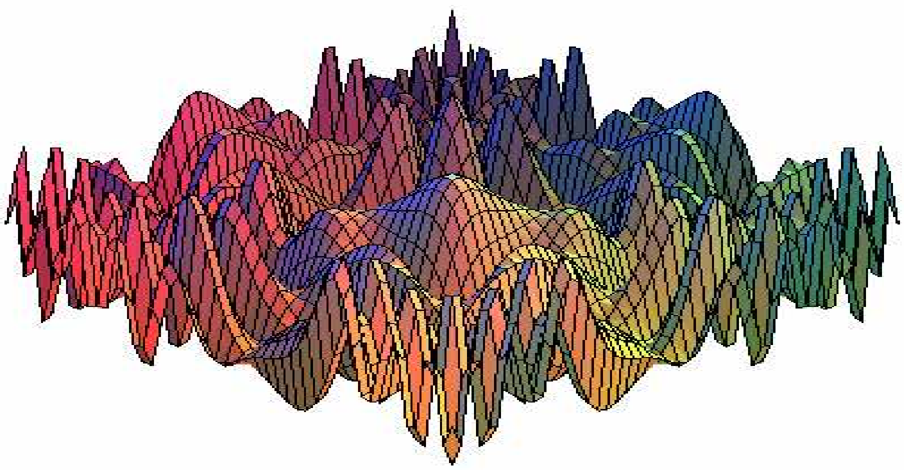
Global Optimization
Software Development and Advanced Applications



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Presentation Topics

- The Relevance of Nonlinear and Global Optimization
- General CGO Model and Some Examples
- Model Development Environments
- GO Software Implementations (LGO and others)
- Illustrative Applications and Case Studies
- Illustrative References
- Software Demonstrations (as time allows, or after talk)

Acknowledgements to all developer partners, clients, and interested colleagues for cooperation, support and feedback

Decision Models and Optimization

- Decision making under resource constraints is a key paradigm in strategic planning, design and operations by government and private organizations
- Examples: environmental management; healthcare; industrial design and production; inventory planning; scheduling, transportation and distribution, and great many others
- Quantitative decision support systems (DSS) tools - i.e., models and solvers - effectively assist decision makers and analysts in finding better solutions

A KISS* Model Classification

Convex (Continuous) Deterministic Models

Linear Programming, Convex Nonlinear Programming, and their numerous special cases

Non-Convex Deterministic Models

Continuous Global Optimization, Combinatorial Optimization, Mixed Integer/Continuous Optimization, and special cases

Stochastic Models

General Stochastic Optimization model; special cases that lead to LP, CP, and general NLP equivalents; and "black box" models

Formally, both the convex and stochastic model-classes can be considered as subsets of the non-convex model class

Combinatorial models can also be formulated as continuous GO models; however, added specifications and insight are helpful

* Keep it Simple, Stupid…

Nonlinear Systems Modeling & Optimization

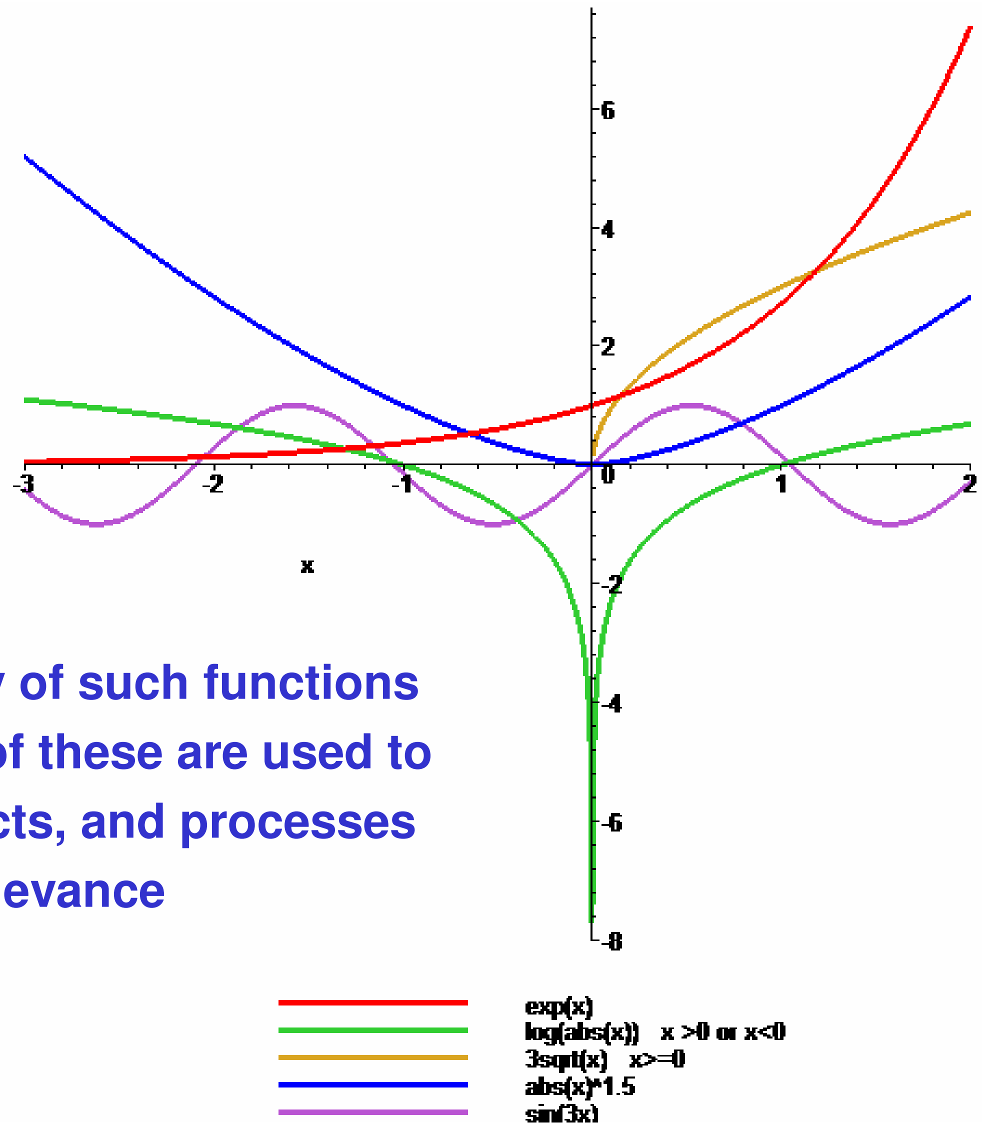
- As the previous slide indicates, nonlinear systems are more of the norm than the exception…
- Nonlinearity is found literally everywhere: in natural formations, objects, organisms, processes, and in their complex interactions
- This fact is reflected by descriptive models in applied mathematics, physics, chemistry, biology, engineering, and economics
- Some of the most frequently used nonlinear function forms: exponential (growth or decay processes,...); logarithmic (growth,…), trigonometric (periodicities,…)

Nonlinear Systems Modeling & Optimization

(continued)

- Composite and more complicated nonlinear functions: special functions, integral equations, linear system of ordinary differential equations, partial differential equations, and so on
- Statistical models: probability distributions, stochastic processes
- “Black box” (deterministic or stochastic) simulation models, closed (confidential) modules, and others, including models with expensive functions

Examples of Basic Nonlinear Functions



A huge variety of such functions exists: many of these are used to describe objects, and processes of practical relevance

Nonlinearity in Nature

[A small collection of great photos from the Web]



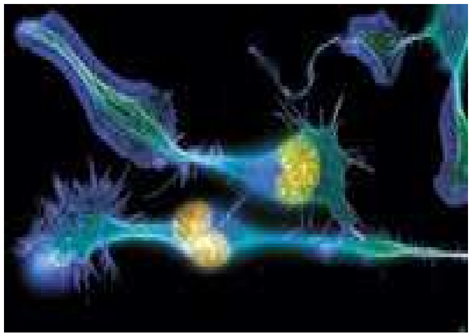


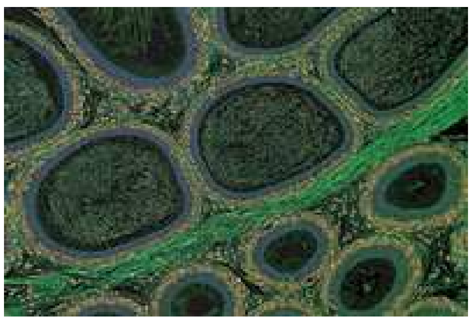

Nature is clearly the most successful of all artists.

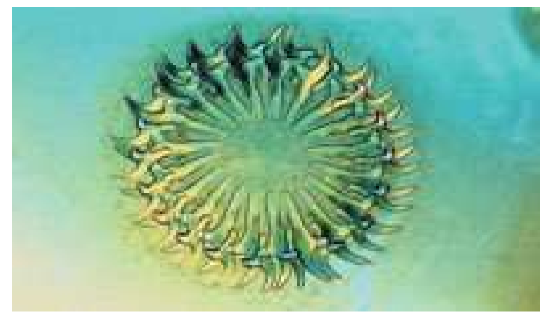
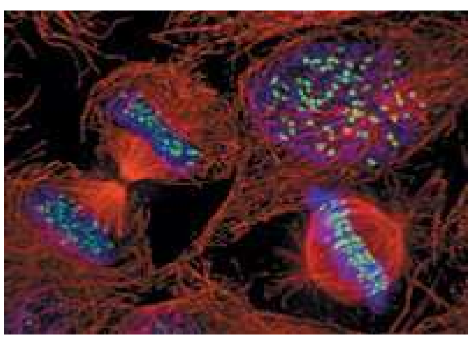
Alvar Aalto, Finnish architect and designer (1898-1976)

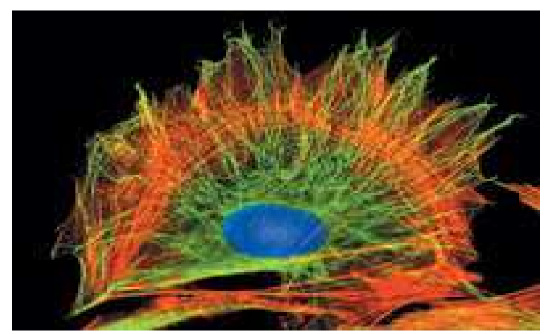
Nonlinear Universe: Further Examples

Credits: Scientific Computing & Instrumentation, 2004



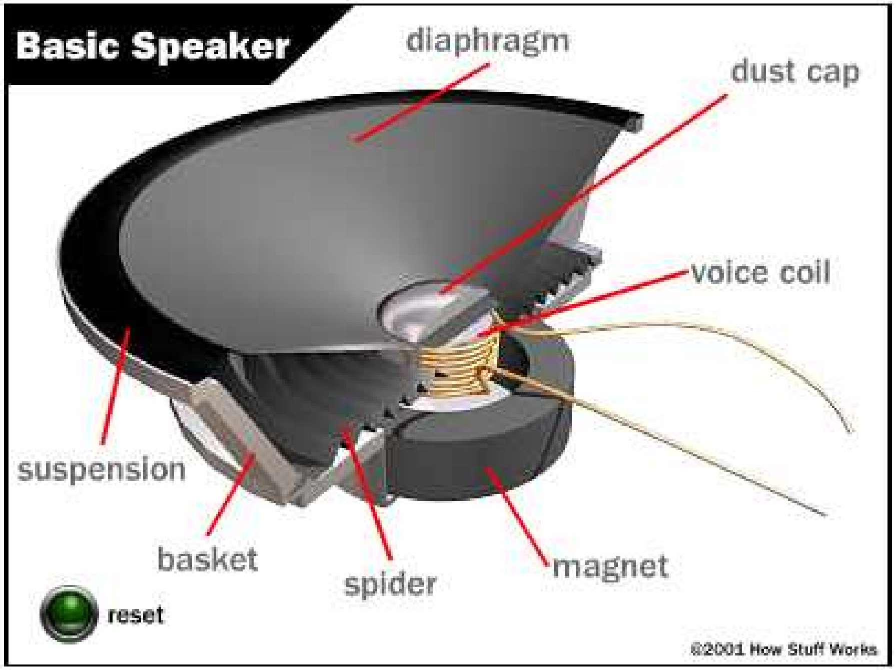





Nonlinearity in Man-Made Systems

Example: Audio Speaker Design

Credits: “How Stuff Works” Website, 2005



Nonlinearity in Man-Made Systems

Example: Automotive Engine Design

Credits: "How Stuff Works" Website & Daimler-Chrysler, 2005

2003 Jeep®
Grand Cherokee

Discovery Spaceship

A Man-Made System with Many Nonlinear Components

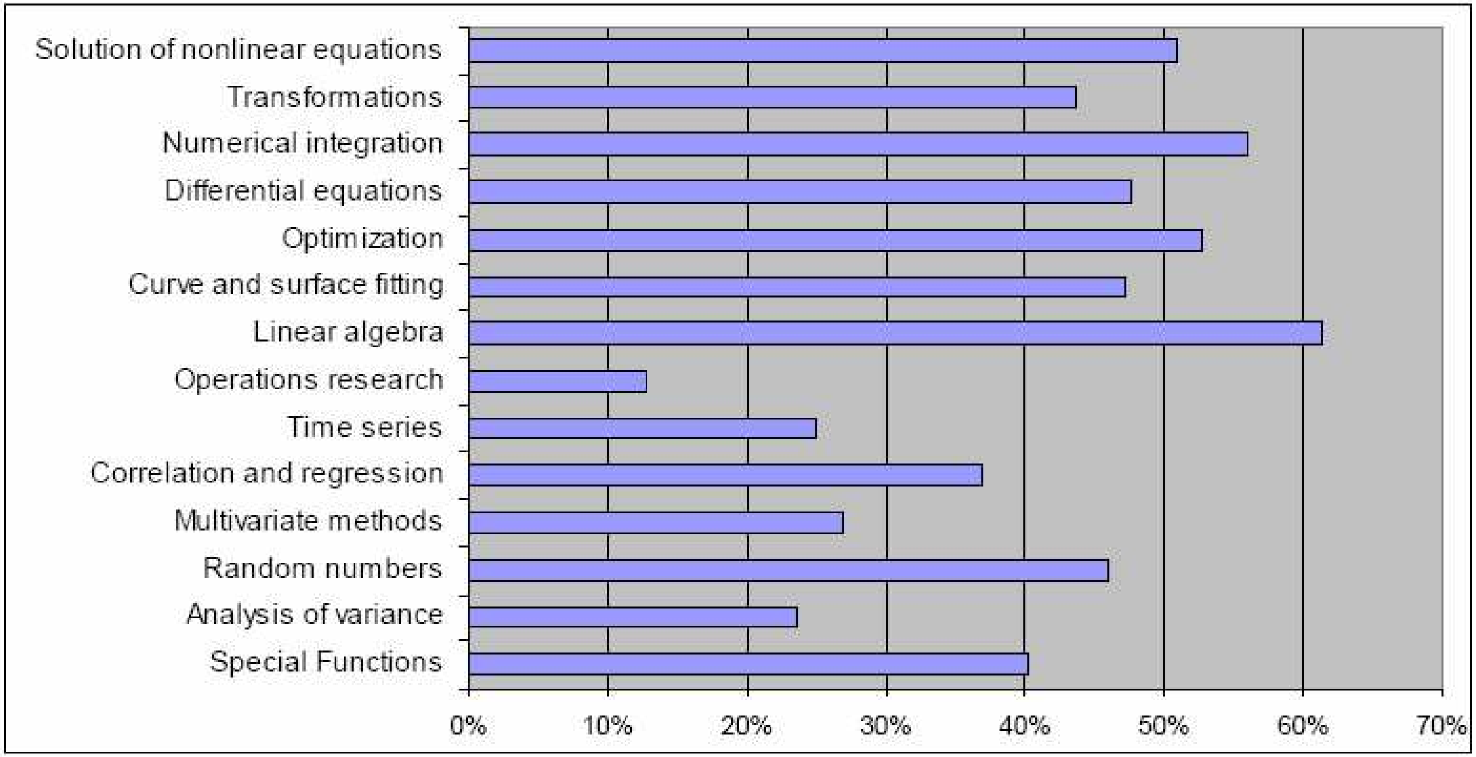
Credits: Robert Sullivan, New York Times, 2006

Need for descriptive system models in combination with control (optimization) methods

NAG Survey on Technical Computing Needs

Functionality use **NB: Many of these uses need NLP/GO solvers!**

Survey participants were asked to report on the use of functionality found in numerical libraries. The following shows the usage of each of the listed functional areas as a percentage of all survey participants. Percentages exceed 100% since most users specified more than one functional area.



The Relevance of Global Optimization

"*Theorists interested in optimization have been too willing to accept the legacy of the great eighteenth and nineteenth century mathematicians who painted a clean world of [linear, or convex] quadratic objective functions, ideal constraints and ever present derivatives.*

The real world of search is fraught with discontinuities, and vast multi-modal, noisy search spaces..."

D. E. Goldberg, genetic algorithms pioneer

The Relevance of Global Optimization

- Optimization in these (and similar) cases is often based on highly nonlinear descriptive models
- Several important and very general model-classes:

  Provably non-convex models

  Black box systems design and operations

  Decision-making under uncertainty

  Dynamic optimization models
- Nonlinear models frequently possess multiple optima: hence, their solution requires a suitable global scope search approach
- The objective of **global optimization** is to find the absolutely best solution, in the possible presence of a multitude of local sub-optima

Continuous Global Optimization Model

$\min f(x)$ $\quad f: R^n \rightarrow R^1$

$g(x) \leq 0$ $\quad g: R^n \rightarrow R^m$

$l \leq x \leq u$ $\quad l, x, u, (l < u)$ are real n-vectors

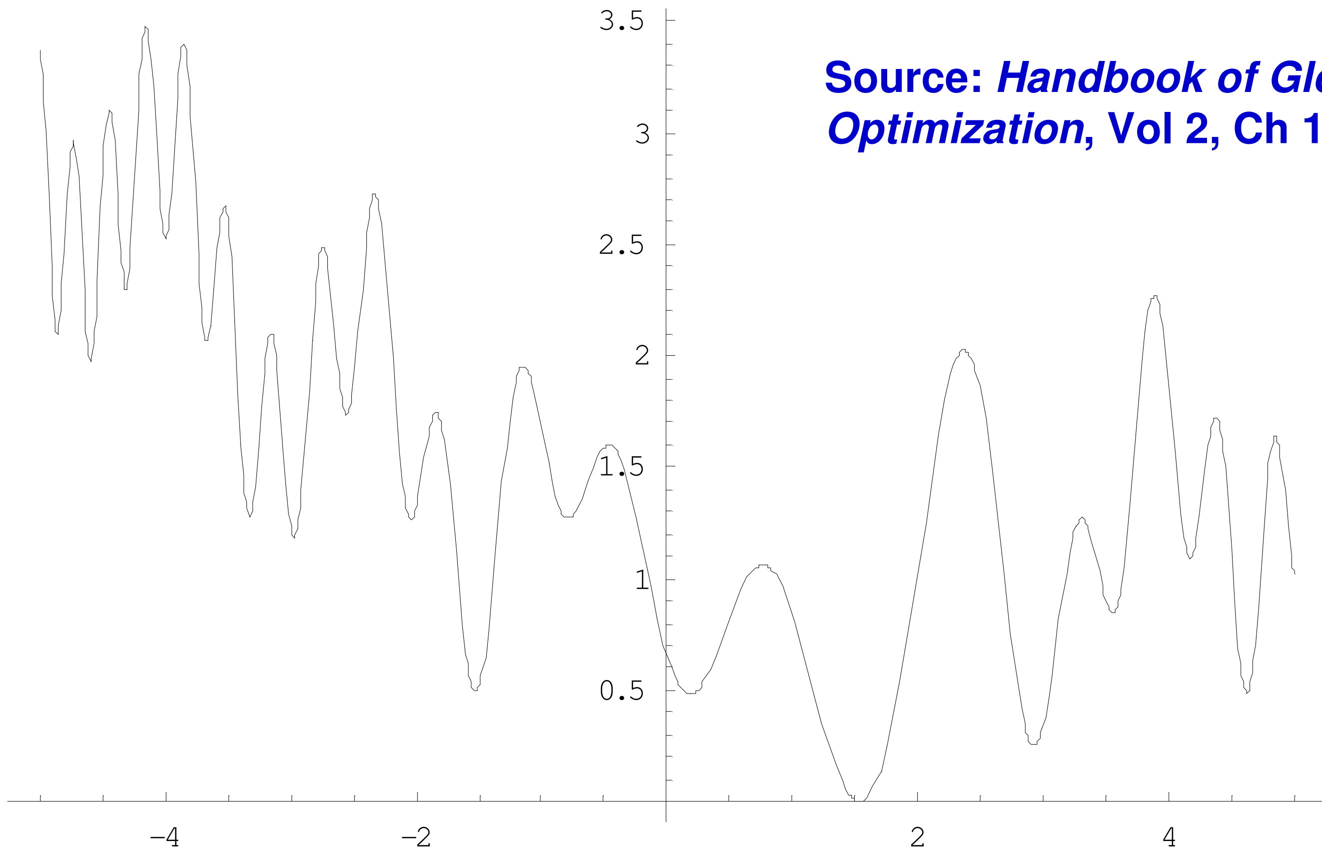
Key ('minimal') analytical assumptions:

- l, u finite
- feasible set $D=\{x_l \leq x \leq x_u: g(x) \leq 0\}$ non-empty
- f, g continuous functions (component-wise)

These assumptions are sufficient to guarantee the existence of the global solution set X^*; also support the application of theoretically rigorous, globally convergent methods

The CGO model covers a very general class of models

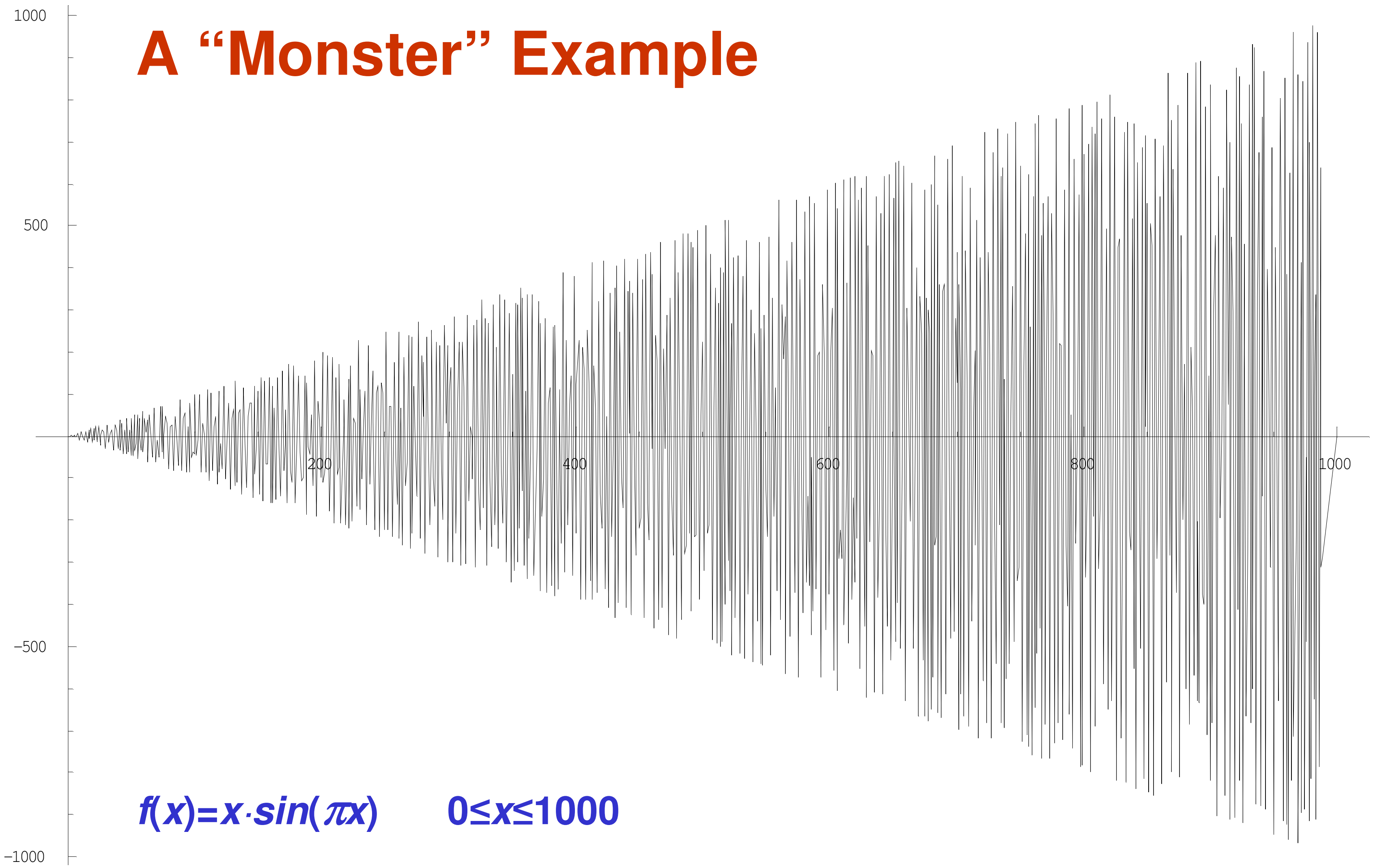
GO models can be difficult...



