Introduction to Gradient-Based Optimisation

Part 1: Introduction, overview, nomenclature

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Outline

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Organisation of the lectures

1. Univariate optimisation
   - Bisection
   - Steepest Descent
   - Newton's method
2. Multivariate optimisation
   - Steepest descent and line-search methods:
   - Wolfe and Armijo conditions,
   - Newton's method, Trust-region methods,
   - Conjugate Gradient, Truncated Newton's, Quasi-Newton methods,
3. Constrained Optimisation:
   - Projected gradient methods,
   - Penalty methods,
   - Exterior and interior point methods, SQP
4. Adjoint methods
   - Reversing time
   - Automatic Differentiation
   - Adjoint CFD codes

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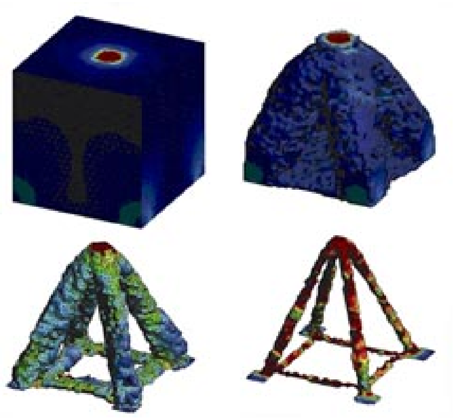
Structure optimisation: topology



(Source: http://www.bloodhoundssc.com/car/structural_design.cfm)

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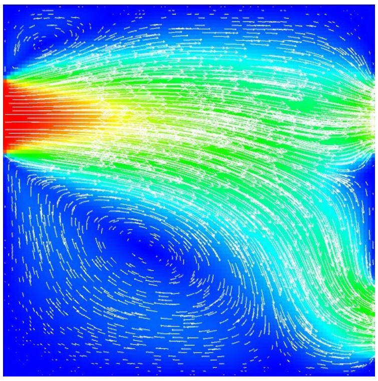
Fluid optimisation: topology



Initial flow field in a box with a single inlet on the left and two outlets on the right

(Source: Othmer, 2006)

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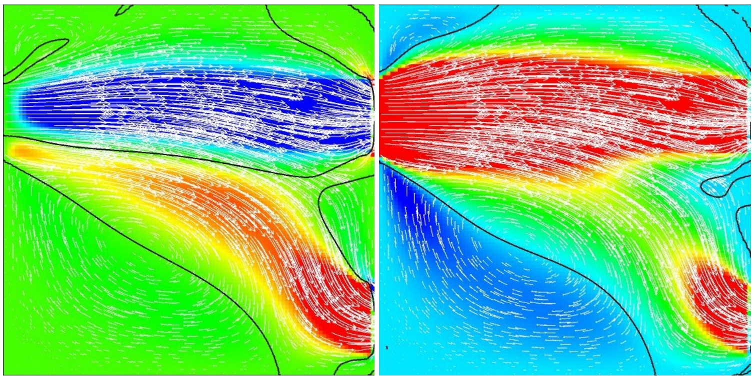
Fluid optimisation: topology



(left): Sensitivity of equal mass flow to porosity,
(right) sensitivity of dissipated power to porosity.

(Source: Othmer, 2006)

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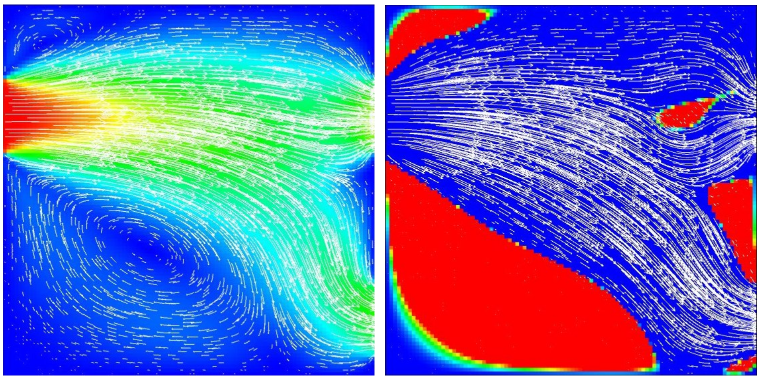
Fluid optimisation: topology



(left): Initial flow field, (right): optimised porosity and velocity field after one iteration to minimise a combination of the two sensitivities.

