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Computational Servers for Global Optimization

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Joint work with Todd Munson

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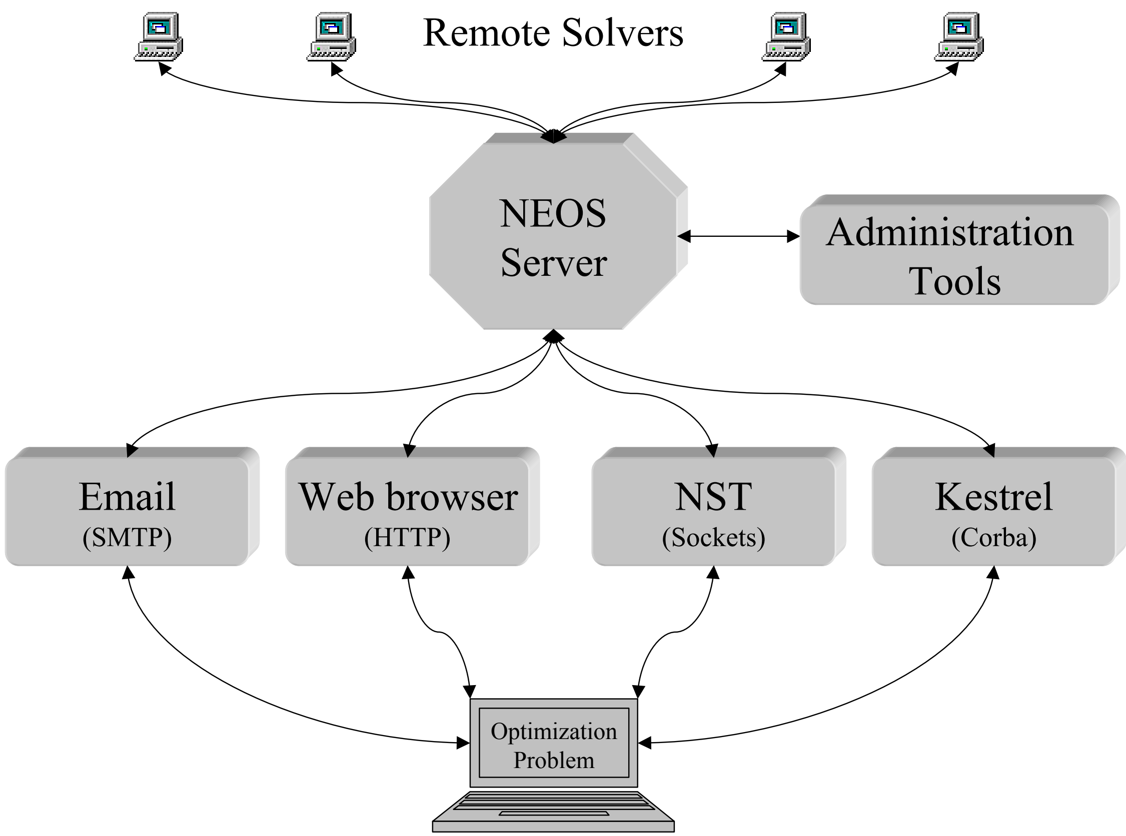
Cocos (Costa Rica)

Cocos has the world's highest concentration of large marine predators, including more sharks per cubic meter of water than anyplace else on the planet.

Outline

- A brief survey of NEOS
- NEOS submissions
- Global optimization issues
  - Comparing solvers
  - Scheduling global optimization jobs
  - Data-mining the NEOS database

Solving Optimization Problems: The NEOS Model



NEOS: Under the Hood

- Modeling languages for optimization: AMPL, GAMS
- Automatic differentiation tools: ADIFOR, ADOL-C, ADIC
- Perl and Corba
- Optimization solvers (40+)
  - Multisolvers: Benchmark, GAMS/AMPL
  - MINCO: MINLP, SBB . . .
  - MILP: FortMP, XPRESS
  - NCO: CONOPT, FILTER, KNITRO, LOQO, MINOS, SNOPT, . . .
  - LP: FortMP, PCx, OOQP, XPRESS, . . .
  - SDP: CSDP, DSDP, MOSEK, PENON, SeDuMi, . . .
  - BCO: BLMVM, L-BFGS-B, TRON, . . .
  - NCP: MILES, PATH
  - GO: ACRS

Research Issues for NEOS

- How do we add solvers?
- How are problems specified?
- How are problems submitted?
- How are problems scheduled for solution?
- How are the problems solved?
- Where are the problems solved?

