Optimization Algorithms and Software at SOL

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SOL and ICME, Stanford University

Computational Linear Algebra and Optimization for the Digital Economy

International Centre for Mathematical Sciences
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Abstract

When a colleague knocks on your door with a mathematical problem, great joy ensues on both sides if you happen to have numerical software that can solve the problem. This is a reason for writing "general-purpose software".

If the software is downloadable, similar happiness ensues when it gets used for unexpected applications. You learn about such cases if your software includes bugs(!) or Google does its usual precise search.

The Systems Optimization Laboratory (SOL) was founded by George Dantzig and Richard Cottle at Stanford University in 1974 to encourage algorithm and software development in traditional Operations Research areas. Dantzig's group built increasingly challenging linear models of the US Economy (the PILOT linear programs), while Alan Manne continued to expand his nonlinear economic models (which began before large-scale optimization software existed). These spurred the development of MINOS at SOL (by the speaker and fellow New Zealander Bruce Murtagh) in parallel with Arne Drud's development of CONOPT at the World Bank and then in Denmark.

In the 1980s, the SOL "Gang of 4" (Gill, Murray, Saunders, and Wright) developed "dense" solvers LSSOL, QPSOL, and NPSOL. After Philip Gill moved to UC San Diego, NPSOL became increasingly important for trajectory optimization at McDonnell-Douglas (now Boeing). This spurred the development of the large-scale optimizers SQOPT and SNOPT.

Many years later, MINOS, CONOPT, and SNOPT remain heavily used solvers within the GAMS and AMPL algebraic modeling systems (and on the NEOS server), and LUSOL remains the reliable "engine" for basis handling in MINOS, SQOPT, SNOPT, and other solvers such as PATH and lp_solve. A unique feature of LUSOL is its Threshold Rook Pivoting option for estimating the rank of a rectangular sparse matrix.

Other solvers developed at SOL include MINRES, MINRES-QLP, LSQR, LSMR, and PDCO. We review the mechanics of the solvers and some unexpected applications that they've been put to work on. We conclude with even more unexpected aspects of optimization reported by radio and TV audiences in New Zealand.

SOL

Systems Optimization Laboratory
Stanford University

SOL

- Founded 1974 by George Dantzig and Richard Cottle
- Dantzig, Alan Manne: economic models (linear & nonlinear)
- Gill, Murray, Saunders, Wright: Software for optimization

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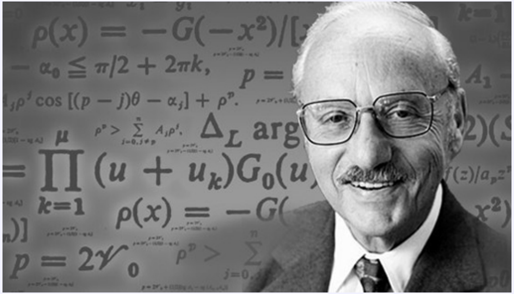
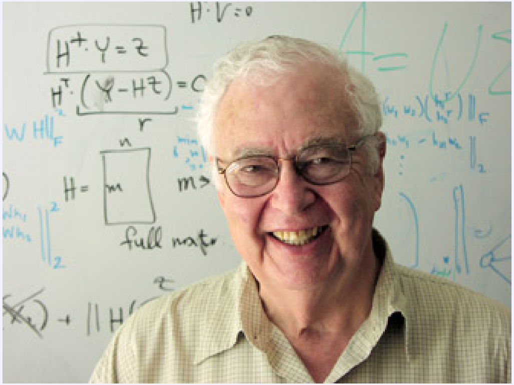


George Dantzig



Gene Golub

SOL

- Founded 1974 by George Dantzig and Richard Cottle
- Dantzig, Alan Manne: economic models (linear & nonlinear)
- Gill, Murray, Saunders, Wright: Software for optimization

SOL

Recent collaborators:

- Chris Paige (McGill), Sou-Cheng Choi (Chicago) — MINRES-QLP
- David Fong (ICME and Facebook) — LSMR
- Xiangrui Meng (ICME and LinkedIn) — LSRN
- Jason Lee, Yuekai Sun (ICME) — PNOPT
- Ding Ma, Nick Henderson, Santiago Akle (ICME) — LUSOL, PDCO

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- Ding Ma, Nick Henderson, Santiago Akle (ICME) — LUSOL, PDCO
- Philip Gill, Elizabeth Wong (UC San Diego)
  Optimization software — NPSOL, QPOPT, SQOPT, SNOPT, SQIC
- Ronan Fleming, Ines Thiele (UCSD, Iceland, Luxembourg)
  Flux balance analysis (FBA), Flux variability analysis (FVA)
  Rank and nullspace of stoichiometric matrices
  (Need LUSOL, PDCO, SQOPT)

Funding: ONR, AFOSR, ARO, DOE, NSF, AHPCRC, . . . ,
DOE DE-FG02-09ER25917, NIH U01-GM102098

Sparse linear equations $Ax = b$ and least squares problems $Ax \approx b$

Sparse direct methods for $Ax = b$ and $Ax \approx b$

- $A = LDU$ — LUSOL (Stanford)
- $A = QR$ — SPQR (Tim Davis, UFL)
- Many sparse solvers — HSL Library (RAL, UK)
  Iain Duff, John Reid, Jennifer Scott, . . .

LUSOL, SPQR, MA27, MA47, MA57, MA67, MA77, . . .
offer rank-revealing capability for sparse matrices
when used with suitable tolerances

Iterative solvers for $Ax \approx b$

Iterative methods for $Ax \approx b$

A may be a sparse matrix
or an operator for computing Av and/or $A^T w$

A maybe Hermitian or complex
A may have any rank

- Symmetric $Ax = b$ — $A =$ □ — MINRES-QLP
- $\min \|Ax - b\|$ — $A =$ ▭ or □ or ▯ — LSQR, LSMR
- Tall skinny $\min \|Ax - b\|$ — $A =$ ▯ (real) — LSRN

LSQR, LSMR for $\min \|Ax - b\|$

Golub-Kahan process generates $U_k = \begin{bmatrix} u_1 & u_2 & \dots & u_k \end{bmatrix}$

$V_k = \begin{bmatrix} v_1 & v_2 & \dots & v_k \end{bmatrix}$

using products Av_j, $A^T u_j$

kth approximation $x_k = V_k y_k$ for some y_k

Choose y_k to minimize something

LSQR, LSMR for $\min \|Ax - b\|$

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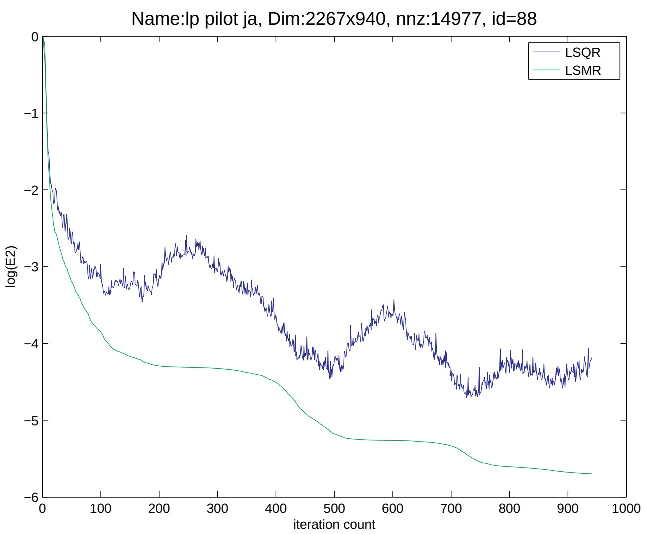
Choose y_k to minimize something

LSQR	$\min \|r_k\|$	residual $r_k = b - Ax_k$
LSMR	$\min \|A^T r_k\|$	residual for $A^T Ax = A^T b$

For LS problems, LSQR, LSMR stop when $\frac{\|A^T r_k\|}{\|r_k\|} \le \alpha \|A\|$
(this is the Stewart backward error)

$\log_{10} \frac{\|A^T r_k\|}{\|r_k\|}$ (typical) LSMR can stop sooner



CG, MINRES for posdef $Ax = b$

Lanczos process generates	$V_k = \begin{bmatrix} v_1 & v_2 & \dots & v_k \end{bmatrix}$ using products Av_j
kth approximation	$x_k = V_k y_k$ for some y_k

