# SQP/SCP-Methods for Nonlinear Programming: Algorithms, Software, and Applications

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**Contents**:

- available software
- SQP and SCP methods for nonlinear programming
- industrial case studies (ship design, control of chemical reactors, design of satellite antennas, ...)
- a large-scale benchmark problem

## Available Software

| | | |
|---|---|---|
| **QL** | - | primal-dual method for quadratic programming |
| **NLPQL** | - | SQP-algorithm for smooth constrained nonlinear programming (calls QL) |
| **DFNLP** | - | Gauss-Newton/quasi-Newton method for constrained least squares, $L_1$, $L_\infty$ and min-max problems (calls NLPQL) |
| **MODFIT** | - | data fitting in explicit functions, Laplace-functions, steady-state systems, and systems of ODEs and DAEs (calls DFNLP) |
| **PDEFIT** | - | data fitting in systems of one-dimensional PDEs and PDAEs (calls DFNLP) |
| **PCOMP** | - | modelling language with automatic differentiation |
| **SCPIP** | - | sequential convex programming method for large-scale nonlinear programming (Ch. Zillober) |

## Available Software (continued)

**EASY-FIT** - GUI for data fitting in dynamical systems, database with 1.200 examples (calls MODFIT, PDEFIT, PCOMP)

## Nonlinear Optimization

**Nonlinear Programming Problem (NLP)**:

$$
\begin{aligned}
& \min \ f(x) \\
& g_j(x) = 0 \quad , \quad j = 1, \ldots, m_e \\
x \in \mathbb{R}^n : \quad & g_j(x) \leq 0 \quad , \quad j = m_e + 1, \ldots, m \\
& x_l \leq x \leq x_u
\end{aligned}
$$

**Assumptions**:

- all model functions are smooth (twice continuously differentiable)
- the problem is highly nonlinear and non-convex
- the problem may become very large ($n >> 100,000, m >> 100,000$)

## SQP Methods (Sequential Quadratic Programming)

**Design Goal:** Fast local convergence speed (nearly quadratic)

- Efficient and robust in case of highly nonlinear, non-convex problems, accurate solutions
- Standard tool in very many applications
- SQP methods are easily tuned to special formulations, e.g.,
  - very many constraints (active set strategy)
  - least squares optimization (Gauss-Newton-type)
  - systems of nonlinear equations (Newton's method)
  - linearly constrained optimization
  - distributed computing

