Communication Lower Bounds and Optimal Algorithms for Programs that Reference Arrays

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Motivation: Why avoid communication?

- Communication = moving data
  - Between levels of memory hierarchy
  - Between processors over network
- Running time of an algorithm is sum of 3 terms:
  - #flops * time_per_flop
  - #words_moved / bandwidth ... communication
  - #messages * latency ... communication
- Time_per_flop $\ll$ 1/bandwidth $\ll$ latency
  - Gaps growing exponentially
- Avoid communication to save time
- Same story for energy: Avoid communication to save energy

Example: Optimal Sequential Matmul

- Naive code
  - for i=1:n, for j=1:n, for k=1:n, $C(i,j) += A(i,k) * B(k,j)$
  - Moves $\Theta(n^3)$ words between cache (size $M < n^2$) and DRAM
- "Blocked" code
  - Write A as $n/b \times n/b$ matrix of $b \times b$ blocks $A[i,j]$
  - Ditto for B, C
  - for i=1:n/b, for j=1:n/b, for k=1:n/b,
    $C[i,j] += A[i,k] * B[k,j]$ ... $b \times b$ matmul
- Thm [Hong,Kung]: Choosing $b \overset{<}{\approx} (M/3)^{1/2}$ attains lower bound:
  #words_moved $= \Omega(n^3/M^{1/2})$
- Where do $1/2$'s come from?

New Theorem, applied to Matmul

- for i=1:n, for j=1:n, for k=1:n, $C(i,j) += A(i,k) * B(k,j)$
- Record array indices in matrix Δ

$$\Delta = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} i & j & k \end{array} \\ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{array}$$

- Let $x = [x_i, x_j, x_k]^T$, $\mathbf{1}$ = vector of 1's
- Solve LP: maximize $\mathbf{1}^T x$ such that $\Delta x \leq \mathbf{1}$
- Solution: $x = [1/2, 1/2, 1/2]$, $\mathbf{1}^T x = 3/2 \equiv s_{HBL}$
- Thm: #words_moved $= \Omega(n^3/M^{s_{HBL}-1}) = \Omega(n^3/M^{1/2})$.
- Attain by blocking index i by $\Theta(M^{x_i}) = \Theta(M^{1/2})$, ditto for j, k

New Theorem, applied to Direct n-Body

- for *i=1:n*, for *j=1:n*, $F(i) += force(P(i), P(j))$
- Record array indices in matrix Δ

$$\Delta = \begin{array}{c} \\ F \\ P(i) \\ P(j) \end{array} \begin{array}{c} \begin{array}{cc} i & j \end{array} \\ \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \end{array}$$

- Let $x = [x_i, x_j]^T$, $\mathbf{1}$ = vector of 1's
- Solve LP: maximize $\mathbf{1}^T x$ such that $\Delta x \le \mathbf{1}$
- Solution: $x = [1, 1]$, $\mathbf{1}^T x = 2 \equiv s_{HBL}$
- Thm: #words_moved $= \Omega(n^2 / M^{s_{HBL}-1}) = \Omega(n^2/M^1)$.
- Attain by blocking index i by $\Theta(M^{x_i}) = \Theta(M^1)$, ditto for j

New Theorem, applied to Random Code

- for *i1=1:n*, ... , for *i6=1:n*,
  $A1(i1, i3, i6) += func1(A2(i1, i2, i4), A3(i2, i3, i5), A4(i3, i4, i6))$
  $A5(i2, i6) += func2(A6(i1, i4, i5), A3(i3, i4, i6))$
- Record array indices in 6×6 matrix Δ
  - one column per index $i1$,...,$i6$
  - one row per distinct set of array subscripts $A1, ..., A6$
  - $\Delta(i, j) = 1$ if array subscript i has index j, else 0
- Let $x = [x_1, ..., x_6]^T$, $\mathbf{1}$ = vector of 1's
- Solve LP: maximize $\mathbf{1}^T x$ such that $\Delta x \leq \mathbf{1}$
- Solution: $x = [2/7, 3/7, 1/7, 2/7, 3/7, 4/7]$, $\mathbf{1}^T x = 15/7 \equiv s_{HBL}$
- Thm: #words_moved $= \Omega(n^6/M^{s_{HBL}-1}) = \Omega(n^6/M^{8/7})$.
- Attained by block sizes $M^{2/7}$, $M^{3/7}$, $M^{1/7}$, $M^{2/7}$, $M^{3/7}$, $M^{4/7}$

Summary of Results (1/3)

- Extend communication lower bound proof from linear algebra to any program with
  - Inner loop iterations indexed by $(i_1, ..., i_d)$
  - Arrays in inner loop subscripted by *linear* functions of indices
  - Ex: $A(i_1, i_2 - i_1, 3i_1 - 4i_2 + 7i_4, ...)$, $B(pntr(i_5 + 6i_6))$, ...
  - Can be dense or sparse, sequential or parallel, ...
- Based on recent generalization of Hölder, Loomis-Whitney, Brascamp-Lieb inequalities by Bennett/Carbery/Christ/Tao
  - Need to count lattice points, not volumes
  - Get linear program with one inequality per subgroup $H \leq \mathbb{Z}^d$
  - Solution of linear program (HBL-LP) is s_{HBL}
  - Thm: #words_moved = $\Omega(\#\text{loop\_iterations}/M^{s_{HBL}-1})$

Summary of Results (2/3)

- Can we write down the lower bound?
  - One inequality per subgroup $H \leq \mathbb{Z}^d$, but still finitely many!
  - Thm (Bad news): Writing down all inequalities in HBL-LP $\iff$ Hilbert's 10th Problem over $\mathbb{Q}$
  - Thm (Good news): Another LP has same solution, is decidable (but expensive, so far)
  - Thm (Better news): Easy to write down HBL-LP explicitly in many cases of interest (eg when subscripts are just subsets of indices)
  - Also easy to get upper/lower bounds on solution s_{HBL}