Choose y_k to minimize something

CG, MINRES for posdef $Ax = b$

Lanczos process generates $V_k = \begin{bmatrix} v_1 & v_2 & \dots & v_k \end{bmatrix}$ using products Av_j

kth approximation $x_k = V_k y_k$ for some y_k

Choose y_k to minimize something

CG	$\min \|x - x_k\|_A$	energy norm of error
MINRES	$\min \|r_k\|$	

They stop when $\dfrac{\|r_k\|}{\alpha\,\|A\|\,\|x_k\| + \beta\,\|b\|} \le 1$ (backward error argument)

CG, MINRES for posdef $Ax = b$

Lanczos process generates	$V_k = \begin{bmatrix} v_1 & v_2 & \dots & v_k \end{bmatrix}$ using products Av_j
kth approximation	$x_k = V_k y_k$ for some y_k

Choose y_k to minimize something

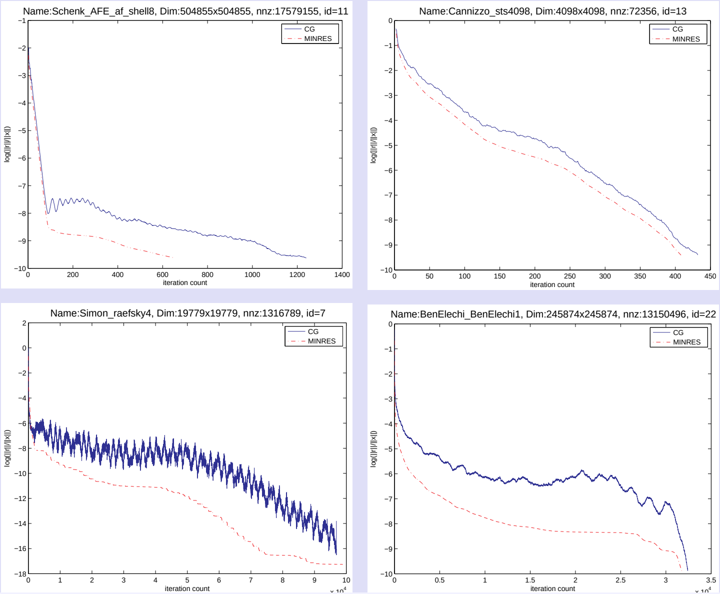
CG	$\min \|x - x_k\|_A$	energy norm of error
MINRES	$\min \|r_k\|$	

They stop when $\dfrac{\|r_k\|}{\alpha \|A\| \, \|x_k\| + \beta \, \|b\|} \le 1$ (backward error argument)

For posdef A, $\|x_k\| \nearrow$ for *both* methods (Steihaug 1983, Fong 2011)

Hence, backward error $\searrow$ for MINRES (but not for CG)

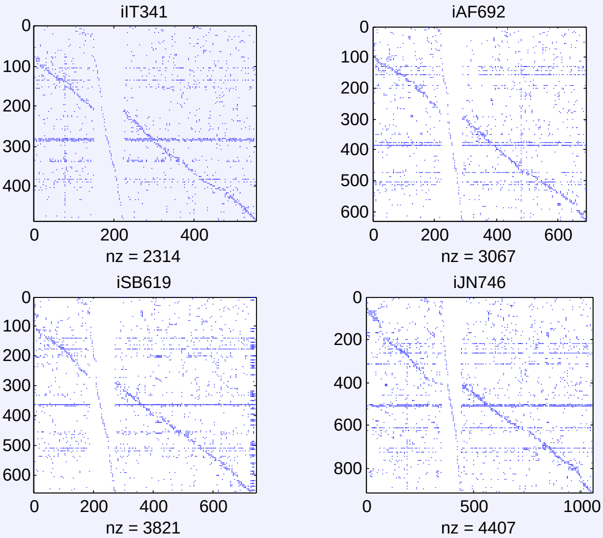
$\log_{10} \|r_k\|/\|x_k\|$ for $A \succ 0$ MINRES can stop sooner



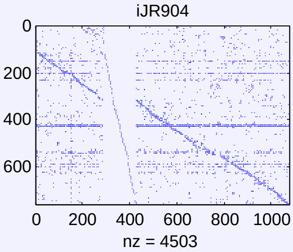
Stoichiometric matrices in systems biology

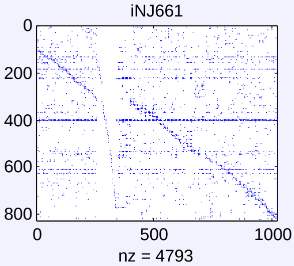
Sparse matrices S
Rows: Chemical species
Cols: Chemical reactions

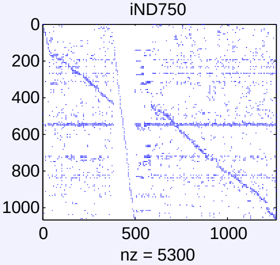
S for models 1, 2, 3, 4 (all similar)

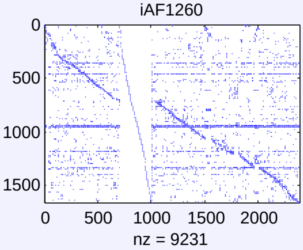


S for Models 5, 6, 7, 8 (all similar)

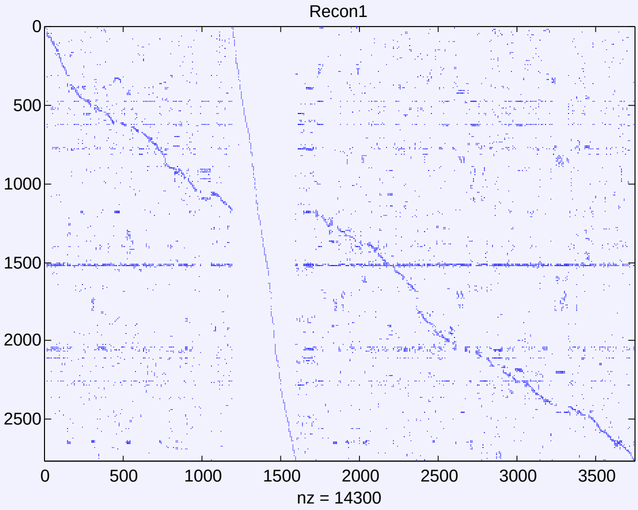




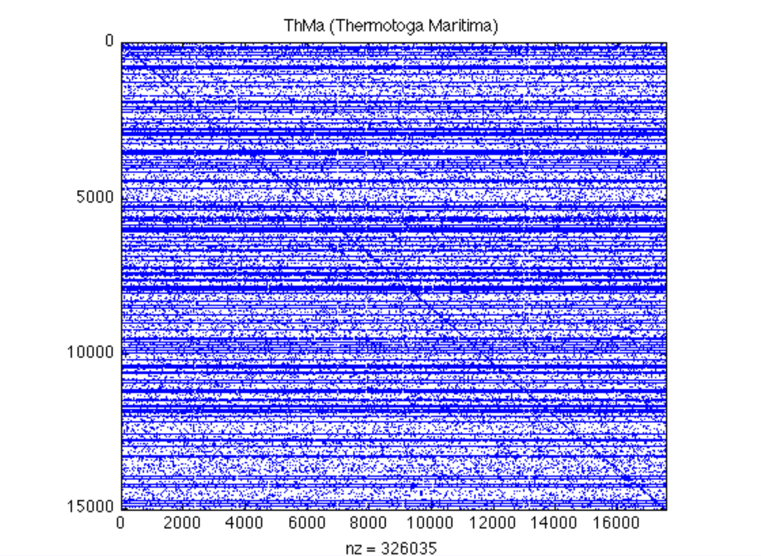




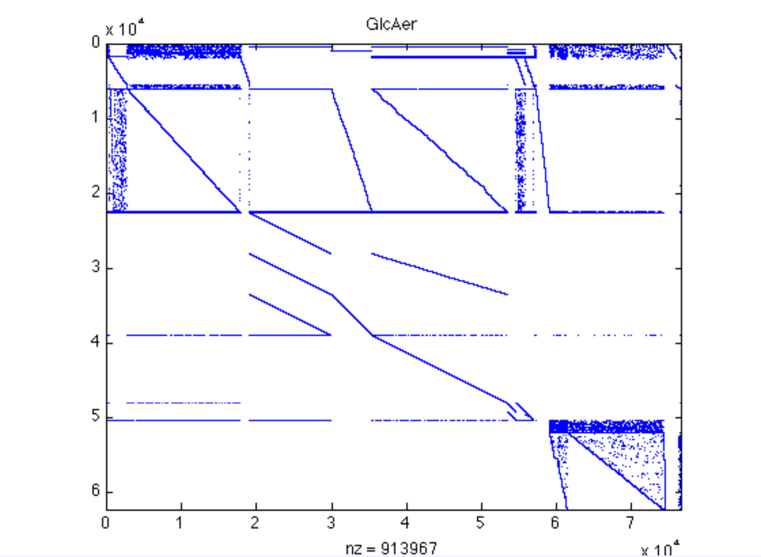
Model 9 (Recon1)