# Case Study: Horn Radiators for Satellite Communication

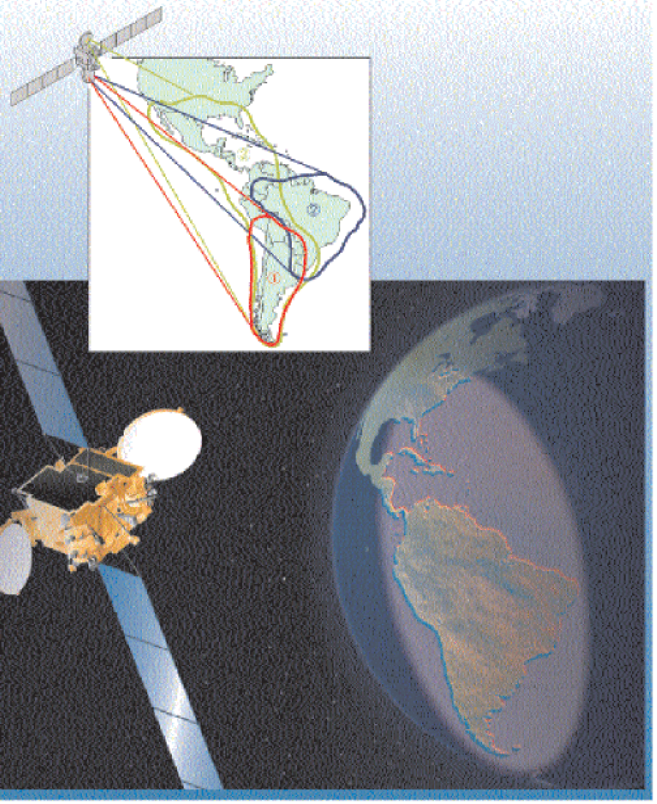
Dornier Satellitensysteme GmbH

Daimler-Benz Aerospace
Dornier

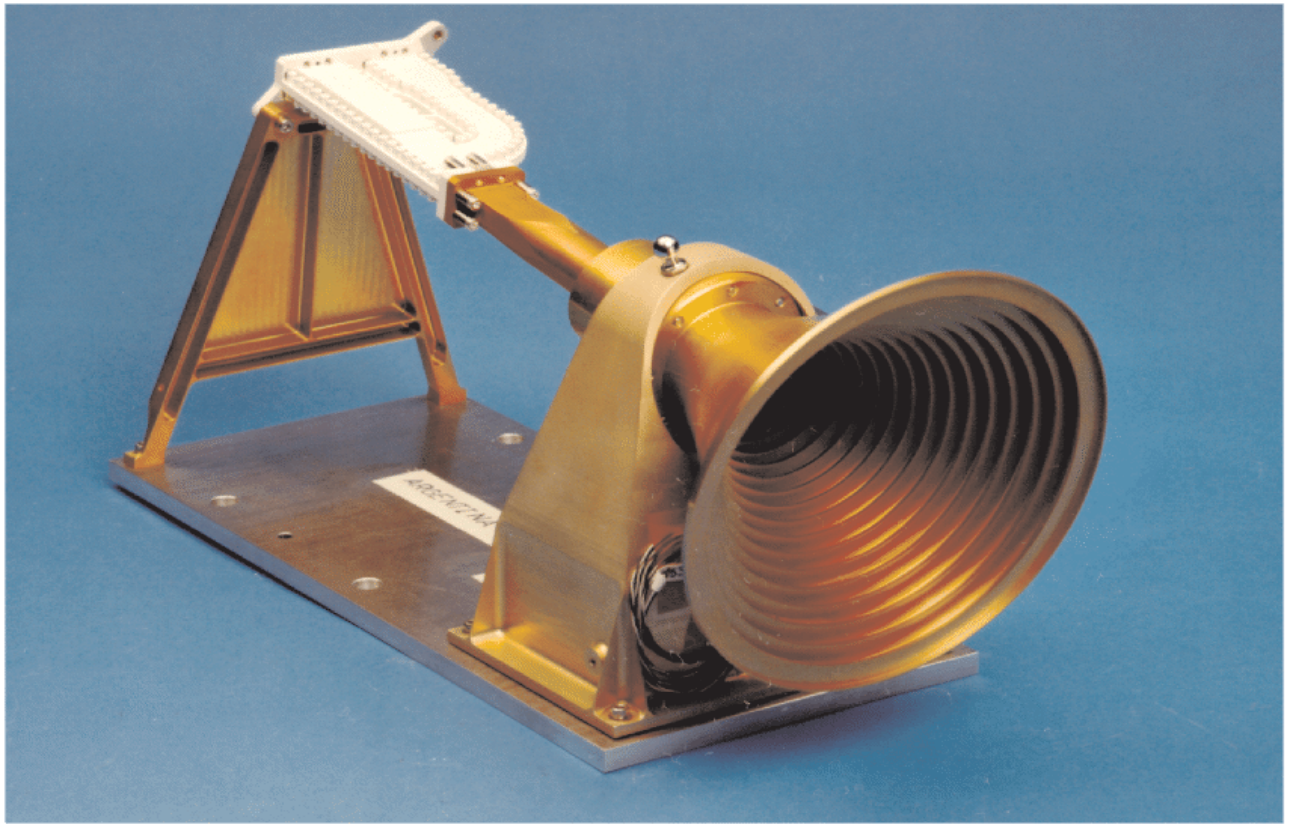
## Nahuel

**Regional communications satellite for Latin America**

- **Customer:** Nahuelsat S.A., Buenos Aires
- **DSS role:** General prime contractor for in-orbit delivery in cooperation with Aerospatiale (satellite) and Alenia (ground segment), subsystems
- **Launch:** 30.01.1997
- **Services:**
  - Data, telephone, telefax
  - TV distribution
  - Direct-to-home TV
- **Coverages:**
  - Argentina (region 1)
  - Brazil (region 2)
  - Latin America and parts of the United States (region 3)
- **Platform:** Spacebus 2000
- **Features:**
  - Transponders in Ku-band (54 MHz) 18 x 55 W
  - Orbit position at 71.8° W and 76.0° W
  - Power 3.1 kW eol
  - Mission lifetime 11 years
- **Size:**
  - Span 22.4 m
  - Mass 1,800 kg at launch



## Case Study: Horn Radiators (continued)



**Nahuel $K_u$-Band**

## Case Study: Horn Radiators (continued)

**Goal**: Compute interior geometry of corrugated horn, so that a given far field distribution of the radio frequency is approximated as accurately as possible (Astrium AG, Hartwanger, S., Wolf 2000)

**Physical Background**: Maxwell's equation for circular horn along constant diameter, homogeneous, isotropic media, ideal conductivity etc.

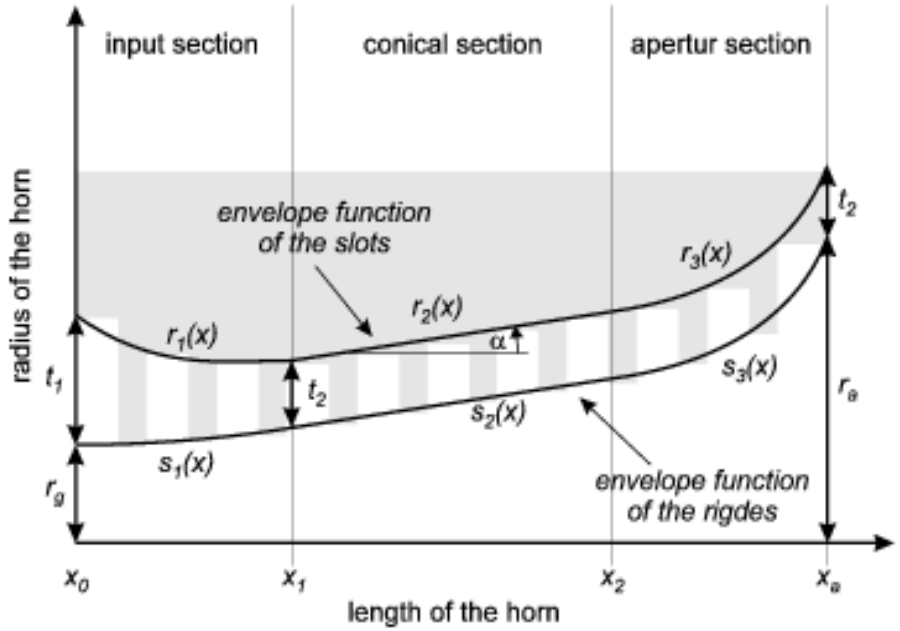
$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\phi^2}+\frac{\partial^2\Psi}{\partial z^2}+k^2\Psi=0$$

