Iterative Refinement in Three Precisions

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Charles University

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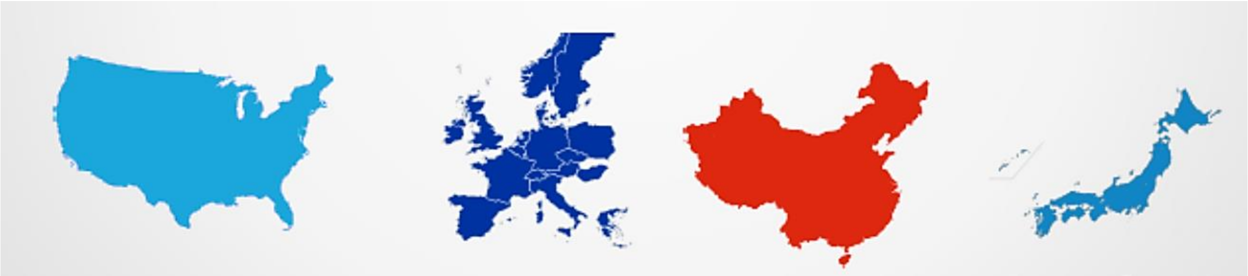
Exascale Computing: The Modern Space Race

- "Exascale": $\mathbf{10^{18}}$ **floating point operations per second**
  - with **maximum energy consumption around 20-40 MWatts**

- Large investment in HPC worldwide



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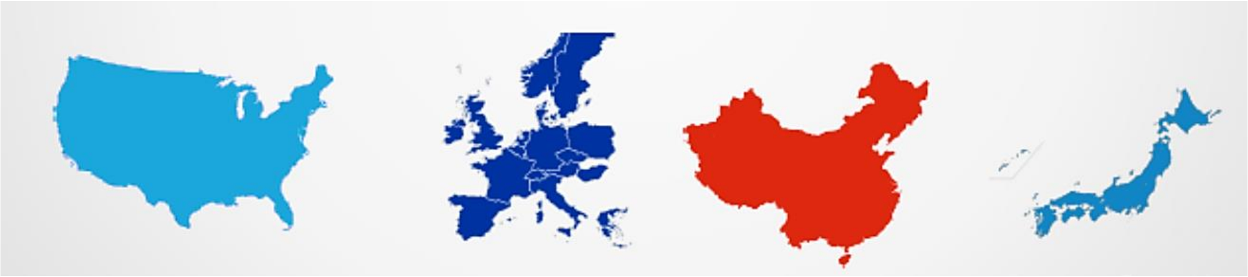

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hardware to algorithms to applications

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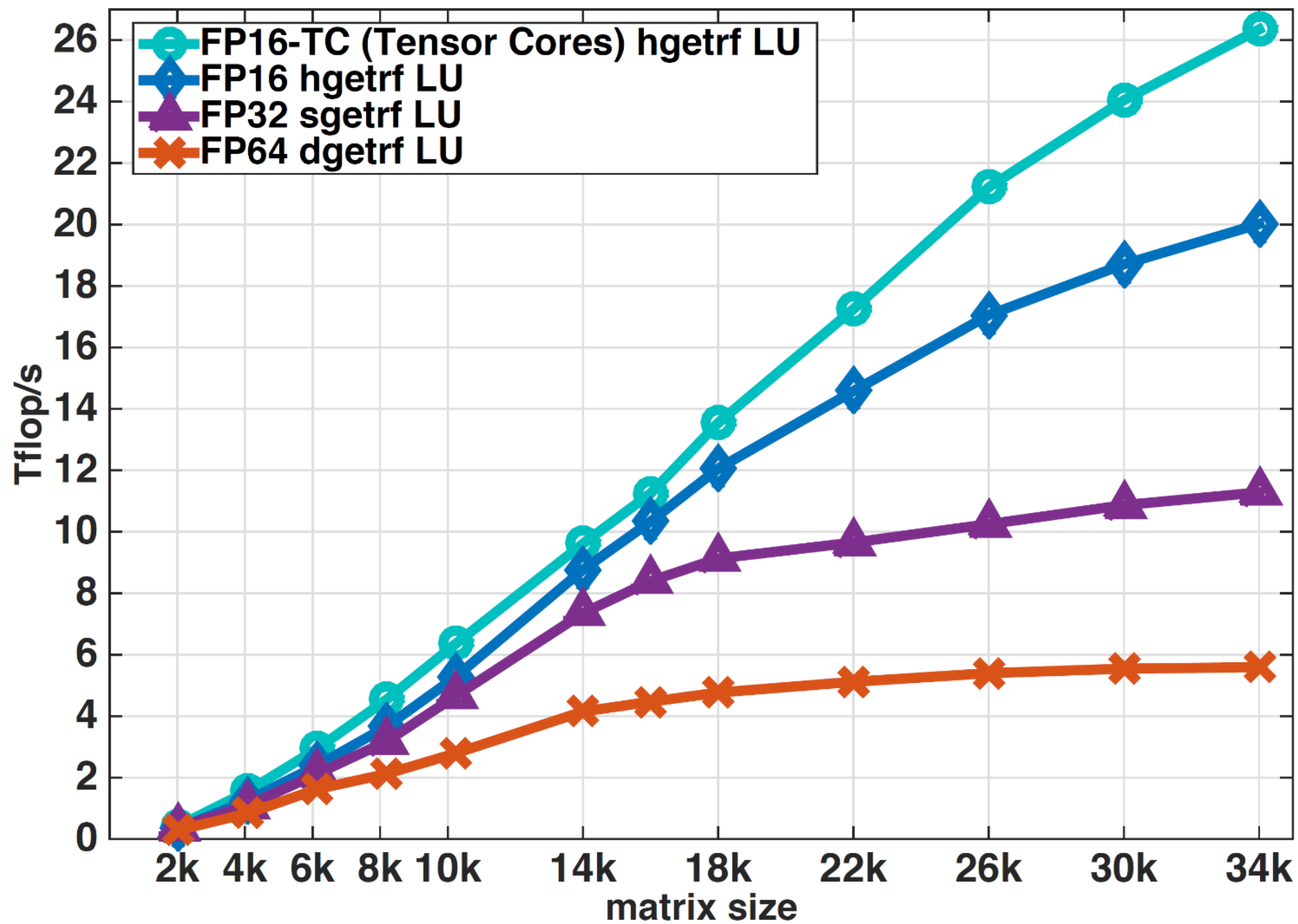
Hardware Support for Multiprecision Computation

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

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

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

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

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

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

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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.

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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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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example: LU solve:

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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

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

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

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

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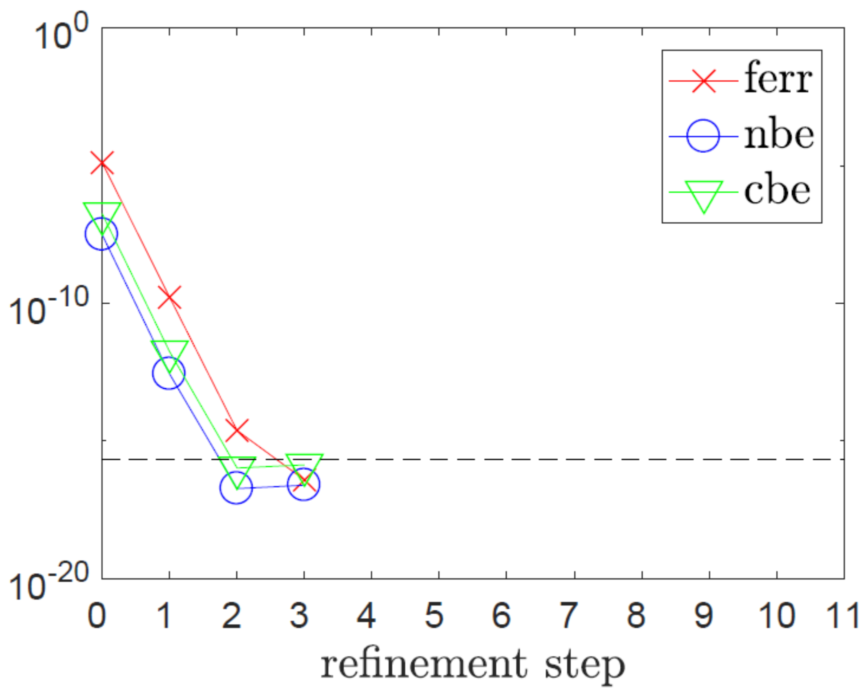
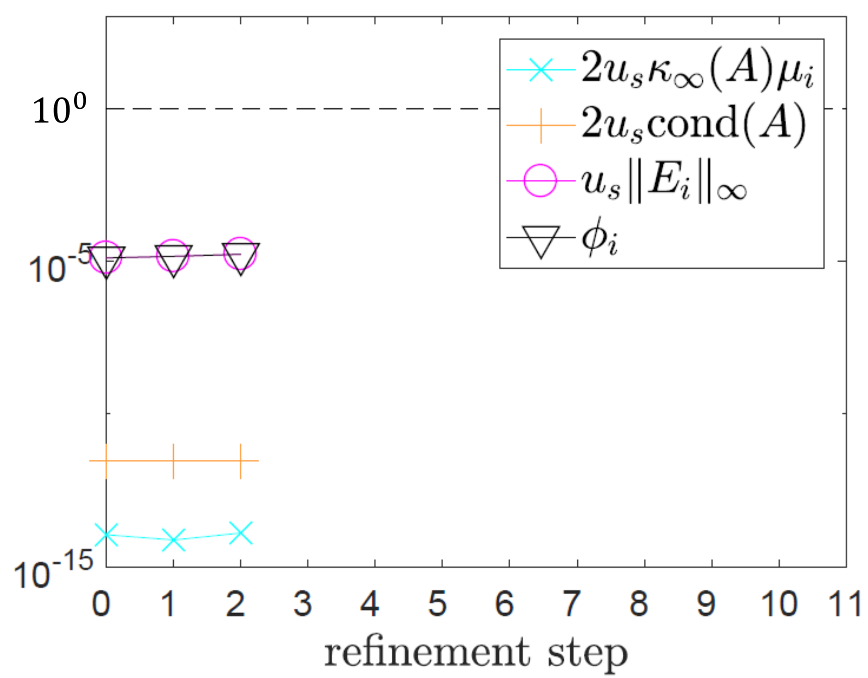
$\Rightarrow$ Benefit of IR3 vs. traditional IR: As long as $\kappa_\infty(A) \leq 10^4$, can use lower precision factorization w/no loss of accuracy!

```
A = gallery('randsvd', 100, 1e3)
b = randn(100,1)
```

