

The Mathematical legacy of ECOSSE

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With help from Sven Leyffer

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Mathematics within ECOSSE

- Centred on Roger Fletcher's group in Dundee

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- Other work done in Edinburgh under Ken McKinnon

Mathematics within ECOSSE

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- Other work done in Edinburgh under Ken McKinnon
- Engineers were also using Maths!

Who am I?

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- First on Jack's list!

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Flexible retrofit design of multiproduct batch plants

Fletcher, Hall and Johns (1991)

Computers and Chemical Engineering **15** 843–852

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- Otherwise, we took the money and ran...
- and went hill-walking...
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- and paved the way for the German invasion



The Dundee group

- Major focus was the solution of mixed-integer nonlinear programming **MINLP** problems

$$\begin{aligned} &\text{minimize } f(\mathbf{x}, \mathbf{y}) \\ &\text{subject to } \mathbf{c}(\mathbf{x}, \mathbf{y}) \geq \mathbf{0} \\ &\quad y_i \in \{0, 1\} \quad \forall i \end{aligned}$$

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- **Why?**

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- What is required in order to solve MINLP problems?



Outer-approximation: Duran and Grossmann (1986)

Choose $\mathbf{y}^{(0)}$; $k = 0$

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Solve $\mathbf{NLP}^{(k)}$
minimize $f(\mathbf{x}, \mathbf{y}^{(k)})$
s.t. $\mathbf{c}(\mathbf{x}, \mathbf{y}^{(k)}) \geq \mathbf{0}$
to obtain $\mathbf{x}^{(k)}$

