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
- 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 support and feedback

Introduction

- **Decision making under resource constraints in 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, see e.g. the 50th Anniversary Issue of *Operations Research*)**
- **Quantitative decision support systems (DSS) tools - i.e., models and solvers - effectively assist decision makers and analysts in finding better solutions**

Classification of Optimization Problems

Convex (Continuous) Deterministic Models

Linear Programming; Nonlinear Programming; numerous special cases

Non-Convex Deterministic Models

Continuous Global Optimization; Combinatorial Optimization; Mixed Integer/Continuous Optimization; special cases

Stochastic Models

Numerous special cases: some of these have LP, CP, and general NLP equivalents, but also includes 'black box' models with non-convex structure.

Note: Formally, both the convex and stochastic model-classes can be considered as subsets of the non-convex models. However, added specifications and insight are, as a rule, very helpful.

The Relevance of Nonlinear Optimization

"Unlike its grubby, uncouth, unreliable nonlinear cousin, linear optimization is clean-shaven, gracious and globally satisfying.

Any civilized being would prefer linear optimization to nonlinear…"

Tom Grossman, *ORMS Today*, August 2001

Note: Tom G. advocates teaching NLP before LP for the *end user*, in business schools and elsewhere…

The Relevance of Nonlinear Optimization (cont'd)

- Nonlinearity is ubiquitous in natural formations, objects, organisms, processes, and in their complex interactions
- This is reflected by descriptive models in applied mathematics, physics, chemistry, biology, engineering, and economics
- Some of the most frequently used nonlinear function forms in physics / chemistry / biology,... are:
exponential function (growth or decay processes,...)
trigonometric functions (periodic motion,…)
statistical models: probability distributions
- More complicated function forms: ordinary and partial differential equations; integral equations; special functions, complete simulation 'boxes' and so on

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**

The Relevance of Global Optimization (cont'd)

"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

Continuous Global Optimization Model

min $f(x)$	f: R^n ô R^1
$g(x) \leq 0$	g: R^n ô R^m
$x_l \leq x \leq x_u$	x, x_l, x_u, ($x_l < x_u$) are real n-vectors

Key ('minimal') analytical assumptions:

- x_l, x_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 are sufficient to guarantee the existence of global solution set

