High Performance Mixed Precision Numerical Linear Algebra

Erin Carson

Charles University

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FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

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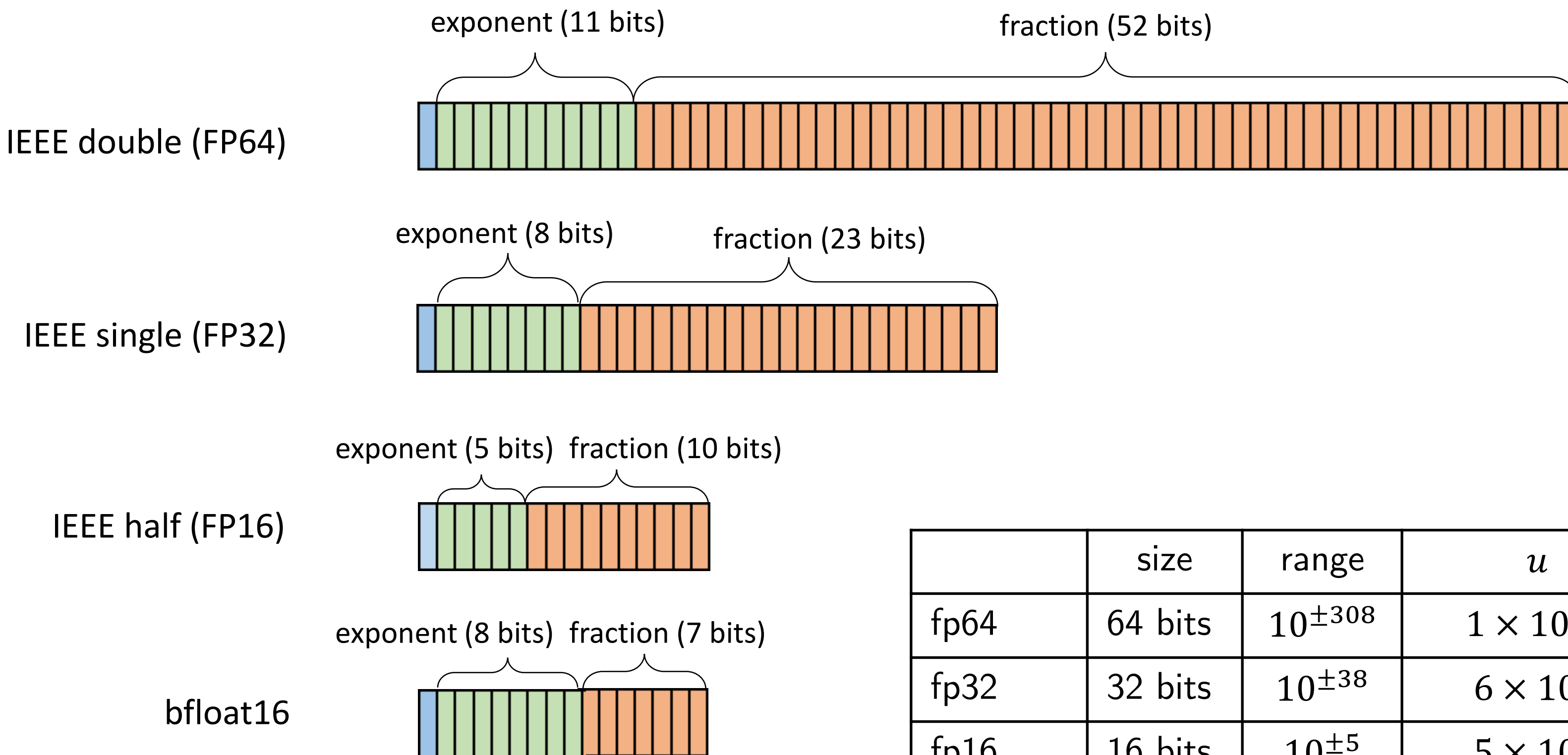
Floating Point Formats

