Error Bounds for Iterative Refinement in Three Precisions

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SIAM Annual Meeting
Portland, Oregon
July 13, 2018

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
- Aurora Exascale supercomputer: (2021) Expected extensive support for reduced-precision arithmetic (32/16/8-bit)

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)

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"Fixed-Precision"

[Jankowski and Woźniakowski, 1977], [Skeel, 1980], [Higham, 1991]

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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	$u_f = u, u_r = u^2$
Fixed precision	$u_f = u = u_r$
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(and **improves** upon existing analyses in some cases)

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

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

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For a stable refinement scheme, in early stages we expect

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

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But close to convergence,

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

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$$\|r_i\|_2 = \mu_i^{(2)} \|A\|_2 \|x - \hat{x}_i\|_2$$

$$x - \hat{x}_i \quad = \quad V\Sigma^{-1}U^T r_i \quad = \quad \sum_{j=1}^{n} \frac{(u_j^T r_i) v_j}{\sigma_j} \qquad\qquad (A = U\Sigma V^T)$$

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- Wilkinson (1977), comment in unpublished manuscript: $\mu_i^{(2)}$ increases with i

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Assume computed solution $\hat{d}_i$ to $Ad_i = \hat{r}_i$ satisfies:

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

Forward Error for IR3

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

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

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

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

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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

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

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

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

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

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

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}	$\text{cond}(A,x)\cdot 10^{-8}$
H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
H	D	D	10^4	10^{-16}	10^{-16}	$\text{cond}(A,x)\cdot 10^{-16}$
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}
S	D	D	10^8	10^{-16}	10^{-16}	$\text{cond}(A,x)\cdot 10^{-16}$
S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}

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

IR3: Summary

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	u_f	u	u_r	max $\kappa_\infty(A)$	Backward error: norm	Backward error: comp	Forward error
LP fact.	H	S	S	10^4	10^{-8}	10^{-8}	$\text{cond}(A,x) \cdot 10^{-8}$
New	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
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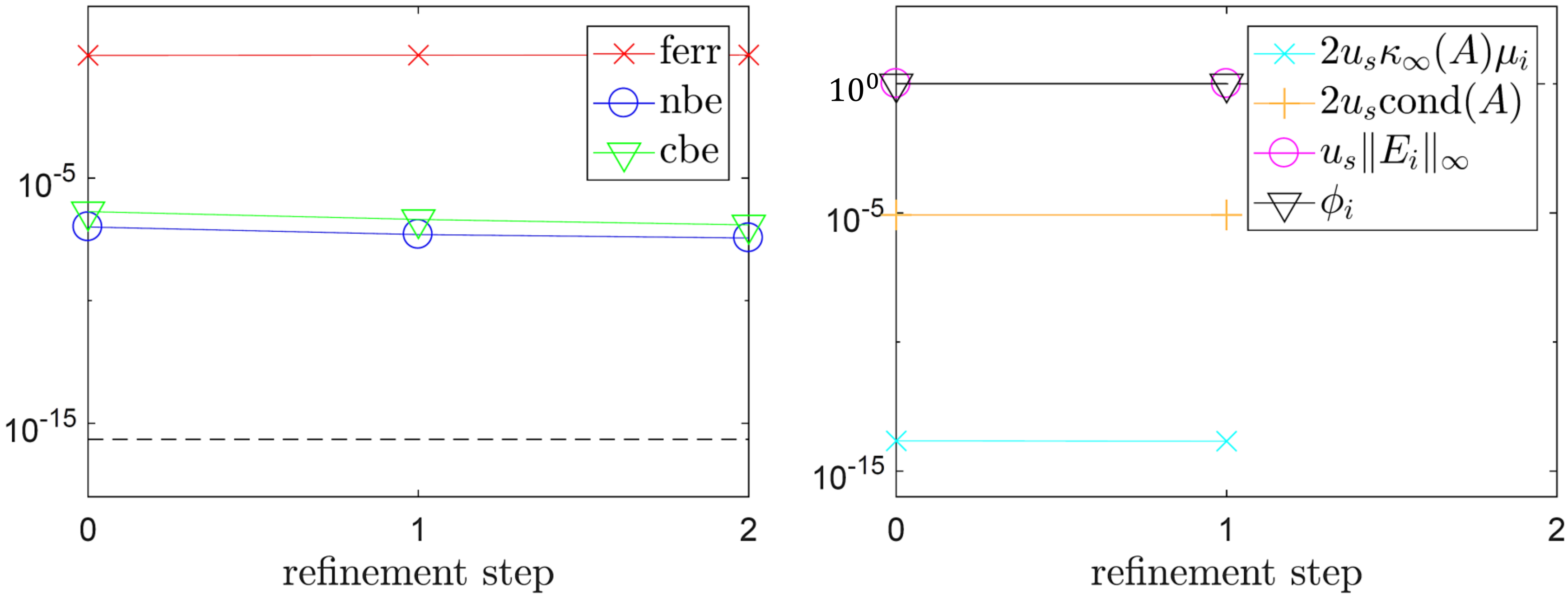
New	S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}

