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# High-Performance GMRES Multi-Precision Benchmark

Design, Performance, and Challenges

Approved for public release

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## Goal & Motivations

- New benchmark is designed to
  - capture typical performance of **“real” applications**
  - allow the use of **mixed precision arithmetic**
- Some current & emerging HP computers provide higher performance for lower precision arithmetic
  - 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)

| | | 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 |
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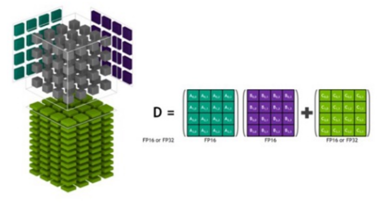

NVIDIA Sparse Tensor Core

## Goal & Motivations

- Growing interests to utilize lower-precision for “real” applications
  - ECP xSDK multi-precision project funded by US DOE
- New benchmark could have wide impacts
  - Capture the computers capabilities for applications by allowing mixed-precision operations
    - Algorithmic & software efforts to utilize lower-precision
  - Motivate hardware vendors to design future HP computers that can obtain high application performance, with mixed-precision arithmetic

| | | GPU Peak Performance (Tflop/s) | | |
|---|---|---|---|---|
| System | GPU | FP64 | FP32 | FP16 |
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| Frontier (ORNL) | AMD MI250X | 26.5 | 26.5 | 191.0 |
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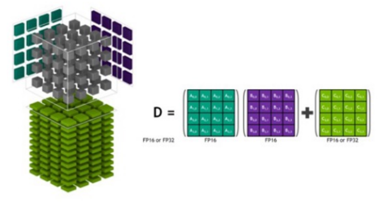
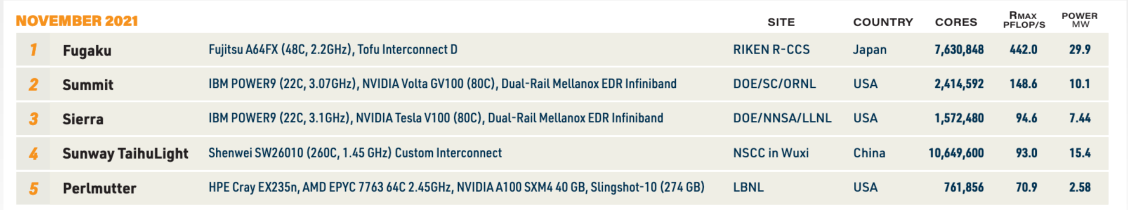


NVIDIA Sparse Tensor Core

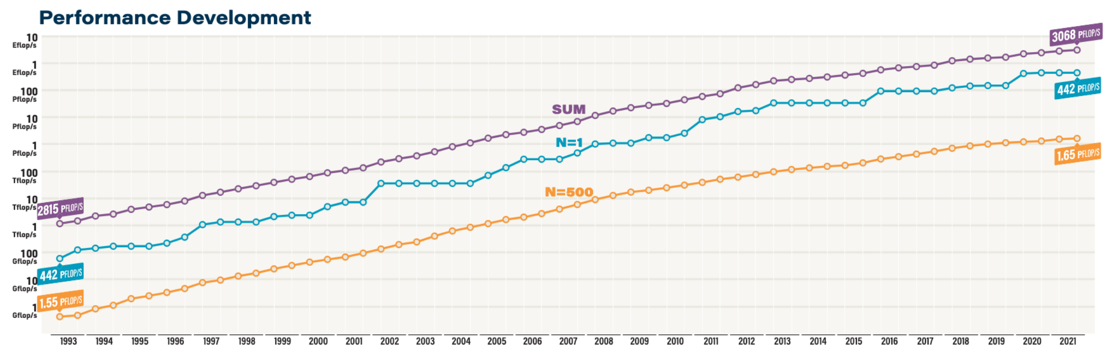
# Existing HP Benchmark 1/3 : High Performance Linpack (HPL)

- HPL measures performance of solving dense linear system in double precision
  - It is based on exact dense LU factorization
- Its performance is dominated by dense matrix-matrix multiply, with a proper implementation.
- Its performance is close to double-precision peak compute performance of the target machine.
- It is used to rank HP computers for Top500 list, providing historical data
- It is also used to stress-test new systems

| | Dense Problem Compute Intensive | Sparse Problem "real" appli. performance |
|---|---|---|
| Uniform Precision | **HPL** | HPCG |
| Mixed Precision | HPL-AL | |



| NOVEMBER 2021 | | | SITE | COUNTRY | CORES | RMAX PFLOP/S | POWER MW |
|---|---|---|---|---|---|---|---|
| 1 | Fugaku | Fujitsu A64FX (48C, 2.2GHz), Tofu Interconnect D | RIKEN R-CCS | Japan | 7,630,848 | 442.0 | 29.9 |
| 2 | Summit | IBM POWER9 (22C, 3.07GHz), NVIDIA Volta GV100 (80C), Dual-Rail Mellanox EDR Infiniband | DOE/SC/ORNL | USA | 2,414,592 | 148.6 | 10.1 |
| 3 | Sierra | IBM POWER9 (22C, 3.1GHz), NVIDIA Tesla V100 (80C), Dual-Rail Mellanox EDR Infiniband | DOE/NNSA/LLNL | USA | 1,572,480 | 94.6 | 7.44 |
| 4 | Sunway TaihuLight | Shenwei SW26010 (260C, 1.45 GHz) Custom Interconnect | NSCC in Wuxi | China | 10,649,600 | 93.0 | 15.4 |
| 5 | Perlmutter | HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10 (274 GB) | LBNL | USA | 761,856 | 70.9 | 2.58 |



## Existing HP Benchmark 2/3 : High Performance Conjugate Gradient (HPCG)

- HPCG is designed to reflect application performance
- It solves a sparse linear system using CG with GMG preconditioner (GS smoother).
  - Composed of computation & communication tasks common in real applications
  - Its performance is more limited by communication latency or bandwidth.
- It is meant to motivate the future HP computers that can achieve high application performance

| | **Dense Problem Compute Intensive** | **Sparse Problem “real” appli. performance** |
|---|---|---|
| Uniform Precision | HPL | **HPCG** |
| Mixed Precision | HPL-AL | |

| HPCG Rank | HPL Rank | System | HPCG (Pflop/s) | HPL (Pflop/s) |
|---|---|---|---|---|
| 1 | 1 | Fugaku (Riken) | 16.0 | 442.0 |
| 2 | 2 | Summit (ORNL) | 2.9 | 148.6 |
| 3 | 5 | Perlmutter (NERSC) | 1.9 | 70.8 |
| 4 | 3 | Sierra (LLNL) | 1.8 | 94.6 |
| 5 | 6 | Selena (NVIDIA) | 1.6 | 63.5 |