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



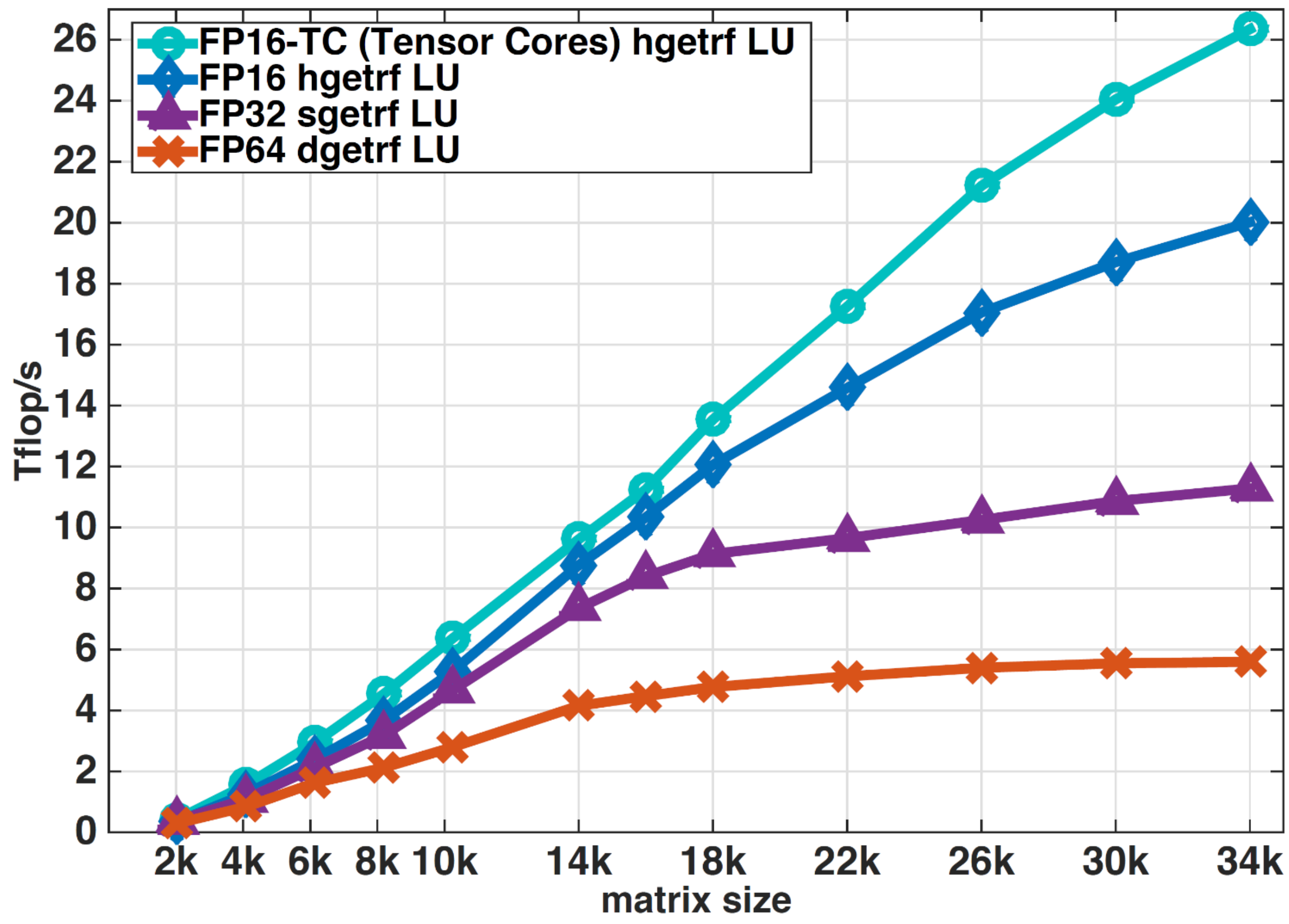
	size	range	u
fp64	64 bits	$10^{\pm 308}$	1×10^{-16}
fp32	32 bits	$10^{\pm 38}$	6×10^{-8}
fp16	16 bits	$10^{\pm 5}$	5×10^{-4}
bfloat16	16 bits	$10^{\pm 38}$	4×10^{-3}

Hardware Support for Multiprecision Computation

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

	Accelerator/CP Family	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
1	NVIDIA Volta	97	19.4	626,503,420	1,049,977,600	11,875,056
2	NVIDIA Ampere	26	5.2	351,252,600	505,841,268	3,435,116
3	NVIDIA Pascal	9	1.8	57,876,640	85,807,525	1,141,300

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1	NVIDIA Pascal	61	12.2	106,025,166	179,951,012	2,738,356
3	NVIDIA Volta	12	2.4	224,559,400	360,593,742	4,488,720

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

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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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  - 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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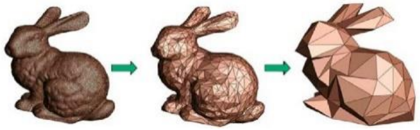
Does it matter?

Inexact computations

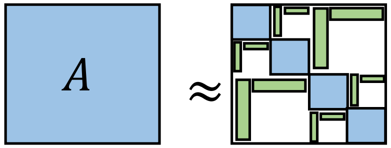
- In real computations we have many sources of inexactness
  - Imperfect data, measurement error
  - Modeling error, discretization error
  - Intentional approximation to improve performance
    - Reduced models, Low-rank representations, sparsification, randomization

Model Reduction

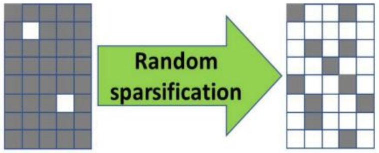


[Schilders, van der Vorst, Rommes, 2008]

Low-rank (hierarchical) approximation



Sparsification, Randomized algorithms



[Sinha, 2018]

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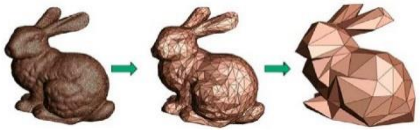

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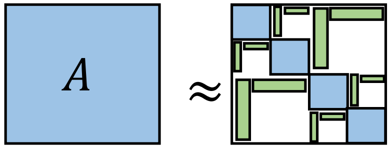

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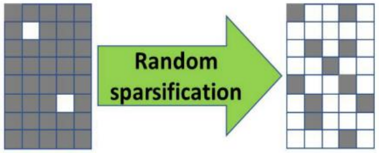
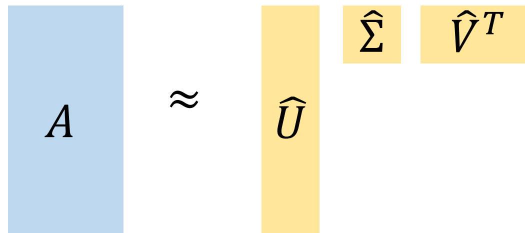


[Sinha, 2018]

