Workshop HPC Methods for Engineering

CINECA (Milan, Italy). June 17th-19th, 2015.

Design optimization and design exploration using an open source framework on HPC facilities

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OPTIMAD

Roadmap

1. Design optimization and design space exploration
2. The optimization loop
3. One practical application
4. Wrap-up

Roadmap

1. **Design optimization and design space exploration**
2. **The optimization loop**
3. **One practical application**
4. **Wrap-up**

Design optimization and design space exploration

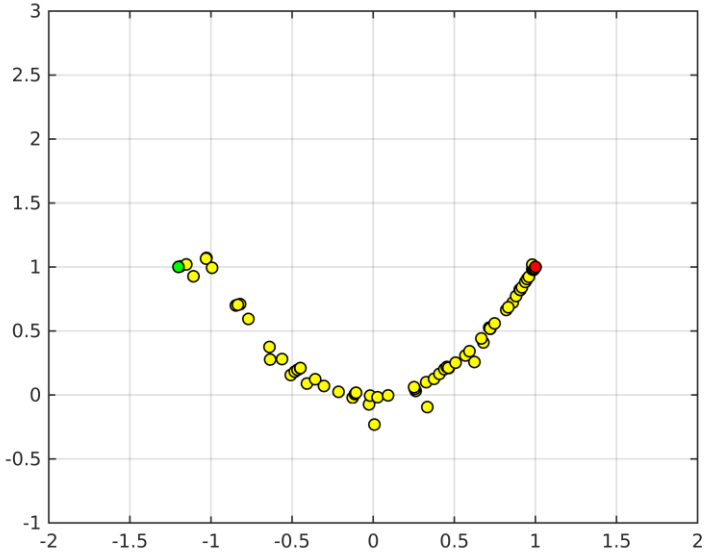
What is optimization?

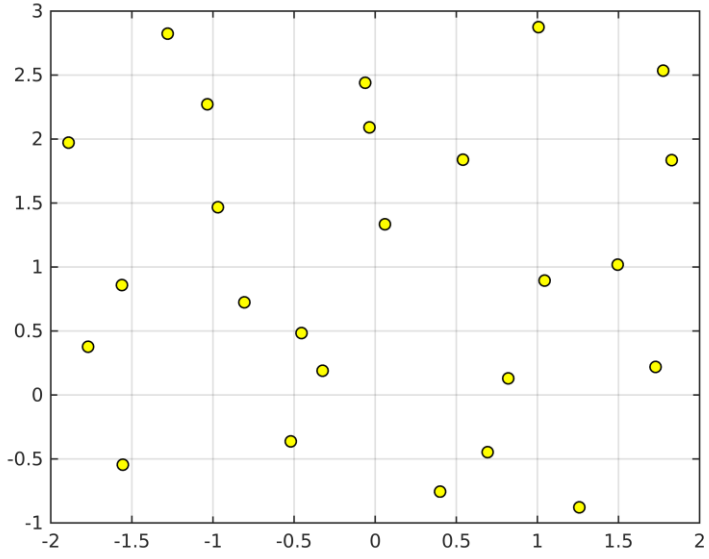
- In plain English, optimization is the act of obtaining the best result under given circumstances.
- This applies to any field (finance, health, construction, operations, manufacturing, transportation, engineering design, sales, public services, mail, and so on).
- The ultimate goal is to minimize, maximize or zeroed an outcome, a process or a function, which we are going to call a quantity of interest or QoI.
- Optimization is not an easy task and it can be time consuming.

Design optimization and design space exploration

Design optimization vs. Design space exploration

Design optimization (DO)	Design space exploration (DSE)
• Converging-Iterative process.	• Diverging-Iterative process.
• DO aims at determining the optimum design.	• DSE aims at searching and characterizing the design space.
• DO strategies have two distinct parts; formulate the problem and converge to the solution.	• Once we know the design space, a better solution can then be found through DO.
• DO depends on a well-posed optimization problem formulation.	• Contrary to DO, in DSE we do not need a well formulated problem.





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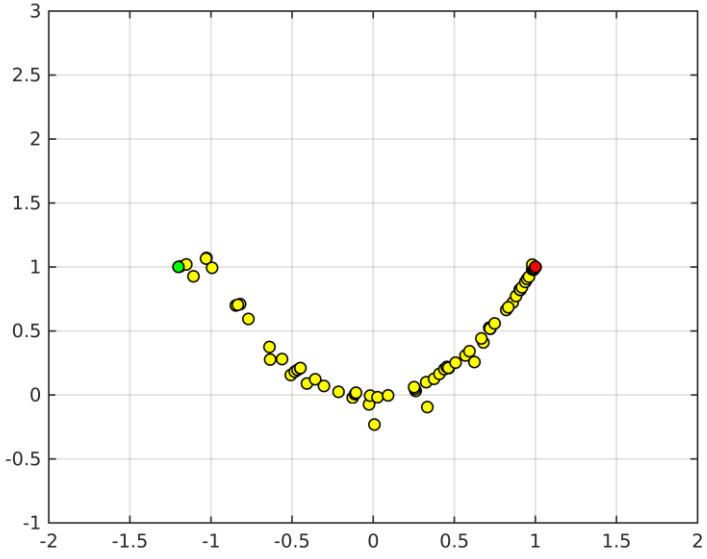

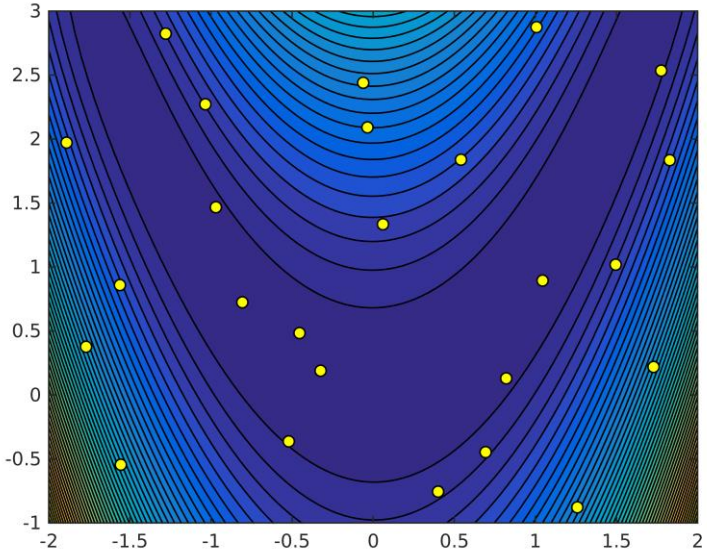

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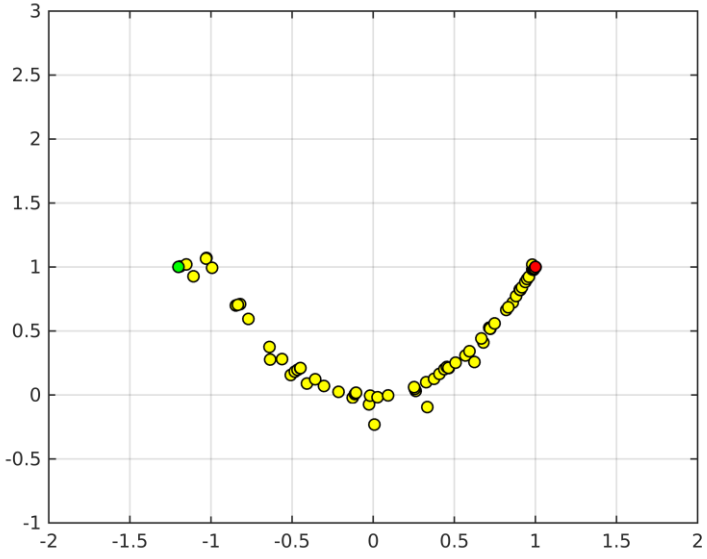
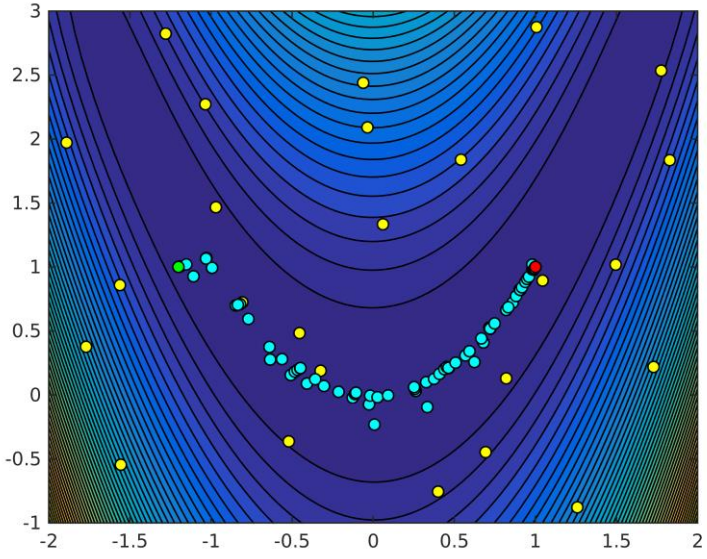


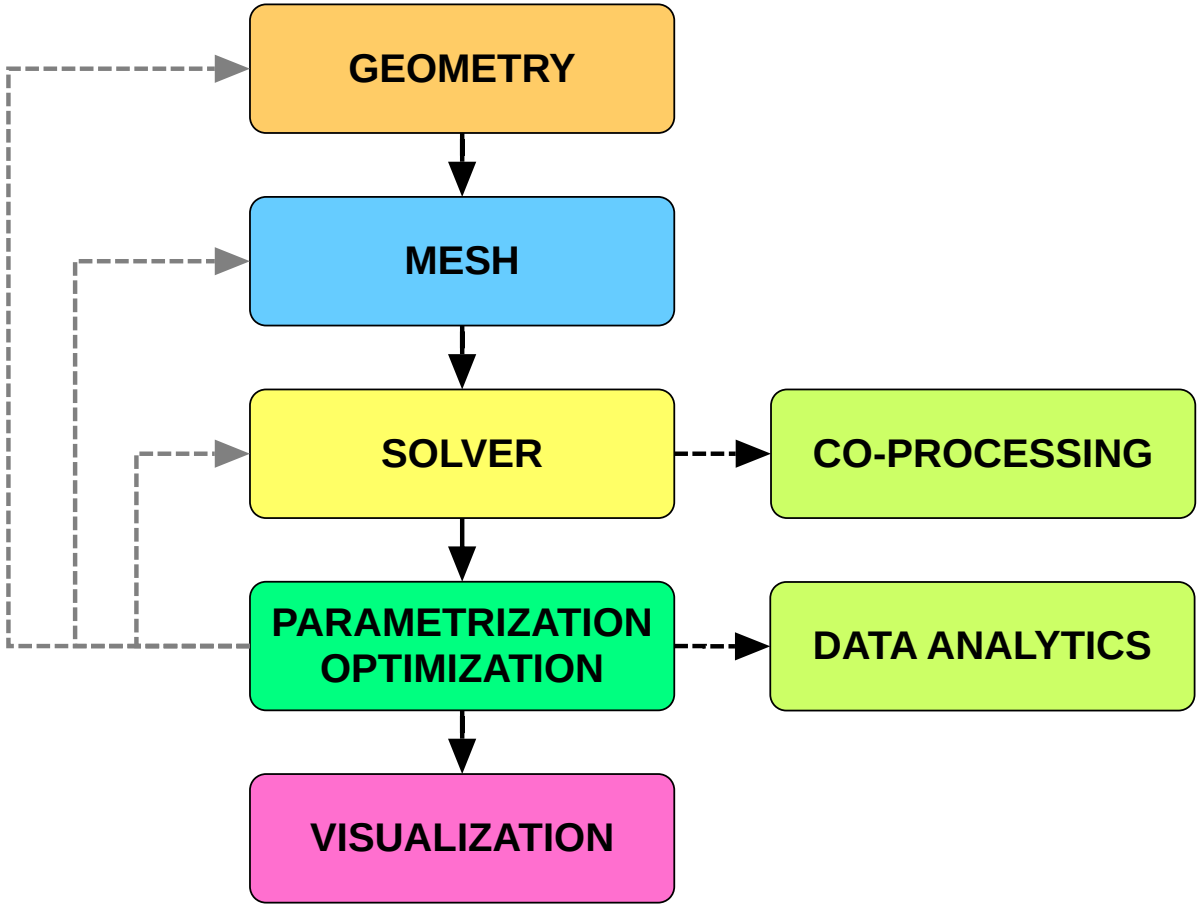


Design space exploration

- The main idea of DSE is to search the design space in a very efficient way at a minimal cost.
- When we conduct DSE we follow a systematic mathematical or statistical approach to acquire model behavior to the maximum extent.
- With DSE we can:
    - Gain a deep statistical understanding of the problem.
    - Explore a wide design space through intelligent sampling.
    - Identify the most important influencing design variables.
    - Create accurate mathematical models.
    - Identify optimal designs.
    - Provide a set of starting points for design optimization.

