Global Optimization with GAMS Applications and Performance

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Introduction & History

- Availability of general purpose global optimization (GO) codes
- Customer demand: currently, about 3000 GAMS systems with NLP capability
- 2001: Start of collaboration GAMS Dev. Corp. and developers of BARON, LGO, and OQNLP
- Outline:
  - GO solvers and their key features
  - GO solvers in a modeling system
  - GO solvers in the market place

GAMS Overview

- Started as a Research Project at the World Bank in 1976
- GAMS went commercial in 1987
- Opened European Office in Cologne, Germany in 1996
- 10,000s of users in over 100 countries
- Unique position between the academic and commercial world

Supported Solvers

BARON	Branch-And-Reduce Optimization Navigator for proven global solutions from The Optimization Firm
BDMLP	LP solver that comes with any GAMS system
CONOPT	Large scale NLP solver from ARKI Consulting and Development
CPLEX	High-performance LP/MIP solver from Ilog
DECIS	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

Continuous GO Model

$\min f(x)$ $\quad$ $f: R^n \rightarrow R^1$

$g(x) \leq 0$ $\quad$ $g: R^n \rightarrow R^m$

$x_l \leq x \leq x_u$ $\quad$ $x, x_l, x_u, (x_l < x_u)$ are real n-vectors

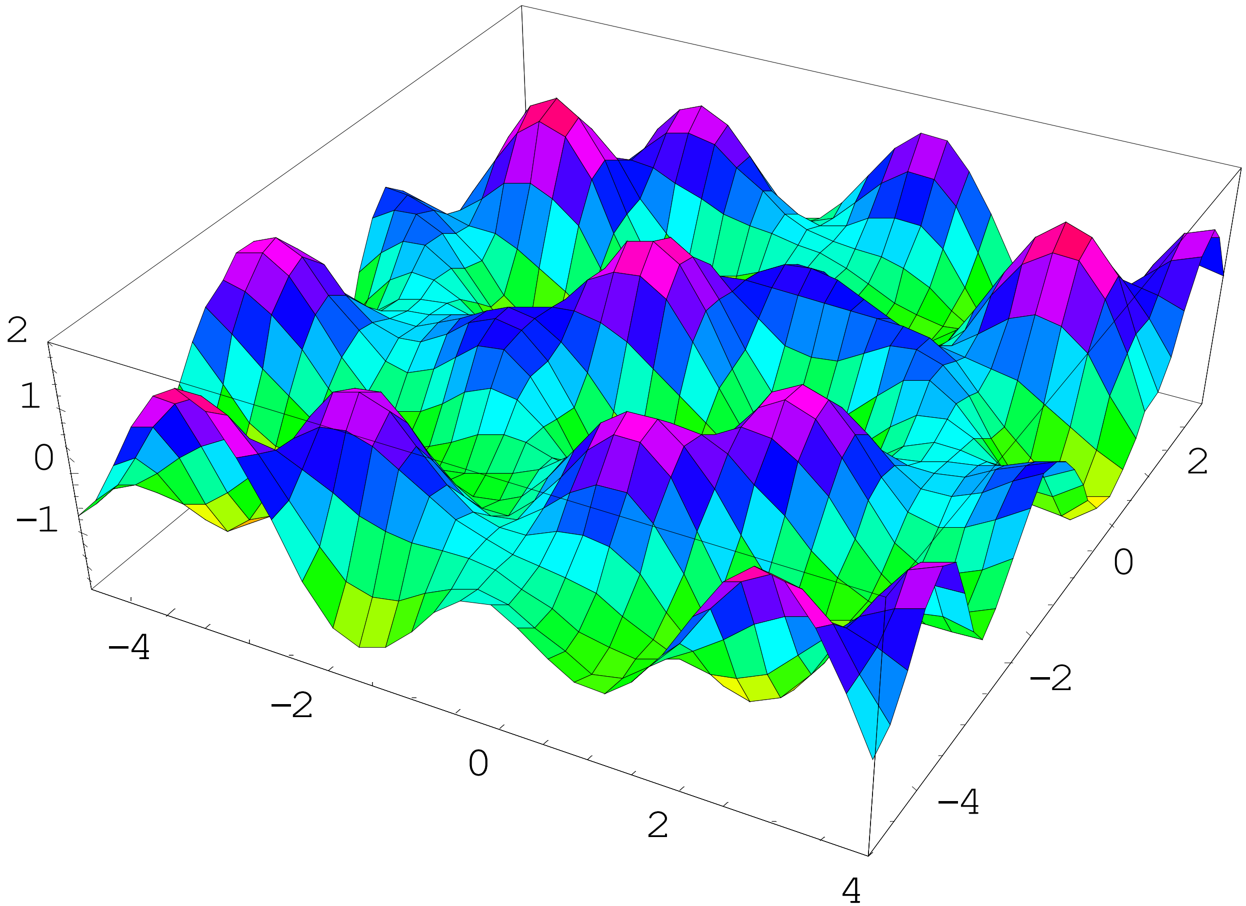
"Minimal" analytical assumptions:

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

This guarantees the existence of global solution set.

