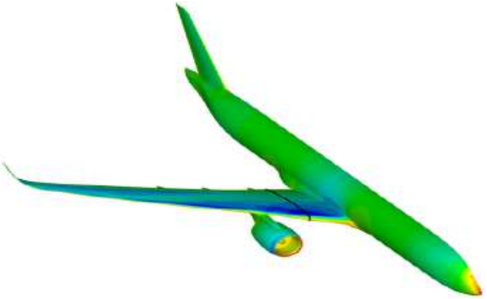
SMT

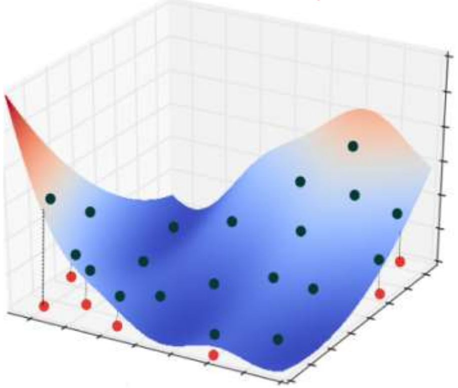
Surrogate Modeling Toolbox

ONERA
THE FRENCH AEROSPACE LAB



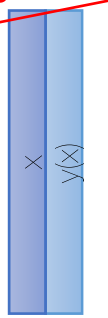
True Function Evaluation

This is costly!



Matrix view of Gaussian Process aka Kriging

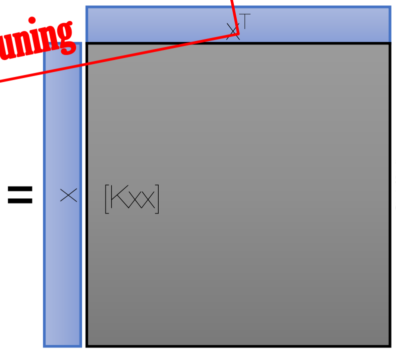
1/ Get your inputs/outputs data

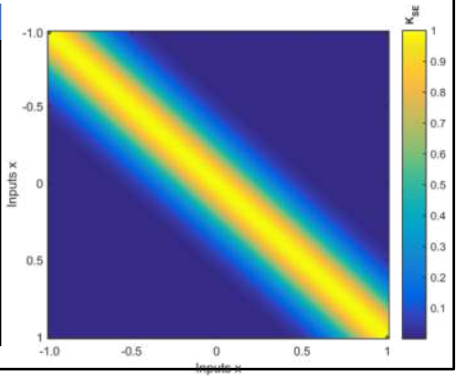


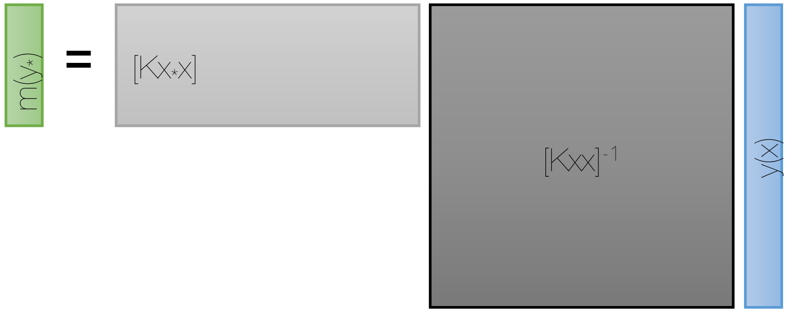
2/ You wan to predict at x*

3/ Choose a Kernel/Construct Kxx and Hyperparameters tuning

$$k(x,x') = \theta_1{}^2 \exp(-\frac{(x-x')^2}{2\theta_2{}^2})$$







$$m(x_*) = K_*[Kxx]^{-1}y$$

4/ compute mean

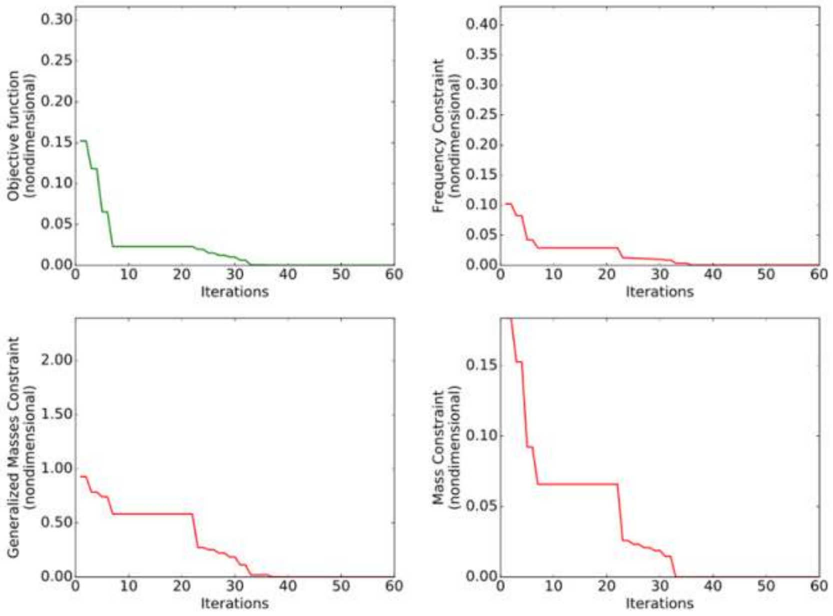
$$var(x_*, x_*') = K_{**} - K_*^T[Kxx]^{-1}K_*$$

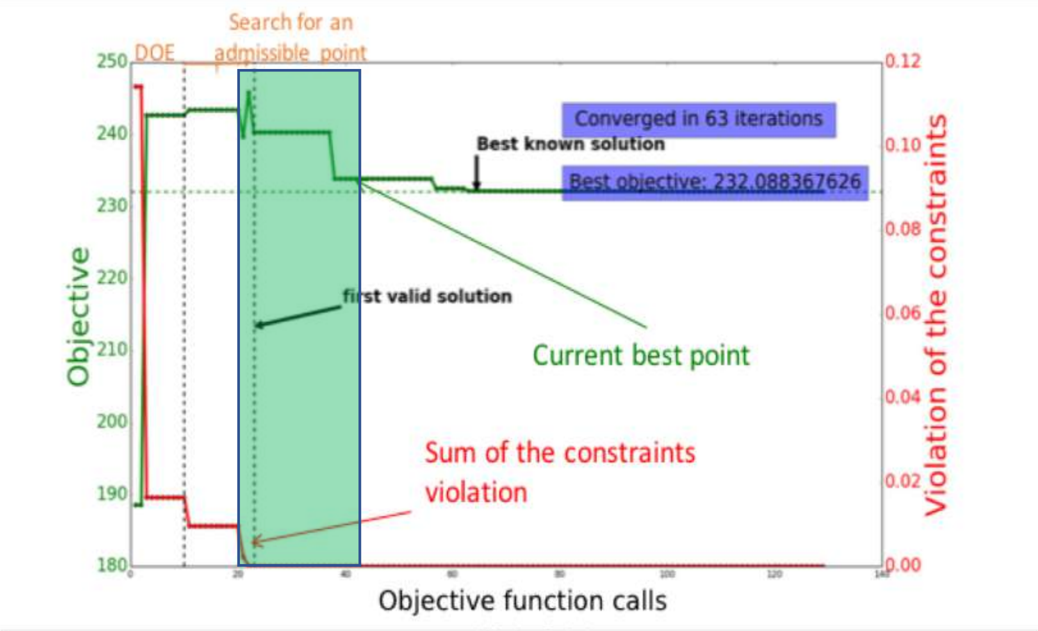
4BIS but IMPORTANT compute variance of estimate

