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NEOS
Optimization Solutions for Scientific Computing Problems

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www-neos.mcs.anl.gov

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A Tale of Two Projects

- NEOS, started in 1994, is a collaborative project that represents the efforts of the optimization community by providing access to a large number (over 50) of solvers from both academic and commercial researchers.

- TAO, started in 1998, focuses on the design and implementation of algorithms and component-based software for the solution of large-scale optimization applications on high-performance architectures.

Note. You only get to hear about NEOS today!

Collaborators

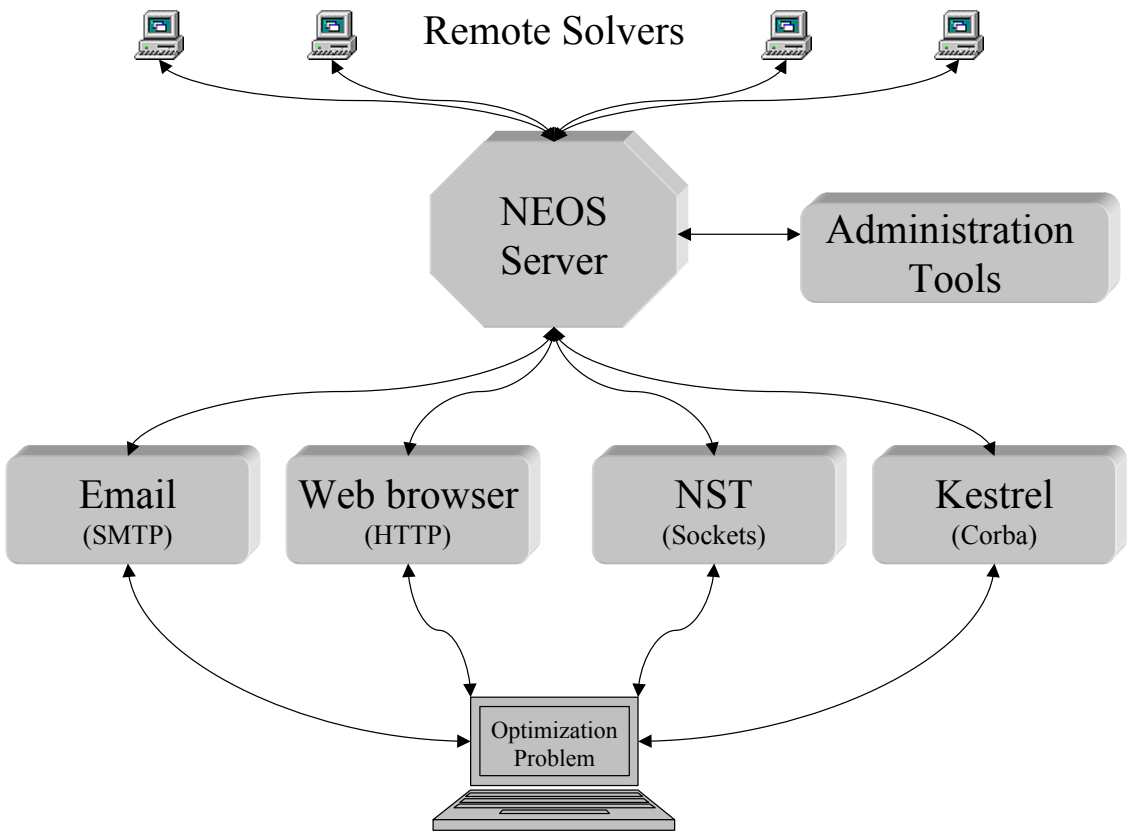
- Steve Benson
- Liz Dolan (NEOS Administrator)
- Mike Gertz
- Lois Curfman McInnes
- Todd Munson
- Dominique Orban
- Jason Sarich

- PETSc and ADIFOR/ADIC Developers
- Optimization Technology Center (Argonne and Northwestern)

Evolution and Revolution: 1980 –

Limited memory methods	1980 –
Modeling languages	1982 –
Interior point methods	1984 –
Automatic differentiation	1989 –
Optimization and Grid computing	1994 –