The CGO model covers a very general class of models

Global Optimization: Historical Perspective

An approximate timeline

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

↓↑

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

↓↑

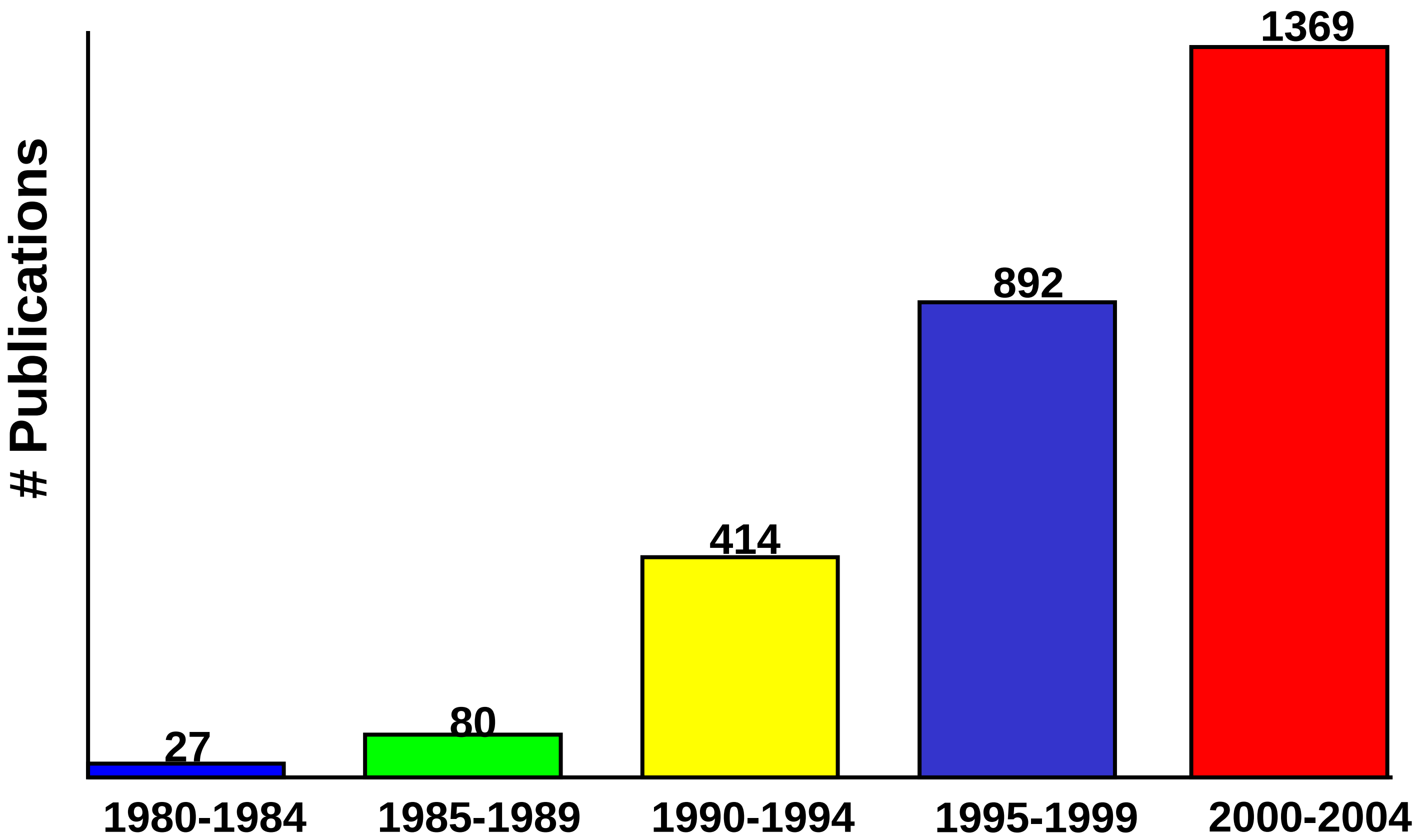
Software (beginnings: 1980's, professional: ~2000+)

↓↑

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

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

Global Optimization: Academic Impact



Cited from: Floudas, C. A.
Global Optimization in the 21st Century: Advances and Challenges
Presented at the Conference on Optimization with Industrial Application
Baku, Azerbaijan, May 2005

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 modeling languages with a focus on optimization: AIMMS, AMPL, GAMS, LINDO/LINGO, LPL, MPL,…
- Fully integrated scientific and technical computing environments: Maple, Mathematica, MATLAB,…
- Relative pros and cons… Select the most appropriate platform considering user needs and requirements (see e.g. the AIMMS website on this subject)

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, LGO, MS-GRG, MS-KNITRO, OptQuest solver engines

- Modeling languages and related solver options:

AIMMS: BARON, LGO

GAMS: BARON, LGO, OQNLP

LINGO: built-in global solver by the developers (LINDO)

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

TOMLAB solvers for MATLAB: CGO, LGO, OQNLP

- Detailed information and references
- Developer websites
- Handbook of GO, Vol. 2, Chapter 15
- Neumaier’s GO website: 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/Lipschitz functions are needed
- Can be applied even to completely "black box" system models
- Globally convergent methods (LGO solver components)

  continuous branch-and-bound

  global adaptive randomized search

  multi-start based adaptive random search

  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**
- **MPL/LGO size-limited demo accompanies the text Hillier & Lieberman, *Introduction to Operations Research* (2005 edition)**
- **Applications and challenges welcome**

GOiA Book and LGO Software Reviews

Peer reviews:

- ***Global Optimization in Action*** **reviewed in** ***Optima*** **(1996),** ***J. of Global Optimization*** **(1998),** ***Optimization Methods and Software*** **(1998)**
- **Book awarded the** ***2000 INFORMS Computing Society Prize;*** **available both for course adoption and to INFORMS members at a special discount**
- **LGO software review in** ***ORMS Today*** **(2000)**
- **MathOptimizer / MathOptimizer Professional reviews in** ***Scientific Computing World*** **(2003)**
- **Maple Global Optimization Toolbox reviews in** ***ORMS Today*** **(2005),** ***Scientific Computing*** **(2006),** ***IEEE Computer Science Magazine*** **(2006)**