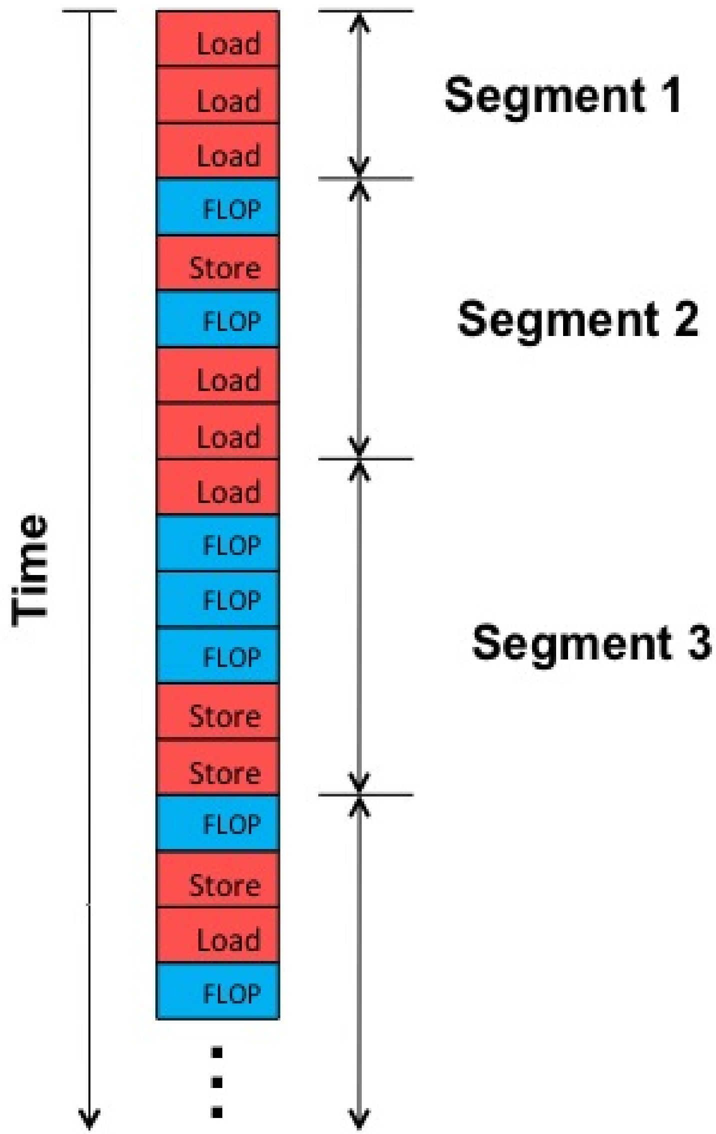
Summary of Results (3/3)

- Can we attain the lower bound?
  - Depends on loop dependencies
  - Best case: none, or reductions (like matmul)
  - Thm: When subscripts are just subsets of indices, the solution x of *dual* HBL-LP tells us the optimal tile sizes $M^{x_1}, \ldots, M^{x_d}$
  - Ex: linear algebra, n-body, "random code", database join, ...
  - Conjecture: always attainable (modulo dependencies)

Outline

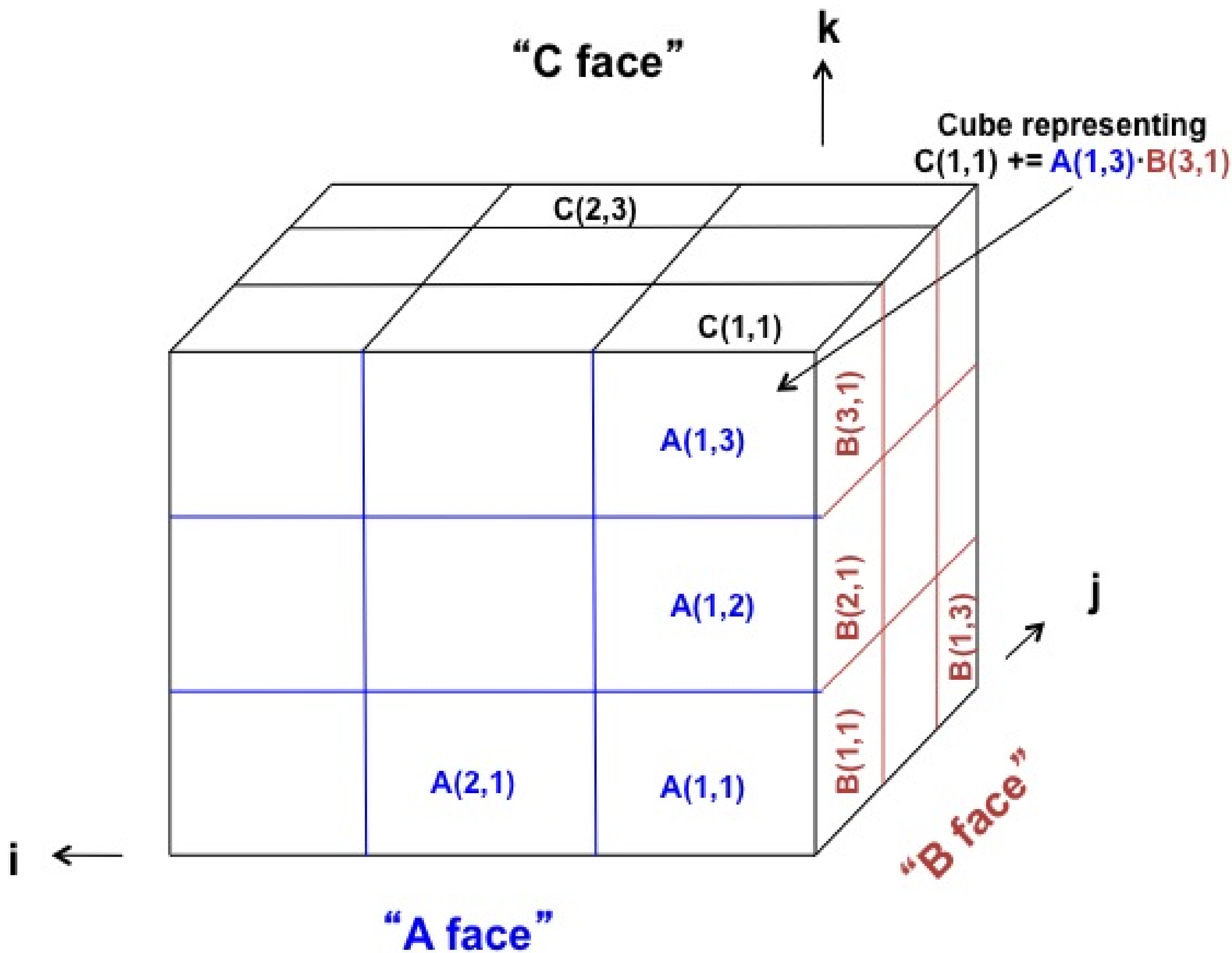
1. Recall lower bound proof for direct linear algebra using Loomis-Whitney
2. Hölder-Brascamp-Lieb Linear Program (HBL-LP)
   - Continuous case, then discrete case
3. Applying lower bound to more general code
4. Decidability of lower bound
   - Where Hilbert's 10th Problem over $\mathbb{Q}$ arises, how to avoid it
5. Special Case: When subscripts are just subsets of indices
   - Why HBL-LP simpler, why dual tells us optimal algorithm
6. Conclusions and Open Problems