Solving Optimization Problems: The NEOS Model



NEOS: Under the Hood

- Mathematical programming languages: AMPL, GAMS
- Automatic differentiation tools: ADIFOR, ADOL-C, ADIC
- Perl and Corba
- Optimization solvers (50+)
  - Benchmark, GAMS/AMPL (Multi-Solvers)
  - MINLP, BonsaiG, XPRESS, ...
  - CONOPT, FILTER, KNITRO, LOQO, MINOS, SNOPT, ...
  - FortMP, PCx, OOQP, XPRESS, ...
  - CSDP, DSDP, MOSEK, PENON, SeDuMi, ...
  - BLMVM, L-BFGS-B, TRON, ...
  - MILES, PATH

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

- Argonne National Laboratory
- Arizona State University
- National Taiwan University
- Northwestern University
- Technical University Aachen
- University of Wisconsin

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 $r_{\min} \leq r_i \leq r_{\max}$ on the radii r_i.

The convexity constraint is expressed as

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

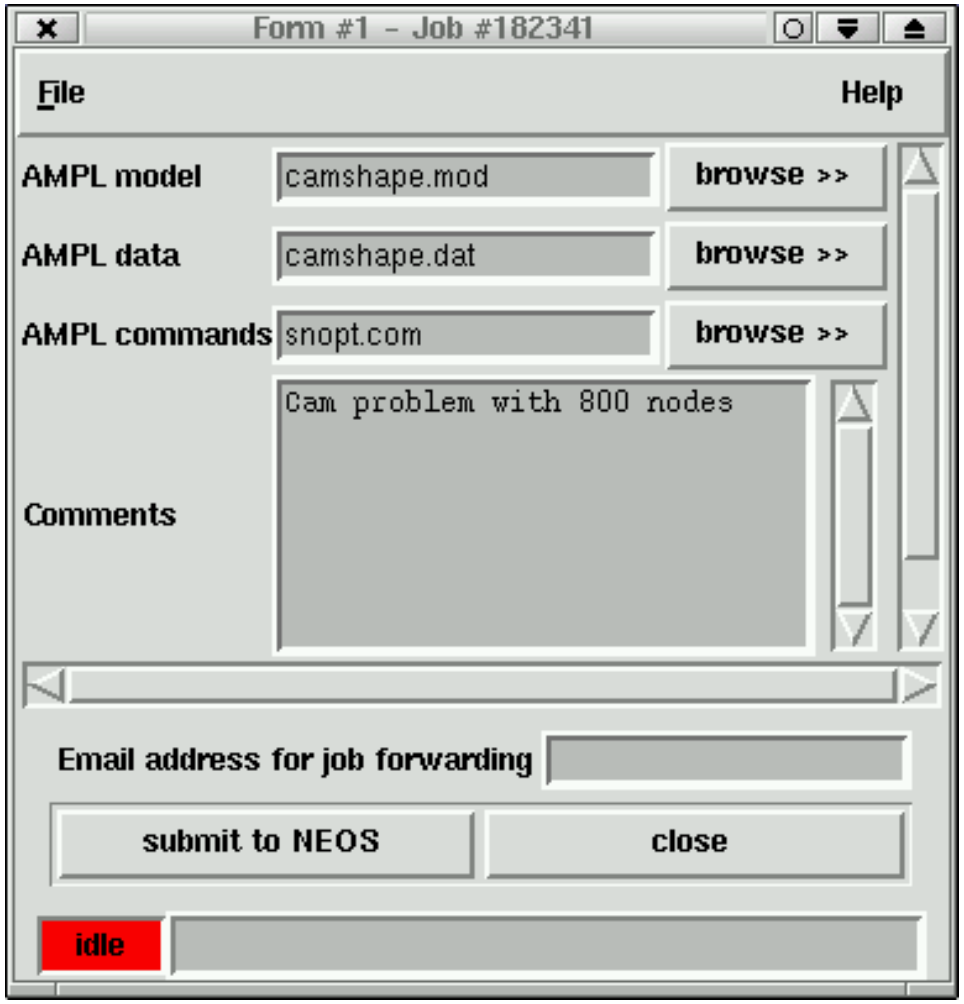
and the curvature requirement is expressed by