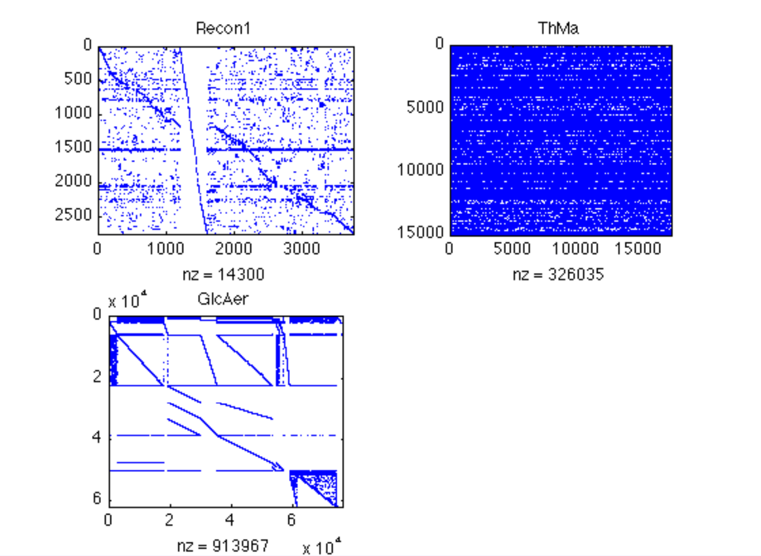
Model 10 (ThMa = Thermotoga maritima)



Model 11 (GlcAer)



S for models 9, 10, 11



Rank of stoichiometric matrices

Conservation analysis for biochemical networks

Need rank(S) and nullspace(S^T)

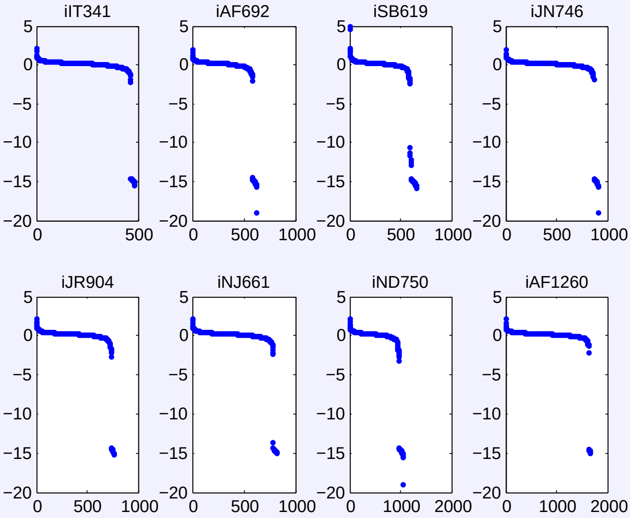
rank(S) by SVD

Singular value decomposition $\quad S = UDV^T$

- $U^TU = I \quad V^TV = I \quad D$ diagonal $\quad \text{rank}(S) = \text{rank}(D)$
- Ideal for rank-estimation but U, V are dense
- model 9 (Recon1) $\quad 2800 \times 3700 \quad$ 17 secs
  model 10 (ThMa) $\quad 15000 \times 18000 \quad$ 11 hours
  model 11 (GlcAer) $\quad 62000 \times 77000 \quad \infty$

Singular values of models 1–8 Dense SVD of S^T

$\log_{10}(\sigma_i)$



rank(S) by QR

Householder QR factorization $\quad SP = QR$

- $P =$ col perm $\quad Q^T Q = I \quad R$ triangular $\quad \text{rank}(S) = \text{rank}(R)$
- Nearly as reliable as SVD
- Dense QR used by Vallabhajosyula, Chickarmane, Sauro (2005)
- Sparse QR (SPQR) now available: Davis (2013)
- model 9 (Recon1) 2800 × 3700 0.1 secs
  model 10 (ThMa) 15000 × 18000 2.5 secs
  model 11 (GlcAer) 62000 × 77000 0.2 secs(!)

rank(S) by LUSOL with Threshold Rook Pivoting

Sparse LU with TRP $\quad P_1 S P_2 = LDU$

- $P_1, P_2 =$ perms $\quad D$ diagonal $\quad \text{rank}(S) \approx \text{rank}(D)$
  L, U well-conditioned
- $L_{ii} = U_{ii} = 1$
  $|L_{ij}|$ **and** $|U_{ij}| \le \texttt{factol} = 4$ (or 2 or 1.2, 1.1, ...)
- LUSOL: Main engine in sparse linear/nonlinear optimizers MINOS, SQOPT, SNOPT
- model 9 (Recon1) 2800×3700 0.1 secs
  model 10 (ThMa) 15000×18000 4.0 secs
  model 11 (GlcAer) 62000×77000 158 secs

rank(S) by LUSOL with Threshold Partial Pivoting

Sparse LU with TPP $\quad P_1 S P_2 = LU$

- $P_1, P_2 =$ perms $\quad$ U trapezoidal $\quad$ $\text{rank}(S) \approx \text{rank}(U)$
  L well-conditioned
- $L_{ii} = 1$
  $|L_{ij}| \le \texttt{factol} = 4$ (or 2 or 1.2, 1.1, ...)
- LUSOL: Main engine in sparse linear/nonlinear optimizers MINOS, SQOPT, SNOPT
- model 9 (Recon1) $\quad 2800 \times 3700 \quad$ 0.1 secs
  model 10 (ThMa) $\quad 15000 \times 18000 \quad$ 0.2 secs
  model 11 (GlcAer) $\quad 62000 \times 77000 \quad$ 0.3 secs

SPQR vs LUSOL with Threshold Rook Pivoting

SPQR: $S = QR$

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

LUSOL: $S = LDU \qquad |L_{ij}|, |U_{ij}| \leq 2.0$

model	nnz(L)	nnz(U)	time
Recon1	4280	16463	0.1
ThMa	30962	346122	4.1
GlcAer	635571	1810491	186.2

LUSOL: $S = LDU \qquad |L_{ij}|, |U_{ij}| \leq 4.0$

model	nnz(L)	nnz(U)	time
Recon1	2701	12896	0.1
ThMa	36350	330485	4.0
GlcAer	427456	1584188	157.9

SPQR vs LUSOL with Threshold Rook Pivoting

SPQR: $S^T = QR$

model	m	n	rank(S')	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	3742	2766	2674	14300	107935	36929	17.2	0.1
ThMa	17582	15024	14983	326035	624640	605888	11hrs	0.7
GlcAer	76664	62212	62182	913967	3573696	4038988	infty	2.7

LUSOL: $S^T = LDU \qquad |L_{ij}|, |U_{ij}| \leq 2.0$

model	nnz(L)	nnz(U)	time
Recon1	12832	7421	0.3
ThMa	501198	358601	37.8
GlcAer	1996892	709448	586.0

LUSOL: $S^T = LDU \qquad |L_{ij}|, |U_{ij}| \leq 4.0$

model	nnz(L)	nnz(U)	time
Recon1	9811	6093	0.2
ThMa	410290	355475	14.8
GlcAer	1823067	711906	791.2