Recall Proof for Direct Linear Algebra (3 Nested Loops)



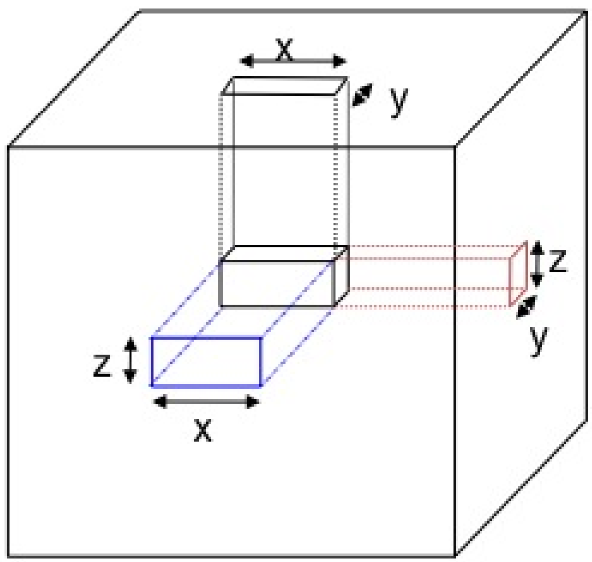
- M = fast memory size
- G = total number of flops
- Break instruction stream into "segments" of M loads/stores
- Data available per segment = 2*M
- Somehow derive upper bound F on #flops possible per segment
- #segments * F ≥ G
- #loads/stores = M * #segments
  ≥ MG/F
- All depends on upper bound F

Geometric Model



If we have at most 2M "A squares", 2M "B squares", and 2M "C squares" on faces, how many cubes can we have?

Loomis-Whitney



\# cubes in black box with
side lengths x, y and z

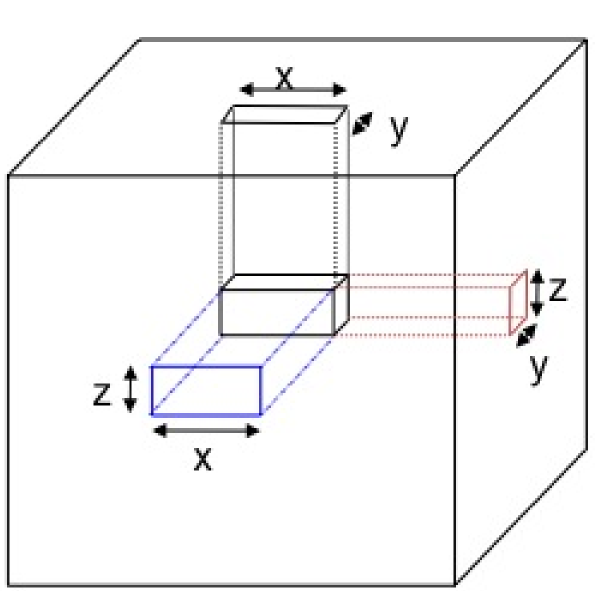
= Volume of black box

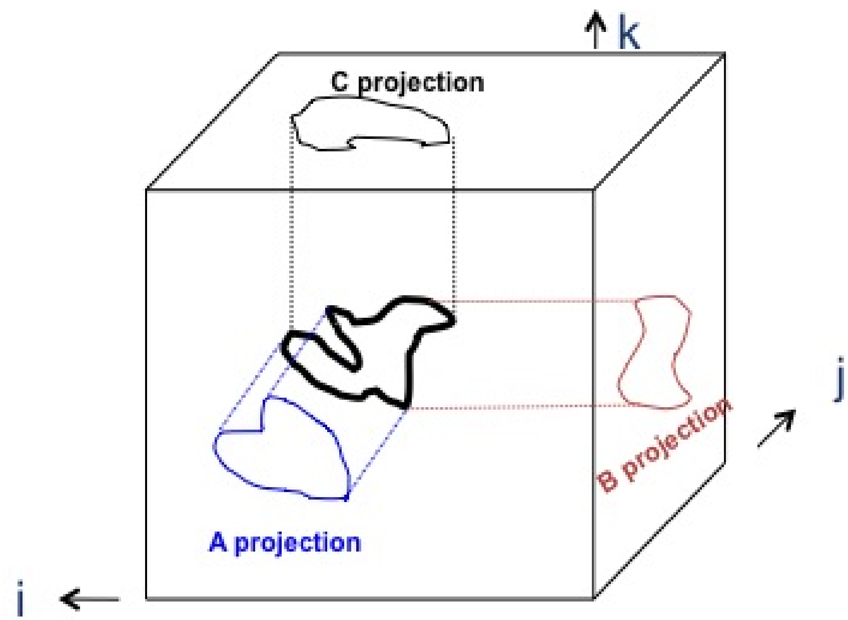
= $x \cdot y \cdot z$

= $(xz \cdot zy \cdot yx)^{1/2}$

= (#A□s · #B□s · #C□s $)^{1/2}$

Loomis-Whitney





cubes in black box with
side lengths x, y and z
= Volume of black box
= x·y·z
= (xz · zy · yx)$^{1/2}$
= (#A□s · #B□s · #C□s)$^{1/2}$

