Global Optimization with GAMS/LGO

Introduction, Usage, and Applications

János D. Pintér PCS Inc., Halifax, NS, Canada

GAMS Global Optimization Workshop Washington, DC Sept 18, 2003

Introduction

- Acknowledgement to GAMS team for contributions to the development of GAMS/LGO for assistance in organizing this GO workshop
- Part of these lecture notes based on Michael Bussieck's related talk at the MPS Conference (Copenhagen, Aug 2003), co-authored with the three other GAMS GO solver developers (Leon Lasdon, Nick Sahinidis, and JDP)
- Nonlinear processes and phenomena surround us
 - → NL models are ubiquitous in the sciences, engineering, and econometrics
 - → NLP/GO modeling and solver needs

Introduction (continued)

- Global optimization is a relatively new field: "noticeable interest" and research efforts only since ~ 1970
- Solid general theoretical foundations since ~ 1980: globally convergent, exact deterministic and stochastic algorithms; as well as a range of heuristic approaches
- Availability of several gradually developed/improved, "professional level" global optimization codes; in addition, a significant variety of "research" codes since ~ 1990
- Collaboration between the GAMS Corp. & the developers of BARON, LGO, and OQNLP → GAMS/GO solvers (~ 2000)

Introduction (continued)

Topics covered

Brief GAMS review

General CGO model statement and related notes

LGO solver: current implementations

LGO solver: key features

GAMS/LGO implementation and usage

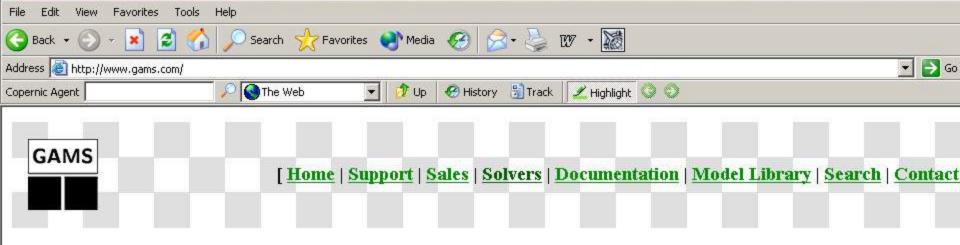
Illustrative numerical example(s)

Existing and prospective applications

Illustrative references

GAMS (General Algebraic Modeling System)

- GAMS: development started as a research project at the World Bank (1976); GAMS Devpt. Corp. (1988)
- GAMS book by Brooke, Kendrick & Meeraus (1988); subsequent revisions; currently, extensive further documentation is available (papers, lectures, models,...)
- GAMS: integrates core model development/parser system and a range of connected solver options
- 10,000+ users in over 100 countries (2003)



Welcome to the GAMS Home Page!

The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming problems. It consists of a language compiler and a stable of integrated high-performance solvers. GAMS is tailored for complex, large scale modeling applications, and allows you to build large maintainable models that can be adapted quickly to new situations.

- An Introduction to GAMS
- Documentation (including FAQ)
- · Contributed Documentation
- Presentations, Books, Posters
- · Contributed Software
- · Courses and Workshops
- The GAMS Mailing List and Newsletter
- Visit our European Web Site
- The GAMS World
- Solution Specialists
- · Other Sites on the Web



 $\overline{} \rightarrow$

GAMS Solver Options

BARON Branch-And-Reduce Optimization Navigator for proven global solutions from The Optimization Firm

BDMLP LP solver that comes with any GAMS system

<u>CONOPT</u> Large scale NLP solver from ARKI Consulting and Development

<u>CPLEX</u> High-performance LP/MIP solver from Ilog

<u>DECIS</u> Large scale stochastic programming solver from Stanford University

DICOPT Framework for solving MINLP models. From Carnegie Mellon University

LGO Lipschitz global optimizer from Pinter Consulting Services

MILES MCP solver from University of Colorado at Boulder that comes with any GAMS system

MINOS NLP solver from Stanford University

MOSEK Large scale LP/MIP plus conic and convex non-linear programming system from EKA Consulting

MPSGE Modeling Environment for CGE models from University of Colorado at Boulder

MPSWRITE MPS file generator that comes with any GAMS System

OQNLP Multi-start method for global optimization from Optimal Methods Inc.

OSL High performance LP/MIP solver from IBM

OSLSE OSL Stochastic Extension for solving stochastic models

PATH Large scale MCP solver from University of Wisconsin at Madison

SBB Branch-and-Bound algorithm from ARKI for solving MINLP models

SNOPT Large scale SQP based NLP solver from Stanford University

XA Large scale LP/MIP system from Sunset Software

XPRESS High performance LP/MIP solver from Dash

GAMS Global Solvers

Available solvers:

BARON Branch-and-reduce solver system

by The Optimization Firm

LGO Global/nonlinear optimization solver suite

by PCS

OQNLP OptQuest/NLP solver system

by OptTek Systems and Optimal Methods

Key differences between the global solver options:

- underlying algorithms
- external solver needs
- optimality guarantees provided
- model forms they can handle
- model sizes they can handle

The Relevance of GO

Optimization is often based on highly nonlinear descriptive models; several important and general model-classes are: "Black box" systems design and operations (experimental design, response surface methods, confidential models,...)

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 GO Model

min f(x)

 $f: R^n \otimes R^1$

 $g(x) \leq 0$

 $g: R^n \bowtie R^m$

$$X_1 \leq X \leq X_U$$

 $x, x_l, x_u, (x_l < x_u)$ are real *n*-vectors

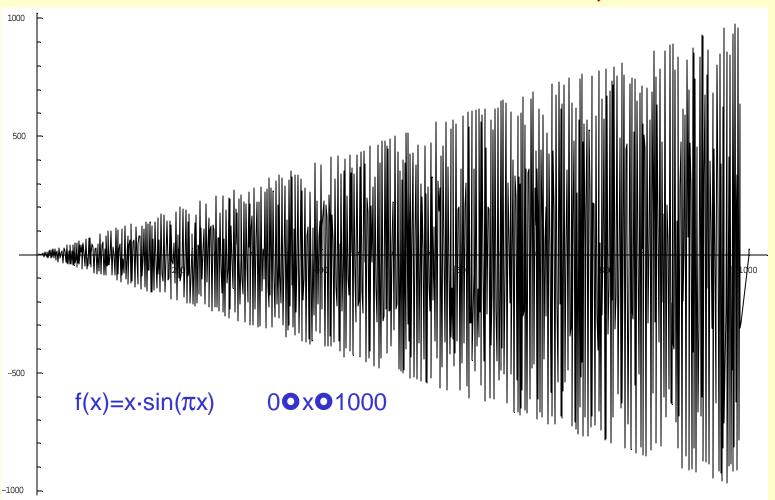
"Minimal" analytical assumptions:

