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# Large-scale Linear and Nonlinear Optimization in Quad Precision

Ding Ma and Michael Saunders MS&E and ICME, Stanford University

US-Mexico Workshop on Optimization and its Applications Mérida, Yucatán, Mexico, Jan 4–8, 2016

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quadMINOS

Mérida, Mexico, Jan 4-8, 2016

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# Coauthor Ding Ma at INFORMS 2014

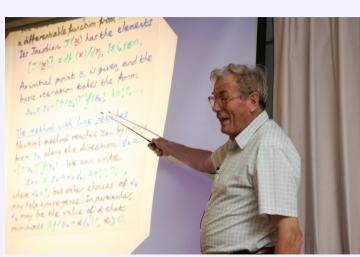




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# Roger Fletcher FRS and Mike Powell FRS





## Abstract

For challenging numerical problems, William Kahan has said that "default evaluation in Quad is the humane option" for avoiding severe unexpected error in floating-point computations. The IEEE 754-2008 standard includes Quad precision (about 34 significant digits) and is provided by some compilers as a software library. For example, gfortran provides a real(16) datatype. This is the humane option for producing Quad-precision software.

We describe experiments on multiscale linear and nonlinear optimization problems using Double and Quad implementations of MINOS. On a range of examples we find that Quad MINOS achieves exceptionally small primal and dual infeasibilities (of order 1e-30) when "only" 1e-15 is requested. The motivation has been large multiscale LP and NLP problems arising in systems biology (flux balance analysis models of metabolic networks). Standard solvers are not sufficiently accurate, and exact simplex solvers are extremely slow. Quad precision offers a reliable compromise.

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### 2 System and Methods

#### 3 DQQ procedure

- ORR procedure
- **(5)** 62 LPnetlib test problems

#### 6 Multiscale NLPs



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# **Motivation**

quadMINOS

# Multiscale LPs in systems biology

#### Normal approach for LP solvers (simplex or interior)

- Scale (to reduce large matrix values)
- Solve with Feasibility/Optimality tols = 1e-6 say
- Unscale

#### Difficulty

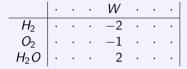
- Unscaling magnifies residuals
- Solution may be far from feasible or optimal

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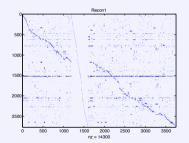
#### Conclusions

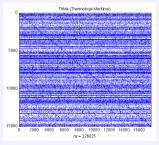
## Stoichiometric matrices S

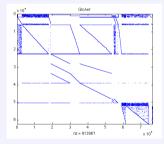
$$2H_2 + O_2 \rightarrow 2H_2C$$



#### $\mathsf{chemicals} \times \mathsf{reactions}$







 $62000\times77000$ 

#### $2800\times3700$

#### $15000\times18000$

#### quadMINOS

#### Mérida, Mexico, Jan 4–8, 2016

# Constraint Based Reconstruction and Analysis (COBRA)

A biochemical network (inherently multiscale) is represented by a stoichiometric matrix S with m rows corresponding to metabolites (chemicals) and n columns representing reactions. S is part of the ODE that governs the time-evolution of concentrations:

$$\frac{d}{dt}x(t) = Sv(t),\tag{1}$$

where  $x(t) \in \mathbf{R}^m$  is a vector of time-dependent concentrations and  $v(t) \in \mathbf{R}^n$  is a vector of reaction fluxes. The objective of maximizing growth rate at steady state leads to an LP:

$$\max_{\substack{v \\ s.t. \\ l \le v \le u,}} c^{T} v$$
(2a)  
(2b)  
(2c)

where growth is defined as the biosynthetic requirements of experimentally determined biomass composition, and biomass generation is a set of reaction fluxes linked in the appropriate ratios.

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ME models (FBA with coupling constraints)

Flux Balance Analysis (FBA) has been used by Ines Thiele (2012) for the first integrated stoichiometric multiscale model of Metabolism and macromolecular Expression (ME) for *Escherichia coli* K12 MG1655. Added coupling constraints

$$c_{\min} \leq \frac{v_i}{v_j} \leq c_{\max}$$
 (3)

become linear constraints

$$c_{\min} v_j \le v_i, \quad v_i \le c_{\max} v_j \tag{4}$$

for various pairs of fluxes  $v_i$ ,  $v_j$ . They are linear approximations of nonlinear constraints and make S in (2b) even less well-scaled because of large variations in reaction rates. Quad precision is evidently more appealing.