Source: ***Handbook of Global Optimization*, Vol 2, Ch 15.**

Obviously, a restricted local view of such a model is not sufficient: truly global scope search is needed

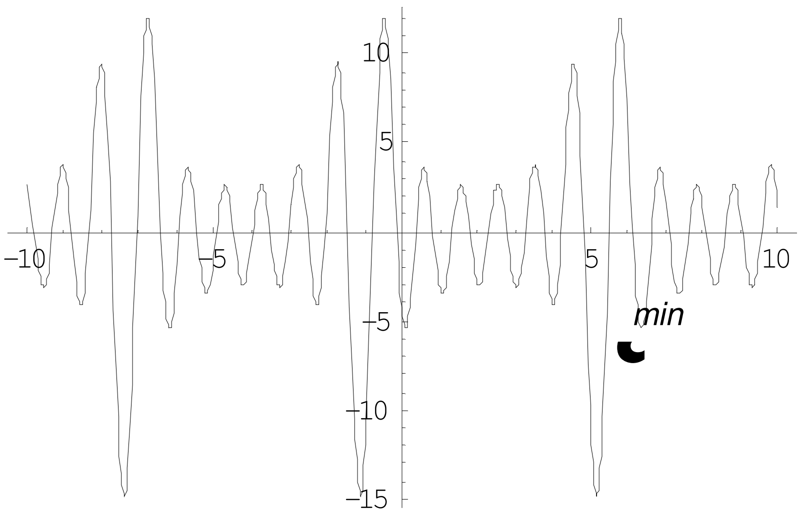
A “Monster” Example



$f(x)=x \cdot sin(\pi x)$ $0 \le x \le 1000$

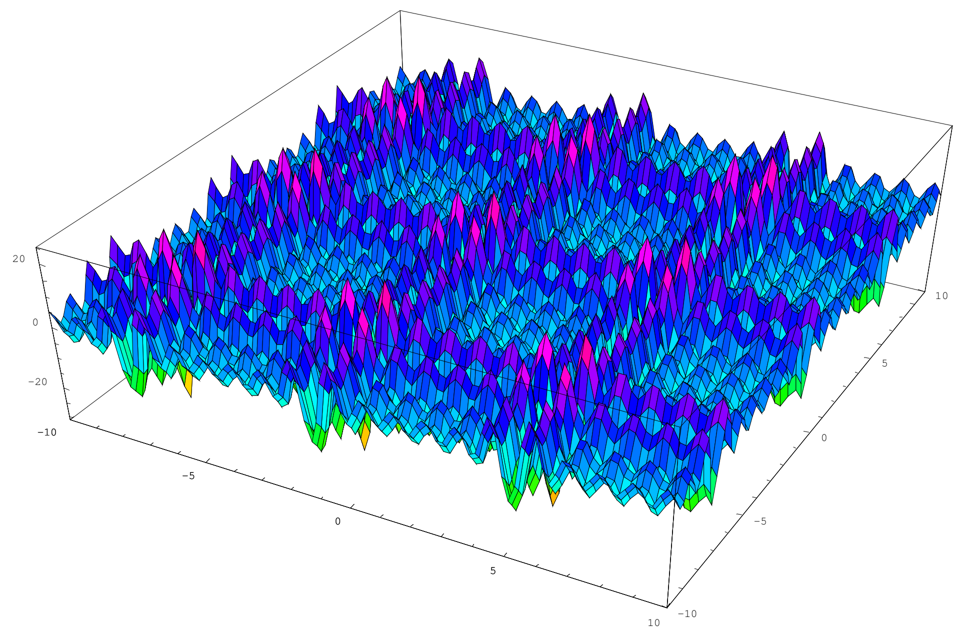
GO models can be arbitrarily difficult to solve, even in (very) low-dimensions…

"Curse of Dimensionality" in GO



$\sum_{k=1,\ldots,5} k \, sin(k+(k+1)x)$

$-10 \le x \le 10.$



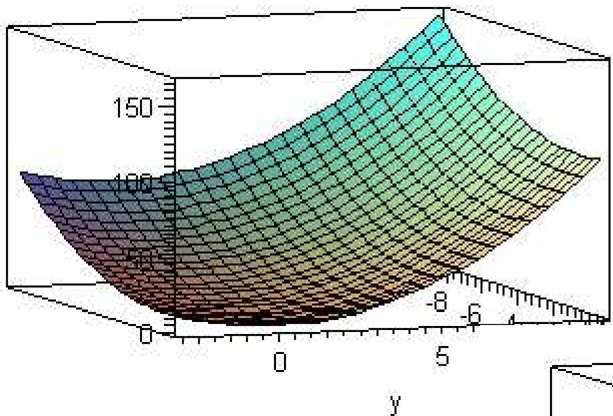
$\sum_{k=1,\ldots,5} k \, sin(k+(k+1)x) + \sum_{k=1,\ldots,5} k \, sin(k+(k+1)y)$

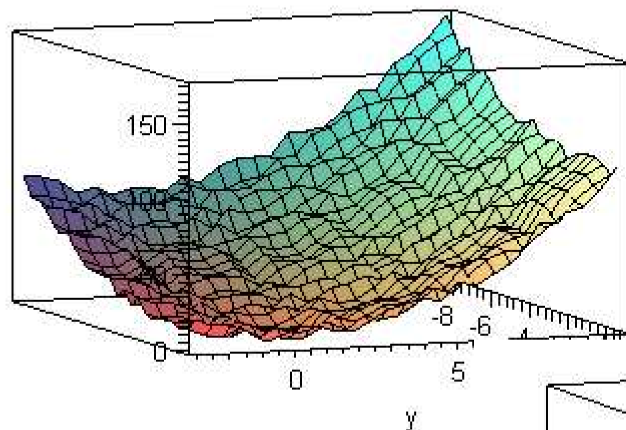
$-10 \le x \le 10, -10 \le y \le 10$..

Shubert's one-dimensional box-constrained optimization model, and its simplest two-dimensional extension

Computational complexity could (and often will) increase exponentially as model size (*n, m*) grows

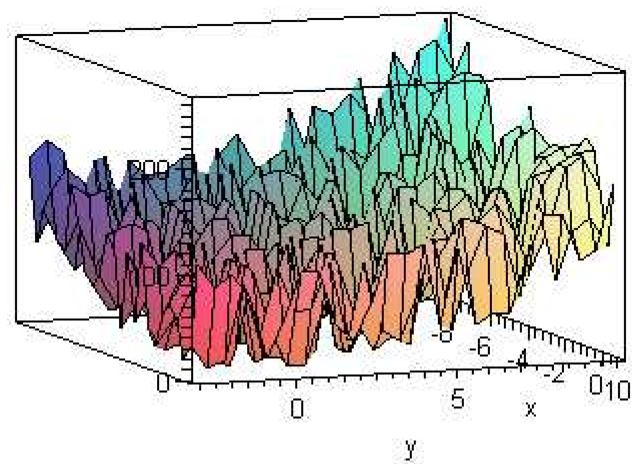
Parameterized Test Functions



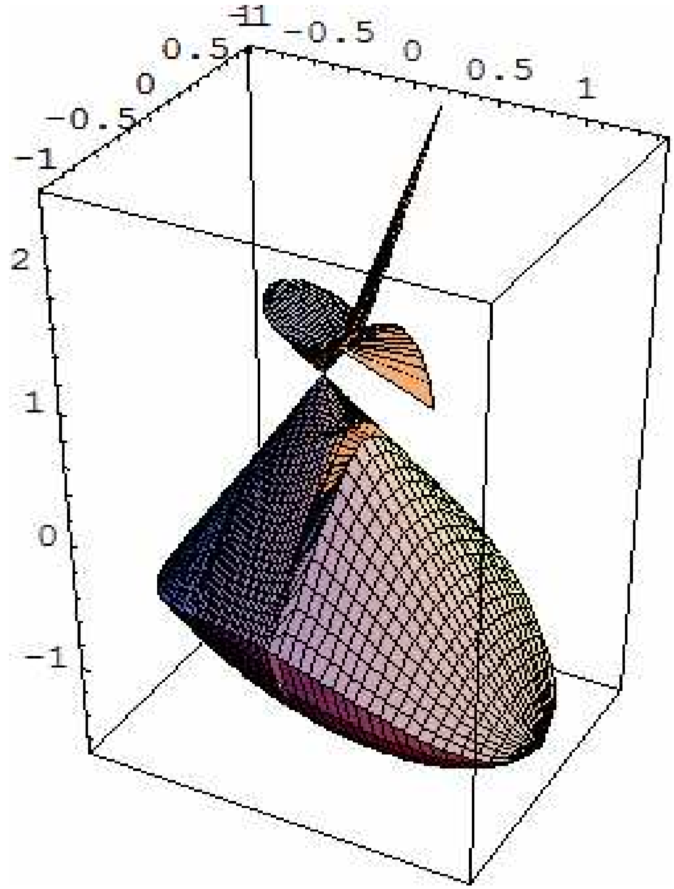


Example:
$x^2+y^2+c \cdot \sin^2(x^2+x+y^2-y)$
x=-8..1, y=-3..10;   c=1, 10, 100

Note: easy to modify in order to generate randomized solution points (as instances)



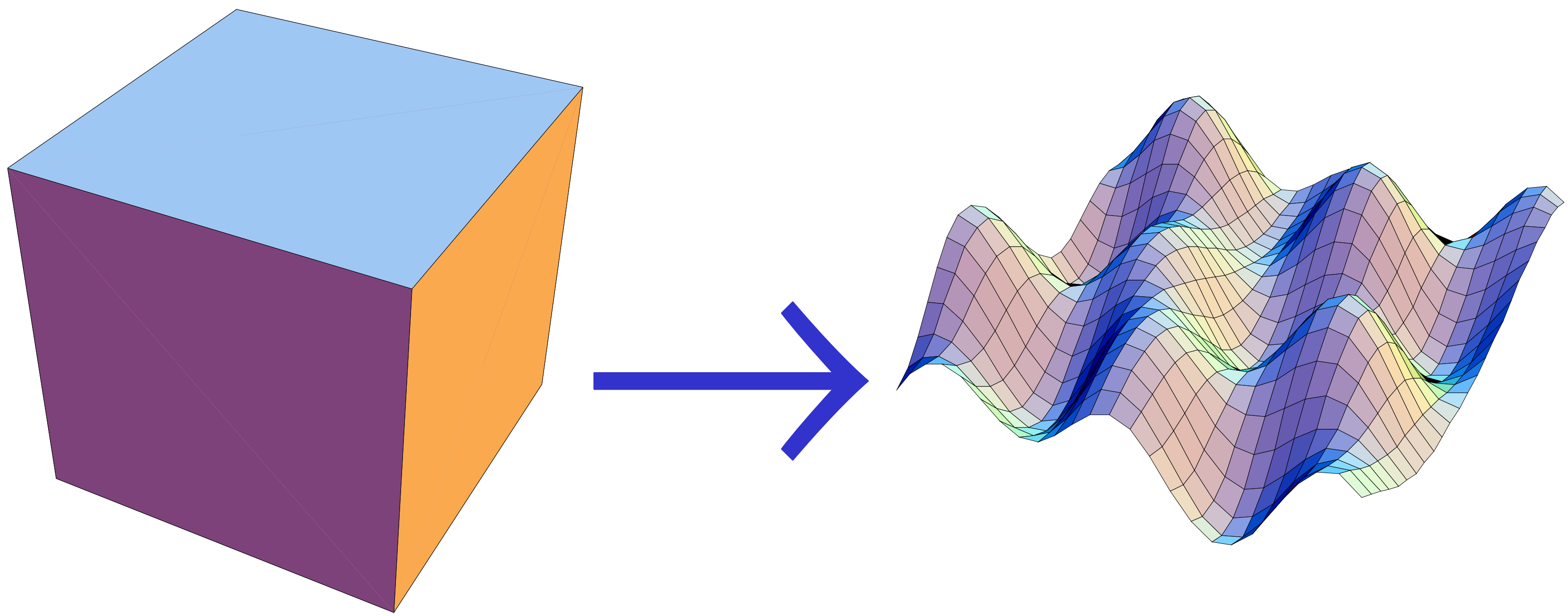
A Tricky Feasible Set



Example: Feasible set in R^3 defined by the constraints

$$x \cdot y \cdot z \le 1, \quad x^2+2y^2+z^2+x \cdot z \le 2, \quad 3x^2+2y^2-(1-z)^2 \le 0$$

The Mixed Integer Global Optimization Challenge



Each binary variable selection (combination) induces a CGO sub-model

The overall complexity is characterized by the combined complexity of combinatorial optimization and continuous global optimization… Hence, massively exponential as model size ($n=n_B+n_C$, m) grows

Global Optimization: A Historical Perspective

An approximate timeline

Theory (beginnings: 1950’s, foundations: 1970’s)

$\downarrow\uparrow$

Methods (beginnings: 1960’s, key results: 1980’s)

$\downarrow\uparrow$

Software (beginnings: 1980’s, professional: ~2000+)

$\downarrow\uparrow$

Applications (needed since ages; only recently tackled by suitable GO tools)

Ideally, all key components of knowledge are developed in close interaction

Global Optimization
Software Development

“Those who say it cannot be done should not interrupt those who are busy doing it.”

Chinese proverb

"It does not matter whether a cat is black or white, as long as it catches mice."

Deng Xiaoping

“I don't want it perfect, I want it Tuesday.”

J.P. Morgan

GO Software Development Environments

- General purpose, “low level” programming languages: C, Fortran, Pascal, … and their modern extensions
- Business analysis and modeling: Excel and its various extensions and add-ons (Excel PSP, @RISK,…)
- Specialized algebraic modeling languages with a focus on optimization: AIMMS, AMPL, GAMS, LINDO/LINGO, LPL, MPL,…
- Integrated scientific and technical computing systems: Maple, Mathematica, MATLAB,…
- Relative pros and cons: instead of “dogmatism”, select the most appropriate platform considering user needs, requirements, and possible options

GO Software: State-of-Art in a Nutshell 1

• Websites (e.g., by Fourer, Mittelmann and Spelucci, Neumaier, NEOS, and others) list discuss dozens of research and commercial codes: examples below

• Excel Premium Solver Platform: Evolutionary, Interval, MS-GRG, MS-KNITRO, MS-SQP, OptQuest solver engines

• Modeling languages and related solver options

AIMMS: BARON, LGO

AMPL: LGO

GAMS: BARON, DICOPT, LGO, OQNLP

LINGO: built-in global solver by the developers; also:
What'sBest! for spreadsheets

MPL: LGO

GO Software: State-of-Art in a Nutshell 2

- Integrated scientific-technical computing environments

Maple: Global Optimization Toolbox

Mathematica: Global Optimization (package),

MathOptimizer, MathOptimizer Professional, NMinimize

Matlab: GADS Toolbox

TOMLAB solvers for MATLAB: CGO, LGO, OQNLP

- Detailed information and references
- Developer websites
- Handbook of GO, Vol. 2, Chapter 15
- Neumaier's GO website, with discussions and links

Further information welcome

LGO (Lipschitz Global Optimizer) Solver Suite: Summary of Key Features

- LGO can analyze and solve complex nonlinear models, under minimal analytical assumptions: computable values of continuous or Lipschitz functions are needed
- LGO can be applied even to completely “black box” system models (defined by continuous functions)
- Globally convergent methods (LGO solver components):

  continuous branch-and-bound

  adaptive random search (single-start)

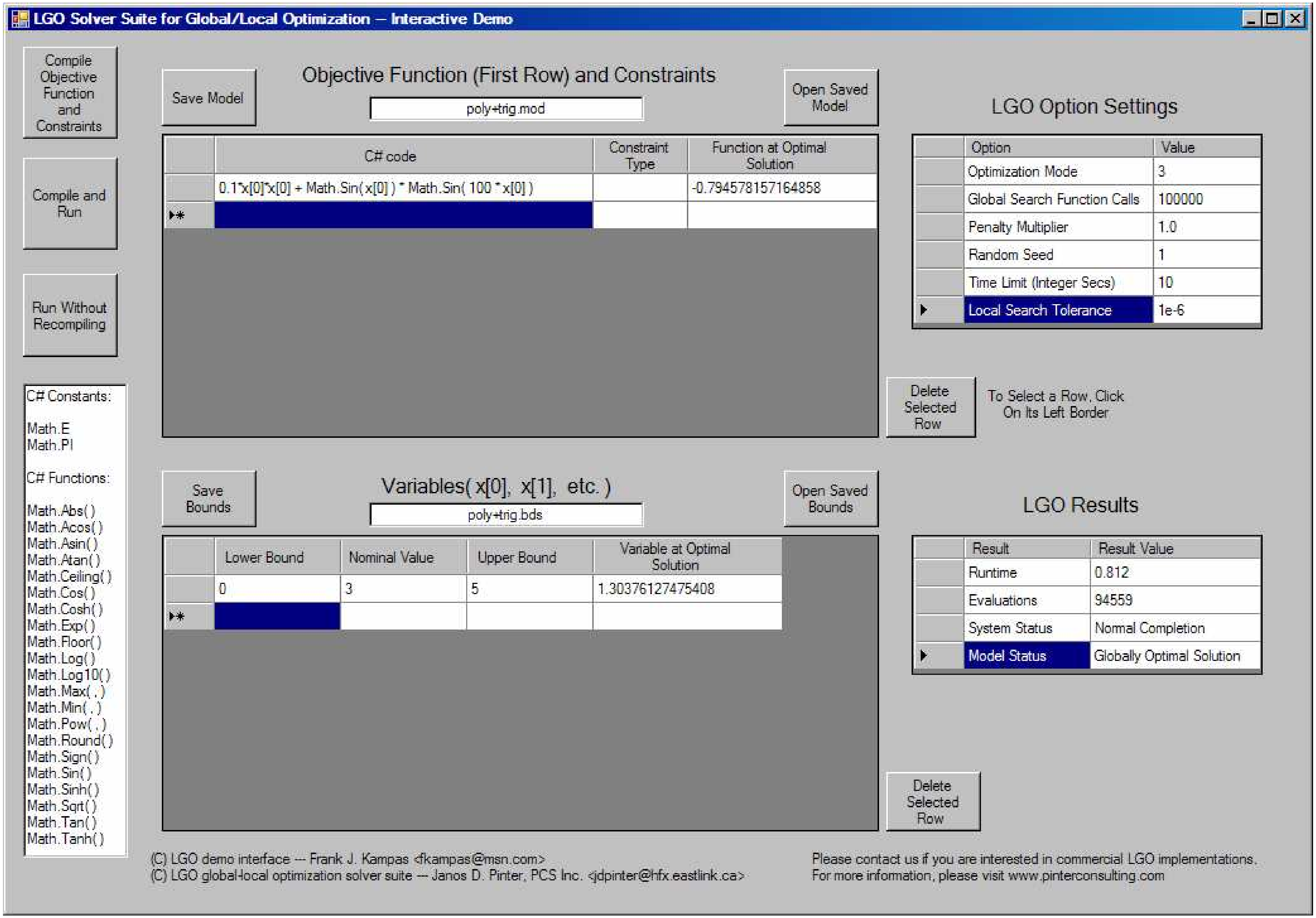
  adaptive random search (multi-start)

  exact penalty function applied in global search phase

LGO: Summary of Key Features (continued)

- Locally convergent method: exact constrained local search (generalized reduced gradient method)
- User Guide(s): mathematical background, detailed description of solver usage, modeling and solver tips
- Tractable model sizes depend only on hardware + time
- LGO reviews in *ORMS Today*, *Opt. Methods and Software*; various other LGO implementations reviewed in *ORMS Today*, *Scientific Computing*, *Scientific Computing World*, *IEEE Control Systems Magazine*, *Int. J. of Modeling, Identification and Control*
- MPL/LGO demo accompanies Hillier & Lieberman OR textbook (2005 edition)

A Simple-to-Use Interactive LGO Demo (C, C#)



Interactive LGO Demo: Example

(Refer to previous slide where this model is solved)

