Iterative Refinement in Three Precisions

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Parallel Solution Methods for Systems Arising from PDEs

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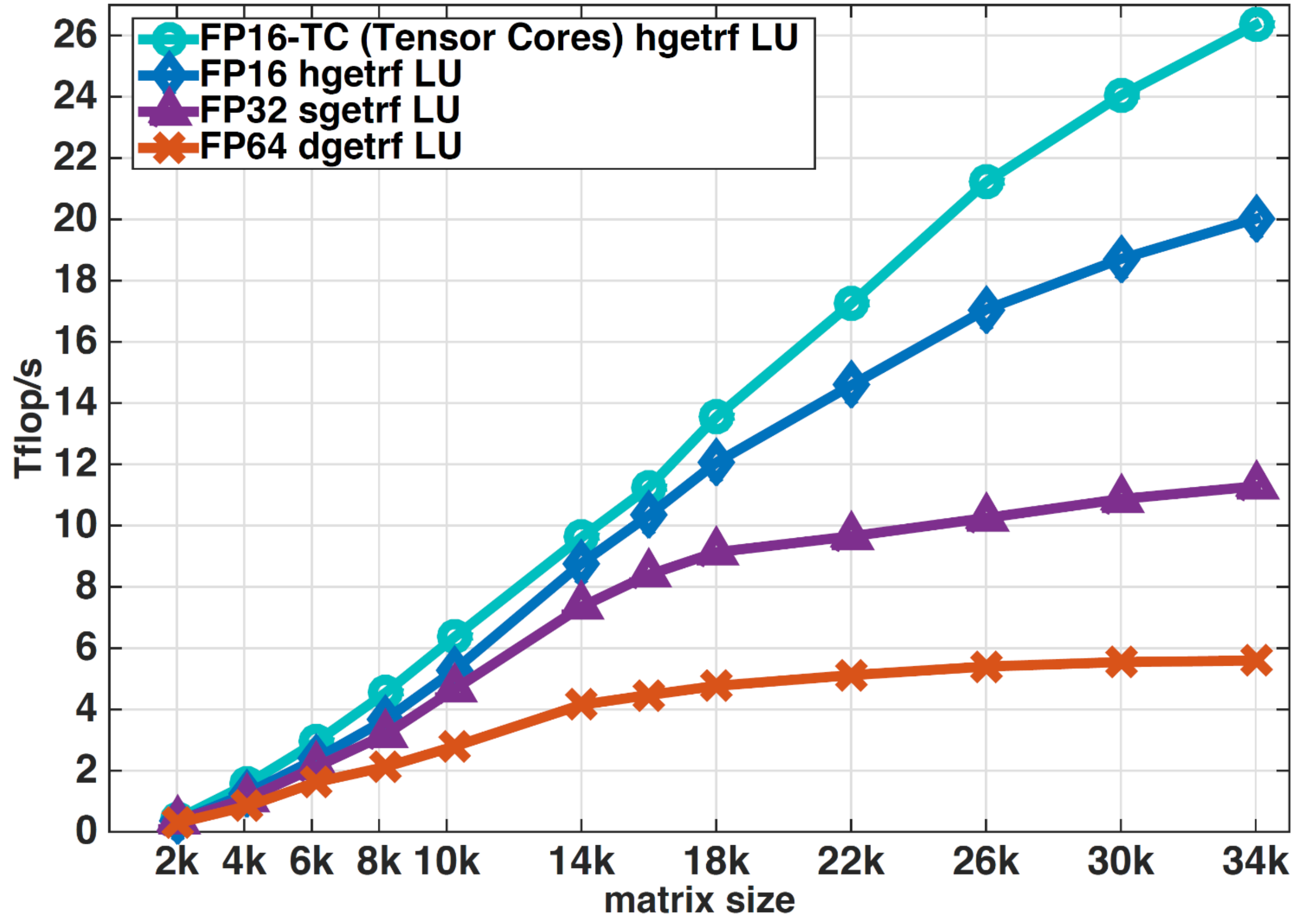
Hardware Support for Multiprecision Computation

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): quantizes 32-bit FP computations into 8-bit integer arithmetic
- 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]

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

for $i = 0\colon \mathrm{maxit}$

$r_i = b - Ax_i$

Solve $Ad_i = r_i$ via $d_i = U^{-1}(L^{-1}r_i)$

$x_{i+1} = x_i + d_i$

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

for $i = 0: \mathrm{maxit}$

$r_i = b - Ax_i$ (in precision u^2)

Solve $Ad_i = r_i$ via $d_i = U^{-1}(L^{-1}r_i)$ (in precision u)

$x_{i+1} = x_i + d_i$ (in precision u)

"Traditional" (high-precision residual computation)

[Wilkinson, 1948] (fixed point), [Moler, 1967] (floating point)

Iterative Refinement for $Ax = b$

$\kappa_\infty(A) = \|A^{-1}\|_\infty \|A\|_\infty$

$\mathrm{cond}(A, x) = \|\, |A^{-1}||A||x| \,\|_\infty / \|x\|_\infty$

As long as $\kappa_\infty(A) \le u^{-1}$,

- relative forward error is $O(u)$
- relative normwise and componentwise backward errors are $O(u)$

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Iterative Refinement for $Ax = b$

Solve $Ax_0 = b$ by LU factorization (in precision $u^{1/2}$)

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"Low-precision factorization"

[Langou et al., 2006], [Arioli and Duff, 2009], [Hogg and Scott, 2010], [Abdelfattah et al., 2016]

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- New analysis **generalizes** existing types of IR:

[C. and Higham, SIAM SISC 40(2), 2018]

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

  (and **improves** upon existing analyses in some cases)

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

Key Analysis Innovations I

Obtain tighter upper bounds:

Typical bounds used in analysis: $\|A(x - \hat{x}_i)\|_\infty \leq \|A\|_\infty \|x - \hat{x}_i\|_\infty$

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For a stable refinement scheme, in early stages we expect

$$\frac{\|r_i\|}{\|A\|\|\hat{x}_i\|} \approx u \ll \frac{\|x-\hat{x}_i\|}{\|x\|} \longrightarrow \boxed{\mu_i \ll 1}$$

