

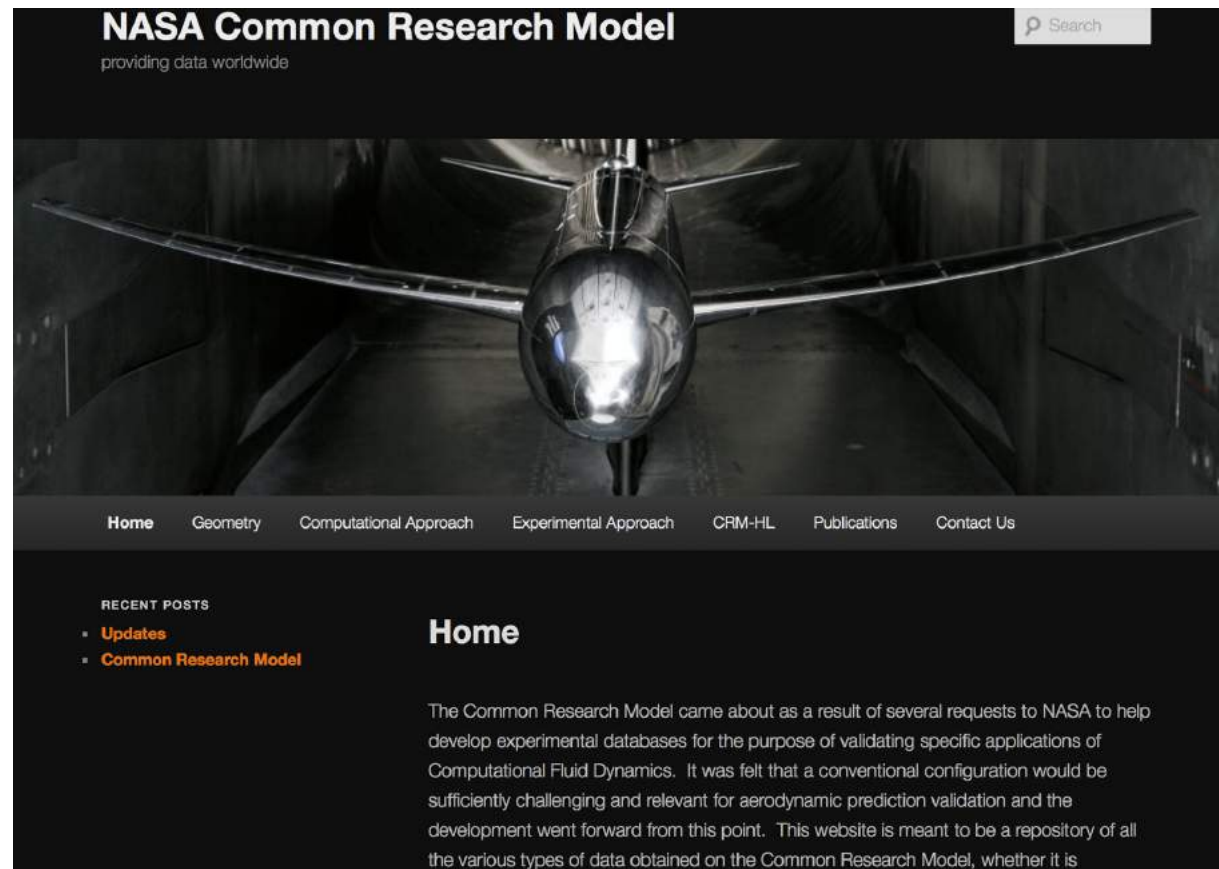


## Reproducible Papers

Prof. J. Morlier

Slide Sources:  
Victoria Stodden CompareML: Structuring Machine Learning Research in Data Driven Science  
Charles Sutton, You and Your Code, Univ. of Edinburgh  
Arnaud Legrand Reproducible Research: Where to Begin With?