for electric ($\Psi = E$) or magnetic ($\Psi = H$) field and suitable boundary conditions

**Conclusion:** A complete orthogonal system of eigenfunctions can be derived for each wave guide

# Case Study: Horn Radiators (continued)

## Design Parameters:



## Case Study: Horn Radiators (continued)

**Optimization Problem**:

$$p \in \mathbb{R}^n : \quad \begin{array}{l} \min \sum_{j=1}^{l_2} (b_2^j(p) - \overline{b}_2^j)^2 + \mu \, b_1^1(p)^2 \\ p_l \leq p \leq p_u \end{array}$$

$$\begin{pmatrix} b_1(p) \\ b_2(p) \end{pmatrix} = \underbrace{\begin{pmatrix} S_{11}^\star(p) & S_{12}^\star(p) \\ S_{21}^\star(p) & S_{22}^\star(p) \end{pmatrix}}_{total\ scattering\ matrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

| | | |
|---|---|---|
| $a_1$ | - | amplitude of mode exciting the horn (first unity vector) |
| $a_2$ | - | amplitudes of reflected modes at horn aperture (far field) |
| $\overline{b}_2^j$ | - | given amplitudes |
| $\mu$ | - | weight for return loss |

## Case Study: Horn Radiators (continued)

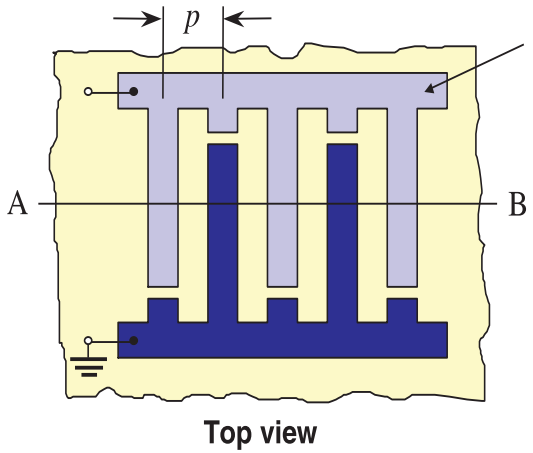
**Numerical Complexity (example)**:

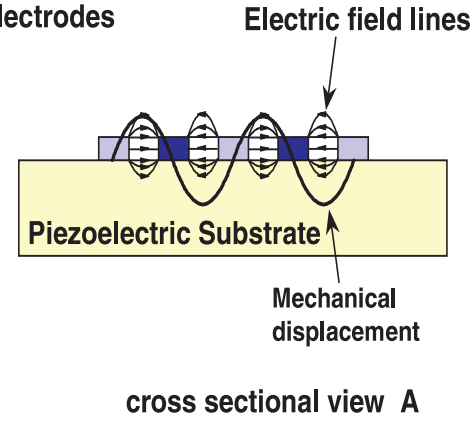
- 70 eigenmodes
- $\mathbf{140 \times 140}$ complex entries for two scattering matrices ($\boldsymbol{E}$, $\boldsymbol{H}$ or $\boldsymbol{U}$, $\boldsymbol{I}$, respectively)
- evaluation of double integrals and Bessel functions for each coeff.
- 40 slots and ridges, i.e., of $\mathbf{2 \cdot 40}$ matrices of size $\mathbf{2 \cdot 140 \times 140}$
- intermediate matrix manipulations, inverse decompositions

| IT | F | SCV | NA | I | ALPHA | DELTA | KT |
|---|---|---|---|---|---|---|---|
| 1 | .16795478D+01 | .00D+00 | 37 | 0 | .00D+00 | .00D+00 | .37D+00 |
| 2 | .14476536D+01 | .57D+00 | 37 | 1 | .10D+01 | .00D+00 | .31D+01 |
| 3 | .11909891D+01 | .68D+00 | 37 | 2 | .10D+00 | .00D+00 | .43D+01 |
| .. | ..... | .... | .. | . | ..... | ..... | ..... |
| 49 | .17397940D-02 | .40D-02 | 37 | 1 | .10D+01 | .00D+00 | .44D-04 |
| 50 | .17219966D-02 | .35D-03 | 37 | 1 | .10D+01 | .00D+00 | .22D-05 |
| 51 | .17225078D-02 | .53D-06 | 37 | 1 | .10D+01 | .00D+00 | .13D-07 |