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But close to convergence,

$$\|r_i\| \approx \|A\|\|x-\hat{x}_i\| \longrightarrow \boxed{\mu_i \approx 1}$$

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Let $\boldsymbol{u_s}$ be the *effective precision* of the solve, with $\boldsymbol{u} \le \boldsymbol{u_s} \le \boldsymbol{u_f}$

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1. $\hat{d}_i = (I + \boldsymbol{u_s} E_i) d_i, \quad \boldsymbol{u_s} \|E_i\|_\infty < 1$

   → normwise relative forward error is bounded by multiple of u_s and is less than 1

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2. $\left\|\hat{r}_i - A\hat{d}_i\right\|_\infty \leq \boldsymbol{u_s}(c_1\|A\|_\infty\left\|\hat{d}_i\right\|_\infty + c_2\|\hat{r}_i\|_\infty)$

   → normwise relative backward error is at most $\max(c_1, c_2)\, u_s$

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E_i, c_1, c_2, and G_i depend on A, $\hat{r}_i$, n, and $\boldsymbol{u_s}$

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Forward Error for IR3

- Three precisions:
  - u_f: factorization precision
  - u: working precision
  - u_r: residual computation precision

$$\kappa_\infty(A) = \|A^{-1}\|_\infty \|A\|_\infty$$
$$\mathrm{cond}(A) = \|\, |A^{-1}||A| \,\|_\infty$$
$$\mathrm{cond}(A,x) = \|\, |A^{-1}||A||x| \,\|_\infty / \|x\|_\infty$$

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Theorem [C. and Higham, SISC 40(2), 2018]

For IR in precisions $\boldsymbol{u_f} \geq \boldsymbol{u} \geq \boldsymbol{u_r}$ and effective solve precision $\boldsymbol{u_s}$, if

$$\phi_i \equiv 2\boldsymbol{u_s} \min(\mathrm{cond}(A), \kappa_\infty(A)\mu_i) + \boldsymbol{u_s}\|E_i\|_\infty$$

is sufficiently less than 1, then the forward error is reduced on the ith iteration by a factor $\approx \phi_i$ until an iterate $\hat{x}_i$ is produced for which

$$\frac{\|x - \hat{x}_i\|_\infty}{\|x\|_\infty} \lesssim 4N\boldsymbol{u_r}\ \mathrm{cond}(A,x) + \boldsymbol{u},$$

where N is the maximum number of nonzeros per row in A.

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Analogous traditional bounds: $\phi_i \equiv 3n\boldsymbol{u_f}\kappa_\infty(A)$

Normwise Backward Error for IR3

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is sufficiently less than 1, then the residual is reduced on the ith iteration by a factor $\approx \phi_i$ until an iterate $\hat{x}_i$ is produced for which

$$\|b - A\hat{x}_i\|_\infty \lesssim N\boldsymbol{u}(\|b\|_\infty + \|A\|_\infty \|\hat{x}_i\|_\infty),$$

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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}
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Fixed	S	S	S	10^8	10^{-8}	10^{-8}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
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New	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
LP fact.	H	D	D	10^4	10^{-16}	10^{-16}	$\mathrm{cond}(A,x) \cdot 10^{-16}$
New	H	D	Q	10^4	10^{-16}	10^{-16}	10^{-16}
Fixed	S	S	S	10^8	10^{-8}	10^{-8}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
Trad.	S	S	D	10^8	10^{-8}	10^{-8}	10^{-8}
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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
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New	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
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$\Rightarrow$ Benefit of IR3 vs. "LP fact.": no $\text{cond}(A,x)$ 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!

```
A = gallery('randsvd', 100, 1e9, 2)
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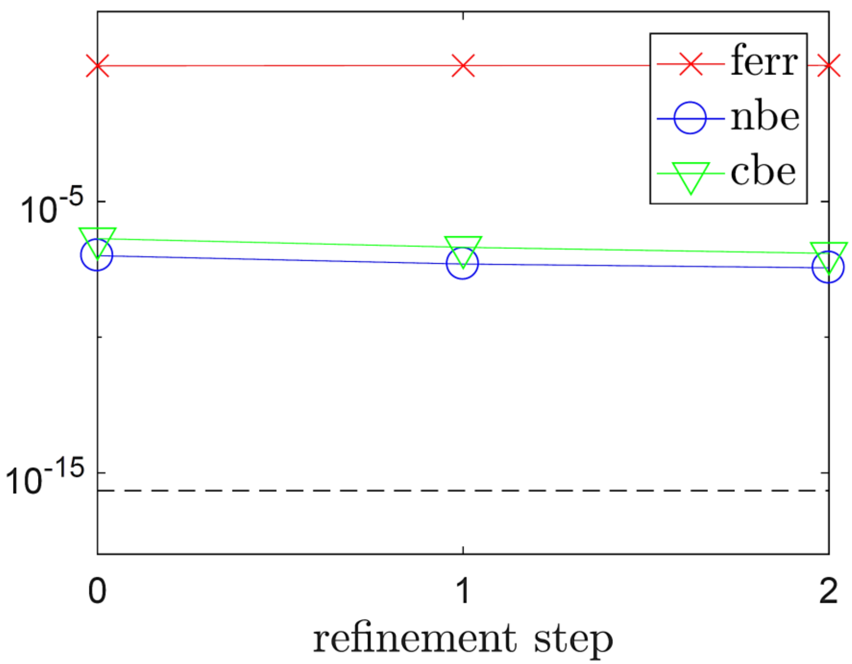
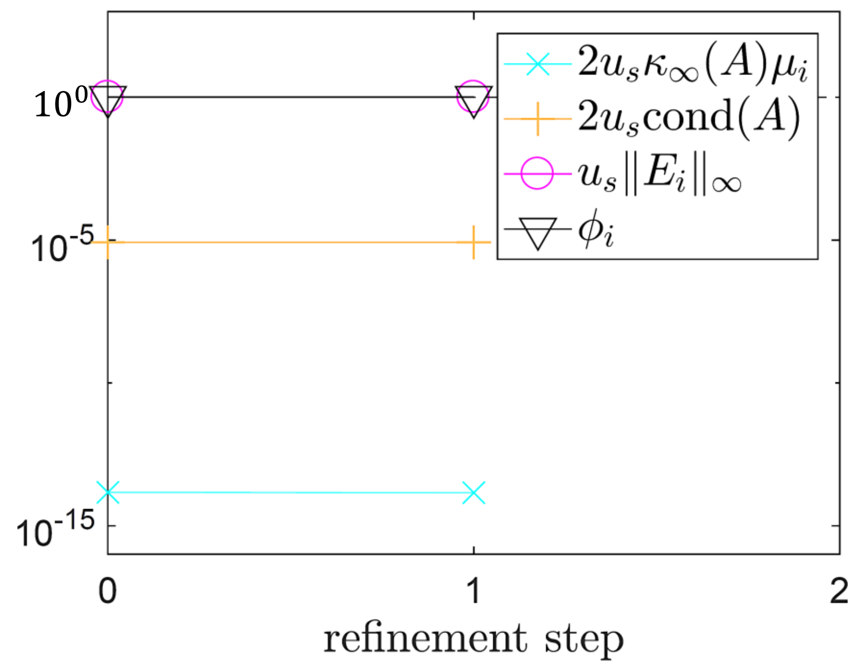
```