## A (Very) Good Example from ... NASA



- Round Robin Test (Test inter Laboratoire en sciences experimentales)
- <http://sem.org/dic-challenge/>
- <https://www.lanl.gov/projects/national-security-education-center/engineering/software/shm-data-sets-and-software.php>
- <http://www.garteur.org>

# MDOlab popularity increases through online a

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




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**VOLUME 53, ISSUE 4 (APRIL)**

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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/10.2514/1.1053318>

## Aerodynamic Shape Optimization Investigations of the Common Research Model Wing Benchmark

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Structural and Multidisciplinary Optimization  
<https://doi.org/10.1007/s00158-018-1912-8>

## EDUCATIONAL ARTICLE



## Open-source coupled aerostructural optimization using Python

John P. Jasa<sup>1</sup>  · John T. Hwang<sup>2</sup> · Joaquim R. R. A. Martins<sup>1</sup>

Received: 2 August 2017 / Revised: 28 November 2017 / Accepted: 15 January 2018  
© Springer-Verlag GmbH Germany, part of Springer Nature 2018

### Abstract

To teach multidisciplinary design optimization (MDO) to students effectively, it is useful to have accessible software that runs quickly, allowing hands-on exploration of coupled systems and optimization methods. Open-source software exists for low-fidelity aerodynamic or structural analysis, but there is no existing software for fast tightly coupled aerostructural analysis and design optimization. To address this need, we present OpenAeroStruct, an open-source low-fidelity aerostructural analysis and optimization tool developed in NASA's OpenMDAO framework. It uses the coupled adjoint method to compute the derivatives required for efficient gradient-based optimization. OpenAeroStruct combines a vortex lattice method and 1-D finite-element analysis to model lifting surfaces, such as aircraft wings and tails, and uses the coupled-adjoint method to compute the aerostructural derivatives. We use the Breguet range equation to compute the fuel burn as a function of structural weight and aerodynamic performance. OpenAeroStruct has proved effective both as an educational tool and as a benchmark for researching new MDO methods. There is much more potential to be exploited as the research community continues to develop and use this tool.

**Keywords** Aerostructural design optimization · Wing design · Multidisciplinary design optimization · Project-based learning · Python

### 1 Summary

In this paper, we discuss OpenAeroStruct,<sup>1</sup> an open-source coupled aerostructural analysis and design optimization tool. OpenAeroStruct couples the vortex-lattice method (VLM) and finite-element analysis (FEA) using six degree-of-freedom (DOF) spatial beam elements with axial, bending, and torsional stiffness. It is mostly implemented in Python, but some of the more intensive computations use Fortran.

<sup>1</sup><https://github.com/mdolab/openaerestruct>

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OpenAeroStruct is developed within the OpenMDAO framework (Heath and Gray 2012), a NASA-developed open-source software framework for multidisciplinary design optimization (MDO). OpenMDAO facilitates derivative computation for gradient-based optimization using the modular analysis and unified derivatives (MAUD) architecture (Hwang and Martins 2018), which unifies the adjoint method with the chain rule and all other methods for computing discrete derivatives (Martins and Hwang 2013). OpenAeroStruct computes derivatives for the aerostructural system using the coupled adjoint method (Martins et al. 2005; Kenway et al. 2014). The aerodynamic forces and structural displacements are transferred between disciplines in a consistent and conservative manner. This process is simplified because the aerodynamic and structural meshes have the same spanwise discretization, so no interpolation is necessary to transfer the loads or displacements. A variety of solvers can be used to converge the coupled aerostructural system, including block Gauss–Seidel, GMRES, or LU decomposition for the lin-



Another nice example

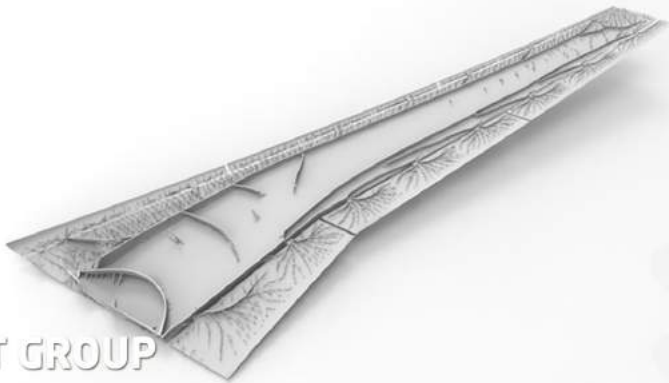
TOPOPT

ABOUT US

PROJECTS

APPS/ SOFTWARE

PUBLICATIONS



TOPOPT GROUP

The TopOpt group at DTU Mechanical Engineering is world leading within development and applications of density based topology optimization. TopOpt is an acronym for Topology Optimization and the group is a joined research effort between the departments of DTU Mechanical Engineering and DTU Civil Engineering with the aim of promoting theoretical extensions and practical applications of the topology optimization method. The group is involved in multidisciplinary research projects sponsored from national and international sources.

