

Communication-Optimal Algorithms

Grey Ballard, Mark Hoemmen

{ballard,mhoemmen}@cs.berkeley.edu

Motivation

"Communication" means

- Parallel: Data movement between processors
- Sequential: Data movement between levels of memory hierarchy
- # words (inverse bandwidth) and # messages (latency)

Communication matters because:

- Much slower than flops, and getting *exponentially slower* over time
- Moving data much more *energy-intensive* than computing on it
- Sparse linear algebra kernels already communication-bound
- Dense linear algebra: strong scaling demands increase relative comm. cost

Iterative Methods

♦ Subject of Mark Hoemmen's 11:30 talk

Based on 2 (or 3) communication-bound kernels

- 1. Sparse matrix-vector multiplication (SpMV)
- 2. (Possibly also preconditioning)
- 3. Orthogonalization (explicit, like Gram-Schmidt, or implicit, like in CG)

Our new algorithms

- Communicate factor of s times less than existing iterative methods (this is optimal)
- Work as long as sparse matrix structure partitions well (true for structured and unstructured meshes, as well as other matrices)

Direct Methods

Summary

- New communication lower bounds for (nearly) all dense or sparse, sequential or parallel, direct linear algebra problems
- New algorithms that attain lower bounds (dense only, sequential and parallel)
- Measured and modeled speedups, not just asymptotics

Dense Matrix Multiplication

Lower bound on: Lower bound

- Ω (# flops / (local/fast memory size)^{1/2} # words
- Ω (# flops / (local/fast memory size)^{3/2} # messages
- Results due to Hong-Kung [HK81], Irony/Tishkin/Toledo [ITT04]
- Attained by usual block algorithm (sequential) and Cannon's algorithm (parallel)

Extensions to (nearly) all direct problems

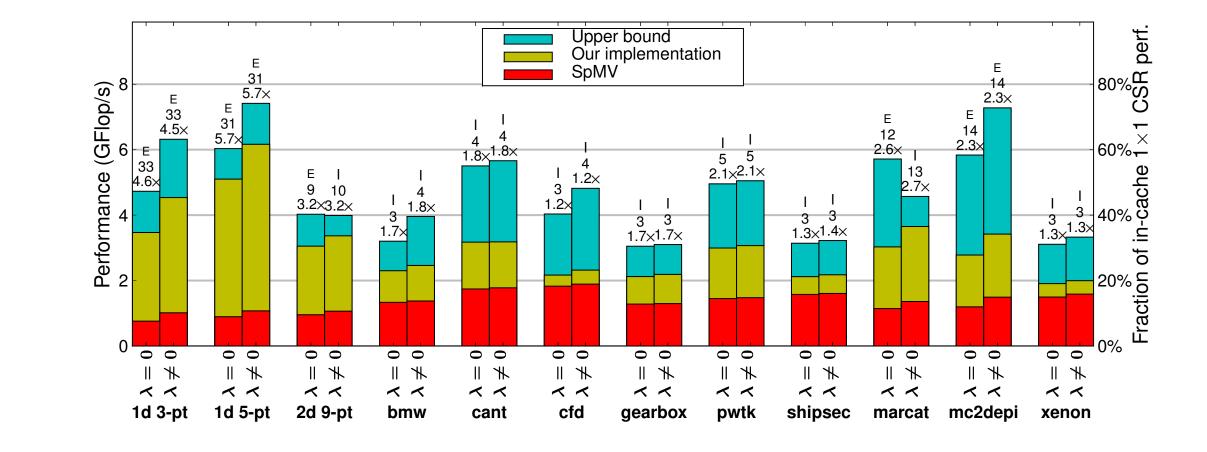
- Theorem: same lower bounds hold for LU, Cholesky, QR, eigenproblems, and SVD
- Sequential or parallel, dense or sparse
- See [BDHS09b] for details and proof
- Existing (Sca)LAPACK routines not both bandwidth and latency optimal
- ScaLAPACK: only Cholesky is optimal; LAPACK: Cholesky bandwidth only
- See [BDHS09a] for details on Cholesky algorithms
- New algorithms to attain lower bounds (up to polylog factors)
- -CAQR (QR factorization): new panel factorization & representation of Q
- -CALU (LU factorization): new pivoting scheme (still stable)
- -Eigenproblems and SVD: constant factor more flops, and randomization (see [DDH07])