SPQR vs LUSOL with Threshold Partial Pivoting

SPQR: $S = QR$

model	m	n	rank(S)	nnz(S)	nnz(Q)	nnz(R)	SVD time (secs)	SPQR time (secs)
Recon1	2766	3742	2674	14300	2750	21093	17.5	0.1
ThMa	15024	17582	14983	326035	844096	10595016	11hrs	2.5
GlcAer	62212	76664	62182	913967	1287	916600	infty	0.2

LUSOL: $S = LU \qquad |L_{ij}|, |U_{ij}| \leq 2.0$

model	nnz(L)	nnz(U)	time
Recon1	721	13585	0.1
ThMa	7779	324483	0.2
GlcAer	533	913781	0.4

LUSOL: $S = LU \qquad |L_{ij}|, |U_{ij}| \leq 4.0$

model	nnz(L)	nnz(U)	time
Recon1	764	13577	0.1
ThMa	7782	323929	0.2
GlcAer	533	913781	0.4

SPQR vs LUSOL with Threshold Partial Pivoting

SPQR: $S^T = QR$

model	m	n	rank(S')	nnz(S)	nnz(Q)	nnz(R)	time (secs) SVD	time (secs) SPQR
Recon1	3742	2766	2674	14300	107935	36929	17.2	0.1
ThMa	17582	15024	14983	326035	624640	605888	11hrs	0.7
GlcAer	76664	62212	62182	913967	3573696	4038988	infty	2.7

LUSOL: $S^T = LU \qquad |L_{ij}| \le 2.0$

model	nnz(L)	nnz(U)	time
Recon1	9304	7813	0.2
ThMa	81506	268938	2.7
GlcAer	337433	703619	126.7

LUSOL: $S^T = LU \qquad |L_{ij}| \le 4.0$

model	nnz(L)	nnz(U)	time
Recon1	9030	6259	0.1
ThMa	77274	268424	2.0
GlcAer	316889	701139	176.5

Rank of stoichiometric S

Perhaps

Sparse LU with TPP	$P_1 S P_2 = LU$

L well-conditioned $\mathrm{rank}(S) \approx \mathrm{rank}(U)$

Then

Sparse LU with TRP	$\bar{P}_1 U \bar{P}_2 = \bar{L}\bar{D}\bar{U}$

$\bar{L}$, $\bar{U}$ well-conditioned $\mathrm{rank}(S) \approx \mathrm{rank}(U) \approx \mathrm{rank}(\bar{D})$

Rank of stoichiometric S

Perhaps

Sparse LU with TPP	$P_1 S P_2 = LU$

L well-conditioned $\qquad \text{rank}(S) \approx \text{rank}(U)$

Then

Sparse LU with TRP	$\bar{P}_1 U \bar{P}_2 = \bar{L}\bar{D}\bar{U}$

$\bar{L}$, $\bar{U}$ well-conditioned $\qquad \text{rank}(S) \approx \text{rank}(U) \approx \text{rank}(\bar{D})$

or

Sparse LU with TPP	$\bar{P}_1 U^T \bar{P}_2 = \bar{L}\bar{U}$

$\bar{L}$ well-conditioned $\qquad \text{rank}(S) \approx \text{rank}(U) \approx \text{rank}(\bar{U})$

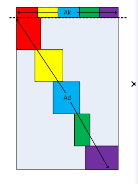
LSQR

in parallel!

LSQR for tomography

Huang, Dennis, Wang, Chen 2013
A scalable parallel LSQR algorithm for solving large-scale linear system for tomographic problems: a case study in seismic tomography
Procedia Computer Science 18:581–590

$$\min \|Ax - b\| \qquad A = $$



261M × 38M
5 billion nonzeros

- 3D stuctural seismology
- Modest-sized dataset from Los Angeles Basin (ANGF)
- Cray XT5 (Kraken) at Oak Ridge National Lab
- Parallelize $y \leftarrow Ax + y$ and $x \leftarrow A^T y + x$
- 2400 cores: 10 times faster than PETSc
- 19200 cores: 33 times faster than PETSc

SOL optimization solvers

Optimization solvers (dense)

- LSSOL (f77): $\min \|Xx - b\|^2$ st $\ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$

  Avoids forming X^TX
  We still don't have a good method for sparse X + constraints

- QPOPT (f77): $\min \frac{1}{2}x^THx$ st $\ell \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$

  H may be indefinite

- NPSOL (f77): $\min \phi(x)$ st $\ell \le \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \le u$

  Philip Gill has recently completed a new NPSOL that includes elastic bounds to handle infeasible QP subproblems (like SQOPT and SNOPT)

Optimization solvers (sparse)

- MINOS (f77): Sparse NLP
  No elastic bounds, but still widely used. f90 version half started.
- SQOPT, SNOPT (f77): Sparse convex QP + general NLP
  Elastic bounds, threadsafe, good for expensive functions
- SNOPT9 (f2003): Gill, S, Wong
  Includes SQIC QP solver
  Switches from SQOPT's reduced-gradient method to KKT-factorization + block-LU updates for problems with many degrees of freedom
- Change 1 line and recompile ⇒ everything in quad precision
  SNOPT9's simplex implementation gives us solutions with astounding accuracy! Great for systems biologists!

NEOS

Free optimization solvers
via Argonne National Lab
(now Univ of Madison, Wisconsin)

NEOS Solver Statistics for 1 year 1 Oct 2012 -- 30 Sep 2013

Total Jobs 1264001

Solver Submissions

MINOS	642263	BDMLP	3747	OOQP	771	sd	33
KNITRO	256367	Couenne	3588	SYMPHONY	692	cplex	29
Gurobi	70179	FilMINT	3424	PATHNLP	666	BiqMac	10
Ipopt	35181	BLMVM	3410	DSDP	627	LGO	3
SNOPT	33197	NMTR	2735	condor	601	lpopt	2
csdp	20142	feaspump	2607	sedumi	585	BDLMP	1
DICOPT	19146	AlphaECP	2538	PSwarm	584		
XpressMP	17761	bpmpd	2317	RELAX4	568		
BARON	14737	PATH	2036	Clp	503		
Cbc	14613	LANCELOT	1972	FortMP	432		
MINTO	13515	MILES	1641	sdplr	415		
scip	12986	sdpt3	1436	Glpk	336		
MOSEK	10837	LRAMBO	1415	ddsip	335		
CONOPT	9871	filterMPEC	1289	nsips	300		
LOQO	9598	SDPA	1244	icos	249		
Bonmin	7320	TRON	1145	bnbs	244		
MINLP	6573	SBB	1085	pensdp	234		
filter	5438	NLPEC	1053	penbmi	226		
concorde	4879	L-BFGS-B	999	PGAPack	216		
LINDOGlobal	4597	qsopt_ex	902	proxy	127		
MUSCOD-II	4425	ASA	858	xpress	36		

NEOS Solver Statistics for 1 year 1 Oct 2012 -- 30 Sep 2013

Total Jobs 1264001

Category	Submissions
nco	982242
milp	100864
minco	57532
lp	42205
sdp	24909
go	17955
cp	12591
bco	5547
co	4889
miocp	4425
kestrel	3981
uco	2735
lno	2407
slp	612
ndo	601
sio	300
socp	75
mip	8
nlp	3
DNLP	2

Input	Submissions
AMPL	1053956
GAMS	152810
SPARSE_SDPA	22083
MPS	10136
TSP	4879
C	4513
Fortran	4114
CPLEX	3723
MOSEL	2182
MATLAB_BINARY	1802
LP	903
ZIMPL	709
SDPA	627
DIMACS	564
SMPS	277
MATLAB	199
SDPLR	198
QPS	164

DICOPT

MINLP solver
Ignacio Grossman, Carnegie-Mellon

MINLP model

- MS student Rui-Jie Zhou transferring from MS&E to EE, mentioned MINOS had been useful
- 2 papers in *Industrial Engineering and Chemistry Research*
  Zhou, Ji-Juan Li, Hong-Guang Dong, Ignacio Grossmann
- Part I (44 pages) Multiscale state-space superstructure for interplant water-allocation and heat-exchange networks design with direct and indirect integration schemes in fixed flow rate (FF) processes
- Part II (42 pages) Extends to fixed contaminant-load (FC) processes and integration of FF and FC processes
- Nonlinear objective
  1500 linear and nonlinear constraints
  1600 variables (some binary)
  GAMS/DICOPT = MINOS + CPLEX or CONOPT + CPLEX