(Source: Othmer, 2006)

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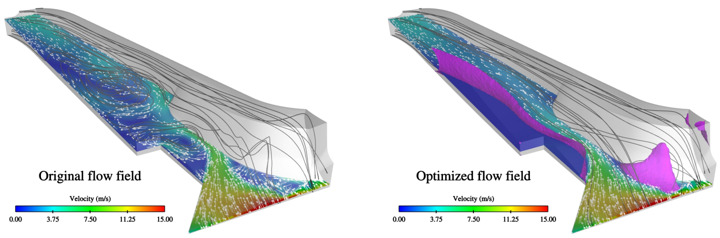
Fluid flow optimisation: topology

Optimisation of an airduct leading to a 90° bend.



before after

Optimisation improved the pressure drop by 49%.

(Source: Müller, Othmer, GACM 2011)

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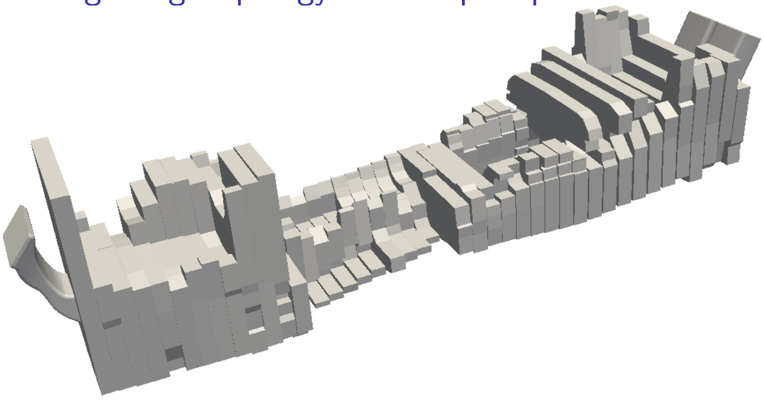
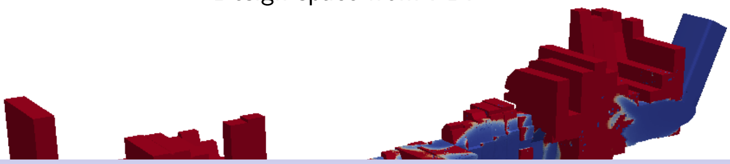
Integrating Topology and Shape Opt: Workflows



Design space from PDP



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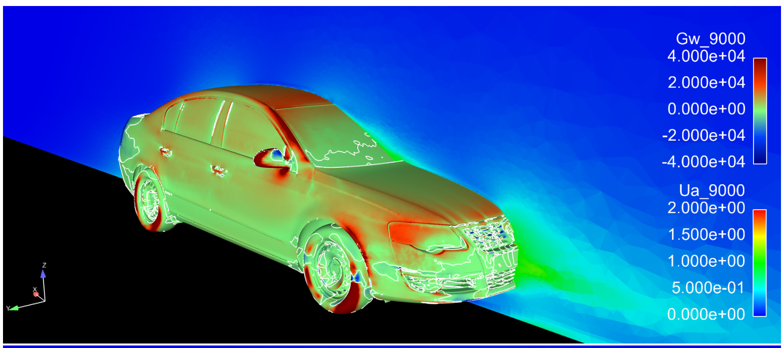
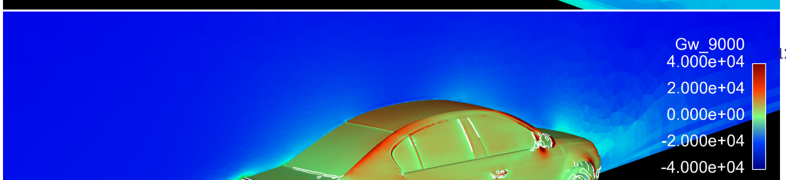
Applications of adjoint solutions

The adjoint solution can directly express the sensitivity of a single cost function, e.g. drag, w.r.t. many design variables, e.g. normal surface displacement of each mesh point:
to reduce drag: red: push in, blue: pull out





