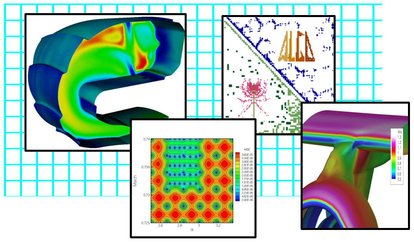


Optimizing
Aerodynamic Design Problems

A. Troeltzsch

Joint work with

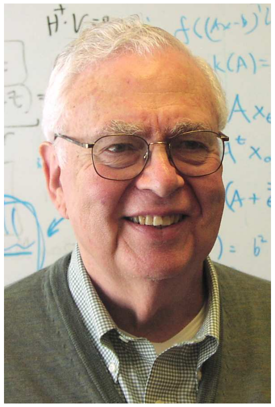
S. Gratton, CERFACS, CNES

Ph. L. Toint, University Namur, Belgium

Thanks to

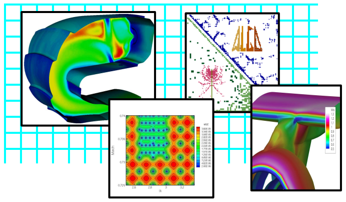
J. Laurenceau, J.-F. Boussuge, CERFACS

M. Meaux, Airbus



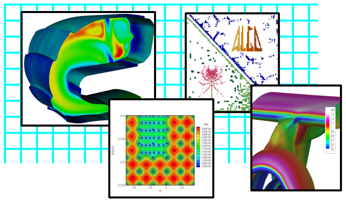
In memory of Gene Golub

(February 29, 1932 - November 16, 2007)



Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



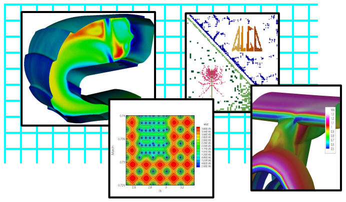
Problem description

(NLP)

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } \quad x \in X \cap \{x \in \mathbb{R}^n : c(x) \leq 0\} \end{aligned}$$

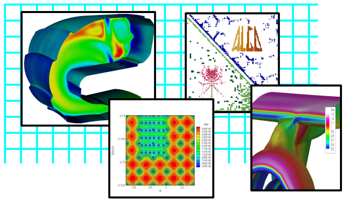
- X is a region where f(x) and c(x) can be evaluated by the underlying CFD simulation
- f, c are expensive black boxes – mins, hours, days, weeks
- nonlinear and nonconvex

- Gradient is available (obtained by Adjoint state system)
- Hessian has to be approximated by the optimizer if necessary



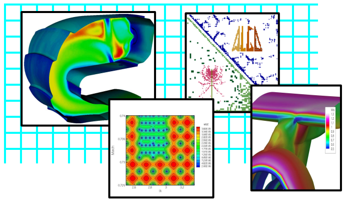
Problem description

- Application: optimize design of a wing shape (collaboration with Airbus)
- Goal: find the best strategy to solve these problems
  - Improve existing strategies
    - Direct minimizer DOT
      - BFGS method, CG method
    - Surrogates approach
      - Kriging and Co-Kriging Model Framework
  - Generalize to constraints
- First step: compare direct solver DOT with a set of well-known optimization codes – free for academic use



Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



Direct minimization

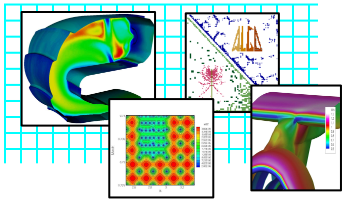
- Direct minimization:
  - approach to minimize the objective function by evaluating directly the true problem function and/or gradient values at each step

- Comparison: DOT with a set of well-known optimizers (L-BFGS-B, TN-BC, Lancelot, IPOPT, DONLP2)

- Important points for fair comparison:
  - Use the same stopping criteria
  - Parameter choice: usage of default values
  - Use the same information of the function (funct. value, first derivatives)

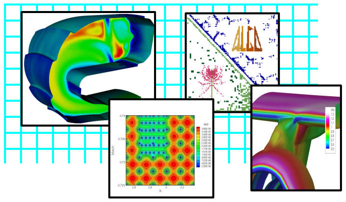
Direct minimization

- Used stopping criteria:
  - Problem solved successfully
    - Infinity norm of projected gradient <= 10e-5
  - Problem not successfully solved
    - Termination by solver:
      - Found no solution
      - Stuck with projected gradient > demanded accuracy
    - Termination by user:
      - Number of iterations > 100000 / 200
      - CPU-Time > 1800 s / 24 h



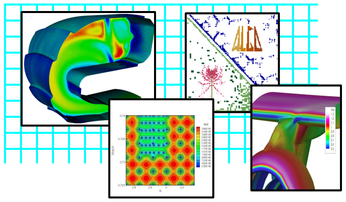
Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



