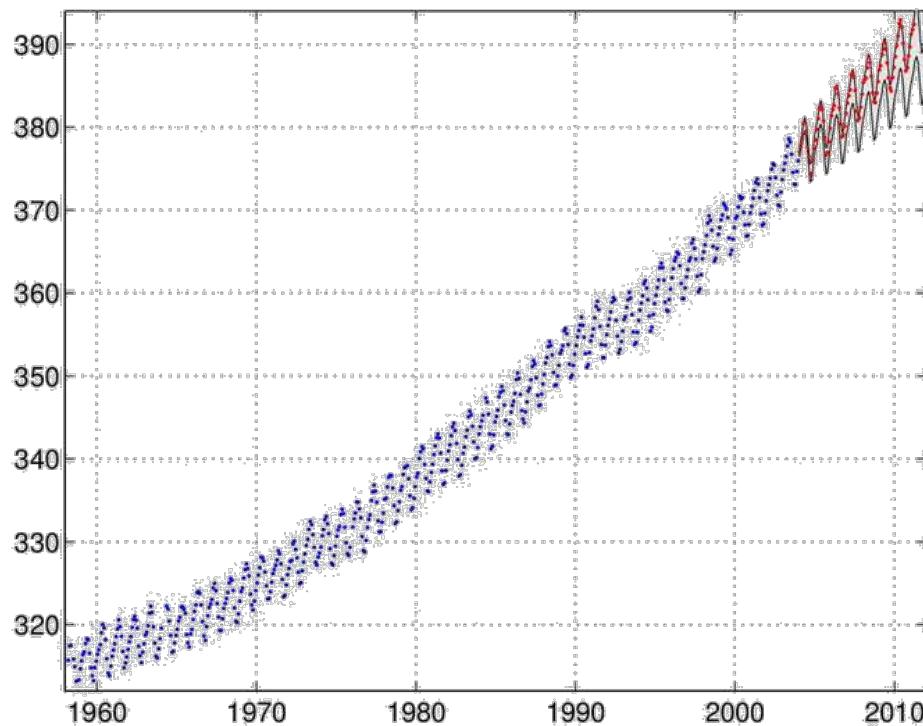
Should we choose a polynomial?

What degree of polynomial should we choose? (overfitting)

For a given degree, what parameters of polynomial should we choose

Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Example – Gaussian Process

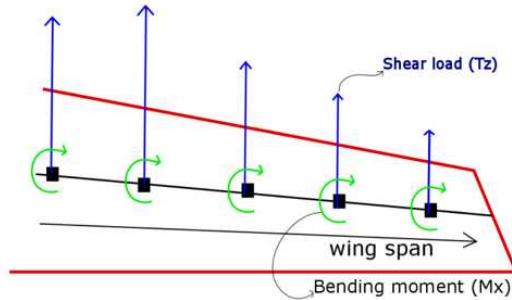


Predicted variance after year 2005 in grey, real data-points in red

Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Multi-Output Gaussian Process

$$\text{Given: } f_1 = g(f_2, x)$$



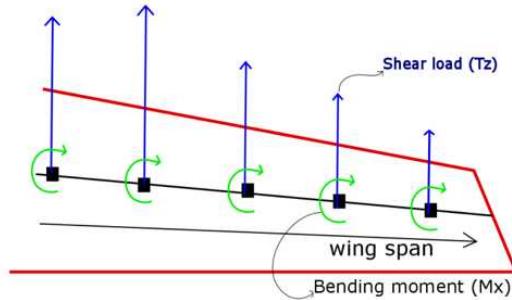
- Earlier examples include **Gradient Enhanced Kriging** (GEK) or **Co-kriging**
- But we want to expand this to integral enhanced kriging, double differential, or any functional relationship between outputs

Forrester, A. I. J., Sobester, A. and Keane, A. J. (2007) Multi-fidelity optimization via surrogate modelling. *Proceedings of the Royal Society A*, 463(2088), 3251–3269, (doi:10.1098/rspa.2007.1900).

LIU, Weiyu. Development of gradient-enhanced kriging approximations for multidisciplinary design optimization. 2003.

Multi-Output Gaussian Process – Flight Test examples

Given: $f_1 = g(f_2, x)$

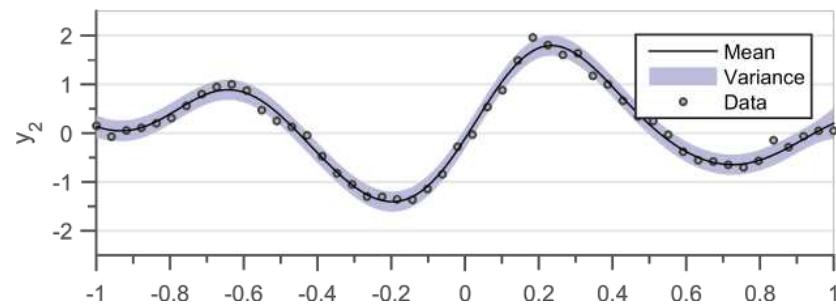
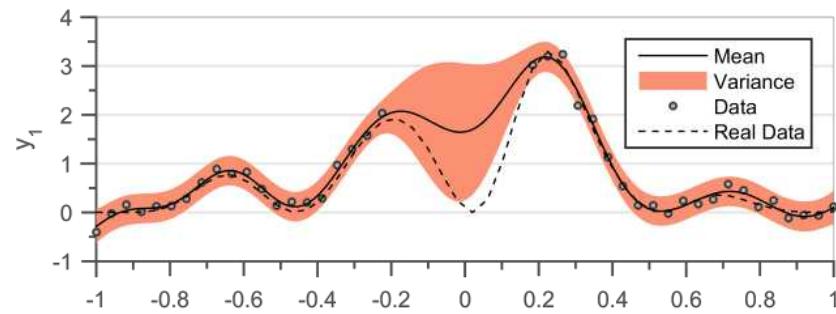


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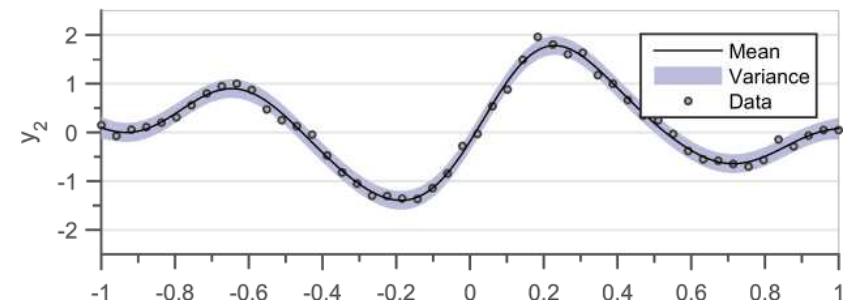
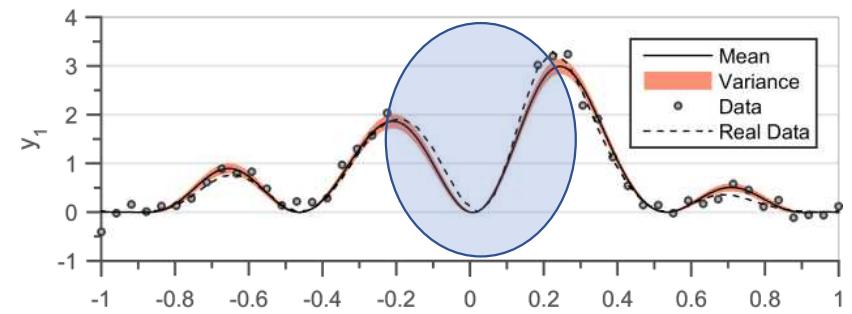
Forrester, A. I. J., Sobester, A. and Keane, A. J. (2007) Multi-fidelity optimization via surrogate modelling. *Proceedings of the Royal Society A*, 463(2088), 3251–3269, (doi:10.1098/rspa.2007.1900).

Liu, Weiyu. Development of gradient-enhanced kriging approximations for multidisciplinary design optimization. 2003.

Example 1: Faulty sensors (using synthetic data) $y_1 = (y_2)^2$

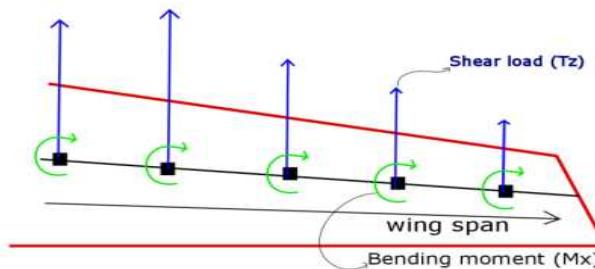


Independent GPs

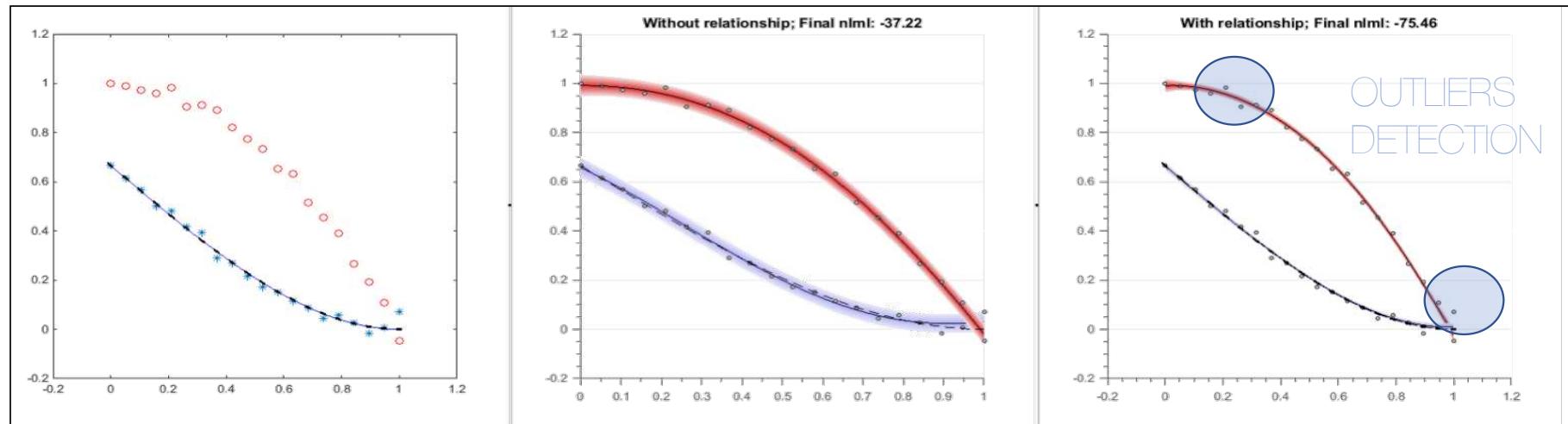


Related GPs

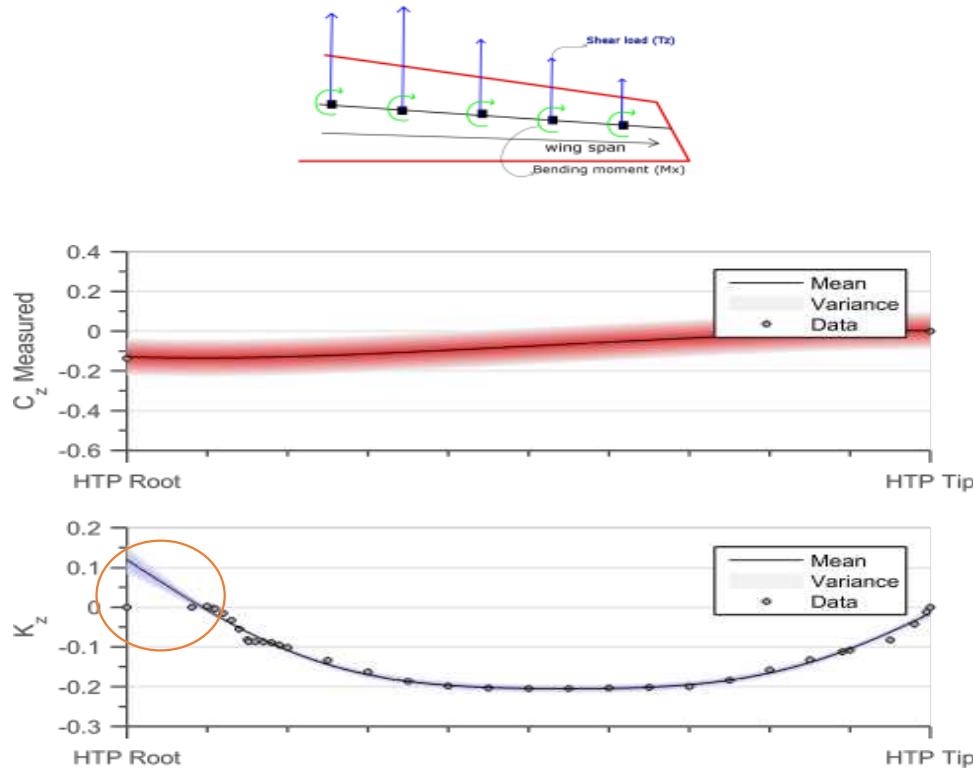
Example 2: use the Relationship between T_z and M_x permits to reduce uncertainties