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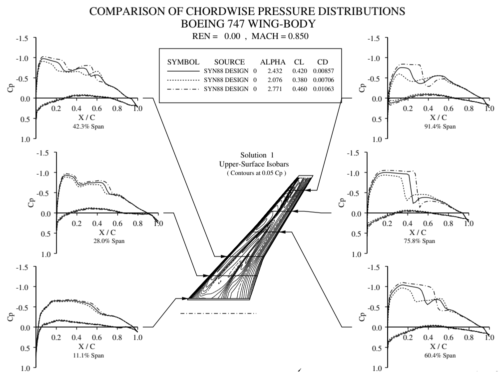
Transonic wing optimisation: wave drag



c_P, Boeing 747 Wing-Body before optimisation

A strong ‘lambda’ shock can be observed on the upper surface.

(Source: Jameson, 1998)

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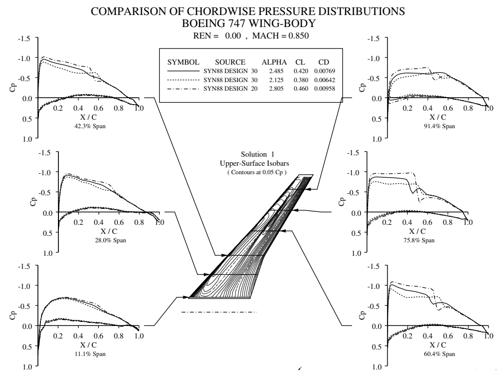
Transonic wing optimisation: wave drag



Pressure distribution after a three-point optimisation

The ‘lambda’-shock has disappeared.

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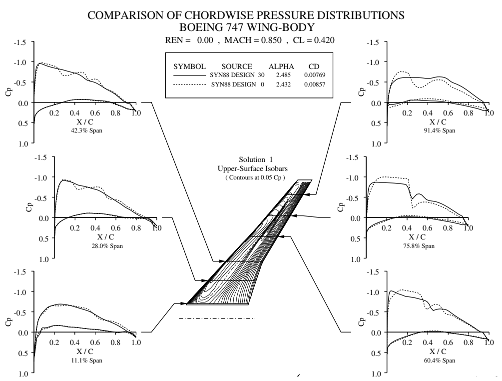
Transonic wing optimisation: wave drag



Pressure distribution: comparison before/after optimisation

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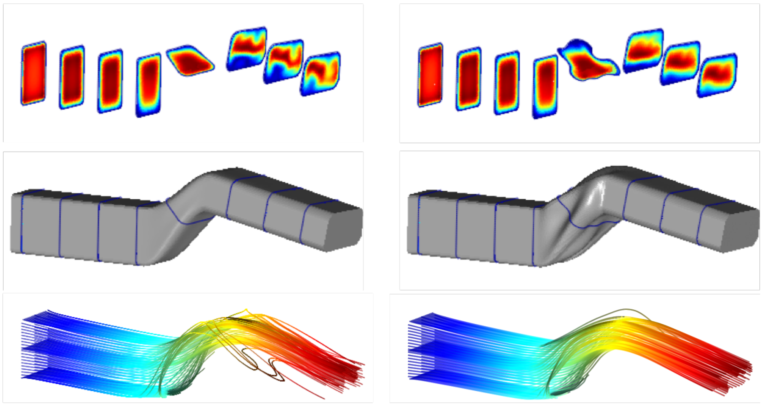
CAD-based shape optimisation



Contour plots of velocity magnitude, shape and streamlines for the initial (left) and optimised (right) ducts. Surface description is taken from and returned to NURBS patches from the CAD description.