CGO covers a very general class of models.

GO Problem in Two Dimensions



Numerical difficulty may increase exponentially, as model size grows

GAMS/GLOBAL Solvers

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

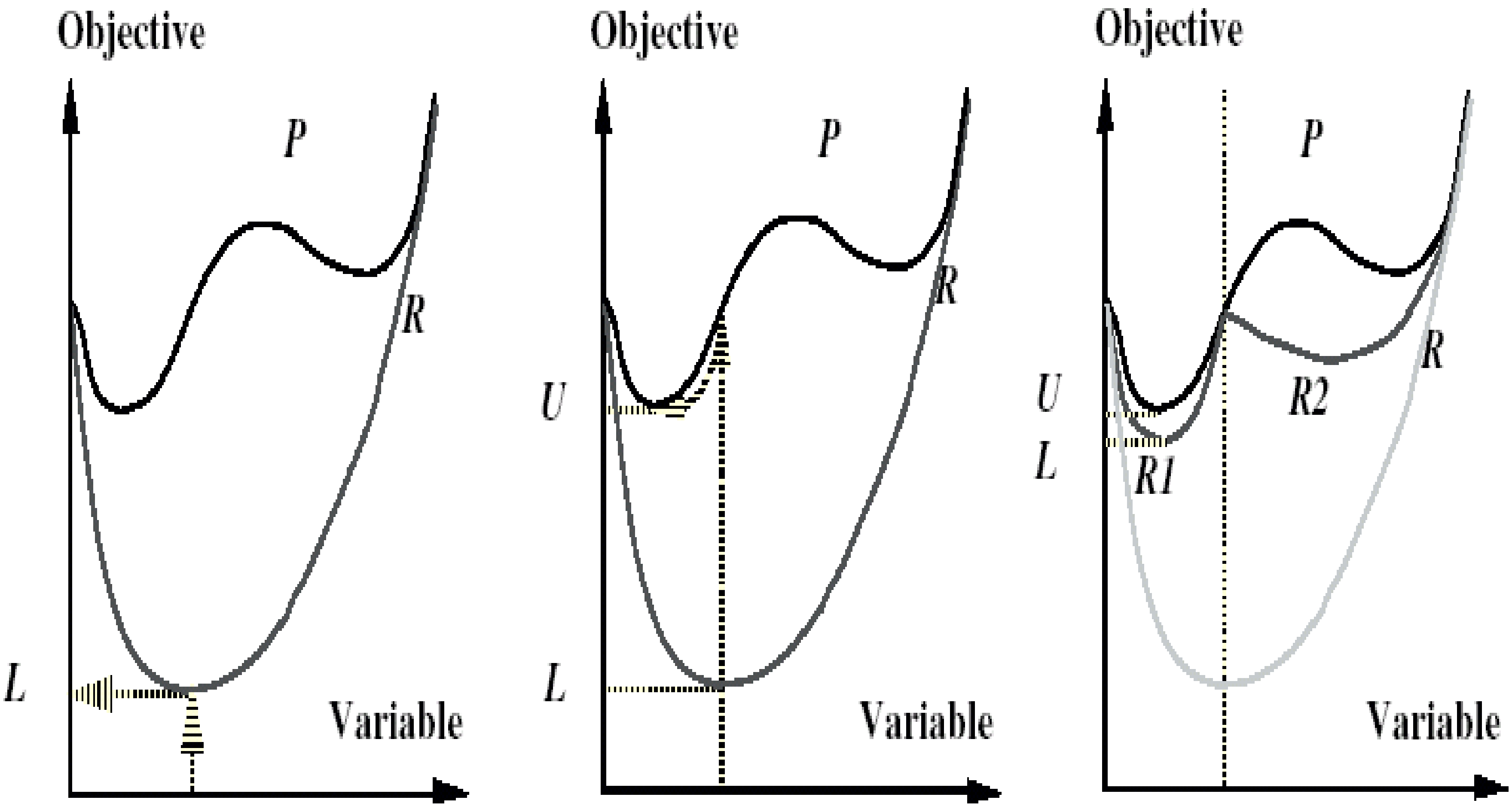
- **BARON** Branch-and-Reduce Optimization Navigator by The Optimization Firm, USA
- **LGO** Global/nonlinear optimization solver suite by Pintér Consulting Services, Canada
- **OQNLP** OptQuest/NLP Multi-start Solver by OptTek Systems and Optimal Methods, USA

"… it winds its way through the hills and valleys of complex optimization problems in search of global solutions."