$\kappa_\infty(A) \approx$ 2e10, $\mathrm{cond}(A,x) \approx$ 5e9

Standard (LU-based) IR with u_f: single, u: double, u_r: double





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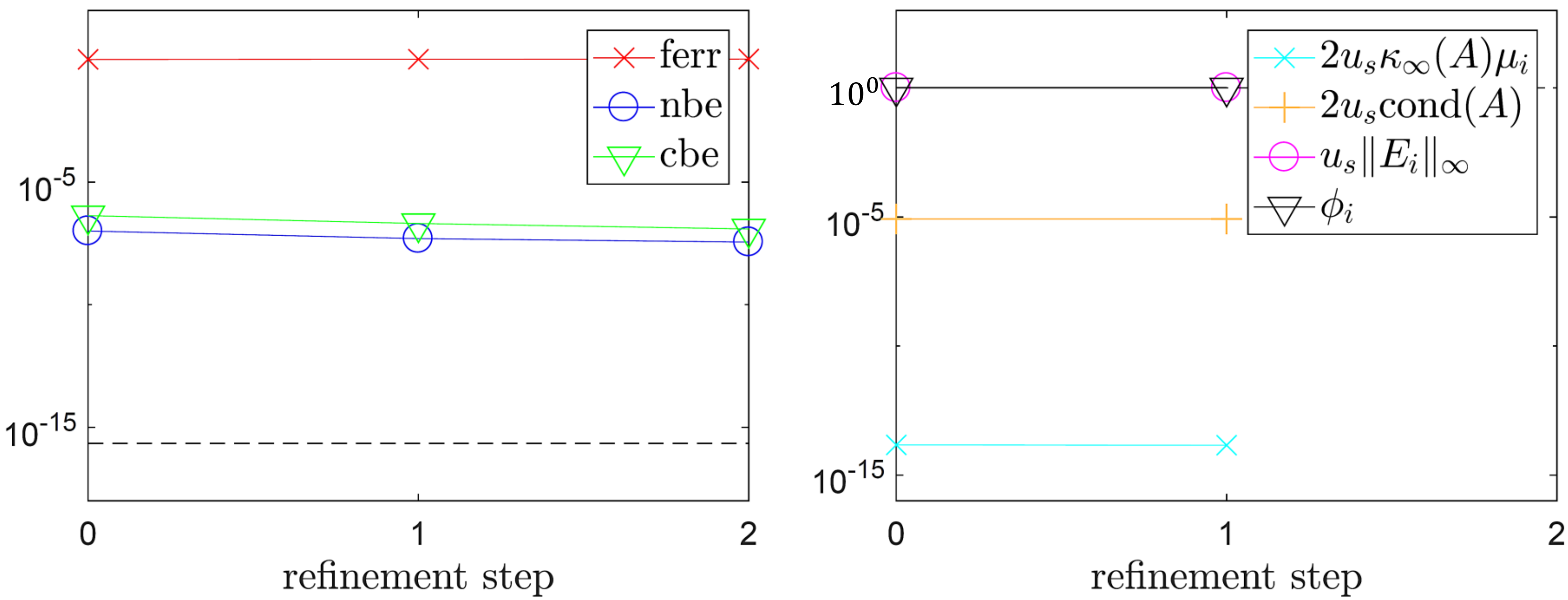

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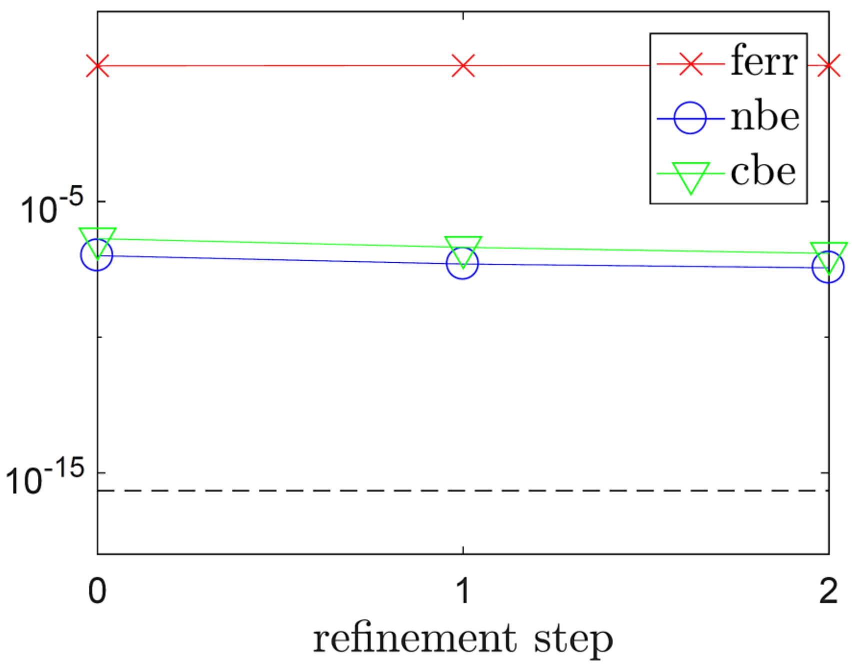