Convergency graphs

Gradient based Optimality, Feasibility

SBO Exploration, Exploitation





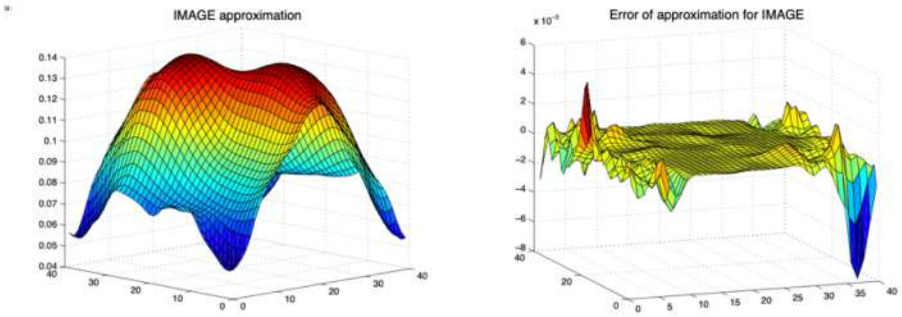
Stopping criteria: tolfun, tolx, maxiter

Stopping criteria: Max Budget (Function calls)

…A long time ago far away

in Onera/Supaero Toulouse

- 2008-2011 D. Bettebghor's PhD first works on Mixture of Experts → How to assemble local surrogates in a global one? IMAGE in matlab



(a) IMAGE approximation (b) Error for IMAGE approximation

- Results of The PhD of M. Boulhel (2013-2016) → KPLS trick → treat HD engineer's problem

Ordinary Kriging $k(x,x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \theta_i |x_i - x_i'|^{p_i}\right)$ d parameters θ_i to evaluate

Covariance kernel ⬇

KPLS $k_{PLS}(x,x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \eta_i |x_i - x_i'|^{p_i}\right)$ with $\eta_i = \sum_{j=1}^{h} \theta_j |w_{i,j}|^{p_i}$

h parameters θ_j to evaluate

- $|w_{i,j}|_{i=1,\cdots,d}$ describes how sensitive the j-th principal component is to each design variable i → PLS
- θ_j describes how sensitive the function is to each principal component (max $h \approx 4$) → MLE
- If $h = d$ → classical kriging (exponential kernels)

- M. Bouhlel left to Michigan as postdoc.We decide to unify our forces with UoM, Nasa Glenn, Supaero/Onera → spirit of reproducible research **RR** developed at the MDOlab (Prof Martins)

Standard papers (no online supplementary materials)

1 Have you ever tried to reproduce some research results ?
2 Have you ever failed ?

what we can do with standard papers:

read the formulas
believe the results
$ check results
$ reproduce the results
$ see the pictures in detail
$ see the graphs in detail

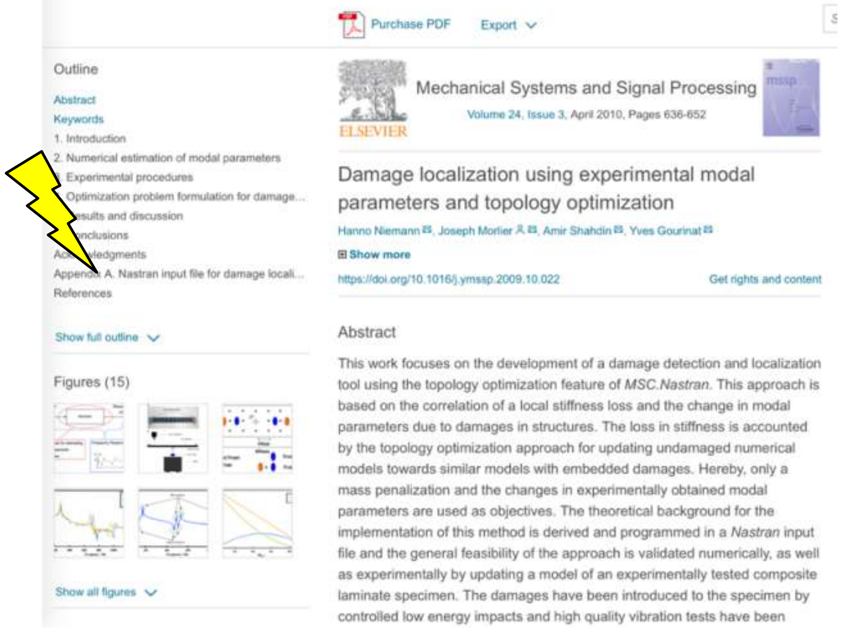
```
FAQ:
How numerical integral is implemented in this paper?
How are estimated the optimization hyperparameters ?
…
What are the postprocessing (stress field) tricks?
…
```

My definition of **RR**

sustainability of the research works
pérennisation des travaux de recherche

“reproducible research” means submitting at minimum:

1. the paper
2. all code & data to reproduce results under open source licenses
3. README files describing code & data



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Outline

Abstract
Keywords
1. Introduction
2. Numerical estimation of modal parameters
Experimental procedures
Optimization problem formulation for damage...
esults and discussion
nclusions
Ac wledgments
Append A. Nastran input file for damage locali...
References

Show full outline

Figures (15)

Show all figures

ELSEVIER

Mechanical Systems and Signal Processing

Volume 24, Issue 3, April 2010, Pages 636-652

Damage localization using experimental modal parameters and topology optimization

Hanno Niemann, Joseph Morlier, Amir Shahdin, Yves Gourinat

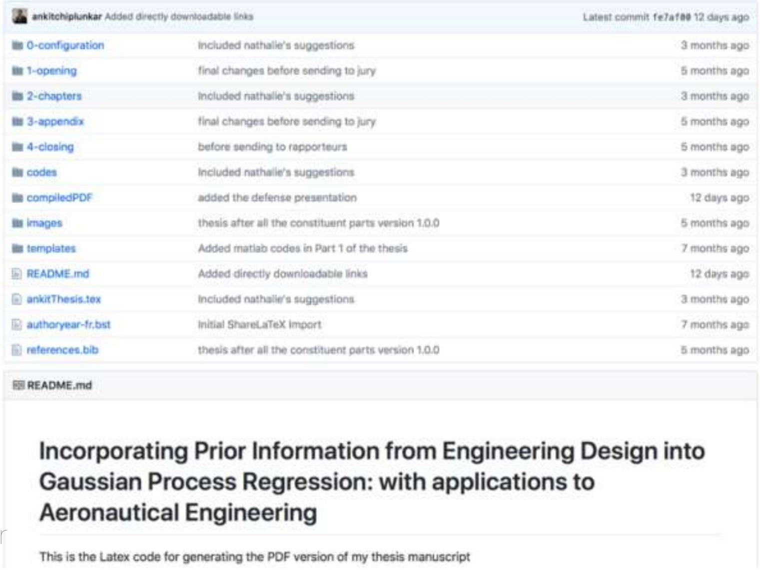
Show more

https://doi.org/10.1016/j.ymssp.2009.10.022   Get rights and content

Abstract

This work focuses on the development of a damage detection and localization tool using the topology optimization feature of *MSC.Nastran*. This approach is based on the correlation of a local stiffness loss and the change in modal parameters due to damages in structures. The loss in stiffness is accounted by the topology optimization approach for updating undamaged numerical models towards similar models with embedded damages. Hereby, only a mass penalization and the changes in experimentally obtained modal parameters are used as objectives. The theoretical background for the implementation of this method is derived and programmed in a *Nastran* input file and the general feasibility of the approach is validated numerically, as well as experimentally by updating a model of an experimentally tested composite laminate specimen. The damages have been introduced to the specimen by controlled low energy impacts and high quality vibration tests have been

https://github.com/ankitchiplunkar/thesis_isae



ankitchiplunkar Added directly downloadable links   Latest commit fe7af00 12 days ago

0-configuration	Included nathalie's suggestions	3 months ago
1-opening	final changes before sending to jury	5 months ago
2-chapters	Included nathalie's suggestions	3 months ago
3-appendix	final changes before sending to jury	5 months ago
4-closing	before sending to rapporteurs	5 months ago
codes	Included nathalie's suggestions	3 months ago
compiledPDF	added the defense presentation	12 days ago
images	thesis after all the constituent parts version 1.0.0	5 months ago
templates	Added matlab codes in Part 1 of the thesis	7 months ago
README.md	Added directly downloadable links	12 days ago
ankitThesis.tex	Included nathalie's suggestions	3 months ago
authoryear-fr.bst	Initial ShareLaTeX Import	7 months ago
references.bib	thesis after all the constituent parts version 1.0.0	5 months ago

