1970-1990



2010-2020



1990-2010



2020+





Recent progress in engineering design with MDO/AI4E

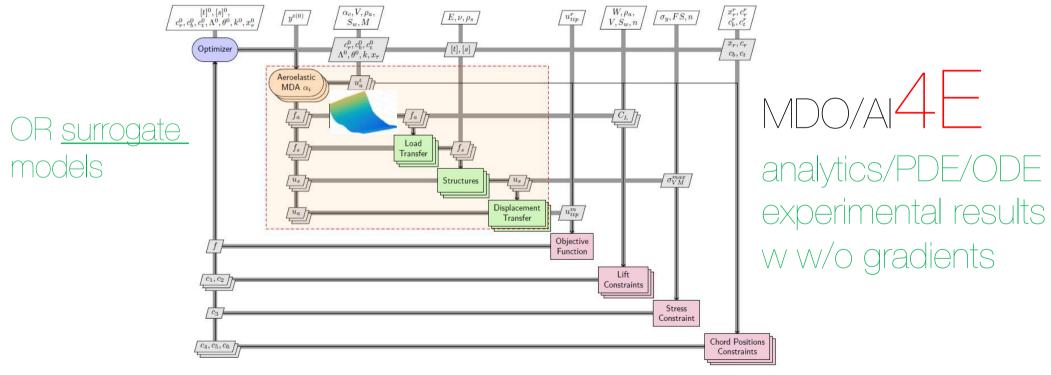
Prof. Joseph Morlier



Multidisciplinary Design Optimization

No MDO without MDA

 Multidisciplinary Design Optimization (MDO) focuses on solving optimization problems spanning across multiple interacting disciplines



seven 12/10/22

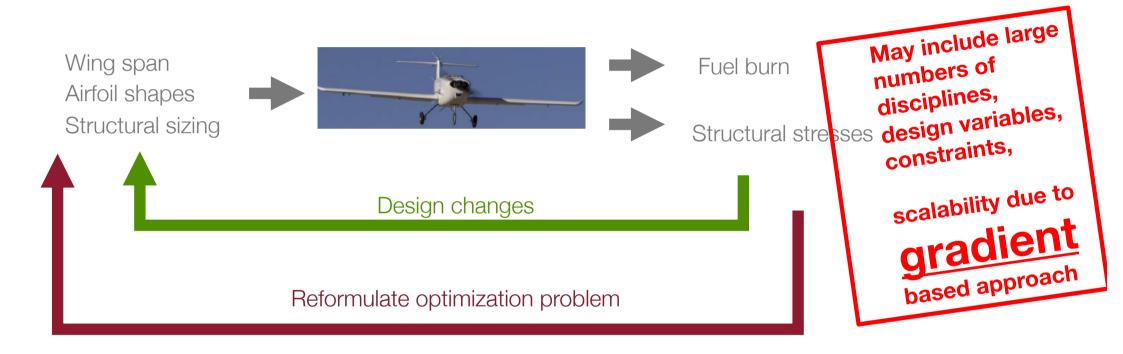
A way to fully automate the design process



Design optimization problem:

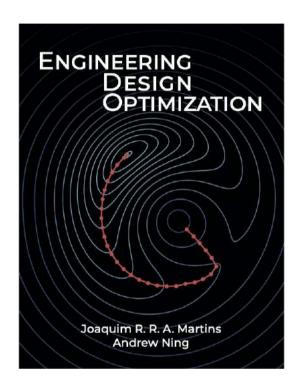
 $\begin{array}{lll} & \text{minimize} & f(x) & \text{objective} \\ & \text{with respect to} & x & \text{design variables} \\ & \text{subject to} & c(x) \leq 0 & \text{constraints} \end{array}$

Nowadays' Engineering Design Optimization is MDO (M:Multidisciplinary)

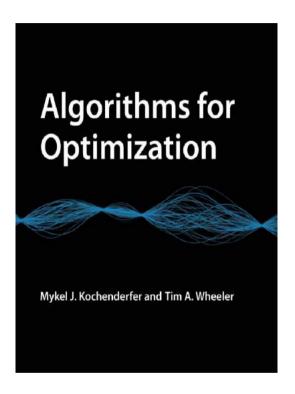


Post-optimality studies

Good Starting Point (x0)



https://github.com/mdobook/resources



https://github.com/sisl/algforopt-notebooks

@Philips: Combining disciplines provides better solutions



Tools/Results » oriented presentation

Duration	Description	Agenda
3'	MDO/AI	New trends
7'	Surrogate	SMT
7'	Ecodesign	Lighter, Stronger, Greener
3'	Conclusions	And future works?

The initial Question was: « Joseph I have a costly multiphysics simulation chain. Can you give me the optimal design at fixed budget? Let's say after the week end (48h of HPC)? »

For theoretical background, have a look to

- 1. Bouhlel, M. A., Hwang, J. T., Bartoli, N., Lafage, R., Morlier, J., & Martins, J. R. (2019). A Python surrogate modeling framework with derivatives. Advances in Engineering Software, 135, 102662.
- 2. N. Bartoli, T. Lefebvre, S. Dubreuil, R. Olivanti, N. Bons, J.R.R.A. Martins, M.-A. Bouhlel, J. Morlier, "Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design ", Aerospace Science and Technology, 90, 85-102., 2019
- 3. 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
- 4. Chiplunkar, E. Rachelson, M. Colombo and J. Morlier. Adding Flight Mechanics to Flight Loads Surrogate Model using Multi-Output Gaussian Processes. AIAA AVIATION 2016
- 5. Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Multidisciplinary design optimization with mixed categorical variables for aircraft design. In AIAA SCITECH 2022 Forum (p. 0082). has been awarded the 2022 AIAA Multidisciplinary Design Optimization Best Paper Award
- 6. Bellier P., , Urbano A., Morlier J. Bil C., and Pudsey A., Impact of Life Cycle Assessment Considerations on Launch Vehicle Design, 73rd International Astronautical Congress (IAC) 2022 Paris, France

Au programme

Duration	Description	Agenda
3'	MDO/AI	New trends
7'	Surrogate	SMT
7'	Ecodesign	Lighter, Greener, stronger
3'	Conclusions	

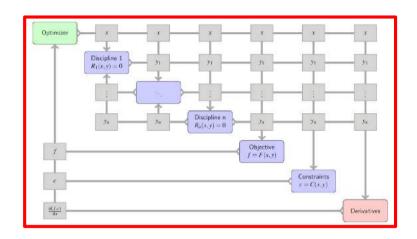


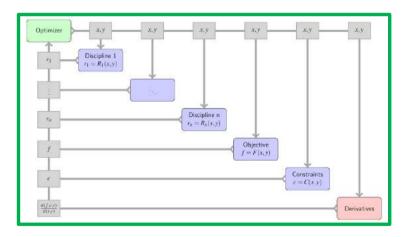
Large-scale MDO?

