Challenges and Opportunities in Mixed Precision Numerical Linear Algebra

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ICL Lunch Talk

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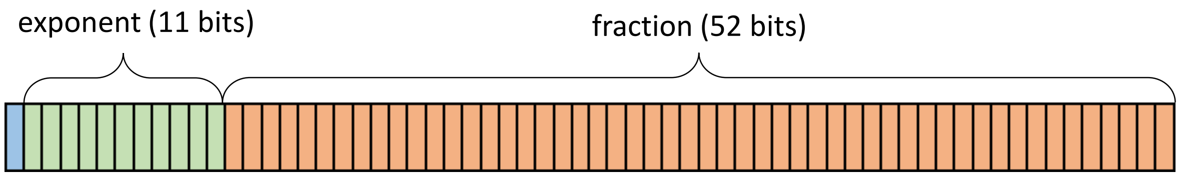
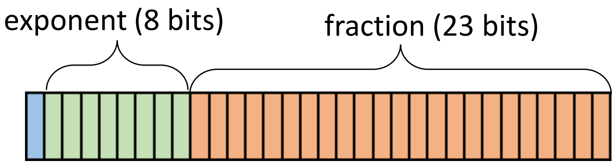
Floating Point Formats

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

IEEE double (FP64)

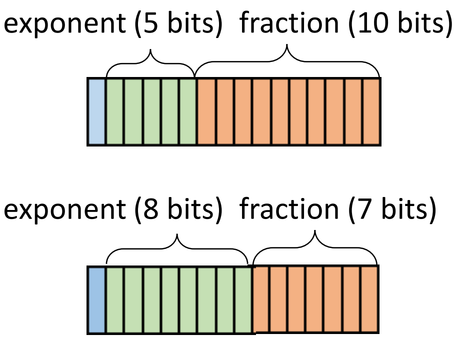


IEEE single (FP32)



IEEE half (FP16)

bfloat16



	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:

- Half precision (FP16) defined as storage format in 2008 IEEE standard
- ARM NEON: SIMD architecture, instructions for 8x16-bit, 4x32-bit, 2x64-bit
- 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!**)
- Google's Tensor processing unit (TPU)
- NVIDIA A100, 2020: tensor cores with multiple supported precisions: FP16, FP64, Binary, INT4, INT8, bfloat16
- NVIDIA H100, 2022: now with quarter-precision (FP8) tensor cores
- Future exascale supercomputers: (~2021) Expected extensive support for reduced-precision arithmetic (32/16/8-bit)

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]

HPL-AI Benchmark

- Like HPL, solves dense Ax=b, results still to double precision accuracy
- Achieves this via mixed-precision iterative refinement

HPL-AI Benchmark

Rank	Site	Computer	Cores	HPL-AI (Eflop/s)	TOP500 Rank	HPL Rmax (Eflop/s)	Speedup
1	RIKEN	Fugaku	7,630,848	2.000	1	0.4420	4.5
2	DOE/SC/ORNL	Summit	2,414,592	1.411	2	0.1486	9.5
3	NVIDIA	Selene	555,520	0.630	6	0.0630	9.9
4	DOE/SC/LBNL	Perlmutter	761,856	0.590	5	0.0709	8.3
5	FZJ	JUWELS BM	449,280	0.470	8	0.0440	10.0
6	University of Florida	HiPerGator	138,880	0.170	31	0.0170	9.9
7	SberCloud	Christofari Neo	98,208	0.123	44	0.0120	10.3
8	DOE/SC/ANL	Polaris	259,840	0.114	13	0.0238	4.8
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15	Calcul Quebec/Compute Canada	Narval	76,320	0.014	84	0.0059	2.4
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- Larger unit roundoff
  - Lose something small when storing: $fl(x) = x(1+\delta), \quad |\delta| \leq u$
  - Lose something small when computing: $fl(x \text{ op } y) = (x \text{ op } y)(1+\delta), \quad |\delta| \leq u$

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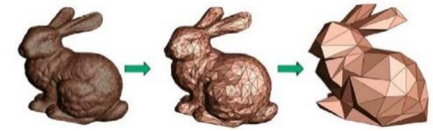
Does it matter?

Inexact computations

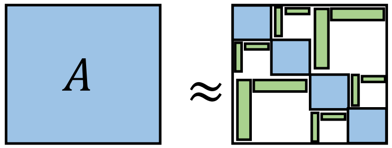
- In real computations we have many sources of inexactness
  - Imperfect data, measurement error
  - Modeling error, discretization error
  - Intentional approximation to improve performance
    - Reduced models, Low-rank representations, sparsification, randomization

Model Reduction



[Schilders, van der Vorst, Rommes, 2008]

Low-rank (hierarchical) approximation



Sparsification, Randomized algorithms

[Sinha, 2018]

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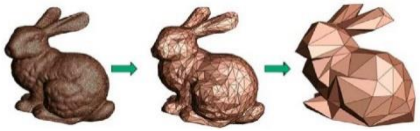

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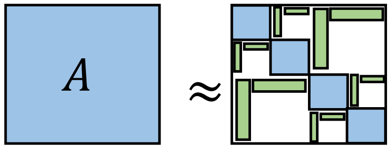

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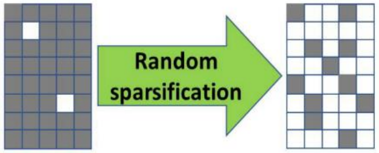
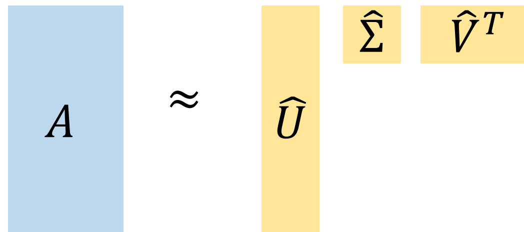


[Sinha, 2018]

