Communication-avoidance
and
Automatic performance tuning

Nick Knight
UC-Berkeley Parlab (Bebop group)

Students and Collaborators (Bebop)

- PIs
  - James Demmel
  - Kathy Yelick
- Students
  - Marghoob Mohiyuddin
  - Shoaib Kamil
  - Vasily Volkov
  - Andrew Gearheart
  - Razvan Carbunescu
  - Grey Ballard
  - Nick Knight
  - Erin Carson
  - Edgar Solomonik
  - Michael Anderson
  - Gilad Arnold
- Collaborators
  - Mark Hoemmen (Sandia)
  - Mike Heroux (Sandia)
  - Jack Dongarra (UTK)
  - Laura Grigori (INRIA)
  - Simplice Donfack (INRIA)
  - Amal Khabou (INRIA)
  - Oded Schwartz (TU-Berlin + UCB)
  - Olga Holtz (UCB)
  - Ming Gu (UCB)
  - Ioana Dumitriu (UW)
  - Julien Langou (UC-Denver)
  - Samuel Williams (LBNL)
  - Aydin Buluc (LBNL)
  - Kamesh Madduri (LBNL)
  - Jong-Ho Byun (UCB)
  - Armando Fox (UCB)
  - Ras Bodik (UCB)
  - Tony Keaveny (UCB)

Talk outline

Developing efficient algorithms

- Strategy: avoiding communication
- Dense linear algebra
  - Heterogeneous comm. complexity
  - Eigenvalue problems
  - 2.5D algorithms
  - Fast matmul comm. complexity
  - CA-pivoting (ask me about it)
- Sparse linear algebra
  - CA-Krylov methods
  - New matrix powers kernel

Automatic performance tuning

- OSKI (Optimized Sparse Kernel Interface)
- Future development

Avoiding communication

Communication =

- Data movement and synchronization
- The dominant performance bottleneck in numerical codes

Comm. lower bounds for direct linear algebra:

- #words moved = Ω(#flops / $M^{1/2}$)
- #messages sent = Ω(#flops / $M^{3/2}$)
- Standard algorithms do *not* attain these bounds!

M = fast/local memory size

We develop:

- *Direct* algorithms that attain these bounds (communication-optimal)
- *Iterative* algorithms that solve problems with optimal communication.

Speedups on today's, future hardware

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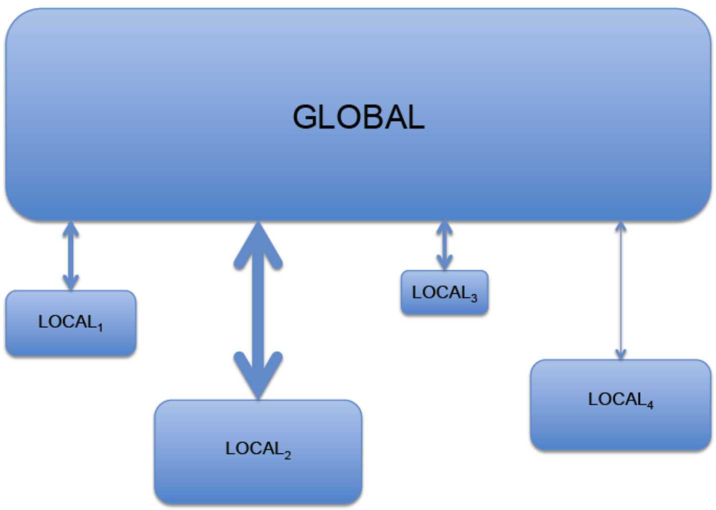
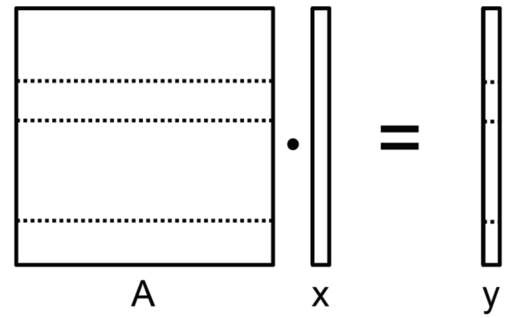
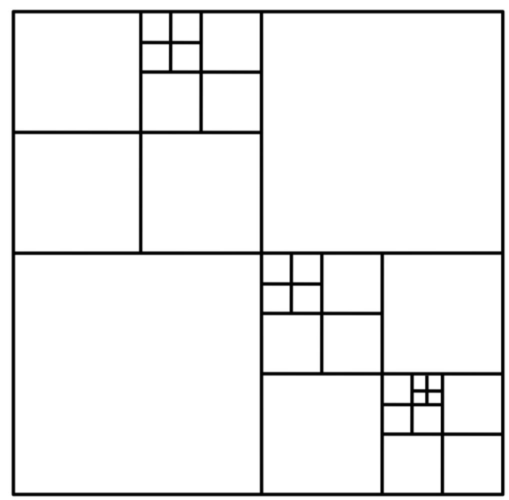
Heterogeneous comm. complexity



Heterogeneous memory model
(Different speeds, bandwidths, latencies)



(dense) matrix-vector multiply



(dense) matrix-matrix multiply

How best to reduce communication costs on heterogeneous machine?