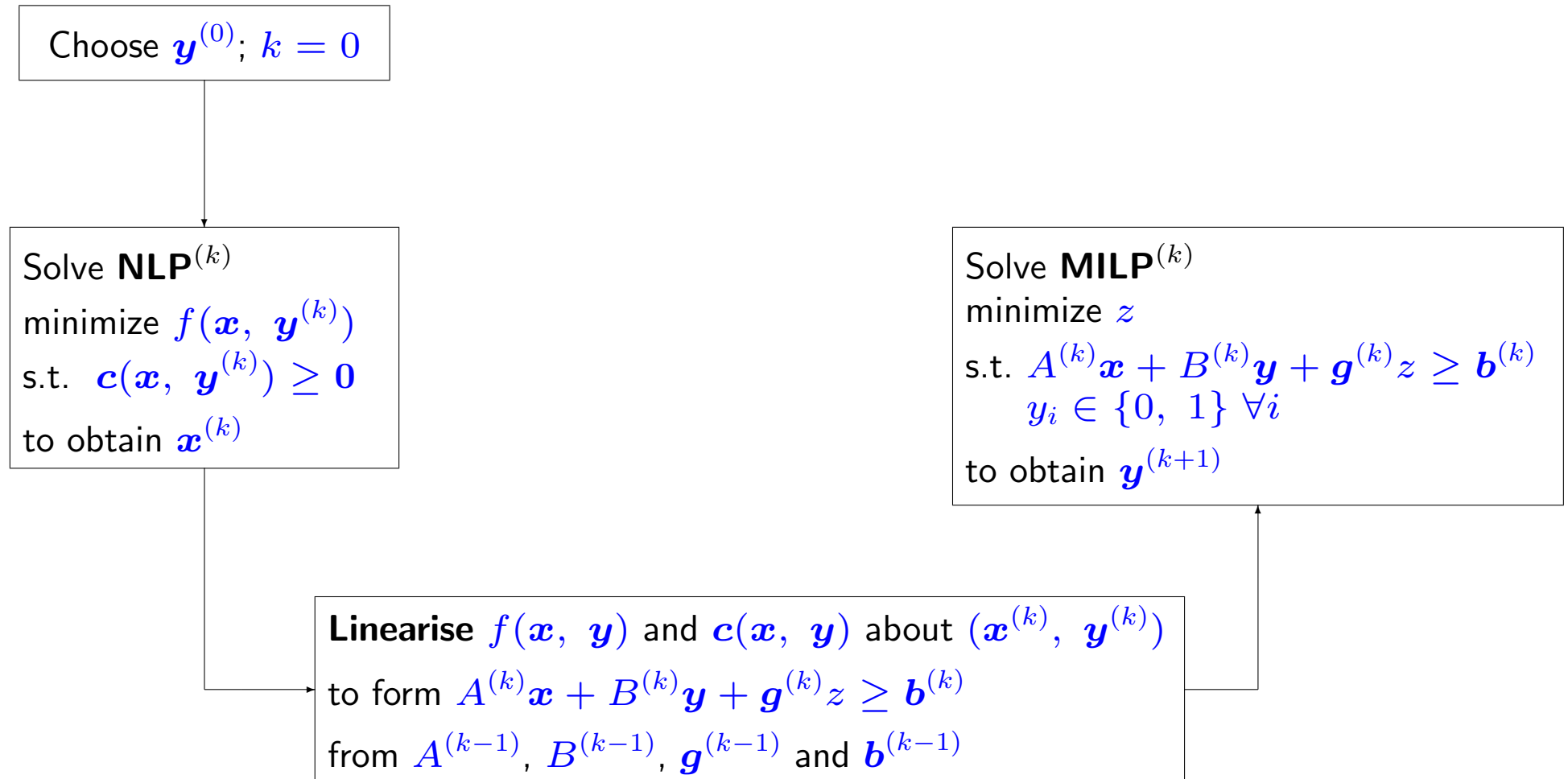
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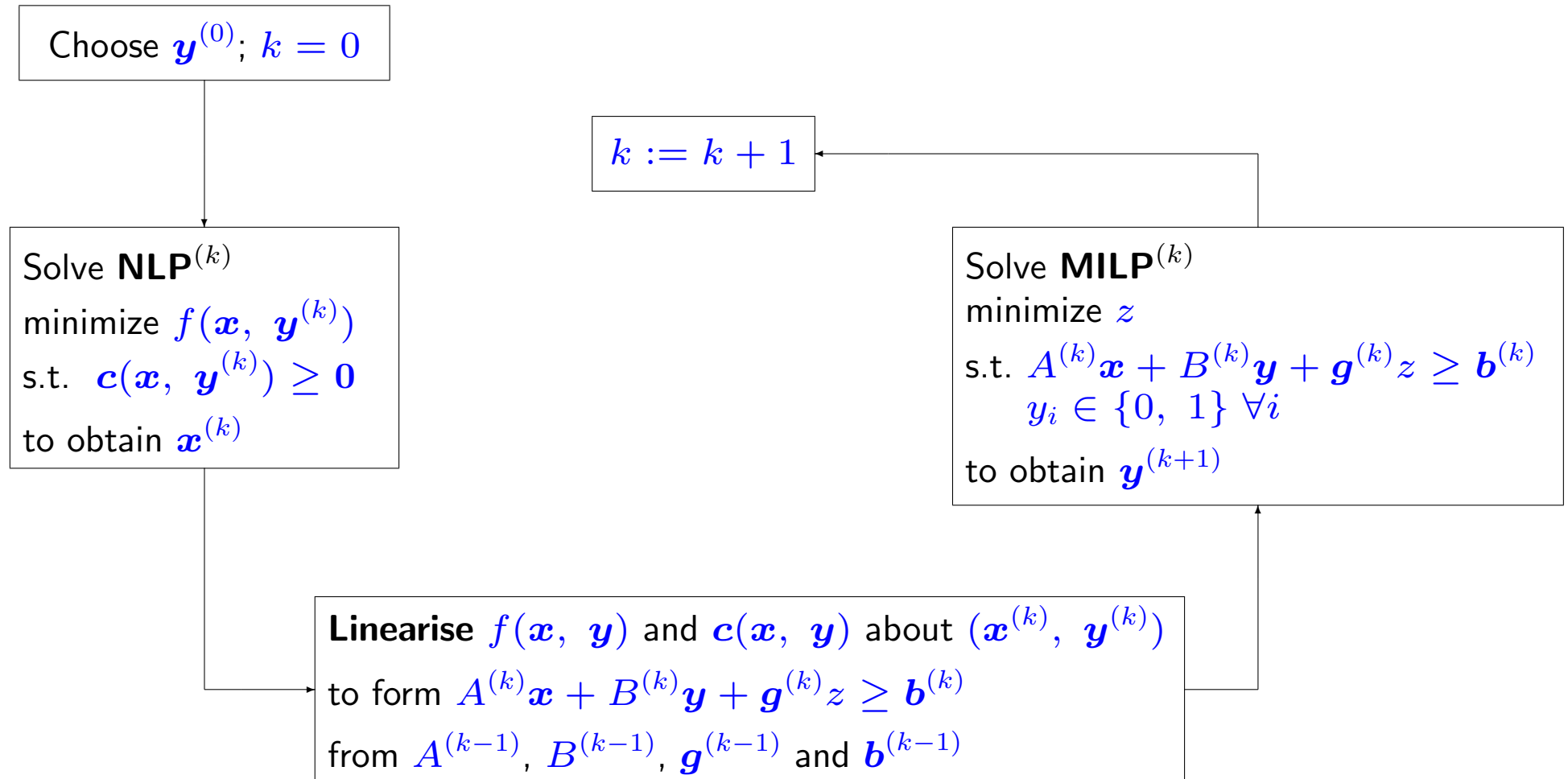
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Linearise $f(\mathbf{x}, \mathbf{y})$ and $\mathbf{c}(\mathbf{x}, \mathbf{y})$ about $(\mathbf{x}^{(k)}, \mathbf{y}^{(k)})$
to form $A^{(k)}\mathbf{x} + B^{(k)}\mathbf{y} + \mathbf{g}^{(k)}z \geq \mathbf{b}^{(k)}$
from $A^{(k-1)}, B^{(k-1)}, \mathbf{g}^{(k-1)}$ and $\mathbf{b}^{(k-1)}$

