Cyberinfrastructure and Optimization

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Topics

Concepts

- Infrastructure & cyberinfrastructure
- Software as a service

Optimization services

- COIN-OR open-source software
- The NEOS Server
- The OS project
- Intelligent optimization systems

Cyberinfrastructure for optimization

- Advanced computing resources
- Cloud computing

What is an infrastructure?

Familiar examples

- Transportation: road, rail, air
- Energy: power grids, pipelines
- Communications: mail, packages, phone

Common characteristics

- Doesn't do things; rather, makes things possible
- Facilitates activities not initially foreseen
- Relies on standards
- Requires broad accessibility

What is a cyberinfrastructure?

Infrastructure for computing

- Internet
- Web
- Supercomputer centers

Infrastructure for computing in some field

- Nanotechnology
- Seismology
- ✤ Optimization . . .

What is cyberinfrastructure research?

Ask the (U.S.) NSF . . .

- National Science Foundation
 Blue-Ribbon Advisory Panel on Cyberinfrastructure
- Revolutionizing Science and Engineering Through Cyberinfrastructure
 - * www.nsf.gov/od/oci/reports/toc.jsp

Organization

- Office of Cyberinfrastructure
- Independent of programs in traditional areas

Workshops

- Over 30 reports
 - * www.nsf.gov/od/oci/reports.jsp
- An Operations Cyberinfrastructure: Using Cyberinfrastructure and Operations Research to Improve Productivity in American Enterprises
 - * http://www.optimization-online.org/OCI/OCI.pdf

Implications for Optimization Research

CI Focus at government agencies

- Big science
- Custom-built, specialized software
- Focused application

CI Focus in the optimization community

- Small science
- General-purpose software
- Broad distribution

Special circumstances of optimization

- Independence of modeling software, solver software, data
- Sensitivity of solver choice to mathematics of problem
- Huge variation in solver performance

Software as a Service ("SaaS")

as a Product

- You install & run on local computers
- You maintain & upgrade

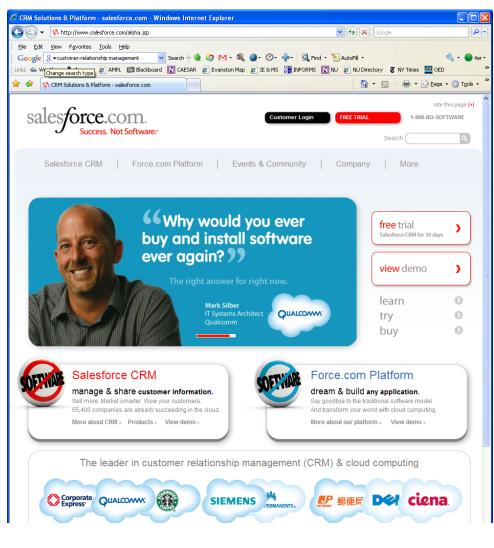
as a Service

- They install on their servers
- ✤ You run on their servers
- They maintain & upgrade

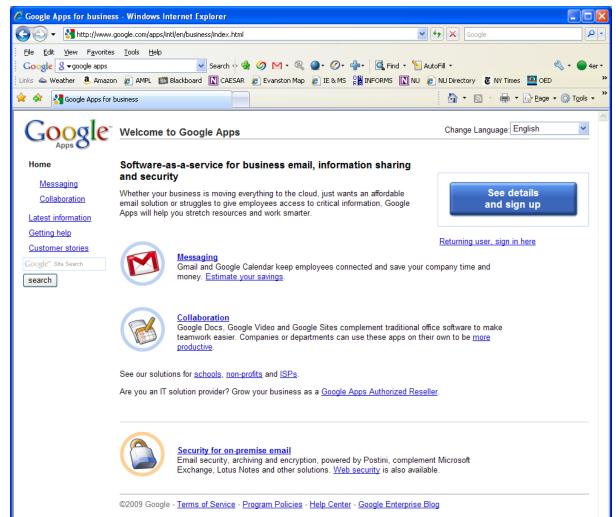
Tax preparation

🧭 TurboTax Free Edition 2008 - Windows Internet Explorer					
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I was legally separated I was widowed	 does taking college classes count as attending college? If it is only me and im in college do I check for "s When it says Someone in my household attended college doe 				
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I paid rent I had more than one job I sold my home I refinanced my home My home My home different states	Answer a Question This message is for julie847. I asked a question and rece				

Customer-relationship management



Communication



Office

🖉 Office - Windows Live - Windows Internet Explorer						
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				can help you	for your degree.	
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Implications for Optimization

Menu of products

- Solvers
- Modeling systems
 - ... independent and interchangeable

Potential impact

- Making products more readily available
- Facilitating comparison of products
- Providing access to advanced computing resources?

