TOMLAB OPTIMIZATION

TOMLAB –Unique Features for Optimization in MATLAB

Bad Honnef, Germany

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Outline of the talk

- The TOMLAB Optimization Environment
  - Background and history
  - Technology available
- Optimization in TOMLAB
- Tests on customer supplied large-scale optimization examples
- Customer cases, embedded solutions, consultant work
- Business perspective
- Box-bounded global non-convex optimization
- Summary

Background

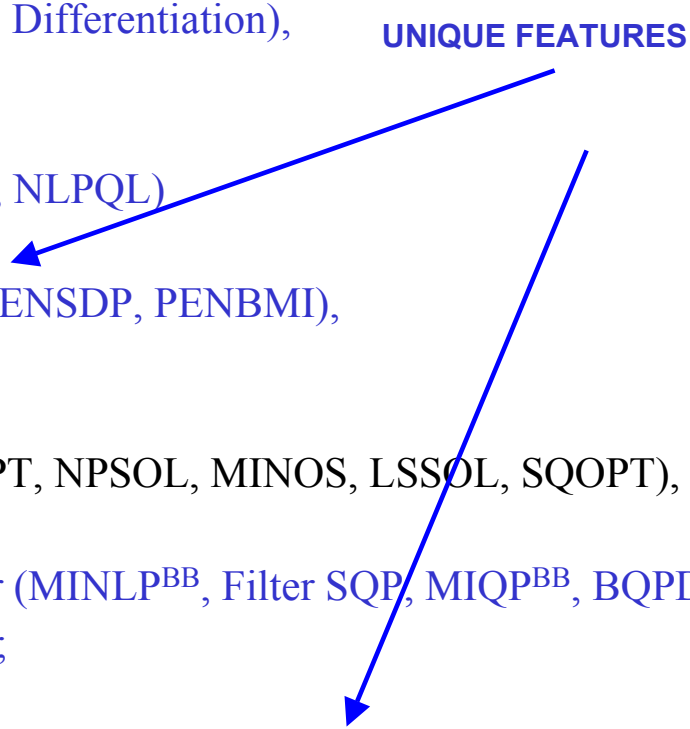
- **MATLAB** – a high-level language for mathematical calculations, distributed by MathWorks Inc.
- Matlab can be extended by **Toolboxes** that adds to the features in the software, e.g.: finance, statistics, control, and ***optimization***
- Why develop the **TOMLAB Optimization Environment?**
  - **A uniform approach to optimization didn't exist in MATLAB**
  - **Good optimization solvers were missing**
  - **Large-scale optimization was non-existent in MATLAB**
  - **Other toolboxes needed robust and fast optimization**
  - **Technical advantages from the MATLAB languages**
    - **Fast algorithm development and modeling of applied optimization problems**
    - **Many built in functions (ODE, linear algebra, …)**
    - **GUI development fast**
    - **Interfaceable with C, Fortran, Java code**

History of Tomlab

- President and founder: Professor Kenneth Holmström
- The company founded 1986, Development started 1989
- Two toolboxes NLPLIB och OPERA by 1995
- Integrated format for optimization 1996
- TOMLAB introduced, ISMP97 in Lausanne 1997
- TOMLAB v1.0 distributed for free until summer 1999
- TOMLAB v2.0 first commercial version fall 1999
- TOMLAB starting sales from web site March 2000
- TOMLAB v3.0 expanded with external solvers /**SOL** spring 2001
- Dash Optimization Ltd's Xpress^{MP} added in TOMLAB fall 2001
- Tomlab Optimization Inc. founded in California December 2001
- **ILOG S.A.'s CPLEX** added to product list fall 2002

2003-2004...

- Around 100 algorithms for optimization.
- Partnerships with;
  - Arki Consulting & Development A/S (CONOPT),
  - Boeing Phantom Works (SOCS, BARNLP, SPRNLP),
  - Cranfield University (MAD, Automatic Differentiation),
  - Dash Optimization Ltd. (Xpress^{MP}),
  - ILOG S.A. (CPLEX),
  - Klaus Schittkowski (NLPJOB, DFNLP, NLPQL)
  - Optimal Methods Inc. (OQNLP),
  - PENOPT GbR (PENNON, PENNLP, PENSDP, PENBMI),
  - Pinter Consulting (LGO)
  - SIEMENS (SENN),
  - Stanford Business Software Inc. (SNOPT, NPSOL, MINOS, LSSOL, SQOPT),
  - Sunset Software Technology (XA),
  - University of Dundee, Fletcher, Leyffer (MINLP^{BB}, Filter SQP, MIQP^{BB}, BQPD),
  - Ziena Optimization Inc. (KNITRO 4.0);
- New Products;
  - Toolbox for Costly (CPU-intensive) Global Black-Box Optimization (CGO)
  - Highly integrated support for AMPL problems
- New home page and InstallShield installations.



Optimization Problems

- General formulation
  - $\min f(x)$
  - S.t. $xL \le x \le xU$

    $bL \le Ax \le bU$

    $cL \le c(x) \le cU$

    a subset of x can be restricted to integer variables.

LP, MILP, QP, MIQP, MIQQ, NLP, MINLP, SDP, BMI, GOAL, L1, LLS, NLLS, GLB, GLC, MINIMAX, LCP, MCP, CGO.

Features in TOMLAB /BASE

- General
  - Entry level optimization solvers and interfaces.
  - Routines for interfacing.

Problem types: LP, MILP, QP, GLB, GLC, MINIMAX, L1, GOAL, LLS, NLLS.

Solver options: 30 including several interfaces.

Features in TOMLAB /CPLEX

- General formulation
  - $\min\ 0.5\ x^T Q\ x + c\ x$
  - S.t. $xL <= x <= xU$

    $bL <= Ax <= bU$

    $x^T H\ x + a\ x <= rU \quad 1 \ldots n$

    a subset of x can be restricted to integer variables.

Problem types: LP, MILP, QP, MIQP, MIQQ.

Solver options: Simplex, Dual simplex, Network simplex, Barrier, Sifting, Concurrent.

Fastest LP, MILP and MIQP solver. Only MIQQ solver.