Model formulation and bounds given in text files *.mod and *.bds

Example 1

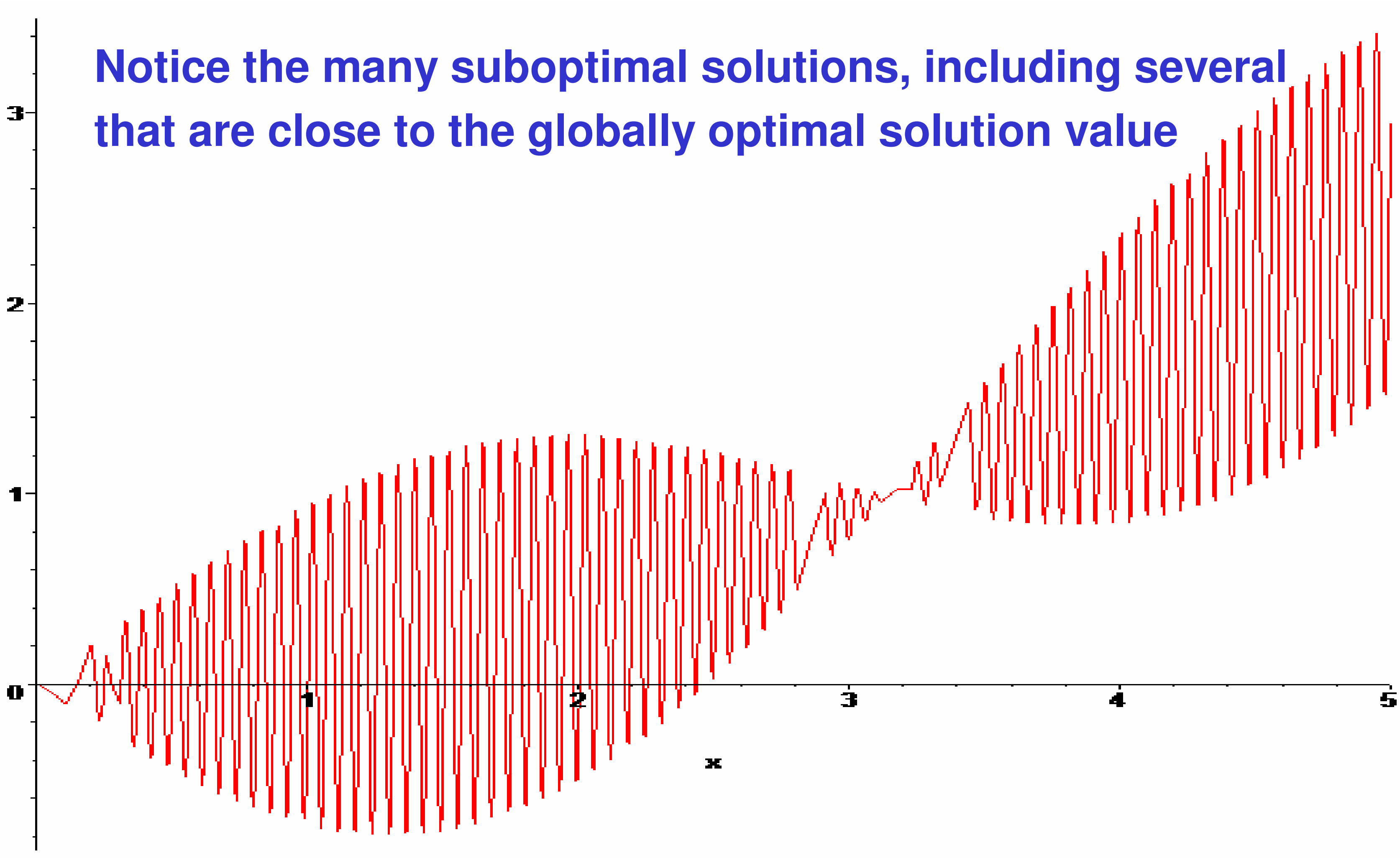
Model: cited from poly+trig.mod

0.1*x[0]*x[0] + Math.Sin(x[0]) * Math.Sin(100*x[0]) objective fct

Bounds: cited from poly+trig.bds

0	lower bound
3	nominal value
5	upper bound

Interactive LGO Demo: Example

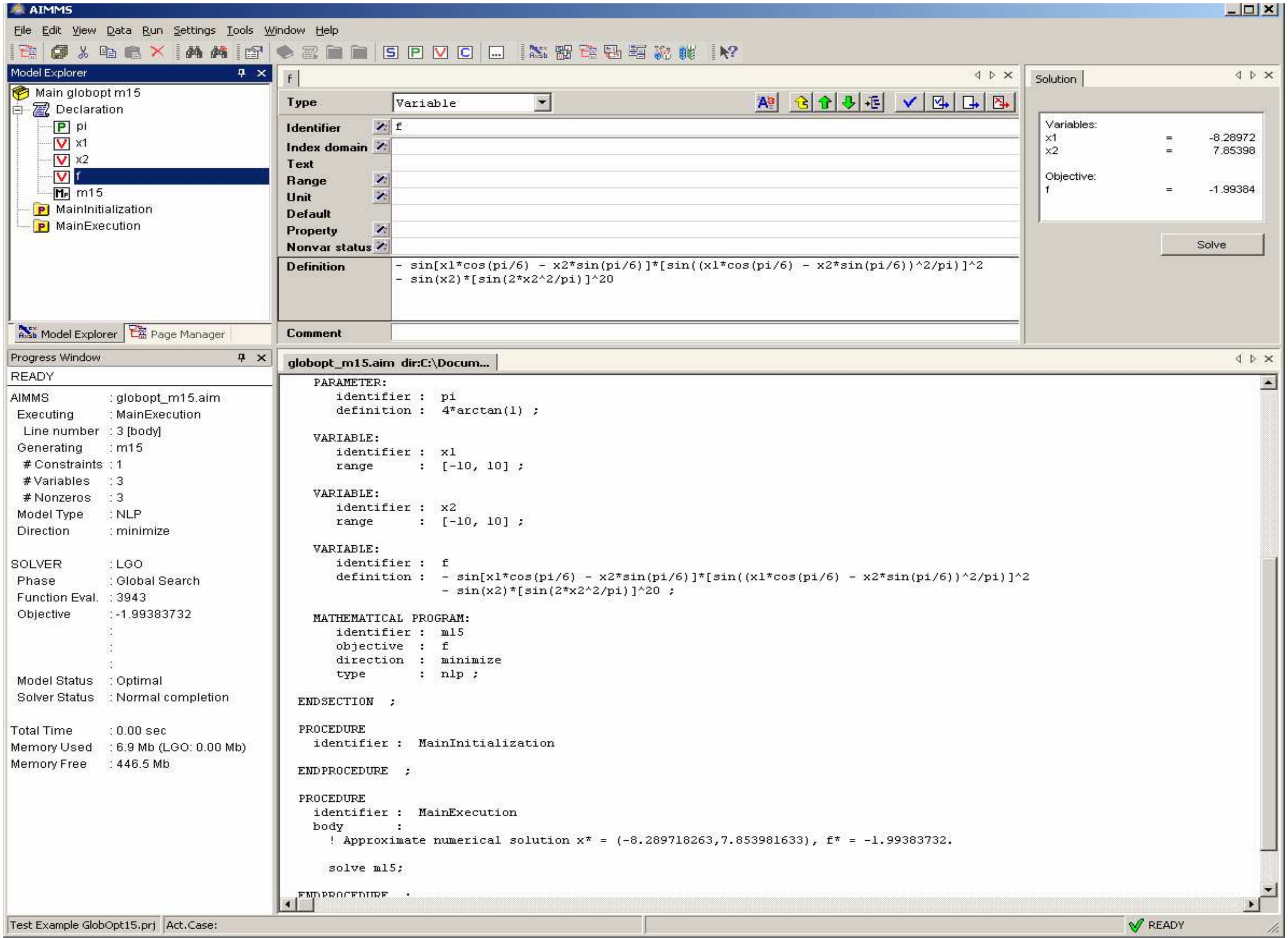


Global solution argument found ~1.30376; optimum value ~-0.79458

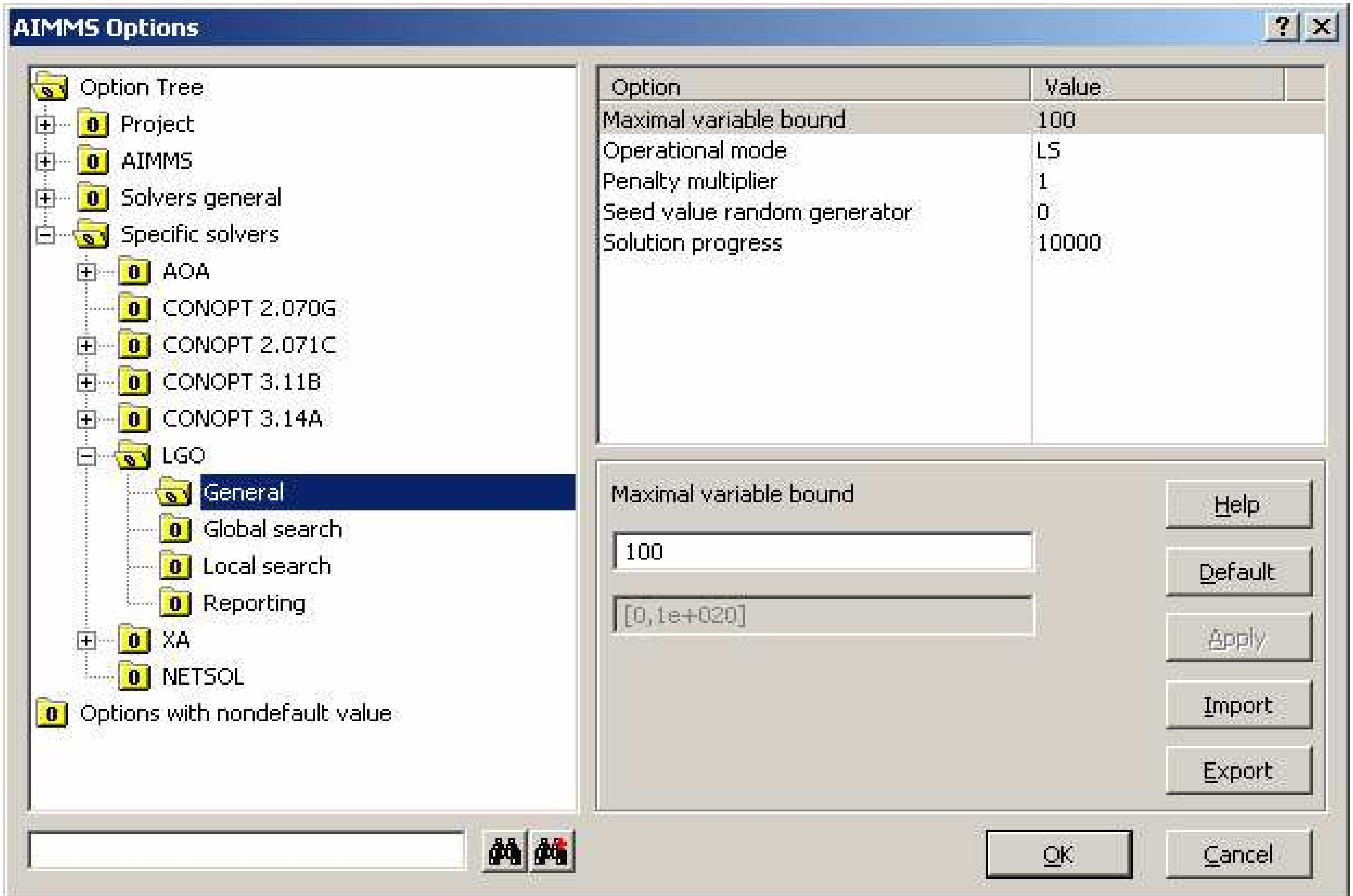
LGO IDE

works in conjunction with C and Fortran compilers

Model Development & Solution by AIMMS/LGO



AIMMS /LGO Solver Link Options



An AMPL Model Solved by LGO

AMPLWin 19990818

File Edit View Send Window Help

New Model Data Save Solve Display Prev Next Find: C M D

Command interface

ampl: ample.out;‖data;‖# Type data here or open a data file...‖sol

reset;‖# !NLPexample.mod‖‖# A parametric NLP model examp

```
== 1 ================
option show_stats 1; option display_eps .000001; print $version;□
AMPL Version 20061130 (MS VC++ 6.0)
Licensed to Janos D. Pinter <jdpinter@hfx.eastlink.ca>.
Trial license expires 20070804.

== 2 ================
reset;
# !NLPexample.mod
# A parametric NLP model example
# J.D. Pinter, 2007
# Model description, background, references etc. can be included here
# Model structure summary
# Number of variables: 2
# Number of bound constraints: 2 (theoretically needed in global optimization,
# Number of general constraints: 2
# Objective: nonconvex, multimodal
# The global minimum value in this example depends on the parameter scale (bel
# and it is bounded from below by 0
# Parameters (as needed to define model)
# Increasing the parameter scale leads to more difficult global optimization t
param scale := 100;
# Model variables
var x{1..2};
# Objective function
minimize Obj: (x[2] - x[1])^2 + scale*(sin(x[1] + x[2]))^2;
subject to
# Bound constraints
Box1l: x[1] >= -8;
Box1u: x[1] <= 10;
Box2l: x[2] >= -17;
Box2u: x[2] <= 4;
# General constraints (in addition to bounds)
Con1: cos(x[1]^2 - x[2]^2) = 0.3;
Con2: x[1] - sin(x[2] - x[1]) <= 2;
# Initial values (typically used by local solvers) can be given here
# data;
# var x :=
#       1  3
#       2 -1
# You can try various (available) solver options
# option solver knitro;
option solver lgo;
# option solver minos;
# Set display precision
option display_round 10;
option display_eps 1e-10;
option display_precisison 10;
# Solve model stated above
solve;
# Display results (in command window)
display Obj;
display _varname, _var;
display _conname, _con;
```

Model I:\AMPL Pro\!NLPexample.mod

```
# !NLPexample.mod
# A parametric NLP model example
# J.D. Pinter, 2007

# Model description, background, references etc. can be included here

# Model structure summary
# Number of variables: 2
# Number of bound constraints: 2 (theoretically needed in global optimization, for all variables
# Number of general constraints: 2
# Objective: nonconvex, multimodal
# The global minimum value in this example depends on the parameter scale (below),
# and it is bounded from below by 0

# Parameters (as needed to define model)
# Increasing the parameter scale leads to more difficult global optimization test models
param scale := 100;

# Model variables
var x{1..2};

# Objective function
minimize Obj: (x[2] - x[1])^2 + scale*(sin(x[1] + x[2]))^2;

subject to

# Bound constraints
Box1l: x[1] >= -8;
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# data;
# var x :=
#       1  3
#       2 -1

# You can try various (available) solver options
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# Set display precision
option display_round 10;
option display_eps 1e-10;
option display_precisison 10;

# Solve model stated above
solve;

# Display results (in command window)
display Obj;
display _varname, _var;
```

gamside: D:\GAMS21.1\modlib\gams.pro.gpr

File Edit Search Windows Utilities Help

No active process

globaltest1

```
--- Starting compilation
--- globaltest1.gms(51) 1 Mb
--- Starting execution
--- globaltest1.gms(45) 1 Mb
--- Generating model m
--- globaltest1.gms(51) 2 Mb
---    10 rows, 12 columns, and 43 non-zeroes.
--- globaltest1.gms(51) 2 Mb
--- Executing LGO

LGO 1.0       Sep  3, 2003 WIN.LG.NA 21.2 001.000.000.VIS

    LGO Lipschitz Global Optimization
    (C) Pinter Consulting Services, Inc.
    129 Glenforest Drive, Halifax, NS, Canada B3M 1J2
    E-mail : jdpinter@hfx.eastlink.ca
    Website: www.dal.ca/~jdpinter

    7 defined, 0 fixed, 0 free
    3 LGO equations and 5 LGO variables

   Iter       Objective      SumInf   MaxInf      Seconds   Errors
  28380   7.634679E-18   0.00E+00  0.0E+00       0.311

--- LGO Exit: Normal completion - Global solution
    0.311 LGO Secs (0.17 Eval Secs, 0.006 ms/eval)
```

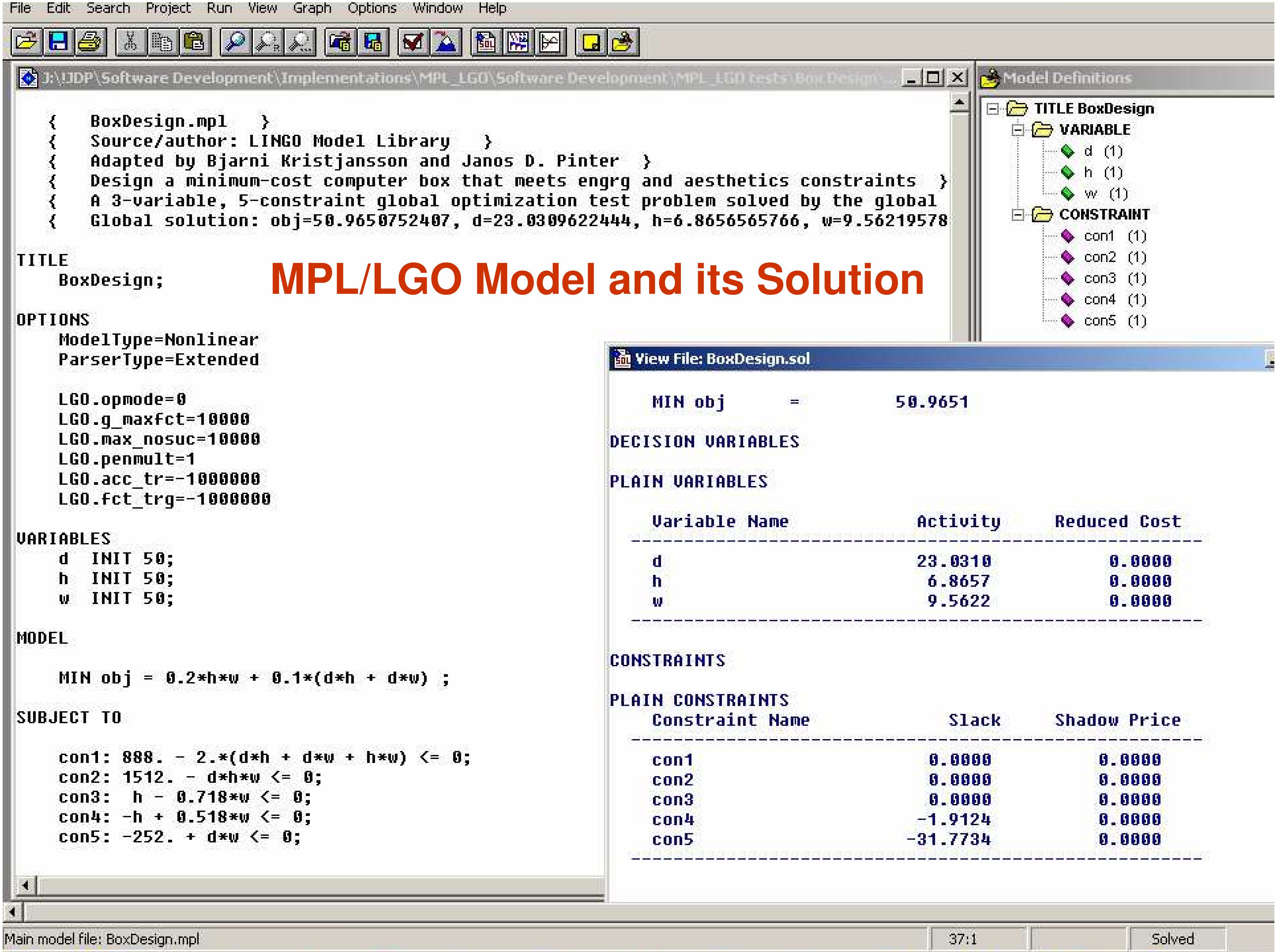
GAMS Preprocessing Step

LGO Solver Result Summary

Close | Open Log | Summary only | Update

1: 1 | Insert

MPL/LGO Model and its Solution



Integrated Scientific and Technical Computing Systems

- Maple, Mathematica, Matlab (and some others; the latter are more specific to certain engineering or scientific fields)
- Model prototyping and development: simple and advanced calculations, programming, documentation, visualization,… supported in ‘live’ interactive documents
- Data import and export features
- Links to external software products, and converters
- Portability across hardware and OS platforms
- ‘One-stop tools’ for interdisciplinary development
- ISTCs are particularly suitable for developing complex, advanced nonlinear models

Getting Started ppt form.nb *

MathOptimizer Model

▪ Getting Started

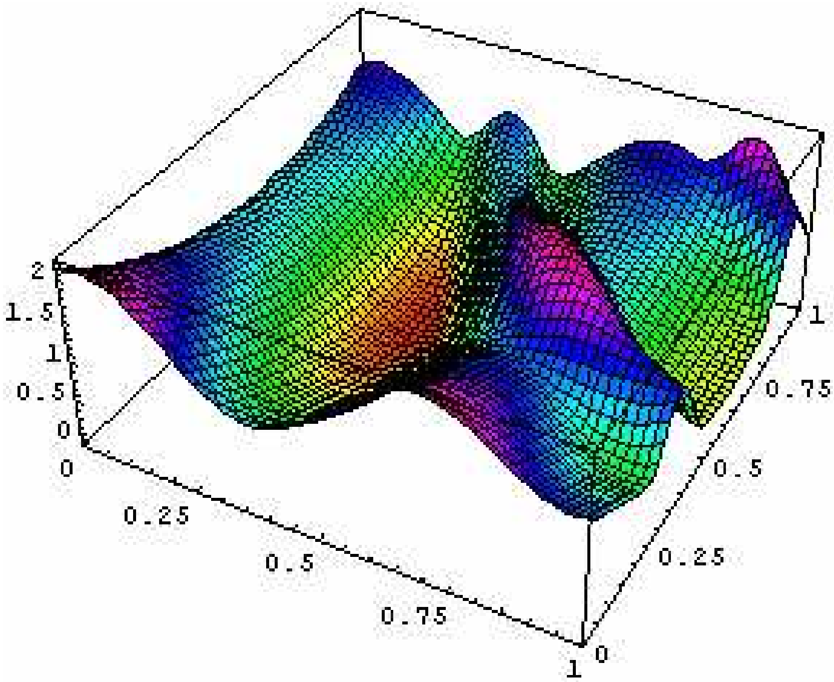
▪ Model Formulation

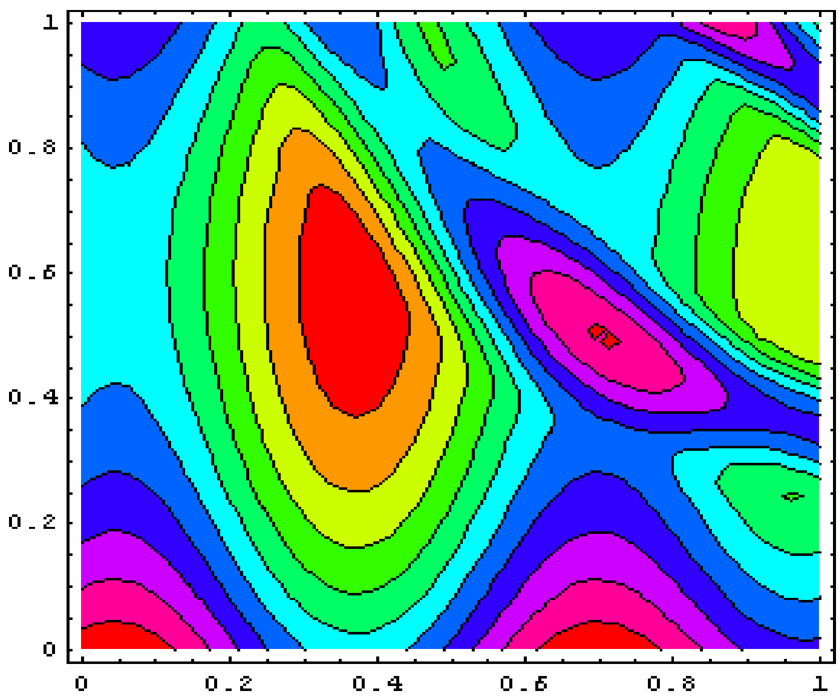
```
vars = {x1, x2};                              (* decision variables *)
varnom = {8., -14.};                          (* nominal values *)
varlb = {-10., -15.};                         (* lower bounds *)
varub = {20., 10.};                           (* upper bounds *)
objf = 10.*(x1^2 - x2)^2 + (x1 - 1)^2;        (* objective function*)
eqs = {x1 - x1*x2};                           (* equality constraints *)
ineqs = {3.*x1 + 4.*x2 - 25.};                (* inequality constraints, ≤0 form *)
```

▪ Numerical Solution

```
Optimize[objf, eqs, ineqs, vars, varnom, varlb, varub,
GlobalSolverMode -> 1, LocalSolverMode -> 1, ReportLevel -> 1]
```

Note that dense nonlinear models (including many GO models) are similarly formulated across platforms: relatively easy model conversions, converters available in several cases (example: GAMS CONVERT utility)





An example from the MathOptimizer User Guide:
Surface and contour plot of randomly generated test function

Mathematica 5.1 - [UserGuide.nb *]

File Edit Cell Format Input Kernel Find Window Help

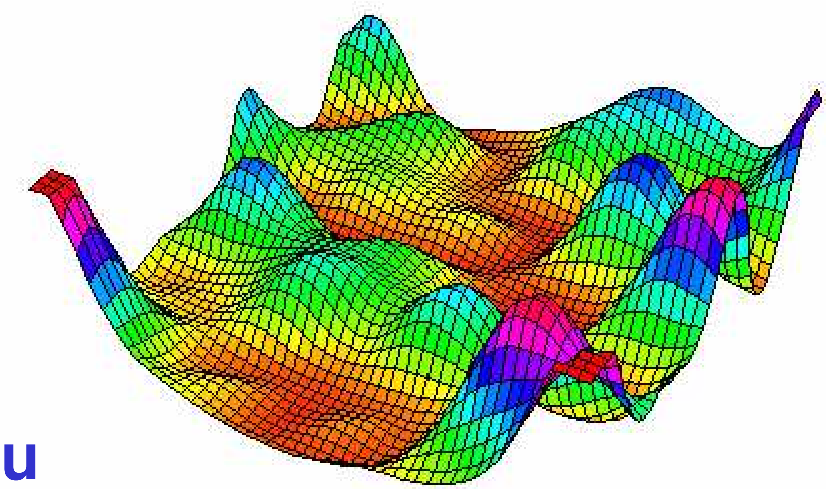
UserGuide.nb *

MathOptimizer Professional

An Advanced Modeling and Optimization System for *Mathematica*,

Using the LGO Solver Engine

User Guide



User Guide can be invoked from Mathematica's online Help menu

Mathematica 5.0 - [MOP Getting Started Example.nb *]

Getting Started with MathOptimizer Professional: Illustrative Examples

■ *Mathematica* Platform and Date

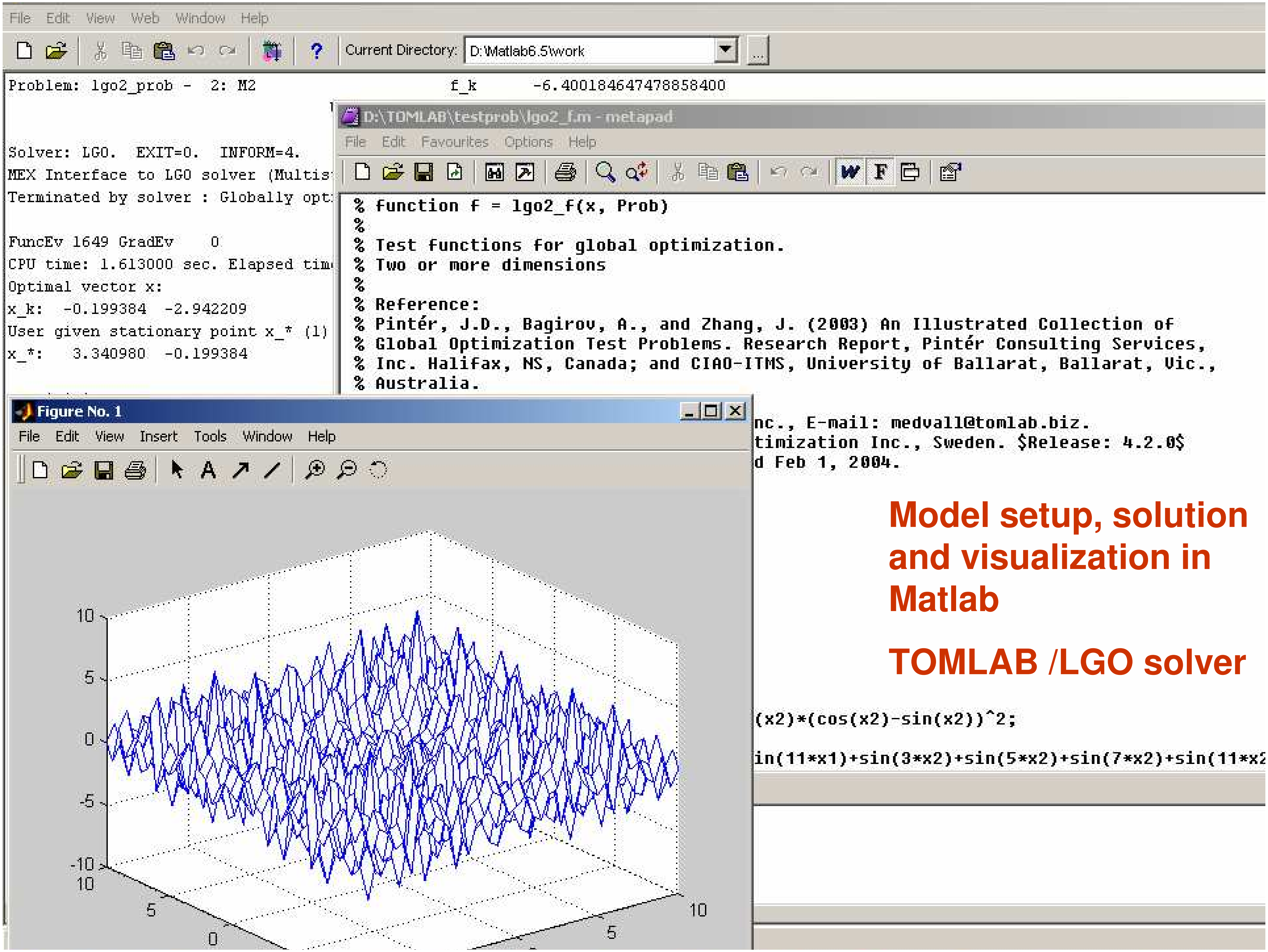
■ Activate MathOptimizer Professional

```
In[1]:= Needs["MathOptimizerPro`callLGO`"];

In[2]:= ?callLGO
```

■ A Simple One-line Example

It is straightforward to define a (small) optimization model, as illustrated by the following example.

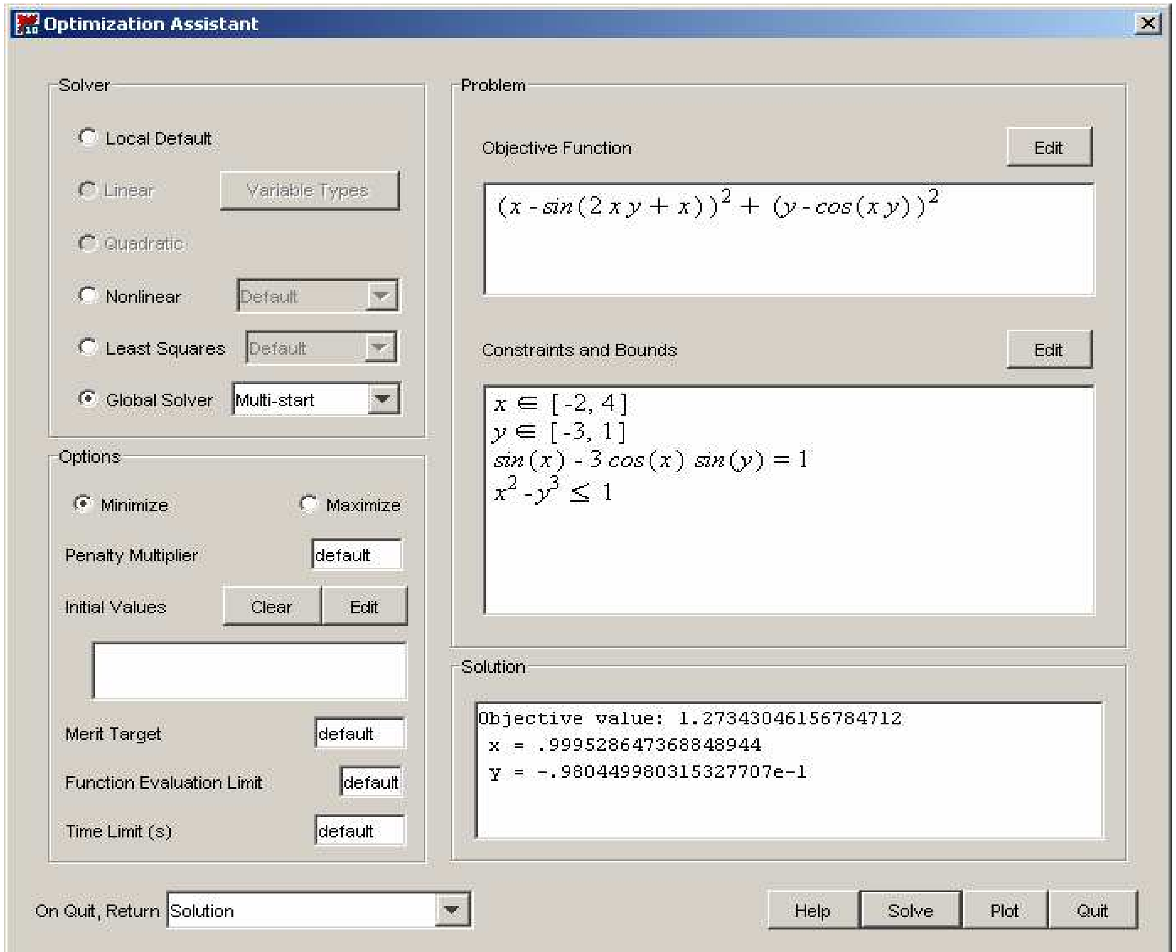
```
In[24]:= callLGO[2*x^2 + y^2, {x + y - 1 == 0, x^2 + 3*y ≤ 2},
           {{x, -2, 1, 3}, {y, -3, 2, 2}}]

Out[24]= {0.673762, {x → 0.381966, y → 0.618034}, 2.79532 × 10^-9}
```