topopt / TopOpt\_in\_PETSc

Watch

13

Star

42

Fork

20

Code

Issues

Pull requests

Projects

Wiki

Insights

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

36 commits

1 branch

0 releases

2 contributors

Branch: master

New pull request

Create new file

Upload files

Find file

Clone or download

Latest commit 4cc931e on 11 Jan

2 months ago

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3 years ago

2 months ago

3 years ago

3 years ago

2 years ago

3 years ago

2 months ago

4 years ago

10 months ago

LETTER

doi:10.1016/j.let.2010.11.001

Giga-voxel computational morphogenesis for structural design

Niels Asger<sup>1</sup>, Erik Andreassen<sup>1</sup>, Boyan S. Lazarov<sup>2</sup> & Ole Sigmund<sup>1</sup>

In the design of industrial products ranging from bearing pads to automobiles and aeroplanes, material is distributed so as to maximize the performance and minimize the cost. Historically, human intuition and insight have driven the evolution of mechanical design, recently assisted by computer-aided design approaches. The computer-aided approach known as topology optimization enables unrestricted design freedom and shows great promise with regard to weight savings, but its applicability has so far been limited to the design of single components or simple structures, owing to the resolution limits of current optimization methods<sup>1,2</sup>. Here we report a computational morphogenesis tool, implemented on a supercomputer, that produces designs with giga-voxel resolution—more than two orders of magnitude higher than previously reported. Such resolution provides insights into the optimal distribution of material within a structure that were hitherto unachievable owing to the challenges of scaling up existing modelling and optimization frameworks. As an example, we apply the tool to the design of the internal structure of a full-scale aeroplane wing. The optimized full-wing design has unprecedented structural detail at length scales ranging from tens of centimetres to millimetres and, intriguingly, shows remarkable similarity to naturally occurring bone structures in, for example, bird beaks. We estimate that our optimized design corresponds to a reduction in mass of 2–5 per cent compared to currently used aeroplane wing designs, which translates into a reduction in fuel consumption of about 40–200 tonnes per year per aeroplane. Our morphogenesis process is generally applicable, not only to mechanical designs, but also to flow systems, antennas, nano-optics and micro-systems<sup>3,4</sup>.

Computational morphogenesis is used in engineering to determine the best possible shapes and material distributions for prescribed structural objectives. A very common goal is to minimize structural weight, subject to constraints on deflections and mechanical stresses. Similar goals are drivers of animal and plant evolution. For plants, the optimal ratio of loading capacity to weight ensures efficient use of limited resources; for animals, it minimizes energy consumption for walking and running. Whereas efficient structures in nature generally result from slow genetic evolution, in engineering fast solutions that also take manufacturing limitations into account are necessary. Topology optimization<sup>5–7</sup> works by redistributing material within a predetermined design domain, not unlike natural bone-growth processes. Here, the design domain is defined as the geometric volume in which material can be distributed, such as the space above the building lot for a high-rise building, or the internal part of a car less the space reserved for passengers, the engine and so on. Through an iterative, deterministic process that involves modelling of the physical system, gradient computations and mathematical programming-based design updates, structural material is gradually redistributed towards the optimal design (Extended Data Fig. 1).

