Avoiding communication in geometric multigrid

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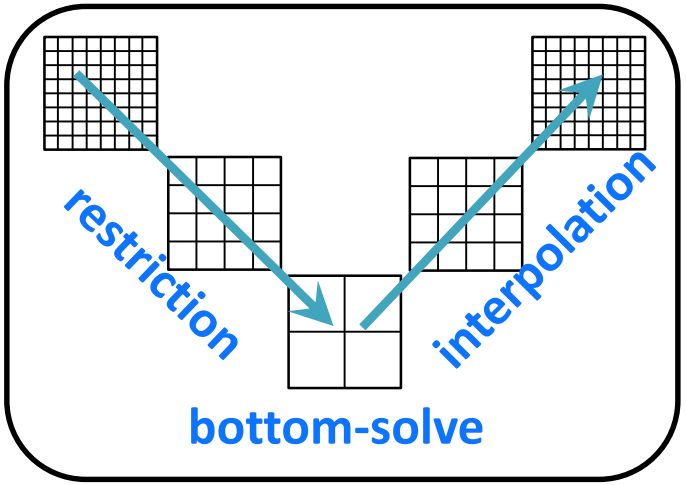
Talk overview

- Coarse grid solver ("bottom solver") often the bottleneck in geometric multigrid methods due to **high cost of global communication**
- Replacing classical solver with ***communication-avoiding*** variant can asymptotically reduce global communication
- **Implementation**, **evaluation**, and **optimization** of a communication-avoiding formulation of the Krylov solver routine (**CA-BICGSTAB**) as a high-performance, distributed-memory bottom solve routine for geometric multigrid
- Bottom solver **speedups**: **4.2x** in miniGMG benchmark, up to **2.5x** in real applications
- First use of communication-avoiding Krylov subspace methods for improving multigrid bottom solve performance

Geometric multigrid

- Numerical simulations in a wide array of scientific disciplines require solving elliptic/parabolic PDEs on a hierarchy of adaptively refined meshes
- Geometric multigrid (GMG) is a good choice for many problems
- Consists of a series of V-cycles ("U-cycles")
  - When further coarsening becomes infeasible, solve distributed coarse grid problem
  - Other options: agglomerate and solve local coarse grid problem, switch to algebraic, etc.



- Krylov subspace methods commonly used for bottom solve routines
  - Only require approximate solve, matrix-free representation
  - GMG + Krylov method available as solver option in many available software packages (e.g., BoxLib, Chombo, PETSc, hypre)

Krylov subspace methods

- Iterative methods based on projection onto expanding subspaces
- In iteration m, approximate solution x_m to $Ax = b$ chosen from the expanding **Krylov Subspace:**

$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\}$$

where $r_0 = b - Ax_0$, subject to orthogonality constraints

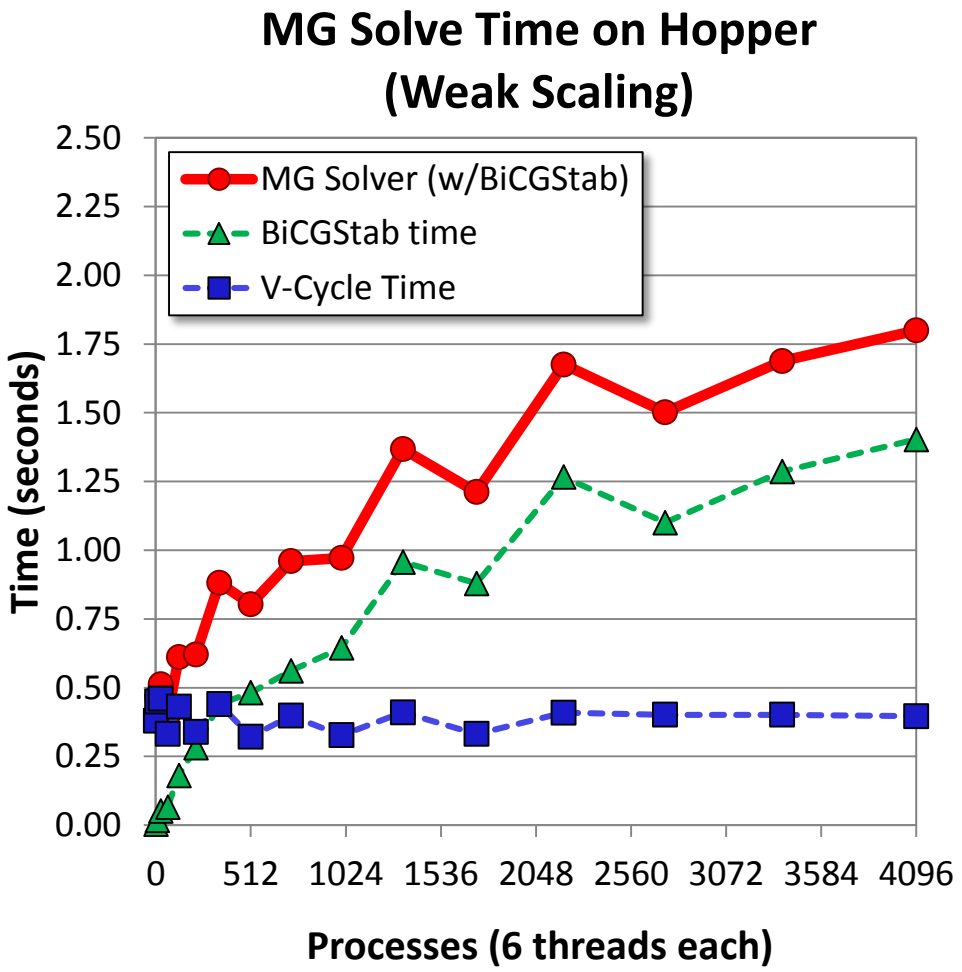
- Main computational kernels in each iteration:
  - **Sparse matrix-vector multiplication** (SpMV) : Compute new basis vector to increase the dimension of the Krylov subspace
    - **P2P communication** (nearest neighbors)
  - **Inner products**: orthogonalization to select "best" solution
    - **MPI_Allreduce** (global synchronization)
- Examples: Conjugate Gradient (CG), Generalized Minimum Residual Methods (GMRES), Biconjugate Gradient (BICG), BICG Stabilized (BICGSTAB)

The miniGMG benchmark

- Geometric multigrid benchmark from (Williams, et al., 2012)
- Designed to **mimic key computational characteristics** of applications, present a **challenge for exascale** architectures
- Uses hybrid MPI+OpenMP
- Finite-volume discretization of variable-coefficient Helmholtz equation ($Lu = a\alpha u - b\nabla \cdot \beta \nabla u = f$) on a cube, periodic boundary conditions
- Global 3D domain, partitioned into subdomains: one 64^3 box per MPI process (reflects memory capacity challenges of real AMR MG combustion applications)
- Piecewise constant interpolation, GSRB smoothing in V-cycle
- When box size reduced to 4^3, restriction terminates, **BICGSTAB** used as bottom solve routine

miniGMG benchmark results

- miniGMG benchmark with BICGSTAB bottom solve
- Machine: Hopper at NERSC (Cray XE6), 4 6-core Opteron chips per node, Gemini network, 3D torus
- Weak scaling: Up to 4096 MPI processes (1 per chip, $24{,}576$ cores total)
  - 64^3 points per process ($N = 128^3$ over 48 cores, $N = 1024^3$ over $24{,}576$ cores)



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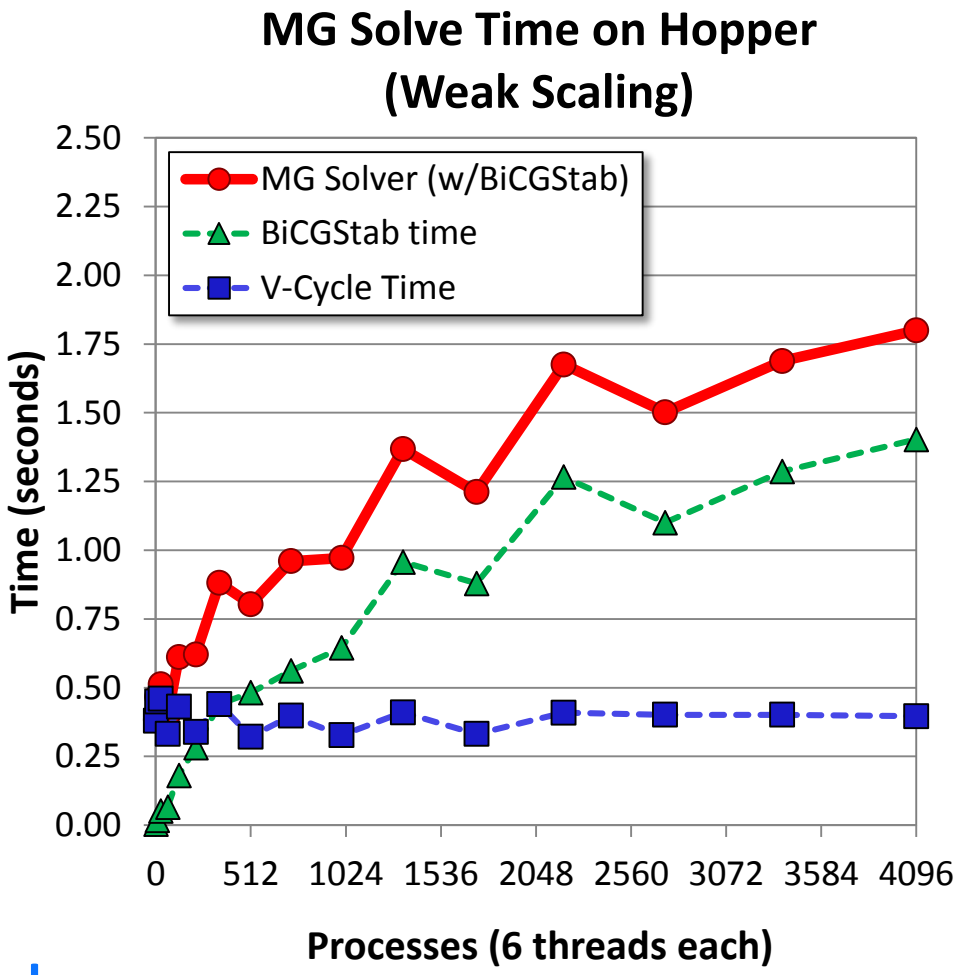
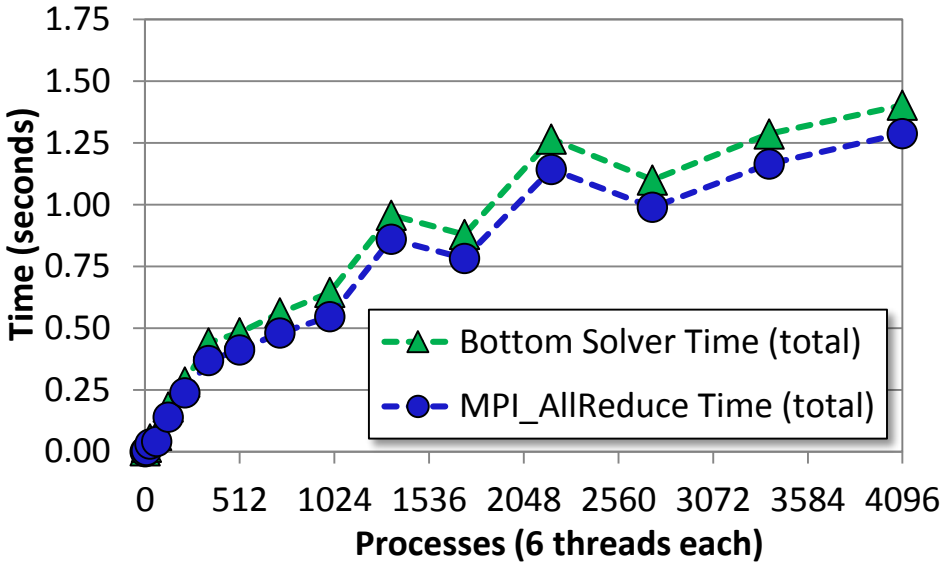


