Object-Parallel Solution of Large-Scale Lasso Problems

Jonathan Eckstein
Rutgers University, NJ, USA

joint work with

György Mátyásfalvi (doctoral student)
Rutgers University, NJ, USA

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Newark and New Brunswick

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Why “Object-Parallel”?

- Current trend: growth in computer power is mainly through increased parallelism
    - Speed of executing a single thread is not improving much
- To solve huge problem instances, including from “big data”, we need scalably parallel algorithms and implementations
- The best ways to exploit parallelism are often dictated by problem instance data structure and are thus highly application-dependent

Suggests we need optimization environments in which

- The application guides the use of parallelism as flexibly as possible
- The underlying algorithms can adapt easily to very different data representations (across distributed memory)

An “Object-Parallel” Approach to Optimization

- An “inside-out” approach:

- User determines the most appropriate data layout for a given application
  - How variables are divided (and perhaps replicated) among processors
  - And similarly for constraints
  - User provides (presumably efficient) calculations of objectives, constraints, and their derivatives using these layouts

- The optimization code is an algorithmic “template” that is applied to the user’s data representation

What Kind of Optimization Algorithms Seem Suitable to Such a Context?

- Methods that use only first derivatives
  - Structure of Hessians may be too complex for users to contemplate
- Methods that do not directly solve linear systems:
  - Structure of factors of matrices like

$$\begin{bmatrix} H & J^{\mathsf{T}} \\ J & 0 \end{bmatrix}$$

  may be too much for users to think about, or may defeat simple parallelism within calculating gradients/Jacobians

- Restrictive, but not impossible:
  - These are largely the same restrictions that apply to most approaches to solving very large-scale problem instances

A Possible General NLP Approach (Digression): Relative-Error First-Order Approximate Augmented Lagrangians

- Quadratic augmented Lagrangian “outer loop”
- Subproblems created within this outer loop are either unconstrained or box-constrained
- Solve the subproblems using an efficient box-constrained first-order method
- Use an approximation criterion so that relatively little effort can be expended on each subproblem…
  - …maybe just a handful of gradient / CG steps

- E & Silva (2013) suggest an algorithm of this form
  - Show global convergence in convex case
  - Encouraging empirical performance results (nonconvex)

Relative-Error Augmented Lagrangians: Background

$$\boxed{\begin{array}{lll} \min & f(x) & \\ \mathrm{ST} & g_i(x) \le 0 & i = 1,\ldots,m_1 \\ & h_i(x) = 0 & i = 1,\ldots,m_2 \\ & l \le x \le u & \end{array}}$$

or just

$$\boxed{\begin{array}{ll} \min & f(x) \\ \mathrm{ST} & g(x) \le 0 \\ & h(x) = 0 \\ & l \le x \le u \end{array}}$$

Basic algorithm:

$$x^k \in \mathop{\arg\min}_{x \in \Re^n,\, l \le x \le u} \left\{ f(x) + \tfrac{1}{2c_k}\left(\sum_{i=1}^{m} \max\left\{0, p_i^{k-1} + c_k g_i(x)\right\}^2 + \left\| q^{k-1} + c_k h(x) \right\|^2 \right) \right\}$$

$$p_i^k = \max\left\{0, p_i^{k-1} + c_k g_i(x^k)\right\} \qquad i = 1,\ldots,m$$

$$q^k = q^{k-1} + c_k h(x^k)$$

- But don’t want to invest too much effort in subproblem minimization when multiplier estimates are poor
- Let $L_c(x,p,q) = f(x) + \tfrac{1}{2c}\left(\sum_{i=1}^{m} \max\left\{0, p_i + c g_i(x)\right\}^2 + \left\| q + c h(x) \right\|^2 \right)$

Relative Error Criterion (E & Silva 2012)

Violation of KKT

$$y^k \in \partial_x L_{c_k}(x^k, p^{k-1}, q^{k-1})$$

$$\frac{2}{c_k}\left|\left\langle w^{k-1} - x^k, y^k \right\rangle\right| + \left\|y^k\right\|^2 \le \sigma\left(\left\|\min\left\{\tfrac{1}{c_k} p^{k-1}, -g(x^k)\right\}\right\|^2 + \left\|h(x^k)\right\|^2\right)$$

Scalar $\sigma \in [0,1)$

$$p_i^k = \max\left\{0, p^{k-1} + c_k g_i(x^k)\right\} \qquad i = 1, \ldots, m$$

$$q^k = q^{k-1} + c_k h(x^k)$$

Weird auxiliary sequence

$$w^k = w^{k-1} - c_k y^k$$

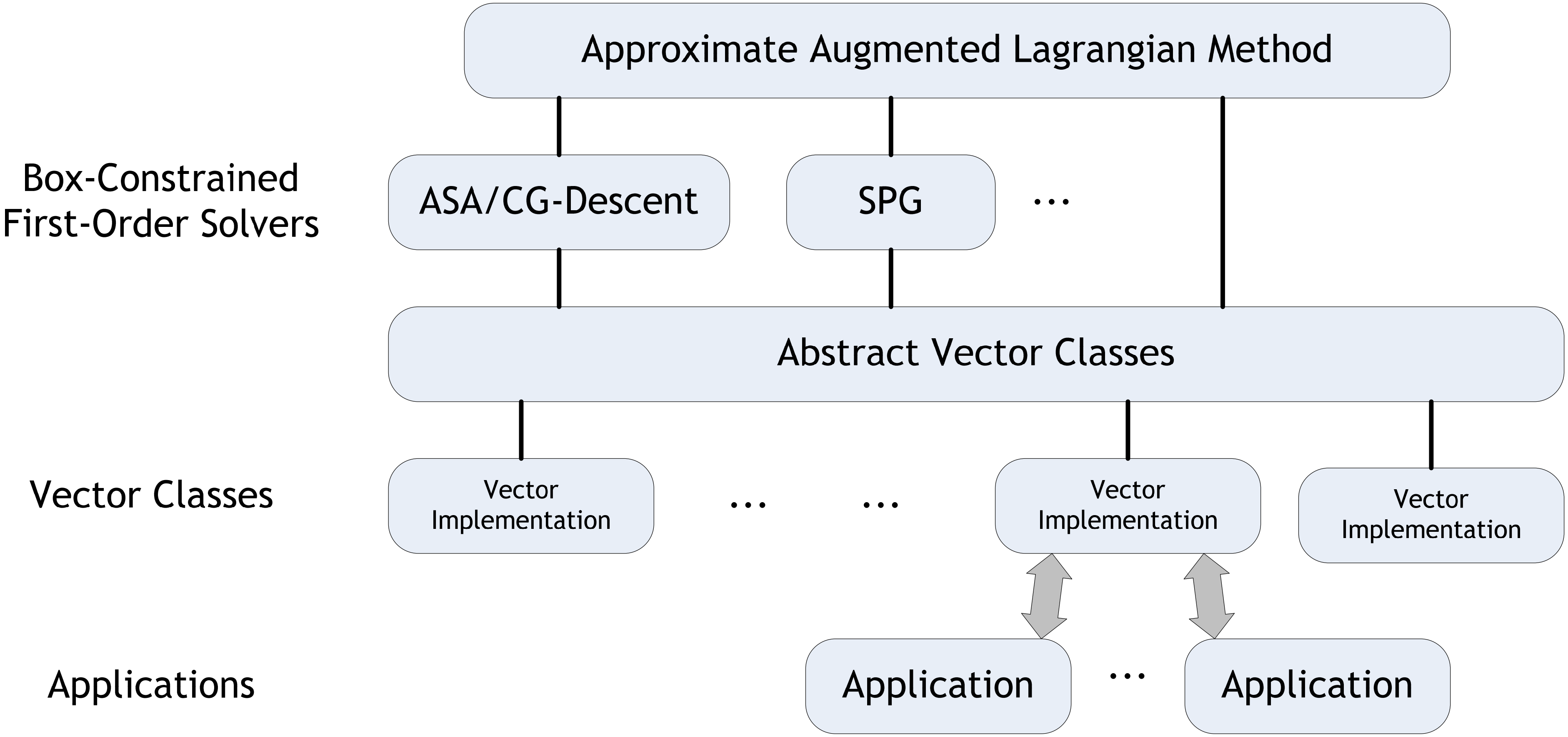
The “FOAAL” Project

- The relative-error augmented Lagrangian approach seems like a reasonably good algorithm in serial — that is, likely to be competitive for at least some problem classes

- So, try to build this approach into object-parallel software:

- FOAAL: First-Order Approximate Augmented Lagrangian

FOAAL Software Architecture (C++)



FOAAL Software Architecture Rationale

- Vector classes encapsulate various vector representations
  - Serial representations of various kinds
  - …including encapsulating various forms of BLAS
  - …including parallel, such as Epetra (Heroux 2004, 2006)

- Abstract vector classes provide operator overloading so that the core optimization algorithms may be expressed with (almost) MATLAB-like simplicity
  - Unlike most high-performance optimization codes, in which the underlying algorithm is obscured by details
  - Without sacrificing much performance
  - Flexibly with respect underlying vector representation
  - Possibly in parallel (upper-level code running synchronously on all processors)

Operator Overloading

- When at least one of **`a`** and **`b`** has a user-defined type, C++ allows the definition of functions like **`operator+`** so that an expression like **`a + b`** implicitly calls **`a.operator+(b)`** etc.