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## Coupling constraints

Two fluxes could be related by

$$0.0001 \le \frac{v_1}{v_2} \le 10000.$$
 (5)

#### Lifting approach (Yuekai Sun, ICME, 2012)

Transform into sequences of constraints involving auxiliary variables with reasonable coefficients. The second inequality in (5) becomes  $v_1 \leq 10000v_2$ , which is equivalent to

$$v_1 \leq 100s_1, \qquad s_1 \leq 100v_2.$$
 (6)

If the first inequality in (5) were presented as  $v_1 \ge 0.0001v_2$ , we would leave it alone, but the equivalent inequality  $10000v_1 \ge v_2$  would be transformed to

 $v_2 \leq 100s_2, \qquad s_2 \leq 100v_1.$ 

# The desirability of Quad precision

"Carrying somewhat more precision in the arithmetic than twice the precision carried in the data and available for the result will vastly reduce embarrassment due to roundoff-induced anomalies."

"Default evaluation in Quad is the humane option."

— William Kahan

# Methods for achieving Quad precision

#### Hand-code calls to auxiliary functions

Even q = qdotdd(v,w) needs several double functions
 twosum, split, twoproduct sum2, dot2

to compute double x, y

and hence quad result q = quad(x) + quad(y)

#### Double-double datatype ( $\approx$ 32 digits)

QD: http://crd-legacy.lbl.gov/~dhbailey/mpdist/ C++ with interfaces to C++ and F90 DDFUN90: entirely F90 Minor changes to source code

#### Quad datatype ( $\approx$ 34 digits)

Some f90 compilers such as gfortran Again minor changes to source code We use this humane approach to Quad implementation

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# **System and Methods**

quadMINOS

## quadMINOS

The GNU GCC compilers make Quad available via 128-bit data types. We have therefore been able to make a Quad version of the Fortran 77 linear and nonlinear optimization solver MINOS using the gfortran compiler<sup>1</sup> with real(8) changed to real(16) everywhere.

Double is implemented in hardware, while Quad is a software library.

Our aim is to explore combined use of the Double and Quad MINOS simplex solvers for the solution of large multiscale linear programs. We seek greater efficiency than is normally possible with exact simplex solvers.

<sup>1</sup>GNU Fortran (GCC) 4.6.2 20111019 on Mac OS X (now version 5.2.0)

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# quadSNOPT

In the f90 implementations of SQOPT and SNOPT, we select one of the modules

snPrecision32.f90
snPrecision64.f90
snPrecision128.f90

For example, snPrecision128.f90:

```
module snModulePrecision
  implicit none
  public
  integer(4), parameter :: ip = 8, rp = 16 ! quad precision
  end module snModulePrecision
```

# quadSNOPT

In the f90 implementations of SQOPT and SNOPT, we select one of the modules

snPrecision32.f90
snPrecision64.f90
snPrecision128.f90

For example, snPrecision128.f90:

```
module snModulePrecision
   implicit none
   public
   integer(4), parameter :: ip = 8, rp = 16 ! quad precision
end module snModulePrecision
```

Later:

```
module sn501p
use snModulePrecision, only : ip, rp
subroutine s5solveLP ( x, y )
real(rp), intent(inout) :: x(nb), y(nb)
```

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# MINOS and quadMINOS

The primal simplex solver in MINOS includes

- geometric-mean scaling of the constraint matrix
- the EXPAND anti-degeneracy procedure
- partial pricing (but no steepest-edge pricing, which would generally reduce total iterations and time)
- Basis LU factorizations and updates via LUSOL

quadMINOS  $\equiv$  MINOS with real(8)  $\rightarrow$  real(16) eps = 2.22e-16  $\rightarrow$  eps = 1.93e-34

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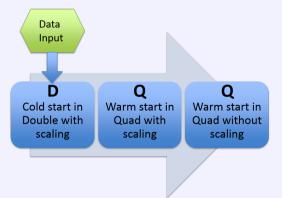
Conclusions

# **DQQ** procedure

# Step D:Double MINOSStep Q1:Quad MINOSStep Q2:Quad MINOS with no scaling

# DQQ procedure

- Cold start Double MINOS with scaling and somewhat strict settings, save basis
- **2** Warm start Quad MINOS with scaling and tighter Featol/Opttol, save basis
- **③** Warm start Quad MINOS without scaling but tighter LU tols