- 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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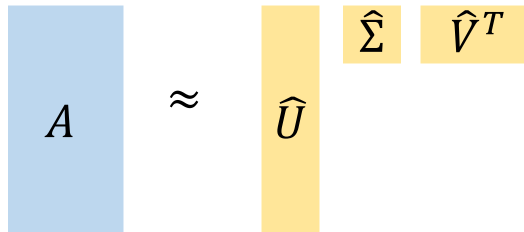
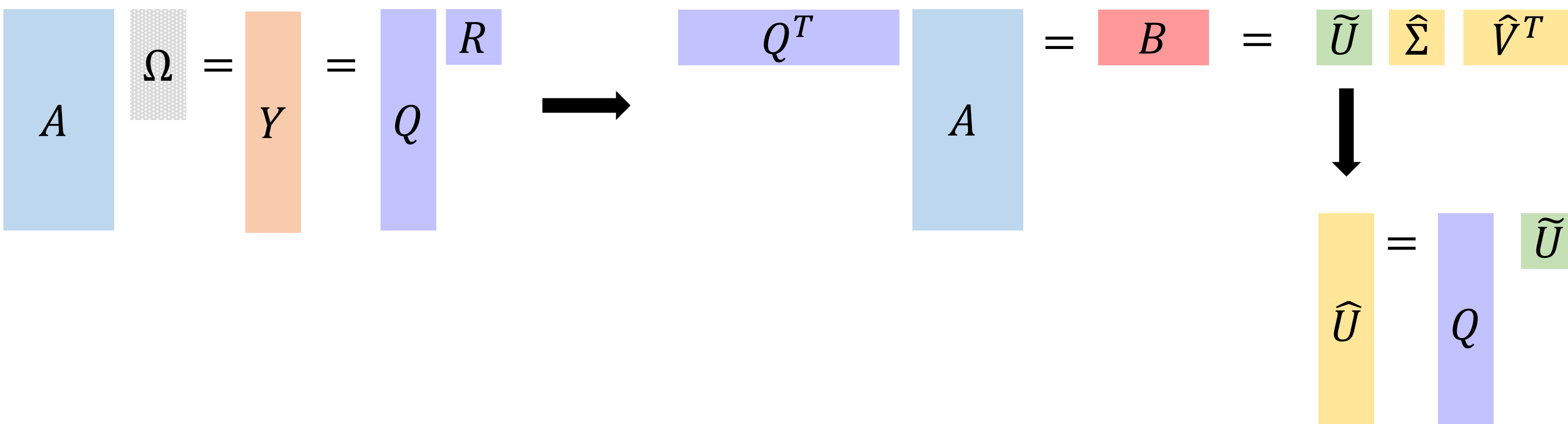


- Randomized SVD:



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

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

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$[\widehat{U}_d,\hat{S}_d,\widehat{V}_d] = \mathrm{rsvd}(A)$: 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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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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$\left\|A - Q_h Q_h^T A\right\|_2 = 3.59\text{e-}06$

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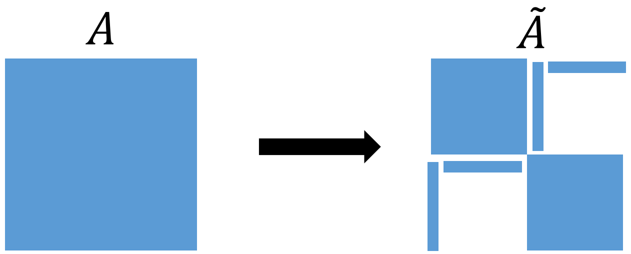
Example: Low-Rank Approximation

- 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

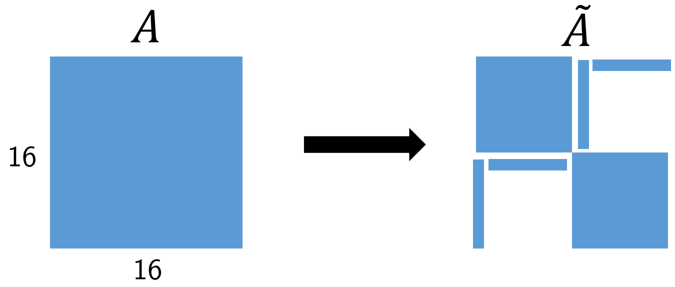
- [Higham, Mary, 2019]: block low-rank LU factorization preconditioner that exploits numerically low-rank structure of the error for LU computed in low precision
- [Higham, Mary, 2019]: Interplay of roundoff error and approximation error in solving block low-rank linear systems using LU
- [Buttari, et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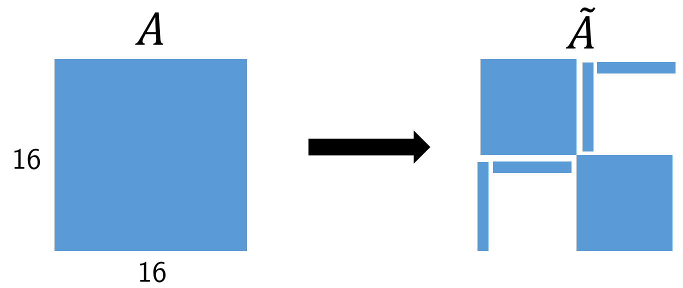
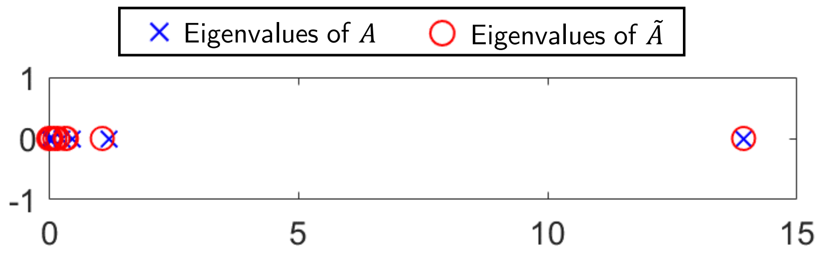


Exact arithmetic SVD:



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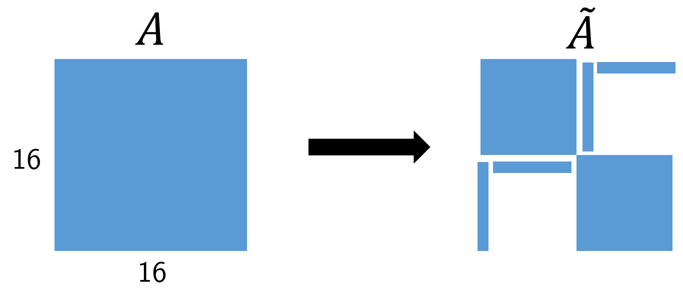

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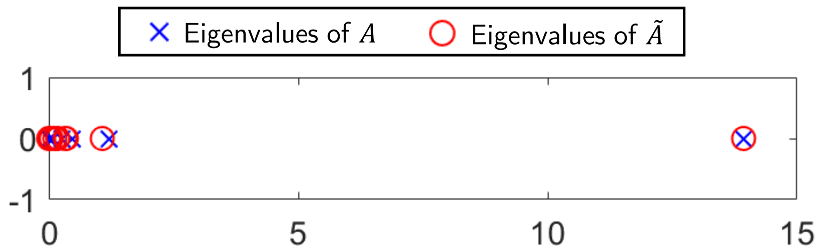
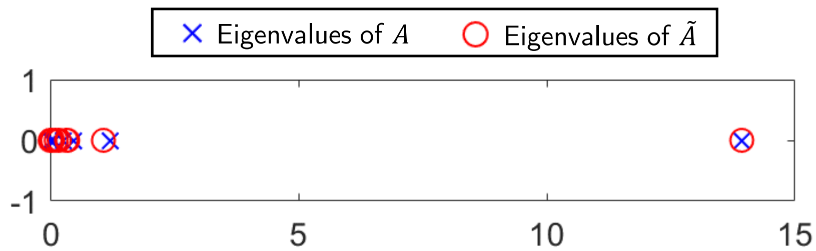