(i,k) is in A projection if (i,j,k) in 3D set
(j,k) is in B projection if (i,j,k) in 3D set
(i,j) is in C projection if (i,j,k) in 3D set

Thm (Loomis & Whitney, 1949)
cubes in 3D set = Volume of 3D set
≤ (area(A projection) ·
area(B projection) ·
area(C projection)) $^{1/2}$

Summary of Lower Bound Proof for 3 Nested Loops

- M = fast memory size, G = total number of flops
- Break instruction stream into segments of M loads/stores
- $\Longrightarrow 2M$ words of data available during segment
- Use Loomis Whitney to bound F = #multiplies/segment by

$$\begin{aligned} F &\leq (\#\text{A\_entries})^{1/2} \cdot (\#\text{B\_entries})^{1/2} \cdot (\#\text{C\_entries})^{1/2} \\ &\leq (2M)^{3/2} = O(M^{3/2}) \end{aligned}$$

- $F \cdot$#segments$\geq G \Longrightarrow$#segments $\geq G/F$
- #loads/stores = $M\cdot$ #segments $\geq MG/F = \Omega(G/M^{1/2})$
- Result independent of dependencies (so works for LU, etc)
- Result independent of G (so works for sparse, parallel etc)
- Bound decreases with $M \Longrightarrow$ replication may help (2.5D algs)

First Extension Strategy

- Loomis-Whitney $\Longrightarrow$ Hölder-Brascamp-Lieb (HBL)
- Volume of $E \subset \mathbb{R}^3 \Longrightarrow$ Volume of $E \subset \mathbb{R}^d$
- Projections from (i,j,k) to (i,j), (i,k), (k,j) $\Longrightarrow$ any linear projections $\phi_1, ..., \phi_m$
- $\text{vol}(E) \leq (\text{area}(E_{ij}))^{1/2} \cdot (\text{area}(E_{ik}))^{1/2} \cdot (\text{area}(E_{jk}))^{1/2} \Longrightarrow$ $\text{vol}(E) \leq C \cdot \prod_{i=1}^{m} \text{vol}(\phi_i(E))^{s_i}$

Where do we get exponents s_i and $C < \infty$?

Continuous HBL

Continuous HBL Linear Program (C-HBL-LP):

$$\dim(\mathbb{R}^d) = d = \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(\mathbb{R}^d)) = \sum_{i=1}^{m} s_i \cdot d_i$$

and for all subspaces $H \le \mathbb{R}^d$, $\dim(H) \le \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(H))$

Note: There exist infinitely many H, but only finitely many possible constraints in C-HBL-LP (at most $(d+1)^{m+1}$)

Thm (B/C/C/T): $s_i \ge 0$ satisfy C-HBL-LP *if and only if* $\exists\, C < \infty$ such that for all $f_i : \mathbb{R}^{d_i} \to [0, \infty)$ in L_{1/s_i}

$$\int_{\mathbb{R}^d} \prod_{i=1}^{m} f_i(\phi_i(x))dx \le C \cdot \prod_{i=1}^{m} (\int_{\mathbb{R}^{d_i}} [f_i(y)]^{1/s_i} dy)^{s_i} = C \cdot \prod_{i=1}^{m} \|f_i\|_{1/s_i}$$

Continuous HBL - Special case (1/3)

$$\dim(\mathbb{R}^d) = d = \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(\mathbb{R}^d)) = \sum_{i=1}^{m} s_i \cdot d_i$$

and for all subspaces $H \le \mathbb{R}^d$, $\dim(H) \le \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(H))$

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$$\int_{\mathbb{R}^d} \prod_{i=1}^{m} f_i(\phi_i(x))dx \le C \cdot \prod_{i=1}^{m} \|f_i\|_{1/s_i}$$

Hölder's Inequality: Choose all ϕ_i = identity, so $\sum_{i=1}^{m} s_i = 1$

$$\|\prod_{i=1}^{m} f_i(x)\|_1 \le C \prod_{i=1}^{m} \|f_i\|_{1/s_i} \qquad \text{... can show } C = 1$$

Continuous HBL - Special case (2/3)

$$\dim(\mathbb{R}^d) = d = \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(\mathbb{R}^d)) = \sum_{i=1}^{m} s_i \cdot d_i \qquad (*)$$

and for all subspaces $H \leq \mathbb{R}^d$, $\dim(H) \leq \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(H))$

Thm (B/C/C/T): $s_i \geq 0$ satisfy C-HBL-LP *if and only if*
$\exists\, C < \infty$ such that for all $f_i : \mathbb{R}^{d_i} \to [0, \infty)$ in L_{1/s_i}

$$\int_{\mathbb{R}^d} \prod_{i=1}^{m} f_i(\phi_i(x))dx \leq C \cdot \prod_{i=1}^{m} \|f_i\|_{1/s_i}$$

Brascamp-Lieb Inequality: Given only (*), C maximized by $f_i(x) = \exp(-x^T A_i x)$ for some s.p.d. A_i (C could be ∞)