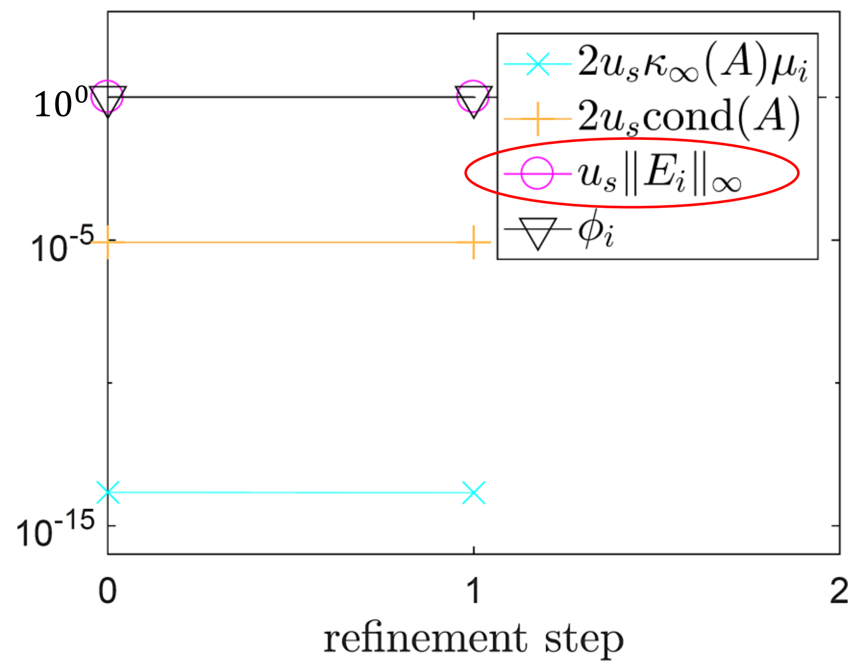

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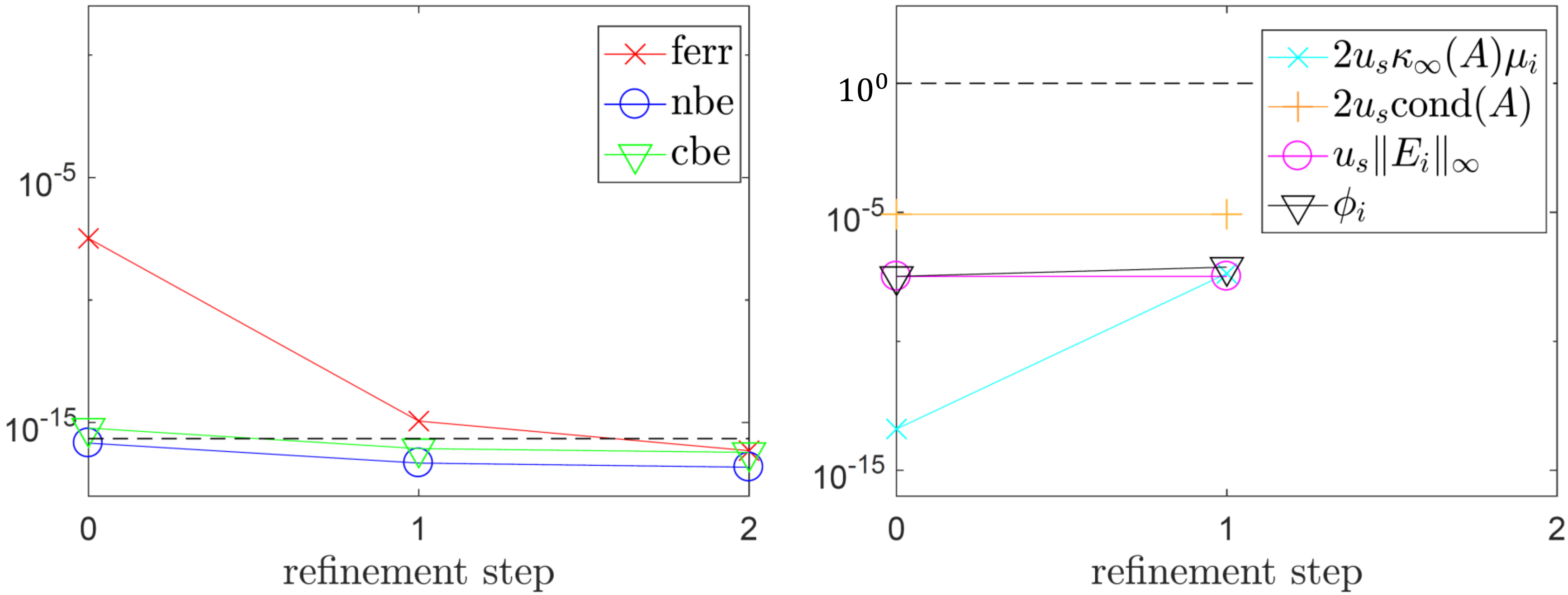

GMRES-Based Iterative Refinement

- Observation [Rump, 1990]: if $\widehat{L}$ and $\widehat{U}$ are computed LU factors of A in precision u_f, then

$$\kappa_\infty\big(\widehat{U}^{-1}\widehat{L}^{-1}A\big) \approx 1 + \kappa_\infty(A)u_f,$$

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<u>GMRES-IR</u> [C. and Higham, SISC 39(6), 2017]

- To compute the updates d_i, apply GMRES to $\overbrace{\hat{U}^{-1}\hat{L}^{-1}A}^{\tilde{A}}d_i = \overbrace{\hat{U}^{-1}\hat{L}^{-1}r_i}^{\tilde{r}_i}$