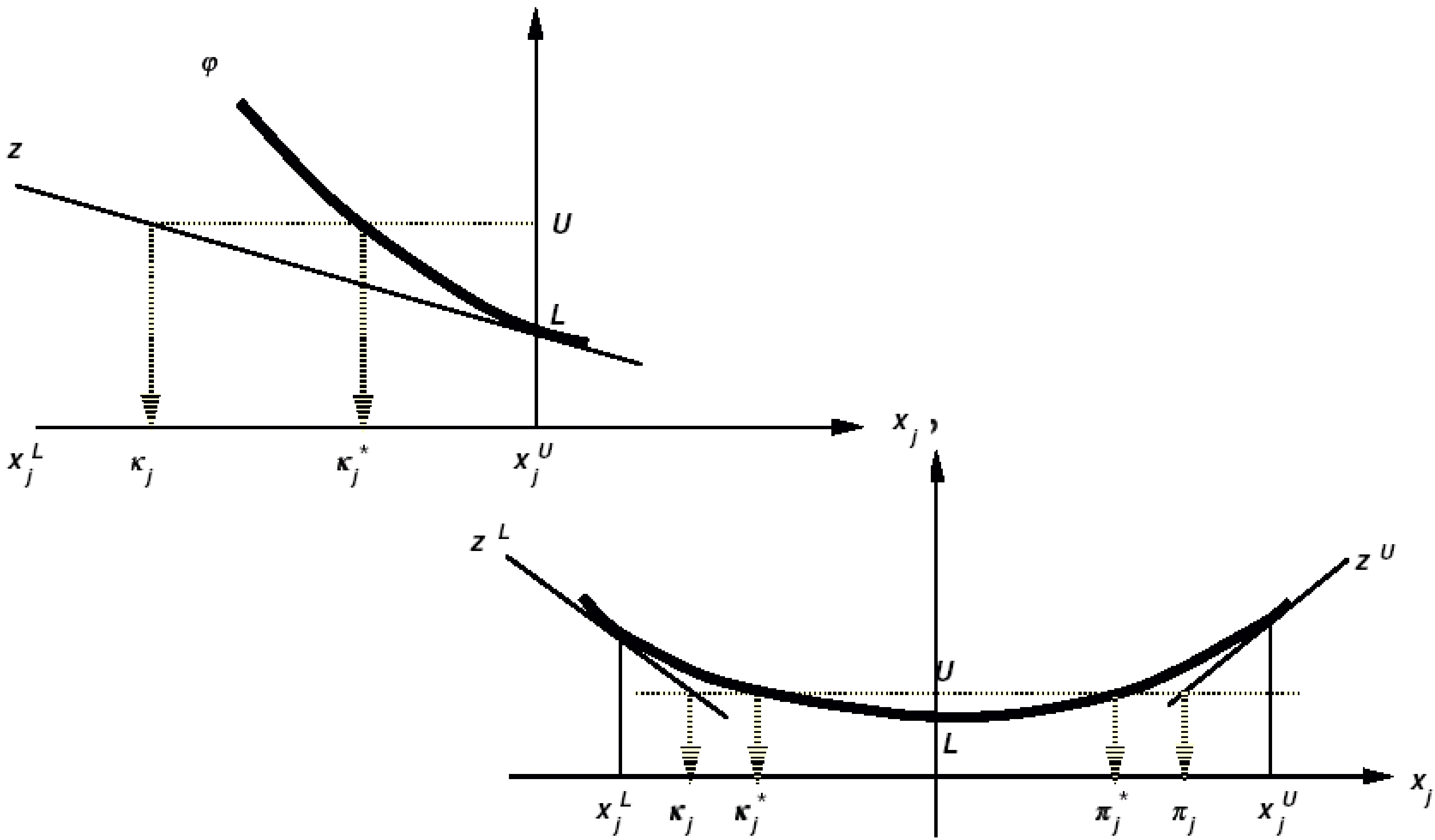
BARON - Branch And Reduce Optimization Navigator

- BARON is a computational system for solving mixed-integer nonlinear non convex optimization problems to global optimality
- Works with relaxed problems by constructing (convex) under-estimators for objective and constraints
- Combining branch-and-bound with range reduction