Description of the methods

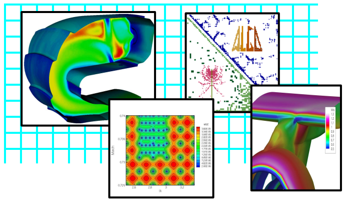
- Selection of the solvers (source code available, no Hessian necessary)
  - **DOT** – BFGS Method, Fletcher Reeves Conjugate Gradient Method
    (Vanderplaats Research & Development, Inc.)
  - **L-BFGS-B** – Limited Memory BFGS Method
    (Richard H. Byrd, Peihuang Lu, Jorge Nocedal, Ciyou Zhu)
  - **TN-BC** – Truncated Newton Method
    (Stephen G. Nash)
  - **Lancelot B** – Trust Region method - SR1, BFGS, PSB update
    (Nicholas I. M. Gould, Andrew Conn, Philippe L. Toint) --- at a price for commercial use
  - **IPOPT** – Interior Point Method
    (Andreas Waechter)
  - **DONLP2** – SQP Method
    (Peter Spellucci)



Description of the methods

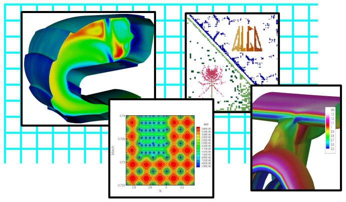
- Algorithmic components of the solvers

	Framework		Linear algebra		needs Hessian approximation
	Line Search	Trust Region	direct	iterative	
DOT BFGS	x		x		yes
DOT FR	x			x	no
L-BFGS-B	x		x		yes
TN-BC	x			x	yes
Lancelot B		x		x	yes
IPOPT	x		x		yes
DONLP2	x		x		yes



Outline

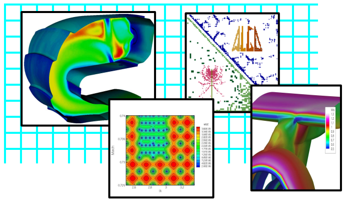
- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



Numerical experiments in CUTEr

- CUTEr: (a Constrained and Unconstrained Testing Environment revisited)
  - Testing environment to compare optimization and linear algebra solvers
  - Contains a large collection of test problems in SIF (Standard Input Format)
  - Provides ready-to-use interfaces to existing solvers (algorithms are not included, have to be implemented)
  - Possible to create new interfaces

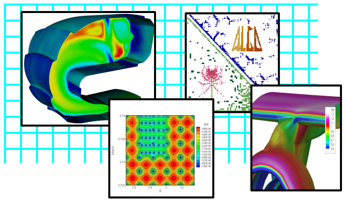
- Overview of used test problems
  - 76 out of 128 bound constrained problems provided by CUTEr
  - Nbr. of variables: 3 to 15625
  - Type of objective function: quadratic (32), sum of squares (19), other (25)



Numerical Experiments in CUTEr

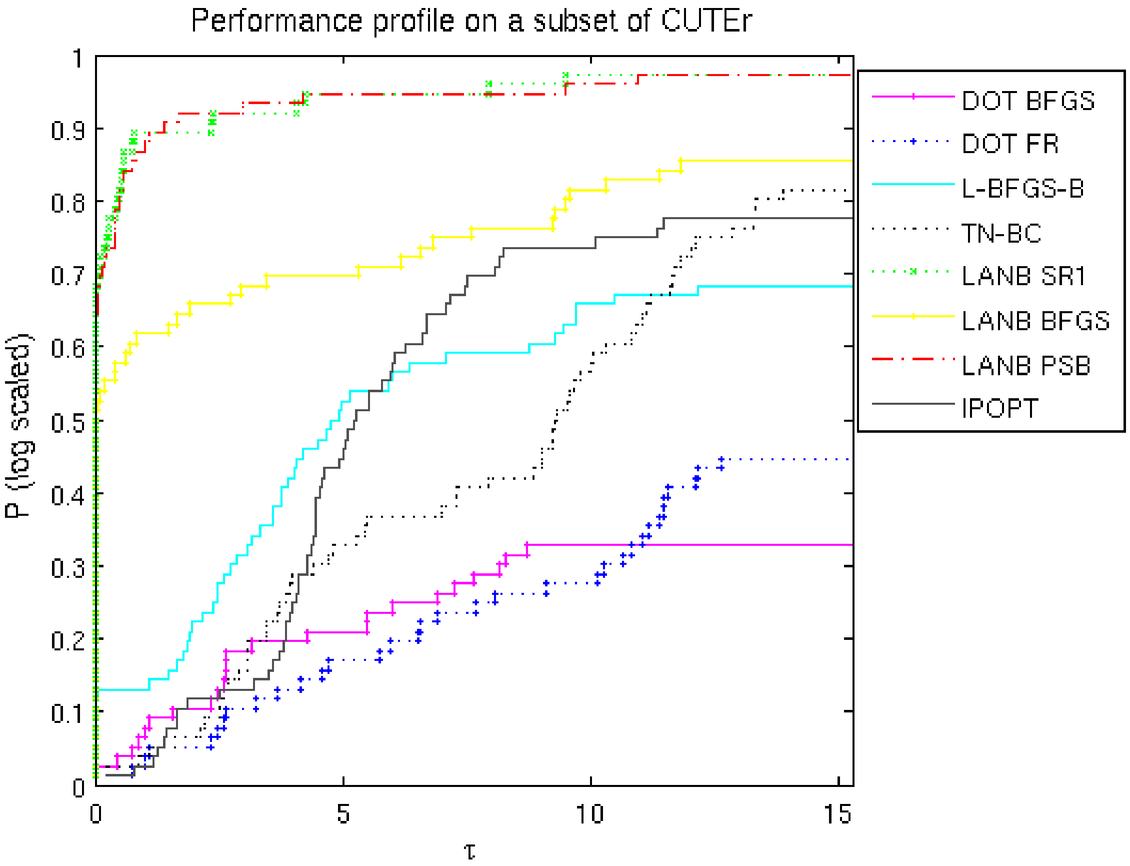
- Results in terms of function + gradient evaluations