- x_l , x_u finite
- feasible set $D=\{x_1 \le x \le x_u: g(x) \le 0\}$ non-empty
- f, g continuous

These guarantee the existence of global solution set X^* Typically, we assume that X^* is finite (at most, countable)

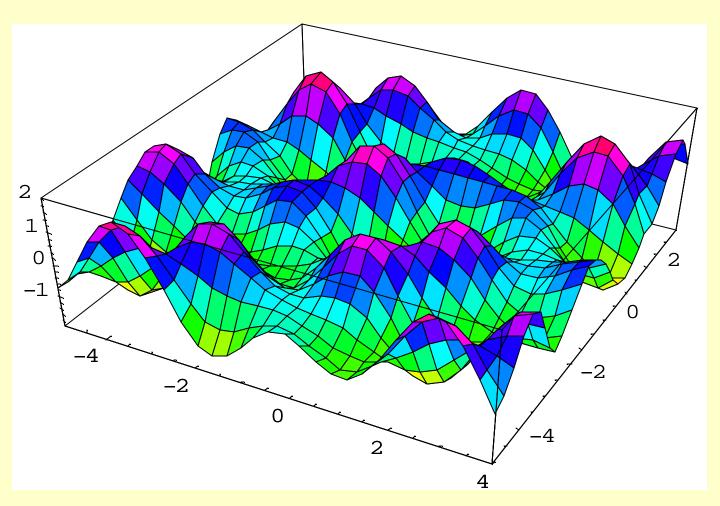
CGO covers a very general class of models, including <u>all</u> combinatorial and mixed integer (MIP) problems

Illustrative GO Model, *n*=1



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

Illustrative GO Model, *n*=2



Numerical difficulty may increase exponentially, as model size (n, m) grows

Solving GO Models

- Practical objective: solution estimates, on the basis of finite sequences of search points and corresponding function values $\{x_1,\ldots,x_k\}, \{f_1,\ldots,f_k\}, \{g_1,\ldots,g_k\}$ (Note: higher order information, as a rule, has no general value in the context of global search)
- If the functions f and g are Lipschitz-continuous, then based on the sample sequence deterministic lower/upper bounds can be derived; hence, a rigorous convergence theory can be developed $(|h(x_1)-h(x_2)| \le L||x_1-x_2||$ for $x_1,x_2 \ \ D$; $L=L(D,h) \ \ D$
- If the model functions are "only" continuous, then stochastic convergence is the best one can aim for: indeed, it can be properly established
- Implementation issues and challenges: "only a few details"...

LGO Solver Suite: General Scope

- The LGO (Lipschitz Global Optimizer) solver suite has been designed and developed with GO models in mind that do not or may not - have an easily identifiable and "exploitable" special structure
- This scope specifically includes "black box" models, and models with computable (perhaps non-analytical) functions: examples will be shown and listed later on
- Note that more structured GO models e.g. with convex, concave or indefinite QP objectives over convex domains also belong to the scope of LGO (as a rule, with a relatively small performance "hit", due to its "broad-minded" methods...)

LGO Solver Suite: Components

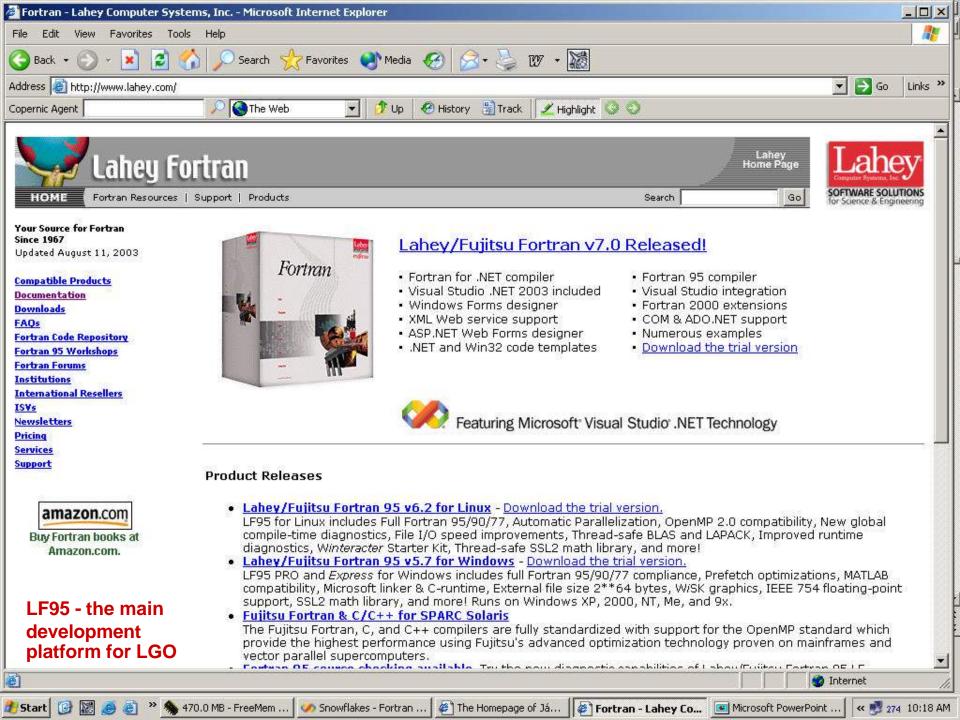
- LGO integrates several global search algorithms
 adaptive partition and search (branch-and-bound)
 adaptive random search
 adaptive multi-start
 and "traditional" local optimization methods
 exact penalty method, box-constrained local search
 generalized reduced gradient method
- This approach flexibly supports the search for global or local solutions in optimization models defined by continuous functions, w/o further necessary analytical conditions

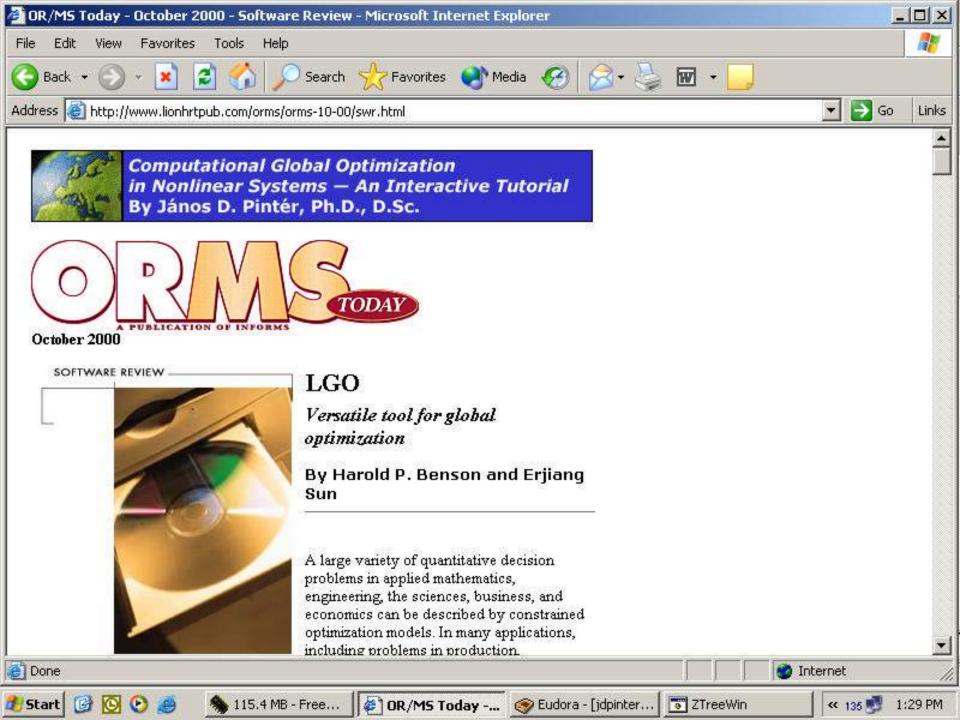
LGO Solver Suite: Characteristics and Implementations