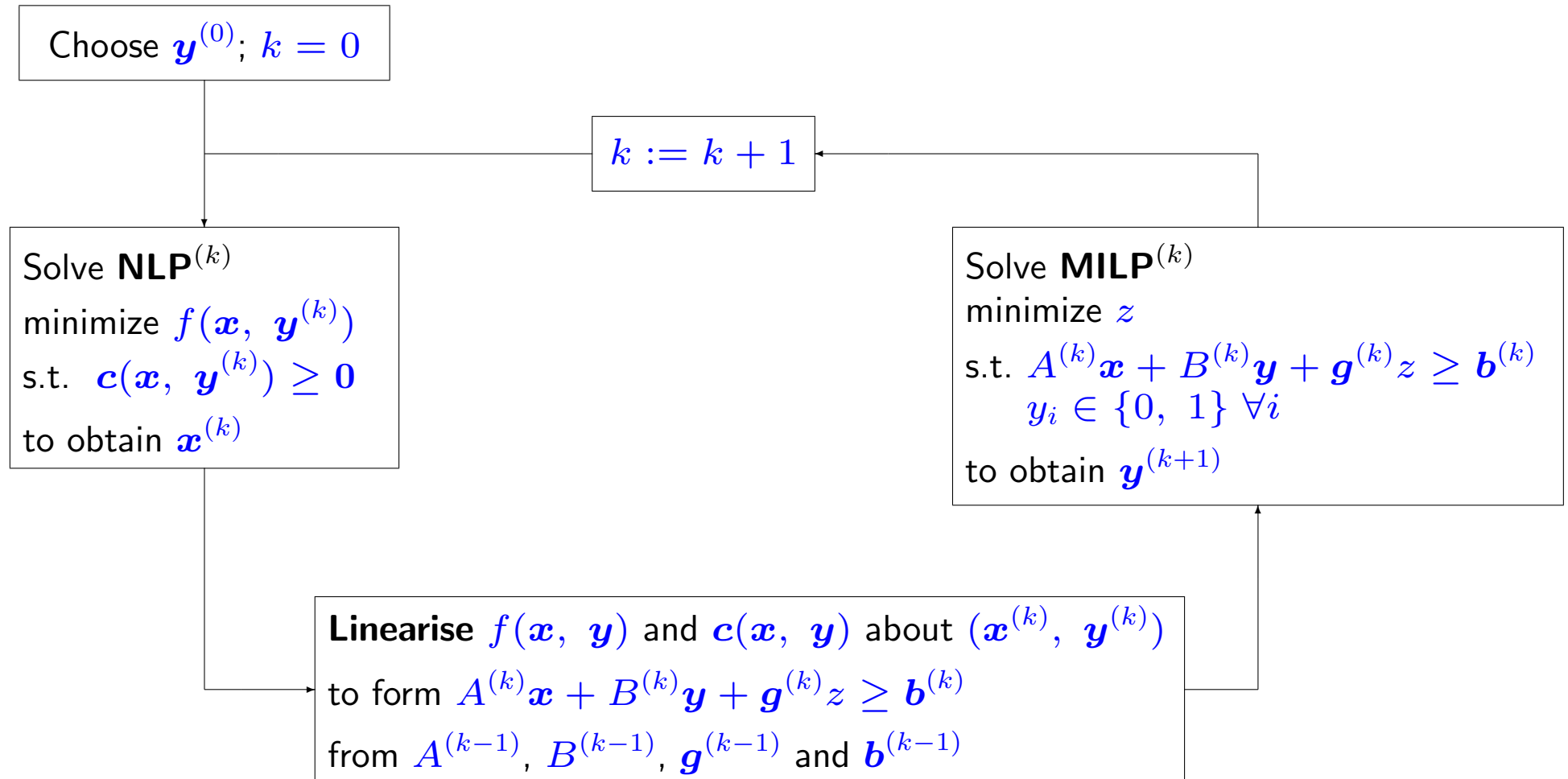
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Components of the first Dundee MINLP solver