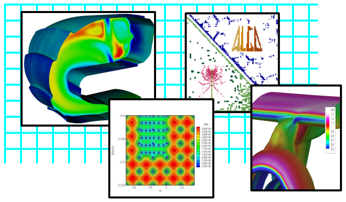
	Nbr. of won test cases
DOT BFGS	2
DOT FR	1
L-BFGS-B	9
TN-BC	1
Lancelot B SR1	49
Lancelot B BFGS	38
Lancelot B PSB	48
IPOPT	0



Numerical Experiments in CUTEr

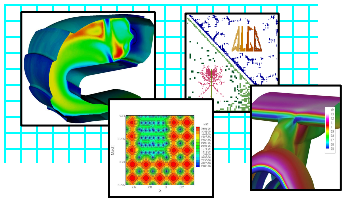
- Results in terms of function + gradient evaluations





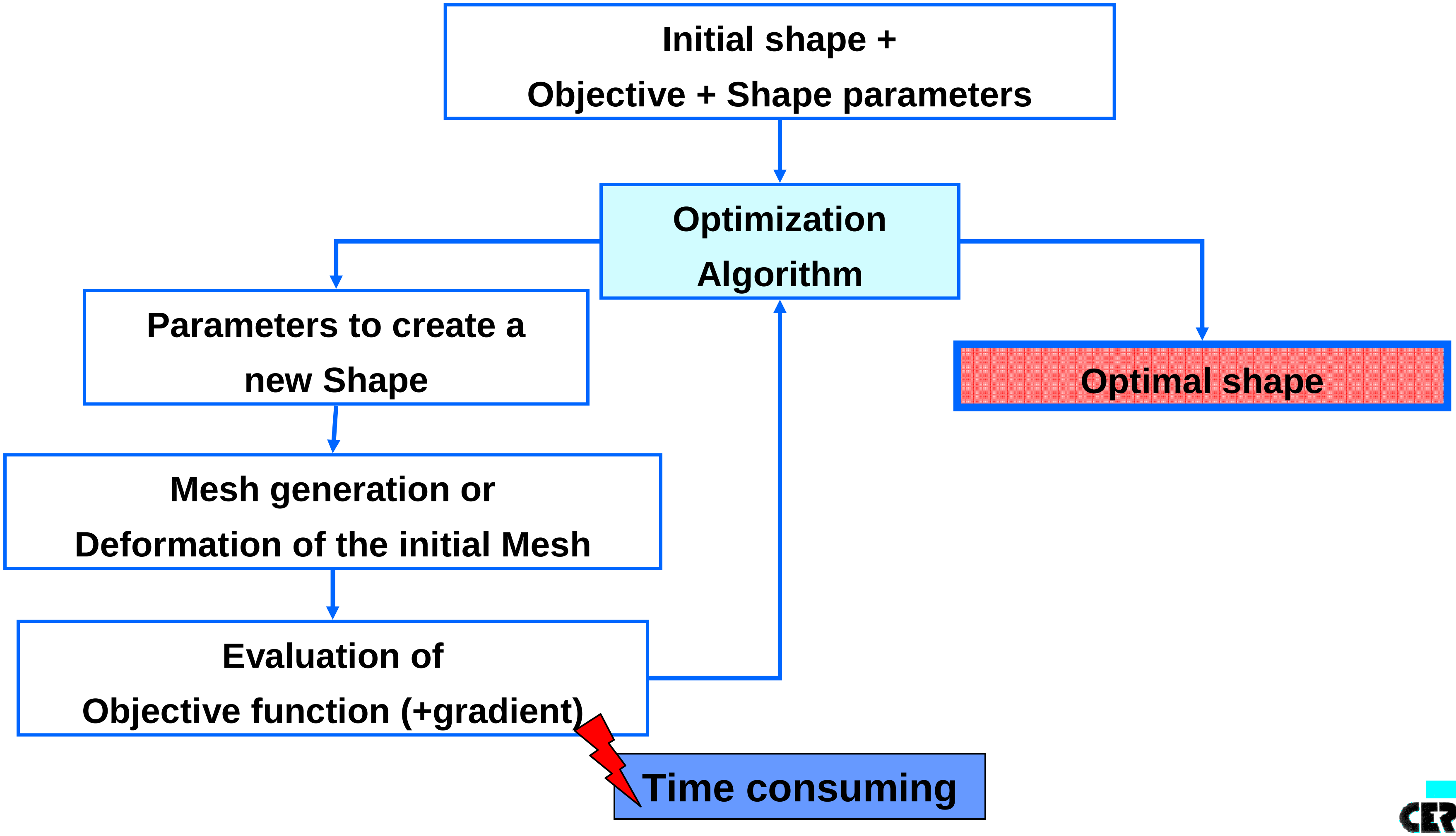
Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



OPTaliA - Numerical shape optimization environment

All steps take place in the same environment (virtually)