Half precision SVD:

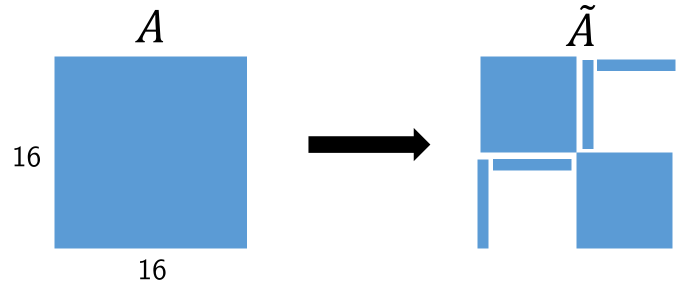


Example: Low-Rank Approximation

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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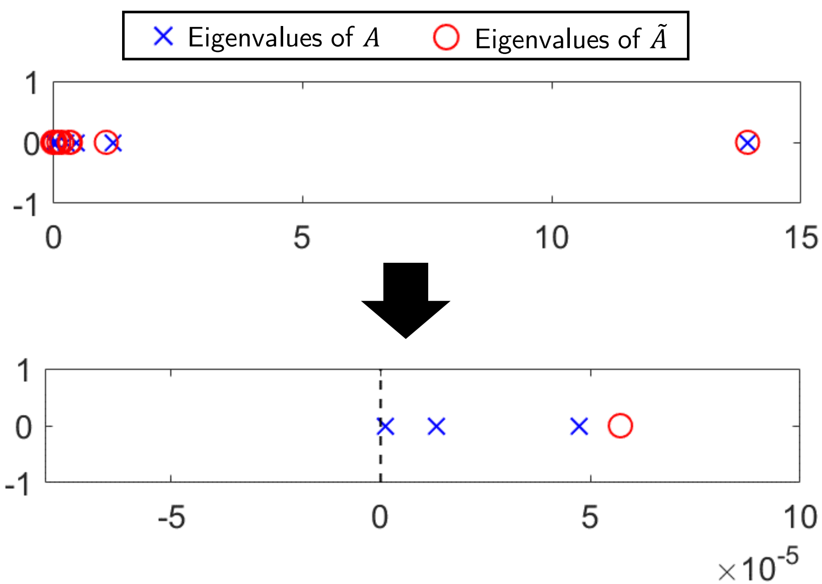

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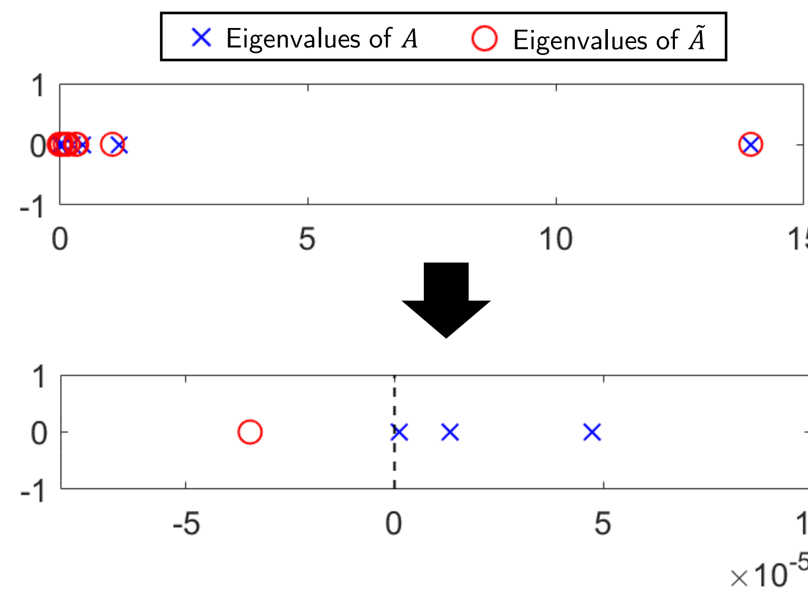

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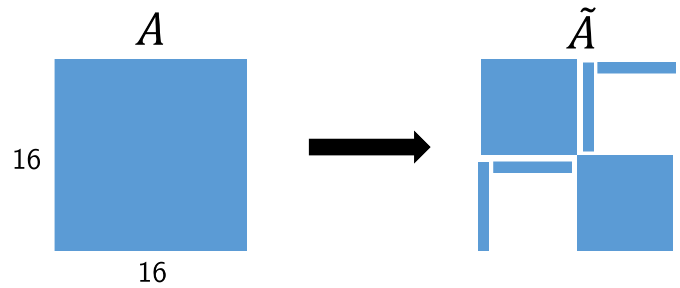

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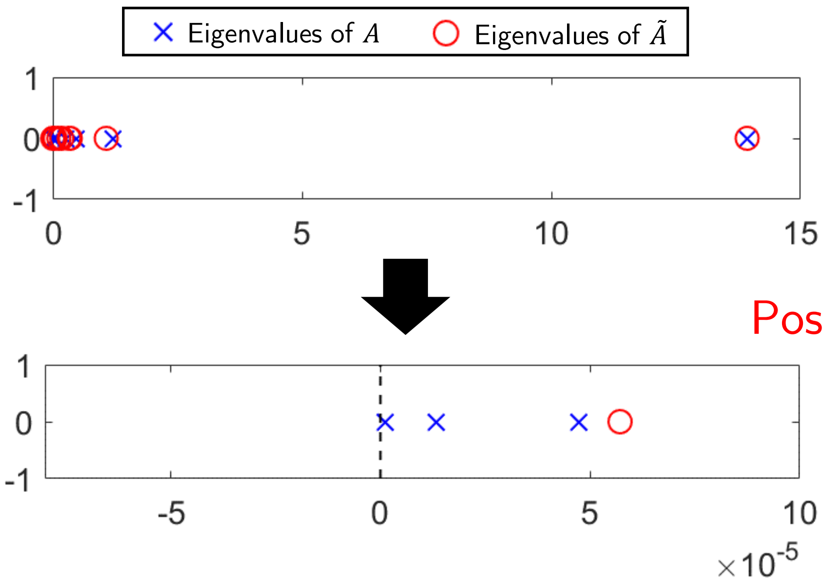

