Parallel distributed-memory simplex for large-scale stochastic LP problems

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ERGO Seminar

June 26th 2012

Overview

- Block-angular structure
- Motivation: stochastic programming and the power grid
- Parallelization of the simplex algorithm for block-angular linear programs

Large-scale (dual) block-angular LPs

$$
\begin{array}{lccccccccccc}
\min & c_0^T x_0 & + & c_1^T x_1 & + & c_2^T x_2 & + & \dots & + & c_N^T x_N & & \\
\text{s.t.} & A x_0 & & & & & & & & & = & b_0, \\
& T_1 x_0 & + & W_1 x_1 & & & & & & & = & b_1, \\
& T_2 x_0 & & & + & W_2 x_2 & & & & & = & b_2, \\
& \vdots & & & & & & \ddots & & & & \vdots \\
& T_N x_0 & & & & & & & + & W_N x_N & = & b_N, \\
& x_0 \geq 0, & & x_1 \geq 0, & & x_2 \geq 0, & & \dots, & & x_N \geq 0. & &
\end{array}
$$

- In terminology of stochastic LPs:
  - First-stage variables (decision now): x_0
  - Second-stage variables (recourse decision): $x_1, \dots, x_N$
  - Each diagonal block is a realization of a random variable (scenario)

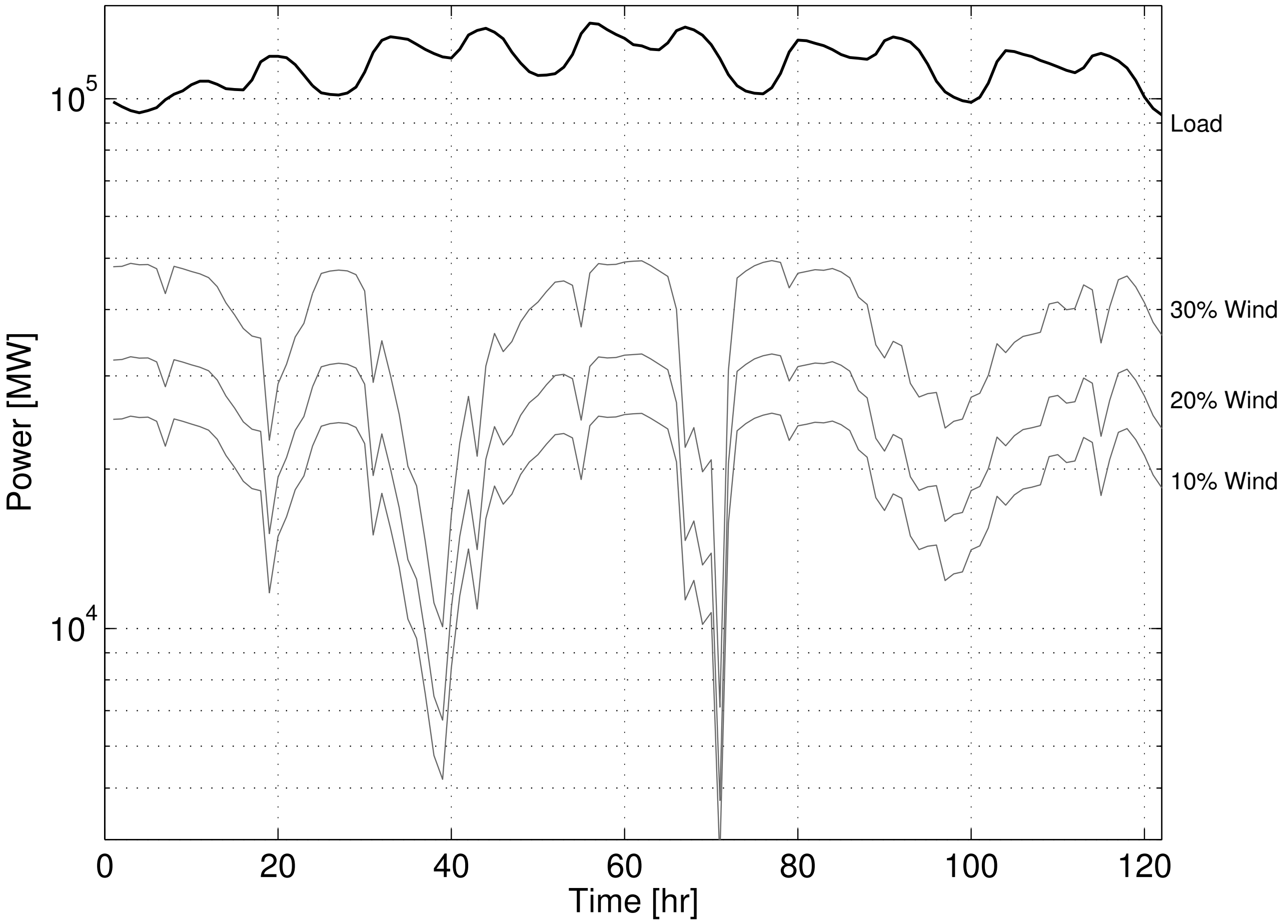
Why?