Traditional stress-based topology optimization of components is well developed and used routinely in all major mechanical engineering industries, including the automotive<sup>8</sup> and aerospace<sup>9</sup> industries. In the automotive industry, this optimization typically results in weight savings of 20%–40% on structural parts and reduced development times compared to designs obtained using intuition or trial and error by skilled engineers, and eliminates the need to build prototypes. Despite its successes, the applicability of the topology optimization approach is still limited to the design of components or smaller structures. The main obstacle in applying it to large structures is resolution, just as the visual quality of a television screen is limited by the number of pixels, the geometric quality and capability of the topology optimization process is limited by the number of voxels (three-dimensional equivalent of pixels) that are used to parameterize the design problem. Current state-of-the-art implementations limit voxel numbers to a few million and hence make their application in the detailed design of high-rise buildings, oil rigs or large aeroplanes impossible. This provides the question of whether giga-voxel resolution computational morphogenesis would lead to radical design changes. If so, we expect these new designs to result in substantial weight savings and reduced environmental impact.

We investigate this question using high-performance computing and demonstrate the potential of giga-voxel resolution computational morphogenesis on a full-scale wing design problem for an aircraft similar to a Boeing 777 (Fig. 1; see also Extended Data Figs 2 and 3, and Supplementary Figs 1 and 2 for high-resolution images). The extension to being able to solve problems with more than one billion voxels requires several non-trivial challenges to be overcome, including the efficient solution of huge systems of linear equations, tailoring of optimization algorithms, and data transfer and visualization (see Methods). Obtaining the optimized designs presented here required access to massive computational resources with run times of 1–5 days on 8,000 CPUs.

The case study that we present considers the design of the load-carrying internal structure for a full aircraft wing based on the publicly available NASA Common Research Model<sup>10,11</sup>. This wing model is similar to the wing of a Boeing 777 and has a half wing span (length of a single wing) of 27 m and an inner and outer chord (the 'width' of the wing at the root and the tip) of 12 m and 3 m, respectively. The fixed-shape wing is discretized into 1.1 billion voxels (corresponding to a mesh of 1,216 × 3,488 × 256 elements) with a maximum element size of 0.8 cm at the root, which is reasonable for a wing structure of this size<sup>12</sup>. From the NASA model, we included two aerodynamic load scenarios, corresponding to angles of attack of 6° and 4° at Mach 0.85 and an altitude of 10,700 m. The outer layer of mesh is fixed to be solid, representing the outer layer of the airfoil; material can then be freely distributed in the internal part of the wing with no further restrictions (Fig. 2a, top). The optimized design, considering a simplified full-wing structure including flaps is shown in Fig. 1, with the top half of the outer layer removed to reveal the optimized interior structure (the following is shown in Extended Data Fig. 2). Remarkably, all of the internal structural details appeared spontaneously as a result of the morphogenesis

ing 88 lines of code

line: 20 November 2010

el programming language that allows  
roas scientific problems with a min-  
. An example is Sigmund's 99 line  
code (Sigmund 2001). The 99 line  
educational purposes and serves as  
le to topology optimization for stu-  
to the field. The use of MATLAB,  
tax, excellent debugging tools, and  
dilling opportunities, allows the user  
al and mathematical background of  
on without being distracted by tech-  
issues. Other examples of simple  
to provide insight in finite element  
optimization include a finite element  
elliptic problems with mixed bound-  
unified grids (Alberty et al. 1999), a  
ms in linear elasticity (Alberty et al.  
mization code for compliant mecha-  
nism conduction problems (Bendsoe and  
; for Pareto-optimal tracing in topol-  
sh 2010), a discrete level-set topol-  
(Challinor 2010), and a Scilab code for  
ization problems based on the level  
99),  
performance programming languages  
an, MATLAB is generally perceived  
comes to computational power. This  
by (1) the fact that many users apply  
a reference to its history as C++.

<sup>1</sup>Department of Mechanical Engineering, Technical University of Denmark, 2800 Lyngby, Denmark; <sup>2</sup>Centre for Aircraft Mechanical System  
Technique, University of Warwick, 2900 Coventry, England

44 | NATURE | VOL. 473 | 9 OCTOBER 2011

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## 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?  
...

For PhDs...

Don't really understand an algorithm unless you can code it.

