High performance numerical linear algebra for the revised simplex method

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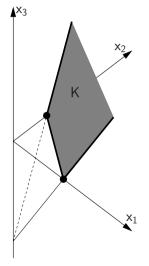




### Background

- Primal simplex algorithm
- Dual simplex algorithm
- NLA challenge
- Hyper-sparsity
- Novel update techniques
- Parallel solution of structured LP problems
- Parallel solution of general LP problems

## Solving LP problems: Characterizing a basis



minimize  $f = \boldsymbol{c}^T \boldsymbol{x}$  subject to  $A\boldsymbol{x} = \boldsymbol{b}$   $\boldsymbol{x} \ge \boldsymbol{0}$ 

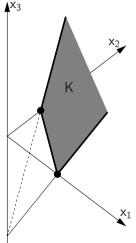
A vertex of the feasible region K ⊂ ℝ<sup>n</sup> has *m* basic components, *i* ∈ B given by Ax = b *n* − *m* zero nonbasic components, *j* ∈ N
where B ∪ N partitions {1,..., n}

• Equations partitioned according to  $\mathcal{B} \cup \mathcal{N}$  as  $B \boldsymbol{x}_{\scriptscriptstyle B} + N \boldsymbol{x}_{\scriptscriptstyle N} = \boldsymbol{b}$ 

with nonsingular basis matrix B

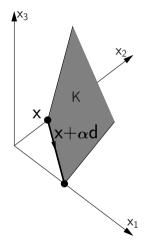
• Points  $\mathbf{x} \in K$  characterized by  $\mathbf{x}_{B} = \widehat{\mathbf{b}} - B^{-1}N\mathbf{x}_{N}$  for some  $\mathbf{x}_{N} \ge \mathbf{0}$ where  $\widehat{\mathbf{b}} = B^{-1}\mathbf{b}$ 

# Solving LP problems: Optimality conditions



minimize 
$$f = c^T x$$
 subject to  $Ax = b$   $x \ge 0$   
• Objective partitioned according to  $\mathcal{B} \cup \mathcal{N}$  as  
 $f = c_B^T x_B + c_N^T x_N$   
 $= \widehat{f} + \widehat{c}_N^T x_N$   
where  $\widehat{f} = c_B^T \widehat{b}$  and  $\widehat{c}_N^T = c_N^T - c_B^T B^{-1} N$   
• Partition yields an optimal solution if there is  
• Primal feasibility  $\widehat{b} \ge 0$   
• Dual feasibility  $\widehat{c}_N \ge 0$ 

### The simplex algorithm: Definition



- At a feasible vertex  $\mathbf{x} = \begin{bmatrix} \hat{\mathbf{b}} \\ \mathbf{0} \end{bmatrix}$  corresponding to  $\mathcal{B} \cup \mathcal{N}$ **1** If  $\hat{c}_{N} > 0$  then stop: the solution is optimal 2 Scan  $\hat{c}_i < 0$  for q to leave  $\mathcal{N}$ **3** Let  $\widehat{\boldsymbol{a}}_q = B^{-1} N \boldsymbol{e}_q$  and  $\boldsymbol{d} = \begin{bmatrix} -\widehat{\boldsymbol{a}}_q \\ \boldsymbol{e}_q \end{bmatrix}$ Scan  $\hat{b}_i/\hat{a}_{ia} > 0$  for  $\alpha$  and p to leave  $\mathcal{B}$ **5** Exchange p and q between  $\mathcal{B}$  and  $\mathcal{N}$ 
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## Solving dual LP problems: Optimality conditions