- Block-angular structure one of the first structures identified in linear programming
  - Specialized solution procedures dating to late 1950s
- Many, many applications
- We're interested in two-stage stochastic LP problems with a finite number of scenarios
  - Optimization under uncertainty
  - Power-grid control under uncertainty

Stochastic Optimization and the Power Grid

- **Unit Commitment**: Determine optimal on/off schedule of thermal (coal, natural gas, nuclear) generators. Day-ahead market prices. (hourly)
  - Mixed-integer
- **Economic Dispatch**: Set real-time market prices. (every 5-10 min.)
  - Continuous Linear/Quadratic
- **Challenge**: Integrate energy produced by highly variable renewable sources into these control systems.
  - Minimize operating costs, subject to:
    - Physical generation and transmission constraints
    - Reserve levels
    - Demand
    - …

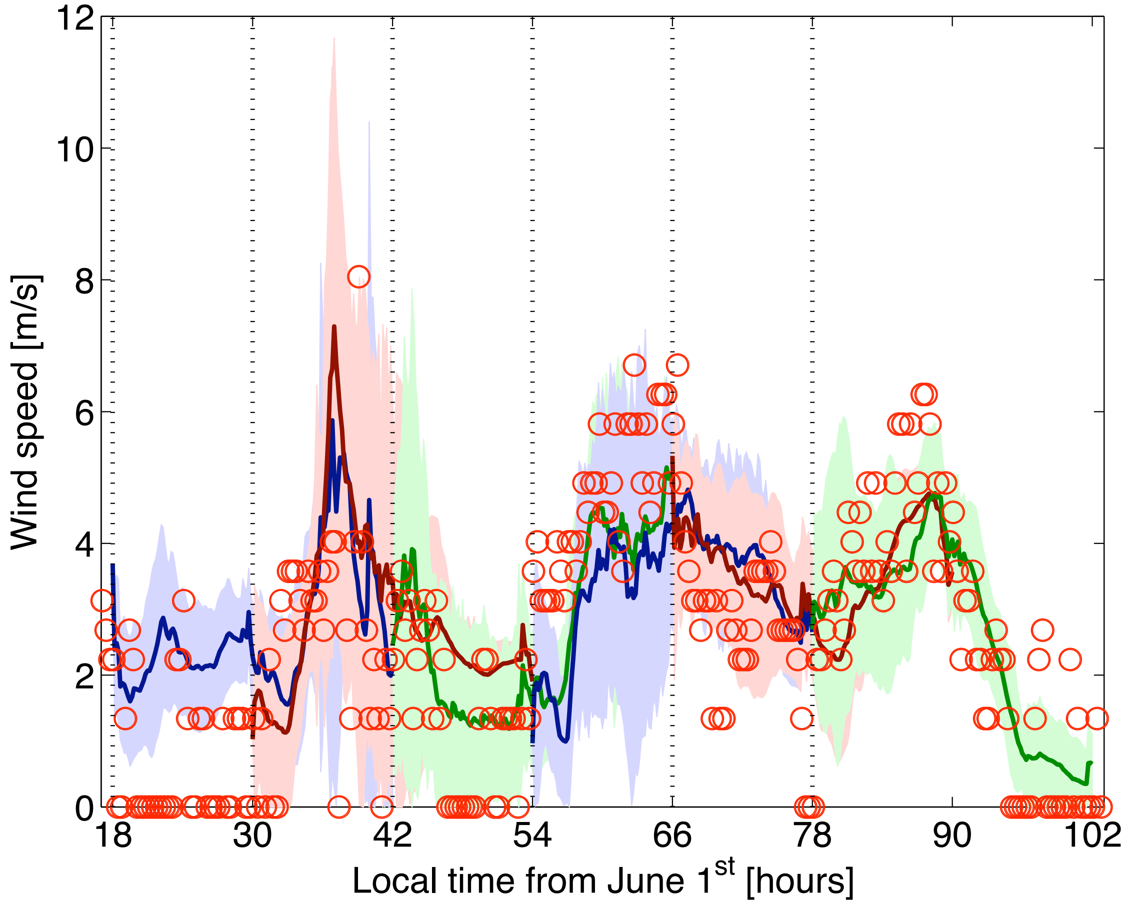
Variability in Wind Energy



Deterministic vs. Stochastic Approach

- To schedule generation, need to know how much wind energy there will be.
- **Deterministic**:
  - Run weather model once, obtain simple predicted values for wind. Plug into optimization problem.
- **Stochastic**:
  - Run ensemble of weather models to generate range of possible wind scenarios. Plug into stochastic optimization problem.
  - These are given to us (the optimizers) as input.