- https://lsdo.eng.ucsd.edu/research
- Prof. John Hwang

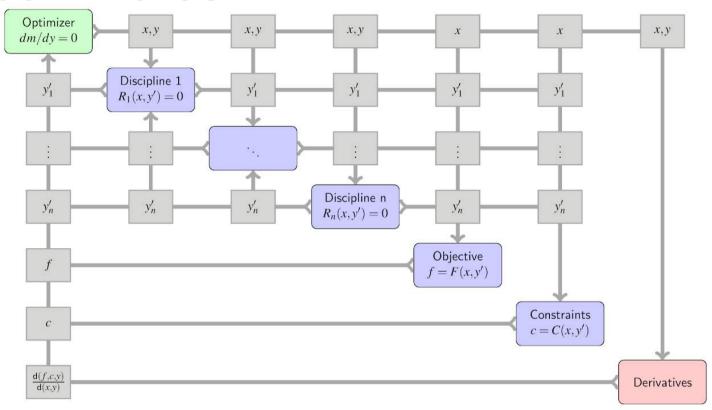
In the reduced-space method, the variables are computed by solvers that are part of the model. In the full-space method, the optimizer is responsible for computing the state variables.

The reduced-space method results in a smaller, easier-to-solve optimization problem, while the full-space method has more inexpensive model evaluations.



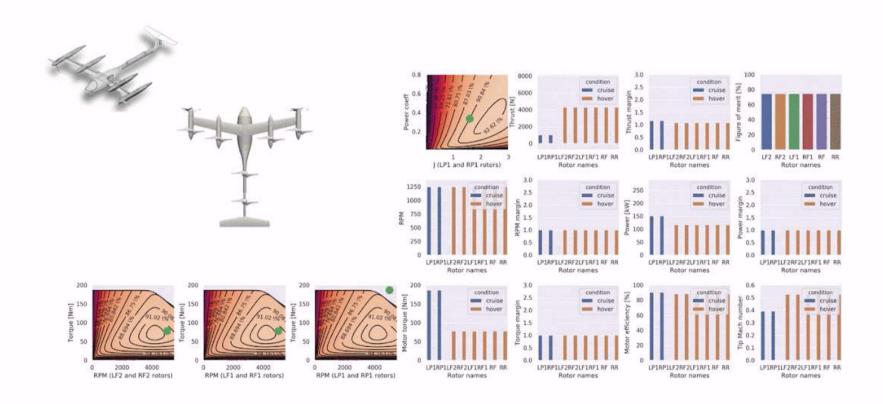


Best of both worlds:



the efficiency of the full-space method and the robustness of the reduced-space method.

Large-scale design optimization is an invaluable tool in the

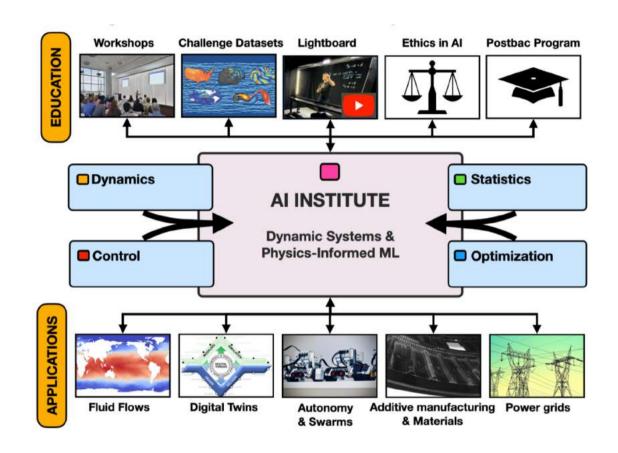


AI4E

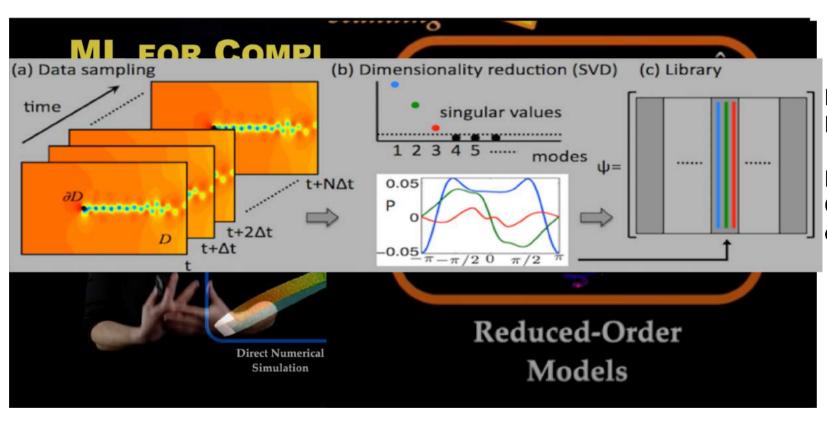
- http://dynamicsai.org
- Prof. J. Nathan Kutz,
- Prof. S. Brunton

"The goal is that anyone anywhere interested in AI for engineering can self-educate. There's no barrier to entry for those who want to learn."

J. Nathan Kutz,



Al can Accelerate CFD



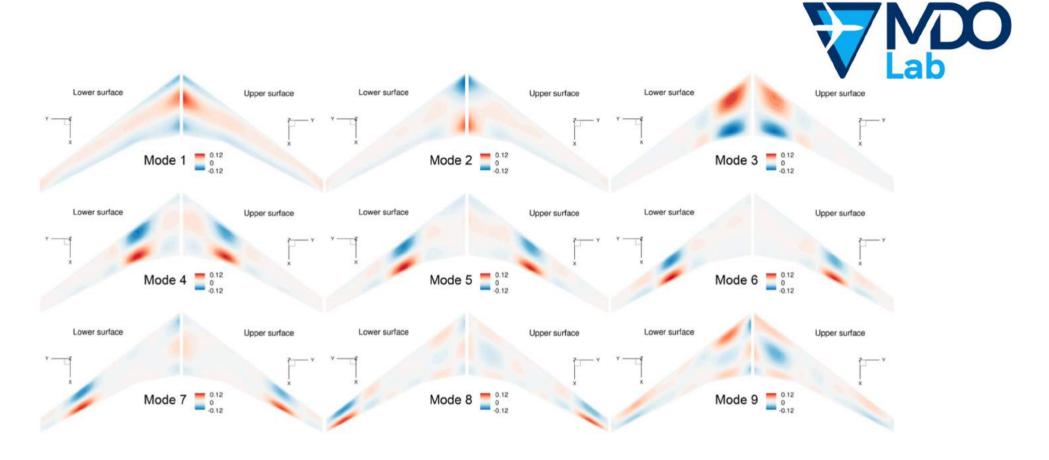
Reduced Order Model ROM for digital twin

K. Willcox UTEXAS
C. Fahrat STANFORD
etc...

SVD, POD, KLD, PCA

Machine Learning in Aerodynamic Shape Optimization

J. Li, X. Du, and J. R. R. A. Martins *Progress in Aerospace Sciences*, 2022



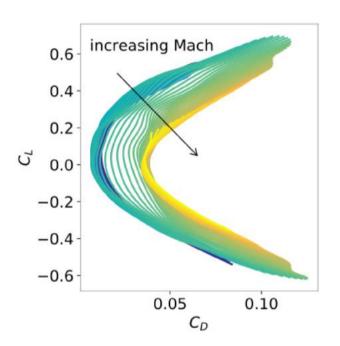
Au programme

Duration	Description	Agenda
3'	MDO	New trends
7'	Surrogate	SMT
7'	Ecodesign	Lighter, Greener, stronger
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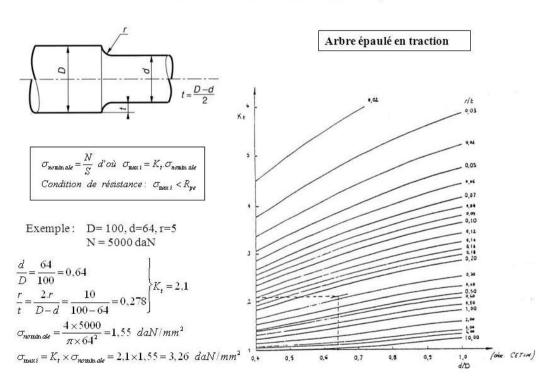


Surrogate: AI4E

Surrogate is the new abacus



Coefficient de concentration de contrainte : K_t .