$$M_x = \int_{\eta}^{\eta_{edge}} (x - \eta) T_z dx$$

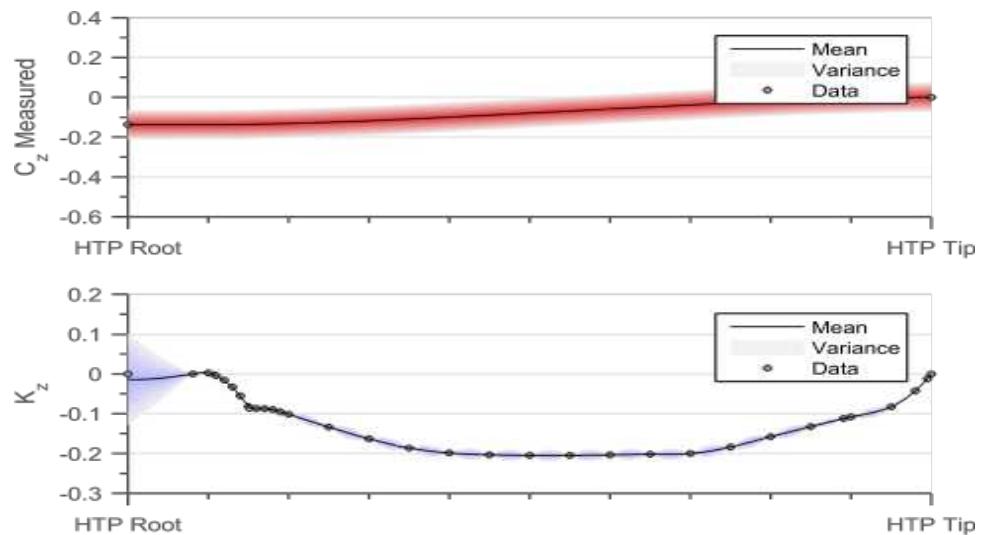


Exemple 3: choosing the good kernel



$$k_{SE}(x, x', \theta) = \theta_1^2 \exp\left[-\frac{d^2}{2\theta_2^2}\right]$$

$$C_z(\eta) = \int_{\eta_{edge}}^{\eta_{root}} k_Z(\eta) d\eta$$



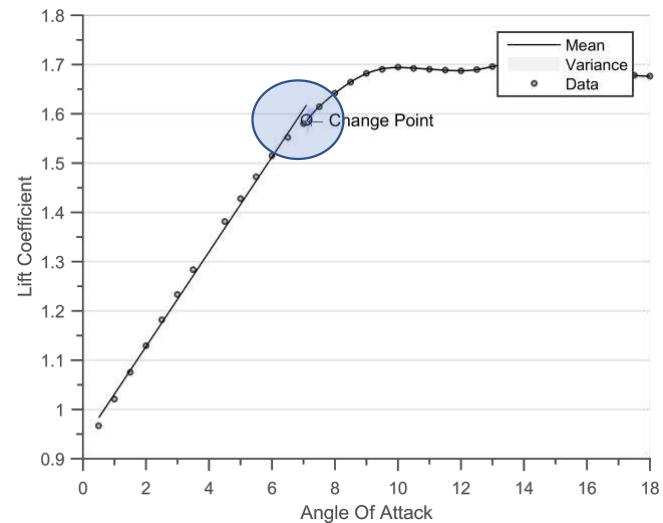
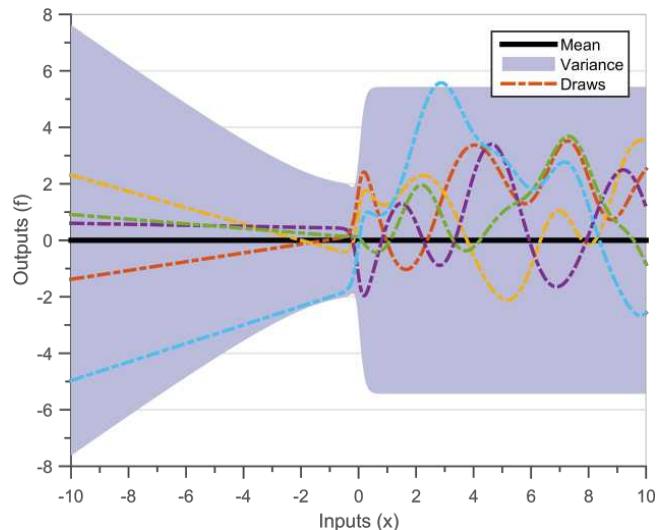
$$k_{Mat2}(x, x', \theta) = \theta_1^2 \left(1 + \frac{\sqrt{5}d}{\theta_2} + \frac{5d^2}{3\theta_2^2}\right) \exp\left[-\frac{\sqrt{5}d}{\theta_2}\right]$$

Constantinescu, Emil M., and Mihai Anitescu. "Physics-based covariance models for Gaussian processes with multiple outputs." *International Journal for Uncertainty Quantification* 3.1 (2013).

3AF-BigData

20

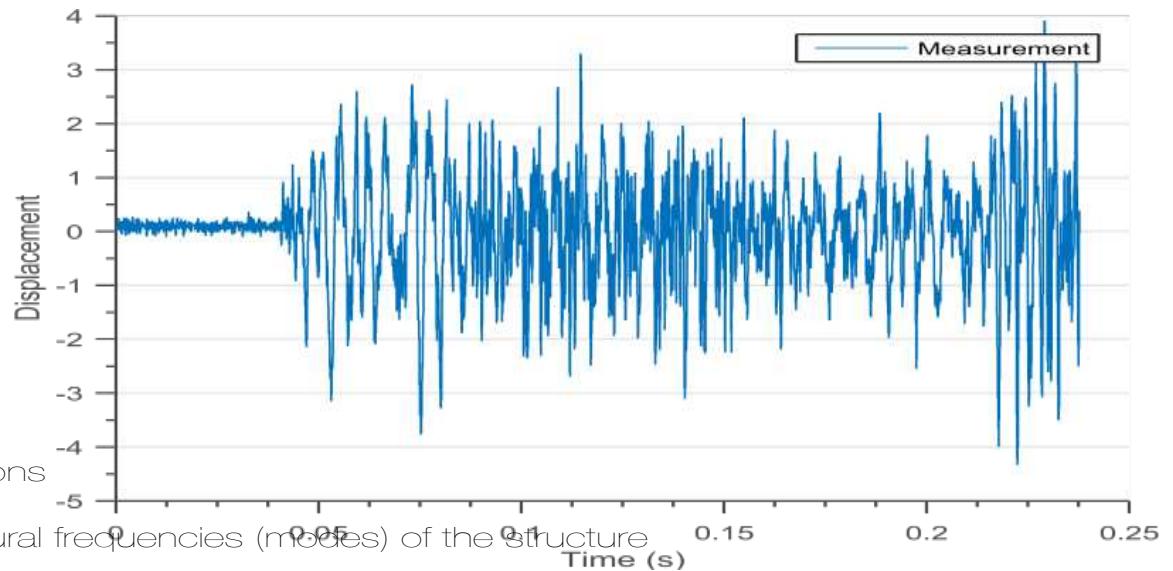
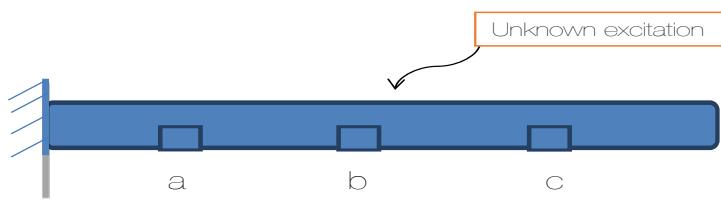
Example 3: Identifying onset of non-linearity



$$k_{CP}(k_1, k_2, x_1, x_2) = \text{sigm}(x_1)k_1\text{sigm}(x_2) + (1-\text{sigm}(x_1))k_2(1-\text{sigm}(x_2))$$

- Estimate change in pattern
- Use global optimization to identify the non-linearity automatically

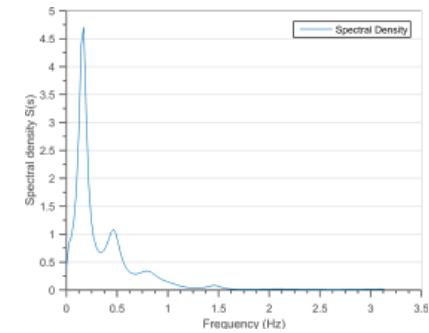
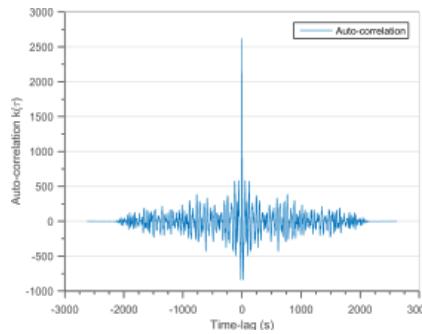
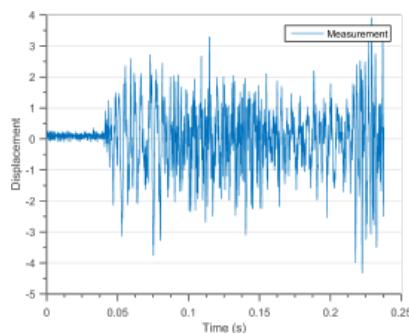
Example 4: Operational Modal analysis



1. Sample is subjected to unknown random excitations
2. Each sensor record time signals
3. Peaks in their power spectral density give the natural frequencies (modes) of the structure

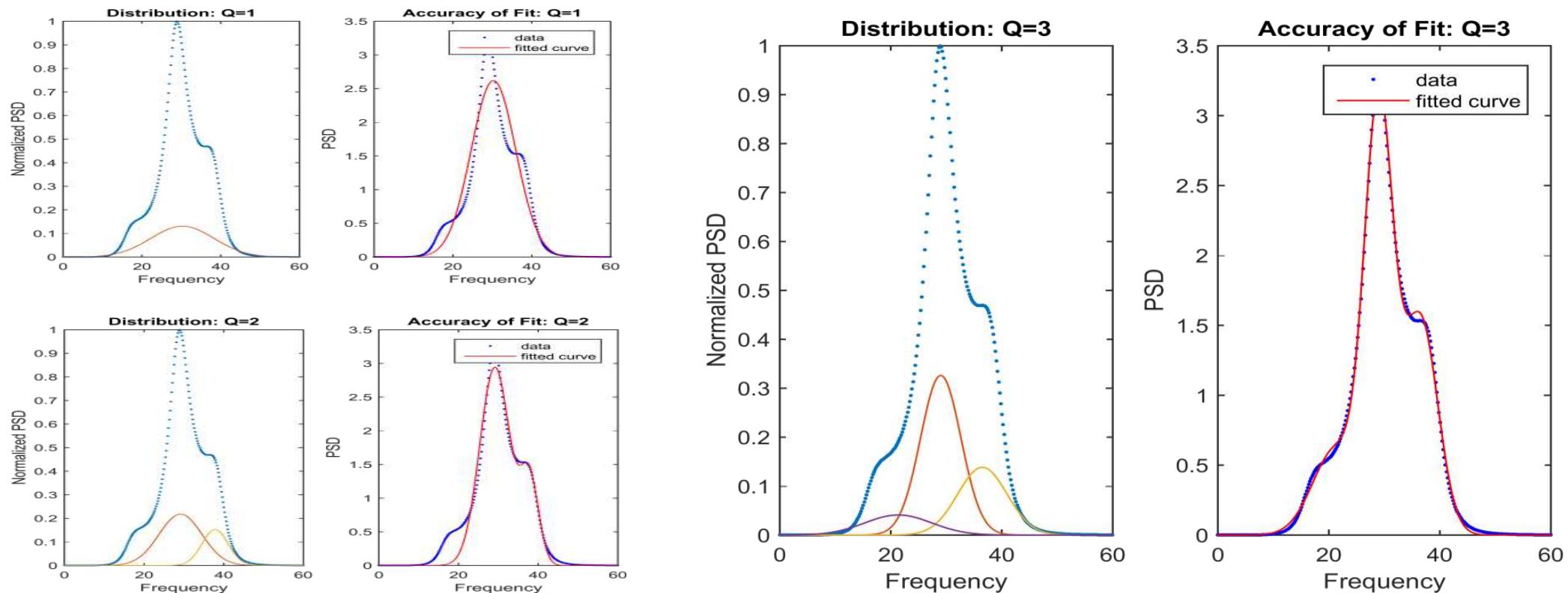
DiazDelaO, F. A., and S. Adhikari. "Structural dynamic analysis using Gaussian process emulators." *Engineering Computations* 27.5 (2010)