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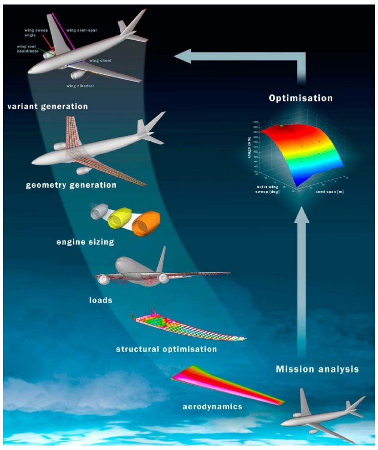
Example: Aircraft

Aim: Maximise aircraft range and minimise fuel consumption
Approach: Variation of wing span, sweep and chord, and MTOW
Methods: 1. Multidisciplinary design & optimisation (MDO)
2. Multi-objective optimisation (MOO)
Results: Trade-off for range versus fuel within the optimal design area



(Source: Vivace Project http://www.vivaceproject.com/content/forum3/6.2%20Vankan.pdf)

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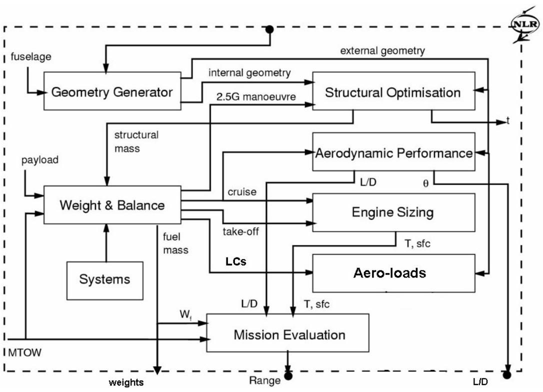
Multi-Disciplinary optimisation of a wing

- comprises the main analyses
- applies relevant load cases
- automates data exchange
- has many design variables
- predicts many design targets



To complex for a human operator: needs an optimisation algorithm

(Source: Vivace Project http://www.vivaceproject.com)

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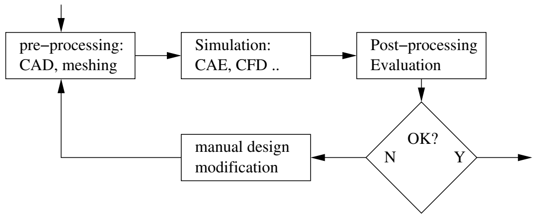
Manual design loop



- manual evaluation of the design, complex judgements possible
- manual changes of parameters, incorporates design constraints
- labour-intensive, only small design spaces possible, design space not fully explored

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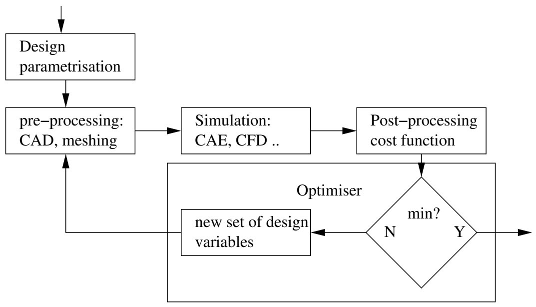
Numerical optimisation



- requires set up of a design parametrisation, if possible respecting design constraints
- the numerical optimiser selects a new set of design variables
- rigorous evaluation of the design space
- **The key element is the optimiser**

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Nomenclature

Model: a computational model of the physical process to be optimised, e.g. a CFD or FEA simulation program.

Parametrisation: definition of how the parameters or design variables affect the model, e.g. variable dimensions that define the shape of an object.

Design space: The range the parameters can take on define the design space.

Cost function, Objective: A scalar function that is to be minimised, e.g. drag of a vehicle. There may be more than one objective.

Optimiser: Algorithm that selects a set of design variables in order to find the minimum

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Taxonomy of optimisation problems

Linear vs. Non-linear: Is the cost function a linear or non-linear function of the design variables. Typically, relevant industrial problems are non-linear

Constrained vs Un-constrained: In constrained opt. an additional constraint that has to be satisfied. E.g. minimise the drag at constant lift (system or PDE-constraint). Geometric constraints are used to ensure manufacturing or assembly.

local vs global: In most industrial applications we seek an improvement of an existing solution, not the best solution in the entire design space.

continuous vs discrete: Changing the wing span is a continuous parameter, deciding between 2 or 4 engines for an aircraft is a discrete parameter.