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- *Towards reliable linear programming*
Fletcher and Hall (1990)
Pitman Research Notes in Mathematics Series 228 89–104
- *Ordering algorithms for irreducible sparse linear systems*
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Annals of Operations Research **43** 15–32



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Hyper-sparsity in the revised simplex method and how to exploit it

Hall and McKinnon (2005)

Computational Optimization and Applications **32(3)** 259–283

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What is hyper-sparsity

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When does hyper-sparsity occur?

- During left-looking implementations of Gaussian elimination
- When applying the revised simplex method to important classes of LP problems



Exploiting hyper-sparsity

- Traditional technique for solving $Lx = b$ by transforming b into x

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do  $k = 1, n$   
   $b := b - b_k l_k$   
end do
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- When x is sparse, the dominant cost is the test for zero
- Efficient identification of vectors l_k to be applied
 - Gilbert and Peierls (1988)
 - Hall and McKinnon (1998–2005)



The Leyffer years (1989–2002)

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- MIQP

Numerical Experience with lower bounds for MIQP branch-and-bound

Fletcher and Leyffer (1998)

SIAM J. Optimization **8(2)** 604–616

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Solving mixed integer nonlinear programs by outer approximation

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Mathematical Programming **66** 327–349

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Mathematical Programming **66** 327–349

- Integrated NLP within branch-and-bound

Integrating SQP and branch-and-bound for mixed integer nonlinear programming

Leyffer (2001)

Computational Optimization & Applications **18** 295–309



The Leyffer years (1989–2002)

- Eventually did some chemical engineering!