## Case Study: Design of SAW (Surface Acoustic Wave) Filters

**Goal**: Guarantee design goals of electronic filters (Epcos AG, Bünner, S., van de Braak 2004)




**Wave Equation**:

$$\left(\Delta - \frac{1}{c^2}\left(\frac{\partial^2}{\partial t^2}\right)\right)\phi(x,y) = 0$$

## Case Study: Design of SAW (Surface Acoustic Wave) Filters

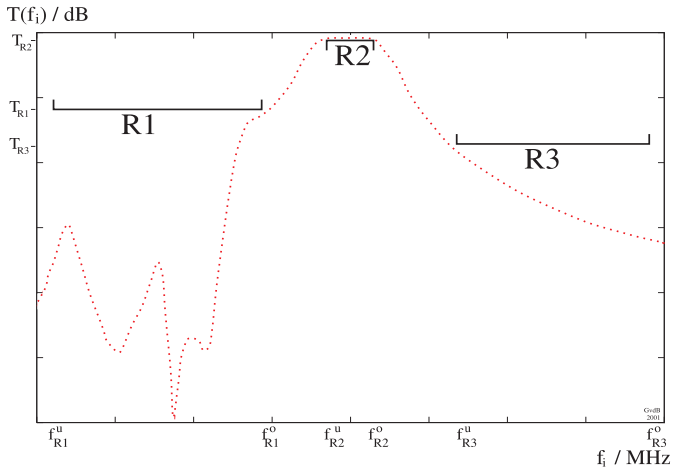
**P-Model**: Evaluate cascading matrices, for example

$$\begin{pmatrix} b_1 \\ b_2 \\ i \end{pmatrix} = \mathrm{P} \begin{pmatrix} a_1 \\ a_2 \\ u \end{pmatrix}, \mathrm{P} = \begin{pmatrix} 0 & 1 & E \\ 1 & 0 & -E^* \\ -2E & 2E^* & 2|E|^2 + i(-\mathcal{H}\{2|E|^2\} + \omega C) \end{pmatrix}$$

| | | |
|---|---|---|
| $\mathcal{H}$ | - | Hilbert transformation |
| $C$ | - | static capacity between two fingers |
| $E$ | - | excitation defined by $E = -i\ 0.5\ \sqrt{\omega W K} \cdot \int_{tr} \sigma_e(x)\ \exp^{-ik\lvert x\rvert}\, dx$ |
| $\omega$ | - | frequency |
| $W$ | - | aperture of IDT |
| $K$ | - | material constant |
| $\sigma_e$ | - | electric load distribution, $k = \frac{\omega}{c}$ |

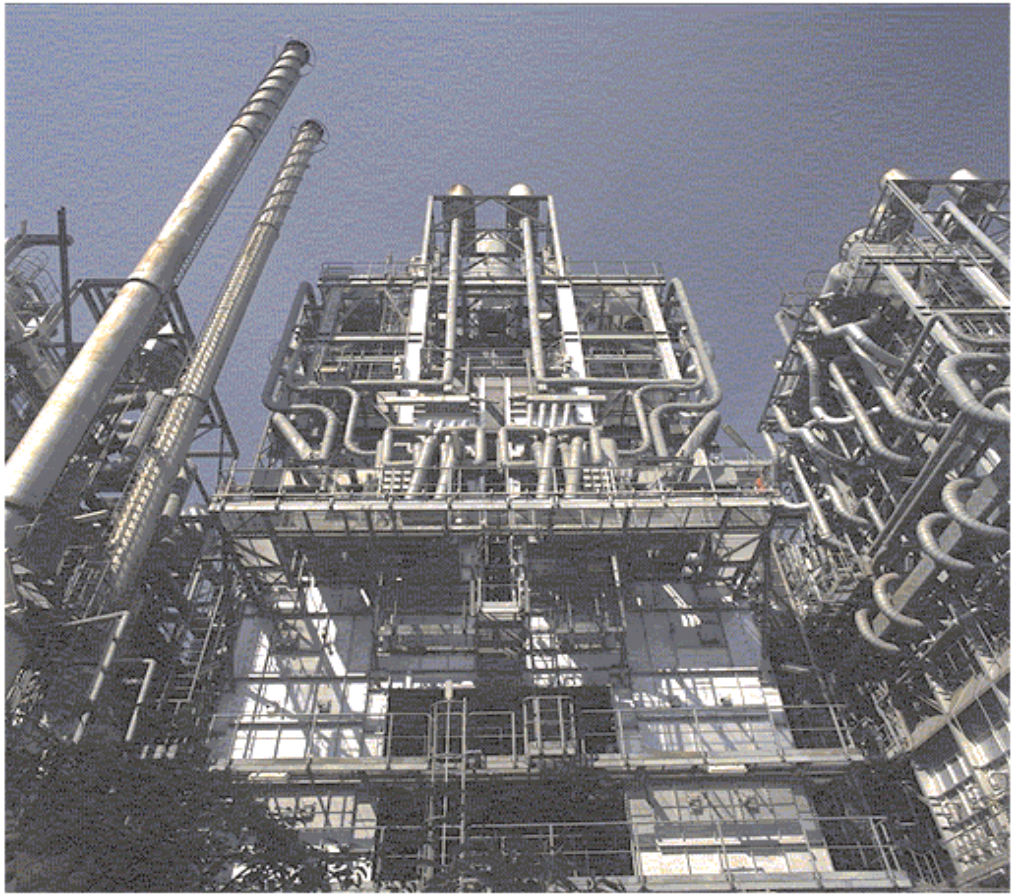
## Case Study: Design of SAW Filters (continued)