$\kappa_\infty(A) \approx$ **1e4**

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

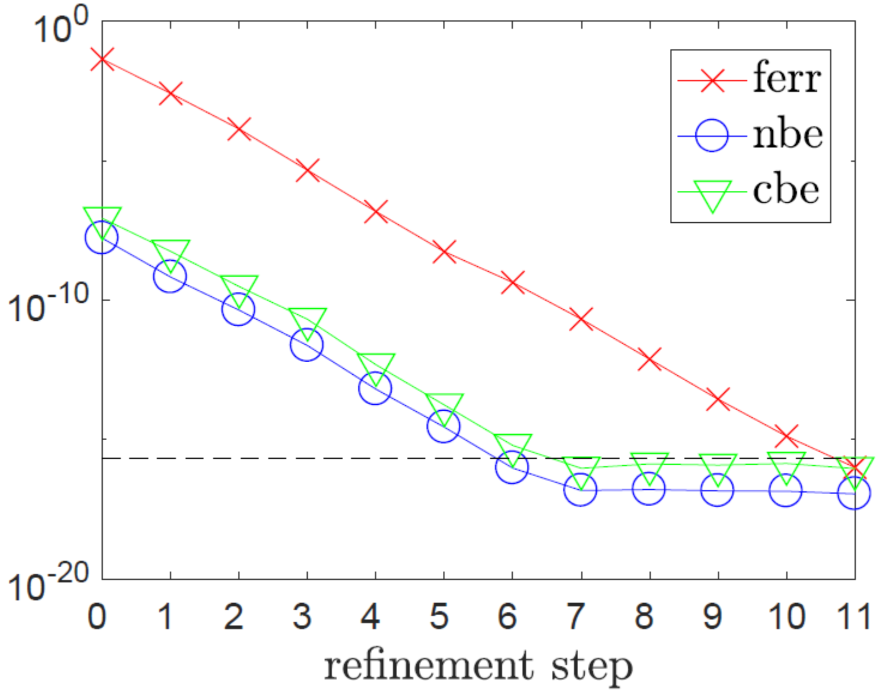


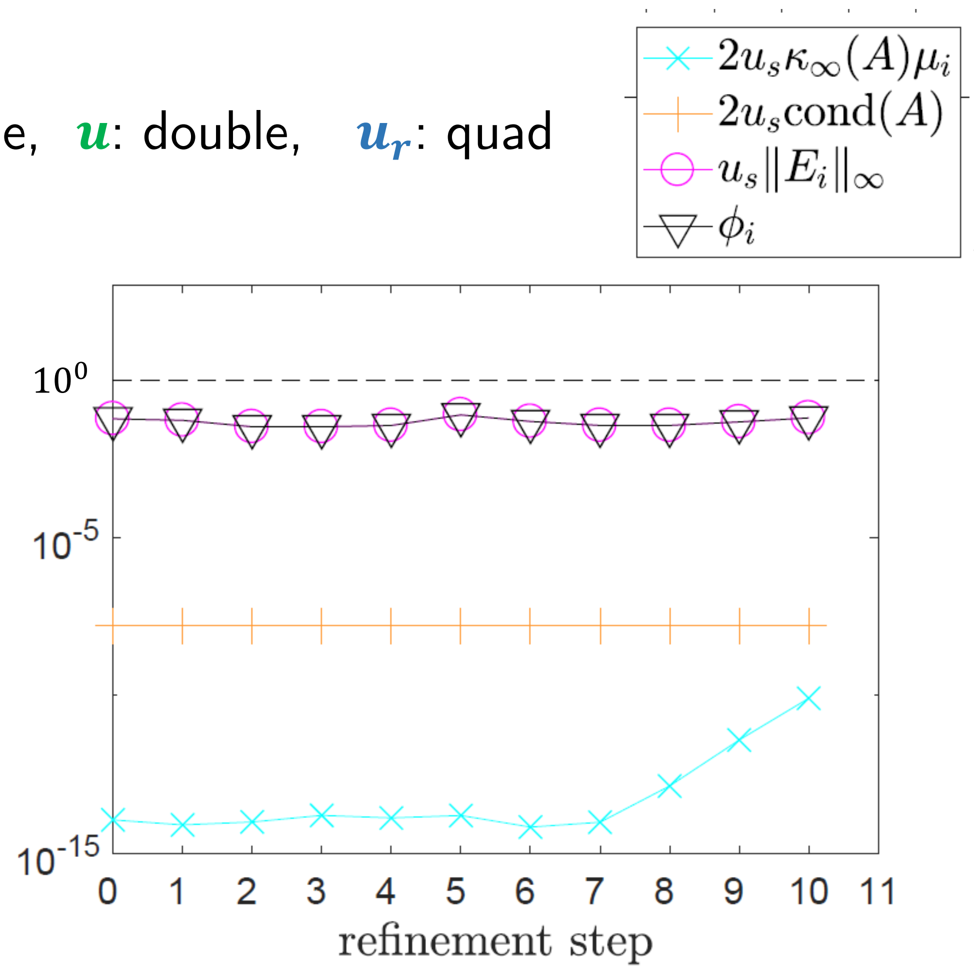


```
A = gallery('randsvd', 100, 1e7)
b = randn(100,1)
```

$\kappa_\infty(A) \approx$ **7e7**

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

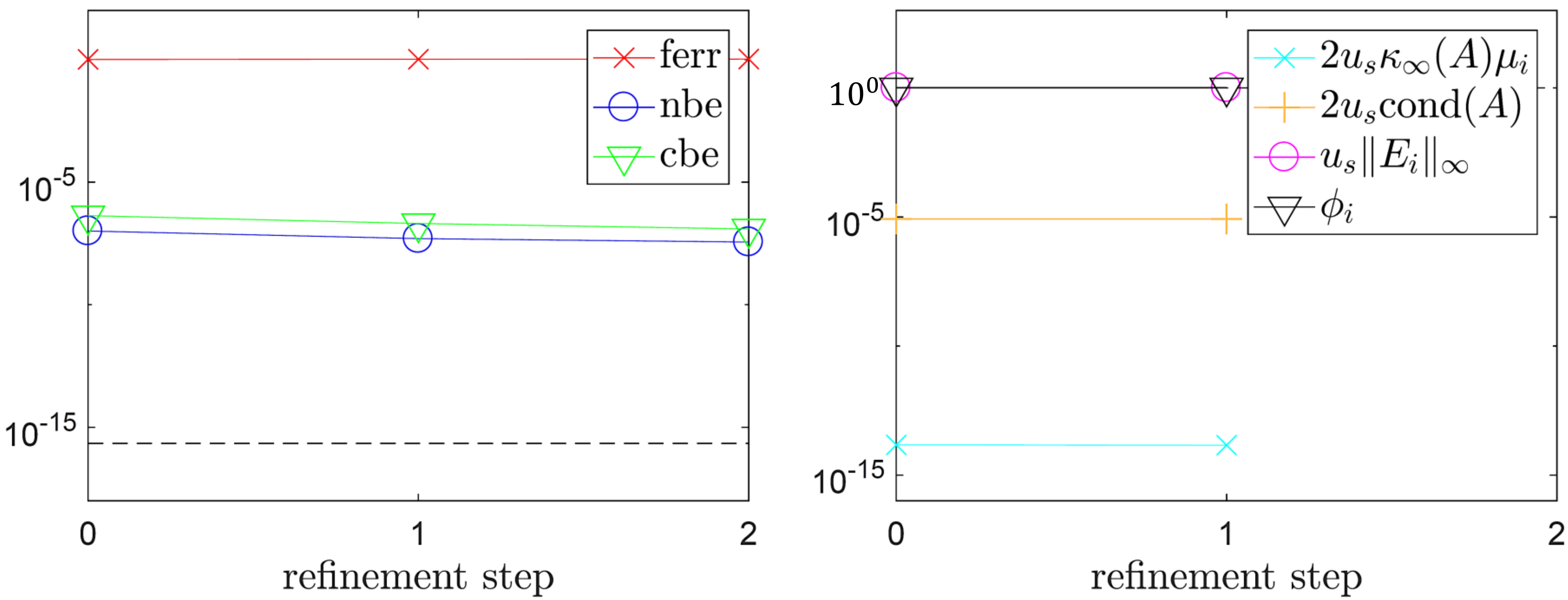




```
A = gallery('randsvd', 100, 1e9)
b = randn(100,1)
```

