Advanced Nonlinear Optimization with *Mathematica*

MathOptimizer and MathOptimizer Professional

János D. Pintér and Frank J. Kampas

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Lecture Topics

- *Mathematica* in Operations Research
- LGO solver suite (with optional IDE demo)
- MathOptimizer (MO)
- MathOptimizer Professional (MOP)
- Illustrative MO and MOP applications
- References
- MO, MOP demonstrations (as time allows, or after talk)

Acknowledgements

- Wolfram Research — R&D support (since ~ 1995)
- Chris Purcell, DRDC — MO development support
- Mark Sofroniou (WR) — Format.m adaptation in MOP

Wolfram Research, Developers of *Mathematica*

Mathematica: Key Features

- integrated environment for modeling and computing
- mathematical knowledge and computational power
- concise and elegant code development in procedural, functional, and rule-based paradigms
- sophisticated interactive notebook documents, from raw ideas to meticulous details: computations, text, graphics, animation, sound,…(cell development steps or units)
- support for rapid prototyping and application development
- portability across hardware platforms (notebook standard)
- integrated, ‘one-stop’ solution

Mathematica in Operations Research

- O.R. is *"The Science of Best"* (Quantitative Decisions)
- INFORMS, IFORS, EURO, MPS, SIAM, … and other organizations; total membership ~$O(10^5)$; visit e.g. www.informs.org
- Integrated computing systems, such as *Mathematica*, have a significant potential in nonlinear systems modeling and optimization
- Systems built by individual building blocks: these are often based on computationally intensive modules. Examples: d.e. systems, integrals, special functions, Monte Carlo simulation, etc.
- Resulting nonlinear model could well be multi-extremal

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The Potentials of *Mathematica* in Operations Research and Related Applications

Author

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URL: http://www.dal.ca/~jdpinter/

Contents

White paper discussing *Mathematica*'s role in operations research

Description

This informal article aims at addressing a broad range of *Mathematica* users. A concise review of the quantitative decision-making, modeling and solution paradigm of Operations Research is provided, with an emphasis on using *Mathematica* in this process.

Subject

- Applied Mathematics > Complex Systems

Keywords

operations research, decision-making, quantitative models and algorithmic solution procedures

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Continuous Global Optimization Model

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

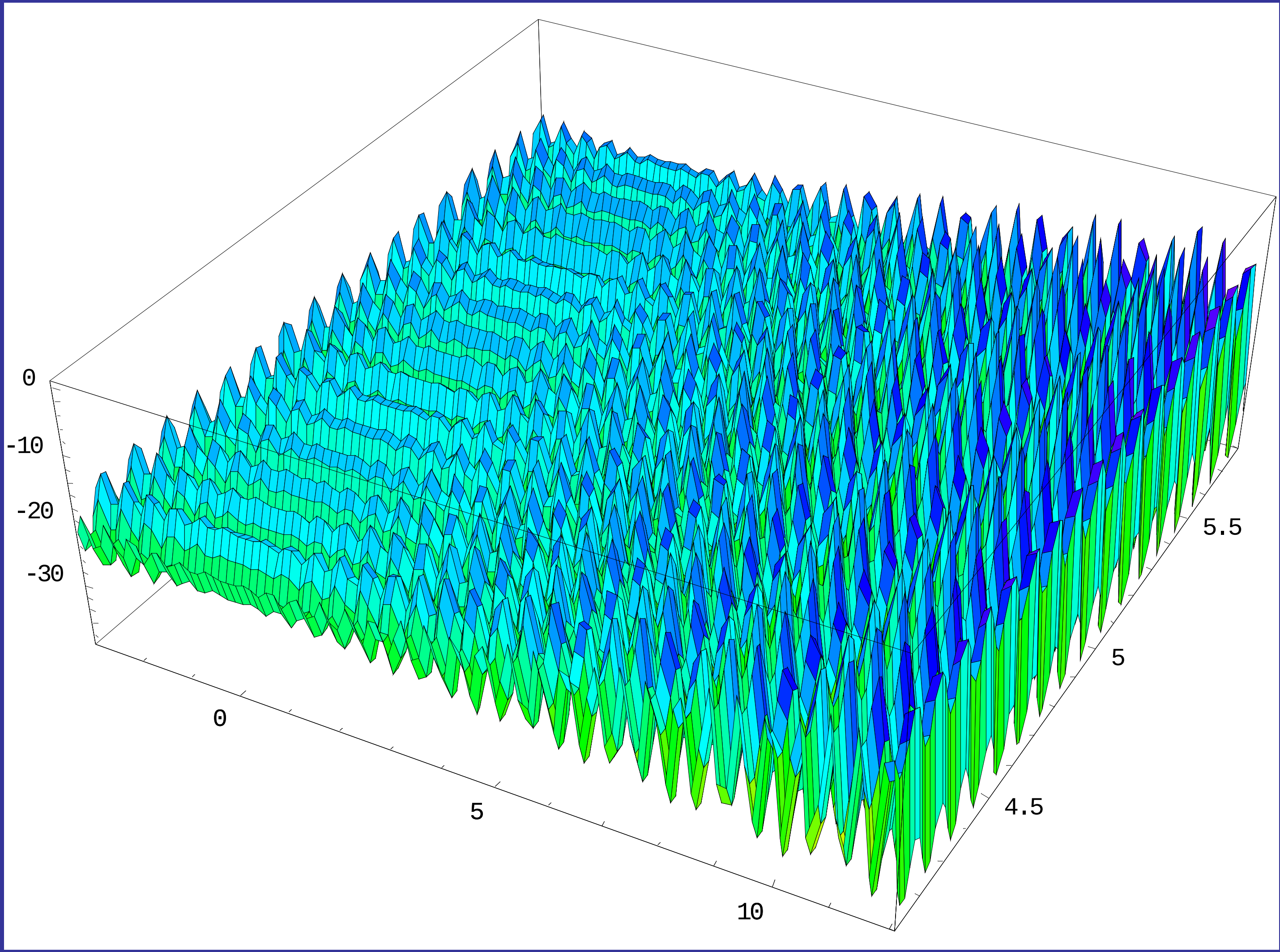
CGO covers a very general class of models
Other (equivalent) model forms are also used

'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 continuous, g continuous (component-wise)

These guarantee that the CGO model has solutions

An Example CGO Problem (by Michalewicz, MOP manual)



The Year 2000 recipient of the INFORMS Computing Society Prize for Research Excellence in the Interface Between Operations Research and Computer Science

Global Optimization in Action

Continuous and Lipschitz Optimization: Algorithms, Implementations and Applications

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by
János D. Pintér
Pintér Consulting Services, Dalhousie University, Halifax, Canada

Book Series: NONCONVEX OPTIMIZATION AND ITS APPLICATIONS : Volume 6

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.

