High-Performance GMRES Mixed-Precision (HPG-MxP) Benchmark with Kokkos-Kernels backend

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Ichitaro Yamazaki, Jennifer Loe, Christian Glusa, Siva Rajamanickam (Sandia National Labs)

Piotr Luszczek, and Jack Dongarra (University of Tennessee, Knoxville)

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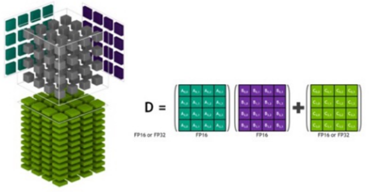
Goal & Motivations

- HPG-MxP is designed to
  - capture typical performance of **“real” applications**
    - Consist of kernels found commonly in these applications
  - allow the use of **mixed precision arithmetic**
  - It’s a mix of HPCG and HPL-MxP
- Some current & emerging HP computers can perform lower precision arithmetic at higher performance
  - Some emerging accelerators may not support double precision
- Lower precision reduces the data transfer volume and may improve application performance
  - Application performance is often limited by communication (latency or bandwidth)
- Such benchmark may be of interests to many decilplines

		GPU Peak Performance (Tflop/s)		
System	GPU	FP64	FP32	FP16
Frontier (ORNL)	AMD MI250X	26.5	26.5	191.0
Fugaku (Riken)	Fujitsu A64 FX	3.4	6.7	13.5
Summit (ORNL)	NVIDIA V100	7.5	19.5	N/A
Perlmutter (NERSC)	NVIIDIA A100	9.7	19.5	312.0
Sierra (LLNL)	AMD MI100	11.5	23.1	184.0
Selena (NVIDIA)	AMD MI250X	26.5	26.5	191.0



NVIDIA Sparse Tensor Core

HP GMRES Mixed-Precision (HPG-MxP)

Input: $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^{n\times 1}$, initial guess $x_0 \in R^{n\times 1}$, relative residual tolerance $rTol$
Output: approximate solution x_m

```
r = b − Ax,
γ = ‖r‖₂
while not converged do
    v₁ = r₀/γ, and h₁,₁ = 0
    for j = 1 : m do
        // GMG preconditioner M, followed by SpMV
        w_j = A M v_j
        // CGS2 orthogonalization
        w_j = w_j − V_j t_j with t_j = V_j^T w_j
        h_{1:j,j} = t_j
        w_j = w_j − V_j t_j with t_j = V_j^T w_j
        h_{1:j,j} = h_{1:j,j} + t_j
        h_{j+1,j} = ‖w_j‖₂
        v_{j+1} = w_j / h_{j+1,j}
    end for
    d̂ = arg min_{y∈ℝ^m} ‖γe₁ − H_{1:m+1,1:m} y‖₂
    x = x + V_m d̂
    r = b − Ax
    γ = ‖r‖₂
end while
```

GMRES in lower precision

Refinement in double precision

	Dense Problem Compute Intensive	Sparse Problem Compute/Comm pattern in "Real" Appls
Uniform Precision	HPL	HPCG
Mixed Precision	HPL-MxP	HPG-MxP

- Mixed-precision Iterative refinement to solve a sparse linear system
  - Lower-precision may be used to solve the sparse linear system
    - GMRES to provide the robustness
      - GMG preconditioner + GS smoother
    - Typically dominates benchmark time
  - Iterative refinement to obtain the double-precision solution
  - How much speedup can we get using lower-precision for communication-bound operations?
  - Benchmark result is penalized if lower-precision increases the iteration count

Mixed-precision GMRES – Iterative Refinement

for solving sparse non-symmetric linear system

- Generalized Minimum Residual (GMRES)
  - A popular Krylov method for solving a non-symmetric system
  - It computes an approximate solution minimizes the residual norm in the computed Krylov projection subspace
- Mixed-precision variant
  - is also a well-established algorithm
  - Growing interests, with lots of numerical theories and performance studies, in recent years

1) *P. Amestoy, A. Buttari, N. Higham, J. L'Excellent, T. Mary, and B. Vieuble. Five-precision GMRES- based iterative refinement. 2021.*

2) *P. Amestoy, A. Buttari, N. Higham, J. L'Excellent, T. Mary, and B. Vieuble. Combining sparse approximate factorizations with mixed precision iterative refinement. Technical report, The University of Manchester, 2022.*