Comparison of certain MINLP algorithms when applied to a model structure determination and parameter estimation problem

Skrifvars, Leyffer and Westerlund (1998)

Computers and Chemical Engineering **22(12)** 1829–1835



The “Filter” method

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For NLP

minimize $f(\boldsymbol{x})$ subject to $\boldsymbol{c}(\boldsymbol{x}) \geq \mathbf{0}$

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minimize $f(\mathbf{x})$ subject to $\mathbf{c}(\mathbf{x}) \geq 0$

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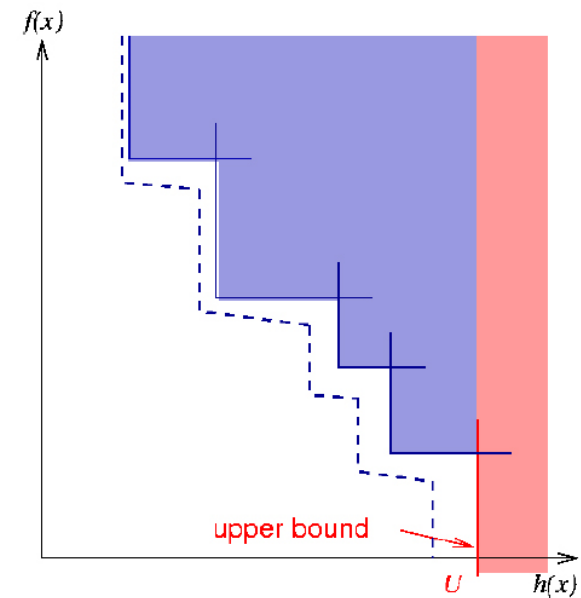
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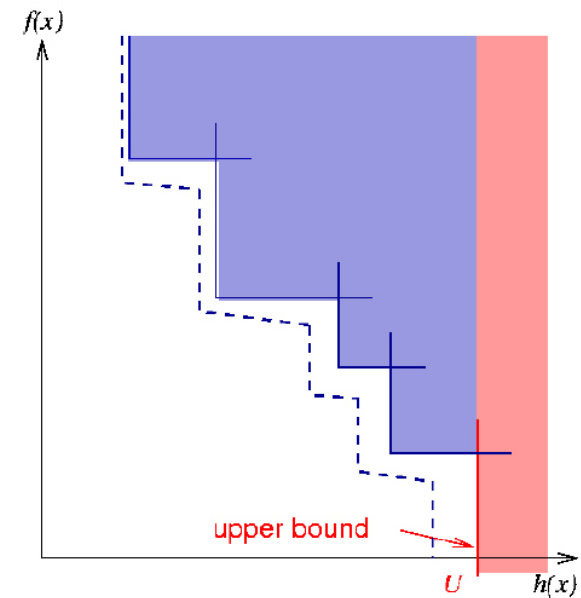
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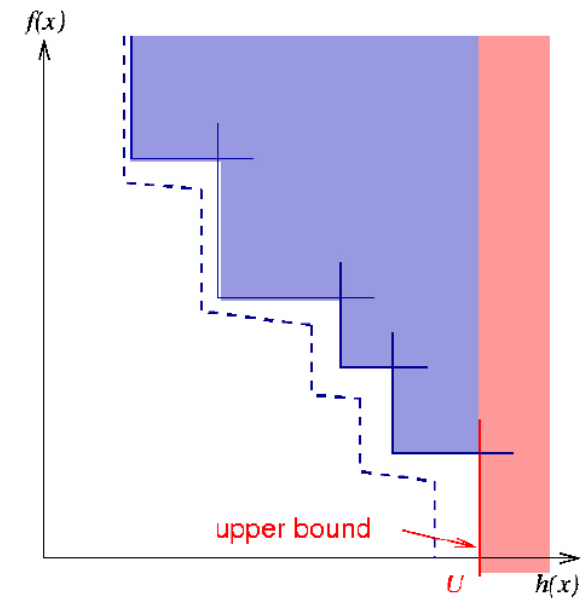