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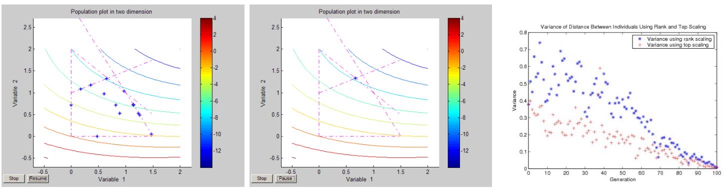
Stochastic optimisation



- Explore the design-space with stochastic sampling
- After initial global exploration, focus on 'promising' areas.
- Typical methods: Genetic Algorithms (GA) and Evolutionary Alg. (EA).

(Source: Matlab.com)

Notes

Meta-modelling/Response surface

- Often combined with stochastic opt. and/or reduced accuracy modelling
- Fit a curve/surface through the sampled points: response surface (RS)
- Search the minimum on the RS
- Update the RS with the new samples

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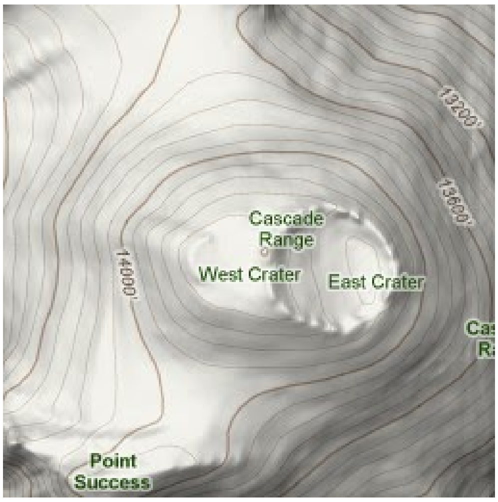
Gradient-based optimisation



- Walk downhill to descend to the minimum,
- May be caught in local minima,
- More complex to deal with constraints, may need gradients of the constraints as well.

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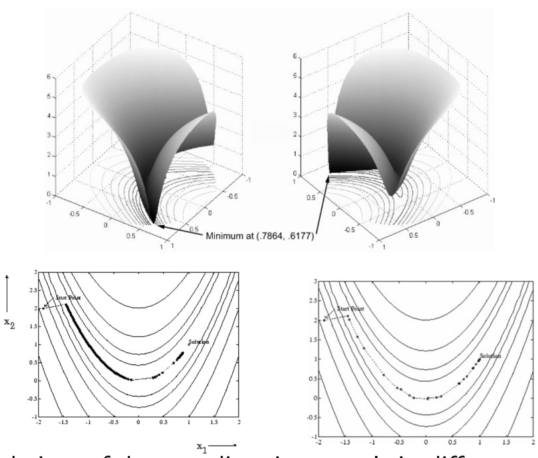
Gradient-based optimisation: Rosenbrock's function



Steepest Descent

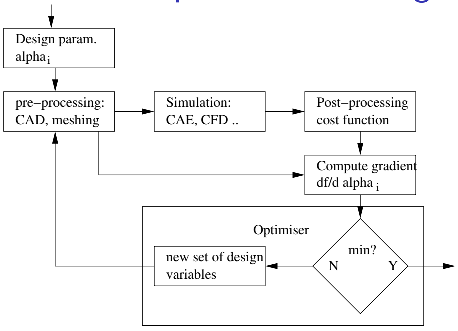
BFGS

Different choices of descent directions result in different convergence rates to the minimum.

(Source: Matlab.com)

Notes

Gradient-based optimisation: design loop



- Computation of the gradient of the cost function J w.r.t the design variables α_i is complex and expensive
- Needs to include how model solution U and mesh coordinates X depends on the α_i:

$$\frac{dJ}{d\alpha_i} = \frac{\partial J}{\partial \alpha_i} + \frac{\partial J}{\partial U}\frac{\partial U}{\partial X}\frac{\partial X}{\partial \alpha_i}$$

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Characteristics of Engineering optimisation problems

Cost of evaluation: Can I afford many evaluations of the model? If so, one could use the existing model discretisation (e.g. CFD code) as a 'black box' by calling it repeatedly.

Gradients: Is it feasible to compute gradients of the cost function w.r.t. design variables?

This leads to two main approaches for numerical optimisation:

- if the evaluation is cheap, e.g. stress analysis, **stochastic methods** are used with black-box models.
- if the evaluation is expensive, e.g. CFD, we have to compute gradients to be able to use **gradient-based** optimisation.

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