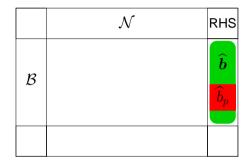
• Consider the **dual problem** 

maximize 
$$f_D = \boldsymbol{b}^T \boldsymbol{y}$$
 subject to  $A^T \boldsymbol{y} + \boldsymbol{s} = \boldsymbol{c}$   $\boldsymbol{s} \ge \boldsymbol{0}$   
• For partition  $\mathcal{B} \cup \mathcal{N}$  of  $\{1, \dots, n\}$   
•  $\boldsymbol{y} = B^{-T}(\boldsymbol{c}_B - \boldsymbol{s}_B)$   
•  $\boldsymbol{s} = \begin{bmatrix} \boldsymbol{s}_B \\ \boldsymbol{s}_N \end{bmatrix}$  for  $\boldsymbol{s}_N = \hat{\boldsymbol{c}}_N + N^T B^{-T} \boldsymbol{s}_B$ ; some  $\boldsymbol{s}_B \ge \boldsymbol{0}$   
• Reduced objective is  $f_D = \hat{f} - \hat{\boldsymbol{b}}^T \boldsymbol{s}_B$ 

- Solution is optimal if there is
  - Dual feasibility  $\widehat{c}_{N} \geq 0$
  - Primal feasibility  $\widehat{\boldsymbol{b}} \ge \boldsymbol{0}$
- Dual simplex algorithm for an LP is primal algorithm applied to the dual problem
- Structure of dual equations allows dual simplex algorithm to be applied to primal simplex tableau

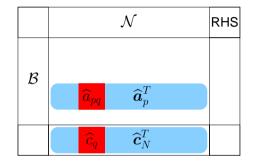
Assume  $\widehat{\boldsymbol{c}}_{\scriptscriptstyle N} \geq \boldsymbol{0}$  Seek  $\widehat{\boldsymbol{b}} \geq \boldsymbol{0}$ 

Scan  $\widehat{b}_i < 0$  for p to leave  $\mathcal{B}$ 

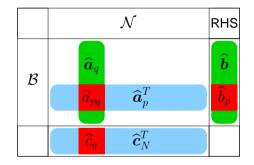


### Assume $\widehat{\boldsymbol{c}}_{N} \geq \boldsymbol{0}$ Seek $\widehat{\boldsymbol{b}} \geq \boldsymbol{0}$

 $\begin{array}{l} \text{Scan } \widehat{b}_i < 0 \text{ for } p \text{ to leave } \mathcal{B} \\ \text{Scan } \widehat{c}_j / \widehat{a}_{pj} < 0 \text{ for } q \text{ to leave } \mathcal{N} \end{array}$ 



Assume  $\widehat{c}_N \geq 0$ Seek  $\widehat{b} \geq 0$ Scan  $\widehat{b}_i < 0$  for p to leave  $\mathcal{B}$ Scan  $\widehat{c}_j / \widehat{a}_{pj} < 0$  for q to leave  $\mathcal{N}$ Update: Exchange p and q between  $\mathcal{B}$  and  $\mathcal{N}$ Update  $\widehat{b} := \widehat{b} - \alpha_P \widehat{a}_q$  $\alpha_P = \widehat{b}_p / \widehat{a}_{pq}$ Update  $\widehat{c}_N^T := \widehat{c}_N^T + \alpha_D \widehat{a}_p^T$  $\alpha_D = -\widehat{c}_q / \widehat{a}_{pq}$ 



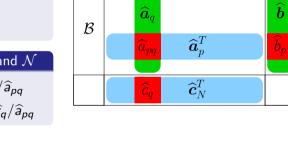
Assume  $\widehat{c}_{N} \geq 0$  Seek  $\widehat{b} \geq 0$ Scan  $\widehat{b}_{i} < 0$  for p to leave  $\mathcal{B}$ Scan  $\widehat{c}_{j}/\widehat{a}_{pj} < 0$  for q to leave  $\mathcal{N}$ Update: Exchange p and q between  $\mathcal{B}$  and  $\mathcal{N}$ 