Model setup, solution and visualization in Matlab

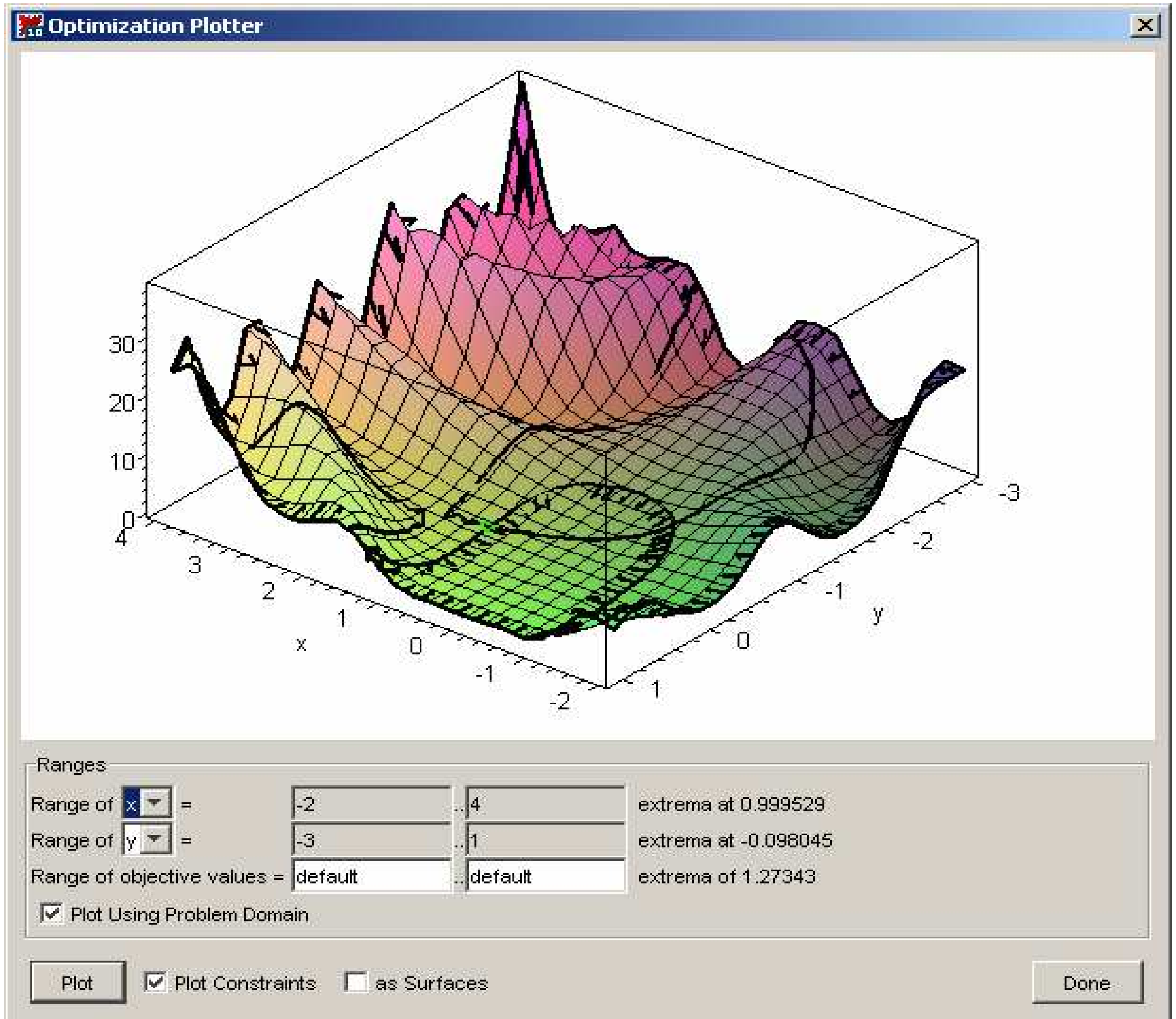
TOMLAB /LGO solver

Maple GO Toolbox: Optimization Assistant



Optimization Methods and Software (2006)

Maple GO Toolbox: Optimization Plotter



Illustrative Case Studies

A (Very) Concise Review

- Many of the actual client case studies reviewed here are based on advanced multi-disciplinary research, in addition to the optimization (solver) component
- All detailed case studies could be presented in full detail, each in a separate lecture… we shall briefly review only a selection of these
- References, demo software examples, publications, and additional details are all available upon request

Illustrative Case Studies reviewed in this talk (as time allows)

- GAMS model libraries: comparative assessment of GAMS/LGO vs. state-of-art local solvers based on hundreds of models
- A “black box” client model (code generated automatically by MathOptimizer Professional)
- Trefethen’s HDHD problem 4, solved by LGO implementations
- Systems of nonlinear equations (Maple GOT)
- Nonlinear model fitting examples (MathOptimizer, Maple GOT)
- Maxi-min experimental design (LGO stand-alone implementation)
- Non-uniform circle packings (MOP)
- Computational chemistry (potential energy) models (MOP)
- Portfolio selection, with a non-convex transfer cost (Maple GOT)

Illustrative Case Studies reviewed in this talk (as time allows)

- Solving differential equations by the shooting method (MOP)
- Data classification and visualization (MOP)
- Circuit design model (Excel PSP/LGO)
- Rocket trajectory optimization (Excel PSP/LGO)
- Industrial design model examples (MO, MOP, Maple GOT)
- Robotics design optimization (LGO stand-alone implementation)
- Laser design (LGO stand-alone implementation)
- Cancer therapy planning (LGO stand-alone implementation)
- Sonar equipment design (MathOptimizer)
- Oil field production optimization (LGO)

- In addition, thousands of standard NLP/GO and other test problems have been used to evaluate solver performance across the various modeling environments reviewed here

“Black Box” Model Received from (MOP) Client…

C:\Documents and Settings\Janos\Desktop\messages\USER_FCT.C - metapad

File Edit Favourites Options Help

```c
#include <stdlib.h>
#include <stdio.h>
#include <math.h>

int __declspec(dllexport) _stdcall USER_FCT( double x[], double fox[1], double gox[])
{
fox[0] = pow(-52.2814830080429 + 0.291083080677605*(sin(x[0])*(1.*(-1.*sin(1.813087*(0.000122738408770829 -
7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(-57.7094469266987*cos(x[0\
]) + 0.000122738408462659*cos(x[0])*cos(x[2])*x[8] + 0.999999992467641*cos(x[0])*sin(x[2])*x[8]) + sin(x[0])*(-
2.30934895009823*sin(x[0]) + cos(x[0])*(0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) + 0.0001227\
38408462659*(57.7154010070919 - 1.*sin(x[2])*x[8]))) + cos(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] -
3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(-2.30934895009823 - 1.*sin(x[0])*(-2.309\
34895009823*sin(x[0]) + cos(x[0])*(0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) + 0.000122738408462659*
(57.7154010070919 - 1.*sin(x[2])*x[8]))))) - 1.*(sin(x[0])*(2.2328632*pow(cos(x[0]),2.) + sin(x[0])*(2.2\
328632*sin(x[0]) + 0.000122738408770829*x[1] + 7.53235849379756e-9*x[6] + x[9])) + cos(1.813087*(0.000122738408770829 -
7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(2.2328632*si\
n(x[0]) + 0.000122738408770829*x[1] + 7.53235849379756e-9*x[6] + x[9] - 1.*sin(x[0])*(2.2328632*pow(cos(x[0]),2.) + sin(x
[0])*(2.2328632*sin(x[0]) + 0.000122738408770829*x[1] + 7.53235849379756e-9*x[6] + x[9]))) - 1.\
*sin(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(-
1.*cos(x[0])*x[4] - 0.000122738408770829*cos(x[0])*x[10]))) + cos(x[0])*(1.*(-1.*sin(1.813087\
*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*
(57.7094469266987*sin(x[0]) - 0.000122738408462659*cos(x[2])*sin(x[0])*x[8] - 0.999999992467641*sin(x[0])*si\
n(x[2])*x[8]) + cos(x[0])*(-2.30934895009823*sin(x[0]) + cos(x[0])*(0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) +
0.000122738408462659*(57.7154010070919 - 1.*sin(x[2])*x[8]))) + cos(1.813087*(0.000122738408\
770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(0.999999992467641*
(48.5067855663717 + cos(x[2])*x[8]) + 0.000122738408462659*(57.7154010070919 - 1.*sin(x[2])*x[8]) - 1.*co\
s(x[0])*(-2.30934895009823*sin(x[0]) + cos(x[0])*(0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) +
0.000122738408462659*(57.7154010070919 - 1.*sin(x[2])*x[8]))))) - 1.*(cos(x[0])*(2.2328632*pow(cos(x[0]),2.) +\
 sin(x[0])*(2.2328632*sin(x[0]) + 0.000122738408770829*x[1] + 7.53235849379756e-9*x[6] + x[9])) + cos(1.813087*
(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7])\
)*(2.2328632*cos(x[0]) - 1.*cos(x[0])*(2.2328632*pow(cos(x[0]),2.) + sin(x[0])*(2.2328632*sin(x[0]) + 0.000122738408770829*x
[1] + 7.53235849379756e-9*x[6] + x[9]))) - 1.*sin(1.813087*(0.000122738408770829 - 7.5323584\
9379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(sin(x[0])*x[4] + 0.000122738408770829*sin(x[0])*x
[10])))) - 0.70817848041004*(0.999991873452302*(-1.*sin(1.813087*(0.000122738408770829 - 7.5\
3235849379756e-9*x[3] - 3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(2.30934895009823*cos(x[0]) +
48.5138690974646*sin(x[0]) + 0.999999992467641*cos(x[2])*sin(x[0])*x[8] - 0.000122738408462659*sin(x[0])*s\
in(x[2])*x[8]) + cos(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] -
9.45607074651404e-18*x[7]))*(0.000122738408462659*(48.5067855663717 + cos(x[2])*x[8]) + 0.999999992467641*(\
-57.7154010070919 + sin(x[2])*x[8])) + sin(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13
*x[5] - 9.45607074651404e-18*x[7]))*(-0.000122738408770829*cos(x[0])*x[1] - 7.53235849379756e\
-9*cos(x[0])*x[6] - 1.*cos(x[0])*x[9]) - 1.*cos(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] -
3.08169898606717e-13*x[5] - 9.45607074651404e-18*x[7]))*(-1.*x[4] - 0.000122738408770829*x[10])) + 0.0040315\
0460189537*(-1.*cos(x[0])*(1.*(-1.*sin(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5]
- 9.45607074651404e-18*x[7]))*(-57.7094469266987*cos(x[0]) + 0.000122738408462659*cos(x[0])\
*cos(x[2])*x[8] + 0.999999992467641*cos(x[0])*sin(x[2])*x[8]) + sin(x[0])*(-2.30934895009823*sin(x[0]) + cos(x[0])*
(0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) + 0.000122738408462659*(57.7154010070919 - 1.*\
sin(x[2])*x[8]))) + cos(1.813087*(0.000122738408770829 - 7.53235849379756e-9*x[3] - 3.08169898606717e-13*x[5] -
9.45607074651404e-18*x[7]))*(-2.30934895009823 - 1.*sin(x[0])*(-2.30934895009823*sin(x[0]) + cos(x[0])*(\
0.999999992467641*(48.5067855663717 + cos(x[2])*x[8]) + 0.000122738408462659*(57.7154010070919 - 1.*sin(x[2])*x[8])))) - 1.
*(sin(x[0])*(2.2328632*pow(cos(x[0]),2.) + sin(x[0])*(2.2328632*sin(x[0]) + 0.00012273840877\
```

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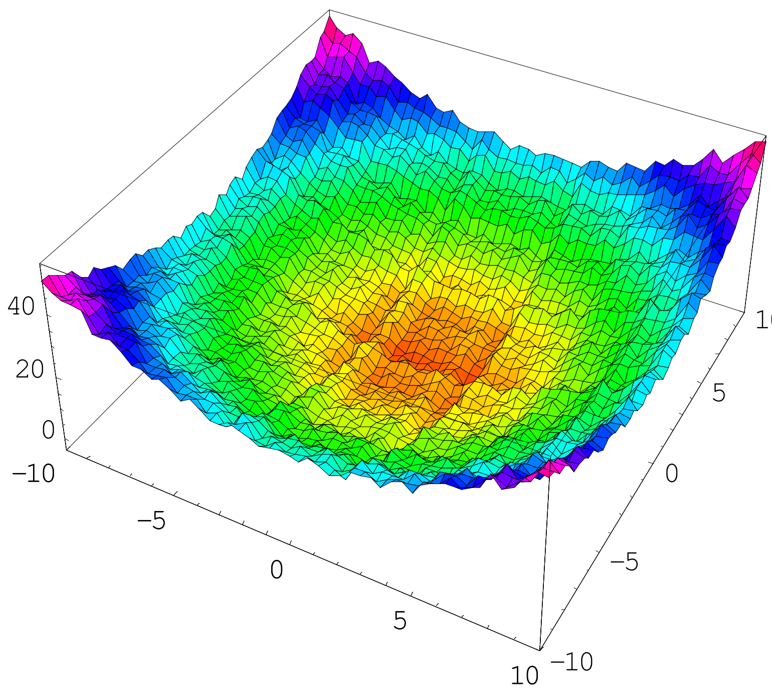
Trefethen's HDHD Challenge, Problem 4 (SIAM News, 2002)

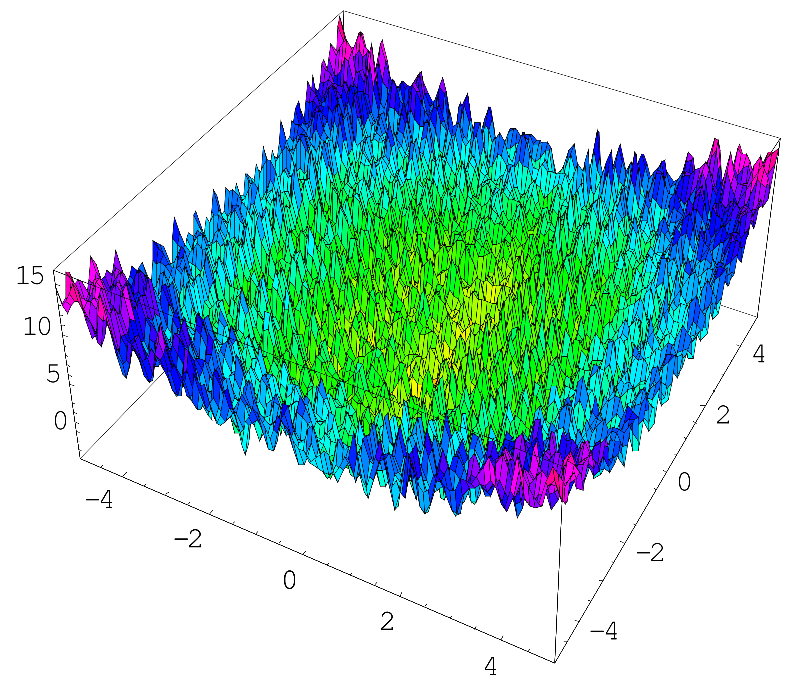
Find the global minimum of the two-variable real function f(x,y) defined below as

$\frac{1}{4}$ [redacted] x [redacted] y [redacted] x [redacted] sin [redacted] $x + y$ [redacted] ã^{y} [redacted] sin [redacted]

sin [redacted]

No explicit variable bounds are provided.



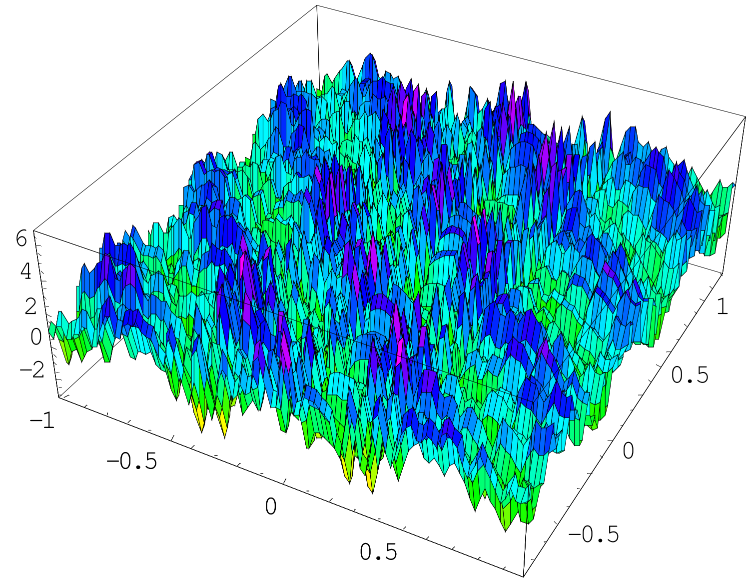


HDHD Challenge, Problem 4 (cont'd)

• This model has been numerically solved by LGO, MathOptimizer, MathOptimizer Pro, TOMLAB /LGO, and the Maple GOT

• The solution found is identical to more than 10 decimals to the announced solution (the latter was originally based on an enormous grid sampling effort combined with local search)

x*~ (-0.024627…, 0.211789…)
f*~-3.30687…
Close-up picture near to global solution: still looks difficult...

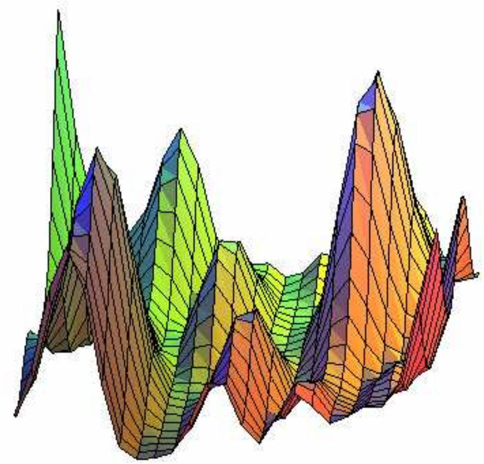


Solving Systems of Nonlinear Equations

Optimization Methods and Software (2006)

Equivalent GO model formulation (assuming that solution exists)

F(x)=0 Û min ||F(x)||



Error function plot

Maple GO Toolbox Example

x-y+sin(2*x)-cos(y)=0
4*x-exp(-y)+5*sin(6*x-y)+3*cos(3*y)=0

A numerical solution:

x = 0.0147589760525313926, y = -0.712474169476650099

l_2-norm error ~ 1.22136735435643598 × 10^{-16}

Note: there could be other solutions; systematic search is possible

Nonlinear Model Calibration in Presence of Noise

An example model (in *Mathematica* notation):

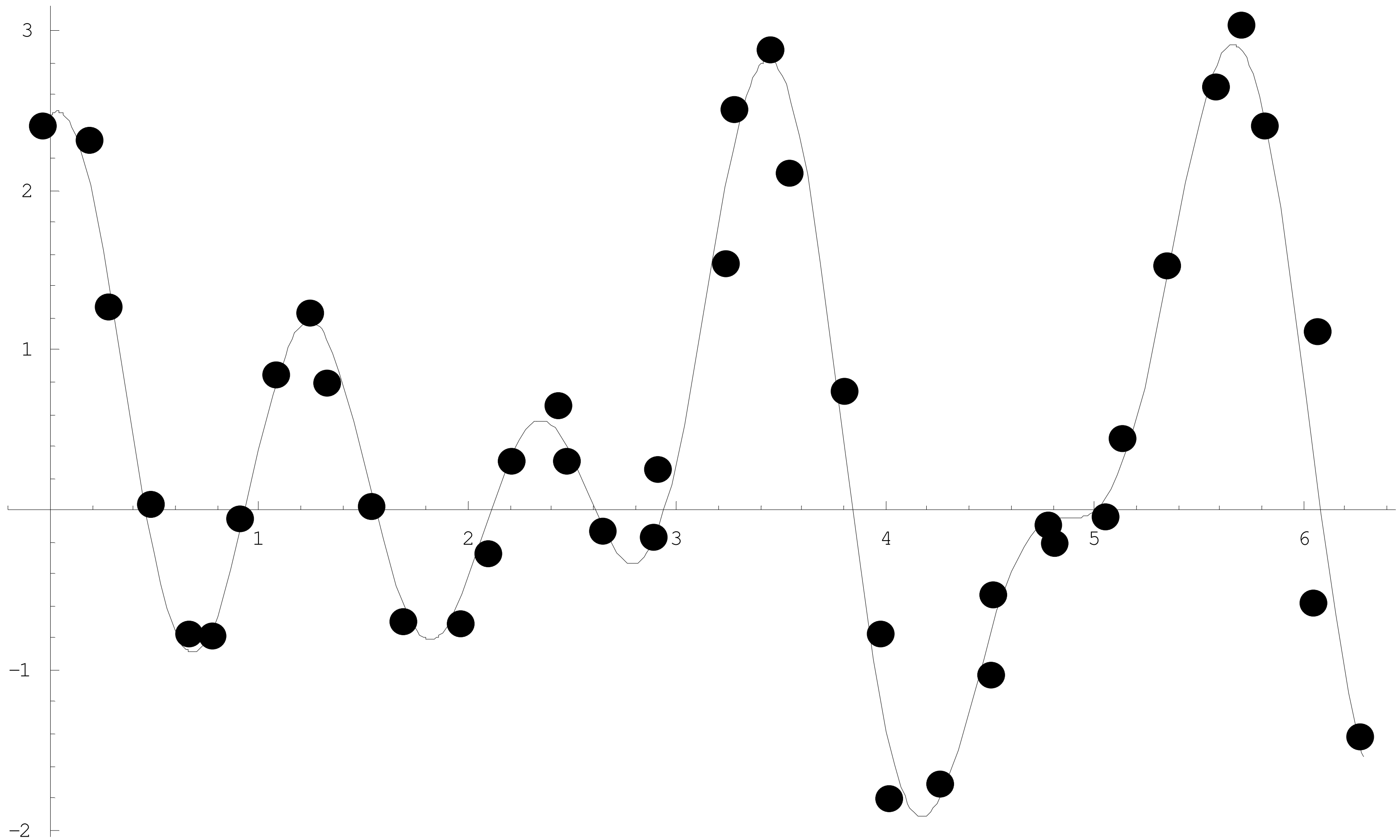
a+Sin[b*(Pi*t)+c]+Cos[d*(3Pi*t)+e]+Sin[f*(5Pi*t)+g]+ξ

The parameters a,b,c,d,e,f,g are randomly generated from interval [0,1]; ξ is a stochastic noise term from *U*[-0.1,0.1]

Subsequently, the optimal parameterization is recovered by using MathOptimizer: superior results, in comparison with Mathematica's corresponding built-in local solver functionality

***Optimization Methods and Software* (2003)**

Calibration of Nonlinear Model in Presence of Noise (cont.)



a+Sin[b*(Pi*t)+c]+Cos[d*(3Pi*t)+e]+Sin[f*(5Pi*t)+g] +ξ

Arrhenius Probe Model Calibration

Credits: Grigoris Pantoleontos et al., Chemical Engineering Department, Aristotle University of Thessaloniki, Greece

ln(y) = A-Ea /RT   Arrhenius formula

temperature dependence of reaction rate coefficient y

A multi-component version of the formula is

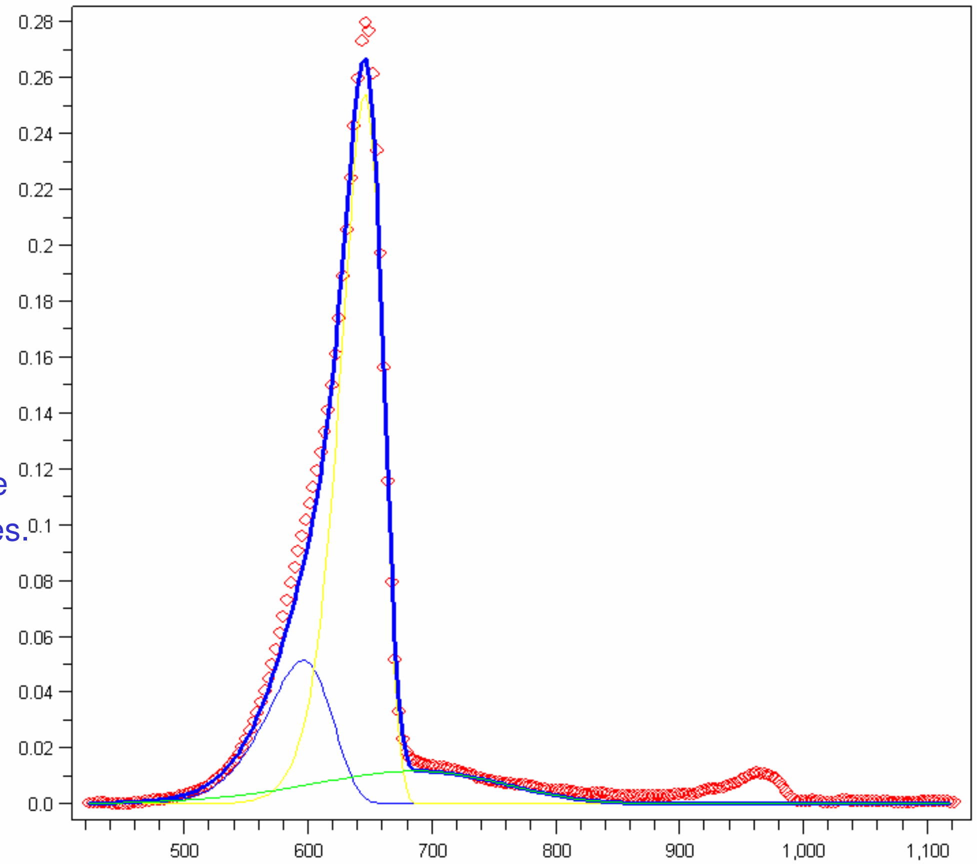
$$y_i = c_i A_i \exp(-E_i/(RTemp[j])) \cdot (1 - R_i[j])$$

Here $R_i[j]$ is calculated from another fairly complicated expression.

The study by GP et al. is aimed at the determination of the parameters c_i, A_i and E_i i=1,2,3 by comparing the computed model output values to the experimental ones.

The figure shows the initially given data points (red circles), the component curves (green, blue, yellow), and the resulting curve (bold blue).

The solution of this computationally intensive example (9 variables to calibrate, very large search region, hundreds of data points, rather difficult interim model functions to compute) took about an hour on a desktop PC.



Maple 10 - I:\Documents and Settings\Janos Pinter\Desktop\Maple materials and info\Suspension model calibration\SuspensionOptimization.mw - [Server 2]

File Edit View Insert Format Table Plot Spreadsheet Sketch Tools Window Help

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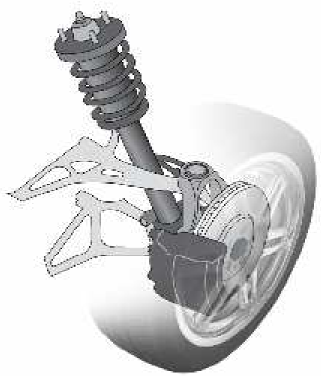
# Suspension System Tuning **Calculation Sheet** *© Maplesoft, a division of Waterloo Maple Inc., 2005* *Added noted by János D. Pintér* *Pintér Consulting Services, Halifax, NS, Canada, 2006*	**Contract:**	685943/N3	Maplesoft command the brilliance
	Customer:	XYZ Engineering, Inc	



Summary

In this example application, we consider the problem of designing a suspension system that exhibits a specified behavior in response to a bump in the road. The problem variables are the spring constant k and the damper constant b. Given the mass of the car on each wheel, m, and the expected amplitude of a typical bump, we have to find values for k and b to generate a system model response that matches the actual (measured) response as close as possible.

The above problem-type can be cast in an optimization model framework: the model objective function is the squared error between the desired and actual response as a function of k and b measured over a discrete set of time moments. After deriving the actual response by solving the system's differential equation, we use numerical optimization to find the values of k and b that minimize the error function.

Due to the typical multi-modal structure of the associated (nonlinear model calibration) error function, the Global Optimization Toolbox is needed to derive the best possible fit to the given actual data set.