$\kappa_\infty(A) \approx$ **2e10**

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



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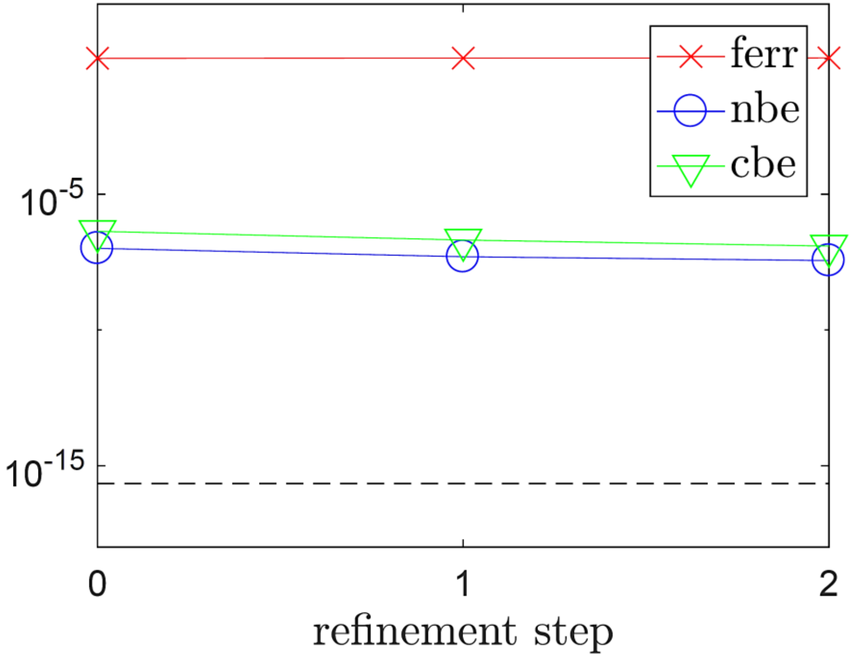

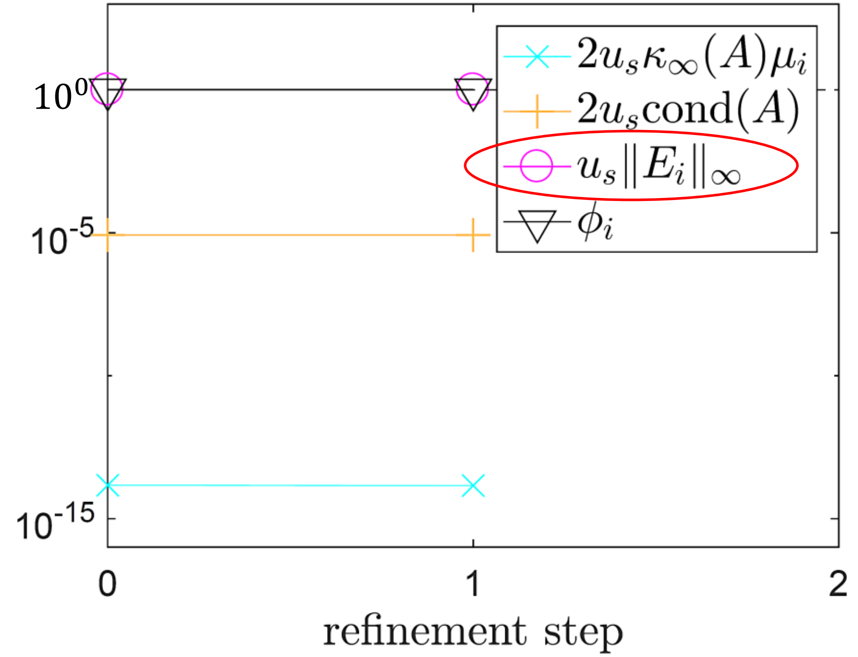

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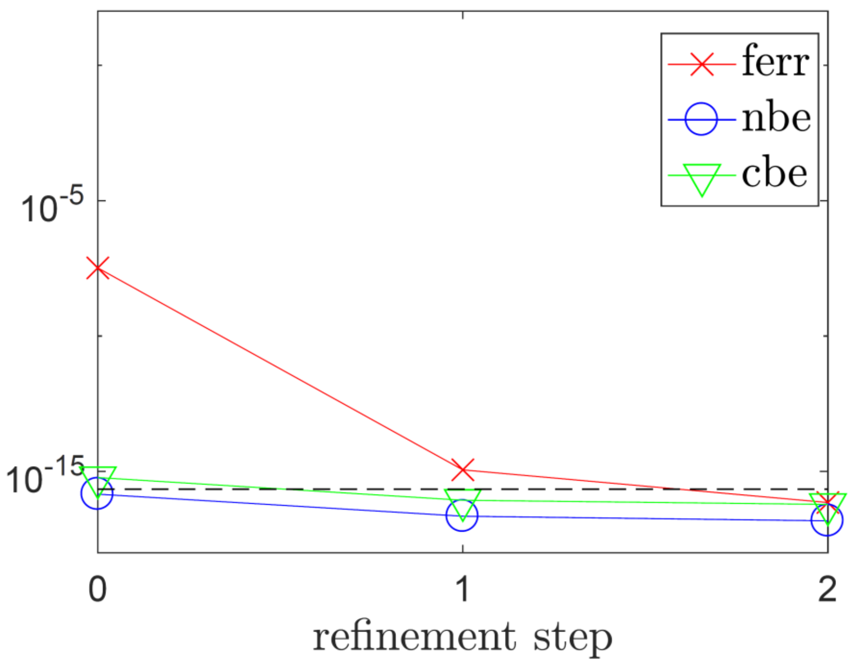
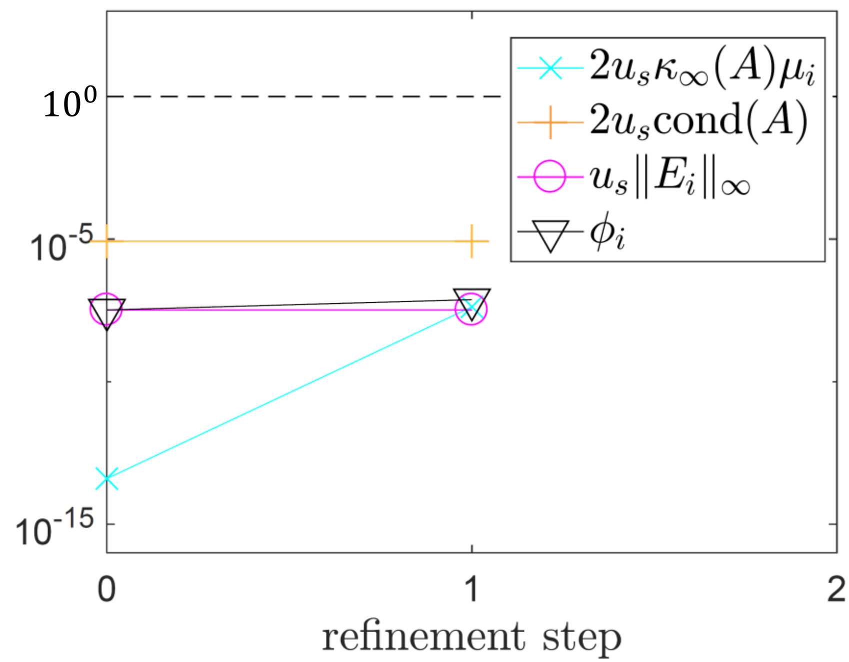
Standard (LU-based) IR with u_f: double, u: double, u_r: quad





GMRES-Based Iterative Refinement

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

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

even if $\kappa_\infty(A) \gg u_f^{-1}$.