$\Rightarrow$ 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!

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

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

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



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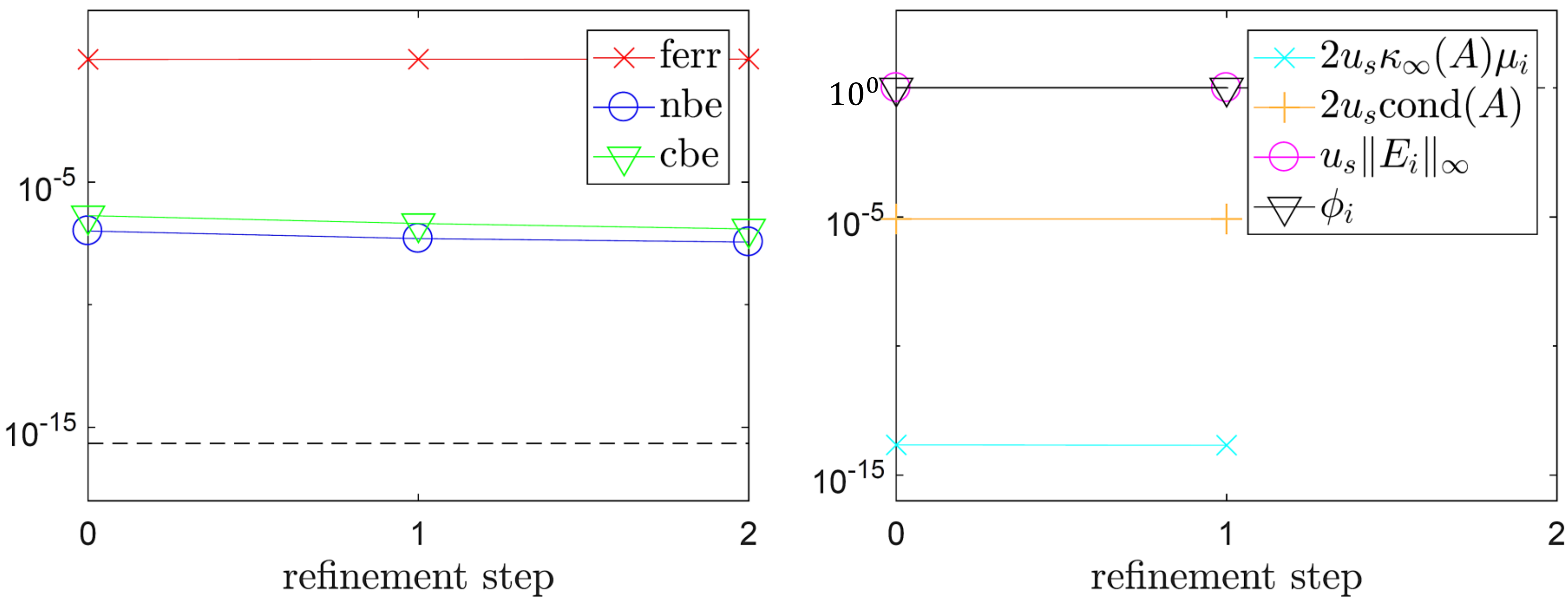
Standard (LU-based) IR with u_f: single, u: double, u_r: quad