▶ Global Optimization Basics

▶ The Global Optimization Toolbox

▶ An Example: Suspension System Model Selection and Target Response

▶ Deriving the Actual Response

▶ Measuring the Error Between the Target and Actual Responses

▶ Minimizing the Error with the Global Optimization Toolbox

▶ Verification of the Result

▶ Illustrative References

Ready | Memory: 0.37M Time: - Text Mode

http://www.maplesoft.com/applications/app_center_view.aspx?AID=1984

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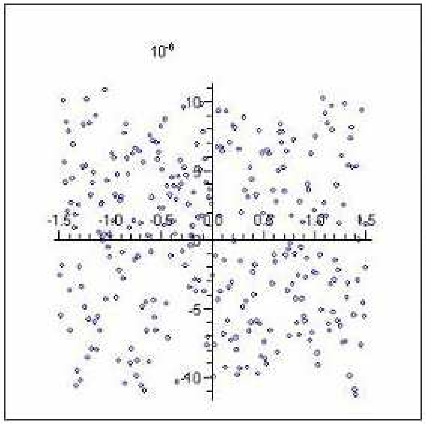
Aspherical Lens Surface Identification - Non-Linear Fitting with the Global Optimization Toolbox



Member Rating:	(rate this application)
Author:	Maplesoft Cybernet Systems Co., Ltd .
Application Type:	Maple Worksheet
Publish date:	August, 2006
Related Products:	Maple 10 Global Optimization
Language:	English
Related Link:	http://www.maplesoft.com/products/toolboxes/glo...
Related Book:	Applied Nonlinear Optimization in Modeling Environments Global Optimization : Scientific and Engineering Case Studies Global Optimization in Action : Continuous and Lipschitz Optimization: Algorithms, Implementations and Applications

Options:

- View HTML version
- Download Maple Code (.zip, 67.9kb)
- E-mail to a colleague

Abstract:

In this Application Demonstration, we investigate Aspherical Lenses and apply non-linear fitting to obtain an accurate representation of the given data in the form of a function, using the GlobalOptimization Toolbox for Maple.

Related Application Categories

Mathematics : Operations Research
Operations Research : Regression
Science : Physics
Statistics & Data Analysis : Regression

Member rating: not rated *(min. 5 ratings required)*
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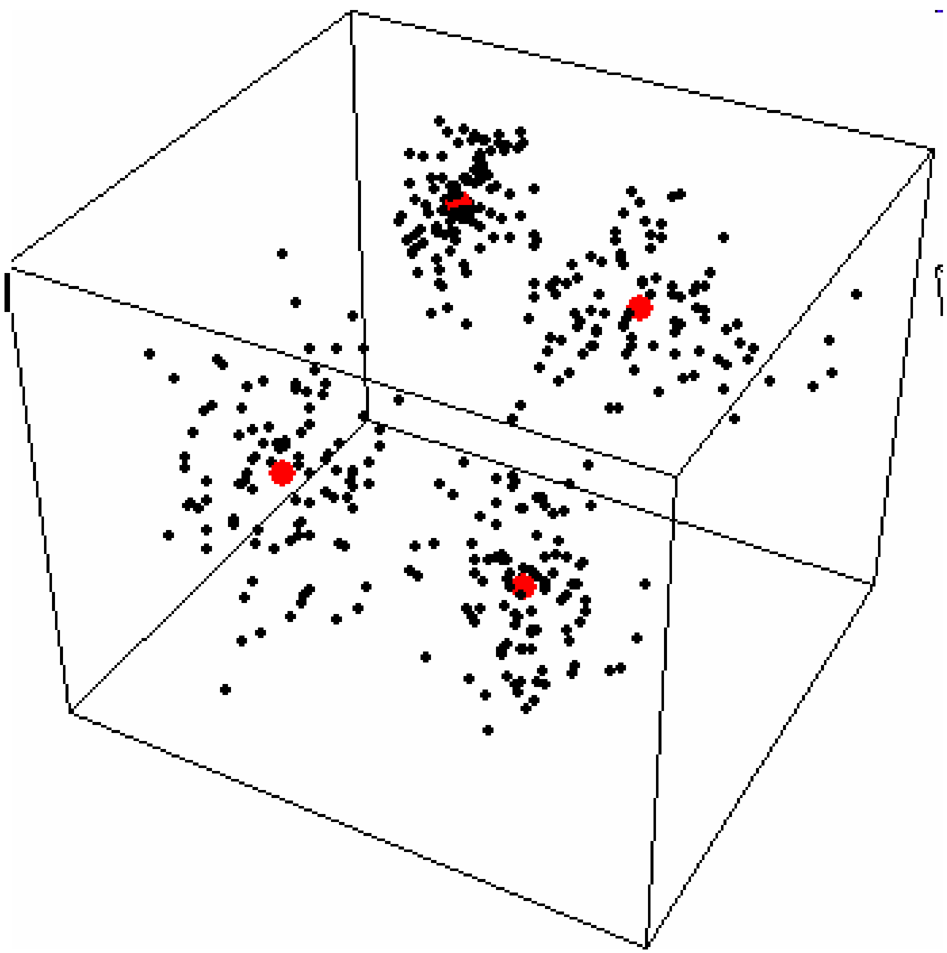
Data Classification (Clustering) by Global Optimization

Example developed and solved using MathOptimizer Professional



Maxi-Min and Related Point Arrangements

In a large variety of applications, one is interested in the 'best possible covering' arrangement of points in a set

- numerical approximation methods
- design of experiments for expensive 'black box' models
- potential energy models (physics, chemistry,…)
- crystallography, viral morphology,...

For illustration, consider a maxi-min model instance

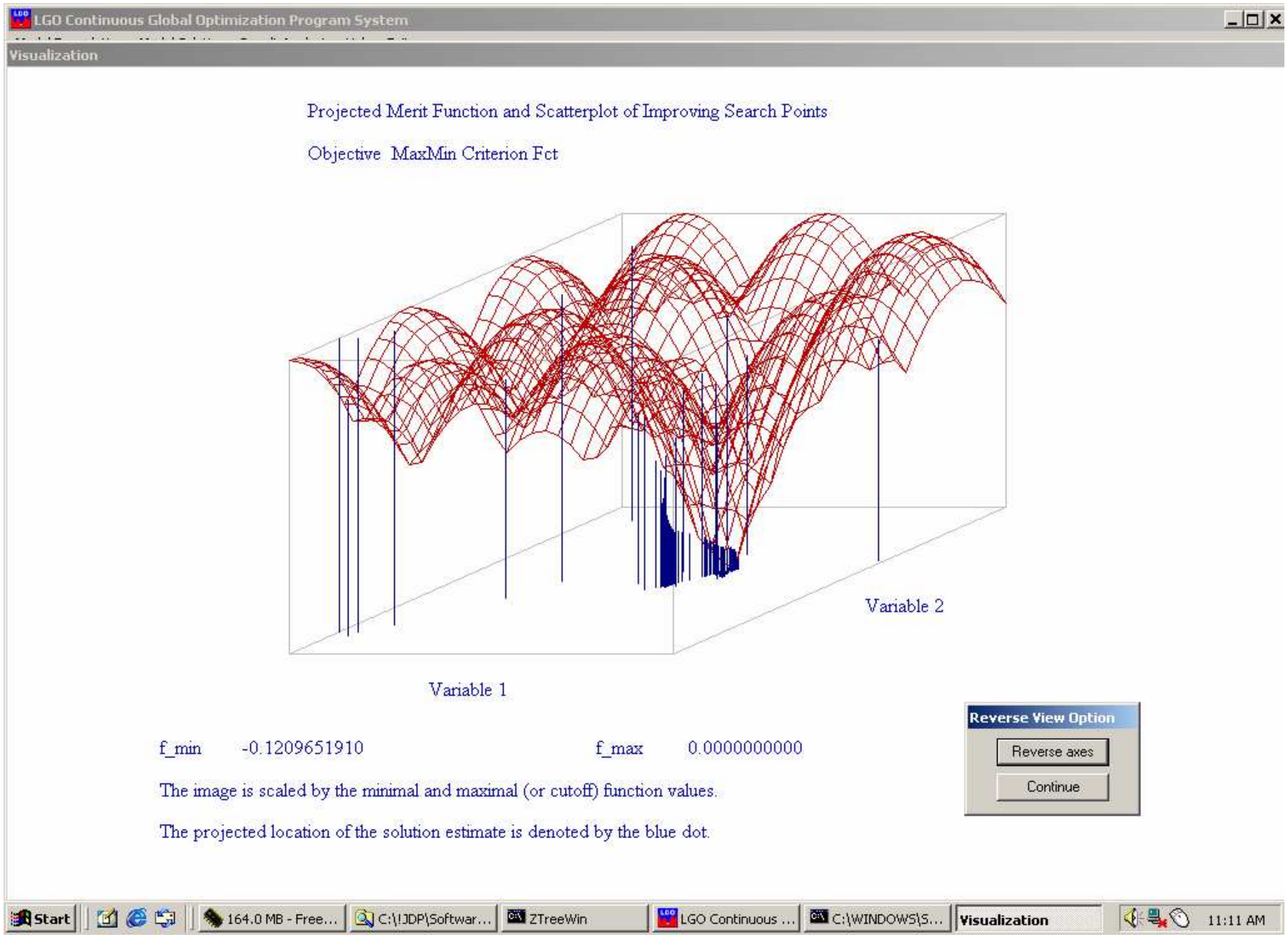
$$\max_{\{x_i\}} \{ \min_{1 \le i<k \le m} ||x_i - x_k|| \} \qquad xl \le x_i \le xu \qquad x_i \in R^d \quad i=1,\ldots,m$$

Additional restrictions, alternative feasible sets, and other quality criteria can also be considered

Permutations   lexicographic point arrangements

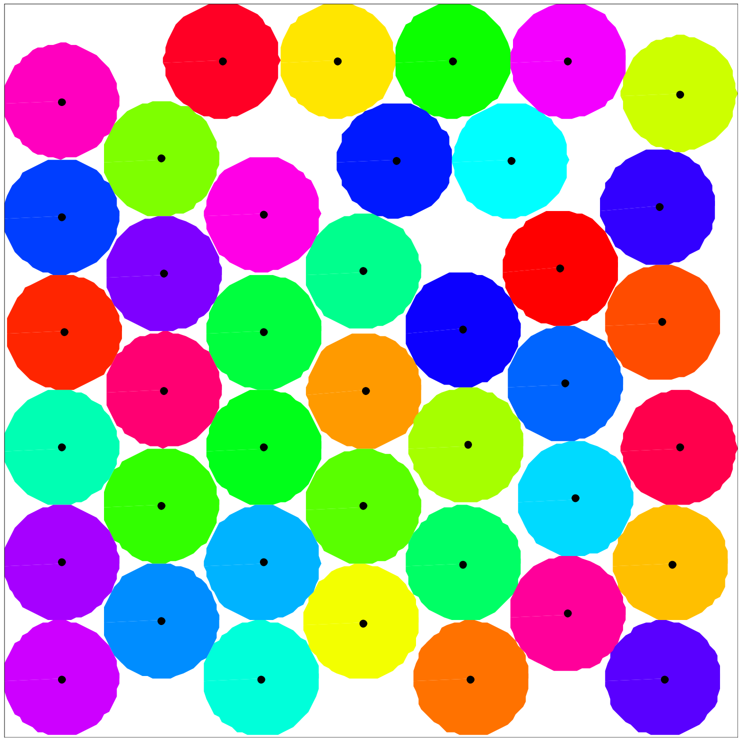
Non-convex models

MaxiMin Point Arrangement Problem



LGO IDE: model visualization (m=13, d=2)

Packing Uniform Size Circles in the Unit Square



Example: 40 circles; optimized radius of circles r~0.787391…
Solution time using MOP: less than 5 minutes (3 GHz PC)
No postulated structural info is exploited: LGO used ‘blindly’

Non-Uniform Size Circle Packings in a Circle

In this example, we study the packing of different size circles in an embedding circle. Since this model formulation typically has infinitely many solutions *per se*, we will additionally try to bring the circles as close together as possible.

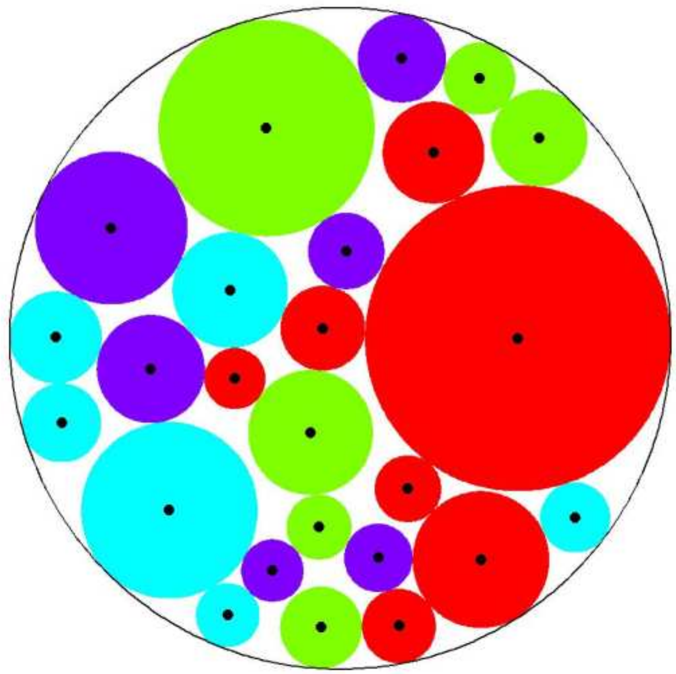
The primary objective (obj1) is to find the circumscribed circle with the smallest radius; the secondary objective (obj2) brings the circles close together (min. average distance among all circle centers).

A scaled linear combination of these two objectives is used. Note that alternative formulations are also possible, and that rotational symmetries of solutions can also be avoided (by added constraints), thereby making the solution of a specific model formulation essentially unique.
Applications: wires packed together in a cable, dashboard design…

***Mathematica in Education and Research* (2005), *The Mathematica Journal* (2006) Co-author: Frank J. Kampas**

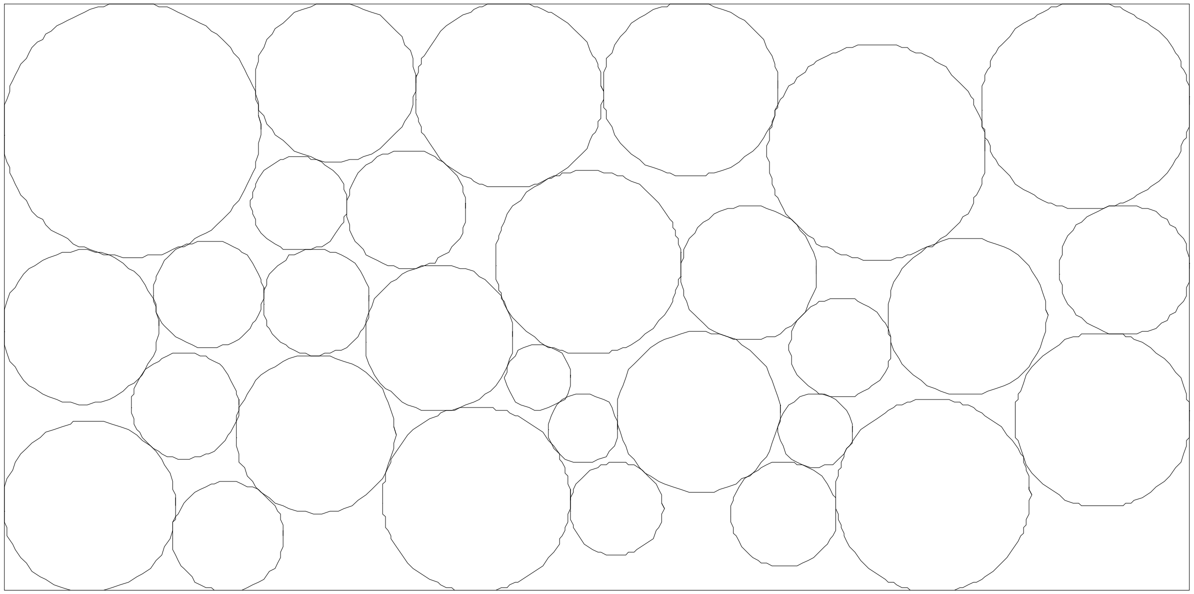
Non-Uniform Size Circle Packings

Optimized Circle Packing for n=25



Embedding circle contains circles with radii $r_k = k^{-0.5}$ k=1,…,25

General Circle Packings in Minimal Volume (Length) Container



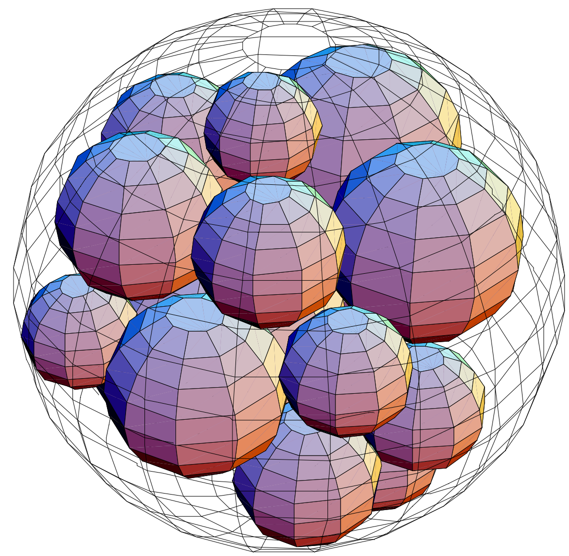
Example: given 30 circles with radii below ; given height of container; find minimal container width

rlist = {1.275, 1.67, 2.05, 1.739, 1.399, 1.18, 0.564, 1.374, 1.237, 0.845, 1.484, 0.868, 0.807, 1.551, 1.274, 0.855, 1.493, 1.281, 1.491, 0.747, 1.085, 1.044, 0.955, 1.404, 1.292, 0.853, 0.76, 0.527, 0.592, 0.887};
best known radius 17.291; MOP default option based radius 18.915 in ~ 20 secs; relative quality ~ 91%
Further structure based refinements possible and recommended

See Pintér and Kampas (2005), Castillo, Kampas, and Pintér (2007), Kampas and Pintér (2006)

Sphere Packings in Optimized Sphere

Given a collection of spheres, find the minimal size sphere that includes all of these, in a non-overlapping arrangement



Example: 15 spheres with radii $r_i=i^{-1/3}$ solved numerically by MOP
Radius of embedding sphere: ~1.96308, 1.5 sec runtime (vs. ~10 min when using the built-in *Mathematica* function NMinimize)

More details: Frank Kampas and JDP talk + several articles
Joint work also with Ignacio Castillo on industrial applications

Potential Energy Models

Point arrangements on the surface of unit sphere

$x_i=(x_{i1},x_{i2},x_{i3})$ — $||x_i||=1$

$x(m)=\{x_1,\ldots,x_m\}$ — m-tuple (point configuration)

$d_{jk}=d(x_j,x_k)\ 1\le j<k\le m$ — Euclidean distance

Model versions considered

$\max \sum_{1\le j<k\le m} \log(d_{jk})$ — Fekete (log-potential)

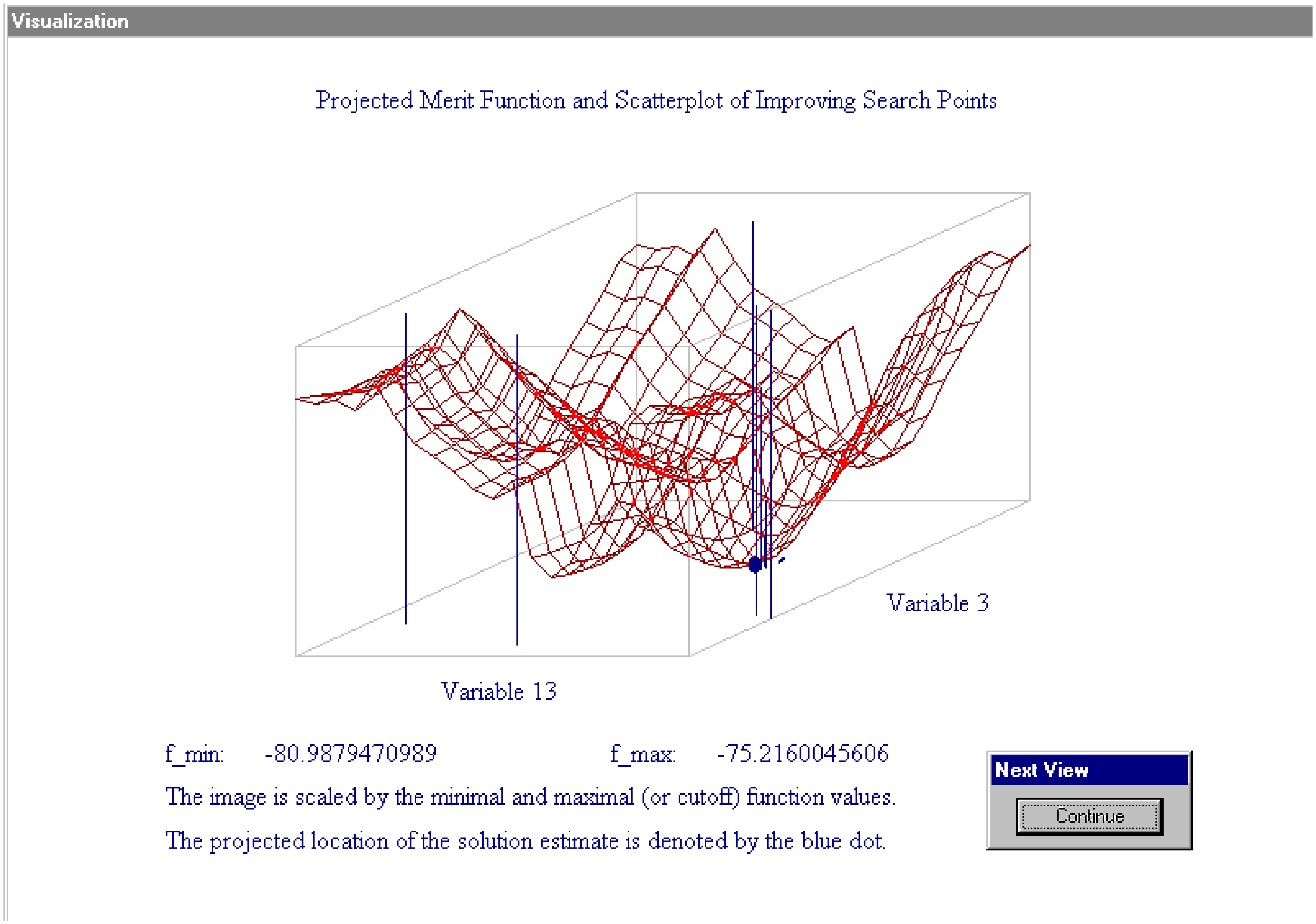
$\min \sum_{1\le j<k\le m} 1/d_{jk}\ \ (d_{jk}>0)$ — Coulomb-Fekete

$\max \sum_{1\le j<k\le m} d_{jk}^{\alpha}$ — Power sum, $0<\alpha<2$

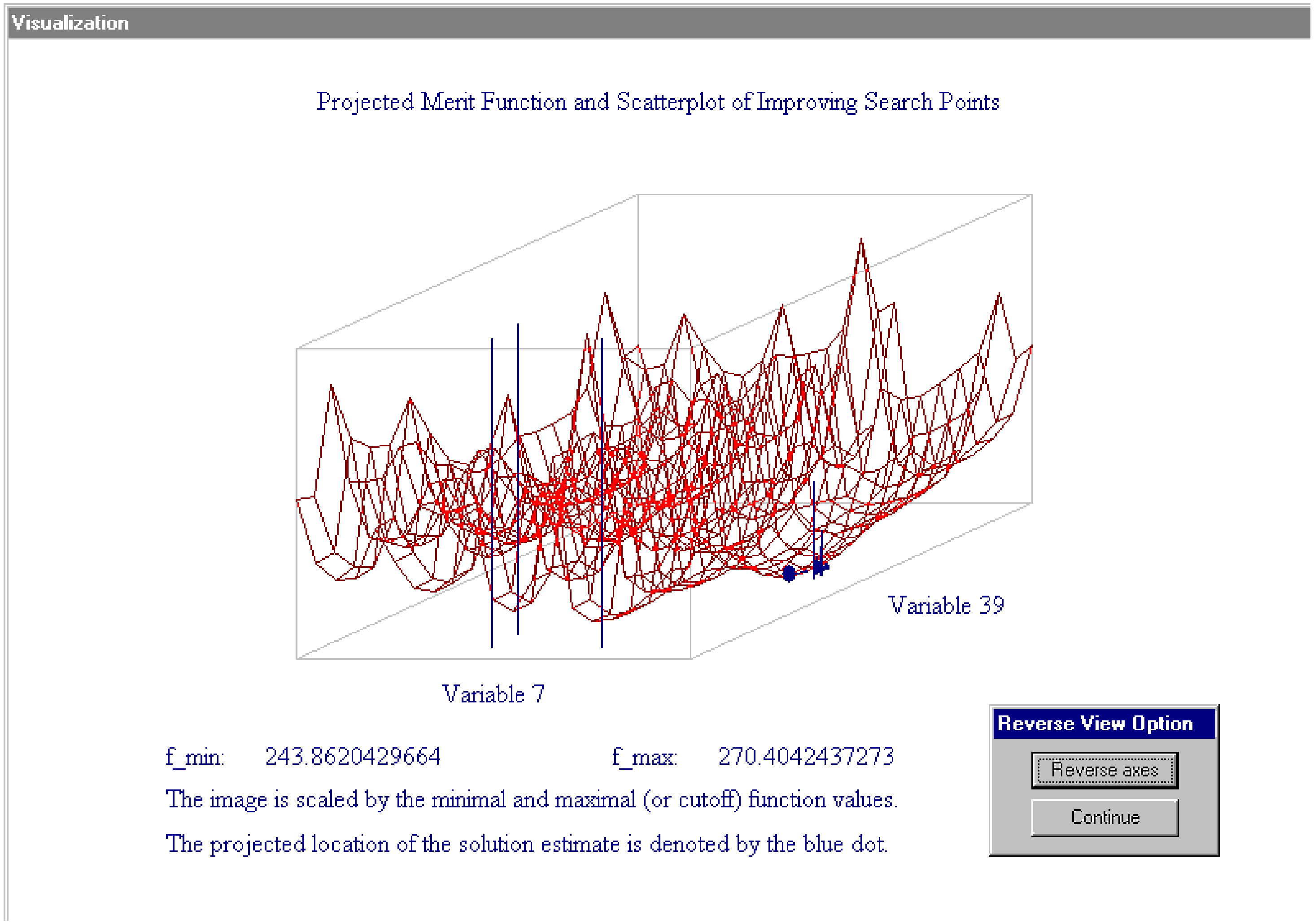
$\max \{\min_{1\le j<k\le m} d_{jk}\}$ — Tammes (hard sphere)

In all cases, the objective function is multi-extremal;
GO (+ expert knowledge) is a valid solution approach
Applications: math, physics, chemistry, biology,...

