Languages and Servers for Optimization Support

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Track 14: Selected Presentations: Features of Current Practice

Large-Scale Optimization

Minimization or maximization

of an objective

that depends on many decision variables

Subject to

many interrelated restrictions (constraints)

on the values of the variables

Large-Scale Optimization Modeling

Central Truth: Optimization Modeling is Hard

Given access to the right technical tools and expertise,
building and analyzing models is most of the work

Subjects of this presentation

Helping people build and analyze models
is the purpose of optimization modeling languages

Giving access to the right technical tools and expertise
is the purpose of optimization servers

Optimization Modeling Languages

Examples

Simple: Diet

Complicated: Fleet sizing

General observations

Essential features

Choices

New developments

The McDonald's Diet Problem

Foods:

QP	*Quarter Pounder*
FR	*Fries, small*
MD	*McLean Deluxe*
SM	*Sausage McMuffin*
BM	*Big Mac*
1M	*1% Lowfat Milk*
FF	*Filet-O-Fish*
OJ	*Orange Juice*
MC	*McGrilled Chicken*

Nutrients:

Prot	*Protein*
Iron	*Iron*
VitA	*Vitamin A*
Cals	*Calories*
VitC	*Vitamin C*
Carb	*Carbohydrates*
Calc	*Calcium*

McDonald's Diet Problem Data

	QP	MD	BM	FF	MC	FR	SM	1M	OJ	
Cost	**1.8**	**2.2**	**1.8**	**1.4**	**2.3**	**0.8**	**1.3**	**0.6**	**0.7**	**Need:**
Protein	28	24	25	14	31	3	15	9	1	**55**
Vitamin A	15	15	6	2	8	0	4	10	2	**100**
Vitamin C	6	10	2	0	15	15	0	4	120	**100**
Calcium	30	20	25	15	15	0	20	30	2	**100**
Iron	20	20	20	10	8	2	15	0	2	**100**
Calories	510	370	500	370	400	220	345	110	80	**2000**
Carbo	34	35	42	38	42	26	27	12	20	**350**

Diet Problem

Formulation: Too General

$$\begin{aligned} &\textit{Minimize} && cx \\ &\textit{Subject to} && Ax = b \\ & && x \geq 0 \end{aligned}$$

Diet Problem

Formulation: Too Specific

$$
\begin{array}{lrrrrrrrrrcr}
\textit{Minimize} & 1.84\,x_{QP} & + 2.19\,x_{MD} & + 1.84\,x_{BM} & + 1.44\,x_{FF} & + 2.29\,x_{MC} & + 0.77\,x_{FR} & + 1.29\,x_{SM} & + 0.60\,x_{1M} & + 0.72\,x_{OJ} & & \\
\textit{Subject to} & 28\,x_{QP} & + 24\,x_{MD} & + 25\,x_{BM} & + 14\,x_{FF} & + 31\,x_{MC} & + 3\,x_{FR} & + 15\,x_{SM} & + 9\,x_{1M} & + 1\,x_{OJ} & \geq & 55 \\
& 15\,x_{QP} & + 15\,x_{MD} & + 6\,x_{BM} & + 2\,x_{FF} & + 8\,x_{MC} & + 0\,x_{FR} & + 4\,x_{SM} & + 10\,x_{1M} & + 2\,x_{OJ} & \geq & 100 \\
& 6\,x_{QP} & + 10\,x_{MD} & + 2\,x_{BM} & + 0\,x_{FF} & + 15\,x_{MC} & + 15\,x_{FR} & + 0\,x_{SM} & + 4\,x_{1M} & + 120\,x_{OJ} & \geq & 100 \\
& 30\,x_{QP} & + 20\,x_{MD} & + 25\,x_{BM} & + 15\,x_{FF} & + 15\,x_{MC} & + 0\,x_{FR} & + 20\,x_{SM} & + 30\,x_{1M} & + 2\,x_{OJ} & \geq & 100 \\
& 20\,x_{QP} & + 20\,x_{MD} & + 20\,x_{BM} & + 10\,x_{FF} & + 8\,x_{MC} & + 2\,x_{FR} & + 15\,x_{SM} & + 0\,x_{1M} & + 2\,x_{OJ} & \geq & 100 \\
& 510\,x_{QP} & + 370\,x_{MD} & + 500\,x_{BM} & + 370\,x_{FF} & + 400\,x_{MC} & + 220\,x_{FR} & + 345\,x_{SM} & + 110\,x_{1M} & + 80\,x_{OJ} & \geq & 2000 \\
& 34\,x_{QP} & + 35\,x_{MD} & + 42\,x_{BM} & + 38\,x_{FF} & + 42\,x_{MC} & + 26\,x_{FR} & + 27\,x_{SM} & + 12\,x_{1M} & + 20\,x_{OJ} & \geq & 350
\end{array}
$$

Diet Problem

Algebraic Model

Given $\mathcal{F}$, a set of foods
$\mathcal{N}$, a set of nutrients

and $a_{ij} \geq 0$, for each $i \in \mathcal{N}$ and $j \in \mathcal{F}$:
units of nutrient i in one serving of food j