ML vs Engineering

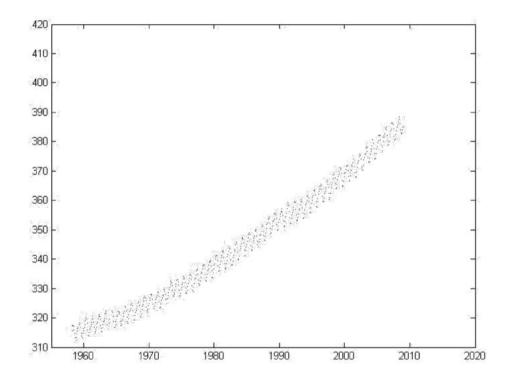
Kriging (Pionneer) Gaussian Processes (link with Al) Developed by Daniel Krige – 1951; formalized by Georges Mathéron in the 60's (Mines Paris) Krige, D. G., 1951, A statistical approach to some basic mine valuation problems on the Witwatersrand: J. Chem. Metal. Min. Soc. South Africa, v. 52, p. 119-139. Matheron, G., 1963b, Principles of geostatistics: Economic Geol., v. 58, p. 1246-1266. Matheron, G., 1963b, Principles of geostatistics: Economic Geol., v. 58, p. 1246-1266.

Qualitative claims such as "ML works OK for interpolation but doesn't work for extrapolation" are wrong.

https://arxiv.org/abs/2110.09485

http://extrapolated-art.com

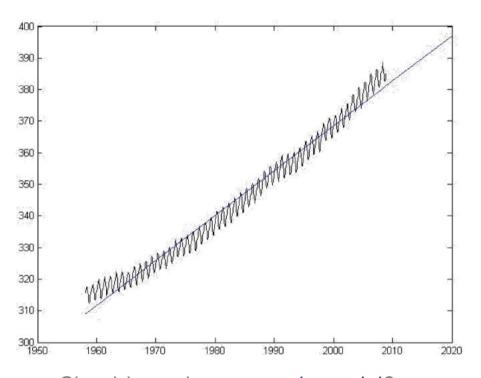
Limit of linear models for prediction



Month-wise data of CO₂ concentration in atmosphere at Hawaii

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

Example – Linear Regression



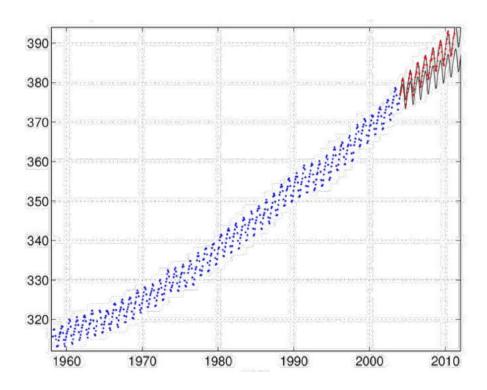
Should we choose a polynomial?

What degree of polynomial should we choose? (overfitting)

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

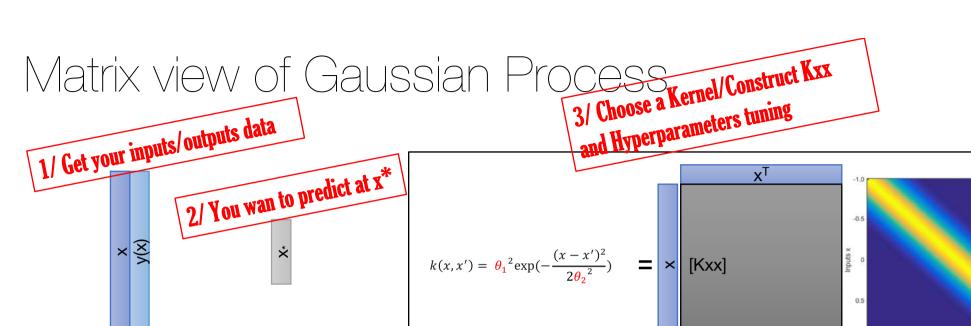
| mage Source: http://mlg.eng.cam.ac.uk/teaching/4f13/1314/

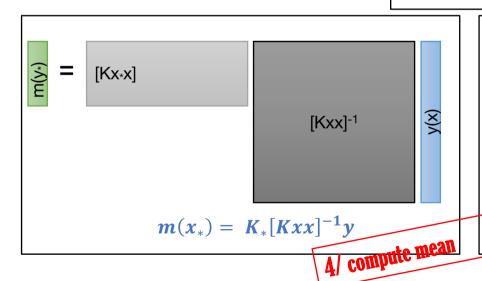
Example – Gaussian Process

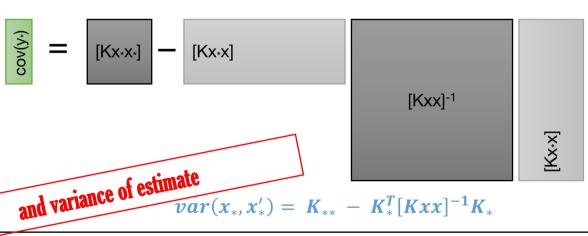


Predicted variance after year 2005 in grey, real data-points in red

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

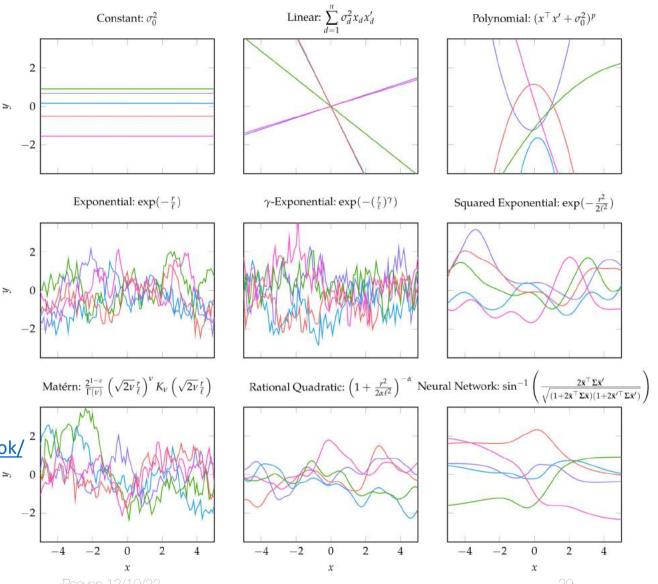






Gaussian Processes

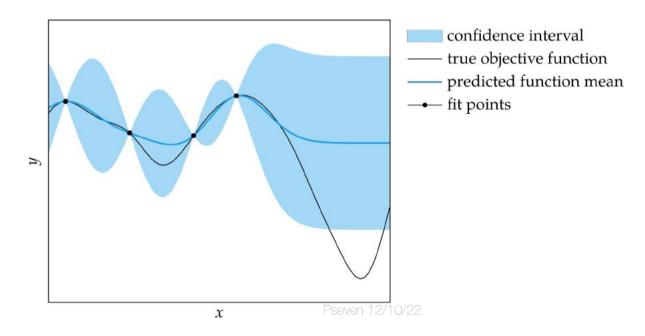
• Examples of the same Gaussian process with different kernel functions