**Optimization Problem**: Apply NLPQL to




$$
\begin{array}{lll}
\max & \min_{i:\, f^u_{R_2} \le f_i \le f^o_{R_2}} T_i(x) & \\
& T_i(x) \le T_{R_1} & , \quad f^u_{R_1} \le f_i \le f^o_{R_1} \\
x \in \mathbb{R}^n : & T_i(x) \ge T_{R_2} & , \quad f^u_{R_2} \le f_i \le f^o_{R_2} \\
& T_i(x) \le T_{R_3} & , \quad f^u_{R_3} \le f_i \le f^o_{R_3} \\
& x_l \le x \le x_u &
\end{array}
$$

# Case Study: Control of a Tubular Reactor



## Case Study: Control of a Tubular Reactor (continued)

**Goal**: Yield optimization of large chemical reactors (BASF AG, Birk, Liepelt, S., Vogel 1999)

1. Steady-state, i.e. no time dependencies
2. Reaction equations modelled by standard simulation package (SPEEDUP)
3. On-line adaption of reactor control data interactively in case of changes of prices, demands, production facilities, quality, etc. (about 5,000 ordinary and algebraic differential equations)
4. Evaluation of gradients by numerical differentiation
5. Iterative execution of NLPQL with warm starts

# Case Study: Control of a Tubular Reactor (continued)

1. $CH_4 \rightarrow \frac{1}{2}C_2H_2 + \frac{3}{2}H_2$
2. $CH_4 + O_2 \rightarrow CO + H_2O + H_2$
3. $CO + \frac{1}{2}O_2 \rightarrow CO_2$
4. $C_2H_2 \rightarrow 2C + H_2$
5. $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$
6. $mC + \frac{n}{2}H_2 \rightarrow C_mH_n$

$$
\begin{aligned}
r_1(z) &= k_1 e^{-\frac{E_1}{RT(z)}} C_1^{\alpha_1} \\
r_2(z) &= k_2 e^{-\frac{E_2}{RT(z)}} C_1 C_2^{\alpha_2} \\
r_3(z) &= k_3 e^{-\frac{E_3}{RT(z)}} C_6 C_2^{0.5} \\
r_4(z) &= k_4 e^{-\frac{E_4}{RT(z)}} C_3^{\alpha_2} \\
r_5(z) &= k_5 e^{-\frac{E_5}{RT(z)}} C_5 C_2^{0.5}
\end{aligned}
$$

$$
\begin{aligned}
\tfrac{\partial}{\partial z} C_1(z) &= (-r_1(z) - r_2(z))/v(z) && , C_1(0) = C_1^0 \\
\tfrac{\partial}{\partial z} C_2(z) &= (-r_2(z) - 0.5r_3(z) - 0.5r_5(z))/v(z) && , C_2(0) = C_2^0 \\
\tfrac{\partial}{\partial z} C_3(z) &= (0.5r_1(z) - r_4(z))/v(z) && , C_3(0) = 0 \\
\tfrac{\partial}{\partial z} C_4(z) &= r_3(z)/v(z) && , C_4(0) = 0 \\
\tfrac{\partial}{\partial z} C_5(z) &= (1.5r_1(z) + r_2(z) + r_4(z) - r_5(z))/v(z) && , C_5(0) = 0 \\
\tfrac{\partial}{\partial z} C_7(z) &= (r_2(z) + r_5(z))/v(z) && , C_7(0) = 0 \\
\tfrac{\partial}{\partial z} C_8(z) &= 2(1-\epsilon)r_4(z)/v(z) && , C_8(0) = 0
\end{aligned}
$$

## Case Study: Control of a Tubular Reactor (continued)

Total mass stream: $\dot{m} = \dot{m}_{CH_4} + \dot{m}_{O_2}$

Speed: $v(z) = \dot{m}/(\rho(z)A)$

Energy balance: $T_z(z) = 1/(\rho(z)v(z)c_p(z)) \sum_{i=1}^{5} r_i(z)\Delta H_i$

Density: $\rho(z) = \sum_{j=1}^{8} C_j(z)M_j$

Heat capacity: $c_p(z) = \dfrac{\sum_{j=1}^{8} c_{p_j}(z)M_jC_j(z)}{\sum_{j=1}^{8} M_jC_j(z)}$

$c_{p_j}(z) = b_j + c_jT(z) + d_jT(z)^2$

Mass stream: $\dot{m}_j(z) = \dot{m}C_j(z)M_j / \sum_{i=1}^{j} C_i(z)M_i$

## SCP Methods (Sequential Convex Programming)

**Design Goal:** Convex 1st-order approximation of problem functions

**Idea**: Insert inverse variables (with or without asymptotes) depending on sign of partial derivative and linearize

$$f^k(x) = \alpha_0^k + \sum_i^+ \frac{\beta_{i,0}^k}{U_i - x_i} - \sum_i^- \frac{\beta_{i,0}^k}{x_i - L_i}$$

$$g_j^k(x) = \alpha_j^k + \sum_i^+ \frac{\beta_{i,j}^k}{U_i - x_i} - \sum_i^- \frac{\beta_{i,j}^k}{x_i - L_i}, \quad j = 1, \ldots, m$$