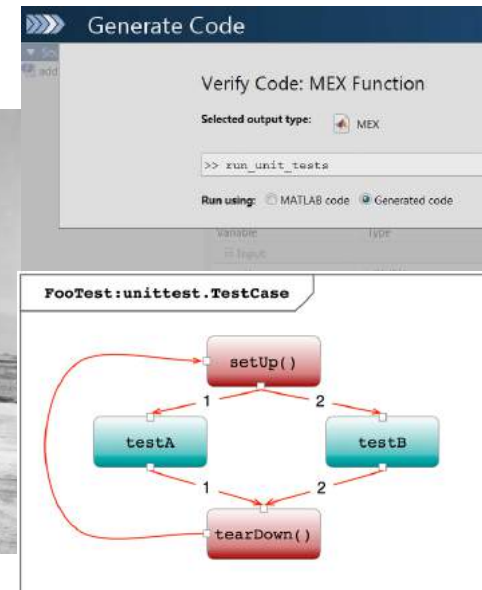
Remember: Software is not your product. → Your product is knowledge:

- ★ New algorithms (often... improvement of existing algorithms)
- ★ New theorems (not often...)
- ★ New models
- ★ New design, optimum, trade-off etc...

## Reproducible research:

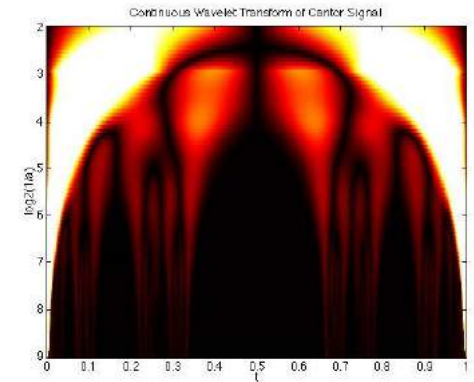
Authors provide all the **necessary data** and the computer **codes** to run the analysis again, **re-creating the results**.

<https://hackernoon.com/barba-group-reproducibility-syllabus-e3757ee635cf>



Lockheed P-80A airplane (1946). Credit: NASA Commons. — A reminder to test your code.

## WAVELAB



Jump to Donoho et al. (2009). This could be the first group to explicitly associate reproducible research with open code and data:

Reproducible computational research, in which all details of computations — code and data — are made conveniently available to others, is a necessary response to [the credibility] crisis.

My favorite quote from Donoho et al. (2009) is: ***“... if everyone on a research team knows that everything they do is going to someday be published for reproducibility, they’ll behave differently from day one.”***

... si tous les chercheurs d'une équipe savaient qu'ils devaient publier avec des contraintes de reproductibilité, ils se comporteraient différemment dès le premier jour



# BUT

In fact, David Donoho, 1998  
paraphrased a Stanford Prof

"Really Reproducible Research" pioneered by Jon Claerbout:

"The idea is: An article about computational science in a scientific publication is *not* the scholarship itself, it is merely **advertising** of the scholarship. The actual scholarship is the complete ... set of instructions [and data] which generated the figures."

L'idée principale est: Un article sur la simulation dans une publication scientifique n'est pas le projet (l'étudiant venant avec sa bourse) en lui-même, c'est simplement la publicité autour de ce projet. Ce projet, lui est l'ensemble ... des instructions [et des données] qui ont généré les figures/tableaux

The screenshot shows the ICERM website header with a search bar and navigation links: Home, Programs & Events, Participate, Proposals, Resources, For Visitors, People, News, Diversity, Support ICERM. The main content area is titled "Reproducibility in Computational and Experimental Mathematics (December 10-14, 2012)".

**Description**

In addition to advancing research and discovery in pure and applied mathematics, computation is pervasive across the sciences and now computational research results are more crucial than ever for public policy, risk management, and national security. Reproducibility of carefully documented experiments is a cornerstone of the scientific method, and yet is often lacking in computational mathematics, science, and engineering. Setting and achieving appropriate standards for reproducibility in computation poses a number of interesting technological and social challenges. The purpose of this workshop is to discuss aspects of reproducibility most relevant to the mathematical sciences among researchers from pure and applied mathematics from academics and other settings, together with interested parties from funding agencies, national laboratories, professional societies, and publishers. This will be a working workshop, with relatively few talks and dedicated time for breakout group discussions on the current state of the art and the tools, policies, and infrastructure that are needed to improve the situation. The groups will be charged with developing guides to current best practices and/or white papers on desirable advances.