- New theoretical results:
  - Model algorithm costs as linear program
  - Solution gives you optimal partition of flops
- New theory → FASTER ALGORITHMS

(SEE POSTER)
Gearhart, Ballard

Eigenvalue problems and SVD

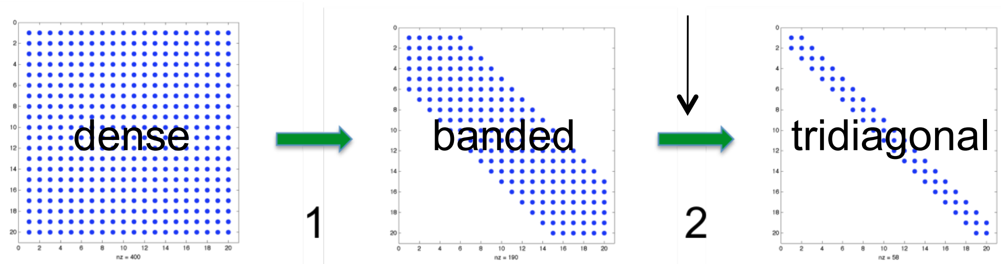
Applications:

- Image processing (M. Anderson's talk yesterday)

Previously:

- Presented three new algorithms at Winter 2010 retreat
- Solve eigenvalue and singular value problems with less communication

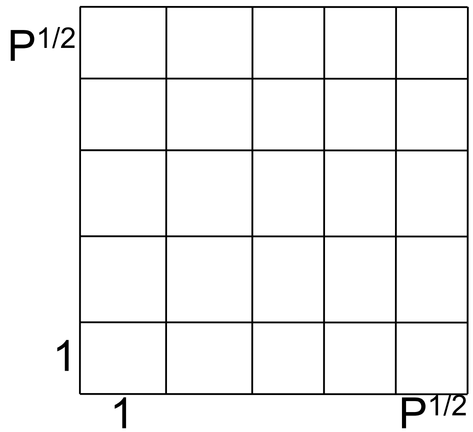
New algorithm for successive band-reduction



- Minimizes bandwidth *and* latency costs in serial
- Parallel SBR and implementations in development

2.5D algorithms I

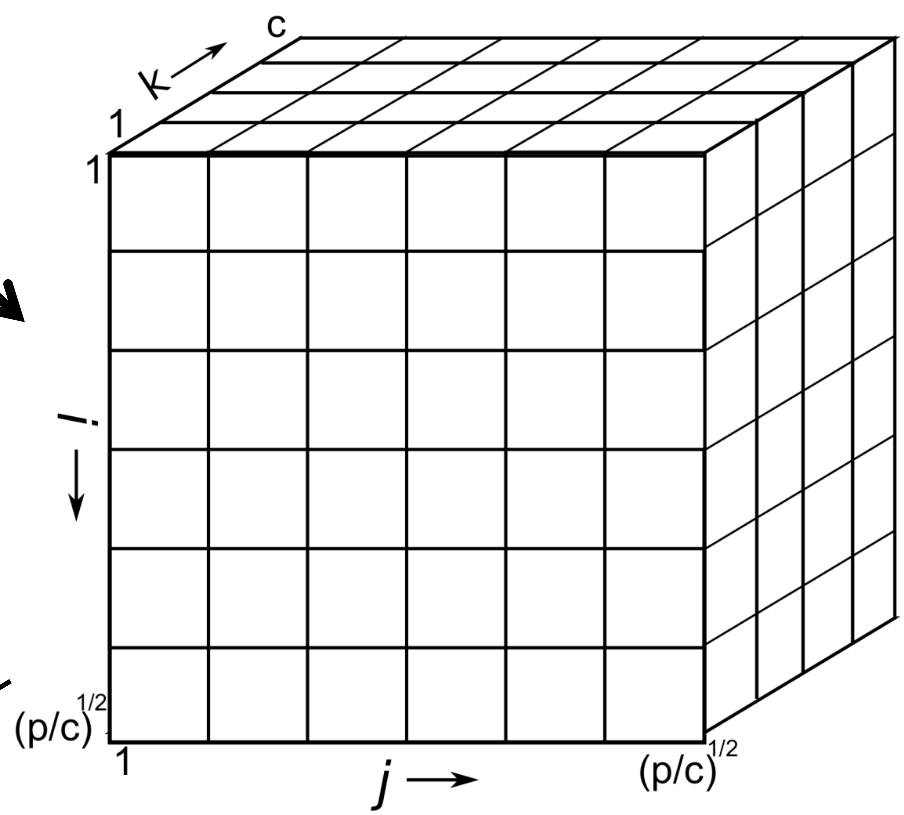
2D processor array



1 copy of data

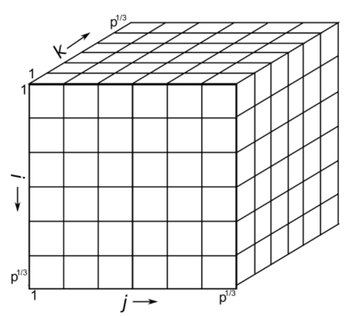
2.5D processor array

dimensions: $(P/c)^{1/2} \times (P/c)^{1/2} \times c$



$1 \le c \le P^{1/3}$ copies of data,
one per `plane' in the *k* direction

Special case: $c = P^{1/3}$ copies
Cube of processors: $P^{1/3} \times P^{1/3} \times P^{1/3}$



2.5D algorithms II

Do you have extra memory available?