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Solve $Ax_0 = b$ by LU factorization

for $i = 0{:}\,\text{maxit}$

$r_i = b - Ax_i$

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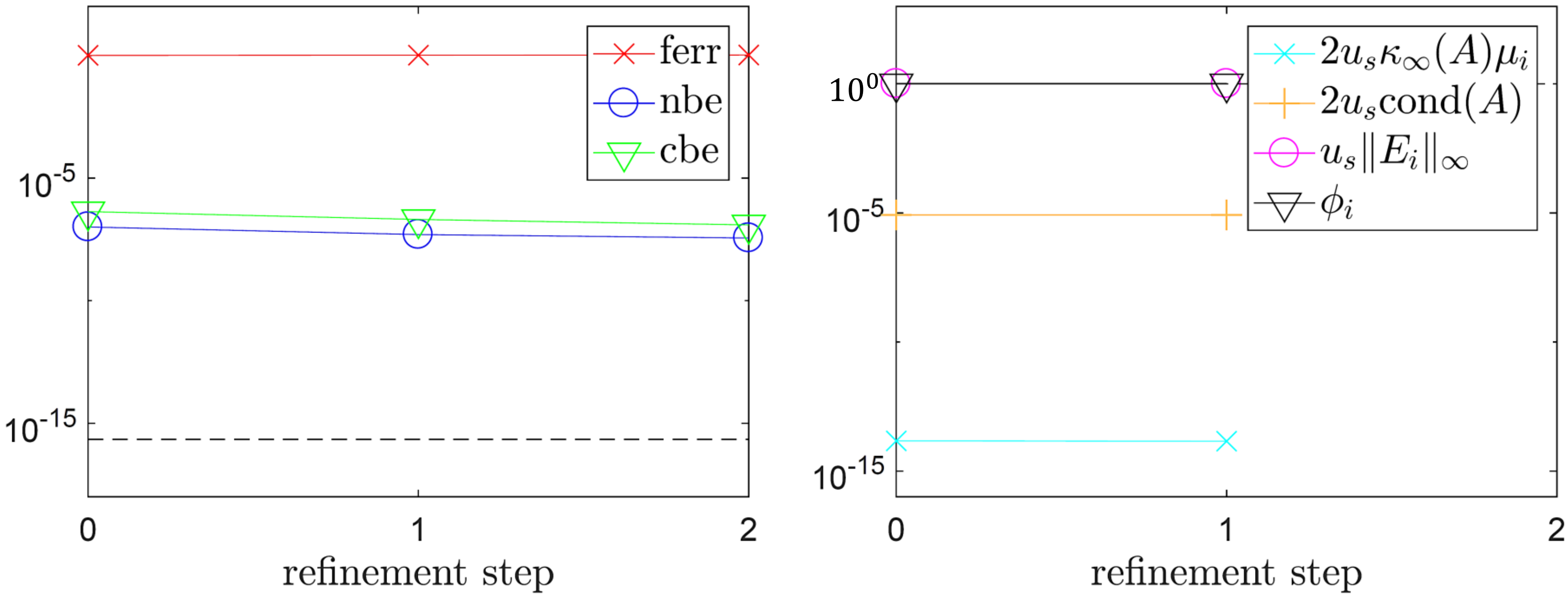

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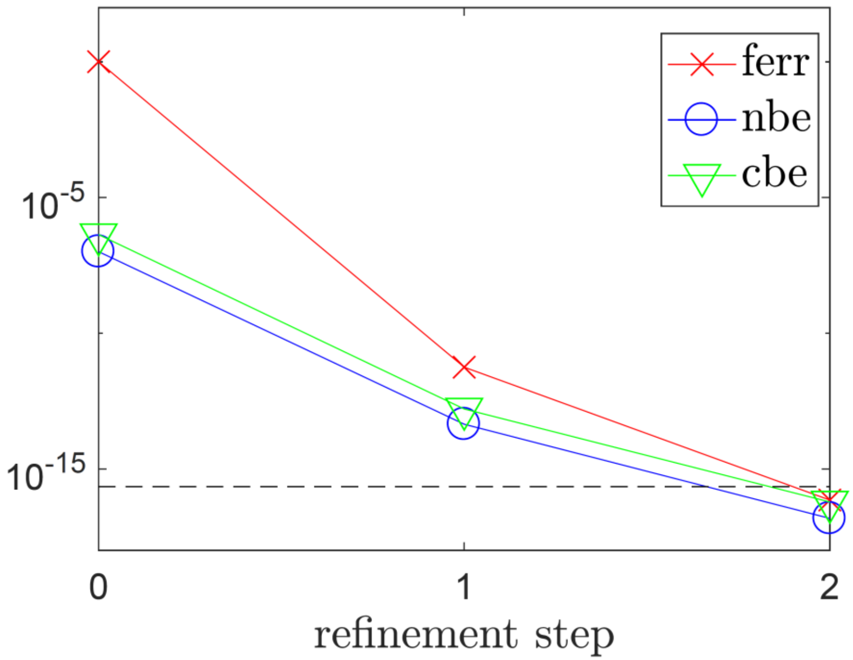

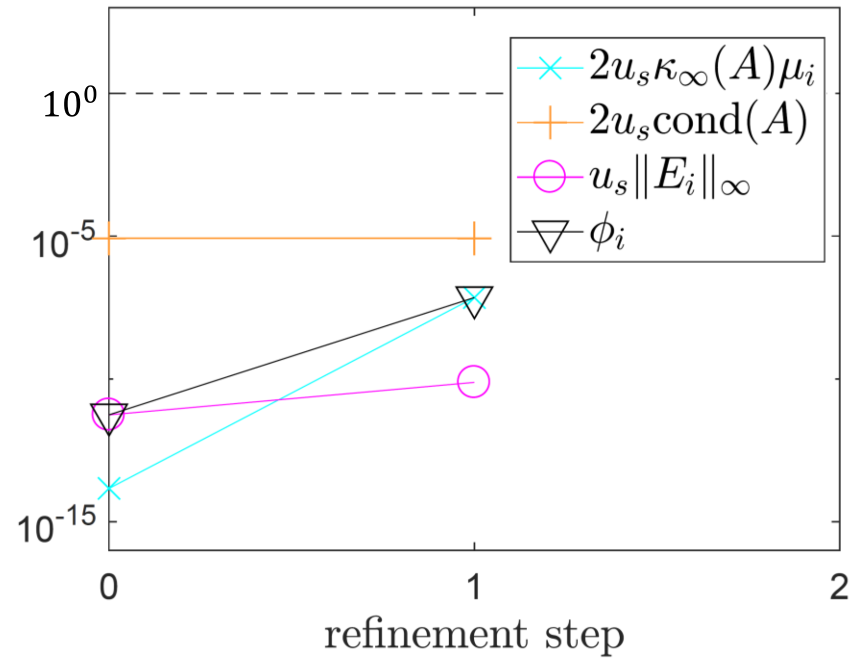

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LU-IR	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
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$\Rightarrow$With GMRES-IR, lower precision factorization will work for higher $\kappa_\infty(A)$

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

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Try IR3! MATLAB codes available at: https://github.com/eccarson/ir3

Comments and Caveats

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  - Smaller $\tau \rightarrow$ more GMRES iterations, potentially fewer refinement steps
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- Why GMRES?
  - Theoretical purposes: existing analysis and proof of backward stability [Paige, Rozložník, Strakoš, 2006]
  - In practice, use any solver you want!