Branch-and-Bound



Range Reduction



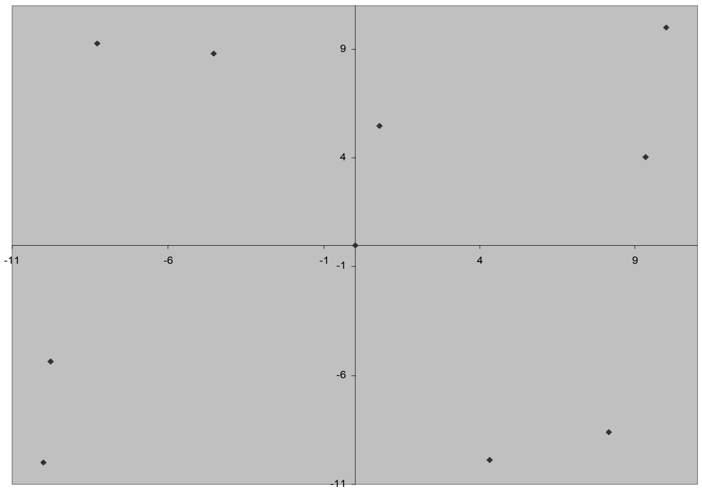
LGO – Lipschitz Global Optimizer

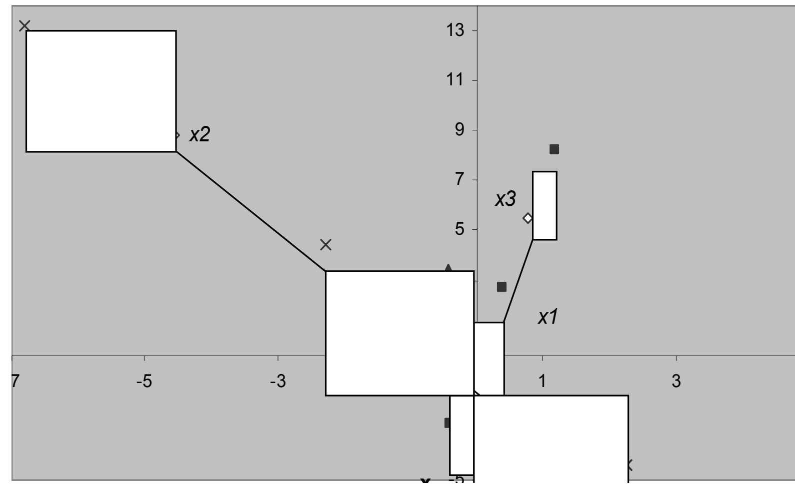
- Global/nonlinear optimization solver suite
- Branch-and-bound based global search, enhanced with a stochastic sampling procedure
- Adaptive global random search, enhanced with a statistical bound estimation technique
- Various local search procedures (function/gradient based)

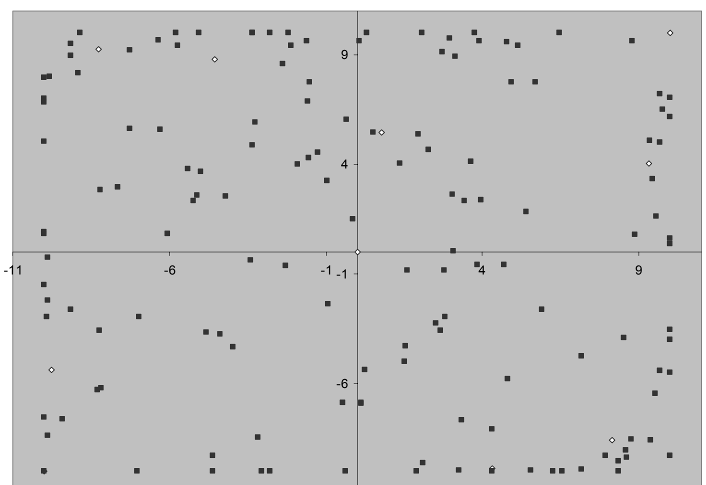
OQNLP
Multi-Start Search Method

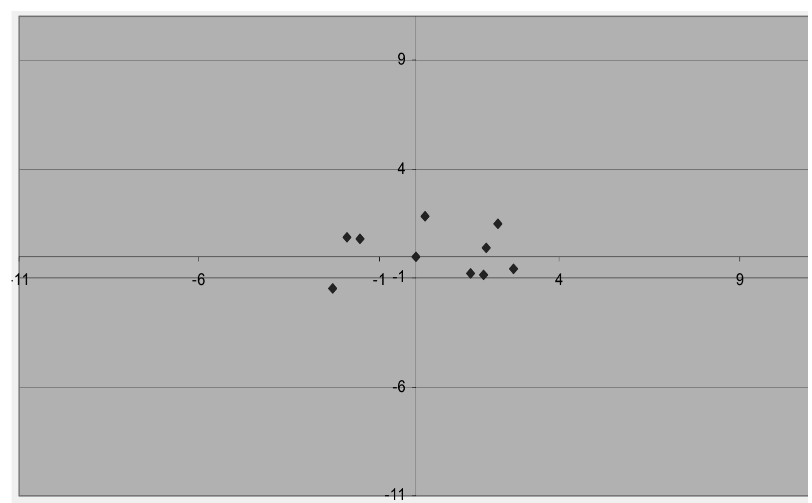
- Intended for nonlinearly constrained, smooth, non-convex NLP's and MINLP's
- It starts any GAMS NLP solver from a set of starting points chosen by the widely used Scatter Search software, OptQuest (Glover, Laguna, Kelly).
- It can also be used to solve any NLP problem where solver failures are common, by automating the process of choosing multiple starting points

Reference Set/Population









OQNLP Algorithm

- While point is evaluated for Scatter Search, NLP solver is called from that point if filter criteria (merit/distance) are satisfied
- User supplied starting point is part of initial reference set which guarantees that OQNLP is at least as good as just the NLP solver

GO Solver Differences

- The three solvers differ in the methods they use. Hence, their requirements, capabilities and the results they provide are different:
- Model requirements
- Problem size
- Solution quality metrics/termination criteria

Difference Matrix

	Model requirements	Problem size	Solution metrics
BARON	**-**	**0**	+
LGO	+	**0**	**0**
OQNLP	**0**	+	**-**