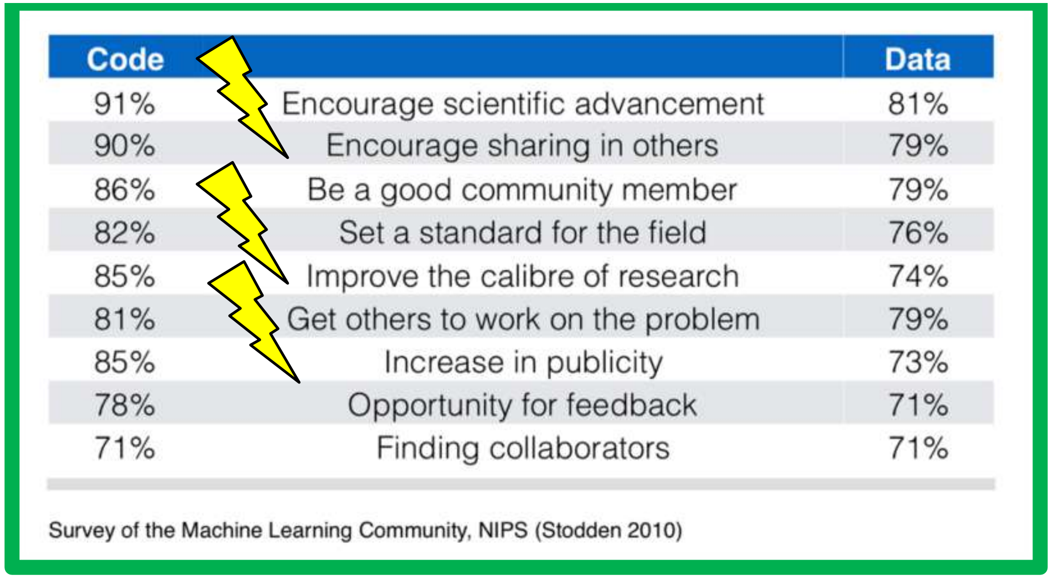
README.md

Incorporating Prior Information from Engineering Design into Gaussian Process Regression: with applications to Aeronautical Engineering

This is the Latex code for generating the PDF version of my thesis manuscript

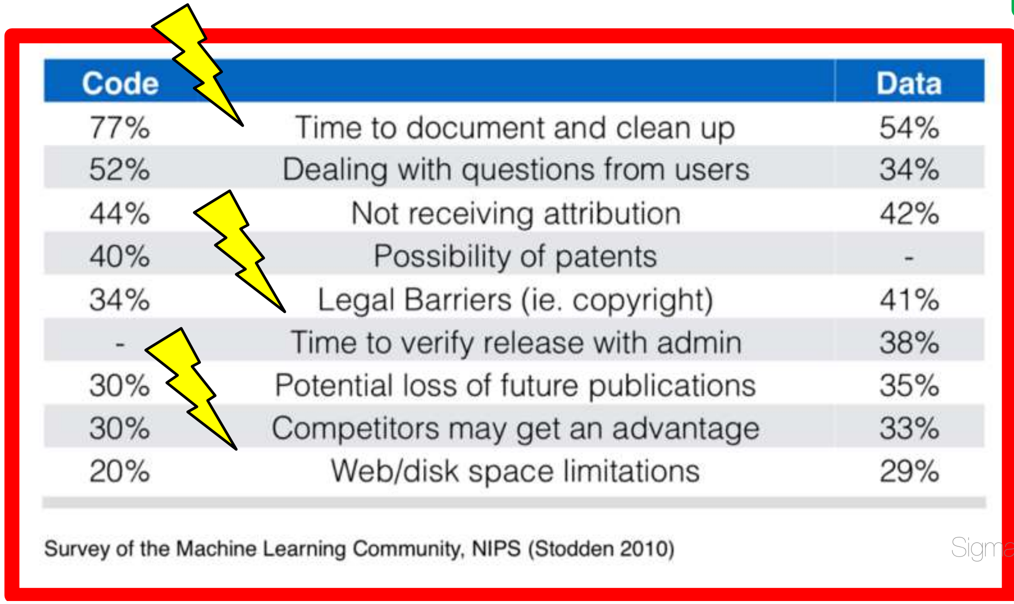
PROs and CONs

- From: Survey of the Machine Learning Community, NIPS (Stodden 2010)



Code		Data
91%	Encourage scientific advancement	81%
90%	Encourage sharing in others	79%
86%	Be a good community member	79%
82%	Set a standard for the field	76%
85%	Improve the calibre of research	74%
81%	Get others to work on the problem	79%
85%	Increase in publicity	73%
78%	Opportunity for feedback	71%
71%	Finding collaborators	71%

Survey of the Machine Learning Community, NIPS (Stodden 2010)



Code		Data
77%	Time to document and clean up	54%
52%	Dealing with questions from users	34%
44%	Not receiving attribution	42%
40%	Possibility of patents	-
34%	Legal Barriers (ie. copyright)	41%
-	Time to verify release with admin	38%
30%	Potential loss of future publications	35%
30%	Competitors may get an advantage	33%
20%	Web/disk space limitations	29%

Survey of the Machine Learning Community, NIPS (Stodden 2010)

The *Reproducible Research Standard* (RRS) (Stodden, 2009)

A suite of license recommendations for computational science:

Release media components (text, figures) under CC BY,

https://web.stanford.edu/~vcs/talks/VictoriaStoddenCommuniaJune2009-2.pdf

Benefit for Scientists

- Openness means increased citation.
- Working reproducibly engenders better science.
- Easier for the scientists to build on his or her own work.
- Showcase of skillset for potential collaborators/funders/employers

Some Labs increases their popularity through online available data

Home > Publications > AIAA Journal > Volume 53, Issue 4 > Aerodynamic Shape Optimization Investigations of the Common Research Model Wing Benchmark

Zhoujie Lyu, Gaetan K. W. Kenway, and Joaquim R. R. A. Martins. "Aerodynamic Shape Optimization Investigations of the Common Research Model Wing Benchmark", AIAA Journal, Vol. 53, No. 4 (2015), pp. 968–985.
https://doi.org/10.2514/1.J053318

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Aerodynamic Shape Optimization Investigations of the Common Research Model Wing Benchmark

Zhoujie Lyu*, Gaetan K. W. Kenway†, and Joaquim R. R. A. Martins‡
Department of Aerospace Engineering, University of Michigan, Ann Arbor, Michigan 48109

*Ph.D. Candidate, Department of Aerospace Engineering. Student Member AIAA.

†Postdoctoral Research Fellow, Department of Aerospace Engineering. Member AIAA.

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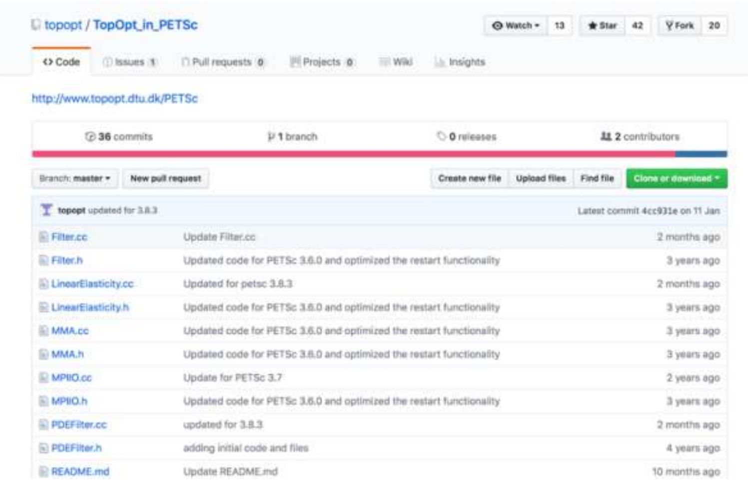
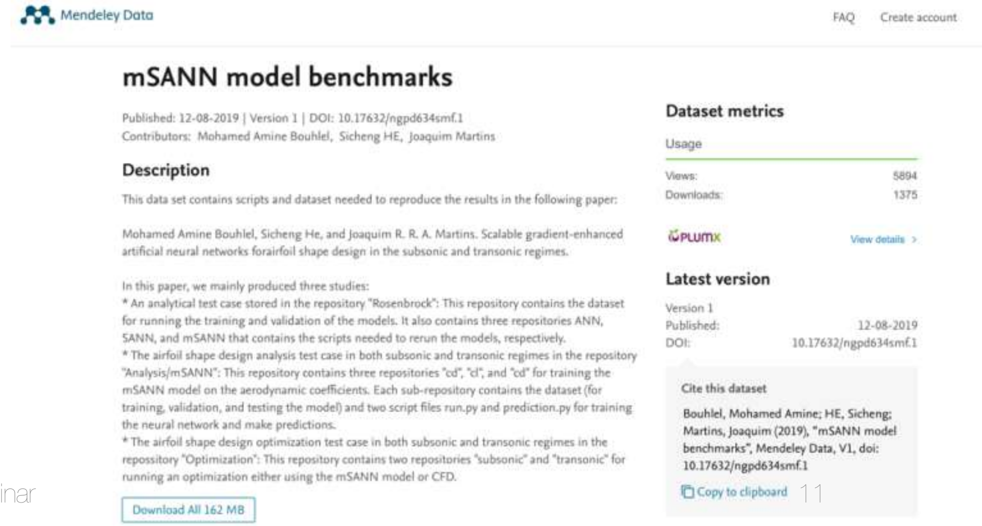