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

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

Job #182341

File

```
182341
Welcome to NEOS!

Parsing:

     1463 bytes written to snopt.mod (AMPL model)
      389 bytes written to snopt.dat (AMPL data)
      642 bytes written to snopt.com (AMPL commands)
       27 bytes written to comments (Comments)
Scheduling:

  You are job #182341, password NcFWGDlX.

  Solver Queues:

    MILP:XPRESS-AMPL: 181964:181993:181994:181995:182000:182001:182006:182009:182021:182022:

    MILP:GLPK-AMPL: 182220:182221:182222:182223:182224:182225:182226:

    NCO:SNOPT-AMPL: 182341:


  Jobs Executing:

    job#182250 executing on harkonnen.mcs.anl.gov---MINCO:MINLP-AMPL.
    job#182161 executing on eos.la.asu.edu---MILP:GLPK-AMPL.
    job#182162 executing on eos.la.asu.edu---MILP:GLPK-AMPL.
    job#182218 executing on eos.la.asu.edu---MILP:GLPK-AMPL.
    job#181750 executing on gallery.iems.northwestern.edu---MILP:XPRESS-GAMS.
    job#182219 executing on eos.la.asu.edu---MILP:GLPK-AMPL.
    job#181805 executing on prado.iems.northwestern.edu---MILP:XPRESS-AMPL.
    job#181806 executing on pergamon.iems.northwestern.edu---MILP:XPRESS-AMPL.
    job#181807 executing on tate.iems.northwestern.edu---MILP:XPRESS-AMPL.
    job#181965 executing on gallery.iems.northwestern.edu---MILP:XPRESS-AMPL.


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

idle

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

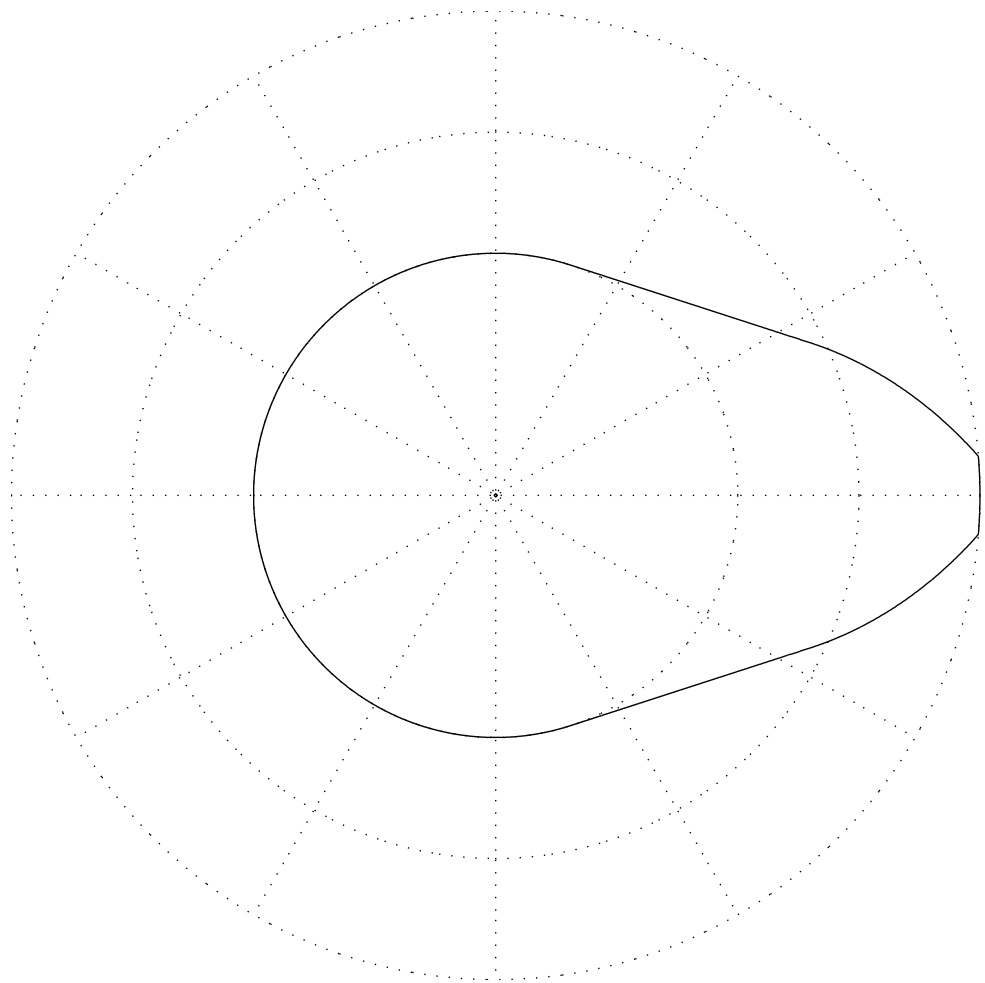
Job #182341

File

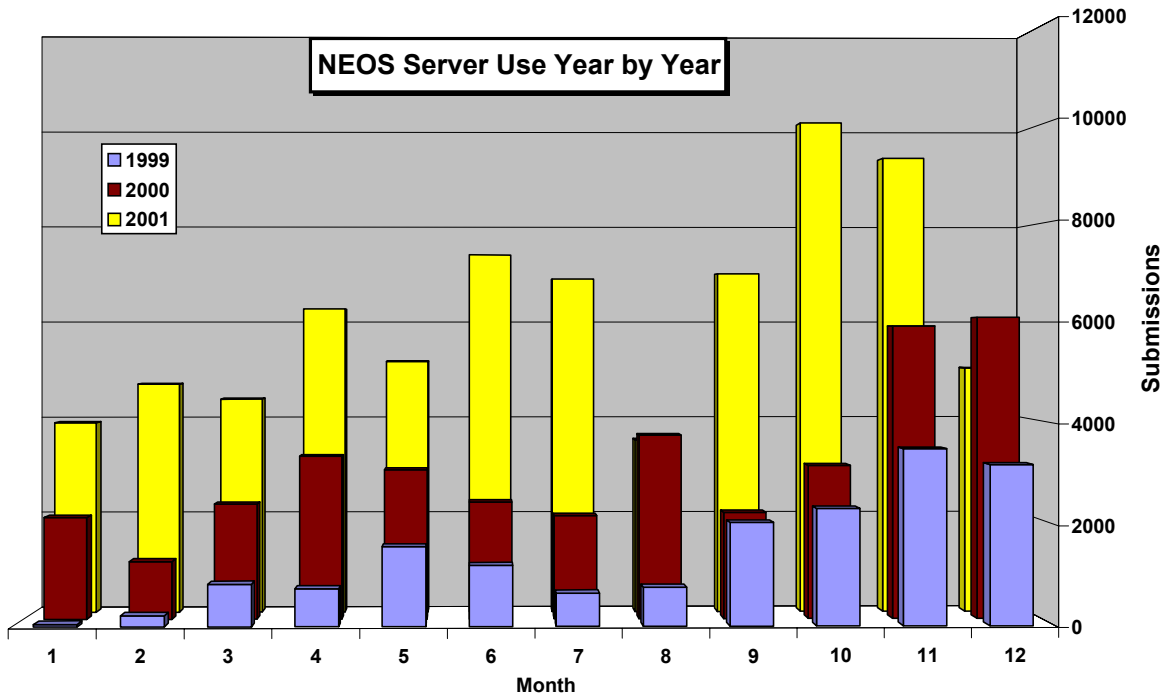
```
EXIT -- optimal solution found


