Communication-Avoiding Algorithms for Linear Algebra and Beyond

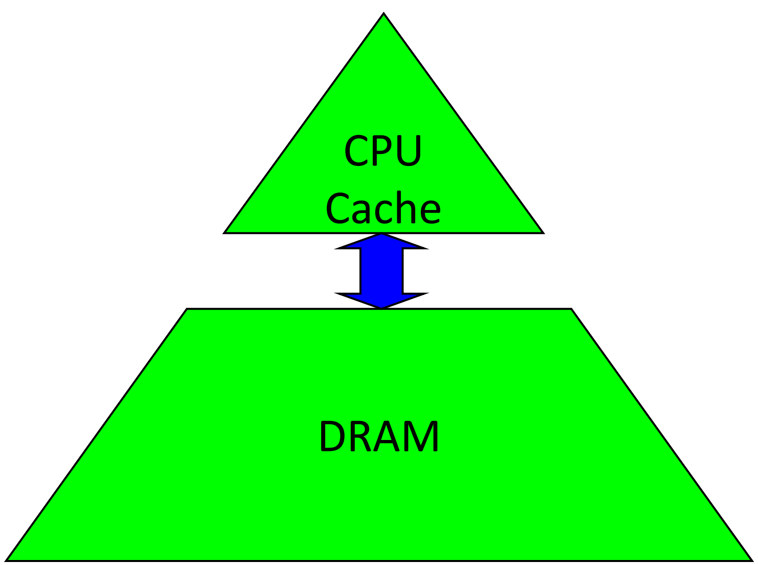
Longer version of slides available at:
www.cs.berkeley.edu/~demmel/SC16_tutorial_final

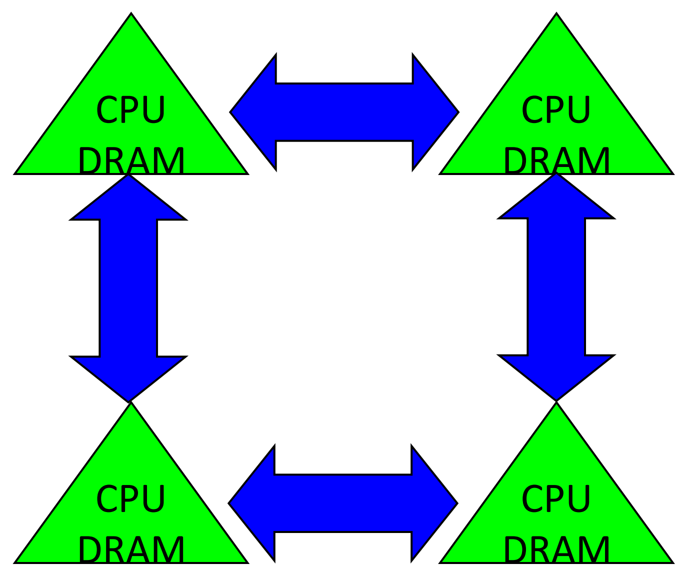
Jim Demmel, EECS & Math Depts, UC Berkeley
and many, many others …

Why avoid communication? (1/2)

Algorithms have two costs (measured in time or energy):

1. Arithmetic (FLOPS)
2. Communication: moving data between
   - levels of a memory hierarchy (sequential case)
   - processors over a network (parallel case).





Why avoid communication? (2/2)

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

  (# words moved / bandwidth and # messages * latency: communication)

- Time_per_flop << 1/ bandwidth << latency
  - Gaps growing exponentially with time
  - Avoid communication to save time
- Similar story for saving energy

Goals

- Redesign algorithms to *avoid* communication
  - Between all memory hierarchy levels
    - L1 $\longleftrightarrow$ L2 $\longleftrightarrow$ DRAM $\longleftrightarrow$ network $\longleftrightarrow$ disk
    - Accommodate heterogeneity
- Attain lower bounds if possible
  - Current algorithms often far from lower bounds
  - Large speedups and energy savings possible

Sample Speedups

- Up to **12x** faster for 2.5D matmul on 64K core IBM BG/P

Ideas adopted by Nervana, "deep learning" startup, acquired by Intel in August 2016

- Up to **2.1x** faster for 2.5D LU on 64K core IBM BG/P
- Up to **11.8x** faster for direct N-body on 32K core IBM BG/P
- Up to **13x** faster for Tall Skinny QR on Tesla C2050 Fermi NVIDIA GPU

SIAG on Supercomputing Best Paper Prize, 2016
Released in LAPACK 3.7, Dec 2016

- Up to **4.2x** faster for MiniGMG benchmark bottom solver, using CA-BiCGStab (**2.5x** for overall solve) on 32K core Cray XE6
  - **2.5x** / **1.5x** for combustion simulation code
- Up to **5.1x** faster for coordinate descent LASSO on 3K core Cray XC30