Initial shape +
Objective + Shape parameters

Optimization
Algorithm

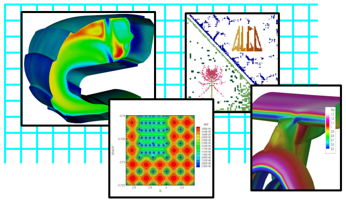
Parameters to create a
new Shape

Mesh generation or
Deformation of the initial Mesh

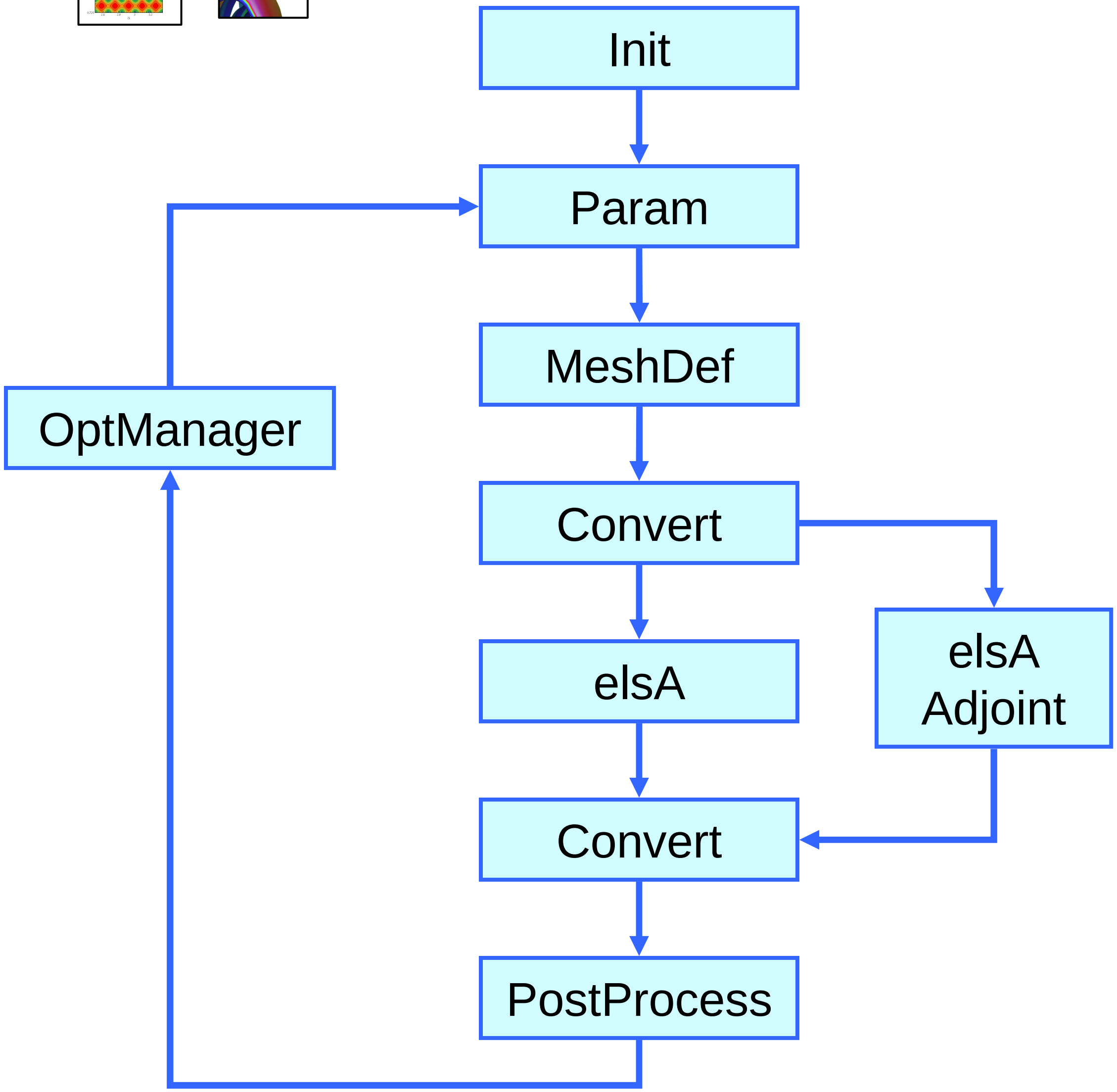
Evaluation of
Objective function (+gradient)