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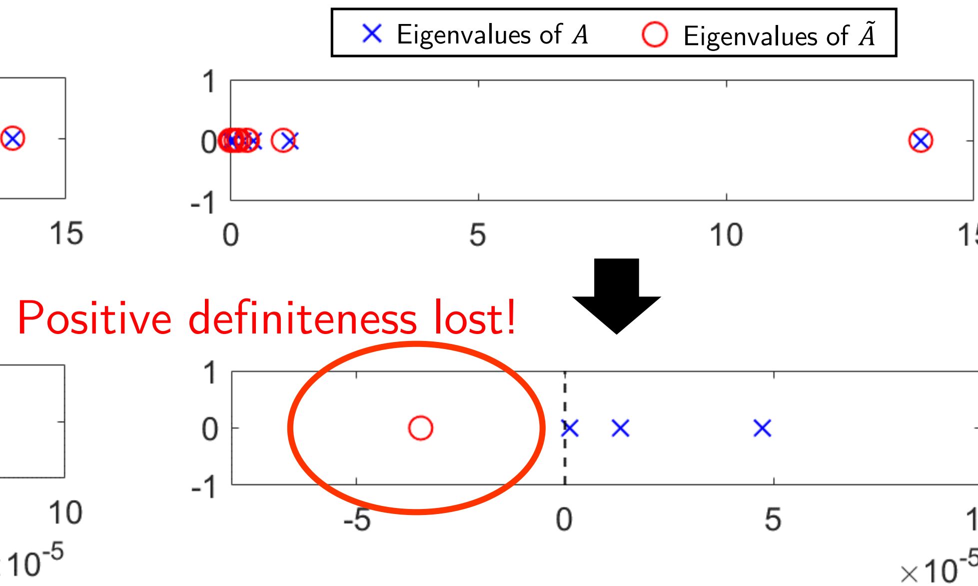
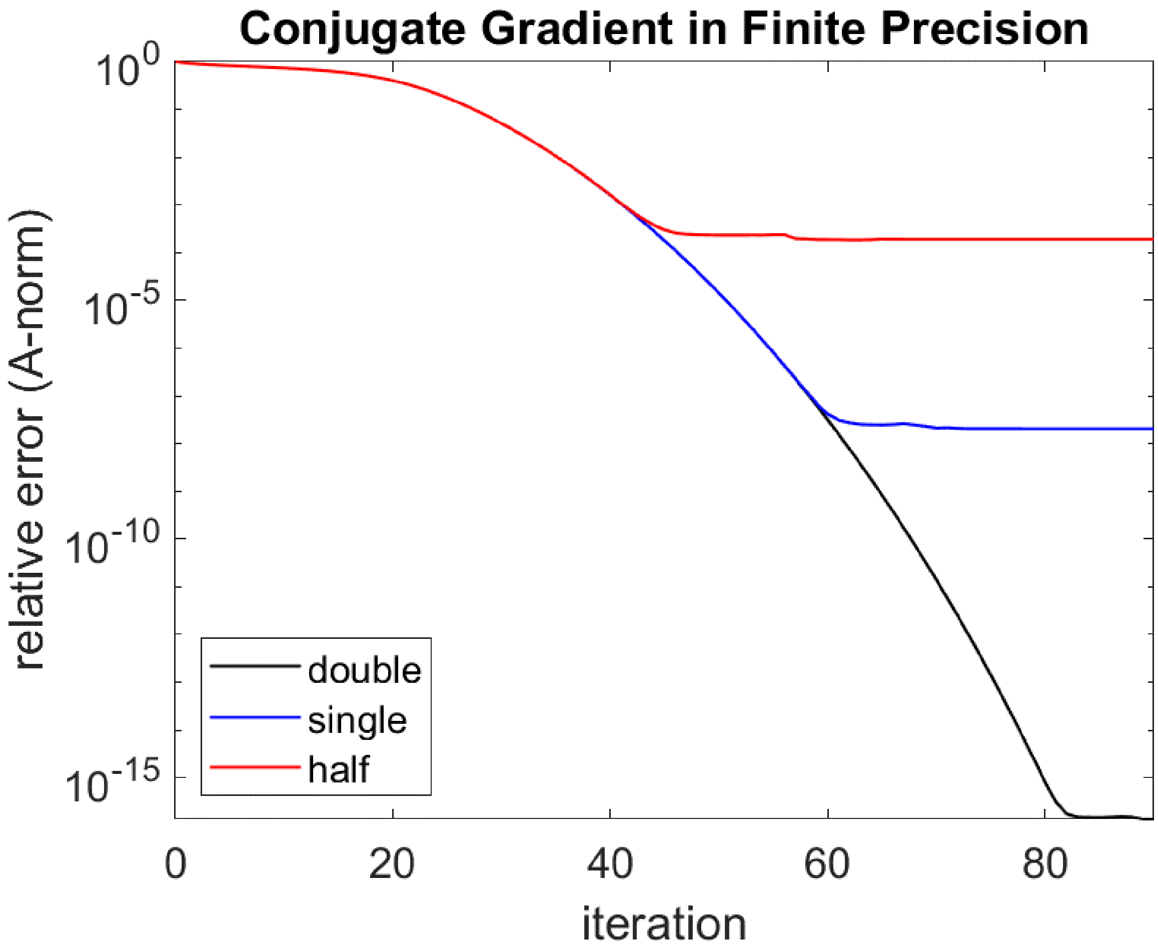


