High Performance Mixed Precision Numerical Linear Algebra

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Charles University

SimRace 2021, IPFEN
December 3, 2021

We acknowledge funding from Charles Univ. PRIMUS project No. PRIMUS/19/SCI/11, Charles Univ. Research Program No. UNCE/SCI/023, and the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Admin.
Floating Point Formats

\[ (-1)^{\text{sign}} \times 2^{(\text{exponent} - \text{offset})} \times 1.\text{fraction} \]

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Use of low precision in machine learning has driven emergence of low-precision capabilities in hardware:

- **AMD Radeon Instinct MI25 GPU**, 2017:
  - single: 12.3 TFLOPS, half: 24.6 TFLOPS
- **NVIDIA Tesla P100**, 2016: native ISA support for 16-bit FP arithmetic
- **NVIDIA Tesla V100**, 2017: tensor cores for half precision;
  - 4x4 matrix multiply in one clock cycle
  - double: 7 TFLOPS, half+tensor: 112 TFLOPS (16x!)
- **NVIDIA A100**, 2020: tensor cores with multiple supported precisions: FP16, FP64, Binary, INT4, INT8, bfloat16
- **Intel AI processors** (Nervana, Xeon)
- **Google's Tensor processing unit** (TPU): as low as 8-bit arithmetic, bfloat16
- **Future exascale supercomputers**: (~2021) Expected extensive support for reduced-precision arithmetic (32/16/8-bit)
Performance of LU factorization on an NVIDIA V100 GPU

[Haidar, Tomov, Dongarra, Higham, 2018]
Mixed Precision Capabilities on Supercomputers

From TOP500:

June 2021

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<th>Accelerator/CP Family</th>
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<td>179,951,012</td>
<td>2,738,356</td>
</tr>
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<td>2.4</td>
<td>224,559,400</td>
<td>360,593,742</td>
<td>4,488,720</td>
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HPL-AI Benchmark

• Highlights confluence of HPC+AI workloads
  • Like HPL, solves dense $Ax=b$, results still to double precision accuracy
  • Achieves this via mixed-precision iterative refinement
    • may be implemented in a way that takes advantage of the current and upcoming devices for accelerating AI workloads
HPL-AI Benchmark

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• HPL-AI Results (June 2021):
  1. Fugaku: 2 EXAFLOP/s (vs. 442 PETAFLOP/s on HPL; 4.5x)
  2. Summit: 1.15 EXAFLOP/s (vs. 149 PETAFLOP/s on HPL; 7.7x)

• More information: https://icl.bitbucket.io/hpl-ai/
• Reference implementation: https://bitbucket.org/icl/hpl-ai/src/
Mixed precision in NLA

- **BLAS**: cuBLAS, MAGMA, [Agullo et al. 2009], [Abdelfattah et al., 2019], [Haidar et al., 2018]
- **Iterative refinement**:
  - Long history: [Wilkinson, 1963], [Moler, 1967], [Stewart, 1973], ...
  - More recently: [Langou et al., 2006], [C., Higham, 2017], [C., Higham, 2018], [C., Higham, Pranesh, 2020], [Amestoy et al., 2021]
- **Matrix factorizations**: [Haidar et al., 2017], [Haidar et al., 2018], [Haidar et al., 2020], [Abdelfattah et al., 2020]
- **Eigenvalue problems**: [Dongarra, 1982], [Dongarra, 1983], [Tisseur, 2001], [Davies et al., 2001], [Petschow et al., 2014], [Alvermann et al., 2019]
- **Sparse direct solvers**: [Buttari et al., 2008]
- **Orthogonalization**: [Yamazaki et al., 2015]
- **Multigrid**: [Tamstorf et al., 2020], [Richter et al., 2014], [Sumiyoshi et al., 2014], [Ljungkvist, Kronbichler, 2017, 2019]
- **(Preconditioned) Krylov subspace methods**: [Emans, van der Meer, 2012], [Yamagishi, Matsumura, 2016], [C., Gergelits, Yamazaki, 2021], [Clark, 2019], [Anzt et al., 2019], [Clark et al., 2010], [Gratton et al., 2020], [Arioli, Duff, 2009], [Hogg, Scott, 2010]

For survey and references, see [Abdelfattah et al., IJHPC, 2021]
Challenges of low precision

• Do error bounds still apply?
  • Error bound with constant $nu$ provides no information if $nu > 1$
  • One solution: probabilistic approach [Higham, Mary, 2019], [Higham, Mary, 2020]
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• Smaller range of representable numbers
  • Limited range of lower precision might cause overflow when rounding
  • Quantities rounded to lower precision may lose important numerical properties (e.g., positive definiteness)
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• Larger unit roundoff
  • Lose something small when storing: $fl(x) = x(1 + \delta), \ |\delta| \leq u$
  • Lose something small when computing: $fl(x \text{ op } y) = (x \text{ op } y)(1 + \delta), \ |\delta| \leq u$
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Does it matter?
Inexact computations

