Global Optimization with GAMS

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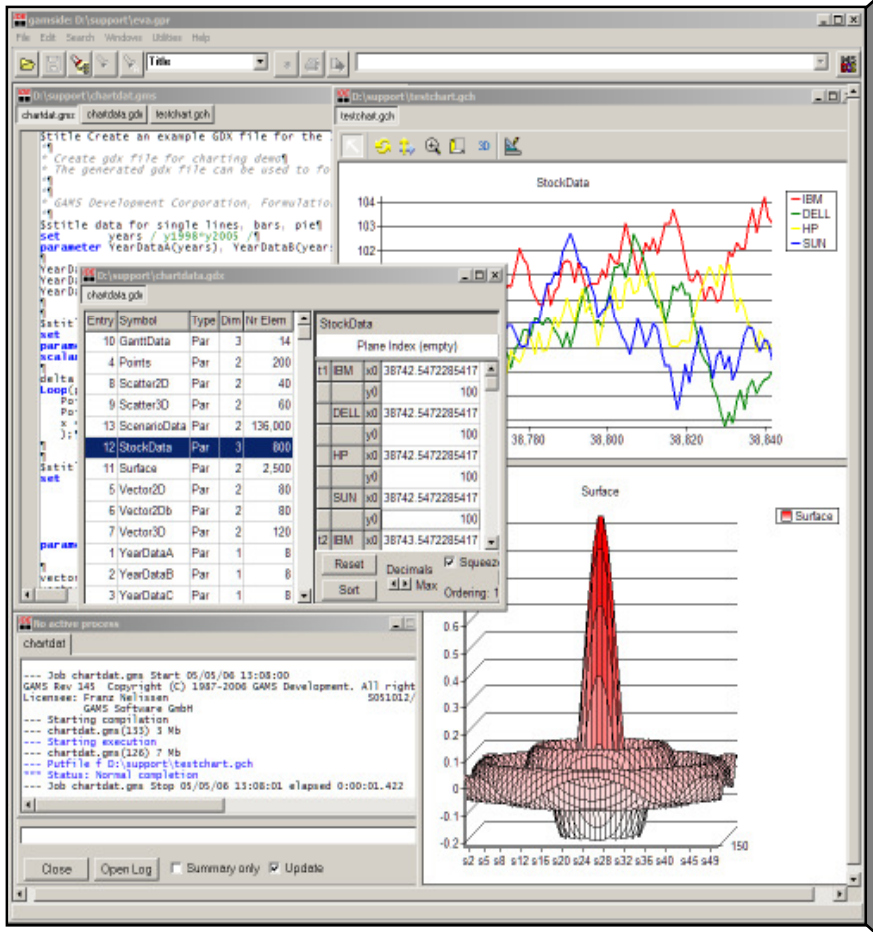
Agenda

- Introduction
- GAMS Global Solvers
- Performance & Quality

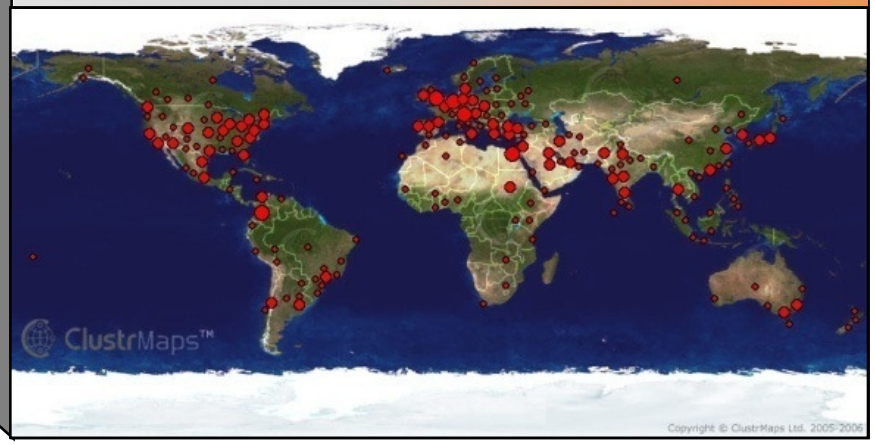
GAMS at a Glance



General **A**lgebraic **M**odeling **S**ystem

- Roots: World Bank, 1976
- Went commercial in 1987
- GAMS Development Corp.
- GAMS Software GmbH