**Organizing Committee**

- » David H. Bailey (Lawrence Berkeley National Laboratory)
- » Jon Borwein (Centre for Computer Assisted Research Mathematics and its Applications)
- » Randall J. LeVeque (University of Washington)
- » Bill Rider (Sandia National Laboratory)
- » William Stein (University of Washington)
- » Victoria Stodden (Columbia University)

Two maps of the Pacific Ocean are shown, with a link "Click for code to create this image."

An interesting example...

Running the same code twice with identical input will produce the same output.

If the computation is done in serial, this assumption is good; **but** with parallel computing, it is not always the case.

Diethelm (2012) ran an experiment using an application of finite-element analysis in computational mechanics. Executing the same simulation (same code, same input data) with varying number of processors gave different results!

## The answer

A vector dot-product, computed in parallel over several partial sums. On each execution, individual processors may complete their portion of the sum in different order. In finite precision, **addition is not associative** and the final sum depends on the **order** of the partial sum

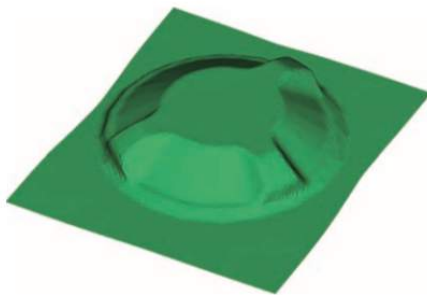


Figure 2. The part to be manufactured. Manufactured from a 0.6-mm thick sheet of steel, the part is about 350-mm long and 400-mm wide. The finite elements used for the simulation have an edge length of 4 mm.

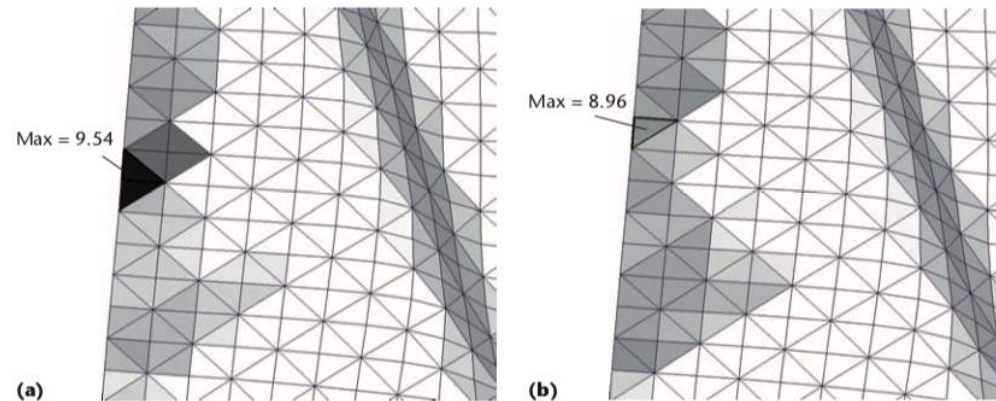


Figure 4. Location of the computed maxima of the sheet thickness change. (a) The simulation with one processor. (b) The second run of the simulation with four processors. The darker the element is colored, the larger the corresponding sheet-thickness change. Elements colored in white have a sheet thickness change of less than 8.5 percent.

# My definition

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

[https://github.com/ankitchiplunkar/thesis\\_isae](https://github.com/ankitchiplunkar/thesis_isae)