Elliptic Fekete model (*m*=25 points)



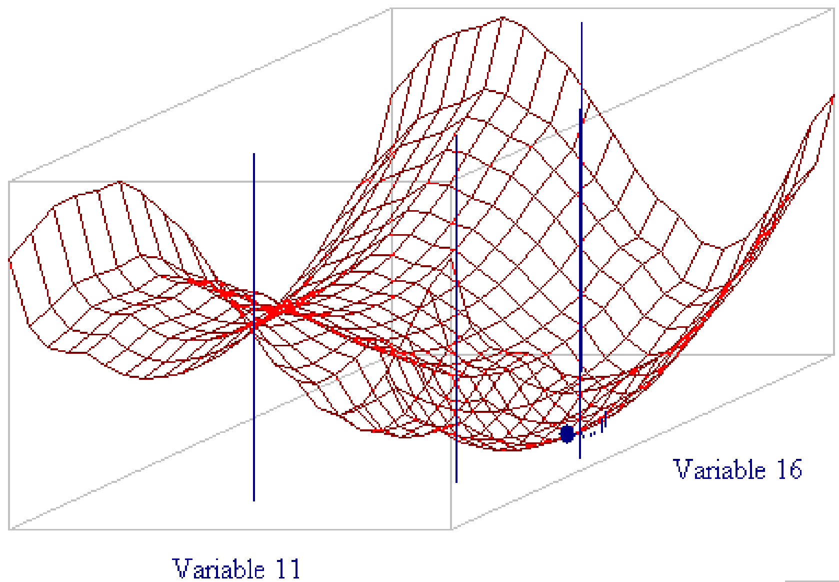
Coulomb-Fekete model (*m*=25 points)



Powersum model (*m*=25 points)

Visualization

Projected Merit Function and Scatterplot of Improving Search Points



f_min: -414.6232862986 f_max: -411.0017200558

The image is scaled by the minimal and maximal (or cutoff) function values.

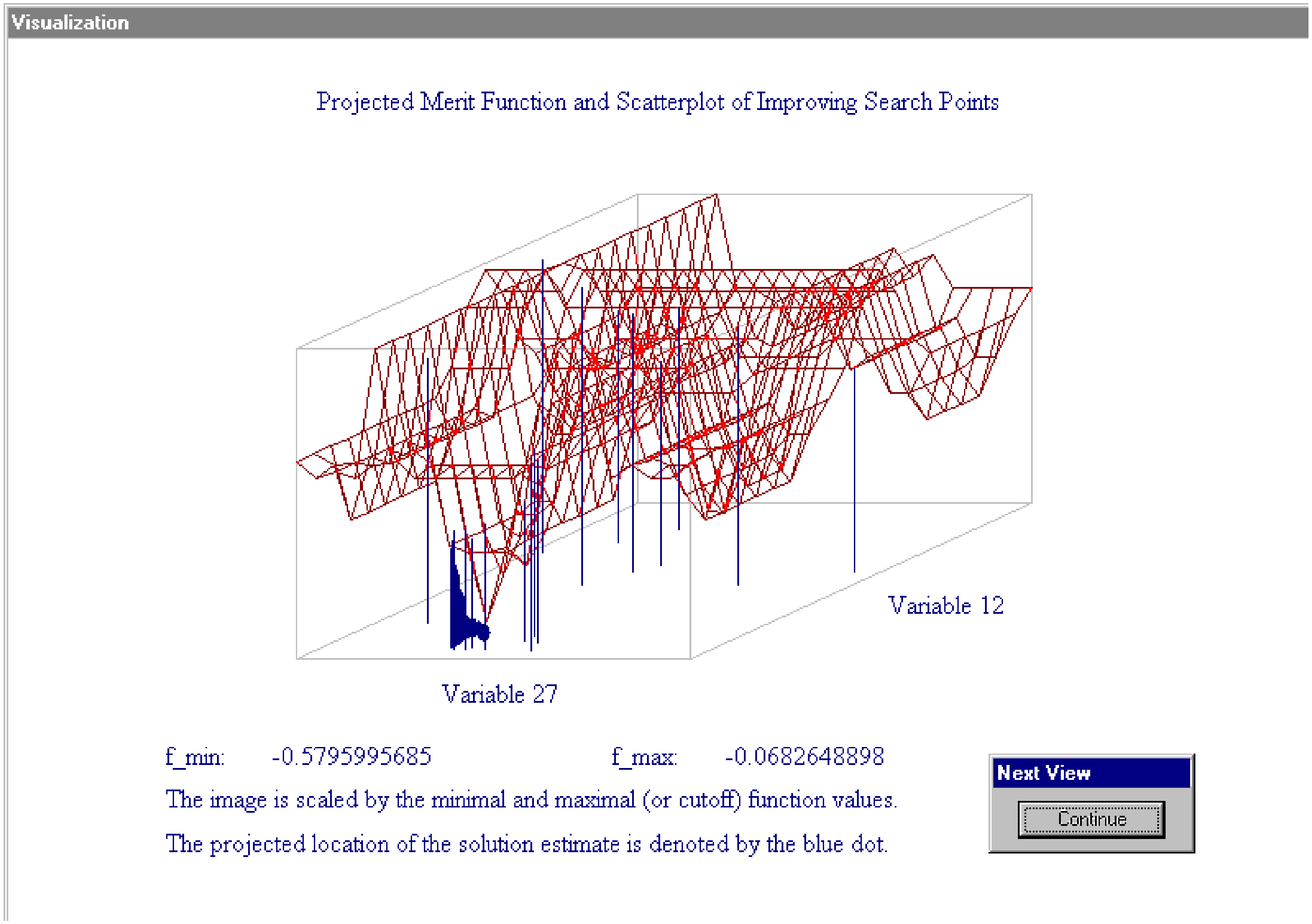
The projected location of the solution estimate is denoted by the blue dot.

Reverse View Option

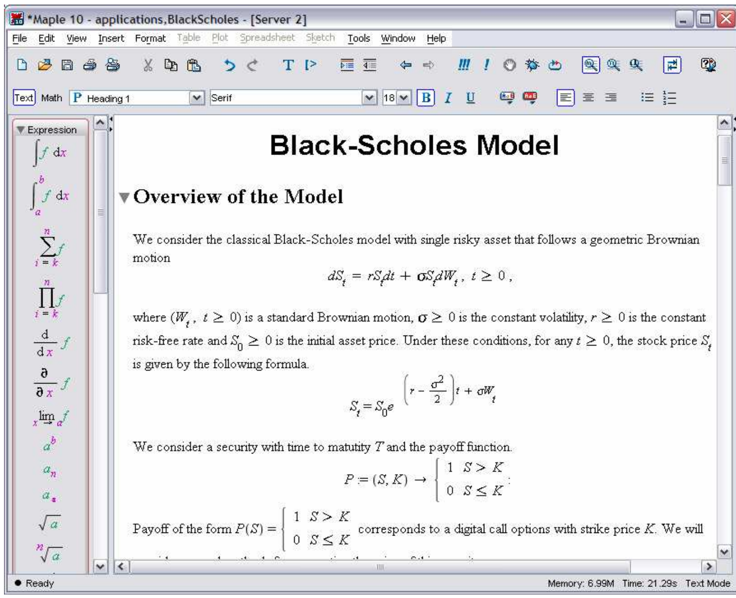
Reverse axes

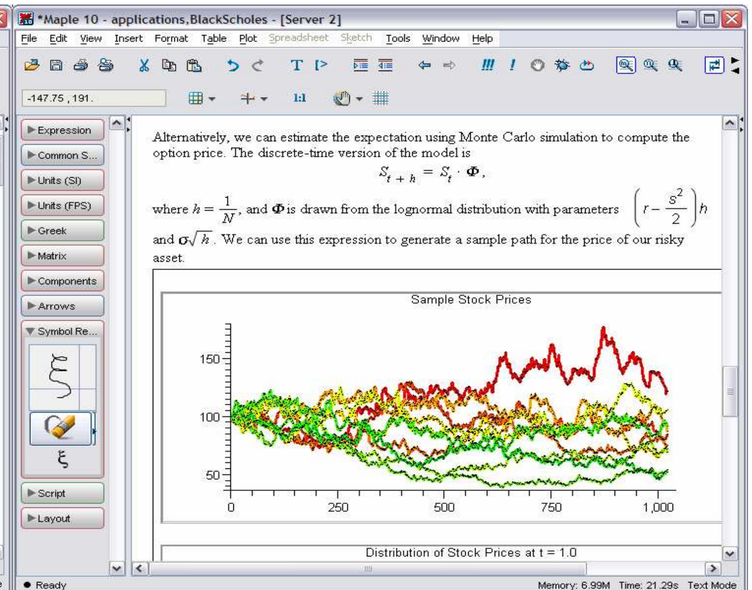
Continue

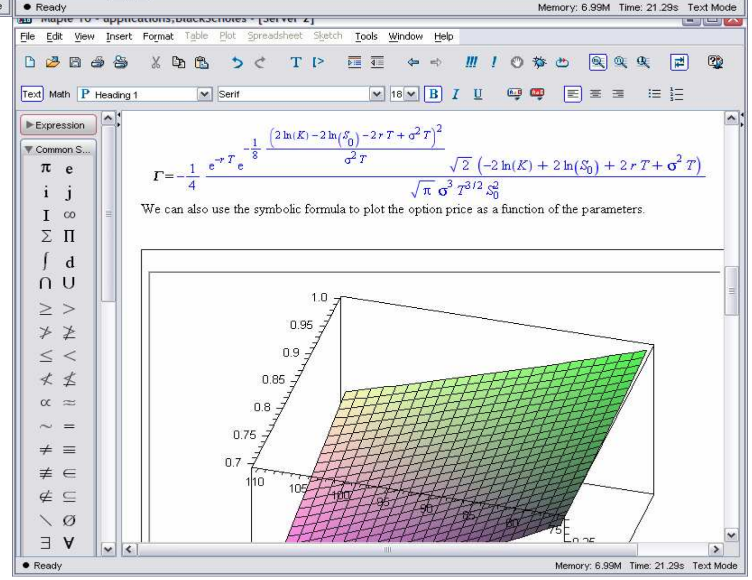
Tammes model (*m*=25 points)



Financial Modeling and Optimization





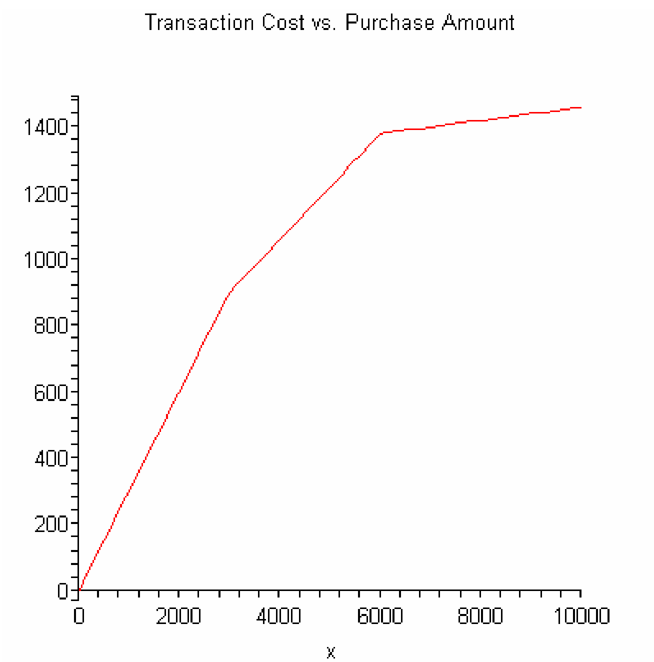


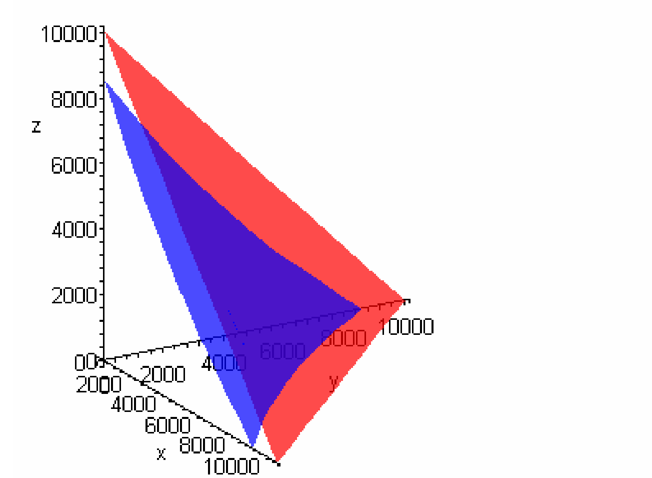
Example:
Model development, solution, and visualization in Maple (Castillo, Lee, Pintér, 2006)

Portfolio Optimization with Transaction Costs

Objective:	**minimize portfolio variance; Q cov. matrix**	$x^T Q x$
Constraints:	**expected return (ER)**	$x^T r \geq ER$
	asset allocation (of capital C)	$\Sigma x_i + \Sigma_i t(x_i) \leq C$

Note: other considerations may (will) make model more complex… GOT can be applied to such more realistic models

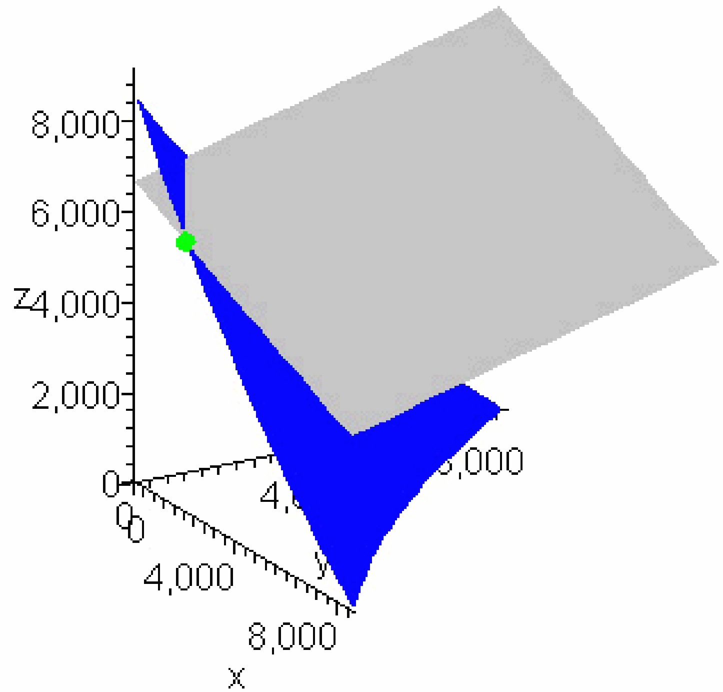




Credits: Jason Schattman, Maplesoft Inc., Waterloo, ON, Canada

Portfolio Optimization under Concave Transaction Costs

(continued)



The figure shows the location of the optimal budget allocation point (in green) on the boundary of the feasible region

The surfaces representing the active budget constraint (blue) and the growth constraint (grey) are also shown (recall KKT theory)

Castillo-Lee-Pintér, Integrated Software Tools for the OR/MS Classroom, *AlgOR* (2007)

Supply Chain Management: Reliability Optimization

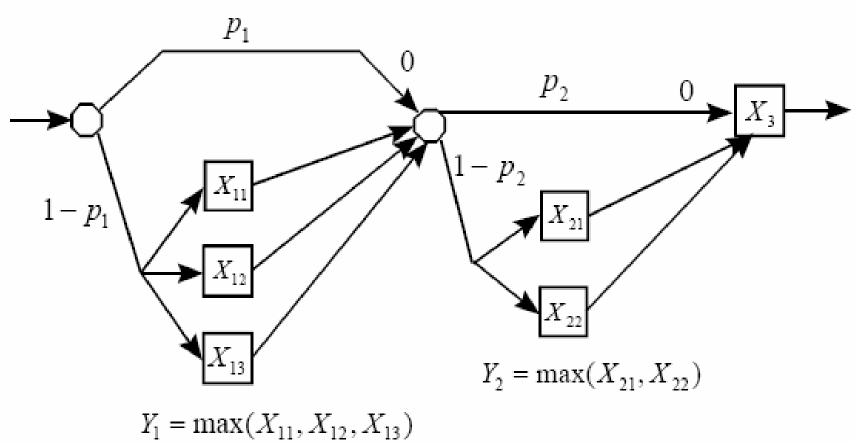


Figure 8: A three-stage assembly-type supply chain. In the first stage, if inventory is not available three components must be ordered from outside suppliers with different leadtimes. In the second stage, when inventory is unavailable, two components must be ordered from suppliers with different leadtime. The last stage always lasts a random length of time and does not require outside components.

Cited from Hum and Parlar (2006); numerical example in Maple e-book

Solving a System of ODEs by the 'Shooting Method'

The SM consists of adjusting the initial conditions of the solution until the boundary conditions are met. Unless the initial conditions are very close to the correct value, singularities are frequently encountered.

Therefore one can use a finite difference approach and solve the resulting system of equations with *MathOptimizer Professional*. Then, based on the initial condition values found, one can find a more precise solution by the SM.

Note: the model shown is received from a user (confidential background).

Tech details in

MOP User Guide

The governing equations

$$\frac{d^2S}{dw^2}+\frac{2}{w}\frac{dS}{dw}=\frac{\Phi_1 S\,C}{(S+1)(C+1)}+\frac{\Phi_2 S\,Z}{(S+1)(C+1)(Z+1)} \qquad 6.2.1)$$

$$\frac{d^2Z}{dw^2}+\frac{2}{w}\frac{dZ}{dw}=-\frac{\Phi_5 H\,C}{(H+1)(C+\alpha)}+\frac{\Phi_4 S\,Z}{(S+1)(C+1)(Z+1)} \qquad 6.2.2)$$

$$\frac{d^2C}{dw^2}+\frac{2}{w}\frac{dC}{dw}=\frac{\Phi_6 S\,C}{(S+1)(C+1)}+\frac{\Phi_7 HC}{(H+1)(C+\alpha)} \qquad (6.2.3)$$

$$\frac{d^2H}{dw^2}+\frac{2}{w}\frac{dH}{dw}=\frac{\Phi_3 H\,C}{(H+1)(C+\alpha)} \qquad (6.2.4)$$

Boundary conditions

$$\left.\frac{dS}{dw}\right|_{w\longrightarrow 0}=0,\quad \left.\frac{dS}{dw}\right|_{w=1}=Sh_s(S_b-S) \qquad \left.\frac{dZ}{dw}\right|_{w\longrightarrow 0}=0,\quad \left.\frac{dZ}{dw}\right|_{w=1}=Sh_z(Z_b-Z)$$

$$\left.\frac{dH}{dw}\right|_{w\longrightarrow 0}=0,\quad \left.\frac{dH}{dw}\right|_{w=1}=Sh_H(H_b-H) \qquad \left.\frac{dC}{dw}\right|_{w\longrightarrow 0}=0,\quad \left.\frac{dC}{dw}\right|_{w=1}=Sh_C(C_b-C)$$

The parameters of the system are given in table (6.1) & table (6.2) [42].

Table (6.1)

sh_s	15.45969	S_b	12.5
sh_z	13.16323	Z_b	1
sh_H	12.5708	H_b	1.5
sh_c	11.24284	C_b	95

Table (6.2)

Φ_1	Φ_2	Φ_3	Φ_4	Φ_5	Φ_6	Φ_7
85.103486	72.337963	59.83288	82.6568	103.04552	2.945e+03	5.0336+03

Circuit Design NLEQ System

Solved by Excel/LGO

Microsoft Excel - CIRCUITD.XLS

objective =con_1^2+con_2^2+con_3^2+con_4^2+factor*con_5^2+factor*con_6^2+con_7^2+factor*con_8^2+con_9^2

Model Variables: LBnd, NomValue, UBnd

Var. Index	x_lb	Variable x	x_ub
1	0	1	10
2	0	2	10
3	0	3	10
4	0	4	10
5	0	5	10
6	0	6	10
7	0	7	10
8	0	8	10
9	0	9	10

767671534	Objective Function: Minimize the total (scaled, l_2 norm) error of equations
	Constraints C1...C9 express physyical system equilibrium conditions
12.062365	C1: prod1*(exp(x5*(g11-g31*x7*rthou-g51*x8*rthou))-one)-g51+g41*x2+cad1 = 0
93.678244	C2: prod1*(exp(x5*(g12-g32*x7*rthou-g52*x8*rthou))-one)-g52+g42*x2+cad2=0
91.053678	C3: prod1*(exp(x5*(g13-g33*x7*rthou-g53*x8*rthou))-one)-g53+g43*x2+cad3=0
174.00957	C4: prod1*(exp(x5*(g14-g34*x7*rthou-g54*x8*rthou))-one)-g54+g44*x2+cad4=0
15.073224	C5: prod2*(exp(x6*(g11-g21-g31*x7*rthou+g41*x9*rthou))-one)-g51+g41*x2+cad5=0
131.4521	C6: prod2*(exp(x6*(g12-g22-g32*x7*rthou+g42*x9*rthou))-one)-g52+g42*x2+cad6=0
-1532.4758	C7: prod2*(exp(x6*(g13-g23-g33*x7*rthou+g43*x9*rthou))-one)-g53+g43*x2+cad7=0
-2763.1953	C8: prod2*(exp(x6*(g14-g24-g34*x7*rthou+g44*x9*rthou))-one)-g54+g44*x2+cad8=0
-5	C9: x1*x3-x2*x4=0

Model Pm	Value
factor=	1.00E+02
rthou=	1.00E-03
one=	1
prod1=	-3
prod2=	-4
cad1=	-3.38889E-05
cad2=	-0.000151406
cad3=	-0.00012015
cad4=	0.000368546
cad5=	15.66836267
cad6=	67.16307487
cad7=	74.74244081
cad8=	126.3450721
g11=	0.485
g12=	0.752
g13=	0.869
g14=	0.982
g21=	0.369
g22=	1.254
g23=	0.703
g24=	1.455
g31=	5.2095
g32=	10.0677
g33=	22.9274
g34=	20.2153
g41=	23.3037
g42=	101.779
g43=	111.461
g44=	191.267
g51=	28.5132
g52=	111.8467
g53=	134.3884
g54=	211.4823

Answer Report LSSQP / Answer Report ES / Feasibility Report IS / Answer Report OQS / Model

Ready

A Time-Discretized Control Model Solved by Excel/LGO

Microsoft Excel - SPACES~1.XLS

Spaceship Navigator

Demonstration spreadsheet model

Frontline Systems and Pinter Consulting Services

Pilot a spaceship from one planet to another using the least amount of fuel. The trip is divided into 9 time blocks, with one engine blast allowed per time block. The pilot must choose the size and direction of each rocket blast for each time block. There are two moving suns whose gravitional fields affect the rocket. The best answer will take advantage of this and use the fields to "slingshot" toward the goal...

This is a non-trivial 17-variable multiextremal model with two complicated nonlinear equality constraints.
Extra difficulty: a large number of locally optimal solutions can be found on the border of the feasible set.

Sun1

xpos	ypos	ship to sun	grav	angle to sun	xgrav	ygrav
200	400	447.2135955	10	1.107148718	4.472136	8.9442719
180	400	406.504936	12.103148	1.125707647	5.2108643	10.923969
160	400	319.5048347	19.591836	1.098593056	8.9113376	17.447868
140	400	118.8074485	141.69113	0.484360388	125.39282	65.977399
120	400	140.630418	101.12801	-1.946257292	-37.083785	-94.0833
100	400	267.3464798	27.982148	-2.237562568	-17.305505	-21.989091
80	400	366.0161194	14.928961	-2.357613614	-10.571339	-10.541378
60	400	450.237664	9.866119	-2.436672084	-7.514658	-6.392982
40	400	522.2734784	7.3321957	-2.4872459	-5.8176991	-4.4626754
20	400	586.9220194	5.8058952	-2.536249019	-4.7742259	-3.3038138

Sun2

xpos	ypos	ship to sun	grav	angle to sun	xgrav	ygrav	Time
0	300	300	22.222222	1.570796327	1.3613E-15	22.2222222	0
10	270	236.9532645	35.620877	1.549626898	0.75401728	35.6128953	1
20	240	124.6547338	128.71005	1.528052239	5.49991839	128.592483	2
30	210	134.7658235	110.12108	-1.606856461	-3.9701203	-110.04949	3
40	180	374.6931255	14.245528	-1.929583627	-5.0021606	-13.33842	4
50	150	507.9881852	7.750376	-2.008551431	-3.2854411	-7.0195587	5
60	120	606.5180477	5.4367898	-2.049128029	-2.5025476	-4.8265866	6
70	90	687.7029927	4.2289073	-2.076151187	-2.04729	-3.7003055	7
80	60	756.9506925	3.4905576	-2.088182762	-1.7264659	-3.0336955	8
90	30	816.0012682	3.0036431	-2.100958261	-1.5188614	-2.5913186	9

sun mass	2000000
pi/2	1.570796
pi	3.14159265

Spac

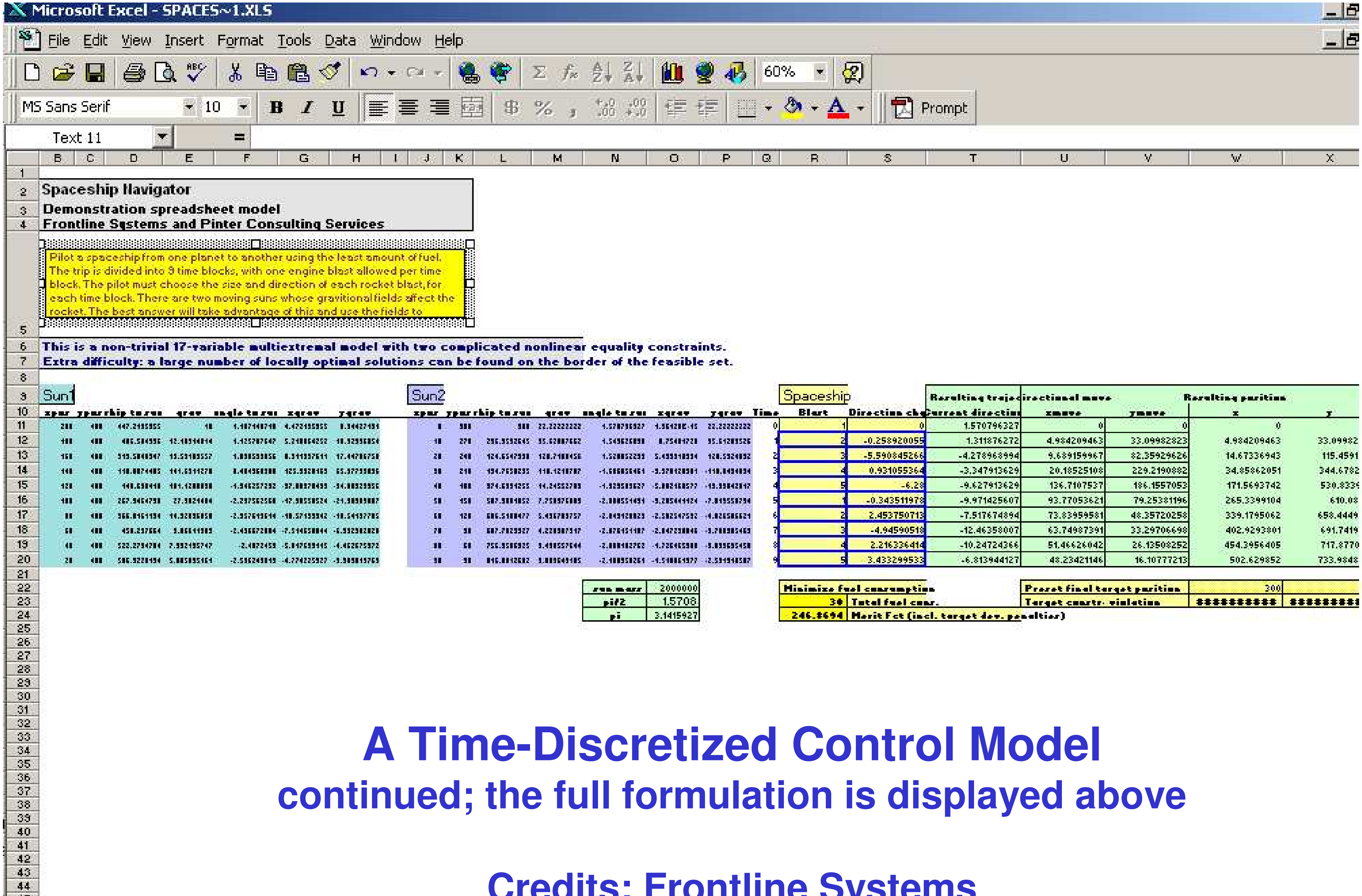
Bla

Minimi

246.8

Answer Report LGO_3 | **SpaceShip Navigator**

Ready



A Time-Discretized Control Model

continued; the full formulation is displayed above

Credits: Frontline Systems

Industrial Design Problems

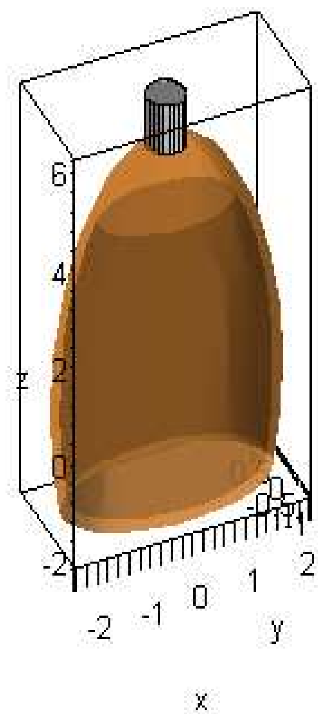
An illustrative application:

Designing an "optimized" parfume bottle using the Maple GOT

Objective:
minimize package volume

Constraints:
Bottle volume ≥ required
Width of the base ≥ required
Aesthetic proportions

Example by Maplesoft



Kinetic Grasp Feasibility Analysis in Robotics Design

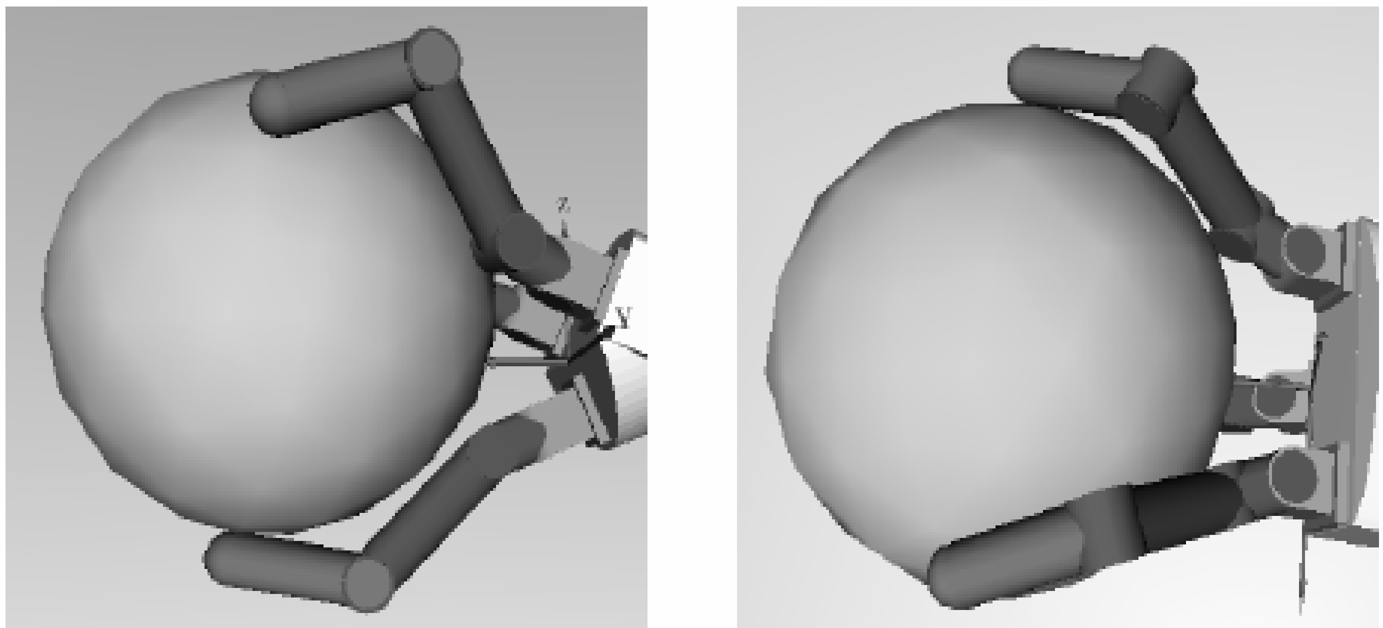


Figure 10: Grasp of the maximum sphere

Credits: Yisheng Guan and Hong Zhang, University of Alberta, Edmonton, Canada

Laser Design

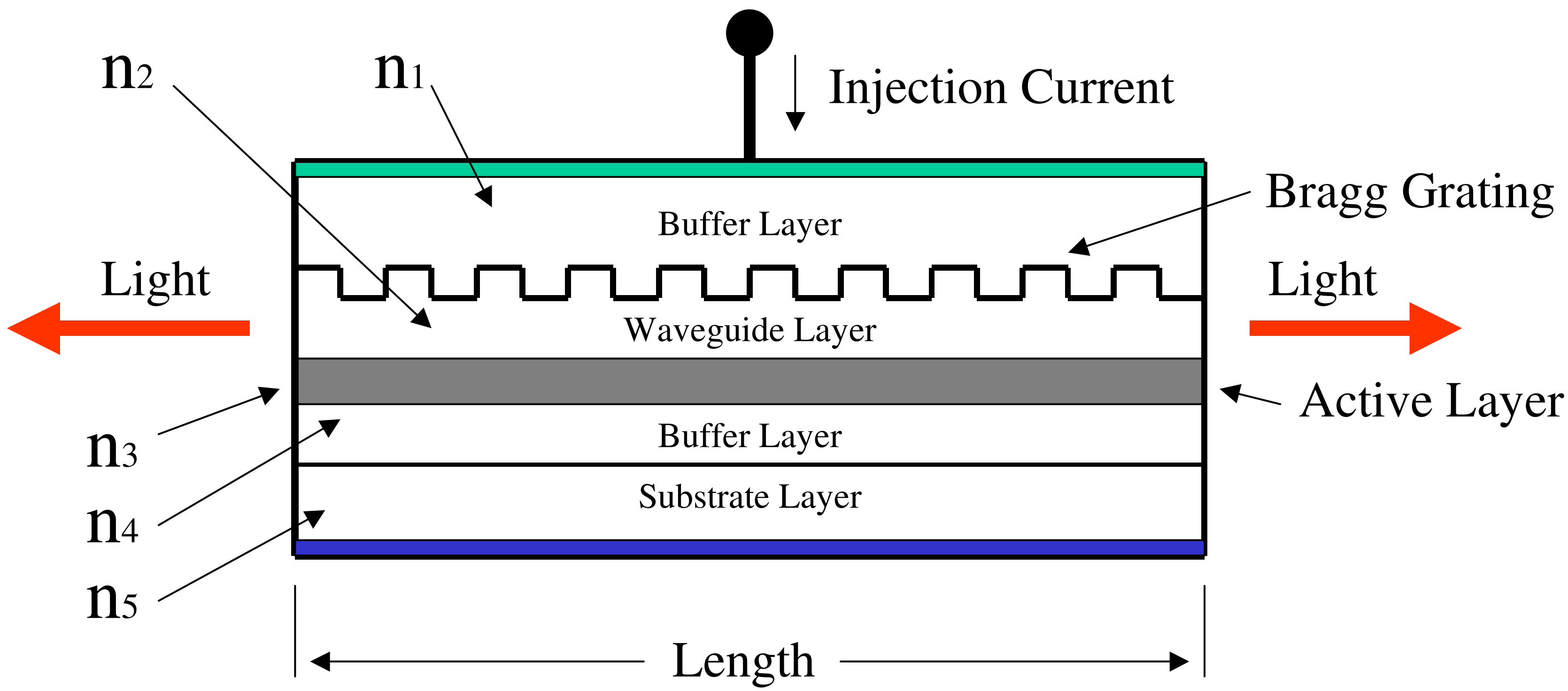
Optimization and Engineering (2003); with G. Isenor & M. Cada

Basic Concepts

The laser is a device that produces a beam of light that is coherent. The beam is produced by a process known as stimulated emission.

The word *laser* is an acronym for the phrase “Light Amplification by Stimulated Emission of Radiation”.

The idea of stimulated emission was proposed by Albert Einstein in 1916. It took another four decades to build the first lasers as a scientific research tool; soon they found numerous significant applications.



$n_{1,2,3,4,5}$ = Index of Refraction $n_5 \leq n_1 < n_4 \leq n_2 < n_3$

Index-coupled distributed feedback laser

Various laser design issues can be analyzed in the framework of global optimization

Example:

$\min f(x)$	field flatness function
$g(x) = 0$	RBC error (boundary condition)
$xl \le x \le xu$	explicit, finite parameter bounds
$x = (KL1, KL2, KL3, \lambda, C_o)$	laser design parameters

Essential difficulty: *f* and *g* are complicated “black box” functions. The LGO IDE software has been used to analyze and solve this model (in several variants).

A very significant improvement (over 90% reduction) of the field flatness function has been attained.

Radiotherapy Planning *Annals of OR*, 2003

Significance of the problem: world-wide interest and R&D activities devoted to cancer therapy by irradiation

Specific area of our research: intensity modulated radiation therapy planning, delivered to cure individual patients

Objective: determine the operations (trajectories) of the leafs in an MLC equipment, to optimally approximate the prescribed dose intensity distribution (in 3 dimensions), thereby

- to provide prescribed radiation intensity to target area or volume (body parts affected by cancer)
- to avoid unwanted radiation as much as possible (especially of organs at risk, as well as other body parts)

For details, cf. our paper (Tervo et al., *Annals of Operations Research,* 2003)

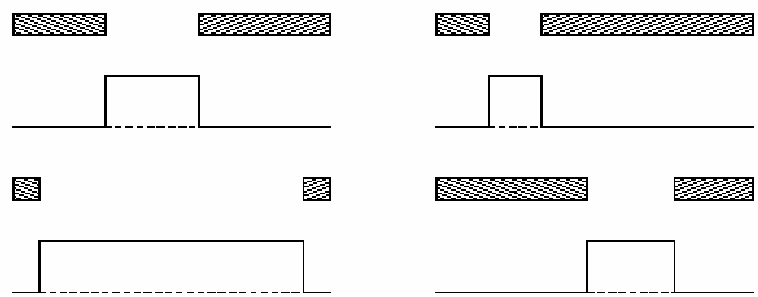
Dose Delivery and Effect Modeling

Sophisticated, computationally intensive mathematical models of dose delivery by MLC equipment have been developed in several versions by researchers at the University of Kuopio, Finland. The key novel feature of this approach is to optimize dose distribution directly via adjusting MLC parameters. Our therapy optimization models are all characterized by

- **tens or hundreds of variables (leaf positions and their coordinated movements, to describe MLC operations),**
- **a large number of relatively simple constraints (feasible leaf positions),**
- **a few significant complex 'black box' constraints; complex objective function (target dose, and limits on unwanted dose in OAR and body tissue).**

Joint operation of leafs in MLC equipment (simplified scheme)

Leaf positions

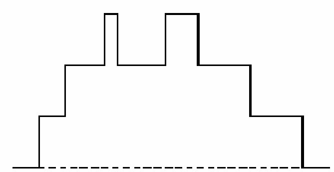


Radiation intensity

A resulting radiation profile

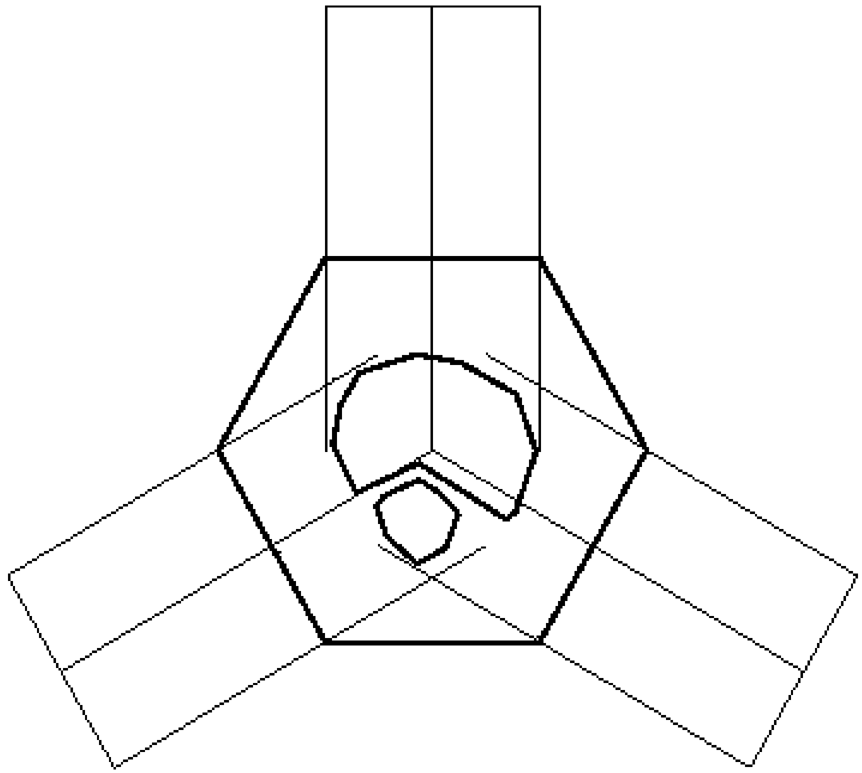
(based on all leaf positions

that determine total exposure)

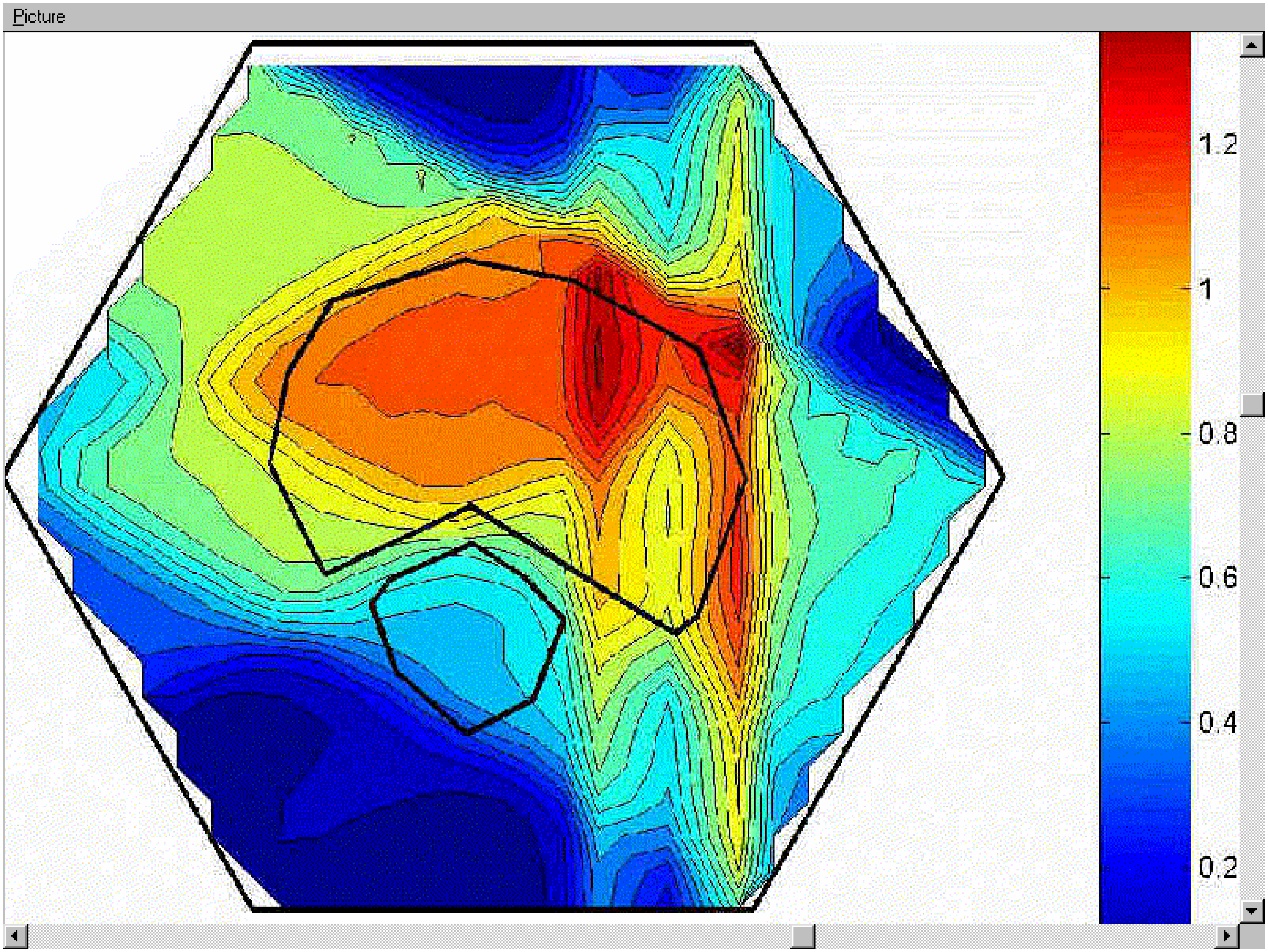


Superposition of overall irradiation effect,
as a function of leaf positions and radiation intensity

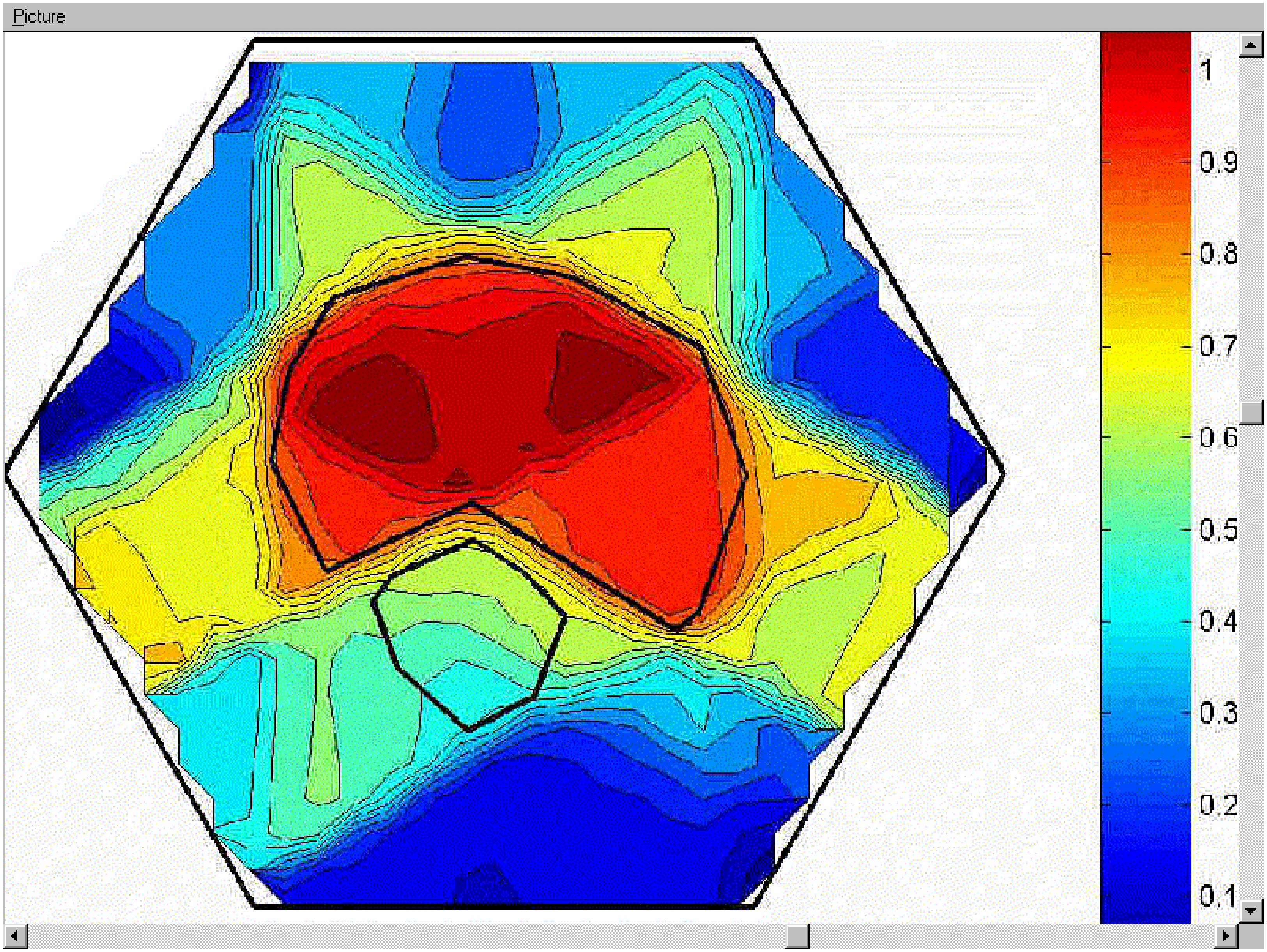
A Numerical Test Example



Illustrative model (2D phantom) used in optimized radiation dose distribution test calculations: overall irradiation area, hypothetical target area, and an organ at risk are shown



Dose distribution found by local optimization of nominal solution



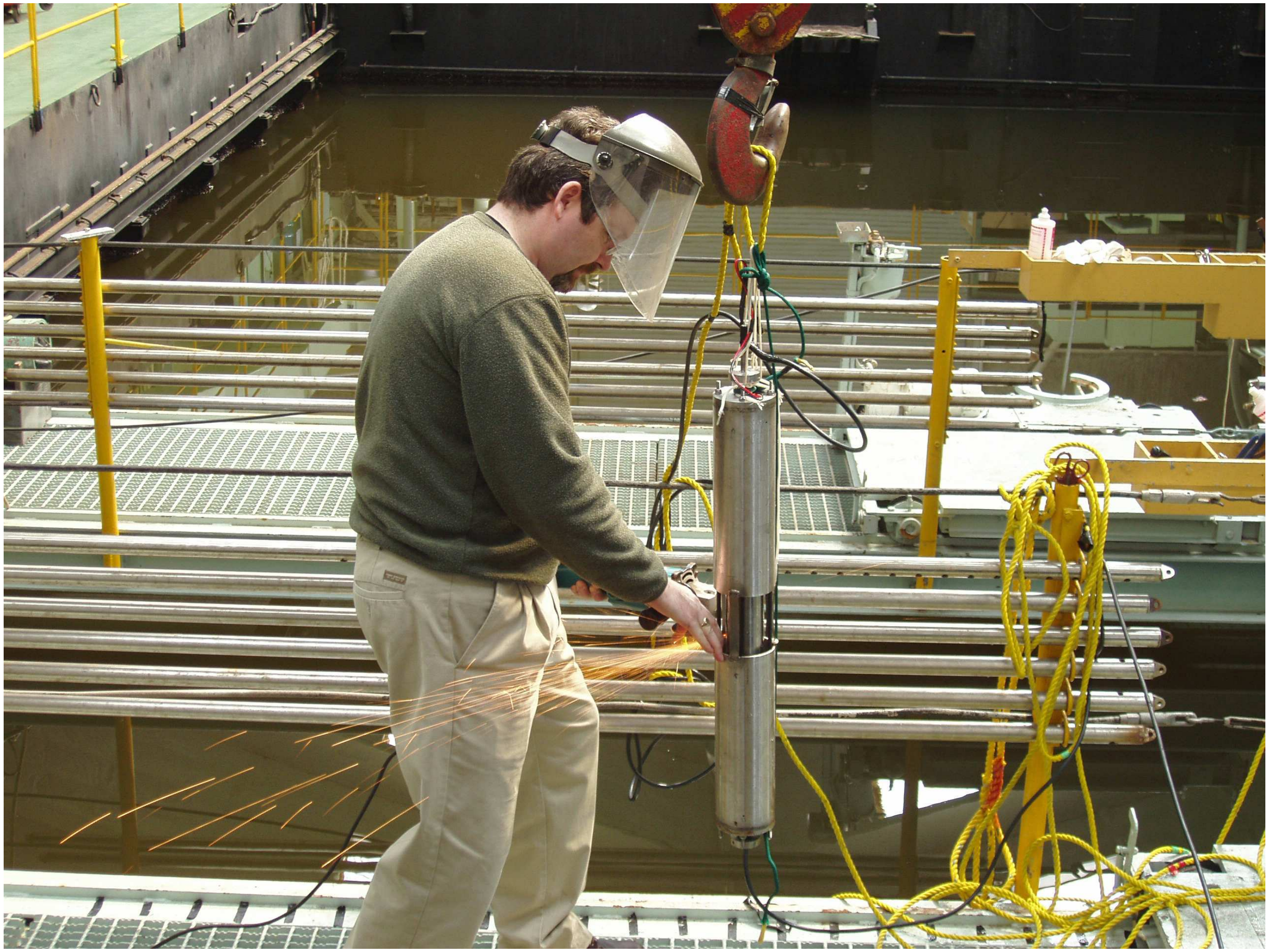
Globally optimized dose distribution

Modeling and Optimization of Transducers

MathOptimizer User Guide, joint presentations with C.J. Purcell

- Traditional engineering design often based on experimental studies: change key parameters and then trace their effect (e.g. by physical experiments and their graphical summaries) – as a rule, expensive and time consuming…
- Parametric studies are ideal tasks for computers: numerical models can (partially) replace experiments
- Parametric models can be directly optimized
- In our study, a combination of detailed system modeling and optimization has been applied; this has resulted in improved (in some cases “surprising” and entirely new) designs

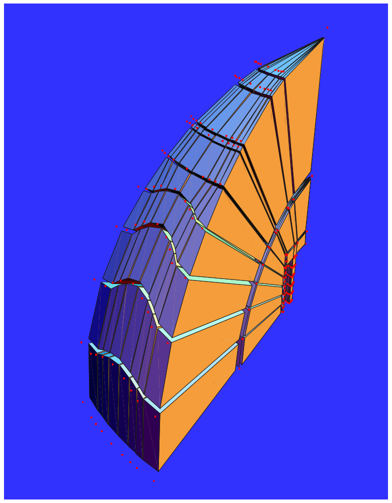
Engineering Design Optimization by Trial and Error

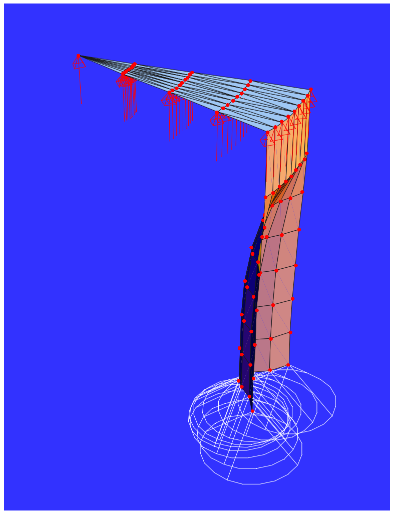


Expensive and time-consuming...