Design optimization and design space exploration

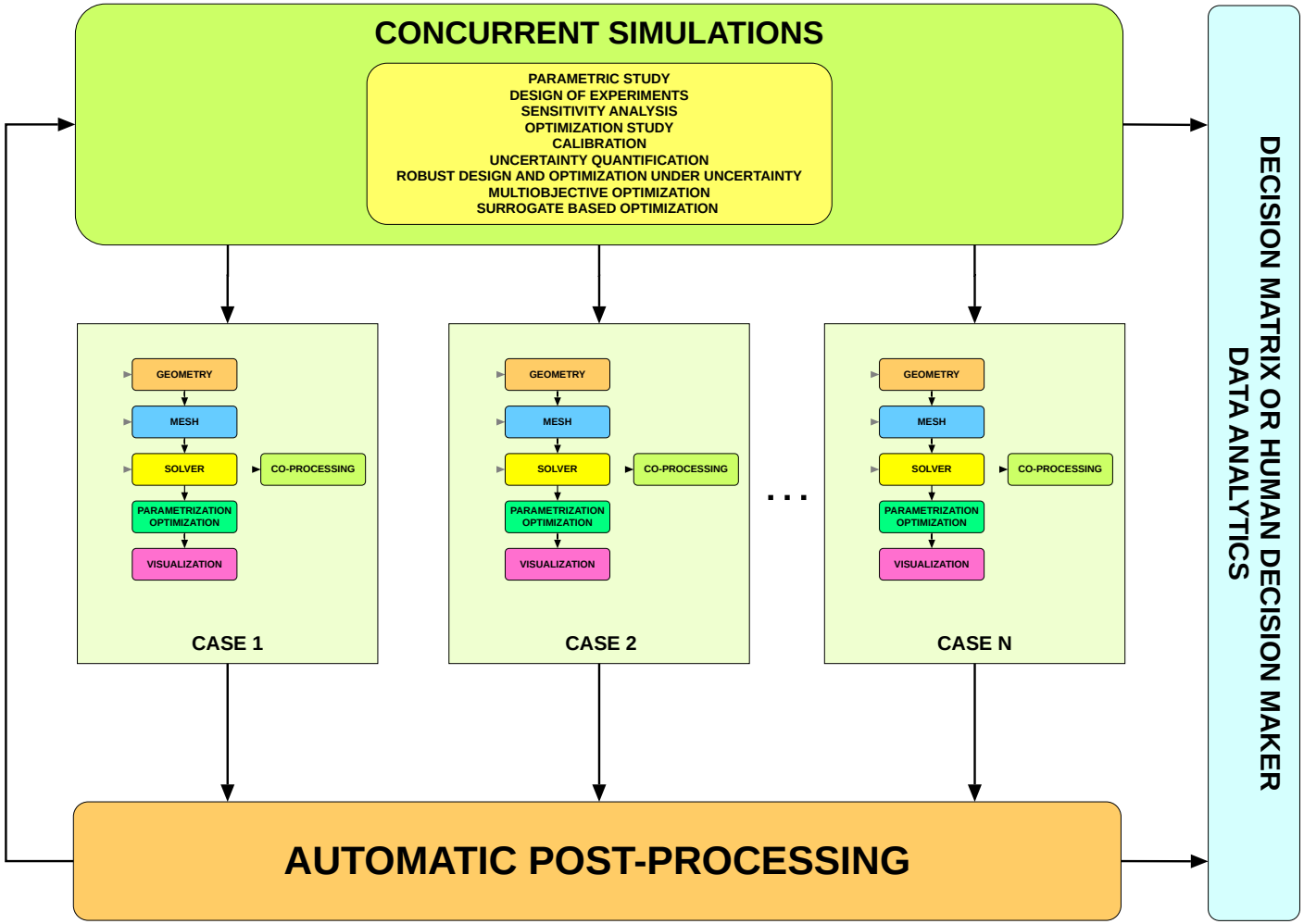
Is DSE expensive?



- Here we use many processors to solve one problem.

Design optimization and design space exploration

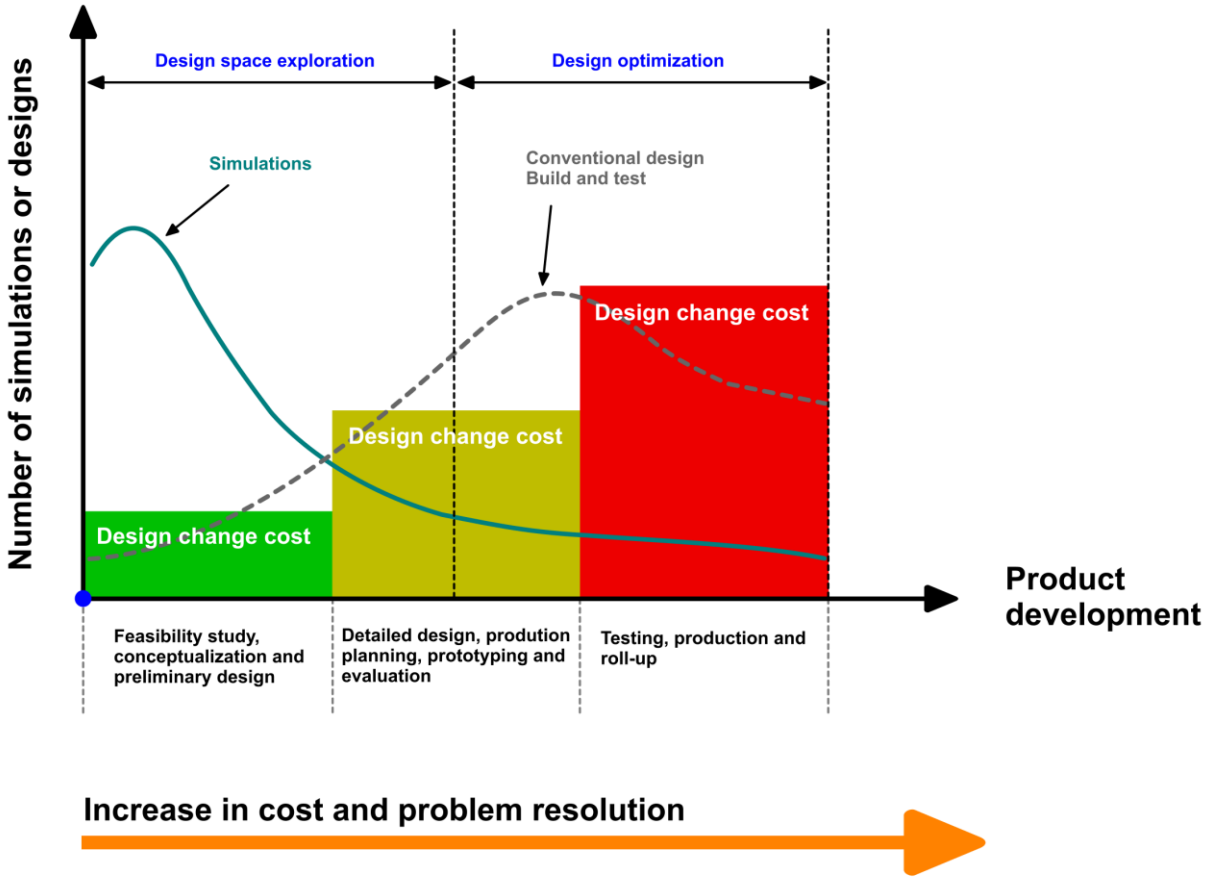
Is DSE expensive?



- Here we use many processors to solve many problems at the same time.
- And at the same time, we solve each problem using many processors.

Design optimization and design space exploration

Design space exploration and product development



- Best strategy in product development:
  - **Simulate early, simulate often.**
  - **Get it right the first time.**

- The benefits of simulating far outweigh its initial costs.

Design space exploration and surrogate based optimization (SBO)

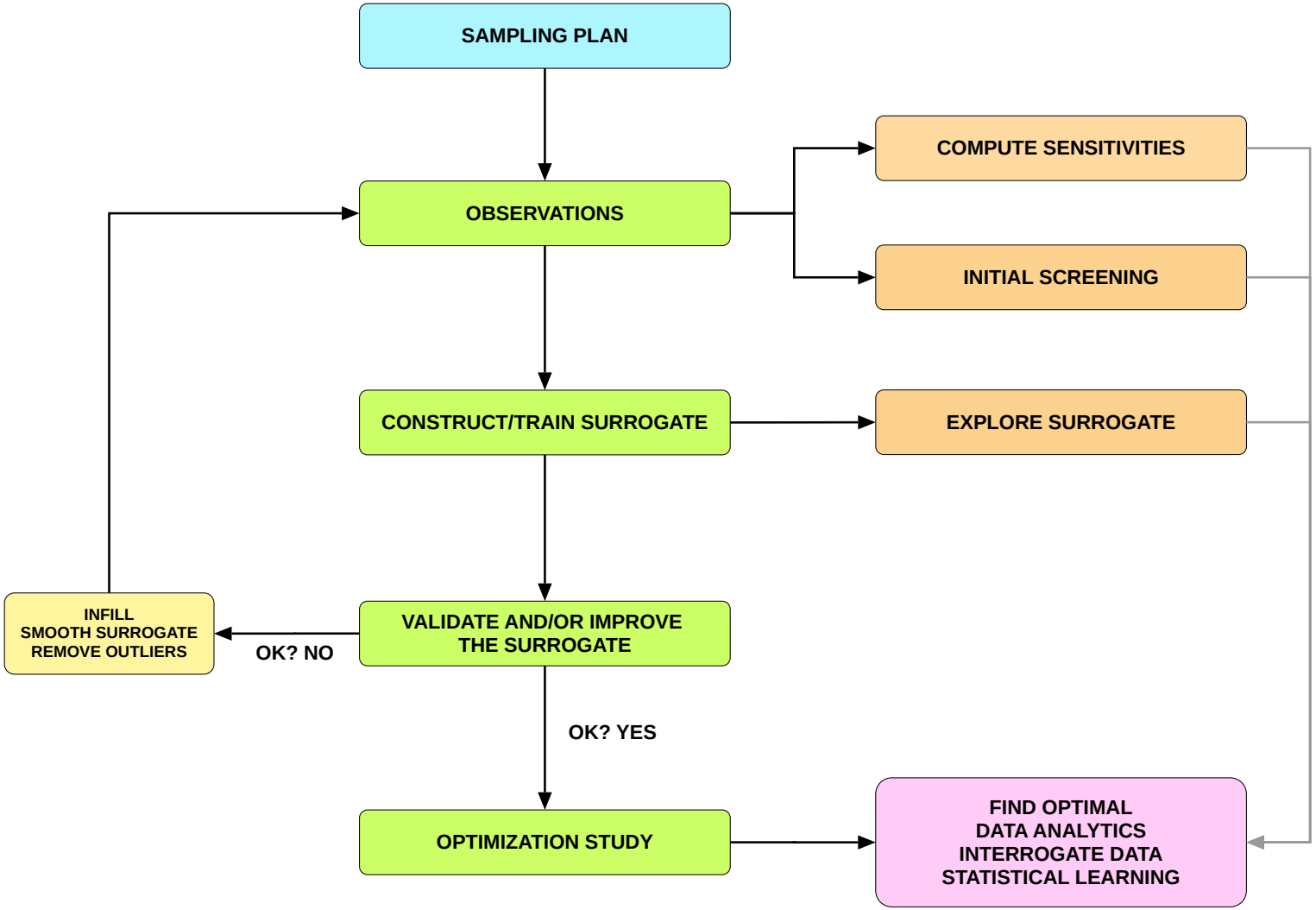
- When we do SBO, we use a surrogate model (also know as meta-model dta-fit, or response surface), to approximate an original high fidelity model (e.g., expensive CFD simulations, costly physical experiments or a mix of both).
- The surrogate acts as data fit or mathematical model to the observations so that new results can be predicted without recurring to expensive and time consuming observations.
- Once the surrogate is constructed, we can use any kind of optimization or calibration method.
- The starting point of the SBO is the DSE study.
- To construct the surrogate there are many methods, just to name a few: kriging interpolation, neural networks, radial basis functions, multivariate adaptive regression splines, polynomial functions, least squares and so on.