Data source : top500.org (Nov, 2021)

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## Existing HP Benchmark 3/3 : HPL - Accelerator Introspection (HPL-AI)

- HPL-AI solves the same dense linear system as HPL, but allows the use of lower-precision
- It uses lower-precision for compute-intensive LU (no pivoting), which dominates benchmark time.
- Iterative refinement is used to obtain the solution with double precision accuracy.
- It achieves much higher performance than HPL on machines with lower-precision at higher performance
  - It measures the computer's capability to perform compute intensive tasks

| | Dense Problem Compute Intensive | Sparse Problem "real" appli. performance |
|---|---|---|
| Uniform Precision | HPL | HPCG |
| Mixed Precision | HPL-AL | |

| HPL-AI Rank | HPL Rank | System | HPL-AI (Pflop/s) | HPL (Pflop/s) |
|---|---|---|---|---|
| 1 | 1 | Fugaku (Riken) | 2.00 | 0.44 |
| 2 | 2 | Summit (ORNL) | 1.41 | 0.15 |
| 3 | 6 | Selena (NVIDIA) | 0.63 | 0.06 |
| 3 | 5 | Perlmutter (NERSC) | 0.59 | 0.07 |
| 5 | 8 | Juwels BM (FZJ) | 0.47 | 0.04 |

Data source : top500.org (Nov, 2021)

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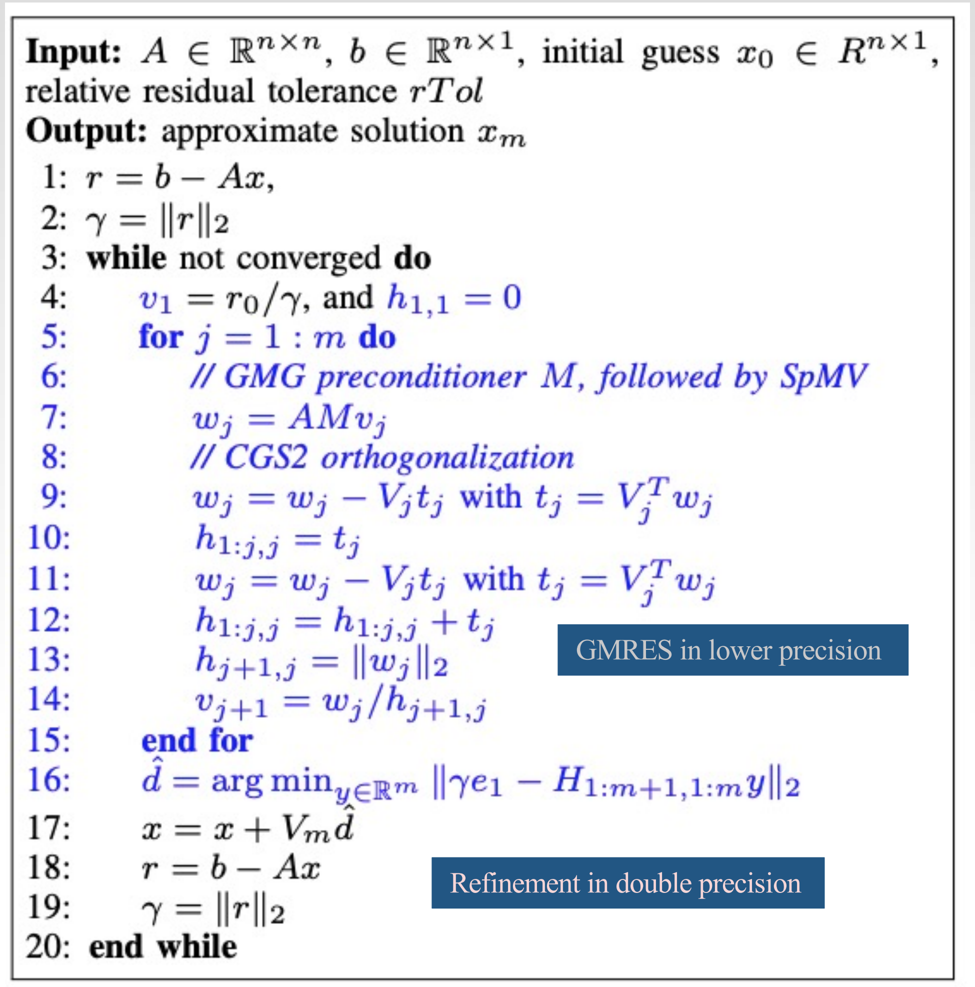
# New HP Benchmark : HP GMRES mixed-precision (HPGMP)



**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 $x_m$

```
1: $r = b - Ax$,
2: $\gamma = \|r\|_2$
3: while not converged do
4:     $v_1 = r_0/\gamma$, and $h_{1,1} = 0$
5:     for $j = 1 : m$ do
6:         // GMG preconditioner $M$, followed by SpMV
7:         $w_j = AMv_j$
8:         // CGS2 orthogonalization
9:         $w_j = w_j - V_j t_j$ with $t_j = V_j^T w_j$
10:        $h_{1:j,j} = t_j$
11:        $w_j = w_j - V_j t_j$ with $t_j = V_j^T w_j$
12:        $h_{1:j,j} = h_{1:j,j} + t_j$
13:        $h_{j+1,j} = \|w_j\|_2$
14:        $v_{j+1} = w_j / h_{j+1,j}$
15:    end for
16:    $\hat{d} = \arg\min_{y \in \mathbb{R}^m} \|\gamma e_1 - H_{1:m+1,1:m} y\|_2$
17:    $x = x + V_m \hat{d}$
18:    $r = b - Ax$
19:    $\gamma = \|r\|_2$
20: end while
```

| | Dense Problem Compute Intensive | Sparse Problem Compute/Comm pattern in "Real" Appls |
|---|---|---|
| **Uniform Precision** | HPL | HPCG |
| **Mixed Precision** | HPL-AL | HPGMP |