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GMRES-IR [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 $i = 0\colon \text{maxit}$

$r_i = b - Ax_i$

Solve $Ad_i = r_i$ via GMRES on $\tilde{A}d_i = \tilde{r}_i$

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

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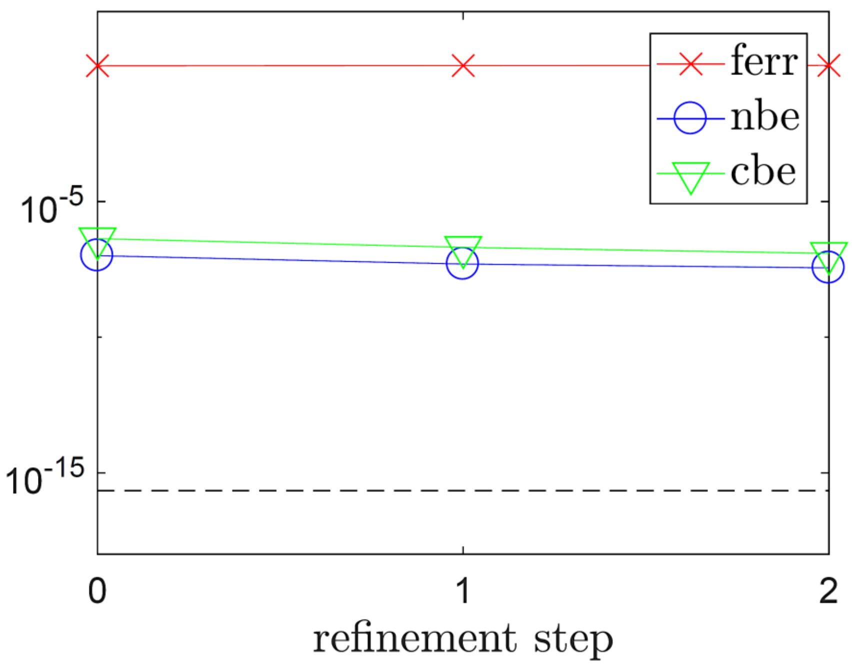
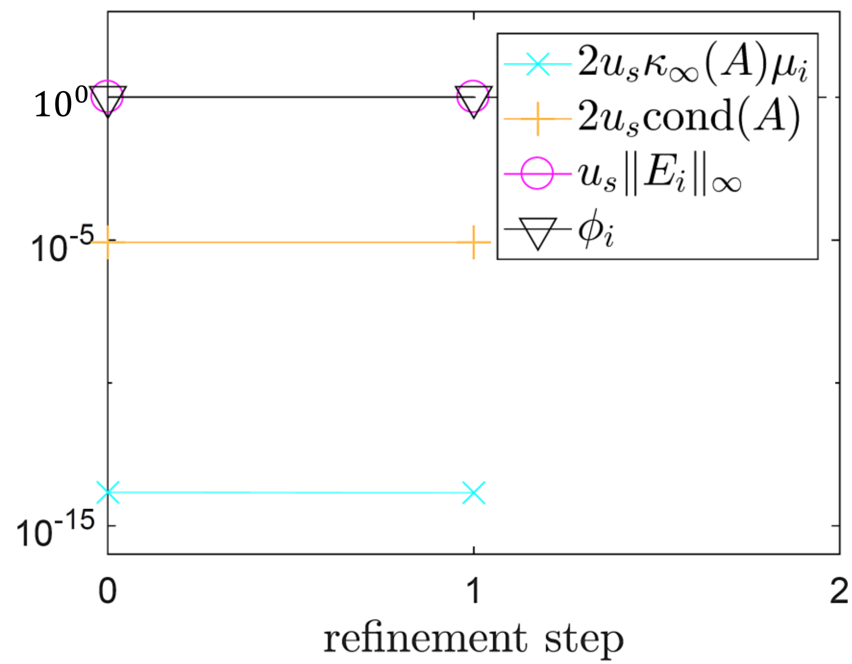
$\boldsymbol{u_s} = \boldsymbol{u}$