Update 
$$\mathbf{b} := \mathbf{b} - \alpha_P \widehat{\mathbf{a}}_q$$
  $\alpha_P = b_P / \widehat{\mathbf{a}}_{Pq}$   
Update  $\widehat{\mathbf{c}}_N^T := \widehat{\mathbf{c}}_N^T + \alpha_D \widehat{\mathbf{a}}_P^T$   $\alpha_D = -\widehat{\mathbf{c}}_q / \widehat{\mathbf{a}}_{Pq}$ 



• Pivotal row 
$$\widehat{\boldsymbol{a}}_{p}^{T} = \boldsymbol{e}_{p}^{T} B^{-1} N$$

• Pivotal column 
$$\widehat{m{a}}_q = B^{-1}m{a}_q$$



 $\mathcal{N}$ 

RHS

### Primal simplex algorithm

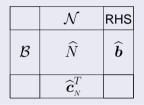
- Traditional variant
- Solution generally not primal feasible when (primal) LP is tightened

### Dual simplex algorithm

- Preferred variant
- Easier to get dual feasibility
- More progress in many iterations
- Solution dual feasible when primal LP is tightened

## Simplex method: Computation

### Standard simplex method (SSM): Major computational component



Update of tableau: 
$$\widehat{N}:=\widehat{N}-rac{1}{\widehat{a}_{pq}}\widehat{a}_{q}\widehat{a}_{p}^{T}$$
 where  $\widehat{N}=B^{-1}N$ 

• Hopelessly inefficient for sparse LP problems

• Prohibitively expensive for large LP problems

### Revised simplex method (RSM): Major computational components

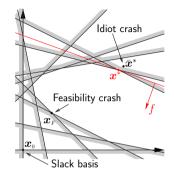
Pivotal row via $B^T \pi_p = e_p$ BTRANand $\widehat{a}_p^T = \pi_p^T N$ PRICEPivotal column via $B \, \widehat{a}_q = a_q$ FTRANRepresent  $B^{-1}$ INVERTUpdate  $B^{-1}$  exploiting  $\overline{B} = B + (a_q - Be_p)e_p^T$ UPDATE

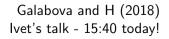
- Given initial  ${\cal B}$  with nonsingular  ${\cal B}$
- Each iteration:
  - Solve  $B\widehat{\boldsymbol{a}}_q = \boldsymbol{a}_q$
  - Solve  $B^T \pi_p = e_p$
  - Column p of B replaced by  $\boldsymbol{a}_q$  to give  $\bar{B} = B + (\boldsymbol{a}_q B\boldsymbol{e}_p)\boldsymbol{e}_p^T$
- Challenge:
  - $\bullet\,$  Choose initial  ${\cal B}$
  - Form PBQ = LU
    - Solve Bx = b for sparse b
  - Solve  $\bar{B} \mathbf{x} = \mathbf{b}$

# NLA Challenge: Choose initial $\mathcal{B}$

### Requirements of initial $\mathcal{B}$

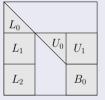
- Must be a useful starting point for the simplex algorithm
- Corresponding matrix B must be
  - Nonsingular
  - Well conditioned
  - Have sparse representation PBQ = LU
- "Slack" basis (B = I) is simple choice  $x_0$
- Standard crash aims for feasible vertex  $x_F$
- "ldiot" crash aims for near-optimal point  $ar{x}^*$





#### Triangularisation

Identify row and column singletons until every active nonzero has positive Markowitz merit



Solve 
$$B\mathbf{x} = \mathbf{r}$$
 as  
 $L_0\mathbf{x}_L = \mathbf{r}_L$   
 $B_0\mathbf{x}_0 = \mathbf{r}_0 - L_2\mathbf{x}_L$   
 $U_0\mathbf{x}_U = \mathbf{r}_U - L_1\mathbf{x}_L - U_1\mathbf{x}_0$ 

- LP basis matrices are typically **highly reducible**:  $\dim(B_0) \ll m$
- For network flow problems B is provably triangularisable