https://www.cs.toronto.edu/~duvenaud/cookbook/

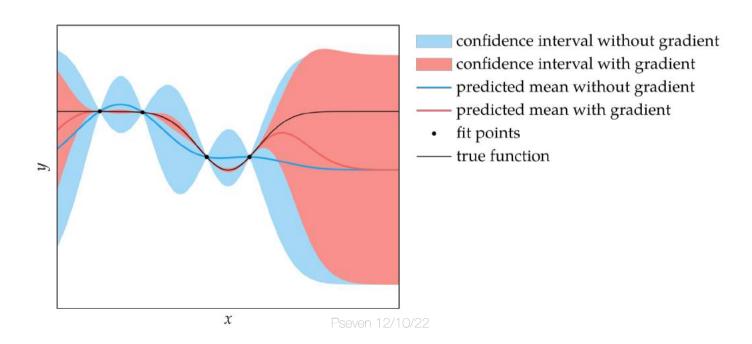
Prediction

- Using variance to compute standard deviation, the predicted mean and standard deviation can be computed at any point
- This enables calculation of the 95% confidence region



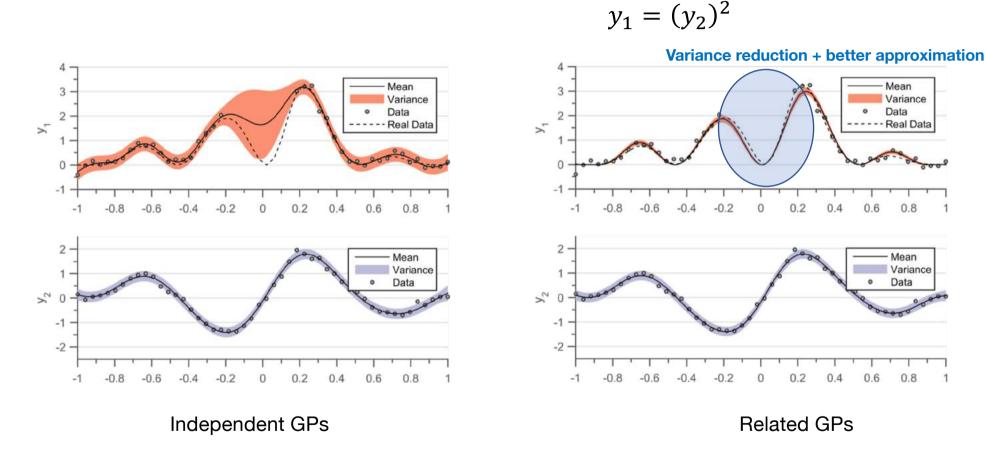
Gradient Measurements

 If function gradient evaluations can be made as well, the process can be extended to include gradient predictions for higher prediction fidelity



Incorporating Prior Information from Engineering Design

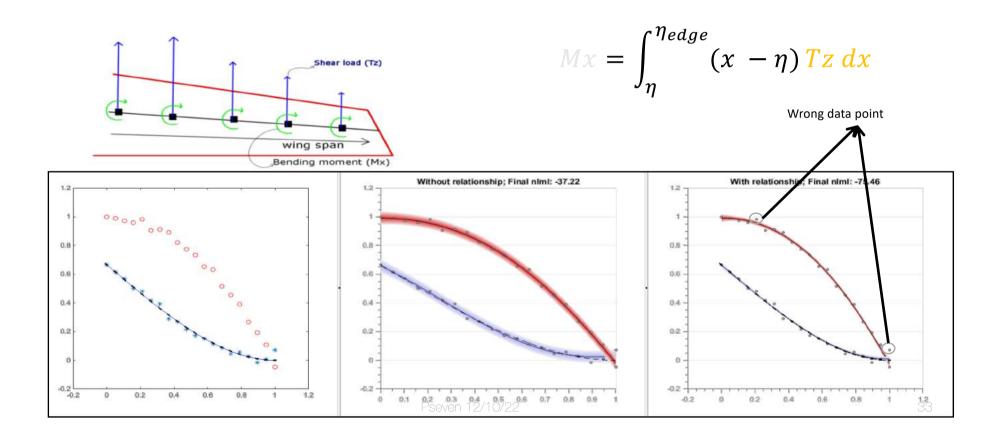
https://github.com/ankitchiplunkar/thesis_isae



before PINN and SciML...

https://github.com/ankitchiplunkar/thesis_isae

Flight test - Relationship between Tz and Mx

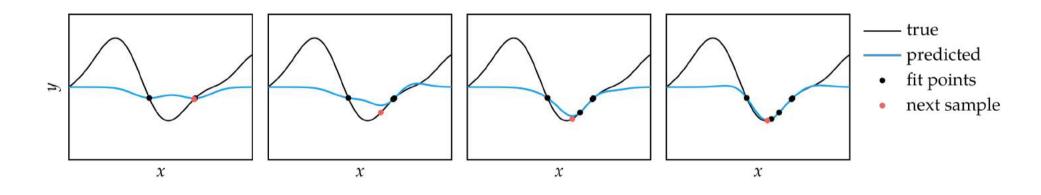


Surrogate Optimization

- Given a surrogate model with both prediction and confidence parameters, an optimization procedure must balance the search for the expected optimal point and decreasing uncertainty
- > balance exploitation with exploration

Prediction-Based Exploration

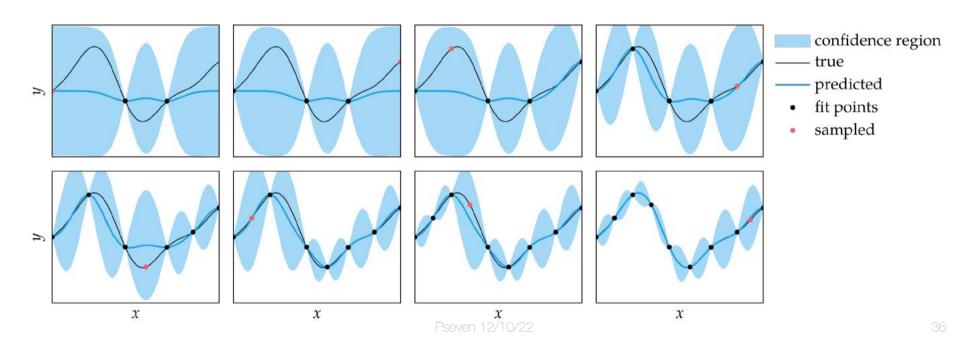
- Focuses exclusively on exploitation, also called greedy approach
- When using a Gaussian process surrogate model, prediction-based exploration simply optimizes over the mean function and ignores uncertainty