Progress in Optimization Services

COIN-OR open-source software

The NEOS Server

The OS Project

Intelligent optimization systems

COIN-OR www.coin-or.org

Computational Infrastructure for Operations Research

- Repository for open-source software for optimization
- Operated by nonprofit COIN-OR Foundation
 - * Origins at IBM (2000)
 - * Currently hosted by INFORMS
- Mission:
 - * Develop, manage & distribute
 - * OR software, models, and data so that
 - * OR professionals can benefit from
 - * peer-reviewed, archived, openly-disseminated software
- Strongest in optimization

Relevance to cyberinfrastructure

- Tools are open for any use
- Each tool has many potential applications
- Presentation, access, maintenance are standardized

Open-Source Software

Things to know

- Free, but subject to licensing restrictions
- Licenses vary considerably
- Equally available to all user classes
- Possibly owned (in part) by
 - * Co-authors
 - * Employer
 - * Granting Agencies
 - * Owner of the machines it was written on

Examples

- GNU Public License, GNU Library Public License
- Eclipse Public License / Common Public License
- Mozilla Public License
- Apache License
- BSD Licenses

Open-Source Software at COIN-OR

Solvers

- Linear continuous & discrete
- Nonlinear continuous & discrete
- Semidefinite
- Stochastic

... source & binary

Infrastructures

- Developer tools
- Optimization utilities
- Interfaces
- Modeling systems and environments
 - ... more later on Optimization Services

Getting Published on COIN-OR

Scope

- Useful to Operations Research professionals
- Not clearly better suited to another repository

Requirements

- Working Code
- Documentation
- Legal

Operational Policies

COIN-OR Requirements

Working code

- The project has some type of "tests"
- The tests are in a form that can be easily supplemented
- No other specific requirements on form or magnitude
 - ... tests ensure the code remains working as it evolves

COIN-OR Requirements (cont'd)

Documentation

- Authors
- Install
 - * How to build, install, and run on at least one platform
 - * Any platform, any computing language
- Readme (FAQs)
 - * What is the project name?
 - * What is the project for?
 - * Who is the maintainer?
 - * How do I contact the maintainer?
 - * How do I run the project once it's built or installed?
 - * How do I report a bug?
- Copying
 - * Licensing information

COIN-OR Requirements (cont'd)

Legal (new format)

- License
 - * Any certified open-source license (see www.opensource.org)
 - * Common/Eclipse Public License recommended (IBM origins)
- Required paperwork
 - * List of authors
 - * Committers' Statements of Respect for Ownership
 - * Contributors' Statement of Ownership and Licensing
- Recommended paperwork
 - * Owner's Confirmation of Licensing
 - * Contributors' Statements of Respect for Ownership
- Optional paperwork
 - * List of authors & their contributions
 - * Committers' permissions from employers
 - * Detailed contributor & contribution logs

NEOS neos.mcs.anl.gov

Network Enabled Optimization System

- Server
 - * free Internet access to over 60 solvers
- Guide
 - * tutorials, case studies, test problems, FAQs

Relevance to cyberinfrastructure

- Facilitates many uses
 - * but does not anticipate particular applications
- Makes all solvers open to anyone
- Supports standard problem representations
- Uses Web standards & protocols
 - * XML files
 - * callable via XML-RPC

NEOS Server

A general-purpose optimization server

- ✤ Over 45 solvers in all
 - * Linear, linear network, linear integer
 - * Nonlinear, nonlinear integer, nondifferentiable & global
 - * Stochastic, semidefinite, semi-infinite, complementarity
- Commercial as well as experimental solvers
- Central scheduler with distributed solver sites
- ✤ 20,000 submissions in a typical month

... has handled over 100,000

A research project

- Currently free of charge
- Supported at Argonne National Laboratory since 1996
- * *Planned move* to Wisconsin Institutes of Discovery in late 2010

Design

Flexible architecture

- Central controller and scheduler machine
- Distributed solver sites

Standard formats

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

Varied submission options

- ✤ E-mail
- ✤ Web form
- Direct call via XML-RPC
 - * from AMPL or GAMS client
 - * from user's client program using NEOS's API
 - ... server processes submissions of new solvers, too