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#### MINOS runtime options for DQQ procedure

	Default	Step D	Step Q1	Step Q2
Scale option	2	2	2	0
Feasibility tol	1e-6	1e-7	1e-15	1e-15
Optimality tol	1e-6	1e-7	1e-15	1e-15
LU Factor tol	100.0	10.0	10.0	5.0
LU Update tol	10.0	10.0	10.0	5.0

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Table: Three pilot models from Netlib, eight Mészáros *problematic* LPs, and three ME biochemical network models. Dimensions of  $m \times n$  constraint matrices A and size of the largest optimal primal and dual variables  $x^*$ ,  $y^*$ .

model	т	п	nnz(A)	$\max  A_{ij} $	$\ x^*\ _{\infty}$	$\ y^*\ _{\infty}$
pilot4	411	1000	5145	3e+04	1e+05	3e+02
pilot	1442	3652	43220	2e+02	4e+03	2e+02
pilot87	2031	4883	73804	1e+03	2e+04	1e+01
de063155	853	1488	5405	8e+11	3e+13	6e+04
de063157	937	1488	5551	2e+18	2e+17	6e+04
de080285	937	1488	5471	1e+03	1e+02	3e+01
gen1	770	2560	64621	1e+00	3e+00	1e+00
gen2	1122	3264	84095	1e+00	3e+00	1e+00
gen4	1538	4297	110174	1e+00	3e+00	1e+00
130	2702	15380	64790	1e+00	1e+09	4e+00
iprob	3002	3001	12000	1e+04	3e+02	1e+00
TMA_ME	18210	17535	336302	2e+04	6e+00	1e+00
GlcAerWT	68300	76664	926357	8e+05	6e+07	2e+07
GlcAlift	69529	77893	928815	3e+05	6e+07	2e+07

Table: Itns and runtimes in secs for Step 1 (Double MINOS) and Steps 2–3 (Quad MINOS). Pinf and Dinf =  $\log_{10}$  final maximum primal and dual infeasibilities. Problem iprob is infeasible. Bold figures show Pinf and Dinf at the end of Step 3. Pinf/ $||x^*||_{\infty}$  and Dinf/ $||y^*||_{\infty}$  are all  $O(10^{-30})$  or smaller, even though only  $O(10^{-15})$  was requested. This is an unexpectedly favorable empirical finding.

model	ltns	Times	Final objective	Pinf	Dinf
pilot4	1571	0.1	-2.5811392602e+03	-05	-13
	6	0.0	-2.5811392589e+03	-39	-31
	0	0.0	-2.5811392589e+03	-	<b>-30</b>
pilot	16060	5.7	-5.5739887685e+02	-06	-03
	29	0.7	-5.5748972928e+02	-	-27
	0	0.2	-5.5748972928e+02	-	<b>-32</b>
pilot87	19340	15.1	3.0171038489e+02	-09	-06
	32	2.2	3.0171034733e+02	-	-33
	0	1.2	3.0171034733e+02	-	<b>-33</b>

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model	ltns	Times	Final objective	Pinf	Dinf
de063155	921	0.0	1.8968704286e+10	-13	+03
	78	0.1	9.8830944565e+09	-	-17
	0	0.0	9.8830944565e+09	-	<b>-24</b>
de063157	488	0.0	1.4561118445e+11	+20	+18
	476	0.5	2.1528501109e+07	-27	-12
	0	0.0	2.1528501109e+07	-	-12
de080285	418	0.0	1.4495817688e+01	-09	-02
	132	0.1	1.3924732864e+01	-35	-32
	0	0.0	1.3924732864e+01	-	<b>-32</b>
gen1	369502	205.3	-1.6903658594e-08	-06	-12
	246428	9331.3	1.2935699163e-06	-12	-31
	2394	81.6	1.2953925804e-06	<b>-45</b>	<b>-30</b>
gen2	44073	60.0	3.2927907828e+00	-04	-11
	1599	359.9	3.2927907840e+00	-	-29
	0	10.4	3.2927907840e+00	-	<b>-32</b>
gen4	45369	212.4	1.5793970394e-07	-06	-10
	53849	14812.5	2.8932268196e-06	-12	-30
	37	10.4	2.8933064888e-06	<b>-54</b>	<b>-30</b>