Deterministic vs. Stochastic Approach



- Single predictions may be very inaccurate, but truth usually falls within range of scenarios.
  - Uncertainty Quantification (Constantinescu, et al. 2010)

Stochastic Formulation

$$
\begin{aligned}
\min_{x \in \mathbb{R}^{n_1}} \quad & c^T x + \mathbb{E}_\xi[Q(x,\xi)] \\
\text{s.t.}\ & Ax = b, \\
& x \geq 0,
\end{aligned}
$$

where

$$
\begin{aligned}
Q(x,\xi) = \min_{y \in \mathbb{R}^{n_2}} \quad & q_\xi^T y \\
\text{s.t.}\ & T_\xi x + W y = h_\xi, \\
& y \geq 0.
\end{aligned}
$$

(some x, y integer)

- Discrete distribution leads to block-angular (MI)LP

Large-scale (dual) block-angular LPs

$$\begin{array}{rcccccccccccl}
\min & c_0^T x_0 & + & c_1^T x_1 & + & c_2^T x_2 & + & \ldots & + & c_N^T x_N & & \\
\text{s.t.} & A x_0 & & & & & & & & & = & b_0, \\
& T_1 x_0 & + & W_1 x_1 & & & & & & & = & b_1, \\
& T_2 x_0 & & & + & W_2 x_2 & & & & & = & b_2, \\
& \vdots & & & & & & \ddots & & & & \vdots \\
& T_N x_0 & & & & & & & + & W_N x_N & = & b_N, \\
& \multicolumn{12}{l}{x_0 \geq 0, \quad x_1 \geq 0, \quad x_2 \geq 0, \quad \ldots, \quad x_N \geq 0.}
\end{array}$$

- In terminology of stochastic LPs:
  - First-stage variables (decision now): x_0
  - Second-stage variables (recourse decision): $x_1, \ldots, x_N$
  - Each diagonal block is a realization of a random variable (scenario)

Difficulties

- May require many scenarios (100s, 1,000s, 10,000s …) to accurately model uncertainty
- "Large" scenarios (W_i up to 100,000 x 100,000)
- "Large" 1st stage (1,000s, 10,000s of variables)
- Easy to build a practical instance that requires 100+ GB of RAM to solve
  - → Requires distributed memory

Plus

- Integer constraints

Existing parallel solution methods

- Based on Benders decomposition
  - Classical approach
  - Asynchronous work by Linderoth and Wright (2003)
- Linear-algebra decomposition inside interior-point methods
  - OOPS (Gondzio and Grothey, 2009)
  - PIPS-IPM (Petra, et al.)
  - Demonstrated capability to efficiently solve large problems from scratch

Focus on warm starts

- With integer constraints, warm starts necessary inside branch and bound
- Real-time control (rolling horizons)
- Neither Benders or IPM approaches particularly suitable …
  - Benders somewhat warm-startable using regularization
  - IPM warm start possible but limited to ~50% speedup
- But we know an algorithm that is…

Idea

- Apply the (revised) simplex method directly to the large block-angular LP
- Parallelize its operations based on the special structure
- Many practitioners and simplex experts (attendees excluded) would say that this won't work

Overview of remainder

- The simplex algorithm
- Computational components of the revised simplex method
- Our parallel decomposition for dual block-angular LPs
- Numerical results
- First experiments with integer constraints

LP in standard form

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & Ax = b \\ & x \geq 0 \end{aligned}$$

Given a basis, projected LP

Given

$$A = \begin{bmatrix} B & N \end{bmatrix}$$

$$c = \begin{bmatrix} c_B & c_N \end{bmatrix}$$

$$x = \begin{bmatrix} x_B & x_N \end{bmatrix}$$

$$\begin{array}{ll} \min & c_B^T B^{-1} b + (c_N^T - c_B^T B^{-1} N) x_N \\ \text{s.t.} & B^{-1}(b - N x_N) \geq 0 \\ & x_N \geq 0 \end{array}$$

Idea of primal simplex

- Given a basis, define current iterates as

$$\hat{x}_B := B^{-1}b$$

$$\hat{x}_N := 0$$

$$\hat{s}_N := c_N - N^T B^{-T} c_B$$

- Assume $\hat{x}_B \geq 0$ (primal feasibility)
- If a component of $\hat{s}_N$ (reduced costs) is negative, increasing the corresponding component of $\hat{x}_N$ will decrease the objective, so long as feasibility is maintained.

Mathematical algorithm

- Given a basis and current iterates, identify index q such that $\hat{s}_q < 0$. **(Edge selection)**
  - If none exists, terminate with an optimal solution.
- Determine maximum step length θ^P such that $\hat{x}_B - \theta^P B^{-1} N e_q \geq 0$. **(Ratio test)**
  - Let p be the blocking index with $(\hat{x}_B - \theta^P B^{-1} N e_q)_p = 0$.
  - If none exists, problem is unbounded.
- Replace the pth variable in the basis with variable q. Repeat.