Range of Solvers

For familiar problem types

- Linear programming
- Linear network optimization
- Linear integer programming
- Nonlinear programming
- Stochastic linear programming
- Complementarity problems

For emerging problem types

- Nondifferentiable optimization
- Semi-infinite optimization
- Global optimization
- Nonlinear integer programming
- Semidefinite & 2nd-order cone programming

... virtually every published semidefinite programming code

Contributors

Open-source solvers

✤ GLPK, CBC, Bonmin (mixed integer)

Research solvers

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

Commercial solvers

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

Commercial modeling languages

- * AMPL
- * GAMS

Hosts

Varied workstations at

- Aachen University of Technology, Germany
- Argonne National Laboratory
- Arizona State University
- Lehigh University
- National Taiwan University
- Universidade do Minho, Portugal
- University of Wisconsin at Madison

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

Support

Large mailing list for questions

- NEOS developers
- Solver developers

Support request buttons on every page



Observations

Donations

- Processor cycles
- Many people's time

Status

- Limited support
- No performance guarantees

... watch for changes with move to WID

OS www.optimizationservices.org

Optimization Services

- Distributed optimization environment
- Unified framework of services & utilities for
 - * modeling languages, servers, registries, agents, interfaces, analyzers, solvers, simulation engines
- Open-source project on COIN-OR

Relevance to cyberinfrastructure

- ✤ A "next generation" NEOS
- *Defines* standards for all activities necessary to support decentralized optimization on the Internet
- Embraces distributed computing standards
 - * Extensible Markup Language (XML)
 - * Service Oriented Architecture
 - * Web Services

OS Goals

Conceive optimization as a service

- Software as a product
 - * in multiple copies on users' machines

* Software as a service

- * residing on a server
- * accessed by numerous client machines over a network

... adapted to special challenges

- Profusion of weak standards for problem description
- Lack of standards for results, queries, instructions
- Variety & complexity of information and behavior
- Disconnect between modeling and solving
 - * mathematical problem types that characterize solvers
 - * model types familiar to customers

OS Framework

Functions

- Representation of instances, results, and solver options
- Communication between clients and solvers
- Registration & discovery of optimization-related services
 * using the concept of Web Services.

Standards & protocols

- Representations of model instances
 - * in text files
 - * in memory
- Interfaces to these representations
 - * get(), set(), calculate() methods
- Protocols for solver registration & discovery
- Protocols for client-server communication

OS on the Internet

Home site: www.optimizationservices.org

- Overview, standards, publications, presentations, FAQs
- Contact information, downloads, licenses

Developer site: www.coin-or.org/projects/OS.xml

Login, register, wiki, source repository, timeline, search

Newsgroup:

groups.google.com/group/optimizationservices

COIN mailing list:

list.coin-or.org/mailman/listinfo/os

OS Integration

Core (OSCommon library)

Modeler side

- * AMPL
- LINGO
- MATLAB

Solver side

- COIN OSI
- AMPL-solver library
- ✤ Linear: CLP, CBC, CPLEX, Impact
- Nonlinear: IPOPT, LINDO, KNITRO, Bonmin
- CppAD (automatic differentiation)

OS Repository

Linear (netlib basic, infeasible, Kennington)

- Individual XML (OSiL format) files available now
- Zip files to come

Mixed integer (mainly from miplib 2003)

Nonlinear

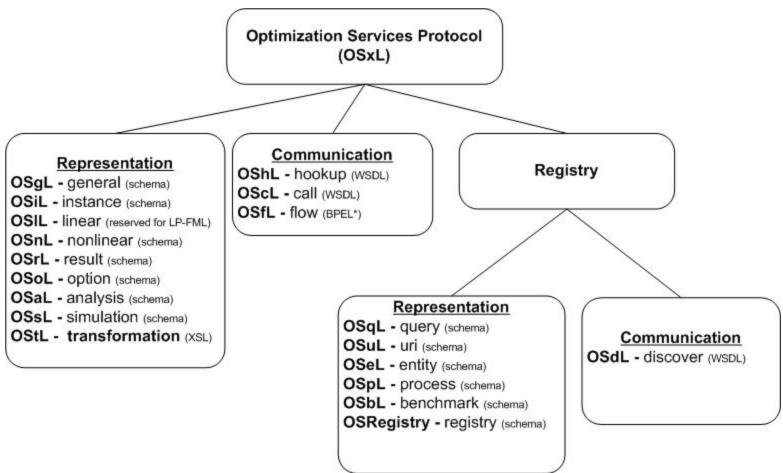
✤ CUTE now, more to come

Stochastic

Thanks to Gus Gassmann

... all known documentation (source, solution, description, type, etc.)