New paradigm: Spectral Mixture

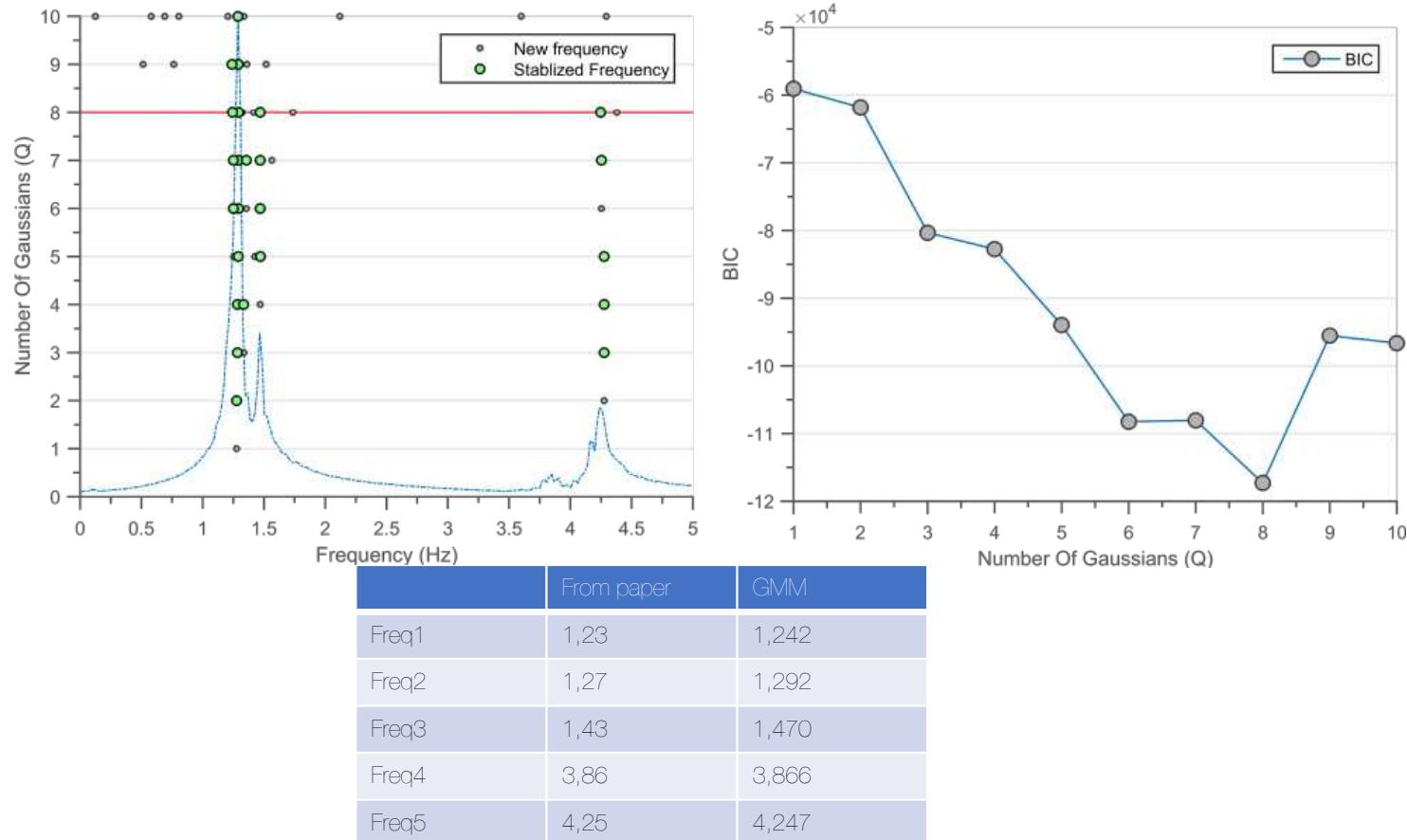


Displacement	Autocorrelation	Power spectral density
$x(t)$	$k(\tau) = \int x(t)x(t - \tau)dt$	$S(s) = \text{Fourier}(k(\tau))$
$M\{\ddot{x}(t)\} + C\{\dot{x}(t)\} + K\{x(t)\} = \{f(t)\}$		
	$k(\tau) = \sum A_i \exp(-\lambda_i \tau) \sin(B_i \tau)$	$S(s) = \frac{\sum a_k(s)^k}{\sum b_l(s)^l}$
Spectral Mixture Covariance		
$x(t) = GP(0, cov_{SM}(t, t'))$	$k_{SM}(d, \mu, \sigma, w) = \sum_{q=1}^Q w_q \cos(2\pi\mu_q) \exp[-2\pi^2 d^2 \sigma_q^2]$	$S_{SM}(s, \mu, \sigma, w) = \sum_{q=1}^Q \frac{w_q}{\sqrt{2\pi\sigma_q^2}} \left(\exp \left[-\frac{(s - \mu_q)^2}{2\sigma_q^2} \right] + \exp \left[-\frac{(-s - \mu_q)^2}{2\sigma_q^2} \right] \right)$

Gaussian Mixture Models



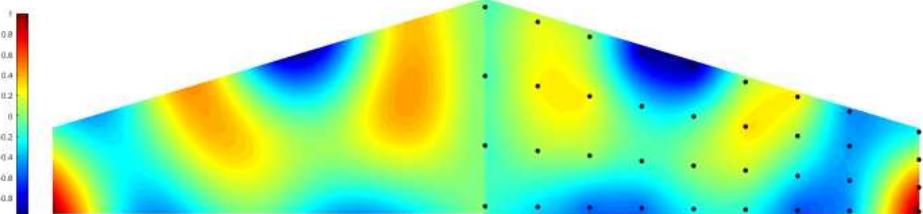
Automatic OMA (Testcase HTC building *)



*Brincker, Rune, and Palle Andersen. "Ambient response analysis of the heritage gourt tower building structure." IMAC, 2000
Data from: <http://www.brinckerdynamics.com/oma-toolbox/>

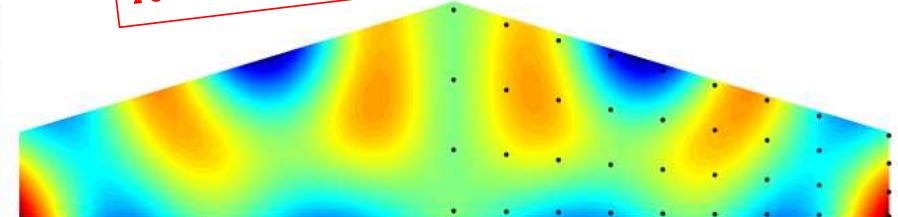
Example 5: Sensor Placement Optimization

- Idea : Reduce in a smart way the number of sensors for GVT by using GP/Kriging for Modeshapes reconstruction
- How: By optimizing the sensor positions and use them as variables in a SPO problem



Comparison between HF FEA results (a) and a Linear Reconstruction with a regular grid of 36 sensors (b), for 9th Mode Shape.

1/ Better Modeshape
reconstruction using GP/Kriging

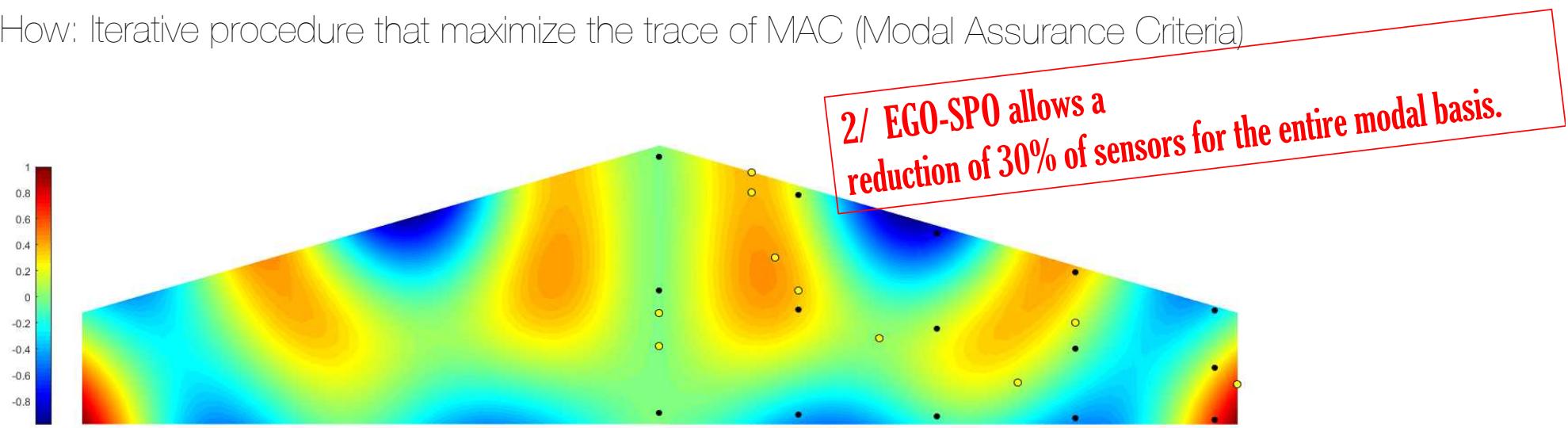


Comparison between HF FEA results (a) and a Kriging Reconstruction with a regular grid of 36 sensors (b), for 9th Mode Shape.

EGO strategy

Jones, D. R., Schonlau, M., & Welch, W. J. (1998). Efficient global optimization of expensive black-box functions. *Journal of Global optimization*, 13(4), 455-492.

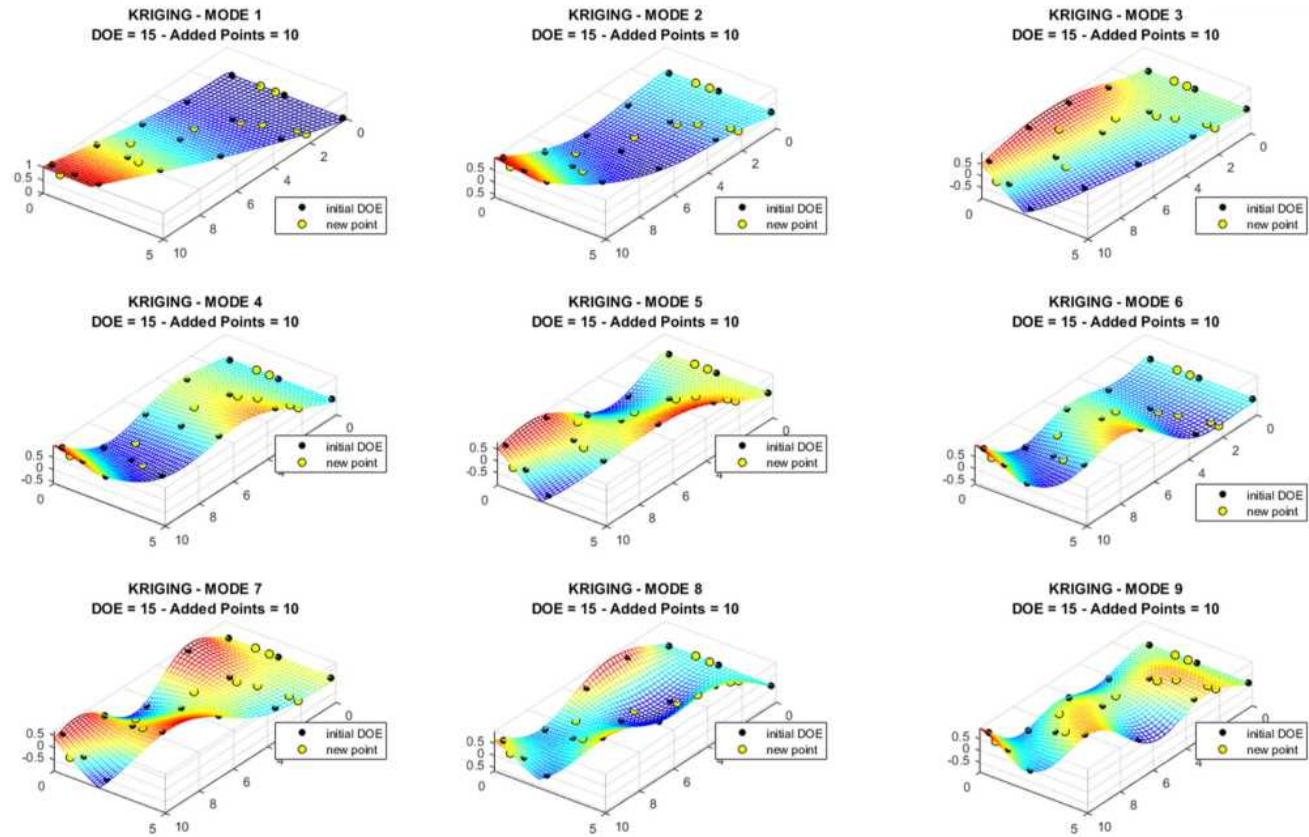
- Idea : Working at fixed budget
- How: Iterative procedure that maximize the trace of MAC (Modal Assurance Criteria)