Advantages with TOMLAB – 1

- No algebraic modeling language offer the unique problem formulations
  - Semi-definite programming problem, general objective, linear and bi-linear matrix inequalities (LMI, BMI)
  - Global black-box optimization, both expensive and non-expensive
- If you know MATLAB (500,000+ users), you know TOMLAB:
  - Reduces training to a minimum
  - Gives novices direct access to the best optimization packages
  - Reduces development time of optimization applications to a minimum
- Multi platform support, TOMLAB is readily available for
  - Windows, Linux, HP, MAC, and SUN systems
- Easily embedded in other products using the MATLAB compiler.
  - Portability

Advantages with TOMLAB – 2

- Uniform and flexible approach to solving your problem
  - Gateway routines automatically convert the problem when using solvers designed for different purposes, e.g. NLP solvers efficiently solving sparse nonlinear least squares problems or a quadratic programming problem
  - Universal driver routine enables the user to switch solver by changing a keyword. Lists for the various problem types, so the user can easily iterate thought all solvers that handle the specific problem
  - Assign routines creating problem structure available for all problem types
  - Multiple solvers can easily be used as backup for one-another, making convergence ~100% safe and robust
- Performance
  - Many solvers implemented in Fortran and C for maximum speed
  - Critical parts of the MATLAB solvers coded in Fortran or C
- Compatibility
  - Automatic Differentiation with `MAD` and `ADMAT`
  - Fully call-compatible with MathWorks' Optimization Toolbox
- User features
  - Dynamic GUI Design – create own database of problems

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Gateway mapping

prob\solv	uc	qp	con	lls	cls	mip	lp	glb	glc	miqp	minlp	sdp	miqq	mcp
uc	x		x					x	x		x	x		
qp		x	x						x	x	x		x	x
con			x						x		x			
lls			x	x	x				x		x			
cls			x		x				x		x			
mip						x			x	x	x		x	
lp		x	x			x	x		x	x	x	x	x	x
glb								x	x					
glc									x					
miqp									x	x	x		x	
minlp									x		x			
sdp												x		
miqq									x		x		x	
mcp														x

Solving an optimization problem - with TOMLAB

1. Define the linear parts and variable types of your problem in matrices and vectors
2. Define the nonlinear parts
   - The following options are available for the gradients, Jacobian and constraints gradients
     - Automatic differentiation (2 MATLAB toolboxes)
     - Numerical differentiation (6 methods)
     - Code them yourself
3. Identify patterns in your problem, Hessian and Constraint patterns, and other information that may be useful to the solver
4. Import your problem to a TOMLAB *Prob* structure array, by using one of the standard assign statements
5. Select solver, and run your problem by using driver routine *tomRun*
6. Debug and modify solver settings, try other solvers and/or sub-solvers

FIND THE BEST SOLVER FOR YOUR PROBLEM!

Large-Scale Optimization Benchmark Tests

- Computer
  - P4 2400 MHz, 1 GB RAM, 3 GB swap
  - Windows 2000, MATLAB 6.5, TOMLAB v4.3
- Definitions
  - n: number of variables
  - m: number of constraints
  - nnz: number of nonzeros
  - d: nnz / (tot. # of elements, e.g. n*m)

Large-Scale LP – Michael Board

Transport problem converted to regular LP

	n	m (all eq.)	nnz(A)	d(A)
1.	674,190	1,671	1,348,380	0.0012
2.	1,483,527	2,488	2,967,054	0.000805
3.	4,841,370	4,407	9,682,740	0.000405

	Board-1		Board-2	
	Iterations	Time	Iterations	Time
Xpress^{MP} (Barrier)	22	58 s	34	179 s
CPLEX (Barrier)	29	44 s	31	196 s
CPLEX (Network)	43,675	5 s	108,356	14 s
MINOS	142,959	576 s	n/a	>45 m
linprog	42	301 s	51	16 m (1)

Board-3: Out of memory, all solvers. (MATLAB limit of 1.4GB)

(1) – Not optimal solution

Large-Scale MILP – Nikos Laoutaris

	n	m	nnz(A)	d(A)
Nikos-1	23,000	7,001	26,000	1.6147e-004
Nikos-2	230,000	70,001	260,000	1.6149e-005

	Nikos-1 Time	Nikos-2 Time
Xpress^{MP}	<1,5 s	<140 s
CPLEX	<1.5 s	<140 s
mipSolve (1)	16,16 s	n/a

Opt Tlbx – no suitable solver available

(1) MINOS 5.5 used as LP sub solver

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Large-Scale QP – Kostas Skouras
Portfolio optimization, Credit Suisse First Boston
dense F (QP term), sparse A (constraints)

	n	m (all eq.)	nnz(F)	d(F)	nnz(A)	d(A)
1.	524	273	524^2	1.0	1572	0.011
2.	4,046	2,119	4046^2	1.0	12138	0.0014

	Kostas-1		Kostas-2	
Solver	Iterations	Time	Iterations	Time
Xpress^{MP} (Barrier)	8	1.68 s	11	203 s
CPLEX (Barrier)	9	1.22 s	11	305 s
SNOPT	20	0.24 s	20	6.17 s
SNOPT - SQOPT	184	1.25 s	Aborted	> 40 min
MINLP - BQPDs	70	1.34 s	Aborted	> 25 min
Opt Tlbx quadprog	529	223 s	n/a – out of memory	

Large-Scale NLP – ABB

Model Predictive Control (MPC) for paper mill production

1246 variables, 495 linear constraints (99 eq.), 300 nonlinear equalities

Density of linear constraint matrix: 0.0029; 1782 nonzeros

Density of nonlinear constraint gradient: 0.017; 6200 nonzeros

feastol=opttol=1E-4, MATLAB 7.0

Solver	Iter	Time	Comment
SNOPT	57	4.75 s	
KNITRO 4.0	169	33.4 s	alg=1 Int/Direct,exact grad, sparse Q-N
KNITRO 4.0	108	14.8 s	alg=2 Interior / CG
KNITRO 4.0	292	62.2 s	alg=3 Active set (feas 1E-12)
FMINCON	n/a	>2.5 hours	Manually terminated
SNOPT	156	12.6 s	feastol=opttol=1E-6

Taiwan Semiconductor Manufacturing Company (TSMC)

- Design improvement projects. Test problem: box constrained nonlinear problem with 63,000 variables.
- Function quite costly. Failed with Optimization Toolbox - fmincon.
- Tried TOMLAB /SNOPT after recoding.
- TOMLAB /KNITRO 3.x solved the problem after optimizing all code in about 2 minutes.
- A full design project was initiated based on the promising results, and a problem with about 480,000 decision variables was solved in about 1 hour.
- Solution implemented with Cadence, Mentor Graphics, and SpringSoft EDA tools. Solution verified from Silicon Data.