Continuous HBL - Special case (3/3)

$$\dim(\mathbb{R}^d) = d = \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(\mathbb{R}^d)) = \sum_{i=1}^{m} s_i \cdot d_i$$

and for all subspaces $H \leq \mathbb{R}^d$, $\dim(H) \leq \sum_{i=1}^{m} s_i \cdot \dim(\phi_i(H))$

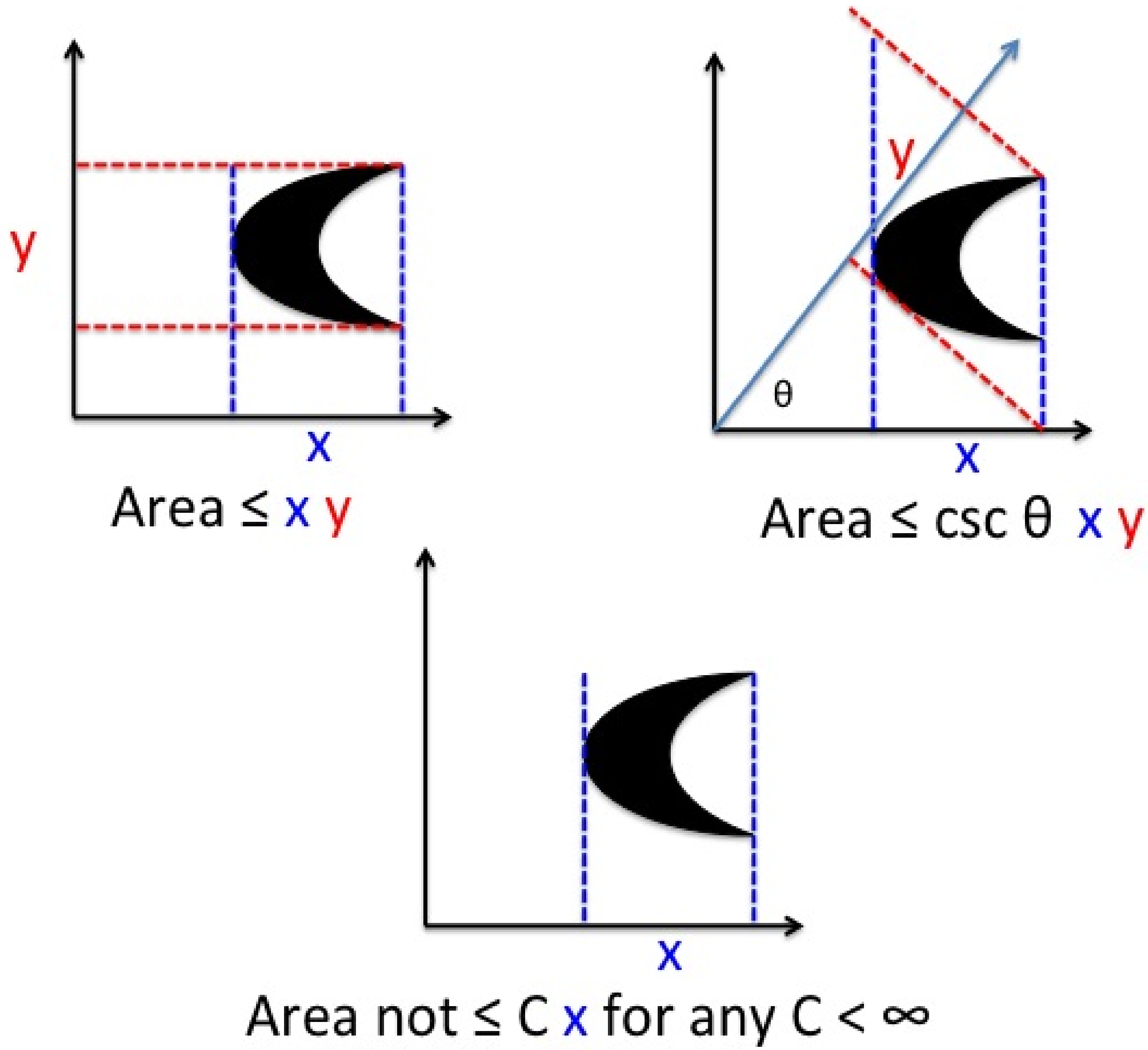
Thm (B/C/C/T): $s_i \geq 0$ satisfy C-HBL-LP *if and only if* $\exists\, C < \infty$ such that for all $f_i : \mathbb{R}^{d_i} \to [0, \infty)$ in L_{1/s_i}

$$\int_{\mathbb{R}^d} \prod_{i=1}^{m} f_i(\phi_i(x))dx \leq C \cdot \prod_{i=1}^{m} \|f_i\|_{1/s_i}$$