In direct linear algebra, we can

use it to avoid communication

by storing $1 \leq c \leq P^{1/3}$ redundant copies of data.

New theory….

- Potential 2.5D communication savings
  - #words moved, by factor of $c^{1/2}$
  - #messages sent, by factor of $c^{3/2}$
  - minimized in 3D case ($c = P^{1/3}$)

→ Tune to find optimal duplication factor c

Flanders ExaScience Lab (Intel Labs Europe) sending visitor this spring.

…. leads to faster algorithms

- New 2.5D matrix-matrix multiplication algorithm
  - Predict up to 5x speedups on future exascale hardware
  - using up to *c*=100 copies
- Also new 2.5D LU algorithm …

(SEE POSTER)
Solomonik

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Fast matmul comm. complexity

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Direct linear algebra does $\Theta(n^\omega)$ flops.

Conventional algorithms: $\omega = 3$
Strassen-like algorithms: $\omega < 3$
eg: $\omega \approx 2.81$ (Strassen's matmul)

New theory ...

- Strassen-like matmuls can communicate less than conventional matmuls.
- # words moved decreases: $\Omega\left(\frac{n^3}{M^{1/2}}\right) = \Omega\left(M\left(\frac{n}{M^{1/2}}\right)^3\right) \longrightarrow \Omega\left(M\left(\frac{n}{M^{1/2}}\right)^\omega\right)$
- # messages M times smaller

… leads to new algorithms

- Result: Strassen-like matmul attains these lower bounds in serial
- Can we attain these bounds in parallel?
  - We believe we can… (current work)
- Rest of sequential direct linear algebra (LU, QR, …) can attain the same bounds.
  - We believe it can in parallel too… (current work)

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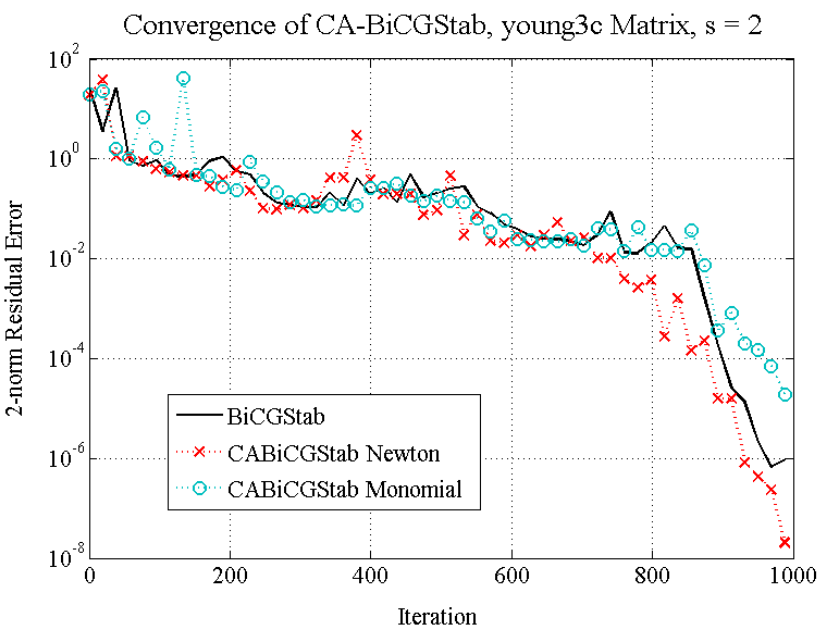
CA-Krylov methods I

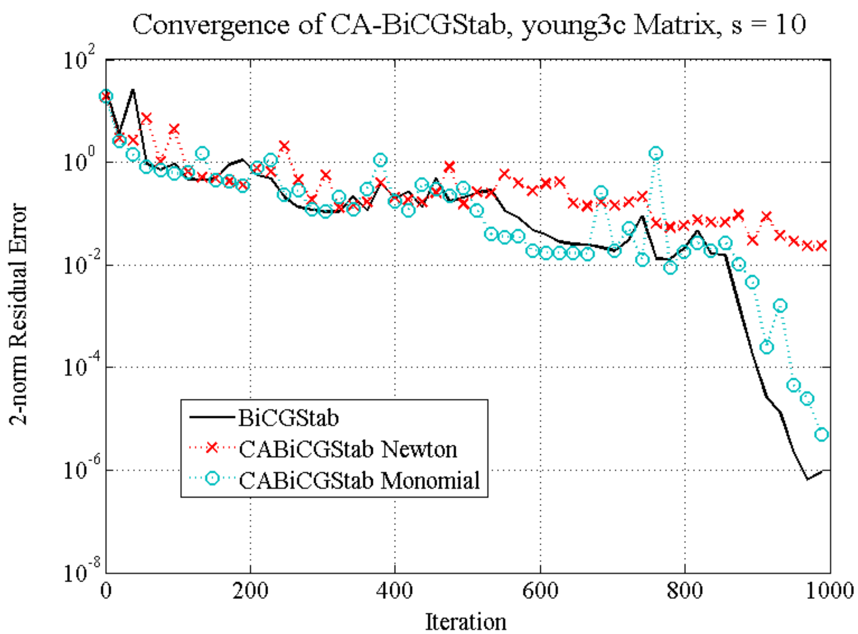
Communication-avoiding biconjugate gradient method