- 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



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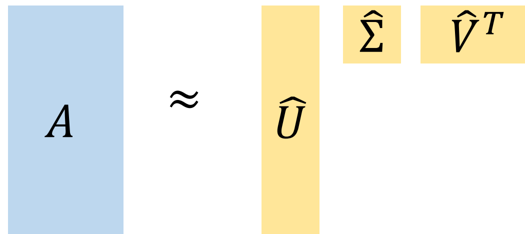
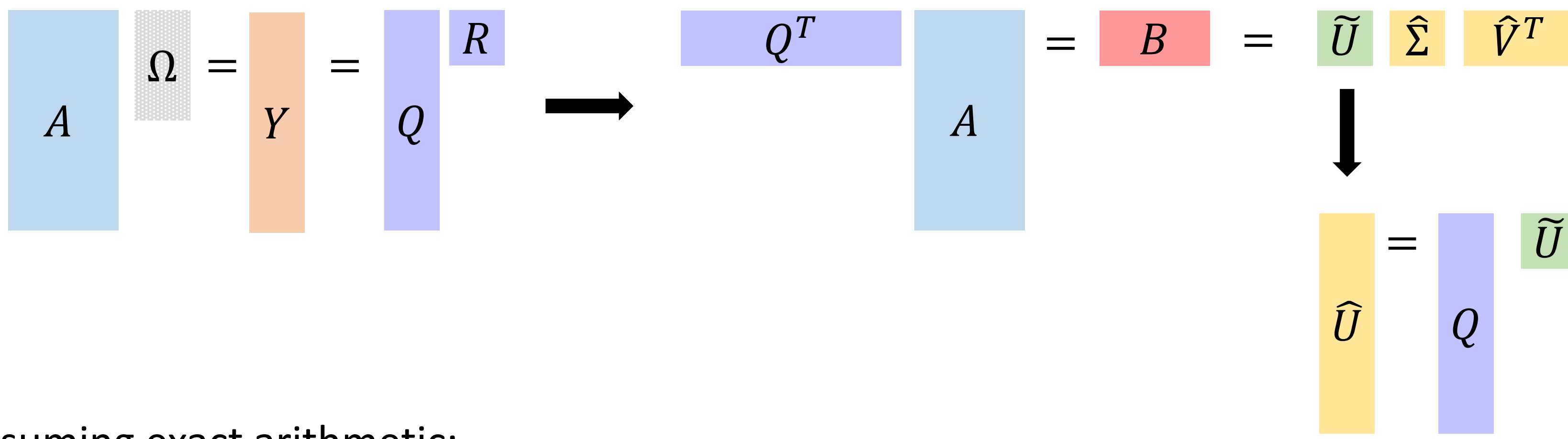


- Randomized SVD:



Assuming exact arithmetic:
If Q satisfies $\|A - QQ^T A\| \le \varepsilon$, then $\|A - \hat{U}\hat{\Sigma}\hat{V}^T\| \le \varepsilon$

What happens in finite precision?

Let's try different types of randsvd matrices from the MATLAB gallery:

```
A = gallery('randsvd',[100,40],1e6,mode); k=15;
```

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

$[\widehat{U}, \hat{S}, \widehat{V}] \quad = \mathrm{rsvd}(A)$: randomized SVD, exact arithmetic

$[\widehat{U}_d, \hat{S}_d, \widehat{V}_d] = \mathrm{rsvd}(A)$: randomized SVD, double precision

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Mode 3: Geometrically distributed singular values

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

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Mode 1: one large singular value

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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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Error bound no longer holds!

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$\|A - Q_h Q_h^T A\|_2$ = 3.59e-06

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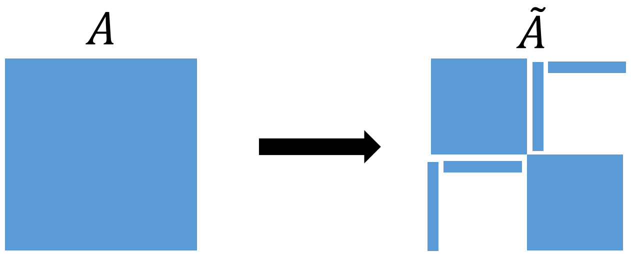
Example: Low-Rank Approximation

- 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

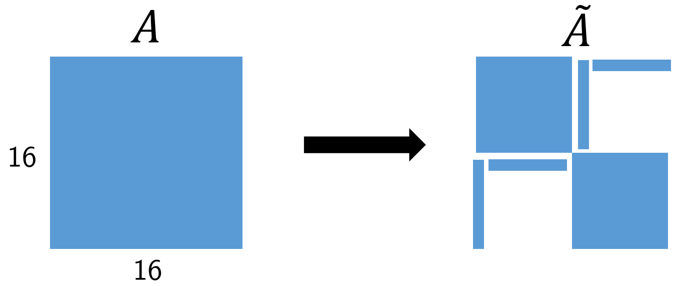
- [Higham, Mary, 2019]: block low-rank LU factorization preconditioner that exploits numerically low-rank structure of the error for LU computed in low precision
- [Higham, Mary, 2019]: Interplay of roundoff error and approximation error in solving block low-rank linear systems using LU
- [Buttari, et 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

Example: Low-Rank Approximation

Inverse multiquadratic kernel:

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

A is SPD. Low-rank approximation of A should also be SPD!