OS Standards



*OSmL: a modeling language and NOT an Optimization Services Protocol

*Letters not currently used: w, z

*BPEL: Business Process Execution Language for flow orchestration.

OSiL: Optimization Problem Instances

Design goals

Simple, clean, extensible, object-oriented

Standard problem types supported

- Linear
- Quadratic
- General nonlinear
- Mixed integer for any of above
- Multiple objective for any of above
- Complementarity

OSiL (cont'd)

Extensions (stable or near-stable)

- User-defined functions
- XML data (within the OSiL or remotely located)
- Data lookup (via XPath)
- Logical/combinatorial expressions and constraints
- Simulations (black-box functions)

OSiL (cont'd)

Prototypes

- Cone & semidefinite programming
- Stochastic
 - * recourse, penalty-based, scenario (implicit or explicit)
 - * risk measure/chance constrained
 - * major univariate, multivariate, user-defined distributions
 - * general linear transformation and ARMA processes
 - * R. Fourer, H.I. Gassmann, J. Ma, and R.K. Martin, "An XML-Based Schema for Stochastic Programs." Forthcoming in *Annals of Operations Research*.

OSrL: Optimization Problem Results

Counterpart to OSiL for solver output

- General results such as serviceURI, serviceName, instanceName, jobID, time
- Results related to the solution such as status (unbounded, globallyOptimal, etc.), substatus, message
- Results related to variables (activities), objectives (optimal levels), constraints (dual values)
- Service statistics such as currentState, availableDiskspace, availableMemory, currentJobCount, totalJobsSoFar, timeLastJobEnded, etc.
- Results related to individual jobs including state (waiting, running, killed, finished), userName, submitTime, startTime, endTime, duration, dependencies, scheduledStartTime, requiredDirectoriesAndFiles.

OSrL (cont'd)

Additional solution support

- Support for non-numeric solutions such as those returned from combinatorial or constraint programming solvers
- Support for multiple objectives
- Support for multiple solutions
- Integration of analysis results collected by the solver

OSoL: Optimization Options

Counterpart to OSiL for solver instructions

- General options including serviceURI, serviceName, instanceName, instanceLocation, jobID, license, userName, password, contact
- System options including minDiskSpace, minMemorySize, minCPUSpeed
- Service options including service type
- Job options including scheduledStartTime, dependencies. requiredDirectoriesAndFiles, directoriesToMake, directoriesToDelete, filesToCreate, filesToDelete, processesToKill, inputFilesToCopyFrom, inputFilesToCopyTo, etc.

Limited standardization of algorithmic options

Currently only initial values

OSoL (cont'd)

Including support for:

- Various networking communication mechanisms
- Asynchronous communication (such as specifying an email address for notification at completion)
- Stateful communication (achieved mainly through the built-in mechanism of associating a network request with a unique jobID)
- Security such as authentication and licensing
- Retrieving separately uploaded information
 (when passing a large file as a string argument is inefficient)
- Extended or customized solver-specific or algorithm-specific options

Other XML Schema-Based Standards

Kept by the OS registry

- OSeL (entity, experimental): static information on optimization services (such as type, developer)
- OSpL (process, near stable): dynamic information on optimization services (such as jobs being solved)
- OSbL (benchmark, experimental): benchmark information on optimization services

For use by the discovery process

- OSqL (query, experimental): specification of the query format used to discover the optimization services in the OS registry
- OSuL (uri/url, experimental): specification of the discovery result (in uri or url) sent back by the OS registry

Other Schema-Based Standards (cont'd)

Formats and definitions

- OSsL (simulation, stable): format for input and output used by simulation services invoked via the Optimization Services to obtain function values
- OSgL (general, near stable): definitions of general elements and data types used by other OSxL schemas. Usually included in the beginning of another OSxL schema through the statement: <xs:include schemaLocation="OSgL.xsd"/>
- OSnL (nonlinear, stable): definitions (operators, operands, etc.) of the nonlinear, combinatorial, and other nodes used in other OSxL's, mainly OSiL

Other WSDL-Based Standards

WSDL

Web Service Definition Language

WSDLs for OS (stable)

- OShL (hook): for invoking solver/analyzer services
- OSdL (discover): for invoking optimization registry services to register and discover services
- OScL (call) for invoking simulation services, usually to obtain function values.