Summary of CA Algorithms

- “Direct” Linear Algebra
  - Lower bounds on communication for linear algebra problems like Ax=b, least squares, Ax = λx, SVD, etc
  - New algorithms that attain these lower bounds
    - Being added to libraries: Sca/LAPACK, PLASMA, MAGMA
    - Large speed-ups possible
  - Autotuning to find optimal implementation
- Ditto for programs accessing arrays (eg n-body)
- Ditto for “Iterative” Linear Algebra => ML

Lower bound for all "direct" linear algebra

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

#words_moved (per processor) = Ω(#flops (per processor) / $M^{1/2}$)

- Parallel case: assume either load or memory balanced

- Holds for
  – Matmul

Lower bound for all "direct" linear algebra

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

#words_moved (per processor) = Ω(#flops (per processor) / $M^{1/2}$)

#messages_sent ≥ #words_moved / largest_message_size

- Parallel case: assume either load or memory balanced
- Holds for
  – Matmul, BLAS, LU, QR, eig, SVD, tensor contractions, …
  – Some whole programs (sequences of these operations, no matter how individual ops are interleaved, eg A^k)
  – Dense and sparse matrices (where #flops << n^3)
  – Sequential and parallel algorithms
  – Some graph-theoretic algorithms (eg Floyd-Warshall)

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- Parallel case: assume either load or memory balanced
- Holds for
  - Matmul, BLAS, LU, QR, eig, SVD, tensor contractions, …
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SIAM SIAG/Linear Algebra Prize, 2012

Ballard, D., Holtz, Schwartz

Approach to generalizing lower bounds

- Matmul

  for i=1:n, for j=1:n, for k=1:n, C(i,j)+=A(i,k)*B(k,j)

=> for (i,j,k) in S = subset of Z^3, access locations indexed by (i,j), (i,k), (k,j)

- Direct N-body

  for i=1:n, for j=1:n, F(i) += func(P(i), P(j))

=> for (i,j) in S = subset of Z^2, access locations indexed by (i), (j)

- More general case

  for i1=1:n, for i2 = i1:m, … for ik = i3:i4

  C(i1+2*i3-i7) = func(A(i2+3*i4,i1,i2,i1+i2,…),B(pnt(3*i4)),…)

  D(something else) = func(something else), …

=> for (i1,i2,…,ik) in S = subset of Z^k

  Access locations indexed by "projections", eg

  ϕ_C (i1,i2,…,ik) = (i1+2*i3-i7)

  ϕ_A (i1,i2,…,ik) = (i2+3*i4,i1,i2,i1+i2,…), …

- Goal: Communication lower bounds and optimal algorithms for *any* program that looks like this

General Communication Lower Bound

- Thm: Given a program with array refs given by projections ϕ_j, then there is an $e \geq 1$ such that

  #words_moved = Ω (#iterations/M^{e-1})

  where e is the the value of a linear program:

  minimize $e = \Sigma_j \, e_j$ subject to

  $\text{rank}(H) \leq \Sigma_j \, e_j * \text{rank}(\phi_j(H))$ for all subgroups $H < Z^k$

  – Proof depends on recent result in pure mathematics by Christ/Tao/Carbery/Bennett
- Thm: This lower bound is attainable, via loop tiling
  – Assumptions: dependencies permit, and iteration space big enough

Avoiding Communication in Iterative Linear Algebra

- k-steps of iterative solver for sparse Ax=b or Ax=λx
  - Does k SpMVs with A and starting vector
  - Many such "Krylov Subspace Methods"
- Goal: minimize communication
  - Assume matrix "well-partitioned"
  - Serial implementation
    - Conventional: O(k) moves of data from slow to fast memory
    - **New**: **O(1) moves of data – optimal**
  - Parallel implementation on p processors
    - Conventional: O(k log p) messages (k SpMV calls, dot prods)
    - **New: O(log p) messages - optimal**
- Lots of speed up possible (modeled and measured)
  - Price: some redundant computation
- Recent extensions to Machine Learning (SGD)

Other on-going work

- Extending “2.5D algorithms”
  - Replicate data to avoid more communication with dist. mem.
- Write-avoiding algorithms for Nonvolatile memories
  - With NVM, writes can be much more expensive than reads
  - Can sometimes do asymptotically fewer writes than reads
- Reproducibility
  - Roundoff makes floating point nonassociative, so different summation orders give different results
  - Have new algorithms that are reproducible, but still cost just one reduction operation, one pass over data
  - IEEE 754 Standard considering adding new instruction
  - BLAS Standard considering adding ReproBLAS

Collaborators and Supporters

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- bebop.cs.berkeley.edu

For more details

- Bebop.cs.berkeley.edu
  - 155 page survey in Acta Numerica (2014)
- CS267 – Berkeley's Parallel Computing Course
  - Live broadcast in Spring 2017
    - www.cs.berkeley.edu/~demmel
    - All slides, video available
  - Prerecorded version broadcast since Spring 2013
    - www.xsede.org
    - Free supercomputer accounts to do homework
    - Free autograding of homework

Summary

Time to redesign all linear algebra, n-body,…
algorithms and software
(and compilers…)

Don’t Communic…