$\sum_i^+$: summation over all indices with positive partial derivatives ($\sum_i^-$ vice versa)

**Important**: Only possible for nonlinear inequality constraints, equality constraints linearized!

## SCP Methods (continued)

**Justification:** Let $f(x)$ and $x_k > L$ given with $f'(x_k) < 0$ and

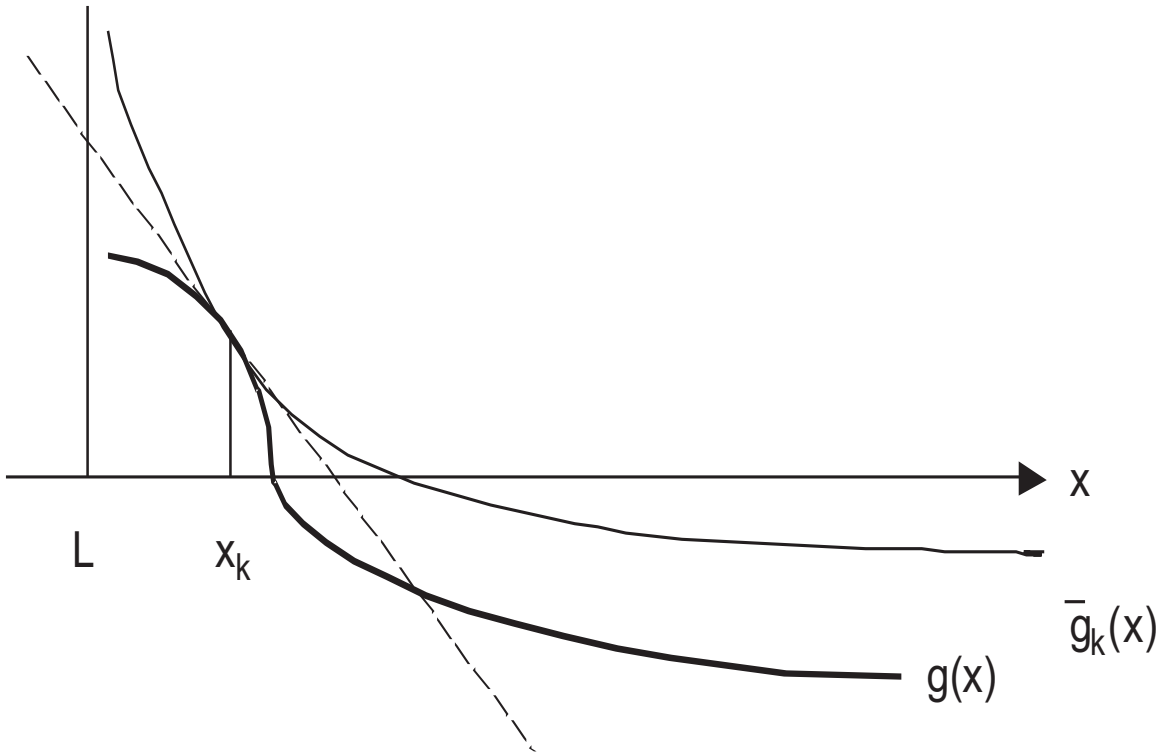
$$f_k(x) = \alpha_k - \frac{\beta_k}{x - L}$$

for $x > L$. From $f(x_k) = f_k(x_k)$ and $f'(x_k) = f'_k(x_k)$ we get

$$f_k(x) = f(x_k) + f'(x_k)(x_k - L) - \frac{f'(x_k)(x_k - L)^2}{x - L}$$

**Conclusion:** $f_k(x)$ is convex for all $x > L$

# Approximation by Moving Asymptote



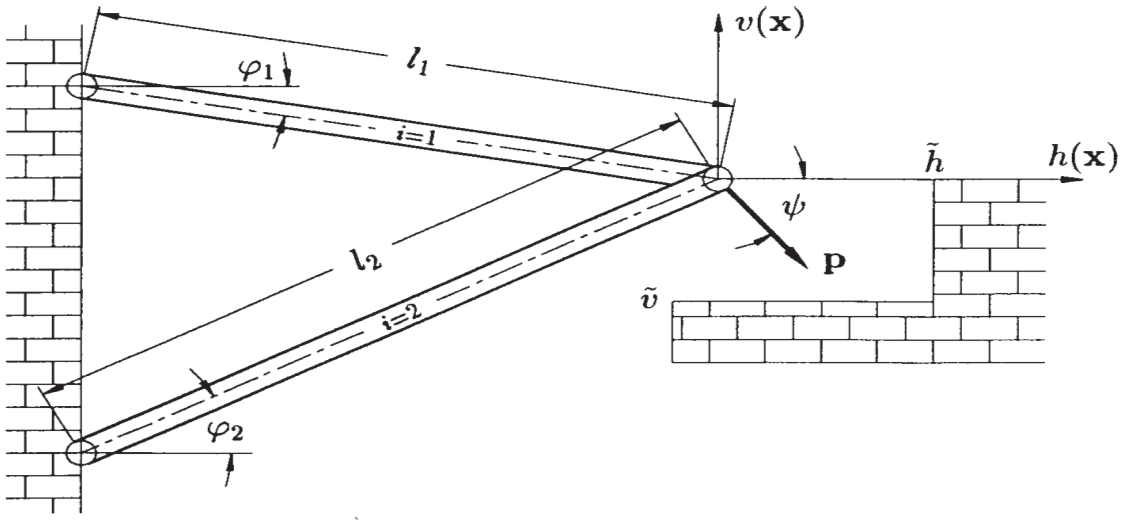
## SCP Methods (continued)

