Global Optimization with GAMS

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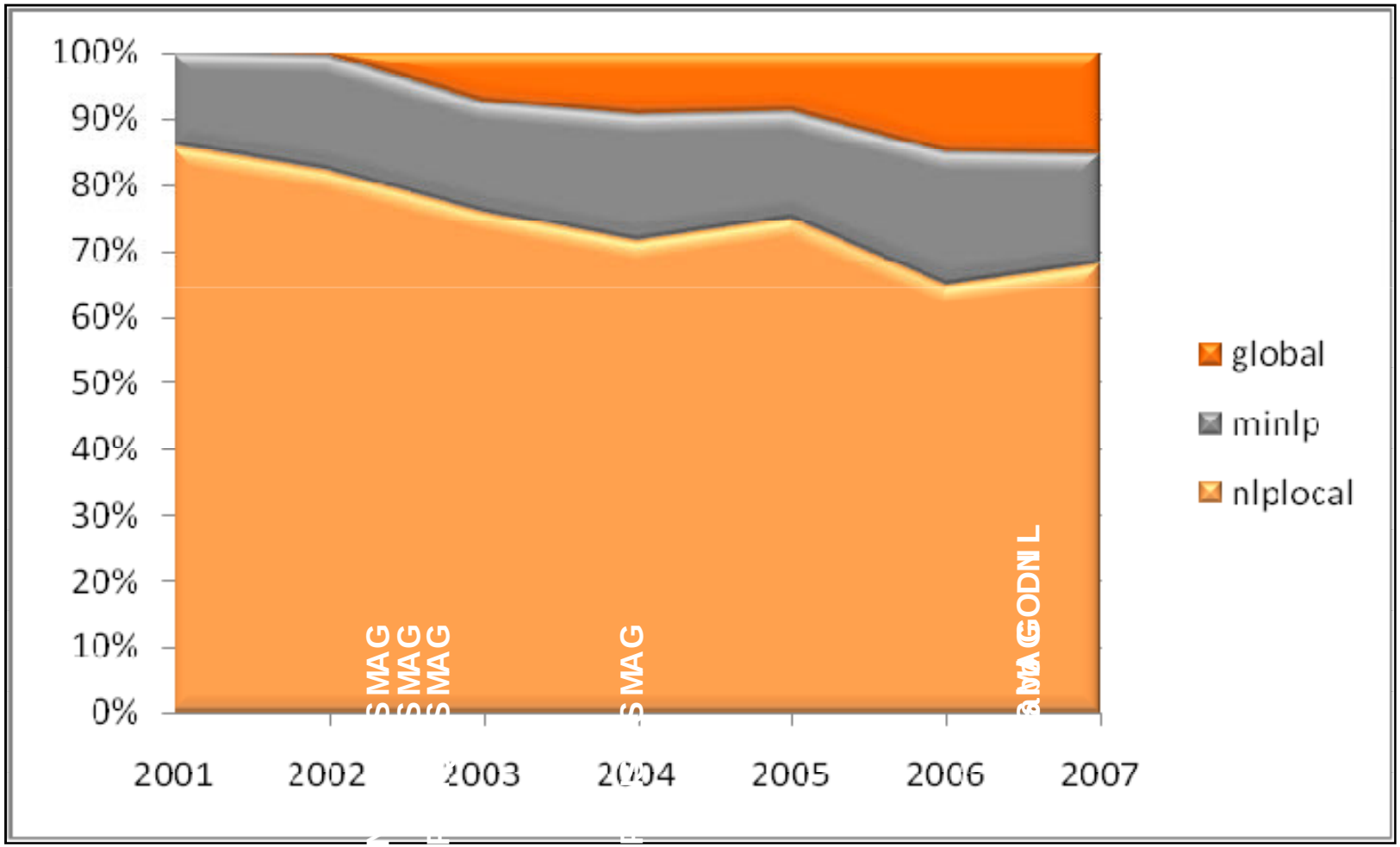
Relevance of GO



Agenda

- Global Optimization Introduction
- GAMS Global Solvers
- Exotic Application of GO
- Performance & Quality