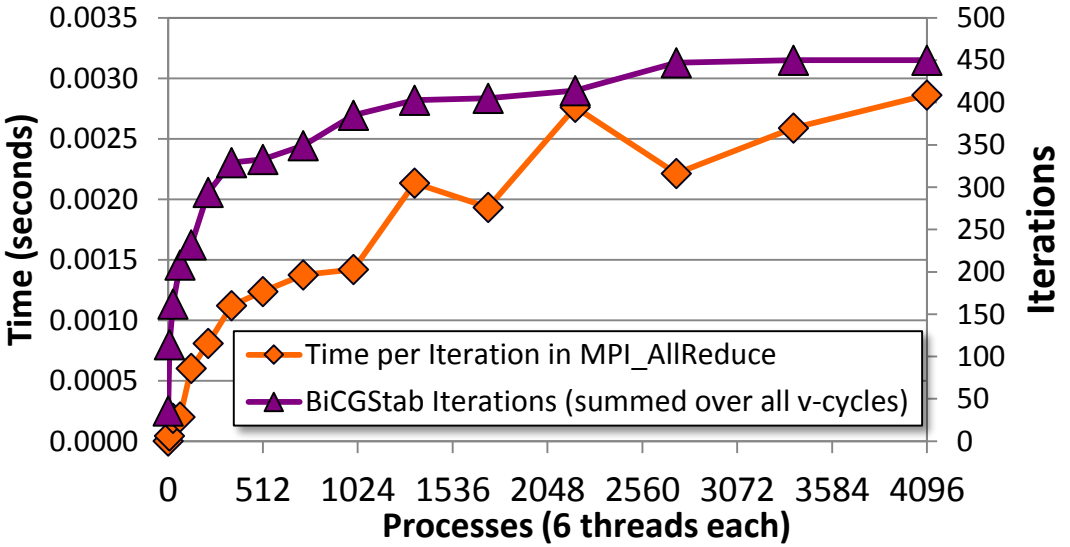
→ **Bottom solve time dominates the runtime of the overall GMG method**

→ **Scales poorly compared to other parts of the V-cycle**

The communication bottleneck

- Same miniGMG benchmark with BICGSTAB on Hopper
- Top: **MPI_AllReduce clearly dominates bottom solve time**
- Bottom: Increase in MPI_AllReduce time due to two effects:
  1. # iterations required by solver increases with problem size
  2. MPI_AllReduce time increases with machine scale (no guarantee of compact subtorus)
- **Poor scalability**: Increasing number of increasingly slower iterations!





The BICGSTAB method

Given: Initial guess x_0 for solving $Ax = b$
Initialize $p_0 = r_0 = b - Ax_0$
Pick arbitrary $\tilde{r}$ such that $(\tilde{r}, r_0) \neq 0$
for $j = 0,1, \ldots,$ until convergence **do**

$\alpha_j = (\tilde{r}, r_j)/(\tilde{r}, Ap_j)$
$x_{j+1} = x_j + \alpha_j p_j$
$q_j = r_j - \alpha_j Ap_j$
Check $\|q_j\|_2 = (q_j, q_j)^{1/2}$ for convergence
$\omega_j = (q_j, Aq_j)/(Aq_j, Aq_j)$
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Inner products in each iteration require global synchronization (MPI_AllReduce)

Communication-avoiding Krylov methods

- Communication-avoiding Krylov subspace methods (CA-KSMS) can **asymptotically reduce parallel latency**
- First known reference: s-step CG (Van Rosendale, 1983)
  - Many methods and variations created since; see Hoemmen's 2010 PhD thesis for thorough overview
- Main idea: Block iterations by groups of s

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- **Outer loop (communication step):**
  - Precompute Krylov basis V (dimension N-by-$O(s)$) required to compute next s iterations ($O(s)$ SpMVs, P2P communication)
  - Encode inner products using Gram matrix $G = V^T V$
    - Requires only one MPI_AllReduce to compute information needed for s iterations -> **decreases global synchronizations by $O(s)$!**

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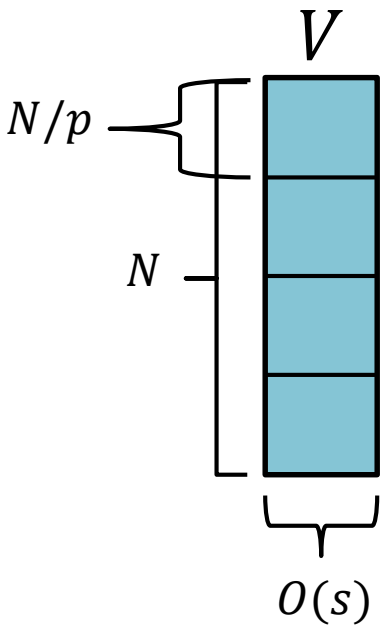
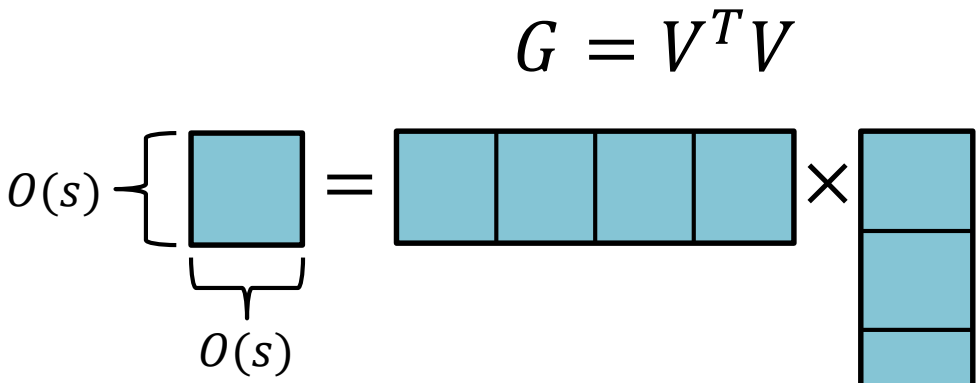
- **Inner loop (computation steps):**
  - Update length-$O(s)$ vectors that represent coordinates of BICGSTAB vectors in V for the next s iterations, use G to recover inner products locally- no further communication required!


V
N/p
N
O(s)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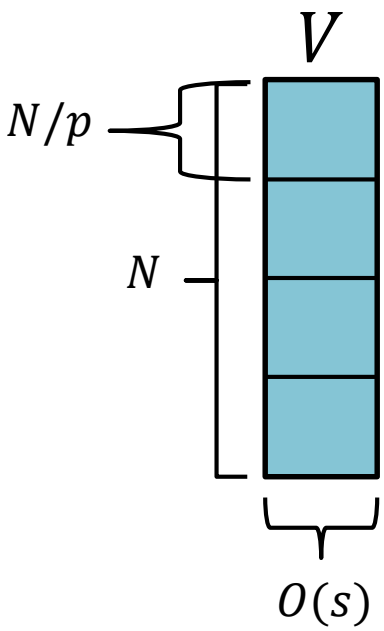
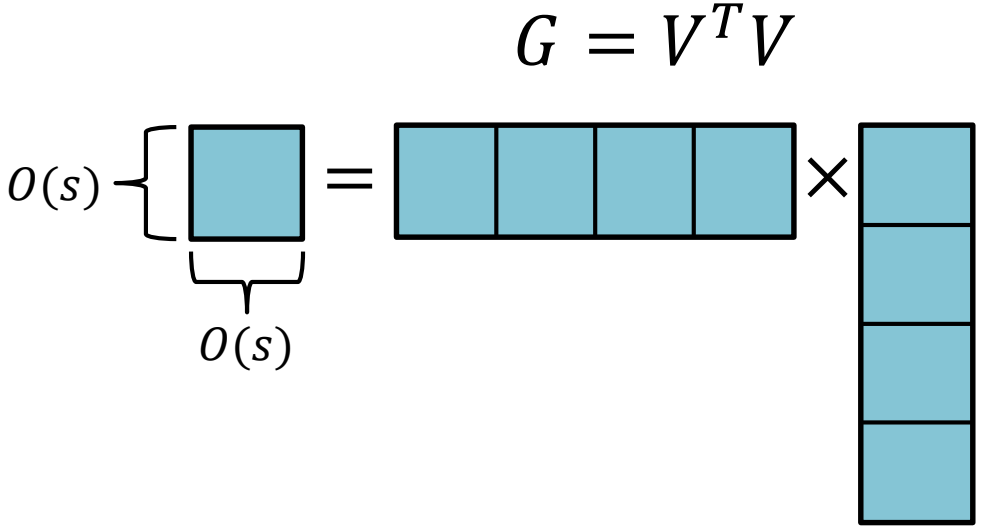
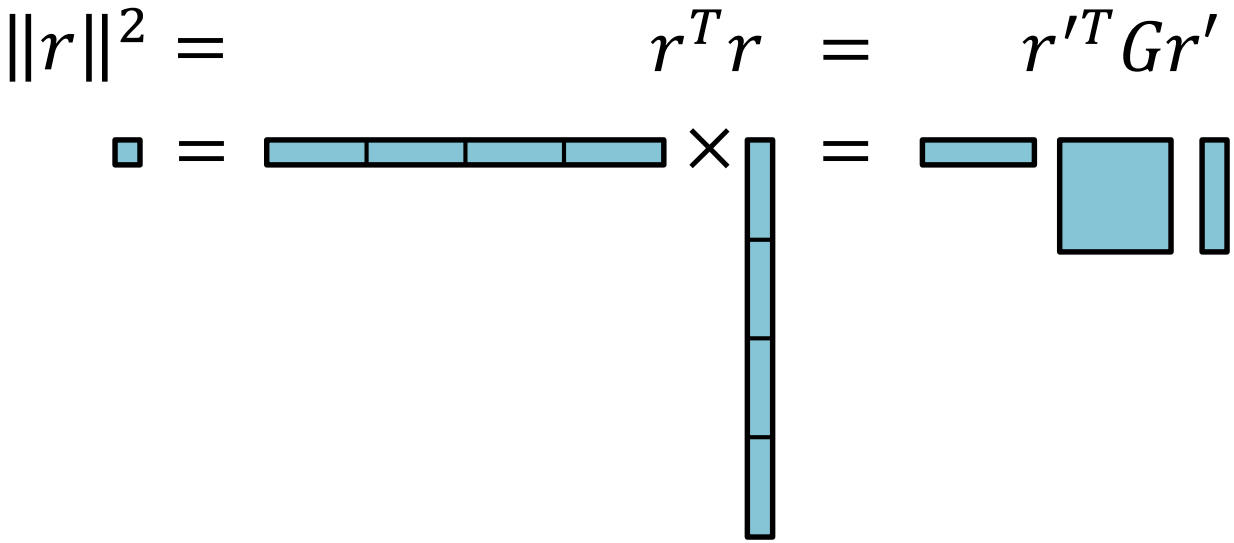
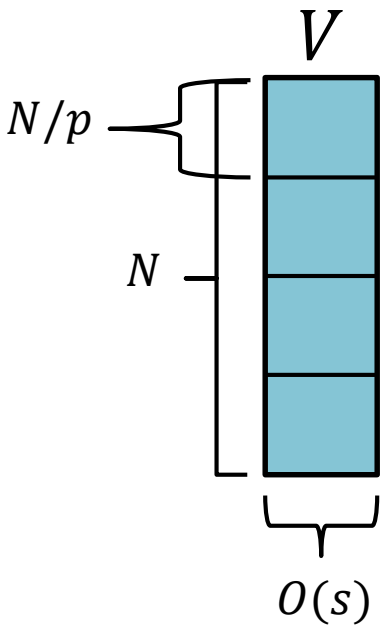
O(s)
=
×
O(s)