- The new benchmark
  - measures computer's capability to perform computation & communication often found in applications (like HPCG)
  - allows use of mixed-precision (like HPL-AI)
- Iterative refinement for solving a sparse linear system
  - Lower-precision may be used to solve the sparse linear system
    - Sparse iterative solver, which typically dominates benchmark time
    - GMRES + GMG + GS smoother (sparse-triangular solve)
  - Double-precision is used to update the solution and to compute the new residual vector

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## 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.*

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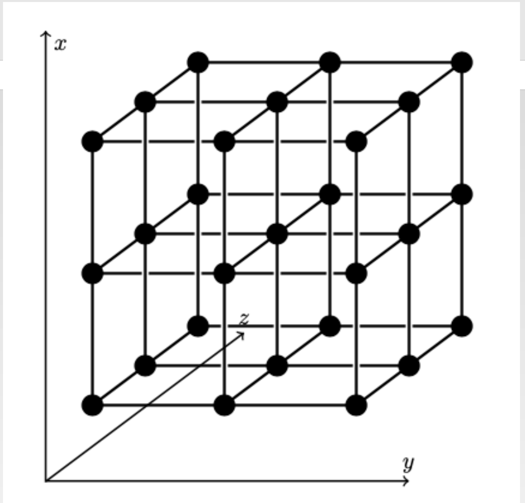
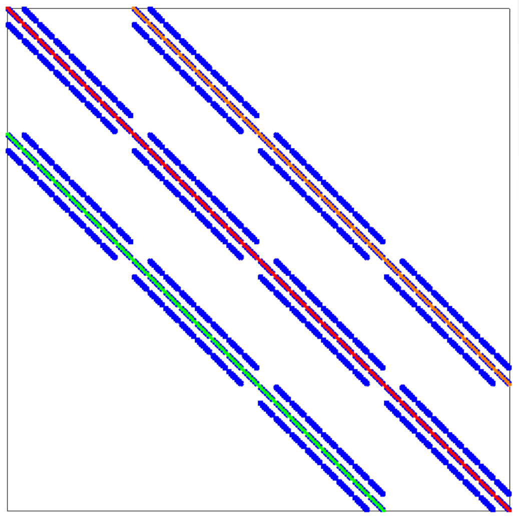
## HPGMP: Problem description

- Regular 3D grid with 27-points stencil
  - Same as HPCG
  - Parameterized for non-symmetric numerical values
    - Represents finite difference discretization of an advection-diffusion problem
  - Right-hand-side vector $b = A*ones$, and initial approximate solution $x$=zeros.
- MPI processes are arranged into a 3D process grid $(p_x\ p_y\ p_z)$
- Participant specifies the dimension of the local subdomain $(n_x\ n_y\ n_z)$ on each MPI
  - the global matrix size is $(n_x p_x\ n_y p_y\ n_z p_z)$



(a) 27-point stencil.



## HPGMP: 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 vector dot-product**, local atomic and **global reduce**
     - Total of 2n(1+m)m Flops / Restart
   - **Blas-2 vector update**, embarrassingly parallel
     - Total of 2n(1+m)m Flops / Restart
3. Geometric Multi Grid (GMG)
   - 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

**Mixture of sparse and dense operations, commonly found in real applications**
- With m = 30, about same number of flops for GMG and CGS2

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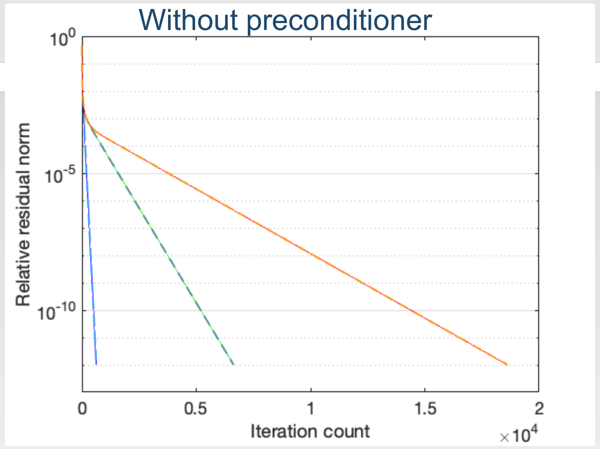
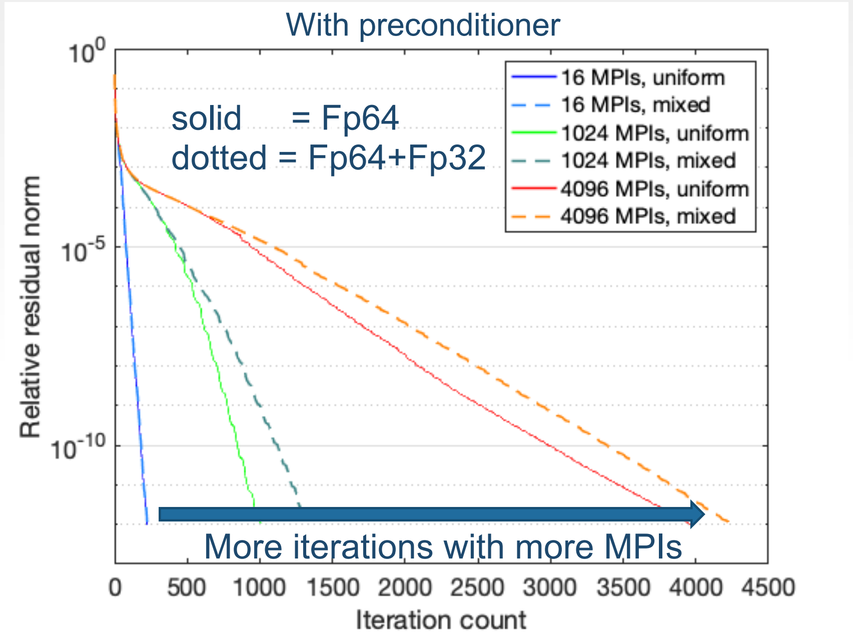
## Q1 : How much flexibility to allow in term of precision?