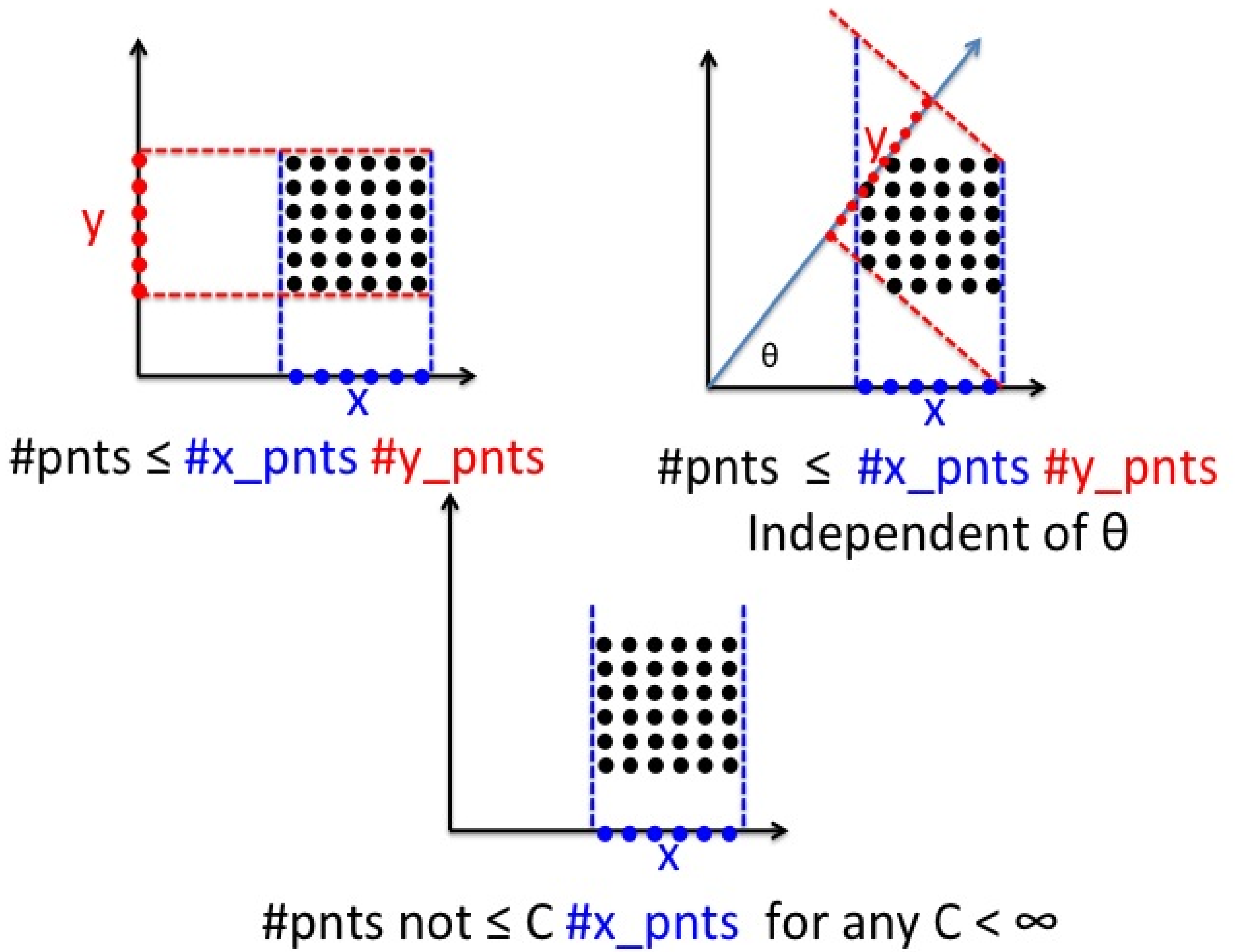
Loomis-Whitney & beyond: Given bounded $E \subset \mathbb{R}^d$, f_i = indicator function of $\phi_i(E)$,

$$\mathrm{vol}(E) \leq C \cdot \prod_{i=1}^{m} (\mathrm{vol}(\phi_i(E)))^{s_i}$$

Illustration of C-HBL-LP



But we want to count lattice points ≡ loop iterations



Second Extension Strategy: Discrete HBL (1/2)

- Count lattice points instead of volumes:
  - Lattice points correspond to loop iterations

$$(i, j, k) \longleftrightarrow C(i, j) += A(i, k) * B(k, j)$$

  - Projected lattice points correspond to array entries

$$(i, j) \longleftrightarrow C(i, j), \quad \text{etc}$$

- Vector space $\mathbb{R}^d \Longrightarrow$ abelian group $\mathbb{Z}^d$ under addition
- Subspaces $H \leq \mathbb{R}^d \Longrightarrow$ subgroups $H \leq \mathbb{Z}^d$
- Linear projection $\phi_i \Longrightarrow$ group homomorphism ϕ_i
- Subspace $\phi_i(H) \Longrightarrow$ subgroup $\phi_i(H)$
- $\dim(H) \Longrightarrow \text{rank}(H)$, $\dim(\phi_i(H)) \Longrightarrow \text{rank}(\phi_i(H))$
- Like C-HBL-LP, but all H, ϕ_i are integer, not real

Second Extension Strategy: Discrete HBL (2/2)

Discrete HBL Linear Program (D-HBL-LP):
for all subgroups $H \le \mathbb{Z}^d$, $\text{rank}(H) \le \sum_{i=1}^m s_i \cdot \text{rank}(\phi_i(H))$

Note: There exist infinitely many H, but only finitely many possible constraints in D-HBL-LP (at most $(d+1)^{m+1}$)

Thm (B/C/<u>C</u>/T): $s_i \ge 0$ satisfy D-HBL-LP *if and only if* for any finite set $E \subset \mathbb{Z}^d$ its cardinality $|E|$ is bounded by

$$|E| \le \prod_{i=1}^{m} |\phi_i(E)|^{s_i} \qquad \ldots \quad C = 1!$$

We want tightest bound when $|\phi_i(E)| \le 2M$, i.e. $|E| \le (2M)^{\sum_{i=1}^m s_i}$
$\Longrightarrow$ Compute $s_{HBL} \equiv \min \sum_{i=1}^m s_i$ subject to D-HBL-LP

Thm: #words_moved $= \Omega(\#\text{iterations}/M^{s_{HBL}-1})$

Some ideas in the proof of Discrete HBL (1/2)

$\forall\, H \le \mathbb{Z}^d$, $\text{rank}(H) \le \sum_{i=1}^m s_i{\cdot}\text{rank}(\phi_i(H)) \Longleftrightarrow |E| \le \prod_{i=1}^m |\phi_i(E)|^{s_i}$

- Necessity
  - For any $H \le \mathbb{Z}^d$, let E_n be $n \times n \times \cdots \times n$ "brick" in H
  - $|E_n| = \Theta(n^{\text{rank}(H)})$ and $|\phi_i(E_n)| = O(n^{\text{rank}(\phi_i(H))})$

$$\begin{aligned}\Theta(n^{\text{rank}(H)}) &= |E_n| \le \prod_{i=1}^m |\phi_i(E_n)|^{s_i} \\ &= O(\prod_{i=1}^m n^{s_i\cdot\text{rank}(\phi_i(H))}) = O(n^{\sum_{i=1}^n s_i\cdot\text{rank}(\phi_i(H))})\end{aligned}$$

