

## FP16 Acceleration in Structured Multigrid Preconditioner for Real-World Applications

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#### Background: Low-Precision Computation

- Half-precision hardware support is now almost ubiquitous.
- We have been witnessing a trend towards lower precision in ML & AI.
- But NOT so prevalent in scientific computation



#### Background: Low Precision + Linear Solver

- Many scientific simulations rely on numerical solutions to PDE problems
- Essential part: linear solver of Ax = b
- Stricter accuracy requirement than AI
- More sensitive to precision



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![](_page_3_Figure_5.jpeg)

### Background: Low Precision + Multigrid

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![](_page_4_Figure_5.jpeg)

### Background: Why multigrid (MG) ?

- Optimal computational complexity O(N) in solving large-scale sparse linear systems.
- Widely used in scientific researches, and industrial software, ...
- Variable smoothers can cover many other "one-level" preconditioners.
  - Jacobi
  - □ Gauss-Seidel (GS)
  - □ Incomplete Lower-Upper (ILU)
  - .....
- **Theoretical foundation**: tolerance of errors introduced by lower-precision <sup>[1]</sup>.
- **Practical benefits**: greater lower-precision speedups than "one-level" preconditioners.
  - A larger proportion of time in workflows

![](_page_5_Figure_11.jpeg)

#### Figure 2: Multigrid overview. V-Cycle is in the solve phase.

![](_page_6_Picture_0.jpeg)

Exponent: 5 bits

Significand: 10 bits

FP16: narrow range & limited accuracy

#### Real world: Large spans, wide gaps, multi scales of values

![](_page_6_Figure_5.jpeg)

## Multigrid: Multi levels, complicated procedures, variable components

![](_page_6_Figure_7.jpeg)

#### Related work: Mix-precision in Multigrid

- **Popular AMG libraries (***hypre***, MueLu, AmgX) lack mix-precision support.**
- Practice ahead of theory for a long time
  - **Most of them use only FP32** as the lowest precision in MG preconditioner. They are safe and efficient with similar #iters of mix-FP32/FP64 to those of full-FP64
  - Utilizing half-precision is scarce. Ginkgo <sup>[6]</sup> is a recent three-precision MG, supporting arbitrary precisions (FP64, FP32, FP16) for matrices and vectors on different levels.
  - Lack of guidelines in how to choose the best configurations. Too many changeable options may overwhelm users.

Ref	Туре	Scaling?	Precond. Precision	Precond. Speedup	E2E Speedup
[1]	GMG	No	FP32	~2.0x	~1.7x
[2]	AMG	No	FP32	1.1x~1.5x	Unclear
[3]	AMG	No	FP32	Unclear	1.19x
[4]	GMG	No	FP32	1.9x	1.6x
[5]	GMG	No	FP32	2.0x	1.18x
[6]	AMG	Yes	FP16, FP32	Unclear	1.05x~1.35x
Ours	AMG	Yes	FP16, FP32	2.7x	1.9x

[1] <u>https://doi.org/10.1109/TPDS.2010.61</u>
[2] https://doi.org/10.1016/j.procs.2010.04.020

[3] https://doi.org/10.1049/cp.2014.0185

[4] <u>https://doi.org/10.1007/978-3-642-33134-3\_68</u>
[5] <u>https://doi.org/10.1016/j.procs.2016.05.502</u>
[6] https://doi.org/10.1016/j.future.2023.07.024

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### Related work: Mix-precision in Multigrid

#### • In our work:

Gains and risks of FP16 Worthwhile combinations

![](_page_8_Picture_3.jpeg)

Guidelines

How to adapt setup and solve phases to FP16

![](_page_8_Picture_6.jpeg)

Algorithms

#### How to avoid precision conversion overhead

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Implementations

#### FP16 Utilization Guidelines

- MG's time:  $T_{tot} = T_{setup} + #iter \cdot T_{single}$ 
  - $T_{\text{setup}}$  is setup time,  $T_{\text{single}}$  is single-iteration time, #iter is number of iterations.
  - $\Box$  T<sub>setup</sub> is only slightly affected by mix-precision.
- Lower-precision reduces  $T_{single}$ , but may increase #iter.
- Rule: **balance** between **performance**  $(T_{\text{single}} \downarrow)$  and **convergence** (#iter  $\uparrow$ )

![](_page_9_Picture_6.jpeg)

#### Guideline 1: Eagerly convert matrices to FP16

- Matrix A is the hotspot of storage.
- The percent of matrix A in storage in Ax = b: memory(A) $percent_A = \frac{(A)}{(A)} + 2$

 $\operatorname{memory}(A) + 2 * \operatorname{memory}(x)$ 

- Statistics of matrices indicate **large percent**<sub>A</sub>.
- The observation strengthens in MG's multi-level context as the coarser matrices are usually denser <sup>[1]</sup>.
- Reducing the lower bounds of memory volumes of matrices by FP16 is the top-priority task.