- We use this feature to allow us to write simple MATLAB-like code for addition, subtraction, and scaling of vectors

- If implemented in the most straightforward way, could be extremely inefficient for large-scale (and parallel) vectors
  - Frequent creation and destruction of temporaries
    - Including parallel layout information
  - Unnecessary copying of memory
  - Excessive load and store operations

“Symbolic Temporaries” Technique

- Suppose **`a`** is a **`double`** and **`w`**, **`x`**, **`y`**, **`z`** are instances of our **`VectorObject`** class
- **`VectorObject`** encapsulates an **`AbstractVector`** pointer
- Consider an assignment statement like

```
w = x + a*y – z;
```

- At run time, this expression builds a relatively compact **`LinearExpression`** object expressing (1,&**`x`**), (a,&**`y`**), (–1,&**`z`**)
- Overloading of the **`=`** operator invokes code to efficiently calculate the result and overwrite **`w`**
- Temporaries are still created, but they are compact and symbolic — their storage is independent of the vector length
- Overhead should be insignificant for large-scale applications (we have confirmed this)

“Symbolic Temporaries” Technique: More Details

`w = x + a*y – z;`

- A **`LinearExpression`** object is a list of pairs of the form (*scalar coefficient*, *pointer to vector*)
- Overload of **`operator*(double&,VectorObject&)`** produces a **`LinearExpression`** of the form (a,&**`y`**)
- Overload of **`VectorObject.operator+(LinearExpression&)`** appends (1,&**`x`**) to the **`LinearExpression`** list
- Overload of **`LinearExpression.operator-(VectorObject&)`** appends (–1,&**`z`**) to the **`LinearExpression`** list
- Overload of **`VectorObject.operator=(LinearExpression&)`** triggers actual calculation with minimum use of temporary memory (deferred evaluation technique)

The `LinearExpression` Class is Enough

First-order optimization methods typically require only a limited range of vector expressions

- Addition, scaling, (subtraction)
- Inner products (just produce a double)
- Projection on simple sets

- Function and gradient calculations:
    - We encapsulate these through a separate **`Problem`** class

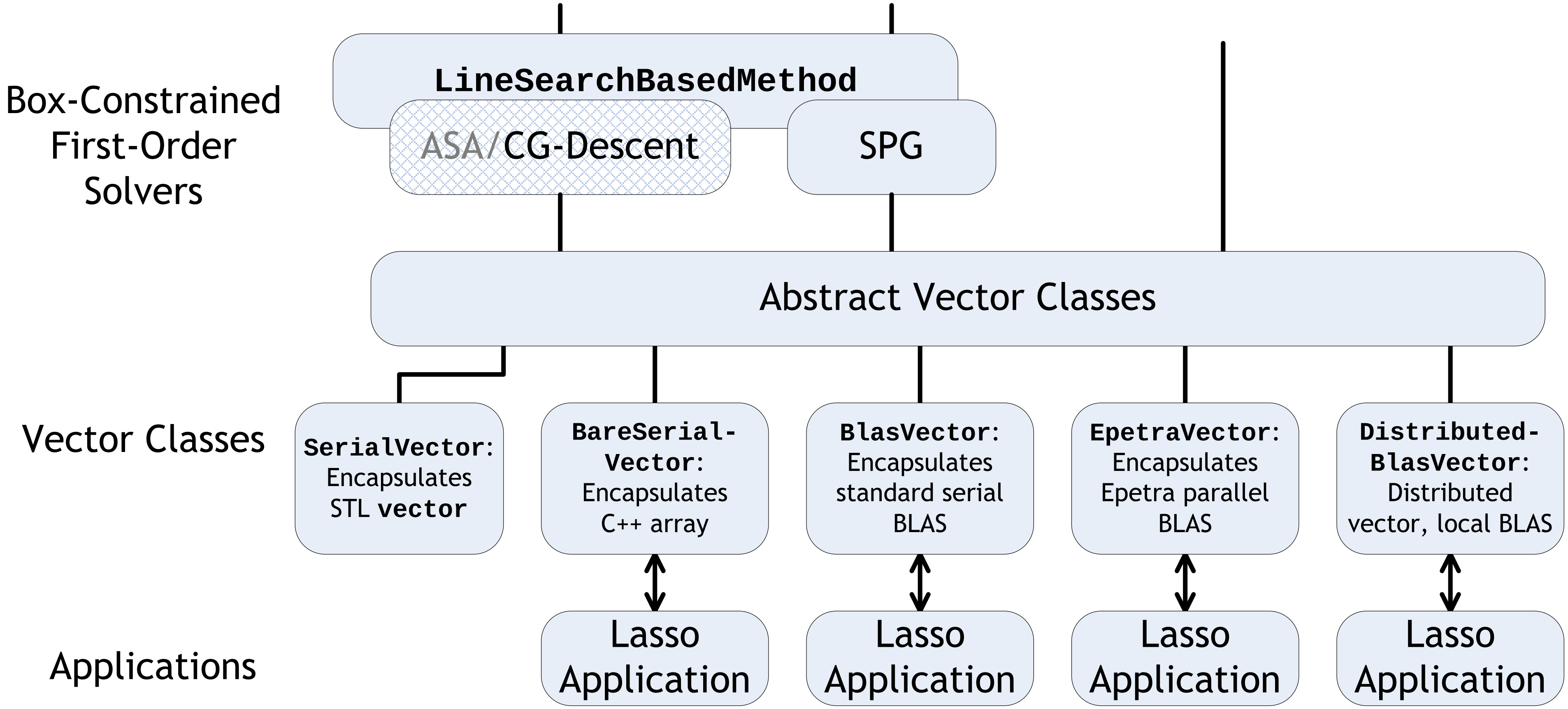
Other operations occur, but are typically on scalars

Support for Line-Search Methods

- We have also built some specialized support for line search
- Automatically cache function values and gradients to avoid both
    - Multiple evaluations at the same point, and…
    - Associated “clutter” in main algorithm code

What We Have Built So Far

- No top-level augmented Lagrangian yet
- Partial implementation of box solvers



Box-Constrained First-Order Solvers

LineSearchBasedMethod

ASA/CG-Descent

SPG

Abstract Vector Classes

Vector Classes

SerialVector: Encapsulates STL **vector**

BareSerial-Vector: Encapsulates C++ array

BlasVector: Encapsulates standard serial BLAS

EpetraVector: Encapsulates Epetra parallel BLAS

Distributed-BlasVector: Distributed vector, local BLAS

Applications

Lasso Application

Lasso Application

Lasso Application

Lasso Application

- Lasso is a convenient (and potentially large-scale) test application for components already built

The Code for SPG Algorithm (with Nonmonotone Line Search)

```
VectorObject& min() {
 while(pGrad.norm_2() > tolerance && iter < maxIter) {
   iter++;
   xPlus = x + lambda*d;
   objValxPlus = Pr->objValGrad(xPlus, gk);
   objValMax = *(max_element(objValArray, objValArray + M));
   if(objValxPlus < objValMax + gamma*lambda*d.inner(g)) {
     descentSteps++;
     objValArray[descentSteps%M] = objValxPlus;
     xk = xPlus;
     b = inner(xk - x, gk - g);
     if(b <= 0) {
       stepSize = stepSizeMax;
     }
     else {
       a = norm_2_sq(xk-x);
       stepSize = smin(stepSizeMax, max(stepSizeMin, a/b));
     }
     x = xk;
     g = gk;
     xk = x - g;
     Pr->projectOnBounds(xk, pxk);
     pGrad = pxk - x;
     xk = x - stepSize*g;
     Pr->projectOnBounds(xk, pxk);
     d = pxk - x;
     lambda = 1;
   }
   else {
     objValx = Pr->objective(x);
     lambda = (-g.inner(d) * lambda*lambda )
       / (2*( objValxPlus - lambda*g.inner(d) - objValx ));
     if (lambda < 0.1 || lambda > 0.9*lambda)
      lambda = lambda/2;
   }
 }
```

Simple Test Application: Lasso

$$\boxed{\min\left\{\tfrac{1}{2}\left\|Ax-b\right\|^2+\nu\left\|x\right\|_1\right\}}$$ (unconstrained, nonsmooth)