Audience: Professors, students, researchers and other professionals in the fields of operations research, management science, industrial and applied mathematics, computer science, engineering, economics and

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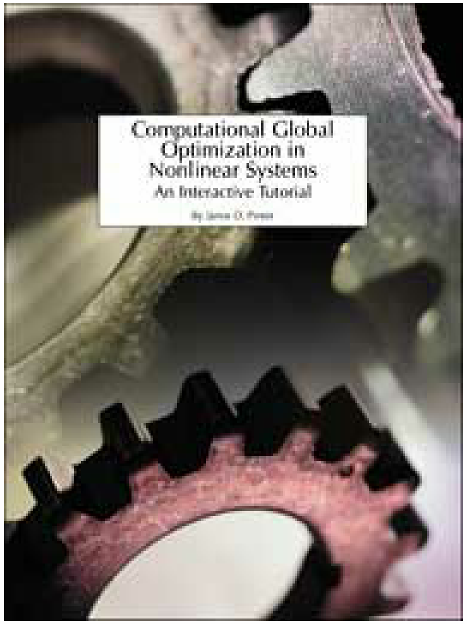
Computational Global Optimization in Nonlinear Systems

An Interactive Tutorial

By
János D. Pintér, Ph.D., D.Sc.



Pages: 61
PDF Price: $15.00
— includes downloadable demo software
Print Price: $19.00
(Plus Shipping & Handling)
— includes demo software on diskette

ORDER INFORMATION

"Computational Global Optimization in Nonlinear Systems," by János Pintér, presents a concise, practical introduction to models and algorithms that enable the analysis and solution of nonlinear decision problems in the presence of multiple optima. Such problems arise in many

MathOptimizer

- Native *Mathematica* package
- Global (MS) and local (CNLP) solver components
- Solver integrator package, with a view towards planned extensions
- User Guide (~75 printed pages): mathematical background, modeling tips, local and global optimization test examples, illustrative applications, references
- User Guide can be directly activated, as part of the on-line help system of *Mathematica*

MathOptimizer: Product Information - Microsoft Internet Explorer

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MathOptimizer

An Advanced Modeling and Optimization System for *Mathematica* Users

MathOptimizer enables the global and local numerical solution of a very general class of optimization problems defined by a finite number of real-valued, continuous functions over a finite *n*-dimensional interval region.

A special emphasis is placed upon nonlinear models, including those that typically have an unknown number of local optima. Nonlinear and global optimization problems are ubiquitous in the sciences, engineering, and economics. Several prominent examples are systems of nonlinear equations and inequalities, nonlinear regression, forecasting models, data classification, minimal energy models, various packing problems, risk management and other stochastic decision problems, and the design and operation of "black box" engineering systems (possibly defined by a complicated, numerically intensive procedure).

MathOptimizer currently consists of two core solver packages and a solver integrator package. The first core solver package is used for approximate global optimization of an aggregated merit (exact penalty) function on a given interval range. This package is based on a globally convergent adaptive stochastic search procedure, and it also incorporates statistical estimation techniques.

The second core solver package is meant for precise local optimization. It is based on the standard nonlinear (convex) programming approach and refines a given initial 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 stand-alone mode. Further solver modules are under development and will be made

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MathOptimizer Professional with LGO Solver Link

- LGO Development since ~ 15 years
- Global solver options: BB, GARS, MS (EPM)
- Local solver options: GRG
- LGO 'silent mode' implementation, with text I/O interface
- LGO IDE, with Windows interface
- Various platform-specific implementations including MathOptimizer Professional for *Mathematica*
- LGO peer-reviewed in ORMS Today (2000)
- LGO demo included in LPI tutorial and in the new edition of the classic textbook Hillier and Lieberman, *Introduction to Operations Research*

ORMS TODAY
A PUBLICATION OF INFORMS
October 2000

SOFTWARE REVIEW

LGO

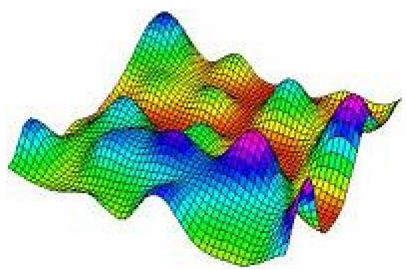
Versatile tool for global optimization

By Harold P. Benson and Erjiang Sun

A large variety of quantitative decision problems in applied mathematics, engineering, the sciences, business, and economics can be described by constrained optimization models. In many applications, including problems in production

MathOptimizer Professional

An Advanced Nonlinear Optimization Environment for *Mathematica* with an External LGO Solver Link



MathOptimizer Professional enables the global and local solution of a general class of continuous optimization problems. The model form considered is:

$$\min f(x) \quad \text{subject to} \quad x \in D \subset R^n \quad D := \{x: xl \le x \le xu \quad g(x) \le 0\}$$

Here $x \in R^n$ is the vector of decision variables (R^n denotes the Euclidean real n-space); $f: R^n \rightarrow R^1$ is a continuous objective function; $D \subset R^n$ is the nonempty set of feasible decisions defined by explicit, finite (with respect to components) lower and upper bounds xl and xu and by a collection of continuous constraint functions $g: R^n \rightarrow R^m$. (Obviously, $g(x) \le 0$ formally covers all cases of $g(x) \sim 0$, where ~ denotes any of the operators =, ≤, and ≥.)