3) *E. Carson and N. Higham. Accelerating the Solution of Linear Systems by Iterative Refinement in Three Precisions. SIAM J. Sci. Comput., 40(2):A817–A847, 2018.*

4) *S. Gratton, E. Simon, D. Titley-Pe´loquin, and P. Toint. Exploiting variable precision in GMRES. ArXiv, abs/1907.10550, 2019*

5) *N. Lindquist, P. Luszczek, and J. Dongarra. Improving the Performance of the GMRES Method using Mixed-Precision Techniques. in Smoky Mountains Conference Proceedings, 2020.*

6) *J. Loe, C. A. Glusa, I. Yamazaki, E. G. Boman, and S. Rajaman- ickam. Experimental evaluation of multiprecision strategies for GMRES on gpus. In 2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), pages 469–478, 2021.*

7) ***K. Turner and H. Walker. Efficient high accuracy solutions with GMRES(m). SIAM J. Sci. Stat. Comput., 13(3):815–825, 1992.***

8) *Etc. etc.*

Also, mixed-precigion MG:

1) *S. McCormick, J. Benzaken, and R. Tamstorf. Algebraic error analysis for mixed-precision multigrid solvers. SIAM J. Sci. Comp., 43(5):S392–S419, 2021.*

HPG-MxP: Main tasks

Same kernels as HPCG, except for CGS2

1. Sparse Matrix Vector Multiply (SpMV)
   - **Point-to-point neighborhood communication** (halo exchange)
     - Exchange 1, n_x, or n_x^2 elements with 7 ~ 26 neighbors
   - Local **SpMV** with 27-pts stencil
     - 54nm Flops / restart
2. Orthogonalization based on Classical Gram Schmidt with reorthogonalization (CGS2)
   - **Blas-2 dense matrix-vector dot-product**, local atomic and **global reduce**
     - Total of 2n(1+m)m Flops / Restart
   - **Blas-2 dense matrix-vector update**, embarrassingly parallel
     - Total of 2n(1+m)m Flops / Restart

Mixture of sparse and dense operations, commonly found in real applications

- With m = 40, about same number of flops for GMG and CGS2

3. Geometric Multi Grid (GMG)
   - Four level with 2^3x smaller coarse grid
   - One forward-sweep of Gauss-Seidel (GS) as pre & post smoother
     - **Halo-exchange**, Local **SpTRSV**
     - Total of 2*(54*73)/64 nm Flops / Restart
   - Residual vector computation
     - **Halo-exchange**, Local **SpMV**
     - Total of 2*(54*73)/64 nm Flops / Restart
   - Restriction & Prolongation operators
     - No communication, Local **SpMV** with a rectangular matrix,
       e.g., one nonzero per row
   - One forward sweep of GS at the final coarse level.
     - **Halo-exchange**, Local **SpTRSV**
     - Total 81 / 512 nm Flops / Restart

HPG-MxP reference implementation

- The reference implementation (solver & benchmark suite) is available
  - https://github.com/iyamazaki/hpcg
  - It is meant to be optimized by participants
- It reuses many of HPCG components
- It is based on C++ template
  - To make it easier to use various precision

```
template<class SparseMatrix_type, class SparseMatrix_type2, class CGData_type, class CGData_type2, class Vector_type>
int GMRES_IR(const SparseMatrix_type & A, const SparseMatrix_type2 & A_lo,
             CGData_type & data, CGData_type2 & data_lo, const Vector_type & b_hi, Vector_type & x_hi,
             const int restart_length, const int max_iter, const typename SparseMatrix_type::scalar_type tolerance,
             int & niters, typename SparseMatrix_type::scalar_type & normr, typename SparseMatrix_type::scalar_type & normr0,
             double * times, bool doPreconditioning);
```

- It also provides CUDA/HIP backends
  - It uses GPUs to generate basis vectors,
    while the tiny least square problem is solved redundantly on each CPU.
  - It uses MPI for data exchange, while solely rely on vendor libraries for the GPU computation
    - **CuBLAS** and **CuSparse** on NVIDIA and **RocBLAS** and **RocSparse** on AMD
    - GS uses general SpMV & SpTRSV
  - Minimum CUDA/HIP code
    - Gather for MPI P2P communication
    - If the vector needs to be casted, then it is done on a CPU (no mixed-precision kernels)

Performance studies of reference implementation : Experimental setups to motivate Kokkos-Kernels backend