- In real computations we have many sources of inexactness
  - Imperfect data, measurement error
  - Modeling error, discretization error
  - Intentional approximation to improve performance
    - Reduced models, Low-rank representations, sparsification, randomization

Model Reduction

[Schilders, van der Vorst, Rommes, 2008]

Low-rank (hierarchical) approximation

\[ A \approx \]

Sparsification, Randomized algorithms

[Sinha, 2018]
Inexact computations

- In real computations we have many sources of inexactness
  - Imperfect data, measurement error
  - Modeling error, discretization error
  - Intentional approximation to improve performance
    - Reduced models, Low-rank representations, sparsification, randomization
- Given that we are already working with so much inexactness, does it matter if we use lower precision?
  - Analysis of accuracy in techniques that use intentional approximation almost always assume that roundoff error is small enough to be ignored
  - Is this true? Is it true even if we use low precision?
Example: Randomized Algorithms

- Given $m \times n \ A$, want truncated SVD with parameter $k$
Example: Randomized Algorithms

• Given $m \times n$ $A$, want truncated SVD with parameter $k$

\[ A \approx \hat{U} \hat{\Sigma} \hat{V}^T \]

• Randomized SVD:

\[ A = Q \Omega Y = QR = Q^T A = B = \hat{U} \hat{\Sigma} \hat{V}^T \]

Assuming exact arithmetic:
If $Q$ satisfies $\|A - QQ^T A\| \leq \varepsilon$, then $\|A - \hat{U} \hat{\Sigma} \hat{V}^T\| \leq \varepsilon$
Let’s try different types of \texttt{randsvd} matrices from the MATLAB gallery:

\[
A = \text{gallery('randsvd',[100,40],1e6,mode); k=15;}
\]

\[
[U,S,V] = \text{svd}(A) : \text{non-randomized SVD, exact arithmetic}
\]

\[
[\tilde{U},\tilde{S},\tilde{V}] = \text{rsvd}(A) : \text{randomized SVD, exact arithmetic}
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\[
[\tilde{U}_d,\tilde{S}_d,\tilde{V}_d] = \text{rsvd}(A) : \text{randomized SVD, double precision}
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[\tilde{U}_h,\tilde{S}_h,\tilde{V}_h] = \text{rsvd}(A) : \text{randomized SVD, half precision}
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What happens in finite precision?

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Mode 3: Geometrically distributed singular values

\[
\|A - USV^T\|_2 = 4.92e-03
\]

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\|A - \bar{U}\hat{S}\hat{V}^T\|_2 = 4.92e-03
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Mode 1: one large singular value

\[
\|A - USV^T\|_2 = 1.00e-06 \\
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Use of low precision leads to an order magnitude loss of accuracy! Roundoff error can’t be ignored!
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<td>|A - Q_h Q_h^T A|_2 = 3.59e-06</td>
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Error bound no longer holds!

Use of low precision leads to an order magnitude loss of accuracy! Roundoff error can’t be ignored!
Example: Low-Rank Approximation

- Block low-rank approximation and hierarchical matrix representations arise in a variety of applications.

- Work on mixed and low precision in block low-rank computations.

- [Higham, Mary, 2019]: Block low-rank LU factorization preconditioner that exploits numerically low-rank structure of the error for LU computed in low precision.

- [Higham, Mary, 2019]: Interplay of roundoff error and approximation error in solving block low-rank linear systems using LU.

- [Buttari, et al., 2020]: Block low-rank single precision coarse grid solves in multigrid.

- [Amestoy et al., 2021]: Mixed precision low rank approximation and application to block low-rank LU factorization.
Inverse multiquadratic kernel:

\[ A(i, j) = \frac{1}{\sqrt{1 + 0.1 \| x - y \|^2}}, \quad x, y \in \mathbb{R}^2 \]

A is SPD. Low-rank approximation of A should also be SPD!
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Exact arithmetic SVD:
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Exact arithmetic SVD:

\[
\begin{array}{ccc}
\times & \times & \times \\
\circ & \circ & \circ \\
\end{array}
\]

Half precision SVD:

\[
\begin{array}{ccc}
\times & \times & \times \\
\circ & \circ & \circ \\
\end{array}
\]

Positive definiteness lost!
Example: Iterative Methods

```matlab
A = diag(linspace(.001,1,100));
[V,~] = eig(A);
b = V'*ones(n,1);
```

![Conjugate Gradient in Finite Precision](chart.png)
Example: Iterative Methods

\[ n = 100, \lambda_1 = 10^{-3}, \lambda_n = 1 \]
\[ \lambda_i = \lambda_1 + \left( \frac{i-1}{n-1} \right) (\lambda_n - \lambda_1)(0.65)^{n-i}, \quad i = 2, \ldots, n - 1 \]

\[
[V, \sim] = \text{eig}(A); \\
b = V' \times \text{ones}(n, 1);
\]
Takeaway

• Low precision can have massive performance benefits but must be used with caution!

