High Performance Software for Nonlinear Optimization
Status and Perspectives
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The NEOS Server
Optimization, Environments, Network Computing

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http://www.mcs.anl.gov/home/more/

NEOS (Network-Enabled-Optimization-System) Server

A novel environment for solving optimization problems.

- Internet-based access to a library of optimization software.
- Submissions via email, a browser, or the `neos-submit` tool.
- Users only need to submit a specification of the problem.
- The NEOS Server provides all other information required by the solver.

NEOS (Network-Enabled-Optimization-System) Server

Optimization software

Software tools

- Perl
- Tcl/Tk

Automatic differentiation

- ADIFOR
- ADOL-C

Heterogeneous distributed computing

- Condor
- Globus

Typical Environment for Nonlinear Optimization

$$\min \{ f(x) : x_l \le x \le x_u, \ c_l \le c(x) \le c_u \}$$

Tasks

- Develop code to evaluate the objective function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and constraint $c : \mathbb{R}^n \mapsto \mathbb{R}^m$
- Decide on the software
- Retrieve the software
- Hand-code the gradients, Hessians, sparsity patterns.
- Compile, debug, compile, debug, ... run
- Interpret the results
- Repeat the process

The NEOS Way

- Develop code to evaluate the objective function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and constraint $c : \mathbb{R}^n \mapsto \mathbb{R}^m$
- Submit problem to the **NEOS** Server
- Interpret the results
- Repeat the process

Advantages

Easy to use
No need to choose or retrieve software
No need to compute derivatives or sparsity patterns

NEOS

A research effort of the Optimization Technology Center, initiated by Argonne National Laboratory and Northwestern University.

NEOS Guide: A Web-based guide to optimization theory and practice.

NEOS Server: An Internet-based client/server application that provides access to a library of optimization software.

NEOS Guide

- Optimization Software Guide
- Optimization Tree
- Case Studies
- Frequently Asked Questions

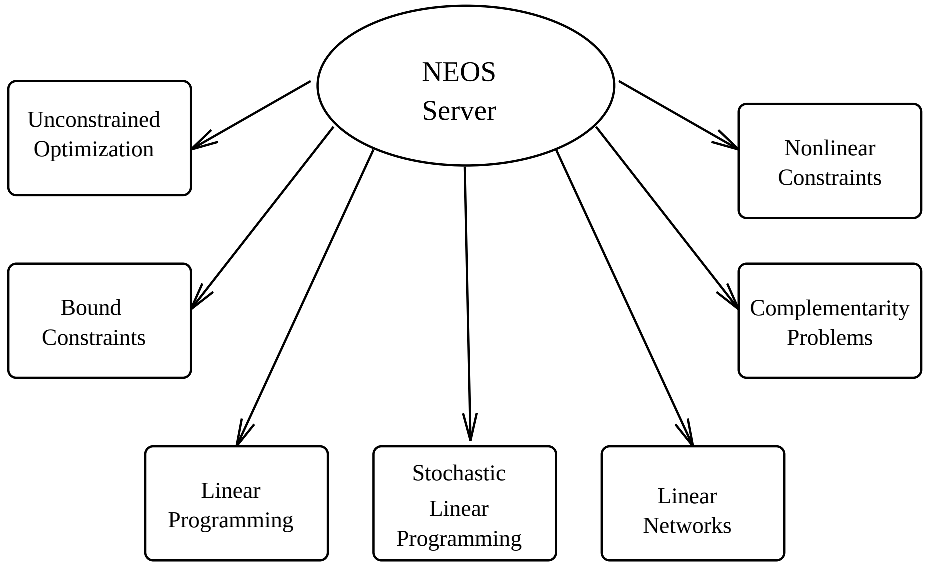
NEOS Collaborations

- Michael Ferris, University of Wisconsin
- Nick Gould, Rutherford Appleton Laboratory
- David Serafini, Rice University
- Jorge Nocedal, Northwestern University
- Joe Czyzyk and Steve Wright, Argonne National Laboratory
- Dan Bienstock, Columbia University
- Phil Gill, University of California, San Diego
- Jorge Moré, Argonne National Laboratory

Outline

- What optimization problems can we solve?
- How are optimization problems specified?
- How are optimization problems submitted?
- How are optimization problems solved automatically?
- How do we add optimization solvers to the NEOS Server?

NEOS Server Solvers



NEOS Server Submissions

NEOS Submission tool

- Socket-based; results returned via `neos-submit`.
- `http://www.mcs.anl.gov/otc/Server/neos/subtool.html`

Web Browser

- Web-based; results returned via browser or email.
- `http://www.mcs.anl.gov/otc/Server/`