- Broad academic & commercial user community and network



Algebraic Modeling Languages

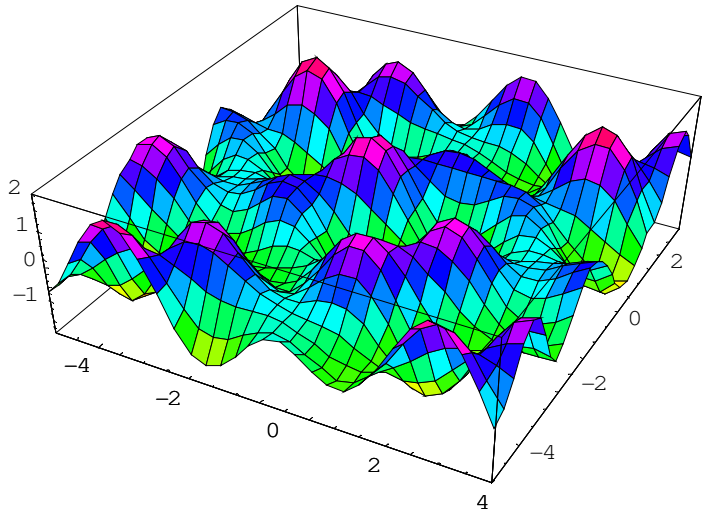
- High-level programming languages for large scale mathematical optimization problems
- Algebraic formulation
  - Syntax similar to mathematical notation
  - Does not contain any hints how to process it
- Do not solve optimization problems directly but call appropriate external algorithms (solvers)

Goals

- Support of decision making process
- Efficient handling of mathematical optimization problems
- Simplify model building and solution process
- Increase productivity and support maintainable models

Global Optimization (GO)

- Practical optimization problems are often nonlinear and non-convex
- They may contain disconnected feasible regions with multiple local optima
- The aim of Global Optimization is to find the best solution of all local optima



Examples for GO Applications

- Chemotherapy and radiotherapy design
- Chemical data and process analysis
- Differential equations
- Engineering design
- Environmental engineering
- Financial model development
- Laser design
- Packing and loading configuration design
- Staff scheduling
- Vehicle routing and scheduling
- …

Algebraic Modeling Language and GO

- AML perfect platform to promote GO
  - Experience with (local) nonlinear optimization
  - Established Quality Assurance
  - Separation of problem formulation and solution technology
  - Model in mathematical algebra
  - In many cases GO solver require other solvers for sub problems