Observations

Contrast to NEOS

- Lightweight repository only
- Emphasis on standards

Status

- Still in formative stages
- Release 2.2 in open source from COIN-OR

... binary distributions also available

Intelligent Optimization Systems

Beyond repositories and registries

- Interactive aids to modeling
- Automatic connection of modelers to solvers

Relevance to cyberinfrastructure

Missing link in optimization as a service

Interactive Aids to Modeling

ANALYZE (Greenberg)

- Alternative views
- Simplification
- Rule-based reporting
- Extended sensitivity analysis
- Infeasibility diagnosis

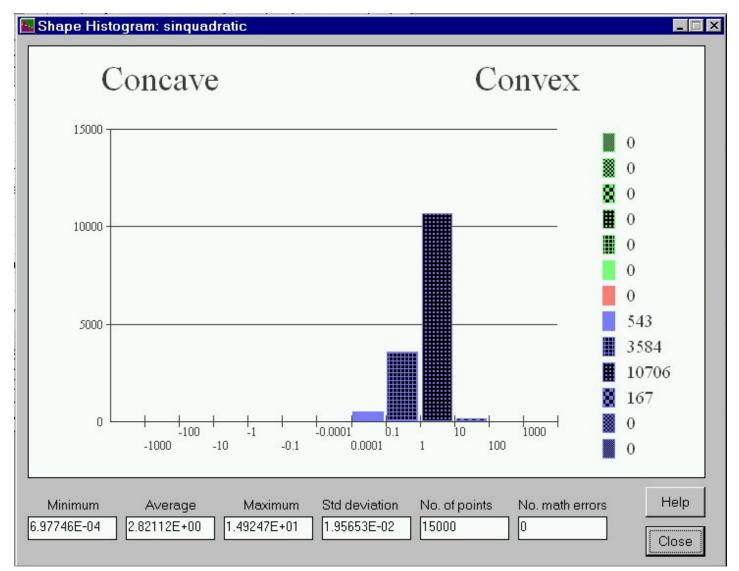
MProbe (Chinneck)

- Analyze feasibility, redundancy, constraint effectiveness
- Tighten bounds, find near-feasible points
- Plot functions
- Analyze function shape (convex? concave? almost linear?)
- Stimate shape of constrained region (convex?)
- Estimate function range and slope
- Estimate objective effect (global? local?)

MProbe Example (1)

Variables V Show only >	<mark>∕orkshop</mark> type: real ▼			Ţ] □ Reverse Selection	1	10 of 17 variables visible				
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mt1	6 F	Real	3	-1.E+00	-1.E+00	8.136667E-01	1.E+00	1.E+00	Nec		
mt2	7 F	Real	1	-1.E+00	-1.E+00	2.635834E-01	1.E+00	1.E+00	Nec		
sinquad2	5 F	Real	1	-1.E+01	-1.E+01	-8.351681E+00	1.E+01	1.E+01	Rec		
sinquad1	4 F	Real	1	-1.E+01	-1.E+01	9.231597E+00	1.E+01	1.E+01	Rec		
z2	3 F	Real	1	-1.E+01	-1.E+01	6.659936E+00	1.E+01	1.E+01	Rec		
z1	2 F	Real	1	-1.E+01	-1.E+01	3.470179E+00	1.E+01	1.E+01	Red		
sinp1	10 F	Real	0	0.E+00	0.E+00	6.348978E+01	1.E+02	1.E+02	Red		
sinp2	11 F	Real	0	0.E+00	0.E+00	8.131882E+01	1.E+02	1.E+02	Rec		
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Freeze varia	able nar	mes/i.d.	1					[Trace		
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change bounds on visible group reset original bounds											
	s	show constraints containing selected variable									
				taining selecte	ed variable nin sampled val						

MProbe Example (2)



Automatic Connection to Solvers

DrAMPL (Orban & Fourer)

- Process model written in AMPL language
- Determine type of problem instance
 - * Linear, quadratic, nonlinear
 - * Continuous, differentiable, integer
 - * Unconstrained, bounded, constrained
 - * Convex, concave
- Compare against database of solver abilities
- Recommend choice of solver