Embedded solutions with TOMLAB

- Philips embeds Tomlab /Xpress in their production planning system for Lumileds' facilities in Malaysia and the Netherlands.
- Gaz de France embeds Tomlab /SNOPT for production planning. Solution based on MCC and distributed for non-MATLAB use.
- US Naval Research Lab: Has developed a package for dynamic optimization and control, DIDO. Tomlab is a required part.
- Halliburton: Embedded in NMRStudio for exploration analysis.
- Optimization platform in DOTS, 3 years EU-project, led by KCL
- NASA/JPL in cooperation with Claremont Grad Univ. for Mars lander data flow analysis
- ABB embeds Tomlab /SNOPT for paper mill production with MPC

Halliburton Energy Services

- **Service provider to the big oil companies.**
- **Tomlab has been compiled and embedded in Halliburton's software NMRStudio for real-time analysis of exploration data.**
- **Optimization is performed in real-time while measurements from the drilling equipment are coming in. Also available for offline analysis.**
- **More robust and faster mathematical analysis is the deliverable, with estimated savings of $200,000 per drilled hole. The system will cut the measurement time in half.**
- **More advanced parameter estimation of very noisy NMR-data (Nuclear Magnetic Resonance) is implemented.**
- **Tomlab's consulting team in the US is continuously improving the models, and optimization methods. A full time position has been introduced at Halliburton to further implement the systems.**

Optimization for the pulp and paper industry

- Tomlab has been selected as the optimization platform for the European Union project DOTS (dynamic optimization of pulp and paper mills) with partners in Finland, France, Germany and Sweden.

- Several problems for the pulp and paper industry:

  Paper quality
  Energy consumption
  White-water System Management (closing up the mill)
  Stabilize regularatory controls

- Tomlab will be an active partner in more EU projects for optimization, with the goal to develop new quality optimization systems.

Unilever multiple fat-blend production planning

- Mixed-integer nonlinear problem
- Solved with standard tools, but too slow (OQNLP, MINLPBB, LGO, glcCluster, glcFast)
- The Tomlab team has developed new algorithms that solve the problems order of magnitude faster

NASA use of TOMLAB

- Claremont University in cooperation with JPL/NASA uses TOMLAB
- Optimizing dataflow from the Mars landers through the orbiters and back to Earth.
- TOMLAB /SNOPT is 10-20 times as fast as MathWorks' Optimization Toolbox, and always finds the right answer.
- Will hopefully be embedded in the mission planning system,

TOMLAB in the market place

- The TOMLAB software sales are growing, factor 2 in 2003. Roughly factor 2 in 2004.
  - Rapidly being established as the standard for optimization in MATLAB
- Recognized for the modeling features.
  - A chapter about Tomlab is published in MODELING LANGUAGES IN MATHEMATICAL OPTIMIZATION (Kluwer Academic Publishers, 2004, Ed. Prof. Josef Kallrath)

Products: Base module + 20 options

Marketing

- Internet site http://tomlab.biz . Full website optimization program to drive in maximum number of users.
- Newsletters to attract users back for more information, testing
- Follow-ups with each registered customer
- Newsgroup coverage. Active participation in Matlab and mathematical newsgroups
- Information messages to mailing lists
- Talks at scientific conferences
- Network of satisfied users and scientists
- Rapid and advanced support in the initial sales process

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LATEST NEWS

Sep 28th 2004
TOMLAB v4.4 released. Major upgrades to several components. Read more >>

Jul 2nd 2004
TOMLAB SAL User's Guide available for customers building embedded solutions.

Jun 1th 2004
TOMLAB Online documentation released for all solver options.

May 21th 2004
TOMLAB Quickguide availble for all problem types. Download from the manuals page.

May 18th 2004
TOMLAB /OQNLP v2.0 released. Many general improvements to the multi-start features. Read more >>

Apr 28th 2004
TOMLAB /PATH now released. Linear and nonlinear mixed complementarity problems can now be solved with TOMLAB. Read more >>

Apr 17th 2004
TOMLAB Base Module and TOMLAB /CPLEX additions. Download TOMLAB v4.3. Read more >>

The TOMLAB Optimization Environment

- For fast and robust large-scale optimization in MATLAB ®

What is TOMLAB?

The TOMLAB Optimization Environment is a powerful optimization platform for solving applied optimization problems in Matlab. TOMLAB provides a wide range of features, tools and services for your solution process. Read more about Tomlab >>

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Are you looking for a solver to embed in your system?

If you register you can test TOMLAB for free for 21 days.

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MOST POPULAR PRODUCTS

TOMLAB /SOL v4.4
TOMLAB /SOL v4.4 efficiently integrates the well-known solvers developed by the Stanford Systems Optimization Laboratory (SOL) with MATLAB and TOMLAB. The toolbox includes the solvers MINOS, LPOPT, QPOPT, NPSOL, NLSSOL, LSSOL, SNOPT, SQOPT.
Read more >>
Buy now >>

TOMLAB /CPLEX v9.0
Solver package CPLEX 9.0, including Matlab interface. State-of-the-art mixed-integer linear and quadratic programming with quadratic constraints (MILP, MIQP, MIQQ), and large-scale simplex and barrier methods for LP and QP. On request we can also provide TOMLAB /CPLEX MEX for CPLEX 7.x and more recent versions.

PARTNERS

BOEING
LINDO SYSTEMS INC
Cranfield UNIVERSITY
THE UNIVERSITY of WISCONSIN MADISON
Pintér Consulting Services, Inc.
ILOG
dash optimization
Systems Optimization Laboratory
UNIVERSITY OF DUNDEE
PENOPT