$b_i > 0$, for each $i \in \mathcal{N}$: units of nutrient i required,

$c_j > 0$, for each $j \in \mathcal{F}$: cost per serving of food j,

Define $x_j \geq 0$, for each $j \in \mathcal{F}$:
number of servings of food j to be purchased

Minimize $\sum_{j \in \mathcal{F}} c_j x_j$

Subject to $\sum_{j \in \mathcal{F}} a_{ij} x_j \geq b_i$, for each $i \in \mathcal{N}$

Diet Problem

Algebraic Model in AMPL

```
set NUTR;   # nutrients
set FOOD;   # foods

param amt {NUTR,FOOD} >= 0;  # nutrient in each food

param n_min {NUTR} > 0;      # lower bounds on nutrients

param cost {FOOD} > 0;       # costs of foods

var Buy {FOOD} integer >= 0; # foods to be purchased

minimize TotalCost: sum {j in FOOD} cost[j] * Buy[j];

subject to Need {i in NUTR}:
   sum {j in FOOD} amt[i,j] * Buy[j] >= n_min[i];
```

Airline Fleet Assignment

```
set FLEETS;
param fleet_size {FLEETS} >= 0;

set CITIES;
set TIMES circular;

set FLEET_LEGS within
   {f in FLEETS, c1 in CITIES, t1 in TIMES,
                 c2 in CITIES, t2 in TIMES:
                         c1 <> c2 and t1 <> t2};

     # (f,c1,t1,c2,t2) represents availability of fleet f
     # to cover the leg that leaves c1 at t1 and
     # whose arrival time plus turnaround time at c2 is t2

param leg_cost {FLEET_LEGS} >= 0;
```

Computed Sets

```
set LEGS :=
   setof {(f,c1,t1,c2,t2) in FLEET_LEGS} (c1,t1,c2,t2);

         # set of all legs that can be covered by some fleet

set SERV_CITIES {f in FLEETS} :=
   union {(f,c1,c2,t1,t2) in FLEET_LEGS} {c1,c2};

         # for each fleet, set of cities that it serves

set OP_TIMES {f in FLEETS, c in SERV_CITIES[f]}
   circular by TIMES :=

      setof {(f,c,c2,t1,t2) in FLEET_LEGS} t1 union
      setof {(f,c1,c,t1,t2) in FLEET_LEGS} t2;

         # for each fleet and city served by that fleet,
         # set of active arrival & departure times,
         # with arrival time padded for turn requirements
```

Underlying Network Model

```
minimize Total_Cost;

node Balance {f in FLEETS, c in SERV_CITIES[f], OP_TIMES[f,c]};
          # for each fleet and city served by that fleet,
          # a node for each possible time

arc Fly {(f,c1,t1,c2,t2) in FLEET_LEGS} >= 0, <= 1,
   from Balance[f,c1,t1], to Balance[f,c2,t2],
   obj Total_Cost leg_cost[f,c1,t1,c2,t2];
          # arcs for fleet/flight assignments

arc Sit {f in FLEETS,
         c in SERV_CITIES[f], t in OP_TIMES[f,c]} >= 0,
   from Balance[f,c,t], to Balance[f,c,next(t)];
          # arcs for planes on the ground
```

Service and Fleet-Size Constraints

```
subj to Service {(c1,t1,c2,t2) in LEGS}:

   sum {(f,c1,t1,c2,t2) in FLEET_LEGS} Fly[f,c1,t1,c2,t2] = 1;

         # each leg must be served by some fleet

subj to FleetSize {f in FLEETS}:

   sum {(f,c1,t1,c2,t2) in FLEET_LEGS:
      ord(t2,TIMES) < ord(t1,TIMES)} Fly[f,c1,t1,c2,t2] +

   sum {c in SERV_CITIES[f]} Sit[f,c,last(OP_TIMES[f,c])]

      <= fleet_size[f];

         # planes used = the number in the air at the
         # last time (arriving "earlier" than they leave)
         # plus number on the ground at the last time
```

Essential Modeling Language Features

Sets and indexing

- Simple sets
- Compound sets
- Computed sets

Variables, objectives and constraints

- Linear, piecewise-linear
- Nonlinear
- Integer

and much more . . .

- Express problems in the many ways that people do
- Support a broad variety of modeling situations
- Drive varied solvers

Modeling Language Features *(cont'd)*

Recognizing other types of models

- Network problems
- Complementarity problems

Exchanging information with solvers

- Solver-specific directives
- Rays of unboundedness, infeasibility diagnostics, and other results

Programming iterative schemes

- Loops over sets; if-then-else tests
- Switching between subproblems

Commercial Modeling Languages

AIMMS `www.aimms.com`

AMPL `www.ampl.com`

GAMS `www.gams.com`

LINGO `www.lindo.com`

MPL `www.maximalsoftware.com`

OPL `www.ilog.com/products/oplstudio/`

. . . what about spreadsheet optimizers?