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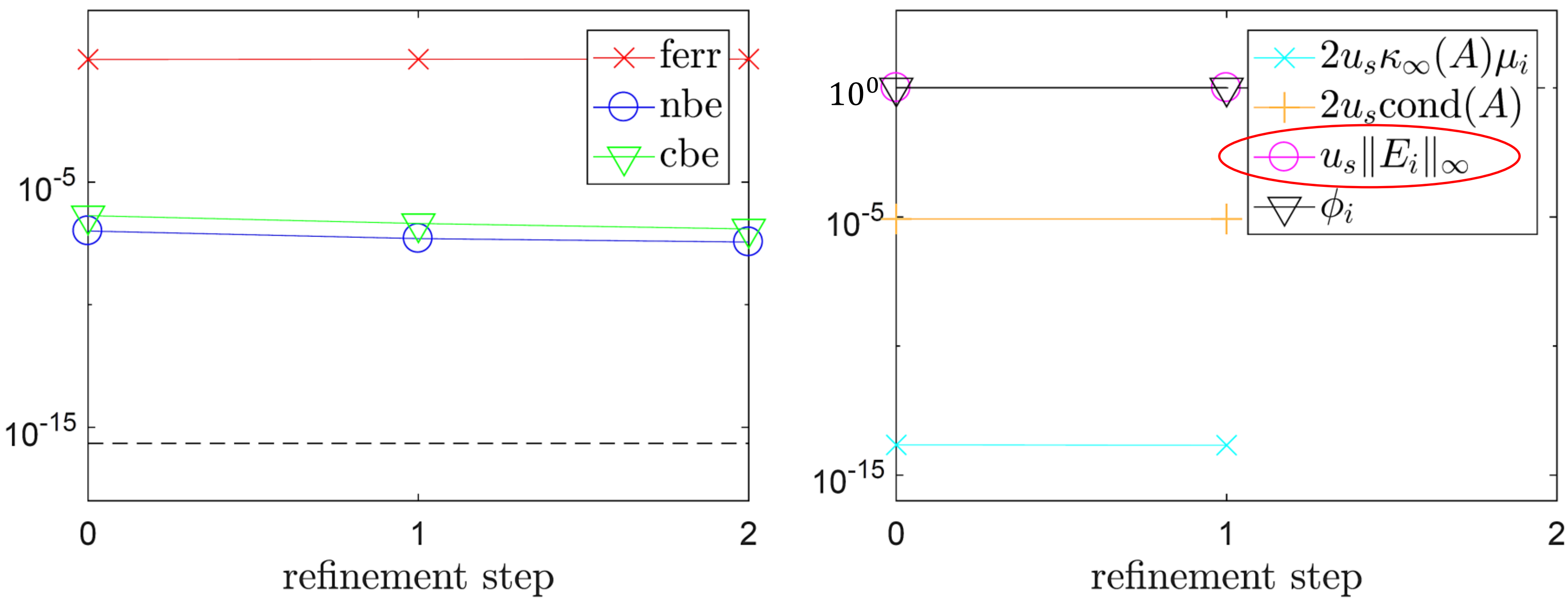