MathOptimizer Professional
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MathOptimizer and MathOptimizer Professional software review
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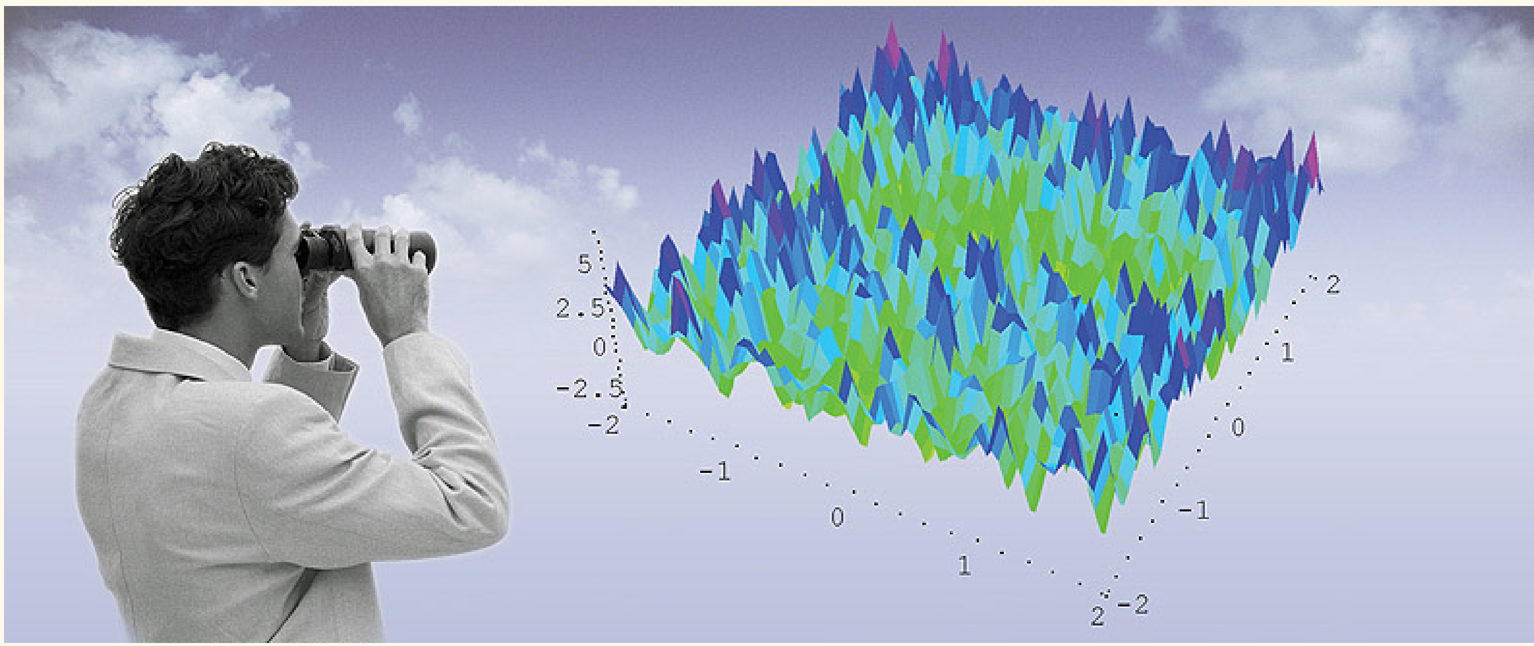
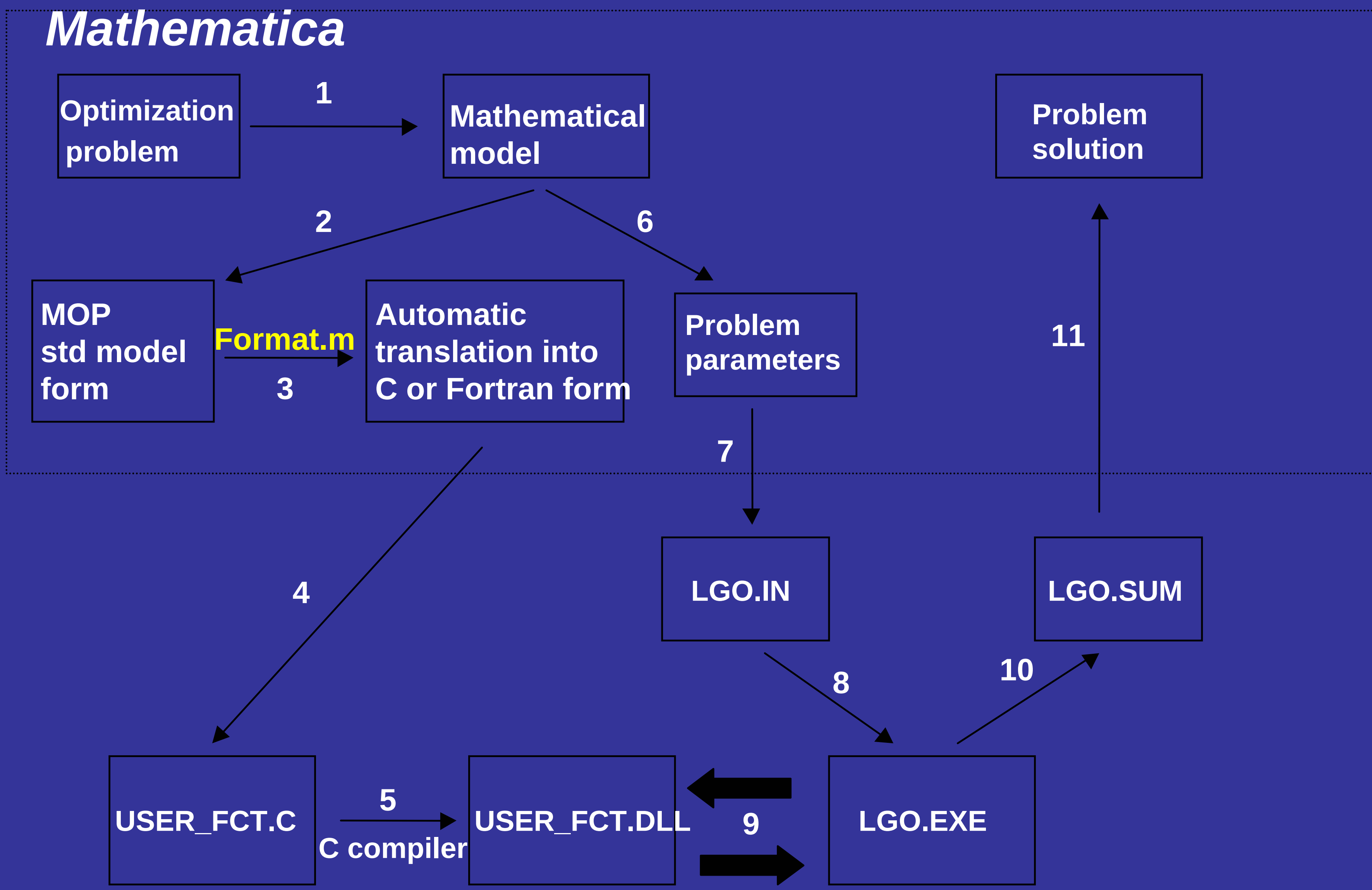


HOW TO GET THE BEST OUT OF OPTIMISATION SOFTWARE



MathOptimizer Professional Operations

* Acknowledgement to Mark Sofroniou

MathOptimizer Professional Options and Parameters

Option Name	Notes and Alternatives
ShowSummary Ø False	Display LGO report (LGO.SUM)
Method Ø MSLS	BBLS, MSLS, LS
MaxEvals Ø ProblemDetermined	Set by user (global search effort)
MaxNoImprov Ø ProblemDetermined	Set by user (global search effort w/o i.)
PenaltyMul Ø 1	Set by user (penalty multiplier)
ModelName Ø LGO Model	Model-dependent name
DllCompiler Ø VC	List of supported compilers
ShowLGOInputs Ø False	Display USER_FCT.C, LGO.IN
LGORandomSeed Ø 0	Set by user
TimeLimit Ø 300	Set by user
TOBJFGL Ø -1000000	Target objfct in global search phase
TOBJFL Ø -1000000	Target objfct in local search phase
MFPI Ø 10^{-6}	Merit fct precision improvement
CVT Ø 10^{-6}	Constraint violation tolerance
KTT Ø 10^{-6}	KTT optimality condition tolerance