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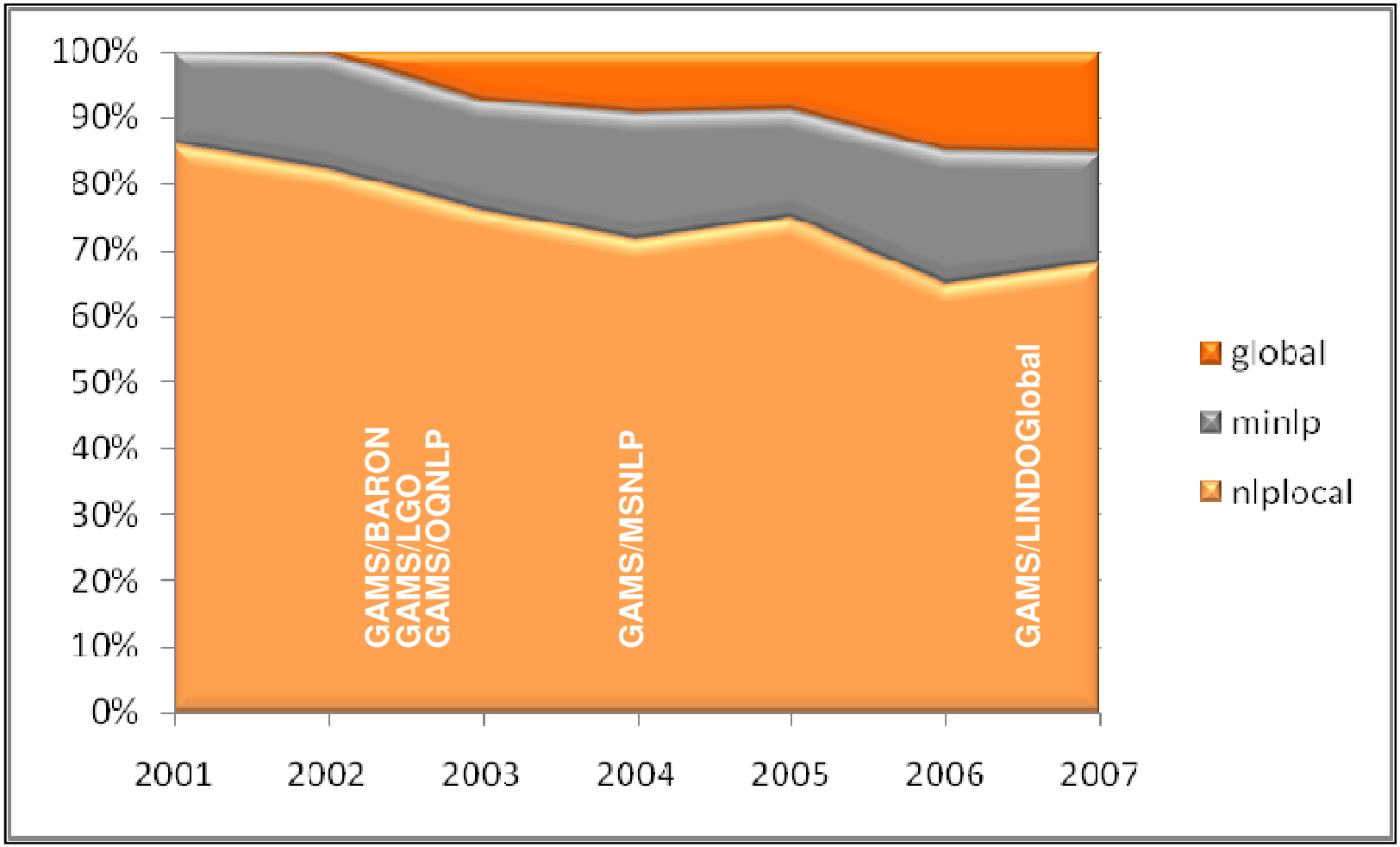
Relevance of GO



GAMS Global Solvers

- **BARON** Branch-and-Reduce Optimization Navigator for proven global solutions by *The Optimization Firm*, USA
- **LGO** Lipschitz Global Optimizer by *Pintér Consulting Services*, Canada
- **OQNLP** OptQuest/NLP Multi-start Solver by *OptTek Systems/Optimal Methods*, USA
- **LINDOGlobal** MINLP solver for proven global solutions by *LINDO Systems*, USA

The solvers differ in the methods they use, in whether they find globally optimal solution with proven optimality, in the size of models they can handle, and in the characteristics of models they accept.

LGO (NLP)

- Integrates several global search algorithms
  - Partition and sampling (branch-and-bound)
  - Adaptive global random search, enhanced with a statistical bound estimation technique
  - Random local search/Multi-start

- Stochastic convergence to global optimum
  - Assumes only Lipschitz-continuity of objective
  - Black box models (external equations)
  - No requirement for other sub solvers

OQNLP (MINLP) / MSNLP (NLP)

- Automates starting point selection
  - Starts local solvers from a set of starting points chosen by the Scatter Search software OptQuest and other point generators
  - Distance and merit filter limit the number of NLP calls
  - Works with any GAMS NLP solver
- Problem size similar to problem size limitation of local NLP solvers
- Scatter Search ensures stochastic convergence towards the global optimum

BARON and LINDOGlobal (MINLP)

- Algorithm
  - Branch-and-bound plus range reduction
  - Under-estimators for objective and constraints
  - require knowledge of algebra
- Deterministic global solution/bounds
  - Relative/absolute gap similar to MIP

- Differences BARON/LINDOGlobal
  - BARON:
    - Can returns the *k* best solutions
    - Multiple LP/NLP solvers to solve sub problems
  - LINDOGlobal
    - Handles models with trigonometric functions (sin, cos, …)
    - Handles some non-smooth functions directly (abs, min, …)

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LP vs. Global, Then vs. Now

LP	Global
Simple certificate of optimality	Solutions: deterministic bounds, stochastic bounds, optimality gap
Established solvers, 1-2 releases/year	Emerging technology, cutting edge research, frequent software updates
Links all look quite similar	Libraries, “captive” links, variety of requirements
Then: users were specialists, expert in modeling and solving	Now: users may be domain experts with little solver knowledge