Reformulated as

$$\boxed{\begin{array}{ll}\min & \tfrac{1}{2}\left\|A(x-y)-b\right\|^2+\nu\cdot 1^{\mathsf{T}}(x+y)\\ \mathrm{ST} & x,y\geq 0\end{array}}$$

- Becomes a box-constrained problem with a smooth objective
- In this form, does not test augmented Lagrangian level, but allows other software components to be tested
- Rest of talk will be about our experiences with (large-scale) Lasso

Overall Setup

- Fundamentally, using spectral projected gradient (SPG) on

$$\boxed{\begin{array}{ll} \min & \tfrac{1}{2}\left\|A(x-y)-b\right\|^2 + \nu\cdot\mathbf{1}^\mathsf{T}(x+y) \\ \mathrm{ST} & x, y \geq 0 \end{array}}$$

- SPG implemented with our operator overloading technique
- Standard serial algorithm
- Parallelism through underlying linear algebra operations
  - o Partly automatic in SPG / parallel vector classes
  - o Partly application-specific (function and gradient evals)
- Main work per iteration is performing matrix multiplications of the form Ax and $A^\mathsf{T}u$:
  - o Objective gradient is $\nabla h(x,y) = \begin{bmatrix} A^\mathsf{T}\big(A(x-y)-b\big)+\nu\mathbf{1} \\ -A^\mathsf{T}\big(A(x-y)-b\big)+\nu\mathbf{1} \end{bmatrix}$

Data Distribution

- For now, assume A is large but has many more columns than rows ($n \gg m$) – fairly typical in Lasso
- Simple idea, sufficient for dense problems and some sparse problems: partition columns among processors, with matching partition of n-vectors:

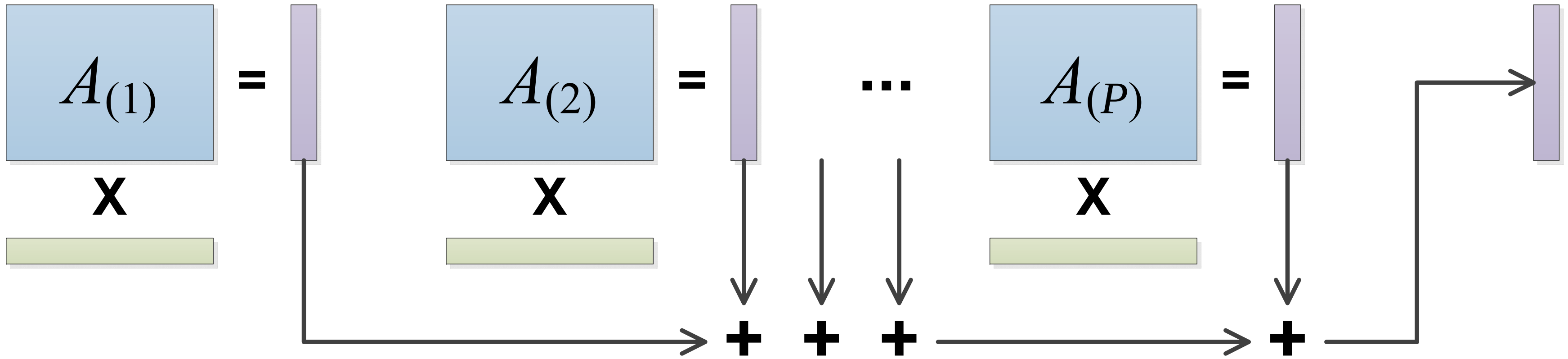
$A_{(1)}$	$\cdots$	$A_{(j)}$	$\cdots$	$A_{(P)}$
$x_{(1)}$ $y_{(1)}$	$\cdots$ $\cdots$	$x_{(j)}$ $y_{(j)}$	$\cdots$ $\cdots$	$x_{(P)}$ $y_{(P)}$

- x and y are segments of a **`DistributedBlasVector`**
- Vectors of length m (like b) are replicated in every processor
  - o Impact small because $n \gg m$

Matrix Multiplications

To multiply $z \in \mathbb{R}^n$ by A: $r = Az$

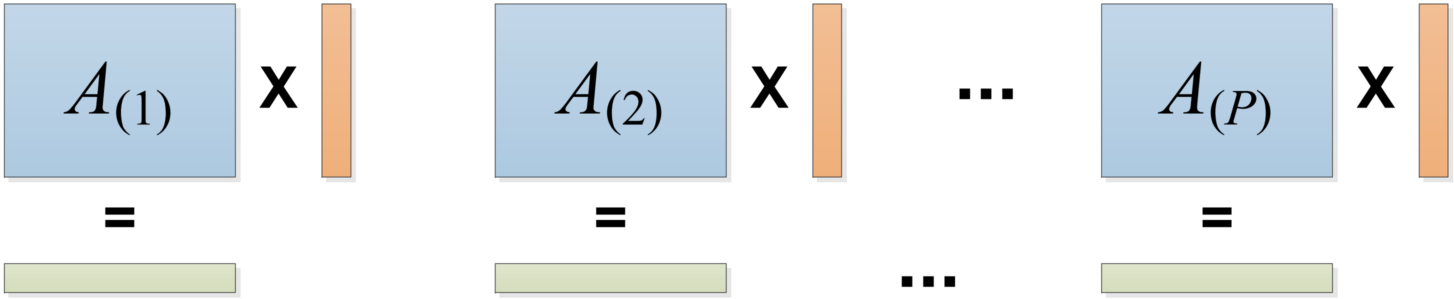
- Each processor performs a local multiplication $r_{(j)} = A_{(j)} z_{(j)}$
  - o For Lasso, first compute $z_{(j)} = x_{(j)} + y_{(j)}$ (in parallel)
- Then do **`Allreduce`** operation (MPI primitive) to compute and broadcast $r = \sum_{j=1}^{P} r_{(j)}$
  - o Requires $\mathrm{O}(\log P)$ rounds of messages, time $\mathrm{O}(m \log P)$



Transpose Matrix Multiplications

To multiply $p \in \mathbb{R}^m$ by A^T: $g = A^\mathsf{T} p$

- Remember, m-vectors are replicated in each processor, so…
- Each processor performs a local multiplication $g_{(j)} = A_{(j)}^\mathsf{T} p$
- Result is g, properly distributed



Balancing Workload

- Key is for each of $A_{(1)},\ldots,A_{(P)}$ to have approximately the same number of nonzero elements
- Then the amount of work in computing $r_{(j)} = A_{(j)}z_{(j)},\ g_{(j)} = A_{(j)}^{\mathsf{T}}p$ will be roughly the same across processors, and the dominant portion of the computation will exhibit near-linear speedup
- Very easy for dense problems: just partition columns as equally as possible and relative imbalance will be $\mathrm{O}(P/n)$
- One approach for sparse problems: heuristically partition the columns in order to balance the number of nonzero elements in each processor