topopt / TopOpt_in_PETSc

http://www.topopt.dtu.dk/PETSc

topopt updated for 3.8.3 — Latest commit 4cc931e on 11 Jan

Filter.cc	Update Filter.cc	2 months ago
Filter.h	Updated code for PETSc 3.6.0 and optimized the restart functionality	3 years ago
LinearElasticity.cc	Updated for petsc 3.8.3	2 months ago
LinearElasticity.h	Updated code for PETSc 3.6.0 and optimized the restart functionality	3 years ago
MMA.cc	Updated code for PETSc 3.6.0 and optimized the restart functionality	3 years ago
MMA.h	Updated code for PETSc 3.6.0 and optimized the restart functionality	3 years ago
MPIIO.cc	Update for PETSc 3.7	2 years ago
MPIIO.h	Updated code for PETSc 3.6.0 and optimized the restart functionality	3 years ago
PDEFilter.cc	updated for 3.8.3	2 months ago
PDEFilter.h	adding initial code and files	4 years ago
README.md	Update README.md	10 months ago



mSANN model benchmarks

Published: 12-08-2019 | Version 1 | DOI: 10.17632/ngpd634smf.1
Contributors: Mohamed Amine Bouhlel, Sicheng HE, Joaquim Martins

Description

This data set contains scripts and dataset needed to reproduce the results in the following paper:

Mohamed Amine Bouhlel, Sicheng He, and Joaquim R. R. A. Martins. Scalable gradient-enhanced artificial neural networks forairfoil shape design in the subsonic and transonic regimes.

In this paper, we mainly produced three studies:
* An analytical test case stored in the repository "Rosenbrock": This repository contains the dataset for running the training and validation of the models. It also contains three repositories ANN, SANN, and mSANN that contains the scripts needed to rerun the models, respectively.
* The airfoil shape design analysis test case in both subsonic and transonic regimes in the repository "Analysis/mSANN": This repository contains three repositories "cd", "cl", and "cd" for training the mSANN model on the aerodynamic coefficients. Each sub-repository contains the dataset (for training, validation, and testing the model) and two script files run.py and prediction.py for training the neural network and make predictions.
* The airfoil shape design optimization test case in both subsonic and transonic regimes in the repossitory "Optimization": This repository contains two repositories "subsonic" and "transonic" for running an optimization either using the mSANN model or CFD.

Dataset metrics

Usage

Views: 5894
Downloads: 1375

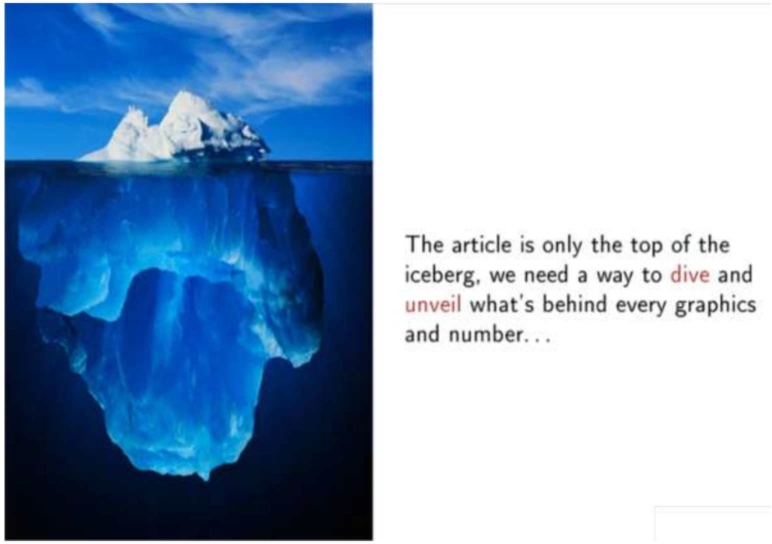
Latest version

Version 1
Published: 12-08-2019
DOI: 10.17632/ngpd634smf.1

Cite this dataset

Bouhlel, Mohamed Amine; HE, Sicheng; Martins, Joaquim (2019), "mSANN model benchmarks", Mendeley Data, V1, doi: 10.17632/ngpd634smf.1

Conclusion for **RR**



The article is only the top of the iceberg, we need a way to dive and unveil what's behind every graphics and number. . .

- Changes in funding agency requirements
- Changes in journal/conferences publication requirements
- Cultural changes in our relation to publication (more work)

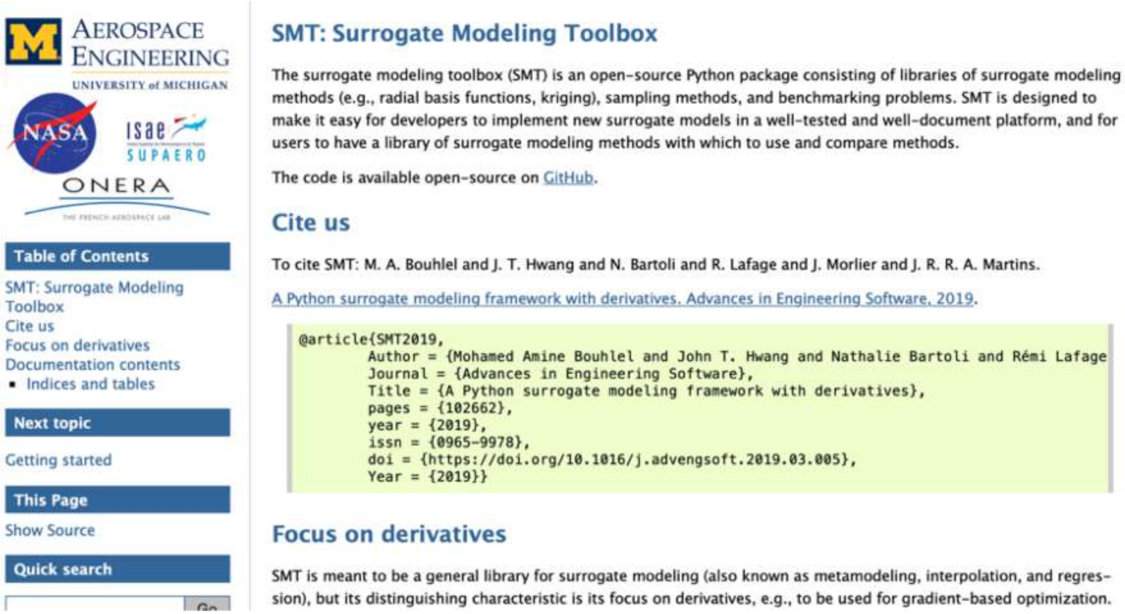
- Reproducible papers are more cited? No Proof at this time

BUT

- **It's Definitely more efficient (not only in the long run and for the community)**
- **It's simply more satisfying…**
- **Train our researchers and students to use better tools, better research methodology,**

→ **https://github.com/alegrand/RR_webinars**

...in 2017 the first SMT version was released



SMT: Surrogate Modeling Toolbox

The surrogate modeling 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-document 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.