V
N/p
N
$O(s)$


$G = V^T V$
$O(s)$
$=$
$\times$
$O(s)$


$\|r\|^2 =$
$r^T r =$
$r'^T G r'$
$=$
$\times$
$=$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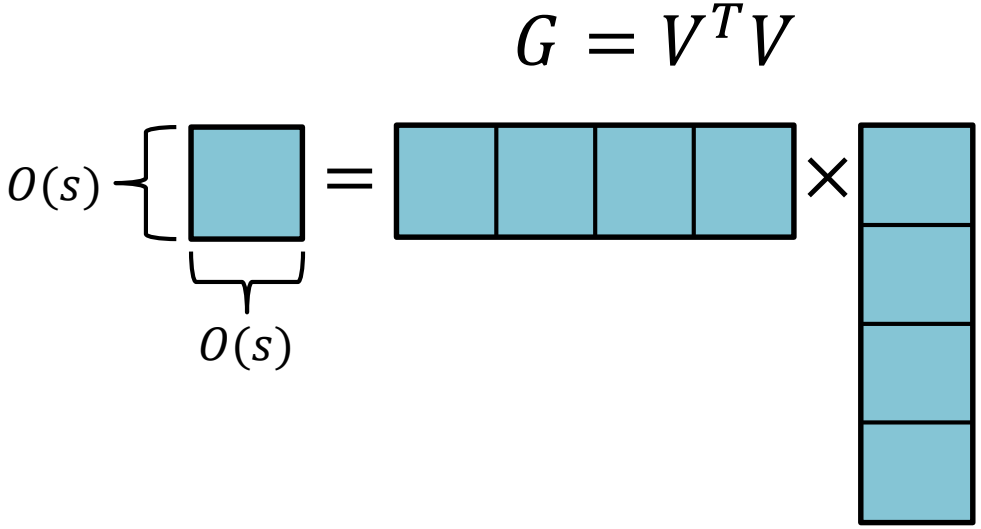
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$O(s)$
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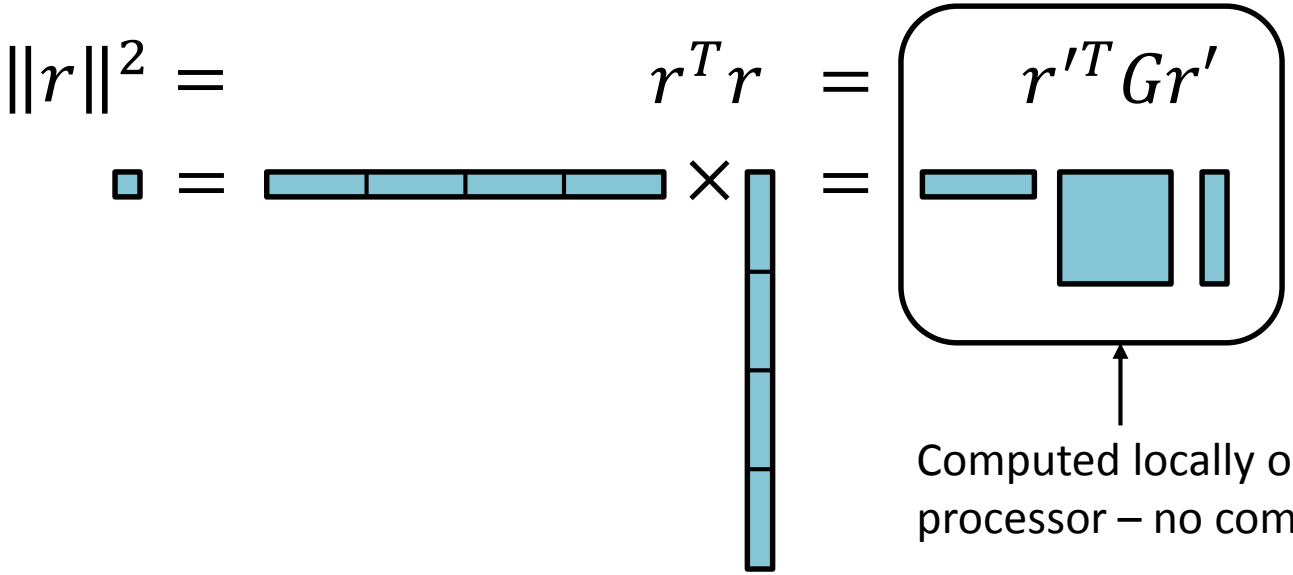
$\|r\|^2 =$
$r^T r =$
$r'^T G r'$
Computed locally on each processor – no communication!

The CA-BICGSTAB method

[C., Knight, Demmel. SISC 35(5), 2013.]

Given: Initial guess x_0 for solving $Ax = b$

Initialize $p_0 = r_0 = b - Ax_0$, pick arbitrary $\tilde{r}$ such that $(\tilde{r}, r_0) \neq 0$

Construct $(4s+1)$-by-$(4s+1)$ matrix T

for $\mathrm{m} = 0, s, 2s, \ldots,$ until convergence **do**

Compute V w/columns a basis for $\mathcal{K}_{2s+1}(A, p_m) + \mathcal{K}_{2s}(A, r_m)$

Compute $[G, g] = V^T[V, \tilde{r}]$

for $j = 0,1, \ldots, s-1$ **do**

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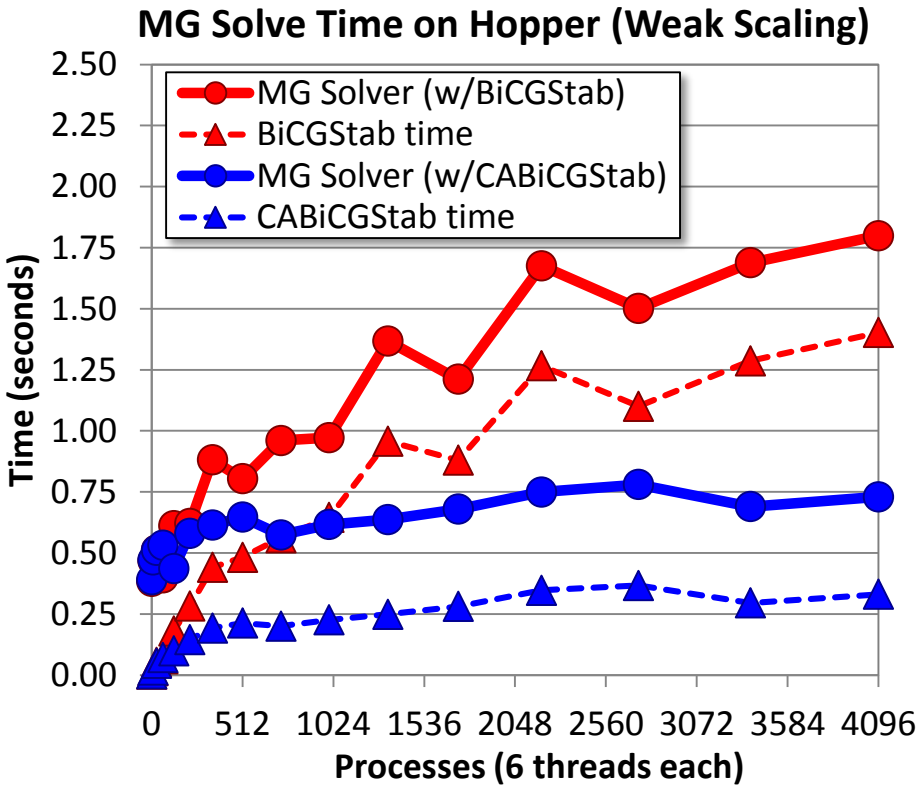
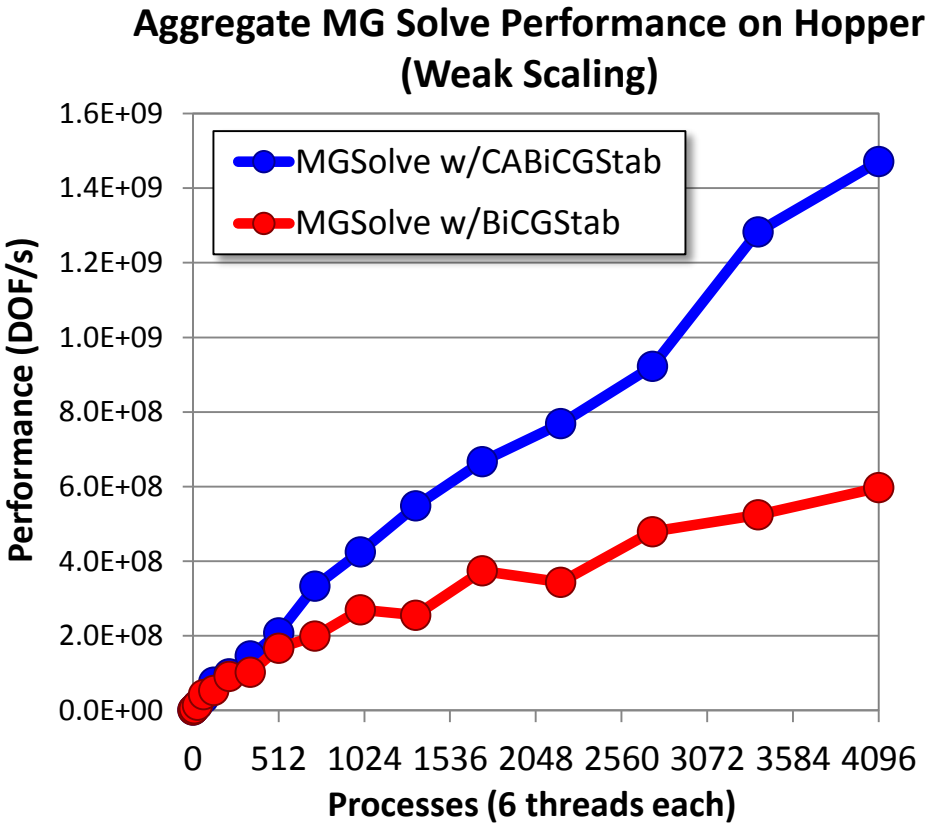
One MPI_AllReduce