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Error-Based Exploration

- Focuses exclusively on exploration
- For Gaussian processes, error-based exploration simply minimizes the maximum standard deviation within a specified domain

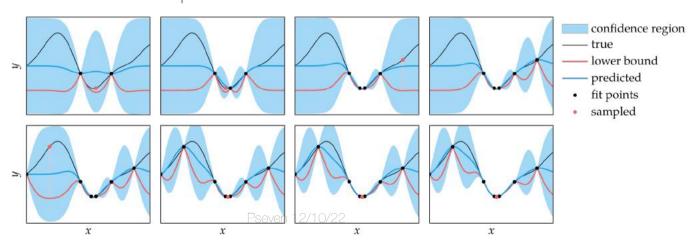


Lower Confidence Bound Exploration

- Tradeoff between exploration and exploitation
- The next sample minimizes the lower confidence bound of the objective function

$$LB(\mathbf{x}) = \hat{\mu}(\mathbf{x}) - \alpha \hat{\sigma}(\mathbf{x})$$

where $a \ge 0$ is the tradeoff parameter



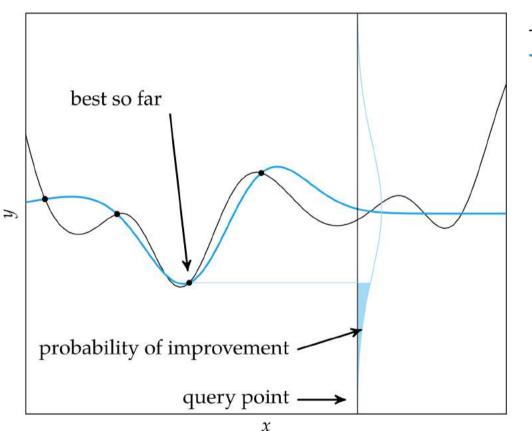
Probability of Improvement Exploration

- Searches at the location with the highest probability of improvement
- Improvement is defined as

$$I(y) = \begin{cases} y_{\min} - y & \text{if } y < y_{\min} \\ 0 & \text{otherwise} \end{cases}$$

• The probability of improvement is defined as

$$\begin{split} P(y < y_{\min}) &= \int_{-\infty}^{y_{\min}} \mathcal{N}(y \mid \hat{\mu}, \hat{\sigma}) dy \\ &= \Phi\bigg(\frac{y_{\min} - \hat{\mu}}{\hat{\sigma}}\bigg) \end{split}$$



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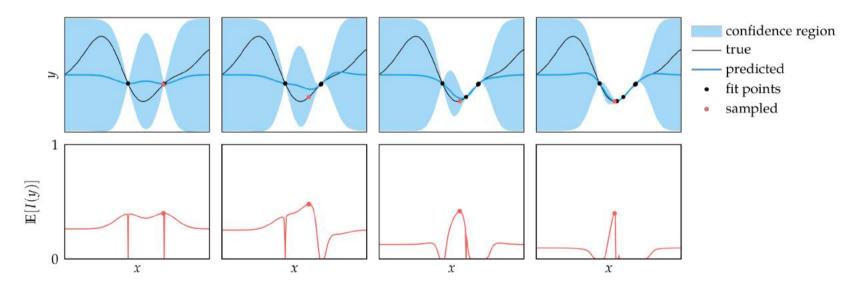
true

predicted

fit points

Expected Improvement Exploration

El Expected
Improvement
exploration seeks to
maximize expected
improvement at each
step



How to build an efficient iterative process?

- Find the global minimum with a limited budget of function evaluations
- Use Bayesian information to detect interesting and promising areas (exploitation/exploration trade-off)
- SEGOMOE optimizer

 Global aspect

 SEGOMOE

 SEGOMOE

 SEGOMOE

 SEGOMOE

 SEGOMOE

 THE FRENCH AEROSPACE LAB

 Gradientbased
 algorithms

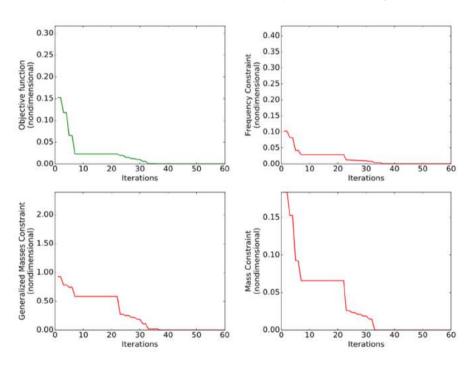
Evaluation cost

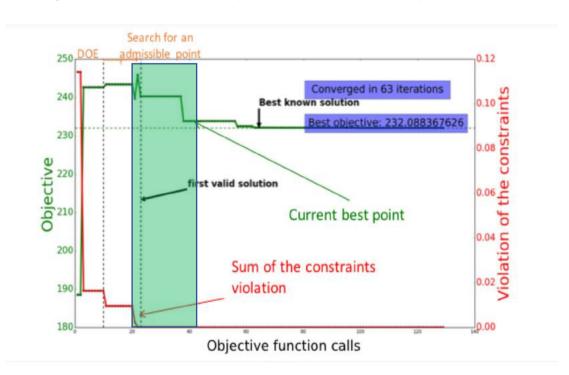
N. Bartoli, T. Lefebvre, S. Dubreuil, R. Olivanti, N. Bons, J.R.R.A. Martins, M.-A. Bouhlel, J. Morlier, "Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design", Aerospace Science and Technology, 90, 85-102., 2019

40

Convergency graphs

Gradient based Optimality, Feasibility SBO Exploration, Exploitation

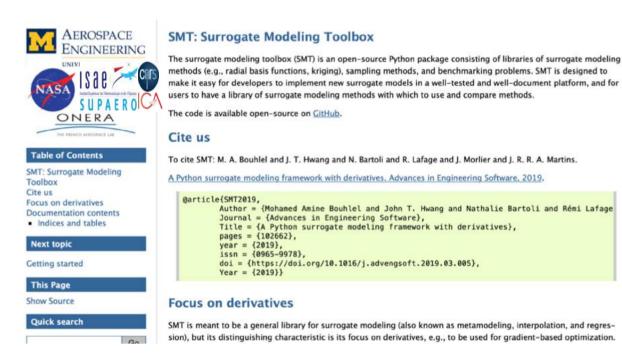




Stopping criteria: tolfun, tolx, maxiter

Stopping criteria: Max Budget (Function calls)

...in 2017 the first SMT version was released



The paper had to wait until 2019...

Bouhlel, M. A., Hwang, J. T., Bartoli, N., Lafage, R., Morlier, J., & Martins, J. R. (2019). A Python surrogate modeling framework with derivatives. *Advances in Engineering Software*, 135, 102662.