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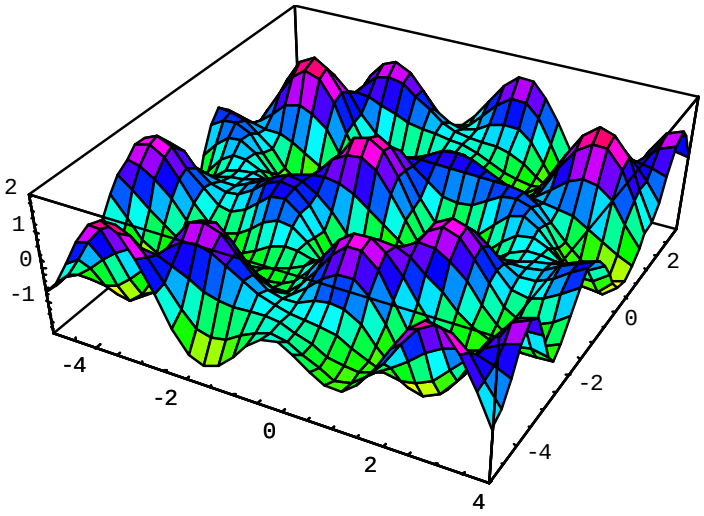
Global Optimization (GO)

- Practical optimization problems are often nonlinear and non-convex, with discrete variables
- 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 System and GO

- AMS perfect platform to promote GO
  - Separation of problem formulation and solution technology
  - Model in mathematical algebra (not black box)
  - Experience with (local) nonlinear optimization

- GO Solvers benefit from GAMS:
  - Search algorithms 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, MSNLP)
    B&B code SBB uses GAMS NLP sub-solvers

Introduction of New Technology (GO)

- Cover large portion of existing algorithmic approaches
  - Deterministic
  - Stochastic
  - Heuristic/Meta-Heuristic
- Have fallback mechanisms
  - Variety of local solvers (program your own multi-start)
  - Multiple solvers implementing same algorithm
- Demonstrate the maturity of the technology
  - Reproducible Examples
  - Books focusing on GO Applications
  - Software Quality Assurance

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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**
  MSNLP — OptQuest/NLP Multi-start Solver by *OptTek Systems/Optimal Methods*, USA
- **LINDOGlobal** — MINLP solver for proven global solutions by *LINDO Systems*, USA

BARON and LINDOGlobal (MINLP)

- Algorithm
  - Branch-and-bound plus range reduction
  - Under-estimators for objective and constraints requires 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 subproblems
  - LINDOGlobal
    - Handles models with trig-functions (sin, cos, …)
    - Handles some non-smooth functions directly (abs, min, …)

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

LGO (NLP)

- Integrates several global search algorithms
  - Partition and search (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 subsolvers

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Linear Fixed-Charge Network Flow Problem

- Single-commodity, uncapacitated, fixed-charge network flow problem

$$\min \sum_{(i,j)\in A}(f_{ij}y_{ij}+c_{ij}x_{ij}), s.t. \sum_{(j,i)\in\delta^-(i)}x_{ji}-\sum_{(i,j)\in\delta^+(i)}x_{ij}=b_i, 0\le x_{ij}\le My_{ij}, y\in\{0,1\}$$

- Problem class includes Steiner Tree Problem
- F. Ortega, L. Wolsey A branch-and-cut algorithm for the single-commodity, uncapacitated, fixed-charge network flow problem. Networks 41 (2003), no. 3, 143—158
- 83 instances (including 24 not proven optimal)

Dicut Inequalities

- Dicut: $\sum_{(i,j)\in\delta^-(S)} y_{ij} \geq 1$ if S⊂V and b(S)>0.
- Separation problem:

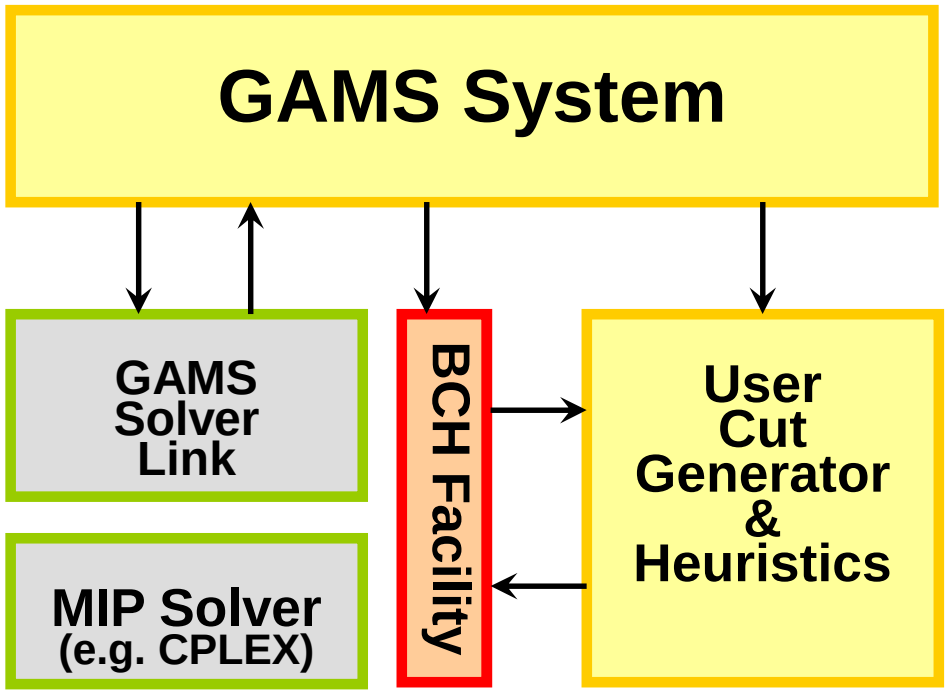
$$\xi = \min \left\{ \sum_{(i,j)\in A} \bar{y}_{ij} z_j (1 - z_i) \;:\; \sum_{i\in V} b_i z_i > 0,\; z_i \in \{0,1\}\ \forall\, i \in V \right\}$$

- Non-convex quadratic binary program:
  - Ortega/Wolsey: Greedy algorithm
  - Let's solve this exactly (small #variables |V|)

Branch-and-Cut-and-Heuristic (BCH) Facility

- **Cut Generator and Heuristic**
  - Represented in terms of original GAMS problem formulation
  - Independent of the specific MIP solver
  - Use any other model type and solver available in GAMS