Design space exploration and surrogate based optimization (SBO)

- Evaluating the QoI at the surrogate level is inexpensive.
- Working at the surrogate level is order of magnitudes faster than using high fidelity models.
- Surrogates can be also used with noisy and incomplete data.
- If you are working with data mining and data analytics surrogates will let you construct predictive models.
- In engineering design, surrogates can be used for design space visualization, initial screening and optimization.

Design optimization and design space exploration

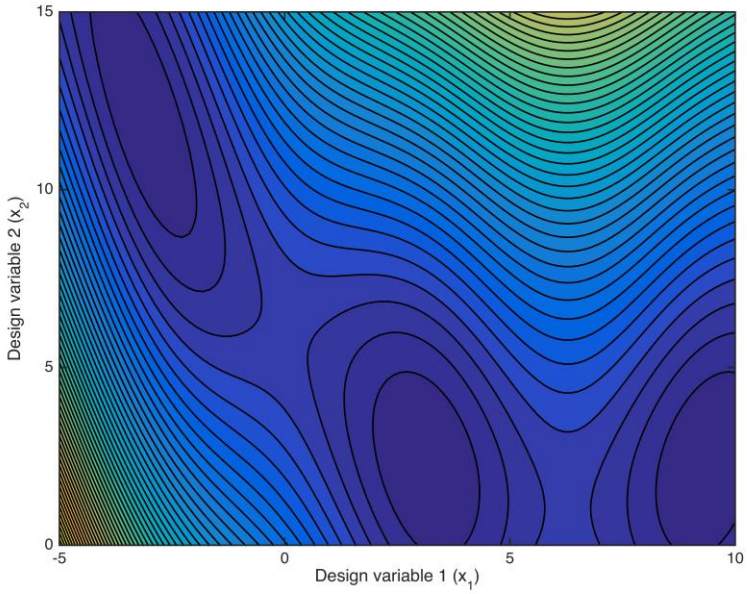
SBO workflow



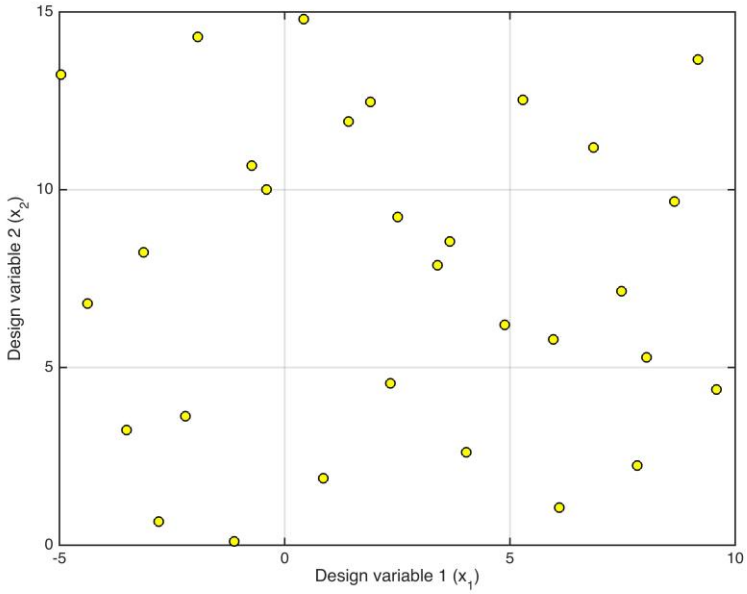
Design optimization and design space exploration

A walkthrough of DSE and SBO

DACE experiment (design and analysis of computer experiments)



Branin function - Analytical

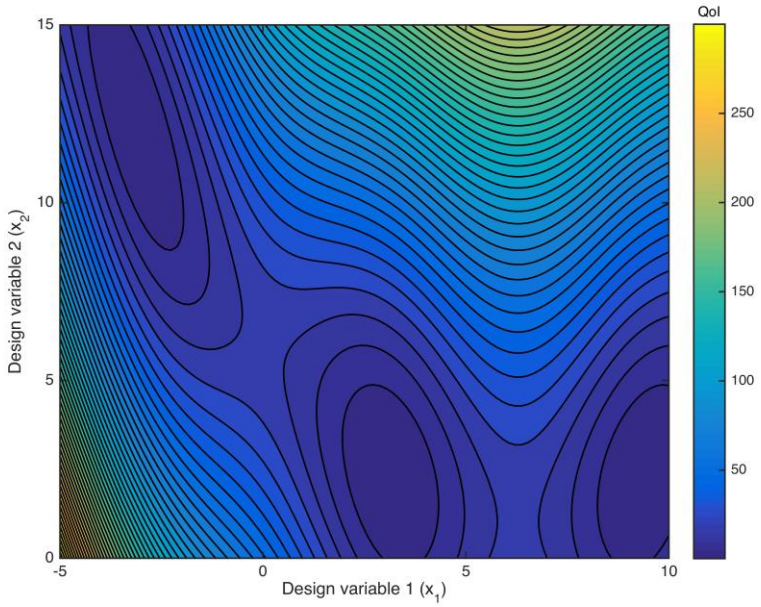


LHS sampling in design space
(30 experiments)

Design optimization and design space exploration

A walkthrough of DSE and SBO

Surrogate – Kriging interpolation



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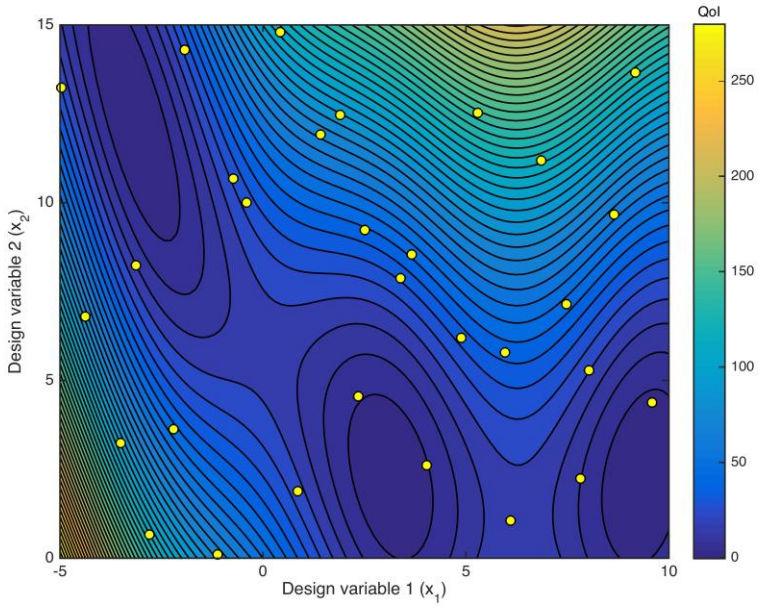
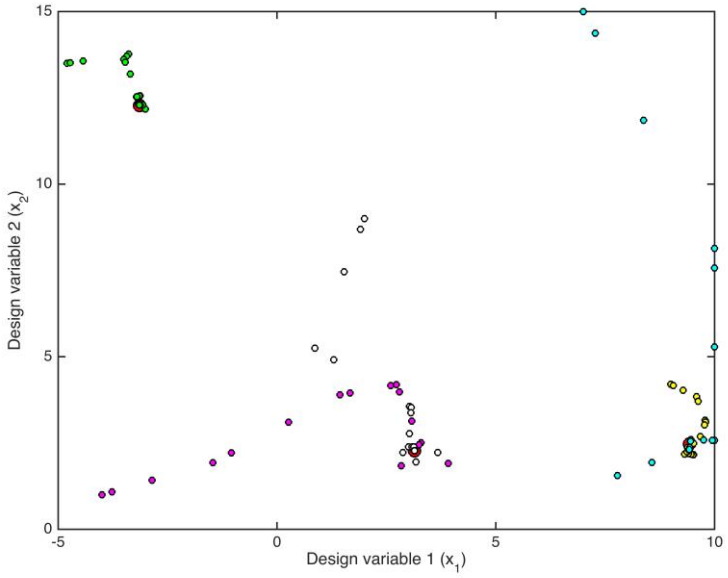


Branin function – Surrogate, meta-model, response surface, you name it

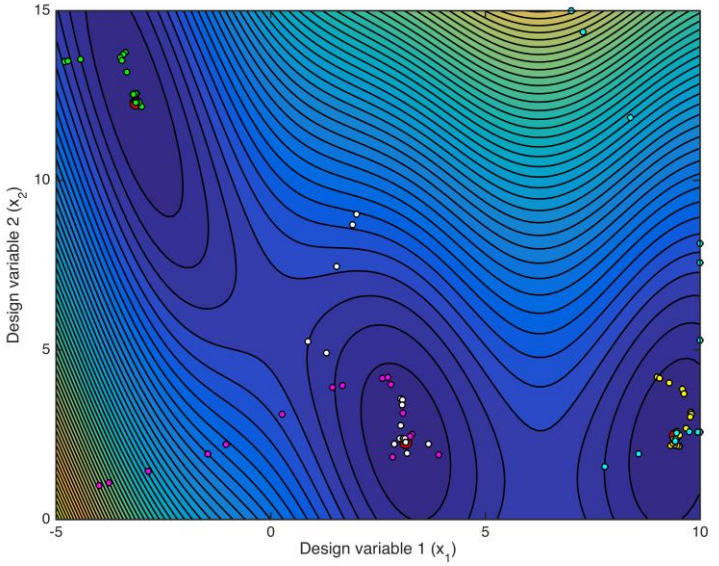
Design optimization and design space exploration

A walkthrough of DSE and SBO

DO (high fidelity simulations) vs. DSE (surrogate based optimization)



Optimization using high fidelity simulations and multi-start (more than 60 experiments)

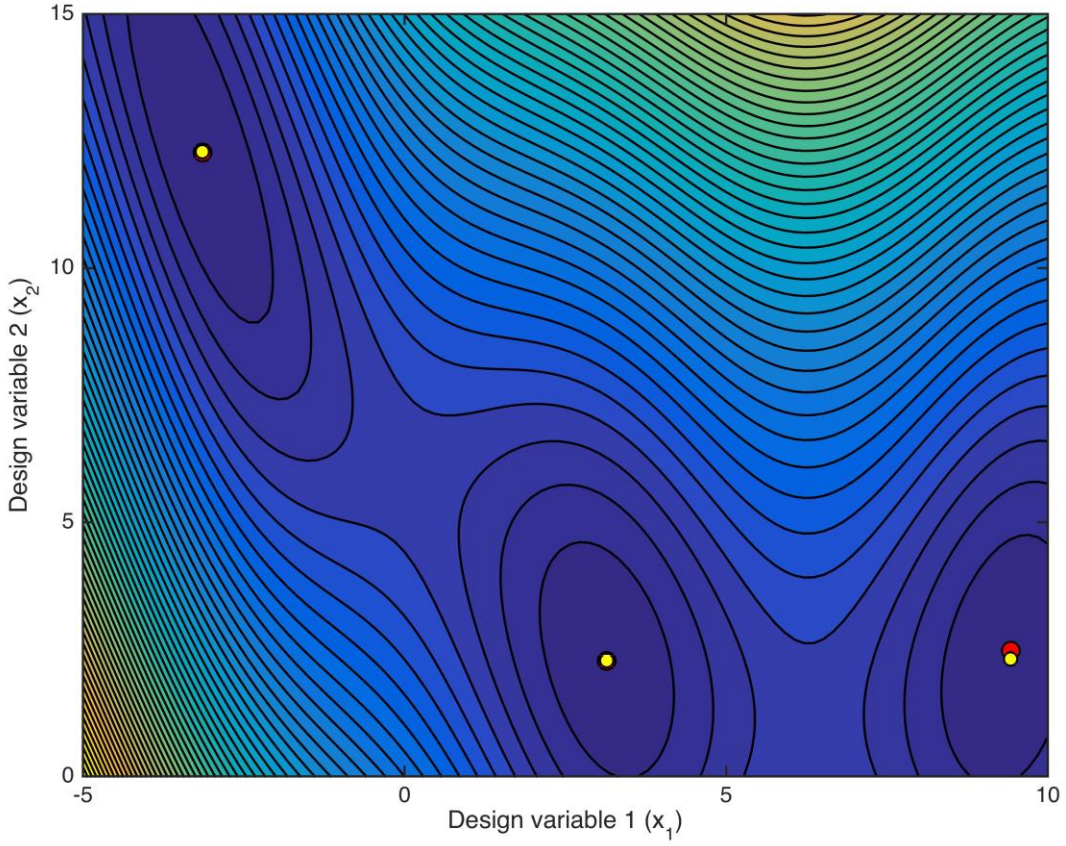


SBO (30 experiments)