Cite us

To cite SMT: M. A. Bouhlel and J. T. Hwang and N. Bartoli and R. Lafage and J. Morlier and J. R. R. A. Martins.

A Python surrogate modeling framework with derivatives. Advances in Engineering Software, 2019.

```
@article{SMT2019,
        Author = {Mohamed Amine Bouhlel and John T. Hwang and Nathalie Bartoli and Rémi Lafage
        Journal = {Advances in Engineering Software},
        Title = {A Python surrogate modeling framework with derivatives},
        pages = {102662},
        year = {2019},
        issn = {0965-9978},
        doi = {https://doi.org/10.1016/j.advengsoft.2019.03.005},
        Year = {2019}}
```

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.

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.

Authors

SMT is developed by:

- Mohamed Amine Bouhlel
- John Hwang
- Nathalie Bartoli
- Rémi Lafage
- Joseph Morlier
- Joaquim Martins

SMT has been developed thanks to contributions from:

- Andres Lopez Lopera
- Emile Roux
- Florent Vergnes
- Frederick Zahle
- Jasper Bussemaker
- Julien Schueller
- Lucas Alber
- Mostafa Meliani
- Nina Moëllo
- Paul Saves
- Raul Carreira Rufato
- Reino Ruusu
- Rémi Vauclin
- Rémy Priem
- Ruben Conde
- Steven Berguin
- Vincent Drouet

Contributors

Thanks to all

anfelopera #5
39 commits 1,873 ++ 1,375 --

m-meliani #6
30 commits 1,444 ++ 503 --

Nov 6, 2016 – May 18, 2021

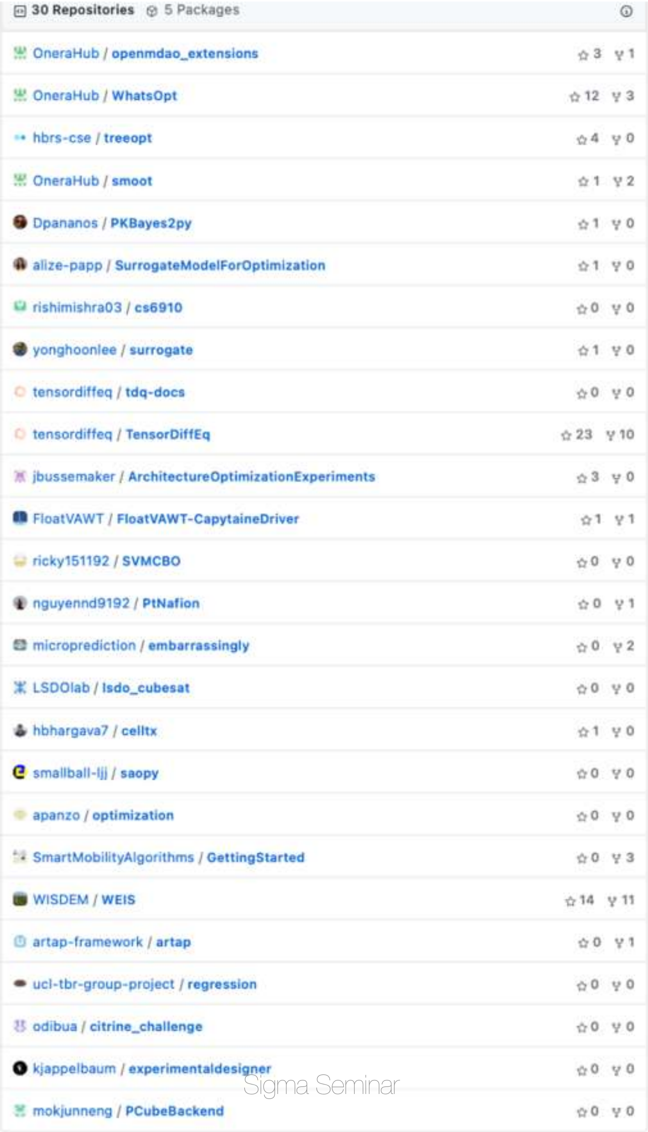
Contributions: Commits

Contributions to master, excluding merge commits and bot accounts

2 commits 2 ++ 2 --

1 commit 127 ++ 1 --

Dependents



30 Repositories 5 Packages

OneraHub / **openmdao_extensions**	☆ 3	⑂ 1
OneraHub / **WhatsOpt**	☆ 12	⑂ 3
hbrs-cse / **treeopt**	☆ 4	⑂ 0
OneraHub / **smoot**	☆ 1	⑂ 2
Dpananos / **PKBayes2py**	☆ 1	⑂ 0
alize-papp / **SurrogateModelForOptimization**	☆ 1	⑂ 0
rishimishra03 / **cs6910**	☆ 0	⑂ 0
yonghoonlee / **surrogate**	☆ 1	⑂ 0
tensordiffeq / **tdq-docs**	☆ 0	⑂ 0
tensordiffeq / **TensorDiffEq**	☆ 23	⑂ 10
jbussemaker / **ArchitectureOptimizationExperiments**	☆ 3	⑂ 0
FloatVAWT / **FloatVAWT-CapytaineDriver**	☆ 1	⑂ 1
ricky151192 / **SVMCBO**	☆ 0	⑂ 0
nguyennd9192 / **PtNafion**	☆ 0	⑂ 1
microprediction / **embarrassingly**	☆ 0	⑂ 2
LSDOlab / **lsdo_cubesat**	☆ 0	⑂ 0
hbhargava7 / **celltx**	☆ 1	⑂ 0
smallball-ljj / **saopy**	☆ 0	⑂ 0
apanzo / **optimization**	☆ 0	⑂ 0
SmartMobilityAlgorithms / **GettingStarted**	☆ 0	⑂ 3
WISDEM / **WEIS**	☆ 14	⑂ 11
artap-framework / **artap**	☆ 0	⑂ 1
ucl-tbr-group-project / **regression**	☆ 0	⑂ 0
odibua / **citrine_challenge**	☆ 0	⑂ 0
kjappelbaum / **experimentaldesigner**	☆ 0	⑂ 0
mokjunneng / **PCubeBackend**	☆ 0	⑂ 0

Applications

- Mixture of experts (MOE) → D. Bettebghor's PhD thesis
- Variable-fidelity modeling (VFM)
- Multi-Fidelity Kriging (MFK) → R. Vauclin's internship
- Multi-Fidelity Kriging KPLS (MFKPLS)
- Multi-Fidelity Kriging KPLSK (MFKPLSK)
- Efficient Global Optimization (EGO) → M. Bouhlel's PhD thesis, M. Meliani's internship
- Mixed-Integer Sampling and Surrogate (Continuous Relaxation) → P. Saves's PhD thesis
- Mixed-Integer Surrogate with Gower Distance →R. Rufato's internship

- Contributing to SMT
    - Developer API for surrogate models
    - Developer API for benchmarking problems
    - Developer API for sampling methods

Benefits of Opensource

Examples of internal reused inside the consortium

Benefits of Opensource

- Coupling with OpenMDAO

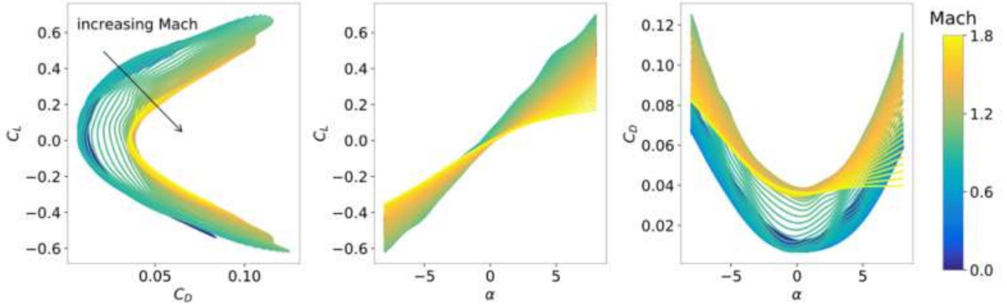


Figure 3. Drag polar and aerodynamic properties for the ESAV aircraft obtained from the CFD-trained surrogate model at an elevation of 30,000 feet with a Mach sweep from 0 to 1.8, and an α sweep from $-8°$to $8°$.