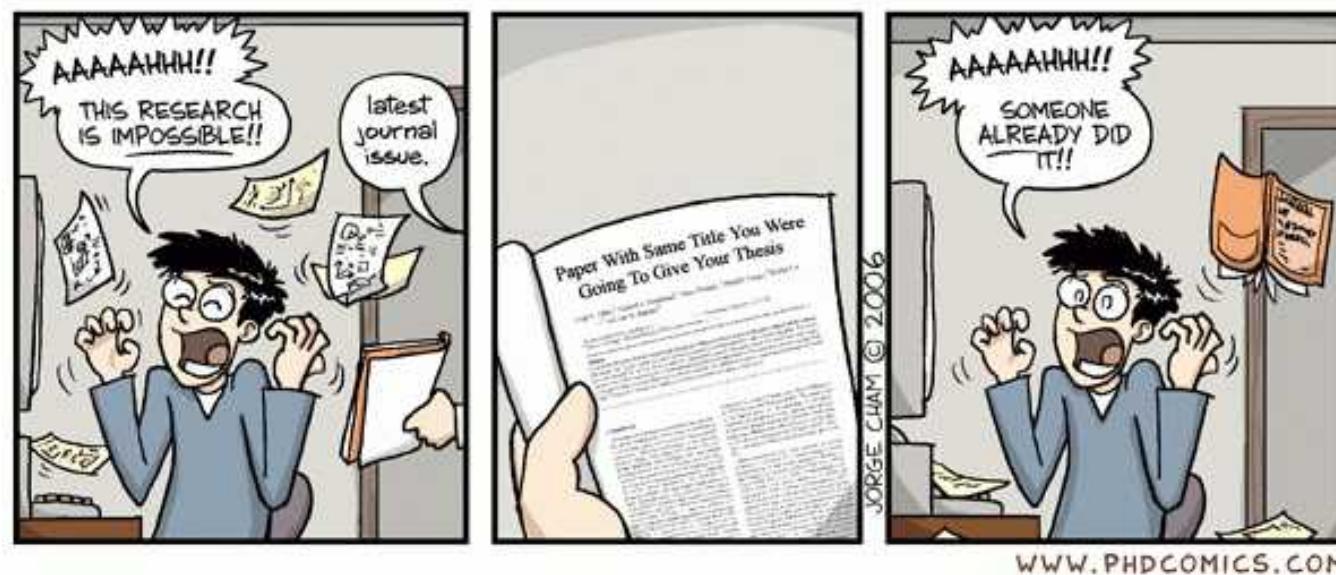
Typical result showing SPO-EGO performance. As example 9th Mode Shape.
(a): HF FEA results. (b): SPO-EGO stategy. The black dots represent the initial DOE (regular grid, 15 sensors).

Results

- Matlab codes (cleaning in profess)
- Compatible with Cliare's inputs



Open questions



- 3D structure

Papers&conf

Chiplunkar, E. Rachelson, M. Colombo and J. Morlier. Approximate Inference in Related Multi-output Gaussian Process Regression. Lecture Notes in Computer Science. 10163, 88-103. 2017

Chiplunkar and J. Morlier. Operational Modal Analysis in Frequency Domain using Gaussian Mixture Models . Proceedings of IMAC XXXV, 2017

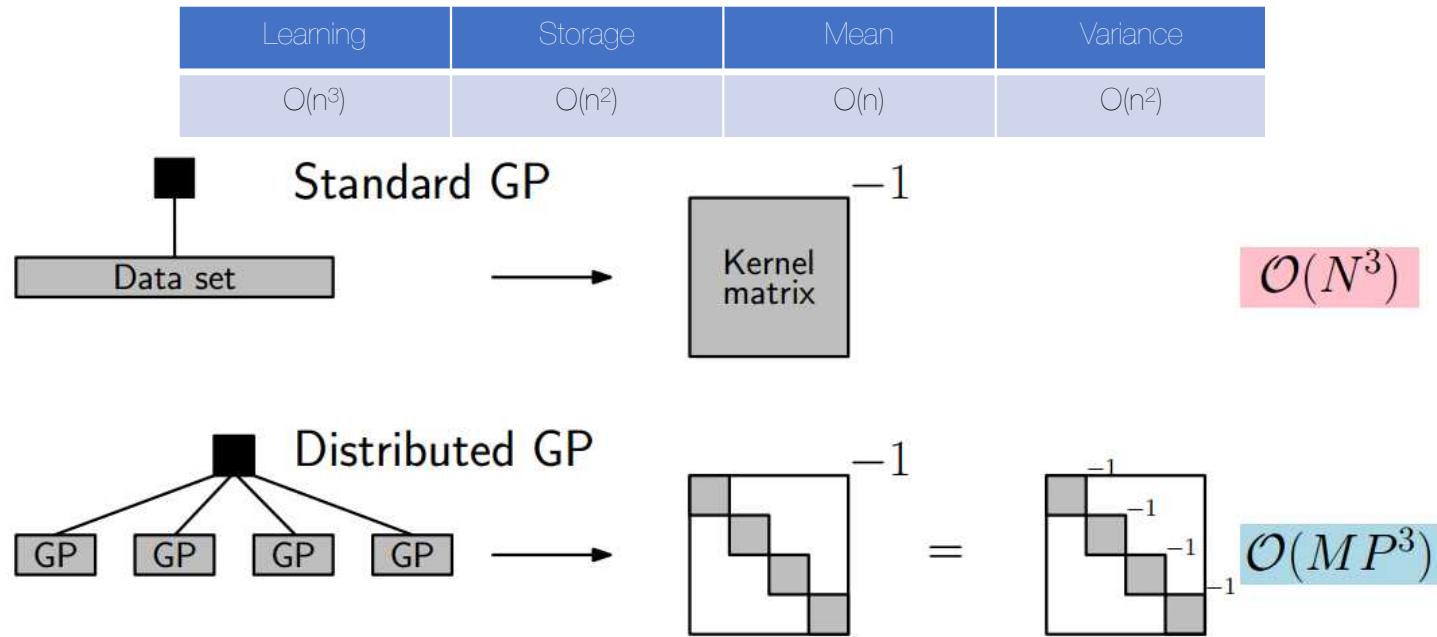
Chiplunkar, E. Bosco and J. Morlier. Gaussian Process for Aerodynamic Pressures Prediction in Fast Fluid Structure Interaction Simulations. Proceedings of WCSMO12 2017

Chiplunkar, E. Rachelson, M. Colombo and J. Morlier. Adding Flight Mechanics to Flight Loads Surrogate Model using Multi-Output Gaussian Processes. AIAA AVIATION 2016

Chiplunkar, E. Rachelson, M. Colombo and J. Morlier. Sparse Physics-Based Gaussian Process for Multi-output Regression using Variational Inferenc. Proceedings of ICPRAM 2016 2016

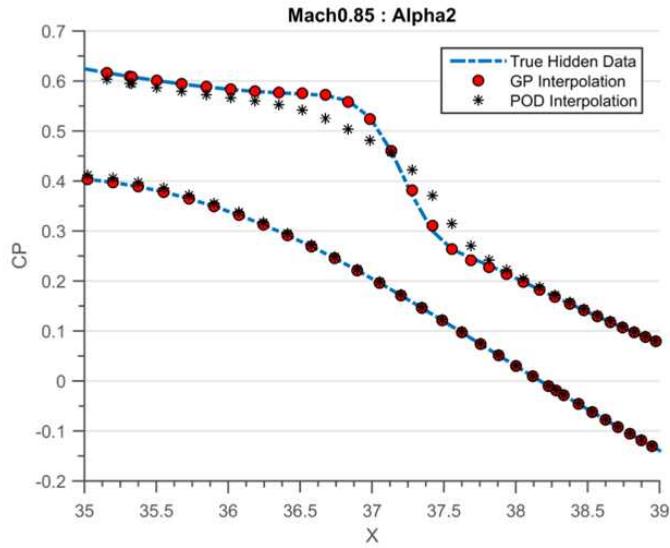
Several Papers in preparation

Link to HPC: Distributed Gaussian Process

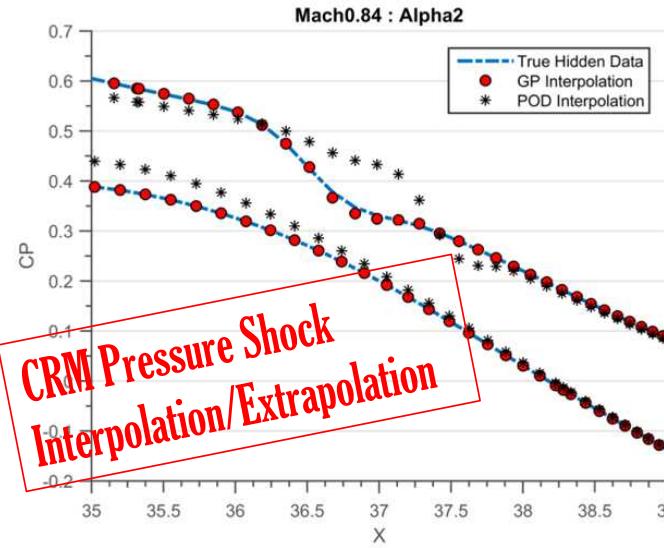


Distributing the dataset into M chunks of size P

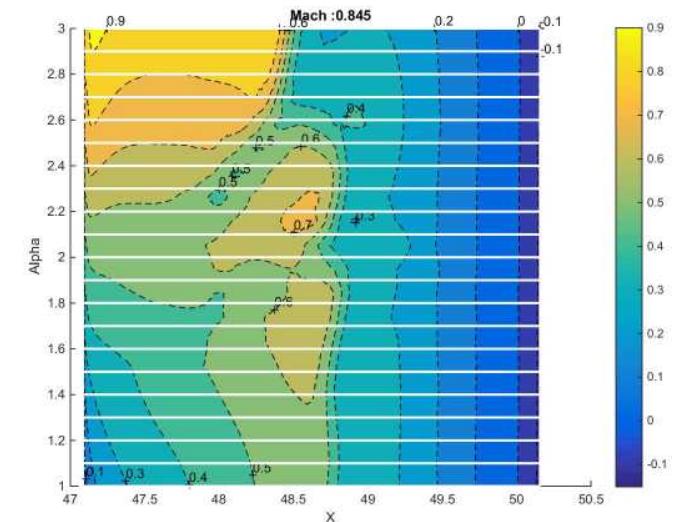
Some others ML applications



(a) Comparison between POD method and Distributed GPs for **interpolation**.



(b) Comparison between POD method and Distributed GPs for **extrapolation**



Outlines

1. Overview of Machine learning techniques
2. Aeroelasticity- Similarity
3. Discrete Continuous Optimization in CSM



Objectives

Build a Python written Open Sources Multi-Fidelity Aircraft Preliminary Design Framework, based on Aero-Structure Optimization

Why Python scripted and open source??



- Collaborative Environment.
- Access to a global user community, who proficiently interact with support and solutions.
- Student projects / PhD

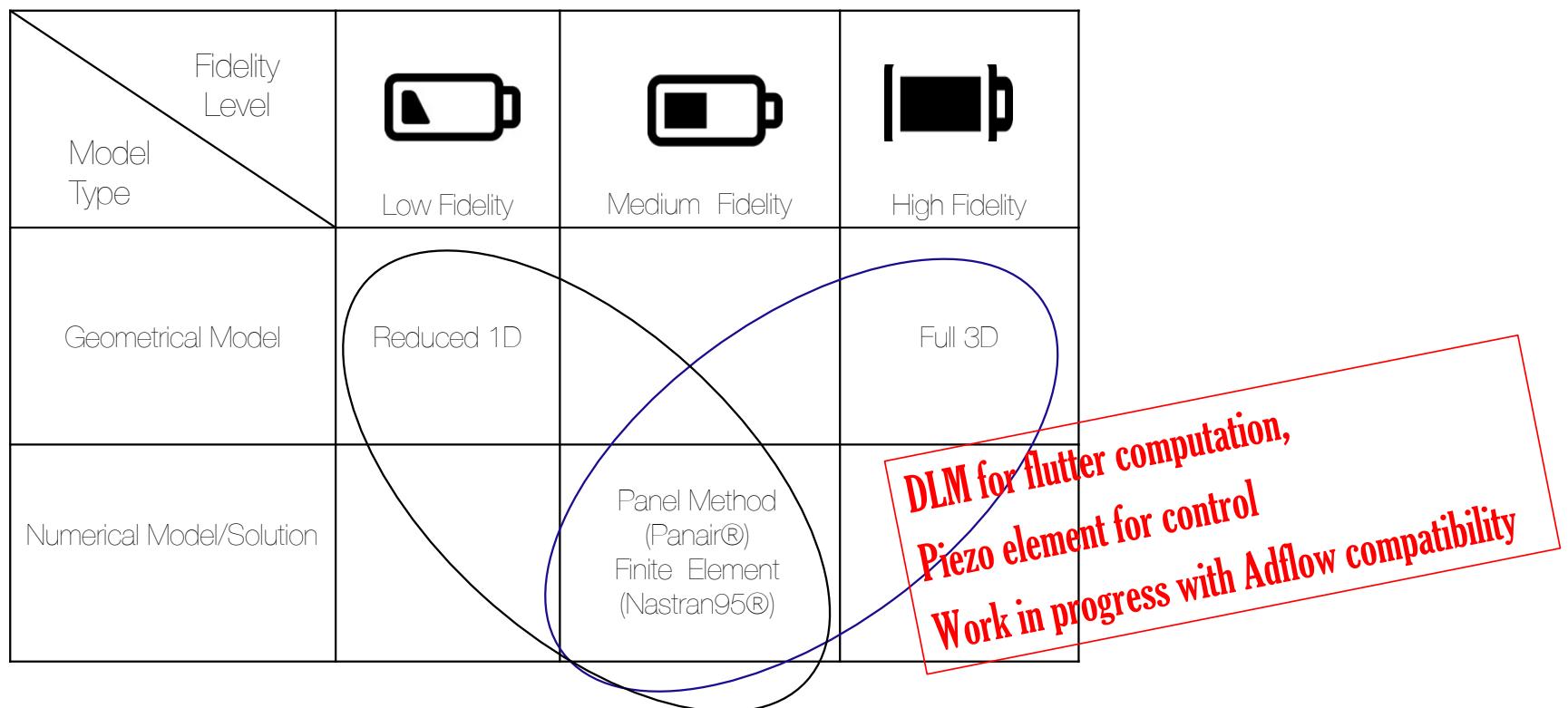
Which Optimization Solutions?