![](_page_10_Figure_7.jpeg)

![](_page_10_Figure_8.jpeg)

#### Guideline 2: Use FP16 from the finest possible level

- Matrices and vectors may have different precisions on different levels.
- 9<sup>n</sup> possible combinations for a *n*-level MG ? Only limited choices are worthwhile !
- MG's features: grid complexity  $C_{\rm G}$  and operator complexity  $C_{\rm O}$

$$C_{\rm G} = \frac{\sum_l m_l}{m_0}$$

![](_page_11_Figure_5.jpeg)

#### Low complexities are common.

- $\Box$  *C*<sub>G</sub> < 1.20, *C*<sub>O</sub> < 1.50 in 80% cases
- $\Box$  C<sub>G</sub> < 1.15, C<sub>O</sub> < 1.22 in 60% cases
- $C_G < 1.15, C_O < 1.22$  in 60% cases Most overheads on the finest level.  $\frac{1000}{100} = 0.06$
- **Common "mistake": use lower** precision on coarser levels.

![](_page_11_Figure_11.jpeg)

#### Guideline 3: Avoid using FP16 for vectors

- The matrix *A* is static throughout the solving. 1.E+07
- The vectors are changing dynamically.
- Difficult to predict which element may overflow or underflow sometime.

![](_page_12_Figure_4.jpeg)

• Safe to keep the precision of vectors  $\geq$  FP32, with **limited performance impact** 

• Recalling Guideline 1 that matrix is the hotspot.

# Guideline 4: Prefer structured matrix formats that do not use per-element index arrays.

- Integers in large matrices are difficult to compress.
  - □ necessary in unstructured formats, such as CSR, CSC, COO
- Index-free format (e.g., SG-DIA<sup>[1]</sup>) without integer arrays are more preferred.
  - □ Can be used in **structured- and semi-structured-specific MGs**, such as SMG, PFMG, SysPFMG, SSAMG from *hypre* (LLNL), RegionMG from *Trilinos* (SNL), and our StructMG, Semi-StructMG, ...
- Upper bound of speedup can be estimated based on minimal memory access volume.

Formet	Byt	tes per Nonz	zero	Upper Bound of Speedup		
Format	FP64	FP32	FP16	FP32/FP16	FP64/FP16	
SG-DIA	8	4	2	$\frac{4}{2} = 2$	4	
CSR (int32)	$12 + 4\delta$	$8 + 4\delta$	6 + 4δ	$\frac{8+4\delta}{6+4\delta} < 1.3$	< 2	
CSR (int64)	$16 + 8\delta$	$12 + 8\delta$	$10 + 8\delta$	$\frac{12+8\delta}{10+8\delta} < 1.2$	< 1.6	

[1] https://doi.org/10.1137/120883153

 $\delta = (\text{#row} + 1)/\text{#nnz}$ .  $\delta = 15\%$  in average of 2216 matrices in SuiteSparse.

### Guidelines => Algorithms

- The above four guidelines instruct the following **algorithmic designs.** 
  - Vectors should be kept in FP32.
  - □ FP16 should compress the memory volumes of matrices as fine-level as possible.
  - Structured or semi-structured grids should have higher priority to discretize the PDE of interest.

#### Algorithms notations

• Variables in different colors are in different precisions:

**iterative precision** usually as **FP64** or **FP32**, is the computation and storage precision of iterative solvers, **determined by users' applications** 

computation precision of preconditioners usually as FP32

storage precision of preconditioners usually as FP16

#### Setup Algorithm: Setup-then-scale

## **?** Idea: prevent FP16 from interfering with multi-level effect

- Essential role: triple matrix products (RAP) that build connections in the hierarchy
- A normal setup is completed first in high precision, followed by scaling (if needed) and truncation.
- *A<sub>i</sub>* and *Q<sub>i</sub>* in high precision are no longer needed after the setup.
  - Limited additional memory overhead.