MINLP model

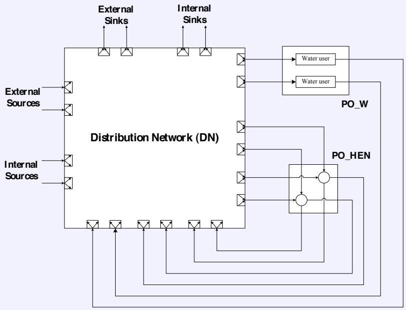


Figure 1. State-space superstructure for stand-alone WAHEN

MINLP model

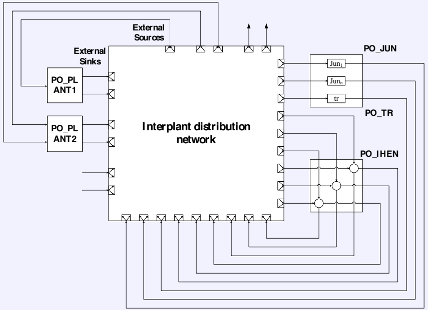


Figure 2. Multi-scale state-space superstructure for interplant WAHEN

MINLP model

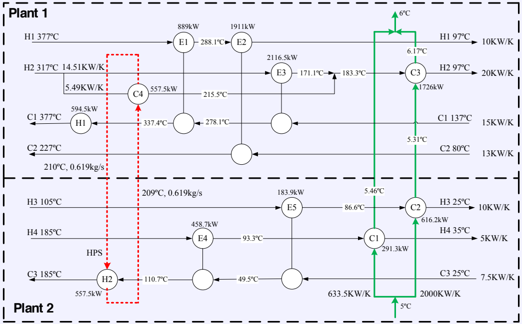


Figure 3. Optimal interplant HEN configuration in Example 1

MINLP model

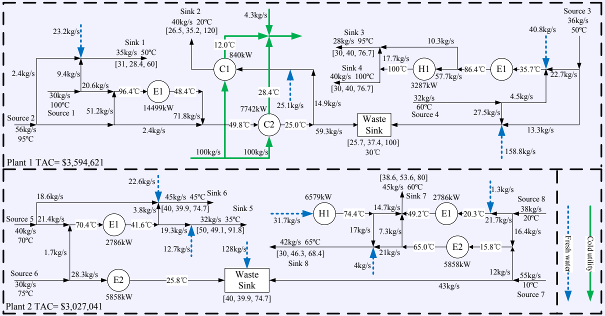


Figure 4. Optimal stand-alone WAHEN designs in Case 1 of Example 2

MINLP model

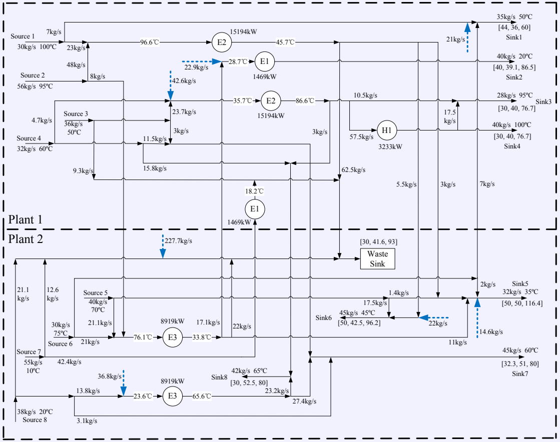
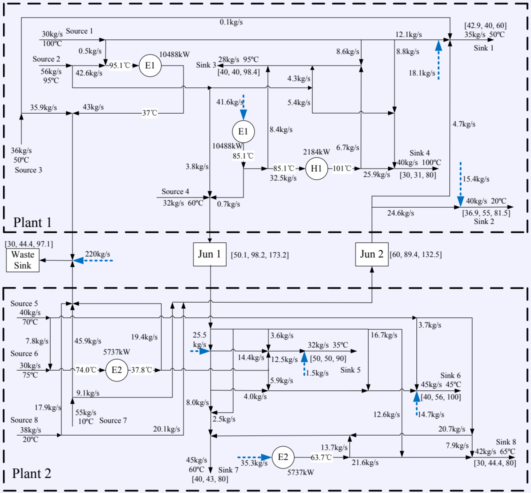


Figure 5. Optimal direct integrated WAHEN design in Case 2 of Example 2

MINLP model


Plant 1
Plant 2
Source 1
Source 2
Source 3
Source 4
Source 5
Source 6
Source 7
Source 8
Sink 1
Sink 2
Sink 3
Sink 4
Sink 5
Sink 6
Sink 7
Sink 8
Waste Sink
Jun 1
Jun 2
E1
E2
H1
10488kW
5737kW
2184kW
220kg/s
[30, 44.4, 97.1]
[50.1, 98.2, 173.2]
[60, 89.4, 132.5]

MINLP model

Lower total annualized cost can be obtained in all examples by solving the corresponding MINLP model

PDCO

Primal-dual interior method for convex optimization

PDCO (Matlab primal-dual convex optimizer)

Nominally

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \phi(x) \\ \text{subject to} & Ax = b, \quad \ell \le x \le u \end{array}$$

$\phi(x)$ is convex with known gradient and Hessian

For example, $\phi(x) = c^T x \quad$ or $\quad \lambda \|x\|_1 \quad$ or $\quad \sum x_j log(x_j)$

A may be a sparse matrix or an operator for Av and $A^T w$

Basis Pursuit (BP)
Basis Pursuit denoising (BPDN) Chen, Donoho, & S (2001)

PDCO (Matlab primal-dual convex optimizer)

To ensure unique solutions, PDCO solves regularized problems:

$$\begin{array}{ll} \underset{x,\,r}{\text{minimize}} & \phi(x) + \frac{1}{2}\|D_1 x\|^2 + \frac{1}{2}\|r\|^2 \\ \text{subject to} & Ax + D_2 r = b, \quad \ell \le x \le u \end{array}$$

where D_1, D_2 are diagonal and positive-definite

- $D_1 = \gamma I$ $\quad\gamma = 10^{-3}$ or 10^{-4}
- $D_2 = \delta I$ for linear programs $\quad\delta = 10^{-3}$ or 10^{-4}
- $D_2 = I$ for least squares
- Jacek prefers D_1, D_2 semi-definite and dynamic!

PDCO for LP feasibility

Regularized least squares with bounds:

$$\begin{array}{ll} \underset{x,\,r}{\text{minimize}} & \frac{1}{2}\|\gamma x\|^2 + \frac{1}{2}\|r\|^2 \\ \text{subject to} & Ax + r = b, \quad \ell \le x \le u \end{array}$$

$\gamma = 10^{-4}$ declare feasible if $\|r\|_\infty \le 10^{-4}$ say

PDCO for LP feasibility

Regularized least squares with bounds:

$$\begin{array}{ll} \underset{x,\,r}{\text{minimize}} & \frac{1}{2}\|\gamma x\|^2 + \frac{1}{2}\|r\|^2 \\ \text{subject to} & Ax + r = b, \quad \ell \le x \le u \end{array}$$

$\gamma = 10^{-4}$ declare feasible if $\|r\|_\infty \le 10^{-4}$ say

Jon Dattorro (2010)

- $10{,}000 \times 200{,}000$ 1.1M nonzeros
  Solve 200,000 times with different b
- Gurobi: average 2 mins
  PDCO (Matlab): average 1 min

PDCO applied to FBA

Flux Balance Analysis = LP problem (Palsson 2006)

FBA

$$\begin{aligned} \underset{v_f, v_r, v_e}{\text{minimize}} \quad & d^T v_e \\ \text{subject to} \quad & S v_f - S v_r + S_e v_e = 0 \\ & v_f, v_r \geq 0, \qquad \ell \leq v_e \leq u \end{aligned}$$

- d optimizes a biological objective
  e.g., maximize replication rate in unicellular organisms
- v_e = exchange fluxes = sources and sinks of chemicals
- PDCO works with $A = \begin{bmatrix} S & -S & S_e \end{bmatrix}$ then $LL^T = AD^2A^T$
  (sparse Cholesky with D increasingly ill-conditioned)
- Solution is $v^* = v_f^* - v_r^*$ and v_e^*