Remote Solvers and Computational Servers

- Argonne National Laboratory
- Northwestern University
- University of Wisconsin

- National Taiwan University
- Technical University Aachen

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Modeling Languages: Shape Optimization of a Cam

Maximize the area of the valve opening in a convex cam,

$$f(r) = \pi r_v \left(\frac{1}{n} \sum_{i=1}^{n} r_i \right),$$

subject to the constraints $r_{\min} \le r_i \le r_{\max}$ on the radii r_i.

The convexity constraint is expressed as

$$2 r_{i-1} r_{i+1} \cos(\theta) \le r_i (r_{i-1} + r_{i+1}), \qquad i = 0, \ldots, n+1,$$

and the curvature requirement is expressed by

$$-\alpha \le \left(\frac{r_{i+1} - r_i}{\theta} \right) \le \alpha, \qquad i = 0, \ldots, n.$$

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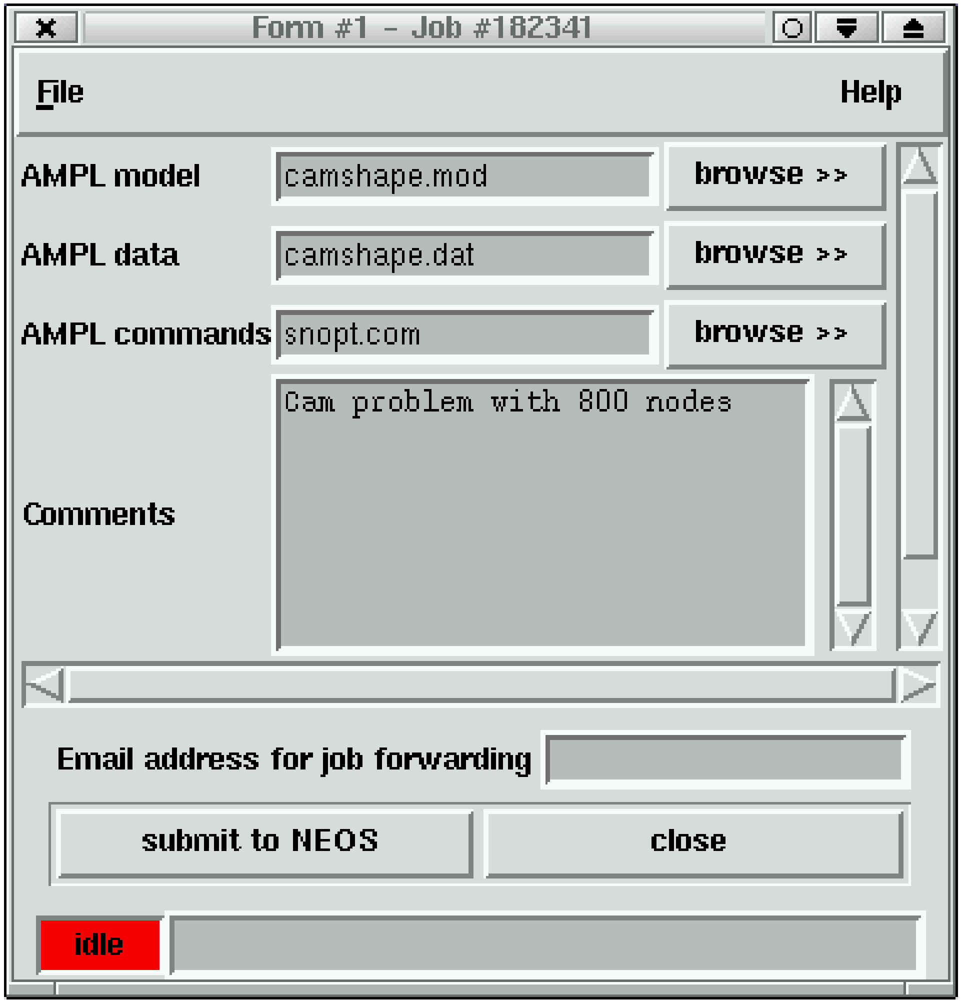