Good motivation for increased performance testing (PT) and quality assurance (QA)

Challenges in PT & QA

- QA is not glamorous – where's the novelty & publications?
  - *Make the tools used public - "open-source" them*
  - *Make it a group project with high priority*
- PT & QA are time-consuming
  - *Create standard libraries of test problems, categorized for convenient access*
  - *Automate the creation of test scripts, the collection of data, and the creation and display of statistics*
- Results can be subjective, misleading, wrong, or useless
  - *Test libraries, automation, and validation reduce subjective element and make results reproducible, hence believable*
  - *Automate the creation and display of useful statistics*

GAMS World

GAMS World

- The Worlds
  - GLOBAL
  - MINLP
  - MPEC
  - MPSGE
  - Performance
  - Translation
- Search
- Contact

Welcome to the GAMS World

This is the home page of the GAMS World, a web site aiming to bridge the gap between academia and industry by providing highly focused forums and dissemination services in specialized areas of mathematical programming.

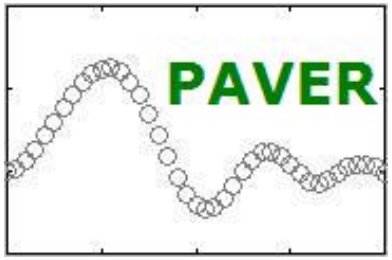
Substantial progress was made in the 1980s and 1990s with the development of algebra based modeling systems, algorithms, and computer codes to solve large and complex mathematical programs. The application of these tools, however, was less than expected. The abstraction, expression, and translation of real world problems into reliable and effective operational systems requires highly specialized and domains specific knowledge. The process of acquisition and dissemination of this knowledge is complex and poorly understood and the number of "good modelers" is much less than we all hoped for. Similarly, the process of transforming a new algorithm into a reliable and effective solution system is a slow and expensive process and there are few "good implementers". This web site hopes to address some of these problems by helping with the collection and dissemination of domain specific information and knowledge that is outside the established channels because of its content or form.

For example, model structures and results get published in commercial and academic papers but it is virtually impossible to reproduce any of those results or lift model components and data from one study to be used in some other study. Algorithm implementers face a similar dilemma when trying to get their hands on real world data models and data to test and refine their systems. This web site offers a few, well focused and maintained services to help with the dissemination of problems and solutions.