- Current benchmark specification allows any precision for the GMRES iteration.
- The benchmark is <u>**not**</u> meant to be a **robust** or **scalable** solver.
  - It is designed to capture application performance
  - Iteration count increases with MPI count
  - It may converge slower, or faster, using lower precision
- We need verification and validation!!
  - The solver should achieve the double precision accuracy
  - If the solver requires more iterations, then the benchmark results should be appropriately penalized



## HPGMP benchmark : two steps

1. **Verification step**:
   - Run both reference & optimized solver
     - Using a fixed problem size on a fixed # of MPI processes
     - To reach double-precision accuracy
   - Record # of iteration needed by both
     - Failure if optimized code did not converge
     - Compute penalty factor
       **$i_p$ = min(1.0, # of optimized iterations / # of reference iteration)**
2. **Benchmark step**:
   - Run optimized solver for a fixed number of iterations
     - Using user-specified problem size and # of MPI processes
     - Until reaching a minimum # of solves or time
   - Compute benchmark Gflop/s
     - **$I_p$ x (# of Gflops / Optimized benchmark time)**

- The benchmark is designed
  - To allow the use of mixed-precision
  - To penalize if the lower-precision results in the loss of accuracy (convergence rate
- Note: we cannot run to double precision accuracy for the large benchmark runs (iteration count increases with # of MPIs)

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## HPGMP: Allowed optimizations

Similar to HPCG

- Hardware specific optimization are allowed
  - Data structures, communication schemes, etc.
- Matrix may be permuted for GS smoother to expose parallelism
  - If the permutation increases the iteration count, benchmark performance is penalized (validation step)
- Algorithm changes are **not** allowed
  - *s*-step (communication-avoiding), pipelined, or randomized variant of GMRES
  - Low-synchronous/single-reduce orthogonalization
  - Iterative-variant of GS smoother
- Knowledge of matrix structure **cannot** be used
  - The matrix should be treated as a general matrix for SpMV
- **Any precision(s) may be used for the sparse solver**
  - **Need to pass the verification, and will be penalized on any increase in iteration count**
- Matrix scaling is **not** allowed
  - The matrix may not be scaled to fit in the numerical range of lower precision
  - It can be used to improve the conditioning of the matrix

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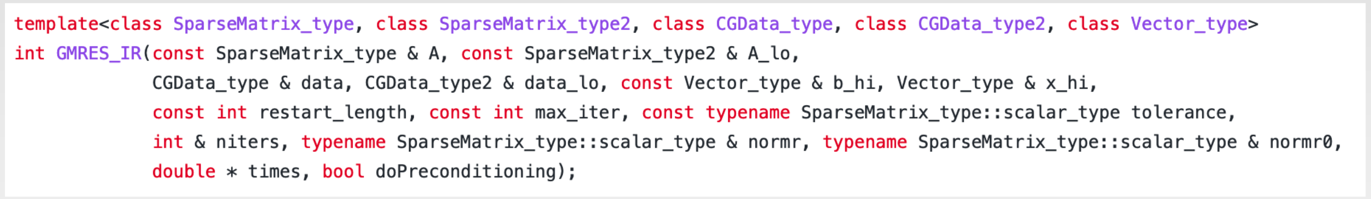
## HPGMP reference implementation

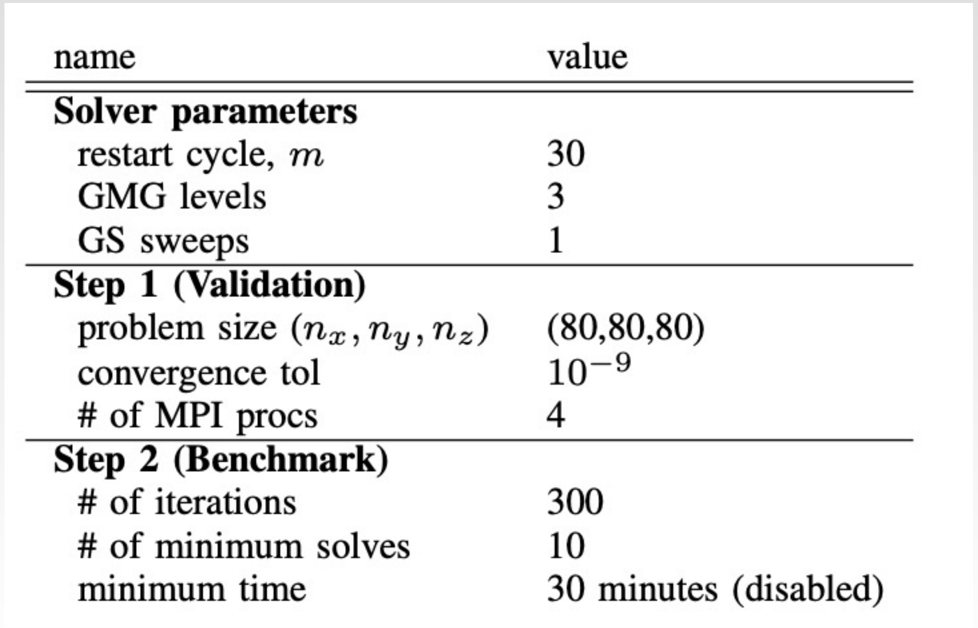
- The reference implementation (solver & benchmark suite) is available
  - https://github.com/iyamazaki/hpcg
  - It is meant to be optimized by participants
- It reuses many of HPCG components
- It is based on C++ template
  - To make it easier to use various precision
- It also provides CUDA/HIP backends
  - 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** for CGS2, **CuSparse** SpMV & SpTRSV for GS and restriction/prolongation, and
      **CUDA library** for memory management
  - No custom CUDA/HIP code
    - MPI message communication is through CPUs
    - If the vector needs to be casted, then it is done on a CPU



```
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);
```

## Performance studies of reference implementation : Experimental setups

- OLCF machines
  - Summit
    - Each node with 2×22-core Power9 CPUs and six NVIDIA V100 GPUs
  - Spock
    - Each node with 1×64-core AMD EPYC 7662 CPU and four AMD MI100 GPUs
  - Crusher
    - Each node with 1×64-core AMD EPYC 7A53 CPU and four AMD MI250X GPUs
- Weak-scaling
  - a fixed problem size per MPI (one MPI / CPU core or GPU)
- Using single-precision for GMRES iterations
  - 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) |