Choosing a Modeling Language

The language itself

- Naturalness
- Power

The modeling system

- Scalability of language translator
- Convenience of user interface

Connections to other systems

- Support for varied solvers
- Database & spreadsheet links
- Callable interfaces
- Application development features

New Directions in Modeling Languages

Model types

- Semi-definite and second-order cone programs
- Combinatorial optimization problems
- Complementarity and equilibrium constrained problems

Solver support

- MPEC solvers
- Constraint programming
- Global optimization

Optimization Servers

Challenges in optimization modeling

- Software challenges
- Solver challenges
- Server challenges

Examples

- NEOS (`www-neos.mcs.anl.gov`)
- WEBOPT (`www.webopt.org`)

Software Challenges

No one way to solve

- Hundreds of *solvers*
- Competing "free" codes and commercial products
- Competing methods

Models built to order

- Competing *modeling systems*
- Each system supports multiple solvers
- Many solvers work with multiple systems

Result: A tangle of software

- Unlike comprehensive statistics/simulation packages

. . . an opportunity for the Internet to offer guidance and access

Solver Challenges

Power

- Faster computers
- More powerful algorithms
- Better implementations of algorithms

Ease of use

- Modeling languages and systems
  (AIMMS, AMPL, GAMS, LINGO, MPL, OPL, . . .)
- Add-ins to general-purpose systems (Excel, MATLAB)
- Object-oriented programming interfaces

Accessibility

- Unpleasant to download and install
- Trial versions have various limitations

. . . few solvers installed at any one site

Server Challenges

Offer optimization as an Internet resource

- One remote *server* offering many solvers
- Any local *client* can submit optimization "jobs"

Support varied clients

- General-purpose software: web browsers, e-mailers
- General optimization software:
  modeling languages & systems
- Specialized tools

History

- Servers for individual solvers
- Servers for individual modeling languages
- ***General-purpose servers***

NEOS www-neos.mcs.anl.gov

A general-purpose optimization server

- About 50 solvers in all
- Commercial as well as experimental solvers
- Central scheduler with distributed solver sites

A research project

- Currently free of charge
- Supported through the Optimization Technology Center of Northwestern Univ & Argonne National Laboratory

Using NEOS

Varied submission options

- E-mail
- Web forms
- TCP/IP socket-based submission tool: Java or tcl/tk
- Direct from optimization modeling environments

Numerous formats

- Low-level formats: MPS, SIF, SDPA
- Programming languages:
  C/ADOL-C, Fortran/ADIFOR
- High-level modeling languages: AMPL, GAMS

Using NEOS *(cont'd)*

Examples

- Used through a web browser
- Used within a modeling environment

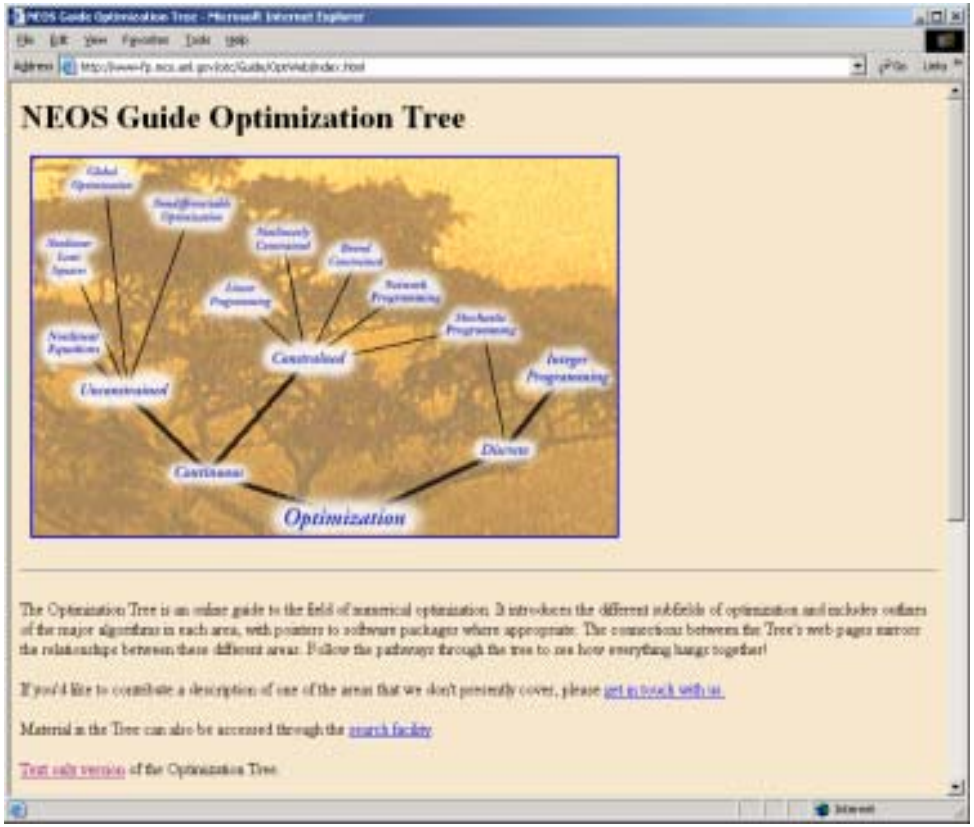
Frequently asked questions

- Who uses NEOS?
- What solvers does it offer?
- How is it supported?