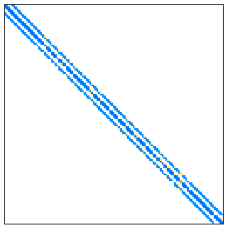
"CA-BiCG"

- Previously seen in poster, summer 2010 retreat
  - BiCG solves sparse, nonsymmetric systems of equations
  - CA-BiCG mathematically-equivalent formulation; takes multiple iterations with communication cost of one iteration of BiCG.
- BiCG vs. GMRES
  - GMRES: faster convergence and more stable, in theory and in practice
  - BiCG: small, constant-size workspace, less work per iteration
  - Stabilized variants (eg, BiCGStab) used in practice
- New communication-avoiding algorithms:
  - BiCG (2-term), CGS, BiCGStab, BiCGStab(*l*)

CA-Krylov methods II







young3c
N=841
nnz=3988
κ=1.15e4

- Reduce communication by factor of s
- CA-BiCGStab follows convergence of standard BiCGStab, even with s=10
- Hard problem! BiCGStab fails to converge in n its.
  - Preconditioning needed

(SEE POSTER)
Knight, Carson

CA-Krylov methods III

Communication-avoiding generalized minimum residual method

"CA-GMRES"

- Previously seen in poster, winter 2010 retreat
- Success story: Parlab → DOE-funded
  - CA-GMRES expected to appear in Spring 2011 Trilinos release
  - Contains tall-skinny QR (TSQR) based on Parlab work
    - Intel TBB + MPI
  - Ongoing work:
    - Incorporate M. Anderson's GPU TSQR (SEE POSTER)
    - New CA-GMRES variants: Flexible GMRES, Recycling GMRES
    - Fault tolerance

New matrix powers kernel

- Previously (Winter 2010):
  - Matrix powers kernel: key to avoiding synchronization in Krylov subspace methods (BiCG, GMRES, etc)
  - $[A, s, x] \rightarrow [x, Ax, A^2x, \ldots, A^sx]$
  - Analyzes system A at runtime

New algorithmic variants required by new CA Krylov methods:

- Both A and A^T
  - $[A, s, x] \rightarrow [[x, Ax, A^2x, \ldots, A^sx], [x, A^Tx, (A^T)^2x, \ldots, (A^T)^sx]]$
  - Multiple source vectors
  - $[A, s, X] \rightarrow [X, AX, A^2X, \ldots, A^sX]$
- Hypergraph partitioning (new communication model)
  - Beats current graph partitioning approach for structured, nonsymmetric matrices. (Up to 80% fewer words moved)
- Extends to (nonlinear) Health App

(SEE POSTER)
Carson, Knight

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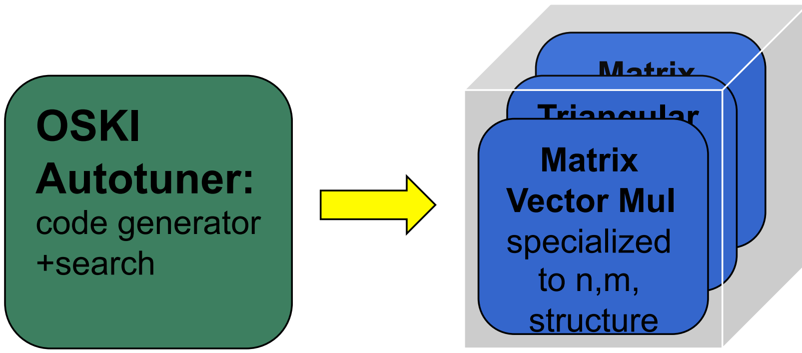
OSKI (Optimized Sparse Kernel Interface)



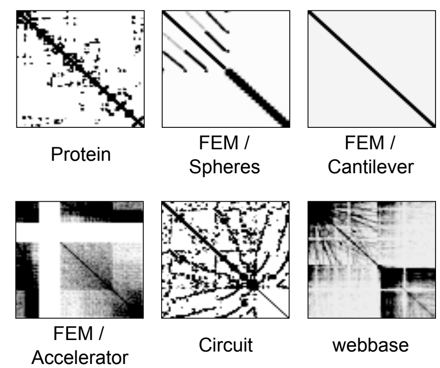
OSKI Library

- Functional portability
  - Python interface (via SEJITS)
  - C code underneath
- Performance portability
  - search/tune at install time

Optimized Sparse Kernel Interface (OSKI):

Autotuned Sparse Matrix-Vector Multiplication (SpMV)