- No external solver needs; combinations with local solvers are possible, and easy to add
- Optimality guarantees provided: exact and stochastic (deterministic, if model Lipschitz constants are known or can be properly over-estimated during optimization)
- Model forms handled: arbitrary continuous model functions
- Model sizes: in principle, arbitrary (depending on processor and RAM), but: "curse of dimensionality"... typical current delivery versions: thousand(s) of variables and constraints
- Customized versions of LGO implemented for several major modeling platforms; used in advanced scientific, engineering, and economic applications for over a decade



LGO modeling and solver system (+ IDE): MS Windows version







LGO Global Solver Engine for Excel - Premium Solver Platform

Innovative Solver for Global Optimization

Frontline Systems is excited to offer the **LGO Global Solver Engine** Version 5.0 for Microsoft Excel. The LGO Global Solver is a new field-installable Solver Engine that **"plugs into" the Premium Solver Platform**. It is designed for global optimization of problems with any continuous (convex or non-convex) functions, with up to 1,000 variables and 1,000 constraints. It also supports **integer variables**, and the new **"alldifferent" constraint** in the Premium Solver Platform V5.0.

Internet

Register What's New Solver Tutorial Solver Technology Select a Product Excel Users

> Developers Academic Users

Press/Analysts

Privacy Policy

Home

- New to Spreadsheet Solvers? Start with our Solver Tutorial
- Learn about LGO Global Solver Product Highlights (on this page)
- Learn about the exciting features built into the Premium Solver Platform
- Learn about the advanced methods used by the LGO Global Solver
- Learn about the ease of use features in the LGO Global Solver
- Users of earlier LGO Global Solvers: Learn the good news about upgrading!
- Users of other Solvers for Excel: Learn about competitive upgrade pricing!



solution. The solver integrator package supports the individual or combined use of the core solver packages, but both of the core packages can also be used in standalone mode. Further solver modules are under development and will be made

(also available from PCS)



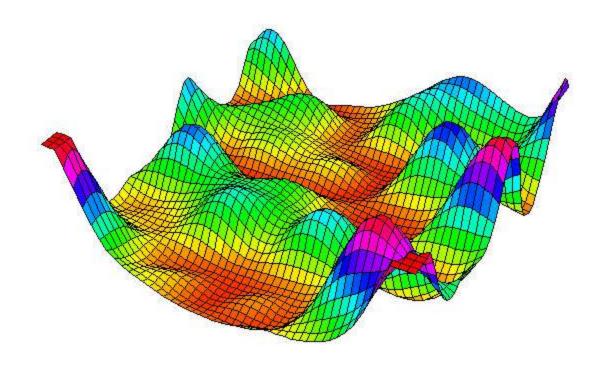


IcarCuida ph +

MathOptimizer Professional

An Advanced Modeling and Optimization System for *Mathematica* Users with an External Solver Link

User Guide



MathOptimizer and MathOptimizer Professional Software review in Scientific Computing World (July - August 2003)



HOME

SUBSCRIBE FOR FREE

NEWS

REVIEWS

FEATURES

PRODUCTS

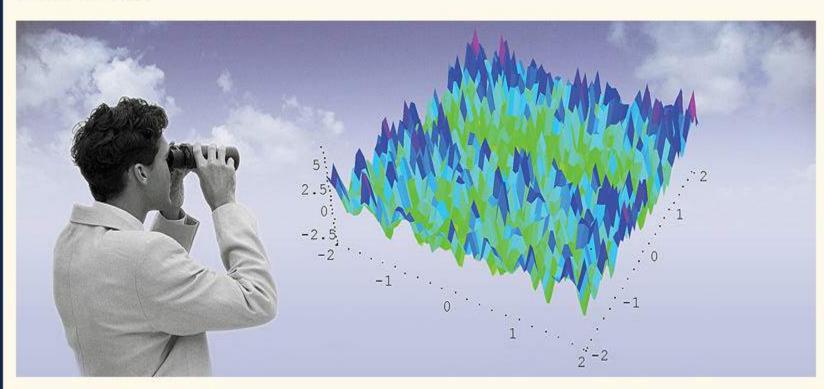
EVENT

MEDIA INFORMATION

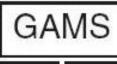
CONTACT US

ABOUT US

OPTIMISATION



HOW TO GET THE BEST OUT OF OPTIMISATION SOFTWARE



www.gams.com

Support

Sales

Solvers

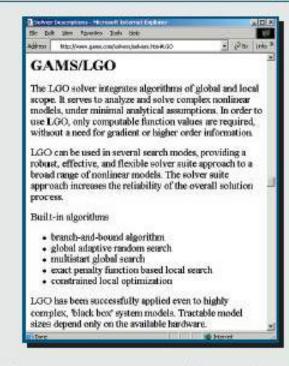
Documentation

Model Library

Search

Contact Us

LGO Global Optimization Solver

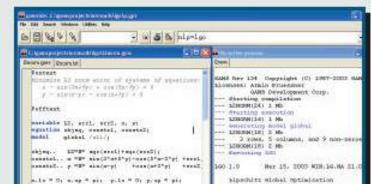


LGO has been successfully applied in many application areas:

Advanced Engineering Design

High performance and reliability of solvers come as a result of technological and theoretical developments in solution technology and modeling systems.

LGO is an integrated solver suite for handling nonlinear optimization models. The LGO solution approach is based on the seamless combination of globally convergent and traditional local search strategies.