GAMS World is featured by GAMS Development Corp. and GAMS Software GmbH

PAVER

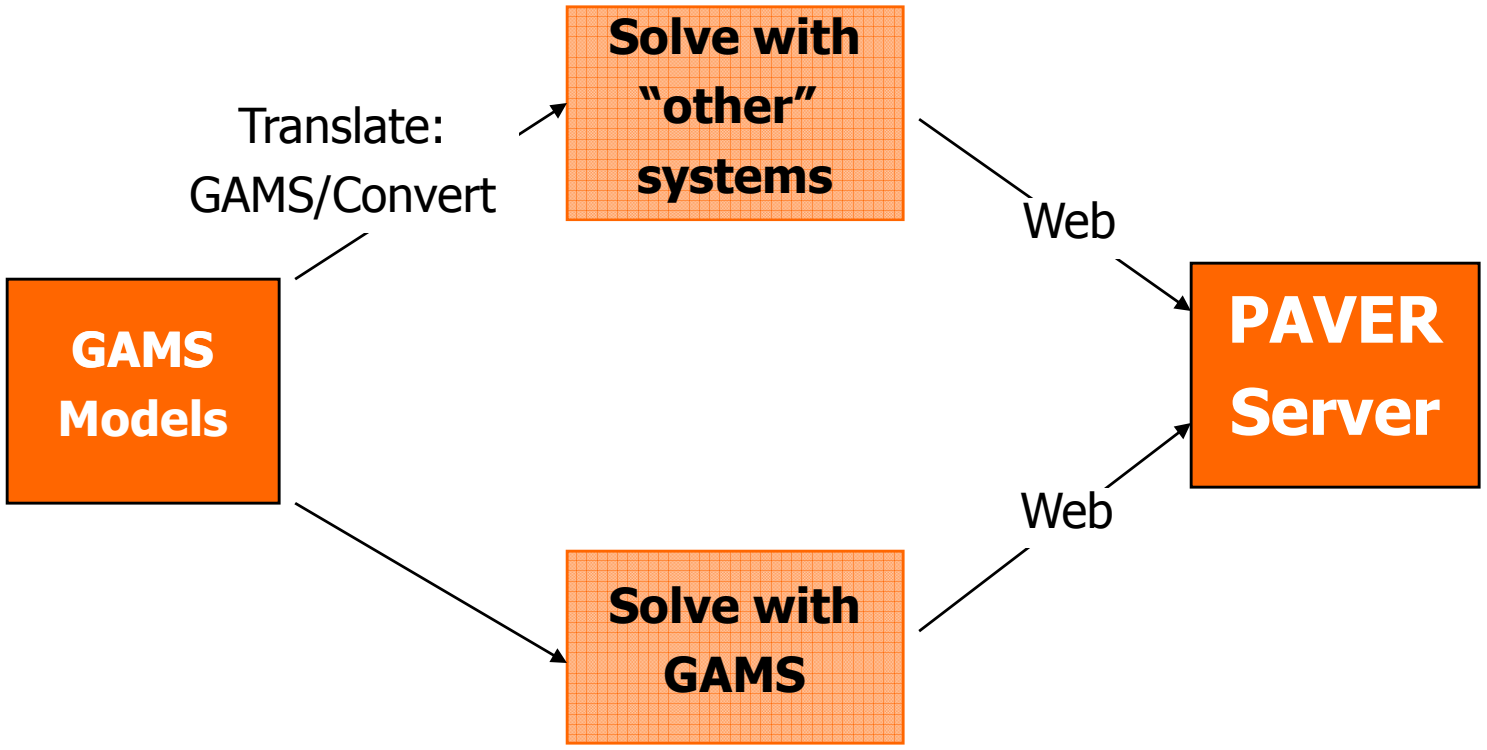
- **P**erformance **A**nalysis and **V**isualization for **E**ffortless **R**eproducibility



- Online server to facilitate performance testing and analysis/visualization
- Results sent via e-mail in HTML format
  - **System independent**

www.gamsworld.org/performance/paver

Open Testing Architecture



Benchmarking pitfalls

- Solvers may contain bugs – really!
  - Wrong solution returned
  - Wrong objective returned
  - False claims of feasibility/optimality
- Solvers will use different termination checks/tolerances
  - Difficult to compare “quality” of solutions
  - Common standard of comparison is lacking
- PAVER does not check validity of input data

GAMS/Examiner

- Purpose: to make an unbiased, independent report on the merit of points
- Points may come from GAMS or a solver
  - GAMS passes the previous solution as initial iterate
  - Solvers pass solutions back to GAMS
- Useful during solver debugging – helps pinpoint problems
  - Most checks are obvious
- Does checks on the scaled and unscaled (original) model
- All solution tolerances can be adjusted, default is tight
- Different points can be checked
- Examiner only *reports*, it doesn't *fix*

GAMS/Bench

- Tool to help facilitate benchmarking of GAMS solvers
- Compares resource usage of solvers selected by the user
- Creates problem matrix once and spawns it to all solvers
- Can create trace files used by PAVER
- Can call GAMS/Examiner for every tested solver
- Comes free with every GAMS system (depends on licensed solvers)