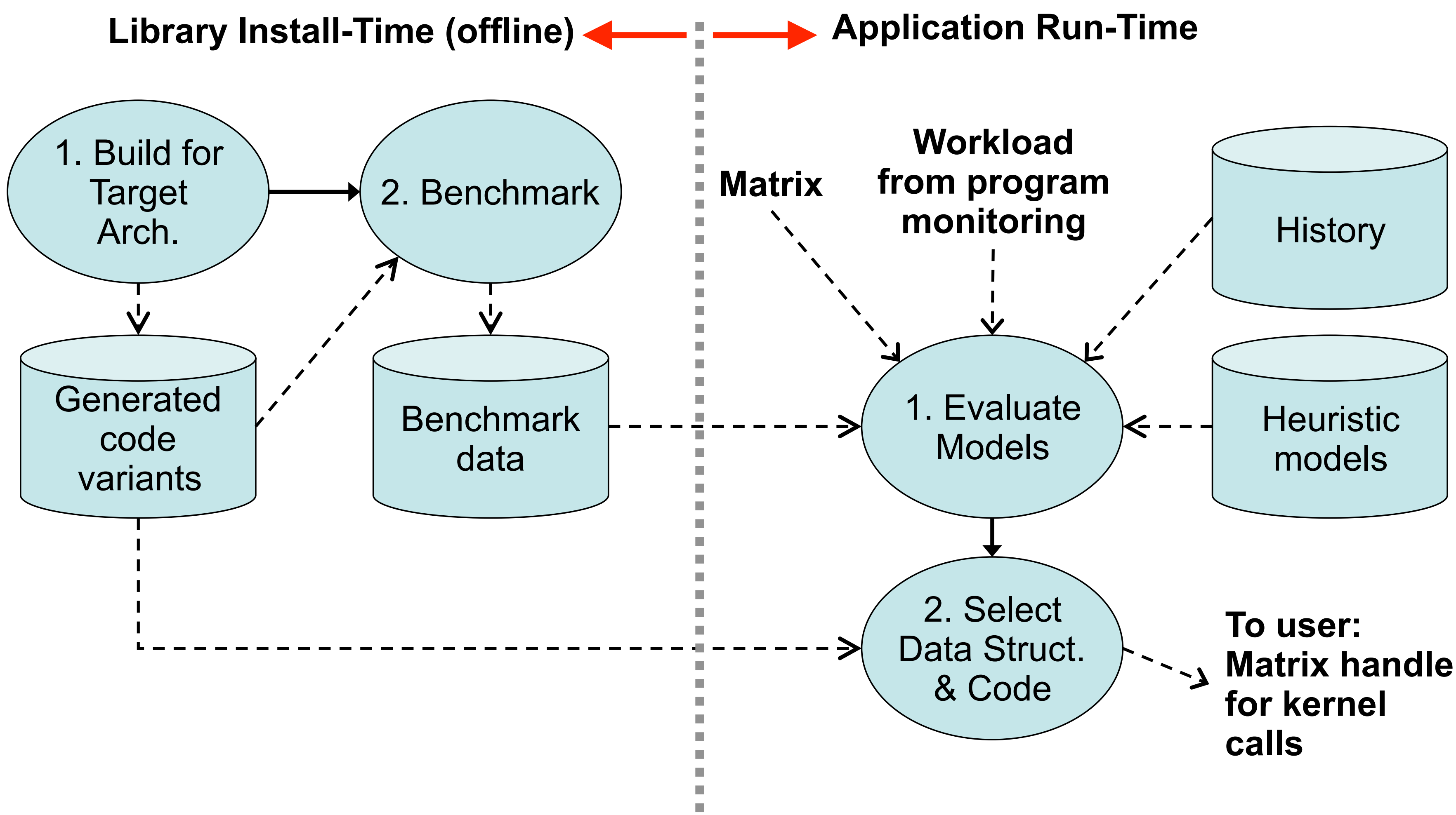
- Huge algorithm design space
- Performance = f(structure,dimension)
  - vs. dense matrix-vector mult: Perf = f(dimension)
  - Runtime tuning necessary



Efficient sparse codes are difficult to write
(SEE POSTER) Arnold, Bodik

OSKI (Optimized Sparse Kernel Interface)

How OSKI tunes:



Extensibility: Advanced users may write & dynamically add “Code variants” and “Heuristic models” to system.

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OSKI development I

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Algorithm design space for next (p)OSKI release:

- Index compression
- Array padding
- Software prefetching
- Software pipelining
- Loop unrolling (depths)
- SpMM (multiple source vectors)
- Variable block splitting
- Switch-to-dense (SpTS)
- Cache interleaving (A^TA)
- Sparse tiling (A^kx)
- Symmetric storage for multicore
- SIMD intrinsics
- Data decomposition (shared/dist)
- NUMA awareness
- Hiding latency
- Reordering (RCM, TSP, …)
- TLB blocking
- Cache-blocking heuristics
- Storage formats:
  - CSB (compressed sparse block)
  - Vector-style (manycore/GPU)
  - *DCSR (delta-coded CSR)*
  - *RPCSR (row-pattern CSR)*
  - *PBR (pattern-based repr.)*
  - *RSDF (row-segmented diagonal fmt.)*

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OSKI development II

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- Requested functionality (from HPC world):
  - Change non-zero pattern of the matrix
    - Matrix may change or be perturbed during computation
  - Assemble a matrix from (possibly overlapping) fragments
    - Common in finite element methods
  - Perform variable block splitting
    - $A = A_1 + A_2$ where A_1 and A_2 have different natural block sizes
- Our (proposed) solutions:
  - List_of_matrices: allows a matrix to be expressed as a sum of matrices ($A = A_1 + ... + A_n$)
    - Easily allows for assembly from fragments and variable splitting
    - Pattern update: represent the changed entry as the addition of another matrix
  - Merge() method: Merges the list $A_1 + ... + A_n$ into a single matrix
    - User can decide when to merge matrices, or…
    - In the future, merging may also be a tuning decision made by OSKI

Questions?