Model Requirements

-	0	+
+	0	0
0	+	-

- BARON
  - Constructs convex under-estimators
  - Knowledge about model algebra
  - No black box evaluators
- LGO
  - Lipschitz-continuity of objective function
  - Black box models
- OQNLP
  - Requirements of local solver used during search
  - Smooth problems (first [and second] order derivatives)

Problem Size

-	o	+
+	o	o
o	+	-

- BARON/LGO
  - Ratio of LP/MIP problem sizes = ratio of local NLP/global NLP sizes
- OQNLP
  - Size of model is limited by size limitation of the local solver

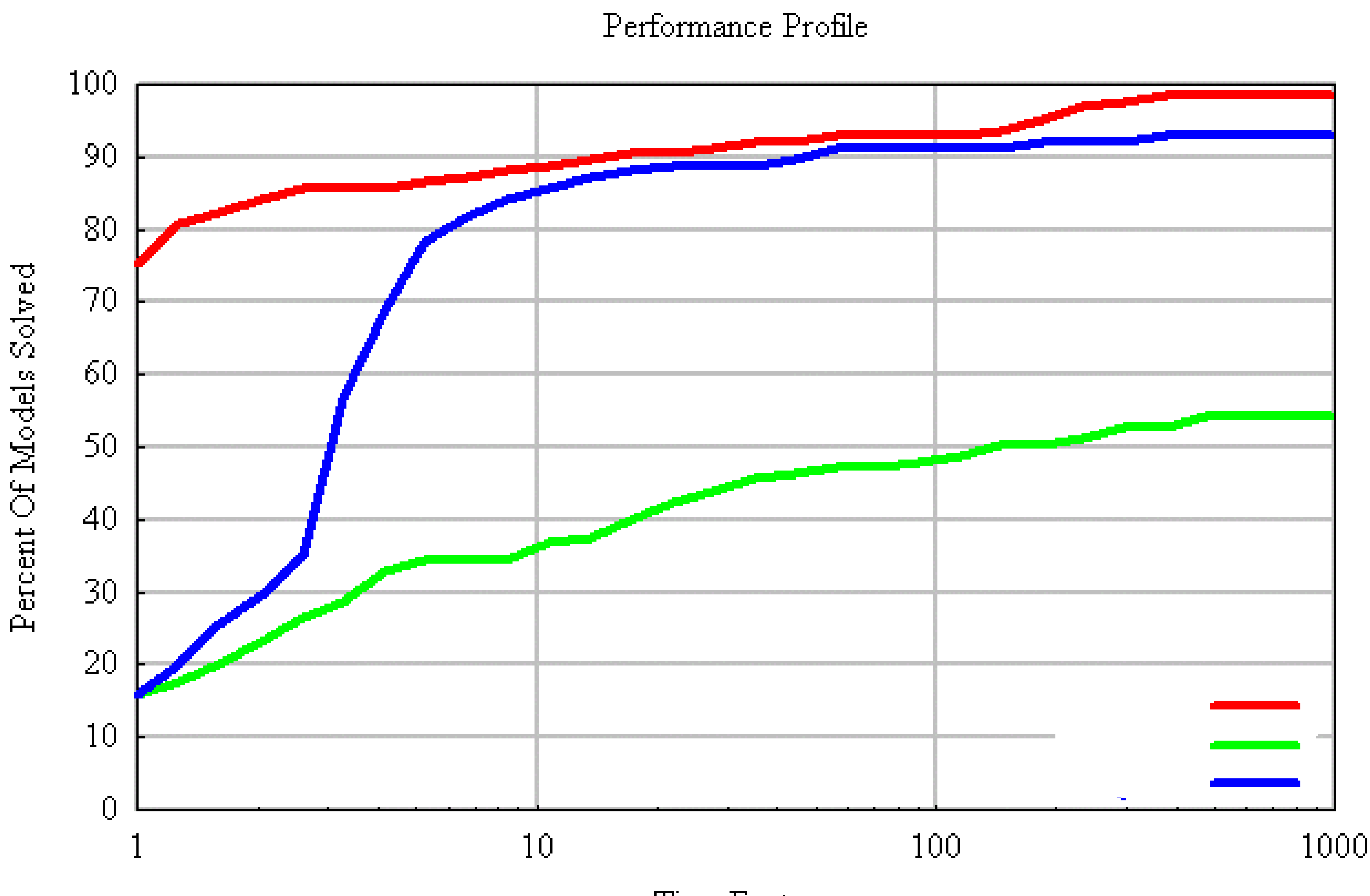
Solution Quality Metrics

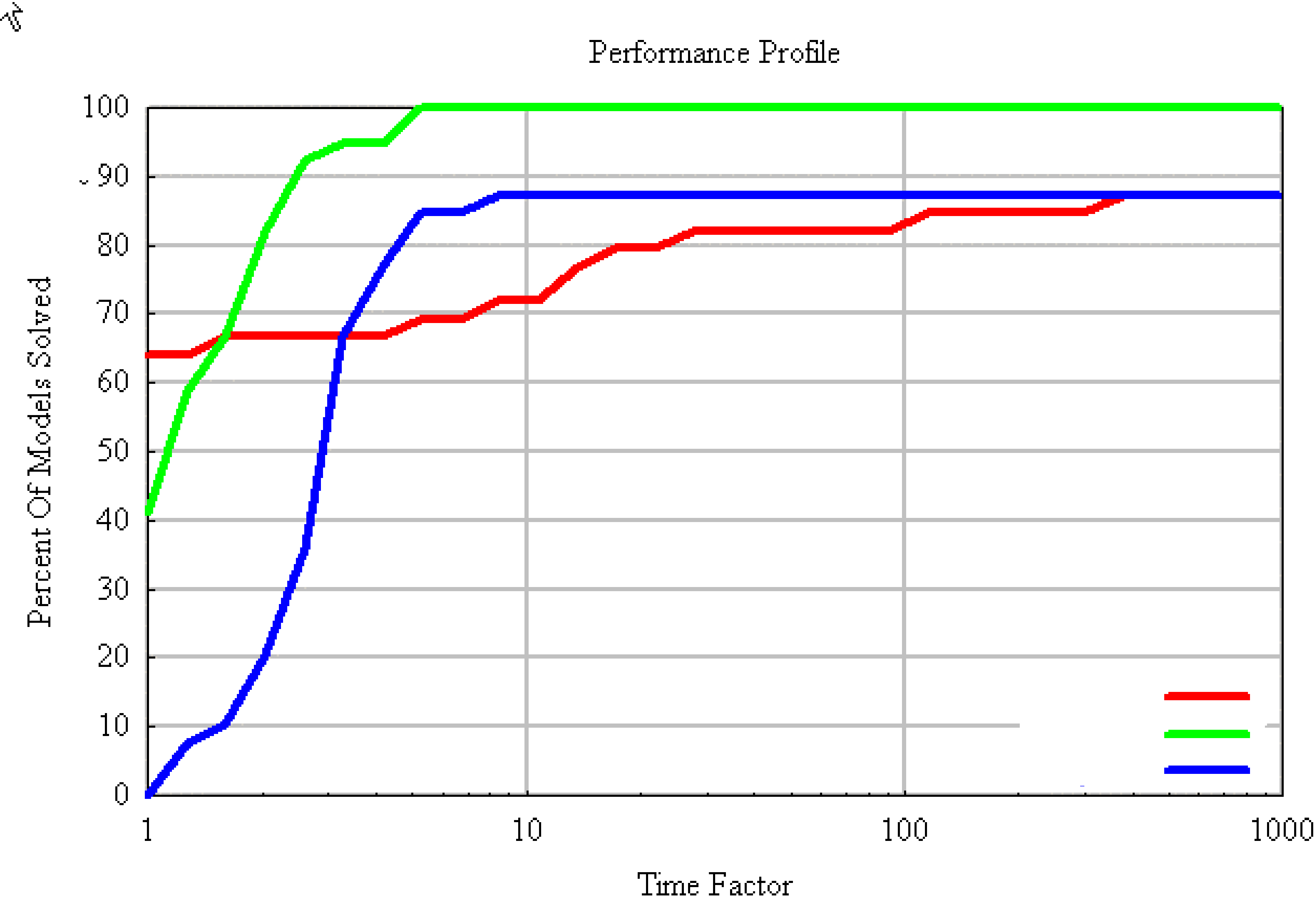
-	o	+
+	o	o
o	+	-

- BARON
  - Deterministic lower bound
  - relative/absolute gap similar to MIP
- LGO
  - Estimated statistical or Lipschitz lower bound
  - Stochastic convergence to global optimum
- OQNLP
  - Scatter Search ensures stochastic convergence towards the global optimum

Which one is the best?

- Models from GlobalLib ($n \leq 500$, $m \leq 500$) (http://www.gamsworld.org/global)
- Performance Profiles (Dolan and More, 2002):
  - Cumulative distribution function for a performance metric
  - Performance metric: ratio of current solver time over best time of all solvers
  - Intuitively: probability of success if given τ times fastest time (τ=ratio)