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



NEOS Submissions: 1999 – 2001



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

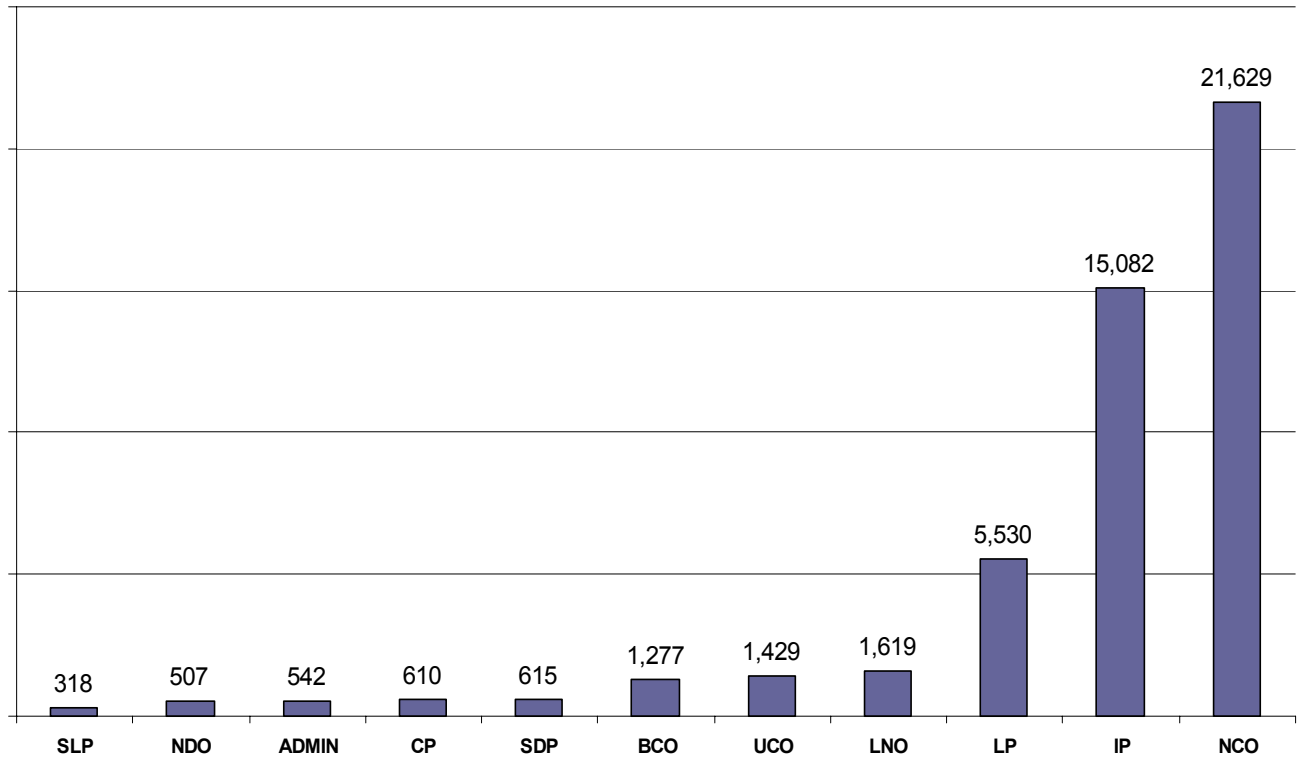
Data Mining the NEOS Database

Grand Challenge: How can we use the NEOS database?

Sample Data

- Number of jobs per time period
- Number of jobs per solver area
- Number of jobs per solver (in a given area)