Alternative Approach for Sparse Problems: Trust Epetra

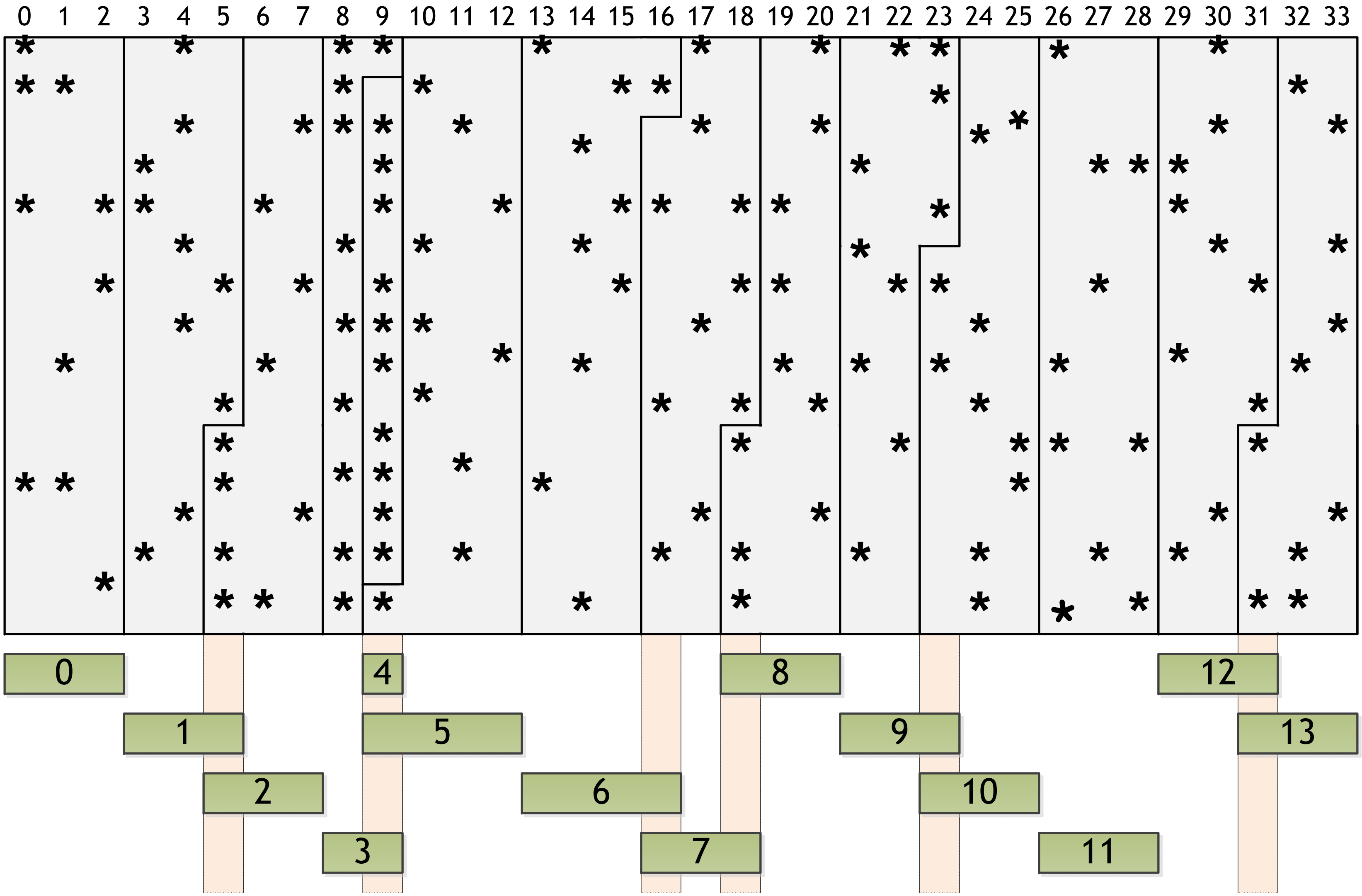
- Represent n-vectors using **`EpetraVector`**
- Partition matrices using Epetra's "Isorropia" sub-package
    - o Can partition by rows **and**/or columns
    - o Could be helpful for matrices that are closer to square
- Use Epetra parallel sparse matrix multiplication

Difficulties with Row/Column Partitioning

- We use matrices derived from real-world datasets
- Derived from UCI repository
- Many are sparse overall, but have a small fraction of relatively dense columns containing a significant fraction of the total nonzeroes
- Rectangular partitions can work poorly such cases

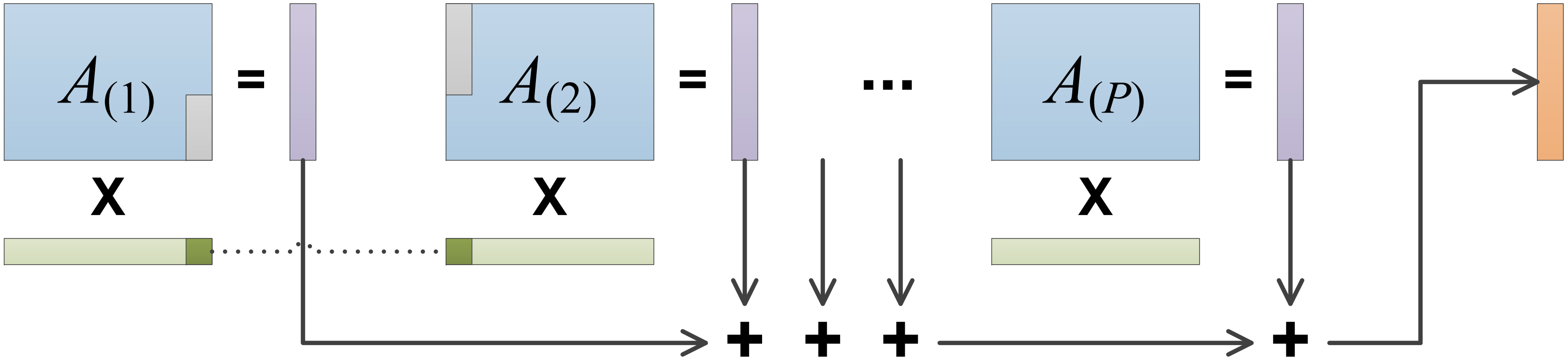
Third Alternative for Sparse Problems

- Sort sparse matrix entries (*row*, *column*, *value*) by *column*
- Partition nonzeros evenly between processors, using this order



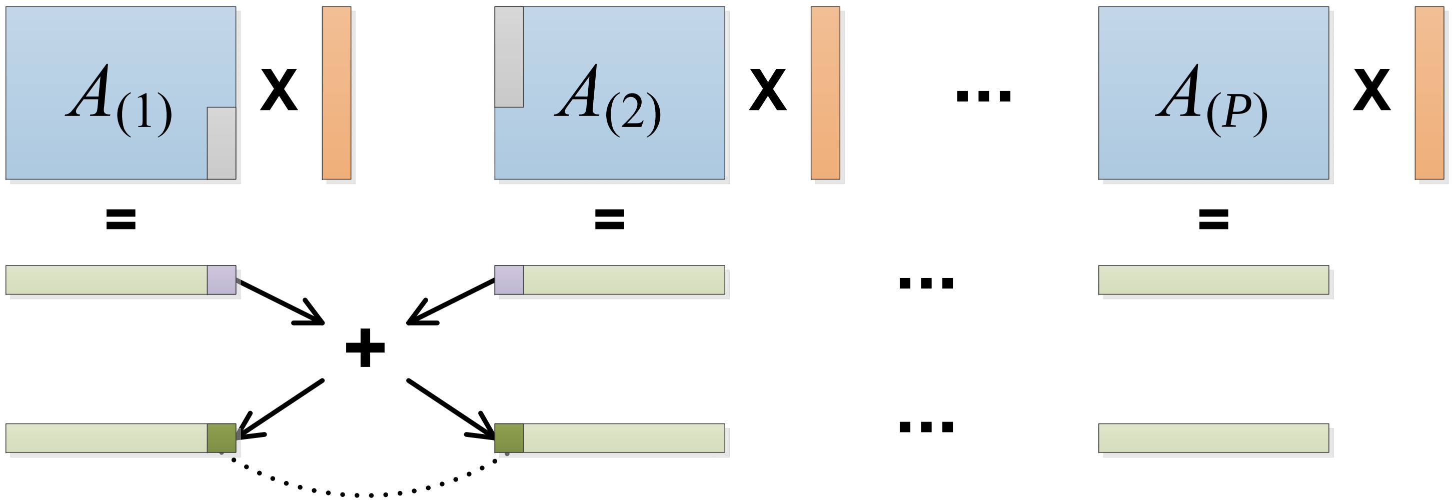
More on the Third Sparse Approach

- For n-vectors, each processor owns all the columns for which it has (*row*, *column*, *value*) triplets
    - o The first and/or last elements might overlap with adjacent processors (with replicated values)
- m-vectors are replicated on each processor as before
- Let $A_{(j)}$ denote the sparse matrix of locally stored triplets, filled out to rectangular shape by zeros
- The multiplication $r = Az$ works exactly the same as before



More on the Third Sparse Approach

- The multiplication $g = A^{\mathsf{T}} p$ consists of the same local multiplication, followed by a scalar sum-reduction and broadcast within each “overlap zone”



Setting Things Up

- For implementation in MPI, we need to set up a “communicator” for each overlap zone
  - Once this is accomplished, implementation is easy
  - Reduction takes $\mathrm{O}(\log V)$ steps, where $V \le P$ is the maximum number of processors in an overlap zone
- Tricky to get communicators set up without introducing an $\Theta(P)$ operation, but can be done in $\mathrm{O}(\log P)$

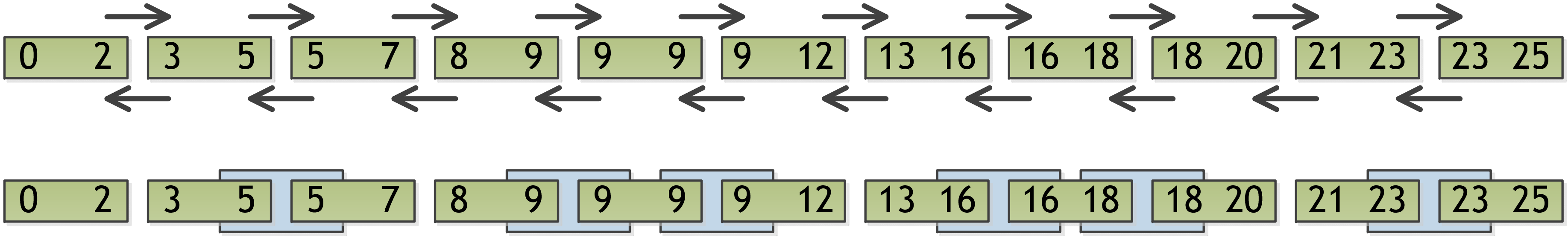
Digression: Parallel Scans

$$\begin{array}{|c|c|c|c|c|c} \hline 1.0 & 2.3 & 4.0 & 2.1 & 0.1 & \cdots \\ \hline \end{array} \rightarrow \begin{array}{|c|c|c|c|c|c} \hline 1.0 & 3.3 & 7.3 & 9.4 & 9.5 & \cdots \\ \hline \end{array}$$