Performance Profile
Percent Of Models Solved
Time Factor
100
90
80
70
60
50
40
30
20
10
0
1
10
100
1000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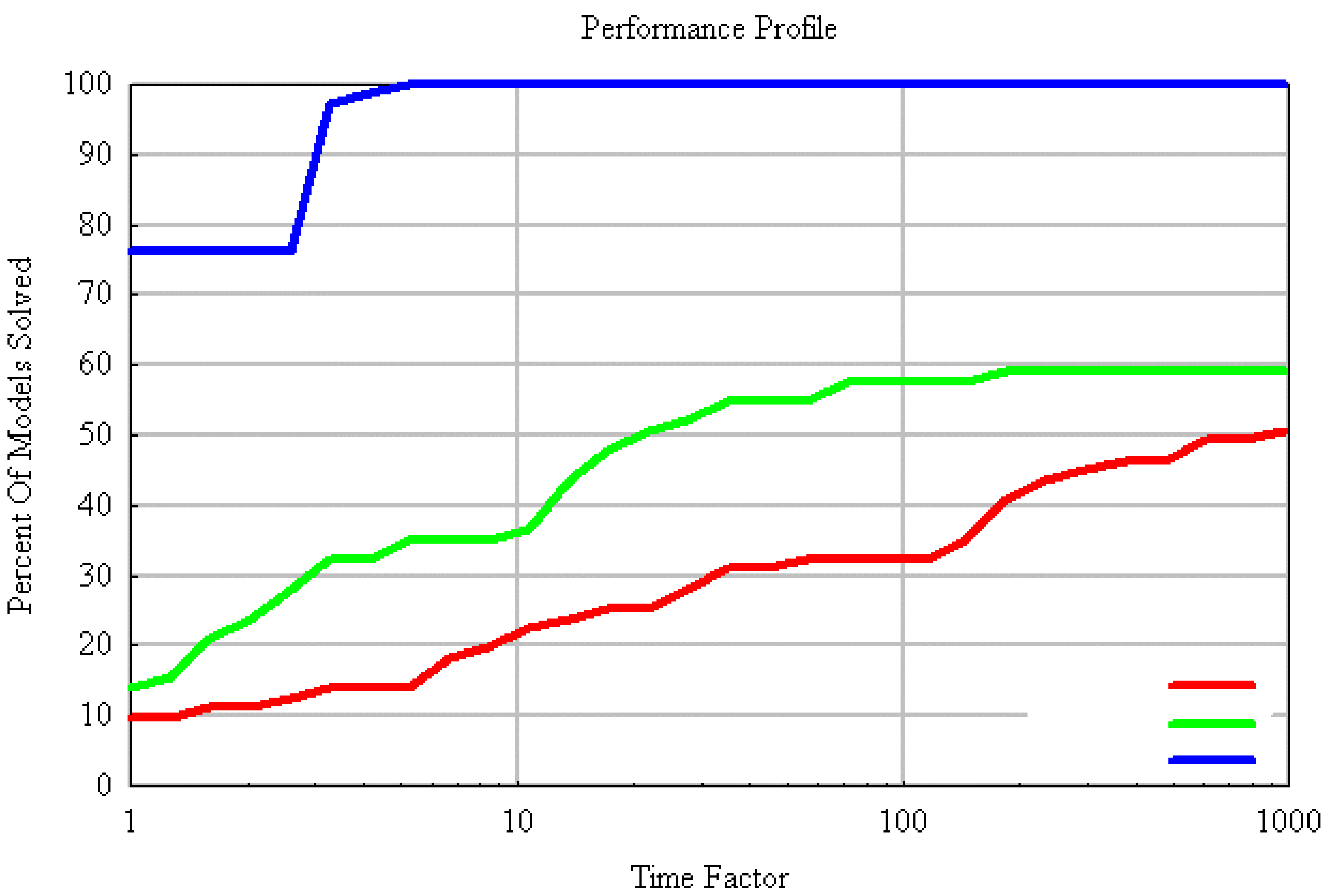
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Time Factor

Comparison Conclusion

- Model selection decides about the "winner"
  - 309 model from GlobalLib (total)
  - Subgroups between 40 and 125 models
- Where does the solver "shine":
  - BARON: Deterministic bounds
  - LGO: Black box models
  - OQNLP: Large models

GO and Modeling Systems

- Nonlinear modeling available in GAMS from the very beginning (large user base)
- Variety of local solvers
  - NLP: MINOS, CONOPT, SNOPT, LSGRG, PATHNLP, MOSEK, TRAMP
  - MINLP: DICOPT, SBB

implementing different methods (SLP, SQP, GRG, B&B, outer approximation…) improve reliability of nonlinear modeling (high expectation)

GO and Modeling Systems

- Seamless exchange of local solvers with global solvers: For example: `Option nlp=oqnlp;`
- GO Solvers benefit from Modeling System Services:
  - Search algorithm have difficulties with equalities

    Defining equation elimination by GAMS
  - Dual solution unavailable, approximate solution

    Optional cleanup up call (CONOPT) from solution found
  - Currently, no MINLP capability (LGO)

    B&B code SBB uses GAMS NLP sub-solvers

GO in the Marketplace

- Benefits of GO:
  - Independence of starting point
  - Global/improved solutions
  - Solution quality metrics
  - Opening new markets
- Risks of GO: raise expectation & fail to deliver
- Minimize risk of new technology for customers
  - Multiple Global Codes (LaGO work in progress)
  - Fallback to Local Solvers (same solver/user interface)
  - Reproducible Quality Assurance Tests

QA Tests for Reducing Risk

- Replication of quality assurance results critical factor for establishing a new solver technology in the commercial world
- Non-reproducible tests damage the reputation of a solver
- Requirement: low cost replication of such results by an independent auditor (user/tester)