# NLA Challenge: Solve $\bar{B}x = r$ using the product form update (PFI)

Each iteration: Exchange p and q between  $\mathcal{B}$  and  $\mathcal{N}$ 

- Column *p* of *B* replaced by  $\boldsymbol{a}_q$  to give  $\bar{B} = B + (\boldsymbol{a}_q B\boldsymbol{e}_p)\boldsymbol{e}_p^T$
- Take B out as a factor on the left

$$\bar{B} = B[I + (B^{-1}\boldsymbol{a}_q - \boldsymbol{e}_p)\boldsymbol{e}_p^T] = BE$$
  
where  $E = I + (\widehat{\boldsymbol{a}}_q - \boldsymbol{e}_p)\boldsymbol{e}_p^T = \begin{bmatrix} 1 & \eta_1 & & \\ \ddots & \vdots & & \\ & \mu & & \\ & \vdots & \ddots & \\ & \eta_m & & 1 \end{bmatrix}$ 

 $\mu = \hat{a}_{pq}$  is the **pivot**; remaining entries in  $\hat{a}_q$  form the **eta vector**  $\eta$ • Can solve  $\bar{B}x = r$  as Bx = r then  $x := E^{-1}x$  as

 $x_{m{p}} := x_{m{p}}/\mu$  then  $m{x} := m{x} - x_{m{p}}m{\eta}$ 

Dantzig and Orchard-Hays (1954)

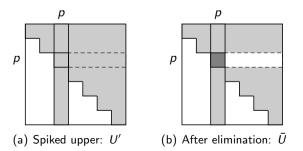
# NLA Challenge: Solve $\bar{B}x = r$ using the Forrest-Tomlin update (FT)

• Given

$$ar{B} = B + (oldsymbol{a}_q - Boldsymbol{e}_p)oldsymbol{e}_p^{T}$$
 where (wlog)  $B = LU$ 

• Multiply  $\bar{B}$  by  $L^{-1}$  to give

$$L^{-1}\bar{B} = U + (L^{-1}\boldsymbol{a}_q - U\boldsymbol{e}_p)\boldsymbol{e}_p^T = U + (\tilde{\boldsymbol{a}}_q - \boldsymbol{u}_p)\boldsymbol{e}_p^T = U' \quad (a)$$
  
• Eliminate entries in row p to give  $R^{-1}U' = \bar{U}$  (b)



- Yields  $\bar{B} = LR\bar{U}$
- Compute  $\widetilde{a}_q$  when forming  $\widehat{a}_q$
- Represent R like E
- FT more efficient than PFI with respect to sparsity

Forrest and Tomlin (1972)

NLA Challenge: Hyper-sparsity

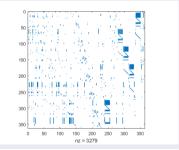
• Given B = LU, solve

$$L\mathbf{y} = \mathbf{r}; \quad U\mathbf{x} = \mathbf{y}$$

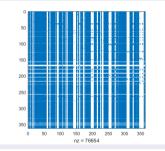
- In revised simplex method, r is sparse: consequences?
  - If *B* is irreducible then *x* is full
  - If B is highly reducible then x can be sparse
- Phenomenon of hyper-sparsity
  - Exploit it when forming x
  - Exploit it when using **x**

#### Inverse of a sparse matrix and solution of $B\mathbf{x} = \mathbf{r}$

#### Optimal B for LP problem stair

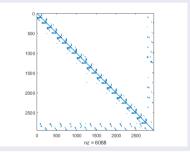


 $B^{-1}$  has density of 58%, so  $B^{-1}\mathbf{r}$  is typically dense

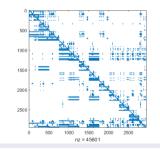


#### Inverse of a sparse matrix and solution of $B\mathbf{x} = \mathbf{r}$

Optimal B for LP problem pds-02



 $B^{-1}$  has density of 0.52%, so  $B^{-1}r$  is typically sparse—when r is sparse