Learn About Your Problem

NEOS Guide

- Optimization tree & software guide
- Frequently asked questions

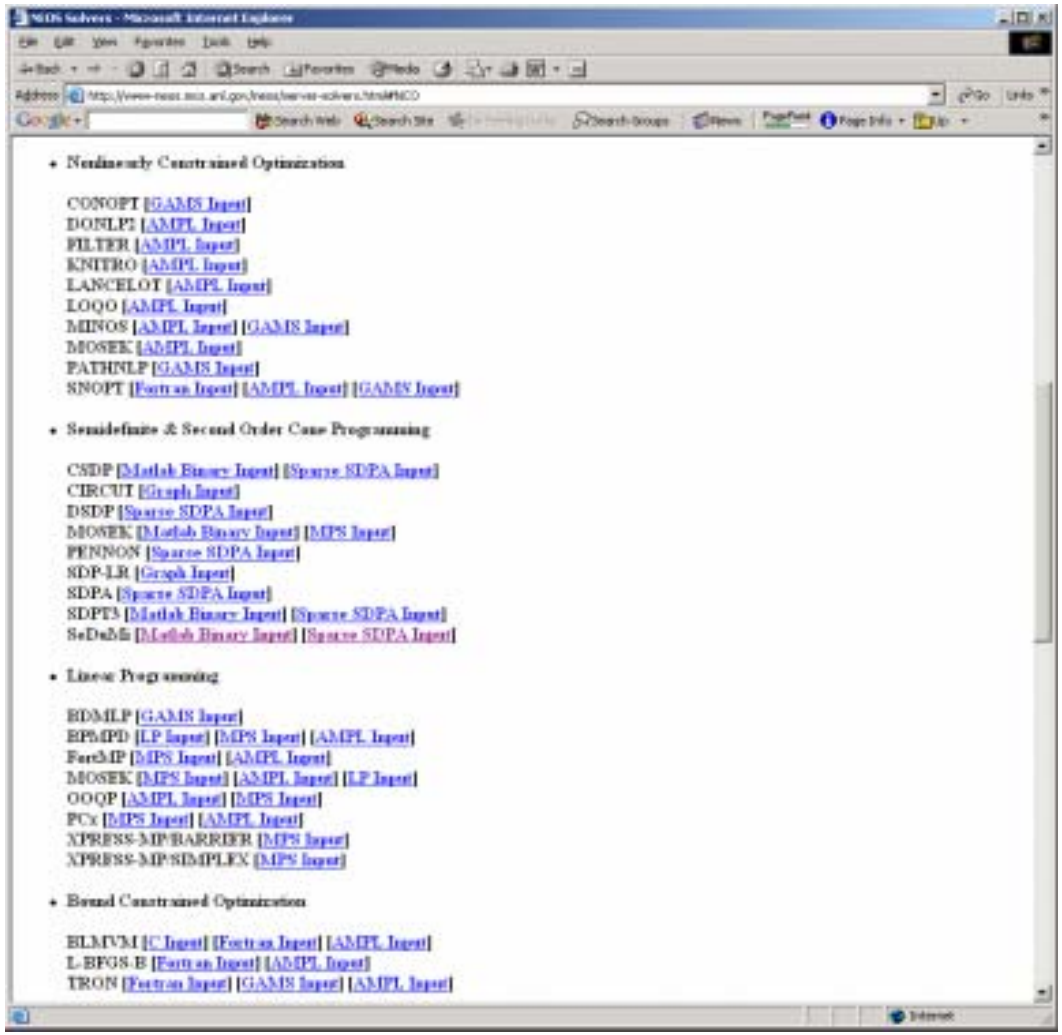


Investigate Solvers

NEOS Server home page

Investigate Solvers

NEOS Server solver listing

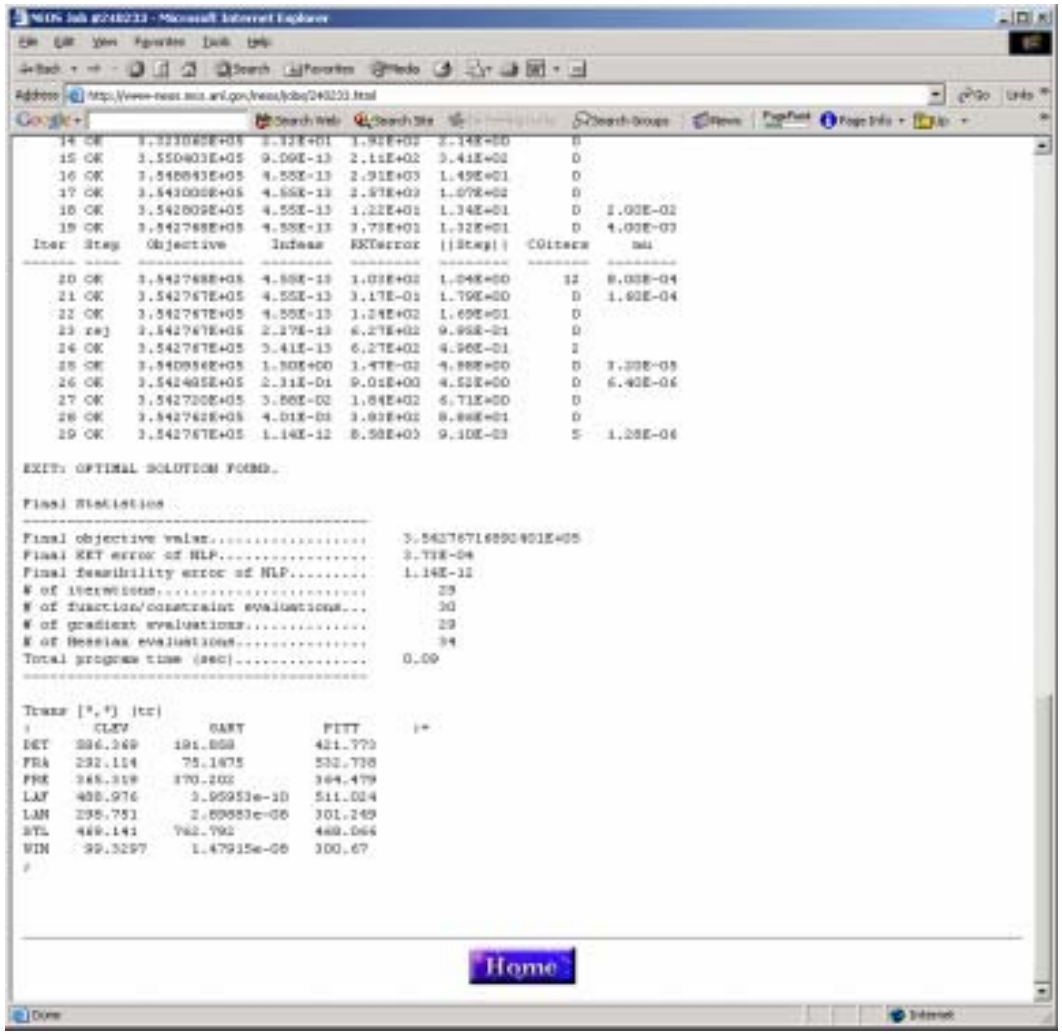


Try a Solver: Web Interface

Submission form for your problem . . .

Try a Solver: Web Interface

. . . listing of your results



```
    14 OK    3.5330482E+05  2.32E-01  1.91E+02  2.14E-00       0
    15 OK    3.5504032E+05  9.09E-13  2.11E+02  3.41E+02       0
    16 OK    3.5488432E+05  4.55E-13  2.91E+03  1.49E+01       0
    17 OK    3.5430008E+05  4.55E-13  2.97E+03  1.07E+02       0
    18 OK    3.5428092E+05  4.55E-13  1.22E+01  1.34E+01       0   2.00E-02
    19 OK    3.5427682E+05  4.55E-13  3.73E+01  1.32E+01       0   4.00E-03
 Iter  Step   Objective      Infeas    KKTerror  ||Step||   COIters     mu
------ ----  -------------  --------  --------  --------  -------  --------
    20 OK    3.5427688E+05  4.55E-13  1.03E+01  1.04E+00      12   8.00E-04
    21 OK    3.5427677E+05  4.55E-13  3.17E-01  1.79E+00       0   1.60E-04
    22 OK    3.5427677E+05  4.55E-13  1.24E+02  1.69E+01       0
    23 rej   3.5427677E+05  2.27E-13  6.27E+02  9.95E-01       0
    24 OK    3.5427677E+05  3.41E-13  6.27E+02  4.96E-01       1
    25 OK    3.5409568E+05  1.50E+00  1.47E-02  4.98E+00       0   3.20E-05
    26 OK    3.5424605E+05  2.31E-01  9.01E+00  4.52E+00       0   6.40E-06
    27 OK    3.5427208E+05  3.86E-02  1.84E+02  6.71E+00       0
    28 OK    3.5427628E+05  4.01E-01  3.83E+01  8.86E-01       0