Some ideas in the proof of Discrete HBL (2/2)

$\forall\, H \leq \mathbb{Z}^d$, $\mathrm{rank}(H) \leq \sum_{i=1}^{m} s_i \cdot \mathrm{rank}(\phi_i(H)) \iff |E| \leq \prod_{i=1}^{m} |\phi_i(E)|^{s_i}$

- Sufficiency (hard part)
  - Suffices to consider extreme points $s = [s_1, ..., s_m]$ of polytope defined by D-HBL-LP
  - Induction over d
  - Def: $H \leq \mathbb{Z}^d$ *critical* if $\mathrm{rank}(H) = \sum_{i=1}^{m} s_i \cdot \mathrm{rank}(\phi_i(H))$
  - Given $V \leq \mathbb{Z}^d$ and s extreme point, then either $\exists$ critical $\{0\} < H < V$ (induction on H) or $s \in \{0,1\}^m$

Applying Bounds to More General Code (1/5)

- General model:

  for all $\mathcal{I} \in \mathcal{Z} \subset \mathbb{Z}^d$, in some order
  $\quad$ inner_loop($\mathcal{I}, A_1(\phi_1(\mathcal{I})), ..., A_m(\phi_m(\mathcal{I}))$)

- Ex: LU inner loop: $A(i,j) = A(i,j) - L(i,k) * U(k,j)$
  - Ok to ignore loop scaling columns of L
  - Ok to overwrite A: $L(i,k) = A(i,k)$ for $i > k$, ditto for U
  - Same idea applies to BLAS, Cholesky, LDL^T, ...
  - Same idea applies to tensor contractions
  - QR, eig, SVD need another idea

Applying Bounds to More General Code (2/5)

- General model:

  for all $\mathcal{I} \in \mathcal{Z} \subset \mathbb{Z}^d$, in some order
  inner_loop($\mathcal{I}, A_1(\phi_1(\mathcal{I})), \ldots, A_m(\phi_m(\mathcal{I}))$)

- Ex: Computing $B = A^k$ (k odd)
  for $i_1 = 1 : \lfloor k/2 \rfloor$, $C = A \cdot B$, $B = A \cdot C$

- Imperfectly nested loops

- Can't just omit $B = A \cdot C$; infinite data reuse possible, so any lower bound $\propto |\mathcal{Z}|$ must be 0; leads to infeasible HBL-LP

- Solution: *impose reads/writes*: let $\hat{A}[1] = A$, then
  for $i_1 = 2 : k$, $\hat{A}[i_1] = \hat{A}[1] * \hat{A}[i_1 - 1]$

- Apply lower bound to new code, subtract added #reads/writes

- #words_moved $= \Omega(kn^3/M^{1/2} - kn^2) = \Omega(kn^3/M^{1/2})$

Applying Bounds to More General Code (3/5)

- General model:

  for all $\mathcal{I} \in \mathcal{Z} \subset \mathbb{Z}^d$, in some order
  inner_loop($\mathcal{I}, A_1(\phi_1(\mathcal{I})), ..., A_m(\phi_m(\mathcal{I}))$)

- Ex: Database join

  for $i_1 = 1 : N_1$, for $i_2 = 1 : N_2$
  if predicate($R(i_1), S(i_2)$) = true,
  output$(i_1, i_2) = func(R(i_1), S(i_2))$

  - Write $\mathcal{Z} = \mathcal{Z}_T \cup \mathcal{Z}_F$, depending on predicate
  - Apply lower bound to $\mathcal{Z}_T$, $\mathcal{Z}_F$ separately, take max
  - #words_moved = $\Omega(\max(|\mathcal{Z}_T|, |\mathcal{Z}|/M))$

Applying Bounds to More General Code (4/5)

- General model:

$$\text{for all } \mathcal{I} \in \mathcal{Z} \subset \mathbb{Z}^d, \text{ in some order}$$
$$\quad \text{inner\_loop}(\mathcal{I}, A_1(\phi_1(\mathcal{I})), \ldots, A_m(\phi_m(\mathcal{I})))$$

- Ex: Dense or sparse QR decomposition, using orthogonal transformations
- Not one "algorithm," many variations: un/blocked Givens/Householder, order in which entries zeroed out, ...
- Blocking orth. trans. ⇒ imperfectly nested loops
  - Challenge: output of first nest input to second, so need to bound data reuse

Applying Bounds to More General Code (5/5)

- Dense or sparse QR decomposition, continued
- Thm 1: #words_moved $= \Omega(\#\text{flops}/M^{1/2})$ if
  - Blocked Householder with any block sizes
  - One Householder transform per column
- Thm 2: #words_moved $= \Omega(\#\text{flops}/M^{1/2})$ if
  - "Forward Progress": each entry zeroed out once
  - Block size must be 1
- Conjecture: Forward Progress sufficient
- Generalizes to eigenvalue problems

Decidability of the Lower Bound (1/3)

- Recall Continuous HBL-LP: $\dim(\mathbb{R}^d) = d = \sum_{i=1}^m s_i \cdot \dim(\phi_i(\mathbb{R}^d))$ and $\forall H \le \mathbb{R}^d$, $\dim(H) \le \sum_{i=1}^m s_i \cdot \dim(\phi_i(H))$
- To write this down, need to solve:
  Given $r_H, r_{H_1}, \ldots, r_{H_m}$, decide if $\exists H \le \mathbb{R}^d$ s.t.
  $\dim(H) = r_H$, $\dim(\phi_1(H)) = r_{H_1}$,..., $\dim(\phi_m(H)) = r_{H_m}$
- Write H as $d \times d$ matrix
- Write each ϕ_i as $d_i \times d$ matrix
- Express rank conditions by (non)zero constraints on minors
- Tarski-decidable
  - Enough to get upper bound on $s_{HBL} \Longrightarrow$ valid lower bound on communication (possibly too low)