Computational algorithm

- Computational concerns:
  - Inverting basis matrix
  - Solving linear systems with basis matrix
  - Matrix-vector products
  - Updating basis inverse and iterates after basis change
  - **Sparsity**
  - Numerical stability
  - Degeneracy
  - …
- A modern simplex implementation is over 100k lines of C++ code.
- Will review key components.

Computational algorithm (Primal Simplex)

`CHUZC:` Scan $\hat{s}_N$ for a good candidate q to enter the basis.
`FTRAN:` Form the pivotal column $\hat{a}_q = B^{-1} a_q$, where a_q is column q of A.
`CHUZR:` Scan the ratios $(\hat{x}_B)_i / \hat{a}_{iq}$ for the row p of a good candidate to leave the basis.
Update $\hat{x}_B := \hat{x}_B - \theta^P \hat{a}_q$, where $\theta^P = (\hat{x}_B)_p / \hat{a}_{pq}$.
`BTRAN:` Form $\pi_p = B^{-T} e_p$.
`PRICE:` Form the pivotal row $\hat{a}_p = N^T \pi_p$.
Update reduced costs $\hat{s}_N := \hat{s}_N - \theta^D \hat{a}_p$, where $\theta^D = \hat{s}_q / \hat{a}_{pq}$.
`If` $\{$growth in representation of $B^{-1}\}$ `then`
    `INVERT:` Form a new representation of B^{-1}.
`else`
    `UPDATE:` Update the representation of B^{-1} corresponding to the basis change.
`end if`

Edge selection

- Choice in how to select edge to step along
  - Rule used has significant effect on the number of iterations
- Dantzig rule ("most negative reduced cost") is suboptimal
- In practice, *edge weights* used, choosing

$$q = \operatorname{argmax}_{\hat{s}_j < 0} |\hat{s}_j| / w_j .$$

  - Exact "steepest edge" (Forrest and Goldfarb, 1992)
  - DEVEX heuristic (Harris, 1973)
- Extra computational cost to maintain weights, but large decrease in number of iterations

Ratio test

- Also have choice in the ratio test
- "Textbook" ratio test: $\theta^P = \min_i \, (\hat{x}_B)_i / \hat{a}_{iq}$
  - Small values of $\hat{a}_{iq}$ cause numerical instability
  - Fails on practical problems
- Instead, use *two-pass* ratio test
  - Allow small infeasibilities in order improve numerical stability
  - See EXPAND (Gill et al., 1989)

Basis inversion and linear solves

- Typically, Markowitz (1957)-type procedure used to form sparse LU factorization of basis matrix
  - LU factorization before "LU factorization" existed
  - Gaussian elimination with pivotal row and column chosen dynamically to reduce fill-in of non-zero elements
  - Uncommon factorization outside of simplex; best for special structure of basis matrices (e.g. many columns of the identity, highly unsymmetric)
- Need to exploit sparsity in right-hand sides when solving linear systems (*hyper-sparsity*, see Hall and McKinnon, 2005)

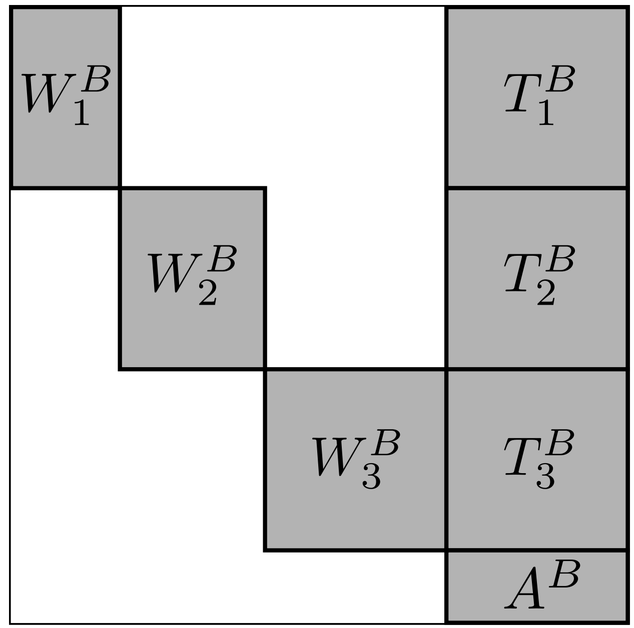
Basis updates

- At every iteration, a column of the basis matrix is replaced.
  - Inefficient to recompute factorization from scratch each time.
- Product-form update: (earliest form, Dantzig and Or-H, 1954)

$$\begin{aligned}\overline{B} &= B + (a_q - Be_p)e_p^T \\ &= B(I + (\hat{a}_q - e_p)e_p^T), \hat{a}_q = B^{-1}a_q. \\ E &:= (I + (\hat{a}_q - e_p)e_p^T)^{-1} = (I + \eta e_p^T). \\ \rightarrow \overline{B}^{-1} &= EB^{-1}\end{aligned}$$