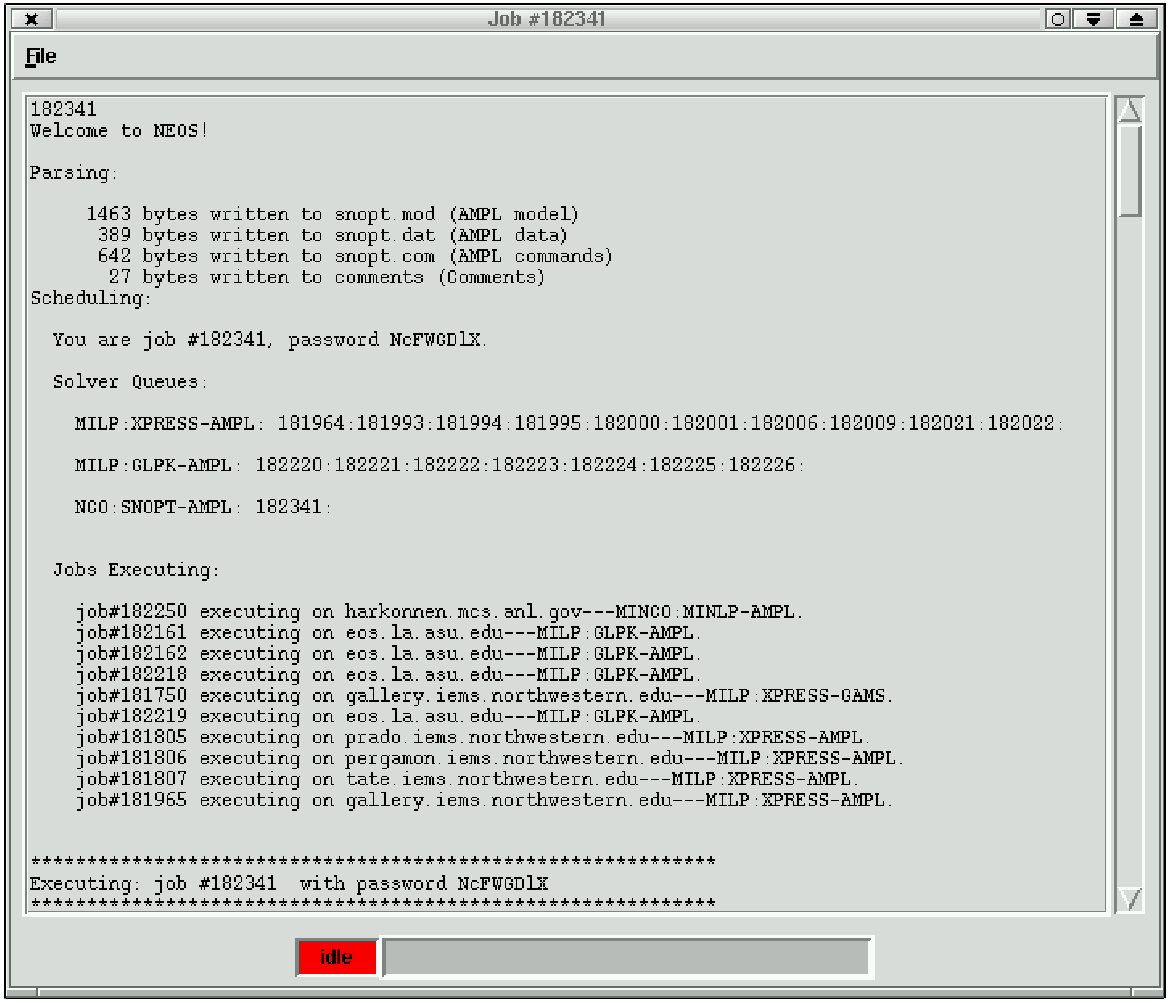
AMPL: Shape Optimization of a Cam

```
maximize valve_area: ((pi*R_v)/n)*sum i in 1..n r[i];

subject to convexity i in 2..n-1:
  - r[i-1]*r[i] - r[i]*r[i+1] + 2*r[i-1]*r[i+1]*cos(d_theta) <= 0;

subject to convex_edge1: - R_min*r[1] - r[1]*r[2] + 2*R_min*r[2]*cos(d_theta) <= 0;
subject to convex_edge2: - R_min^2 - R_min*r[1] + 2*R_min*r[1]*cos(d_theta) <= 0;
subject to convex_edge3: - r[n-1]*r[n] - r[n]*R_max + 2*r[n-1]*R_max*cos(d_theta) <= 0;
subject to convex_edge4: - 2*R_max*r[n] + 2*r[n]^2*cos(d_theta) <= 0;

subject to curvature i in 1..n-1:
   -alpha*d_theta <= (r[i+1] - r[i]) <= alpha*d_theta;

subject to curvature_edge1: -alpha*d_theta <= (r[1] - R_min) <= alpha*d_theta;
subject to curvature_edge2: -alpha*d_theta <= (R_max - r[n]) <= alpha*d_theta;
```