Vector updates for s iterations computed locally

Speedups for synthetic benchmark

- Time (left) and performance (right) of miniGMG benchmark with **BICGSTAB** vs. **CA-BICGSTAB** with $s = 4$ (monomial basis) on Hopper
- At 24K cores, CA-BICGSTAB's asymptotic reduction of calls to MPI_AllReduce **improves bottom solver by 4.2x, overall multigrid solve by nearly 2.5x**





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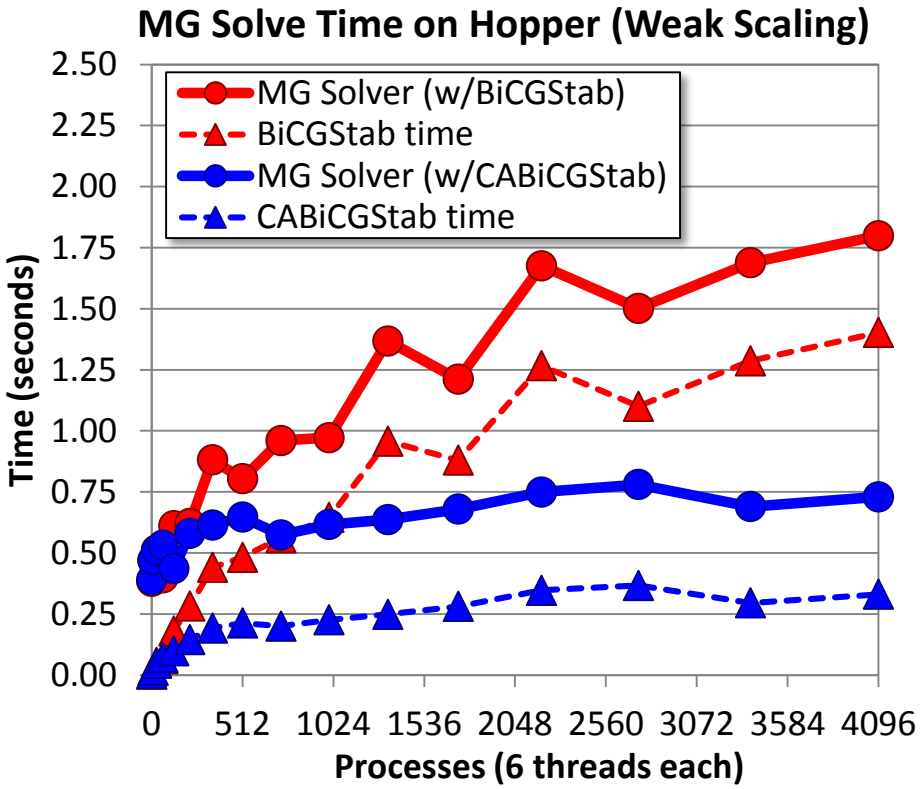
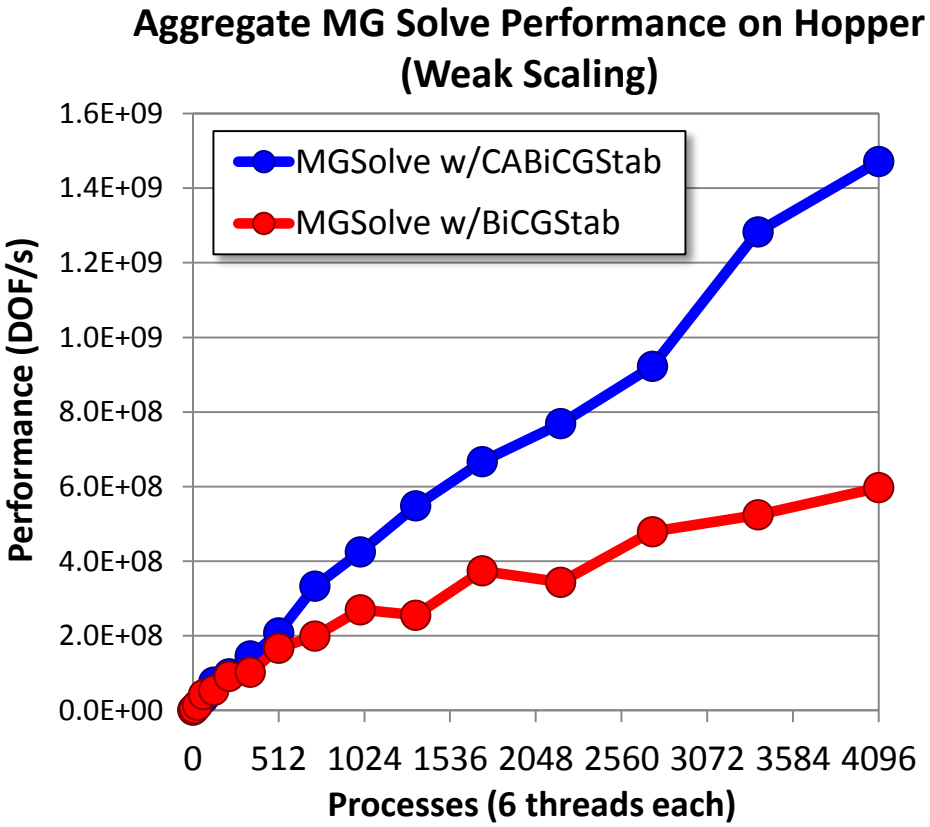
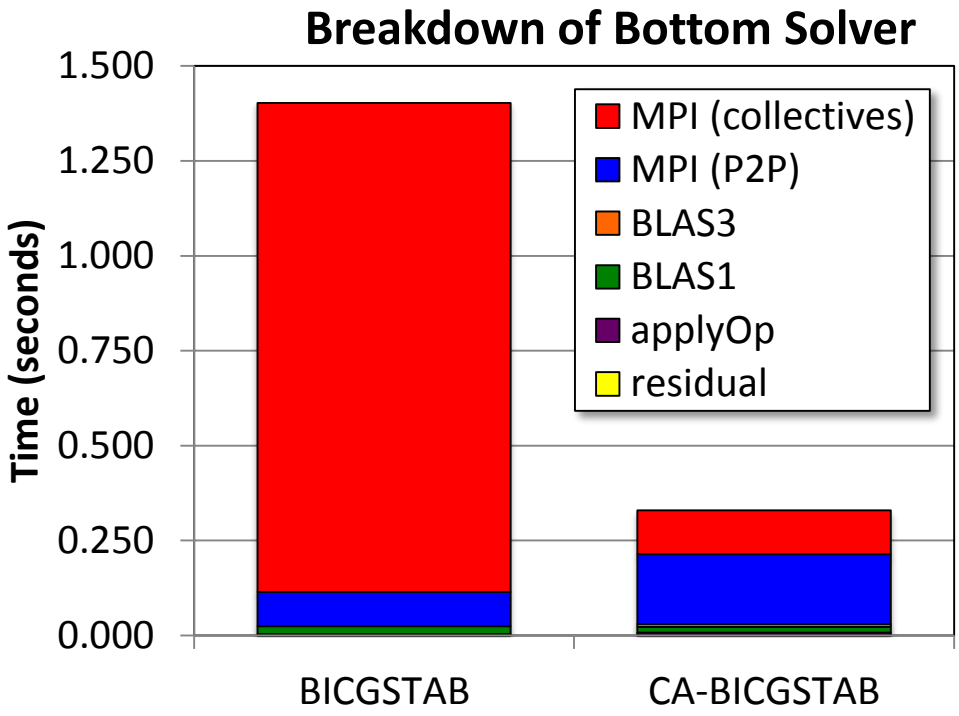
- Aggregate MG solve performance using CA-BICGSTAB much closer to **linear in DOF/s**





Benchmark timing breakdown

- Plot: Net time spent across all bottom solves at $24{,}576$ cores, for BICGSTAB and CA-BICGSTAB with $s = 4$



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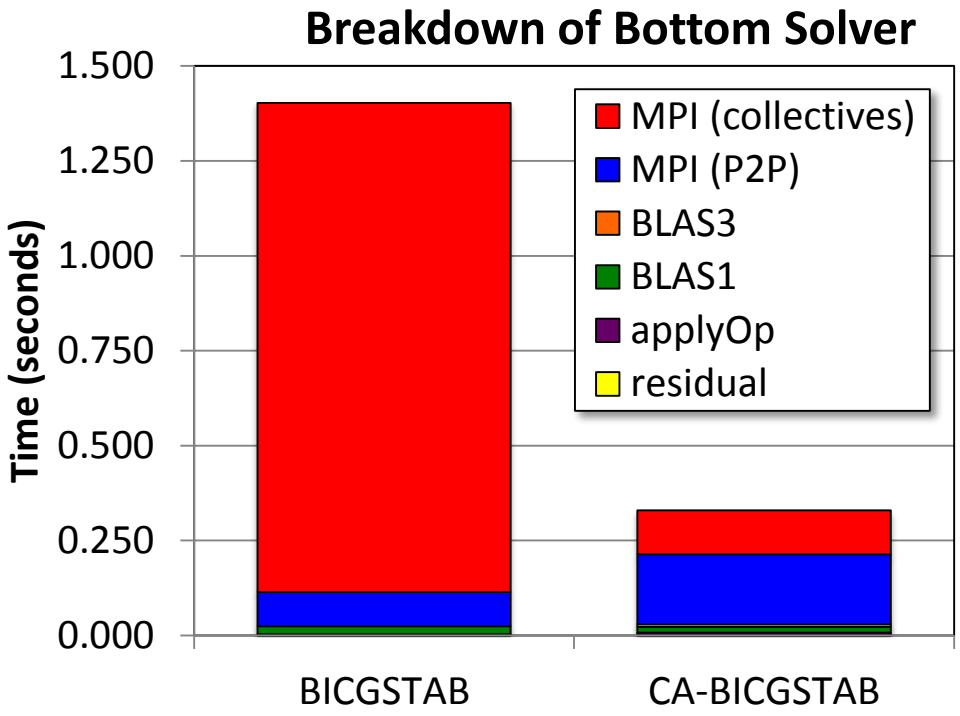
  - Less than theoretical 24x since messages in CA-BICGSTAB are larger, not always latency-limited