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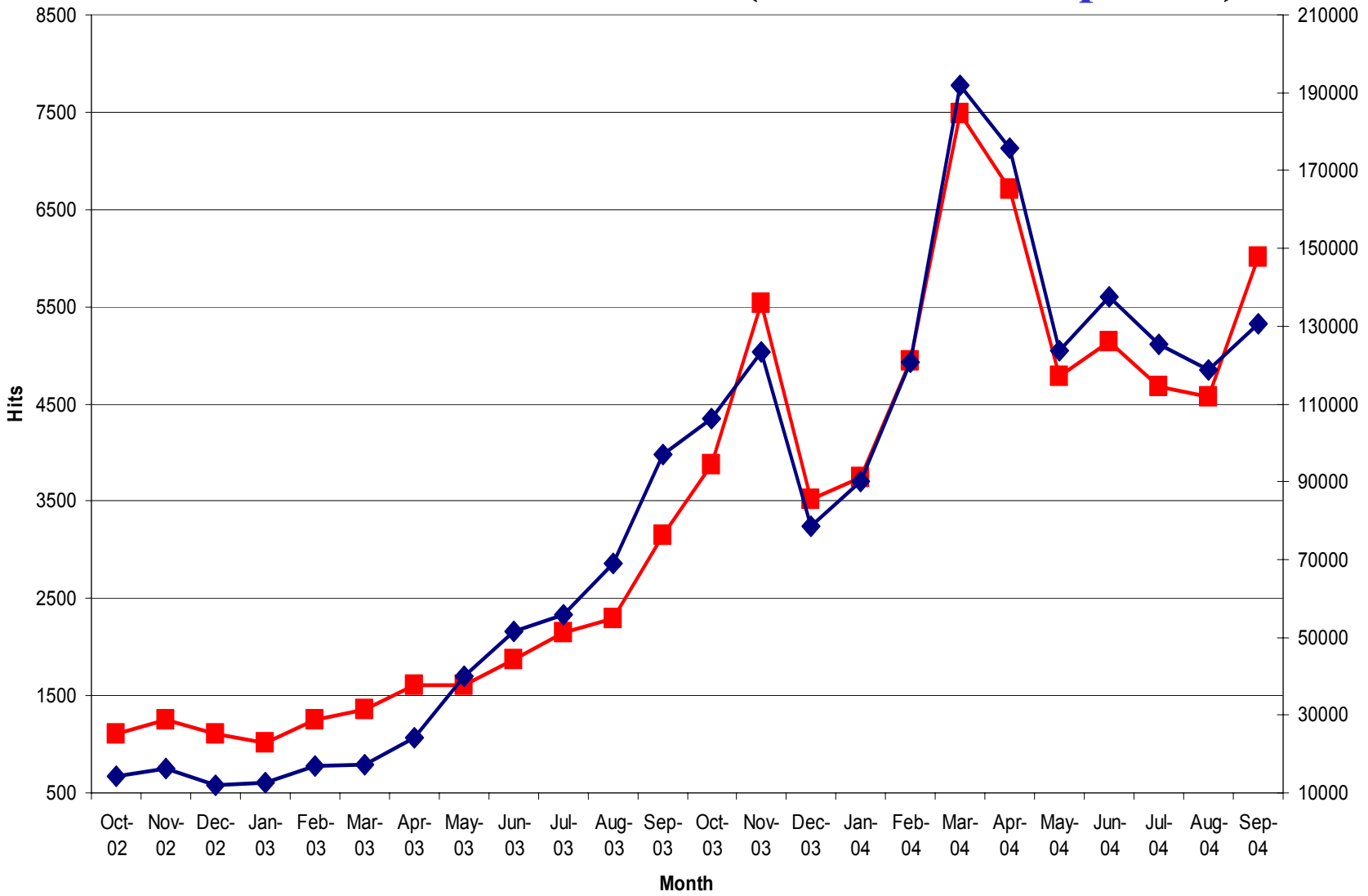
TOMLAB Website Traffic (total and site specific)



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Georgia Tech Aerospace Initial Test Problem - SNOPT

- Problem with n = 752, m = 755 was evaluated. Initial problem was solved in about 15 min.
- Turns out the major feasibility tolerance was set to 1e-9 using numerical derivatives. Problem now solved in about 44.25 s.
- Adding ConsPattern: 20.6 s.
- Modifying objective function: 18.8 s.
- Modifying constraint calculation: 15.4 s.
- Removing redundant constraints, re-writing to a QP problem: 0.6 s.
  - 255 constraints were fixing the decision variables.
- Switching to SQOPT: 0.45 s.

EXAMPLE OF ADVANCED USER SUPPORT DURING THE SALES PROCESS

User feedback October 12. 2004

- The evaluation went very well; I was highly impressed with the simplicity with which I could replace Optimization Toolbox with Tomlab
- The sales documentation online probably does not do enough to make clear how easy it is to run the Tomlab solvers instead of Optimization Toolbox; I had expected a lot of recoding but there was none!
- I've also been pleased with the performance, especially using npsol. At least a 20x speedup over fmincon for my application

Box-bounded global optimization

$$\min_x \quad f(x)$$

$$\text{s/t} \quad -\infty < x_L \le x \le x_U < \infty$$

$$x_L,\ x, x_U \in R_d,\quad f(x) \in R$$

No derivative information available.

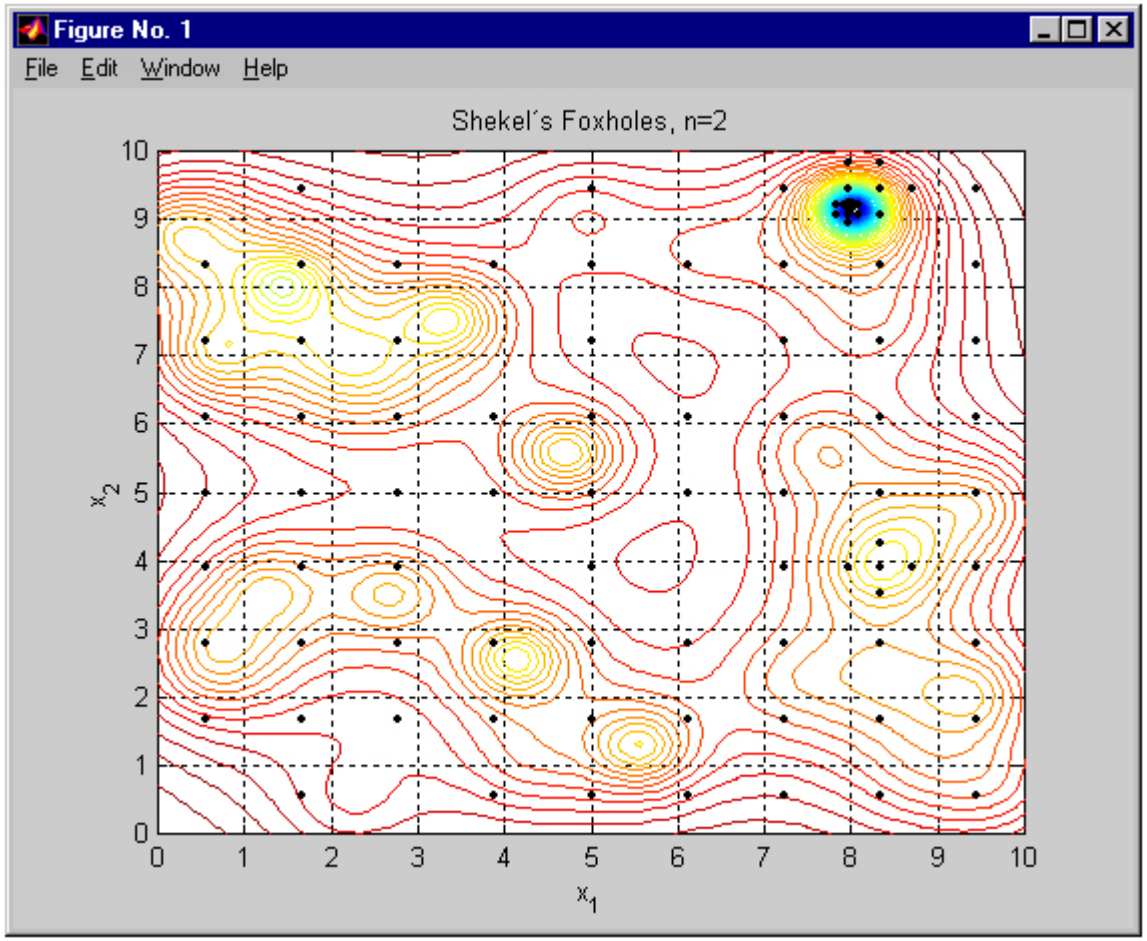
$f(x)$ is either non-costly or costly.