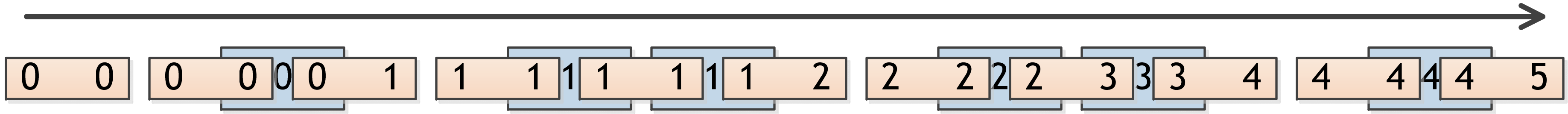
- For any associative operator, this operation can be performed in $\mathrm{O}(\log P)$ communication, $\mathrm{O}((n/P)\log P)$ time
- Can design the operator to restart accumulation “from scratch” at certain points (implementing “segments”)

Digression: Details of Setting up Communicators

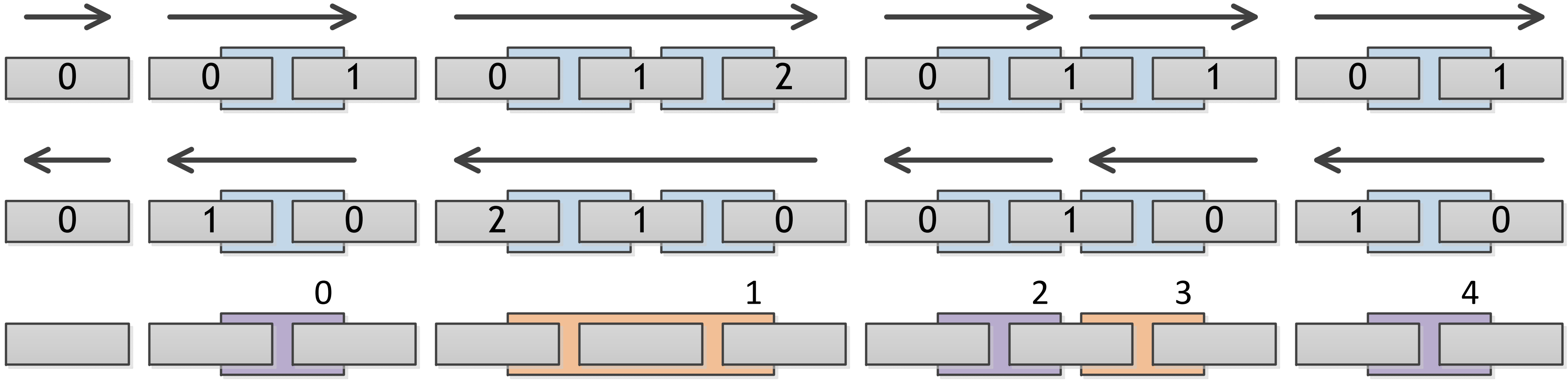
1. One message left, one message right to identify neighbors



2. Sum-scan to assign a unique number to each overlap group

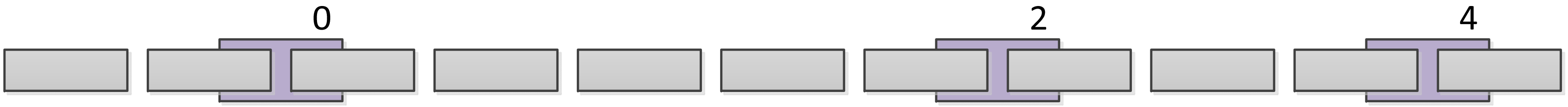


3. Scan forward and back with a customized operator so each processor knows full extent of left and right group

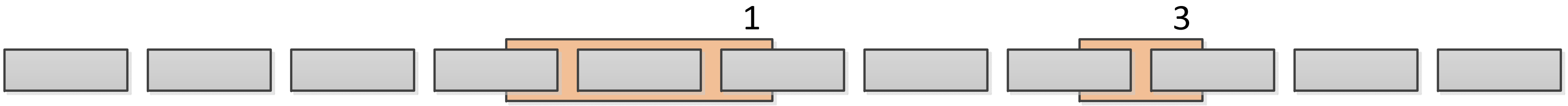


Continued Digression: Detail of Setting Up Communicators

4. Call **`MPI_Comm_create`** to make all even-numbered groups



5. Call **`MPI_Comm_create`** to make all odd-numbered groups



- Each call subdivides an existing communicator
- Each processor in at most one communicator
- All processors call **`MPI_Comm_create`** synchronously
- Those with nothing to do create and destroy a trivial communicator

This procedure avoids using tempting routines like **`MPI_Comm_split`**, which perform gather / scatter operations that can introduce $O(P)$ communication, hurting scalability

Computational Experiments

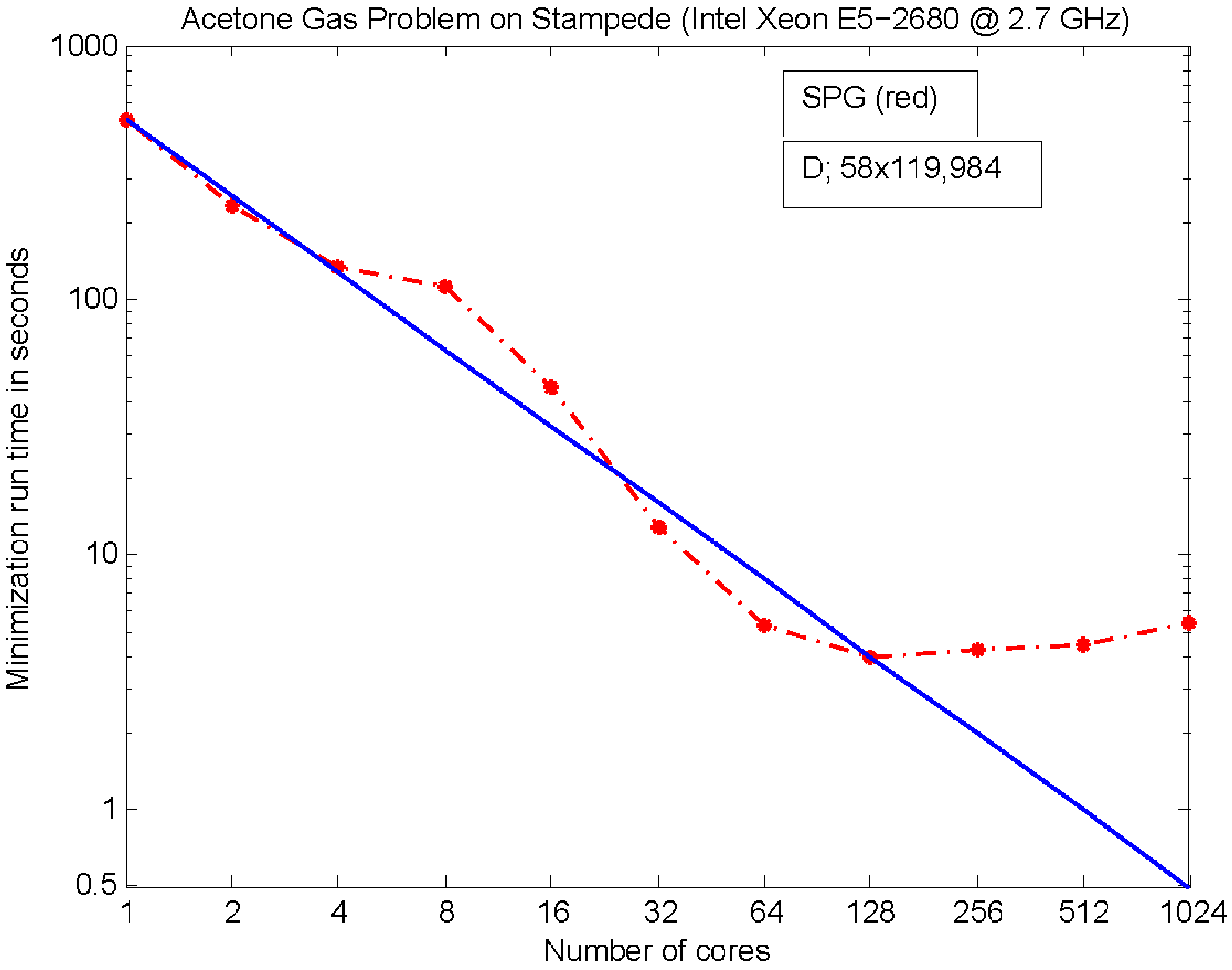
- SPG is a numerically sensitive algorithm
  - o Minor changes (even version of BLAS) can cause some variation (not gigantic) in the number of iterations