GAMS/LGO Solver Operations

GAMS Model

Model description/preprocessing GAMS/LGO

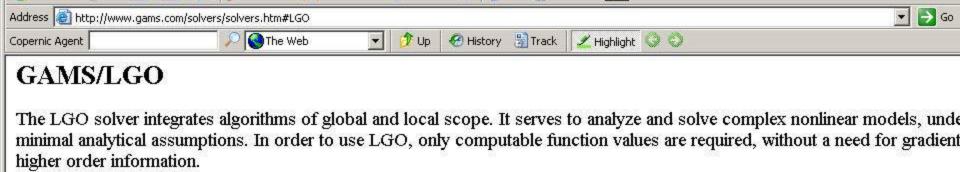
Solver options Solution report

LGO Solver Suite

Global search methods for multiextremal models

Local search methods for convex nonlinear models

Optional calls to other GAMS solvers and to external program systems



LGO can be used in several search modes, providing a robust, effective, and flexible solver suite approach to a broad range of

Search 🌟 Favorites 💕 Media 🪱

nonlinear models. The solver suite approach increases the reliability of the overall solution process.

LGO Solver Components

- branch-and-bound based global search
- multistart global search
- exact penalty function based local search
- constrained local optimization

Favorites Tools

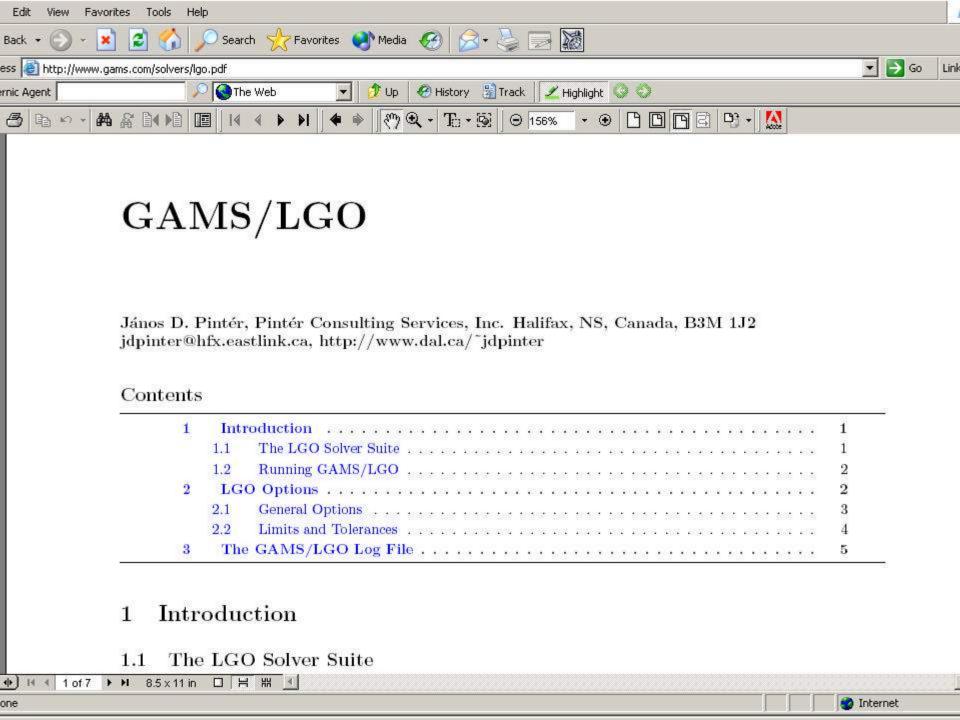
LGO has been successfully applied even to highly complex, 'black box' system models. Tractable model sizes depend only on available hardware.

Illustrative Application Areas

- advanced engineering design
- · econometrics and finance
- · medical research and biotechnology
- chemical and process industries
- scientific modeling







GAMS/LGO

General Options

Option	Description	Default
Opmode	Specifies the search mode used.	3
	0 Local search from the given nominal	
	solution without a preceding global	
	search (LS)	
	1 Global branch-and-bound search and	
	local search (BB+LS)	
	2 Global adaptive random search and	
	local search (GARS+LS)	
	3 Global multistart random search and	
	local search (MS+LS)	1000
Tlimit	Time limit in seconds. This is	1000
	equivalent to the GAMS option	
	reslim. If specified, this overrides the	
_	GAMS reslim option.	
Log_time	Iteration log time interval in seconds.	0.5
	Log output occurs every log_time	
	seconds.	_
Log_iter	Iteration log time interval. Log output	1
	occurs every log_iter iterations.	
Log_err	Iteration log error output. Error reported	10
	(if applicable) every log_err	
_	iterations.	
Debug	Debug option. Prints out complete LGO	0
	status report to listing file.	
	0: No	
	1: yes	
CallConopt	Number of seconds given for cleanup	10
	phase using CONOPT. CONOPT	
	terminates after at most CallConopt	
	seconds. The cleanup phase determines	
TT = 1	duals for final solution point. Prints out all available GAMS/LGO	
Help		
	solver options in the log and listing	
	files.	

GAMS/LGO

Limits and Tolerances

Option	Description	Default
G_maxfct	Maximum number of merit function	1000
_	evaluations before termination of global	*(n+m)
	search phase (BB, GARS, or MS). The	
	difficulty of global optimization models	
	varies greatly: for difficult models,	
	g_maxfct can be increased to	
	1.0E+6, or even larger values, as	
	needed.	
Max_nosuc	Maximum number of merit function	200
	evaluations in global search phase (BB,	*(n+m)
	GARS, or MS) where no improvement	
	is made. Algorithm terminates upon	
	reaching this limit.	
Penmult	Constraint penalty multiplier. Global	1
	merit function is defined as objective +	
	the violated constraints weighted by	
	penmult.	
Acc_tr	Global search termination criterion	-1.0E10
	parameter (acceptability threshold). The	
	global search phase (BB,GARS, or MS)	
	ends, if an overall merit function value	
	found in the global search phase is less	
	than acc_tr.	
Fct_trg	Partial stopping criterion in second local	-1.0E10
	search phase.	
Fi_tol	First local search merit function	1.0E-6
	improvement.	
Con_tol	Maximal constraint violation in local	1.0E-6
	search.	
Kt_tol	Kuhn-Tucker local optimality condition	1.0E-6
	tolerance.	
Irngs	Random number seed.	0
Var_lo	Smallest lower bound	-1.0E10
Var_up	Largest uppder bound	1.0E10
Bad_obj	Default value for objective function	1.0E10
	given evaluation errors.	

An Illustrative Test Model (N.L. Trefethen)

A Hundred-dollar, Hundred-digit Challenge

Each October, a few new graduate students arrive in Oxford to begin research for a doctorate in numerical analysis. In their first term, working in pairs, they take an informal course called the "Problem Solving Squad." Each week for six weeks, I give them a problem, stated in a sentence or two, whose answer is a single real number. Their mission is to compute that number to as many digits of precision as they can.

Ten of these problems appear below. I would like to offer them as a challenge to the SIAM community. Can you solve them? I will give \$100 to the individual or team that delivers to me the most accurate set of numerical answers to these problems before May 20, 2002. With your solutions, send in a few sentences or programs or plots so I can tell how you got them. Scoring will be simple: You get a point for each correct digit, up to ten for each problem, so the maximum score is 100 points.