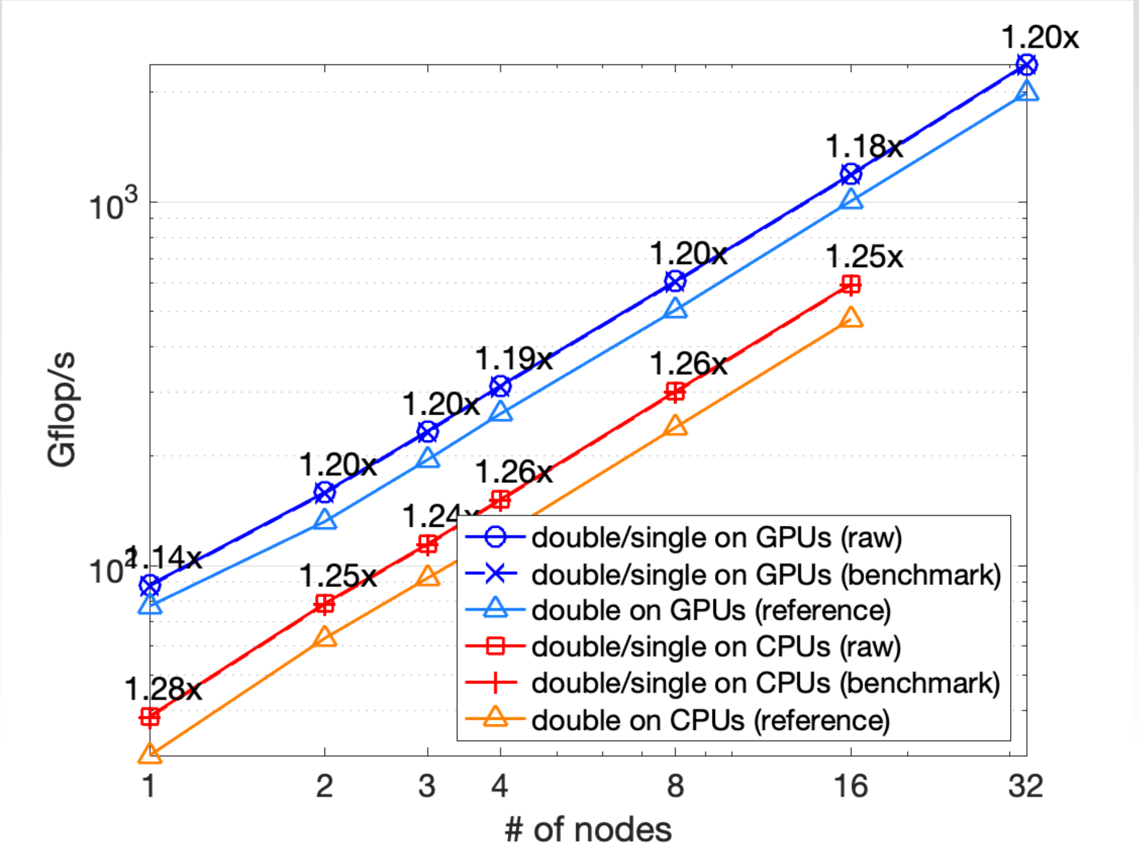
Some of the parameter values are selected for convenience.

## 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
  - 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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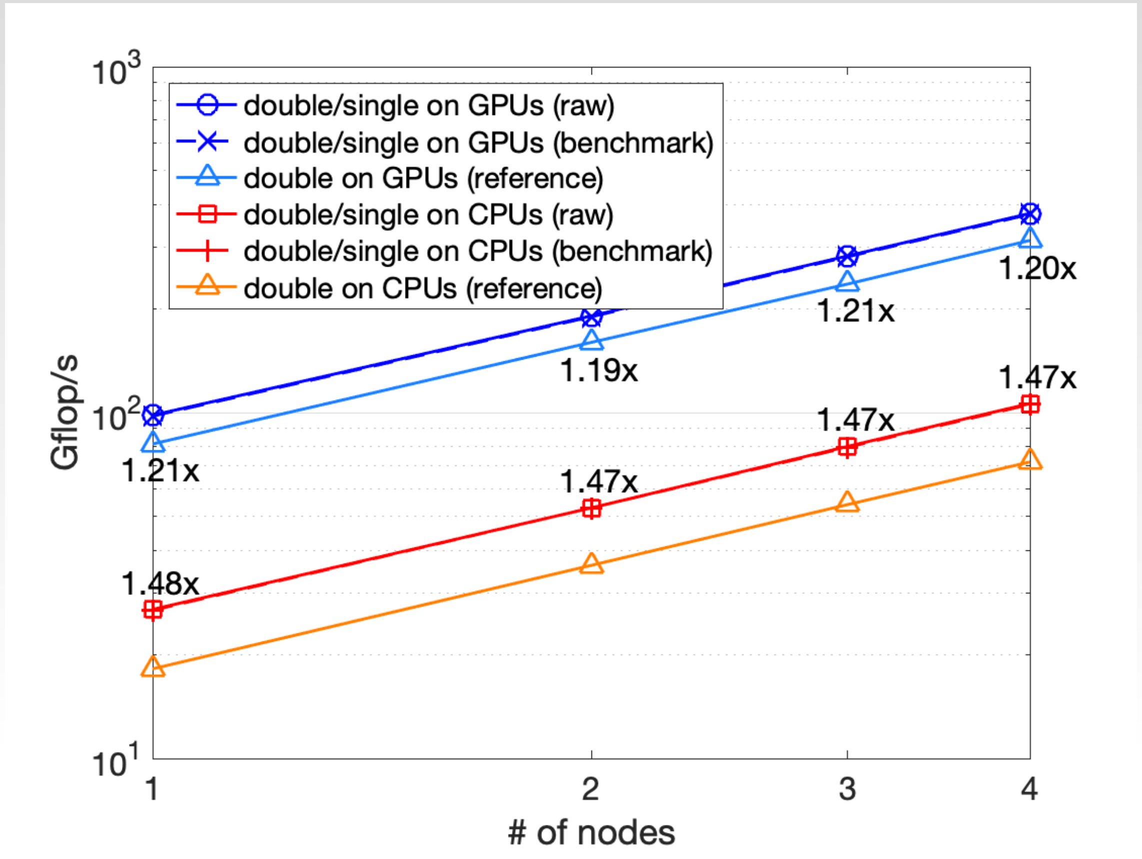
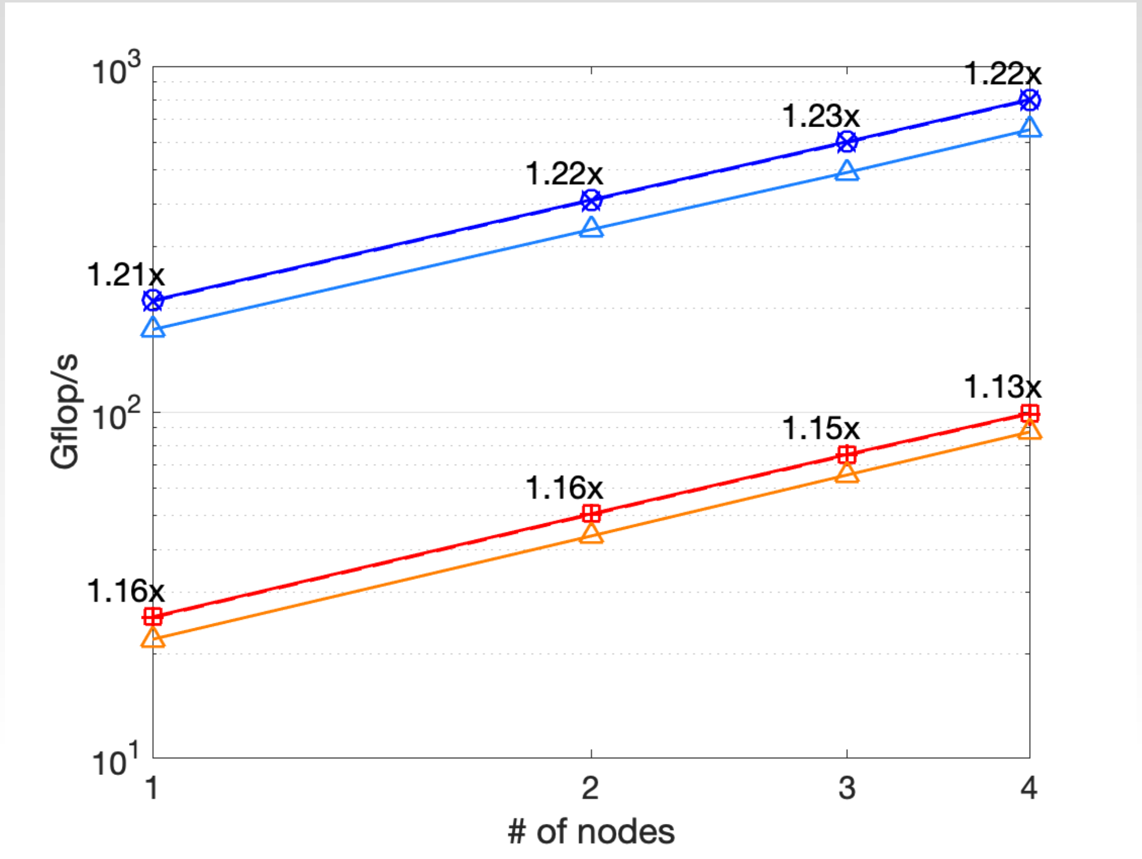
## Performance of reference implementation on Spock & Crusher
## AMD EPYC CPUs + AMD MI100/250X GPUs