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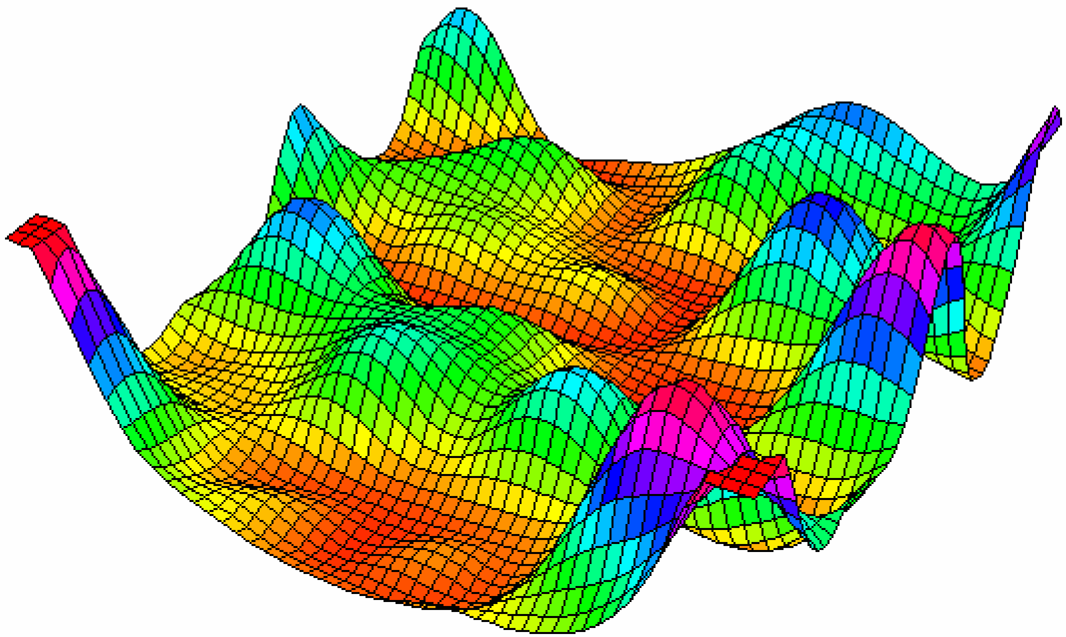
MathOptimizer Professional

An Advanced Modeling and Optimization System

for *Mathematica* Users with an External Solver Link

User Guide



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UserGuide.nb *

- Ratschek and Rokne Test Problem
- SinPoly Test Problem
- SinPoly2 Test Problem
- A Non-Convex Test Problem-Class
- Michalewicz Test Problem, and its Constrained Extensions
- Trefethen's HDHD 2002 Challenge, Problem 4
- A Simple Industrial Design Problem
- Circuit Design Test Problem
- Systems of Equations and Inequalities: An Example
- Portfolio Selection
- Catenary (Hanging Chain) Model
- Hilbert Test Problem
- Box Test Problem
- Non-Uniform Circle Packings
- Models with Integer Variables
- A Nonlinear Boundary-Value Differential Equation
- Numerical Solution to a Differential Equation (Watson Problem)

MOP User Guide: a partial list of illustrative examples (test challenges and new GO applications)

Note: the auto-generated C or Fortran files can be used also in other tests and applications

100%

Illustrative Numerical Results: Circle Packing Problems

General model form

Optimized non-overlapping object packings in an embedding object

Examples studied and solved by MO and/or MOP

- Equal size circles in unit square: radius is maximized
- Equal size circles in unit circle: radius is maximized
- Non-uniform size circles: optimize circumscribing radius and tightness

All are difficult GO problems: k objects → $k(k\text{-}1)/2$ non-convex constraints, $O(k)$ additional constraints, and $O(2k)$ variables; proofs known only for a few cases (interval method applied to k=28: special B&B + 57-hr runtime…)

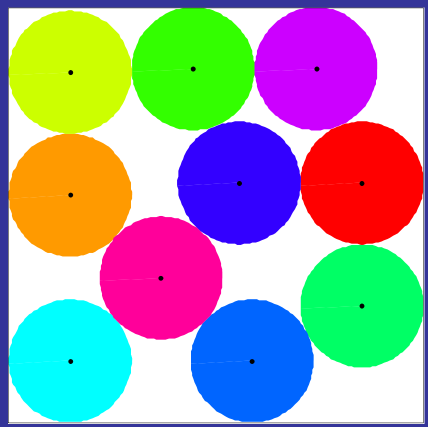
MO and MOP compares favourably to built-in *Mathematica* optimization functions and all third-party packages that we could try; notebooks available

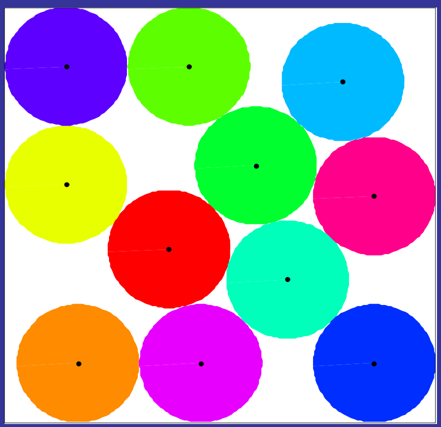
Illustrative Results: Circles in Unit Square

Results compare well to best known (w/o “tweaking”, for “small” values *k*);

see e.g. www.packomania.com (by E. Specht)