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

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

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





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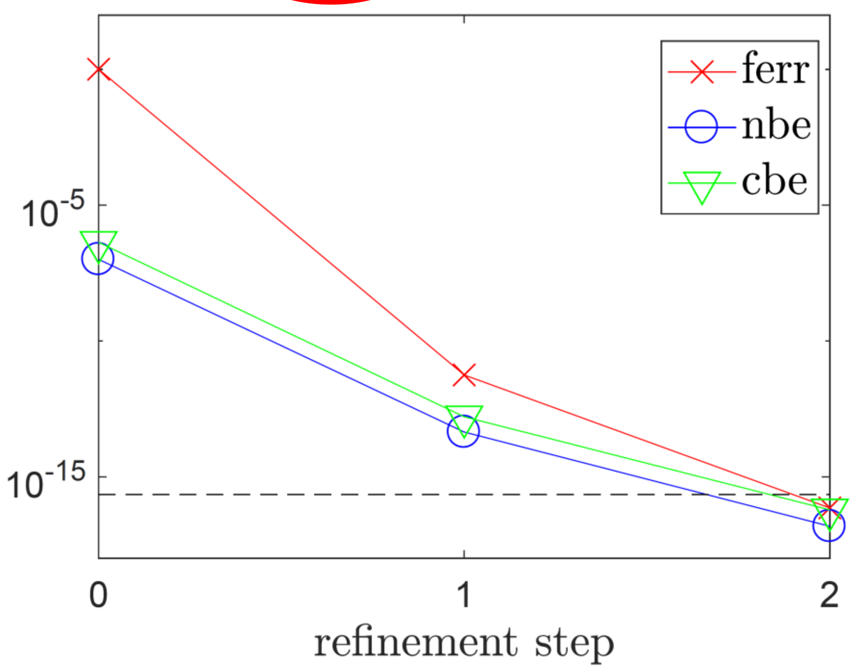
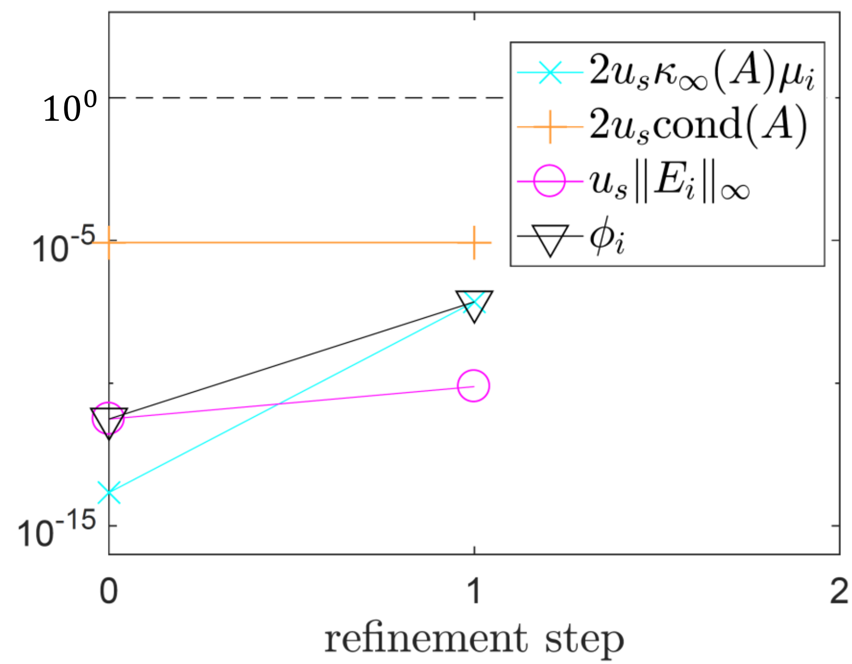
```

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

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





Number of GMRES iterations: (2,3)

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

GMRES-IR: Summary

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

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

GMRES-IR: Summary

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

Comments and Caveats

- Convergence tolerance τ for GMRES?
  - Smaller $\tau \rightarrow$ more GMRES iterations, potentially fewer refinement steps
  - Larger $\tau \rightarrow$ fewer GMRES iterations, potentially more refinement steps

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  - If A is ill conditioned and LU factorization is performed in very low precision, it can be a poor preconditioner
    - 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!

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

Least Squares Iterative Refinement

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

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

Results for 3-precision IR for linear systems **also applies to least squares problems**

Least Squares Iterative Refinement

- To apply the existing analysis, we must consider:
  1. How is the condition number of $\tilde{A}$ related to the condition number of A?
  2. What are bounds on the forward and backward error in solving the correction equation $\tilde{A}d_i = \tilde{r}_i$?