PDCO applied to Entropy problem

$$\text{EP} \qquad \underset{v_f, v_r}{\text{minimize}} \quad v_f^T(\log v_f + c - e) + v_r^T(\log v_r + c - e)$$
$$\text{subject to} \quad Sv_f - Sv_r = -S_e v_e^*$$
$$v_f, v_r > 0$$

- $c =$ any vector, $e = (1, 1, \ldots, 1)^T$
  $v_e^* =$ optimal exchange fluxes from FBA
- Entropy objective function is strictly convex
- Solution v_f^*, v_r^* is thermodynamically feasible
  (satisfies energy conservation and 2nd law of thermodynamics)

Fleming, Maes, S, Ye, Palsson (2012)

PDCO applied to LR-NMR problems

Laplace Inversion of Low-Resolution NMR Relaxometry Data

Biotech and Environmental Engineering, Ben Gurion Univ, Israel

Determine composition of olive oil, rapeseed oil, biodiesel, . . .

$$s(t) \approx \int_0^\infty e^{-t/T_2}\, x(T_2)\, dT_2 \qquad x = \text{probability density}$$

Standard method (discretize):

$$\min_{x \ge 0} \left\| \begin{pmatrix} A \\ \lambda I \end{pmatrix} x - \begin{pmatrix} s \\ 0 \end{pmatrix} \right\|_2^2$$

- A = discrete Laplace transform (fast operator)
- λ = Tikhonov regularization
- Could apply PDCO to handle $x \ge 0$
- Distorts solution by broadening peaks

PDCO applied to LR-NMR problems

Laplace inversion via basis pursuit denoising:

$$\text{BPDN} \qquad \begin{array}{ll} \underset{x,\,r}{\text{minimize}} & \alpha\,\|x\|_1 + \tfrac{1}{2}\,\|\lambda x\|_2^2 + \tfrac{1}{2}\,\|r\|_2^2 \\ \text{subject to} & Ax + r = s \quad : \; y \\ & x \geq 0 \end{array}$$

- A = discrete Laplace transform (fast operator)
- PDCO solves $\min \left\| \begin{pmatrix} DA^T \\ I \end{pmatrix} \Delta y - \begin{pmatrix} Dw \\ t \end{pmatrix} \right\|$ using LSMR, where posdef diagonal D becomes increasingly ill-conditioned
- α helps resolve close adjacent peaks

$\alpha = 0$

$\alpha > 0$

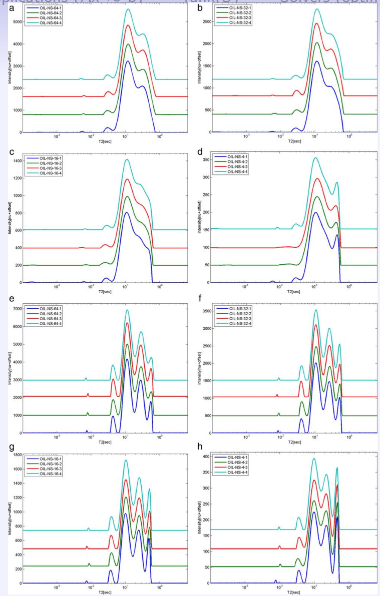


Figure 6 Comparison of WinDXP (a)–(d) and PDCO using the universal regularization values for α_1 and α_2 (e)–(h) solutions on a real LR-NMR dataset acquired from an oil sample. The results are ordered by descending number of scans (descending SNR).

PDCO applied to LR-NMR problems

- Berman, Leshem, Etziony, Levi, Parmet, S, Wiesman 2013
  Novel ^1H low field nuclear magnetic resonance applications for the field of biodiesel
  Biotechnology for Biofuels 6:55, 20pp
- Berman, Levi, Parmet, S, Wiesman 2013
  Laplace inversion of low-resolution NMR relaxometry data using sparse representation methods
  Concepts in Magnetic Resonance Part A 42A:3, 72–88

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Problem setup (normal numerical people):

```
[U,S,V] = svd(A);
```

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Problem setup (normal numerical people):

```
[U,S,V] = svd(A);
```

Astounding line of code (one coauthor):

```
[S,V,D] = svd(A);          (!)
```

SQOPT in quad precision

Flux Balance Analysis (FBA) on Thermotoga maritima

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \le v \le u$$

S rows and cols	18210×17535
Nonzero S_{ij}	33602
max and min $\|S_{ij}\|$	2×10^4 and 3×10^{-6}

SQOPT in double precision (15 digits)

```
Feasibility tol       1e-6
Optimality  tol       1e-6
```

SQOPT in quad precision (32 digits)

```
Feasibility tol       1e-15
Optimality  tol       1e-15
```

Flux Balance Analysis (FBA) on Thermotoga maritima

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \le v \le u$$

S rows and cols	18210×17535
Nonzero S_{ij}	33602
max and min $\lvert S_{ij} \rvert$	2×10^4 and 3×10^{-6}

SQOPT in double precision (42 secs)

```
SQOPT  EXIT  10 -- the problem appears to be infeasible

Problem name                        ThMa
No. of iterations                  18500   Objective value      8.2286249495E-07
No. of infeasibilities                 9   Sum of infeas        1.9606461069E-03
No. of degenerate steps            11611   Percentage                      62.76
Max x       (scaled)        3482 8.2E+00   Max pi      (scaled)    18210 9.8E-01
Max x                       5134 5.9E+00   Max pi                  18210 1.0E+00
Max Prim inf(scaled)       32832 1.3E-03   Max Dual inf(scaled)    16417 1.0E+00
Max Primal infeas          32832 5.6E-06   Max Dual infeas         32669 2.3E+02
```

Flux Balance Analysis (FBA) on Thermotoga maritima

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \le v \le u$$

S rows and cols	18210×17535
Nonzero S_{ij}	33602
max and min $\lvert S_{ij} \rvert$	2×10^4 and 3×10^{-6}

Restart SQOPT in quad precision (36 secs)

```
SQOPT  EXIT   0 -- finished successfully

Problem name                        ThMa
No. of iterations                    498   Objective value      8.7036461686E-07
No. of infeasibilities                 0   Sum of infeas        0.0000000000E+00
No. of degenerate steps              220   Percentage                      44.18
Max x       (scaled)        3482 8.2E+00   Max pi      (scaled)      2907 1.3E+00
Max x                       5134 5.9E+00   Max pi                   15517 1.1E+00
Max Prim inf(scaled)       16475 5.2E-28   Max Dual inf(scaled)     13244 1.9E-32
Max Primal infeas          16475 5.2E-29   Max Dual infeas          13244 4.8E-33
```

Flux Balance Analysis (FBA) on GlcAer

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \le v \le u$$

S rows and cols	68300×76664
Nonzero S_{ij}	926357
max and min $\lvert S_{ij} \rvert$	8×10^5 and 5×10^{-5}

SQOPT in quad precision — cold start, no scaling (30786 secs)

```
SQOPT  EXIT   0 -- finished successfully

Problem name                     GlcAer
No. of iterations                 84685   Objective value      -7.0382454070E+05
No. of degenerate steps           62127   Percentage                       73.36
Max x                     61436 6.3E+07   Max pi                   25539 2.4E+07
Max Primal infeas         72623 3.0E-21   Max Dual infeas          17817 2.7E-21
```

Flux Balance Analysis (FBA) on GlcAer

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \le v \le u$$

S rows and cols	68300×76664
Nonzero S_{ij}	926357
max and min $\lvert S_{ij} \rvert$	8×10^5 and 5×10^{-5}

SQOPT in quad precision — cold start, with scaling (4642 secs)

```
SQOPT  EXIT   0 -- finished successfully

Problem name                    GlcAer
No. of iterations                37025   Objective value      -7.0382454070E+05
No. of degenerate steps          28166   Percentage                       76.07
Max x        (scaled)      59440 3.7E+00   Max pi       (scaled)      40165 8.1E+11
Max x                      61436 6.3E+07   Max pi                     25539 2.4E+07
Max Prim inf(scaled)       81918 7.0E-16   Max Dual inf(scaled)       59325 1.5E-17
Max Primal infeas          81918 1.3E-07   Max Dual infeas            27953 2.0E-22
```