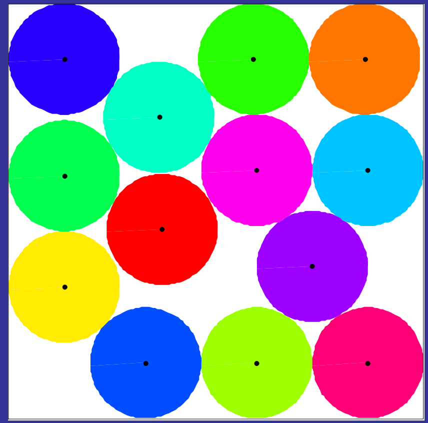
k=10
r~0.148204

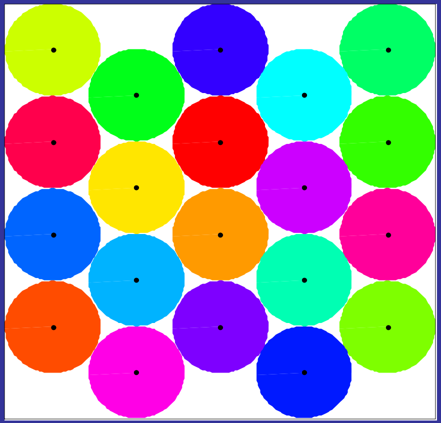




k=11
r~0.142399

k=13
r~0.133993





k=20
r~0.111382

MOP runtimes:
secs to mins

Illustrative Results: Circles in Unit Square

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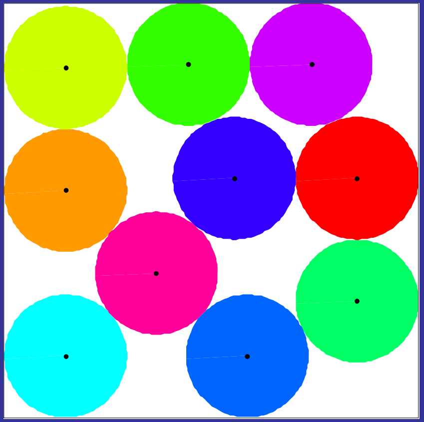
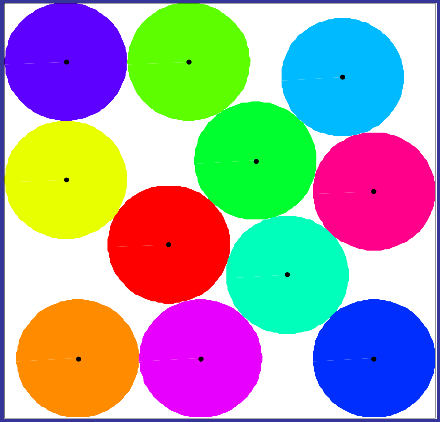
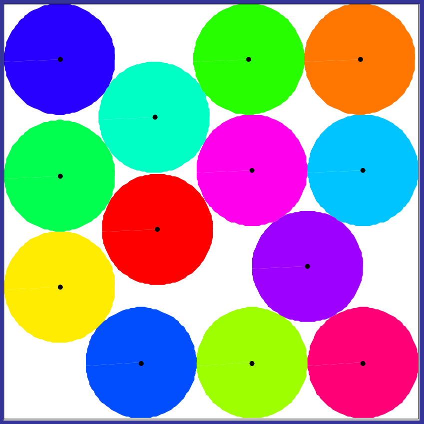
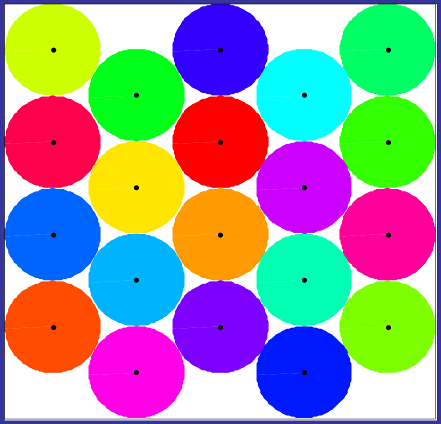




k=11
r~0.142399

k=13
r~0.133993

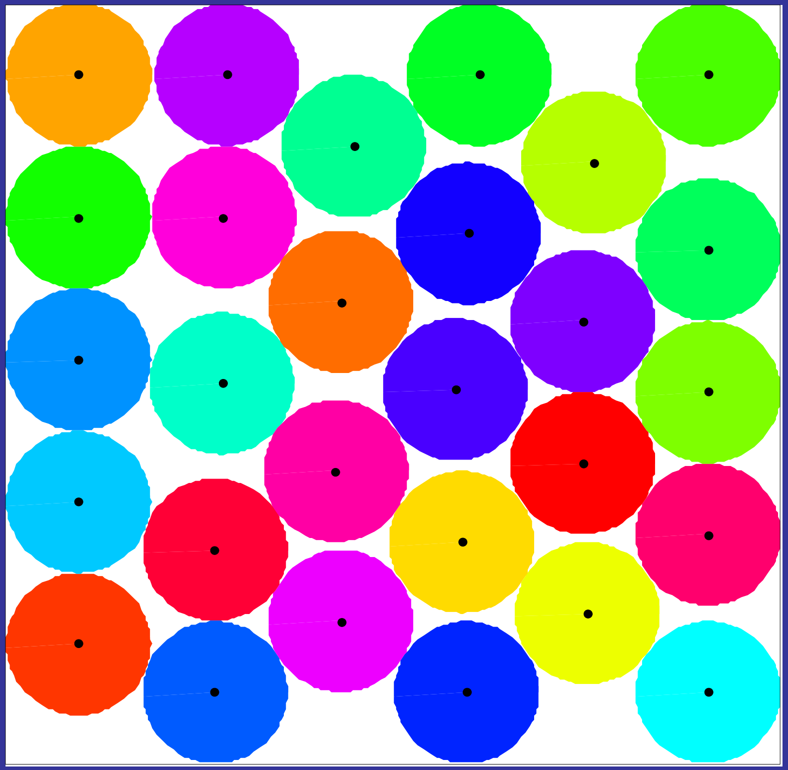




k=20
r~0.111382

MOP runtimes:
secs to mins

Illustrative Results: 28 Circles



k=28 *r*~0.0936719714 vs. guaranteed *ropt*~0.093672833833
Runtime: 1052 Seconds (P4 1.6 GHz)

Generalized Circle Packings

Circles with radii $r(i)=i^{-1/2}$, for $i=1,\ldots,k$ (other models also considered)

Obj1=radius of the embedding circle centered at the origin (standardization)

Obj2=average distance between the centers of all of the pairs of circles

Obj=0.5*(Obj1+Obj2)

Added model standardization:

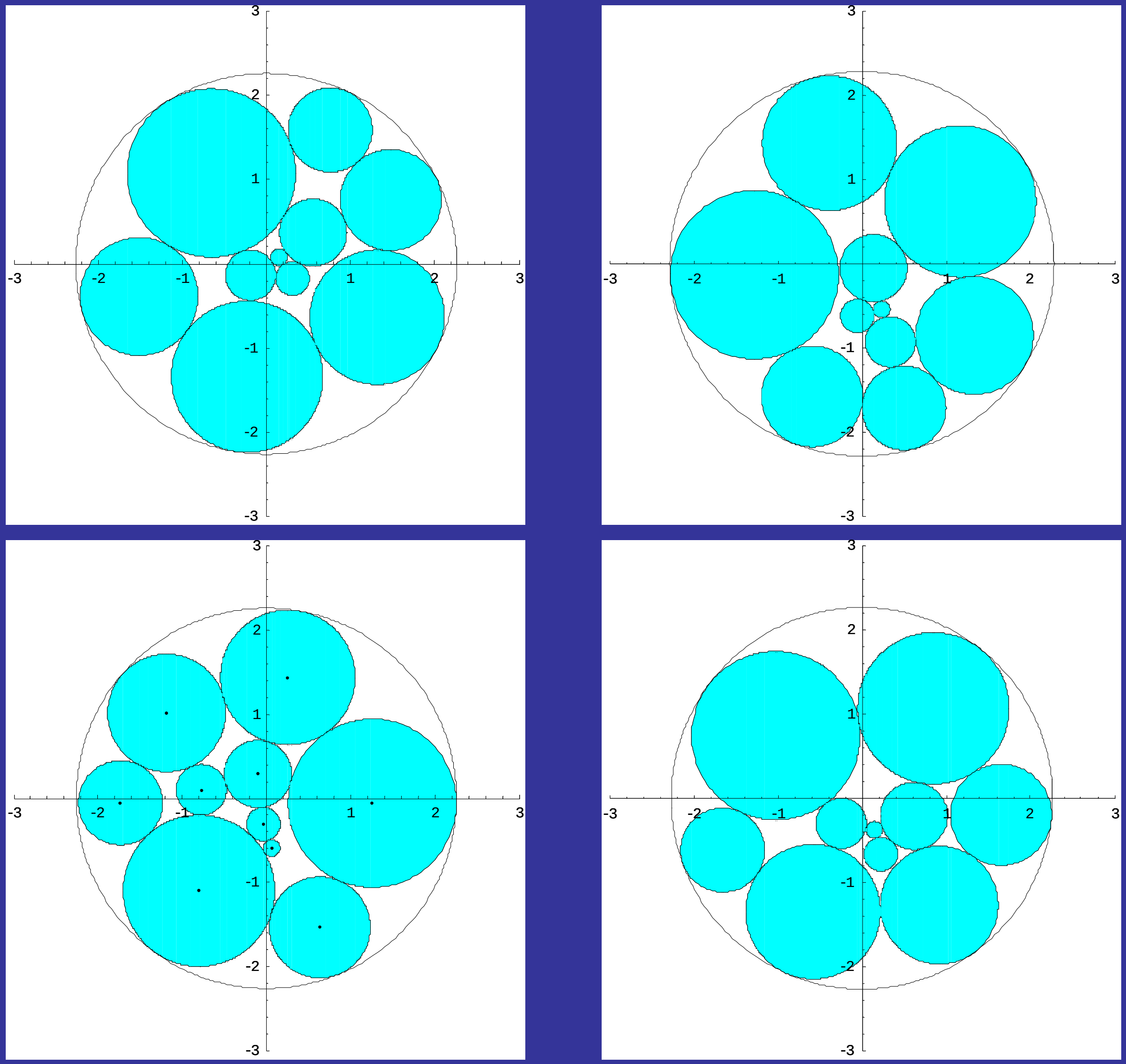
position of circle 1, relative position of circles 2, 3

Solutions found by *MathOptimizer Professional*, up to k=40

Runtimes: ~1.5 sec (n=3) to ~ 7 hours (k=40) (P4, 1.6 GHz desktop PC)

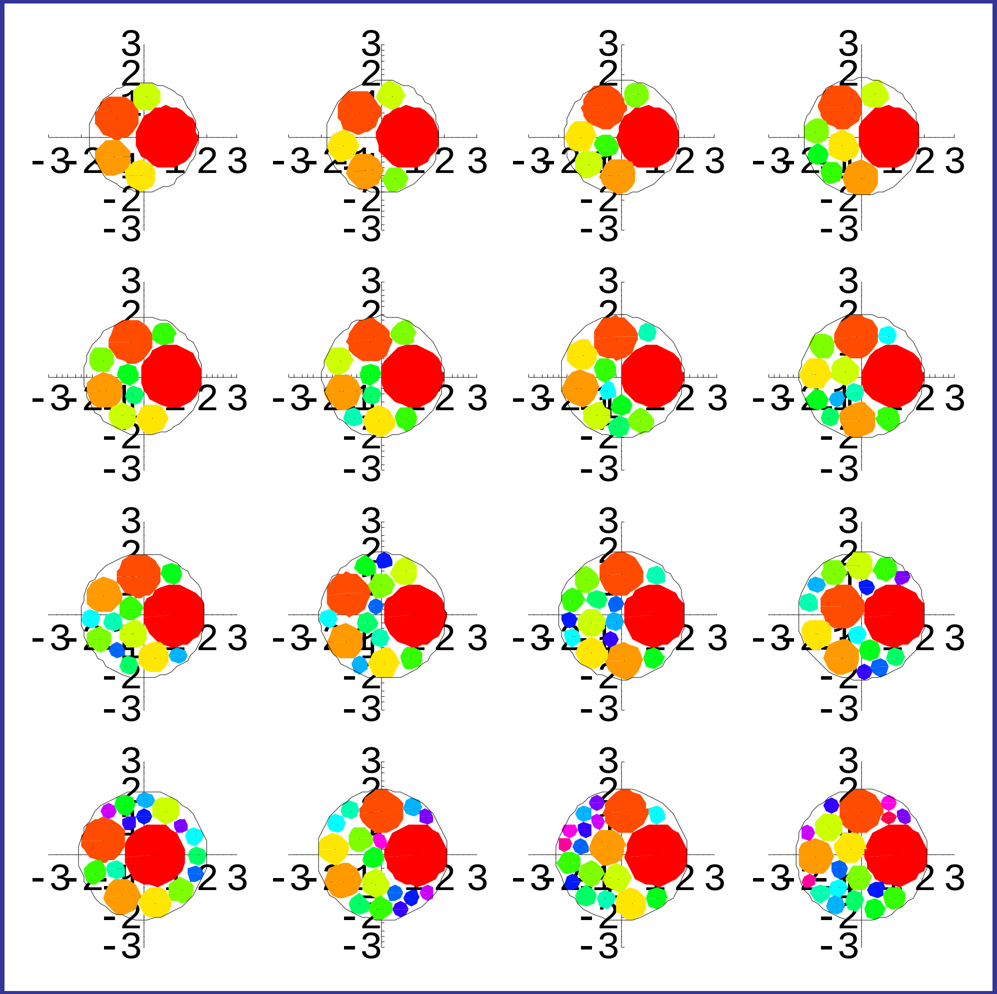
Note: built-in *Mathematica* optimization functions could *not* produce good quality solutions