GAMS/Bench Output

```
Primal constraints satisfied (tol = 1e-006)
alan,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.158,0,8,9,4,24,3,NA,1,1,2.92500000000001,2.925,0.078,167,0,1,#
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beuster,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.158,0,115,158,52,398,159,NA,8,3,128002.432361333,13002.3195417608,601,2904299,0,378,#
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csched1,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.172,0,23,77,63,174,8,NA,1,1,-30639.2578450033,-30639.2578557346,26.922,114747,0,145,#
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eg_int_s,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.197,0,28,8,3,220,196,NA,13,3,NA,NA,601.875,0,0,0,#
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ex1226,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.22,0,6,6,3,15,2,NA,1,1,-17,-17,0.031,91,0,2,#
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ex1252,MINLP,LINDOGLOBAL,CONOPT,CPLEX,39231.224,0,44,40,15,118,36,NA,1,1,128893.741013226,128893.741010754,17.813,194740,0,325,#
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```
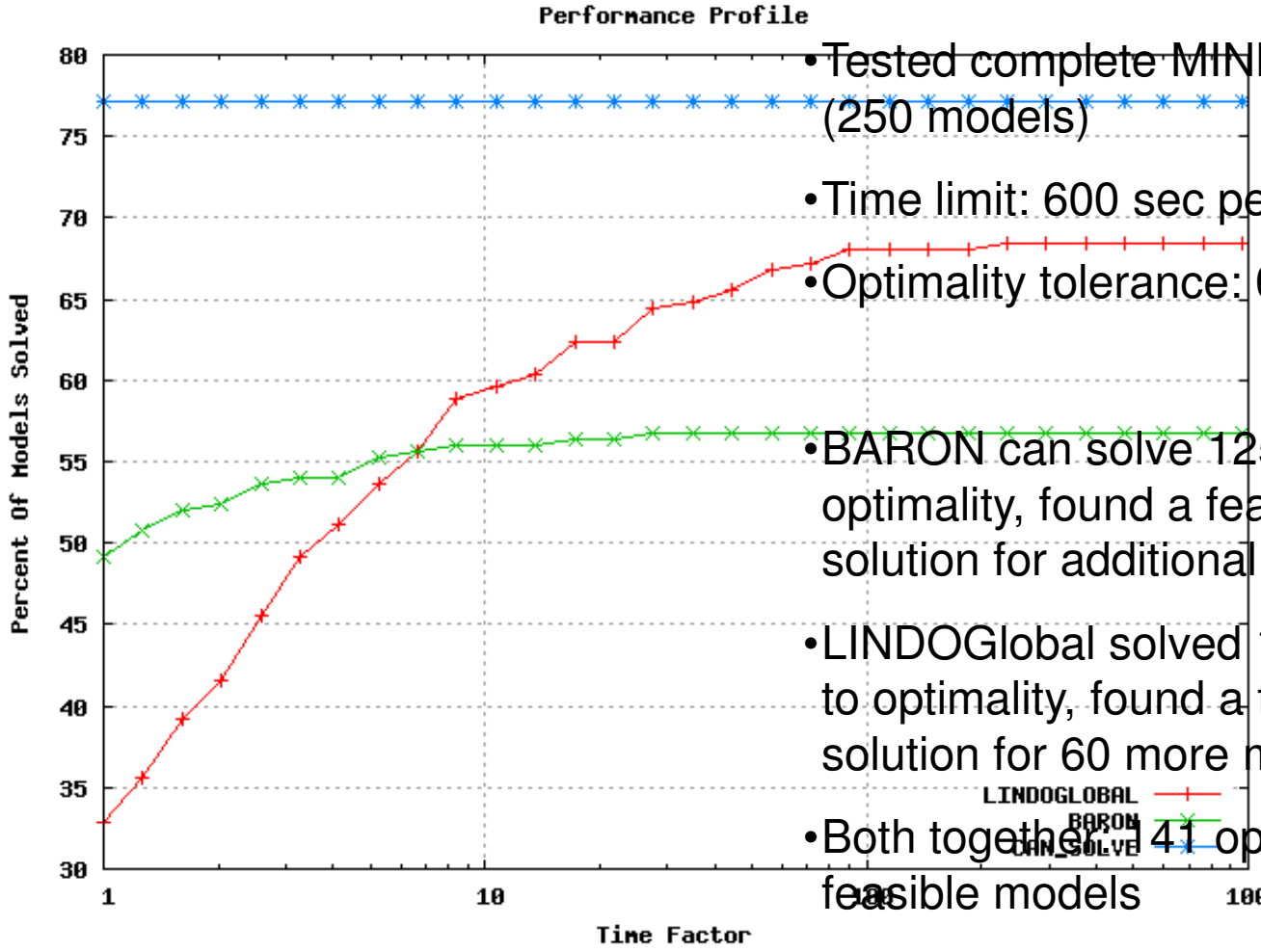

PAVER: LINDOGlobal vs. BARON



- Tested complete MINLP Library (250 models)
- Time limit: 600 sec per model
- Optimality tolerance: 0
- BARON can solve 125 models to optimality, found a feasible solution for additional 40 model
- LINDOGlobal solved 131 models to optimality, found a feasible solution for 60 more models
- Both together 141 optimal and 53 feasible models

PAVER: Solver Square

Solver Square Comparison - All Models - Microsoft Internet Explorer

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Solvers used :	Solver A
	Solver B
Modeltype(s)	MINLP

Result Totals in Percent:

Solver	% models optimal	% models feasible	% models infeasible	% models unbounded	% models fail
Solver A	-	71.72	1.01	-	27.27
Solver B	-	87.88	8.08	-	4.04

Result Totals in Number of Models:

	optimal	feasible	infeasible	unbounded	fail	total Solver A
optimal	-	-	-	-	-	-
feasible	-	67	2	-	2	71
infeasible	-	1	-	-	-	1
unbounded	-	-	-	-	-	-
fail	-	19	6	-	2	27
total Solver B	-	87	8	-	4	99

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PAVER: Square (cont.)

Solver Square Comparison - All Models - Microsoft Internet Explorer

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Solver Resource Times

- Models for each solver pair outcome. Listed are the solver resource times in seconds, as well as the ratio of resource times for the two solvers if both solved optimally.
- Also listed are the objective values using both solvers. The better solution found is listed in boldface. A solution is considered better, if the relative objective function difference is greater than 1.00E-05.
