Iterative Linear Algebra in the Exascale Era

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MINISTRY OF EDUCATION,
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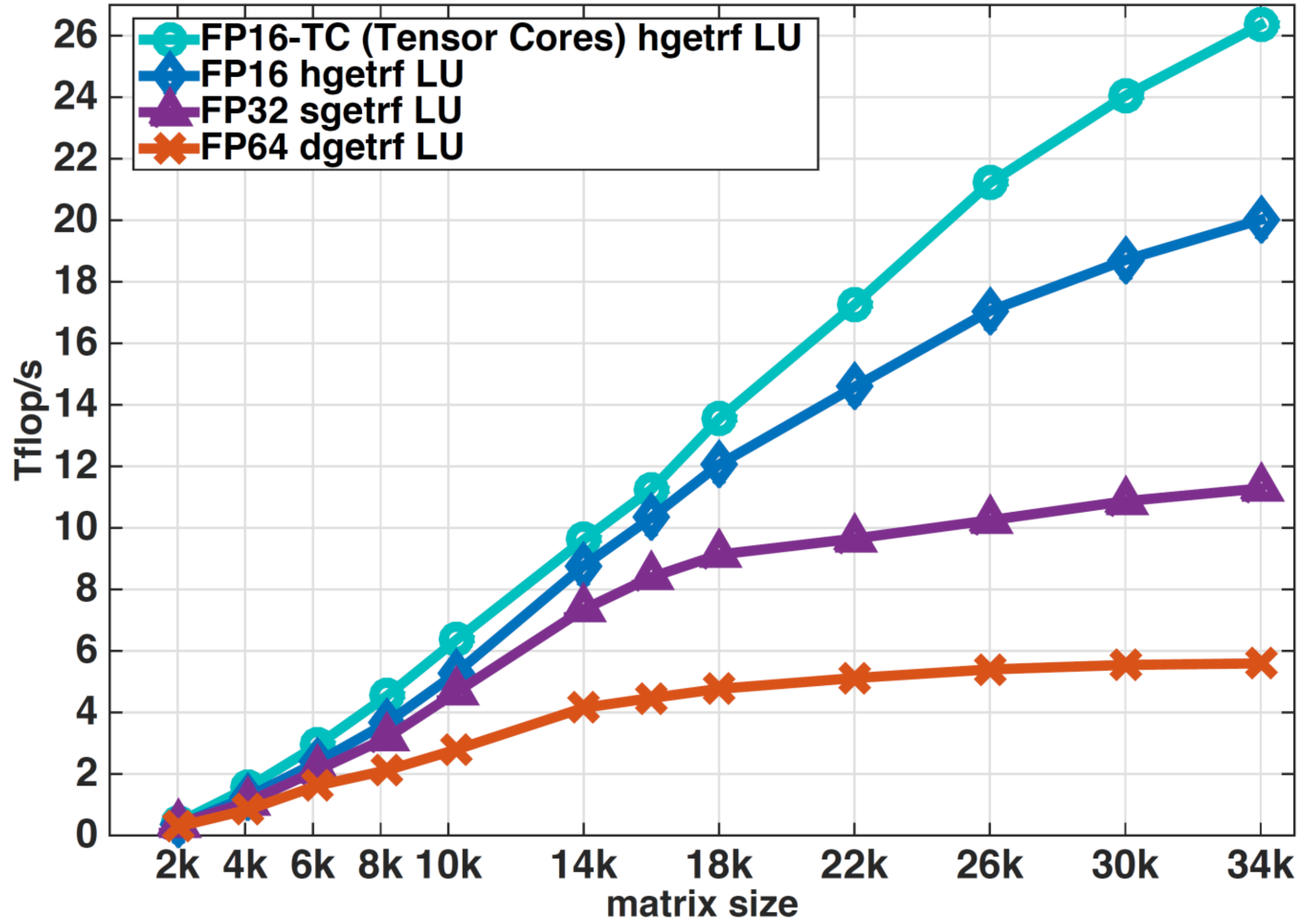
Hardware Support for Multiprecision Computation

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

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

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"Traditional" (high-precision residual computation)

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

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

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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.

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

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- Wilkinson (1977), comment in unpublished manuscript: $\mu_i^{(2)}$ increases with i

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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

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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.