**Mechanical Systems and Signal Processing**  
Volume 24, Issue 3, April 2010, Pages 636-652

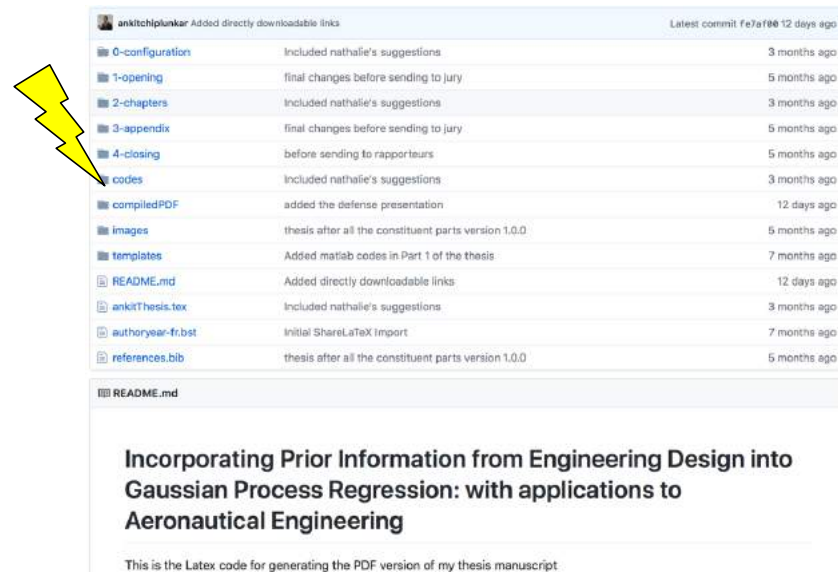
## Damage localization using experimental modal parameters and topology optimization

Hanno Niemann, Joseph Morlier, Amir Shahdin, Yves Gourinat

<https://doi.org/10.1016/j.ymssp.2009.10.022>

**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



File	Description	Latest commit
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
ankiThesis.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

Code is not a paper but...

- <https://distill.pub>
- <https://www.software.ac.uk/resources/guides/which-journals-should-i-publish-my-software>
- <https://www.journals.elsevier.com/softwarex/>

## 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)



## Response from Within the Sciences

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

The pledge:



<http://lorenabarba.com/gallery/reproducibility-pi-manifesto/>

I will teach my graduate students about reproducibility.

All our research code (and writing) is under version control.

We will always carry out verification and validation (V&V reports are posted to figshare)

For main results in a paper, we will share data, plotting script & figure under CC-BY

We will upload the preprint to arXiv at the time of submission of a paper.

We will release code at the time of submission of a paper.

We will add a "Reproducibility" declaration at the end of each paper.

I will keep an up-to-date web presence.

→ Higher confidence in our (students) work can create a competitive advantage

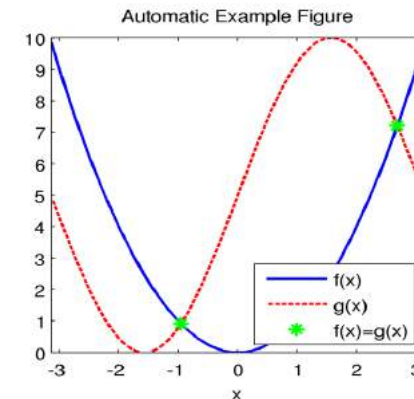
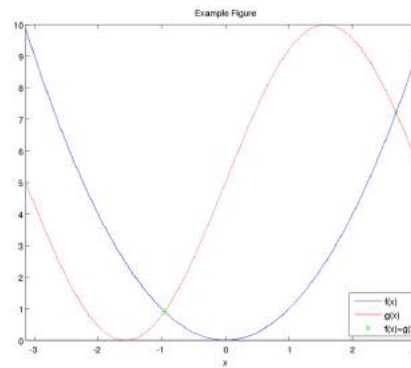
→ Our research will become deeper more visible & reusable (even for us)

Finally...



Reach HQ standards

- Manuscript
- Presentation



What is the best way to present your results?

En France, depuis 2013

<http://www.runmycode.org/home/?/CompanionSite/>

[https://www.lemonde.fr/sciences/article/2013/07/15/pour-une-recherche-reproductible-publiez-vos-codes-et-donnees\\_3447825\\_1650684.html](https://www.lemonde.fr/sciences/article/2013/07/15/pour-une-recherche-reproductible-publiez-vos-codes-et-donnees_3447825_1650684.html)

<https://www.fun-mooc.fr/courses/course-v1:inria+41016+session01bis/about>



## Conclusion

- Changes in funding agency requirements
- Changes in journal/conferences publication requirements (SMO?)
- Cultural changes in our relation to publication (more work)
- Reproducible papers are more cited? No Proof at this time



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

# 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](https://github.com/alegrand/RR_webinars)

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