Email

- Email-based; results returned via email.
- `neos@mcs.anl.gov`

Specifying Constrained Optimization Problems

$$\min\left\{f(x) : x_l \leq x \leq x_u,\ c_l \leq c(x) \leq c_u\right\}$$

$$f(x) = \sum_{i=1}^{n_f} f_i(x)$$

Dimensions: `n, m`

Number of element functions: `nf`

Initial point: `initpt(n,x)`

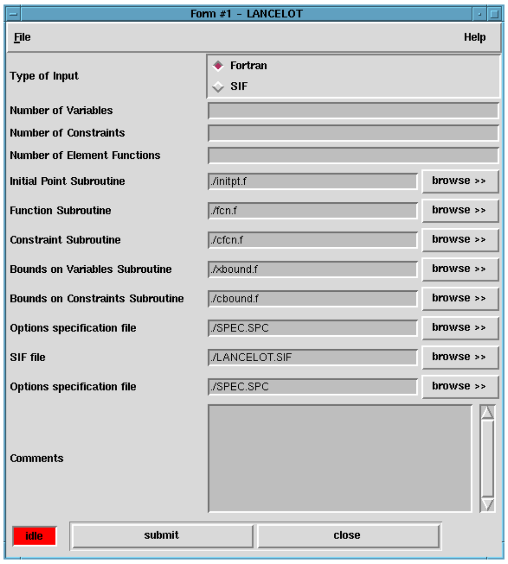
Objective function: `fcn(n,x,nf,fvec)`

Constraint function: `cfcn(n,x,m,c)`

Bounds on the variables: `xbound(n,xl,xu)`

Bounds on the general constraints: `cbound(m,cl,cu)`

NEOS Submission Tool – LANCELOT



NEOS Email Submission – NMTR

Send the following message to `neos@mcs.anl.gov`

```
type UCO
solver NMTR
n = 100
begin.initpt
```

Subroutine `initpt(n,x)` to evaluate the starting point

```
end.initpt
begin.fcn
```

Subroutine `fcn(n,x,f)` to evaluate $f : \mathbb{R}^n \mapsto \mathbb{R}$

```
end.fcn
```

NEOS Submission – `initpt`

```
subroutine initpt(n,x)
integer n
double precision x(n)

integer nx, ny
nx = 10
ny = 10
call odc_init(nx,ny,x)
end

subroutine odc_init(nx,ny,x)

.....

end
```

NEOS Submission – `fcn`

```
subroutine fcn(n,x,f)
integer n
double precision f
double precision x(n)

integer nx, ny
double precision lambda
lambda = 0.008
nx = 10
ny = 10
call dodc(nx,ny,x,f,lambda)
end

subroutine dodc(nx,ny,x,f,lambda)

.....

end
```

Performance: Optimal Design with Composites Problem

Determine a minimizer $v : \mathbb{R}^2 \mapsto \mathbb{R}$ of the problem

$$\min\{f_\lambda(v) : v \in H_0^1(\mathcal{D})\},$$

where

$$f_\lambda(v) = \int_{\mathcal{D}} \left\{ \psi_\lambda \left(\|\nabla v(x)\| \right) + v(x) \right\} dx$$

$$\psi_\lambda(t) = \begin{cases} \frac{1}{2}\mu_2 t^2, & 0 \le t \le t_1, \\ \mu_2 t_1 (t - \frac{1}{2} t_1), & t_1 \le t \le t_2, \\ \frac{1}{2}\mu_1 (t^2 - t_2^2) + \mu_2 t_1 (t_2 - \frac{1}{2} t_1), & t_2 \le t, \end{cases}$$

$$t_1 = \left(2\lambda \frac{\mu_1}{\mu_2} \right)^{\frac{1}{2}}, \qquad t_2 = \left(2\lambda \frac{\mu_2}{\mu_1} \right)^{\frac{1}{2}}.$$

Discretization of the ODC Problem

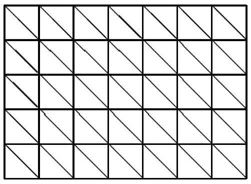
A finite element formulation leads to

$$\min \{ f(x) : x \in \mathbb{R}^n \}$$

with `nx*ny` variables. The mapping $f : \mathbb{R}^n \to \mathbb{R}$ is a partially separable function

$$f(x) = \sum_{i=1}^{m} f_i(x),$$

where $f_i : \mathbb{R}^n \to \mathbb{R}$ only depends on 3 variables.



Performance of the NEOS Solver vmlm

Optimal design problem

`dodc(nx,ny,x,nf,fvec,lambda)`

	Function			Function and Gradient		
n	`niters`	`nfgev`	`time`	`niters`	`nfgev`	`time`
2,500	230	237	139	232	239	22
10,000	427	436	1042	427	433	165
40,000	865	871	8399	877	885	1461

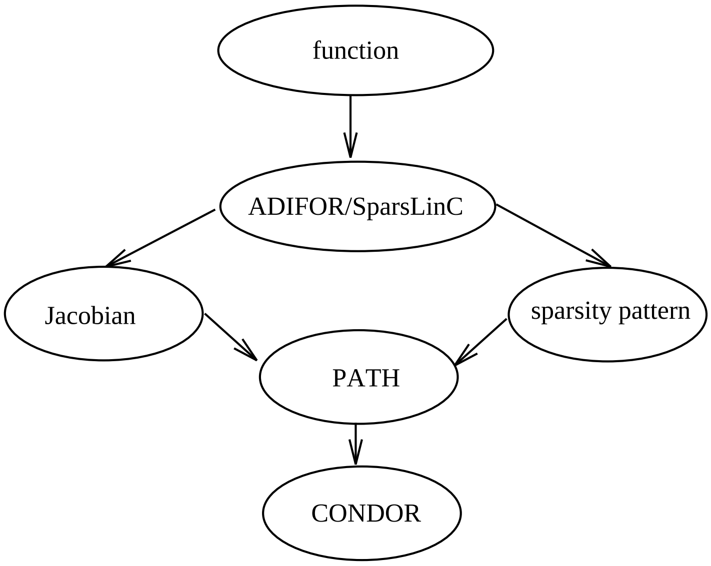
Computing time for the function/gradient grows linearly with n

Issues for Problem-Solving Environments

What if ...