- **Design Principle:**

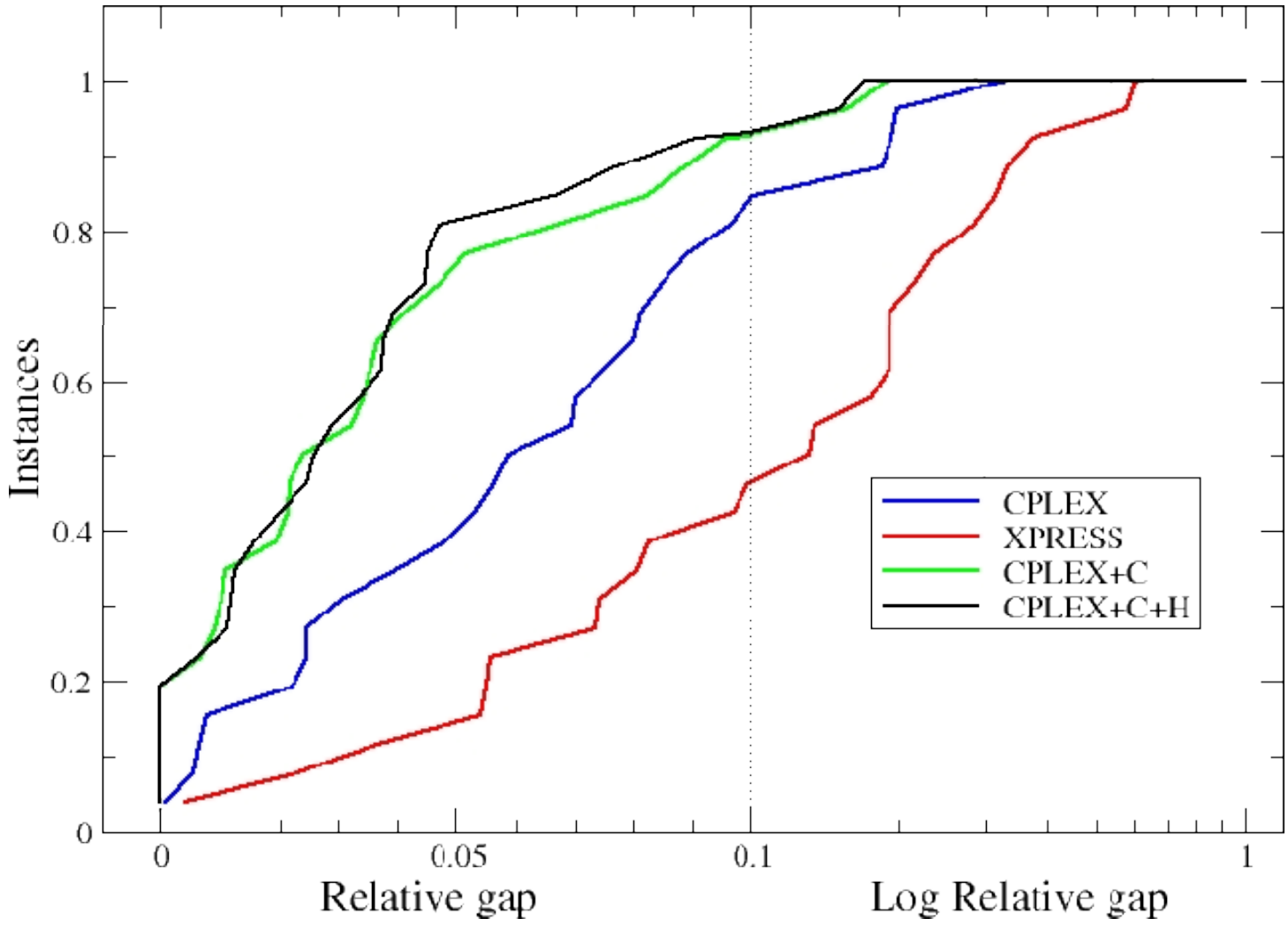


Local versus Global

- Berlin52 – from SteinLib
  - 52 nodes (1 source, n'=15 sinks), 1326 edges

	CPLEX 9 (no BCH)	BCH + SBB (local)	BCH + BARON (global)
# cuts	0	139	610
# nodes	168449	1	1
Time	1000	1000	223
Gap	45%	39%	0%

Unsolved Instances - Gap



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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, proven track record, 1-2 releases/year	Emerging technology, cutting/bleeding edge research, frequent software updates
Links all look quite similar	Libraries, shared source, “captive” links
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)

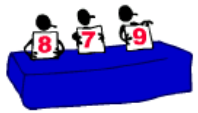
Challenges in PT & QA

- 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*
- QA & PT 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*

GAMSWorld Libraries

- Collections of all kinds of models (~1e3 models)
- Large and varied set of both theoretical and practical models
- Helps algorithm developers to test their source
- Helps users do PT

www.gamsworld.org



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Performance Libraries

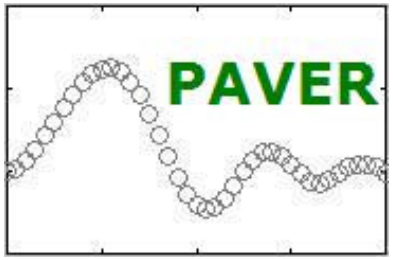
The purpose of the collections is to provide users with an established and varied set of both theoretical and practical test models. Users can make use of our automation tools for collecting performance measurements on an established set of models.