- Originally used to invert the basis matrix! (column by column)
- Today, LU factors updated instead (e.g, Forrest and Tomlin, 1972)

Decomposition – Structure of the basis matrix



$$
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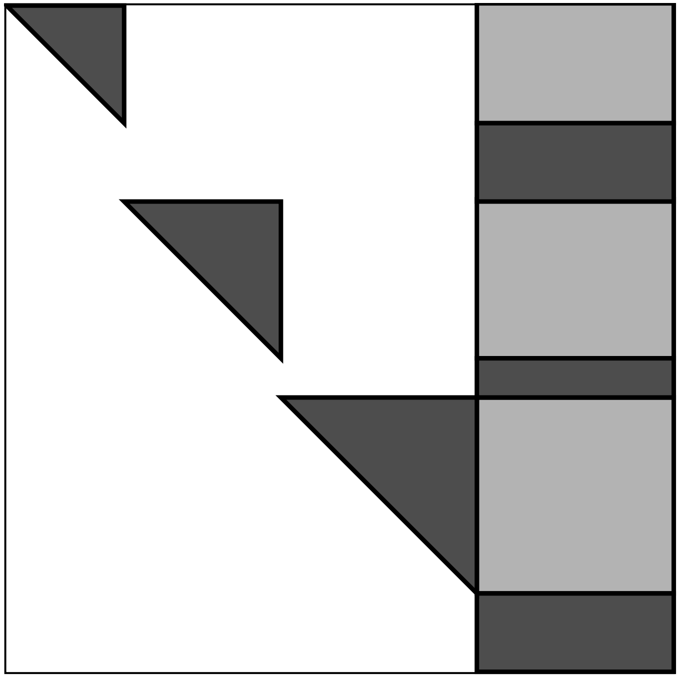
\end{array}
$$

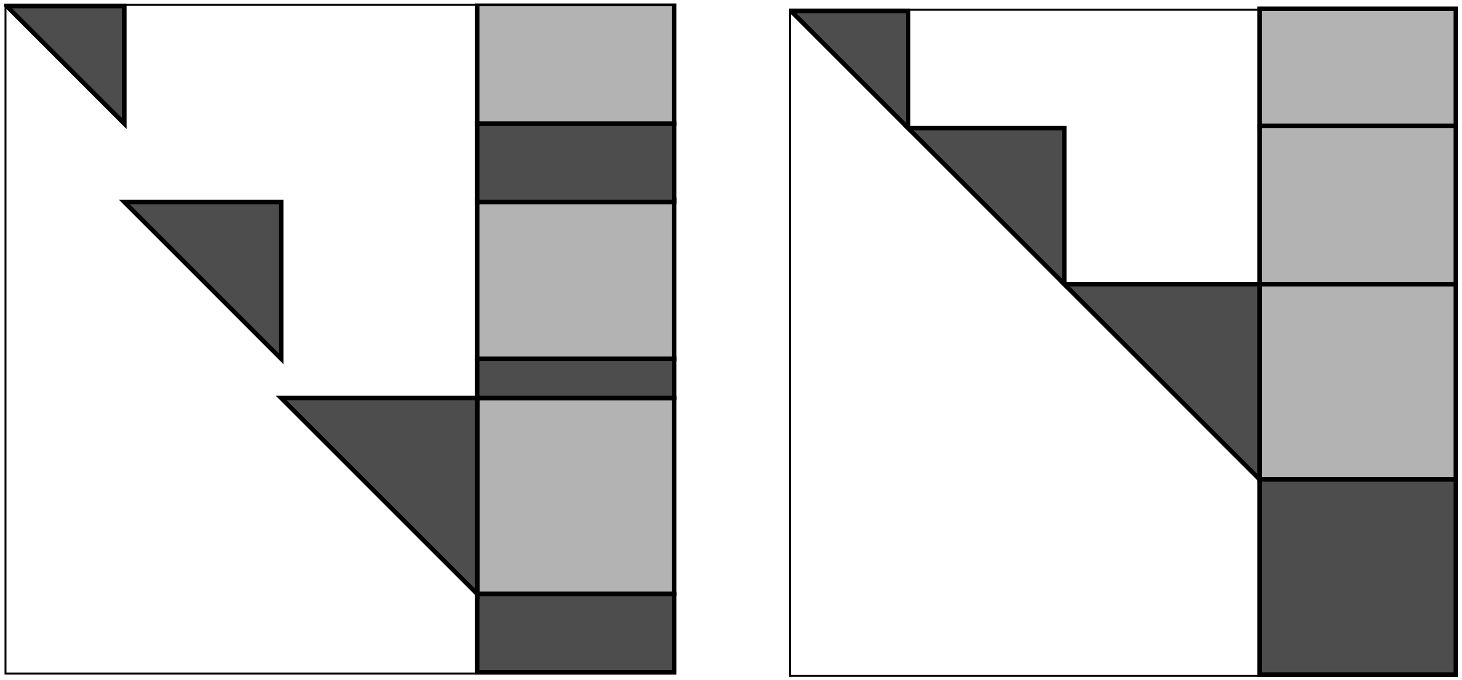
Key linear algebra

- Observation: Eliminating lower-triangular elements in diagonal blocks causes no structure-breaking fill-in
- Observation: May be performed in parallel