Illustrative Results: Circle Packings



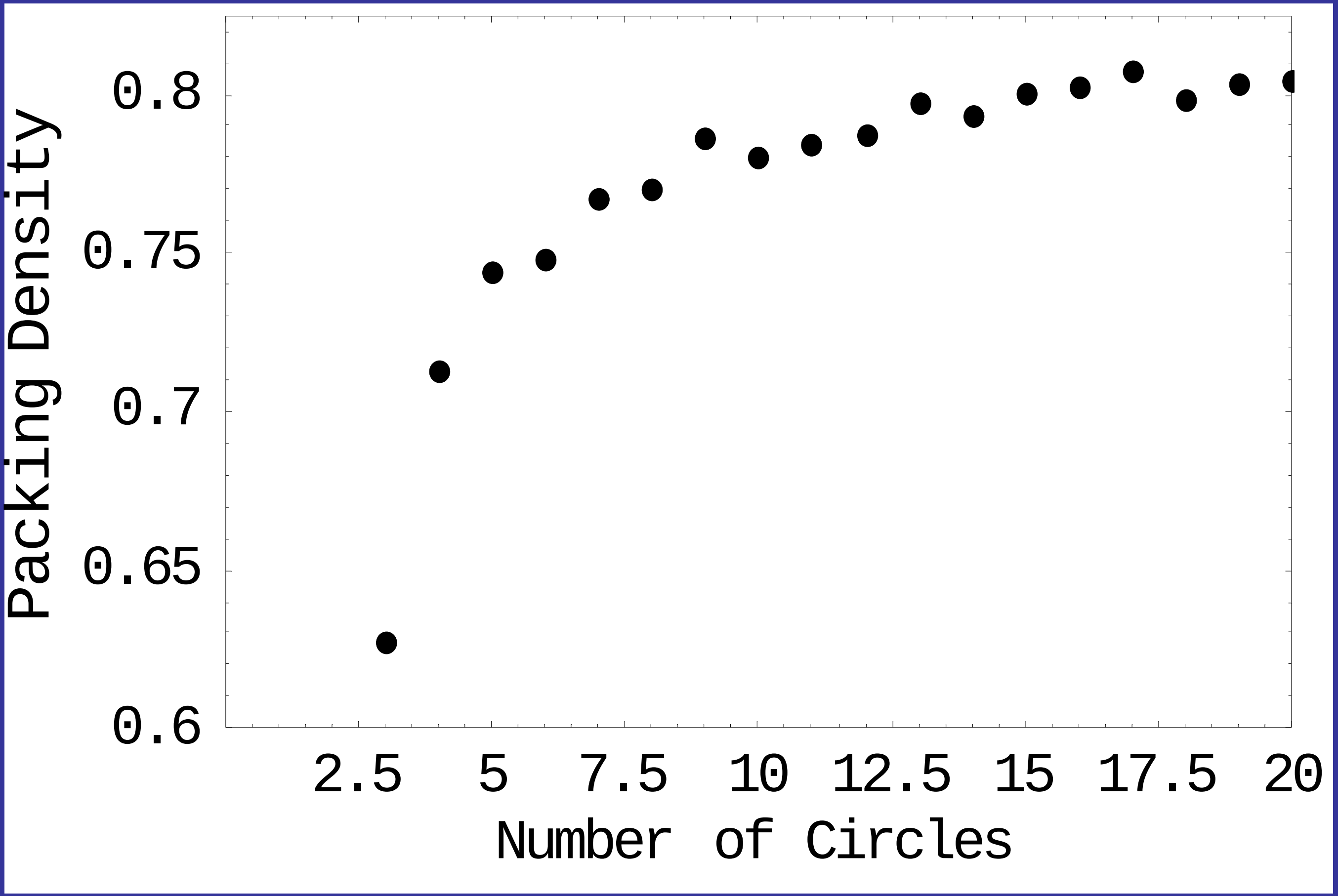
Several 10-circle arrangements of nearly equivalent quality

Illustrative Results: Circle Packings



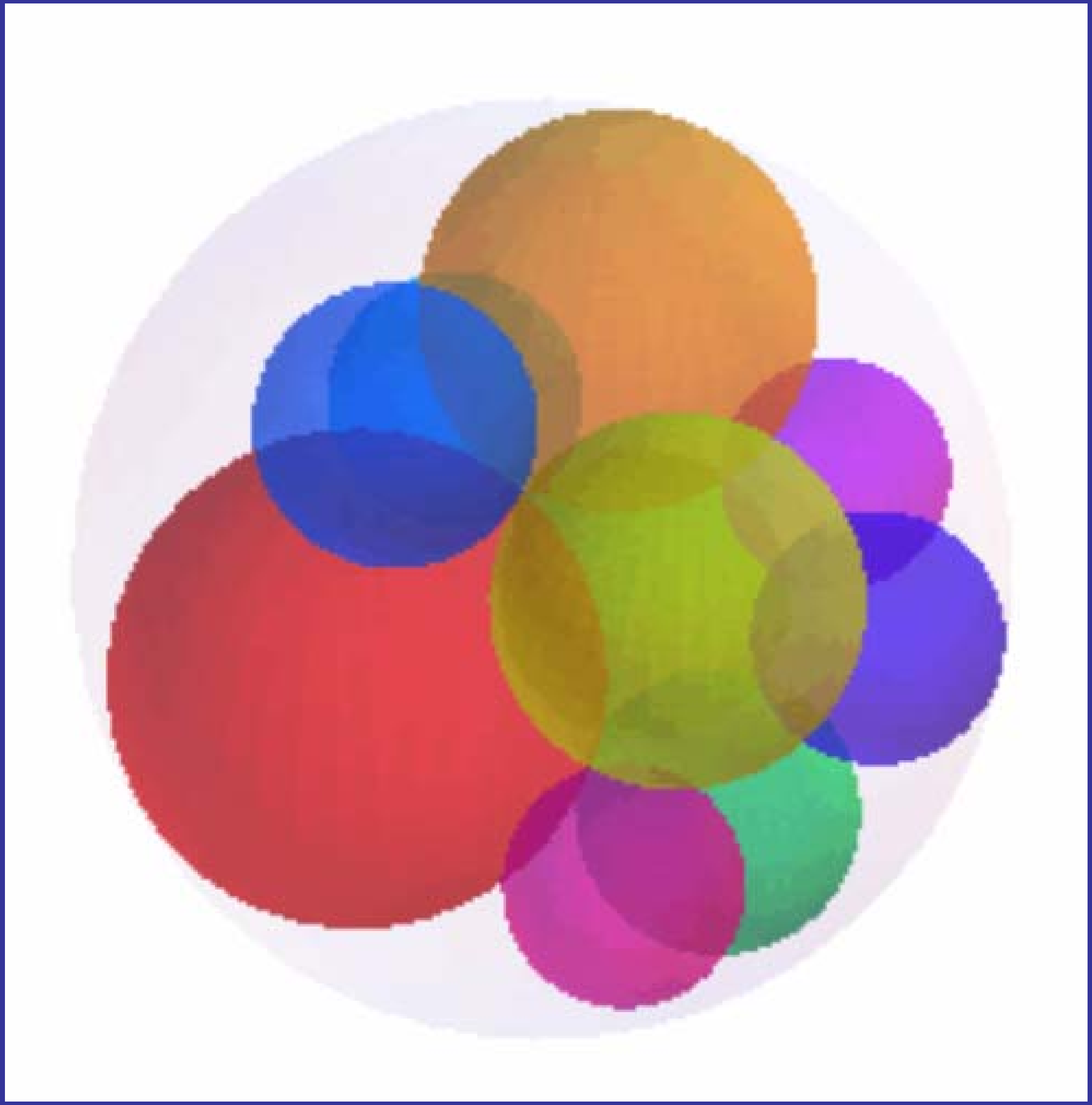
Optimized arrangements for circles with radii $k^{-1/2}$ k=5,…,20