    29 OK    3.5427677E+05  1.14E-12  8.58E+03  9.10E-03       5   1.28E-06

EXIT: OPTIMAL SOLUTION FOUND.

Final Statistics
----------------------------------------
Final objective value.....................    3.5427677168901E+05
Final KKT error of NLP....................    3.73E-04
Final feasibility error of NLP............    1.14E-12
# of iterations...........................       29
# of function/constraint evaluations...       30
# of gradient evaluations..................       29
# of Hessian evaluations...................       34
Total program time (sec)..................    0.09
----------------------------------------

Trans [*,*] (tr)
:      CLEV          OART          PITT      :*
DET    886.269     191.858         421.773
FRA    232.114      75.1875        532.738
PHX    345.319     370.203         364.479
LAX    408.976       3.95953e-10   511.024
LAN    235.751       2.69685e-08   301.249
STL    469.141     762.792         468.066
WIN     99.3297      1.47915e-08   300.67
;
```

Home

Try a Solver: Kestrel Interface

Applying a local solver to an AMPL model

```
AMPL Version 20040202 (MS VC++ 6.0)

ampl: model gs2000b.mod; data gs2000b.dat;
ampl: option solver minos;
ampl: solve;

Presolve eliminates 100 constraints.
Adjusted problem:
4290 variables:
        4260 binary variables
        30 linear variables
733 constraints, all linear; 36340 nonzeros
1 linear objective; 30 nonzeros.

MINOS 5.5:

Sorry, the student edition is limited to 300 variables and
300 constraints.  You have 4290 variables and 733 constraints.

exit code 1
<BREAK>
```