- Solver resource time ratios for a particular model are listed only if one solver has resource greater than 5.00E-02.

Solver A: feas -- Solver B: feas Back to top

Modelname	Solver A	Solver B	Ratio (Solver A/Solver B)	Obj (Solver A)	Obj (Solver B)
alan	0.0973	0.0100	9.730	3.60000000	**2.92500000**
batch	0.2478	0.5100	0.486	285506.50824405	285506.50000000
batchdes	0.1094	0.0400	2.735	167427.65711470	167427.70000000
du-opt	1.9718	0.5200	3.792	31.02527833	**3.55634000**
du-opt5	2.0975	1.7000	1.234	40.77273140	**8.07365800**
eg_all_s	28.3584	19.7400	1.437	11.23946680	**7.92018200**
eg_disc2_s	63.1667	5.3400	11.829	6.92006923	**5.64210100**
eg_disc_s	88.8061	9.3800	9.468	10.42127936	**5.76054000**
eg_int_s	106.3869	7.7900	13.657	7.88724302	**7.46308000**
elf	0.0573	15.3200	0.004	1.67500000	**0.19166670**
ex1221	0.0270	0.0000	---	7.66718007	7.66718000
ex1222	0.0629	99999.0000	0.000	1.07654308	1.07654300

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PAVER: Solver Resource Time

Resource Time Comparison - All Models - Microsoft Internet Explorer

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Solvers used :	Solver A
	Solver B
Modeltype(s)	MINLP

	Total	Obj Solver A better	Obj same	Obj Solver B better
Solver Solver Ainfinitely faster :	4	4	-	-
Solver Solver A much faster :	13	1	4	8
Solver Solver A faster :	1	-	1	-
Solvers perform the same :	10	-	7	3
Solver Solver B faster :	31	-	23	8
Solver Solver B much faster :	12	-	4	8
Solver Solver B infinitely faster :	20	-	-	20
Both solvers failed to solve optimally :	8	-	8	-
Total models: :	99	5	47	47

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PAVER: Resource Time (cont.)

Resource Time Comparison - All Models - Microsoft Internet Explorer

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Solver Solver A much faster - Obj of Solver A better:

Modelname	Solver A	Solver B	Ratio (Solver A / Solver B)	Obj Solver A	Obj Solver B
synheat	0.2878	2.0600	0.140	1.54997335E+05	1.60435500E+05

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Solver Solver A much faster - Obj same for both solvers:

Modelname	Solver A	Solver B	Ratio (Solver A / Solver B)	Obj Solver A	Obj Solver B
batch	0.2478	0.5100	0.486	2.85506508E+05	2.85506500E+05
ex1222	0.0629	99999.0000	0.000	1.07654308E+00	1.07654300E+00
ex4	1.1326	3.8400	0.295	-8.06413616E+00	-8.06413600E+00
util	0.6693	14.2400	0.047	9.99578750E+02	9.99578800E+02

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Something completely different

The GAMS Beta Distribution 22.8 is available for download

http://beta.gams-software.com

- New Solver Libraries, e.g.
  - CPLEX 11.1
  - Coin-OR Solvers
- Experimental Solvers offering in-core communication
- Two new Model Libraries
- New utilities (gdx2xls, invert, xlstalk)
- …

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