Extension to 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 to Least Squares Problems

- (Björck,1967): Least squares problem can be written as a linear system with square matrix of size $(m+n)$:
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    - Many possibilities...requirements of theory vs. what works in practice

GMRES-IR for Least Squares

- Ex: block diagonal preconditioner ([Murphy, Golub, Wathen, 2000], [Ipsen, 2001])

$$\begin{bmatrix} \alpha I & 0 \\ 0 & \frac{1}{\alpha}\hat{R}^T\hat{R} \end{bmatrix} = \begin{bmatrix} \sqrt{\alpha} I & 0 \\ 0 & \frac{1}{\sqrt{\alpha}}\hat{R}^T \end{bmatrix} \begin{bmatrix} \sqrt{\alpha} I & 0 \\ 0 & \frac{1}{\sqrt{\alpha}}\hat{R} \end{bmatrix} \equiv M_1 M_2$$

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- Assuming QR factorization is exact,

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is nonsymmetric, diagonalizable, with eigenvalues $\left\{1, \frac{1}{2}\left(1 \pm \sqrt{5}\right)\right\}$.

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- If we take split preconditioner

$$M_1^{-1} \tilde{A} M_2{}^{-1} = \begin{bmatrix} I & A\hat{R} \\ \hat{R}^{-T}A^T & 0 \end{bmatrix}$$

we will have a well-conditioned system

  - However, split-preconditioned GMRES is not backward stable
  - Potentially useful in practice, not but in theory

GMRES-IR for Least Squares

- One option:

$$M = \begin{bmatrix} \alpha I & \hat{Q}_1 \hat{R} \\ \hat{R}^T \hat{Q}_1^T & 0 \end{bmatrix}$$

- Then we can prove that for the left-preconditioned system,

$$\kappa\left(M^{-1}\tilde{A}\right) \leq \left(1 + \boldsymbol{u_f} c\, \kappa(A)\right)^2$$

where $c = O(m^{7/2})$, where we note this bound is pessimistic.

- Thus even if $\kappa(A) \gg \boldsymbol{u_f}^{-1}$, the preconditioned system can still be reasonably well conditioned

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- Thus even if $\kappa(A) \gg \boldsymbol{u_f}^{-1}$, the preconditioned system can still be reasonably well conditioned
- GMRES run on $\tilde{A}$ with left-preconditioner M gives

$$\boldsymbol{u_s} \|E_i\|_\infty \equiv \boldsymbol{u}\, f(m+n)\kappa_\infty(M^{-1}\tilde{A})$$

where f is a quadratic polynomial

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$$\kappa\left(M^{-1}\tilde{A}\right) \leq \left(1 + \boldsymbol{u_f} c\, \kappa(A)\right)^2$$

where $c = O(m^{7/2})$, where we note this bound is pessimistic.

- Thus even if $\kappa(A) \gg \boldsymbol{u_f}^{-1}$, the preconditioned system can still be reasonably well conditioned

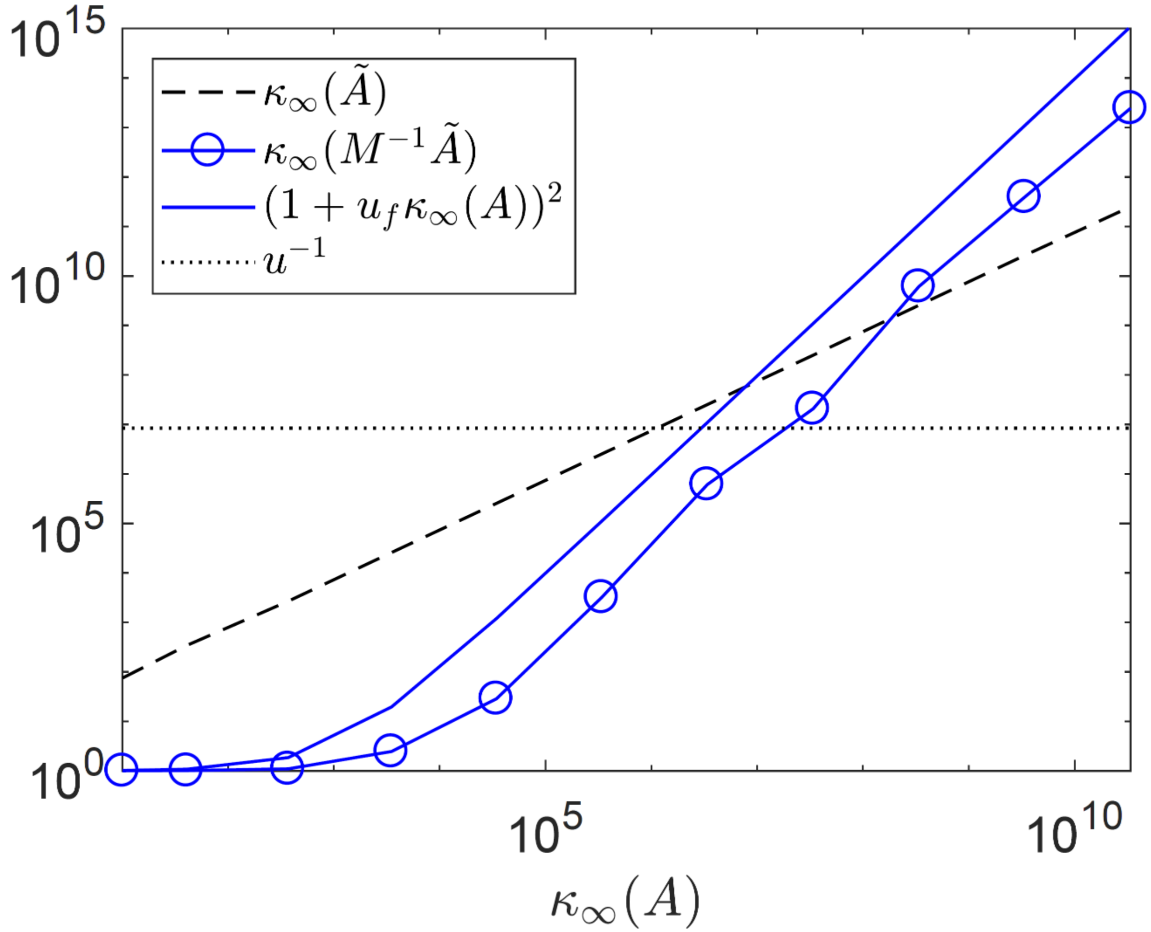
- GMRES run on $\tilde{A}$ with left-preconditioner M gives