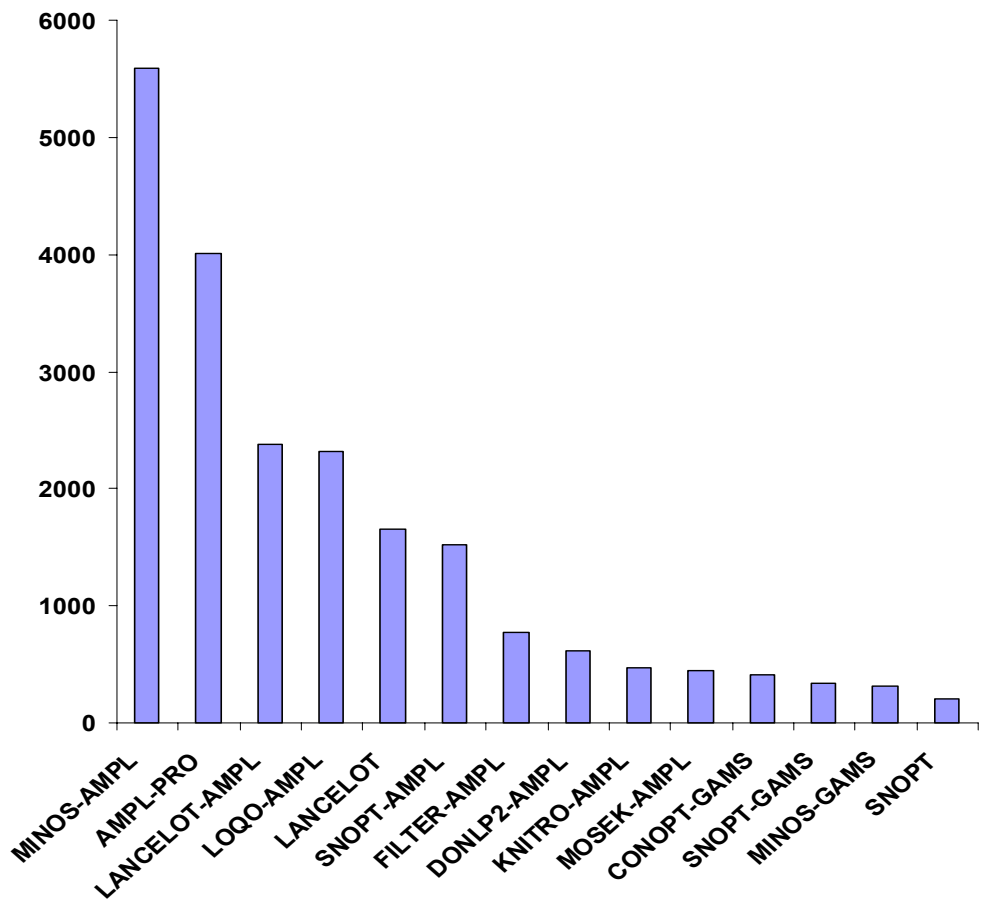
NEOS Jobs: June 2000 – June 2001



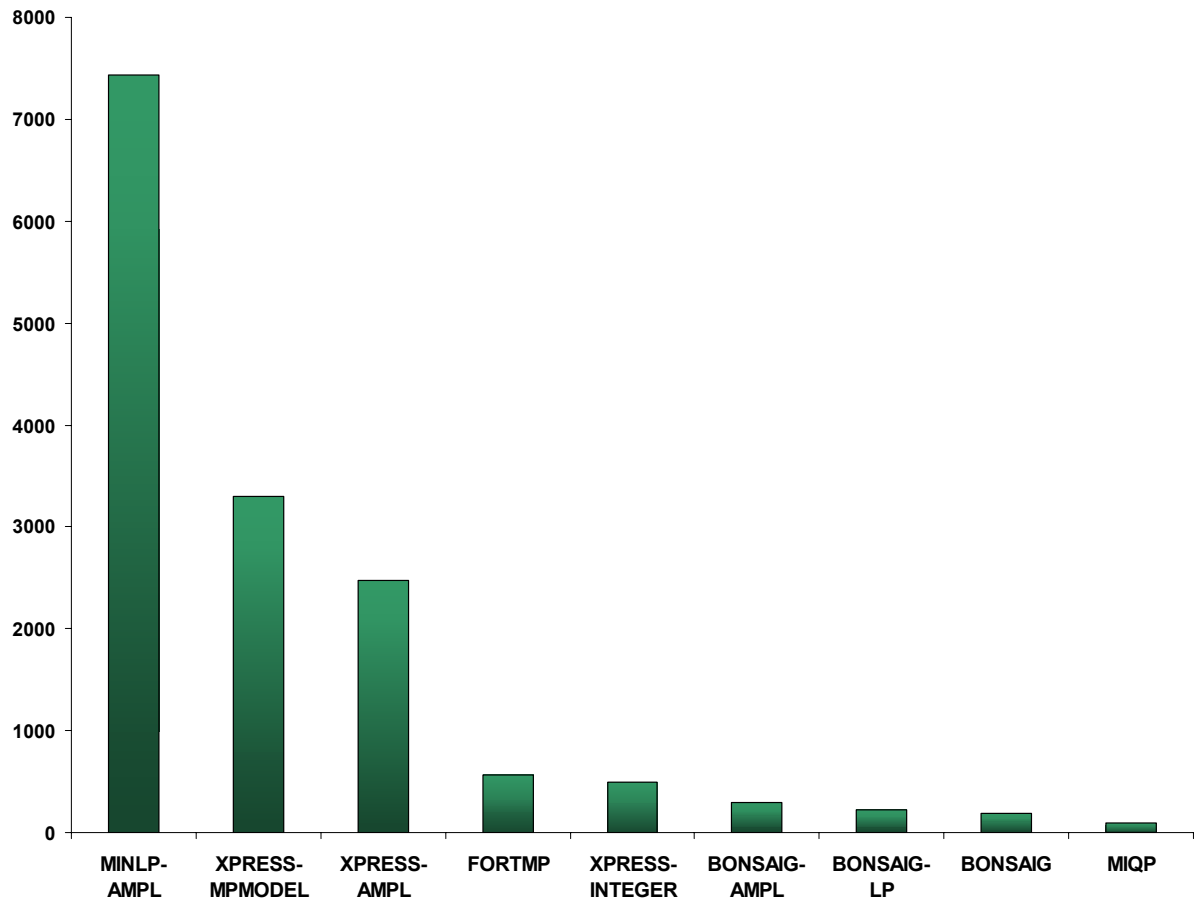
SLP	Stochastic Linear Programming	SDP	Semidefinite Programming	LP	Linear Programming
NDO	Nondifferentiable Optimization	BCO	Bound Constrained Optimization	IP	Integer Programming
ADMIN	Administrative Solvers	UCO	Unconstrained Optimization	NCO	Nonlinearly Constrained Optimization
CP	Complementarity Problems	LNO	Linear Network Optimization		