**Algorithm 1:** MG\_setup\_for\_FP16 **Input:** matrix A **Output:** matrices  $A_0, A_1, ..., A_L$  on hierarchical grids and smoothers  $S_0, S_1, ..., S_L$ , and  $Q_0, Q_1, ..., Q_L$  if needed 1 for  $i = 0, 1, \dots, L - 1$  do  $A_{i+1} \leftarrow R_i A_i P_{i+1}$  // Galerkin coarsening 3 end 4 for i = 0, 1, ..., L do if need to scale then // truncation after scaling 5  $Q_i \leftarrow \frac{1}{G_i}$  extract\_diagonals( $\underline{A_i}$ ); 6  $A_i \leftarrow Q_i^{-1/2} A_i Q_i^{-1/2};$ 7  $A_i \leftarrow A_i;$ 8  $Q_i \leftarrow Q_i;$ 9 else // direct truncation 10  $A_i \leftarrow A_i$ 11 end 12  $S_i \leftarrow \text{smoother\_setup}(A_i);$ // setup smoothers 13 17 14 end

#### Solve Algorithm: Recover-and-rescale on the fly

- Solve phase consists of the iterative solver and the MG preconditioner.
- Everything is normal about iterative solvers.
  - Researches of mix-precision iterative solvers are orthogonal to this study.

- A stationary iterative solver illustrates how an FP16-accelerated preconditioner is employed.
  - Other solvers (CG, GMRES, etc.) are similar.

Algorithm 2: Stationary iterative method.

**Input:** matrix  $\underline{A}$ , right-hand-side  $\underline{b}$ , initial solution  $\underline{x}$ **Output:** approximated solution  $\underline{x}$ 

- 1 Initialize preconditioner: MG\_setup\_for\_FP16(<u>A</u>);
- 2 while not converged do

### Solve Algorithm: Recover-and-rescale on the fly

## **?** Idea : FP16 in storage of matrices (hotspots) to reduce memory access volumes

• Nothing in iterative precision inside the MG.

- □ Matrices are stored in FP16 and need restoration.
- □ Vectors' precision is unchanged, usually as FP32.
- If  $A_i$  was scaled, it must be recovered and rescaled
  - □ **Recover:**  $A_i \rightarrow A_i$  (precision promotion)
  - □ **Rescale:**  $A_i \rightarrow Q_i^{1/2} A_i Q_i^{1/2}$  (to original values)
- **On-the-fly:**  $A_i$  in FP32 are **NOT** explicitly maintained<sup>20</sup>

Algorithm 3: MG\_solve\_with\_FP16

```
Input: right-hand-size b
    Output: approximated solution x
 1 Initialize: f_0 \leftarrow b;
 <sup>2</sup> for i = 0, 1, ..., L - 1 do // forward part of V-Cycle
         for j = 0, 1, ..., v_1 - 1 do // pre-smoothing v_1 times
 3
             u_i \leftarrow \text{smoother\_solve}(S_i, f_i, u_i);
         end
 5
         if scaled in setup then // compute residual
 6
             \underline{r_i} \leftarrow \underline{f_i} - \underline{Q_i}^{1/2} \underbrace{A_i} \underline{Q_i}^{1/2} \underline{u_i};
 7
         else
 8
          r_i \leftarrow f_i - A_i u_i;
 9
         end
10
         if i < L - 1 then // restrict residual to next level
11
              f_{i+1} \leftarrow \text{Restrict}(r_i);
12
         end
13
14 end
15 for i = L − 1, ..., 1, 0 do // backward parf of V-Cycle
         for j = 0, 1, ..., v_2 - 1 do // post-smoothing v_2 times
16
             u_i \leftarrow \text{smoother\_solve}(S_i^T, f_i, u_i);
17
         end
18
         if i > 0 then // interpolate error to next finer grid
19
              u_{i-1} \leftarrow u_{i-1} + \text{Interpolate}(u_i);
20
         end
22 end
                                                                      19
\underline{x} \leftarrow \underline{u_0};
```

#### Practical Remarks

## Additional overhead of *Q<sub>i</sub>*? Why not scale-then-setup ?

- Setup-then-scale has two fold advantages over scale-then-setup.
  - Scaling inside MG without users' involvement
  - Scale-then-setup performs triple matrix products (RAP) in FP16 range even if with FP64 precision.
- In practice, *Q<sub>i</sub>* is cost-efficient compared to more #iter.