Optimal shape

Time consuming



OPTaliA – Optimization Scenario



Init

Param

MeshDef

Convert

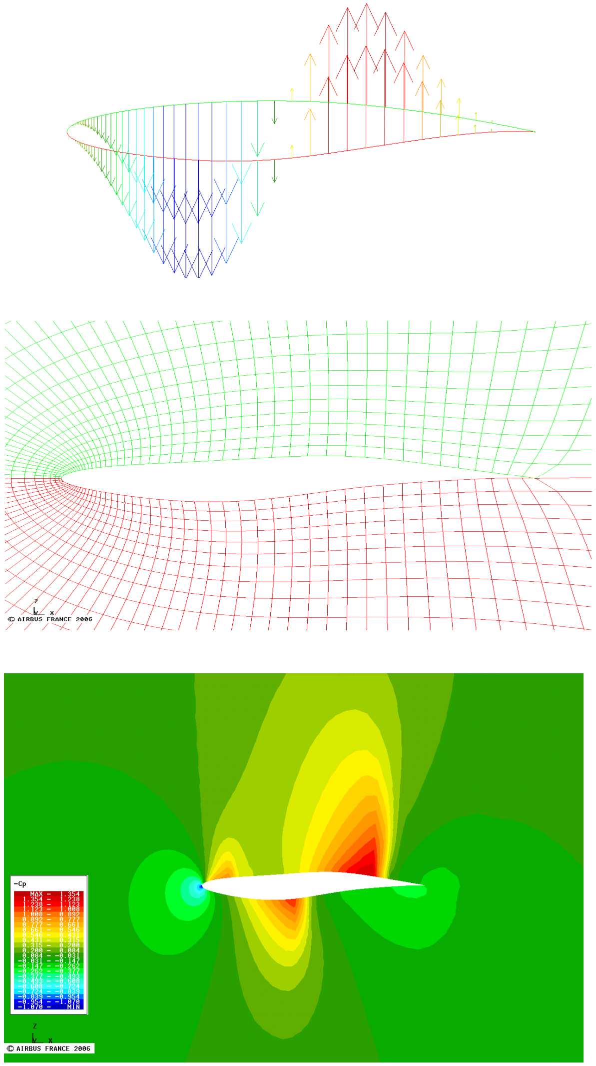
elsA

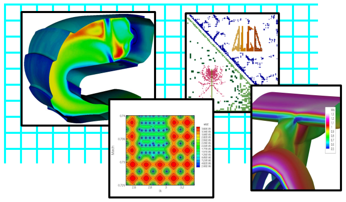
elsA Adjoint

Convert

PostProcess