- Convergence condition: $\left\| \left[(x,y) - \nabla h(x,y) \right]_+ - (x,y) \right\|_\infty \le 10^{-6}$

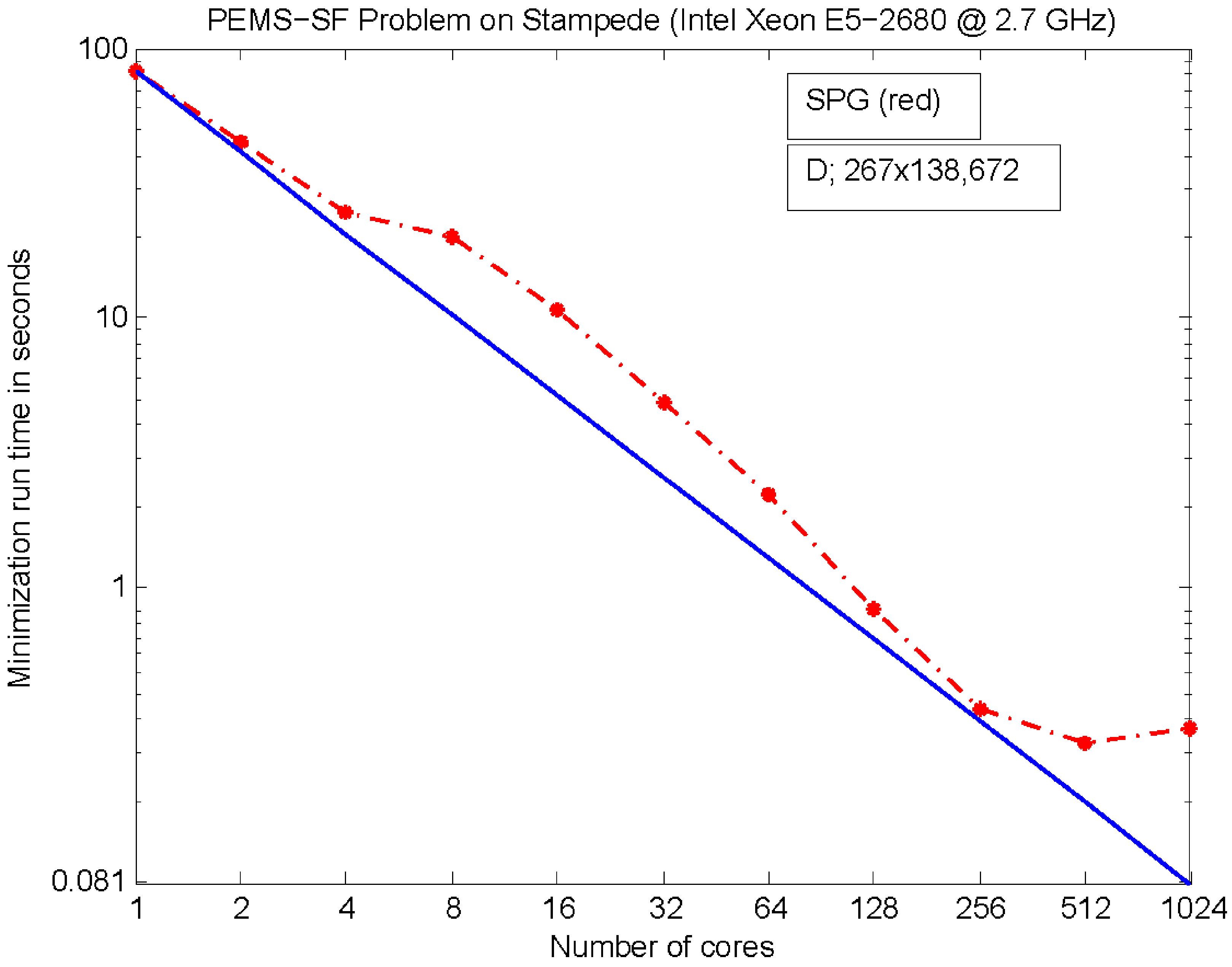
- Some data adapted from UCI machine learning Repository
- Other data randomly generated

- Computer system: TACC Stampede
  - o Xeon E5 cores, 2.7 GHz clock
  - o Xeon Phi accelerators, but not used by our code
  - o Infiniband fat-tree interconnect, MPI

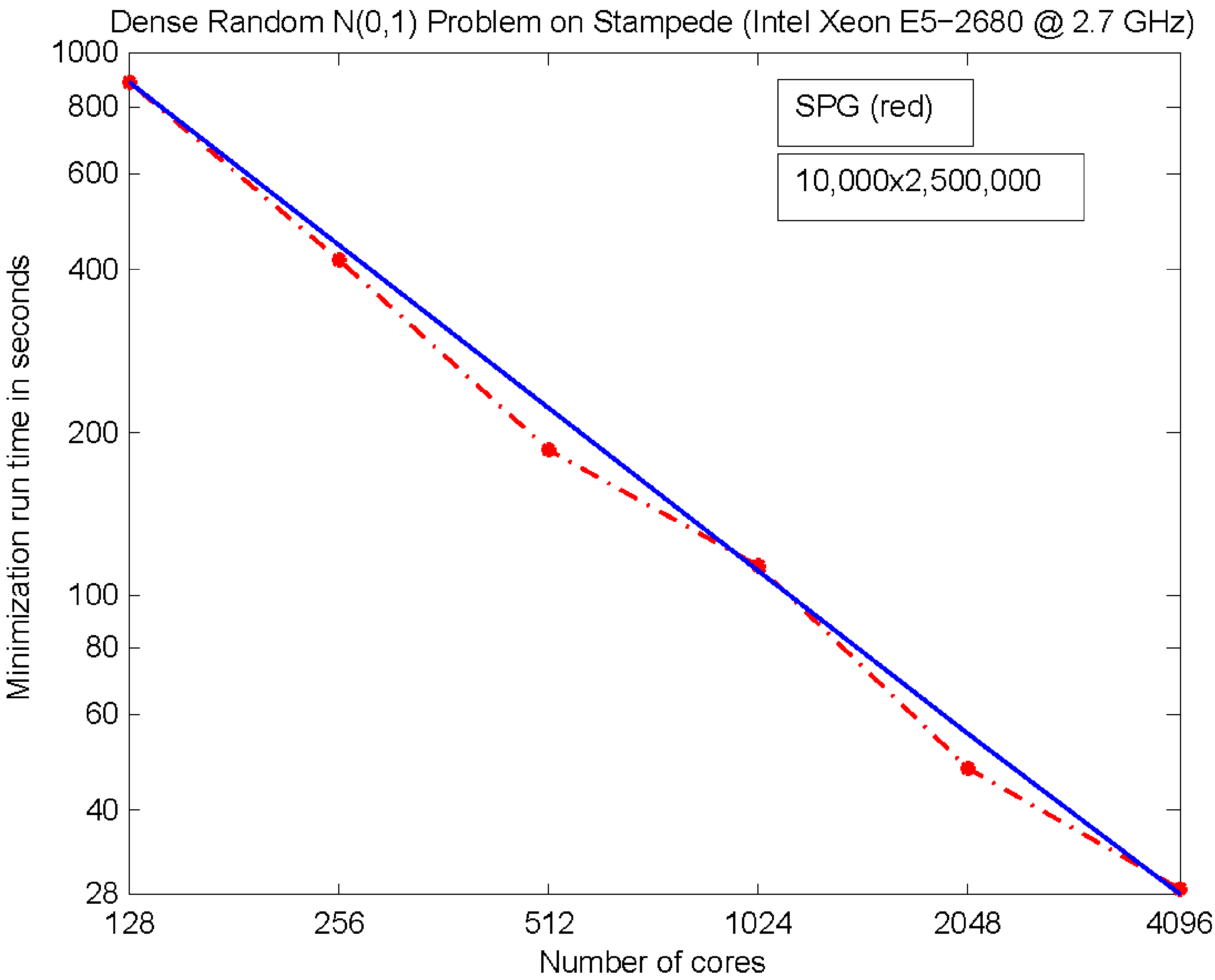
Dense: Detecting Acetone in Gas Samples (from UCI Repository)