Forward Error for IR3

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

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

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

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

Normwise Backward Error for IR3

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

$$\phi_i \equiv (c_1 \kappa_\infty(A) + c_2)\boldsymbol{u_s}$$

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

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

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 $\approx 10^{-34}$

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}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
	S	S	D	10^8	10^{-8}	10^{-8}	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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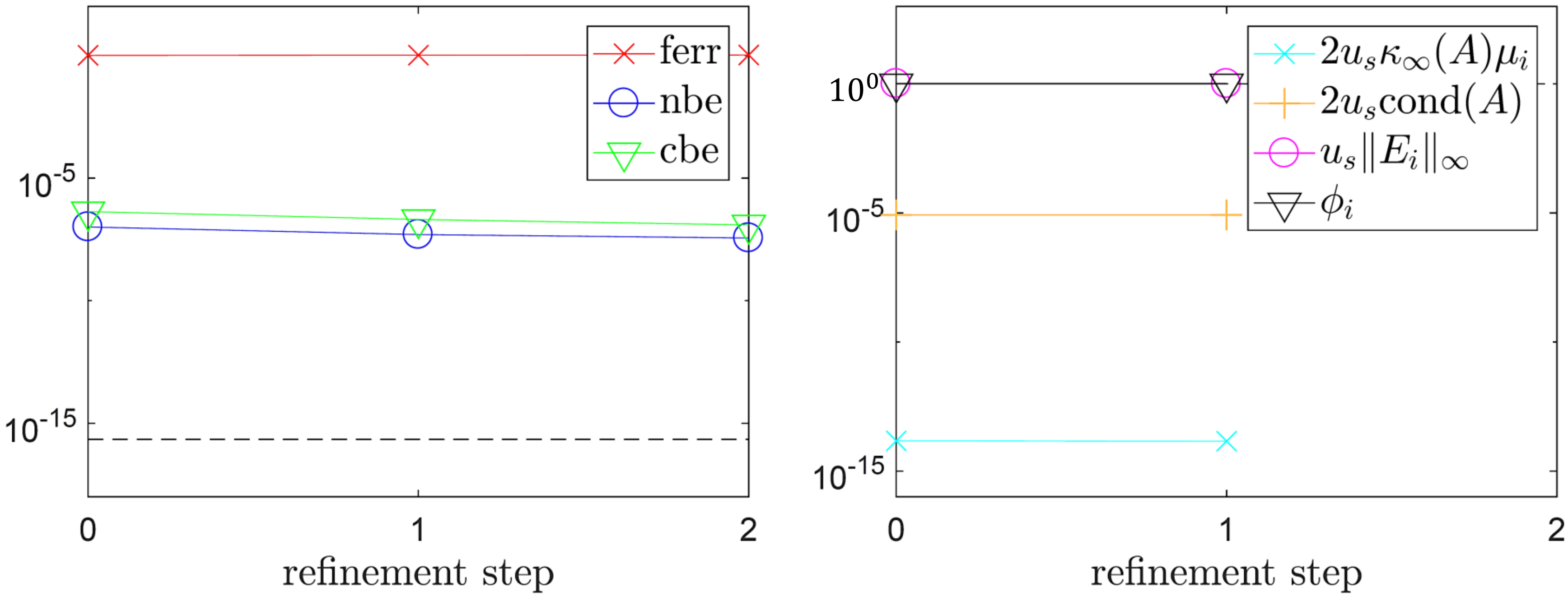
$\Rightarrow$ Benefit of IR3 vs. traditional IR: As long as $\kappa_\infty(A) \le 10^4$, can use lower precision factorization w/no loss of accuracy!