... some obvious, some difficult

Example ("Dr. AMPL")

Analysis

```
Problem type
-Problem has bounded variables
-Problem has no constraints
Analyzing problem using only objective
 -This objective is quadratic
 -Problem is a QP with bounds
 -0.833013 <= objective <= 0.8359
Problem convexity
Nonlinear objective looks convex on its domain.
Detected 0/0 nonlinear convex constraints,
          0/0 nonlinear concave constraints.
```

Example ("Dr. AMPL")

Solver recommendations

```
### Specialized solvers, based on all properties ###
        MOSEK
        OOOP
### Specialized solvers, excluding "hard" properties ###
        BLMVM
        FortMP
        L-BFGS-B
        MINLP
        MOSEK
        OOQP
        PathNLP
        SBB
        TRON
### General-purpose solvers ###
        KNITRO
        LANCELOT
        LOQO
```

Challenges

Detection & transformation

- Identify tractable problem types
- Convert to forms that solvers can handle
- Convert the results back

Examples

- Generalized variable domains
 - * arbitrary unions of points & intervals
- Separable piecewise-linear functions
- Complementarity constraints
- Logical and combinatorial constraints
 - ***** <c1> or <c2>, <c1> implies <c2>
 - * counting, all-different
- Second-order cone constraints

Cyberinfrastructure for Optimization

Advanced computing resources

Cloud computing

Advanced Computing Resources

Platforms offering special power

- Multiple processors
- Huge storage devices
- Fast networks
 - ... and algorithms to take advantage of them

Relevance to cyberinfrastructure

- Facilitates many uses sometimes unanticipated
- ✤ Infrastructure already in existence
 - * supercomputer centers
 - * computational grids

Types of Advanced Computing

High-performance computing

- Large numbers of specialized processors
- Specialized interconnections

Distributed computing (MW)

- Standard computers
- Working together through Internet connections

High-throughput computing (Condor)

- Otherwise idle computers
- Networked by special software

Sample Research

From the metaNEOS project (1997–2001)

- 1010-variable deterministic equivalent of a 107-scenario stochastic program on a computational grid of about 800 workstations, in about 32 hours of wall-clock time
- a previously intractable quadratic assignment problem using an average of 650 worker machines over a oneweek period, providing the equivalent of almost 7 years of computation on a single workstation
- a mixed-integer nonlinear programming problem with parallel efficiency of up to 80% on 600 million searchtree nodes

Resulting Applications

Essentially none

- Impractical to write new software for each application
- No access to software from previous studies

Needs

Advanced computing + software services

- Put optimization software on high-performance platforms
- Make it generally available through NEOS or OS

Advanced computing for optimization

- Solving on demand
- ✤ Flexible resource allocation

... a new paradigm

Cloud Computing

Current significance

- Software-as-a-service by another name
- Cyberinfrastructure for building software services

What it means for optimization providers

- Coordination
 - * NEOS scheduler
 - * OS registry
- Resources
 - * Windows Azure
 - * IBM's various options
 - * Amazon EC2

Cloud Coordination

NEOS

- * Central *registry*
- Central scheduler
- ✤ You supply solvers and hardware

OS

- * Central *registry* only
- You supply scheduler, solvers and hardware
 ... *lighter-weight solution*

Cloud Resources

Several commercial offerings

- * Central *hardware*
- Central *development software*
- You supply solvers

Current examples . . .

Cloud Resources (1)

Microsoft Windows Azure

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Windows	° Azure [°] Pla	atform			Account Su	oport
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	an	d price.			iet Tools & SDK	
	tructure that supports your				Sign up now	
peak times. Getting t	Forecasting the highest po ne right servers in place at the Microsoft cloud. The V	the right time, managing a	and maintaining the system	ms. Custo	mer Quotes	
platform that lets ye to invest upfront on e	bu focus on solving busin expensive infrastructure. Pa you don't. We handle all t	ess problems and addre y only for what you use, s	ssing customer needs. N cale up when you need ca	lo need pacity onment	3M	
	ndows Azure platform ha	•		valu	Azure is of great le to 3M ause it takes the abase management	
Since the Windows A	zure platform is so flexible,	the use cases are unlimit	ed.	pied	ce off our plate. ??	
 Emerging startu on the Windows 	ps: If you're building the n Azure platform and use yo	ext Internet hit, the last thi ur hard–won VC funding o	ng you want is a fail whale on polishing up your proc	e. Count	lim Graham lechnical Manager, 3M	
	ees: Deploying an update to everywhere to handle the h s.					
	ftware Vendors: Want to o tion? Use the Windows Azu les.					