Example: Iterative Methods

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

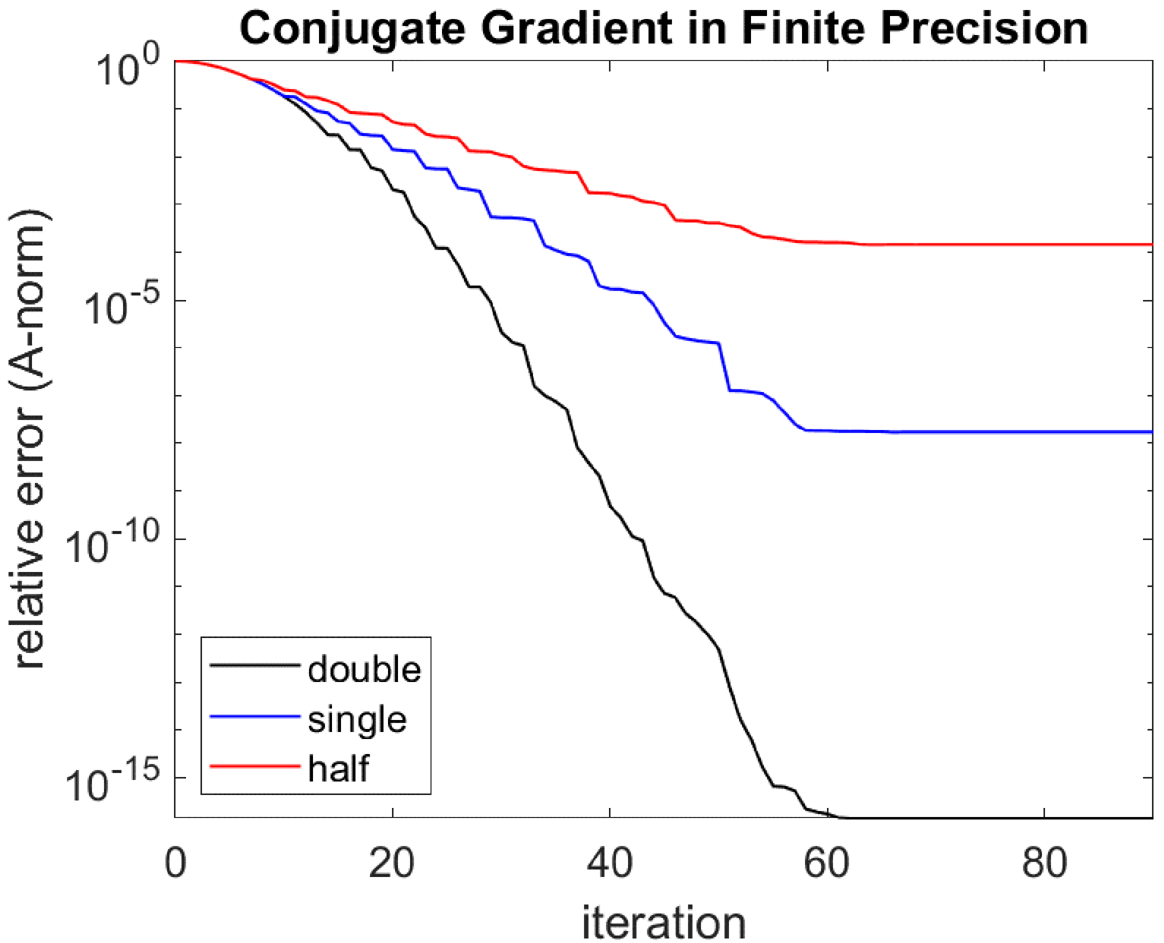


Example: Iterative Methods

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

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

```
[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

$$u_f \geq u \geq u_r$$

$\boldsymbol{u_s}$ is the *effective precision* of the solve, with $\boldsymbol{u} \leq \boldsymbol{u_s} \leq \boldsymbol{u_f}$

- For triangular solves with LU factors: $\boldsymbol{u_s} = \boldsymbol{u_f}$
- For GMRES preconditioned by LU factors, $\boldsymbol{u_s} = \boldsymbol{u}$ [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 $\approx 10^{-34}$

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

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New	S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}

$\Rightarrow$ 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-IR: Solve for d_i via GMRES on $U^{-1}L^{-1}Ad_i = U^{-1}L^{-1}r_i$

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}
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LU-IR	H	D	Q	10^4	10^{-16}	10^{-16}	10^{-16}
GMRES-IR	H	D	Q	10^{12}	10^{-16}	10^{-16}	10^{-16}

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

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

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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!

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

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

Extension: Least Squares Problems

- Want to solve