• Mathematically equivalent to existing methods and stable in practice

Based on two new kernels

- Matrix powers kernel: use (possibly) redundant computation to compute a basis of span{ $v, Av, A^2v, \ldots, A^sv$ }
- TSQR: orthogonalize this basis accurately in 1 reduction
- See [MHDY09] for implementation and performance details of a GMRES algorithm using these two kernels

Matrix powers kernel performance results



• Matrix powers kernel on a variety of sparse matrices, symmetric and nonsymmetric

- Red (on bottom) is *tuned* $A \cdot x$, green (next) is matrix powers kernel, blue (top) is upper bound
- Performance relative to *in L2 cache* $A \cdot x$ ("instruction throughput measured peak")

New algorithm - Communication-Avoiding LU (CALU)

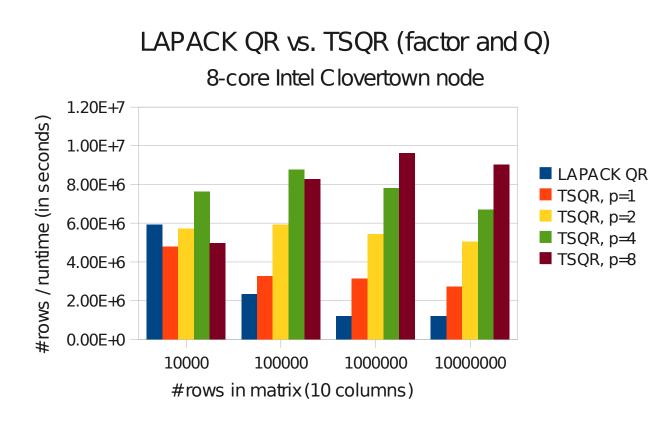
- Factor panel once with "Tall Skinny LU" (like a block reduction) to choose pivots
- Swap pivot rows to top and factor *again* without pivoting $O(n^2)$ extra computation
- Measured speedup of parallel TSLU: up to $5.58 \times$ on Cray XT4
- Measured speedup of parallel CALU (size $10^4 \times 10^4$): $1.31 \times$ on Cray XT4
- See [DGX08] for details, models, and more performance results

New algorithm - Communication-Avoiding QR (CAQR)

- Panel factorization: "Tall Skinny QR" (TSQR) block reduction with QR as operator
- Measured speedup of parallel TSQR: up to $6.7 \times$ on 16 procs of a Pentium III cluster
- Modeled speedup of parallel CAQR: up to $9.7 \times$ on an IBM Power5 system
- See [DGHL08] for details, models, and more performance results
- Standalone TSQR useful for iterative methods (orthogonalize basis vectors)

TSQR performance results

- Single node of 8-core Intel Clovertown (we have cluster and out-of-core versions too)
- Includes factorization and assembling explicit Q factor
- Best number of threads for LAPACK QR (Intel MKL and stock LAPACK): 1
- Even better measured and modeled speedups on clusters



- Two different bases computed:
- 1. $\lambda = 0$ is "power basis" v, Av, A^2v, \ldots
- **2.** $\lambda \neq 0$ is "Newton basis" v, $(A \lambda_1 I)v$, $(A \lambda_2 I)(A \lambda_1 I)v$, ...

Credits

- Research supported by Microsoft (Award #024263) and Intel (Award #024894) funding and by matching funding by U.C. Discovery (Award #DIG07-10227).
- Joint work with J. Demmel, L. Grigori, O. Holtz, J. Langou, M. Mohiyuddin, O. Schwartz, H. Xiang

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