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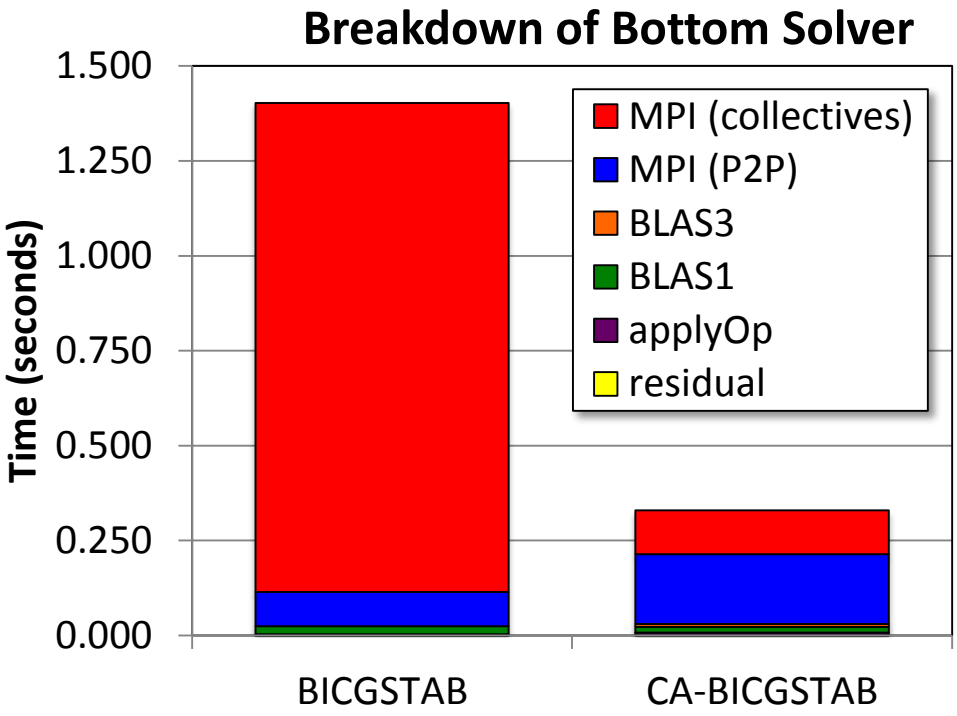
- **P2P (blue) communication doubles** for CA-BICGSTAB
  - Basis computation requires twice as many SpMVs (P2P) per iteration as BICGSTAB

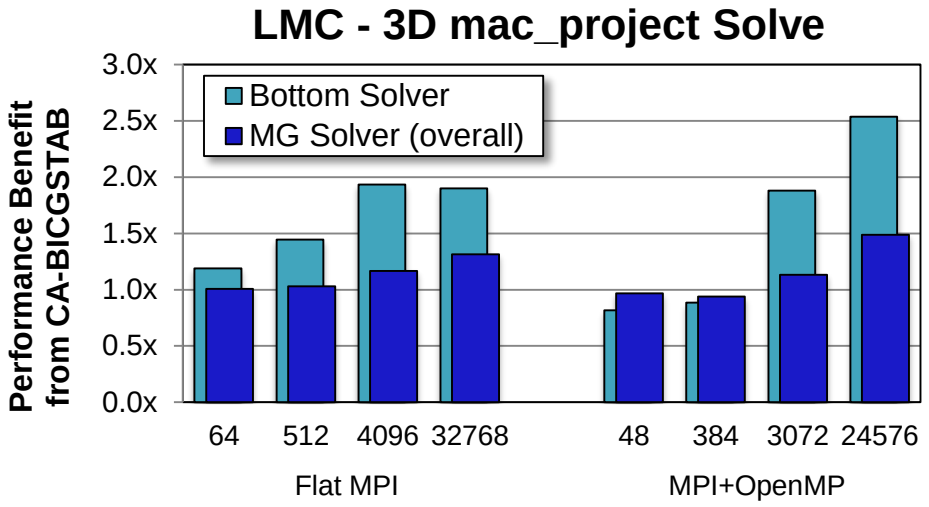


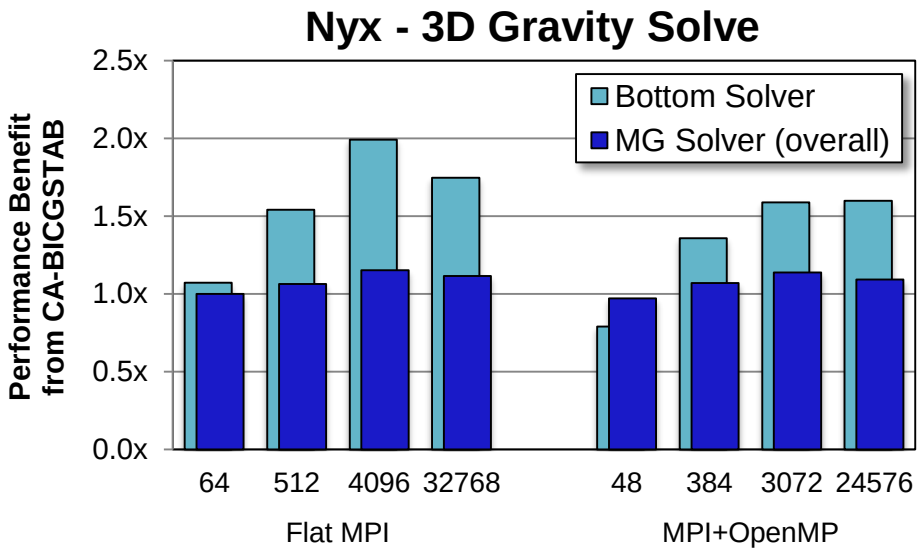
Speedups for real applications

- CA-BICGSTAB bottom-solver implemented in BoxLib (AMR framework from LBL)
- Compared GMG with BICGSTAB vs. GMG with CA-BICGSTAB for two different applications:

Low Mach Number Combustion Code (LMC): gas-phase combustion simulation

Nyx: 3D N-body and gas dynamics code for cosmological simulations of dark matter particles





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- Up to **2.5x speedup in bottom solve; up to 1.5x in MG solve**

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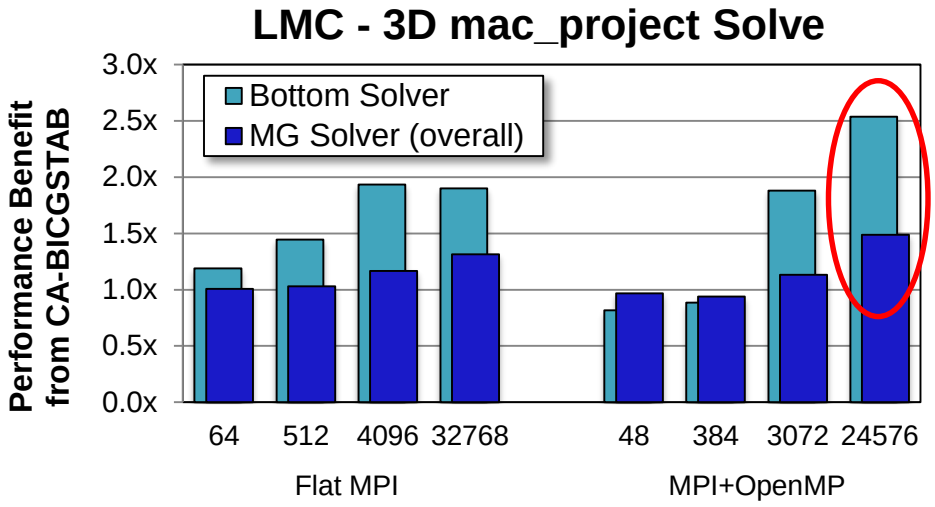