More Dense: Highway Lane Occupancy (UCI Repository)



Dense: Randomly Generated Data



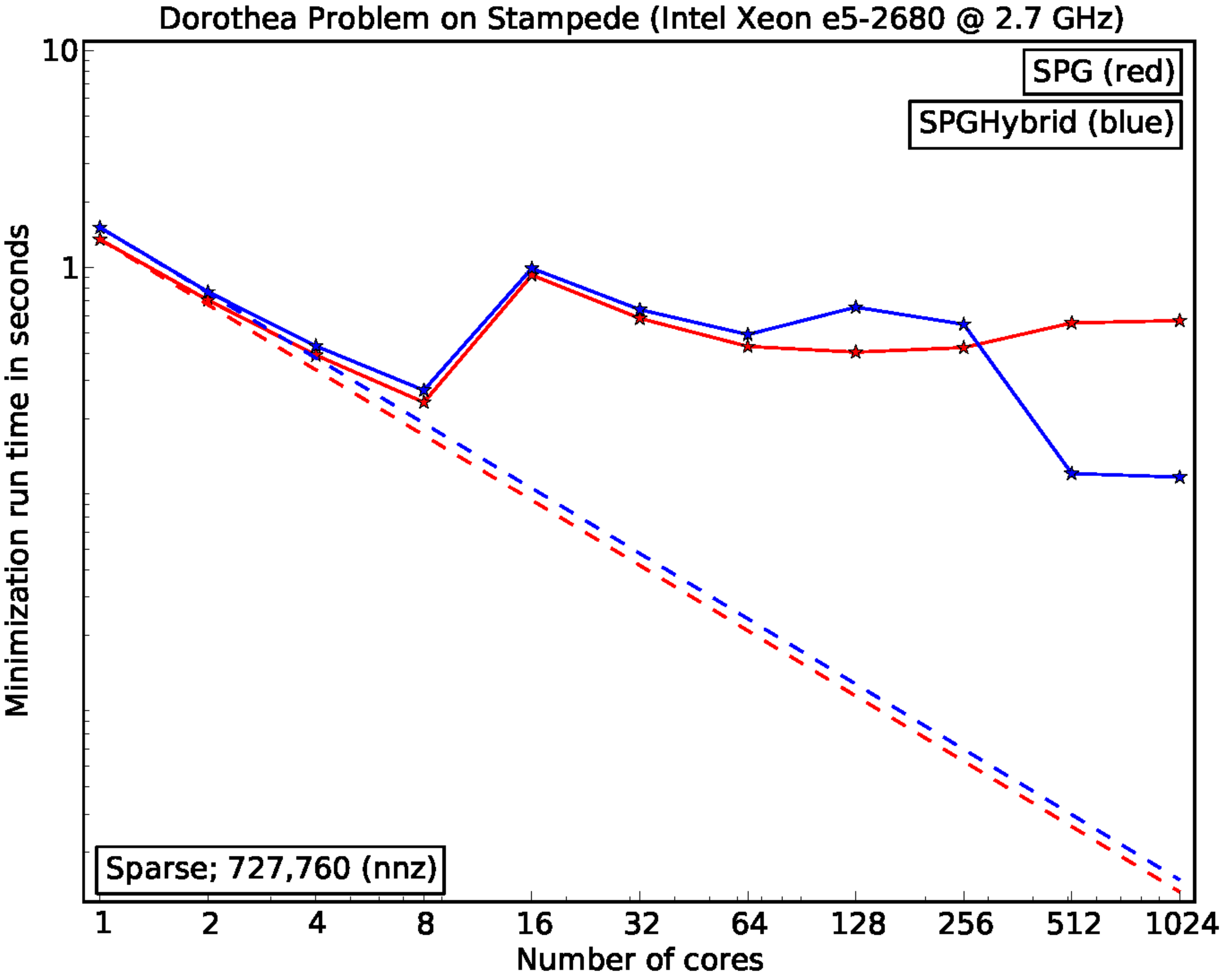
Sparse Problems

- “SPG” : our method with balanced nonzero partition
- “SPGHybrid” : our method with heuristic column partition
- “SPGEpetra” : our method with Epetra partitioning of matrix and vectors
- “ACDC” : Richtárik / Takáč random parallel coordinate descent
    - With small setting of proximal parameter – far below threshold required by (probabilistic) convergence theory
    - Does not have its own termination test; we terminate when it is close to the optimal value computed by SPG

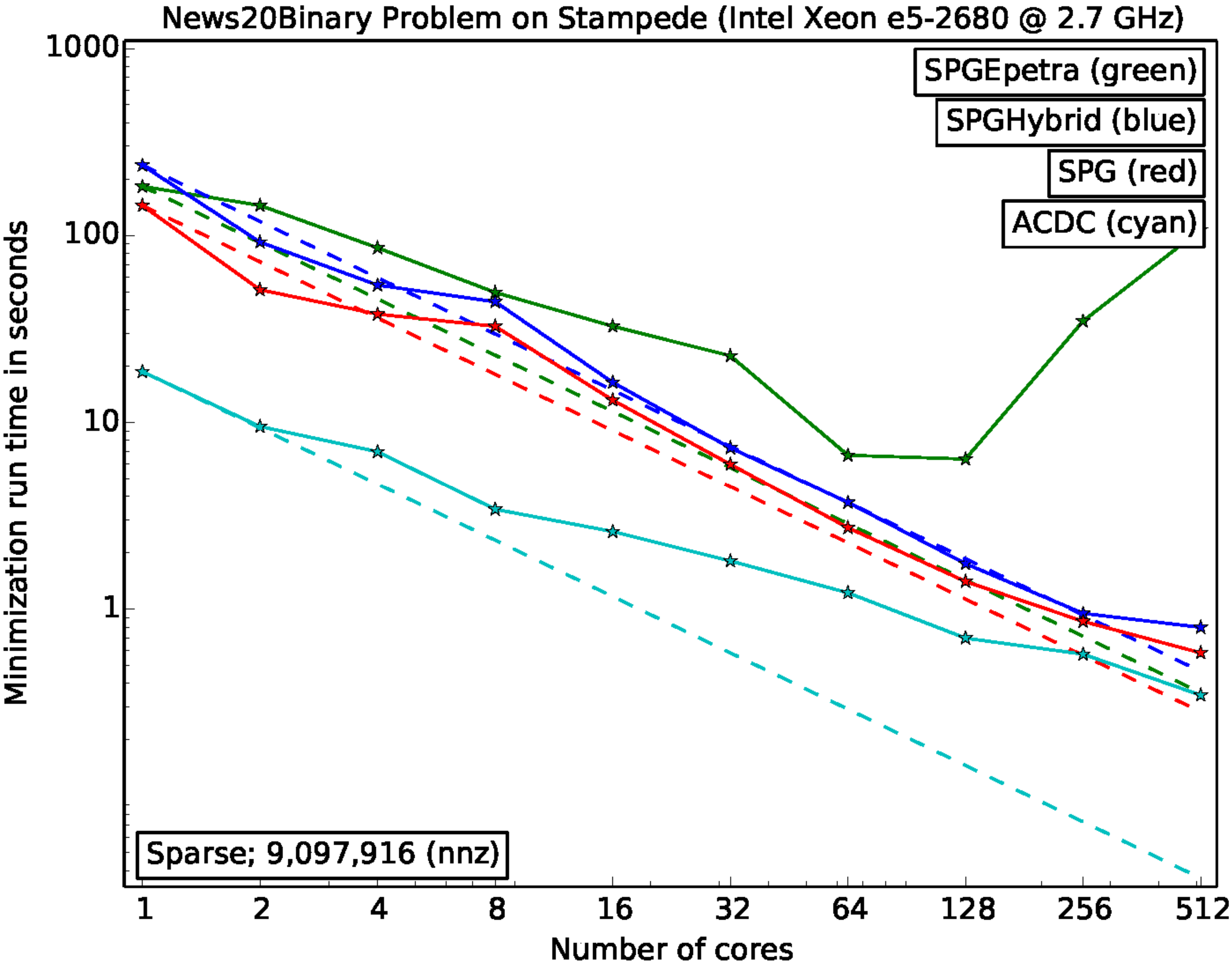
Current datasets: (working on getting more)

- Drug discovery: 1,950 × 100,000, 728K nonzeroes
- News articles: 19,996 × 1,355,191, 9.1M nonzeroes
- Randomly generated: 10,000 × 2,500,000, 250M nonzeroes