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model	ltns	Times	Final objective	Pinf	Dinf
130	1229326	876.7	9.5266141574e-01	-10	-09
	275287	7507.1	-7.5190273434e-26	-25	-32
	0	0.2	-4.2586876849e-24	<b>-24</b>	<b>-33</b>
iprob	1087	0.2	2.6891551285e+03	+02	-11
	0	0.0	2.6891551285e+03	+02	-31
	0	0.0	2.6891551285e+03	+02	<b>-28</b>
TMA_ME	12225	37.1	8.0051076669e-07	-06	-05
	685	61.5	8.7036315385e-07	-24	-30
	0	6.7	8.7036315385e-07	-	-31
GlcAerWT	62856	9707.3	-2.4489880182e+04	+04	-05
	5580	3995.6	-7.0382449681e+05	-07	-26
	4	60.1	-7.0382449681e+05	-19	<b>-21</b>
GlcAlift	134693	14552.8	-5.1613878666e+05	-03	-01
	3258	1067.1	-7.0434008750e+05	-09	-26
	2	48.1	-7.0434008750e+05	<b>-20</b>	-22

DRR procedure

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# **DRR procedure**

# Step D:Double MINOSStep R1:RefinementStep R2:Refinement with no scaling

# Plausible alternative to DQQ

# DRR procedure

- **()** Cold start Double MINOS with scaling and somewhat strict settings
- **2** Warm start with scaling and Iterative Refinement and tighter Featol/Opttol
- **③** Warm start with no scaling but Iterative Refinement and tighter LU tols

• We need Quad residuals for  $Bx_B = b - Nx_n$  after LU and for By = a,  $B^T y = c_B$  each iteration

# DRR procedure

- **(**) Cold start Double MINOS with scaling and somewhat strict settings
- **2** Warm start with scaling and Iterative Refinement and tighter Featol/Opttol
- **③** Warm start with no scaling but Iterative Refinement and tighter LU tols

- We need Quad residuals for  $Bx_B = b Nx_n$  after LU and for By = a,  $B^T y = c_B$  each iteration
- Quad r = a By needs  $r \leftarrow r y_k B_k$  (qaxpy) Compiler converts B to Quad every iteration

# DRR procedure

- **()** Cold start Double MINOS with scaling and somewhat strict settings
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- Quad r = a By needs  $r \leftarrow r y_k B_k$  (qaxpy) Compiler converts B to Quad every iteration
- Quad  $r = c_B B^T y$  needs Quad dotproducts (qdot) Again, compiler converts B to Quad every iteration

# DRR procedure

- Old start Double MINOS with scaling and somewhat strict settings
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- **③** Warm start with no scaling but Iterative Refinement and tighter LU tols

- We need Quad residuals for  $Bx_B = b Nx_n$  after LU and for By = a,  $B^T y = c_B$  each iteration
- Quad r = a By needs  $r \leftarrow r y_k B_k$  (qaxpy) Compiler converts B to Quad every iteration
- Quad  $r = c_B B^T y$  needs Quad dotproducts (qdot) Again, compiler converts B to Quad every iteration
- James Ho (1975) SRR procedure?

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# LPnetlib test problems

#### Unexpectedly high accuracy in Quad

quadMINOS

### 62 classic LP problems (ordered by file size)

afiro stocfor1 adlittle scagr7 sc205 share2b recipe vtpbase share1b bore3d scorpion capri brandy scagr25 sctap1 israel

scfxm1 bandm e226 grow7 etamacro agg scsd1 standata beaconfd gfrdpnc stair scrs8 shell scfxm2 pilot4 scsd6

ship04s seba grow15 fffff800 scfxm3 ship041 ganges sctap2 grow22 ship08s stocfor2 pilotwe ship12s 25fv47sierra czprob

pilotja ship081 nesm ship121 cvcle greenbea greenbeb 80bau3b d2q06c woodw d6cube pilot wood1p pilot87

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# DRR procedure on LPnetlib problems

Pinf = max Primal infeasibility  
Dinf = max Dual infeasibility/
$$(1 + ||y^*||_{\infty})$$

MINOS stops when	$Pinf \leq F$	easibility tol	Default 1e-6
	$Dinf \leq O$	Optimality tol	Default 1e-6