     - We now have a QR factorization rather than an LU factorization, and the augmented system has structure which can be exploited

Augmented System Condition Number

- Result of Björck (1967):

The matrix

$$\tilde{A}_\alpha = \begin{bmatrix} \alpha I & A \\ A^T & 0 \end{bmatrix}$$

has condition number bounded by

$$\sqrt{2}\kappa_2(A) \le \min_\alpha \kappa_2\left(\tilde{A}_\alpha\right) \le 2\kappa_2(A), \qquad \max_\alpha \kappa_2\left(\tilde{A}_\alpha\right) > \kappa_2(A)^2$$

and $\min_\alpha \kappa_2\left(\tilde{A}_\alpha\right)$ is attained for $\alpha = 2^{-\frac{1}{2}}\sigma_{min}(A)$.

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- Scaling does not change the solution to least squares problem; further, if α is a power of the machine base, it doesn't affect rounding errors
  $\Rightarrow$ Safe to assume that $\kappa_2(\tilde{A})$ is the same order of magnitude as $\kappa_2(A)$

LS-IR in 3 precisions

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For $i = 0, \dots$

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

$$h = U^{-T} g_i$$

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = [Q_1, Q_2]^T f_i$$

$$\Delta r_i = Q\begin{bmatrix} h \\ d_2 \end{bmatrix}$$

$$\Delta x_i = U^{-1}(d_1 - h)$$

precision u

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Update $x_{i+1} = x_i + \Delta x_i,\ r_{i+1} = r_i + \Delta r_i$ → precision u

Returning to IR3 Analysis...

The backward error for the correction solve:

$$\left(\tilde{A} + \Delta\tilde{A}\right)\hat{d}_i = \tilde{r}_i, \qquad \left\|\Delta\tilde{A}\right\|_\infty \leq c_{m,n}\boldsymbol{u_f}\left\|\tilde{A}\right\|_\infty$$