NEOS Submission Tool (NST) Form



NST: The Queues



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NST: Job Submission

Job #182341

File

```
*****************************************************************
Executing: job #182341  with password NcFWGDlX
*****************************************************************

job_client.pl: alarm in 604800 seconds
job_client.pl: connecting to louvre.iems.northwestern.edu:4000
job_client.pl: connected
job_client.pl: sending request
.
job_client.pl: 1141 bytes sent
job_client.pl: receiving data

comms-daemon.pl: downloading user data
comms-daemon.pl: uncompressing...
comms-daemon.pl: untarring...
comms-daemon.pl: launching NCO:SNOPT-AMPL driver...
---------Begin Standard output/error--------
SNOPT driver (NEOS)
Checking the AMPL files
Executing algorithm...
Composing results
---------End Standard output/error----------
*****************************************************************
```

idle

NST: Final Results

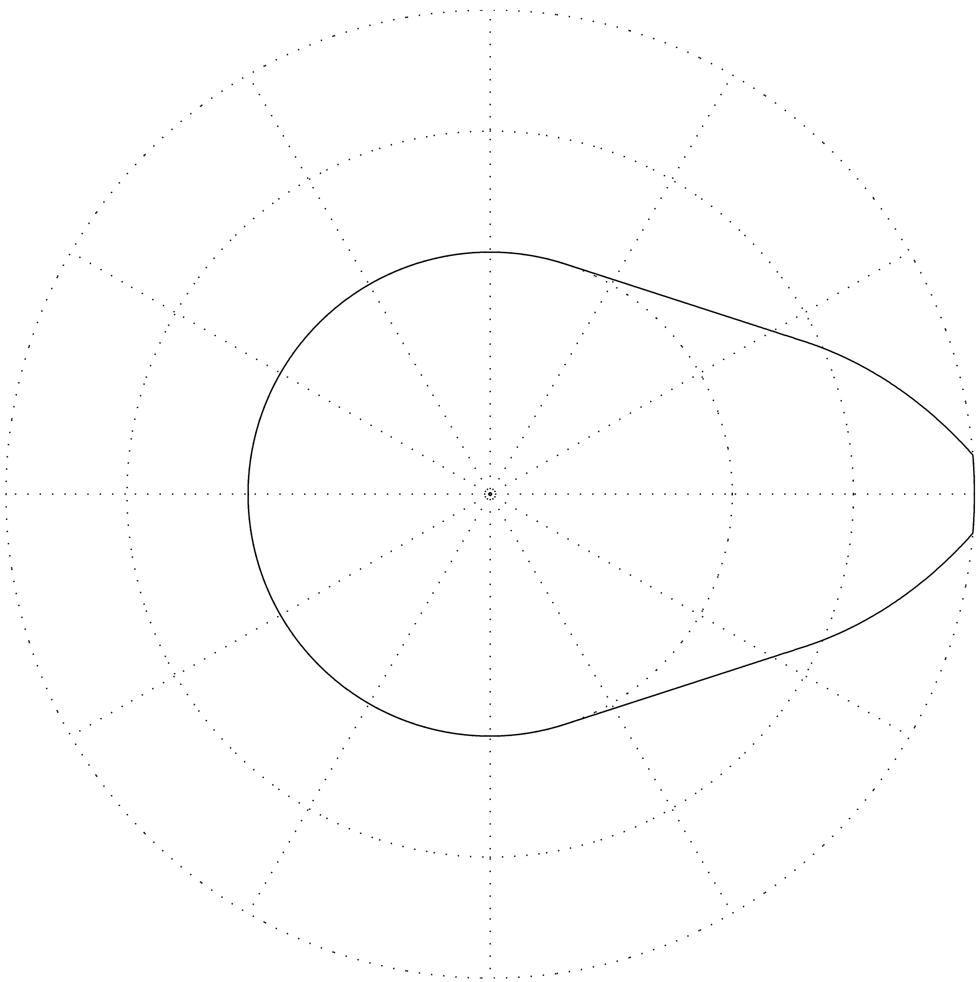
Job #182341

File

```
EXIT -- optimal solution found


No. of iterations                 552   Objective value      4.2289623305E+00
No. of major iterations             1   Linear objective     4.2289623305E+00
Penalty parameter           0.000E+00   Nonlinear objective  0.0000000000E+00
No. of calls to funobj              0   No. of calls to funcon              3
No. of superbasics                  9   No. of basic nonlinears           784
No. of degenerate steps            87   Percentage                      15.76
Norm of x                     3.8E+01   Norm of pi                    1.0E+03
Max Primal infeas           0 0.0E+00   Max Dual infeas           798 5.9E-03
Nonlinear constraint violn    1.3E-07

Solution not printed

Time for MPS input                          0.00 seconds
Time for solving problem                    1.38 seconds
Time for solution output                    0.00 seconds
Time for constraint functions               0.02 seconds
Time for objective function                 0.00 seconds
SNOPT times:
read:         0.05
solve:        1.94
write:        0.00
total:        1.99
SNOPT 6.1-1(5)(Nov 2001):
Optimal solution found.
552 iterations, objective 4.22896233
Nonlin evals: constrs = 3, Jac = 2.
_ampl_time + _total_solve_time = 14.63
```