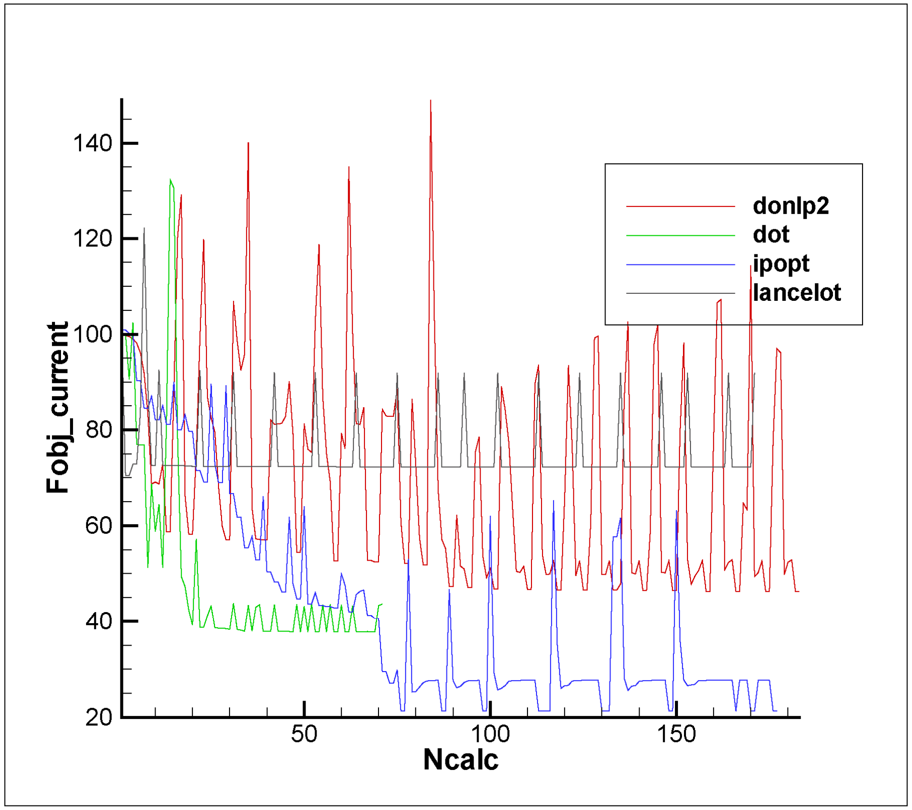
OptManager





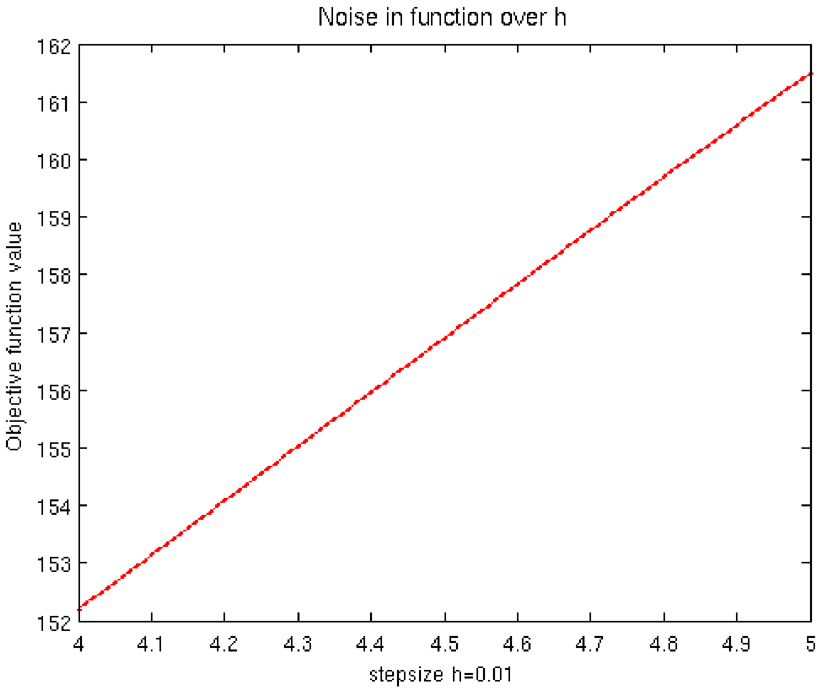
Numerical Experiments in OPTaliA

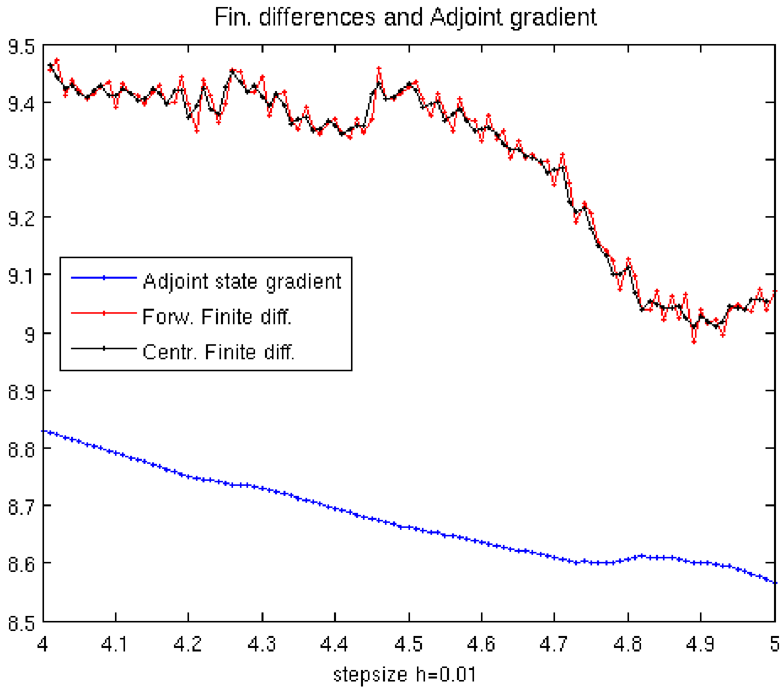
- Convergence history (each func evaluation) of true Airbus function (n=6)