- A subroutine does not compile?
- The calling sequence is wrong?
- The function evaluation blows up at the starting point?
- The function evaluation blows up at an iterate?
- The function evaluation is garbage?
- The function is non-differentiable?
- The user wants to write out information?

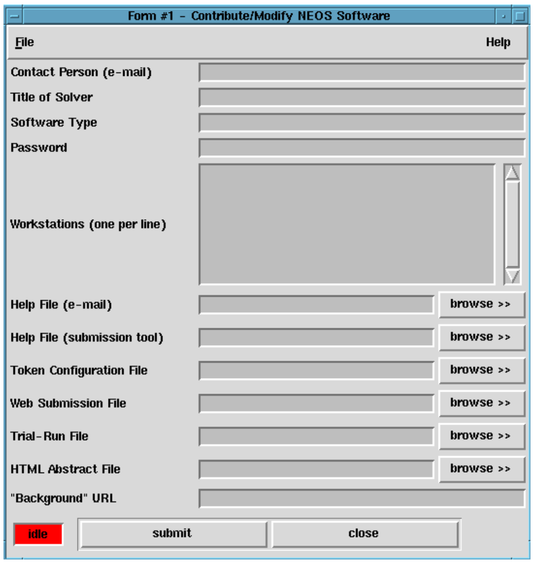
Handling Complementarity Problems: PATH



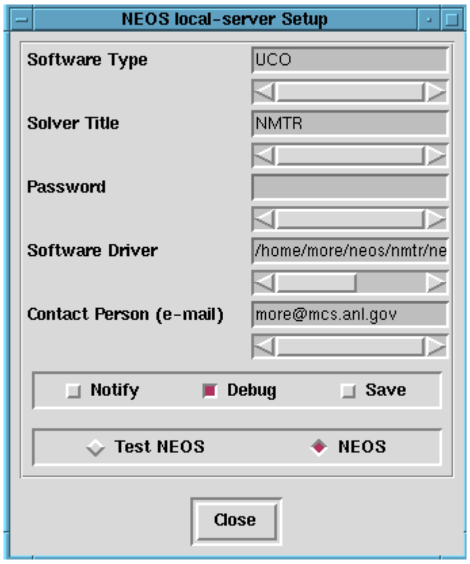
NEOS Server Issues

- Registering software – The NEOS Submission Tool
- Registering software – The NEOS Communications Tool
- Monitoring traffic – The NEOS Monitor
  - Job number
  - Type of job and interface used to submit job
  - Date and user name

Registration of Software: NEOS Submission tool



Registration of Software: NEOS Communications tool

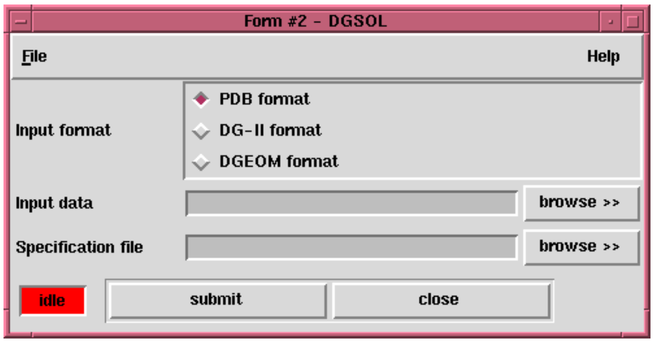


Registration of Software: Adding Solvers

Problem: Determine $x_1, \ldots, x_m$ in $\mathbb{R}^3$ such that

$$l_{i,j} \le \|x_i - x_j\| \le u_{i,j}, \qquad (i,j) \in \mathcal{S}$$

Data: $(i, j, l_{i,j}, u_{i,j}), \qquad (i,j) \in \mathcal{S}$



Uses of the NEOS Server

- Solving large optimization problems
- Education and information on optimization technology
- Classroom exercises
- Testing optimization software
- Comparing optimization software
- Prototype problem solving environment

Future Directions for the NEOS Server

- Handling C-programs (ADOL-C and ADIC)
- Distributed computing (remote procedure calls)
- Global optimization
- Problem-solving environment

Additional Information

J. Czyzyk, M. Mesnier, and J. Moré,
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MCS-P654-0397, March 1997.

NEOS Server `http://www.mcs.anl.gov/otc/Server/`
NEOS Guide `http://www.mcs.anl.gov/otc/Guide/`