Extra Slides

Summary of Performance Optimizations

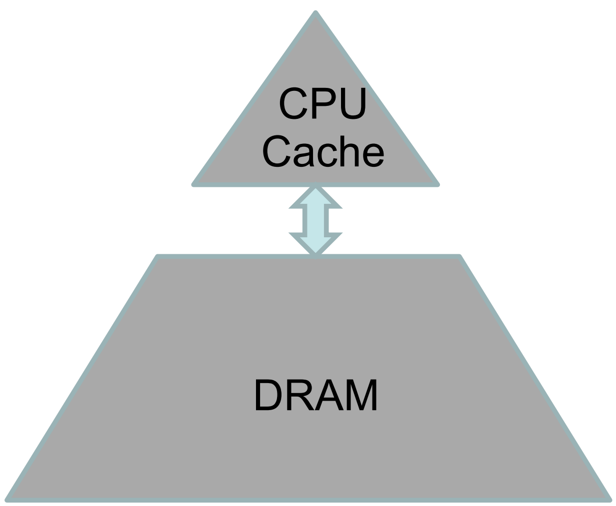
- Optimizations for SpMV
  - **Register blocking (RB)**: up to **4x** over CSR
  - **Variable block splitting**: **2.1x** over CSR, 1.8x over RB
  - **Diagonals**: **2x** over CSR
  - **Reordering** to create dense structure + **splitting**: **2x** over CSR
  - **Symmetry**: **2.8x** over CSR, 2.6x over RB
  - **Cache blocking**: **2.8x** over CSR
  - **Multiple vectors (SpMM)**: **7x** over CSR
  - And combinations…
- Sparse triangular solve
  - Hybrid sparse/dense data structure: **1.8x** over CSR
- Higher-level kernels
  - **$A \cdot A^T \cdot x$, $A^T \cdot A \cdot x$**: **4x** over CSR, 1.8x over RB
  - **$A^2 \cdot x$**: **2x** over CSR, 1.5x over RB
  - $[A \cdot x, A^2 \cdot x, A^3 \cdot x, .. , A^k \cdot x]$

Why Avoid Communication?

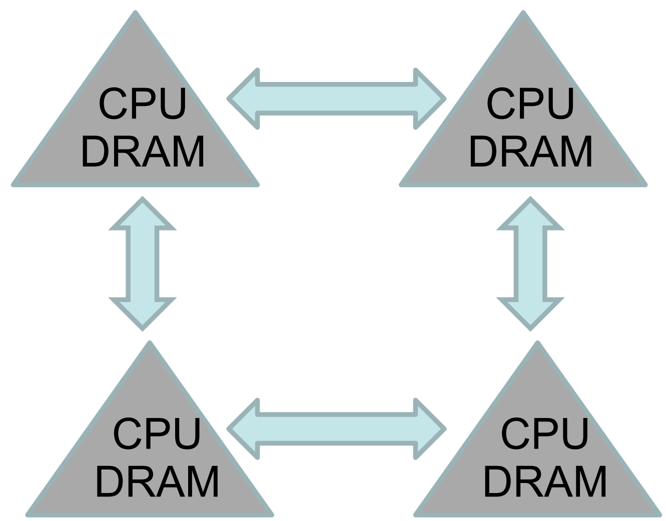
Algorithms have two costs:

1. Arithmetic (flops)
2. Communication: moving data between

- levels of a memory hierarchy (sequential)



- processors (parallel)
  - messages (distributed mem)



  - cache-coherency (shared mem)
  - data transfers (bus-based)

Why Avoid Communication?

- Running time of an algorithm is sum of 3 terms:
  - # flops * time_per_flop
  - # words moved / bandwidth ⎫
  - # messages * latency ⎭ communication

- Time_per_flop << 1/ bandwidth << latency
  - Gaps growing exponentially with time (FOSC, 2004)

Annual improvements			
Time_per_flop		Bandwidth	Latency
59%	Network	26%	15%
	DRAM	23%	5%

- Goal : reorganize linear algebra to *avoid* communication
  - Between all memory hierarchy levels
    - L1 ⟷ L2 ⟷ DRAM ⟷ network, etc
  - Not just *hiding* communication (speedup ≤ 2x)
  - Arbitrary speedups possible

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Avoiding Communication

- Let M = "fast" memory size (per processor). Then,

$$\#\ \text{words moved (per processor)} = \Omega\left(\frac{\#\ \text{flops per processor}}{M^{1/2}}\right)$$

$$\#\ \text{messages sent (per processor)} = \Omega\left(\frac{\#\ \text{flops per processor}}{M^{3/2}}\right)$$

- Parallel case: assume either load- or memory- balanced
- Trivial lower bound: #words moved ≥ #inputs + #outputs

- Holds for:
  - BLAS, LU, QR, EVD/SVD, tensor contractions, …
  - Some whole programs (sequences of these operations, no matter how individual ops are interleaved, e.g., A^k)
  - Sequential and parallel algorithms
  - Some graph theoretic algorithms (e.g., Floyd-Warshall)