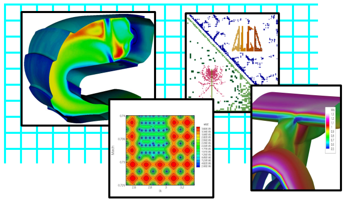


Numerical Experiments in OPTaliA

- Function and gradient of a one-dimensional Airbus function

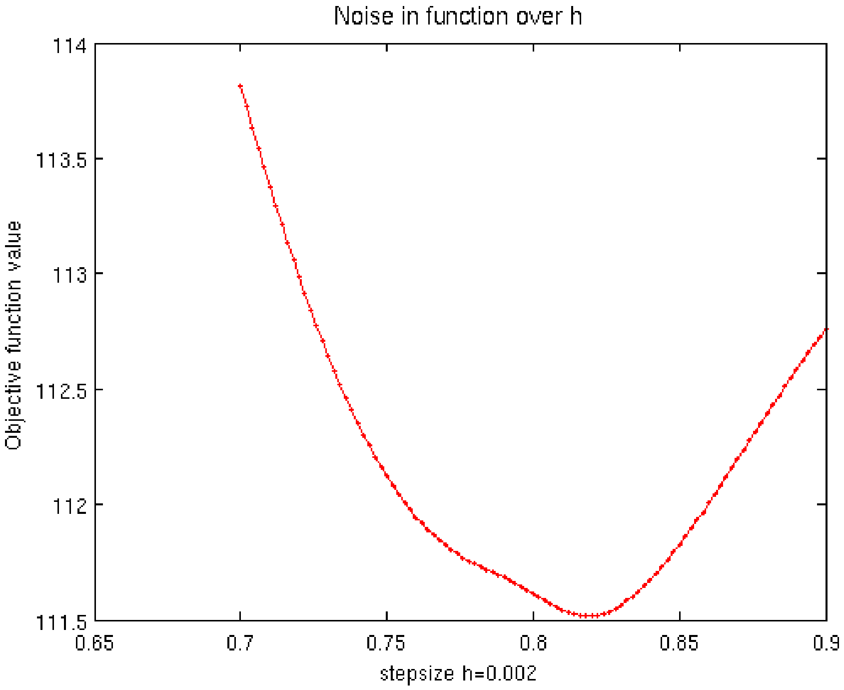


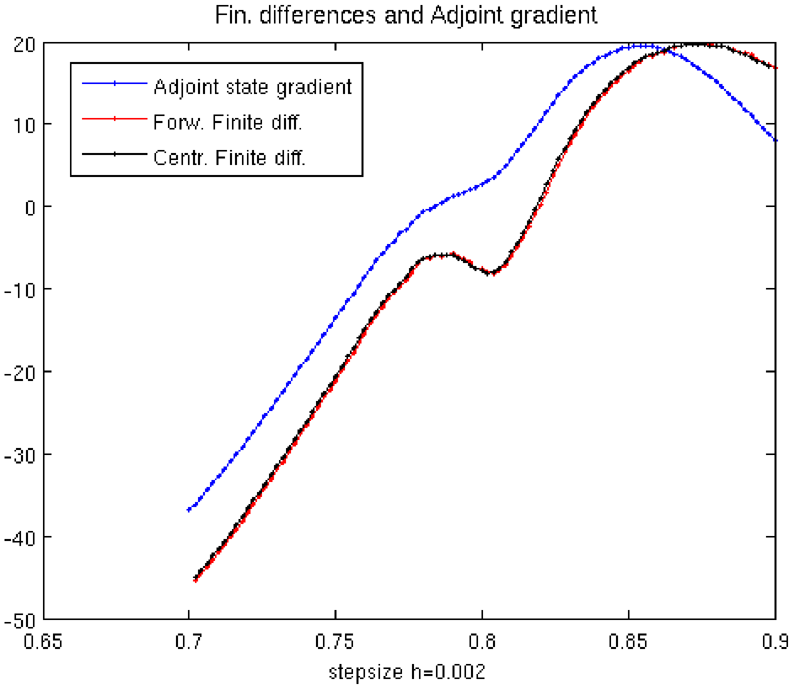


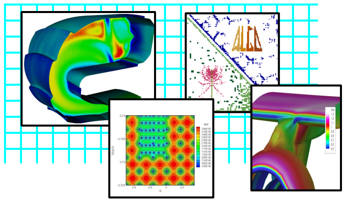


Numerical Experiments in OPTaliA

- Function and gradient of a one-dimensional Airbus function

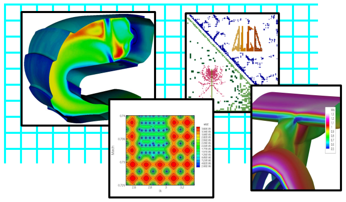






Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook



Conclusions

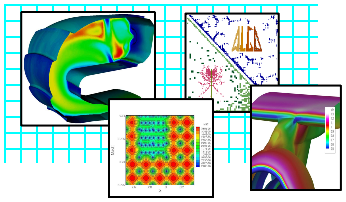
- Behaviour of solvers on true aerodynamic functions different from academic test cases

- Many local minima

- Noise detected in function and gradient, due to
  - Single precision in CFD simulation
  - Truncation of simulation process

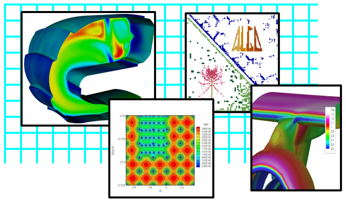
- Gradient can be inexact, depending on objective function and parameters in CFD simulation (angle of attack, mach number, coefficients in the adjoint state system)

- Use of surrogates necessary to solve these kind of problems



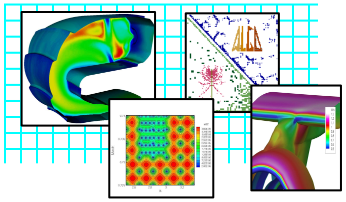
Outline

- Problem description
- Bound-constrained direct minimization
- Description of the methods
- Numerical Experiments in CUTEr (academic testing env.)
- Numerical Experiments in OPTaliA (industrial optimization env.)
- Conclusions
- Outlook