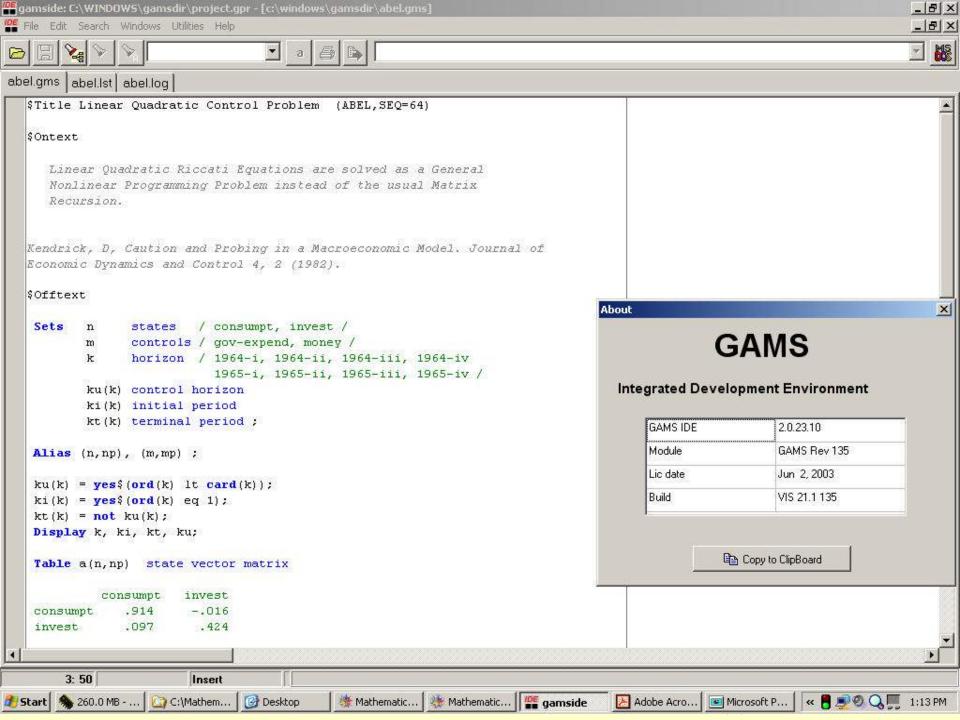
Fine print? You are free to get ideas and advice from friends and literature far and wide, but any team that enters the contest should have no more than half a dozen core members. Contestants must assure me that they have received no help from students at Oxford or anyone else who has already seen these problems.

Hint: They're hard! If anyone gets 50 digits in total, I will be impressed. The ten magic numbers will be published in the July/ August issue of SIAM News, together with the names of winners and strong runners-up.—Nick Trefethen, Oxford University.

The Hundred-dollar, Hundred-digit Challenge Problems

- 1. What is $\lim_{\kappa \to 0} \int_{\kappa}^{1} x^{-1} \cos(x^{-1} \log x) dx$?
- 2. A photon moving at speed 1 in the x-y plane starts at t = 0 at (x,y) = (0.5, 0.1) heading due east. Around every integer lattice point (i,j) in the plane, a circular mirror of radius 1/3 has been erected. How far from the origin is the photon at t = 10?
- 3. The infinite matrix A with entries $a_{11} = 1$, $a_{12} = 1/2$, $a_{21} = 1/3$, $a_{13} = 1/4$, $a_{22} = 1/5$, $a_{31} = 1/6$, etc., is a bounded operator on ℓ^2 . What is ||A||?
- 4. What is the global minimum of the function

 $\exp(\sin(50x)) + \sin(60e^y) + \sin(70\sin(x)) + \sin(\sin(80y)) - \sin(10(x+y)) + \frac{1}{4}(x^2+y^2)$?



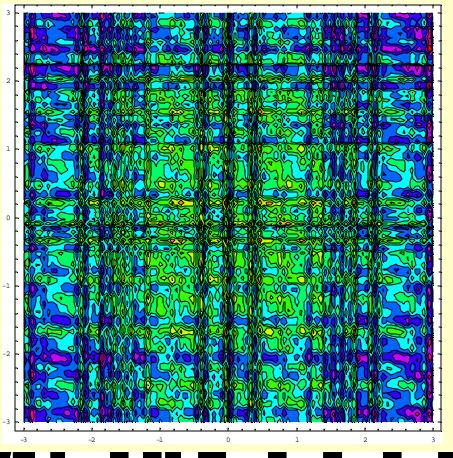
Trefethen's Problem 4 (continued)

```
$title Trefethen's HDHD 2002 Challenge, Problem 4
Sontext
Trefethen's GO model: a 2-var, 0-cons problem, with many local optima
Source: SIAM News, Jan - Feb 2002 issue
Solution: x^* \sim (-0.0244030796, 0.2106124272); f(x^*) \sim -3.306868647
Sofftext
variables f, x1, x2;
equations objf;
objf.. f = e = 0.25*(x1*x1+x2*x2) + exp(sin(50.*x1)) + sin(60.*exp(x2))
        +\sin(70.*\sin(x1)) + \sin(\sin(80.*x2)) - \sin(10.*(x1+x2));
model trefethen 4 / all /;
x1.lo = -3;
x1.1 = -2;
x1.up = 3;
x2.lo = -3;
x2.1 = 2;
x2.up = 3;
solve trefethen4 using nlp minimizing f;
                                                  // nlp=lgo option is set
```

Trefethen's Problem 4 (continued)

- Solution found by LGO:
 x* ~ (-0.0244030796, 0.2106124272);
 f(x*) ~ -3.306868647
- This solution is identical to at least 10 decimal digits to the "true" solution reported by SIAM News (July-August 2002)
- LGO runtime << 1 second (P4 desktop PC)

Trefethen's Problem 4 Contour Plot of Objective Function



Thousands of local optima; a single global solution...