- Optimization with aeroelastic constraints
- Applications to BWB, and scaled aircrafts
- New testcases for comparing Gradient vs Surrogate based optimization



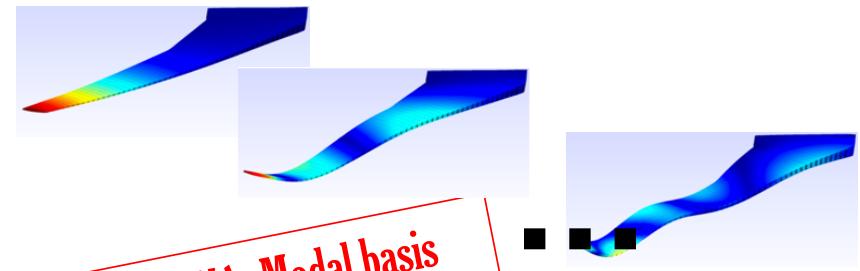
Multifidelity Fidelity



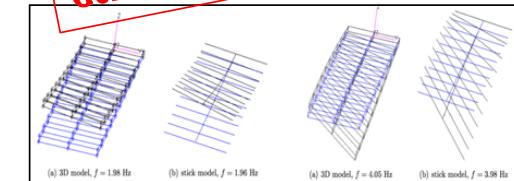
CAD= Airconics+ OpenNastran

All types of body shape may be reproduced, here some wing examples:

Aerodynamic Surface	Airframe	Wing Type
		CRM
		BWB
		GOLAND



Aircraft DNA: Modal basis



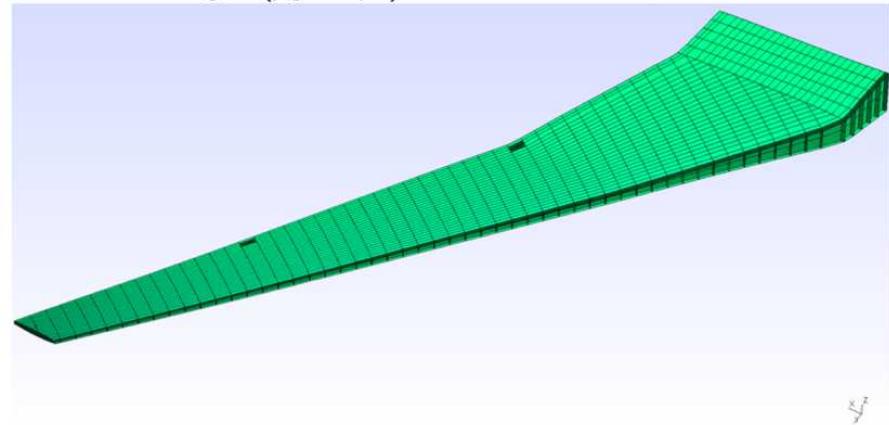
2. Example: Mode tracking strategy



- Blind identification
- From ONERA Chatillon's optimized CRM (thanks to C. Blondeau)

FROM A GIVEN MODAL BASIS AND GEOMETRY, CAN WE UPDATE A FEM ?

Reference Design* (jig shape): For all elements $t_r = 8.89\text{mm}$



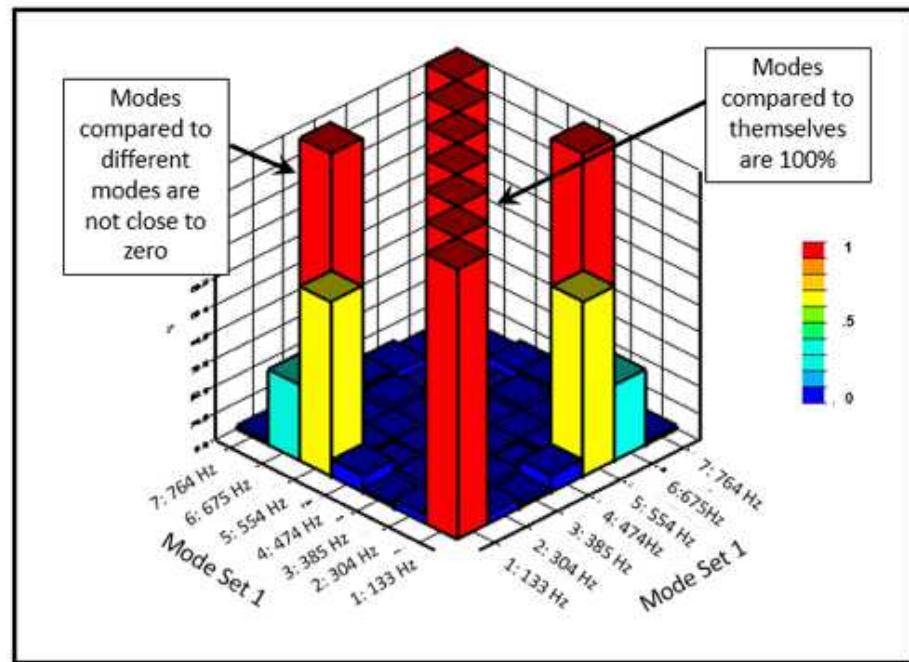
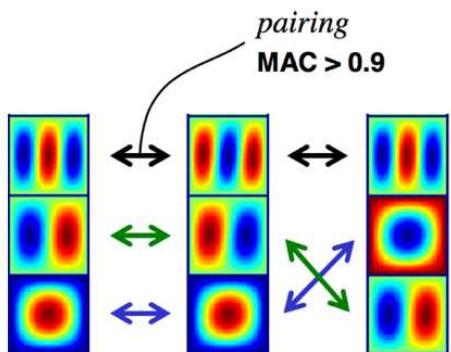
Model provided by T. Achard and C. Blondeau*

Mode pairing

MAC (Modal Assurance Criterion) usually used for Experimental/Numerical correlation (late 70s)

$$\mathbf{K} \cdot \mathbf{V} = \lambda \cdot \mathbf{M} \cdot \mathbf{V}$$

$$MAC(V_1, V_2) = \frac{(V_1^T V_2)^2}{(V_1^T V_1)(V_2^T V_2)}$$



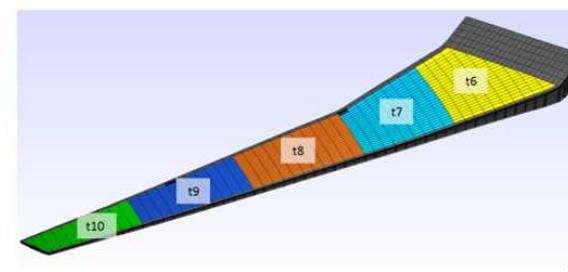
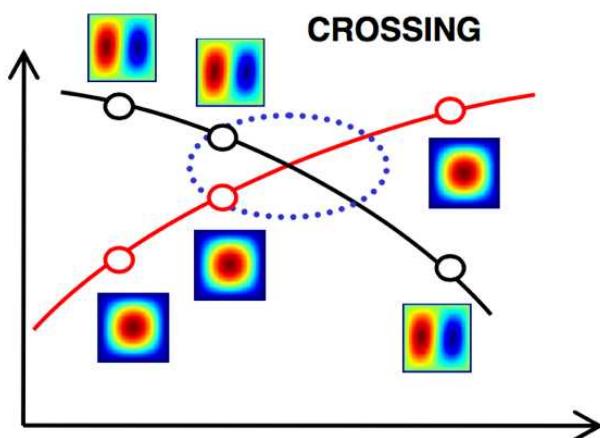
Reference aircraft: r
Scaled model: m

Thickness initialization :Vector of size
10 t1-t10 (meter):

```
array([
0.01863388, 0.01661411, 0.012
73371, 0.01495363, 0.00847329
,
0.01743593, 0.02332176, 0.020
23447, 0.02068164, 0.0213995 ])
```

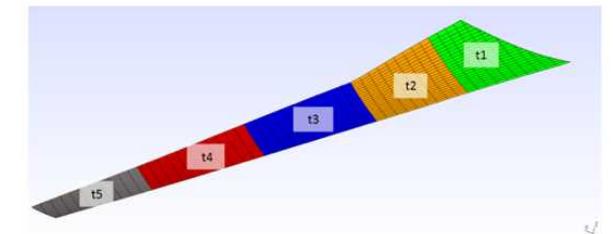
Modes pairing/tracking: Problem definition

Objective Function	Dimension	Bounds
Mode shape difference minimization $\min(N - \text{trace}(\text{MAC}([\Phi_r], [\Phi_m])))$	\mathbb{R}	
Design Variables		
Skin thicknesses vector	$[t]$	\mathbb{R}^{10}
		$[0.0889, 26.67]$ mm
Constraints		
Reduced frequency matching	$\ \omega_r - \omega_m\ = 0$	\mathbb{R}
Mass matching	$M_r - M_m = 0$	\mathbb{R}
Generalized masses matching	$\ m_r - m_m\ = 0$	\mathbb{R}