Our current collection consists of the following libraries:

- FCNetLib - MIP
- GLOBALLib - NLP
- LINLib - LP, MIP, and QCP
- MINLPLib - MINLP
- PrincetonLib - NLP
- AMPLBookLib - LP, MIP, and NLP
- MPLLib - LP, NLP
- XPRESSLib - LP, NLP

PAVER

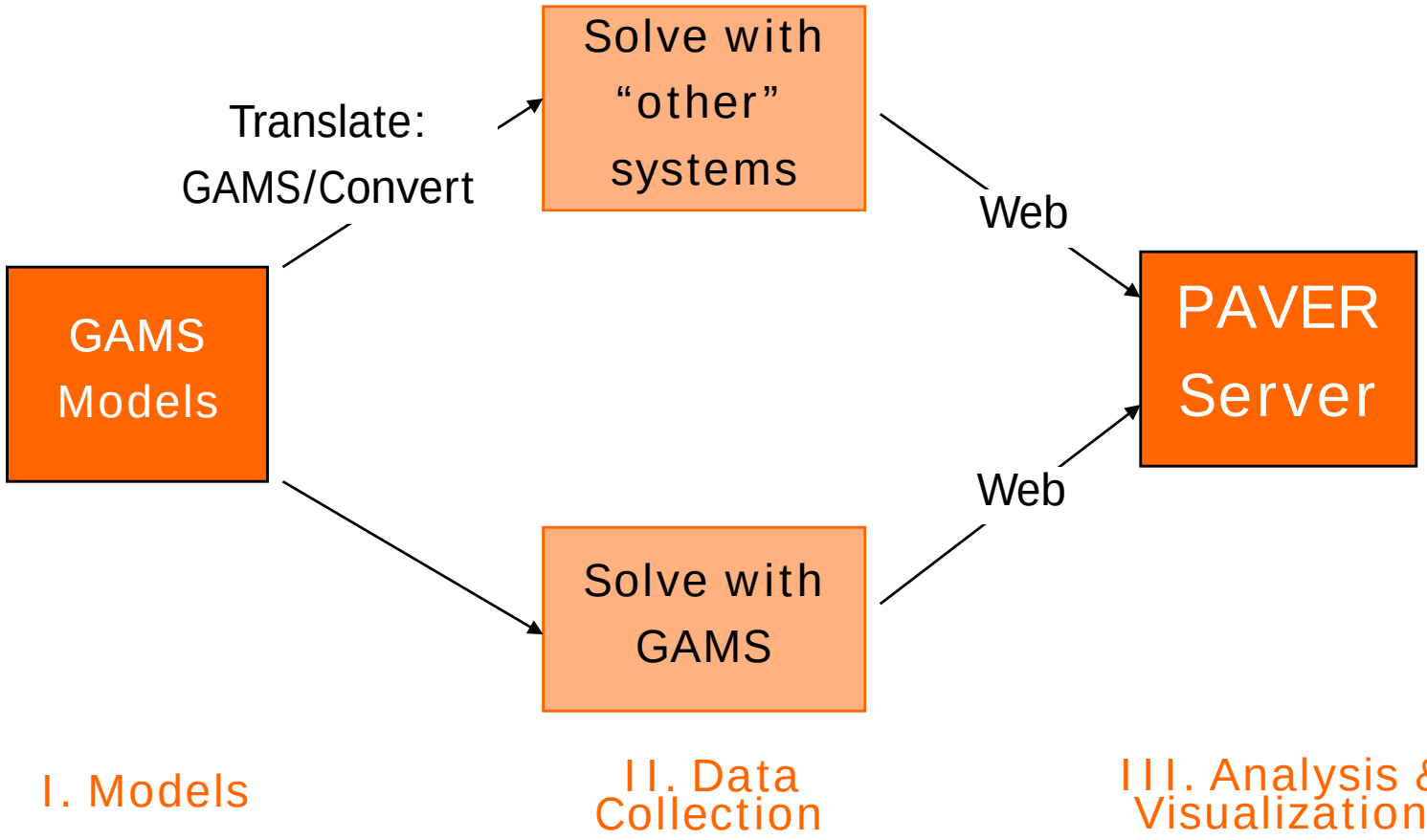
- **P**erformance **A**nalysis and **V**isualization for **E**ffortless **R**eproducibility