Flux Balance Analysis (FBA) on GlcAer

$$\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \leq v \leq u$$

S rows and cols	68300×76664
Nonzero S_{ij}	926357
max and min $\lvert S_{ij} \rvert$	8×10^5 and 5×10^{-5}

SQOPT in quad precision — warm start, no scaling (28 secs)

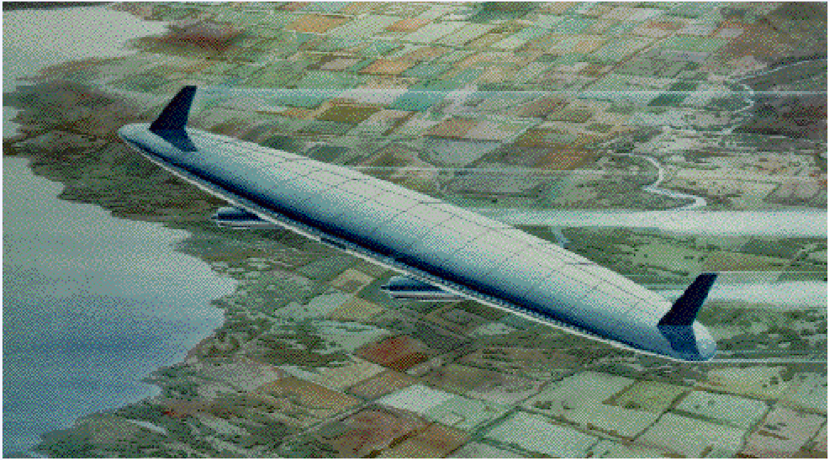
```
SQOPT  EXIT   0 -- finished successfully

Problem name                   GlcAer
No. of iterations                   1   Objective value     -7.0382454070E+05
No. of degenerate steps             0   Percentage                       0.00
Max x                   61436 6.3E+07   Max pi                  25539 2.4E+07
Max Primal infeas      141186 7.1E-21   Max Dual infeas         14993 8.9E-23
```

Aerospace Applications

NASA Aerospace Applications

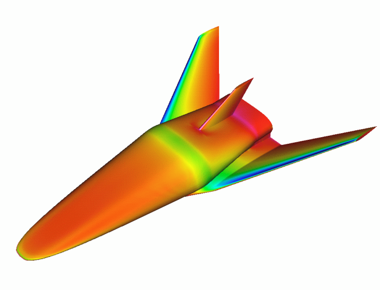
- David Saunders
  - 1970 Visit Stanford for 1 month (now 43 years)
  - 1973 Serra House, RA, MS (thanks to Gene)
  - 1974–present NASA Ames
- Projects
  - OAW Oblique All-Wing supersonic airliner
  - HSCT Supersonic airliner
  - CTV SHARP shuttle design
  - MSL Heat shield for landing Mars rover Curiosity
  - CEV Heat shield for Apollo-type capsule to ISS/moon

OAW oblique all wing airliner



HSCT high speed civil transport

CTV crew transfer vehicle



SHARP design (Slender Hypervelocity Aerothermodynamic Research Probes)

Aerothermal performance constraint in (Velocity, Altitude) space, used during trajectory optimization with UHTC materials (Ultra High Temperature Ceramics) to avoid exceeding material limits

- Trajectory optimization with SNOPT
- Could always abort to Kennedy, Boston, Gander, or Shannon
- 4000-mile cross-range capability during reentry

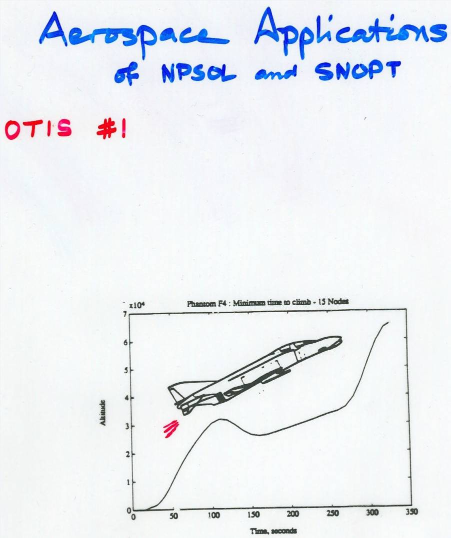
Image credit: David Kinney, NASA Ames Research Center

CEV crew exploration vehicle

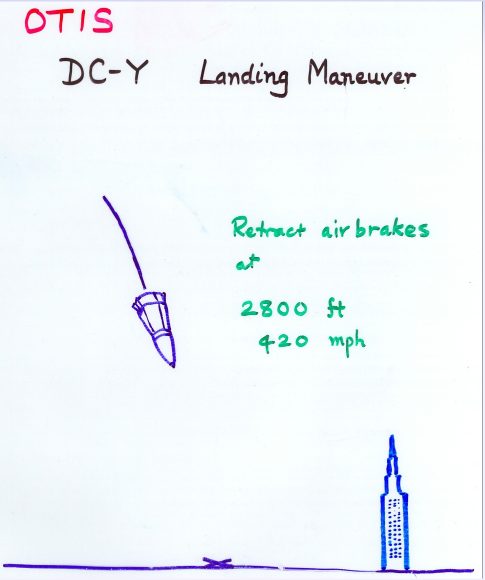
McDonnell-Douglas Aerospace Applications

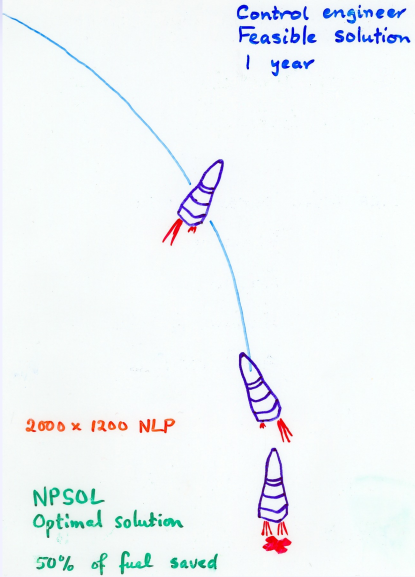
- Philip Gill, Rocky Nelson
  1979–1988 SOL QPSOL, LSSOL, NPSOL
  1988–2007 UC San Diego QPOPT, SQOPT, SNOPT
  McDonnell-Douglas Space Systems, LA (now Boeing)
- Projects
  F-4 Minimum time-to-climb
  DC-Y SSTO Minimum-fuel landing maneuver

F-4 minimum time-to-climb



DC-Y single-stage-to-orbit


OTIS
DC-Y Landing Maneuver
Retract air brakes
at
2800 ft
420 mph


Control engineer
Feasible solution
1 year
2000 x 1200 NLP
NPSOL
Optimal solution
50% of fuel saved

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
- 2nd optimization: starting altitude = variable
- New constraint needed:

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
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Optimum starting altitude = 1400ft(!)

DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
- 2nd optimization: starting altitude = variable
- New constraint needed: Don't exceed 3g

Optimum starting altitude = 1400ft(!)

Come back Alan Shephard!