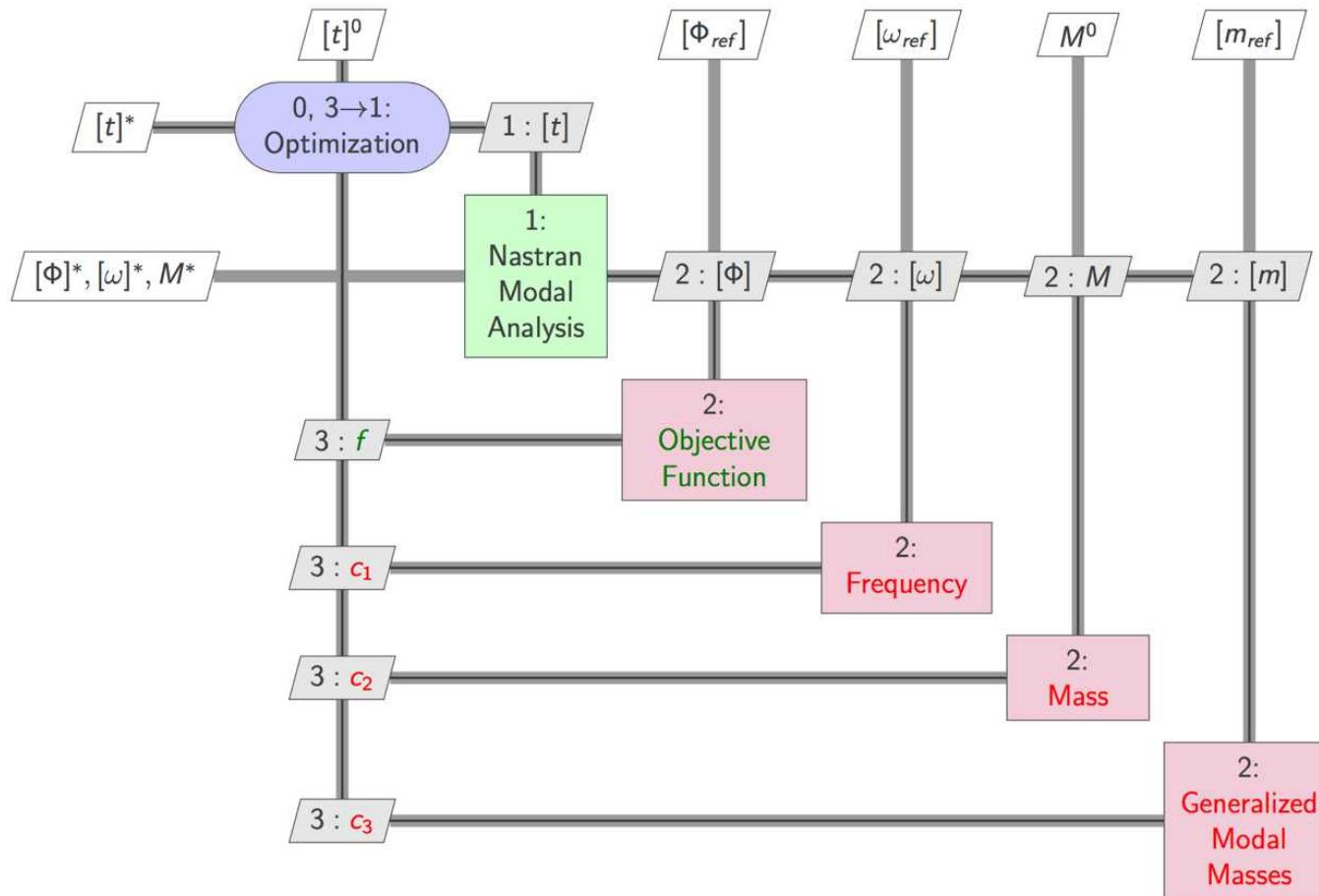


→ Upper skin panels

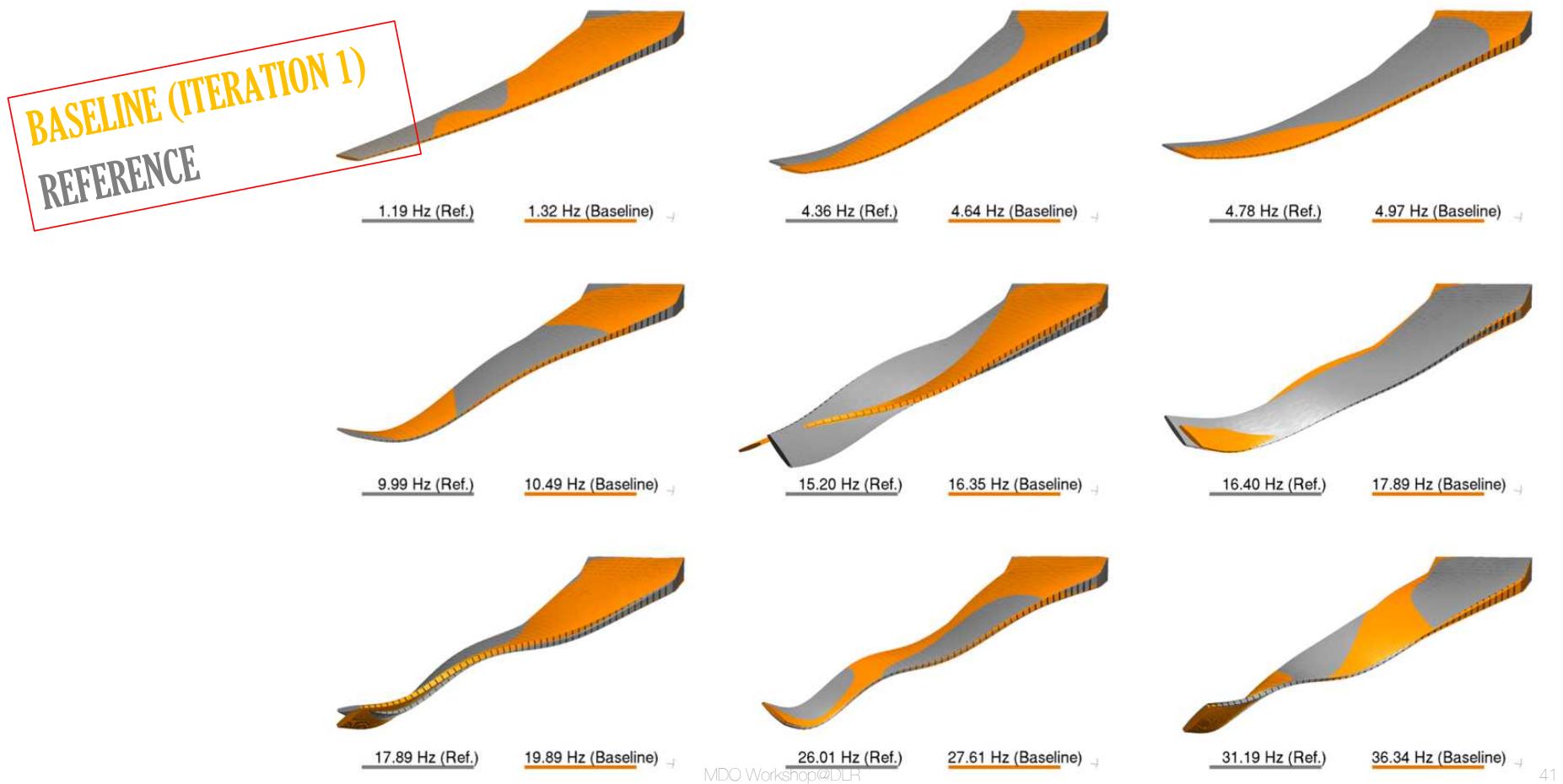
Lower skin panels ←



Modal Optimization

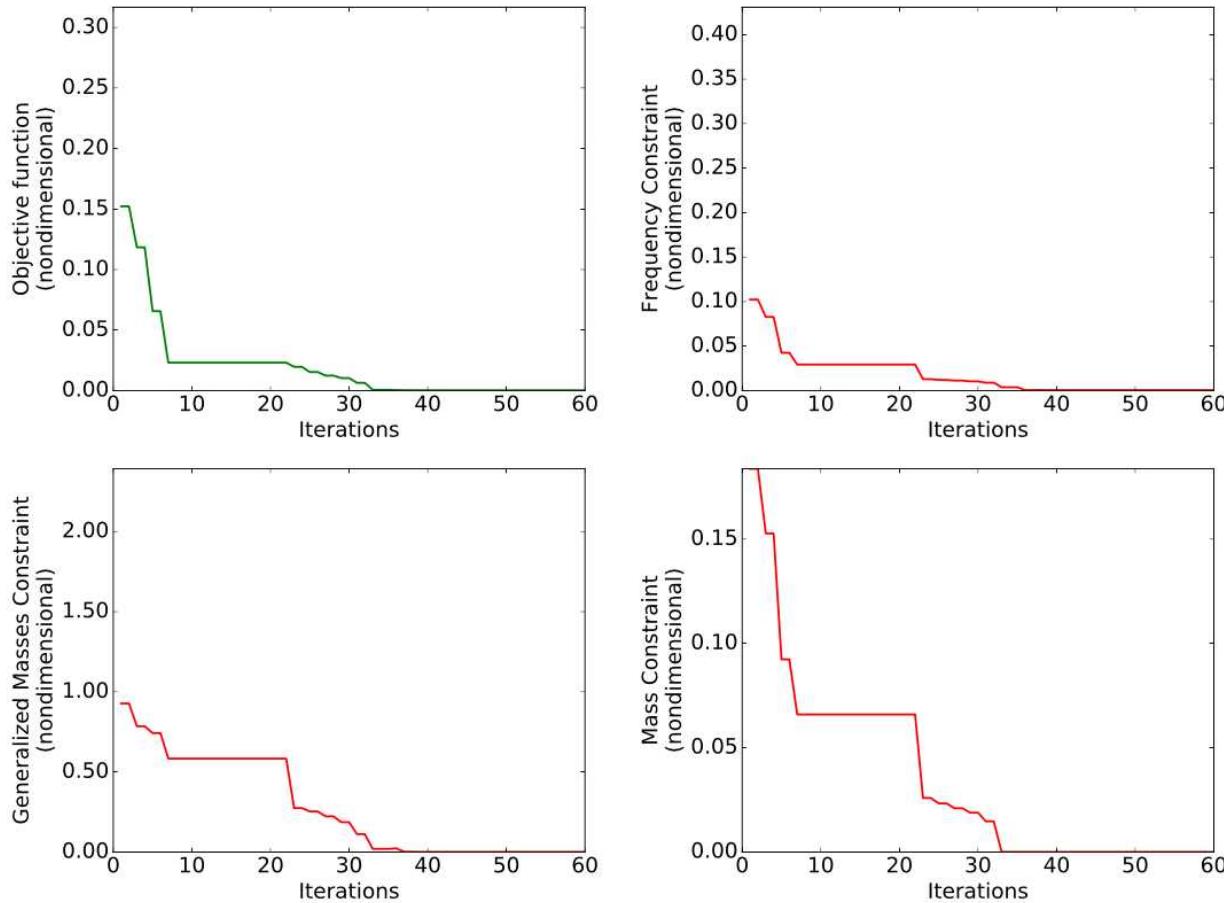


1st Validation CRM Blind Updating



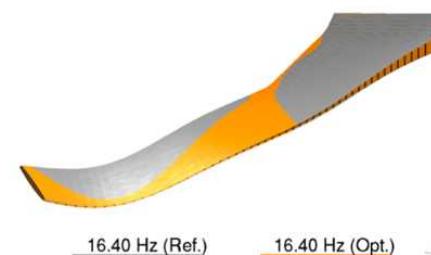
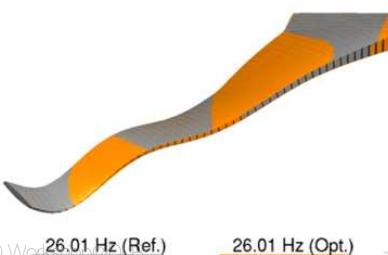
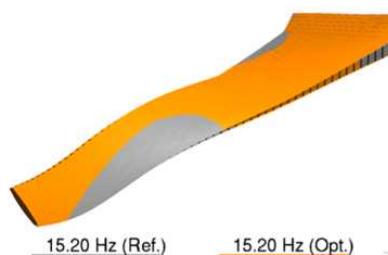
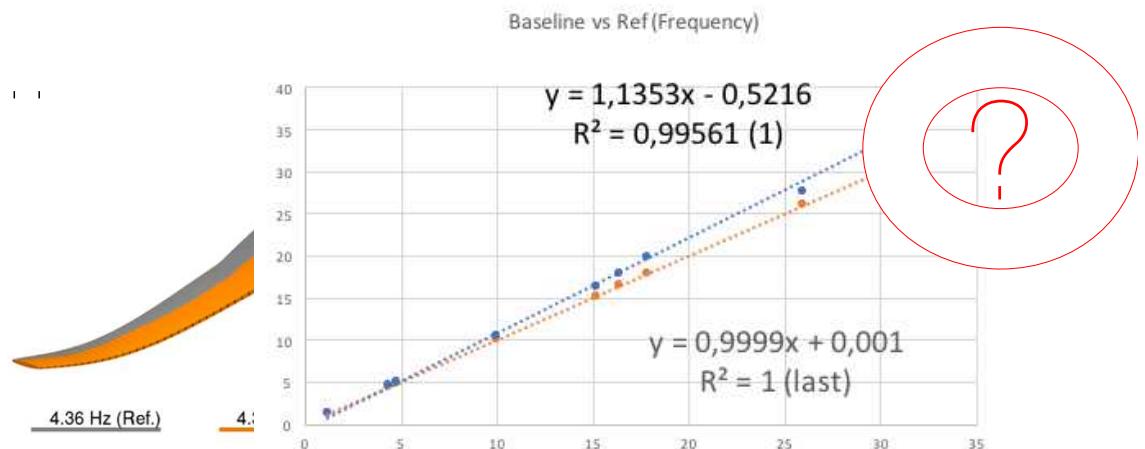
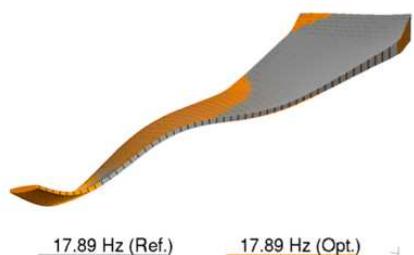
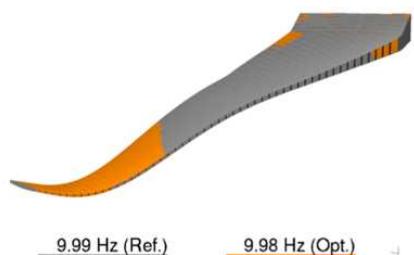
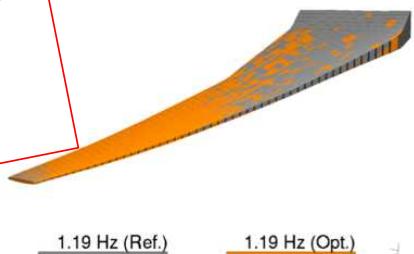
Results of the Optimization (SLSQP)

Optimality
Feasibility



Graphically AT CONVERGENCE...