Advanced GO Applications

An Illustrative List

The list below is primarily based on actual (PCS client) case studies and projects, and a few articles / reports

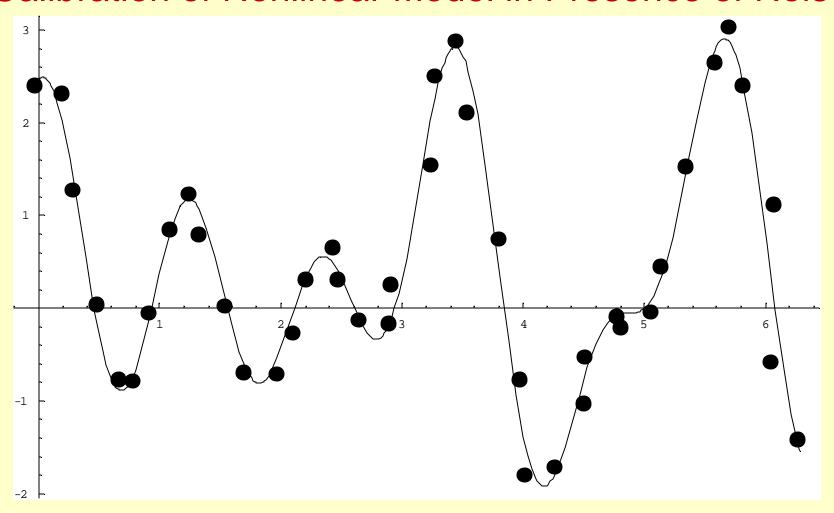
- Chemotherapy and radiotherapy design
- Computational physics and chemistry
- Chemical data and process analysis
- Data classification (clustering) and visualization
- Differential equations (numerical solution)
- Engineering design
- Experimental design
- Environmental engineering
- Financial model development

Application Examples (Continued)

- Laser design
- Model fitting to experimental data (in various calibration or forecasting contexts)
- Packing and loading configuration design
- Resource / population (fish stock,...) management
- Robotics (grasp) design
- Staff scheduling
- Systems of (nonlinear) equations and inequalities
- Vehicle routing and scheduling
- Waste-water engineering system design and some other areas

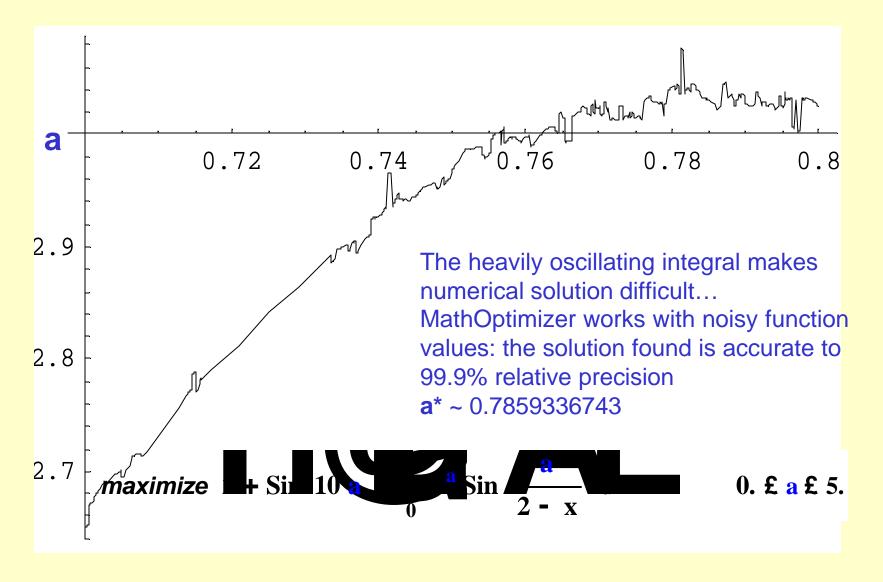
Several advanced applications are highlighted on the next slides

Calibration of Nonlinear Model in Presence of Noise

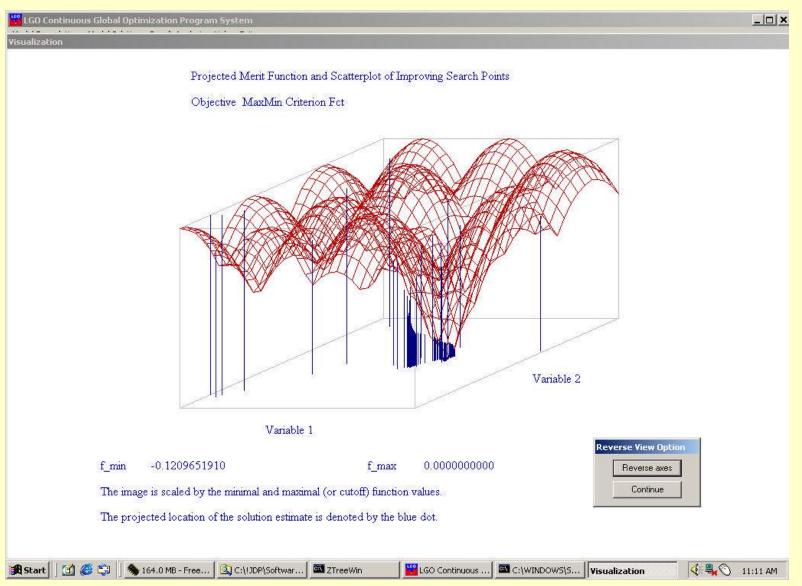


a+Sin[b*(Pi*t)+c]+Cos[d*(3Pi*t)+e]+Sin[f*(5Pi*t)+g] +ξ Globally optimized model fit (found by MathOptimizer)

HDHD Challenge, Problem 9: Parametric Integration



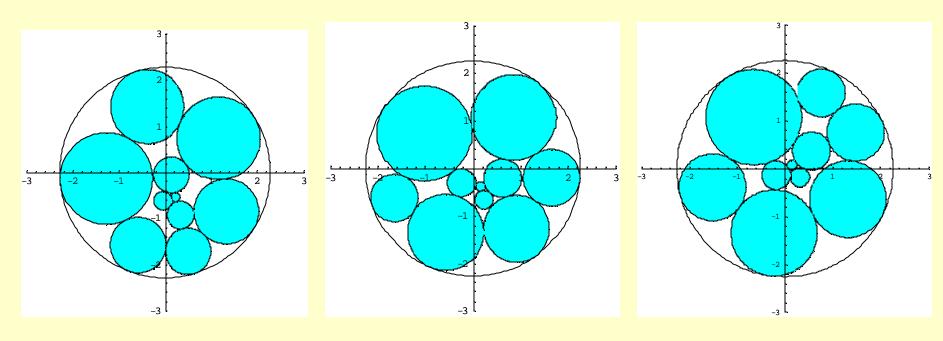
MaxiMin Point Arrangement Problem (U. of Tilburg, NL)