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

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

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



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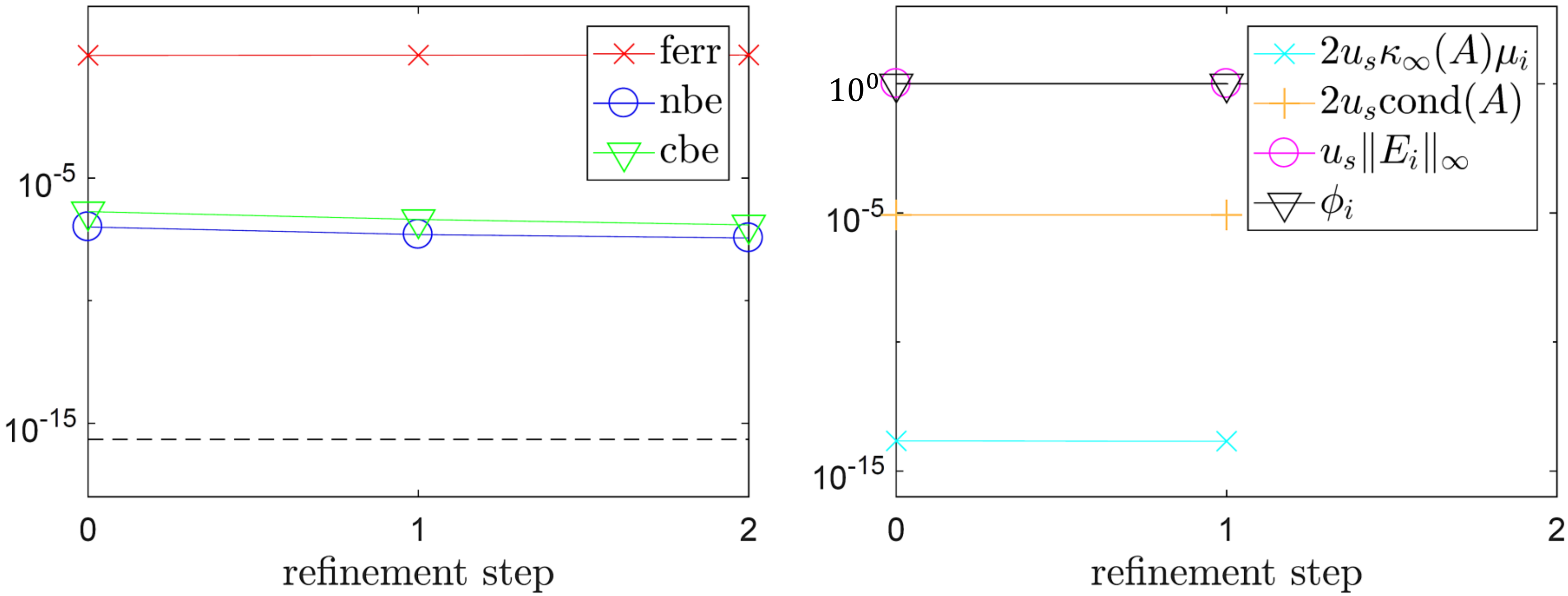

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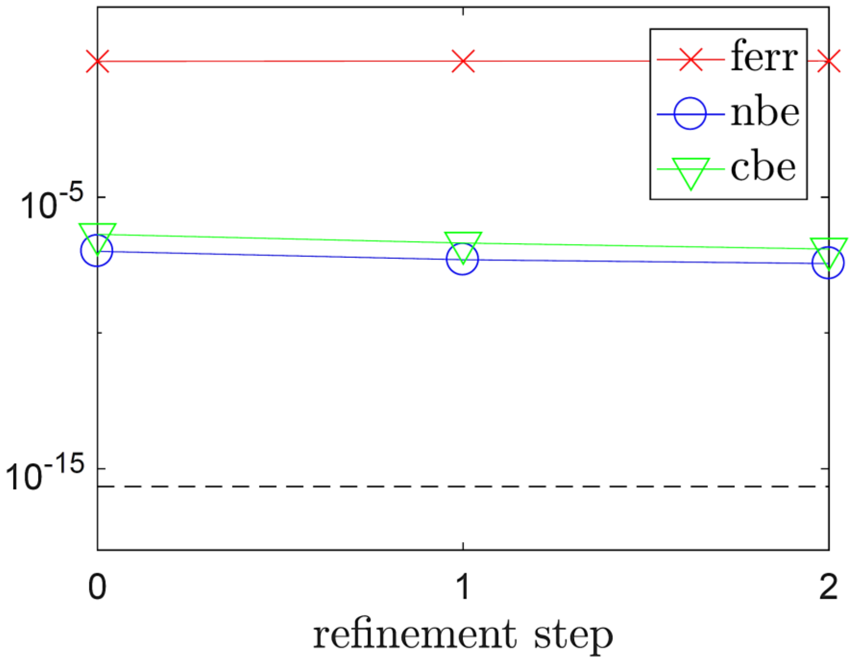