Key linear algebra – Implicit LU factorization

1. Factor diagonal blocks in parallel
2. Collect rows of square bottom-right *first-stage* system
3. Factor first-stage system



Implementation

- New codebase "PIPS-S"
  - C++, MPI
  - Reuses many primitives (vectors, matrices) from open-source CoinUtils
  - Algorithmic implementation written from scratch
  - Implements both primal and dual simplex

Implementation - Distribution of data

- Before reviewing operations, important to keep in mind distribution of data
- Targeting distributed-memory architectures (MPI) in order to solve large problems.
- Given P MPI processes and $N\,(\geq P)$ second-stage scenarios, assign each scenario to one MPI process.
- Second-stage data and iterates only stored on respective process. ➔Scalable
- First-stage data and iterates duplicated in each process.

$$
\begin{array}{rccccccccccl}
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  `INVERT:` Form a new representation of B^{-1}.

`else`

  `UPDATE:` Update the representation of B^{-1} corresponding to the basis change.

`end if`

Implementation - Basis Inversion (INVERT)

- Want to reduce non-zero fill-in both in diagonal blocks and on the border
  - Determined by choice of row/column permutations
- Modify existing LU factorization to handle this, by giving as input the augmented system
$$\begin{bmatrix} W_i^B & T_i^B \end{bmatrix},$$
and restricting column pivots to the W_i^B block.
- Implemented by modifying `CoinFactorization` (John Forrest) of open-source CoinUtils package.
- Collect non-pivotal rows from each process, forming first-stage system. Factor first-stage system identically in each MPI process.

Implementation – Linear systems with basis matrix (FTRAN)

- Obtain procedure to solve linear systems with basis matrix by following math for inversion procedure; overview below:

1. Triangular solve for each scenario (parallel)
2. Gather result from each process (communication)
3. Solve first-stage system (serial)
4. Matrix-vector product and triangular solve for each scenario (parallel)

Implementation - Linear systems with basis transpose (BTRAN)

1. Triangular solve and matrix-vector product for each scenario (parallel)
2. Sum contributions from each process (communication)
3. Solve first-stage system (serial)
4. Triangular solve for each scenario (parallel)

Implementation - Matrix-vector product with non-basic columns (PRICE)

$$\begin{bmatrix} W_1^N & & & & T_1^N \\ & W_2^N & & & T_2^N \\ & & \ddots & & \vdots \\ & & & W_N^N & T_N^N \\ & & & & A^N \end{bmatrix}^T \begin{bmatrix} \pi_1 \\ \pi_2 \\ \vdots \\ \pi_N \\ \pi_0 \end{bmatrix} = \begin{bmatrix} (W_1^N)^T \pi_1 \\ (W_2^N)^T \pi_2 \\ \vdots \\ (W_N^N)^T \pi_N \\ (A^N)^T \pi_0 + \sum_{i=1}^N (T_i^N)^T \pi_i \end{bmatrix}$$

- Parallel procedure evident from above:

1. Compute $(W_i^N)^T \pi_i, (T_i^N)^T \pi_i$ terms (parallel)
2. Form $\sum_{i=1}^N (T_i^N)^T \pi_i$ (communication, `MPI_Allreduce`)
3. Form $(A^N)^T \pi_0$ (serial)

Implementation - Edge selection and ratio test

- Straightforward parallelization
- Each process scans through its local variables, then `MPI_Allreduce` determines the maximum/minimum across processes and its corresponding owner

Implementation - Basis updates

$$\overline{B}^{-1} = E_k \ldots E_2 E_1 B^{-1}$$

$$E_i = (I + \eta_i e_{p_i}^T)$$

- Consider operations to apply "eta" matrix to a right-hand side:

$$E_i x = (I + \eta_i e_{p_i}^T)x = (x + x_{p_i}\eta)$$

- What if *pivotal element* x_{p_i} is only stored on one MPI process?
  - Would need to perform a broadcast operation for every eta matrix; huge communication overhead
- Developed a procedure that requires only one communication per sequence of eta matrices.