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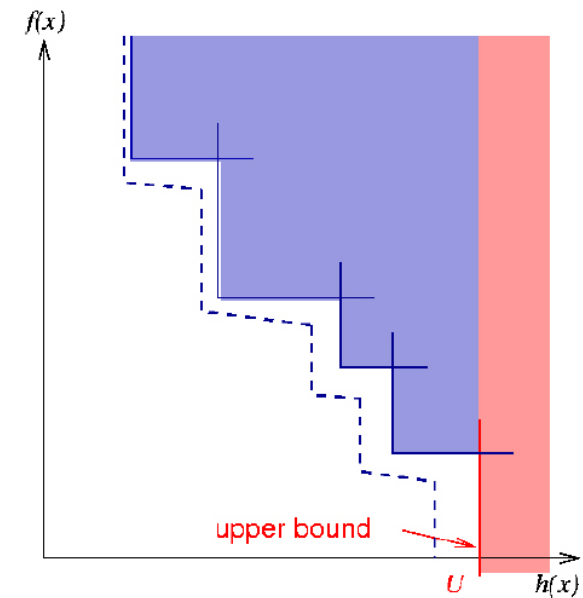
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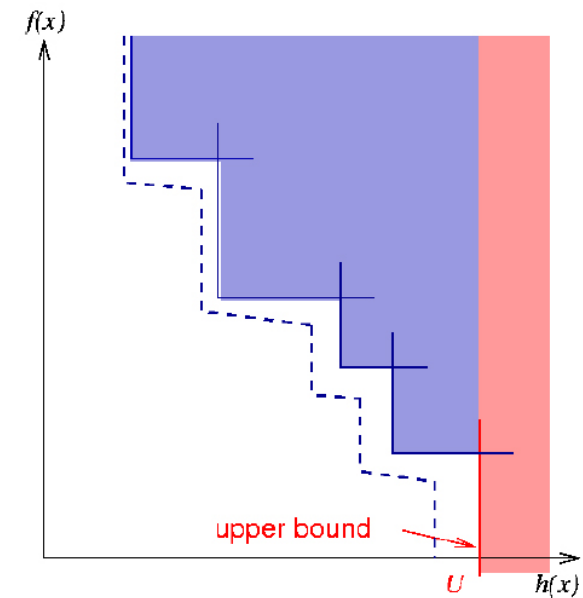
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- First presented by Fletcher in a plenary talk at SIAM Optimization (May 1996)



Legacy

- Convergence proof and extensions generated a sequence of landmark papers
 - *Nonlinear programming without a penalty function*
Fletcher and Leyffer (2002)
Mathematical Programming **91** 239–270
 - *On the global convergence of a filter-SQP algorithm*
Fletcher, Leyffer and Toint (2002)
SIAM J. Optimization **13(1)** 44–59
 - *Global convergence of trust-region SQP-filter algorithms for general nonlinear programming*
Fletcher, Gould, Leyffer, Toint, and Wächter (2002)
SIAM J. Optimization **13(3)** 635–659

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- Extended (with Fletcher, Gould and Toint) to algebraic inequalities, nonlinear systems of equations and nonlinear least squares
- With Fletcher and Toint, won the SIAM Lagrange prize in 2006



After ECOSSE?

- Work on mathematical programs with equilibrium constraints (MPEC) was motivated by Bill Morton's multi-phase flow example presented at an ECOSSE meeting)

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The Return of the Filter

Dundee/SIAM

How the Grinch Solved MPECs

Dundee

Filter Methods By Dummies (*)

Argonne

MPECs: Much Ado About Nothing?

ISMP-00

The M&M of Optimization: Modeling and Methods

Argonne

QPPAL: A Friendly Solver for Large-Scale QPs

INFORMS

(*) actually a misprint: should have been “For” 😊



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- Where are they now?
 - Marcel Mongeau: maître de conférences at Université Paul Sabatier, Toulouse
 - Colin Millar: DJ?



Future work?

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- Now a major field of optimization

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Thanks Jack!