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2.5D algorithms

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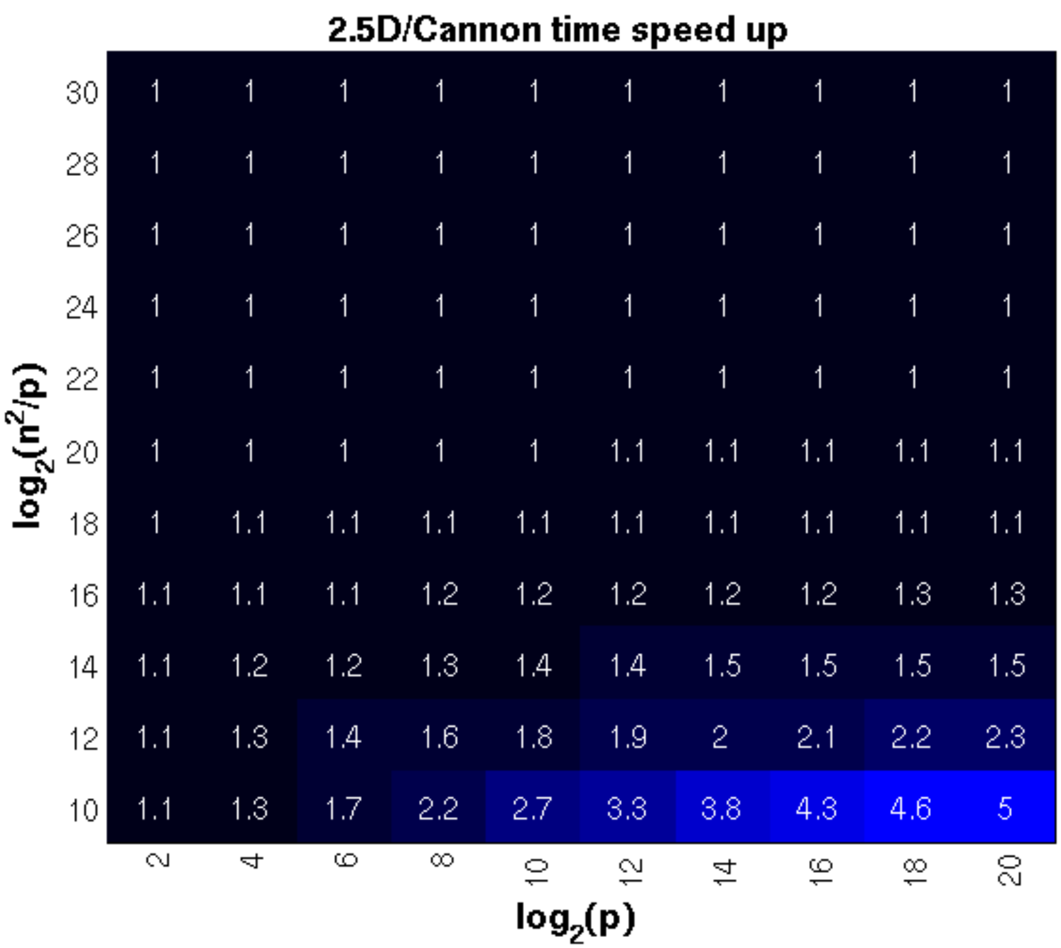
- P processors: # words moved = $\Omega\left(\frac{n^3/P}{M^{1/2}}\right)$ (intuition: make M bigger!)
- 2D algorithms: distribute matrices (2D arrays) across $\sqrt{P} \times \sqrt{P}$ (logical) 2D grid of processors
  - If one copy of data, $M = \frac{n^2}{P}$
  - What if you have extra memory?
- 3D algorithms: distribute matrices across $P^{1/3} \times P^{1/3} \times P^{1/3}$ processor cube,
  - $P^{1/3}$ duplicate copies of data (M increased by a factor of $P^{1/3}$)
  - This decreases lower bounds for:
    - # words moved by a factor of $P^{1/6}$
    - # messages sent by a factor of $P^{1/2}$
- 2.5D algorithms:
  - $1 \leq c \leq P^{1/3}$ copies of data: smooth transition between 2D to 3D bounds.
  - Flexibility

SEE POSTER

2.5D algorithms

Predicted exascale speedups



Model Parameters:

- 1×10^{18} flops/s (`exa-')
- 24 PB total memory
- 2^{20} nodes → 24 GB/node
- 100 GB/s interconnect bandwidth (overestimate?)
- 100 ns network latency

2.5D algorithms

2.5D Best choice of c for efficiency

$\log_2(n^2/p)$ \ $\log_2(p)$	2	4	6	8	10	12	14	16	18	20
30	1	1	1	1	1	1	1	1	1	1
28	2	3	4	4	4	4	4	4	4	4
26	2	3	4	6	10	16	15	16	15	16
24	2	3	4	6	10	16	25	40	64	57
22	2	3	4	6	10	16	25	40	64	102
20	2	3	4	6	10	16	25	40	64	102
18	2	3	4	6	10	16	25	40	64	102
16	2	3	4	6	10	16	25	40	64	102
14	2	3	4	6	10	16	25	40	64	102
12	2	3	4	6	10	16	25	40	64	102
10	2	3	4	6	10	16	25	40	64	102