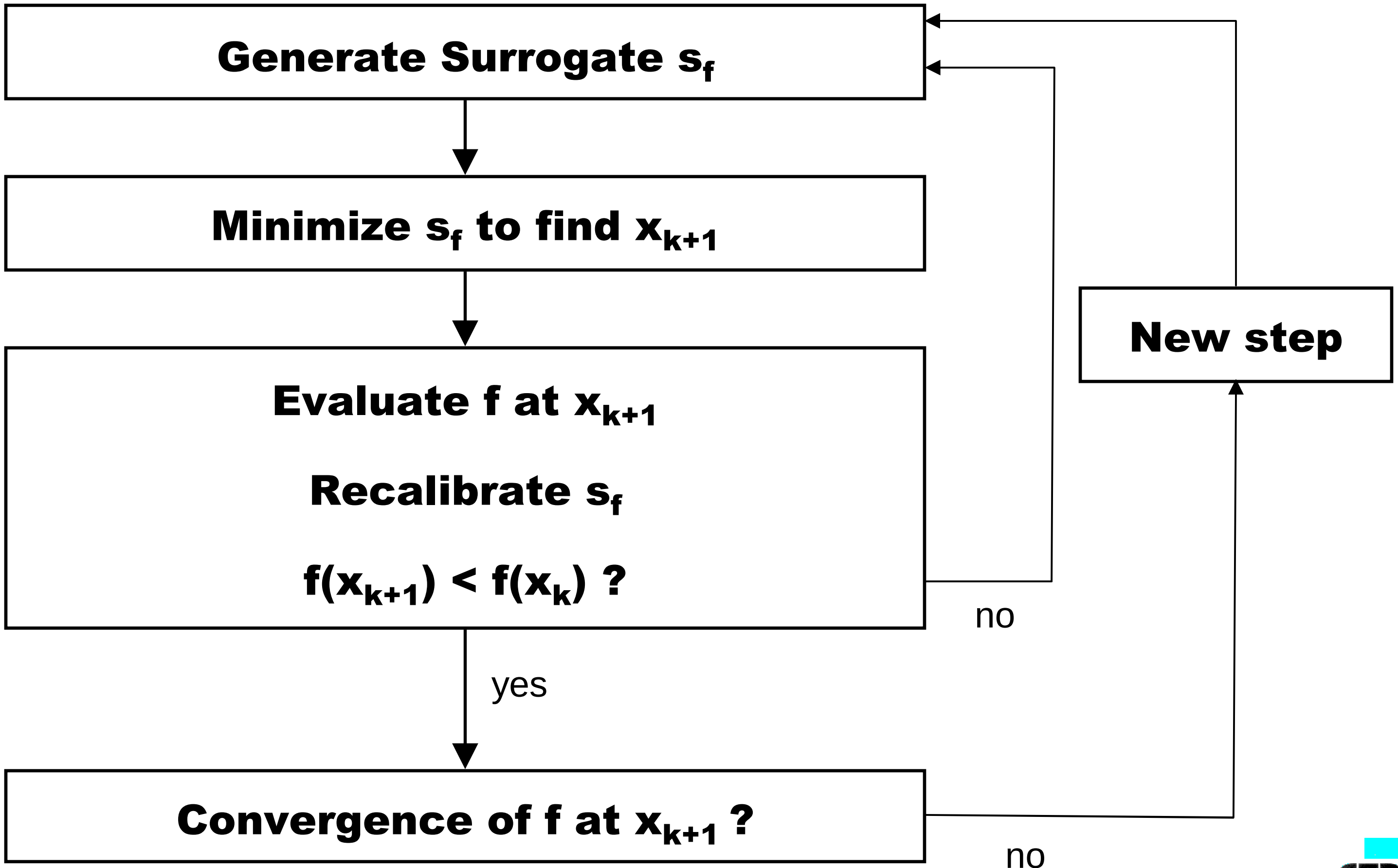


Optimization Using Surrogates

- Idea: replace expensive function by a surrogate / model which is (well enough) representing the function
- Advantages: surrogates much cheaper, continuous, differentiable
- Enables the use of sophisticated optimization routines and possibly of more global optimization techniques
- Two general types: Functional models (generated by fitting into sampled data), Physical models (based on simplification of the particular physical system)



General Surrogate Optimization Framework



Generate Surrogate s_f

Minimize s_f to find x_{k+1}

Evaluate f at x_{k+1}

Recalibrate s_f

$f(x_{k+1}) < f(x_k)$?

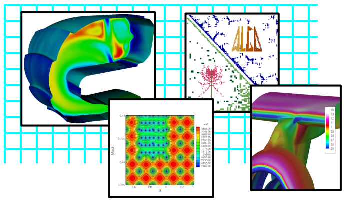
no

yes

Convergence of f at x_{k+1} ?

no

New step

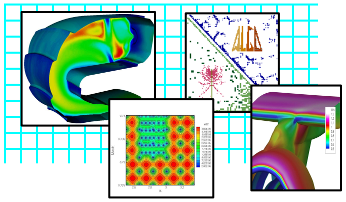


Optimization Using Surrogates

- Compare / improve state-of-the-art techniques to handle design optimization with surrogates
  - SMF – Surrogate Management Framework

    [Booker, Dennis, Frank, Serafini, Torczon, and Trosset, A Rigorous Framework for Optimization of Expensive Functions by Surrogates (1999)]
  - TR – Trust Region Framework

    [Conn, Gould, Toint (2000), NASA AIAA papers Alexandrov, Lewis (2000)]



Optimization Using Surrogates

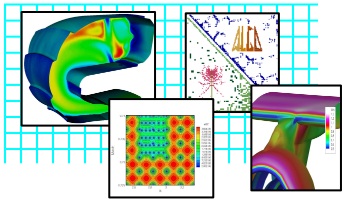
- Surrogates to consider:
  - Response Surface Model

    [R.H. Myers, D.C. Montgomery, Response Surface Methodology, second edition, John Wiley & Sons, Inc., 2002]
  - Neural network

    [Howard Demuth, Mark Beale, Neural Network Toolbox User's Guide, The Mathworks, Inc., 1994]
  - Kriging

    [Lophaven, S.N., Nielsen, H.B., Sondergaard, J., DACE: a Matlab Kriging toolbox, version 2.0, 2002]
  - Radial Basis Function

    [Mark A. Abramson, Matlab Toolbox: RBF version 1.0 User’s Guide, 2006]

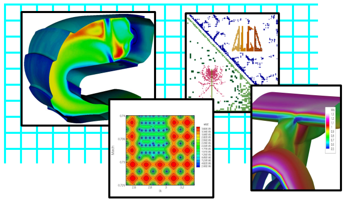


Optimization Using Surrogates

- Surrogates are necessary and very useful in the context of Aerodynamic Design Optimization

- Better surrogates provide better predictions of the real function value and hence fewer expensive function evaluations are needed

- Task:
  - Find suitable surrogate and suitable inner solver which minimizes the surrogate inside a good outer algorithm which minimizes the real function



Thank you for your attention!