Design optimization and design space exploration

A walkthrough of DSE and SBO

DO (high fidelity simulations) vs. DSE (surrogate based optimization)

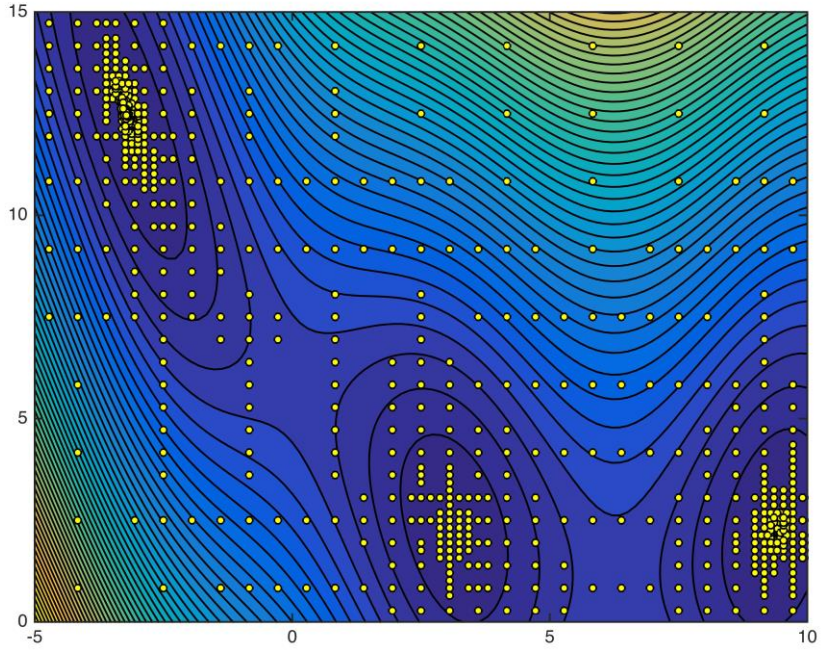


Red dots: high fidelity simulations
Yellow dots: surrogate based optimization

Design optimization and design space exploration

A walkthrough of DSE and SBO

- This function is highly non-linear and multimodal.
- Local methods will have problems in finding all the optimal points.
- Global methods can find all all the optimal points.



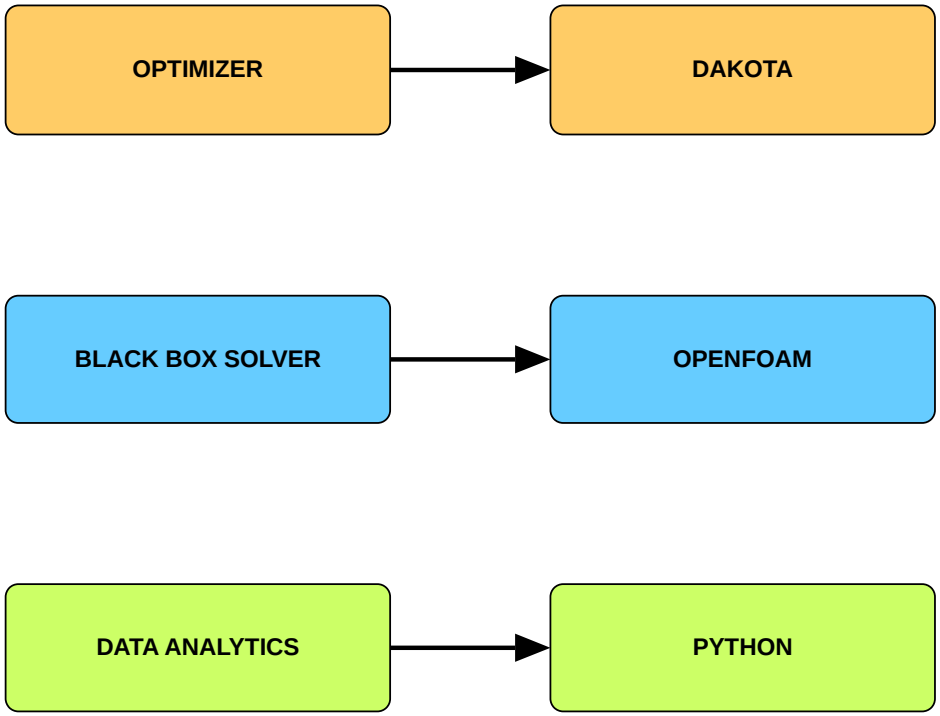
Derivative free global method – DIRECT (division of rectangles)
1000 function evaluations at surrogate level

Roadmap

1. ~~Design optimization and design space exploration~~
2. **The optimization loop**
3. One practical application
4. Wrap-up

The optimization loop

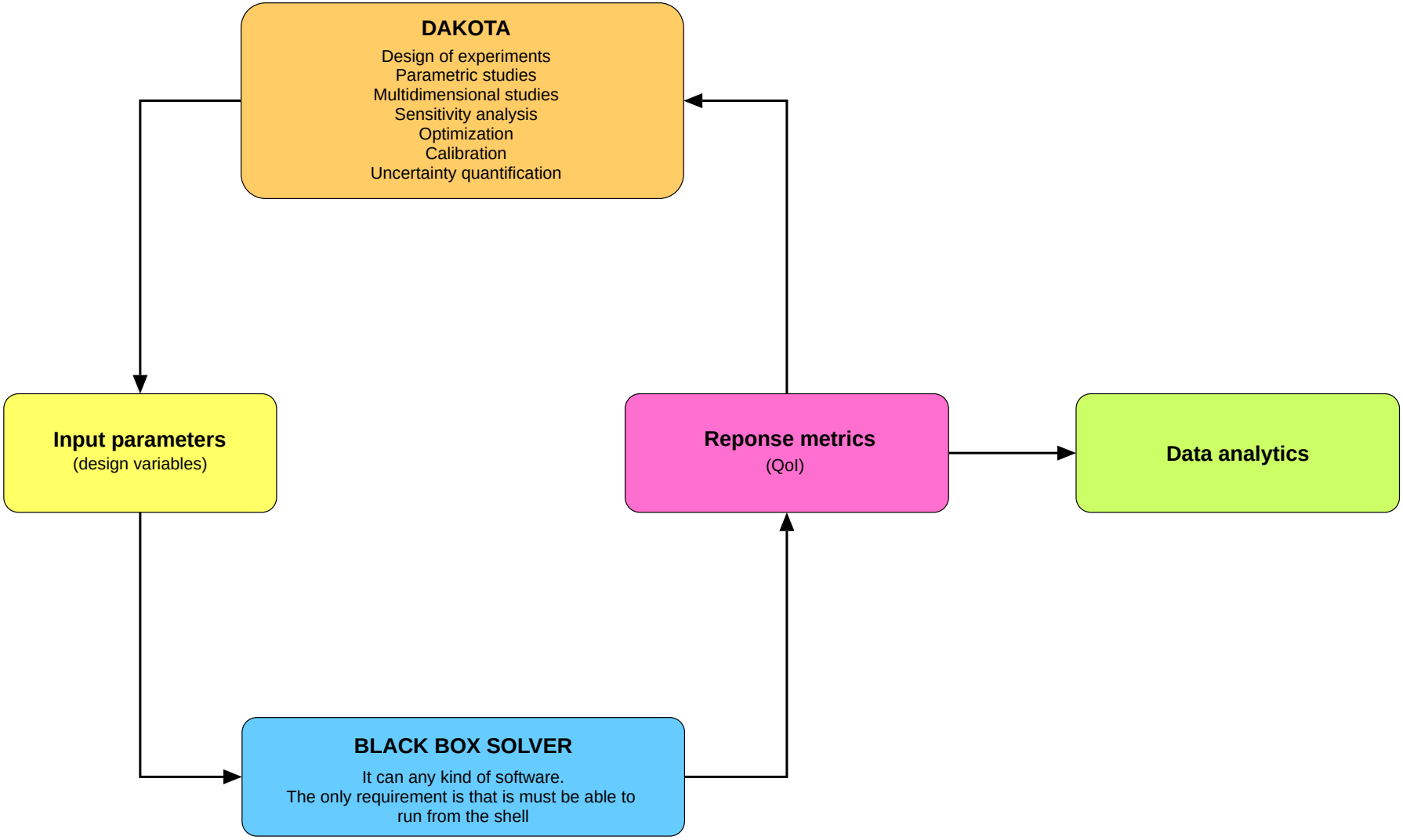
Optimization loop – Tools in use



- Why DAKOTA?
- Why not matlab, scilab, octave, Java, Python?

The optimization loop

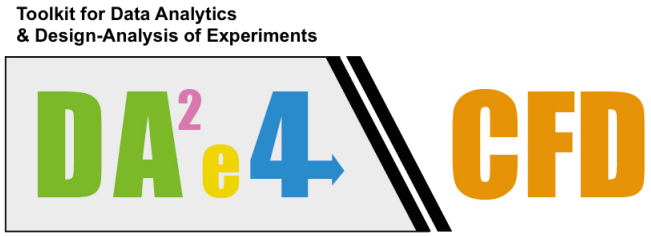
Optimization loop – The big picture



The optimization loop

Optimization framework

DAKOTA is a general-purpose software toolkit for performing optimization, uncertainty quantification, parameter estimation, design of experiments, and sensitivity analysis on high performance computers.
https://dakota.sandia.gov/



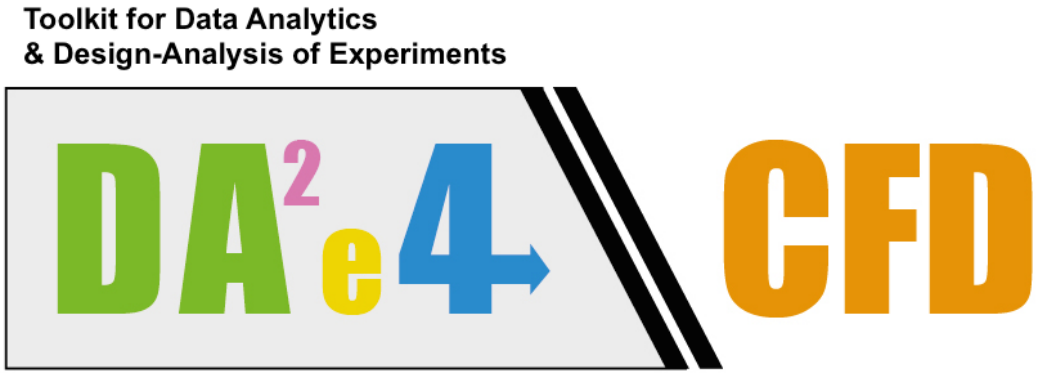
DAe for CFD is a toolkit for data analysis and inspection, interactive data visualization and statistical learning of data obtained from engineering design space exploration and design optimization studies.
https://github.com/joelguerrero/dae4cfd

CAMILO (Computer Aided ManIpulation by Level set for Optimization) is tool to manipulate 3D object shapes, based on Free Form Deformation (FFD) and Level Set (LS) techniques.
http://www.optimad.it/products/camilo/

DICE (Dynamic Interface for Computation and Evaluation) is a framework for a simplified creation of user interfaces and utilities in the area of numerical simulations.
http://dicehub.net/

The optimization loop

Optimization framework



Web-based interactive data visualization and analysis toolkit.