- Test machines
  - Summit (OLCF)
    - Each node with 2×22-core Power9 CPUs and six NVIDIA V100 GPUs
  - Frontier (OLCF)
    - Each node with 1×64-core AMD EPYC CPUs and four AMD MI250X GPUs
  - Perlmutter (NERSC)
    - Each node with 1×64-core AMD EPYC CPUs and four NVIDIA A100 GPUs
- Weak-scaling
  - a fixed problem size per MPI (one MPI / CPU core or GPU)
- Using single-precision for GMRES iterations
  - 2.0x reduction in dense matrix storage
  - 1.6x reduction in sparse matrix storage
- Performance of the reference implementation
  - Meant to motivate interests

name	value
Solver parameters	
restart cycle, m	30
GMG levels	3
GS sweeps	1
Step 1 (Validation)	
problem size (n_x, n_y, n_z)	(80,80,80)
convergence tol	10^{-9}
# of MPI procs	4
Step 2 (Benchmark)	
# of iterations	300
# of minimum solves	10
minimum time	30 minutes (disabled)

Some of the parameter values are selected for convenience.

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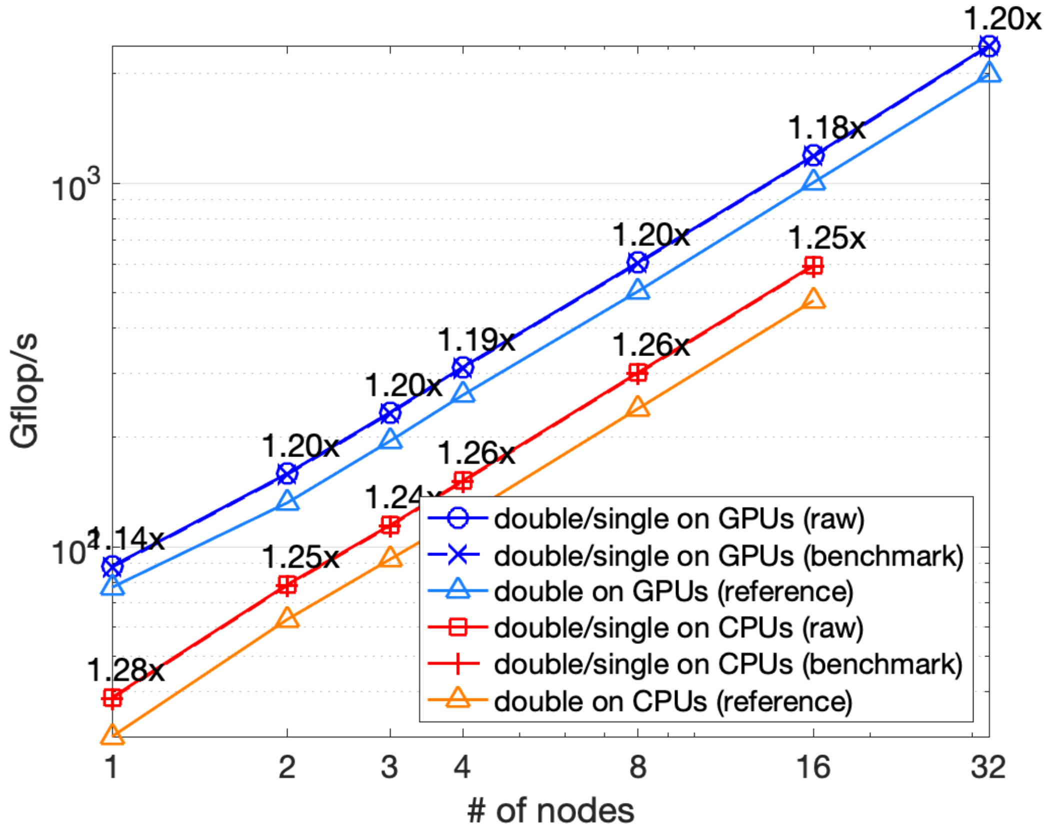
Performance of reference implementation on Summit
IBM Power9 CPUs + NVIDIA V100 GPUs

- Speedup of 1.2x using a non-optimized reference
- Most of the solver time is spent in SpTRSV for GMG
  - It has limited parallelism, and
    its performance may be more dominated by latency
  - it is harder to get speedup using lower precision
  - Reference implementation uses CuSparse SpMV & SpTRSV
    (no coloring)