![](_page_19_Figure_6.jpeg)

#### Kernel: SIMD to amortize fcvt overhead

- **Mix-precision kernel** introduces additional **overhead of precision conversion (fcvt)**.
- Based on structured-specific MGs that use AOS (array of structure) format. Nonzero entries within a row are stored contiguously.

AOS (in FP16)

![](_page_20_Figure_5.jpeg)

- AOS is good enough for full-FP32
  - Only one ldr instruction for each 4-byte entry to prepare for multiplication.
- For matrices in FP16, data preparation has 4-times-high arithmetic intensity
  - One ldr, one fcvt for each 2-byte entry

![](_page_20_Picture_10.jpeg)

#### Kernel: SIMD to amortize fcvt overhead

- Transforming from AOS to SOA enables vectorization
- Floating-point conversion overhead is amortized.
- Only one ldr, and two fcvt for every eight 2-byte entries when SIMD length is 128-bit.
   AOS (in FP16)

![](_page_21_Figure_4.jpeg)

#### Experiments

#### Problems

- Covering scalar- and vector-type PDE, different and complex numerical features
- □ 3 benchmark problems: laplace27, laplace27\*10<sup>8</sup>, solid-3D
- □ 5 real-world problems: rhd, rhd-3D, oil, oil-4C, weather

Problem	Туре	Domains
laplace27	Scalar -type PDE	Benchmark problem in HPCG
laplace27*10 <sup>8</sup>		Coefficients of laplace27 multiplied by 10 <sup>8</sup>
Rhd		Radiation hydrodynamics
Oil		Petroleum reservoir simulation. SPE1 and SPE10 benchmarks are combined via OpenCAEPoro.
Weather		Atmospheric dynamics, from GRAPES-MESO of 2-km resolution of Chinese region in Dec 2018
rhd-3T	Vector	Radiation hydrodynamics. 3T: three temperatures (radiation, electron, and ion).
oil-4C	-type	Petroleum reservoir simulation. 4C: four components (oil, water, gas, and dissolved gas in oil).
solid-3D	PDE	Linear elasticity in solid mechanics. 3D: three displacements associated with each element

![](_page_23_Figure_0.jpeg)

![](_page_23_Figure_1.jpeg)

Numerical distributions of nonzero entries.

Problem	Real- world ?	Out-of- FP16 ?	Distance	Anisotropy	Cond. Number	Precision	Solver	C <sub>G</sub>	<b>C</b> <sub>0</sub>
laplace27	No	No	Within	None	3e+03	FP64/FP32/FP16	CG	1.14	1.14
laplace27*10 <sup>8</sup>	No	Yes	Far	None	3e+03	FP64/FP32/FP16	CG	1.14	1.14
rhd	Yes	Yes	Far	Low	1e+08	FP64/FP32/FP16	CG	1.14	1.14
oil	Yes	No	Within	High	1e+04	FP64/FP32/FP16	GMRES	1.14	1.14
weather	Yes	Yes	Near	High	1e+05	FP32/FP32/FP16	GMRES	1.31	1.44
rhd-3T	Yes	Yes	Far	High	1e+15	FP64/FP32/FP16	CG	1.14	1.14
oil-4C	Yes	Yes	Near	High	1e+05	FP64/FP32/FP16	GMRES	1.14	1.14
solid-3D	No	Yes	Far	Low	1e+07	FP64/FP32/FP16	CG	1.14	1.26

#### Experiments

- Solvers
  - Users' applications determine the **iterative precisions**.
  - StructMG<sup>[1]</sup> is used. Other structured-specific MGs can also be used, such as *hypre*'s SMG, PFMG, SysPFMG, SSAMG, ...
  - **Only one V-cycle is applied, with one pre- and post-smoothing.**

- Machinaa	System	ARM	X86	
Ivrachines	Processor	Kunpeng 920-6426	AMD EPYC-7H12	
$\square$ ARM and X86 platforms	Frequency	2.60 GHz	2.60~3.30 GHz	
	Cores per node	128 (64 per socket)	128 (64 per socket)	
Results are similar on two platforms.	L1/L2/L3 per core	64 KB/512 KB/1 MB	32 KB/512 KB/4 MB	
ADM '41 NEON OC '41 AVXO	Stream Triad BW	138 GB/s	100 GB/s	
• ARM with NEON, $x86$ with $AVX2$	Memory per Node	512 GB DDR4-2933	256 GB DDR4-3200	
Best results among various	Max Nodes	64	64	
Dest results among various	Network	100Gbps InfiniBand	100Gbps InfiniBand	
MPI/OpenMP ratios reported.	MPI/Compiler	OpenMPI-4.1.4/gcc-9.3.0	Intel-OneAPI-2021.6	

#### Results & Analysis

• The results will be presented in a **local-to-global perspective**.