Try a Solver: Kestrel Interface

Applying a NEOS solver to an AMPL model . . .

```
ampl: option solver kestrel;
ampl: option kestrel_options 'solver=loqo';
ampl: option loqo_options 'minlocfil outlev=1';
ampl: solve;

Job has been submitted to Kestrel

Kestrel/NEOS Job number    : 368607
Kestrel/NEOS Job password  : OxBpVYMb

Check the following URL for progress report :

http://www-neos.mcs.anl.gov/neos/
neos-cgi/check-status.cgi?job=368607&pass=OxBpVYMb

In case of problems, e-mail neos-comments@mcs.anl.gov
```

Try a Solver: Kestrel Interface

. . . and receiving a solution from NEOS . . .

```
LOQO 6.06: minlocfil

 1    0.000000e+00   2.1e-01   -4.266000e+05   3.1e+02
 2    2.840664e+03   9.8e-04   -4.206215e+05   1.5e+01
 3    2.796511e+03   4.8e-04   -3.078341e+05   6.2e-01
 4    1.769055e+03   4.2e-04   -2.948373e+04   0.0e+00            DF
 5    3.024840e+02   5.2e-05   -3.871922e+03   0.0e+00            DF
 6    3.705130e+01   5.9e-06   -2.158849e+02   0.0e+00            DF
 7    2.220340e+01   3.1e-06   -1.070050e+01   0.0e+00            DF
 8    1.685976e+01   1.4e-06    2.596295e+00   0.0e+00            DF
 9    1.534094e+01   6.7e-07    9.491761e+00   0.0e+00         PF DF
10    1.445050e+01   2.1e-07    1.284805e+01   0.0e+00    1    PF DF
11    1.405725e+01   8.3e-09    1.333832e+01   0.0e+00    1    PF DF
12    1.400313e+01   4.9e-10    1.396657e+01   0.0e+00    3    PF DF
13    1.400016e+01   2.5e-11    1.399833e+01   0.0e+00    4    PF DF
14    1.400001e+01   1.2e-12    1.399992e+01   0.0e+00    5    PF DF

LOQO 6.06: optimal solution (14 QP iterations, 14 evaluations)

primal objective 14.00000783
  dual objective 13.99991642
```

Try a Solver: Kestrel Interface

. . . where it can be browsed interactively

```
ampl: option display_eps .000001;

ampl: display MinType, MaxType;
:                                              MinType  MaxType :=
Division Shipping                                0        1
Division Logistics_and_Supply_Chain              1        2
Division Information_Technology                  1        1
Division Production                              0        1
Division Production_Scheduling                   1        2
Division Production_Scheduling_Research          1        2
Division Operations_Management                   0        1
Division Finance                                 3        4
Division Support                                 0        1
Office   Americas                               7        8
Office   EMEA                                   1        2
Office   Far_East                               1        2
Gender   F                                       3        4
Gender   M                                       7        8
;
```

Frequently Asked Questions

Who uses NEOS?

- What do they use it for?
- Where are they from?
- How much do they use it?

What solvers does NEOS offer?

- Who supplies them?
- Where are they hosted?

How is NEOS supported?

- Who answers user questions?

Who Uses NEOS? *(a sample)*

- We are using NEOS services for duty-scheduling for ground handling activities in a regional airport environment.
- We used NEOS to solve nonlinear optimization problems associated with models of physical properties in chemistry.
- Our company is working with various projects concerning R&D of internal combustion engines for cars and brakes for heavy vehicles.
- I am dealing with ultimate limit-state analyses of large dams by means of a non-standard approach ("direct method"); this requires solving problems of linear and non-linear programming. The NEOS server is an extraordinary tool to perform parametric tests on small models, in order to choose the best suited solver.
- I have used NEOS with LOQO solver to optimize an interpolator. . . . My domain is digital receivers where the receiver clock is not changed to match the transmitter clock.

Who Uses NEOS? *(more)*

- I have been able to build and solve a prototype combinatorial auction MIP model using AMPL and NEOS in a fraction of the time it would have required me to do this had I needed to requisition a solver and install it locally.
- Our idea is trying to design antennas by using the computer. . . . We have tried various solvers on NEOS to see if this is possible at all.
- I am using the LOQO solver and code written in AMPL to perform numerical optimization of a spinor Bose-Einstein condensate.
- We are using the NEOS Server for solving linear and nonlinear complementarity problems in engineering mechanics and in robotics.
- I have been working on a system for protein structure prediction. . . . I had need to incorporate a nonlinear solver to handle packing of sidechain atoms in the protein.

Where are They From?

2004 through 24 April: Identifiable domain and >= 20 submissions

(com)	3502
(edu)	13610
(gov)	2510
(net)	12310
(mil)	90

Northwestern	1338
Argonne	2194

Belgium(be)	4918
Brazil(br)	2558
Canada(ca)	4514
Switzerland(ch)	1098
Chile(cl)	158
Colombia(co)	218
Cyprus(cy)	20
Czech Republic(cz)	554
Germany(de)	1834
Spain(es)	1548
Finland(fi)	270
Micronesia(fm)	36
France(fr)	2730
Greece(gr)	776
Hong Kong(hk)	...

NEOS Users

What Countries are They From?