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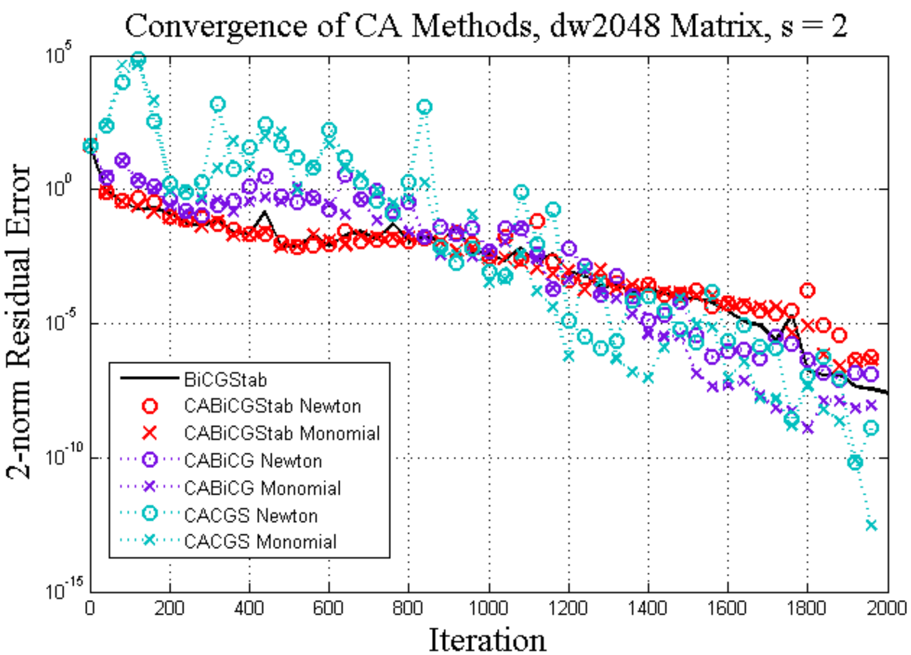
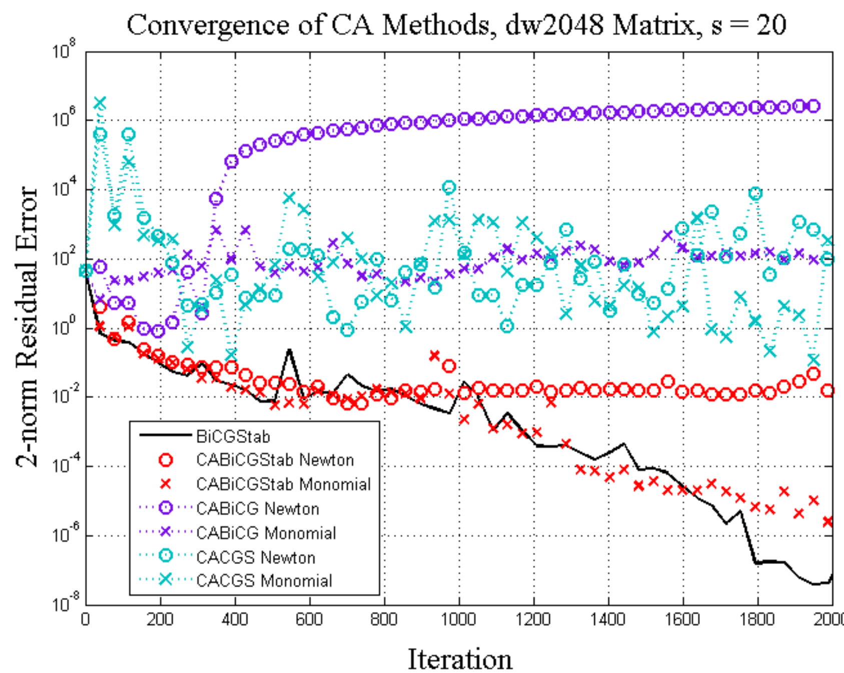
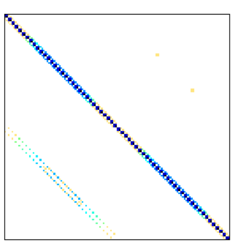
CA-Krylov methods II

CA-BiCGStab convergence







Name	n	NNZ	Pattern Symmetry	Value Symmetry	Condition Number	Application
dw2048	2048	10114	No	No	5.3015e3	Electromagnetics Problem (H. Dong, 1993)

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Fast matmul comm. complexity

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- M = fast memory size
- Conventional matrix-matrix multiplication (matmul)
  - # flops = $2n^3$
  - # words moved = $\Omega\left(\frac{n^3}{M^{1/2}}\right) = \Omega\left(M\left(\frac{n}{M^{1/2}}\right)^3\right)$, attainable
  - # messages = $\Omega\left(\frac{n^3}{M^{3/2}}\right) = \Omega\left(\left(\frac{n}{M^{1/2}}\right)^3\right)$, attainable
- Strassen's matmul
  - # flops = $\Theta(n^\omega)$ where $\omega = \log_2(7) \approx 2.81$
  - # words moved = $\Omega\left(M\left(\frac{n}{M^{1/2}}\right)^\omega\right)$, attainable too
  - # messages = $\Omega\left(\left(\frac{n}{M^{1/2}}\right)^\omega\right)$, attainable too
- Applies to all other Fast matmul algorithms we know
  - How broadly does it apply?
    - We know rest of linear algebra can be done in $O(n^\omega)$ flops and attain these #words moved and #messages, in serial.
    - If these are valid lower bounds, then they are tight