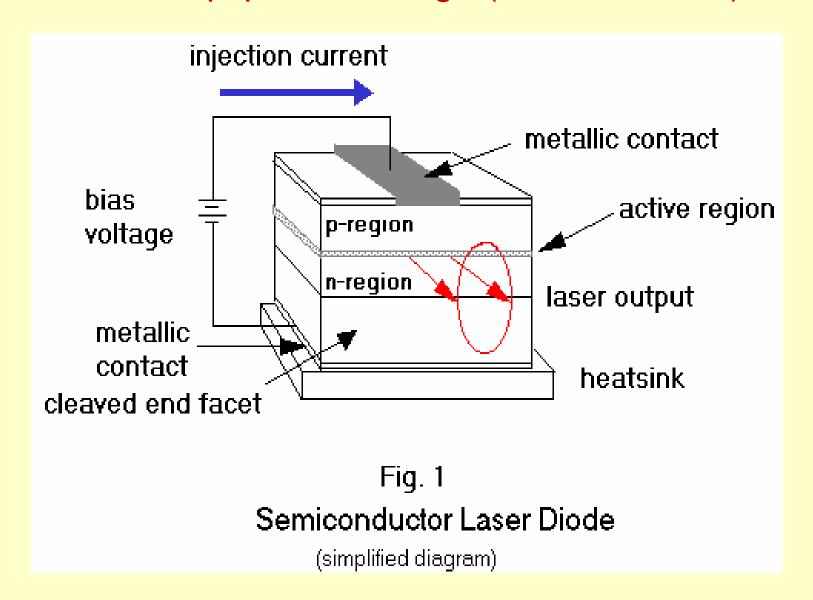
LGO IDE: model visualization (m=13, d=2)

Non-Uniform Circle Packings

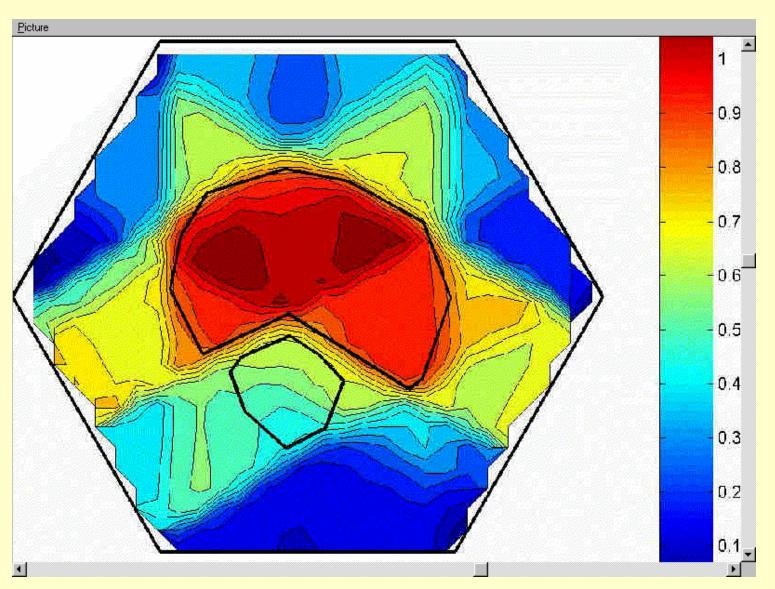
On the pictures shown below, 10 circles - with radii 0.1, 0.2,..., 1.0 - are arranged; equal consideration is given to the "tightness" of the configuration and the radius of the embedding circle (emb_c_rad)



Laser Equipment Design (NRC, Canada)

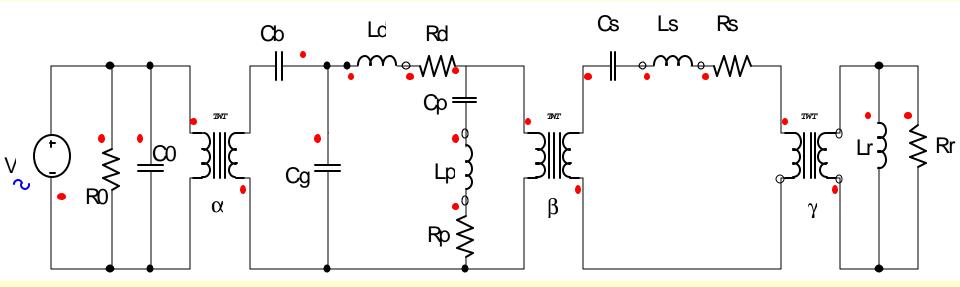


Intensity Modulated Radiotherapy (U. of Kuopio, FI)



Globally optimized dose distribution

Sonar Transducer Design: Numerical Model (DRDC)

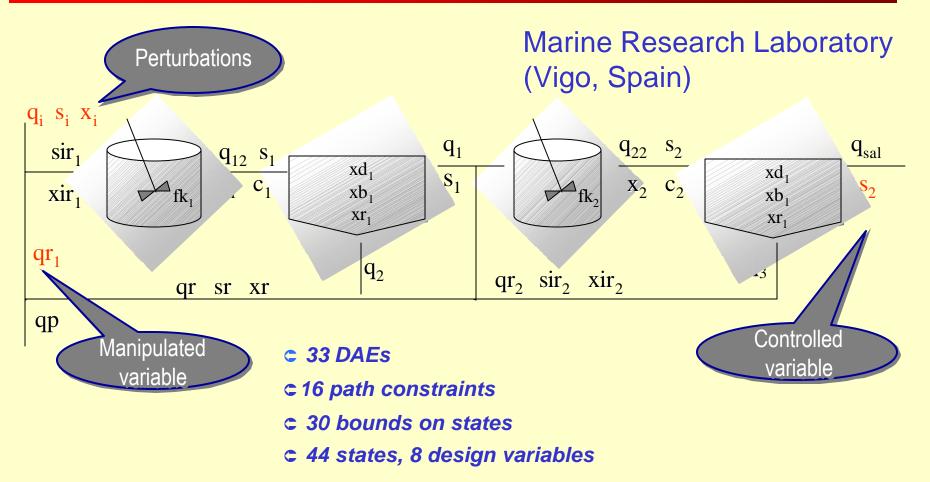


This electric circuit simulates a piezoelectric sonar projector

The optimization problem consists of finding a set of 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

Integrated Design and Operation of Waste-Water Plant



Objective: to find the design of the units, the operating conditions and the parameters of the controller which minimize a weighted sum (C) of economic terms (f_{econ}) and a controllability measure (ISE)

This model has been analyzed and solved using an LGO DLL version

Conclusions

- Brief Review:
 GAMS, GO, LGO
 LGO solver modes
 Illustrative applications
- Benefits of Global Optimization:
 Globally sought (hence, often improved) solutions
 Added modeling freedom: more realistic models, new possibilities and markets
- Models welcome; additional documentation available Workshops, consulting services offered

Illustrative References

- Over one hundred GO books
- Kluwer AP Non-Convex Opt. And its Appls. series: 60+ volumes (2003)
- Handbook of GO, Vols. 1-2
- J. of Global Optimization
- J. of Heuristics
- Many thousands of research articles and reports