2004 through 24 April

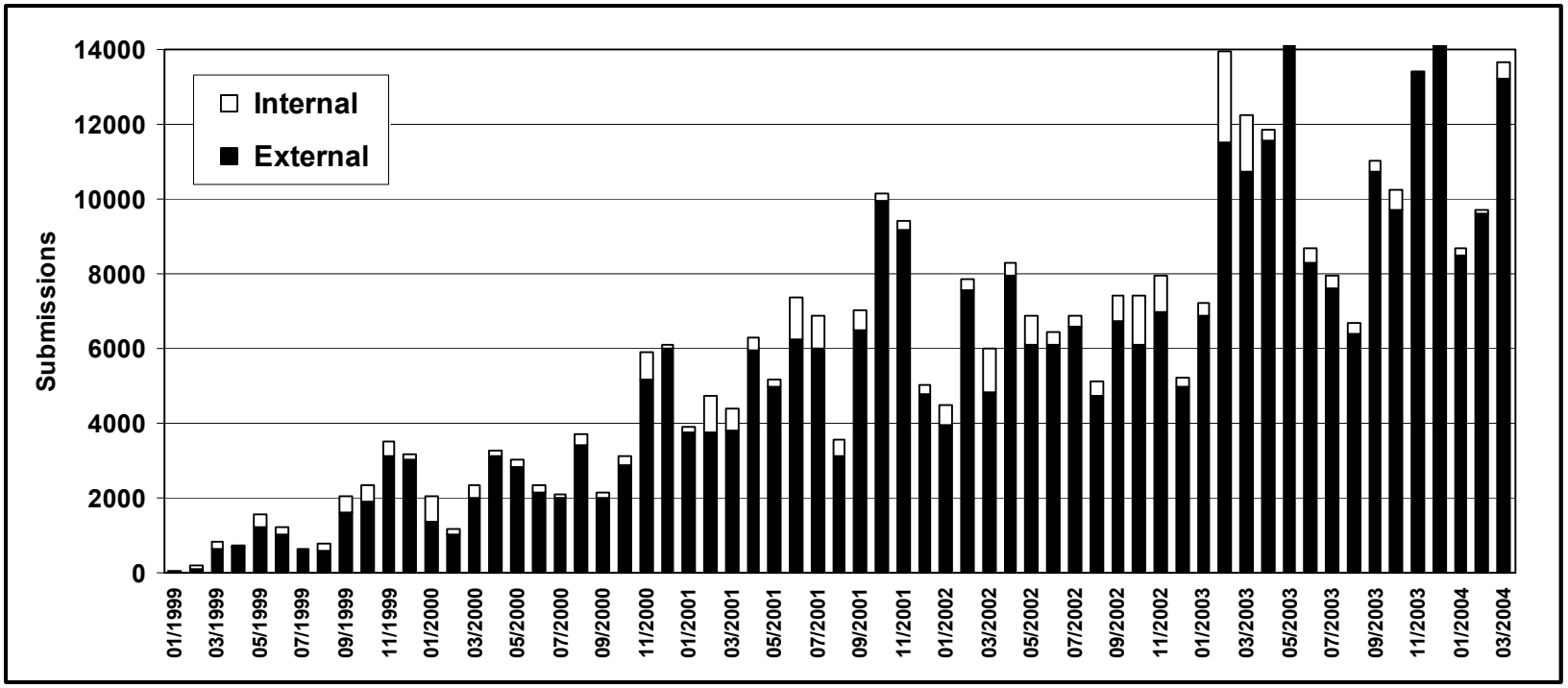
Belgium(be)	4918
Brazil(br)	2558
Canada(ca)	4514
Switzerland(ch)	1098
Chile(cl)	158
Colombia(co)	218
Cyprus(cy)	20
Czech Republic(cz)	554
Germany(de)	1834
Spain(es)	1548
Finland(fi)	270
Micronesia(fm)	36
France(fr)	2730
Greece(gr)	776
Hong Kong(hk)	466
Hungary(hu)	182

Israel(il)	1022
Italy(it)	1646
Japan(jp)	32
Luxembourg(lu)	40
Mexico(mx)	252
Malaysia(my)	912
Netherlands(nl)	4254
Norway(no)	82
New Zealand (nz)	20
Poland(pl)	302
Sweden(se)	3562
Singapore(sg)	236
USSR (former)(su)	834
Turkey(tr)	526
Taiwan(tw)	62
United Kingdom(uk)	4870
Venezuela(ve)	2042

NEOS Users

How Much Do They Use It?

Submissions by month, 1/1999 through 3/2004



. . . 15 / hour over past year

. . . 20 / hour in peak months

Who Supplies Them?

Some commercial solver vendors

- Xpress, FortMP (mixed integer)
- CONOPT, KNITRO, MOSEK (nonlinear)

Universities and their researchers

- BonsaiG (mixed integer)
- DONLP2, FILTER,
  LANCELOT, LOQO, MINOS, SNOPT (nonlinear)

Open-Source Enthusiasts

- GLPK (mixed integer)

with thanks to . . .

- Modeling language vendors (AMPL, GAMS)
- *Hans Mittelmann,* University of Arizona

NEOS Solvers

Where are They Hosted?

Varied workstations at

- Aachen University of Technology
- Argonne National Laboratory
- Arizona State University
- National Taiwan University
- Northwestern University
  (with support from Sun Microsystems)
- University of Wisconsin at Madison

. . . new hosts are readily added anywhere on the Internet

How is NEOS Supported?