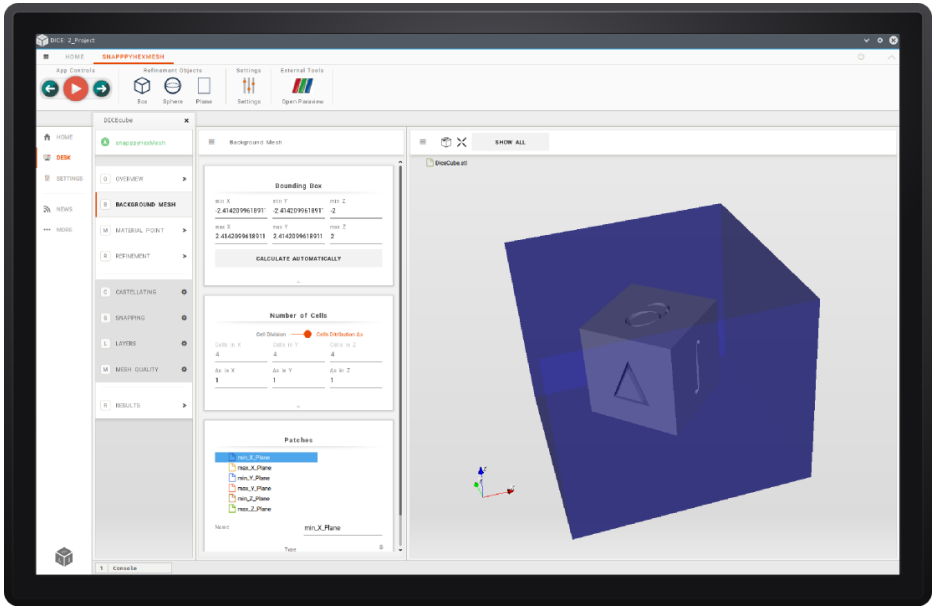
The goal is to enhance people's ability to understand and communicate data through the design of new interactive systems for data visualization and analysis. The data to be used can be obtained from any discipline (social sciences, econometrics, marketing, health care, physics, social web, etc.), but we will focus our attention on data obtained from engineering design exploration and design optimization studies.

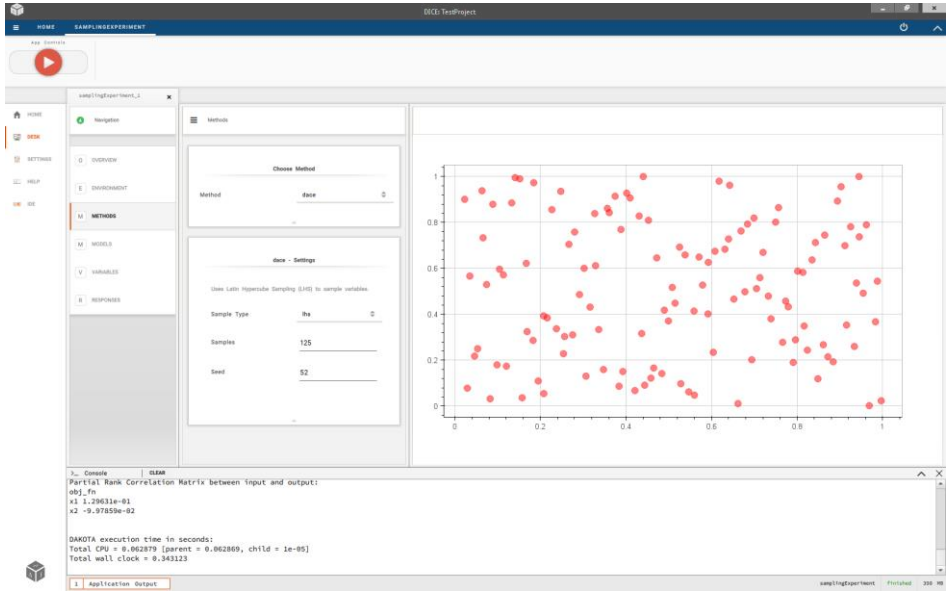
We aim at studying the perceptual, cognitive and social factors affecting data analysis in order to improve the efficiency at which expert analysts work, and to lower barriers for non-experts. The tools are implemented in Python, javascript and html5, and are able to run from any device (PC, tablet, smart-phone).

The optimization loop

Framework for tools integration (GUI)

DICE (Dynamic Interface for Computation and Evaluation)





Roadmap

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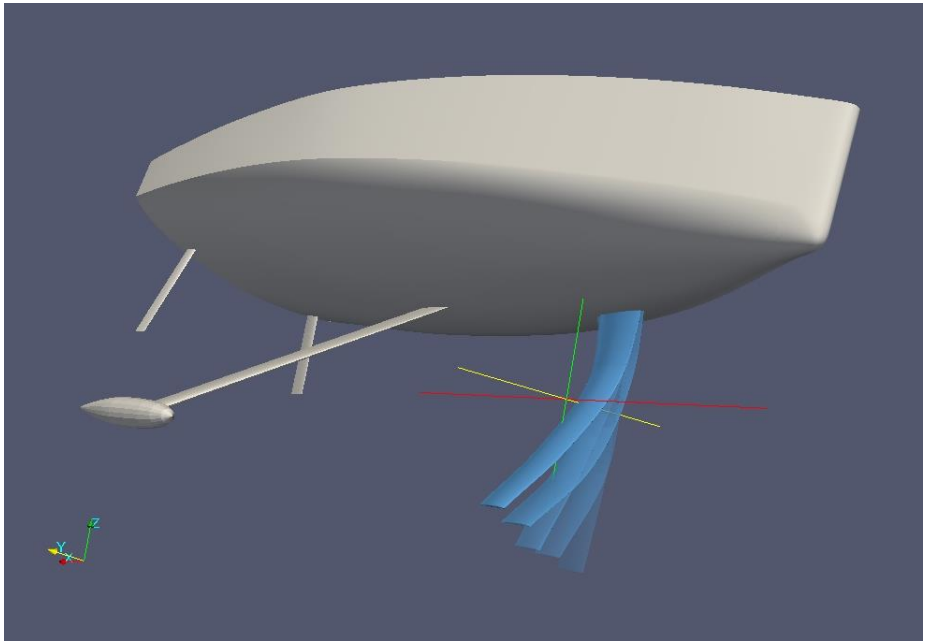
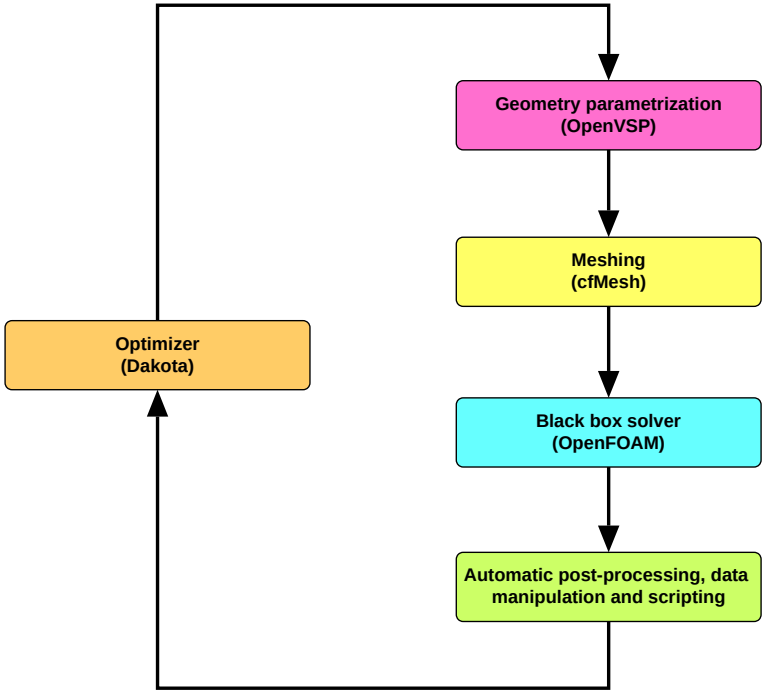
Practical applications

Sailing yacht daggerboard optimization

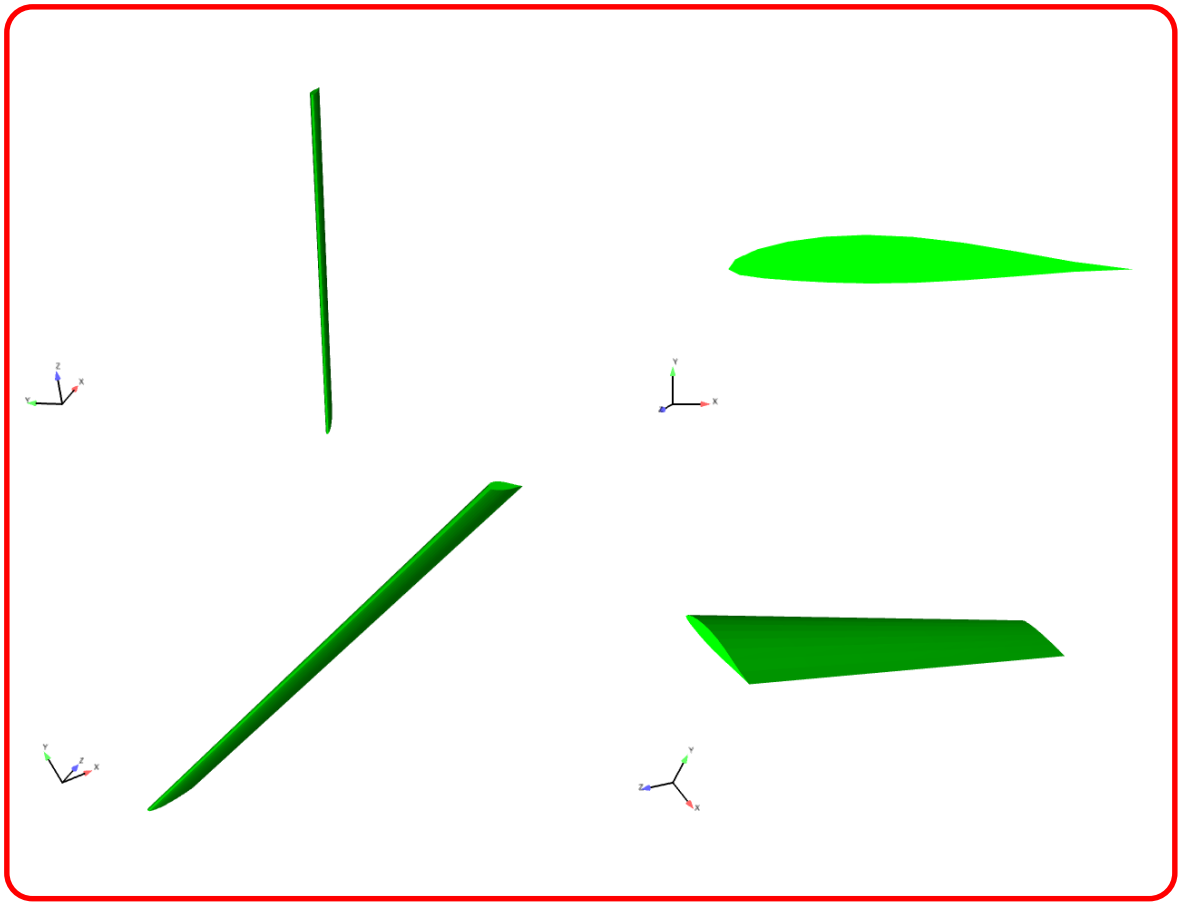
- In this case we aim at optimizing the shape of a daggerboard. The goals are maximize the vertical force and minimize the drag coefficient.
- There are 12 design variables and 1 non-linear constraint (the lateral force on the daggerboard). All design variables are bounded and for the non-linear constraint we use an inequality.
- The design variables control the airfoil shape (NACA 6-Series and NACA 4-Series) and the daggerboard shape and flexion.
- To conduct the MOO we use the MOGA method and SBO.
- We also perform online data analytics using Python.