Local

Global

A controlled variables experiment to verify algorithmic effect.

Kernel performance to demonstrate amortizing FP conversion overhead Overall speedups in a single processor Scalability tests

#### Results & Analysis: Algorithmic Effect

- Descending curves of residual norms in a controlled variable comparison.
- 5 problems feature distinct numerical ranges and distributions.
- Idealized problems cannot distinguish candidates.
- FP16 delays convergence in complicated problems.
- Setup-then-scale is better than scale-thensetup in complicated problems.

![](_page_26_Figure_6.jpeg)

## Results & Analysis: Kernel Optimization Effect

- Two essential kernels: SpTRSV and SpMV
- Baselines: 'MG-fp32/fp32'
  - □ full-FP32 kernels of AOS format, **without** fcvt
  - $\square$  ~3.5x and ~1.8x faster than ARMPL on ARM
  - $\sim$  ~2.2x and ~1.2x faster than MKL on x86
- **Max-fp16/fp32':** maximum speedups in theory
- 'MG-fp16/fp32(naive)': straightforward extensions of baselines
  - severe bandwidth efficiency degradation
- 'MG-fp16/fp32(opt)': SOA format with SIMD
  - time reduction proportional to memory volume reduction
  - very close to the theoretical upper bounds

![](_page_27_Figure_12.jpeg)

#### Results & Analysis: End-to-end Improvement

- Setup-then-scale introduces limited setup overhead.
- Speedups are case-dependent.
  - **3.70x** in laplace27: close to the upper-bound (4.0x).
  - The additional  $Q_i$  reduce speedups.
  - □ Vector-type PDEs are more favored by FP16.
  - Increases of #iter in rhd, rhd-3T, weather slow down speeds.
- Speedups are 2.4x, 2.2x, 1.7x, 1.7x, 1.9x, 1.8x,
   2.3x, 2.4x per iteration for eight problems.

![](_page_28_Figure_8.jpeg)

#### Results & Analysis: Scalability Test

#### Mix-precision weakens scalability

- □ FP16 in storage: computation time  $\downarrow$ , comm. proportion  $\uparrow$ .
- □ In most cases, leveraging FP16 acceleration at the cost of scalability is **still worthwhile**.
- Parallel efficiencies reach 96%, 89%, 63%, 99%, 98%, 71%, 93%, 62% of the full-iterative-precision to counterpart.
- Nearly perfect scalability in medium and large sizes.
  - Given enough workloads per core, speedups are as expected based on reduction of memory volumes.
- Degraded scalability in small sizes.
  - □ E.g., rhd, rhd-3T, solid-3D
  - **SIMD underutilization** when too few workloads per core.

![](_page_29_Figure_10.jpeg)

#### Discussion (skipped, see the article)

- **1.** More numbers of times of V-cycle or smoothing, more significant speedups.
- 2. BF16 may probably be less suitable than FP16 for linear solvers.
- **3.** Transformation from AOS to SOA extends to GPU.
- 4. A simple rollback is effective when underflow is severe.

#### Conclusion

- Average 2.7x speedups in MG preconditioner and 1.9x in E2E workflow of 8 problems.
- All is about **balance** between **performance**  $(T_{\text{single}} \downarrow)$  and **convergence** (#iter  $\uparrow$ ).
  - □ Performance: FP16 in matrices' storage, and recover-and-rescale on the fly
  - Convergence: setup-then-scale avoids damaging multi-level quality
- Guidelines, algorithms, and implementations form the balance together.
  - Guidelines and algorithms also apply to unstructured multigrids with CSR format.
  - Kernel implementations can be ported to *hypre*'s (semi-)structured-specific multigrids, such as SMG, PFMG, SysPFMG, SSAMG, ...

![](_page_32_Picture_0.jpeg)

### Thanks for your listening! Q&A