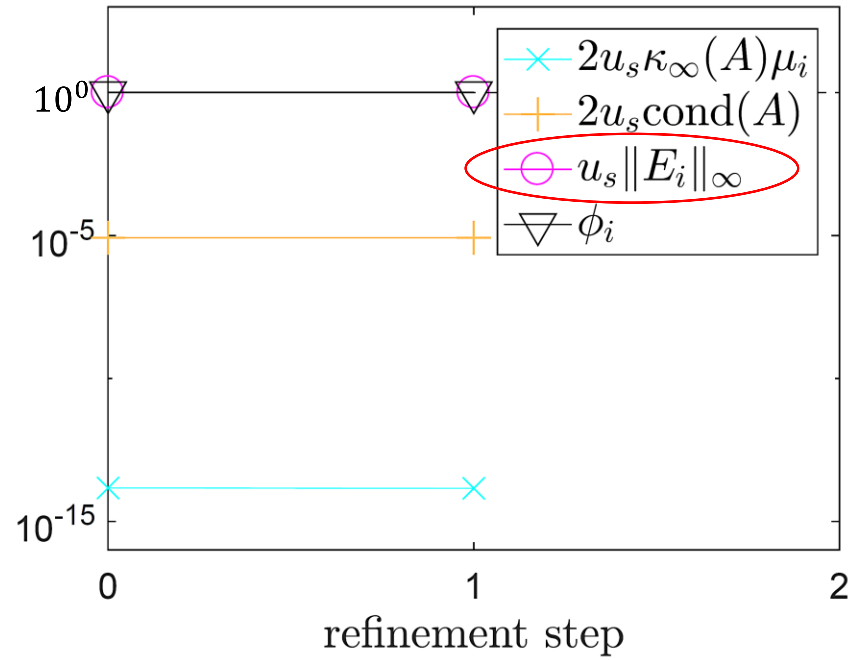

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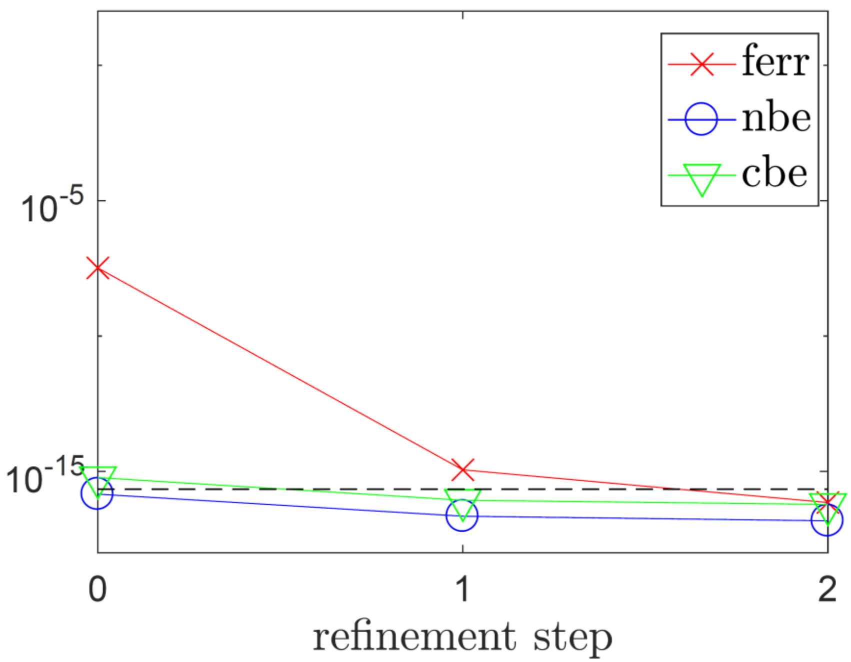