• Many opportunities for using mixed and low precision computation in scientific applications

• Need to develop a theoretical understanding of how mixed precision algorithms behave; need to revisit analyses of algorithms and techniques that ignore finite precision
Iterative Refinement for $Ax = b$

Iterative refinement: well-established method for improving an approximate solution to $Ax = b$

$A$ is $n \times n$ and nonsingular; $u$ is unit roundoff

Solve $Ax_0 = b$ by LU factorization (in precision $u_f$)

for $i = 0$: maxit

$r_i = b - Ax_i$ (in precision $u_r$)

Solve $Ad_i = r_i$ (in precision $u_s$)

$x_{i+1} = x_i + d_i$ (in precision $u$)
Iterative Refinement in 3 Precisions

- 3-precision iterative refinement [C. and Higham, 2018]

\[ u_f = \text{factorization precision}, \quad u = \text{working precision}, \quad u_r = \text{residual precision} \]

\[ u_f \geq u \geq u_r \]

\( u_s \) is the effective precision of the solve, with \( u \leq u_s \leq u_f \)

- For triangular solves with LU factors: \( u_s = u_f \)
- For GMRES preconditioned by LU factors, \( u_s = u \) [C. and Higham, 2017]

- New analysis generalizes existing types of IR:

<table>
<thead>
<tr>
<th>Traditional</th>
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</thead>
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<tr>
<td>Fixed precision</td>
<td>( u_f = u = u_r )</td>
</tr>
<tr>
<td>Lower precision factorization</td>
<td>( u_f^2 = u = u_r )</td>
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- Enables new types of IR: (half, single, double), (half, single, quad), (half, double, quad), etc.
Standard (LU-based) IR in three precisions \((u_s = u_f)\)

Half \(\approx 10^{-4}\), Single \(\approx 10^{-8}\), Double \(\approx 10^{-16}\), Quad \(\approx 10^{-34}\)

<table>
<thead>
<tr>
<th>(u_f)</th>
<th>(u)</th>
<th>(u_r)</th>
<th>(\max \kappa_{\infty}(A))</th>
<th>Backward error</th>
<th>Forward error</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(10^4)</td>
<td>(10^{-8})</td>
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Standard (LU-based) IR in three precisions ($u_s = u_f$)

Half $\approx 10^{-4}$, Single $\approx 10^{-8}$, Double $\approx 10^{-16}$, Quad $\approx 10^{-34}$

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### IR3: Summary

Standard (LU-based) IR in three precisions ($\bm{u}_s = \bm{u}_f$)

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$\Rightarrow$ Benefit of IR3 vs. "LP fact.": no $\text{cond}(A, x)$ term in forward error
### IR3: Summary

**Standard (LU-based) IR in three precisions ($u_s = u_f$)**

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$\Rightarrow$ Benefit of IR3 vs. traditional IR: As long as $\kappa_\infty(A) \leq 10^4$, can use lower precision factorization w/no loss of accuracy!
### GMRES-IR: Summary

GMRES-based IR in three precisions ($u_s = u$)

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⇒ With GMRES-IR, lower precision factorization will work for higher $\kappa_\infty(A)$
**GMRES-IR: Summary**

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$\kappa_\infty(A) \leq u^{-1/2} u_f^{-1}$

⇒ With GMRES-IR, lower precision factorization will work for higher $\kappa_\infty(A)$
GMRES-IR: Summary

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⇒ As long as \(\kappa_{\infty}(A) \leq 10^{12}\), can use half precision factorization and still obtain double precision accuracy!
GMRES-IR: Summary

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\[\kappa_\infty(A) \leq u^{-1/2} u_f^{-1}\]

⇒ As long as \(\kappa_\infty(A) \leq 10^{12}\), can use half precision factorization and still obtain double precision accuracy!

Recent work: 5-precision GMRES-IR [Amestoy, et al., 2021]
**GMRES-IR: Summary**

GMRES-based IR in three precisions \((u_s = u)\)

<table>
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<tr>
<th></th>
<th>(u_f)</th>
<th>(u)</th>
<th>(u_r)</th>
<th>(\max \kappa_\infty(A))</th>
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<th>Forward error</th>
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<td>comp</td>
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\[ \kappa_\infty(A) \leq u^{-1/2} u_f^{-1} \]

\[ \Rightarrow \text{As long as } \kappa_\infty(A) \leq 10^{12}, \text{ can use half precision factorization and still obtain double precision accuracy!} \]

Recent work: 5-precision GMRES-IR [Amestoy, et al., 2021]

\[ \kappa_\infty(A) \leq u^{-1/3} u_f^{-2/3} \]
Performance Results (MAGMA)

- [Haidar, Tomov, Dongarra, Higham, 2018]

(a) Matrix of type 3: positive $\lambda$ with clustered singular values, $\sigma_i=(1, \ldots, 1, \frac{1}{\text{cond}})$. 
Performance Results (MAGMA)

- [Haidar, Tomov, Dongarra, Higham, 2018]

(b) Matrix of type 4: clustered singular values, $\sigma_i=(1, \cdots, 1, \frac{1}{\text{cond}})$. 
The rise of multiprecision hardware

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• As numerical analysts, we must determine when and where we can exploit lower-precision hardware to improve performance
Thank you!

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