idle

Shape Optimization of a Cam



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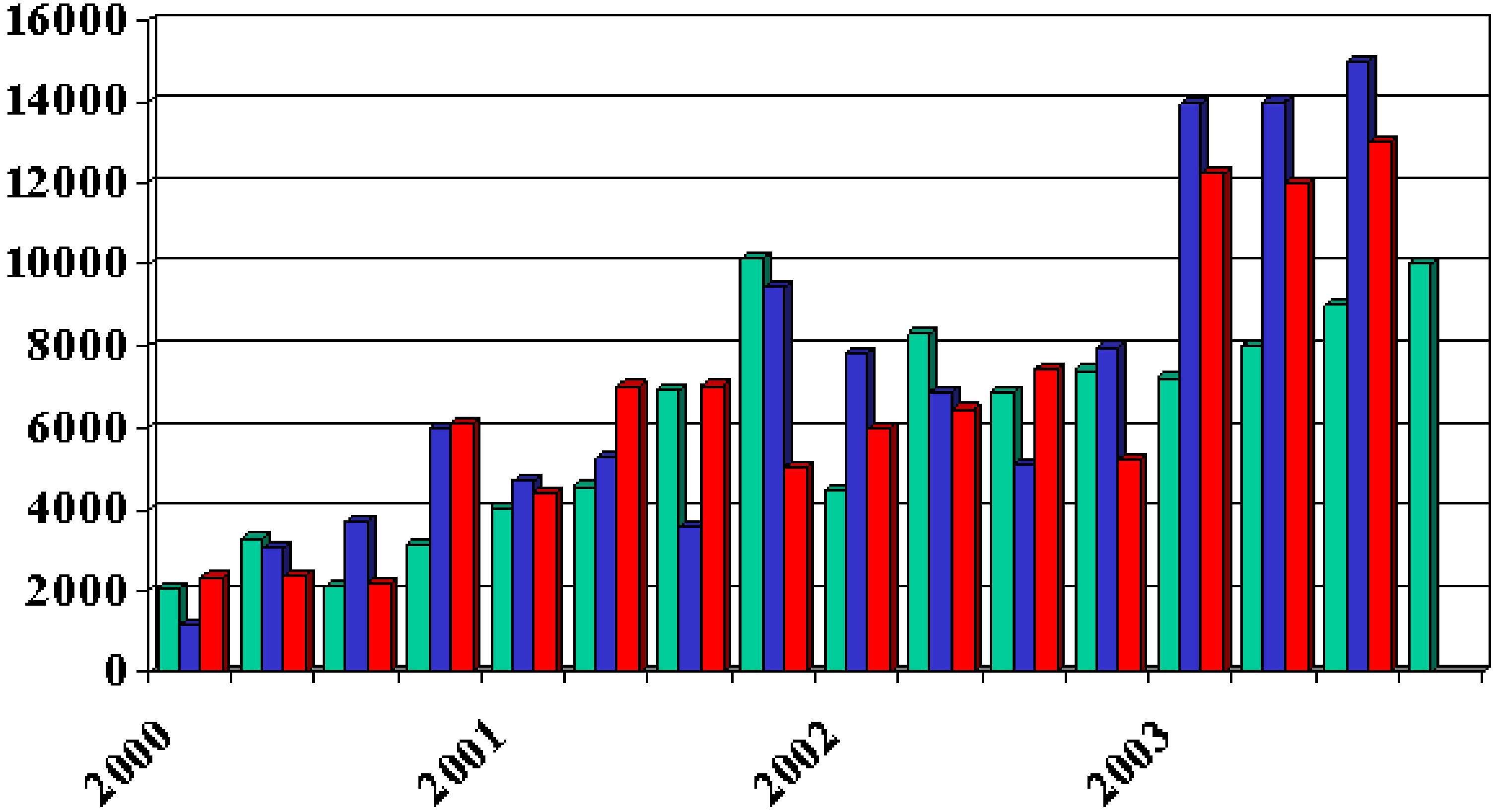
NEOS Submissions: 2000 – 2003



NEOS Users and Uses – 2000

- Estimating the value at risk of financial institutions
- Optimal shift schedules for ground-handling activities
- Unilateral contact problems in engineering mechanics
- Distance geometry and multidimensional scaling
- Portfolio selection and scheduling
- Designing a yagi antenna
- Resource requirements for broadband networks
- Image reconstruction of space objects
- Optimization of weights for routing in the Internet
- Designing large, distributed communication networks
- Circuit simulation at Philips Research Laboratories

NEOS Users and Uses – 2001

- Optimizing design parameters for high-voltage power systems
- Predicting recent observations of Bose-Einstein condensates
- Predicting globular protein folding
- Showing characteristics of multi-person co-operation
- Studying the brain's representation system
- Modeling electricity markets
- Designing fractional delay filters for LAN/WAN's
- Scheduling thermo and hydro energy resources
- Building a crew-scheduling system for an airline in Indonesia
- Solving the modified Cahn-Hilliard free energy equation
- Applying optimization to farming in Switzerland

NEOS Users and Uses – 2002

- Determining the boiling points of alkanes
- Studies of the complexity of phase retrieval
- Energy technology scenarios with endogenous learning
- Design of a telecommunications network
- Grid-enabling high performance machines at Sandia
- Measuring efficiency using carbon dioxide emissions
- Estimating wavenumbers with complex pressure measurements
- Building a prototype combinatorial auction model for GM
- Analyzing economic policy in industrial competition
- Setting up an optimization system for radiation oncology
- Minimizing wastage in splitting polyfilm mill rolls