ModelMaker

- *Mathematica* package for developing advanced finite element models (FEM)
- Numeric and symbolic parameterized models can be developed
- Models and results presented in interactive *Mathematica* document (notebook) format
- Built-in, extensible documentation
- Supports other FEM packages (such as Mavart, Mavart3D, MavartMag, Atila,…)
- Developed since 1994 by C. Purcell, DRDC



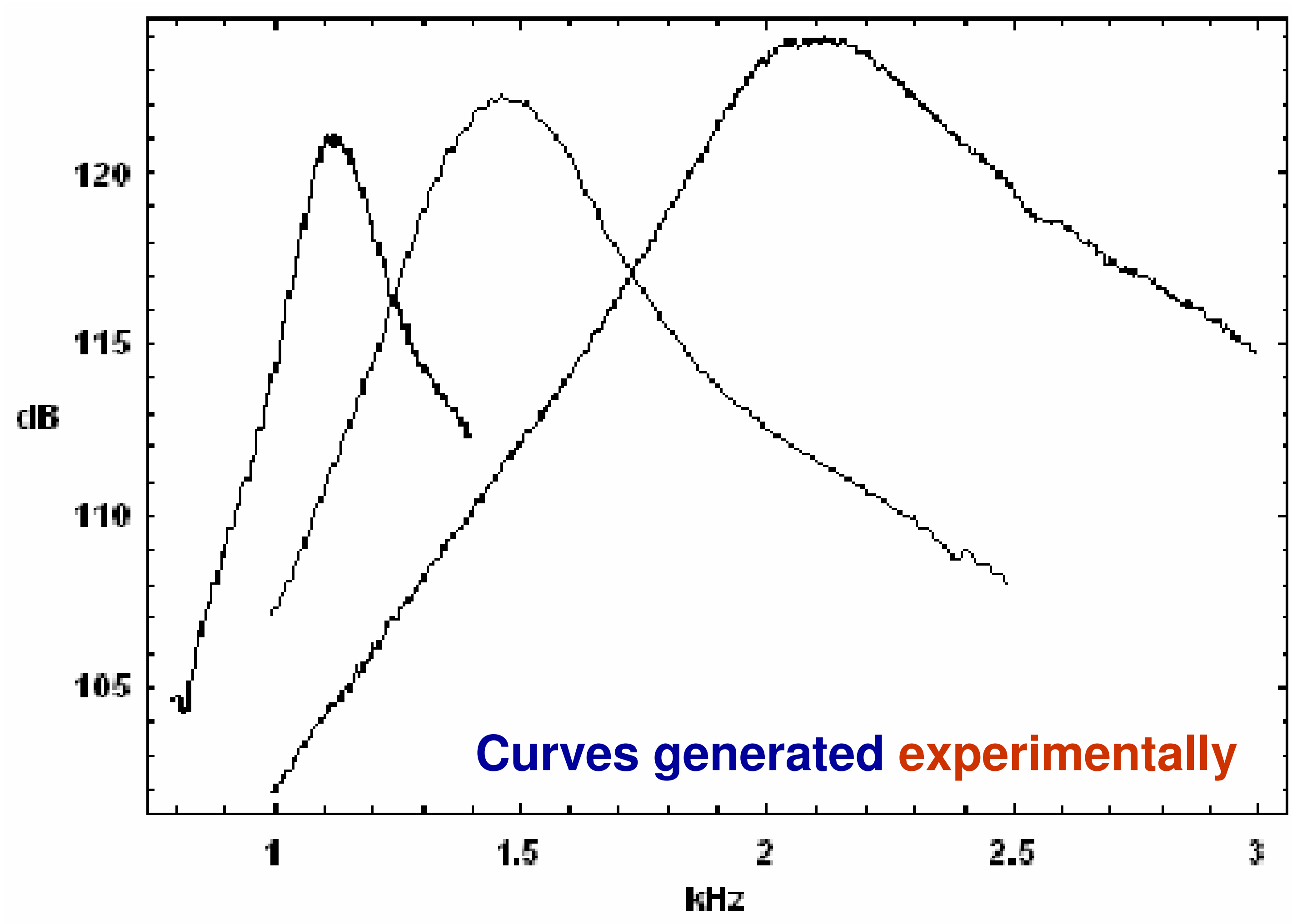


Example: Folded Shell Projector

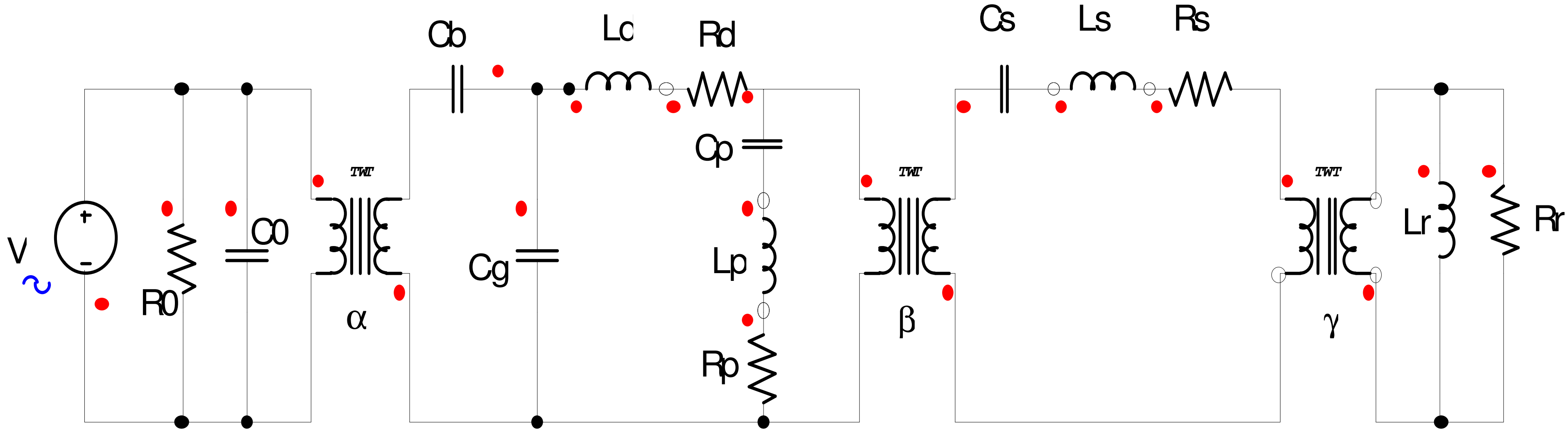
FSP is a sonar projector (or in-air loudspeaker) with overall cylinder shape with corrugations on the sides

Experimental Design

Three FSPs with varying transformer ratio (a key design parameter): optimization needed...



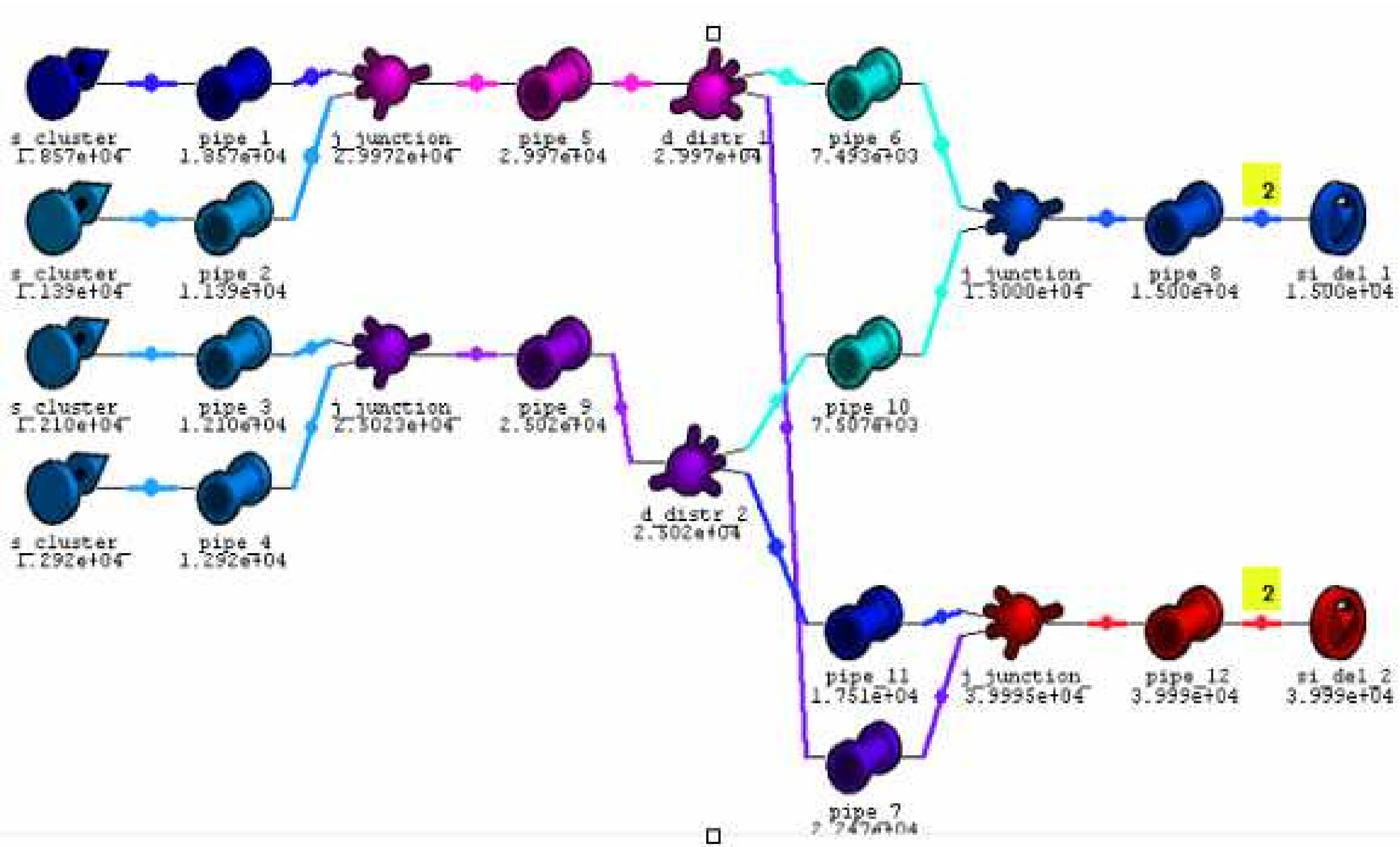
Sonar Transducer Design: Numerical Model



This electric circuit simulates a piezoelectric sonar projector

The optimization problem consists of finding circuit design parameters such that the sonar projector gives a broad efficiency *vs.* frequency. This model has been solved using MathOptimizer. The results have been applied to the actual design of sonar equipment, leading to improved designs.

Oil Field Production Analysis and Optimization



Credits: T. Mason, P. Zwietering, C. Emelle, et al. Shell R&D, Rijswijk, The Netherlands

2 Description of the Optimization Problem

Our test model considers the blending of gas produced from five fields $(F_1, ..., F_5)$ to supply different quality gas at six processing plants $(P_1, ..., P_6)$ through a converging-diverging gas gathering/distribution network, as shown in Figure 1 below:

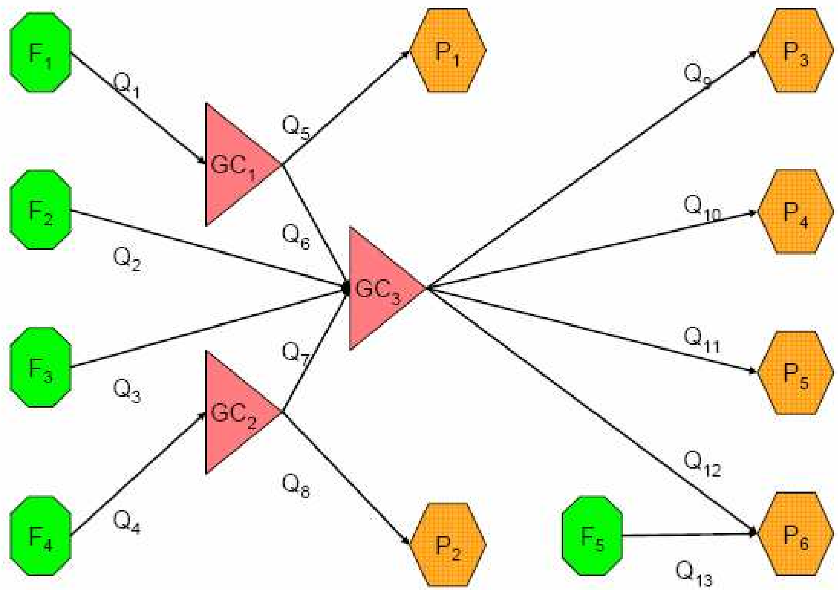
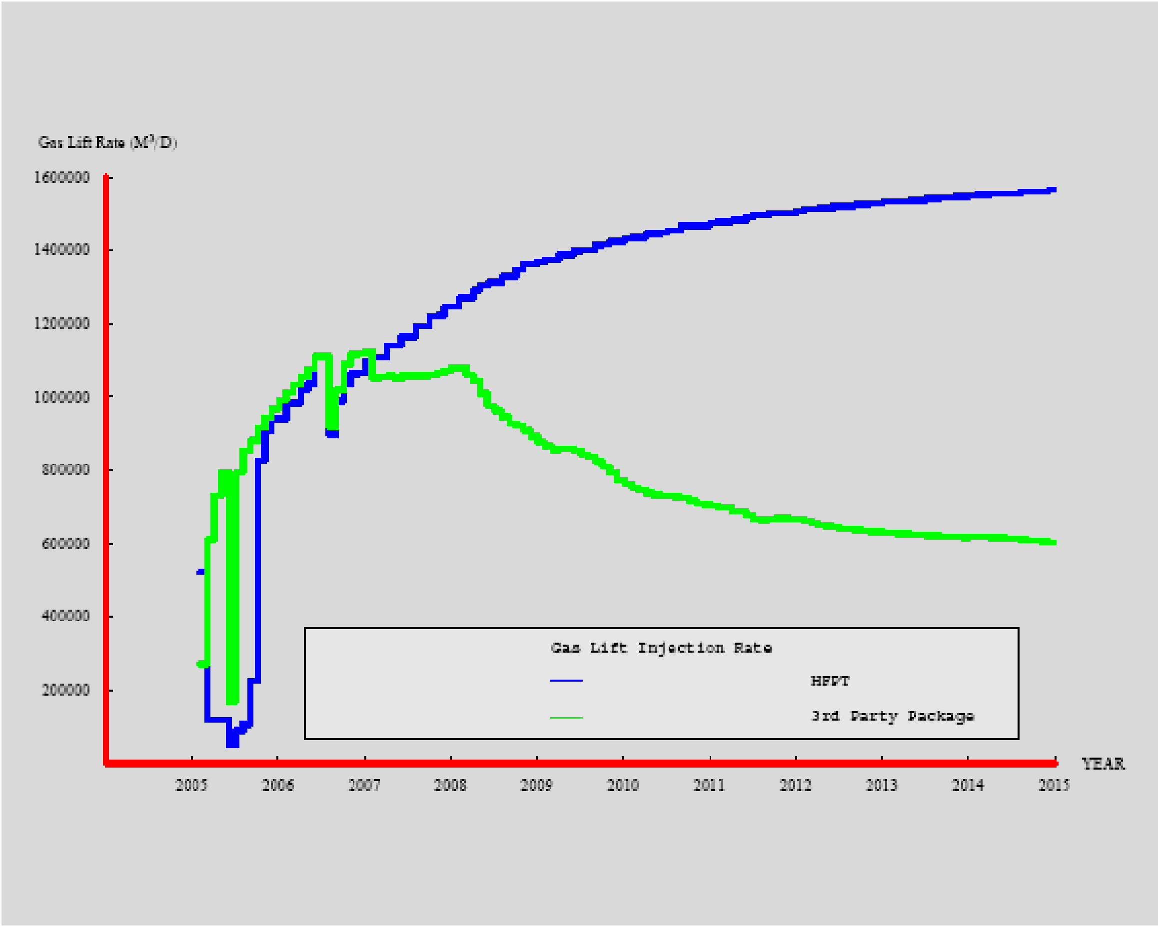


Figure 1: Schematic of the Gas Blending Network

Source: Mason et al. EURO 2006 presentation and JIMO 07 joint paper

Oil Field Production Analysis and Optimization: The Global Optimization Advantage



Improved gas lift (production) using HFTP/LGO at Shell IEP

EURO 2006 talk, JIMO 2007 paper by T. Mason, C. Emelle, J. van Berkel, A. Bagirov, F. Kampas, and JDP

Global Optimization Software Users

- Universities
- Research organizations
- Advanced industries, R&D departments
- Scientific, engineering, econometrist and financial modelers
- Consulting organizations
- GO software is used worldwide

Global Optimization Applications and Perspectives: Illustrative References

Authors/Editors	Application Areas, with Information on Software (in works denoted by +S)
Grossmann, 1996	Chemical Engineering Design + S
Pardalos, Shalloway & Xue, 1996	Computational Chemistry and Biology
Pintér, 1996	Environmental Modeling/Mgmt, and others + S
Corliss and Kearfott, 1999	Rigorous Optimization in Industry + S
Floudas et al., 1999	Handbook of Test Problems
Papalambros and Wilde (2000)	Engineering Design
Edgar, Himmelblau & Lasdon, 2001	Chemical Engineering Design/Operations+ S
Gao, Ogden & Stavroulakis, 2001	Physics (Mechanics)
Pardalos and Resende, 2002	Topical chapter by Floudas (Chem. Engrg)
Schittkowski, 2002	Model Fitting (Calibration) + S
Tawarmalani and Sahinidis (2002)	Chemical Engineering Design/Operations+ S
Diwekar (2003)	Environmental Modeling/Mgmt + S

Global Optimization Applications and Perspectives: Illustrative References

Authors/Editors	Application Areas, with Details on Software (in works denoted by +S)
Locatelli, Schoen et al. 2000+	Computational Chemistry and Biology + S
Stojanovic, 2003	Financial Modeling + S
Zabinsky, 2003	Engineering Design + S
Neumaier, 2004	See topical review sections + S
Bartholomew-Biggs, 2005	Financial Modeling and Optimization
Liberti & Maculan, 2005	Chapters on Software Implementations + S
Nowak, 2005	MINLP Software Devpt & Tests + S
Pintér, 2006	Global Optimization with Maple + S
Pintér, 2006	GO: Sci & Engrg Case Studies + S
Pintér, 2007	Applied NLO in Modeling Environments + S
Kampas & Pintér, 2007	Modeling & Opt. Using Mathematica + S

Further information is welcome

Note: Keep an eye also on other literature not written by GO researchers — numerous examples discussed by engineers and scientists who need GO…

Global Optimization

obal Search, As Timely As Ever

"Consider everything. Keep the good. Avoid evil whenever you notice it."
(1 Thess. 5:21-22)

New - COCONUT
Introduction - Techniques
Software (global) - Software (local) - Test Problems
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is is a comprehensive archive of online information on (almost exclusively non-commercial) global optimization, and somewhat less comprehensive on local timization, collected by Arnold Neumaier on the web server http://www.mat.univie.ac.at/~neum/glopt.html of the Computational Mathematics group at the iversity of Vienna, Austria. Later on this page there is a Table of Contents of this Site.

ease help to keep the archive up to date by informing me at Arnold.Neumaier@univie.ac.at about new or missing electronic documents related to public domain rk on global optimization, and about links that are no longer working.

lated, but not formally part of this site is the COCONUT web site with many links specifically devoted to the activities of the European COCONUT project, wi goal of integrating various existing complete approaches to global optimization into a uniform whole.

pen Positions in Global Optimization

stdoctoral position in Computer Science ans Interval Mathematics (University of Nantes)

stdoctoral position in Computer Science (Ecole Normale Superieure, Lyon, France)

st Positions in Global Optimization

Mathematics

Global Optimization in Action
Continuous and Lipschitz Optimization: Algorithms, Implementations and Applications
Series: Nonconvex Optimization and Its Applications, Vol. 6
Pintér, János D.
1996, 512 p., Hardcover
ISBN: 0-7923-3757-3

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About this book

In science, engineering and economics, decision problems are frequently modelled by optimizing the value of a (primary) objective function under stated feasibility constraints. In many cases of practical relevance, the optimization problem structure does not warrant the global optimality of local solutions; hence, it is natural to search for the globally best solution(s).
Global Optimization in Action provides a comprehensive discussion of adaptive partition strategies to solve global optimization problems under very general structural requirements. A unified approach to numerous known algorithms makes possible straightforward generalizations and extensions, leading to efficient computer-based implementations. A considerable part of the book is devoted to applications, including some generic problems from numerical analysis, and several case studies in environmental systems analysis and management. The book is essentially self-contained and is based on the author's research, in cooperation (on applications) with a number of colleagues.

This e-book includes hands-on demos of the LGO IDE

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Global Optimization
Scientific and Engineering Case Studies
Series: Nonconvex Optimization and Its Applications, Vol. 85
Pintér, János D. (Ed.)
2006, Hardcover
ISBN: 0-387-30408-8

Not yet published. Available: April 2006

approx. US$99.95

Print version
Recommend to others

All books by this editor
Pintér, János D.

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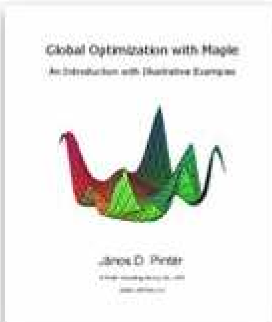
About this book

Optimization models based on a nonlinear systems description often possess multiple local optima. The objective of global optimization (GO) is to find the best possible solution of multiextremal problems. This volume illustrates the applicability of GO modeling techniques and solution strategies to real-world problems.

The contributed chapters cover a broad range of applications from agroecosystem management, assembly line design, bioinformatics, biophysics, black box systems optimization, cellular mobile network design, chemical process optimization, chemical product design, composite structure design, computational modeling of atomic and molecular structures, controller design for induction motors, electrical engineering design, feeding strategies in animal husbandry, the inverse position problem in kinematics, laser design, learning in neural nets, mechanical engineering design, numerical solution of equations, radiotherapy planning, robot design, and satellite data analysis. The solution strategies discussed encompass a range of practically viable methods, including both theoretically rigorous and heuristic approaches.

Written for:

Researchers and practitioners in academia, research and consulting organizations, and industry mapleconnect™



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Global Optimization with Maple™

Product Description:

This electronic book presents Maple as an advanced model development and optimization environment. A special emphasis is placed on solving multiextremal models using the Global Optimization Toolbox™ for Maple™. Following a brief topical introduction, an extensive collection of detailed numerical examples and illustrative case studies is presented.

The following topics are covered:

- A brief introduction to Operations Research / Management Science (ORMS)
- Maple as an integrated platform for developing ORMS studies and applications
- A review of the key global optimization concepts
- The Global Optimization Toolbox™ (GOT) for Maple™, including a concise discussion of the core LGO™ solver technology
- Model development tips
- Detailed "hands-on" numerical examples of using the GOT, from a simple illustration of the key tools and options to more advanced challenges
- Illustrative case studies from the sciences and engineering.

Intended Audience:

This electronic book will be of interest to practitioners, researchers, academics, and students in the sciences and engineering.

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Description | Contents | Series

Applied Nonlinear Optimization in Modeling Environments

Janos D Pinter *Pinter Consulting Services Inc, Nova Scotia, Canada*

Series: Operations Research Series

List Price: $129.95
Cat. #: 1623
ISBN: 0849316235
Publication Date: 9/15/2005
Number of Pages: 320
Availability: Not Yet Published

(forthcoming)

CRC Press

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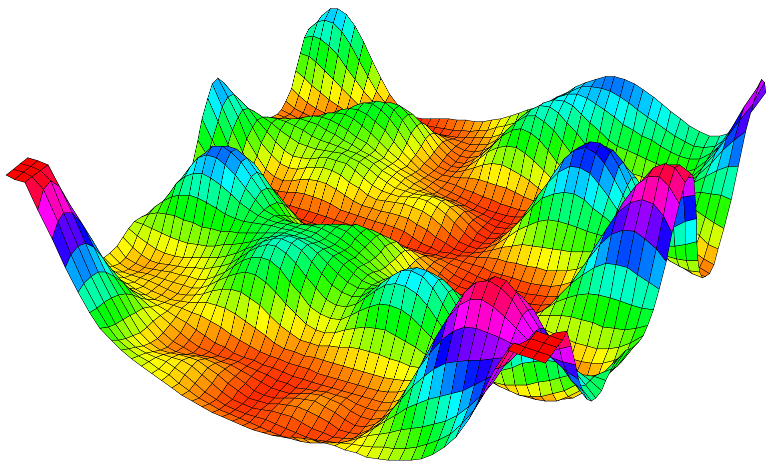
- Offers a practically driven discussion of continuous nonlinear optimization strategies
- Provides an overview of several prominent model development systems
- Presents professional nonlinear solver implementations (developed by the author and his partners): currently, these include the stand-alone (compiler-based) LGO solver suite, an embedding integrated development environment (LGO IDE), and customized solver versions for Excel, GAMS, Maple, MATLAB, and Mathematica
- Illustrates the use of these tools with examples from numerical analysis, natural sciences, engineering design and operations, econometrics, and financial analysis
- Provides both example code and runtime executable demo files

In a unique treatment that reviews prominent modeling environments and solution approaches, numerical tests and real-world applications, this work presents a practically motivated discussion of nonlinear (global and conve optimization. From this book, readers will gain a solid practical understanding of readily applicable methods and tools in an important and rapidly emerging field.

Advanced Optimization

Scientific, Engineering, and Economic Applications with Mathematica Examples



Frank J. Kampas and János D. Pintér

ELSEVIER SCIENCE (forthcoming)

Conclusions

- Global optimization is a subject of growing importance: it is relevant in many areas in the sciences, engineering, and economics
- Development and application of sophisticated, complex numerical models: the use of global scope optimization methodology is often essential
- Professionally developed and supported GO solver options are available for a growing number of platforms
- Further developments of modeling tools, algorithms, and software in progress

Conclusions

Some Key Challenges and Future Work

- Integrate exact and heuristic methods
- Handle problems with (very) costly functions
- Handle problems w/o an exploitable structure
- Stochastic optimization: simulation and optimization
- Dynamic models: d.e. solvers and optimization

Several Key Application Areas of GO

- Advanced engineering
- Chemical and process industries
- Defense, security
- Econometrics and finance
- Math/physics/chemistry/biology
- Medical and pharmaceutical R&D

Interest in R&D and Business Cooperation

- Customized model, algorithm, software, DSS development and related consulting services
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Thanks for your attention!

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