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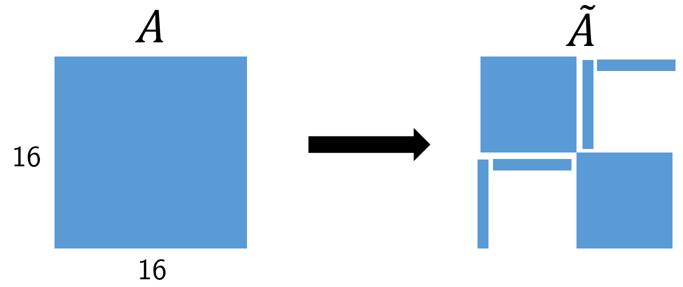
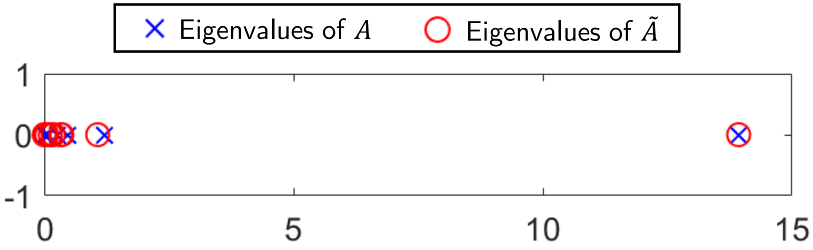


Exact arithmetic SVD:



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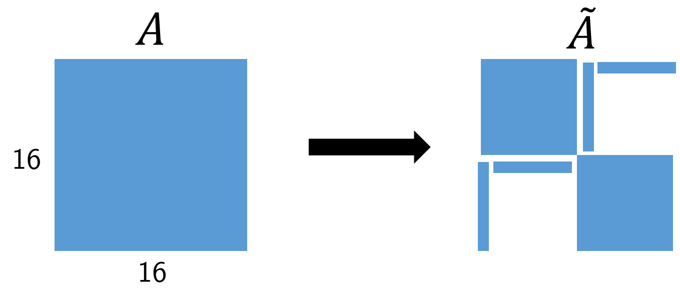

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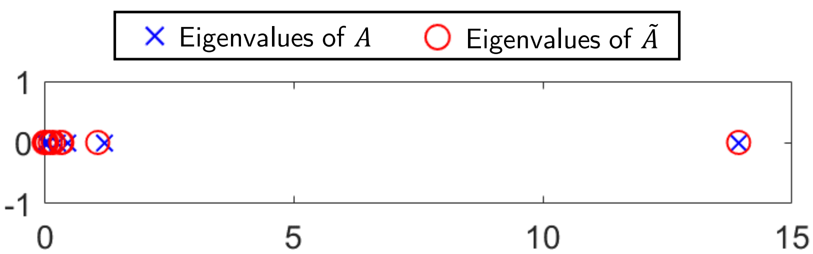

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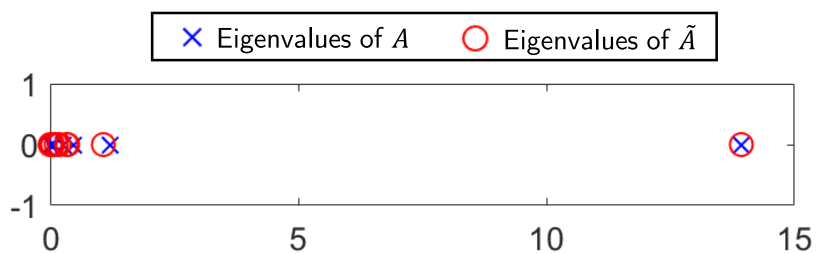

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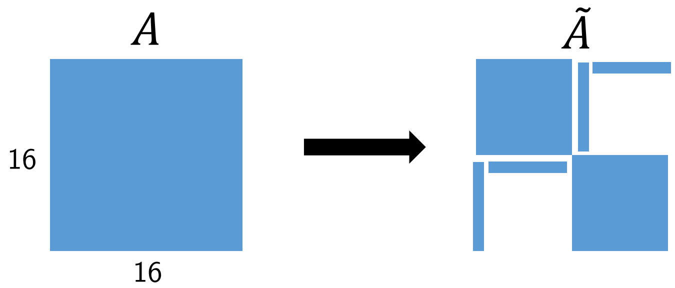

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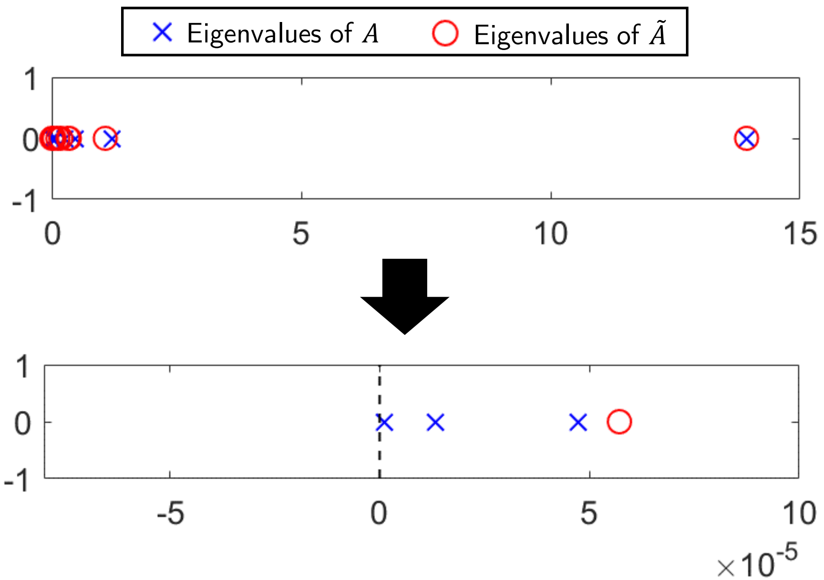