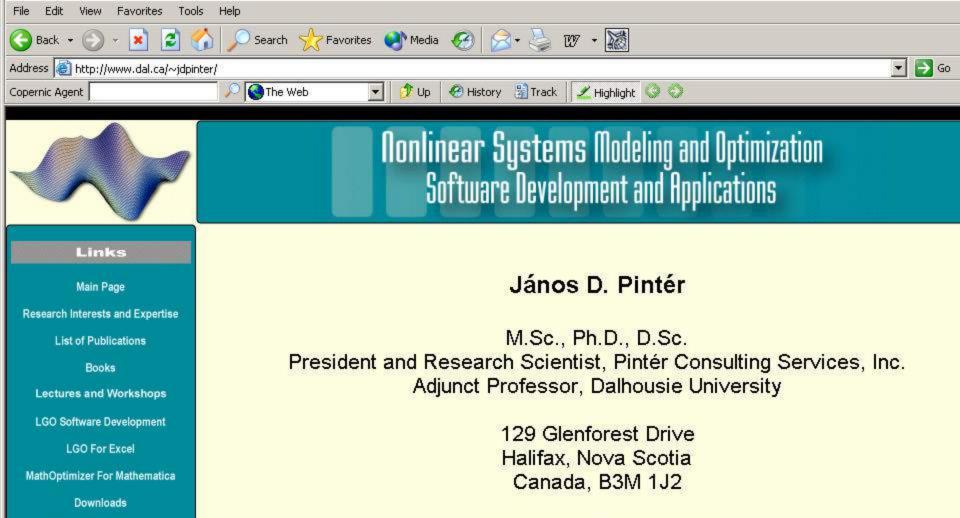
. . .

Illustrative References (cont'd)

Some recent work by JDP & colleagues

- Chapter 15 in Handbook of Global Optimization, Vol. 2
- Radiotherapy: Tervo et al; Annals of Opns. Res. (2003)
- Model calibration: JDP; Opt. Methods & Software (2003)
- Laser design: Isenor, JDP & Cada, Opt. & Engrg. (2003)
- MathOptimizer / MathOptimizer Pro applications:
 Kampas and JDP; The Mathematica Journal (to appear)
- Global Optimization: Selected Case Studies JDP, ed.; Kluwer AP (forthcoming)
- Nonlinear optimization in modeling environments (in ed. Vol.)
- Numerical GO tests: Khompatraporn, JDP & Zabinsky;
 J. of Glob. Opt. (to appear)
- GAMS/LGO: JDP and Pruessner (work in progress)
- MathOptimizer and ModelMaker: JDP and Purcell (w.i.p.)

. . .



Phone: 1-(902)-443-5910

Fax: 1-(902)-431-5100 (work and software orders only)

E-mail: jdpinter@is.dal.ca
URL address: http://www.dal.ca/~jdpinter/



Selected Professional Links

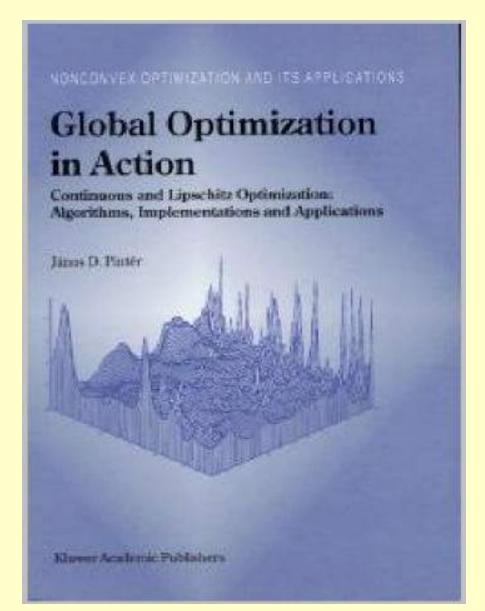
Personal Interests

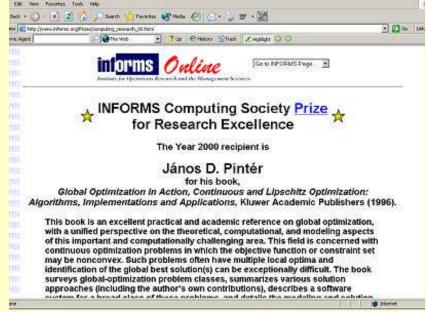
Dalhousie University Homepage

Website Design

Contact







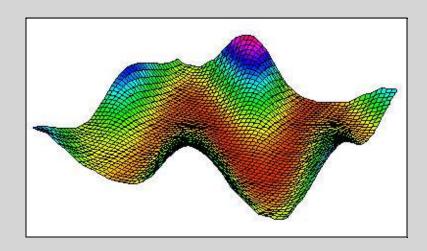
Research monograph: theoretical background of LGO solvers; applications



"Easygoing" e-book; GO review, includes demos of the LGO IDE

Global Optimization

Scientific and Engineering Applications with Mathematica® Examples

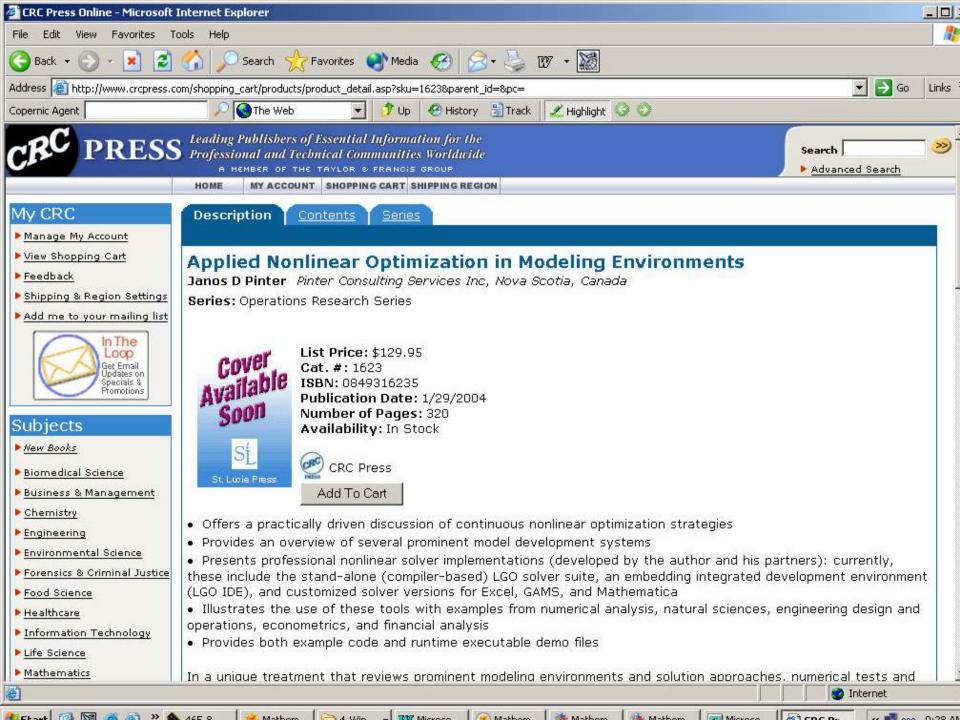


János D. Pintér

ELSEVIER

SCIENCE

Joint work with Frank J. Kampas (forthcoming, 2004)



Thanks for your attention!