Numerical Experiments

- Comparisons with highly-efficient serial solver Clp
- Presolve and internal rescaling disabled (not implemented in PIPS-S)
- 10^{-6} feasibility tolerances used
- Preview of conclusions before the numbers:
  - Clp 2-4x faster in serial
  - Significant speedups (up to 100x, typically less) over Clp in parallel
  - Solves problems that don't fit in memory on a single machine

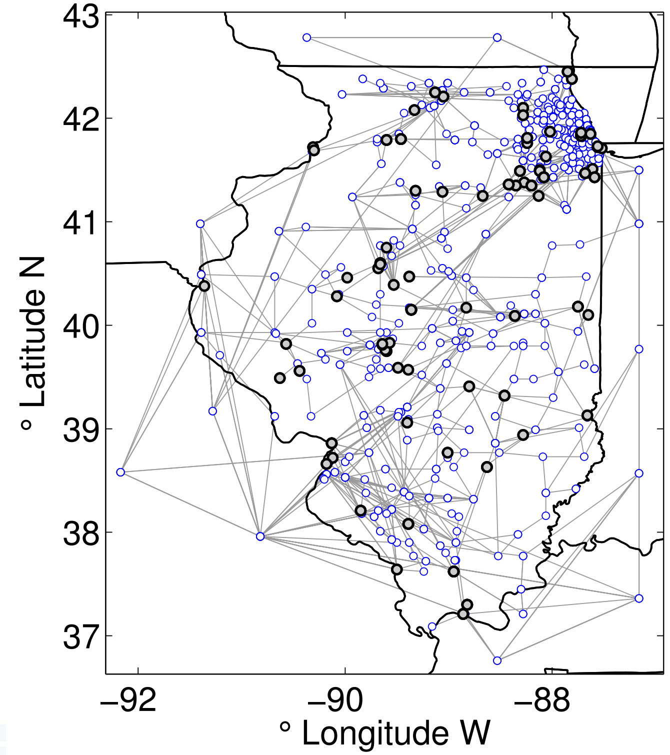
Test problems

Test Problem	1st Stage Vars.	1st Stage Cons.	2nd-Stage Scenario Vars.	2nd-Stage Scenario Cons.	Nonzero Elements A	Nonzero Elements W_i	Nonzero Elements T_i
Storm	121	185	1,259	528	696	3,220	121
SSN	89	1	706	175	89	2,284	89
UC12	3,132	0	56,532	59,436	0	163,839	3,132
UC24	6,264	0	113,064	118,872	0	327,939	6,264

- Storm and SSN used by Linderoth and Wright
- UC12 and UC24 developed by Victor Zavala
- Scenarios generated by Monte-Carlo sampling

UC12 and UC24

- Stochastic Unit Commitment models with 12-hour and 24-hour planning horizons over the state of Illinois.
- Includes (DC) transmission constraints.



Architectures

- “Fusion” high-performance cluster at Argonne
  - 320 nodes
  - InfiniBand QDR interconnect
  - Two 2.6 Ghz Xeon processors per node (total 8 cores)
  - Most nodes have 36 GB of RAM, some have 96 GB
- “Intrepid” Blue Gene/P supercomputer
  - 40,960 nodes
  - Custom interconnect
  - Each node has quad-core 850 Mhz PowerPC processor, 2 GB RAM

Large problems with advanced starts

- Solves "from scratch" not particularly of interest
- Consider large problems that require "high-memory" (96GB) nodes of Fusion cluster
  - 20-40 Million total variables/constraints
- Advanced starting bases in the context of:
  - Using solution to subproblem with a subset of scenarios to generate a starting basis for extensive form
    - Storm and SSN
    - Not included in time to solution
  - Simulate branch and bound (reoptimize after modifying bounds)
    - UC12 and UC24

Storm and SSN – 32,768 scenarios

Test Problem	Solver	Nodes	Cores	Iter./ Sec.
Storm	Clp	1	1	2.2
	PIPS-S	1	1	1.3
	"	1	4	10.0
	"	1	8	22.4
	"	2	16	47.6
	"	4	32	93.9
	"	8	64	158.8
	"	16	128	216.6
	"	32	256	260.4
SSN	Clp	1	1	2.0
	PIPS-S	1	1	0.8
	"	1	4	4.1
	"	1	8	10.5
	"	2	16	22.9
	"	4	32	46.8
	"	8	64	92.8
	"	16	128	143.3
	"	32	256	180.0

UC12 (512 scenarios) and UC24 (256 scenarios)

Test Problem	Solver	Nodes	Cores	Avg. Iter./Sec
UC12	Clp	1	1	0.73
	PIPS-S	1	1	0.34
	"	1	8	2.5
	"	2	16	4.7
	"	4	32	8.8
	"	8	64	14.9
	"	16	128	20.9
	"	32	256	25.8
UC24	Clp	1	1	0.87
	PIPS-S	1	1	0.36
	"	1	8	2.4
	"	2	16	4.4
	"	4	32	8.2
	"	8	64	14.8
	"	16	128	23.2
	"	32	256	28.7

Very big instance

- UC12 with 8,192 scenarios
  - 463,113,276 variables and 486,899,712 constraints
- Advanced starting basis from solution to problem with 4,096 scenarios
- Solved to optimal basis in 86,439 iterations (4.6 hours) on 4,096 nodes of Blue Gene/P (2 MPI processes per node)
- Would require ~1TB of RAM to solve in serial (so no comparison with Clp)

Performance analysis

- Simple performance model for execution time of an operation:

$$\max_p \{t_p\} + c + t_0,$$

where t_p is the time spent by process p on its local second-stage calculations, c is the communication cost, and t_0 is the time spent on the first-stage calculations.