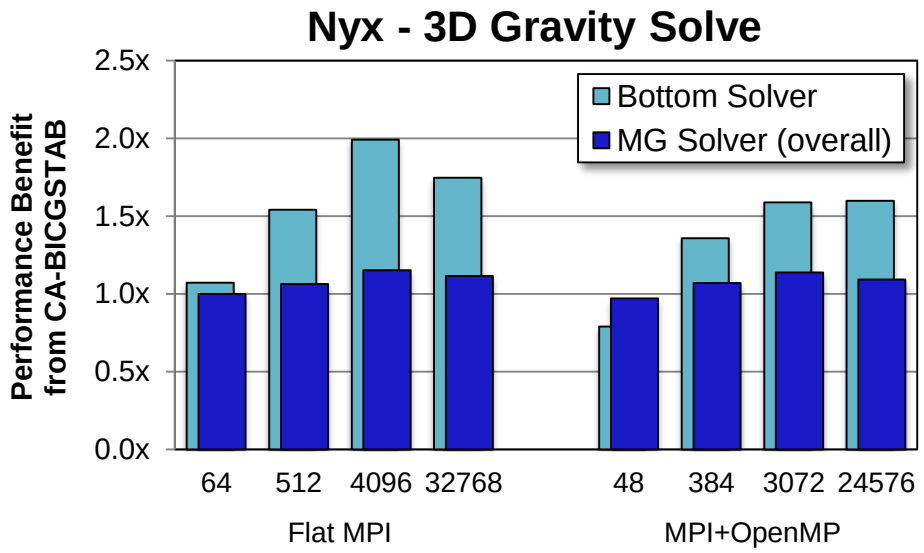

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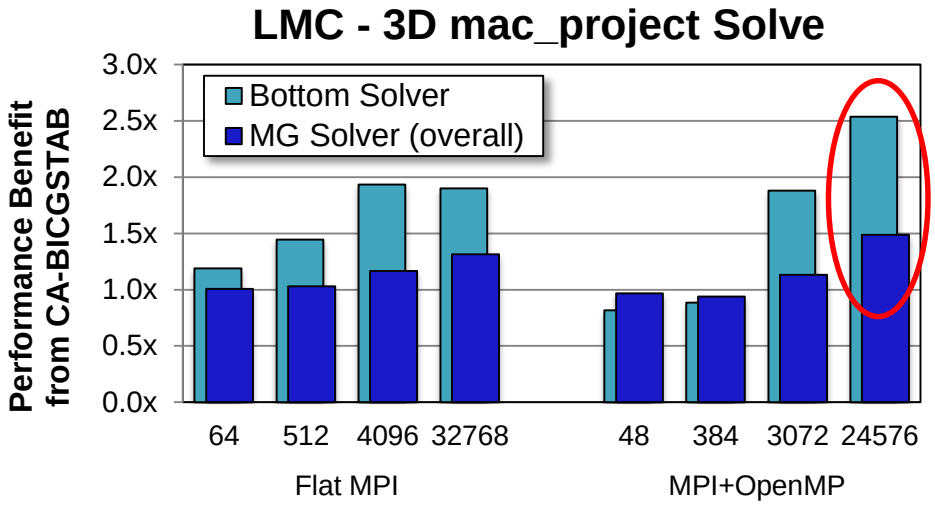
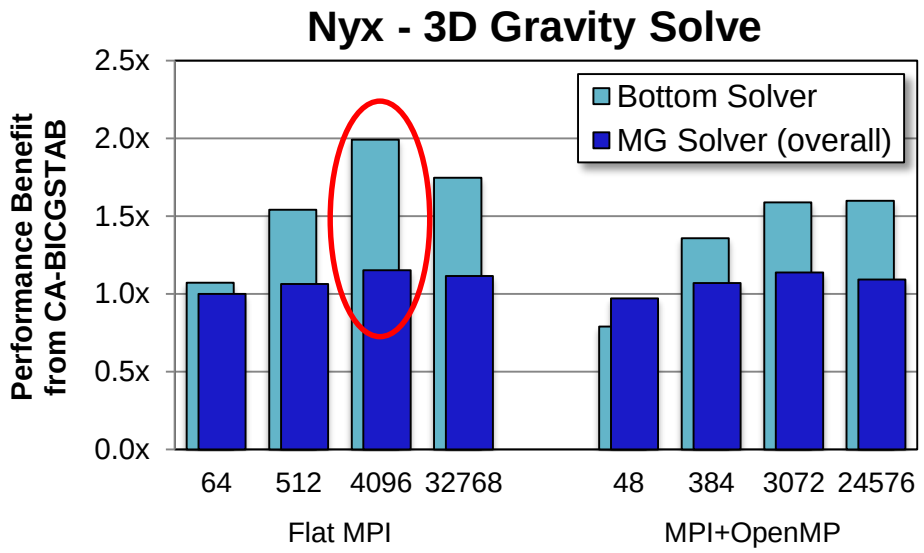
Nyx: 3D N-body and gas dynamics code for cosmological simulations of dark matter particles

- Up to **2x speedup in bottom solve, 1.15x in MG solve**





Discussion and challenges

- For practical purposes, choice of s limited by finite precision error
  - **As s is increased, convergence slows** – more required iterations can negate any speedup per iteration gained
  - Can use better-conditioned Krylov bases, but this can incur extra cost (esp. if A changes b/t V-cycles); ongoing work
  - In our tests, $s = 4$ with the monomial basis gave similar convergence for BICGSTAB and CA-BICGSTAB

- Some bottom-solves are "harder" – take more iterations to converge – than others
  - Implemented "**telescoping s**" approach
    - Outer loops begin using $s = 1$, increase up in subsequent outer loops up to $s = 4$
    - Ensures that easy solves don't incur extra costs of computing V and $G = V^T V$, hard solves see asymptotic benefits

Discussion and challenges

- Timing breakdown shows we **must consider tradeoffs** between bandwidth, latency, and computation when optimizing for **particular problem/machine**
  - Blocking BICGSTAB inner products most beneficial when:
    - MPI_AllReduces in bottom solve are dominant cost in GMG solve, GMG solves are dominant cost of application
    - Bottom solve requires enough iterations to amortize extra costs (bigger MPI messages, more P2P communication)
  - **CA-BICGSTAB can also be optimized to reduce P2P communication or reduce vertical data movement** when computing Krylov bases ("matrix powers kernel")

Design space and related approaches

- **Parallelizing multigrid methods**
  - Concurrent iterations, multiple coarse corrections, full domain partitioning, block factorization, etc.
- **Solving the coarse grid problem**
  - Type of solver: direct (e.g., LU), stationary iterative (e.g., Jacobi), Krylov, switch to algebraic
  - Coarse grid agglomeration - use only a subset of available processors
- **Reducing communication cost in Krylov subspace methods**
  - Pipelining: overlap nonblocking reductions with matrix-vector multiplications (Ghysels, Ashby, Meerbergen, Vanroose, 2013)
  - Tiling approach to reduce communication bottleneck in Chebyshev iteration smoothers (Ghysels, Kłosiewicz, Vanroose, 2012)
  - Overlap global synchronization points with SpMV and preconditioner application (Gropp, 2010)
  - Delayed reorthogonalization: avoid synchronization due to reorthogonalization (ADR in SLEPc) (Hernandez, Román, Tomás, 2007)

Summary and future work

- Implemented, evaluated, and optimized CA-BICGSTAB as a high-performance, distributed-memory bottom solve routine for geometric multigrid solvers
  - GMG+CABICGSTAB available as option in miniGMG, BoxLib, and CHOMBO frameworks

Summary and future work

- Implemented, evaluated, and optimized CA-BICGSTAB as a high-performance, distributed-memory bottom solve routine for geometric multigrid solvers
  - GMG+CABICGSTAB available as option in miniGMG, BoxLib, and CHOMBO frameworks
- **Expands the design space**: trade collective latency for bandwidth, trade s fine-grained operations for one coarse-grained operation that expresses more parallelism

Summary and future work

- Implemented, evaluated, and optimized CA-BICGSTAB as a high-performance, distributed-memory bottom solve routine for geometric multigrid solvers
  - GMG+CABICGSTAB available as option in miniGMG, BoxLib, and CHOMBO frameworks
- **Expands the design space**: trade collective latency for bandwidth, trade s fine-grained operations for one coarse-grained operation that expresses more parallelism
- Future work:
  - **Exploration of design space** for other Krylov solvers, other architectures, other applications
  - Implementation of different polynomial bases for Krylov subspace to **improve convergence** for higher s values
  - **Improve accessibility** of communication-avoiding Krylov methods through scientific computing libraries and frameworks

Thank you!

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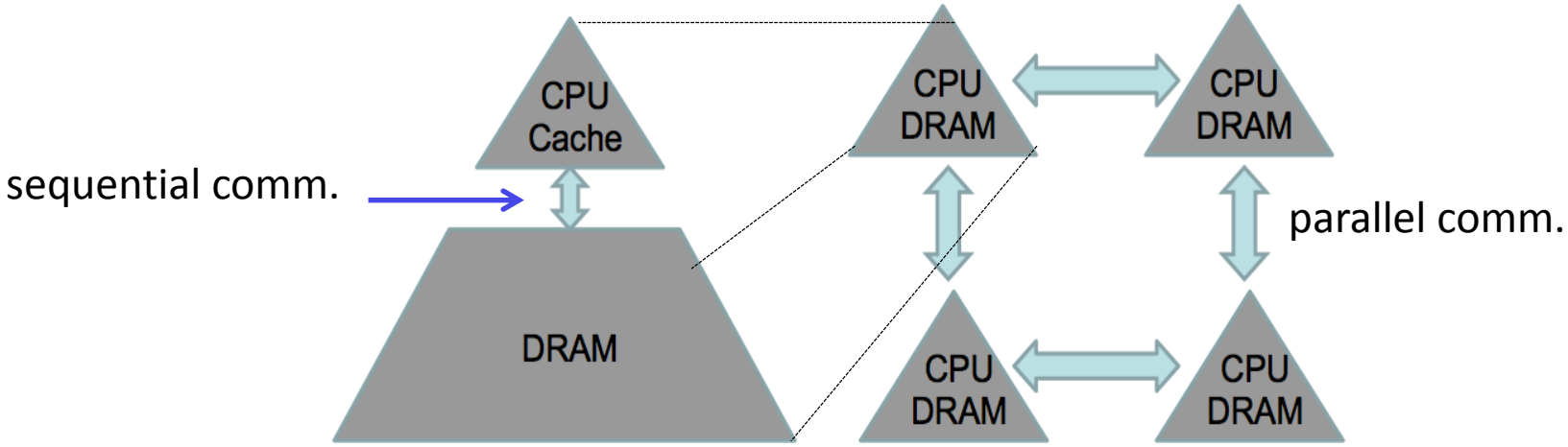
Extra Slides

Communication is expensive!

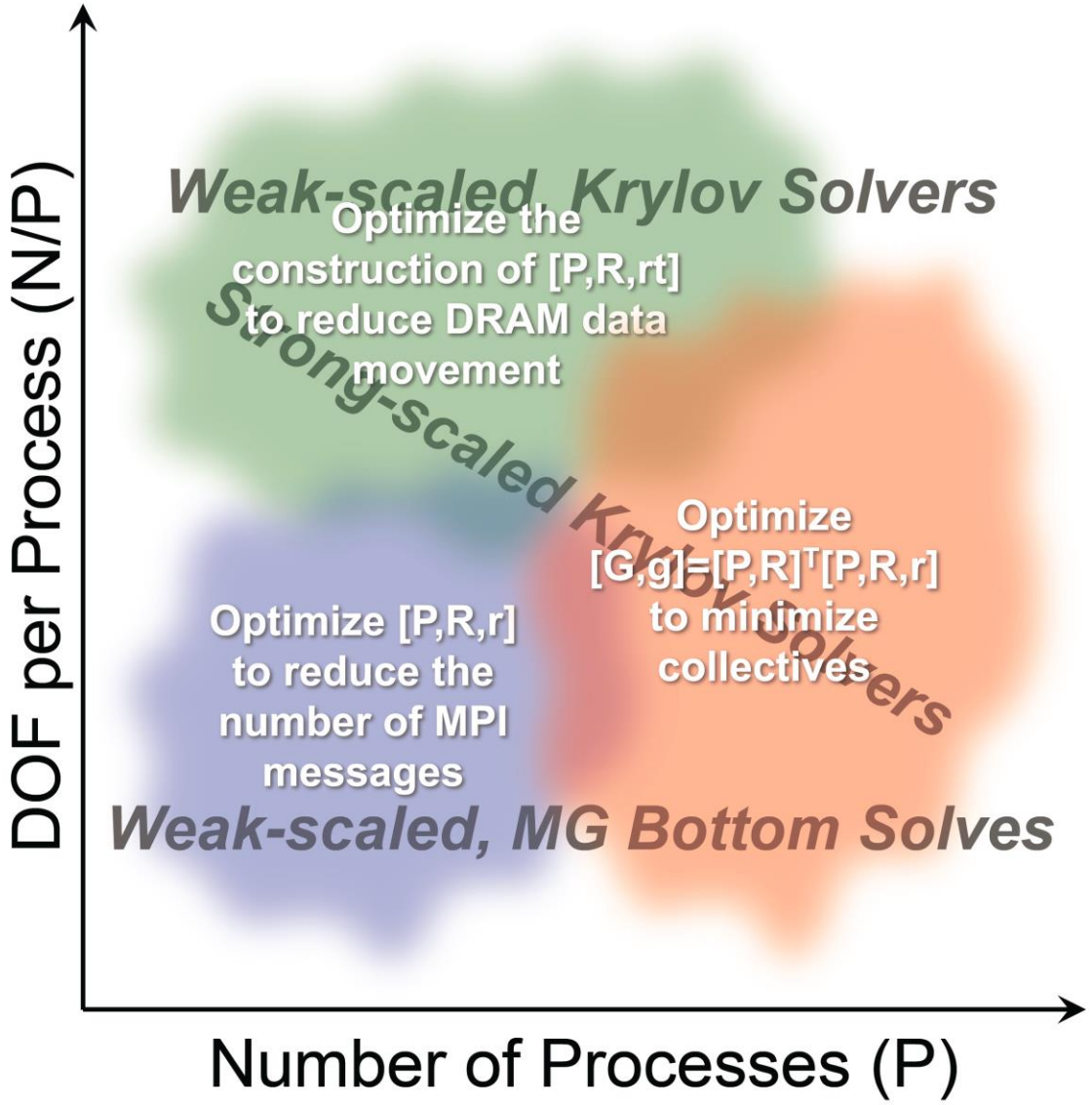
- Algorithms have two costs: **communication** and **computation**
  - **Communication : moving data** between levels of memory hierarchy (sequential), between processors (parallel)