#### Plot $log_{10}(Pinf)$ and $log_{10}(Dinf)$ for steps D, R1, R2

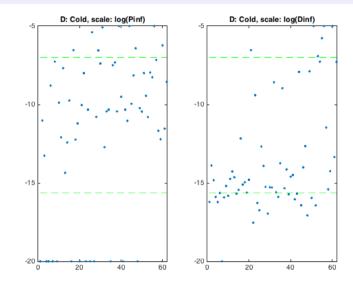
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#### Primal/dual infeasibilities:

#### Step D: Double MINOS, cold start, scale

Scale option 2 Feasibility tol 1e-7 Optimality tol 1e-7 LU Partial Pivoting LU Factor tol 10.0 LU Update tol 10.0 Quad refinement 0

 $\epsilon = 2.2e-16$ 



DRR procedure

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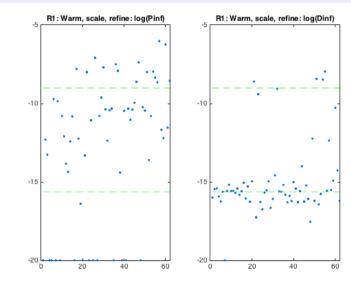
#### Primal/dual infeasibilities:

#### Step R1: Double MINOS, warm start, scale, refine

Scale option 2 Feasibility tol 1e-9 Optimality tol 1e-9

LU Partial Pivoting LU Factor tol 1.9 LU Update tol 1.9 Quad refinement 1

 $\epsilon = 2.2e-16$ 



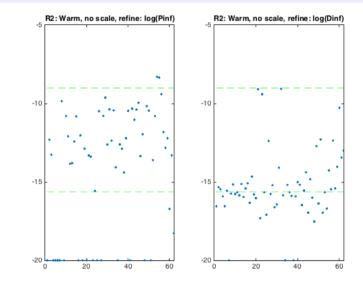
LPnetlib tests

#### Primal/dual infeasibilities:

#### Step R2: Double MINOS, warm start, no scale, refine

Scale option 0 Feasibility tol 1e-9 Optimality tol 1e-9 LU Partial Pivoting LU Factor tol 1.9 LU Update tol 1.9 Quad refinement 1

 $\epsilon = 2.2e-16$ 



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### DQQ procedure on LPnetlib problems

$$Pinf = max Primal infeasibility$$
  
 $Dinf = max Dual infeasibility/(1 + ||y^*||_{\infty})$ 

### Plot $\log_{10}(\text{Pinf})$ and $\log_{10}(\text{Dinf})$ for steps D, Q1, Q2

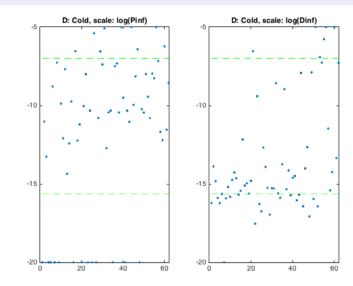
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### Primal/dual infeasibilities:

### Step D: Double MINOS, cold start, scale (repeat)

Scale option 2 Feasibility tol 1e-7 Optimality tol 1e-7 LU Partial Pivoting LU Factor tol 10.0 LU Update tol 10.0 Expand freq 100000

 $\epsilon = 2.2e-16$ 

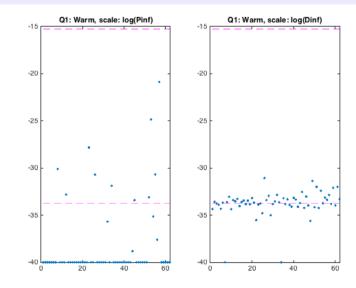


### Primal/dual infeasibilities:

### Step Q1: Quad MINOS, warm start, scale

Scale option 2 Feasibility tol 1e-15 Optimality tol 1e-15 LU Partial Pivoting

LU Factor tol 10.0 LU Update tol 10.0





DQQ procedure

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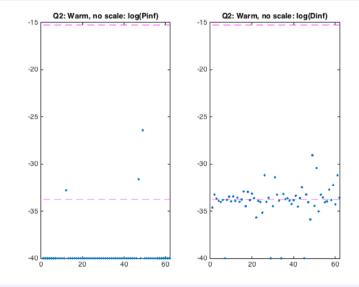
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### Primal/dual infeasibilities:

### Step Q2: Quad MINOS, warm start, no scale

Scale option 0 Feasibility tol 1e-15 Optimality tol 1e-15 LU Partial Pivoting LU Factor tol 5.0 LU Update tol 5.0