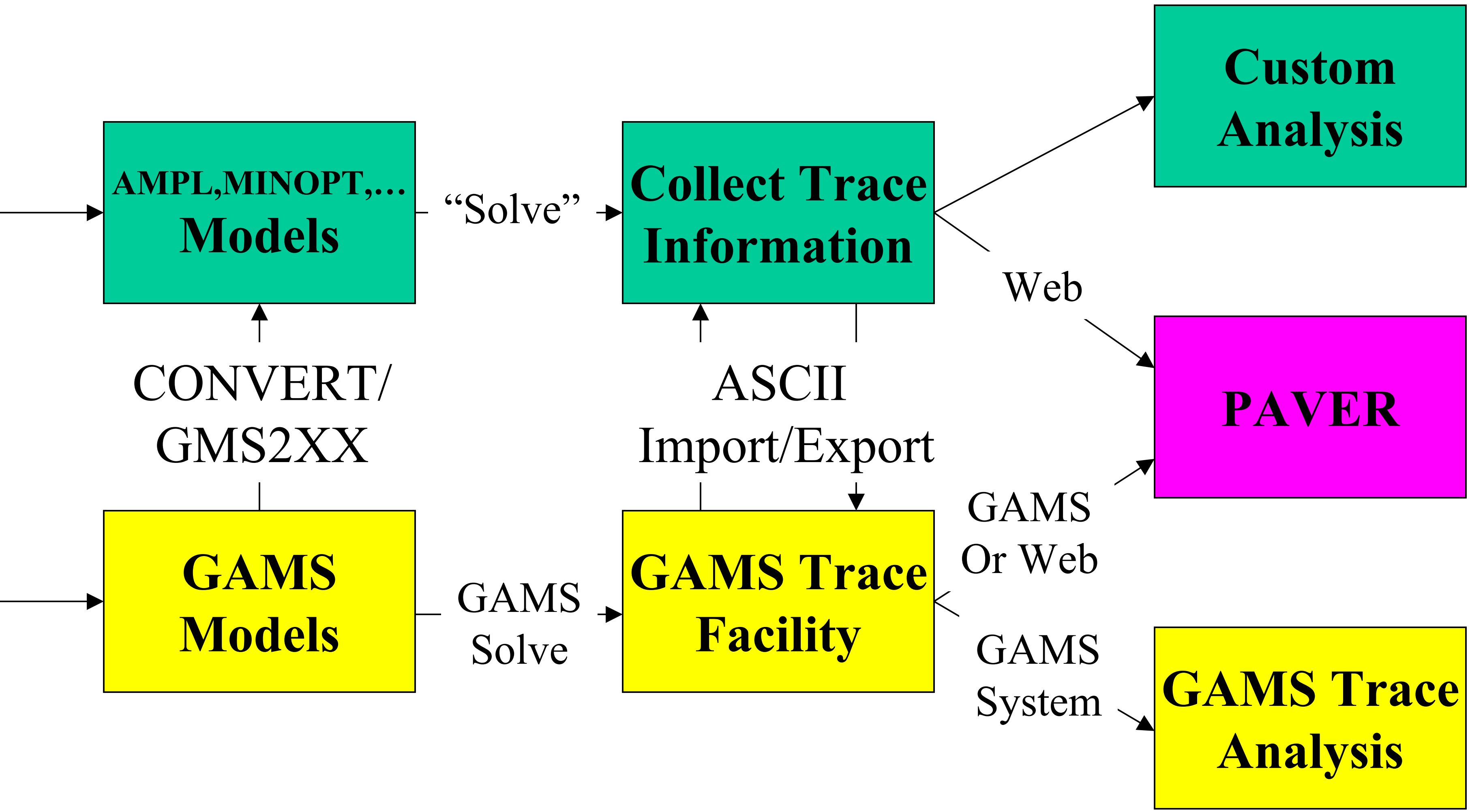
Effective Testing

- Test cases
  - Widely available collection of standardized test model instances
- Data collection tools
  - Automatic collection of solution and statistics
  - Capture test environment setting (hardware, software)
- Data analysis tools
  - Standard quality and performance measurements

Open Testing Architecture

- Test models
  - Open source GAMS models
  - Automatic translation into different formats, e.g. AMPL
  - Web/Email interface for this translation service
- Trace facility API
  - ASCII import/export of trace files
- Analysis tools
  - open source GAMS programs
  - Web interface for PAVER (**P**erformance **A**nalysis and **V**isualization for **E**ffortless **R**eproducibility)

Open Testing Architecture



Conclusions

- Introduction and addition of three well known global optimization codes into the GAMS solver portfolio.
- Commitment to quality assurance in the optimization world (critical for success in the commercial environment).
- Presentation will be available at **`http://www.gams.com/presentations`**

Illustrative References

- GAMS solver documentation Web pages
- Edgar, Himmelblau and Lasdon (2001) *Optimization of Chemical Processes*, McGraw-Hill.
- Pintér (1996) *Global Optimization in Action*, Kluwer Academic Publishers.
- Tawarmalani and Sahinidis (2002) *Convexification and Global Optimization…*, Kluwer Academic Publishers.
- The Web sites of the solver developers provide further professional details