	Time in seconds with GPUs				TFlop/s with GPUs			
	GMG	SpMV	CGS2	**Total**	**GMG**	SpMV	CGS2	**Total**
Uniform	**51.5**	3.8	2.5	**60.2**	**0.30**	1.20	4.13	**0.50**
Mixed	**44.5**	2.4	1.8	**50.1**	**0.35**	1.87	5.73	**0.61**
Speedup	**1.16**	1.56	1.39	**1.20**	**1.15**	1.56	1.39	**1.20**

Performance on 8 Summit nodes with GPUs
(about same total # of flops for GMG or CGS2)



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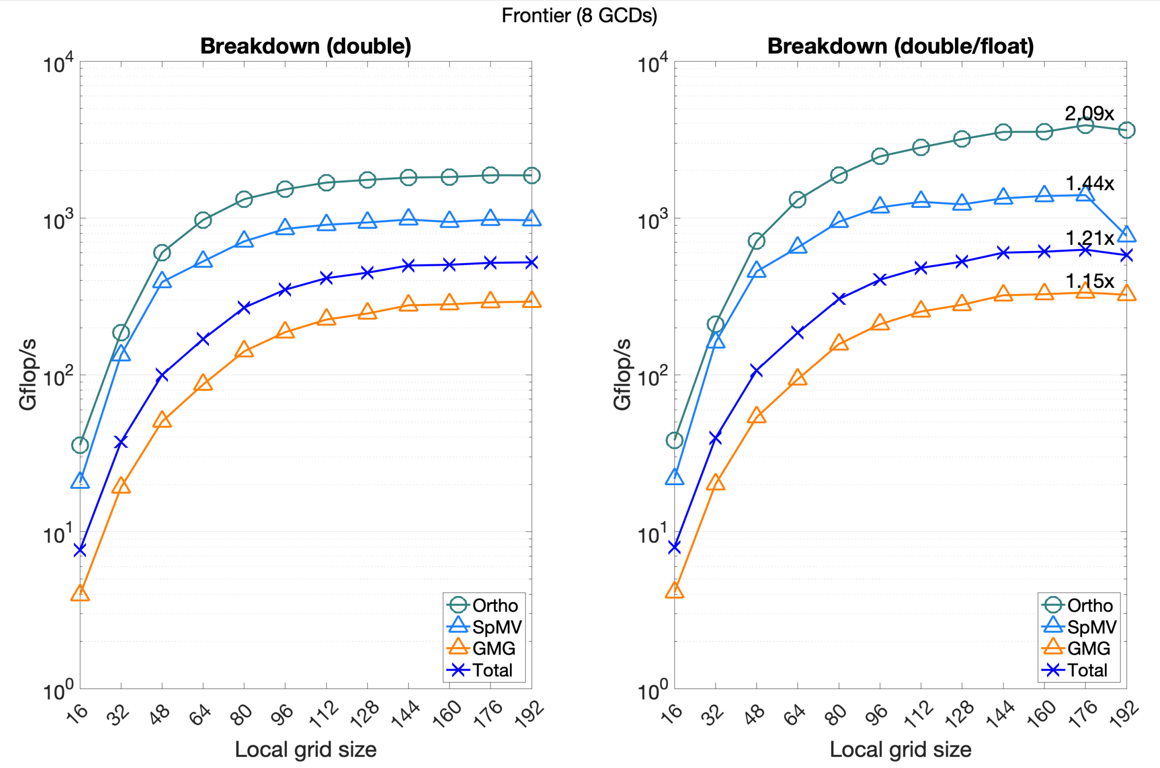
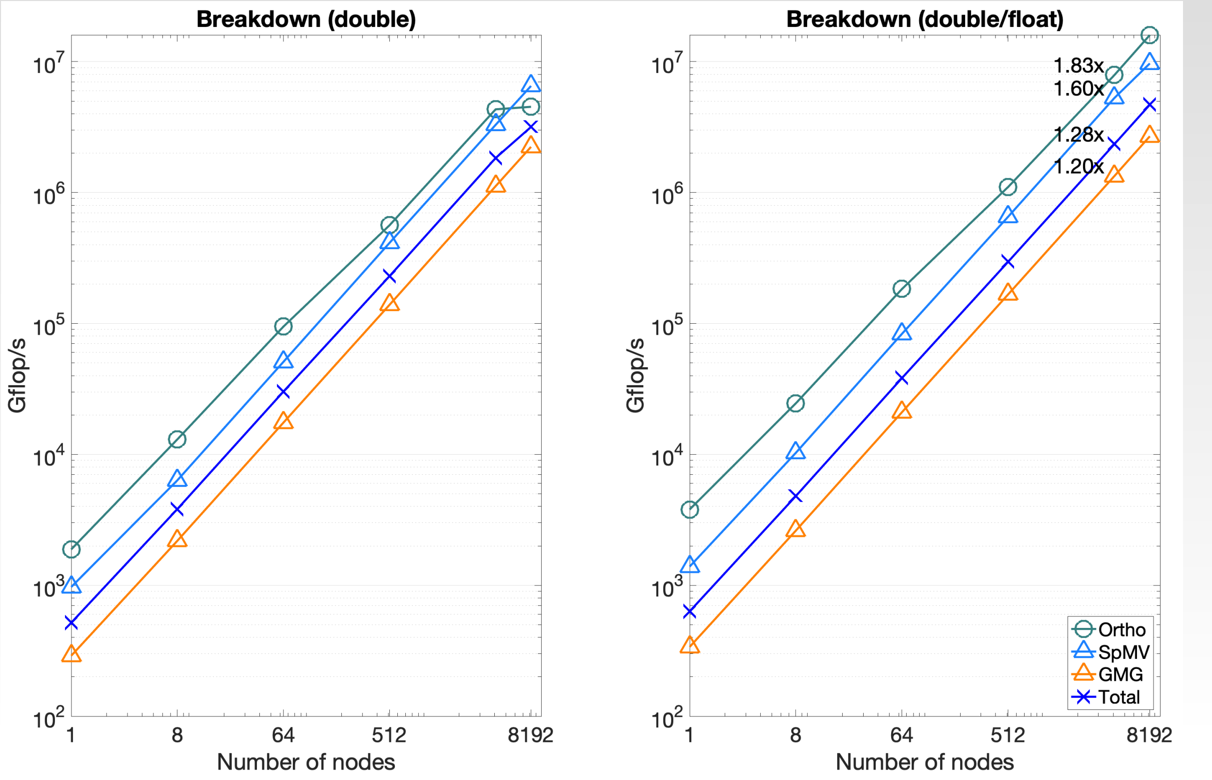
Performance of reference implementation on Frontier (at larger scale)
AMD EPYC CPUs + AMD MI250X GPUs