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# Multiscale NLPs

# Systems biology FBA problems with variable $\mu$ (Palsson Lab, UC San Diego, 2014)

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# ME models with nonlinear constraints

As coupling constraints are often functions of the organism's growth rate  $\mu$ , Lerman et al. (UCSD) consider growth-rate optimization nonlinearly with the single  $\mu$  as the objective instead of via a linear biomass objective function. Nonlinear constraints of the form

$$\frac{v_i}{v_j} \le \mu \tag{7}$$

represented as

$$\mathbf{v}_i \leq \mu \mathbf{v}_j \tag{8}$$

are added to (2b), where  $v_i, v_j, \mu$  are all variables. Constraints (8) are linear if  $\mu$  is fixed at a specific value  $\mu_k$ . Lerman et al. employ a binary search to find the largest  $\mu_k \in [\mu_{\min}, \mu_{\max}]$  that keeps the associated LP feasible. Thus, the procedure requires reliable solution of a sequence of related LPs.

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# tinyME

Nonlinear FBA formulation, Laurence Yang, UCSD, Dec 2014

- Tiny example:  $\approx 2500 \times 3000$
- $\mu = x_1$  and the first columns of A, B are empty
- Constraints are linear if  $\mu$  is fixed suggests binary search on sequence of LPs 25 LP subproblems would give 8 digits (really need quad Simplex)
- Instead, apply quad MINOS LCL method = Linearly Constrained Lagrangian 6 NLP subproblems (with linearized constraints) give 20 digits

# Quadratic convergence of major iterations (Robinson 1972)

quadMINOS 5.6 (Nov 2014)

Begin t	inyME-NI	LP cold	l sta	art NL	P with	mu = mu0	
Itn 304 linear constraints satisfied.							
Calling funcon. mu = 0.80000000000000000000000000000000000							
nnCon,	nnJac, 1	neJac		1073		1755	2681
funcon	sets	2681	$\operatorname{out}$	of	2681	constraint	gradients.
funobj	sets	1	$\operatorname{out}$	of	1	objective	gradients.

Major	minor	step	objective H	Feasible	Optimal	nsb	ncon penalty
1	304T	0.0E+00	8.00000E-01	6.1E-03	2.1E+03	0	4 1.0E+02
2	561T	1.0E+00	8.00000E-01	2.6E-14	3.2E-04	0	46 1.0E+02
3	40T	1.0E+00	8.28869E-01	5.4E-05	3.6E-05	0	87 1.0E+02
4	7	1.0E+00	8.46923E-01	1.2E-05	2.9E-06	0	96 1.0E+02
5	0	1.0E+00	8.46948E-01	4.2E-10	2.6E-10	0	97 1.0E+02
6	0	1.0E+00	8.46948E-01	7.9E-23	1.2E-20	0	98 1.0E+01

EXIT -- optimal solution found

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#### EXIT -- optimal solution found

Problem name	tinyME		
No. of iterations	912	Objective value	8.4694810579E-01
No. of major iterations	6	Linear objective	0.000000000E+00
Penalty parameter	1.000000	Nonlinear objective	8.4694810579E-01
No. of calls to funobj	98	No. of calls to func	on 98
No. of superbasics	0	No. of basic nonline	ars 786
No. of degenerate steps	0	Percentage	0.00
Max x (scaled)	12 5.6E-01	Max pi (scaled)	103 8.3E+05
Max x	1020 6.1E+01	Max pi	103 9.7E+03
Max Prim inf(scaled)	0 0.0E+00	Max Dual inf(scaled)	9 2.9E-14
Max Primal infeas	0 0.0E+00	Max Dual infeas	9 1.3E-18
Nonlinear constraint vio	ln 1.9E-20		

funcon called with nstate = 2
Final value of mu = 0.84694810578563166175146802332321527

Time for solving problem 13.50 seconds

quadMINOS

Mérida, Mexico, Jan 4–8, 2016

Conclusions

### ME 2.0

### Large FBA and FVA problems, Laurence Yang, UCSD, Sep 2015

FBA model iJL1678:	71,000 imes 80,000 LP
Quad MINOS cold start:	$\sim$ 3 hours
FVA problems:	min and max individual variables $v_j$