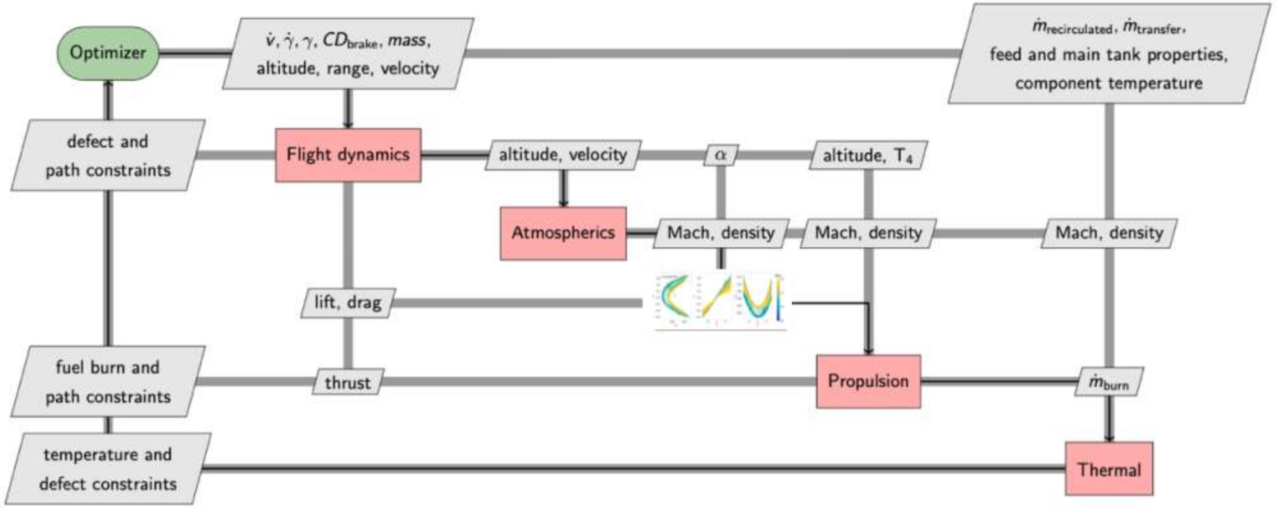
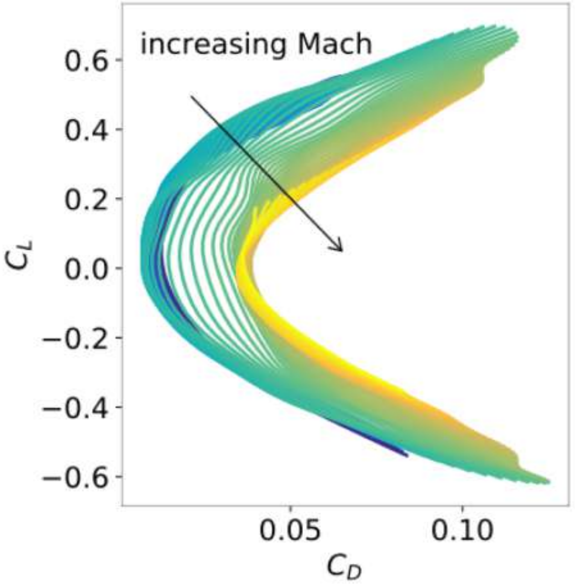
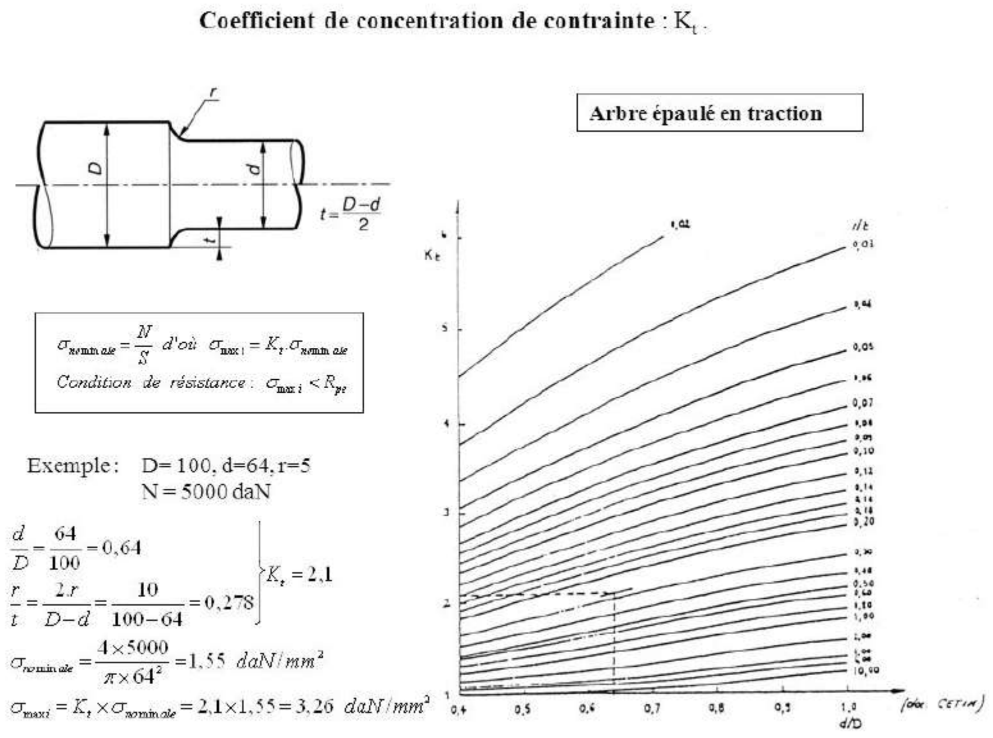


Figure 6. XDSM diagram [60] of the fully-coupled problem, including the optimizer, design variables, and constraints.

Surrogate is the new abacus




Coefficient de concentration de contrainte : K_t .

Arbre épaulé en traction

$$\sigma_{nominale} = \frac{N}{S} \text{ d'où } \sigma_{maxi} = K_t . \sigma_{nominale}$$

Condition de résistance : $\sigma_{maxi} < R_{pe}$

Exemple : D= 100, d=64, r=5
N = 5000 daN

$$\left.\begin{array}{l} \frac{d}{D} = \frac{64}{100} = 0,64 \\ \frac{r}{t} = \frac{2.r}{D-d} = \frac{10}{100-64} = 0,278 \end{array}\right\} K_t = 2,1$$

$$\sigma_{nominale} = \frac{4 \times 5000}{\pi \times 64^2} = 1,55 \ daN/mm^2$$

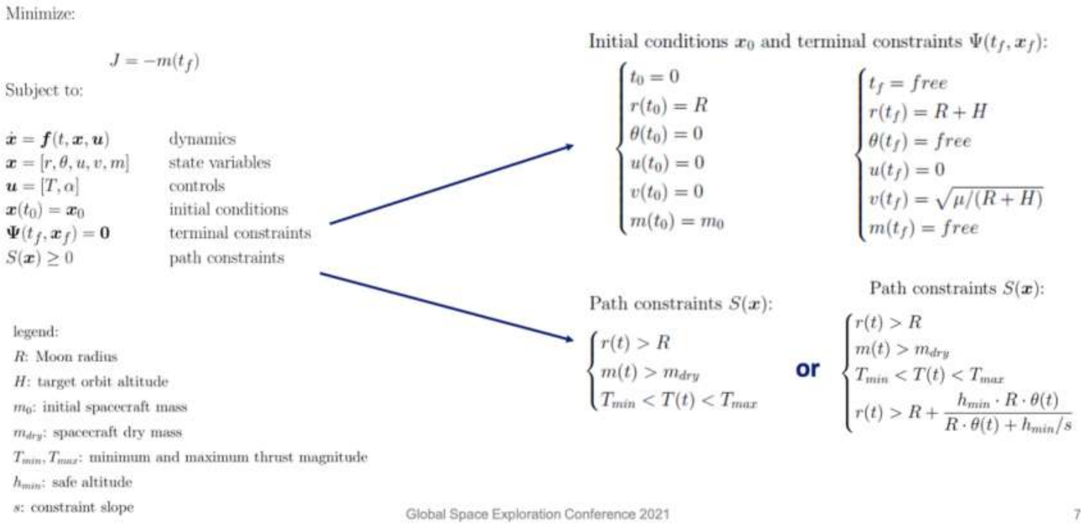
$$\sigma_{maxi} = K_t \times \sigma_{nominale} = 2,1 \times 1,55 = 3,26 \ daN/mm^2$$

Surrogate is the new abacus

Multidisciplinary Optimal Control Library

- Coupling with OpenMDAO /dymos

Beauregard, L., Urbano, A., Lizy-Destrez, S., & Morlier, J. (2021). Multidisciplinary Design and Architecture Optimization of a Reusable Lunar Lander. *Journal of Spacecraft and Rockets*, 1-14.