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
- Model formulation and solution in Maple (GOT) using Maple GUI Assistants
- Solving a system of nonlinear equations (Maple GOT)
- Nonlinear model fitting (MathOptimizer, Maple GOT)
- A “black box” client model (code generated automatically by MathOptimizer Professional)
- Numerical GO challenges (Trefethen’s problems 4 and 9, solved by various LGO implementations)
- Emergency service centre location (MOP)
- 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)
- Wastewater treatment system design (LGO)
- Environmental (groundwater) assessment and management (LGO)

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

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)**

Maxi-Min and Other 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 { min ||x_i - x_k || } $\quad$ ***xl≤x_i£xu*** $\quad$ ***$x_i \in R^d$*** $\quad$ ***i*=1,…,*m***

{ x_i } $\quad$ $1 \leq i < k \leq m$

Additional restrictions, alternative feasible sets, and other quality criteria can also be considered; non-convex models

Permutations ô lexicographic point arrangements

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**

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£j<k£m	Euclidean distance

Model versions considered

max $\text{Â}_{1£j<k£\mathrm{m}}$ log(d_{jk})	Fekete (log-potential)
min $\text{Â}_{1£j<k£\mathrm{m}}$ 1/d_{jk} (d_{jk}>0)	Coulomb-Fekete
max $\text{Â}_{1£j<k£m}$ d_{jk}^{a}	Power sum, 0<a<2
max {min $_{1£\mathrm{j}<\mathrm{k}£\mathrm{m}}$ 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,...

Potential Energy Models: Conclusion

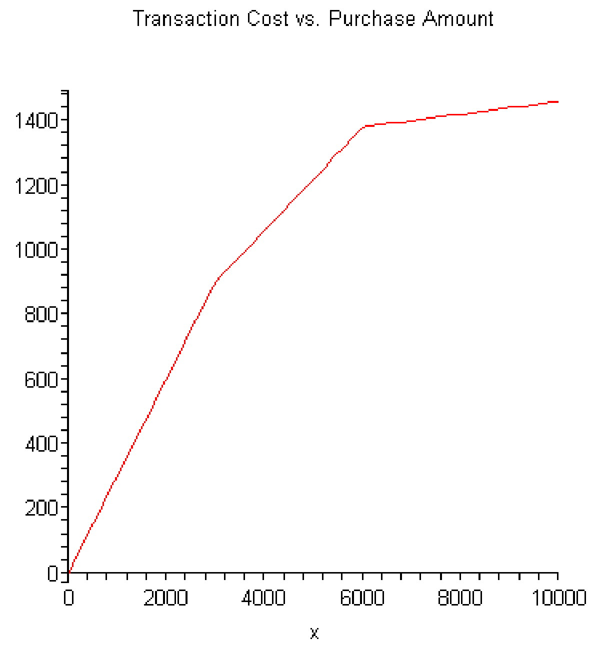
Putative global optima are taken (used for comparison) from the Web site of AT&T Bell Laboratories: those results have been derived by extensive numerical experiments

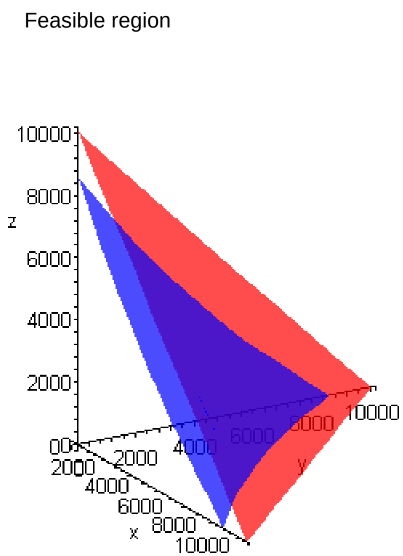
The illustrative LGO results successfully approximate the corresponding best known results to more than 99.99 precision for the log-potential, Coulomb, and power sum models; LGO solution time ~ 10-15 sec (on P4)

Hard sphere model solution quality is only ~90% of best: obviously, longer runs, good - or even randomly chosen - initial solutions could be used to improve this result (we have obtained much better results recently)

***Annals of Opns. Res.* (2001); *J. Comp. Appl. Math.* (2001)**
Co-authors of *JCAM* paper: W. Stortelder and J. de Swart

Portfolio Optimization under Concave Transaction Costs





In practice, brokers ask for commission rates and offer volume discounts. Under this assumption, the Markowitz portfolio model becomes non-convex.