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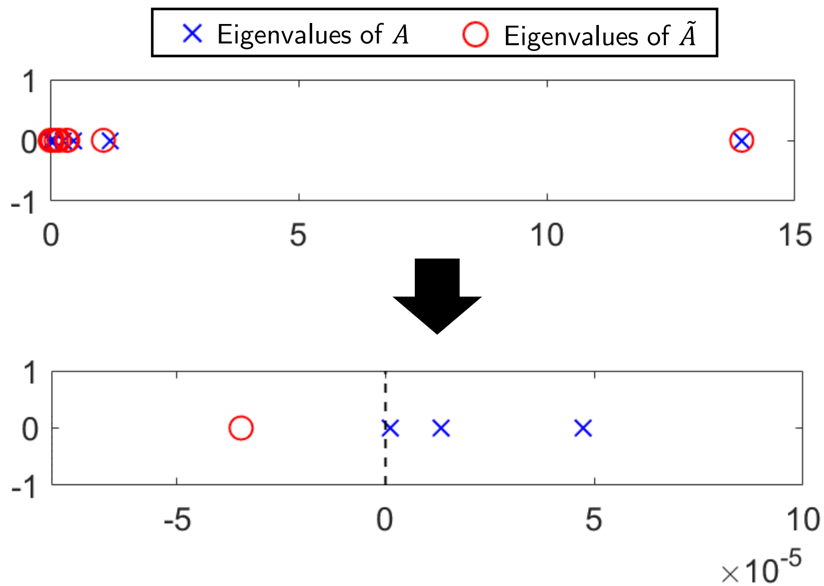

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