Dimension d is not too large, say 1-20.

Solution of non-costly subproblems

- DIRECT algorithm (Jones et al. 1993) efficient strategy, global convergence proof
- No tuning parameters
- Dividing space into rectangles
- Estimating all possible Lipschitz constants
- Handles nonsmooth, nonlinear, nonconvex, multimodal functions
- Fast, robust and efficient implementation of the DIRECT algorithm in glbFast

DIRECT algorithm – initial phase



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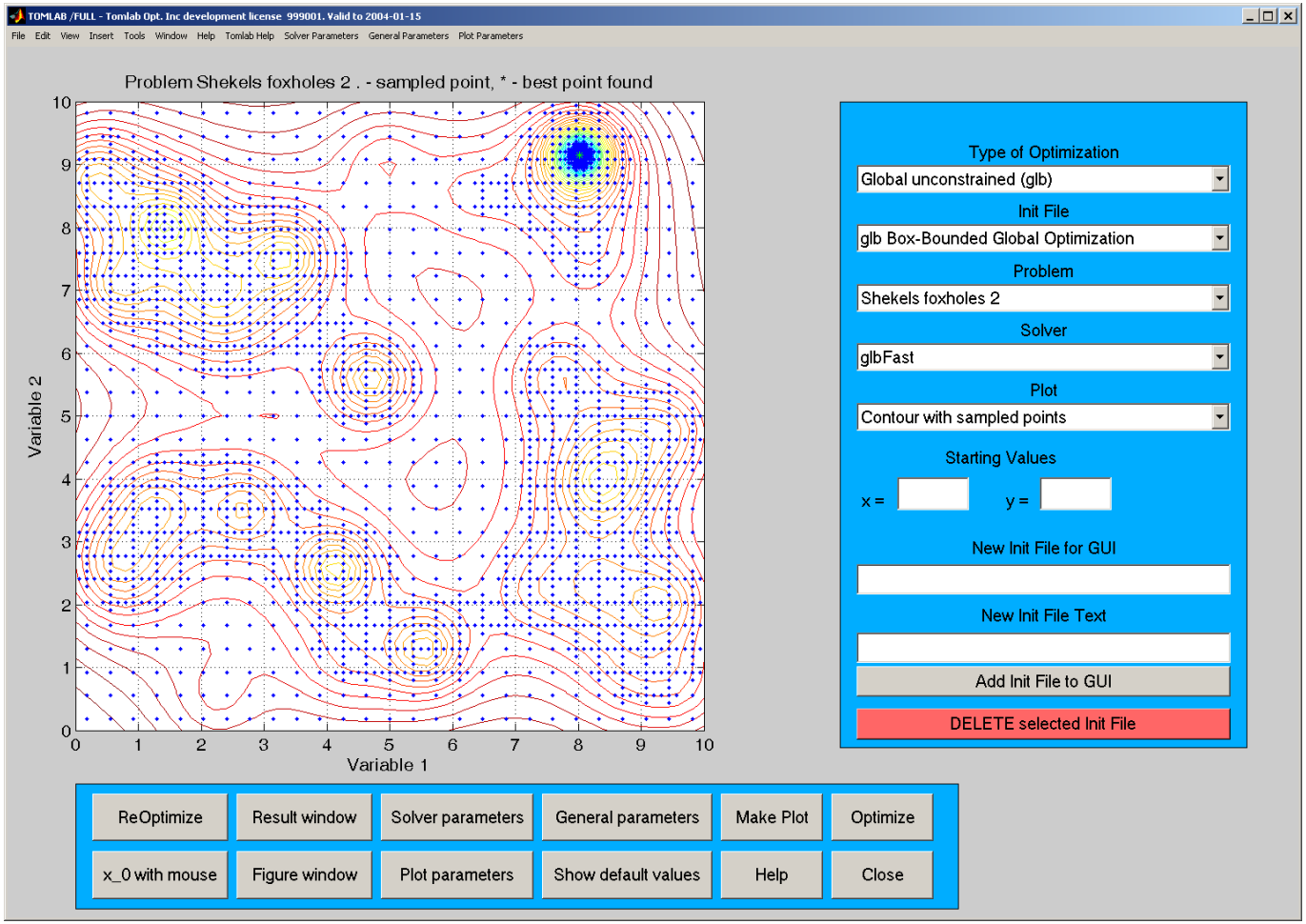
TOMLAB GUI – global optimization



Constrained box-bounded global optimization

$$\min_x \; f(x)$$

$$\text{s/t} \quad -\infty < x_L \le x \le x_U < \infty$$

$$b_L \le Ax \le b_U$$

$$c_L \le c(x) \le c_U$$

$$x_L, x, x_U \in R_d, \quad f(x) \in R$$

$$b_L, b_U \in R_m, \quad c(x), c_L, c_U \in R_p,$$

No derivative information available.

$c_i(x)$ either costly or non-costly.

Subset of x could be integer valued.

Non-costly constrained optimization

- glcFast - Fast and efficient implementation of the extended DIRECT algorithm (Jones 2001) that handles constraints and some x integer valued.
- glcSolve – Matlab version of the extended DIRECT algorithm

glcCluster

- Hybrid-clustering algorithm for constrained box-bounded global mixed-integer non-convex optimization.
- Uses all sampled points in the constrained DIRECT algorithm (glcFast) as input to a new clustering algorithm.
- The clustering algorithm finds a set of suitable starting points for local search.
- Local search by any NLP solver, e.g. NPSOL.
- The best point found from the local searches, if any better, is then used in a second DIRECT search with glcFast.