SMT structure — Surrogate herefreeased this 1

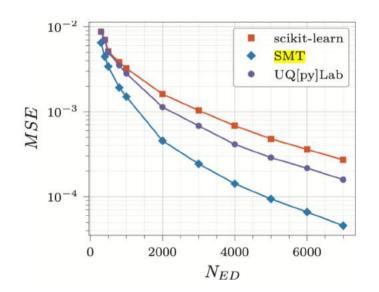
of components estimation in KPLS surrogate models (#325) Add_propagate_uncertainty_option in MFK method (#320); when True the variance of lower fidelity levels are taken into account. Add ordered variables management in mixed integer surrogates (#326, #327), Deprecation warning: INT type is deprecated and superseded by ORD type. Update version for the GOWER distance model. (#330) Implement generalization of the homoscedastic hypersphere kernel from Pelamatti et al. (#330) Radial basis functions Svante Wold (1978) Cross-Validatory Estimation of the Number of Components in Inverse-distance weighting Factor and Principal Components Models, Technometrics, 20:4, 397-Regularized minimal-energy tensor-product splines 405, DOI: 10.1080/00401706.1978.10489693 Useful for low dimensional problem Least-squares approximation Second order polynomial approximation useful for kriging in high dimension Kriging Kriging with partial least square (KPLS) Gradient-enhanced KPLS Focus on derivatives Gradient-enhanced neural networks Marginal Gaussian process

Compare +

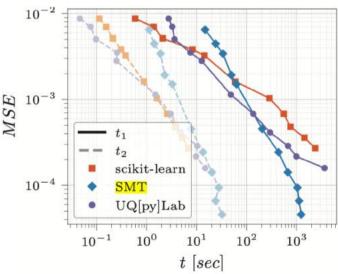
Bouhlel, M. A., Hwang, J. T., Bartoli, N., Lafage, R., Morlier, J., & Martins, J. R. (2019). A Python surrogate modeling framework with derivatives. Advances in Engineering Software, 135, 102662.

Proceedings of the 32nd European Safety and Reliability Conference (ESREL 2022)

reaches a better accuracy (up to almost an order of magnitude) than the other toolboxes.

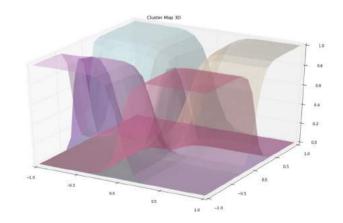


 As evidence, the SMT package
 SMT tends to perform quickly than the other packages for higher *NED* in calibrating the Kriging model, but not in its evaluation.



ALE

- Mixture of experts (MOE) if 1 expert, comparison of all experts
- Variable-fidelity modeling (VFM)
- Multi-Fidelity Kriging (MFK)
- Multi-Fidelity Kriging KPLS (MFKPLS)
- Multi-Fidelity Kriging KPLSK (MFKPLSK)
- Efficient Global Optimization (EGO)
- Mixed-Integer Sampling and Surrogate (Continuous Relaxation)
- Mixed-Integer Surrogate with Gower Distance



How to approximate highly non linear function?

- •Handle heterogeneity and non linearity (all phases in the flight mission, buckling factor for composite fuselage)
- •Combine multiple surrogate models divide-and- conquer strategy

AI4E

- Mixture of experts (MOE)
- Variable-fidelity modeling (VFM)
- Multi-Fidelity Kriging (MFK)
- Multi-Fidelity Kriging KPLS (MFKPLS)
- Multi-Fidelity Kriging KPLSK (MFKPLSK)
- Efficient Global Optimization (EGO)
- Mixed-Integer Sampling and Surrogate (Continuous Relaxation)
- Mixed-Integer Surrogate with Gower Distance

How to handle multi-information sources?

ullet Access to different information sources that approximate y(x) with varying accuracy and cost Hierarchical relationships among information sources: low-fidelity / high-fidelity

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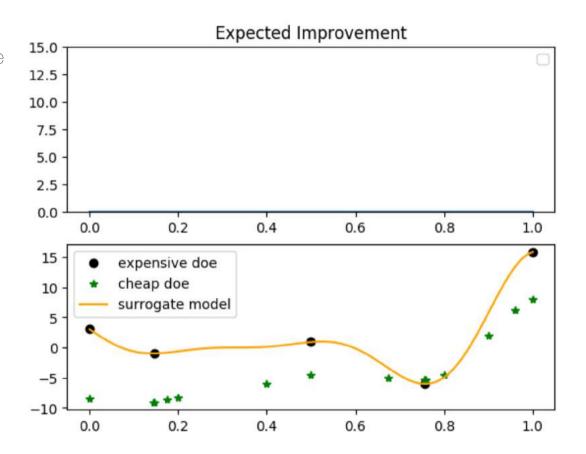
Why multifidelity?

What if Several levels of fidelity of the same simulation are available?

(in aerodynamics **multifidelity** means: Liflting line theory, Vortex lattice method, and RANS CFD simulation tools available)

Raw approach luse ow fidelity for exploration and high fidelity for exploitation

Our approach combines Bayesian optimization with multifidelity



AI4E

- Mixture of experts (MOE)
- Variable-fidelity modeling (VFM)
- Multi-Fidelity Kriging (MFK)
- Multi-Fidelity Kriging KPLS (MFKPLS)
- Multi-Fidelity Kriging KPLSK (MFKPLSK)
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- Mixed-Integer Sampling and Surrogate (Continuous Relaxation)
- Mixed-Integer Surrogate with Gower Distance

Bayesian optimization (EGO without constraint) for continuous and mixed variables



Included some dedicated Jupyter Notebooks

SMT_EGO_application.ipynb

SMT_MixedInteger_application.ipynb

SMT_Noise.ipynb

SMT_Tutorial.ipynb

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AI4E

- Mixture of experts (MOE
- Variable-fidelity modeling (VFM)
- Multi-Fidelity Kriging (MFK)
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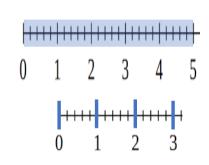
Focus on mixed integer

Variables types:

Continuous (x) Ex: wing length

Integer (z) Ex: winglet number

Categorical (u) Ex: Plane shape





Categorical variables: n variables,

n=2

u1= shape

u2= color

<u>Levels:</u> L_i levels for I in 1,...n,

 $L_1 = 3$, $L_2 = 2$.