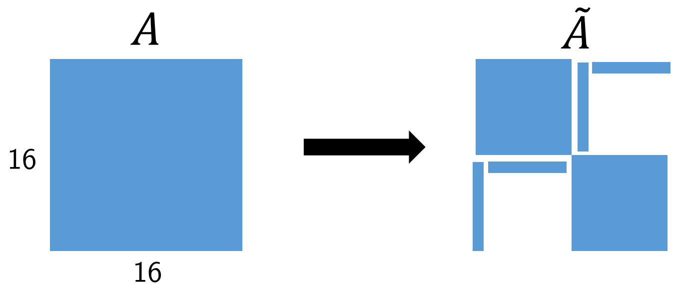

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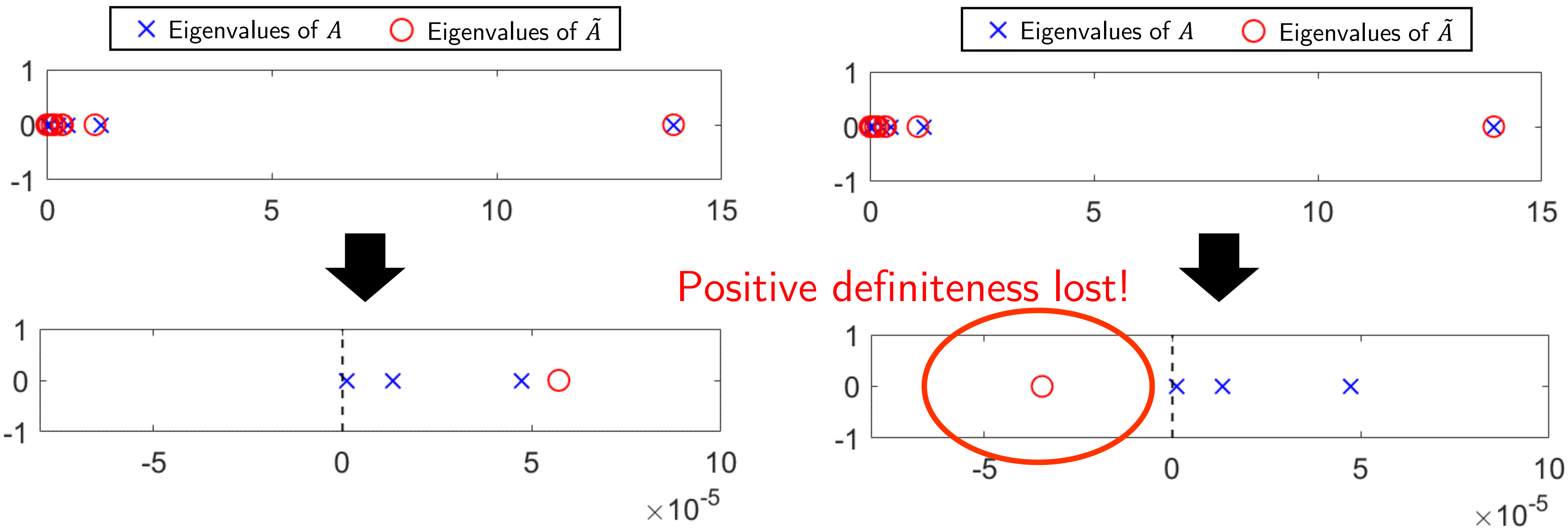
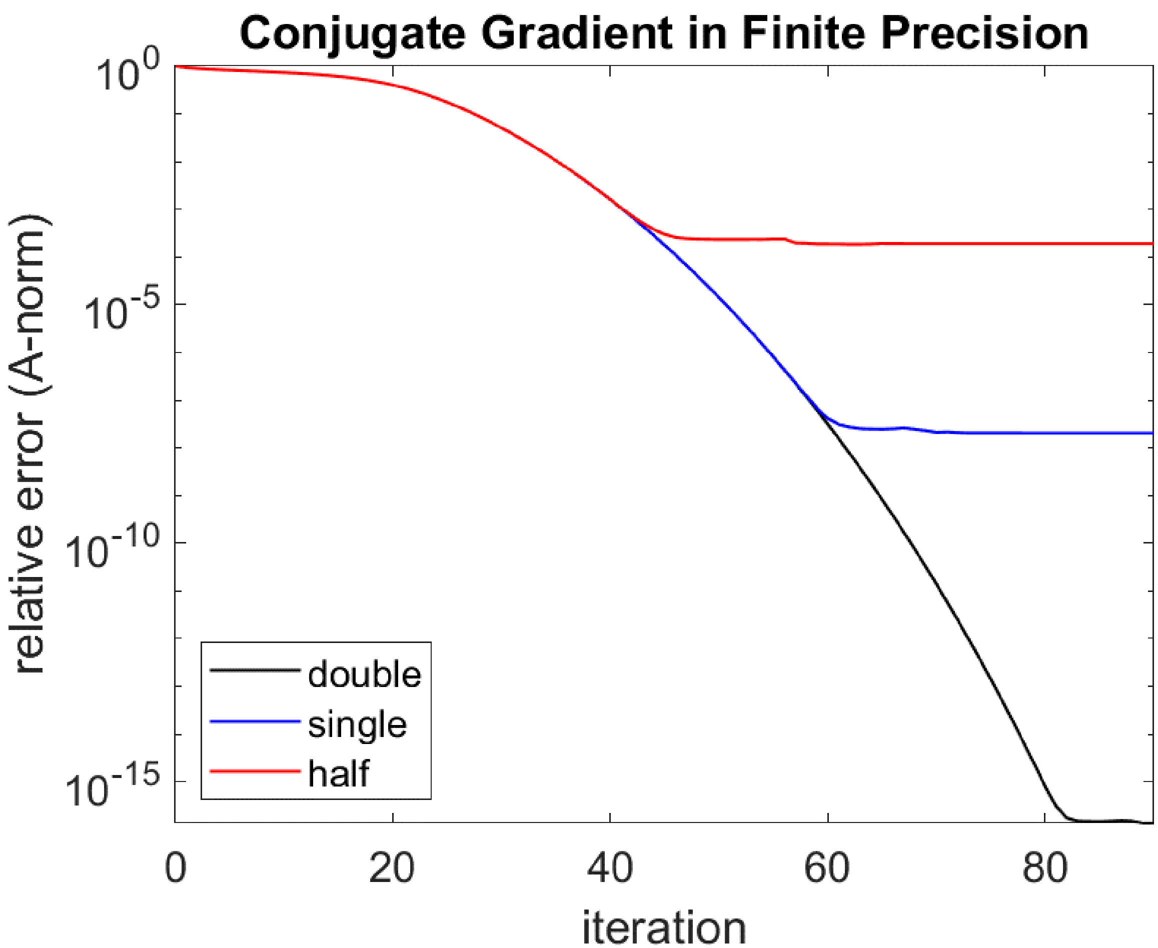