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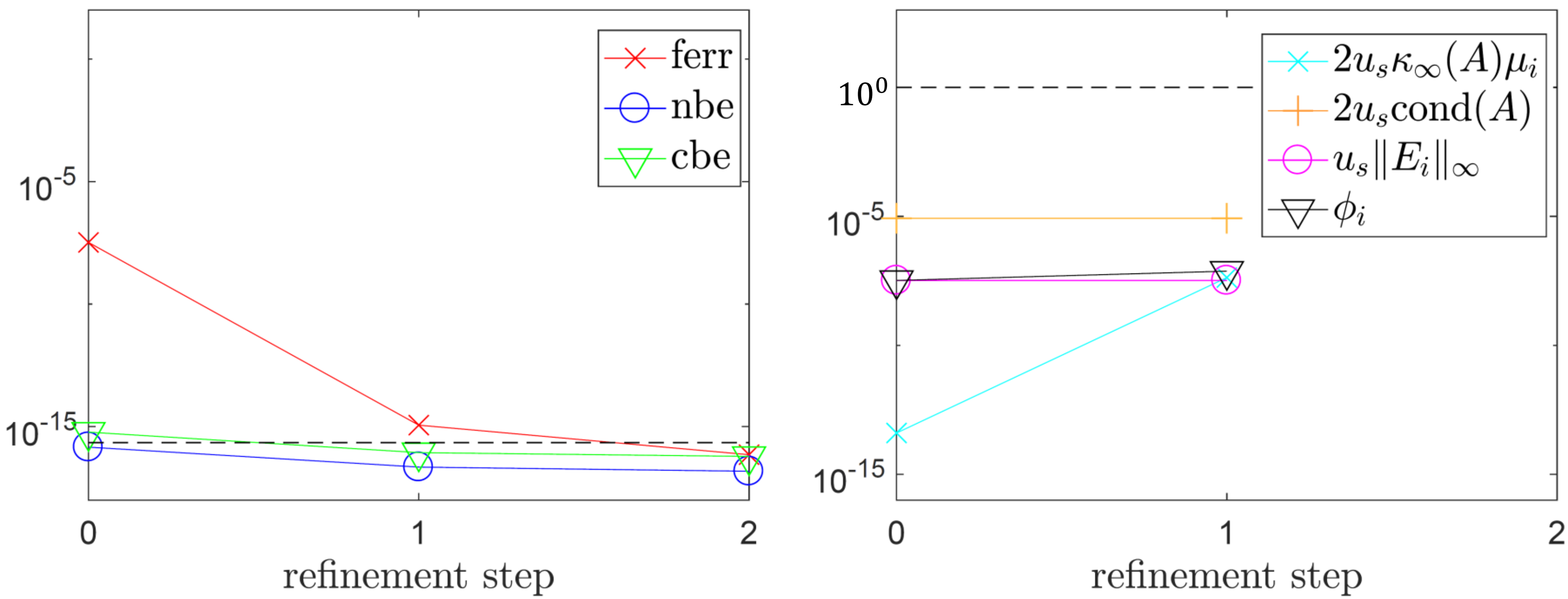
Standard (LU-based) IR with u_f: double, u: double, u_r: quad



GMRES-Based Iterative Refinement

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

$$\kappa_\infty\left(\hat{U}^{-1}\hat{L}^{-1}A\right) \approx 1 + \kappa_\infty(A)u_f,$$

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

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

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Solve $Ax_0 = b$ by LU factorization