- Speedups, similar to those on Summit
  - AMD MI250X GPUs on Crusher have same peak performance using double and single

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## Experimental studies with 16-bit floating precisions

- Kokkos-Kernels backends as an "optimized" implementation
  - Portable implementation of LA operations on different node architectures
    - Perlmutter (NVIDIA A100) and Crusher (AMD 250X), or Fugaku (A64 FX)
  - Allows the use of FP16 or BF16, and mixed-precision operations
- We look at performance (time / iteration) and convergence (# iterations needed for convergence)
  - FP16 for GMRES iterations, except accumulations are stored in FP32 (e.g., Hessenberg matrix for LSP, and norms for convergence check, on CPU)
  - Both performance & convergence depend on how mixed-precision operations are implemented through software stacks and on hardware

| | | GPU Peak Performance (Tflop/s) | | |
|---|---|---|---|---|
| System | GPU | FP64 | FP32 | FP16 |
| | | | | |
| Crusher (ORNL) | AMD MI250X | 26.5 | 26.5 | 191.0 |
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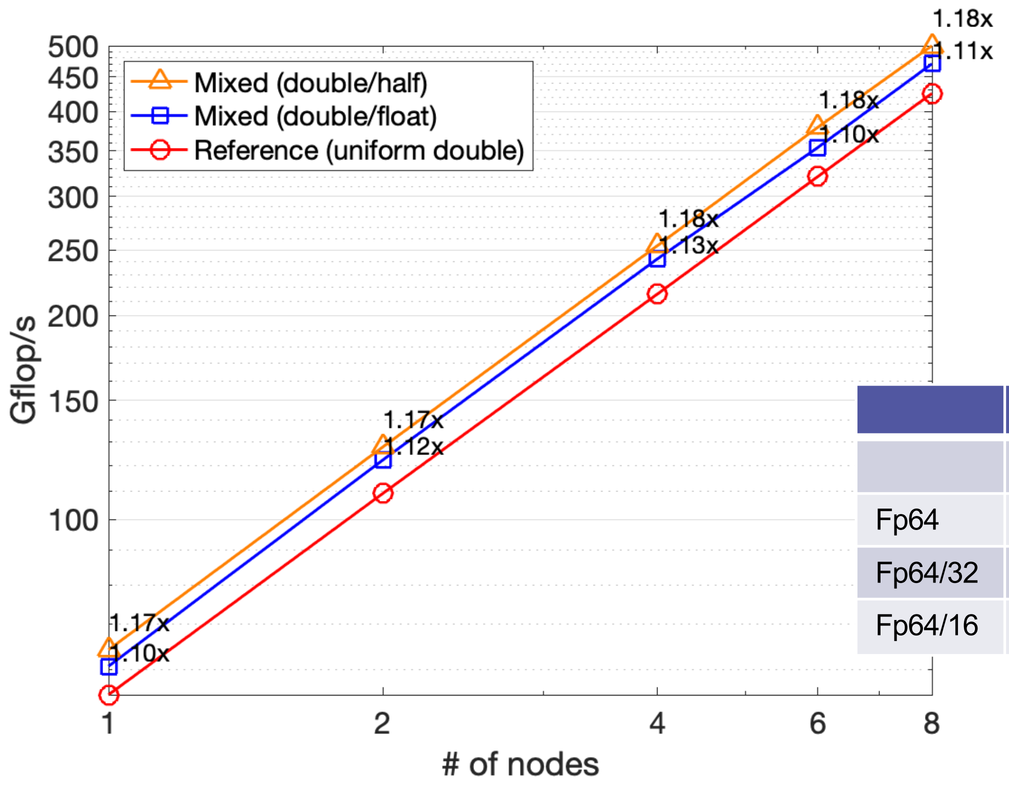
Special thanks to Kokkos-Kernels team, Brian Kelley, Evan Harvey, and Vinh Dang