In the numerical example shown here, the feasible region corresponding to the concave cost function (left figure) is non-convex (right figure, blue boundary, as opposed to the linear constraint (red boundary) based on linear costs. The Maple GOT solves this problem easily, unlike the local solver.

Example provided by Jason Schattmann, Maplesoft; Castillo-Lee-Pinter (2006)

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

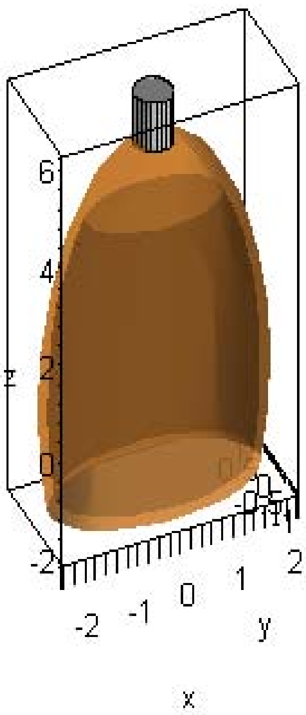
Industrial Design Problems

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

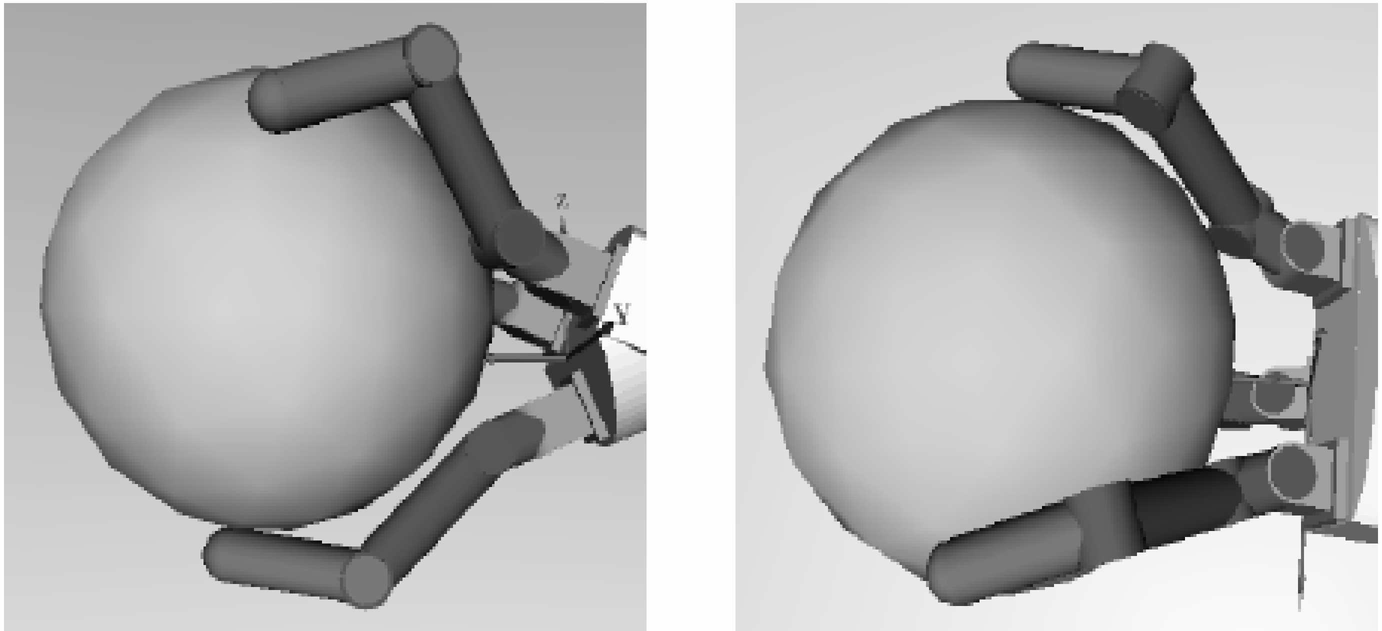


Figure 10: Grasp of the maximum sphere

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

Radiotherapy Planning: Summary

GO (LGO IDE implementation) has been applied as part of R&D project on intensity modulated therapy planning