Levels(u1)= square, circle,

rhombus

Levels(u2)= blue, green

Categories: $\prod_{i=1}^{n} L_i$, 2*3=6

- Blue square
- Blue circle
- Blue rhombus
- Green square
- Green circle
- Green rhombus

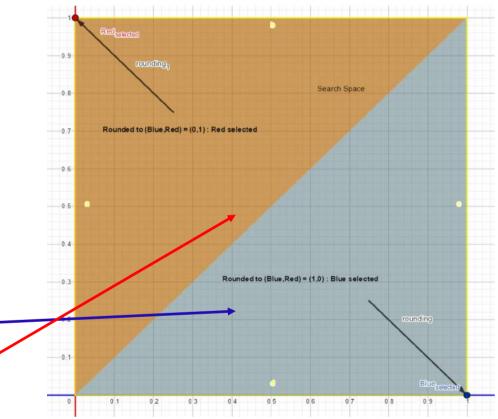
Focus on mixed integer

Continuous relaxation

E. C. Garrido-Merchán, and D. Hernández-Lobato. "Dealing with categorical and integer-valued variables in Bayesian Optimization with Gaussian processes". Neurocomputing, vol. 380 (2020), pages 20-35

Example with 1 categorical variable and two levels

- Red color
- Blue color
- → Categorical variable replaced by two continuous variables denoted by X₁ and X₂
- If $X_1 > X_2 = > (1., 0.) = >$ Blue color
- If $X_1 < X_2 => (0.,1.) => Red color$



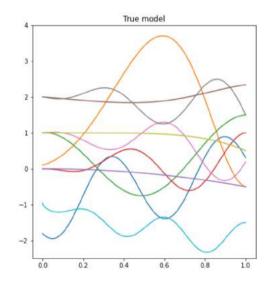
Focus on mixed integer

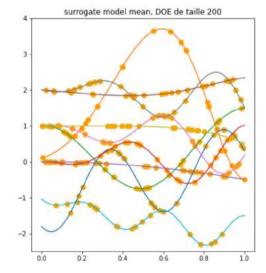
Continuous relaxation

Validation problem $n_{var} = 2$ Variable types: continuous and categorical with 10 levels. $n_{var,relaxed} = 11$

Toy function surrogate

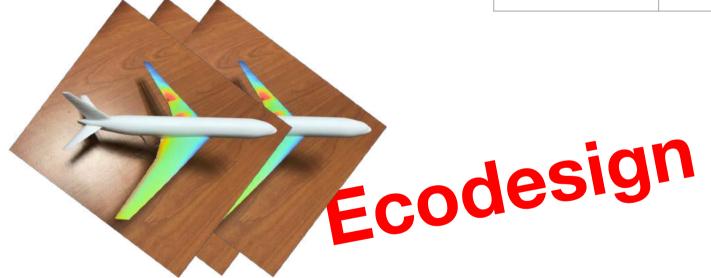
$$f(x,z) = \begin{cases} \cos{(3.6\pi(x-2))} + x - 1 & \text{if} \quad z = 1, \\ 2\cos{(1.1\pi)} \exp{(x)} - \frac{x}{2} + 2 & \text{if} \quad z = 2, \\ \cos{(2\pi x)} + \frac{1}{2}x & \text{if} \quad z = 3, \\ x \left(\cos{(3.4\pi(x-1))} - \frac{x-1}{2}\right) & \text{if} \quad z = 4, \\ -\frac{x^2}{2} & \text{if} \quad z = 5, \\ 2\cos{(\frac{\pi}{4}\exp{(-x^4)})^2} - \frac{x}{2} + 1 & \text{if} \quad z = 6, \\ x\cos{(3.4\pi x)} - \frac{x}{2} + 1 & \text{if} \quad z = 7, \\ x(-\cos{(7\frac{\pi}{2}x)} - \frac{x}{2}) + 2 & \text{if} \quad z = 8, \\ -\frac{x^5}{2} + 1 & \text{if} \quad z = 9, \\ -\cos{(5\frac{\pi}{2}x)^2} \sqrt{x} - \frac{\ln{(x+0.5)}}{2} - 1.3 & \text{if} \quad z = 10. \end{cases}$$



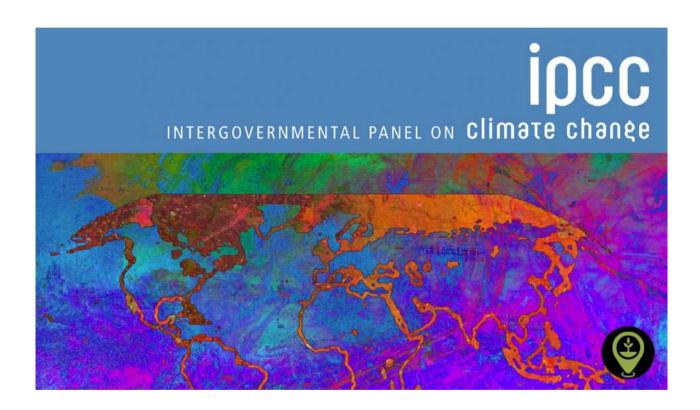


Au programme

Duration	Description	Agenda
3'	MDO	New trends
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3'	Conclusions	



Aerospace sustainability: combining the growth of (new) Aerospace activities with the urgent need to reduce global environmental impact



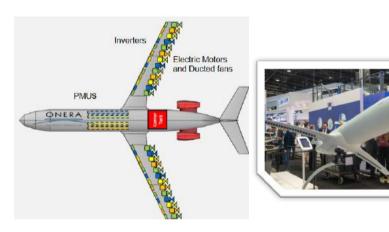
MDO for greener aircraft

- POLYTECHNIQUE MONTRÉAL UNIVERSITÉ D'INGÉNIERIE
 - ONERA

THE FRENCH AEROSPACE LAB

- √ 30% reduction of CO2 emissions by 2035
- ✓ Distributed electric propulsion aircraft: propulsive efficiency
- ✓ 150 passengers over 2750nm
- √ Transonic cruise speed (M0.78)





P. Schmollgruber, C. Doll, J. Hermetz, R. Liaboeuf, M. Ridel, I. Cafarelli, O. Atin-ault, C. Francois, and B. Paluch. "Multidisciplinary Exploration of DRAGON: an ONERA Hybrid Electric Distributed Propulsion Concept". In: AIAA Scitech 2019, 2019

Optimization problem: DRAGON

Table 4 Definition of the "DRAGON" optimization problem.

	Function/variable	Nature	Quantity	Range
Minimize	Fuel mass	cont	1	
with respect to	Fan operating pressure ratio	cont	1	[1.05, 1.3]
	Wing aspect ratio	cont	1	[8, 12]
	Angle for swept wing	cont	1	[15, 40] (°)
	Wing taper ratio	cont	1	[0.2, 0.5]
	HT aspect ratio	cont	1	[3,6]
	Angle for swept HT	cont	1	[20, 40] (°)
	HT taper ratio	cont	1	[0.3, 0.5]
	TOFL for sizing	cont	1	[1800., 2500.] (m)
	Top of climb vertical speed for sizing	cont	1	[300., 800.](ft/min)
	Start of climb slope angle	cont	1	[0.075., 0.15.](rad)
	Total continuous variables		10	
	Architecture	cat	17 levels	{1,2,3,,15,16,17}
	Turboshaft layout	cat	2 levels	{1,2}
	Total categorical variables		2	
	Total relaxed variables		29	
subject to	Wing span $< 36 (m)$	cont	1	
	TOFL < 2200 (m)	cont	1	
	Wing trailing edge occupied by fans $< 14.4 (m)$	cont	1	
	Climb duration $< 1740 (s)$	cont	1	
	Top of climb slope > $0.0108 (rad)$	cont	1	
	Total constraints		5)

n = 12Variable types: continuous (10), categorical (2) n' = 29

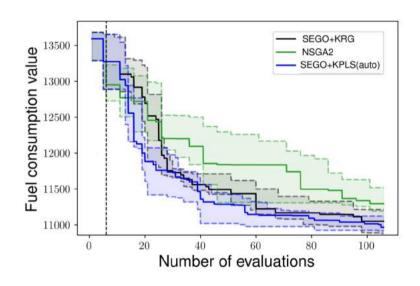
5 inequality constraints (MC)Fuel mass to minimize