Minimize:

$$J = -m(t_f)$$

Subject to:

$\dot{\boldsymbol{x}} = \boldsymbol{f}(t, \boldsymbol{x}, \boldsymbol{u})$	dynamics
$\boldsymbol{x} = [r, \theta, u, v, m]$	state variables
$\boldsymbol{u} = [T, \alpha]$	controls
$\boldsymbol{x}(t_0) = \boldsymbol{x}_0$	initial conditions
$\boldsymbol{\Psi}(t_f, \boldsymbol{x}_f) = \boldsymbol{0}$	terminal constraints
$S(\boldsymbol{x}) \geq 0$	path constraints

legend:

R: Moon radius

H: target orbit altitude

m_0: initial spacecraft mass

m_{dry}: spacecraft dry mass

T_{min}, T_{max}: minimum and maximum thrust magnitude

h_{min}: safe altitude

s: constraint slope

Initial conditions $\boldsymbol{x}_0$ and terminal constraints $\Psi(t_f, \boldsymbol{x}_f)$:

$$\begin{cases} t_0 = 0 \\ r(t_0) = R \\ \theta(t_0) = 0 \\ u(t_0) = 0 \\ v(t_0) = 0 \\ m(t_0) = m_0 \end{cases} \qquad \begin{cases} t_f = free \\ r(t_f) = R + H \\ \theta(t_f) = free \\ u(t_f) = 0 \\ v(t_f) = \sqrt{\mu/(R+H)} \\ m(t_f) = free \end{cases}$$

Path constraints $S(\boldsymbol{x})$:

$$\begin{cases} r(t) > R \\ m(t) > m_{dry} \\ T_{min} < T(t) < T_{max} \end{cases}$$

or

Path constraints $S(\boldsymbol{x})$:

$$\begin{cases} r(t) > R \\ m(t) > m_{dry} \\ T_{min} < T(t) < T_{max} \\ r(t) > R + \dfrac{h_{min} \cdot R \cdot \theta(t)}{R \cdot \theta(t) + h_{min}/s} \end{cases}$$

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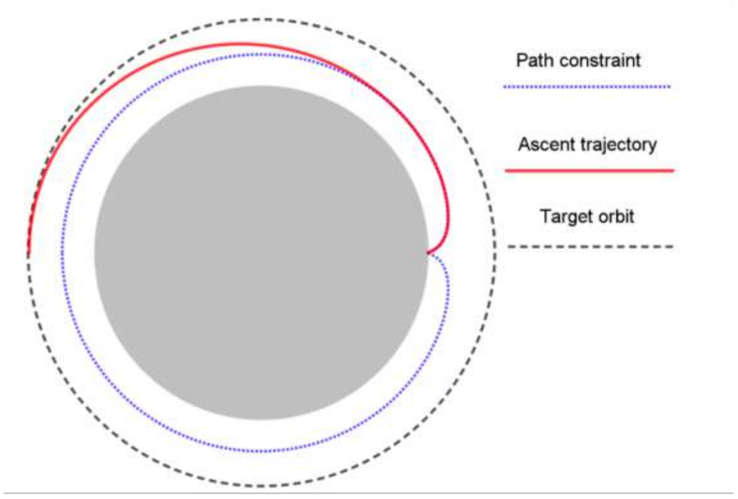
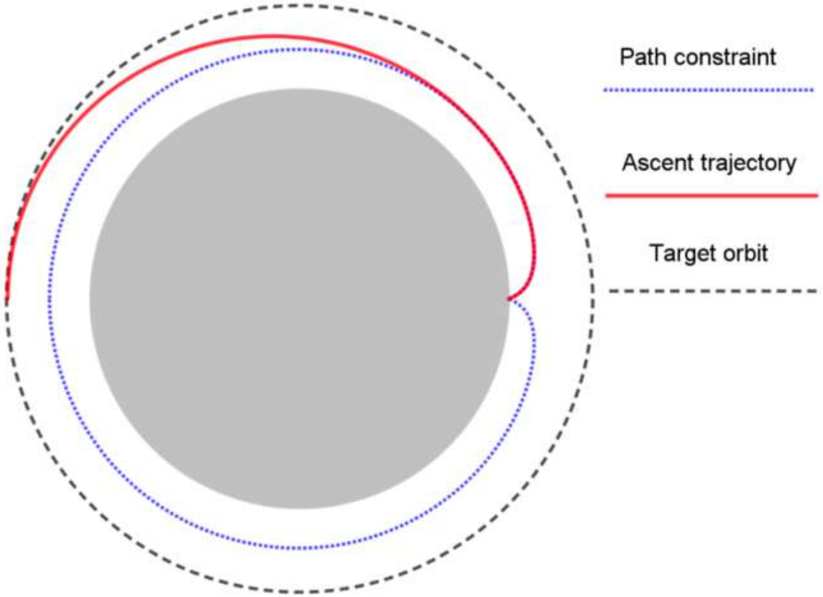
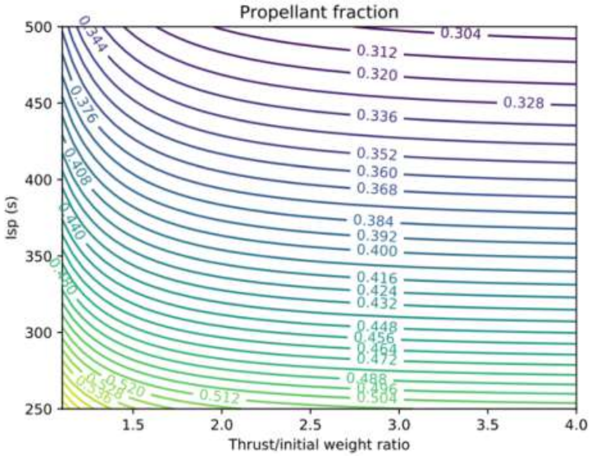
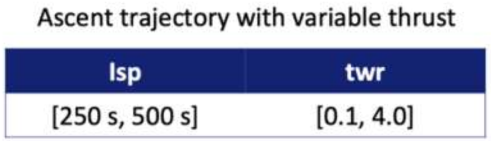


Surrogate is the new abacus

- MDO + Optimal control i.e. « learn « the optimal control and uses it in the mdo loop