for $i = 0$: maxit

$r_i = b - Ax_i$

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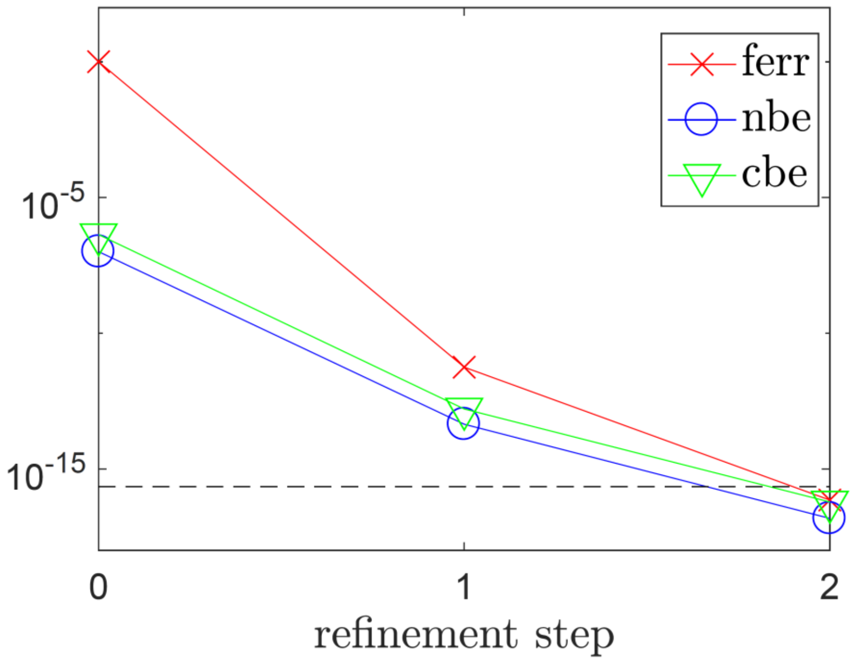
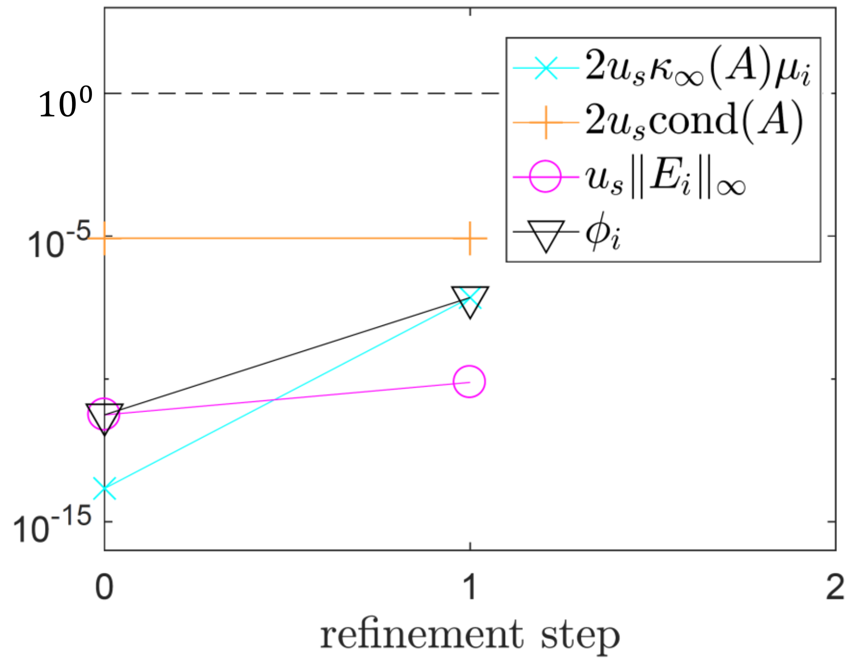
$\kappa_\infty(A) \approx$ 2e10, $\mathrm{cond}(A,x) \approx$ 5e9, $\kappa_\infty(\tilde{A}) \approx$ 2e4

GMRES-IR with u_f: single, u: double, u_r: quad





GMRES-IR: Summary

Benefits of GMRES-IR:

	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}
GMRES-IR	S	D	Q	10^{16}	10^{-16}	10^{-16}	10^{-16}
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}

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

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⇒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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$\Rightarrow$ If $\kappa_\infty(A) \leq 10^{12}$, can use lower precision factorization w/no loss of accuracy!

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

Performance results? Stay tuned for the next talk by Azzam Haidar;
3-precision approach on NVIDIA V100

Comments and Caveats

- Convergence tolerance τ for GMRES?
  - Smaller $\tau \rightarrow$ more GMRES iterations, potentially fewer refinement steps
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    - e.g., if $\tilde{A}$ still has cluster of eigenvalues near origin, GMRES can stagnate until n^{th} iteration, regardless of $\kappa_\infty(A)$ [Liesen and Tichý, 2004]

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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!

Thank You!

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