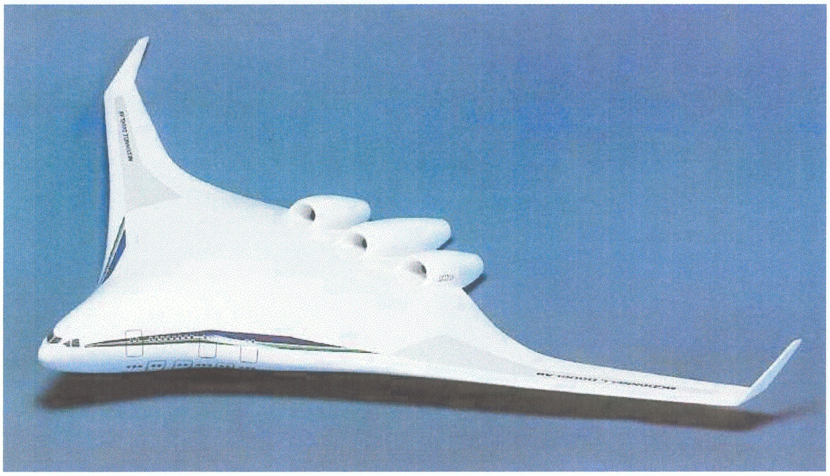
Stanford Aerospace Applications

- Ilan Kroo Stanford Aircraft Aerodynamics and Design Group
  Blended Wing-Body Transonic airliner

Stanford Aerospace Applications

- Ilan Kroo Stanford Aircraft Aerodynamics and Design Group
  Blended Wing-Body Transonic airliner
- Antony Jameson, Juan Alonso Aerospace Computing Lab
  MDO Multidisciplinary Design Optimization
  ASO Aerodynamic Shape Optimization

Blended wing airliner



Blended wing airliner

Ilan Kroo, Michael Holden, Aero/Astro Dept, Stanford 1999

- Compute control for stable flight of 17ft-span flying model
- Collocation model:
  minimize wing weight (or move CG as far aft as possible)
  subject to flutter constraints
- 9000 nonlinear equations
  9000 state variables, 7 design variables

MINOS 5.5:

26	major iterations
4000	minor iterations (first 3000 = LP)
1500	constraint + Jacobian evaluations
= 60000	function evaluations
3 days	on SGI Octane

News Flash, 3 March 2007

- Mike Ross Naval Postgraduate School, Monterey
  DIDO: A package for solving optimal control problems
  Implemented in MATLAB
  Calls TOMLAB/SNOPT for the optimization

- GMT 062:19:26
  The International Space Station was successfully maneuvered
  using DIDO/TOMLAB/SNOPT
  Found zero propellant solutions (globally optimal)
  Saved NASA $1M fuel cost

America's Cup Yacht Race

AC 95: NPSOL was used in different ways by both AC95 finalists

- For Team Dennis Conner, NPSOL was used with Boeing's TRANAIR CFD system for optimal hull design of Young America
- For Team NZ, Andy Philpott (University of Auckland) used NPSOL to maximize the velocity around the course of 11 potential hull designs. One design appeared significantly faster and was chosen to become Black Magic

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AC 2013 (San Francisco Bay): NZ Herald blog

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- (Score 8–5) Come on whale, where are you?

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AC 2013 (San Francisco Bay): NZ Herald blog

- (Score 8–5) Come on whale, where are you?
- (Score 8–6) Dratted whales, we can't trust them anymore
- I haven't had so much fun since the cat died
- ...
- (Score 8–9) In the immortal words, 'bugga'

Optimization in NZ

In New Zealand, the radio/TV guide is called *The Listener*.
Every week a Life in New Zealand column publishes clippings describing local events.
The first sender receives a $5 Lotto Lucky Dip. The following clippings illustrate some characteristics of optimization problems in the real(?) world.

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Every week a Life in New Zealand column publishes clippings describing local events.
The first sender receives a $5 Lotto Lucky Dip. The following clippings illustrate some characteristics of optimization problems in the real(?) world.

Robust solutions

RECOVERY CARE gives you financial protection from specified sudden illness.
You get cash if you live . . . and cash if you don't.

No objective function

People have been marrying and bringing up children for centuries now. Nothing has ever come of it. (Evening Post, 1977)

Multiple objectives

"I had the choice of running over my team-mate or going onto the grass, so I ran over my team-mate then ran onto the grass", Rymer recalled later.

Obvious objective

He said the fee was increased from $5 to $20 because some people had complained it was not worth writing a cheque for $5.

Equilibrium condition

"The pedestrian count was not considered high enough to justify an overbridge", Helen Ritchie said. "And if there continues to be people knocked down on the crossing, the number of pedestrians will dwindle."

Constraints

ENTERTAINERS, DANCE BAND, etc. Vocalist wanted for New Wave rock band, must be able to sing.

DRIVING INSTRUCTOR Part-time position. No experience necessary.

HOUSE FOR REMOVAL in excellent order, $800. Do not disturb tenant.

Exactly one feasible solution

MATTHEWS RESTAURANT, open 365 nights. Including Mondays.

Buying your own business might mean working 24 hours a day. But at least when you're self-employed you can decide which 24.

Peters: Oh, it's not that I don't want to be helpful. But in this case the answer is that I don't want to be helpful. (Listener, 1990)

Sergeant J Johnston said when Hall was stopped by a police patrol the defendant denied being the driver, but after it was pointed out he was the only person in the car he admitted to being the driver.

His companion was in fact a transvestite, X, known variously as X or X.

Bound your variables

By the way, have you ever seen a bird transported without the use of a cage? If you don't use a cage it will fly away and maybe the same could happen to your cat. Mark my words, we have seen it happen.

Redundant constraints

If you are decorating before the baby is born, keep in mind that you may have a boy or a girl.

EAR PIERCING while you wait

CONCURRENT TERM FOR BIGAMY

(NZ Herald, 1990)

Infeasible constraints

I chose to cook myself to be quite sure what was going into the meals.

We apologize to Wellington listeners who may not be receiving this broadcast.

The model 200 is British all the way from its stylish roofline to its French-made Michelin tyres. (NZ Car Magazine)

BALD, 36 yr old, handsome male seeking social times and fun with bald 22 years and upwards female Napier Courier, 28/2/02

$\geq$ or $\leq$?

BUY NOW! At $29.95 these jeans will not last long!

NOT TOO GOOD TO BE TRUE! We can sell your home for much less than you'd expect! (NZ Property Weekly)

The BA 146's landing at Hamilton airport was barely audible above airport background noise, which admittedly included a Boeing 737 idling in the foreground.

Yesterday Mr Palmer said "The Australian reports are not correct that I've seen, although I can't say that I've seen them".

It will be a chance for all women of this parish to get rid of anything that is not worth keeping but is too good to throw away. Don't forget to bring your husbands.

$\geq$ or $\leq$?

The French were often more blatant and more active, particularly prop X and number eight Y, but at least one
All Black was seen getting his retaliation in first.

WHAT EVERY TEENAGER SHOULD KNOW — PARENTS ONLY

"Love Under 17" Persons under 18 not admitted.

"Keeping young people in the dark would not stop them having sex—in fact it usually had the opposite effect," she said.

NELSON, approximately 5 minutes from airport. Golf course adjacent. Sleeps seven all in single beds. Ideal for honeymoons. (Air NZ News, 1978)

Hard or soft constraints

> The two have run their farm as equal partners for 10 years, with Jan in charge of grass management, Lindsay looking after fertilizer, and both working in the milk shed. "We used to have our staff meetings in bed. That got more difficult when we employed staff!" (NZ country paper)

Elastic constraints

The Stationary Engine Drivers Union is planning rolling stoppages.

When this happens there are set procedures to be followed and they are established procedures, provided they are followed.

APATHY RAMPANT? Not in Albany—the closing of the electoral rolls saw fully 103.49 percent of the area's eligible voters signed up.

Auckland City ratepayers are to be reminded that they can pay their rates after they die.

(Auckland Herald, 1990)

He was remanded in custody to appear again on Tuesday if he is still in the country.

Convergence

"There is a trend to open libraries when people can use them", he says.

Mayor for 15 years, Sir Dove-Myer wants a final three years at the helm "to restore sanity and stability in the affairs of the city".

Applications

(Yachting) It is not particularly dangerous, as it only causes vomiting, hot and cold flushes, diarrhoea, muscle cramping, paralysis, and sometimes death . . . (Boating New Zealand, 1990)

(Ecological models) CAR POLLUTION SOARS IN CHRISTCHURCH—BUT CAUSE REMAINS MYSTERY

Nappies wanted for window cleaning. Must be used.

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(Optimal control) Almost half the women seeking fertility investigations at the clinic knew what to do to get pregnant, but not when to do it.

Binary variables

0 or 1 Sometimes neither is optimal

Binary variables

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Integer variables

0 or 1 or 2 . . .

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Integer variables

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When Taupo police arrested a Bay of Plenty man
for driving over the limit,
they discovered he was a bigamist.

Nelson Mail, 5/04

Always room for improvement

The owner Craig Andrew said the three main qualities for the job were speed, agility and driving skills. "Actually, Merv has none of those, but he's still the best delivery boy we've had", he said.

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SCICME

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Final thoughts

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that we don't learn from history
– G. W. F. Hegel

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Special thanks!

Jacek Gondzio
Rachael Tappenden
EPSRC, Maxwell Institute