## Performance (time / iteration) using FP16 on Perlmutter (Six NVIDIA A100 GPUs / node)

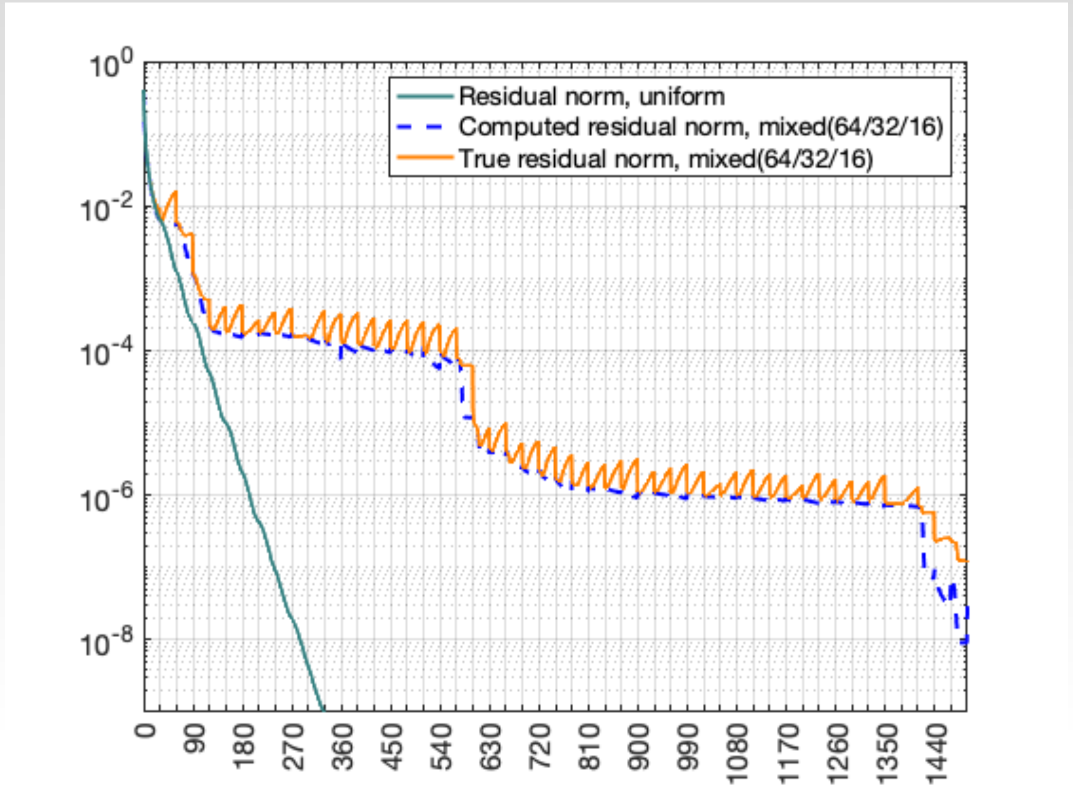


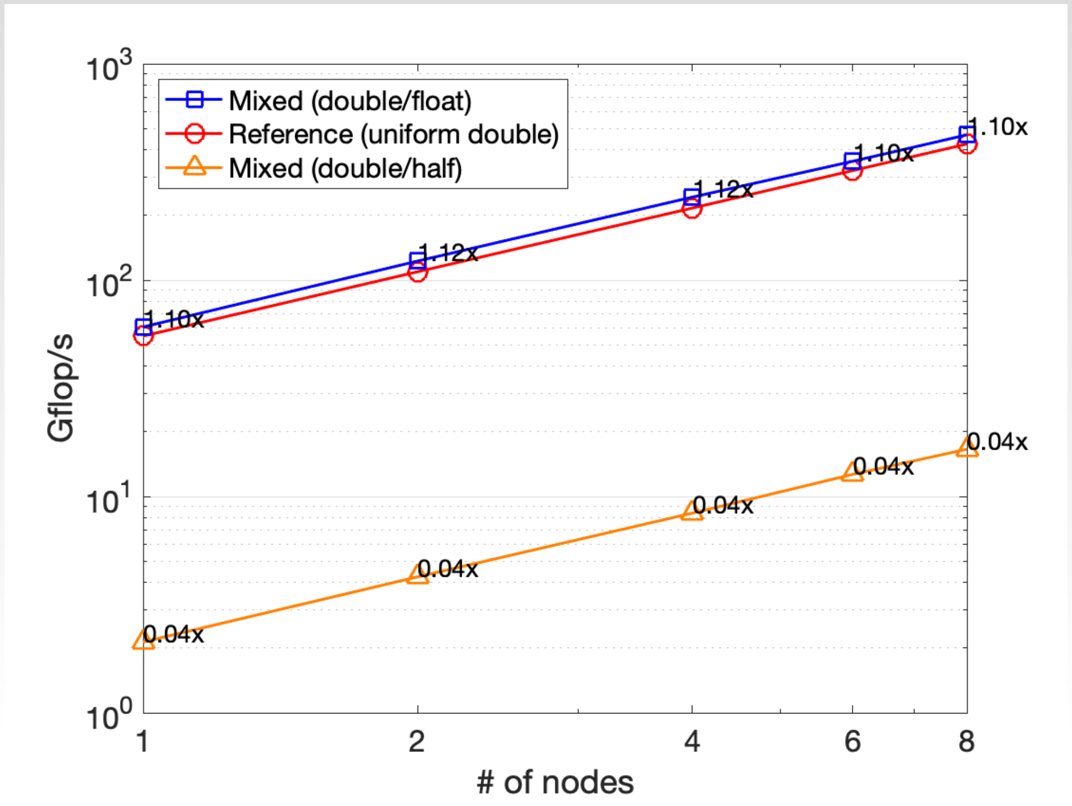
- using FP16 did help reducing the iteration time
  - Performance & speedup dominated by GMG
  - We used clustered GS from Kokkos-Kernels

| | 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)