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$$\max(c_1, c_2)\,\boldsymbol{u_s} = O(\boldsymbol{u_f})$$

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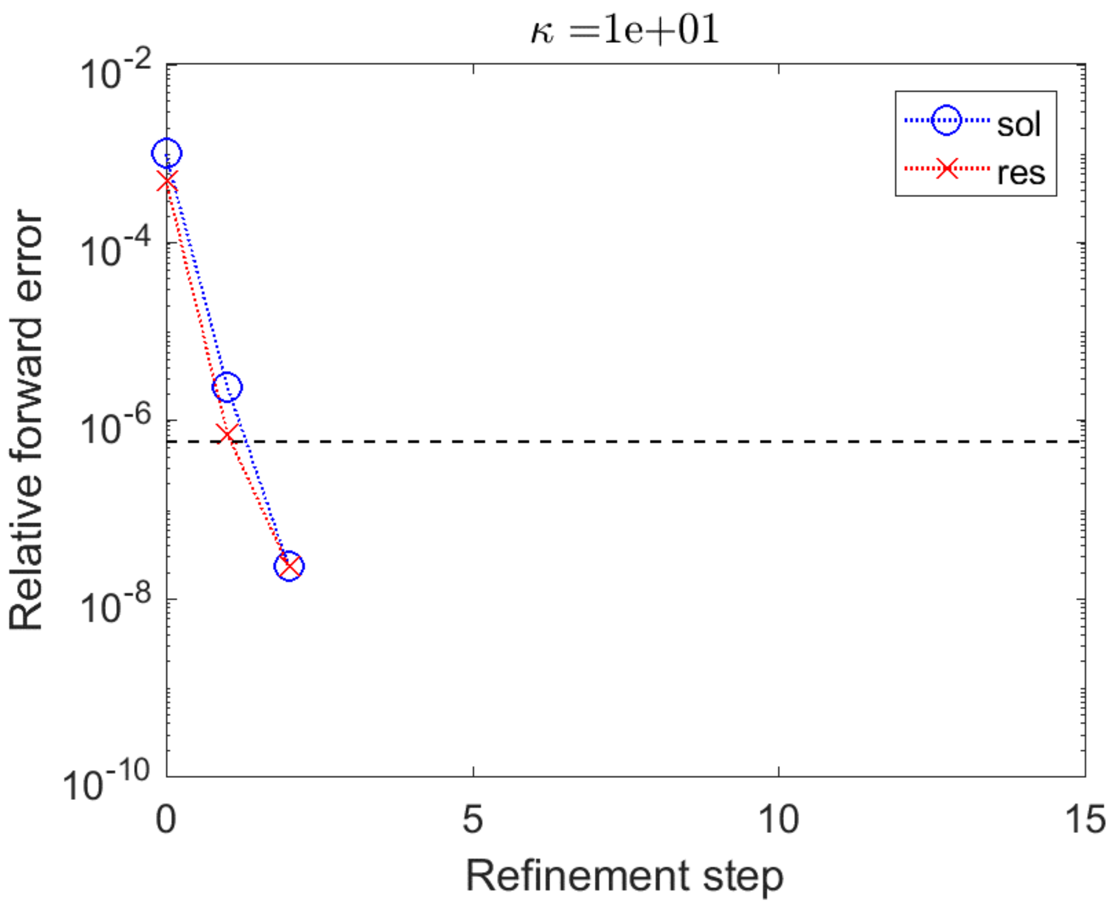
```
A = gallery('randsvd', [100, 10], kappa,3)
b = randn(100,1); b = b./norm(b)
```

Standard (QR-based) least squares IR with
u_f: half, u: single, u_r: double



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m = 100, n = 10

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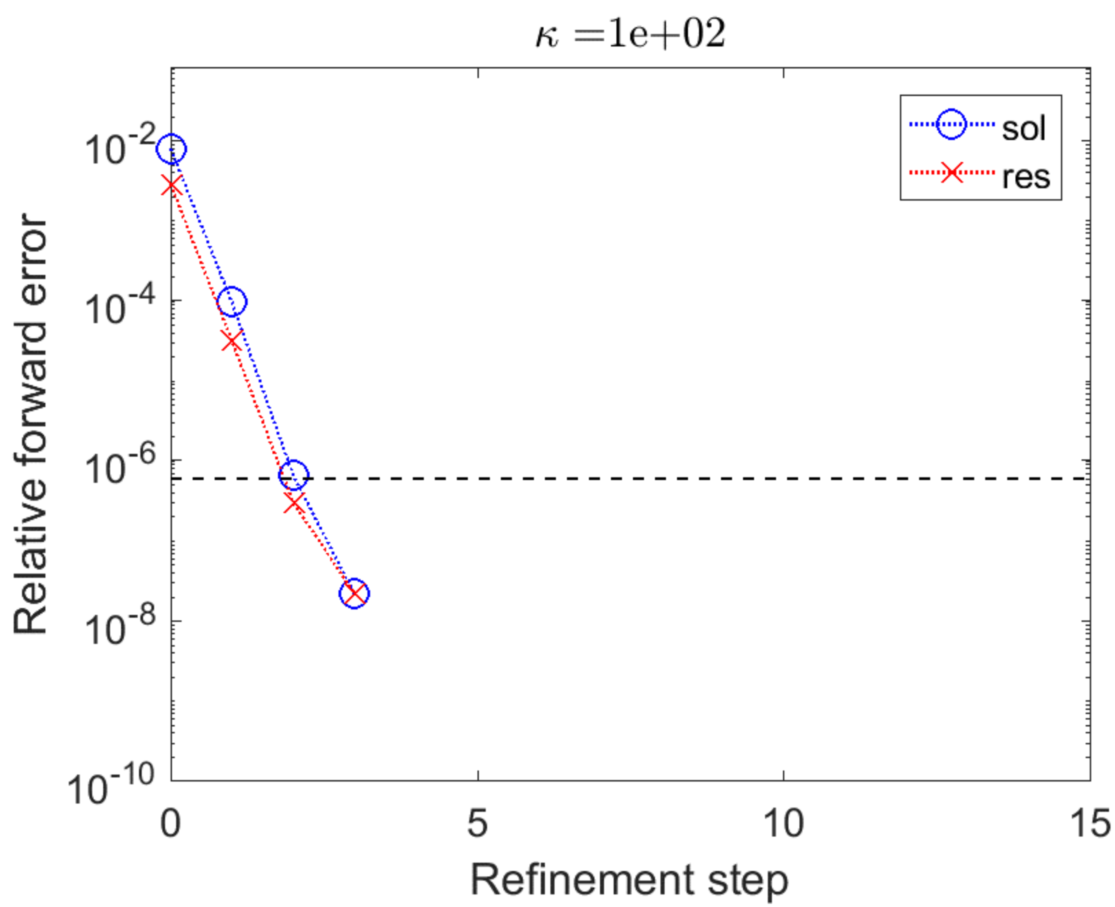

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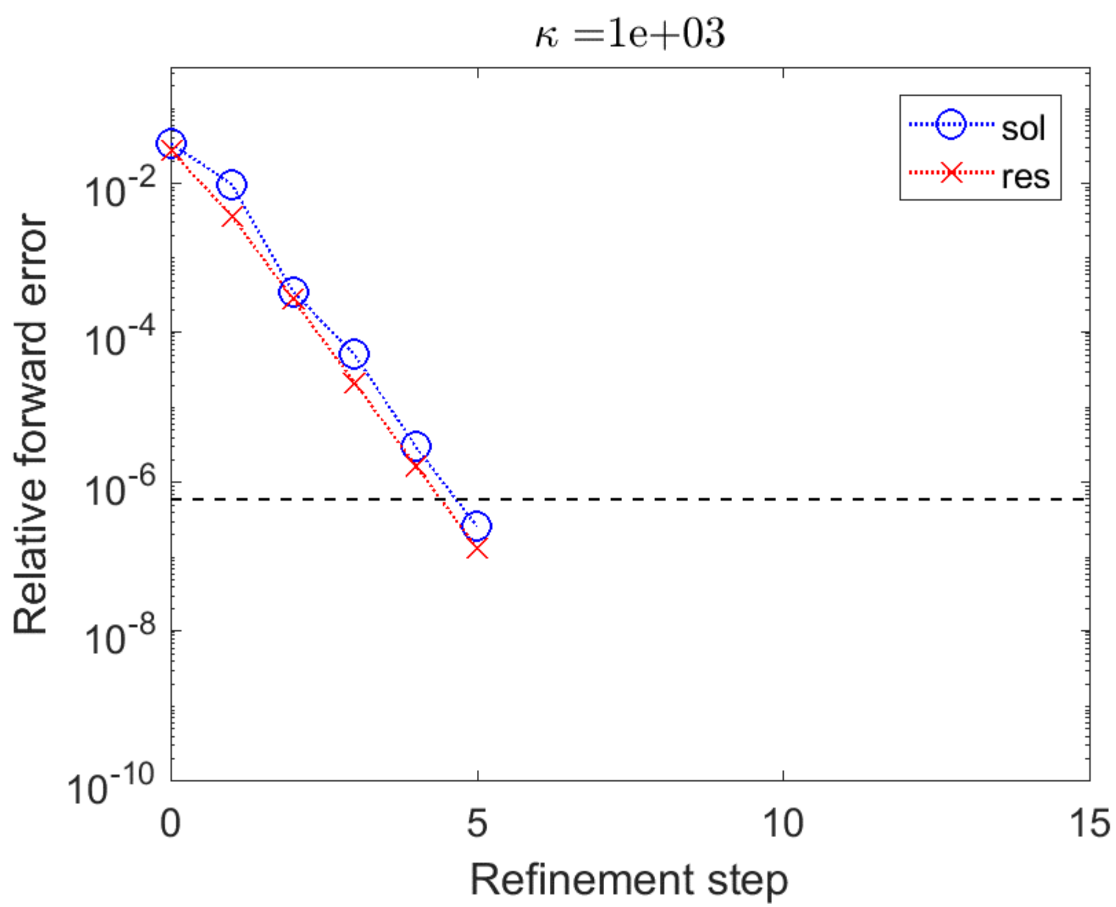

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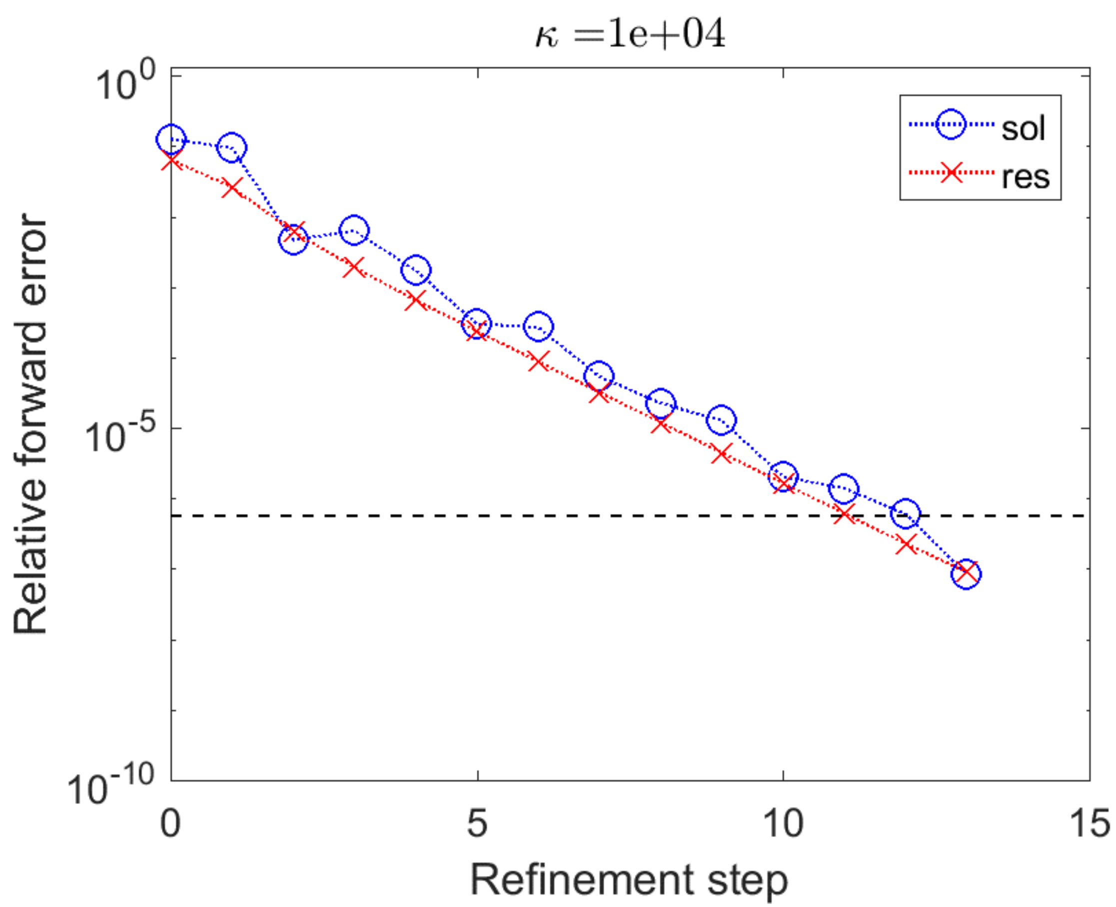

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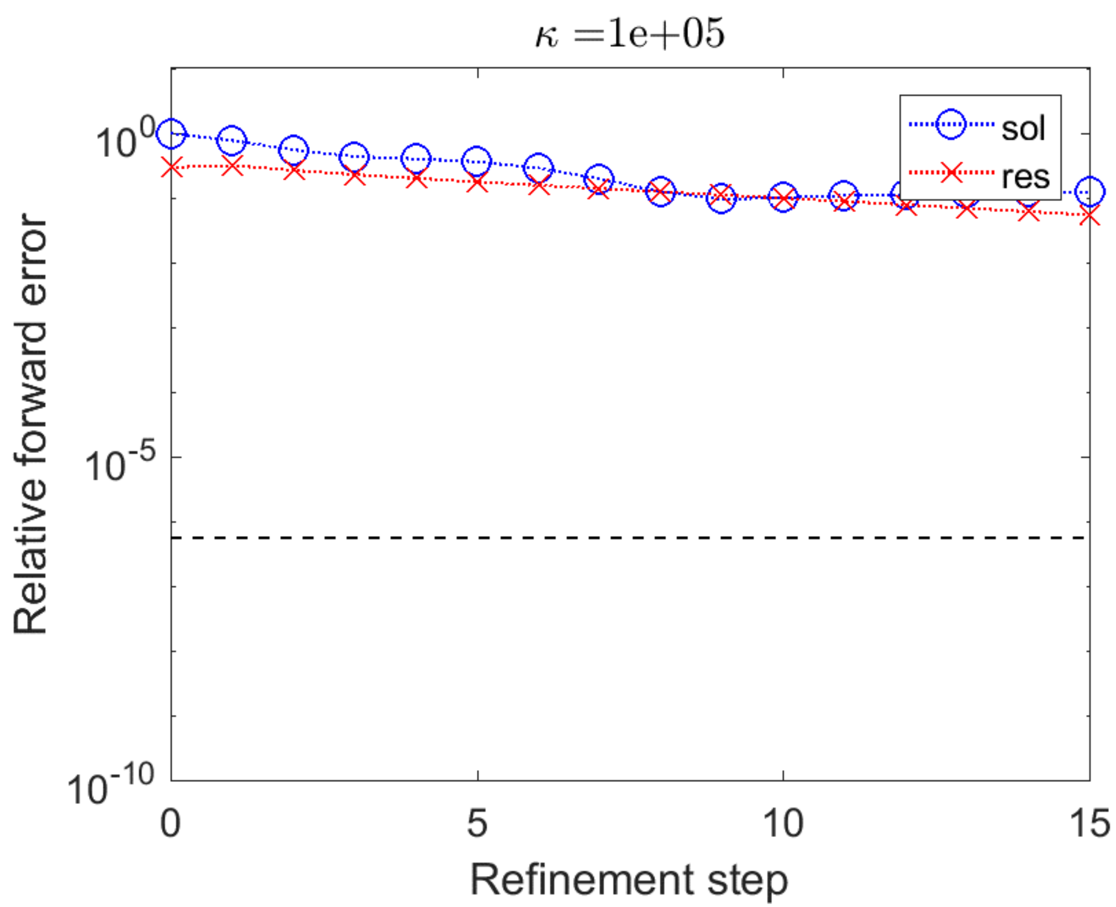

GMRES-IR for Least Squares

- Similar to the linear system case, we can use a lower precision factorization for even more ill-conditioned problems if we improve the effective precision of the solver

- Again, don't want to compute an LU factorization of the augmented system

- How can we use existing QR factors to construct an effective and inexpensive preconditioner for the augmented system?

- Note that augmented system is a saddle-point system; lots of existing work (block diagonal, triangular, constraint-based, ...)

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,

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

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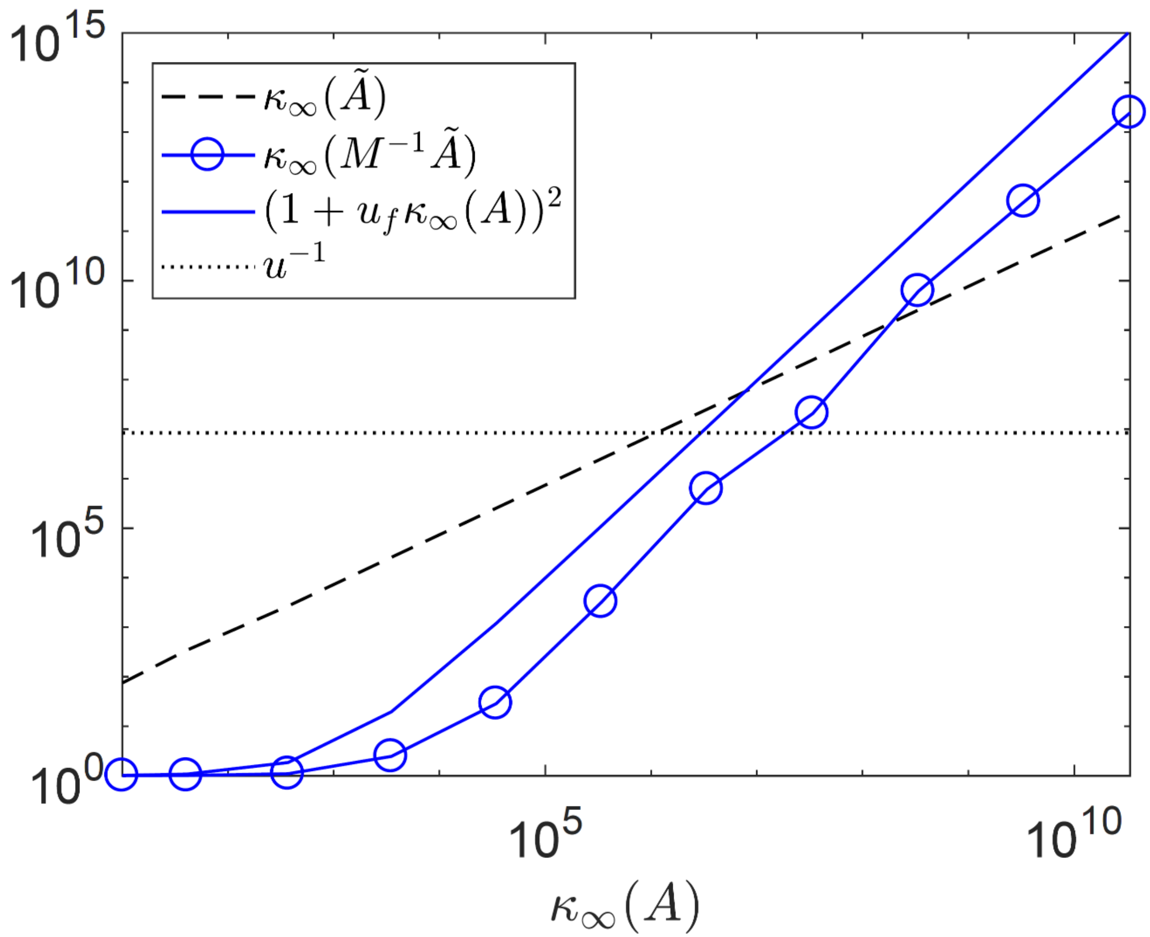
- So for GMRES-based LSIR, $\boldsymbol{u_s} \equiv \boldsymbol{u}$; expect convergence of forward error when $\kappa_\infty(A) < \boldsymbol{u}^{-1/2} \boldsymbol{u_f}^{-1}$