Decidability of the Lower Bound (2/3)

- What about Discrete HBL-LP?
  $\forall H \le \mathbb{Z}^d$, $\mathrm{rank}(H) \le \sum_{i=1}^{m} s_i \cdot \mathrm{rank}(\phi_i(H))$
- To write this down, need to solve:
  Given $r_H, r_{H_1}, ..., r_{H_m}$, decide if $\exists H \le \mathbb{Z}^d$ s.t.
  $\mathrm{rank}(H) = r_H$, $\mathrm{rank}(\phi_1(H)) = r_{H_1}$,..., $\mathrm{rank}(\phi_m(H)) = r_{H_m}$
- Can encode with minors as before
- Thm: Whether any given system of polynomial equations with rational coefficients has a rational solution or not can be encoded by right choice of $\phi_1, ..., \phi_m$.
- Cor: Being able to write down D-HBL-LP $\Longleftrightarrow$
  $\exists$ decision procedure for Hilbert's 10th Problem over $\mathbb{Q}$
  - Over $\mathbb{Q}$ instead of $\mathbb{Z}$ because all conditions homogeneous

Decidability of the Lower Bound (3/3)

- What about Discrete HBL-LP?
  $\forall H \leq \mathbb{Z}^d$, $\text{rank}(H) \leq \sum_{i=1}^{m} s_i \cdot \text{rank}(\phi_i(H))$
- Constraints define polytope $\mathcal{P}$ in space of $[s_1, ..., s_m] \in \mathbb{R}^m$
- Enough to get any subset of subgroups H defining $\mathcal{P}$
- Let $(H_1, H_2, H_3, ...)$ be any enumeration of all $H \leq \mathbb{Z}^d$
- Let $\mathcal{P}_i$ be polytope defined by $(H_1, ..., H_i)$
- "Simple" decidability algorithm:

$$i = 0, \text{ repeat } i = i + 1 \text{ until } \mathcal{P}_i = \mathcal{P}$$

- Thm: Decidable whether a vertex of $\mathcal{P}_i$ in $\mathcal{P}$
  - Similar induction idea as before
- Better algorithm: which subgroups H to try first?

Special Case: When subscripts are just subsets of indices (1/3)

- Ex: linear algebra, N-body, database join, ...
  - Matmul: (i, j, k) are indices, subscripts $A(i, k)$, $B(k, j)$, $C(i, j)$
- Much simpler:
  - Easy to write down Discrete HBL-LP to get lower bound
  - Easy to attain lower bound (modulo dependencies): Dual of Discrete HBL-LP gives optimal block sizes
  - Basis of examples at start of talk
- Extends to subsets of unimodular transformations of indices
  - Ex: subsets of $(i, 2i + j, 3i + 2j + k)$

Special Case: When subscripts are just subsets of indices (2/3)

- $i_1, ..., i_d$ be indices, ϕ_1,...,ϕ_m be projections
- Let $\Delta_{j,k} = 1$ if i_k in range of ϕ_j, else 0
- Thm: Let $s = [s_1, ..., s_m]$ minimize $\mathbf{1}^T s \equiv s_{HBL}$ such that $s^T \Delta \geq \mathbf{1}^T$. Then
  #words_moved = Ω(#loop_iterations/$M^{s_{HBL}-1}$)
- Proof idea
  - Constraints $s^T \Delta \geq 1$ are subset of Discrete HBL-LP, for all H spanned by $(0, ..., 0, 1, 0, ..., 0)$ (k-th entry = 1)
  - Show this subset implies $\text{rank}(H) \leq \sum_{j=1}^{m} s_j \text{rank}(\phi_j(H))$ for all $H \leq \mathbb{Z}^d$

Special Case: When subscripts are just subsets of indices (3/3)

- $i_1, ..., i_d$ be indices, $\phi_1,...,\phi_m$ be projections
- Let $\Delta_{j,k} = 1$ if i_k in range of ϕ_j, else 0
- Dual LP: Let $x = [x_1, ..., x_d]$ maximize $\mathbf{1}^T x \equiv s_{HBL}$ such that $\Delta x \le \mathbf{1}^T$.
- Thm: The solution x of the Dual LP gives the optimal block sizes to minimize communication: i_k blocked by M^{x_k}
- Proof idea
  - Each constraint in $\Delta x \le \mathbf{1}$ bounds number of entries of each array by M
  - $\mathbf{1}^T x = s_{HBL}$ says number of inner loop iterations per block is $M^{s_{HBL}}$.
- Extends to parallel case, "n.5D" algorithms

Some improved algorithms that avoid communication

- Work of many people!
  - Up to **12x** faster for 2.5D matmul on 64K core IBM BG/P
  - Up to **3x** faster for tensor contractions on 3K core Cray XE6
  - Up to **6.2x** faster for APSP on 24K core Cray XE6
  - Up to **2.1x** faster for 2.5D LU on 64K core IBM BG/P
  - Up to **11.8x** for direct N-body on 32K core IBM BP/P
  - Up to **13x** for TSQR on Tesla C2050 Ferma NVIDIA GPU
  - Up to **6.7x** faster for symeig(band A) on 10 core Intel Westmere
  - Up to **2x** faster for 2.5D Strassen on 38K core Cray XT4
- Communicate asymptotically $<$ existing algorithms in theory
  - SVD, LDL^T, 2.5D QR, Nonsymmetric eigenproblem
  - QR with column pivoting, other pivoting schemes
  - Sparse Cholesky, for suitable graphs

Conclusions

- Possible to derive decidable communication lower bounds for many widely used algorithms that access arrays
- Possible to achieve these bounds in many cases, leading to faster algorithms
- Open problems
  - Make derivation of lower bounds efficient, automate it
  - Conjecture: Always attainable, modulo loop dependencies
  - Implement in compilers

Key to Success

Key to Success

Don't Communic...