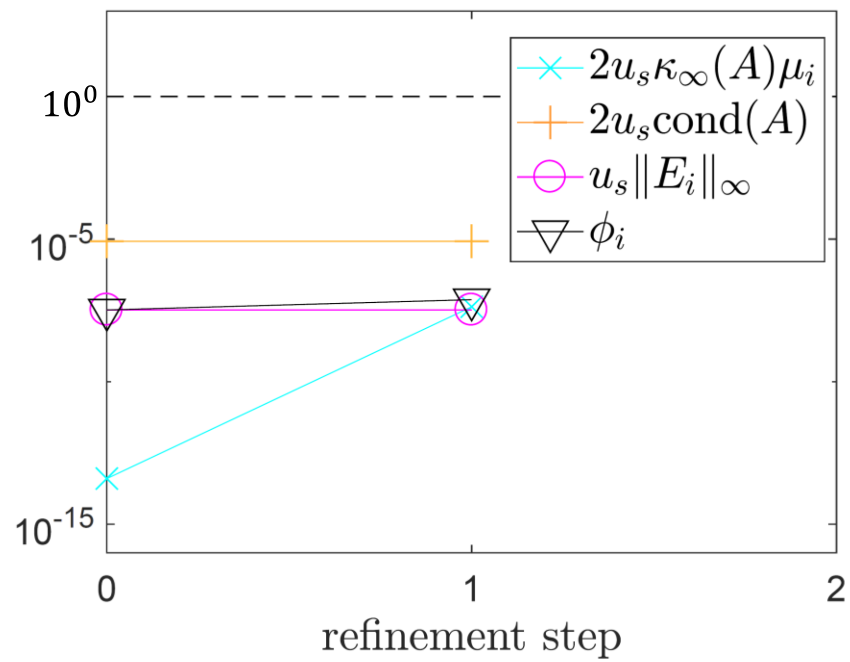

GMRES-Based Iterative Refinement

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

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

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

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

$r_i = b - Ax_i$

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

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

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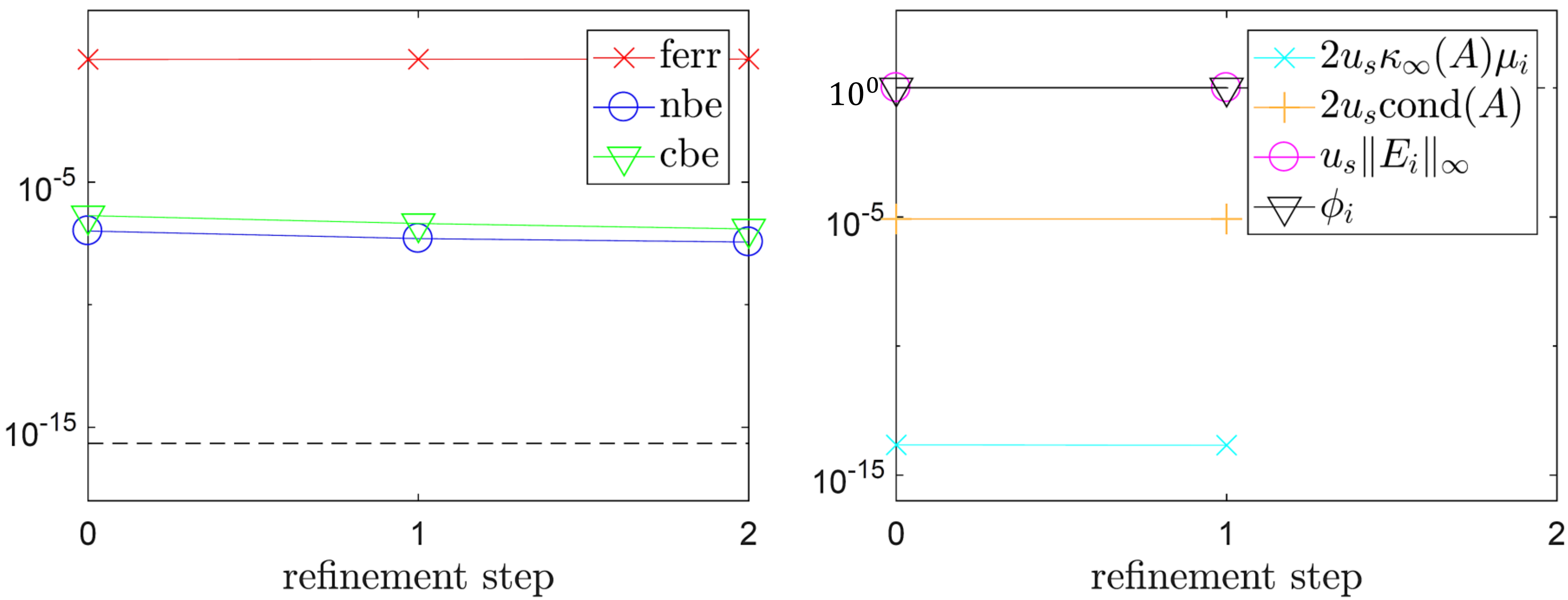