		Double C	PLEX	Quad MINOS	
Reaction	Protein	<i>v</i> <sub>min</sub>	<i>v</i> <sub>max</sub>	<i>v</i> <sub>min</sub>	<i>v</i> <sub>max</sub>
translation_b0169	RpsB	30.71 <mark>5011</mark>	30.71 <mark>2581</mark>	30.719225	30.719225
translation_b0025	RibF	0.212807	0.211712	0.210161	0.210161
$translation_b0071$	LeuD	0.303 <mark>304</mark>	0.765585	0.303634	0.303634
translation_b0072	LeuC	0.303 <mark>304</mark>	0.681146	0.303634	0.303634

DRR procedur

LPnetlib test

Multiscale NL

Philosophy

Conclusions

# Philosophy

quadMINOS

# Philosophy

• Humor is mankind's greatest blessing.



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 System and Methods
 DQQ procedure
 DRR procedure
 LPnetlib tests
 Multiscale NLPs
 Philosophy

 • Humor is mankind's greatest blessing.
 - Mark Twain

 • There are three rules for writing a great English novel. Unfortunately noone knows what they are.
 - Somerset Maugham (?)

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- Mark Twain

#### Conclusions

# Philosophy

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- There are three rules for writing a great English novel.
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   Somerset Maugham (?)

We will cover some variations which may be useful.

We will cover some variations, which may be useful.

We will cover some variations that may be useful.



# Philosophy

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• If the glove won't fit, you must acquit.





- Mark Twain

#### Multiscale NLPs

#### Conclusions

# Philosophy

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We will cover some variations that may be useful.

- If the glove won't fit, you must acquit.
- If the comma's omitted, the which is wicked.





Philosophy

Conclusions

# Philosophy



Thanks for the quick reply.

Thanks for your quick reply.

Peter, thanks for your quick reply.

Philosophy

Conclusions

# Philosophy

٩ Jan 5 ٩ Tues, Jan 5

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quadMINOS

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– Dalai Lama

• Can humour (not satire) be the antidote to extremism? It would be great to think so.



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- You have to think anyway, so why not think big? Donald Trump



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- Can humour (not satire) be the antidote to extremism? It would be great to think so.
- You have to think anyway, so why not think big? Donald Trump
- Metabolic networks will keep getting bigger (genome-scale up to whole human).
- Urge chip-makers to implement hardware quad precision.

DRR procedur

LPnetlib tests

Multiscale N

Philosophy

Conclusions

# Conclusions

quadMINOS

### Conclusions

Just as double-precision floating-point hardware revolutionized scientific computing in the 1960s, the advent of quad-precision data types (even in software) brings us to a new era of greatly improved reliability in optimization solvers.

### References

- Y. Sun, R. M. T. Fleming, I. Thiele, and M. A. Saunders. Robust flux balance analysis of multiscale biochemical reaction networks, *BMC Bioinformatics* 14:240, 2013, 6 pp.
- Ding Ma and Michael Saunders (2015). Solving multiscale linear programs using the simplex method in quadruple precision, Proceedings of NAO-III, Muscat, Oman, Jan 2014, Springer.

### Conclusions

Just as double-precision floating-point hardware revolutionized scientific computing in the 1960s, the advent of quad-precision data types (even in software) brings us to a new era of greatly improved reliability in optimization solvers.

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### Special thanks

- George Dantzig, born 101 years ago (8 Nov 1914)
- William Kahan, IEEE floating-point standard, including Quad, Boulder.pdf (2011)
- GNU gfortran
- Ronan Fleming, Ines Thiele (Luxembourg)
- Bernhard Palsson, Josh Lerman, Teddy O'Brien, Laurence Yang (UCSD)
- Ed Klotz (IBM CPLEX), Yuekai Sun, Jon Dattorro (Stanford)
- Frank Curtis, Jose Luis Morales, Katya Scheinberg, Andreas Wächter



Is quadMINOS available?	Yes, in the openCOBRA toolbox
http:/	//opencobra.github.io/cobratoolbox/
• Can quadMINOS be called from Matla	b or Tomlab? Yes via system call (not Mex)
Is quadMINOS available in GAMS?	Soon Yes
• How about AMPL?	No, but should be feasible
Is there a quadSNOPT?	Yes, in f90 SNOPT9 we can change 1 line
• Can CPLEX / Gurobi / Mosek / he	Ip? Yes, they can provide Presolve and Warm start, especially from GAMS
• Will Quad hardware eventually be stan	dard? We hope so but Kahan is pessimistic