$$\min_x \|b - Ax\|_2$$

where $A \in \mathbb{R}^{m \times n}$ $(m > n)$ has rank n

- Commonly solved using QR factorization:

$$A = QR = [Q_1, Q_2] \begin{bmatrix} U \\ 0 \end{bmatrix}$$

where Q is an $m \times m$ orthogonal matrix and U is upper triangular.

$$x = U^{-1} Q_1^T b, \qquad \|b - Ax\|_2 = \left\|Q_2^T b\right\|_2$$

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- As in linear system case, for ill-conditioned problems, iterative refinement often needed to improve accuracy and stability

Extension: Least Squares Problems

- For inconsistent systems, must simultaneously refine both solution and residual
- (Björck,1967): Least squares problem can be written as a linear system with square matrix of size $(m+n)$:

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

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- Refinement proceeds as follows:

1. Compute "residuals"

$$\begin{bmatrix} f_i \\ g_i \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} - \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r_i \\ x_i \end{bmatrix} = \begin{bmatrix} b - r_i - Ax_i \\ -A^T r_i \end{bmatrix}$$

2. Solve for corrections

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} \Delta r_i \\ \Delta x_i \end{bmatrix} = \begin{bmatrix} f_i \\ g_i \end{bmatrix}$$

3. Update "solution":

$$\begin{bmatrix} r_{i+1} \\ x_{i+1} \end{bmatrix} = \begin{bmatrix} r_i \\ x_i \end{bmatrix} + \begin{bmatrix} \Delta r_i \\ \Delta x_i \end{bmatrix}$$

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$$\begin{bmatrix} r_{i+1} \\ x_{i+1} \end{bmatrix} = \begin{bmatrix} r_i \\ x_i \end{bmatrix} + \begin{bmatrix} \Delta r_i \\ \Delta x_i \end{bmatrix} \qquad \tilde{x}_{i+1} = \tilde{x}_i + d_i$$