**Convex Separable Subproblem**:

$$
\begin{aligned}
& \min \ f_k(x) \\
& g_j^k(x) = 0 \quad , \quad j = 1, \ldots, m_e \\
x \in \mathbb{R}^n : \quad & g_j^k(x) \leq 0 \quad , \quad j = m_e + 1, \ldots, m \\
& L_i \leq x_i \leq U_i \quad , \quad i = 1, \ldots, n
\end{aligned}
$$

**Motivation**: Mechanical engineering, i.e. statically determinated structures are linear in reciprocal variables (Fleury 1989, Svanberg 1987, Zillober 1994)

## Example (2-bar-truss)




**Design Variables**: $x_i = Ea_i/l_i$ with elasticity modulus $E$, cross sectional area $a_i$ and length $l_i$, $i = 1, 2$

**Displacement**:

$$h(x) = |p|(\cos\psi(s_1^2/x_2 + s_2^2/x_1) - \sin\psi(s_1c_1/x_2 + s_2c_2/x_1))/\gamma$$

## SCP Methods (continued)

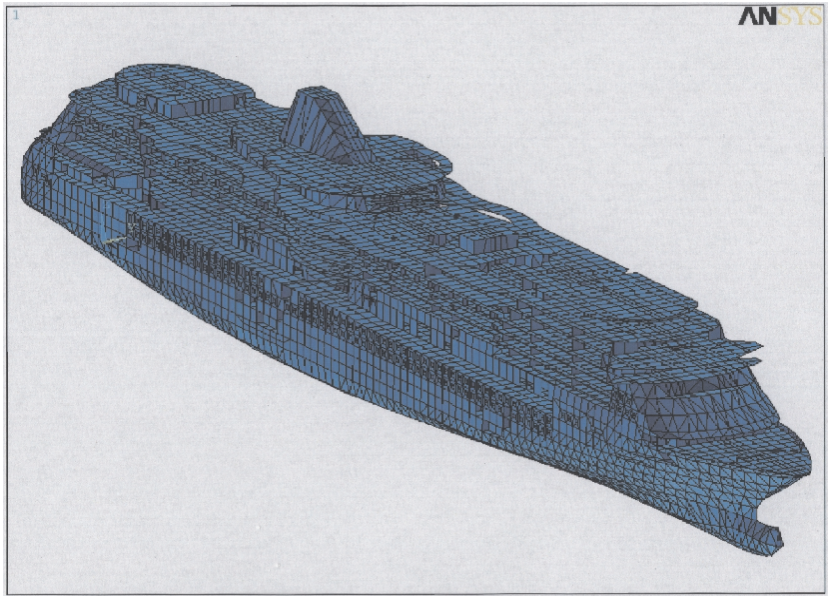
**Subproblem Solution**:

- Regularization of objective function leads to strictly convex, separable, often very large NLP (diagonal and positive definite Hessian)
- Numerical solution by interior point method possible with $n \times n$ or $m \times m$ systems of equations
- Exploiting sparsity patterns in systems of linear equations

(Zillober 2002)

## Case Study: Ship Design

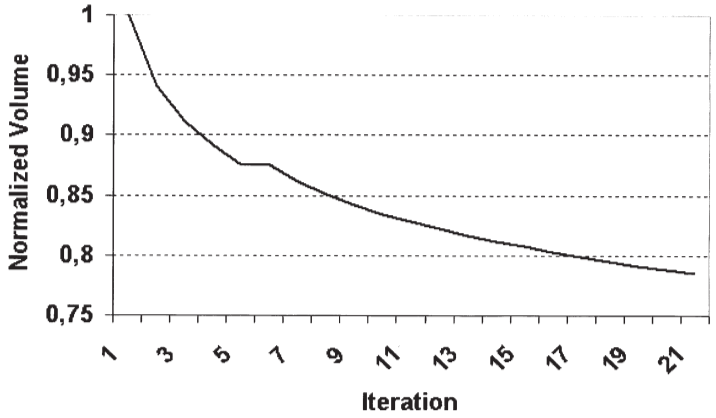
**Goal**: Minimize the weight of a ship structure (cruise ship *Radiance of the Seas*, Meyer Werft)



# Case Study: Ship Design (continued)

## Data and FE-Discretization:

| | | | | | |
|---|---|---|---|---|---|
| length overall | - | 293,20 m | breadth moulded | - | 32,20 m |
| number of decks | - | 15 | draught | - | **8,15 m** |
| tonnage | - | 90,090 BRZ | deadweight | - | 8,900 t |
| speed | - | Over 24 kn | total power output | - | 78.600 HP |
| passenger capacity | - | 2,100 | crew | - | 858 |
| shell elements | - | 32,946 | beam elements | - | 33,637 |
| load cases | - | 2 (sagging, hogging) | design variables | - | 415 |
| stress constraints | - | 4,980 | (shell thickness) | | |