Tomlab /CGO - Costly box-bounded global optimization

- f(x) takes considerable CPU time, e.g. 30 minutes
- f(x) is often a complex computer program, or the result of an advanced simulation, e.g. Monte-Carlo simulation or trading strategy evaluation.
- f(x) often noisy, no derivatives known or usable.

Basic algorithm for costly global optimization

- Find initial set of $n \geq d+1$ sample points x. Experimental design problem.
- Compute costly f(x) for initial set of points.
- Iteration until *target f(x)* achieved or no time left:
- 1. Use the n sampled points to build a response surface model as an approximation of f(x) surface.
- 2. Optimize a *cheap* function of the approximating surface to obtain a new trial point to compute the costly f(x) for.
- 3. Compute and validate new (x, f(x)), increase n.

RBF algorithm

- Interpolation of all sampled point by radial basis function interpolation.
- Cycle of target values on surface gives trade off between local and global search.
- Global convergence proof (Gutmann 2001).
- Target value achievement balanced against size of new interpolation coefficient – gives well-conditioned interpolation matrix as size increases.
- Efficient numerical implementation for cubic and thin plate spline RBFs.

RBF algorithm - improvements

- Efficient numerical implementation of interpolation updates.
- Efficient trial point computations of interpolation coefficients and values, i.e. f(x) for non-costly global optimization subproblem.
- Each RBF iteration takes only order of seconds.
- Scaling of x to unit hypercube.
- Reduce influence of large f(x).
- Removal of too close points, keeping the best.
- Warm start of RBF (and/or EGO).

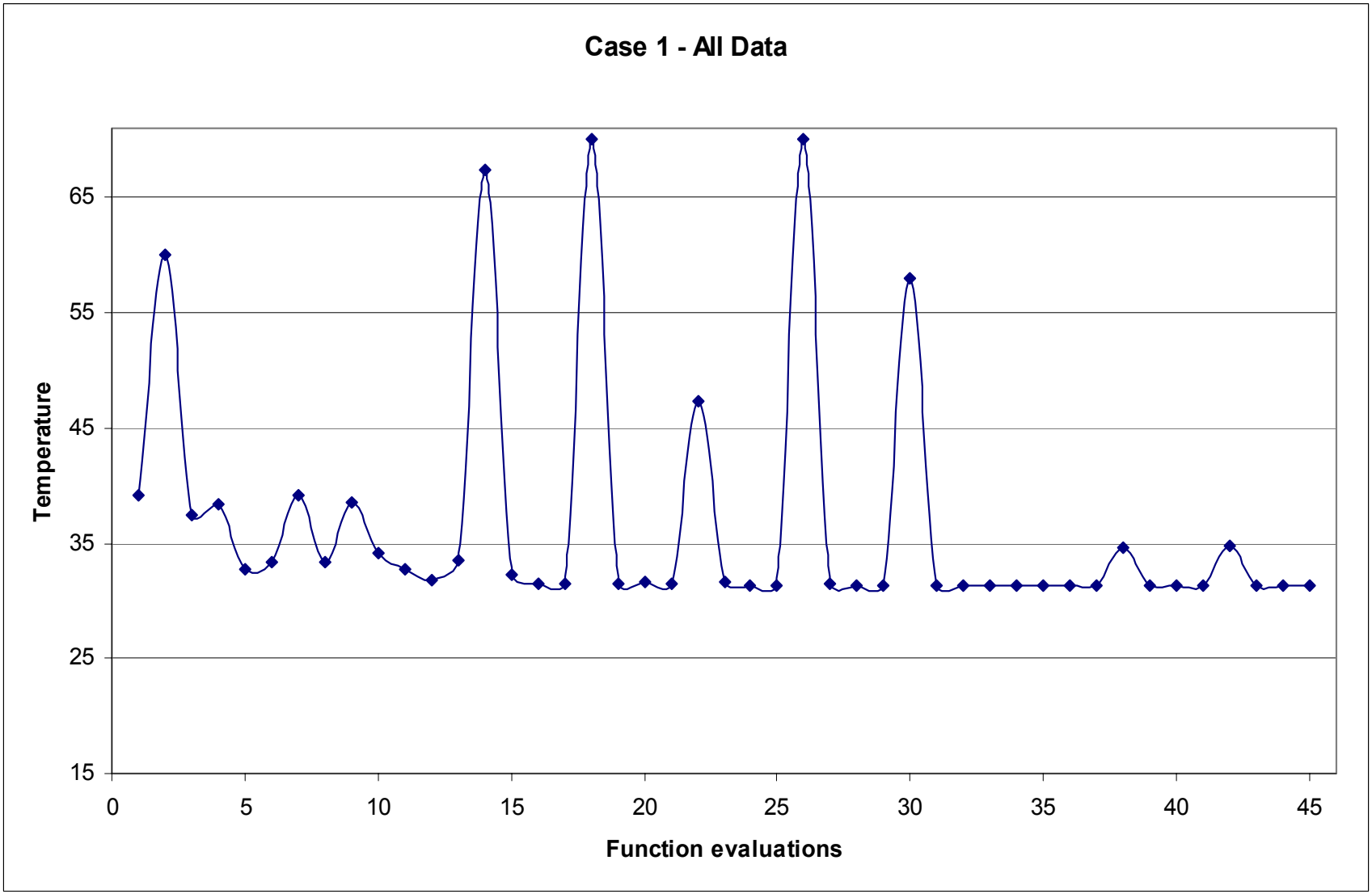
Tomlab /CGO – more improvements

- Extended RBF and EGO algorithm to handle mixed-integer problems (to be presented at Informs Annual Conference October 2004)
- Extended RBF and EGO algorithm to handle non-costly constraints.
- Added more types of local-global search strategies for RBF algorithm