$$\boldsymbol{u_s} \|E_i\|_\infty \equiv \boldsymbol{u}\, f(m+n)\kappa_\infty(M^{-1}\tilde{A})$$

where f is a quadratic polynomial

- So for GMRES-based LSIR, $\boldsymbol{u_s} \equiv \boldsymbol{u}$; expect convergence of forward error when $\kappa_\infty(A) < \boldsymbol{u}^{-1/2}\boldsymbol{u_f}^{-1}$

```
gallery('randsvd', [100,10], kappa(i), 3)
```
QR factorization computed in half precision; preconditioned system computed exactly

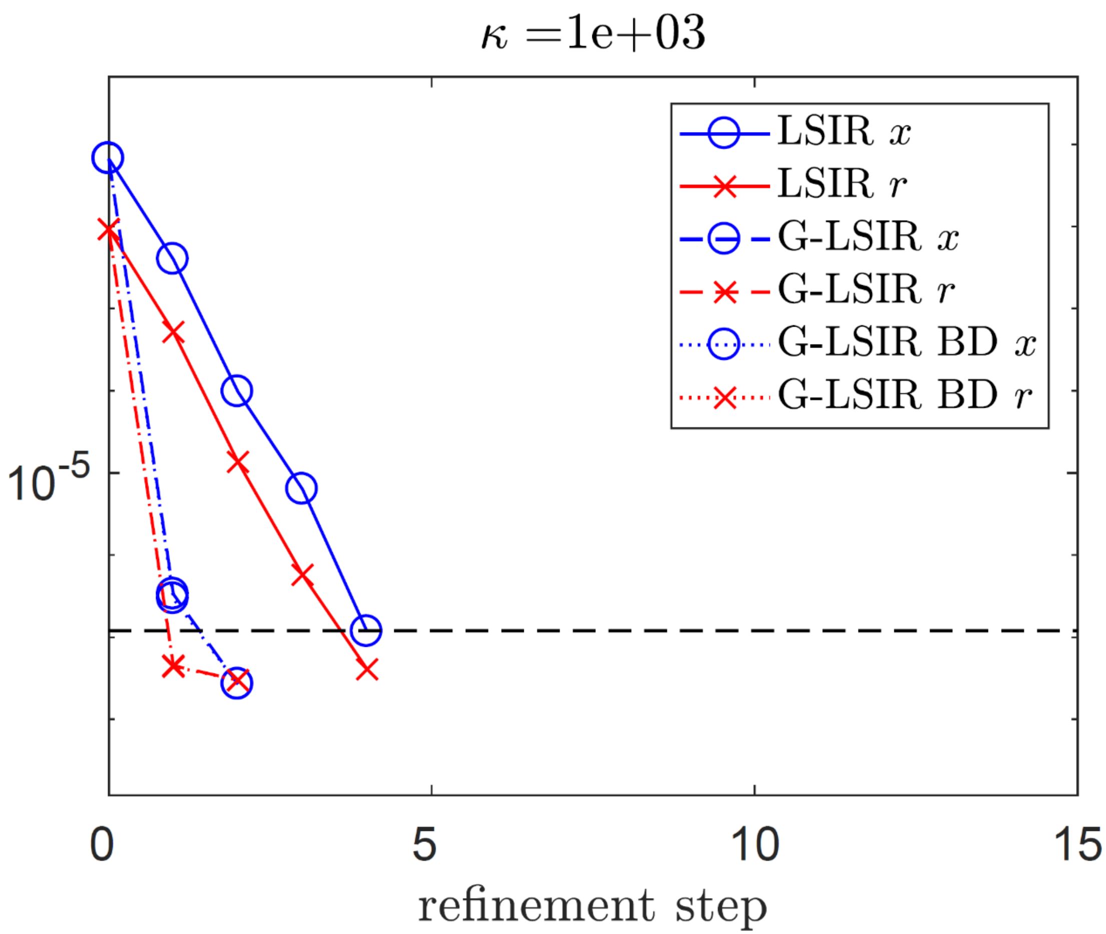


```
A = gallery('randsvd', [100, 10], kappa, 3)
b = randn(100,1); b = b./norm(b)
```