Ascent trajectory with variable thrust

Isp	twr
[250 s, 500 s]	[0.1, 4.0]

https://github.com/mid2SUPAERO/LaTOM

Benefits of Opensource

Examples of external reused out of the consortium

OpenSource: reuse of the code - KPLS

chemical process design

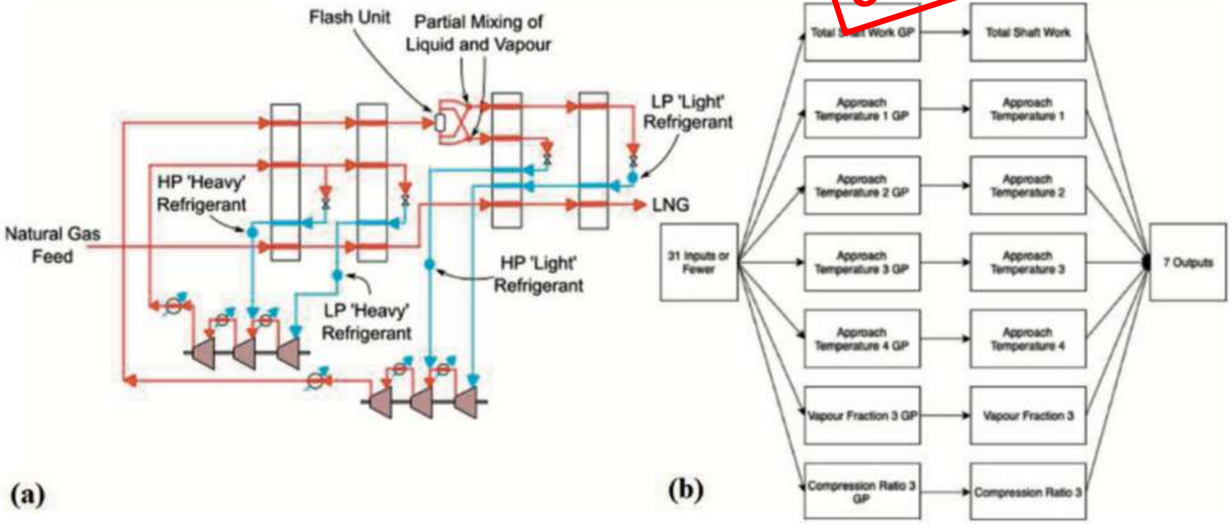
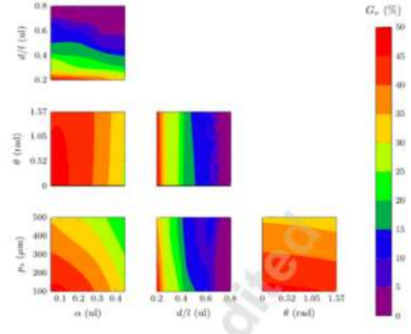


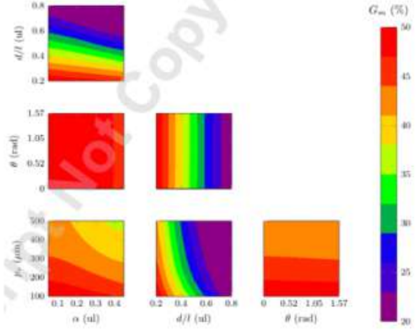
Figure 1: The CryoMan Cascade cycle (a), and its KPLS based surrogate model (b).

Savage, T., Almeida-Trasvina, H. F., del Río-Chanona, E. A., Smith, R., & Zhang, D. (2020). An adaptive data-driven modelling and optimization framework for complex chemical process design. In Computer Aided Chemical Engineering (Vol. 48, pp. 73-78). Elsevier.

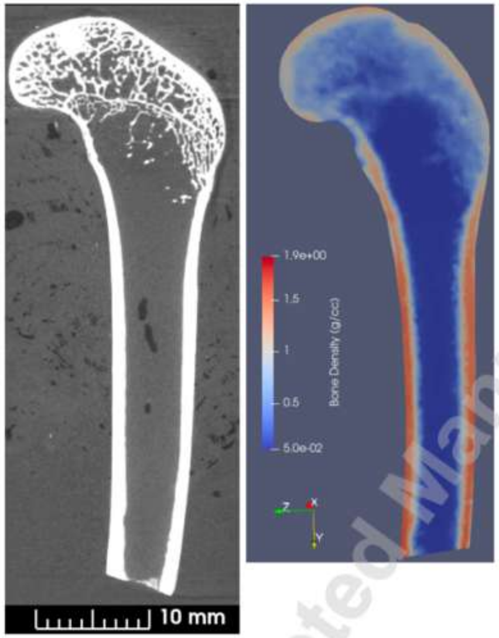
OpenSource: reuse of the code KPLS



(a) Volume growth



(b) Mass growth



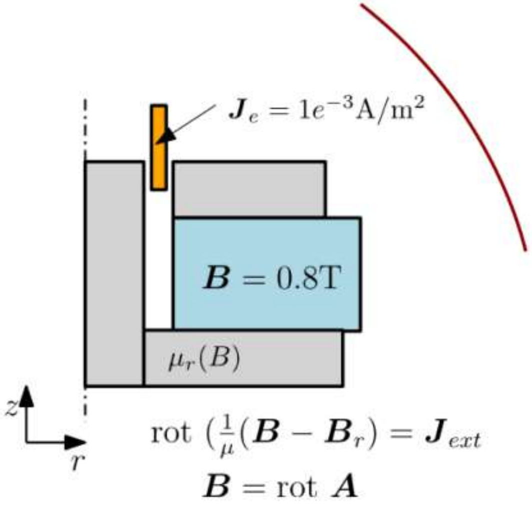
(a) CT scan (b) FEA femur model

Biomedical

Cohen, D. O., Aboutaleb, S. M., Wagoner Johnson, A. J., & Norato, J. A. (2021). BONE ADAPTATION-DRIVEN DESIGN OF PERIODIC SCAFFOLDS. Journal of Mechanical Design, 1-21.

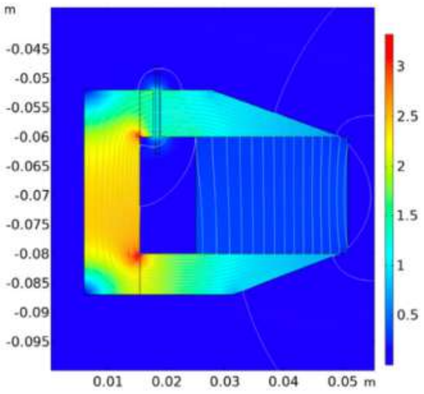
OpenSource: reuse of the code in other packages

Optimization of a loudspeaker



$$\mathrm{rot}\ \left(\frac{1}{\mu}(\boldsymbol{B} - \boldsymbol{B}_r)\right) = \boldsymbol{J}_{ext}$$

$$\boldsymbol{B} = \mathrm{rot}\ \boldsymbol{A}$$



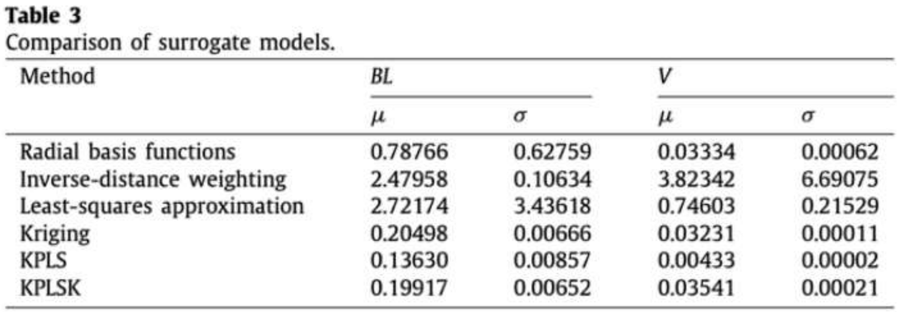


Table 3
Comparison of surrogate models.

Method	BL		V	
	μ	σ	μ	σ
Radial basis functions	0.78766	0.62759	0.03334	0.00062
Inverse-distance weighting	2.47958	0.10634	3.82342	6.69075
Least-squares approximation	2.72174	3.43618	0.74603	0.21529
Kriging	0.20498	0.00666	0.03231	0.00011
KPLS	0.13630	0.00857	0.00433	0.00002
KPLSK	0.19917	0.00652	0.03541	0.00021

Karban, P., Pánek, D., Orosz, T., Petrášová, I., & Doležel, I. (2021). FEM based robust design optimization with Agros and Ārtap. Computers & Mathematics with Applications, 81, 618-633.

Conclusions

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

AIRCRAFT 3RD GENERATION MDO FOR INNOVATIVE COLLABORATION OF HETEROGENEOUS TEAMS OF EXPERTS

Given its focus on **derivatives**, SMT is synergistic with the OpenMDAO framework. **It can provide the derivatives that OpenMDAO requires from its components to compute the coupled derivatives of the multidisciplinary model.**

SMT is a natural framework for Bayesian Optimization (**DV<100 through KPLS**)

SMT core capabilities has been adapted for efficient **mixed variables / multifidelity / multiObjectives**