- Use solution of  $L \mathbf{x} = \mathbf{b}$ 
  - To illustrate the phenomenon of hyper-sparsity
  - To demonstrate how to exploit hyper-sparsity
- Apply principles to other triangular solves in the simplex method

**Recall:** Solve Lx = b using

function ftranL(
$$L$$
,  $\boldsymbol{b}$ ,  $\boldsymbol{x}$ )  
 $\boldsymbol{r} = \boldsymbol{b}$   
for all  $j \in \{1, \dots, m\}$  do  
for all  $i : L_{ij} \neq 0$  do  
 $r_i = r_i - L_{ij}r_j$   
 $\boldsymbol{x} = \boldsymbol{r}$ 

When **b** is **sparse** 

• Inefficient until r fills in

**Better:** Check  $r_j$  for zero

$$\begin{aligned} \mathbf{function ftranL}(L, \mathbf{b}, \mathbf{x}) \\ \mathbf{r} &= \mathbf{b} \\ \mathbf{for all } j \in \{1, \dots, m\} \ \mathbf{do} \\ & \mathbf{if } r_j \neq 0 \ \mathbf{then} \\ & \mathbf{for all } i : L_{ij} \neq 0 \ \mathbf{do} \\ & r_i &= r_i - L_{ij}r_j \\ \mathbf{x} &= \mathbf{r} \end{aligned}$$

### When *x* is **sparse**

- Few values of  $r_j$  are nonzero
- Check for zero dominates
- Requires more efficient identification of set X of indices j such that r<sub>j</sub> ≠ 0

Gilbert and Peierls (1988) H and McKinnon (1998–2005)

# NLA Challenge: Hyper-sparsity

#### Recall: major computational components

- FTRAN: Form  $\widehat{a}_q = B^{-1} a_q$
- BTRAN: Form  $\pi_p = B^{-T} \boldsymbol{e}_p$
- **PRICE**: Form  $\widehat{\boldsymbol{a}}_p^T = \pi_p^T N$

### BTRAN: Form $\pi_p = B^{-T} \boldsymbol{e}_p$

- Transposed triangular solves
- $L^T \mathbf{x} = \mathbf{b}$  has  $x_i = b_i \mathbf{I}_i^T \mathbf{x}$ 
  - Hyper-sparsity:  $\boldsymbol{I}_i^T \boldsymbol{x}$  typically zero
  - Also store *L* (and *U*) row-wise and use FTRAN code

PRICE: Form 
$$\widehat{\boldsymbol{a}}_p^T = \pi_p^T N$$

- Hyper-sparsity:  $\pi_p^T$  is sparse
- Store N row-wise
- Form *a*<sup>T</sup><sub>p</sub> as a combination of rows of N for nonzeros in π<sup>T</sup><sub>p</sub>

H and McKinnon (1998-2005)

NLA Challenge: Novel update techniques

### NLA Challenge: Alternative product form update

- **Recall:** Column *p* of *B* is replaced by  $\boldsymbol{a}_q$  to give  $\bar{B} = B + (\boldsymbol{a}_q B\boldsymbol{e}_p)\boldsymbol{e}_p^T$ 
  - Traditional PFI takes B out as a factor on the left so  $\bar{B} = BE$
- Idea: Why not take it out on the right!

$$ar{B} = [I + (oldsymbol{a}_q - Boldsymbol{e}_p)oldsymbol{e}_p^TB^{-1}]B = TB$$
  
where  $T = I + (oldsymbol{a}_q - oldsymbol{a}_{p'})oldsymbol{\widehat{e}}_p^T$ 

• *T* is formed of known data and readily invertible (like *E* for PFI) Naturally compute  $\hat{e}_p$  when solving  $B^T \pi_p = e_p$ 