LANS
laboratoryforadvancednumericalsoftware

Nonlinearly Constrained Solvers: June 2000 – June 2001



Integer Programming Solvers: June 2000 – June 2001



Selected Recent Developments

- ◇ Kestrel
- ◇ Performance profiles
- ◇ GAMS to AMPL translator

Notes

- ⋆ Kestrel provides a flexible interface between NEOS, and the mathematical programming languages AMPL and GAMS
- ⋆ Performance profiles provide a rational framework for comparing solvers
- ⋆ The GAMS to AMPL translator is courtesy of GAMS Development Corp.

Kestrel: Scheduling

```
merlin% ampl
ampl:  model camshape.mod;
ampl: data camshape.dat;
ampl: option show_stats 1;
ampl: option solver kestrel;
ampl: option kestrel_options "solver=snopt";
ampl: option snopt_options "outlev=2 timing=1";
ampl: solve;

Presolve eliminates 3 constraints.
Adjusted problem:
800 variables, all nonlinear
1600 constraints; 3997 linear nonzeros
        801 nonlinear constraints
        799 linear constraints
1 linear objective; 800 nonzeros.

Setting $presolve_fixeps >= 2.95e-06 could change presolve results.

Job has been submitted to Kestrel
Kestrel/NEOS Job number     : 182060
Kestrel/NEOS Job password   : aSrEFDay
Check the following URL for progress report :
     http://www-neos.mcs.anl.gov/neos/neos-cgi/check-status.cgi?job=182060&pass
aSrEFDay
In case of problems, e-mail :
     neos-comments@mcs.anl.gov


Intermediate Solver Output:
Checking the AMPL files
Executing algorithm...
SNOPT 6.1-1(5)(Nov 2001): outlev=2
timing=1
```

Kestrel: Solution

```
xterm

EXIT -- optimal solution found

Problem name                    problem
No. of iterations                   3166   Objective value      4.2230935639E+00
No. of major iterations                9   Linear objective     4.2230935639E+00
Penalty parameter              0.000E+00   Nonlinear objective  0.0000000000E+00
No. of calls to funobj                 0   No. of calls to funcon             18
No. of superbasics                     5   No. of basic nonlinears           784
No. of degenerate steps              176   Percentage                       5.56
Norm of x                          3.8E+01   Norm of pi                   7.8E+02
Max Primal infeas              0 0.0E+00   Max Dual infeas          2114 2.1E-01
Nonlinear constraint violn         7.8E-06

Solution not printed

Time for MPS input                              0.00 seconds
Time for solving problem                        9.45 seconds
Time for solution output                        0.01 seconds
Time for constraint functions                   0.07 seconds
Time for objective function                     0.00 seconds
SNOPT times:
read:        0.05
solve:      12.38
write:       0.06
total:      12.49
Finished call

SNOPT 6.1-1(5)(Nov 2001):
Optimal solution found.
3166 iterations, objective 4.223093564
Nonlin evals: constrs = 18, Jac = 17.
ampl:
```

NEOS Team

- ⋆ Michael Bussieck (GAMS)
- ⋆ Liz Dolan (Argonne/NU)
- ⋆ Steve Dirkse (GAMS)
- ⋆ Michael Ferris (Wisconsin)
- ⋆ Bob Fourer (Northwestern)
- ⋆ David Gay (Lucent)
- ⋆ Philip Gill (UC San Diego)
- ⋆ Nick Gould (Rutherford)
- ⋆ Jean-Pierre Goux (Artelys)
- ⋆ Chih-Jen Lin (Taiwan)
- ⋆ Jeff Linderoth (Axioma)
- ⋆ Sven Leyffer (Dundee)
- ⋆ Hans Mittelmann (Arizona)
- ⋆ Todd Munson (Argonne)
- ⋆ Jorge Nocedal (Northwestern)
- ⋆ Michael Saunders (Stanford)
- ⋆ Bob Vanderbei (Princeton)
- ⋆ Steve Wright (Wisconsin)

Emeritus: Mike Mesnier (Intel)

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.