- On modern computers, communication is expensive, computation is cheap
  - Flop time << 1/bandwidth << latency
  - Communication bottleneck a barrier to achieving scalability
  - Communication is also expensive in terms of energy cost
- For scalability, we **must redesign algorithms to avoid communication**

Coarse Grid Agglomeration

- Unite subdomains onto a subset of the available processors once ratio of interior nodes to boundary nodes falls below some threshold
- Pros: Reduces communication required to perform operations at this level and lower levels
- Cons: Leaves processors idle, requires lots of data movement (scatter/gather) to perform data redistribution
  - **Words moved = $2 \cdot O(n^2)$ for scatter/gather, versus $\frac{\#\ its}{s} \cdot O(s^2 \log p)$ for MPI_AllReduce in CA coarse grid solves**
- This approach could be combined with coarse grid solve – do agglomeration at some level, then coarse grid solve at this level or lower
  - Expect CA-KSMs to have less speedup over KSMs in this case, since communication in bottom solve less expensive due to more processors
    - But not clear that this would always be the winning approach in terms of overall runtime
- **Best approach will depend on the parallel environment and application!**


Weak-scaled, Krylov Solvers
Optimize the construction of [P,R,rt] to reduce DRAM data movement
Strong-scaled Krylov Solvers
Optimize [G,g]=[P,R]T[P,R,r] to minimize collectives
Optimize [P,R,r] to reduce the number of MPI messages
Weak-scaled, MG Bottom Solves
DOF per Process (N/P)
Number of Processes (P)

Krylov Subspace Methods

- A **Krylov Subspace** is defined as

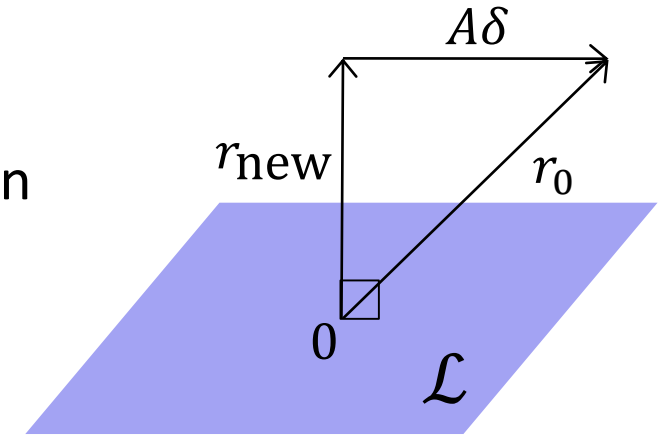
$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\}$$

- A **Krylov Subspace Method** is a projection process onto the subspace $\mathcal{K}$ orthogonal to $\mathcal{L}$
  - The choice of $\mathcal{L}$ distinguishes the various methods
    - Examples: Conjugate Gradient (CG), Generalized Minimum Residual Methods (GMRES), Biconjugate Gradient (BICG), BICG Stabilized (BICGSTAB)

For linear systems, in iteration m, approximates solution x_m to $Ax = b$ by imposing the condition

$$x_m = x_0 + \delta, \ \delta \in \mathcal{K}_m \quad \text{and} \quad r_0 - A\delta \perp \mathcal{L}_m,$$

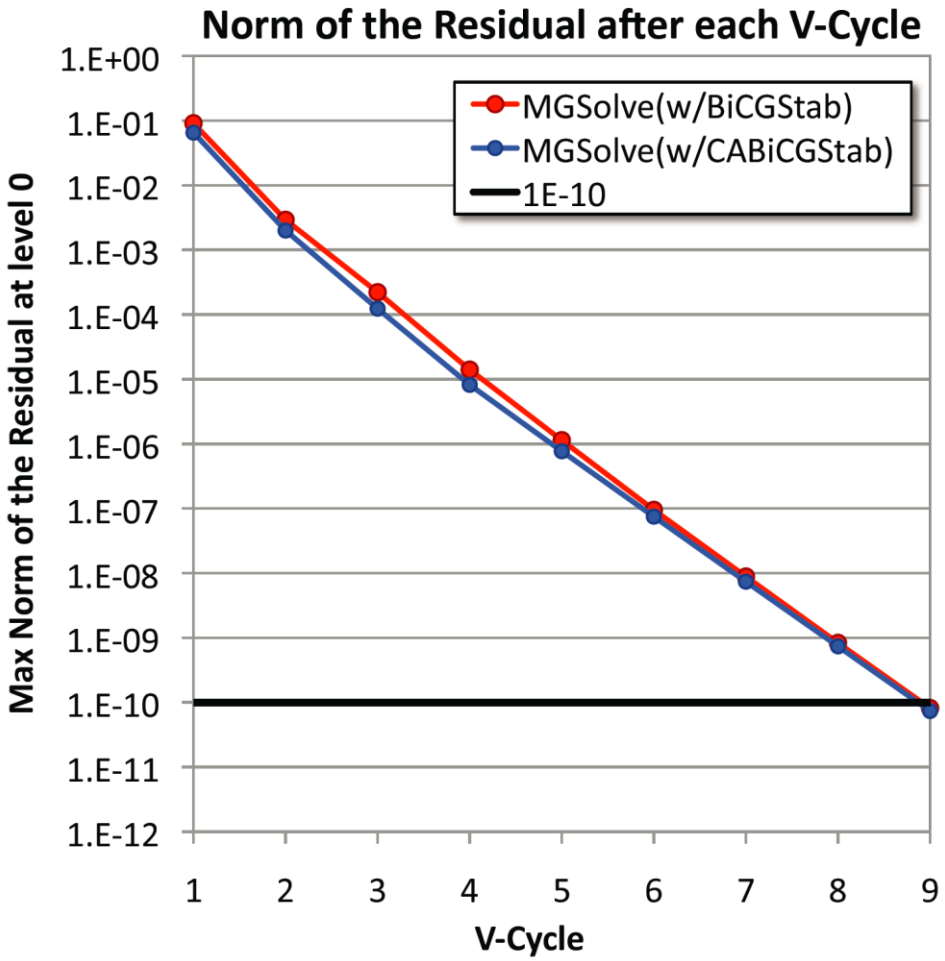
where $r_0 = b - Ax_0$



Hopper

- Cray XE6 MPP at NERSC
- Each compute node that four 6-core Opteron chips each with two DDR3-1333 mem controllers
- Each superscalar out-of-order core: 64KB L1, 512KB L2. One 6MB L3 cache per chip
- Pairs of compute nodes connected via HyperTransport to a high-speed Gemini network chip
- Gemini network chips connected to form high-BW low-latency 3D torus
  - Some asymmetry in torus
  - No control over job placement
  - Latency can be as low as 1.5 microseconds, but typically longer in practice

Convergence rates with $s = 4$



Related Work: s-step methods

Authors	KSM	Basis	Precond?	Mtx Pwrs?	TSQR?
Van Rosendale, 1983	CG	Monomial	Polynomial	No	No
Leland, 1989	CG	Monomial	Polynomial	No	No
Walker, 1988	GMRES	Monomial	None	No	No
Chronopoulos and Gear, 1989	CG	Monomial	None	No	No
Chronopoulos and Kim, 1990	Orthomin, GMRES	Monomial	None	No	No
Chronopoulos, 1991	MINRES	Monomial	None	No	No
Kim and Chronopoulos, 1991	Symm. Lanczos, Arnoldi	Monomial	None	No	No
Sturler, 1991	GMRES	Chebyshev	None	No	No

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Joubert and Carey, 1992	GMRES	Chebyshev	No	Yes*	No
Chronopoulos and Kim, 1992	Nonsymm. Lanczos	Monomial	No	No	No
Bai, Hu, and Reichel, 1991	GMRES	Newton	No	No	No
Erhel, 1995	GMRES	Newton	No	No	No
de Sturler and van der Vorst, 2005	GMRES	Chebyshev	General	No	No
Toledo, 1995	CG	Monomial	Polynomial	Yes*	No
Chronopoulos and Swanson, 1990	CGR, Orthomin	Monomial	No	No	No
Chronopoulos and Kinkaid, 2001	Orthodir	Monomial	No	No	No

Related Work: s-step methods

- Many previously derived s-step Krylov methods
  - First known reference is (Van Rosendale, 1983)
- Motivation: minimize I/O, increase parallelism
- Empirically found that monomial basis for $s > 5$ causes instability
- Many found better convergence using better conditioned polynomials based on spectrum of A (e.g., scaled monomial, Newton, Chebyshev)

- Hoemmen et al. (2009) first to produce CA implementations that also avoid communication for general sparse matrices (and use TSQR)
  - Speedups for various matrices for a fixed number of iterations
    - Shows that $\left(\frac{\text{time per } s \text{ iterations KSM}}{\text{time per outer iteration CA}-\text{KSM}}\right)$ can be $O(s)$

Parallel Multigrid Methods

- **Concurrent iterations**
  - Reduces time per multigrid iteration by performing relaxation sweeps on all grids simultaneously
- **Multiple coarse corrections**
  - Accelerates convergence by projecting the fine grid system onto several different coarse grid spaces
- **Full domain partitioning**
  - Reduces communication during refinement stage
- **Block factorization**
  - Use a special selection of coarse and fine points to expose parallelism

The BICGSTAB method

Given: Initial guess x_0 for solving $Ax = b$

Initialize $p_0 = r_0 = b - Ax_0$

Pick arbitrary $\tilde{r}$ such that $(\tilde{r}, r_0) \neq 0$

for $j = 0,1, \ldots,$ until convergence **do**

$\alpha_j = (\tilde{r}, r_j)/(\tilde{r}, Ap_j)$

$x_{j+1} = x_j + \alpha_j p_j$

$q_j = r_j - \alpha_j Ap_j$

Check $\|q_j\|_2 = (q_j, q_j)^{1/2}$ for convergence

$\omega_j = (q_j, Aq_j)/(Aq_j, Aq_j)$

$x_{j+1} = x_{j+1} + \omega_j q_j$

$r_{j+1} = q_j - \omega_j Aq_j$

Check $\|r_{j+1}\|_2 = (r_{j+1}, r_{j+1})^{1/2}$ for convergence

$\beta_j = (\alpha_j/\omega_j)(\tilde{r}, r_{j+1})/(\tilde{r}, r_j)$

$p_{j+1} = r_{j+1} + \beta_j(p_j - \omega_j Ap_j)$

end for

Inner products in each iteration require global synchronization (MPI_AllReduce)

Multiplication by A requires nearest neighbor communication (P2P)

CA-BICGSTAB derivation: Basis change

Suppose we are at some iteration m. What are the dependencies on r_m, p_m, and x_m for computing the next s iterations?