- Speedups, similar to those on Summit
  - AMD MI250X GPU on Frontier has same peak compute performance using double and single
    - Peak 530-1600 Gflop/s for Ortho and 450-1100 Gflop/s for SpMV (800 GB/s)
    - 14 PFlop/s HPCG on Frontier
  - SpMV (with P2P) seems to scale better than Ortho (all-reduce)

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HPG-MxP with Kokkos-Kernels backend (as an "optimized" implementation)

- Kokkos-Kernels backends
  - Optimized version of GS (e.g., coloring) [Devici'16, Kelley'22]
    - TPL to vendor BLAS/Sparse kernels
    - Reference spends most of time in GS
    - KK GS may get closer to SpMV on big enough matrix?
  - Mixed-precision operations, including FP16 or BF16
    - Reference explicitly type-casts (on host) before uniform-precision kernels
  - Portable implementation of LA ops on different node architectures
    - FP16/BF16 supports on host.

```
template <class ExecutionSpace, class AViewType, class XViewType,
          class YViewType>
void gemv(const ExecutionSpace& space, const char trans[],
          typename AViewType::const_value_type& alpha, const AViewType& A,
          const XViewType& x, typename YViewType::const_value_type& beta,
          const YViewType& y) {
```

		GPU Peak Performance (Tflop/s)		
System	GPU	FP64	FP32	FP16
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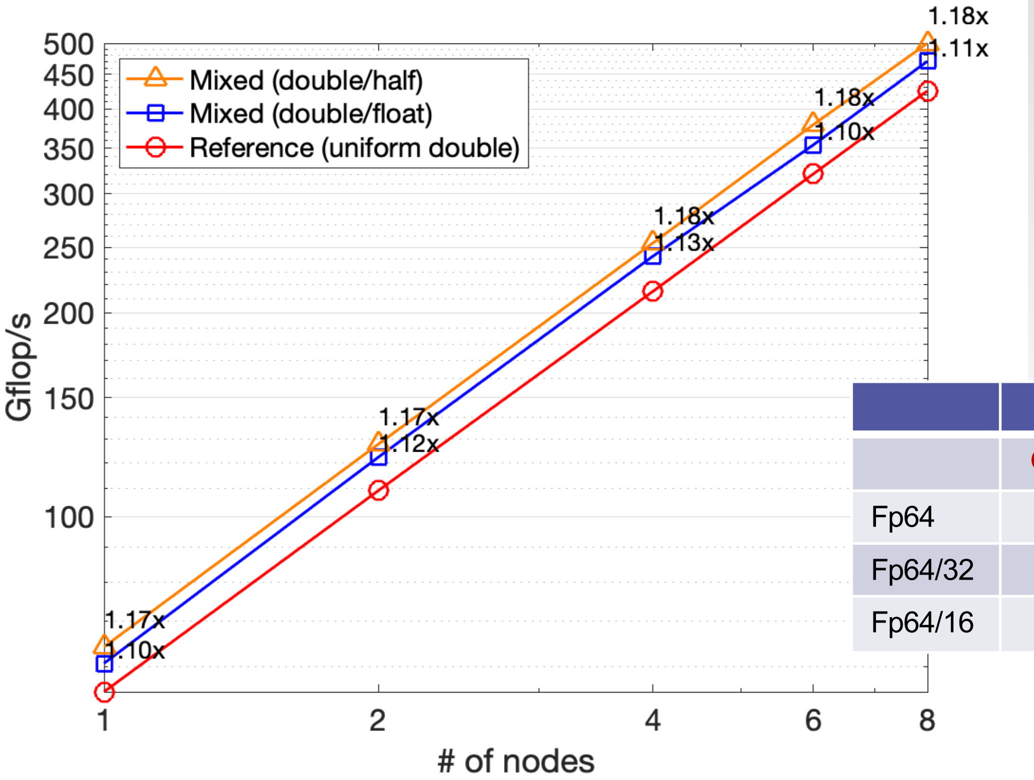
	fp64	fp32	fp16	bf16
maximum	$1.80 \cdot 10^{308}$	$3.40 \cdot 10^{38}$	$6.55 \cdot 10^{4}$	$3.39 \cdot 10^{38}$
minimum	$2.22 \cdot 10^{-308}$	$1.17 \cdot 10^{-38}$	$5.96 \cdot 10^{-8}$	$1.18 \cdot 10^{-38}$
epsilon	$2.22 \cdot 10^{-16}$	$1.19 \cdot 10^{-7}$	$9.77 \cdot 10^{-4}$	$7.81 \cdot 10^{-3}$

Special thanks to Kokkos-Kernels team,
Brian Kelley, Evan Harvey, and Vinh Dang

Performance (time / iteration) using FP16 on Perlmutter (Four NVIDIA A100 GPUs / node) using mixed-precision FP16/FP32 KK interface (FP16 for GMRES iterations, but accumulations are stored in FP32)



- using FP16 did help reducing the iteration time
  - Performance & speedup still dominated by GS
  - We used clustered GS from Kokkos-Kernels
  - Iteration count went up, and benchmark results were 25x slower using FP16

	Time in milliseconds / iter				GFlop/s				Speedup			
	GMG	SpMV	CGS	Total	GMG	SpMV	CGS	Total	GMG	SpMV	CGS	Total
Fp64	8.80	0.67	3.88	13.4	42.3	162.1	64.9	55.1	--	--	--	--
Fp64/32	8.11	0.47	3.55	12.1	45.8	232.6	71.0	60.7	1.08	1.43	1.09	1.10
Fp64/16	8.02	0.40	3.04	11.5	46.4	274.4	82.7	64.2	1.10	1.69	1.27	1.17

Performance on one Perlmutter node with GPUs (about same total # of flops for GMG or CGS2)

Final remarks

- Kokkos-Kernels backend for HPG-MxP
  - Optimized GS, mixed-precision interface, and portable kernels
  - Looking at performance on current HPC system (Frontier, Perlmutter, and maybe Aurora)
    - GS performance and speedups
    - Potential of BF16/FP16 precision
      - Store just matrices in FP16 for GS

Thank you !!

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Acknowledgments

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Discussion