Example: Iterative Methods

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

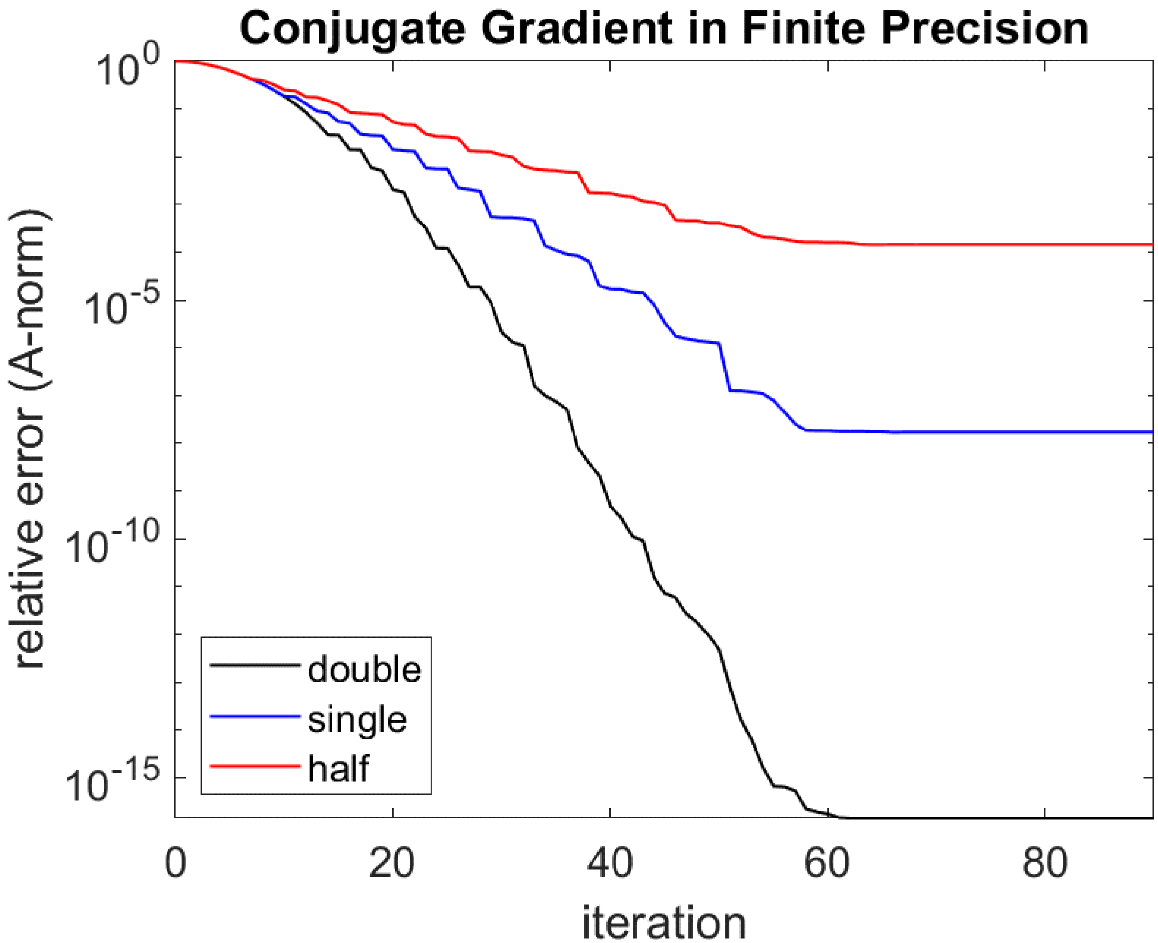


Example: Iterative Methods

$n = 100, \lambda_1 = 10^{-3}, \lambda_n = 1$

$\lambda_i = \lambda_1 + \left(\frac{i-1}{n-1}\right)(\lambda_n - \lambda_1)(0.65)^{n-i}, \quad i = 2, \ldots, n-1$

```
[V,~] = eig(A);
b = V'*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 $i = 0\colon \mathrm{maxit}$

$r_i = b - Ax_i$ (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 = factorization precision, u = working precision, u_r = 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:

Traditional	$u_f = u, u_r = u^2$
Fixed precision	$u_f = u = u_r$
Lower precision factorization	$u_f^2 = u = u_r$

- Enables **new** types of IR: (half, single, double), (half, single, quad), (half, double, quad), etc.

IR3: Summary

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

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

u_f	u	u_r	max $\kappa_\infty(A)$	Backward error norm	Backward error comp	Forward error
H	S	S	10^4	10^{-8}	10^{-8}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
H	D	D	10^4	10^{-16}	10^{-16}	$\mathrm{cond}(A,x) \cdot 10^{-16}$
H	D	Q	10^4	10^{-16}	10^{-16}	10^{-16}
S	S	S	10^8	10^{-8}	10^{-8}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
S	S	D	10^8	10^{-8}	10^{-8}	10^{-8}
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Fixed	S	S	S	10^8	10^{-8}	10^{-8}	$\text{cond}(A,x)\cdot 10^{-8}$