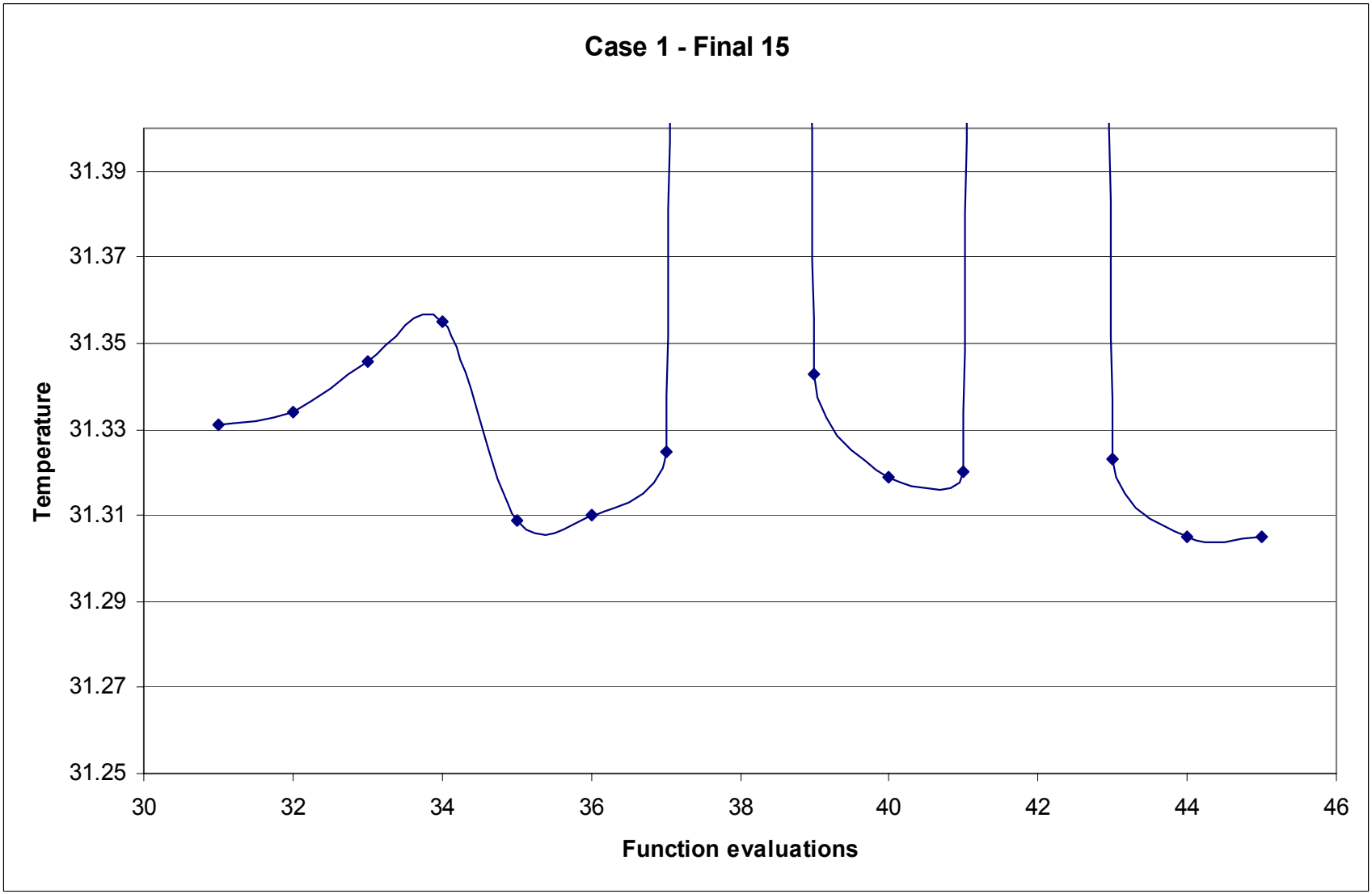
TOMLAB /CGO – 2 dim test case

- Testing with Coolit, a CFD (Computation Fluid Dynamics) software from DAAT Inc.
- Function evaluations between 15 minutes and 4 hours.
- One continuous and one integer variable.
- 13 points used for initialization.
- glcFast global subsolver for local and global problem.
- 45 function evaluations establish a good optimum.

TOMLAB /CGO – 2 dim test case



TOMLAB /CGO – 2 dim test case – final 15



TOMLAB /CGO – 3 dim test case

- Testing with Coolit, a CFD (Computation Fluid Dynamics) software from DAAT Inc.
- Function evaluations between 15 mins and 1 hour.
- Two continuous and one integer variable.
- 5 corner points used for initialization (Gutmann).
- TOMLAB /OQNLP subsolver for local and global problem.
- Still good progress after 115 function evaluations.

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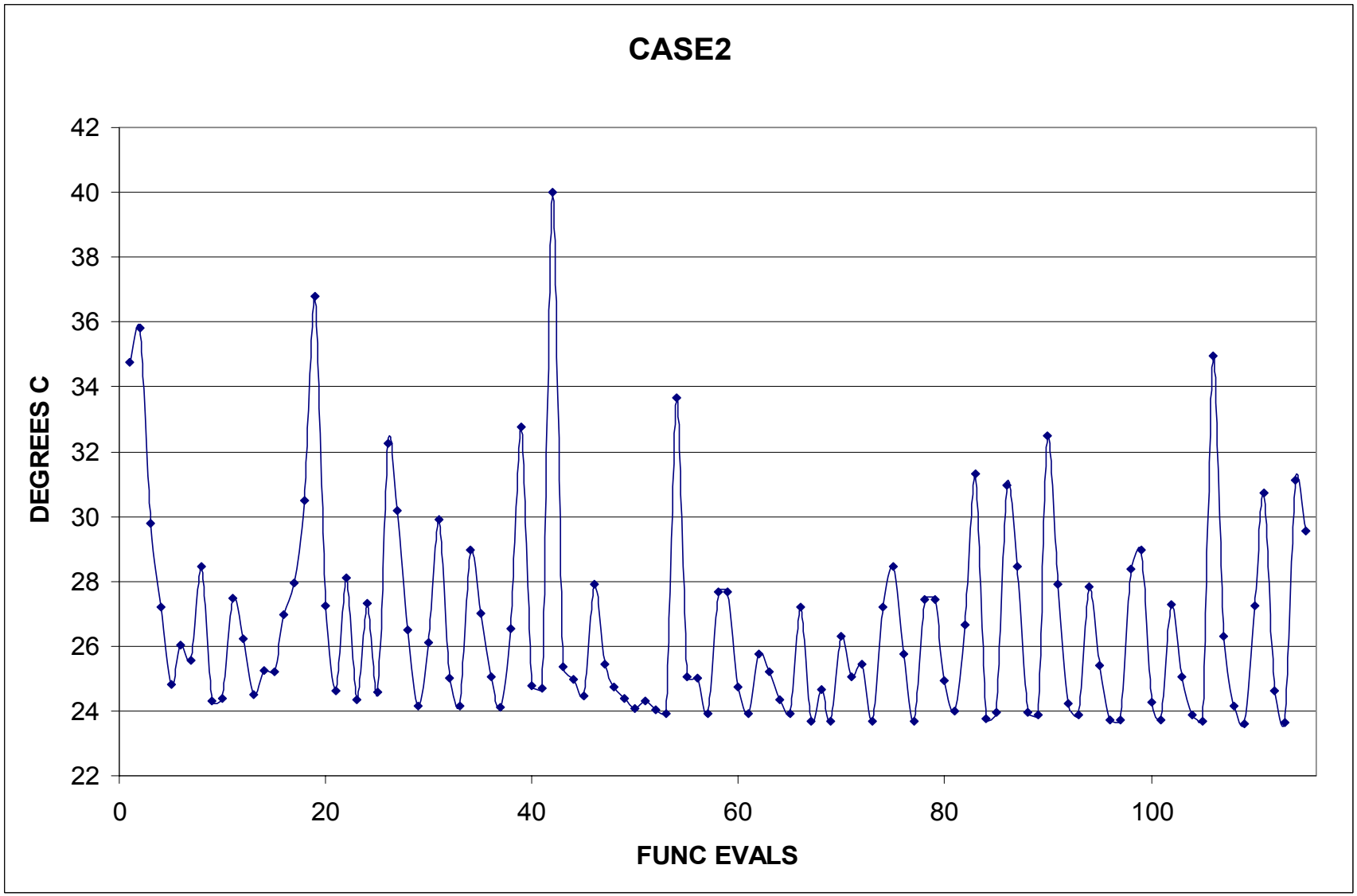
TOMLAB /CGO – 3 dim test case