### NLA Challenge: Middle product form update

- **Recall:** Column p of B is replaced by  $\boldsymbol{a}_q$  to give  $\bar{B} = B + (\boldsymbol{a}_q B\boldsymbol{e}_p)\boldsymbol{e}_p^T$
- Idea: Substitute B = LU and take factors L on the left and U on the right!

$$\begin{split} \bar{B} &= LU + (\boldsymbol{a}_q - B\boldsymbol{e}_p)\boldsymbol{e}_p^T \\ &= LU + LL^{-1}(\boldsymbol{a}_q - B\boldsymbol{e}_p)\boldsymbol{e}_p^T U^{-1}U \\ &= L[I + (\widetilde{\boldsymbol{a}}_q - U\boldsymbol{e}_p)\widetilde{\boldsymbol{e}}_p^T]U \\ &= LMU \quad \text{where} \quad M = I + (\widetilde{\boldsymbol{a}}_q - \boldsymbol{u}_p)\widetilde{\boldsymbol{e}}_p^T \end{split}$$

• *M* is formed of known data and readily invertible (like *E* for PFI) Naturally compute  $\tilde{a}_q$  when solving  $B \hat{a}_q = a_q$  and  $\tilde{e}_p$  when solving  $B^T \pi_p = e_p$ 

- Update Forrest-Tomlin representation of B after multiple basis changes
- Don't have data to perform a sequence of standard FT updates
- Have to perform elimination corresponding to multiple spikes

Huangfu and H (2013)

NLA Challenge: Parallel solution of structured LP problems

# NLA Challenge: Parallel solution of stochastic MIP problems

Two-stage stochastic LPs have column-linked block angular (BALP) structure

- Variables  $x_0 \in \mathbb{R}^{n_0}$  are first stage decisions
- Variables  $\mathbf{x}_i \in \mathbb{R}^{n_i}$  for i = 1, ..., N are second stage decisions Each corresponds to a scenario which occurs with modelled probability
- The objective is the expected cost of the decisions
- In stochastic MIP problems, some/all decisions are discrete

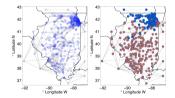
# NLA Challenge: Parallel solution of stochastic MIP problems

- Power systems optimization project at Argonne
- Integer second-stage decisions
- Stochasticity from wind generation
- Solution via branch-and-bound
  - Solve root using parallel IPM solver PIPS

Lubin, Petra et al. (2011)

• Solve nodes using parallel dual simplex solver PIPS-S



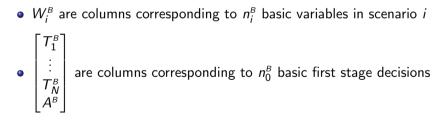


Convenient to permute the LP thus:

### PIPS-S: Exploiting problem structure

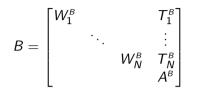
• Inversion of the basis matrix B is key to revised simplex efficiency

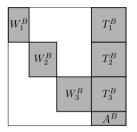
$$B = \begin{bmatrix} W_1^B & & T_1^B \\ & \ddots & & \vdots \\ & & W_N^B & T_N^B \\ & & & A^B \end{bmatrix}$$



### PIPS-S: Exploiting problem structure

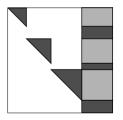
• Inversion of the basis matrix B is key to revised simplex efficiency





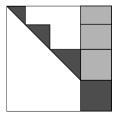
- B is nonsingular so
  - $W_i^{\scriptscriptstyle B}$  are "tall": full column rank
  - $\begin{bmatrix} W_i^B & T_i^B \end{bmatrix}$  are "wide": full row rank
  - $A^{\scriptscriptstyle B}$  is "wide": full row rank
- Scope for parallel inversion is immediate and well known

• Eliminate sub-diagonal entries in each  $W_i^{\scriptscriptstyle B}$  (independently)