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$\Rightarrow$ Benefit of IR3 vs. "LP fact.": no $\mathrm{cond}(A,x)$ term in forward error

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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 ($u_s = u$)

	u_f	u	u_r	max $\kappa_\infty(A)$	Backward error norm	Backward error comp	Forward error
LU-IR	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
GMRES-IR	H	S	D	10^8	10^{-8}	10^{-8}	10^{-8}
LU-IR	S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}
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→ $\kappa_\infty(A) \leq u^{-1/2} u_f^{-1}$

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

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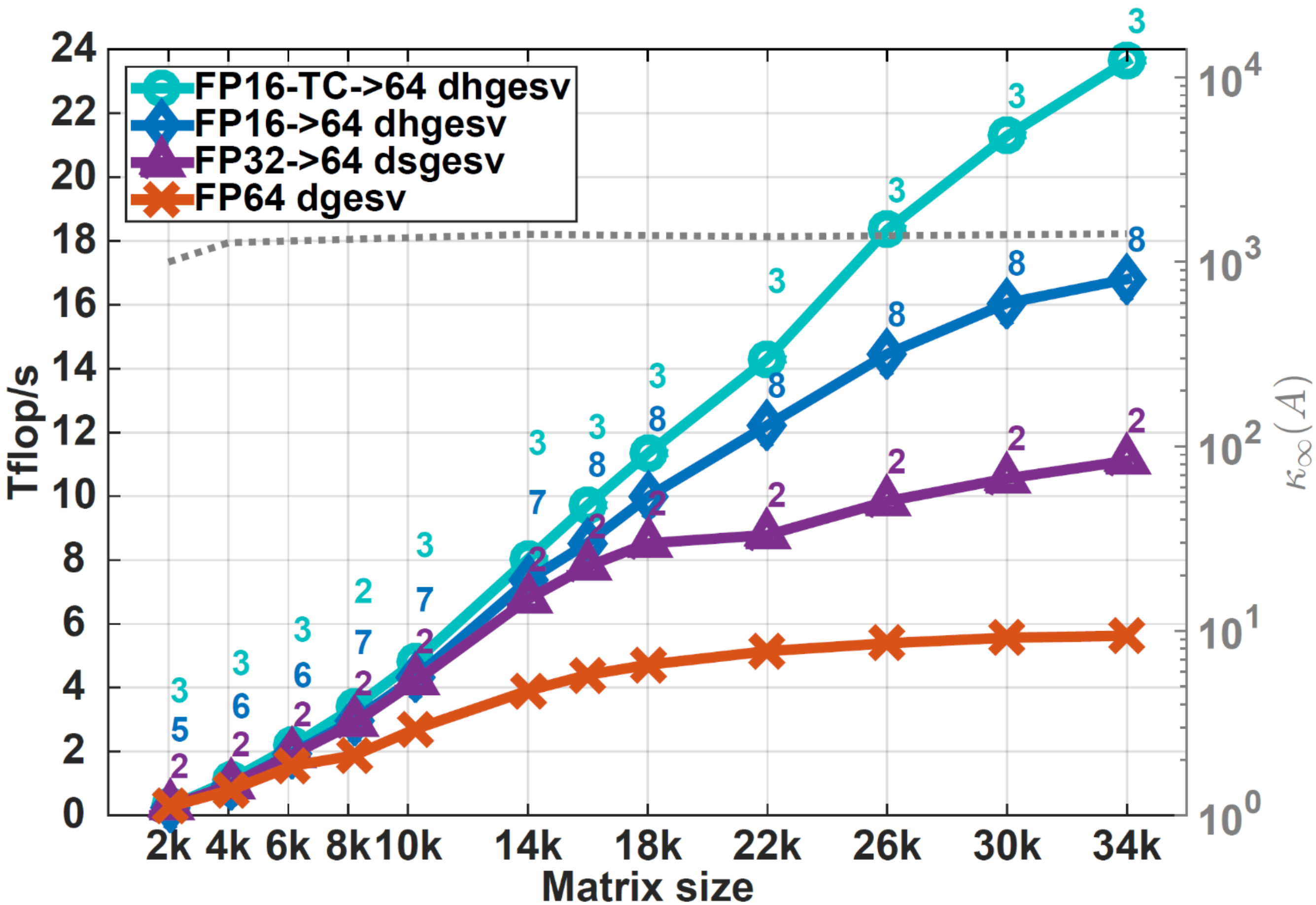
Recent work: 5-precision GMRES-IR [Amestoy, et al., 2021]

→ $\kappa_\infty(A) \leq u^{-1/3}\, u_f^{-2/3}$

Performance Results (MAGMA)

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



(a) Matrix of type 3: positive λ with clustered singular values, σ_i=(1, $\cdots$, 1, $\frac{1}{cond}$).

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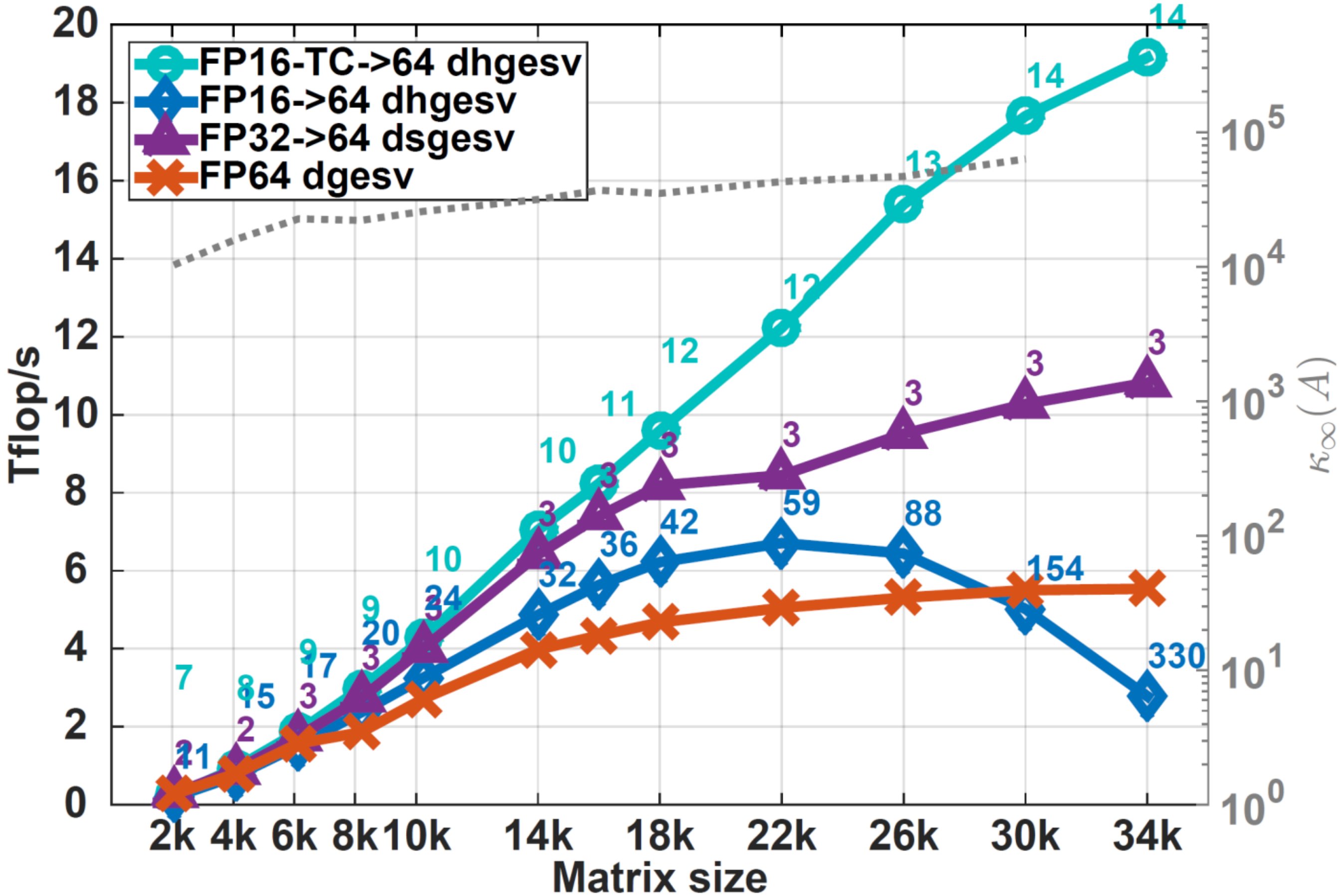

(b) Matrix of type 4: clustered singular values, $\sigma_i=(1, \cdots, 1, \frac{1}{cond})$.

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

Thank you!

carson@karlin.mff.cuni.cz

www.karlin.mff.cuni.cz/~carson/