- Limits to scalability:
  - Load imbalance: $\max_p\{t_p\} - \frac{1}{P}\sum_{i=1}^{P} t_p$
  - Communication cost: c
  - Serial bottleneck: t_0
- Instrumented matrix-vector product (PRICE) to compute these quantities

Matrix-vector product with non-basic columns (PRICE)

$$\begin{bmatrix} W_1^N & & & & T_1^N \\ & W_2^N & & & T_2^N \\ & & \ddots & & \vdots \\ & & & W_N^N & T_N^N \\ & & & & A^N \end{bmatrix}^T \begin{bmatrix} \pi_1 \\ \pi_2 \\ \vdots \\ \pi_N \\ \pi_0 \end{bmatrix} = \begin{bmatrix} (W_1^N)^T \pi_1 \\ (W_2^N)^T \pi_2 \\ \vdots \\ (W_N^N)^T \pi_N \\ (A^N)^T \pi_0 + \sum_{i=1}^N (T_i^N)^T \pi_i \end{bmatrix}$$

1. Compute $(W_i^N)^T \pi_i, (T_i^N)^T \pi_i$ terms (parallel)
2. Form $\sum_{i=1}^N (T_i^N)^T \pi_i$ (communication, `MPI_Allreduce`)
3. Form $(A^N)^T \pi_0$ (serial)

Performance analysis – "Large" instances

Test Problem	Nodes	Cores	Load Imbal. (μs)	Comm. Cost (μs)	Serial Bottleneck (μs)	Total Time/Iter. (μs)
Storm	1	1	0	0	1.0	13,243
	1	8	88	33	0.8	1,635
	2	16	40	68	0.9	856
	4	32	25	105	0.9	512
	8	64	26	112	1.0	326
	16	128	11	102	0.9	205
	32	256	34	253	0.8	333
SSN	1	1	0	0	0.8	2,229
	1	8	18	23	0.8	305
	2	16	25	54	0.8	203
	4	32	14	68	0.7	133
	8	64	12	65	0.7	100
	16	128	10	87	0.6	106
	32	256	8	122	0.6	135

Performance analysis – "Large" instances

Test Problem	Nodes	Cores	Load Imbal. (μs)	Comm. Cost (μs)	Serial Bottleneck (μs)	Total Time/Iter. (μs)
UC12	1	1	0	0	6.8	24,291
	1	8	510	183	6.0	4,785
	2	16	554	274	6.0	2,879
	4	32	563	327	6.0	1,921
	8	64	542	355	6.0	1,418
	16	128	523	547	6.0	1,335
	32	256	519	668	5.8	1,323
UC24	1	1	0	0	11.0	28,890
	1	8	553	259	9.8	5,983
	2	16	543	315	9.7	3,436
	4	32	551	386	9.6	2,248
	8	64	509	367	9.5	1,536
	16	128	538	718	9.5	1,593
	32	256	584	1413	9.5	2,170

Performance analysis

- First-stage calculation bottleneck relatively insignificant
- Load imbalance depends on problem
  - Caused by exploiting hyper-sparsity
- Communication cost significant, but small enough to allow for significant speedups
  - Speedups on Fusion unexpected
  - High-performance interconnects (Infiniband)

Back to what we wanted to solve - Preliminary results

- First-stage variables in UC12 are binary on/off generator states
- With 64 scenarios (3,621,180 vars., 3,744,468 cons., 3,132 binary)
  - LP Relaxation: 939,208
  - LP Relaxation + `CglProbing` cuts: 939,626
  - Feasible solution from rounding: 942,237
  - Optimality Gap: 0.27% (0.5% is acceptable in practice)
  - Starting with optimal LP basis:
    - 1 hour with PIPS-S on 4 nodes (64 cores) of Fusion
    - 4.75 hours with Clp in serial
- Further decrease in gap by better primal heuristics and more cut generators
- UC12 can be “solved” at the root node!
  - Reported in literature for similar deterministic model

Conclusions

- Simplex method is parallelizable for dual block-angular LPs
- Significant speedups over highly-efficient serial solvers possible on a high-performance cluster on appropriately sized problems
- Sequences of large-scale block-angular LPs can now be solved efficiently in parallel
- Path forward for block-angular MILPs
  - Solve stochastic unit commitment problem at root node?
  - Parallel simplex inside parallel branch and bound?

Conclusions

- Communication intensive optimization algorithms can successfully scale on today's high-performance clusters
  - Each simplex iteration has ~10 collective (broadcast/all-to-all) communication operations.
  - Observed 100s of iterations per second.
  - Communication cost is order of 10s/100s of *micro*seconds
    - Used to be order of milliseconds

Thank you!