- 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



PT/QA 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)
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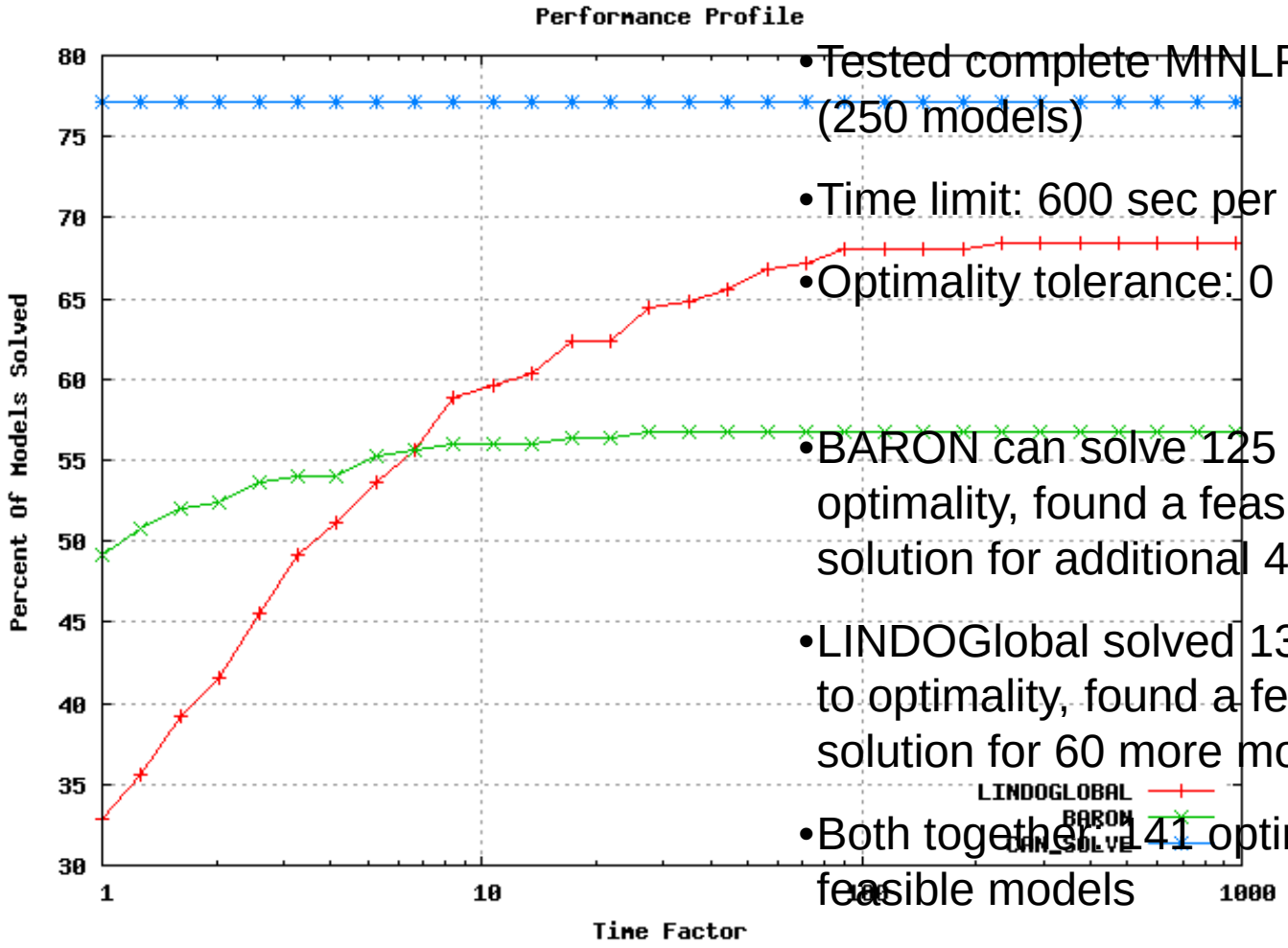
PAVER: LINDOGlobal vs. BARON



- 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

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