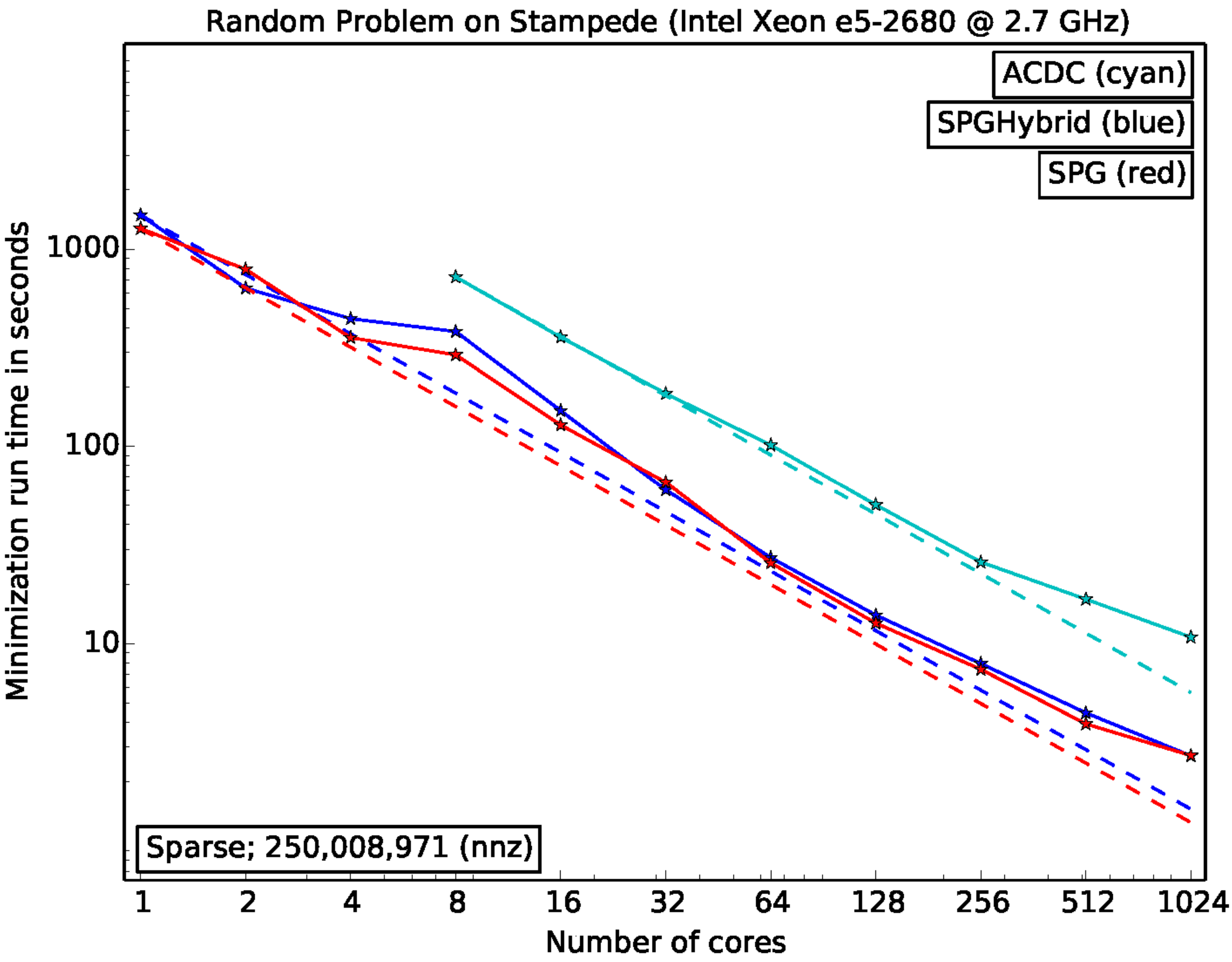
Sparse: Drug Discovery (Small)



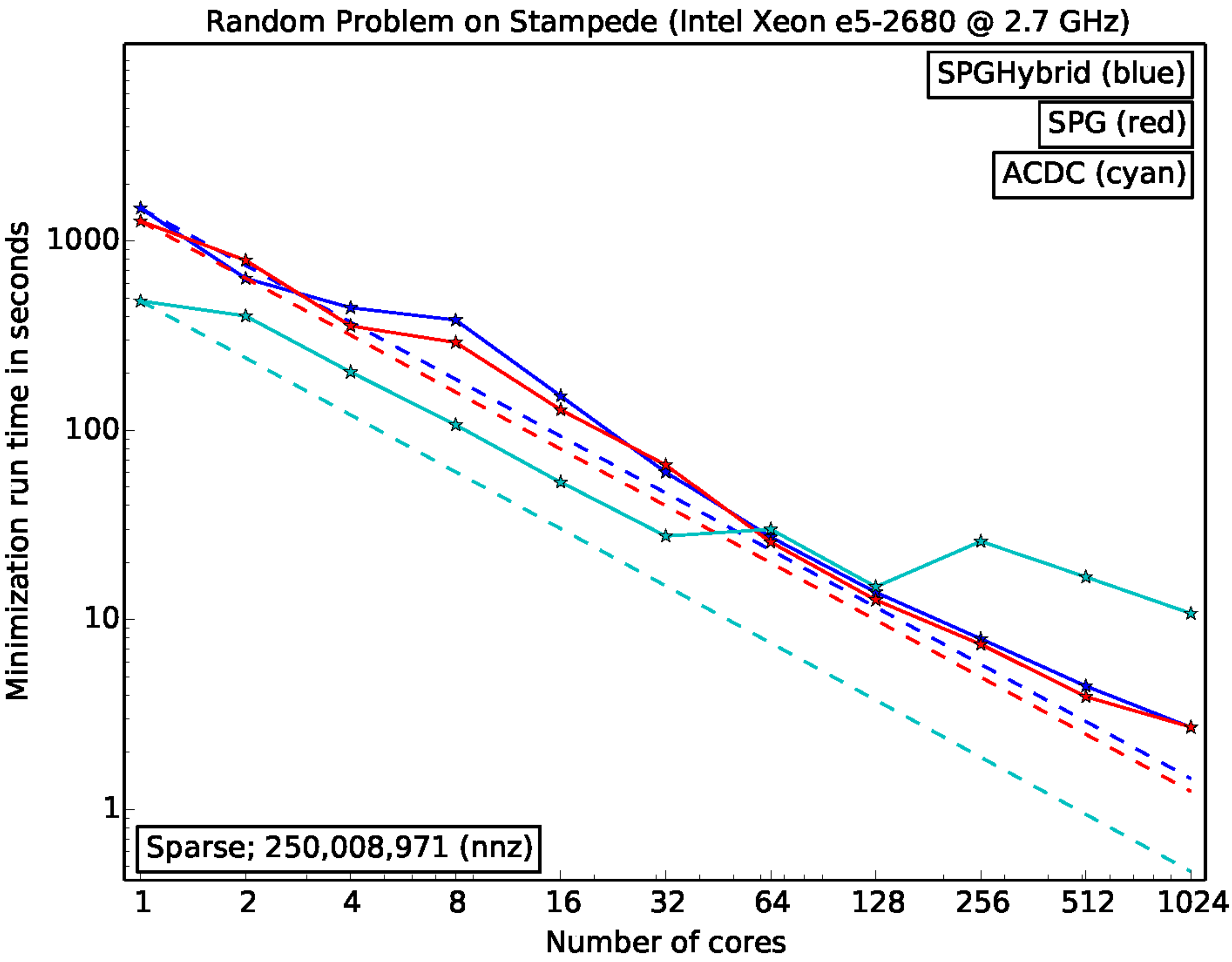
Sparse: News Articles



Sparse: Randomly Generated (Fairly Large)



Sparse: Randomly Generated (Varying Parameters for ACDC)



Discussion of Experimental Results

- Dense code scales well

- Balanced nonzero distribution seems to work best and scales quite well

- But only beats heuristic column balancing by a small amount (will this remain true for larger real datasets?)
  - However, it also has lower setup time (not shown here), so it's preferable to heuristic column balancing

- Epetra does not scale well on these datasets ☹

- Not dominated by ACDC in a parallel setting
  - ACDC specifically designed for Lasso-like problems
  - Our fundamental method is generic…
  - … yet reasonably competitive in parallel

The “Object-Parallel” Approach…

… allowed application development to focus on efficiency of objective/gradient evaluations

- But not more complicated things like structure of matrix factors
- We could organize the data to optimize efficiency of the most compute-intensive operations
- We tried four different data representations and two different data layouts for x and y …
- … but the SPG code remained identical
- Parallelism applied to underlying operations of serial method: iteration count largely independent of number of processors.

Same principles could apply to problems with general constraints, through approximate augmented Lagrangian method

- But also need to consider application constraint structure

The “Object-Parallel” Approach: Summary

Approach to parallel optimization by combining several well-established principles:

- Efficient first-order methods (continuing to develop)
- Object-oriented programming

- And eventually, augmented Lagrangians (for problems with general constraints)
    - … with new “loose” approximation criteria