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- Refinement proceeds as follows:

1. Compute "residuals"

$$\begin{bmatrix} f_i \\ g_i \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} - \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r_i \\ x_i \end{bmatrix} = \begin{bmatrix} b - r_i - Ax_i \\ -A^T r_i \end{bmatrix}$$

2. Solve for corrections

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} \Delta r_i \\ \Delta x_i \end{bmatrix} = \begin{bmatrix} f_i \\ g_i \end{bmatrix}$$

3. Update "solution":

$$\begin{bmatrix} r_{i+1} \\ x_{i+1} \end{bmatrix} = \begin{bmatrix} r_i \\ x_i \end{bmatrix} + \begin{bmatrix} \Delta r_i \\ \Delta x_i \end{bmatrix}$$

$$\tilde{r}_i = \tilde{b} - \tilde{A}\tilde{x}_i$$

$$\tilde{A}d_i = \tilde{r}_i$$

$$\tilde{x}_{i+1} = \tilde{x}_i + d_i$$

Results for 3-precision IR for linear systems **also applies to least squares problems [C., Higham, Pranesh, 2020]**

Extension: Multistage Mixed Precision IR

- Many different variants of mixed precision IR
  - "standard IR" (SIR): LU solves
  - SGMRES-IR: preconditioned GMRES entirely in working precision
  - GMRES-IR: preconditioned GMRES with extra precision

cost, reliability

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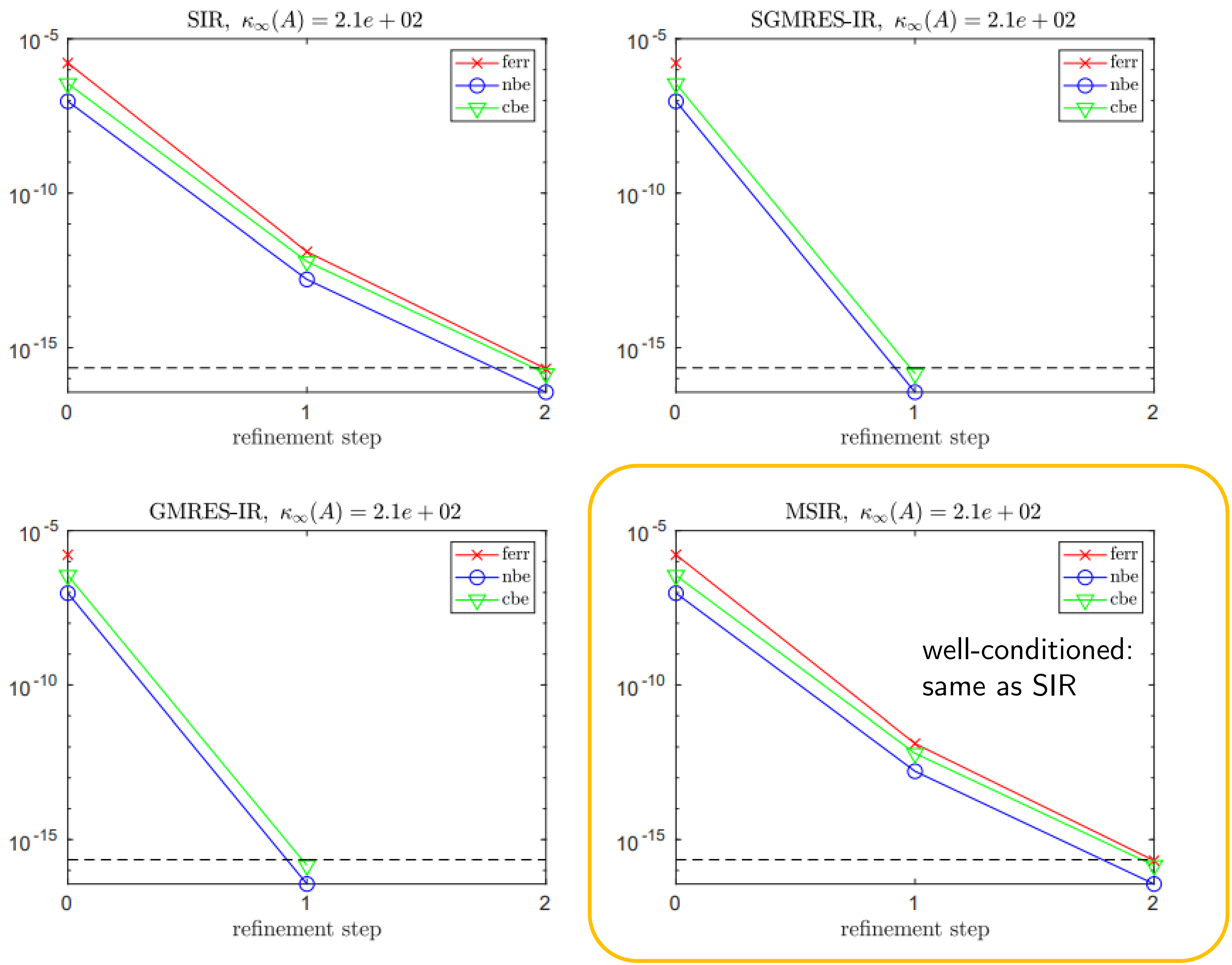
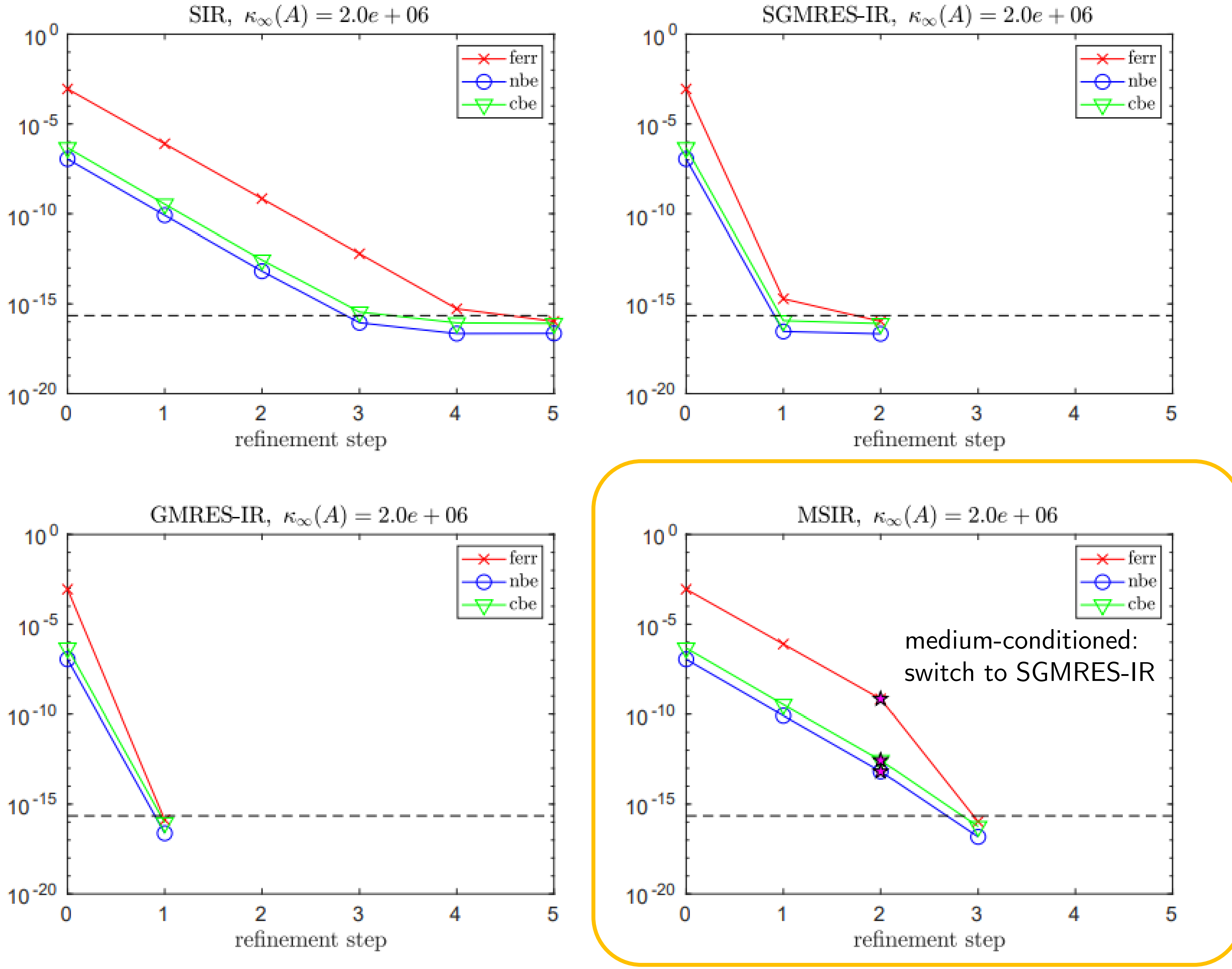
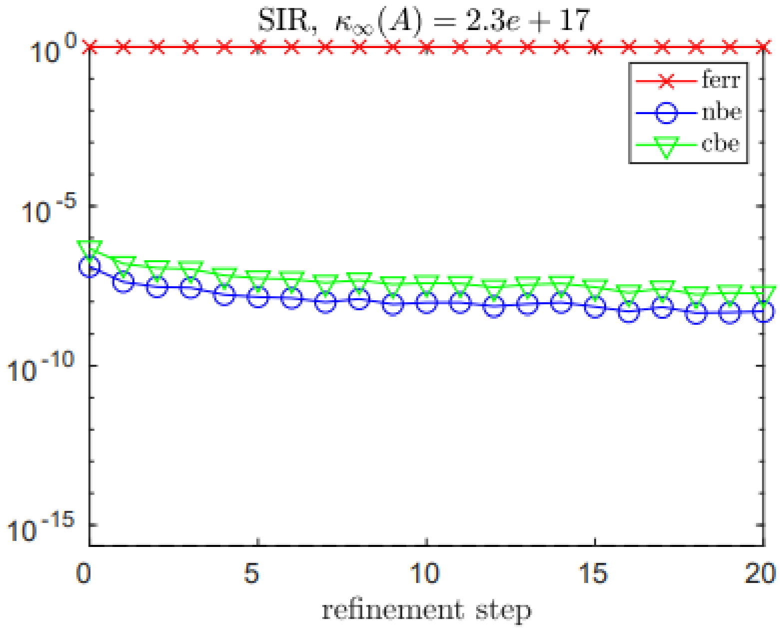
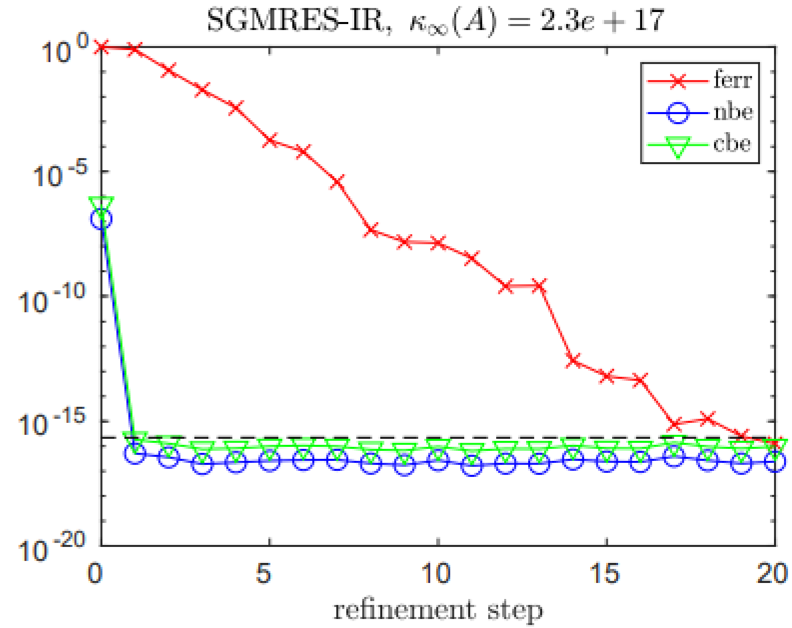
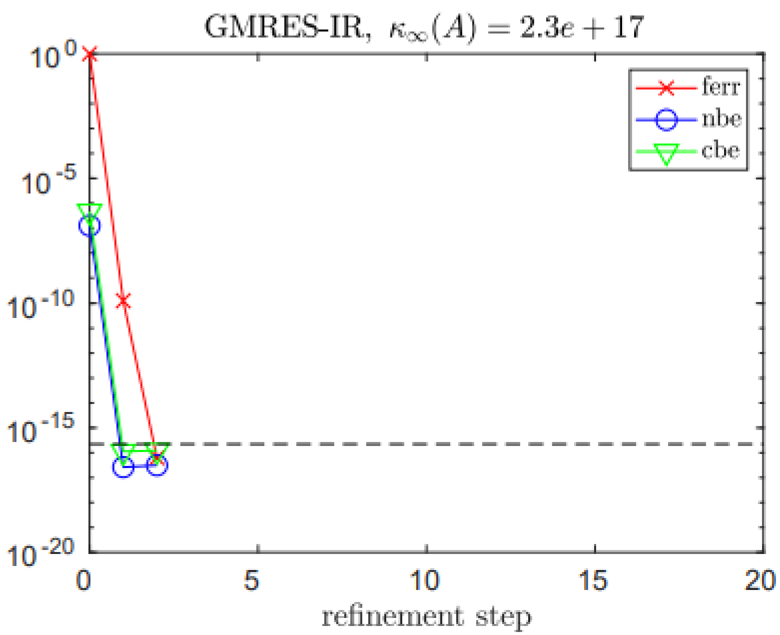
→ **Multistage Iterative Refinement (MSIR)** [Oktay, C., NLAA, 2022]