BASELINE (ITERATION Last)
REFERENCE



MDO Workbench

Open questions



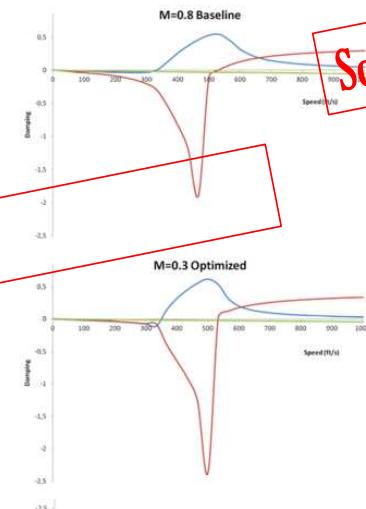
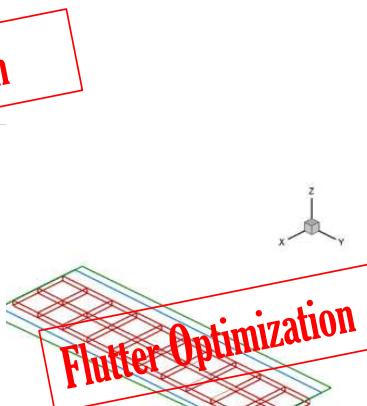
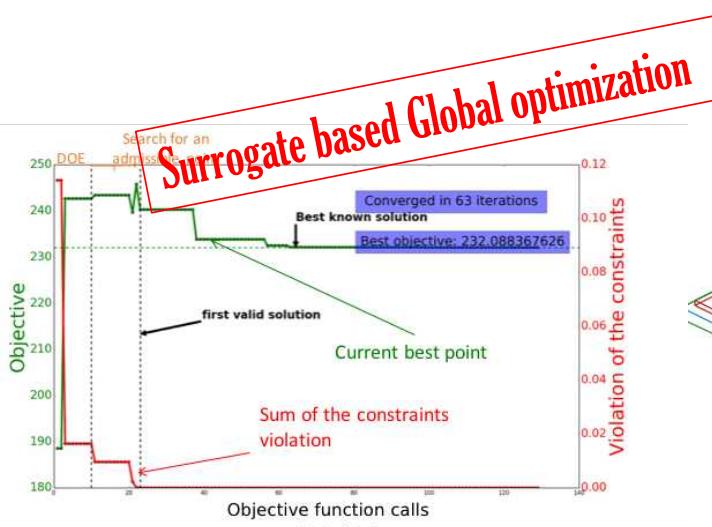
- AIRBUS CIFRE on Flutter Multidisciplinary including Control Law tuning (so called co-design)

Papers&conf

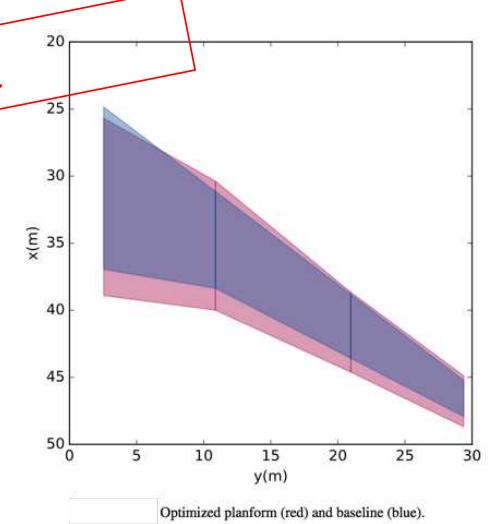
J. Mas Colomer et al Similarity Maximization of a Scaled Aeroelastic Flight Demonstrator via Multidisciplinary Optimization.
AIAA SCITECH 2017

J. Mas Colomer, et al, Static and Dynamic Aeroelastic Scaling of the CRM Wing via Multidisciplinary Optimization. WCSMO12
2017

Several Papers in preparation



Scaled Aircraft



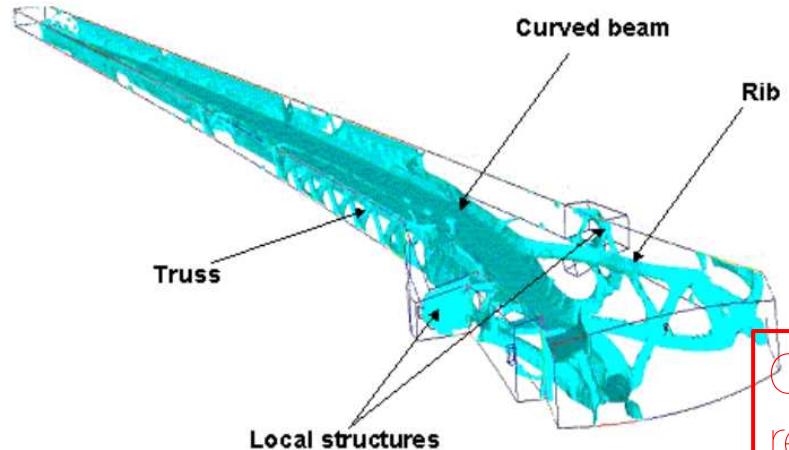
Outlines

1. Overview of Machine learning techniques
2. Aeroelasticity- Similarity

3. Discrete Continuous Optimization in CSM

Starting point*, Open at least 2 questions ??

*L.Krog, S.Grihon, A.Marasco, Smart design of structures through topology optimisation, 8th World Congress on Structural and Multidisciplinary Optimization, June 1 - 5, 2009, Lisbon,



Identified features:

- **Curved beam** for carrying bending loads
- Large **rib-like** structure connecting the gear rib area to the forward root joint
- **Truss-like** spar structures
- **Local structures** around gear-rib and pylon areas

Can we do pattern (structural element) recognition?
Can we process an optimization from a catalog of structural elements?

Pixels?

When the size of the FE model is increasing, the SIMP optimization problem is ...

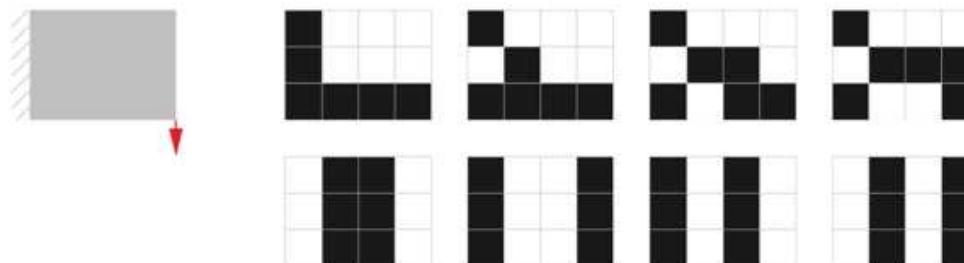


Chris Columbus *et al*, Pixels, movie 2015



Pixels

- Finding a solution by checking all the possible combinations IS impossible since the number of topologies nT increases exponentially with the number of finite elements n
- $nT = 2^n$,



The legal (top) and some illegal (bottom) topologies with 4 by 3 elements

Division into elements (pixels or voxels) and binary decision for each
or example 10,000 elements --> 210,000 possible configurations!

Intuitive Problem? Quadratic Form

- Objective function; Strain energy

$$\min c(\mathbf{x}) = \mathbf{U}^T \mathbf{F} = \mathbf{U}^T \mathbf{K} \mathbf{U}$$

$$x_e = \frac{\rho_e}{\rho_0} \text{ with } \quad (4)$$

with $\mathbf{K} = \mathbf{K}_0 \sum_{e=1}^N x_e^p$ one can write:

$$\min c(\mathbf{x}) = \sum_{e=1}^N (x_e)^p \mathbf{u}_e^T \mathbf{k}_0 \mathbf{u}_e \quad (5)$$

- Constraints: mass target

$$\frac{V(\mathbf{x})}{V_0} = f = \text{const} \Leftrightarrow \sum_{e=1}^N V_e x_e - V_0 f = 0 = h(\mathbf{x})$$

$$0 < \rho_{\min} \leq \rho_e \leq 1$$

$$\frac{\partial c}{\partial \rho_e} = -p (\rho_e)^{p-1} \mathbf{u}_e^T \mathbf{k}_0 \mathbf{u}_e$$

Transform discrete variables continuously
 (TO USE gradient-based algorithms)
 Cheap derivatives!

Visiting scholar at UoM

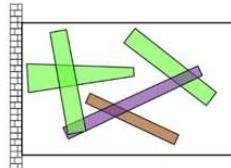
Can we do pattern (structural element) recognition?
Lead an optimization rom a catalog of structural elements?

Struct Multidisc Optim (2016) 53:1243–1260
DOI 10.1007/s00158-015-1372-3

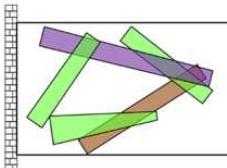
RESEARCH PAPER

A new topology optimization approach based on Moving Morphable Components (MMC) and the ersatz material model

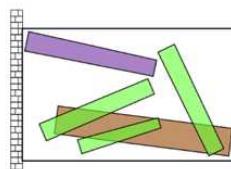
Weisheng Zhang¹ · Jie Yuan¹ · Jian Zhang¹ · Xu Guo¹



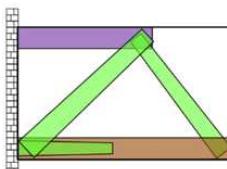
Components: the basic building blocks for MMC based topology optimization



Topology 1



Topology 2



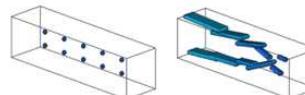
Topology 3

Struct Multidisc Optim
DOI 10.1007/s00158-016-1466-6

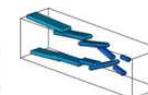
RESEARCH PAPER

A geometry projection method for the topology optimization of plate structures

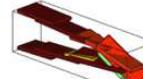
Shanglong Zhang¹ · Julián A. Norato¹ · Arun L. Gain² · Naesung Lyu³



(a) Initial Design



(b) Iteration 10



(c) Iteration 20



(d) Iteration 30



(e) Iteration 40



(f) Iteration 50



(g) Iteration 100



(h) Iteration 150



Explicit Topology Optimization

MDO Workshop@DLR

Optimization algorithm

Nodal movement

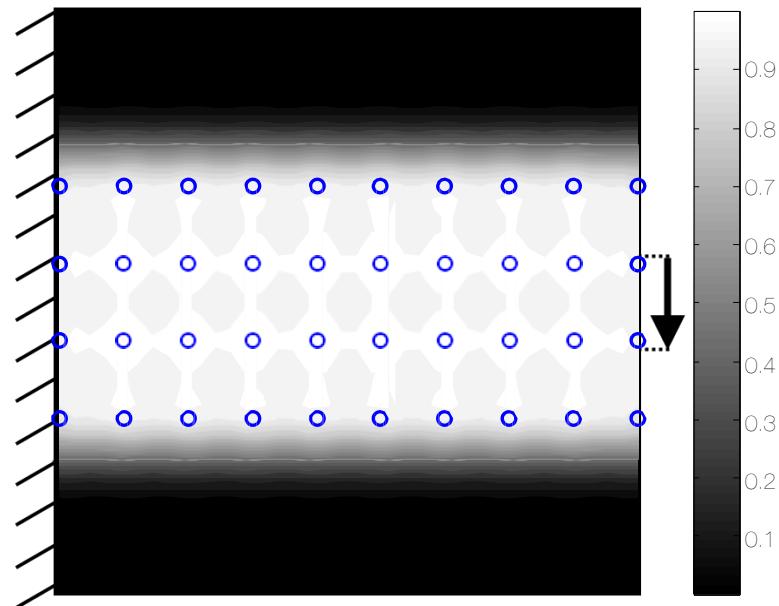
- Optimization algorithm based on decoupling
- Movement of nodes
 - Direction of the movement
- Measure performance of structure by compliance
 - Move mass nodes in the direction of decreasing compliance

$$C = \mathbf{f}^T \mathbf{u} \quad \frac{\partial C}{\partial x_j^I}$$

Original Work

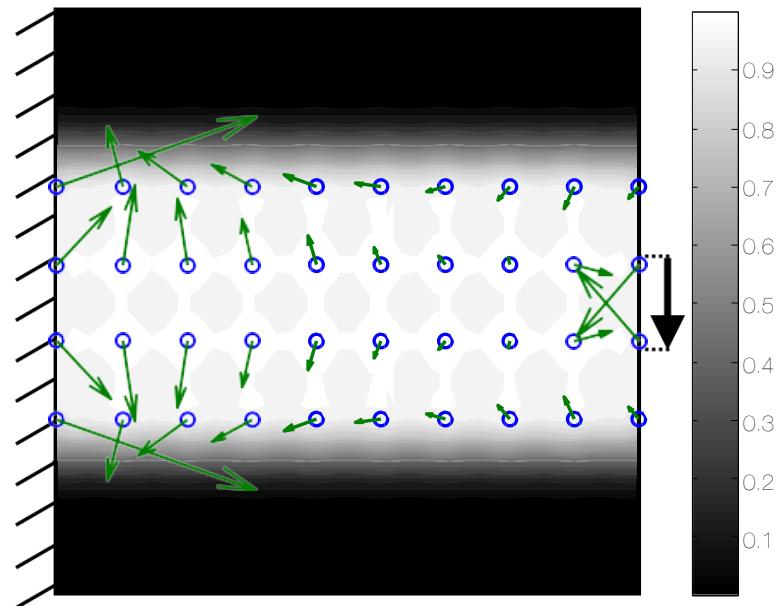
Optimization algorithm

Example of compliance sensitivity



Optimization algorithm

Example of compliance sensitivity

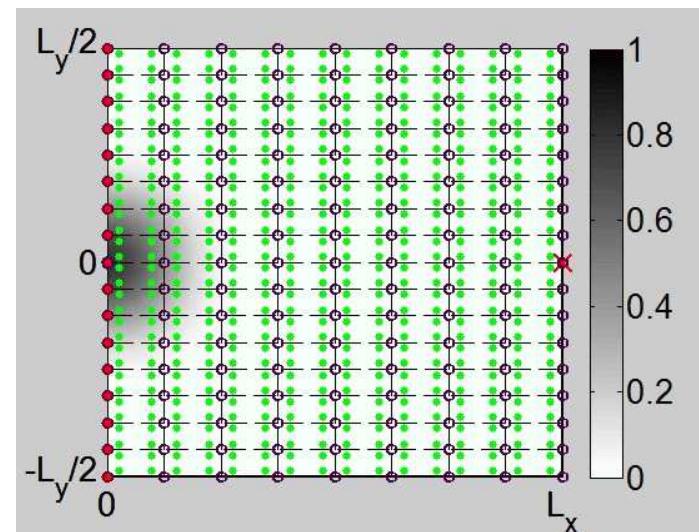


Moving Node Approach (MNA)