Significant GO challenge; further numerical model extensions are studied by the research team of the University of Kuopio, including dynamic treatment plans

Annals of Operations Research **(2003); co-authors:**
J. Tervo, P. Kolmonen, T. Lyyra-Laatinen, and T. Lahtinen

Chemotherapy studies, involving a different modeling approach + LGO: collaboration in progress with J. McCall et al., Robert Gordon University, Aberdeen

Modeling and Optimization of Transducers

***MathOptimizer User Guide, WTC 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**

Simulation and Optimization in Environmental Management

- **This example is based on excerpts from the PhD thesis of Larry M. Deschaine, PE *Mathematical Simulation and Optimization of Subsurface Environmental Contamination Events* (Chalmers Technical University)**
- **The work summarized in the thesis is implemented in an advanced DSS, and has led to significant practical results in contamination analysis and remediation**
- **Excel GUI, numerical solvers and algorithms 'under the hood': the latter tools include LGO and MathOptimizer**
- **The DSS is fully adaptable and expandable**

Integrated DSS Development for Environmental Assessment and Management

Key DSS components

- **Pollution impact model to describe pollutant transport in air, water, or soil: physical and bio/geo-chemical processes in material flow and transport**
- **In general, the actual description leads to PDE systems that need to be solved numerically**
- **Impact assessment and monitoring: needed to verify description above**
- **Optimized remediation design: select best long-term strategy and technology to reduce pollution effects to 'acceptable' level, at minimal cost**
- **Implementation: combines numerically intensive computations (simulation, PDE solvers,...) and optimization techniques**

Conclusions and Future Work

- 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
- Professional quality solver options are available for a growing number of platforms
- Further developments of modeling tools, algorithms, and software in progress

Global Optimization (Software) Clients

- **Universities**
- **Research organizations**
- **Advanced industries, R&D departments**
- **Scientific, engineering, econometrist and financial modelers**
- **GO software developed by PCS and its partners used in more than 25 countries**
- **Consulting services and workshops are also offered**

Some Illustrative References

- **Over one hundred GO books; thousands of papers**
- ***Handbook of Global Optimization*, Vols. 1-2;**
- ***J. of Global Optimization* and other journals**
- **Web sites by Neumaier and others**
- ***Global Optimization in Action* (Kluwer AP, 1996)**
- ***Computational Global Optimization…* : a short tutorial book, accompanied by LGO IDE demo + examples (Lionheart Publishing, 2001)**
- ***Global Optimization: Scientific and Enginering Case Studies* (Edited volume; Springer, 2006)**
- **Chapter 15 in *Handbook of GO*, Vol. 2, 2002**
- **Two forthcoming books, numerous journal articles**
- **LGO and other User Guides (since 1995)**

Further Information

- Please visit the following software vendor sites for technical information and further details:
- AIMMS www.aimms.com
- Excel PSP www.solver.com
- GAMS www.gams.com
- Maple www.maplesoft.com
- Mathematica www.wolfram.com
- MPL www.maximalsoftware.com
- TOMLAB www.tomlab.biz

Acknowledgements

LGO solver versions	Lahey Computer Systems
AIMMS /LGO	Paragon Decision Technology
Excel PSP /LGO	Frontline Systems
GAMS /LGO	GAMS Development Corp.
Maple Global Optimization Toolbox	Maplesoft
MathOptimizer	Wolfram Research
MathOptimizer Professional	Frank J. Kampas and WR
MPL /LGO	Maximal Software
TOMLAB /LGO	TOMLAB AB

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Frank Kampas (MathOptPro cooperation, and packing models)
Charlie Khompatraporn & Zelda Zabinsky (evaluation of GO software)
Oscar Linares (discussions re: model calibration examples)
Frontline Systems (spaceship model)
Chris Purcell (MathOptimizer development and engrg applications)
Chris Purcell & Richard Fleming (transducer design)
Helmuth Ratschek and Jon Rokne (circuit design model)
Jason Schattmann (portfolio model)
Walter Stortelder & Jacques de Swart (log-potential model)
Jouko Tervo & colleagues (radiotherapy research)
L. N. Trefethen (HDHD numerical challenges)
Joint articles and reports are available upon request (in most cases)

Thanks for your attention!

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