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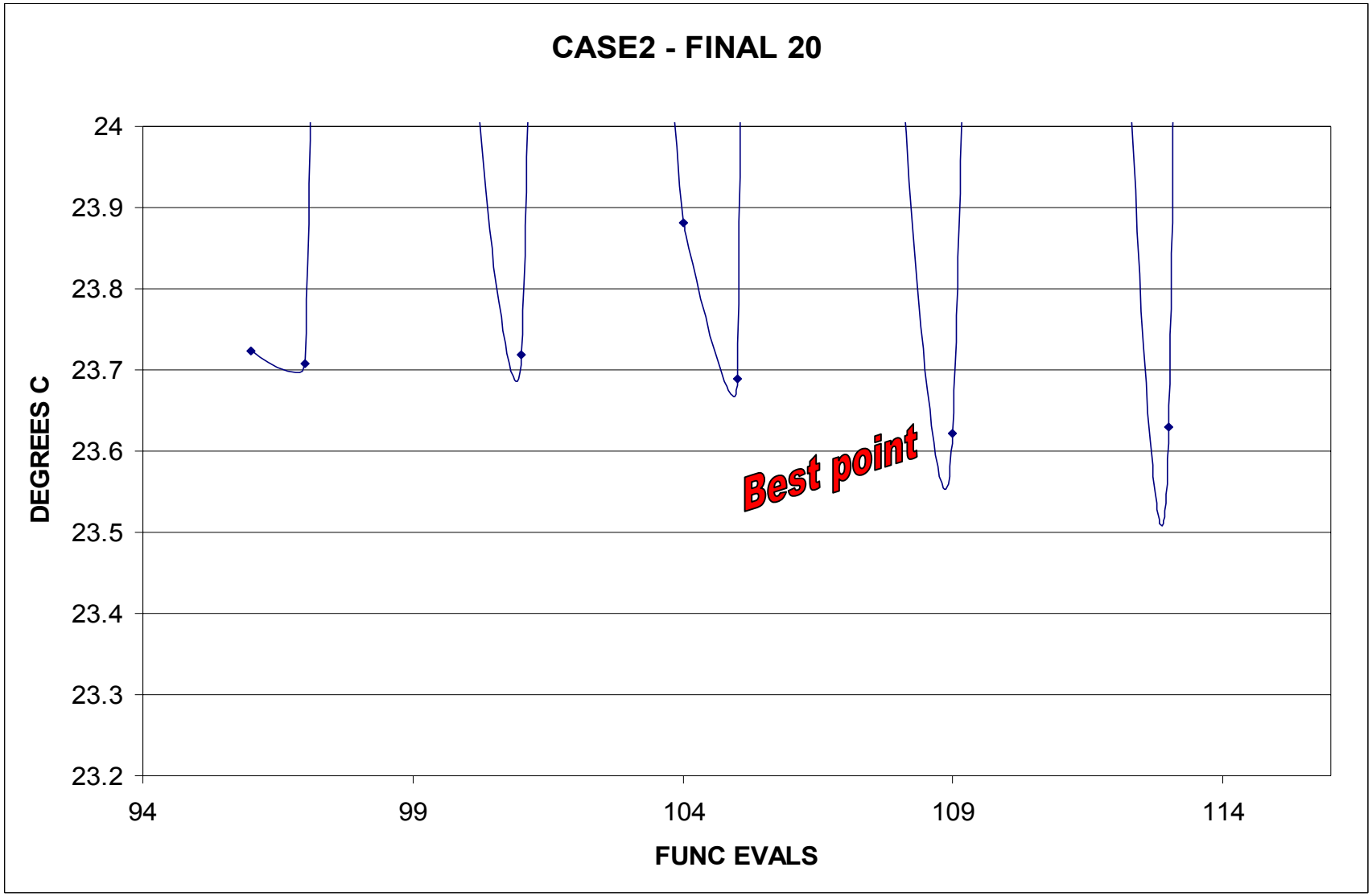
TOMLAB /CGO – 3 dim test case – final 20



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Global Optimization - Solvers

glbSolve glbFast		DIRECT algorithm, box-bounded, both Matlab and fast MEX Fortran version.
glcSolve glcFast		DIRECT by Jones (2001) for nonlinear and integer constraints, box-bounded, Matlab and fast MEX Fortran version.
glcCluster		DIRECT, combined with clustering techniques and local search from best cluster points found.
ego		Efficient Global Optimization (EGO) for costly functions (Jones et. al 1998)
rbfSolve		Algorithm for costly (expensive) functions using radial basis interpolation (RBF) and response model techniques.

Summary

- Tomlab is a powerful environment for all sorts of optimization in MATLAB
- Tomlab can be embedded in products. On-going work to make Tomlab more independent on MATLAB.
- The Tomlab team is interested in cooperating in challenging optimization projects