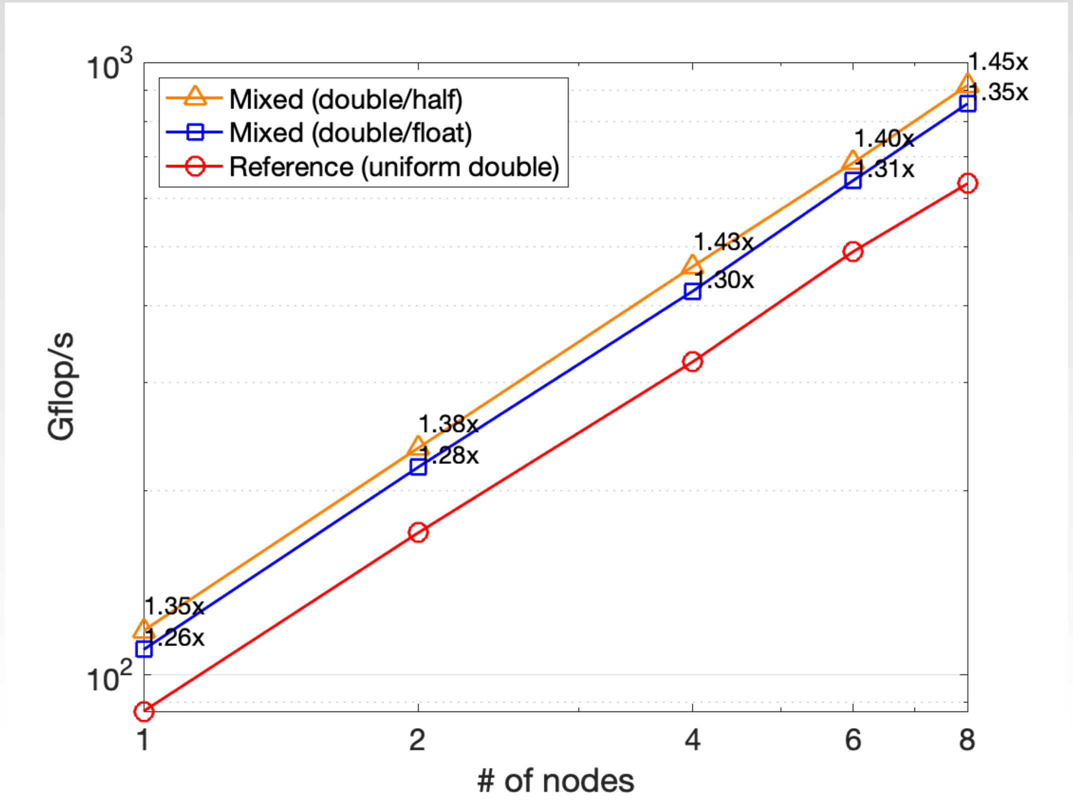
## Performance (time / iteration) using FP16 on Perlmutter (Four NVIDIA A100 GPUs / node)

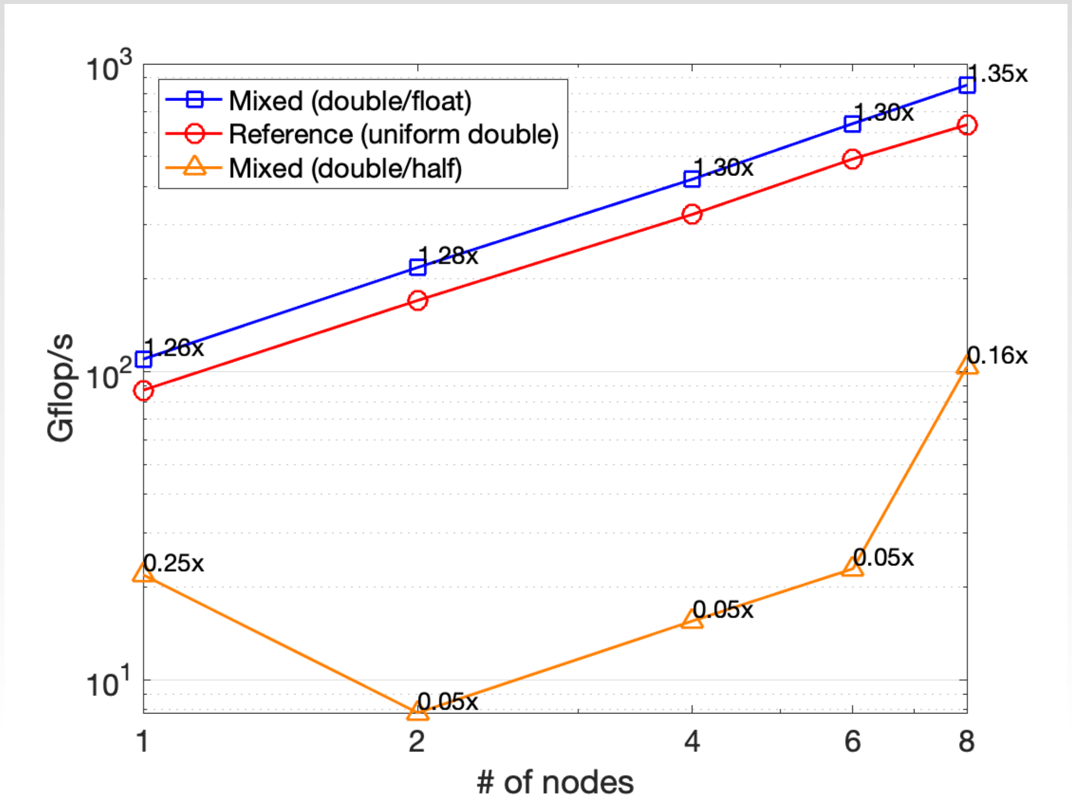




- Number of iterations increased using FP16
  - Bad from solver point (longer time to solution)
  - Good from benchmark point (captured and penalized benchmark results)

## Performance (time / iteration) using FP16 on Crusher (Six AMD MI250X GCDs / node)





- Number of iterations increased using FP16
  - Bad from solver point (longer time to solution)
  - Good from benchmark point (captured and penalized benchmark results)

## Final remarks

- Developing a new benchmarks
  - Captures the performance of applications
  - Allows the use of mixed lower precision arithmetic
  - Please see our SC'22 workshop paper
- Reference implementation is publicly available
  - Working with Kokkos-Kernels backend as "optimized" version, for numerical & performance tests with more mixed-precision
    - Optimizing Kernel performance, with FP16
    - Improving stability (following/breaking current specifications)
  - Running on current top-ranked HP computers, at larger-scale, and beyond
  - Comparing with application performance
  - etc.

Open for feedbacks & collaborations !!

EXASCALE COMPUTING PROJECT

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