- Key idea:

Move material => optimal layout

- Regular discretization = precision
- Material distribution -> mass nodes



The variables (5 per Node)

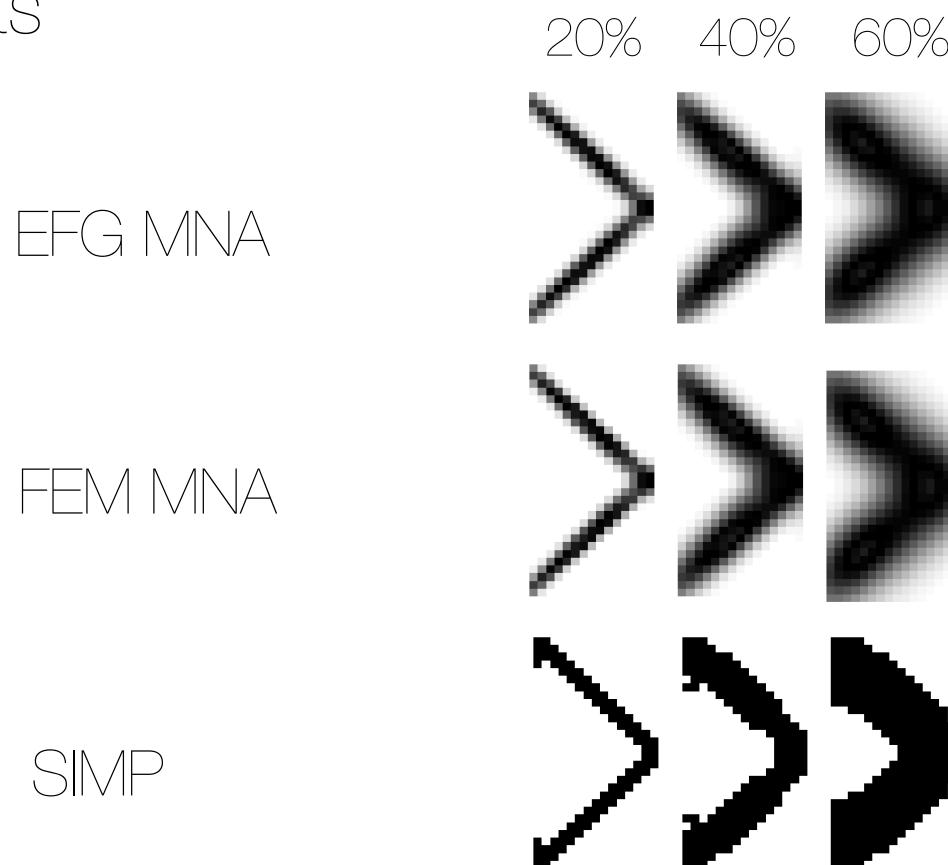
Optimization variables :

- Positions (x,y)
- Orientation (θ)
- Dimensions (L_x,L_y)



Deformable Structural Members

Results

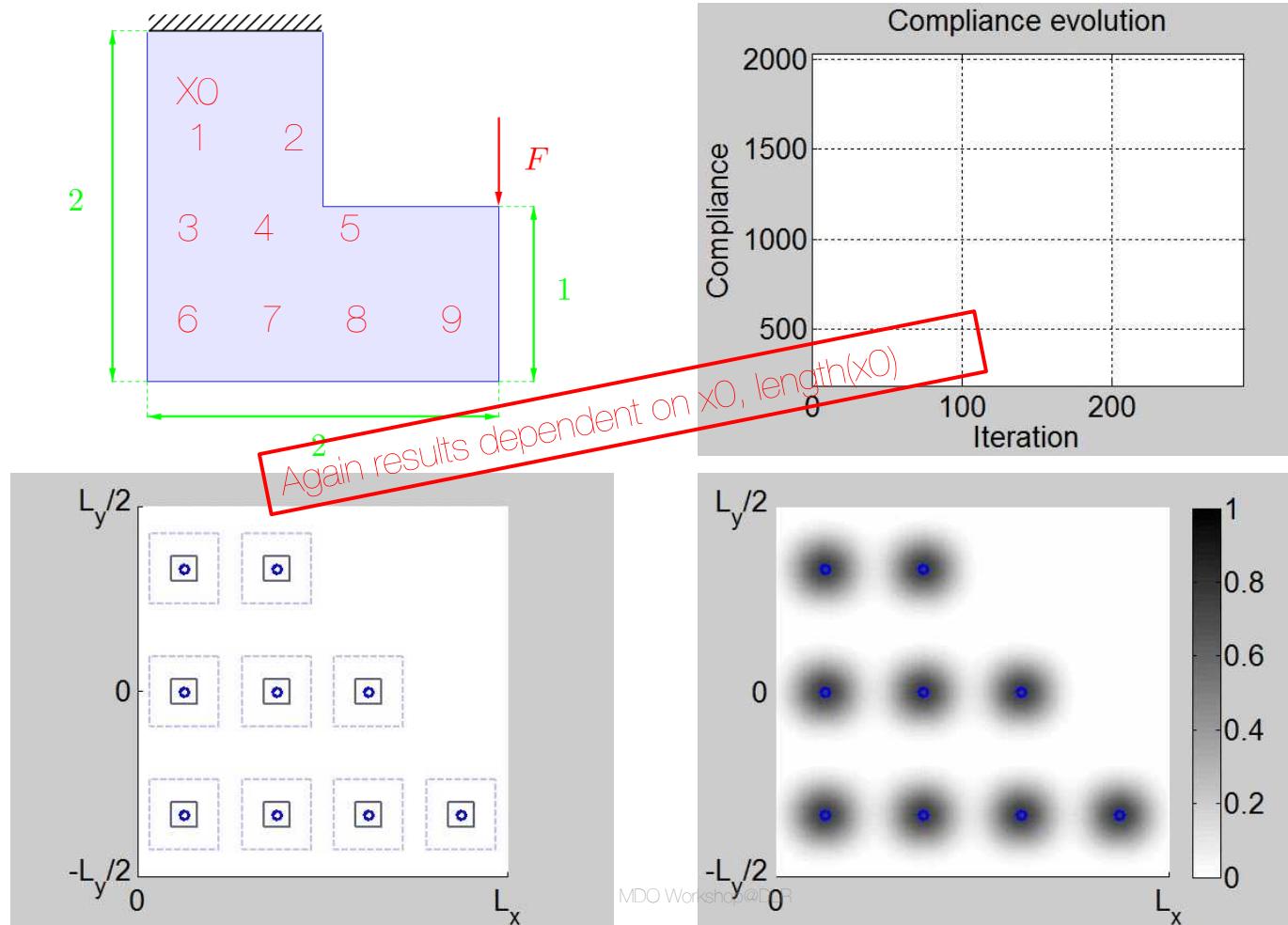


O. Sigmund, "A 99 line topology optimization code written in matlab", Structural and multidisciplinary optimization, vol. 21, no. 2, pp. 120-127, 2001.

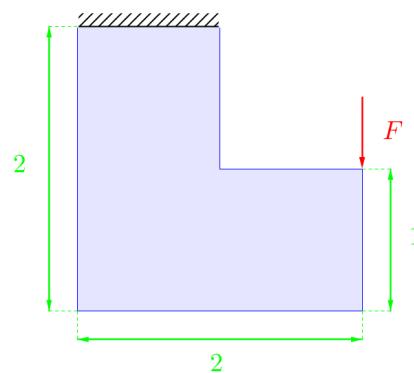
E. Andreassen, A. Clausen, M. Schevenels, B. S. Lazarov, and O. Sigmund, "Efficient topology optimization in matlab using 88 lines of code", Structural and Multidisciplinary Optimization, vol. 43, no. 1, pp. 1-16, 2011.

Length(x_0)

Our Results on L-Shape 9*5 variables



Results on L-Shape (Best solution using a multistart approach)



MNA



$C = 127$

SIMP



$C = 94$

```
disp('MNA')
topmna(x0,nelx,nely,volfrac,3,[ratio;aspect],tolchange);

disp('SIMP')
top88(nelx,nely,volfrac,3,2,1)
```

MDO Workshop@DLR

TopMNA include Few hyperparameters, starting from a « dense » regular grid with Fusion/merging/Recognition of beam elements

Papers&conf

PJ. Barjhoux et al. Mixed Variable Structural Optimization: toward an Efficient Hybrid Algorithm, WCSMO12, 2017

G. Raze et al, Optimisation topologique sans maillage : vers la reconnaissance d'éléments structuraux, CSMA 2017

Several Papers in preparation



Open questions



Conclusions

- New Surrogate and ML technics for an automated optimal design process
 - structural/aeroelastic constraints at the early stage of the MDO loop
 - A new step toward a catalogue based-multimaterial structures design
- Teach/apply our (simplified) methodologies in 2 MDO courses (MsC level) at SUPAERO with ONERA/AIRBUS
- We also have interesting stuff in FSI-nonlinear transient analysis, Isogeometric (IGA) Shell Structures Optimization ...

<http://www.institut-clement-ader.org/pageperso.php?id=jmorlier>

- Thanks to My co-workers: Joaquim Martins, Nathalie Bartoli, Emmanuel Benard, Claudia Bruni Emmanuel Rachelson, Nicolas Gourdain, John Hwang, Mohamed Bouhlel, Thierry Lefebvre, Youssef Diouane, Sylvain Dubreuil, Christian Gogu and PhDs Pierre-Jean Barjhoux, Simone Coniglio, Elisa Bosco, Joan Mas Colomer, Ankit Chiplunkar, and MsC Ghislain Haine, ...

Surrogate
modeling in HD,
focus on
derivatives

Visit :
<https://github.com/SMTorg/SMT>



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Focus on derivatives
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SMT: Surrogate Modeling Toolbox

The surrogate model toolbox (SMT) is an open-source Python package consisting of libraries of surrogate modeling methods (e.g., radial basis functions, kriging), sampling methods, and benchmarking problems. SMT is designed to make it easy for developers to implement new surrogate models in a well-tested and well-documented platform, and for users to have a library of surrogate modeling methods with which to use and compare methods.

The code is available open-source on [GitHub](#).

Focus on derivatives

SMT is meant to be a general library for surrogate modeling (also known as metamodeling, interpolation, and regression), but its distinguishing characteristic is its focus on derivatives, e.g., to be used for gradient-based optimization. A surrogate model can be represented mathematically as

$$y = f(\mathbf{x}, \mathbf{xt}, \mathbf{yt}),$$

where $\mathbf{xt} \in \mathbb{R}^{n_{XT}}$ contains the training inputs, $\mathbf{yt} \in \mathbb{R}^m$ contains the training outputs, $\mathbf{x} \in \mathbb{R}^n$ contains the prediction inputs, and $\mathbf{y} \in \mathbb{R}^m$ contains the prediction outputs. There are three types of derivatives of interest in SMT:

1. Derivatives (dy/dx): derivatives of predicted outputs with respect to the inputs at which the model is evaluated.
2. Training derivatives (dy/dt): derivatives of training outputs, given as part of the training data set, e.g., for gradient-enhanced kriging.
3. Output derivatives (dy/dy): derivatives of predicted outputs with respect to training outputs, representing how the prediction changes if the training outputs change and the surrogate model is re-trained.

Not all surrogate modeling methods support or are required to support all three types of derivatives; all are optional.