• Apply elimination operations to each  $T_i^B$  (independently)

 Accumulate non-pivoted rows from the W<sup>B</sup><sub>i</sub> with A<sup>B</sup> and complete elimination



### Scope for parallelism

- Parallel Gaussian elimination yields **block LU** decomposition of B
- Scope for parallelism in block forward and block backward substitution
- Scope for parallelism in PRICE

### Implementation

- Distribute problem data over processes
- Perform data-parallel BTRAN, FTRAN and PRICE over processes
- Used MPI

Lubin, H, Petra and Anitescu (2013)

### **PIPS-S:** Results

On Fusion cluster: Performance relative to clp										
	Dimension	Cores	Storm	SSN	UC12	UC24				
	$m+n=O(10^6)$	1 32	0.34 8.5		0.17 2.4					
	$m+n=O(10^7)$	256	299	45	67	68				

### On Blue Gene

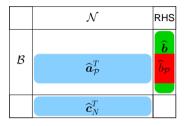
- Instance of UC12
- $m + n = O(10^8)$
- Requires 1 TB of RAM
- Runs from an advanced basis

Cores	Iterations	Time (h)	lter/sec
1024	Exceeded	execution t	ime limit
2048	82,638	6.14	3.74
4096	75,732	5.03	4.18
8192	86,439	4.67	5.14

NLA Challenge: Parallel solution of general LP problems

## NLA Challenge: Parallel solution of general LP problems

- Perform standard dual simplex minor iterations for rows in set  $\mathcal{P}~(|\mathcal{P}|\ll m)$
- Suggested by Rosander (1975) but never implemented efficiently in serial



- Task-parallel multiple BTRAN to form  $m{\pi}_{\mathcal{P}}=B^{-T}m{e}_{\mathcal{P}}$
- Data-parallel PRICE to form  $\widehat{a}_{p}^{T}$  (as required)
- Task-parallel multiple FTRAN for primal, dual and weight updates
- Novel update techniques for minor iterations

Huangfu and H (2011-2014)

# NLA Challenge: HiGHS (2011-date)

#### Overview

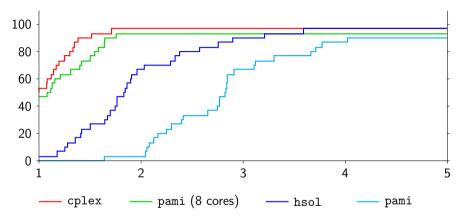
- Written in C++ to study parallel simplex
- Dual simplex with steepest edge and BFRT
- Forrest-Tomlin update
  - complex and inherently serial
  - efficient and numerically stable

### Concept

- High performance serial solver (hsol)
- Exploit limited task and data parallelism in standard dual RSM iterations (sip)
- Exploit greater task and data parallelism via minor iterations of dual SSM (pami)
- Test-bed for research
- Work-horse for consultancy

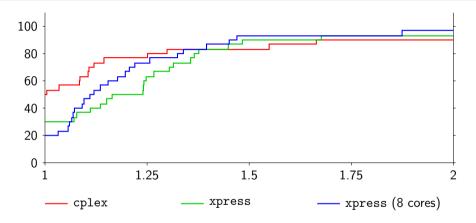
Huangfu, H and Galabova (2011-date)

### HiGHS: cplex vs pami vs hsol



- pami is less efficient than hsol in serial
- pami speedup more than compensates
- pami performance approaching cplex

### HiGHS: Impact



- pami ideas incorporated in FICO Xpress (Huangfu 2014)
- Xpress has been the fastest simplex solver for most of the past five years

### To close

#### Conclusions

- Revised simplex method offers NLA challenges
- Novel techniques of practical value are hard to find but get noticed
- Look for alternative algorithms for fast (approximate) solution of LPs

### Slides:

http://www.maths.ed.ac.uk/hall/NLAO18

#### Code:

https://github.com/ERGO-Code/HiGHS

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