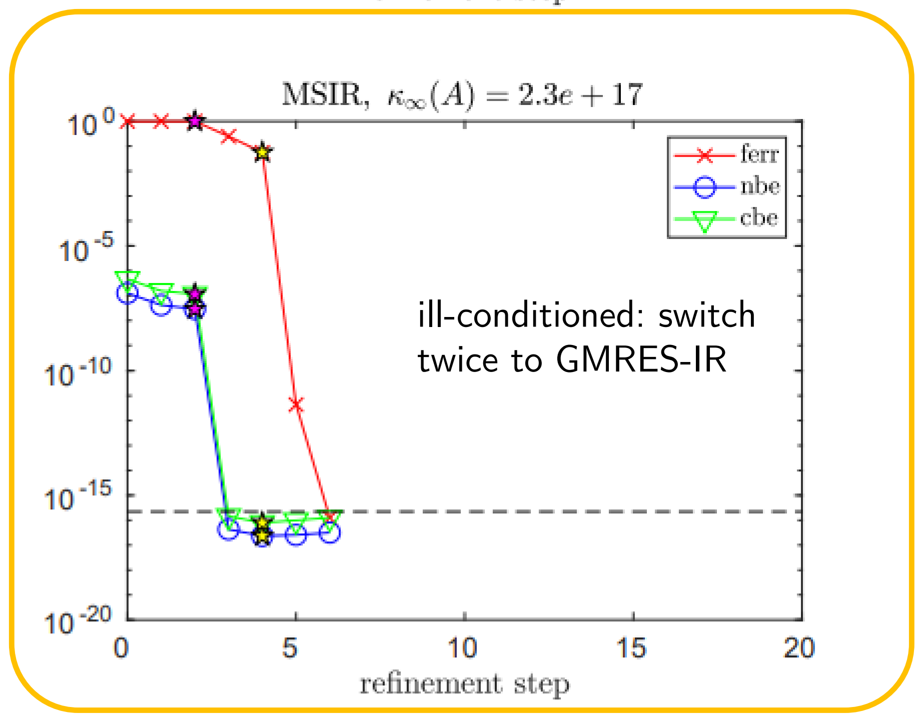

SIR, $\kappa_\infty(A) = 2.1e + 02$
SGMRES-IR, $\kappa_\infty(A) = 2.1e + 02$
GMRES-IR, $\kappa_\infty(A) = 2.1e + 02$
MSIR, $\kappa_\infty(A) = 2.1e + 02$
ferr
nbe
cbe
10^{-5}
10^{-10}
10^{-15}
0
1
2
refinement step
well-conditioned:
same as SIR


SIR, $\kappa_\infty(A) = 2.0e+06$
SGMRES-IR, $\kappa_\infty(A) = 2.0e+06$
GMRES-IR, $\kappa_\infty(A) = 2.0e+06$
MSIR, $\kappa_\infty(A) = 2.0e+06$
ferr
nbe
cbe
10^{0}
10^{-5}
10^{-10}
10^{-15}
10^{-20}
0
1
2
3
4
5
refinement step
medium-conditioned:
switch to SGMRES-IR


SIR, $\kappa_\infty(A) = 2.3e + 17$
ferr
nbe
cbe
refinement step


SGMRES-IR, $\kappa_\infty(A) = 2.3e + 17$
ferr
nbe
cbe
refinement step


GMRES-IR, $\kappa_\infty(A) = 2.3e + 17$
ferr
nbe
cbe
refinement step


MSIR, $\kappa_\infty(A) = 2.3e + 17$
ferr
nbe
cbe
ill-conditioned: switch
twice to GMRES-IR
refinement step

Extension: SPAI-GMRES-IR

- Existing analyses of GMRES-IR assume we use full LU factors
- In practice, often want to use sparse preconditioners (ILU, SPAI, etc.)
- [C., Khan, arXiv:2202.10204, 2022]: analysis of GMRES-IR with SPAI preconditioning)
  - Convergence to limiting accuracy as long as $n u_f \mathit{cond}(A^T) \lesssim n\varepsilon \lesssim u^{-1/2}$

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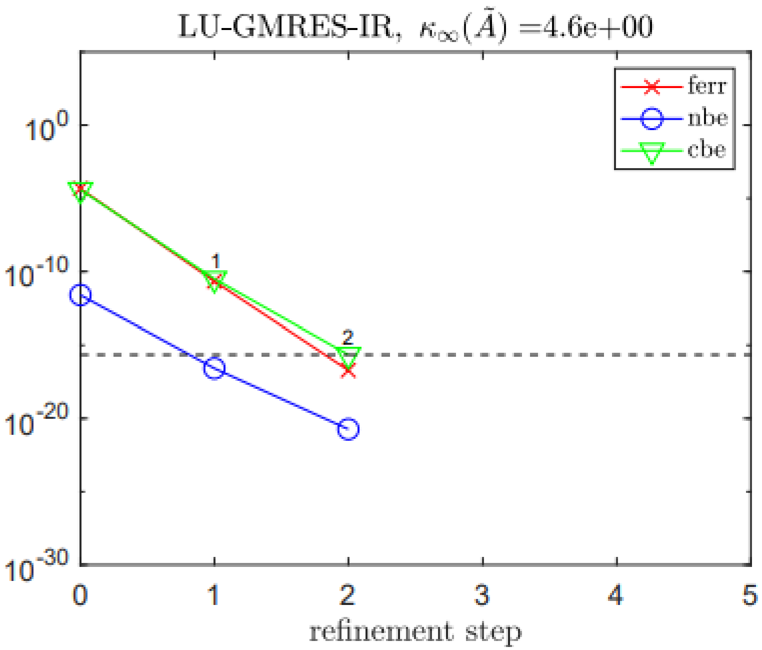
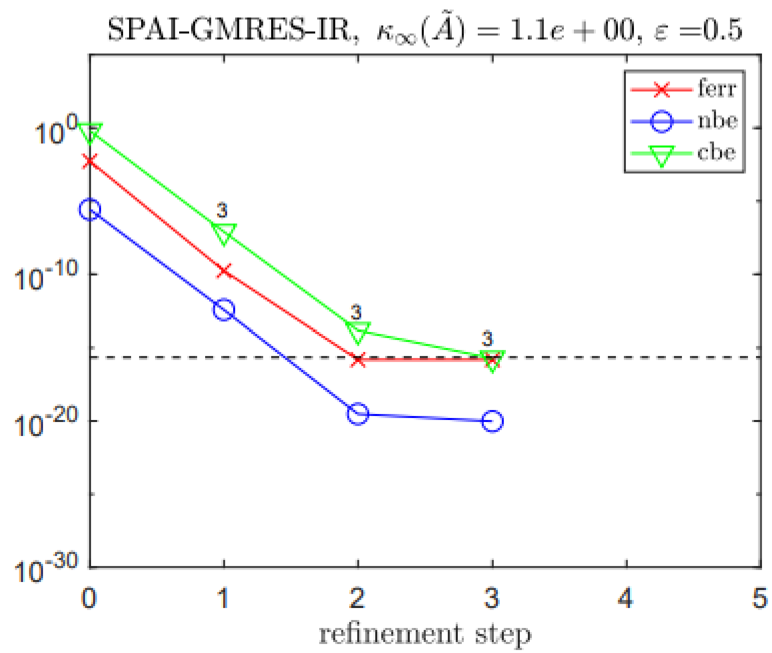
matrix: steam1, (u_f, u, u_r) = (single, double, quad)



nnz$(L+U)$ = 21,657



nnz(M) = 2,248

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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