Density of Circle Packings



Packing density for circles with radii $n^{-1/2}$ n=3,…,20

‘Tightest’ 8-Sphere Packing Found by MOP



Microsoft Excel - opt-compt.xls

A Comparison of *Mathematica* Global Solvers on Circle Packing Problems

Dell P4 3 GHz; Windows XP

All packages used in default mode

Software Package	4 circles	5 circles	6 circles
MathOptimizerPro	**1.71**	**1.7516**	**1.81008**
	0.5 secs	**0.765 secs**	**1.391 secs**
MathOptimizer	**1.71**	**1.7734**	**1.83052**
	18.875 secs	**58.219 secs**	**151.82 secs**
Nminimize	**1.7516**	**1.7734**	**1.84734**
	1.469 secs	**2.5 secs**	**3.766 secs**
MultiplierMethod	**1.7617**	**1.765**	**1.87752**
	0.609 secs	**1.109 secs**	**2.328 secs**
Global Optimization			
Global Search	**2.7515**	**2.8361**	**2.74901**
	1.594 secs	**1.922 secs**	**3.125 secs**
Global Penalty Function	**1.9464**	**2.1398**	**2.81465**
	0.375 secs	**0.609 secs**	**0.938 secs**
MultiStart Min	**2.2708**	**3.2047**	**3.86576**
	0.297 secs	**0.203 secs**	**0.328 secs**

Hardware and Software Platforms

- MO: All *Mathematica* (v. 4 and above) platforms
- MOP: Currently, personal computers, Windows 2000/XP; *Mathematica* (v. 4 and above)*;* MS Visual C/C++ , Borland C/C++, Lahey Fortran 90/95; Salford FTN77 and 95. Other compiler links and platforms will also be made available as needed

Licensing

- single and multiple professional licenses
- s/m non-profit research licenses with discounts
- university department and site licenses

Concluding Notes

MathOptimizer supports the solution of essentially “all” continuous nonlinear optimization models in *Mathematica.* This specifically includes complex “black box” native *Mathematica* systems such as e.g. ModelMaker. *S*olution quality compares favorably to other solvers.

MathOptimizer Professional combines the modeling capabilities of *Mathematica* with the speed and quality of an external solver suite. This allows the solution of large and complex nonlinear optimization models, with an efficiency comparable to compiler-based ‘number-crunching’ solvers. Models with up to a few thousand variables and constraints can be handled today.

Recommended MO and MOP application areas: education, model development and prototyping, industrial R&D, interdisciplinary R&D.

Product demonstrations available; test models and application examples are welcome.

Illustrative MO and MOP References

- JDP *MathOptimizer User Guide* (~ 70 pp.) and
- JDP & FJK *MathOptimizer Professional User Guide* (150 pp.)
  Mathematical background, usage, applications
- JDP, *Opt. Methods and Software*, 2003 Model calibration
- JDP & FJK, *Developer Conference 2003* presentation MOP
- JDP & CJP, *Developer Conference 2003* talk MO and MM
- FJK & JDP, *IMS 2004* Generalized circle packings
- FJK & JDP, *The Mathematica Journal* 2004 (to appear)
  Configuration (collision and packing) models solved by MO and MOP, with comparisons to other global solvers

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Title

Optimization of Finite Element Models with *MathOptimizer* and ModelMaker

Authors

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Organization: PCS Inc. and Dalhousie University
URL: http://www.dal.ca/~jdpinter/

Christopher J. Purcell
Organization: Defence R&D Canada

Conference

2003 *Mathematica* Developer Conference

Conference location

Champaign

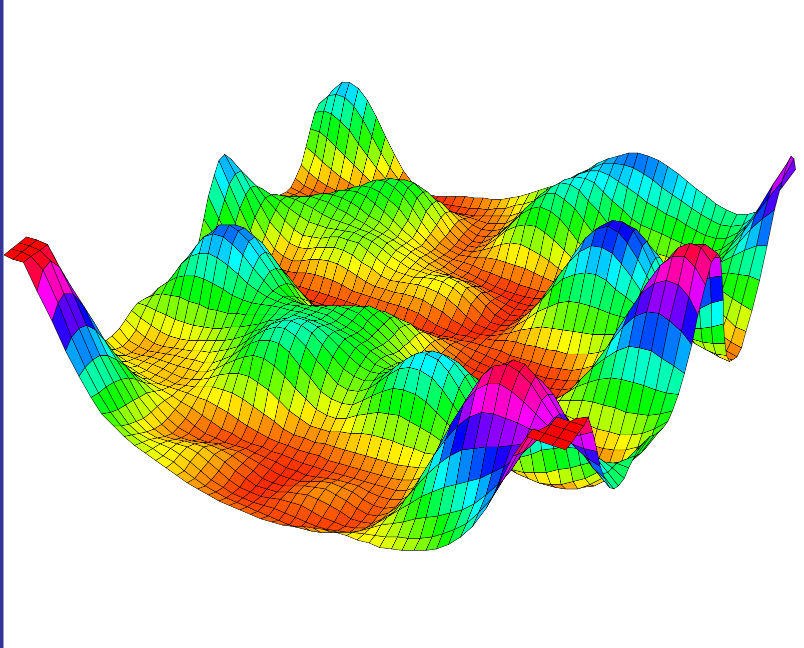
Description

Quantitative decisions related to engineering, economic and scientific investigations are frequently made using optimization concepts and tools. The decision-maker or modeler typically wants to find the "absolutely best" decision, which corresponds to the minimum or maximum of a suitable objective function and satisfies certain feasibility constraints. The objective function expresses overall system performance, and the constraints originate from physical, technical, or economic considerations.

This paper describes two *Mathematica* packages: *MathOptimizer*, a general-purpose nonlinear (global and local) optimizer, and ModelMaker, a parametric finite-element modeller. As an example, we presented the optimized design of a tuning fork, where the design objective function involves a finite element calculation. This simple example illustrates a typical

Advanced Optimization

Scientific, Engineering and Economic Applications with Mathematica Examples



Frank J. Kampas and János D. Pintér

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(forthcoming)

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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

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 re world applications, this work presents a practically motivated discussion of nonlinear (global and convex) optimization. From this book, readers will gain a solid practical understanding of readily applicable methods and tools in an important and rapidly emerging field.

Related Titles

Product Development and Support

Pintér Consulting Services, Inc.
jdpinter@hfx.eastlink.ca http://www.dal.ca/~jdpinter

and

Frank Kampas <fkampas@msn.com>

Product demonstrations are available
Test models and application examples are welcome

Thanks for your attention!