Practical applications

Sailing yacht daggerboard optimization



12 Design variables (dv):

- 3 airfoil dv – c_l (dv1, dv2, dv3)
- 3 airfoil dv – A (dv4, dv5, dv6)
- 3 wing chord dv (dv7, dv8, dv9)
- 2 wing dihedral dv (dv10, dv11)
- 1 wing sweep dv (dv12)

2 Objective functions (of)

- Drag (of1)
- Vertical force (of2)

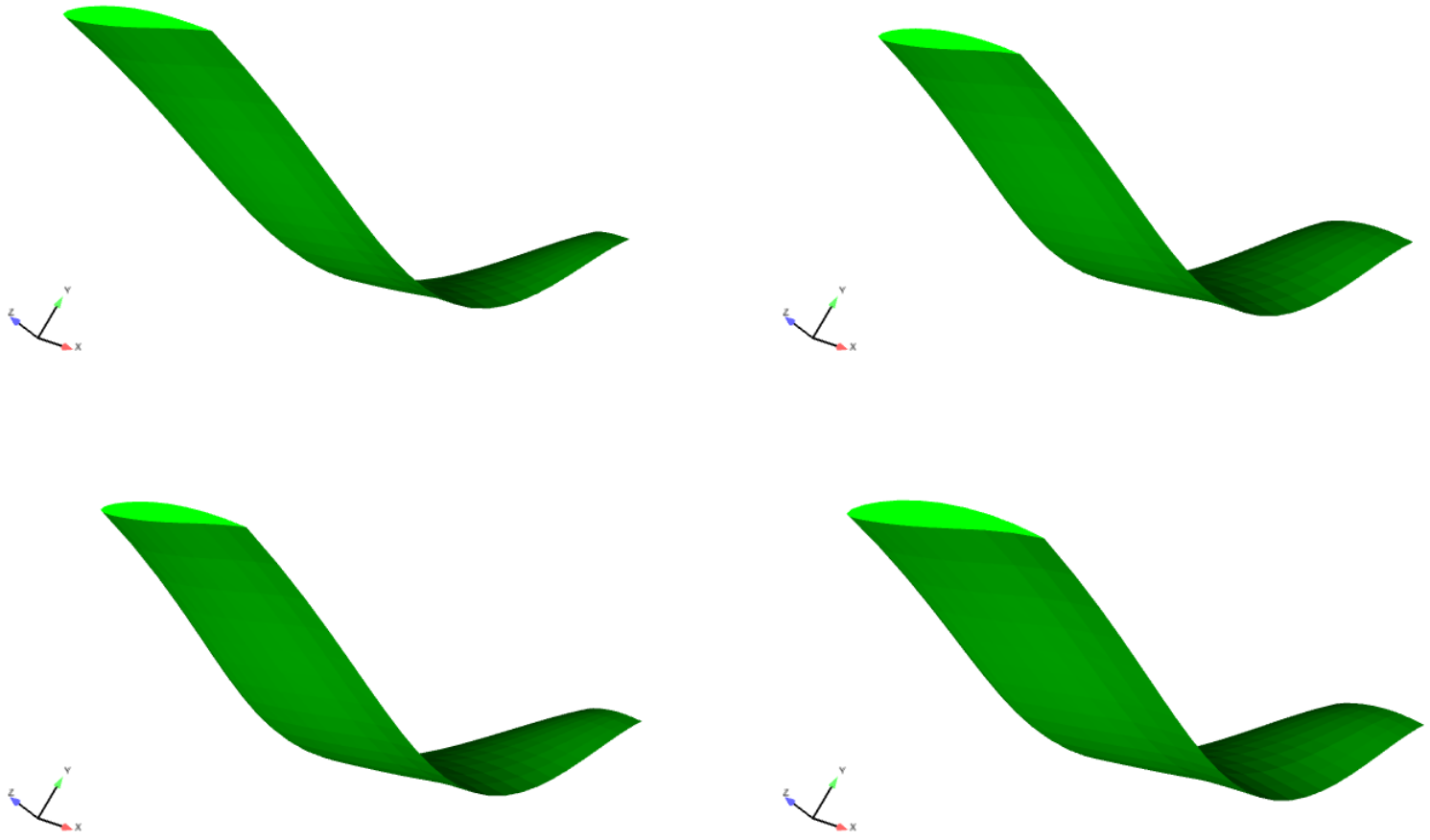
1 non-linear constraint (of)

- Lateral force (of3)

Daggerboard – Initial geometry

Practical applications

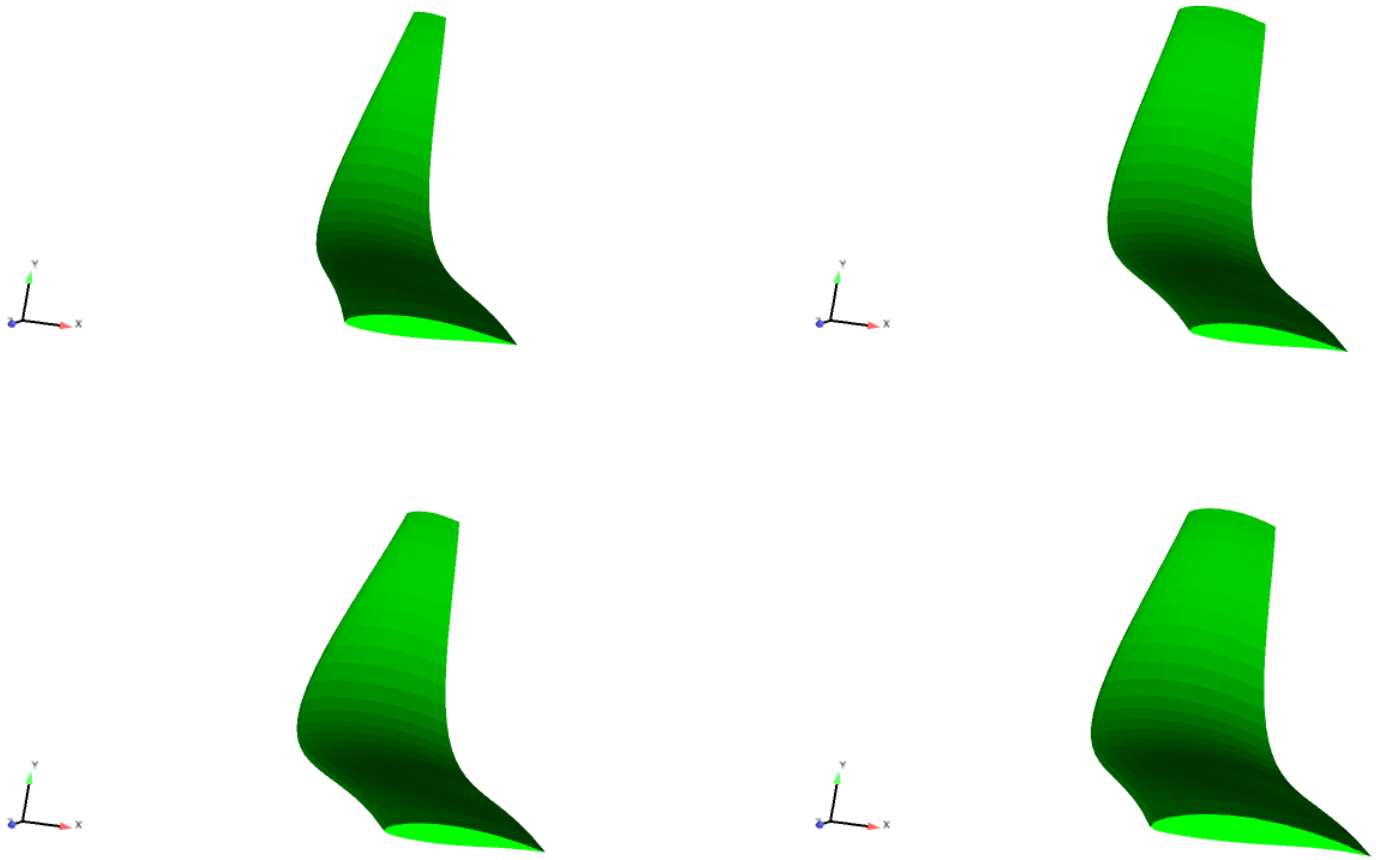
Sailing yacht daggerboard optimization



Daggerboard – Optimized geometry (4 non-dominated solutions)

Practical applications

Sailing yacht daggerboard optimization



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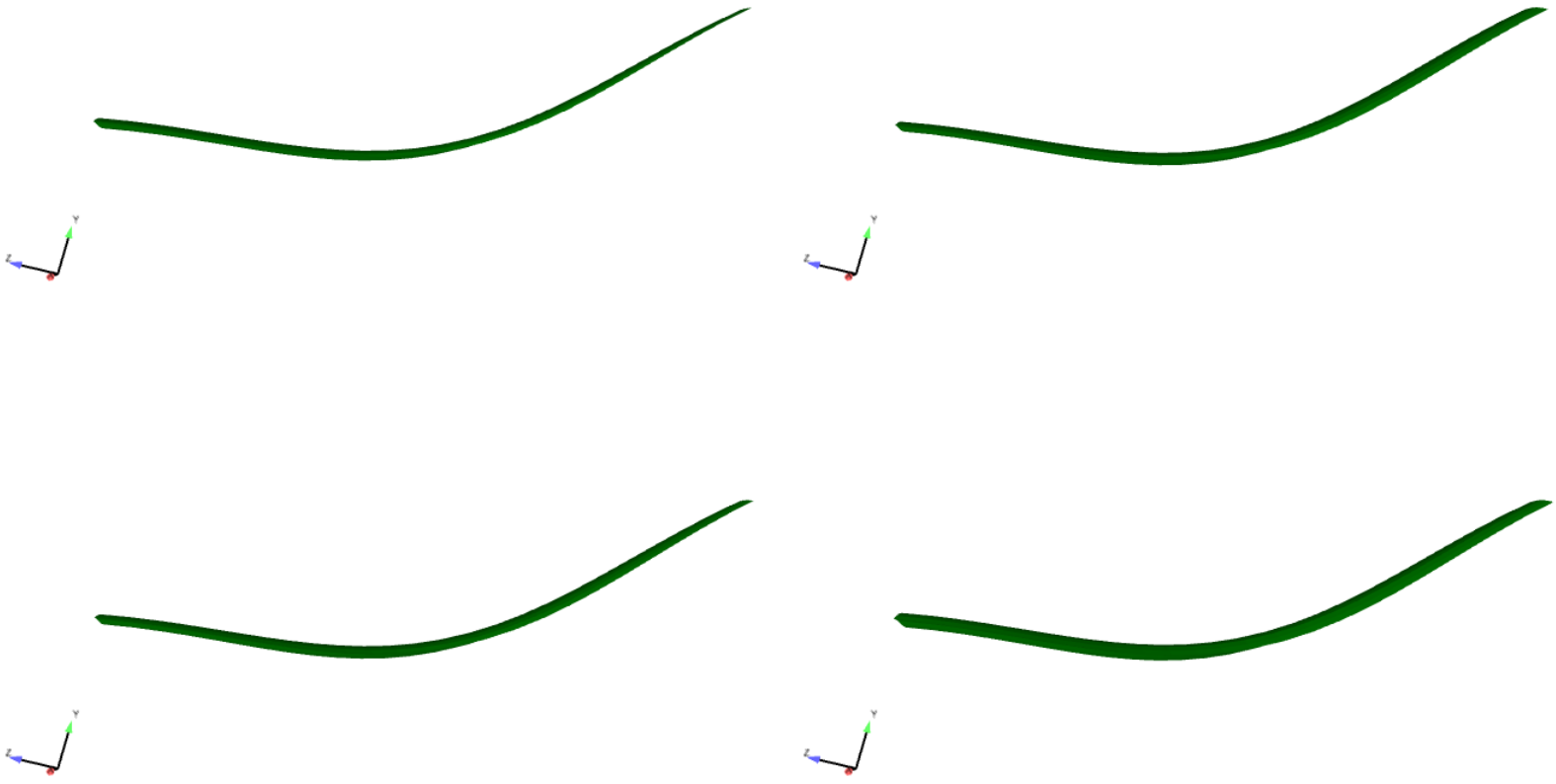