m n

GMRES-LSIR and "Standard" LSIR with

u_f: half, u: single, u_r: double



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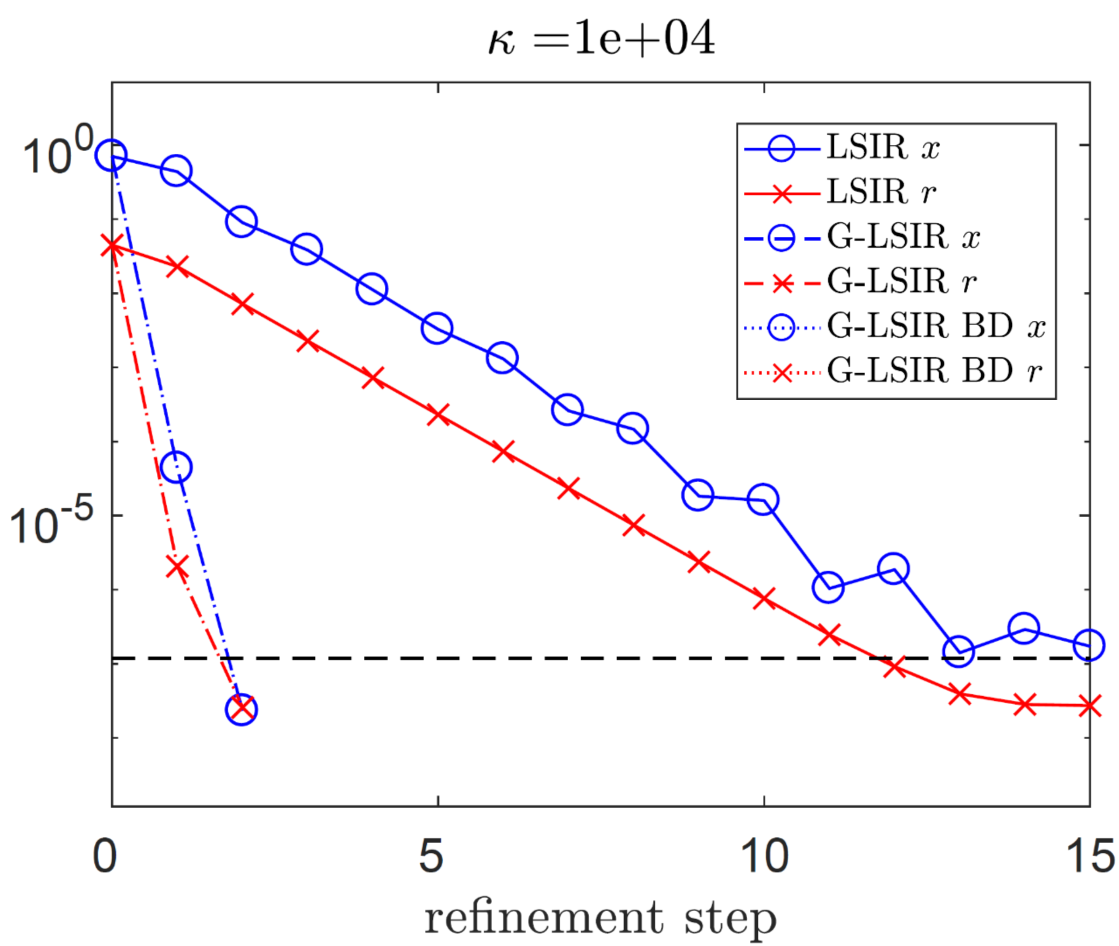

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```

GMRES-LSIR and "Standard" LSIR with

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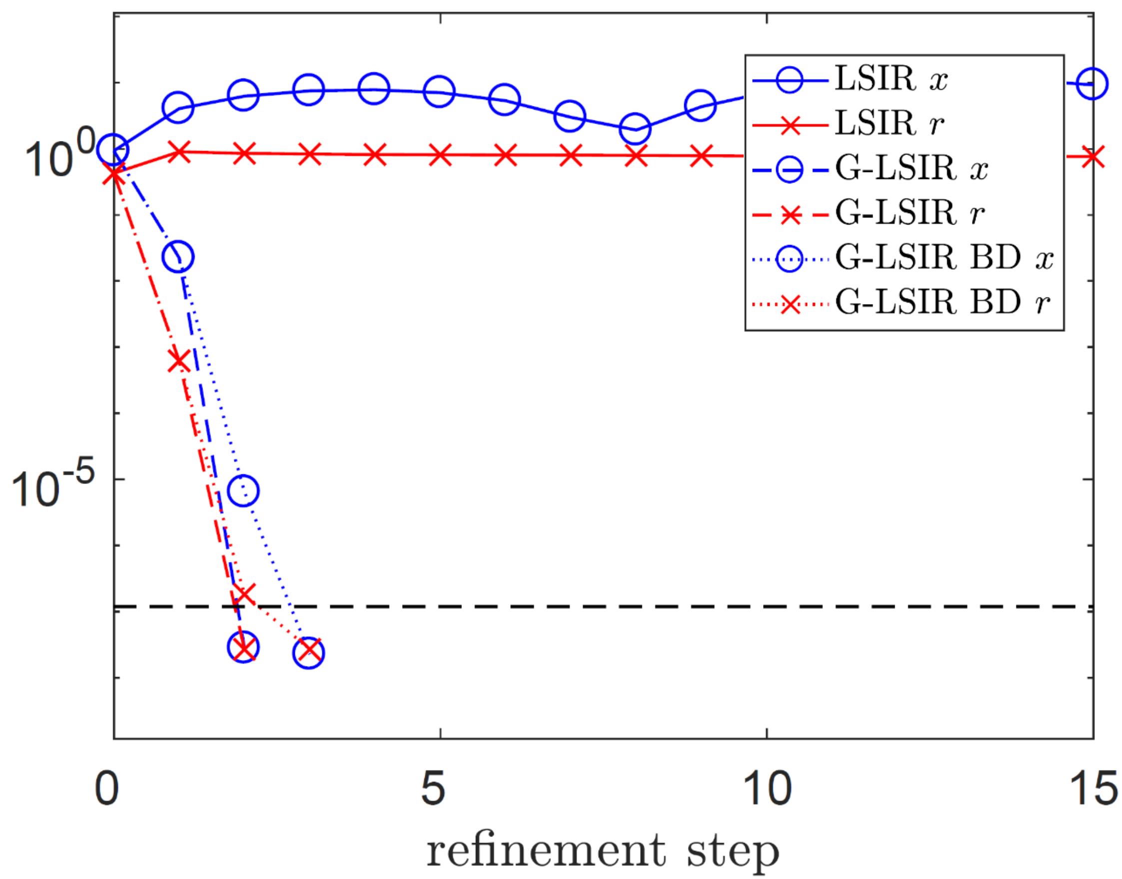
κ =1e+06



The rise of multiprecision hardware

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- Lower-precision arithmetic is faster and more energy efficient, but the potential for its use depends heavily on the particular problem and algorithm
- As numerical analysts, we must determine when and where we can exploit lower-precision hardware to improve performance

Thank You!

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