## Case Study: Topology Optimization

**Power Law Approach**:

$$x \in \mathbb{R}^n, u \in \mathbb{R}^m : \begin{array}{c} \min\ u^T f \\ V(x) \leq pV_0 \\ K(x)u = f \\ 0 < x \leq 1 \end{array}$$

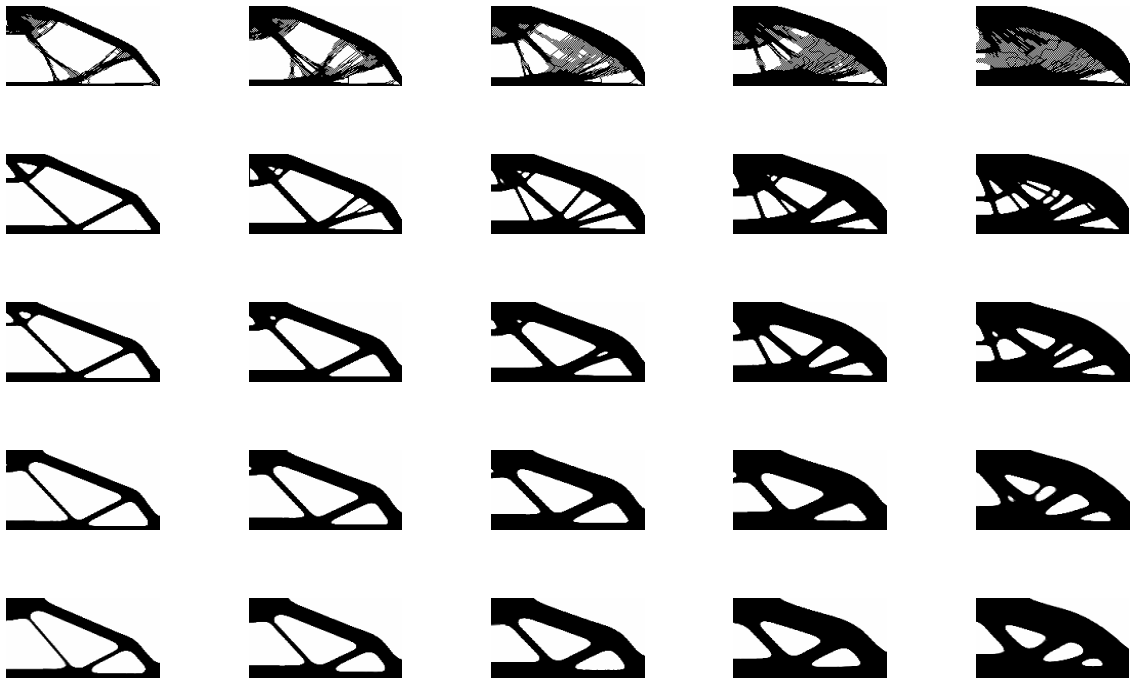
| | | |
|---|---|---|
| $x$ | - | relative densities |
| $u$ | - | displacements |
| $K(x)$ | - | stiffness matrix |
| $f$ | - | external loads |
| $V(x)$ | - | volume |

$$K(x) = \sum_{i=1}^{n} x_i^3 \, k_i^0$$

Conclusion: Hessian of objective function is dense!

## Case Study: Topology Optimization (continued)

**Test Case**: Half beam with varying volume restrictions and filter radii



## Case Study: Topology Optimization (continued)

**Results**: Half beam

| $n_x$ | $n_y$ | $n$ | $n_{it}$ | $f(x)$ | $\|\nabla_x L(x,u)\|$ | $r_f$ |
|---|---|---|---|---|---|---|
| 600 | 400 | 240,000 | 22 | 52.63 | 1.3E-3 | 8 |
| 600 | 400 | 240,000 | 26 | 54.25 | 6.5E-4 | 0 |
| 1,050 | 700 | 735,000 | 38 | 54.39 | 4.6E-4 | 10 |
| 1,260 | 840 | 1,058,400 | 43 | 56.55 | 1.3E-5 | 0 |

| | | |
|---|---|---|
| $n_x$, $n_y$ | - | number of elements in $x$- and $y$-direction |
| $n$ | - | number of optimization variables |
| $n_{it}$ | - | number of iterations |
| $f(x)$ | - | final objective function value |
| $\|\nabla_x L(x,u)\|$ | - | norm of final gradient of Lagrangian function |
| $r_f$ | - | filter radius |

**Hardware:** SUN Fire V880 (8 processors, 750 MHz)

## Conclusions

**State-of-the-Art**:

- Constrained and smooth optimization problems can be solved routinely by SQP and, in special situations, even more efficiently by SCP methods.
- Very large scale optimization problems with nonlinear constraints can be solved by SCP methods.
- Optimization became an integrated design tool especially in mechanical structural optimization.

## Conclusions (continued)

**Future Challenges:**

1. efficient methods for certain classes of global optimization problems

2. efficient methods for non-convex mixed-integer nonlinear optimization

3. integrated design by C++ toolbox