Sample User Comments

- . . . I adore the gladiatorial aspect: put your solver up on NEOS, and let it fight, naked, against the world's finest . . .
- . . . these models may end up in a software application that will do some good for our company . . . Please keep up this excellent work. It is making a very real and very positive difference.
- I am wondering if I understand what NEOS is offering. Do you provide a free solver and the use of hardware? I want to solve a SOCP with 3200 constraints and 22 variables.
- . . . NEOS is a great service. I'm currently finishing up my Ph.D. at the University of . . . and without NEOS I probably would not be writing right now.

Performance Profiles

Definition. A *performance profile* is the distribution function of a performance metric.

- Compute the performance ratio

$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,s} : 1 \le s \le n_s\}}.$$

- Compute the probability distribution function

$$\rho_s(\tau) = \frac{1}{n_p}\text{size}\Big\{p \in \mathcal{P} : r_{p,s} \le \tau\Big\}$$

Properties of Performance Profiles

The performance profile $\rho_s : \mathbb{R} \mapsto [0,1]$ is a non-decreasing, piecewise constant function, continuous from the right at each breakpoint.

- ◇ Not sensitive to the data on a small number of problems
- ◇ Not sensitive to small changes in the data
- ◇ Information on the size of improvement is provided
- ◇ Does not depend on the subjective choice of a parameter
- ◇ Can be used to compare more than two solvers.