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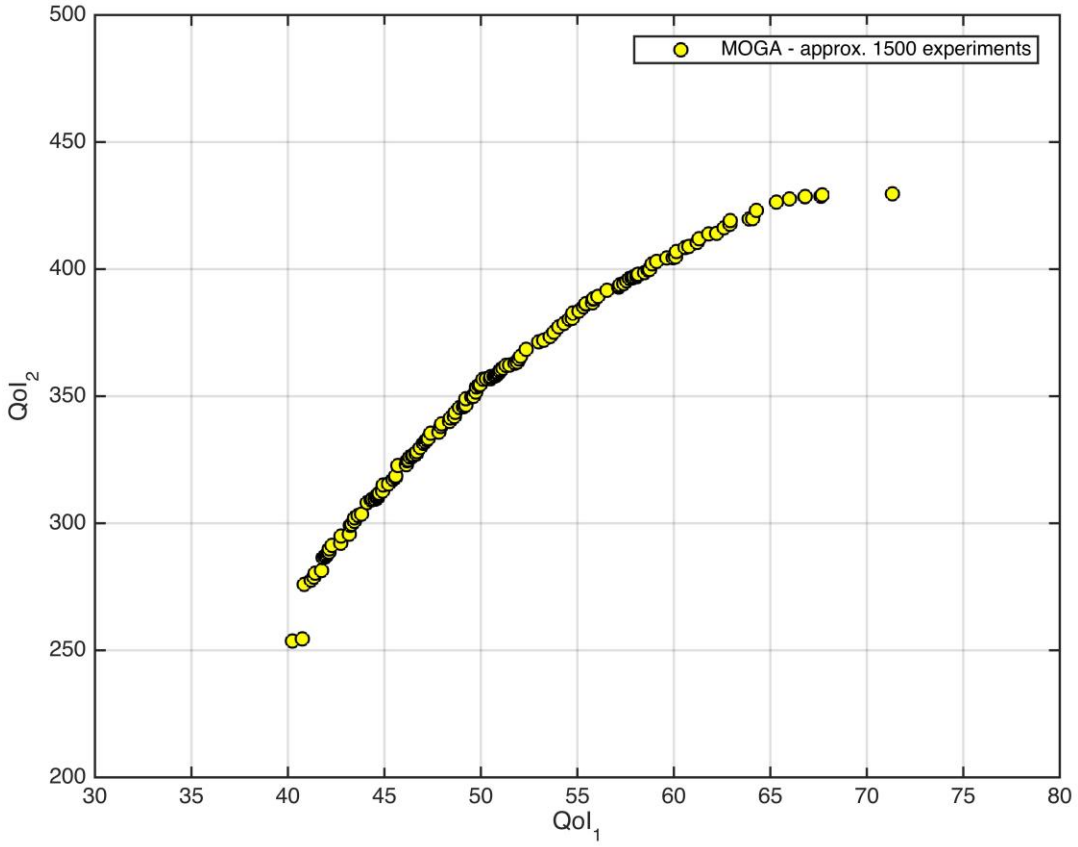
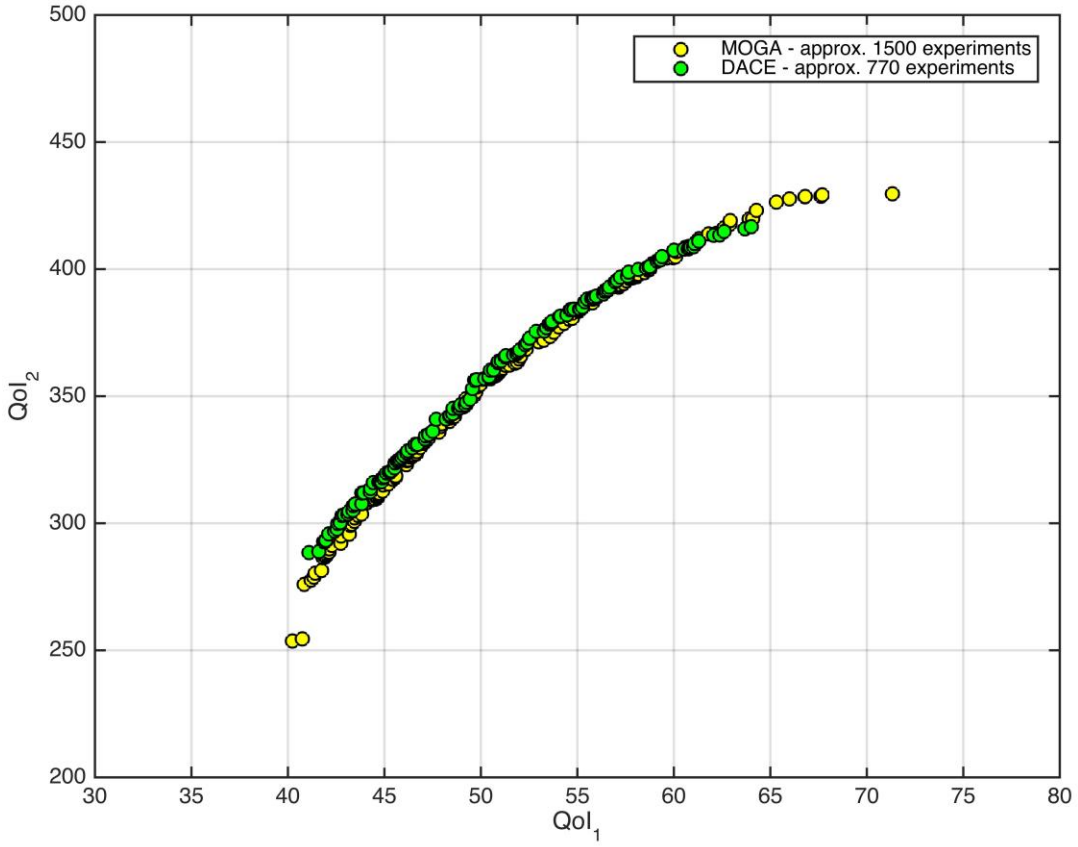


Pareto front
(QoI 1 = drag, QoI 2 = vertical force)

Practical applications

Sailing yacht daggerboard optimization



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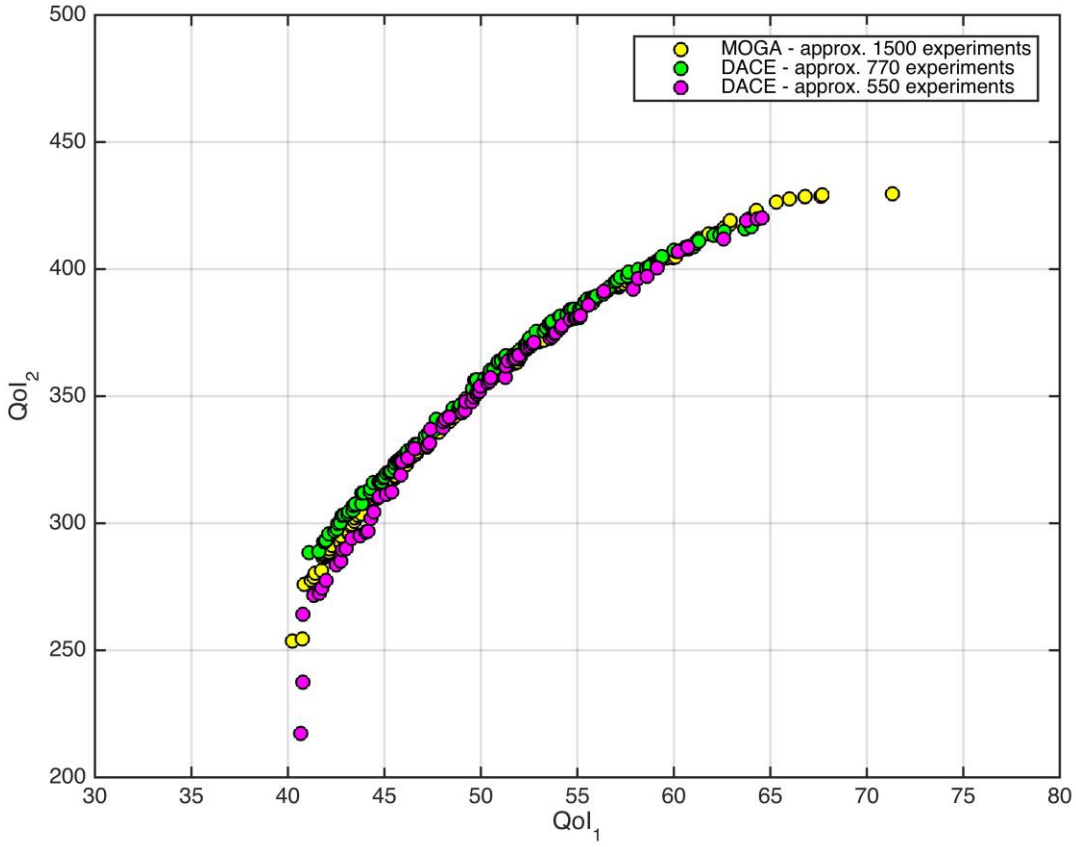

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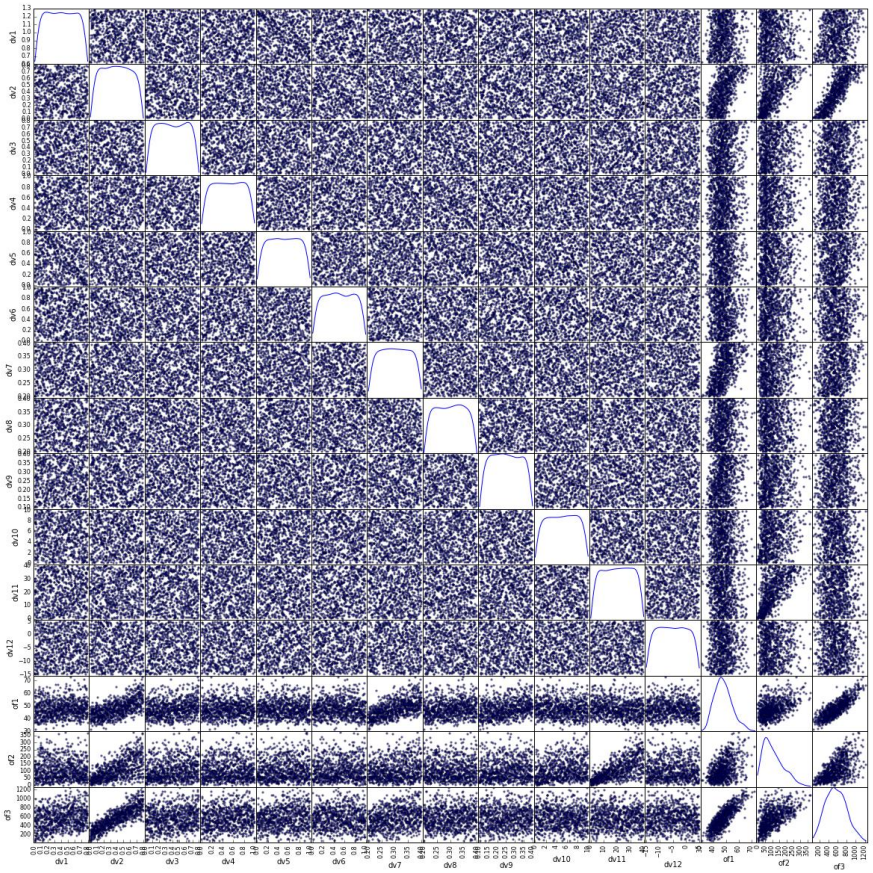
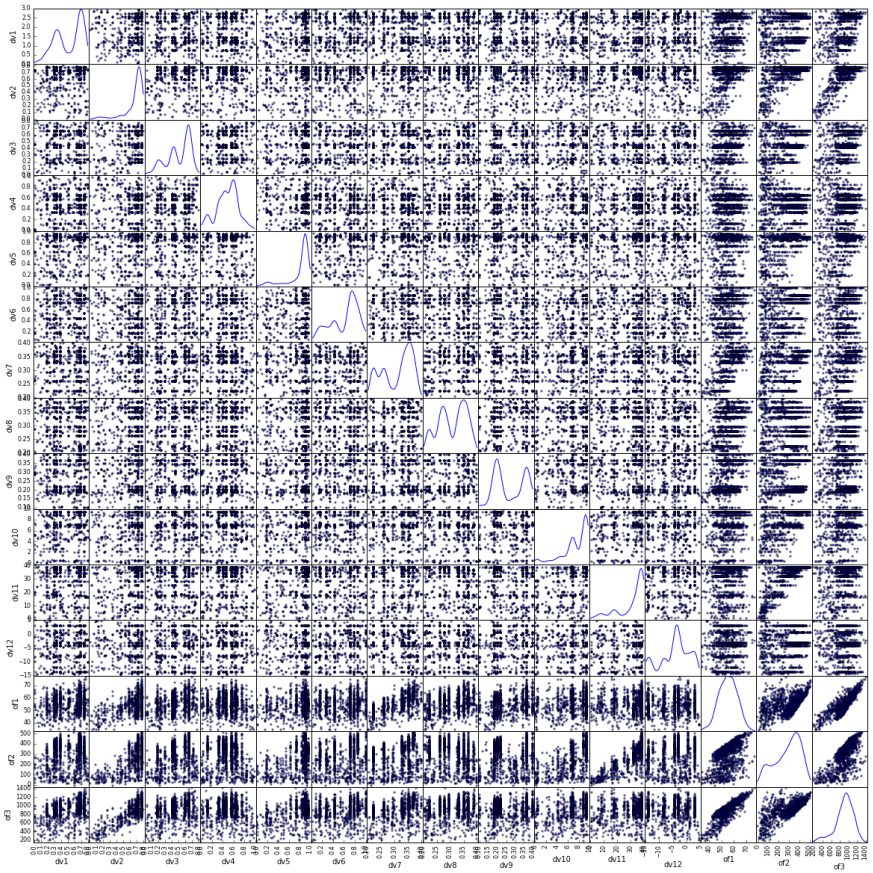