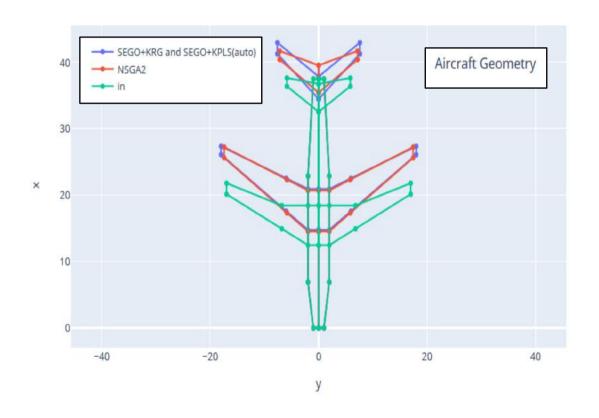


Optimization results: DRAGON

Options for SEGO-KPLS From n' = 29 to d(auto) $d \sim 1.6$

Convergence plots for DRAGON





6/ Pseven 12/10/2:

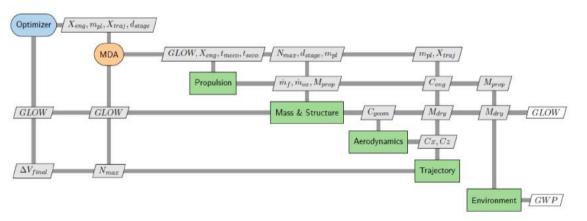
MDO for ECOlauncher design

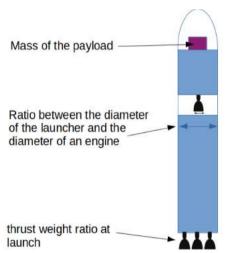


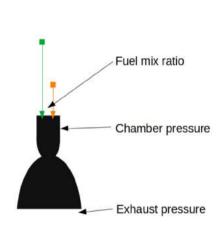
Objective function: GLOW

 $\textbf{Design variables}: X_{eng}, m_{pl}, X_{traj}, d_{stage}$

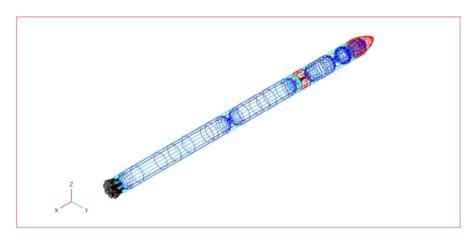
Constraints : $\Delta V_{final} \geq 0$

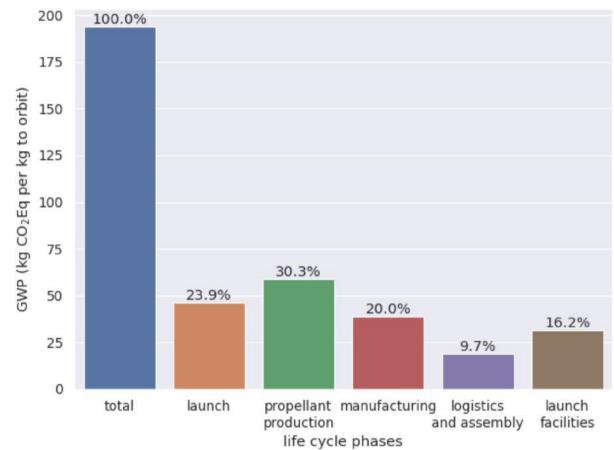






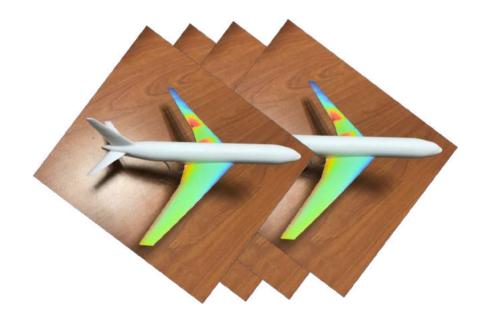






Early LCA results demonstrate that manufacturing take into account 20% of Global Warming Potential (wrt 1% in Aircraft)

Time to conclude



Duration	Description	Agenda
10'	MDO	Examples
10'	Surrogate	SMT
10'	Ecodesign	Lighter and Greener
4'	Conclusions	And future works?

Conclusions

« Learning » an industrial (&costly) simulation code is interesting to easily exchange data only (without having access to the code in a collaborative project)





- 1. SMT is a natural framework for Bayesian Optimization (DV>+100 thanks **KPLS**
- 2. SMT core capabilities has been adapted for efficient mixed variables / multifidelity / multiObjectives but is not a Global {Constrained} Optimizer (SEGO-MOE is...)
- 3. Combining MDO/AI can solve Engineering problem up to +100 DV, and lots of constraints (thanks to KS function) (SEGO-MOE can do this!)
- 4. By including Ecodesign constraints we can accelerate the path toward greener aerospace vehicules.

Bonus:



Web application for MDO

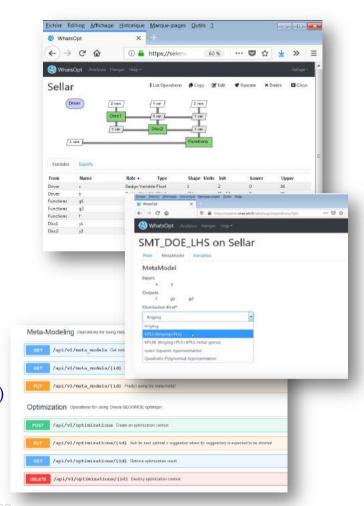
- MDA management
- Code generation
 - MDO Frameworks (OpenMDAO, GEMSEO)
 - DOE run
 - Surrogate models (SMT)
 - Sensitivity analysis (SAlib)
 - Uncertainty quantification (<u>OpenTURNS</u>)
 - Distant code execution (Thrift)
 - Parallel execution (DOE with Linux MPI)
- Import / Export of Data
- Results visualisation

Surrogate Models

- Creation of metamodels from database
- Creation of metamodels from MDA or discipline

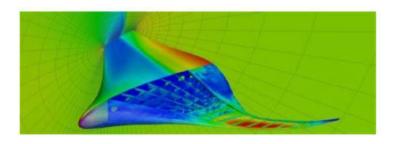
External access

- External server (<u>https://ether.onera.fr/whatsopt</u>) allows acces to:
- Metamodels capabilities
- SEGOMOE optimizer



Popularization ONFRA-SUPAFRO

https://www.linkedin.com/pulse/optimizationmdo-connecting-people-joseph-morlier/



http://mdolab.engin.umich.edu

Optimization [MDO] for connecting people?



- Thanks to all my Students and Colleagues at SUPAERO, ONERA, AIRBUS, ICA
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- Paul Saves, Thomas Bellier

12/10/22