```
gallery('randsvd', [100,10], kappa(i), 3)
```

QR factorization computed in half precision; preconditioned system computed exactly



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GMRES-LSIR and "Standard" LSIR with

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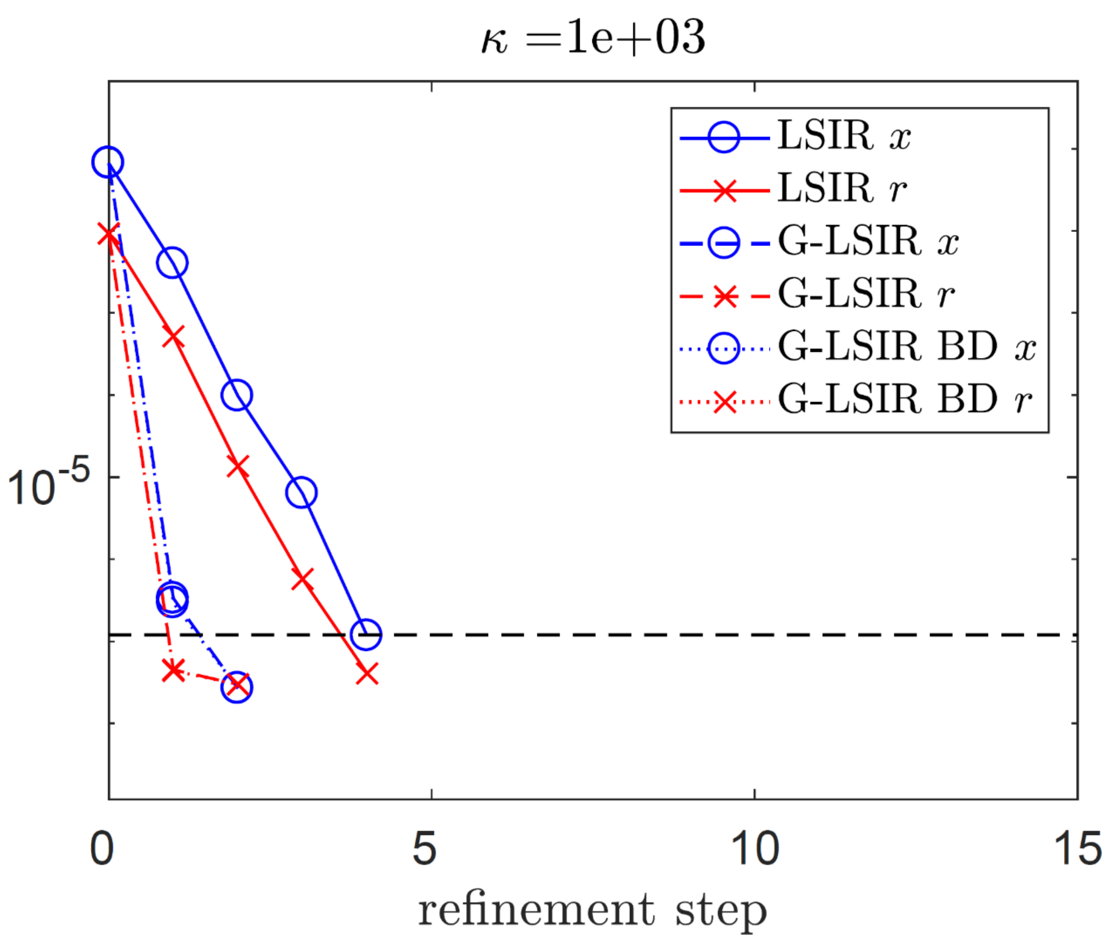

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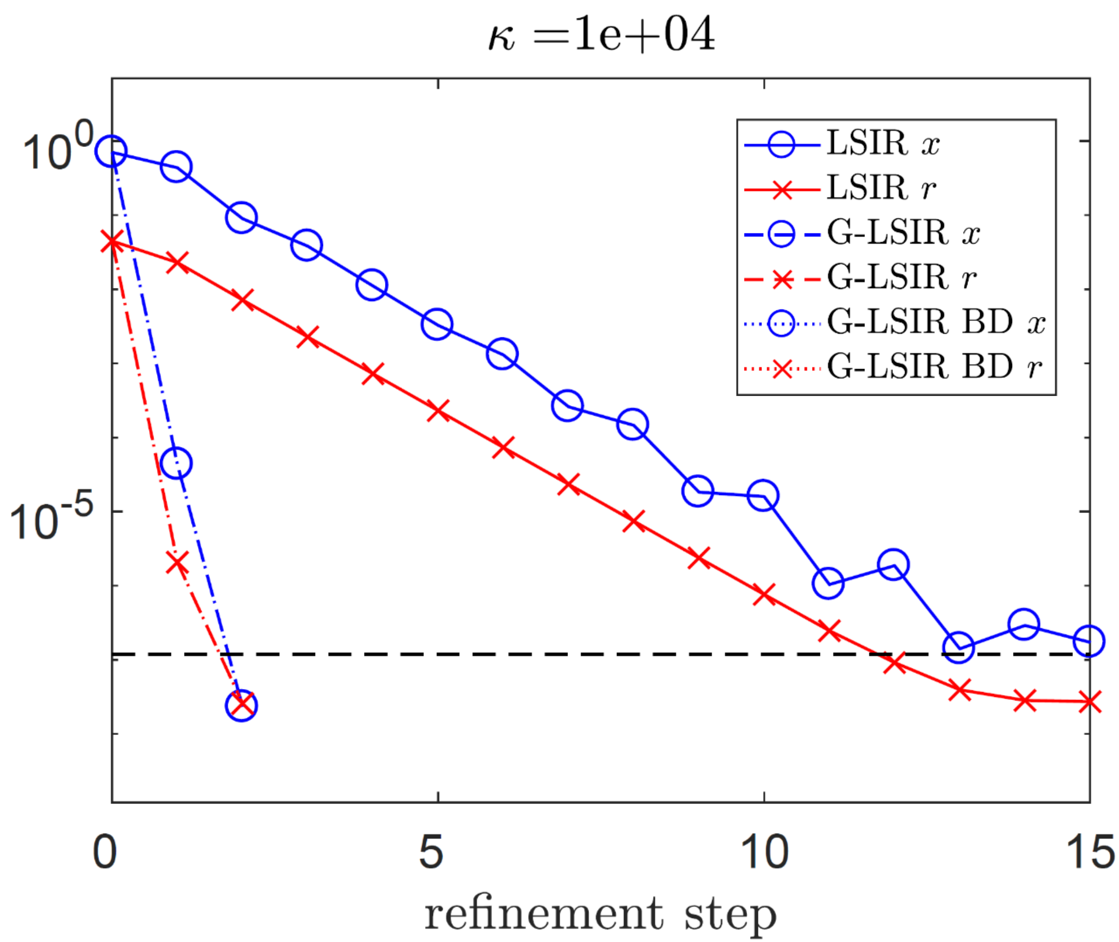

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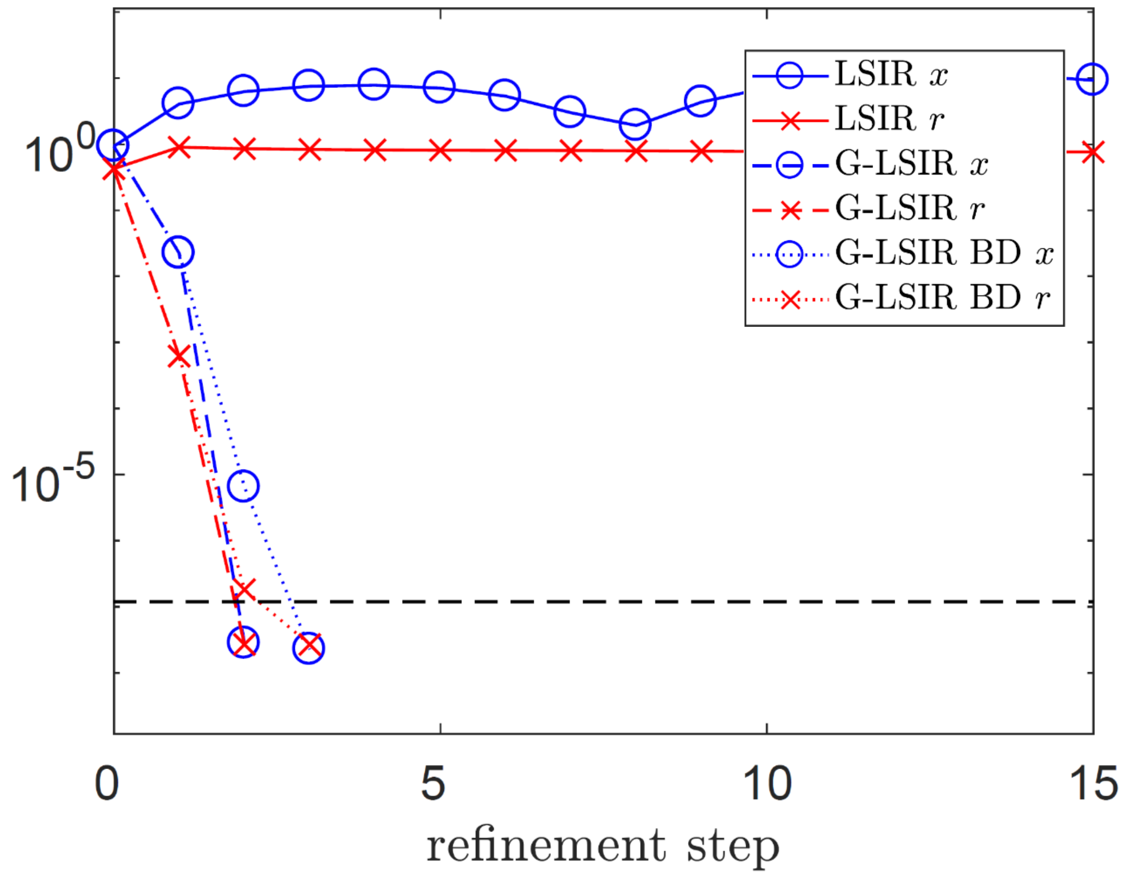
$\kappa = $1e+06



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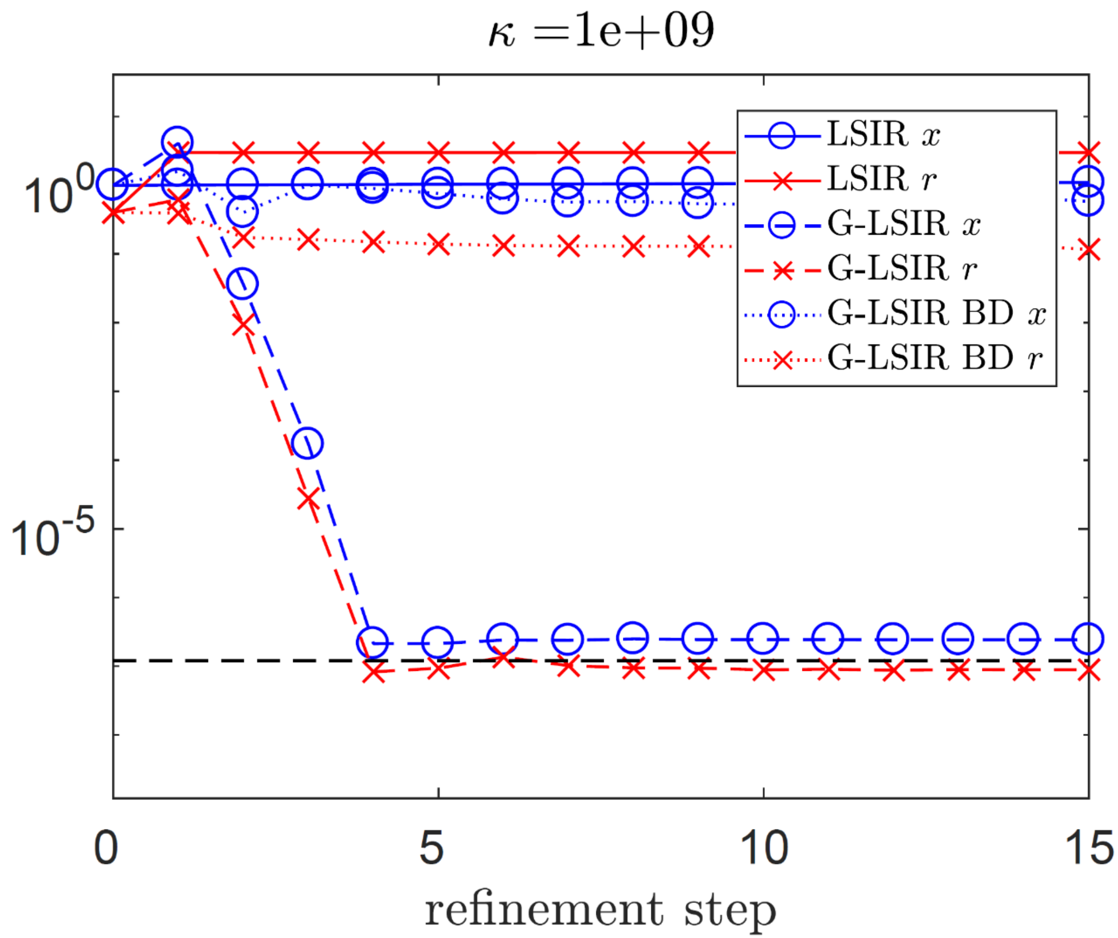

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- As numerical analysts, we must determine when and where we can exploit lower-precision hardware to improve performance

Thank You!

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