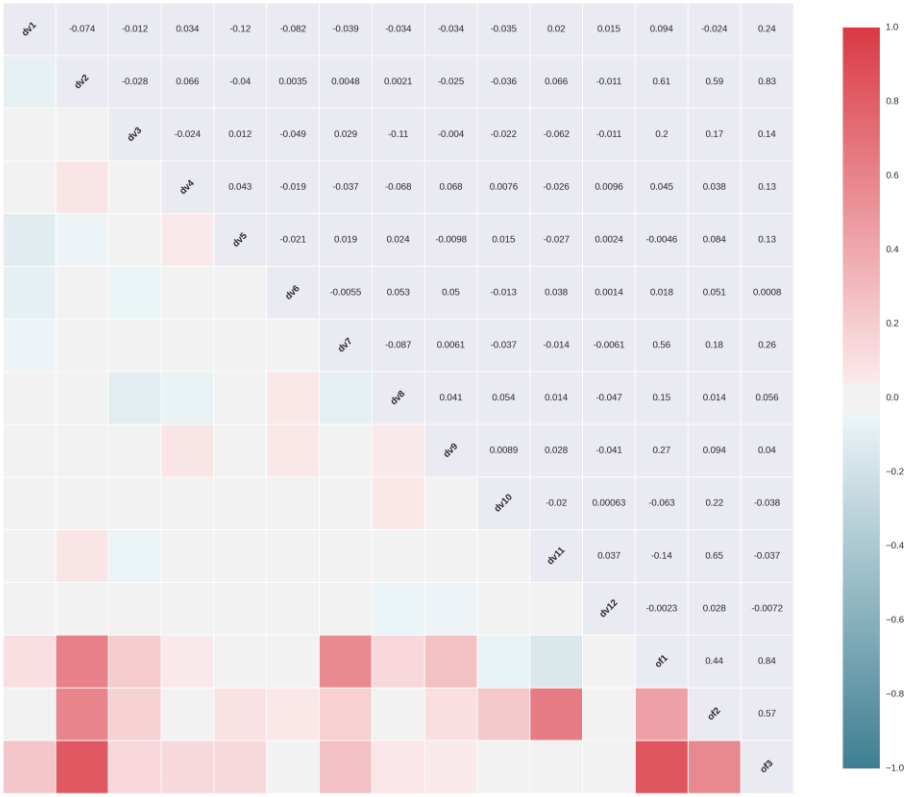
Scatter plot matrix – DACE 700



Scatter plot matrix – MOGA

Practical applications

Sailing yacht daggerboard optimization

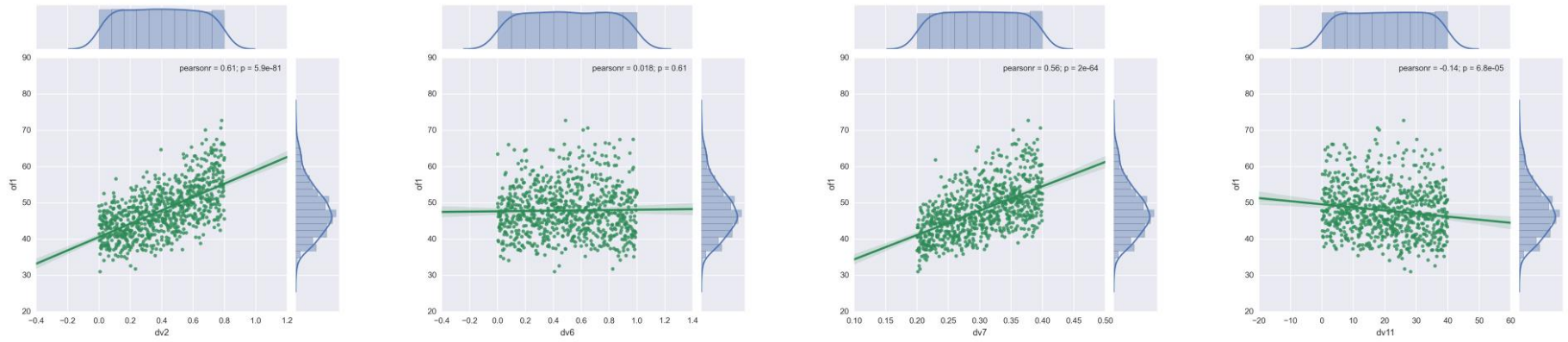


Correlation matrix – DACE 700

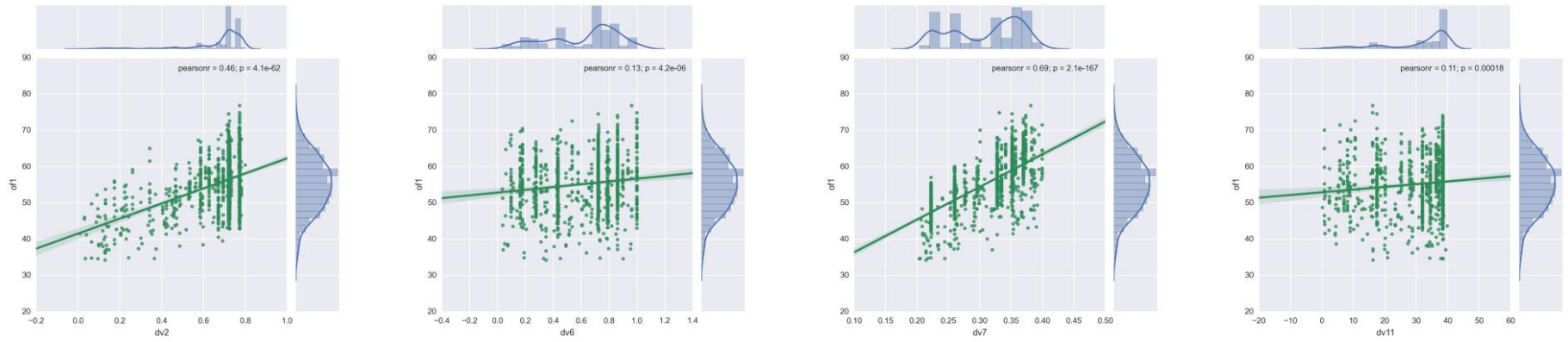
Correlation matrix – MOGA

Practical applications

Sailing yacht daggerboard optimization



QoI (of1) vs. DV (dv2, dv6, dv7, dv11) – DACE 700



QoI (of1) vs. DV (dv2, dv6, dv7, dv11) – MOGA

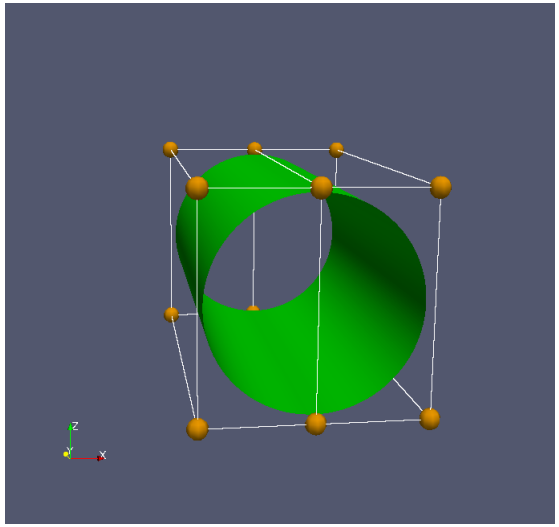
Roadmap

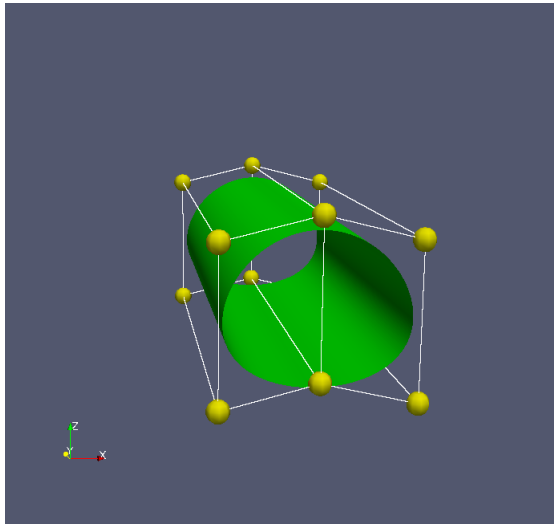
1. ~~Design optimization and design space exploration~~
2. ~~The optimization loop~~
3. ~~One practical application~~
4. **Wrap-up**

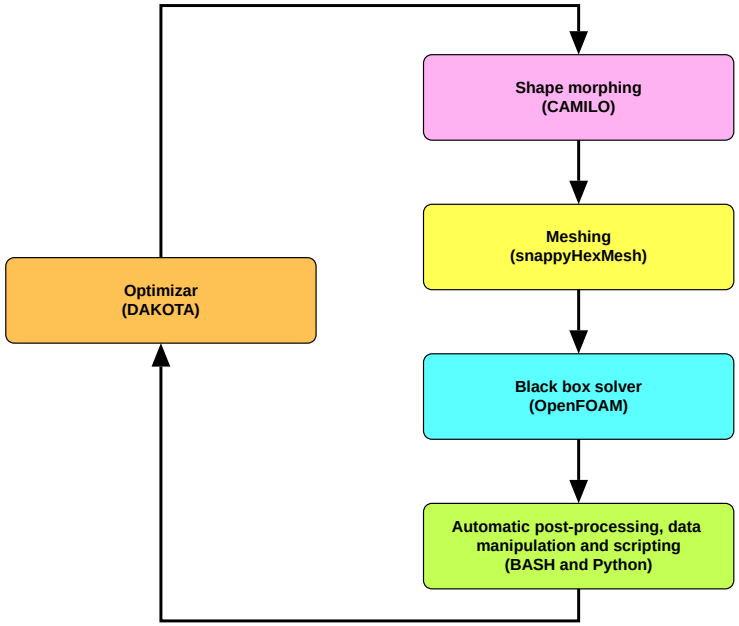
Wrap-up

Live case

- In the live case we aimed at optimizing the shape of a blunt body.
- To reach our goal we conducted a DO case and a DSE case.
- The goal was to minimize the drag coefficient.
- For shape morphing we used a free-form deformation tool with one lattice







Wrap-up

Key takeaways

- We have effectively used an optimization framework entirely based on open-source technology.
- The framework can be easily automated and used in HPC environments.
- The tools used are capable of performing and completing general purpose applications, as well as complex engineering tasks.
- Engage in DSE by simulating early and simulating often.

Wrap-up

Ongoing work

- Currently we are working in adding advanced dataset exploration and machine learning tools to the framework.
- Uncertainty quantification.
- Dynamic multidimensional detective.
- Web-based interactive data analysis and visualization tools.
- Real time rendering.
- Visualization of multidimensional surrogates.
- Substituting all the scripts with a GUI.
- All the visualization will be implemented using Python and D3.js

Wrap-up

Future developments (or good intentions)

- Mesh smoothing and mesh morphing.
- An intuitive GUI for code coupling.
- A web interface for data analytics.
- Efficient mesh morphing tools.
- Adjoint optimization.

Thank you for your attention

Questions?