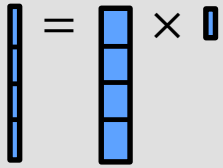
By induction, for $j = \{0,1, \dots s-1\}$

$$\begin{aligned} p_{m+j+1}, r_{m+j+1}, x_{m+j+1} - x_m &\in \mathcal{K}_{2s+1}(A, p_m) + \mathcal{K}_{2s}(A, r_m) \\ q_{m+j} &\in \mathcal{K}_{2s}(A, p_m) + \mathcal{K}_{2s-1}(A, r_m) \\ p_{m+j} &\in \mathcal{K}_{2s-1}(A, p_m) + \mathcal{K}_{2s-2}(A, r_m) \end{aligned}$$

Let P and R be bases for $\mathcal{K}_{2s+1}(A, p_m)$ and $\mathcal{K}_{2s}(A, r_m)$, respectively.

For the next s iterations ($j = \{0,1, \dots s-1\}$),

$$\begin{aligned} r_{m+j+1} &= [P, R] r'_{j+1} & p_{m+j+1} &= [P, R] p'_{j+1} \\ x_{m+j+1} - x_m &= [P, R] x'_{j+1} & q_{m+j} &= [P, R] q'_j \end{aligned}$$

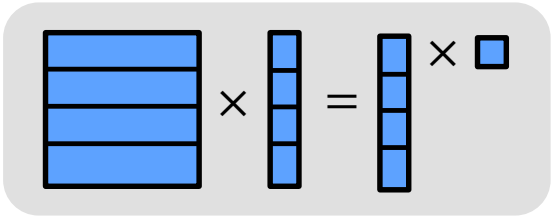


i.e., length-$(4s+1)$ vectors r'_{j+1}, p'_{j+1}, x'_{j+1}, and q'_j are coordinates for the length-N vectors r_{m+j+1}, p_{m+j+1}, x_{m+j+1}-x_m, and q_{m+j} respectively, in bases $[P, R]$.

CA-BICGSTAB derivation: Coordinate updates

The bases P, R are generated by polynomials satisfying 3-term recurrence represented by $(4s+1)$-by-$(4s+1)$ tridiagonal matrix T satisfying

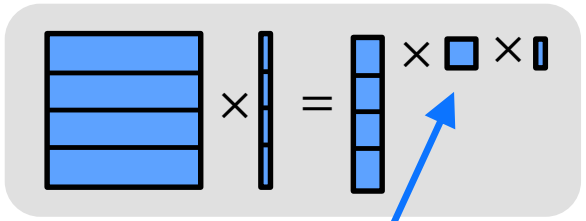
$$A\left[\underline{P}, 0_{N,1}, \underline{R}, 0_{N,1}\right] = [P, R]T$$



where $\underline{P}, \underline{R}$ are P, R resp. with last columns omitted

Multiplications by A can then be written:

$$A\left[q_{m+j}, p_{m+j}\right] = A[P, R]\left[q'_j, p'_j\right] = [P, R]T\left[q'_j, p'_j\right]$$



Update BICGSTAB vectors by updating their coordinates in $[P, R]$:

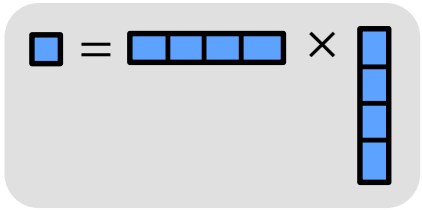
$$\begin{aligned} x'_{j+1} &= x'_j + \alpha_{m+j}\, p'_j \\ q'_j &= r'_j - \alpha_{m+j}\, T p'_j \\ x'_{j+1} &= x'_{j+1} + \omega_{m+j}\, q'_j \\ r'_{j+1} &= r'_j - \omega_{m+j}\, T q'_j \\ p'_{j+1} &= r'_{j+1} + \beta_{m+j}\,(p'_j - \omega_{m+j}\, T p'_j) \end{aligned}$$

Each process stores T locally, redundantly compute coordinate updates

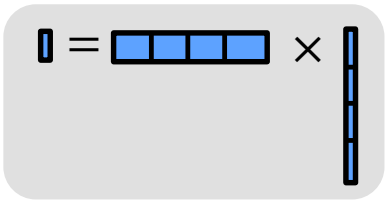
CA-BICGSTAB derivation: Inner products

Last step: rewriting length-N inner products in the new Krylov basis. Let

$$G = [P, R]^T [P, R]$$

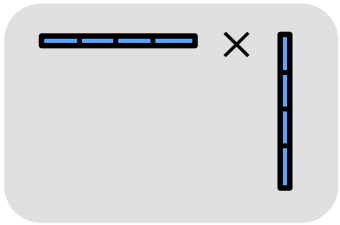


$$g = [P, R]^T \tilde{r}$$

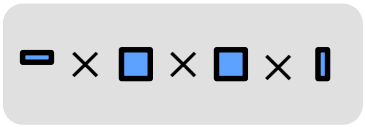


where the "Gram Matrix" G is $(4s+1)$ -by-$(4s+1)$ and g is a $(4s+1)$ vector. (Note: can be computed with **one MPI_AllReduce** by $[P, R]^T [P, R, \tilde{r}]$).

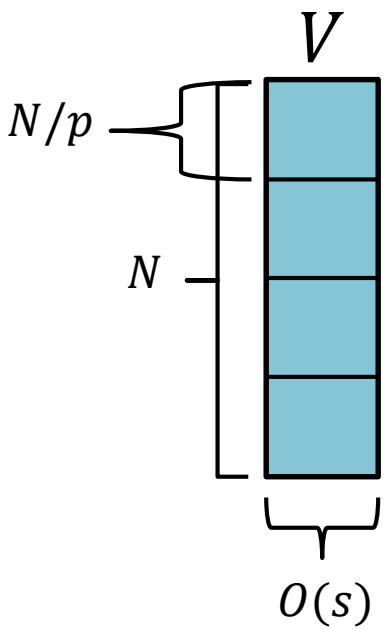
Then **all the dot products for s iterations of BICGSTAB can be computed locally** in CA-BICGSTAB using G and g by the relations

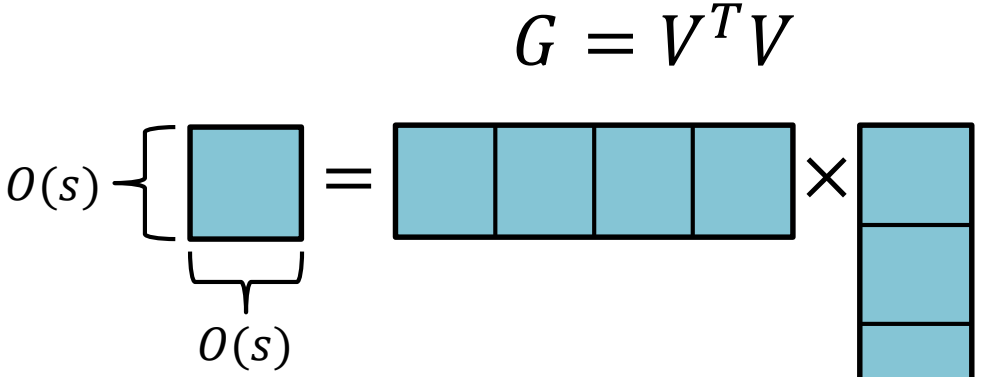


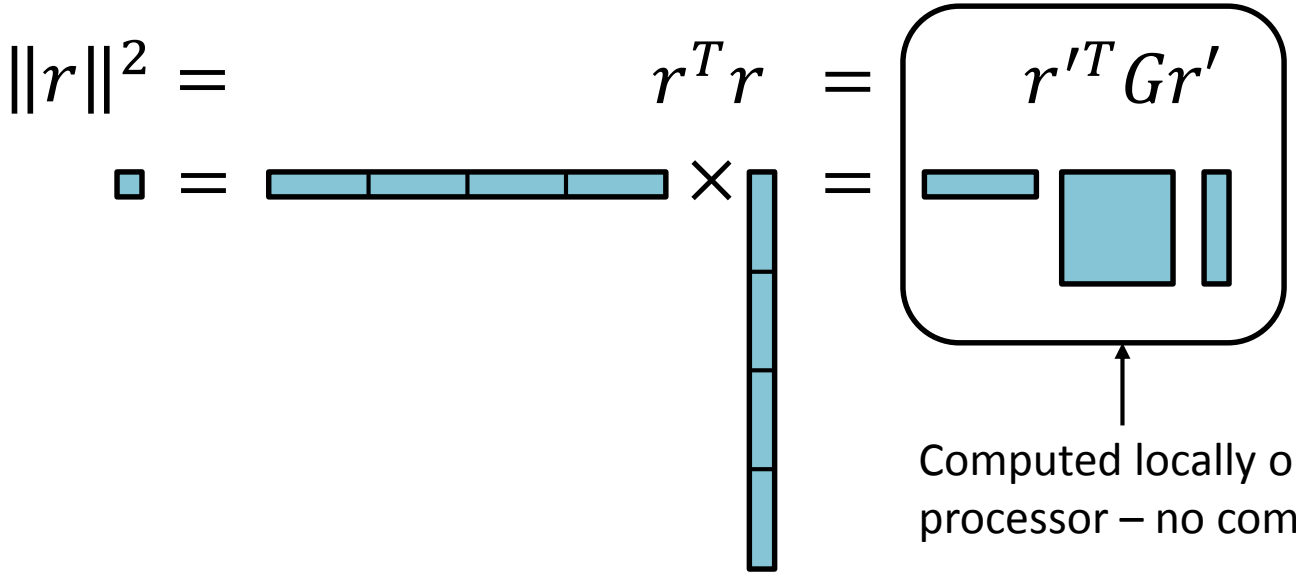
$$\begin{aligned}
(\tilde{r}, r_{m+j}) &= (g, r'_j) \\
(\tilde{r}, r_{m+j+1}) &= (g, r'_j) \\
(\tilde{r}, Ap_{m+j}) &= (g, Tp'_j) \\
(q_{m+j}, Aq_{m+j}) &= (q'_j, GTq'_j) \\
(Aq_{m+j}, Aq_{m+j}) &= (Tq'_j, GTq'_j)
\end{aligned}$$



Note: norms for convergence checks can be estimated with no communication in a similar way, e.g., $\|r_{m+j+1}\|_2 = (r_{m+j+1}, r_{m+j+1}) = (r'_{j+1}, Gr'_{j+1})$.


V
N/p
N
$O(s)$


$G = V^T V$
$O(s)$
$=$
$\times$
$O(s)$


$\|r\|^2 =$
$r^T r =$
$r'^T G r'$
$=$
$\times$
$=$
Computed locally on each processor – no communication!