Grants

- U.S. Department of Energy, Office of Advanced Scientific Computing, Mathematical, Information, and Computational Sciences Division subprogram, Contract W-31-109-Eng-38
- National Science Foundation, Challenges in Computational Science Program, grant CDA-9726385
- National Science Foundation, Information Technology Research Program, grant CCR-0082807

Donations

- Processor cycles
- Many people's time ***. . . but no user charges as yet***

WEBOPT www.webopt.org

"Web enabled" optimization tools & models

- More than just methods
- For research & professional training as well as industrial deployment

Mission: to address societal issues by

- Forming a network of scientists in Europe and India to exchange skills and best practices
- Creating optimization based solution strategies through web technology
- Disseminating knowledge and information
- Developing partnership with industry

Services

Access to solvers and modeling systems

- FortMP, FortSP, CPLEX
- MPL, AMPL

Optimization-based decision support systems

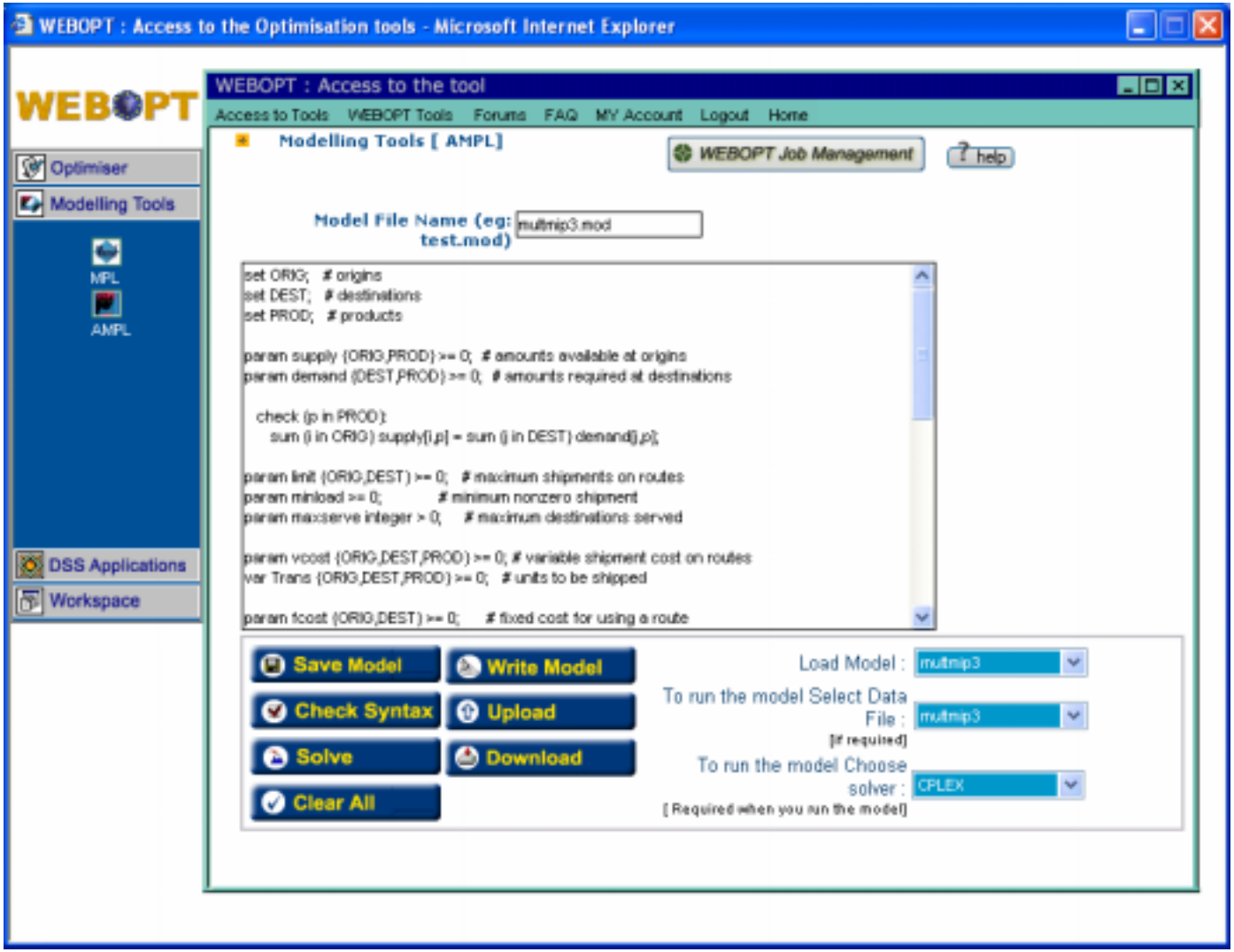
- Supply chain management
- Portfolio optimization

Remote workspace

- Model and data files
- Solver Control and solution files
- Data and log files

WEBOPT

Graphical Interface



New Directions in Optimization Servers

Automated user help

- Problem analysis
- Solver choice

Automated benchmarking

Extension of services

- Clones
- Web service paradigms

Charges for service

- Determining prices
- Scaling up