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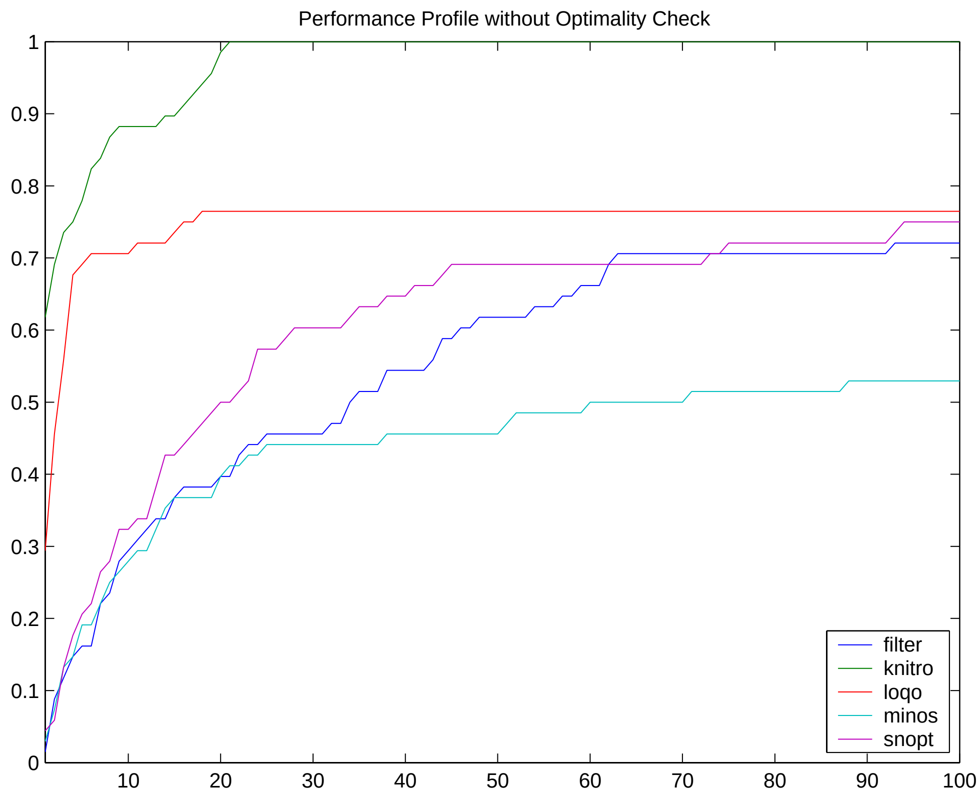
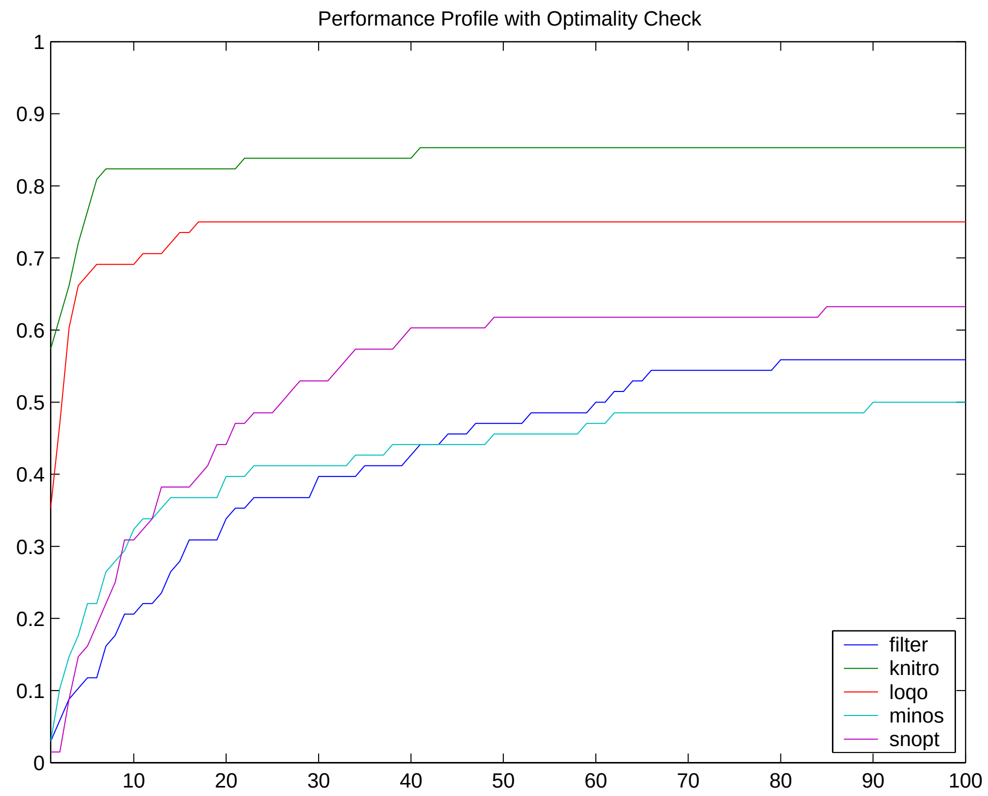
Performance Profiles and Optimality Conditions





Optimality conditions enforced on the graph on the right

Scheduling in a Computational Server

Standard scheduling

- By job number
- Time limit of 150 hours per job.
- At most p jobs per machine, where p is machine-dependent.

Proposed scheduling for global optimization

- Two queues
- Jobs on queue #1 get τ minutes of computing time.
- Queue #2 is for jobs that ask for more than τ minutes.

Question. What should τ be?

Data-Mining the NEOS Database

Assumption. Problems that satisfy property $\mathcal{P}$ are of interest.

Question. What should property $\mathcal{P}$ be?

Neumaier

- All nonlinearly constrained problems such that two solvers returned different solutions
- All nonlinearly constrained problems such that two solvers claimed that the problem was infeasible

Recent References

◇ R. Fourer and J.-P. Goux, Optimization as an Internet resource, Interfaces 31 (2001), 130-150.

◇ E. Dolan, NEOS Server 4.0 Administrative Guide, Technical Report ANL/MCS-TM-250, Mathematics and Computer Science Division, Argonne National Laboratory, May 2001.

◇ E. Dolan and J. Moré, Benchmarking optimization software with performance profiles, Mathematical Programming 91 (2002), 201-213.

◇ E. Dolan, R. Fourer, J. Moré, and T. Munson, Optimization on the NEOS Server, SIAM News 35 (2002), 5, 8–9.

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