Excel Solver for the Cloud ... coming soon?

Cloud Resources (2)

IBM solutions, technologies, consulting, design



Many offerings . . .

CPLEX not there yet

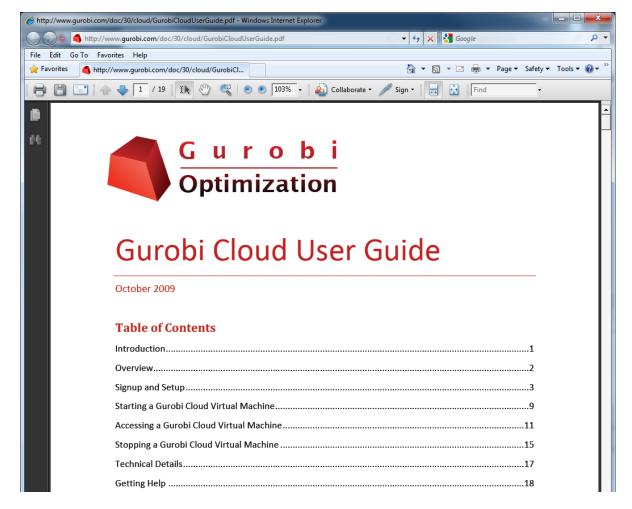
Cloud Resources (3)

Amazon EC2

mazon Elastic Compute Cloud (Ama	zon EC2) - Windows Inte	rnet Explorer				-			
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Amazon EC2 Details	provides resiza	able compute capacity in	the cloud. It is designed	July 1 op 1	For Amazon EC2				
EC2 Overview	web-scale com	puting easier for develop	oers.						
EC2 FAQs		Amazon EC2's simple web service interface allows you to obtain and							
 EC2 Pricing 	configure capacity with minimal friction. It provides you with complete control of your computing resources and lets you run on Amazon's								
Amazon EC2 SLA	proven comput	proven computing environment. Amazon EC2 reduces the time required							
 EC2 Instance Types 		boot new server instance apacity, both up and dow		ou to					
 EC2 Instance Purchasing Options 	requirements of by allowing yo	change. Amazon EC2 cha u to pay only for capacity	nges the economics of co that you actually use. Ar	nazon					
 Reserved Instances 		developers the tools to be emselves from common fa		ations					
 Spot Instances 									
 Windows Instances 	This page cont	ains the following catego	ories of information. Click	to jump down:					
	↓ Amaz	on EC2 Functionality	/	↓ Pricing					
Amazon EC2 Features	↓ Servi	ce Highlights		↓ Resources					
Elastic Block Store	↓ Features ↓ Detailed Description								
Amazon CloudWatch	↓ Instance Types ↓ Intended Usage and Restrictions								
 Auto Scaling 	↓ Opera	ating Systems and S	oftware						
 Elastic Load Balancing 									
 High Performance Computing 	Amazon	EC2 Functionali	ty						
	Amazon EC2 p	resents a true virtual con	nputing environment, allo	wing you to use web ser	vice interfaces to launch				

Cloud Resources (3)

Gurobi solver on Amazon EC2



Cloud Resources (3)

Gurobi solver on Amazon EC2 (prices)

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	This license i Compute Clo unlimited. Th is started. Us virtual machii hours. Additi Cloud. All bill High-I High-I	Server – Unlimited- is associated with a p pud (EC2) platform. The latest version of Gu ie is charged from the ne is terminated. Part onal costs of \$0.20/G ing is handled by Ama Memory Extra Large Memory Double Ext	eInstance	e Amazon Elastic sers and uses is ch time an instance rted to when the are billed as full	\$4 per hour \$6 per hour \$8 per hour	H

Cloud Optimization Prices

Gurobi prices

- High-memory extra-large instance \$4/hour
- High-memory double extra-large instance \$6/hour
- High-memory quadruple extra-large instance \$8/hour
- Data transfer in or out \$0.20/gigabyte

General principles

- Rent machine time, not CPU time
- Adaptable to mixed modeling and solving

Practical issues

- Will there be day, week, month discounts?
- How can both a modeling system and solver be provided?

... need to divide the revenues