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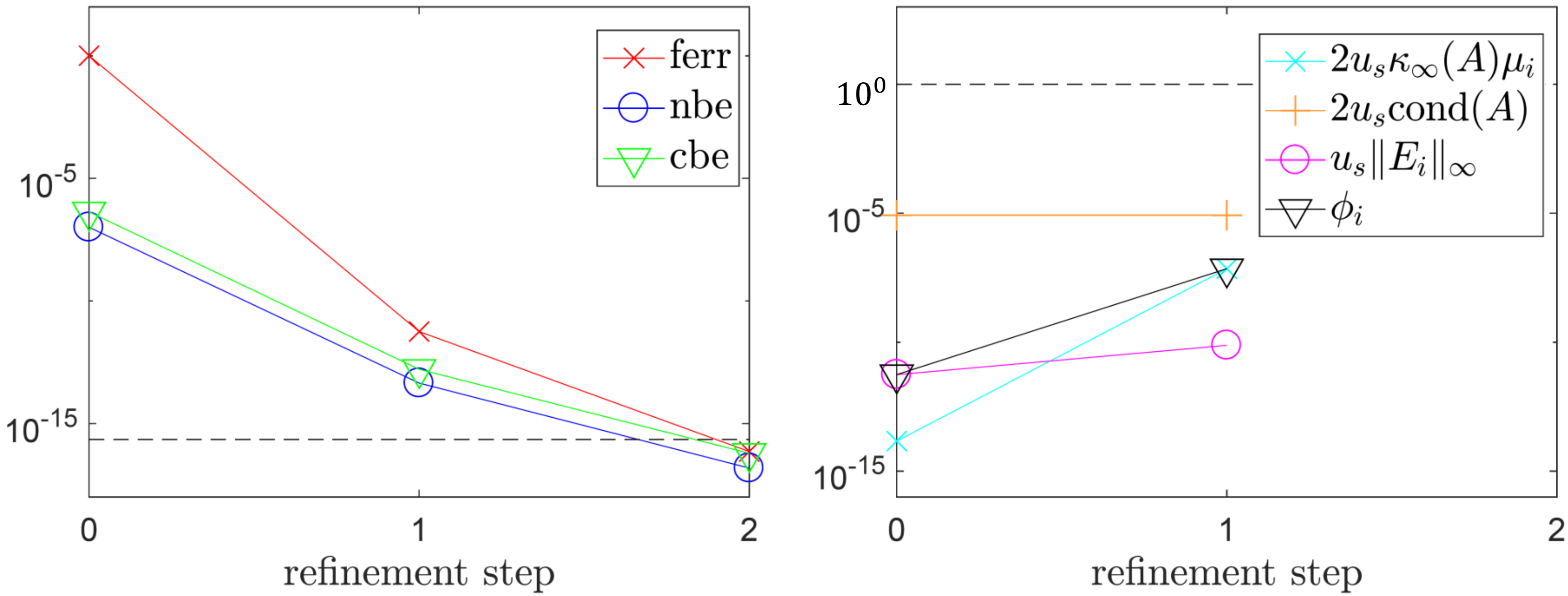
$\kappa_\infty(A) \approx$ 2e10, $\text{cond}(A,x) \approx$ 5e9, $\kappa_\infty(\tilde{A}) \approx$ 2e4

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}
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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 $\kappa_\infty(A)$

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

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

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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

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

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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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- 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.

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

- 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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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

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

and $\min_\alpha \kappa_2(\tilde{A}_\alpha)$ 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 $\kappa_2(A)$

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Compute QR factorization $A = QR = [Q_1, Q_2]\begin{bmatrix} U \\ 0 \end{bmatrix} \longrightarrow$ precision u_f

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For $i = 0, \ldots$

Compute residuals $\begin{bmatrix} f_i \\ g_i \end{bmatrix} = \begin{bmatrix} b - r_i - Ax_i \\ -A^T r_i \end{bmatrix}$ → precision u_r

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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

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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:

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

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As long as $\kappa_\infty(\tilde{A}) \lesssim \boldsymbol{u_f^{-1}}$, expect normwise and componentwise backward errors to be $O(\boldsymbol{u})$

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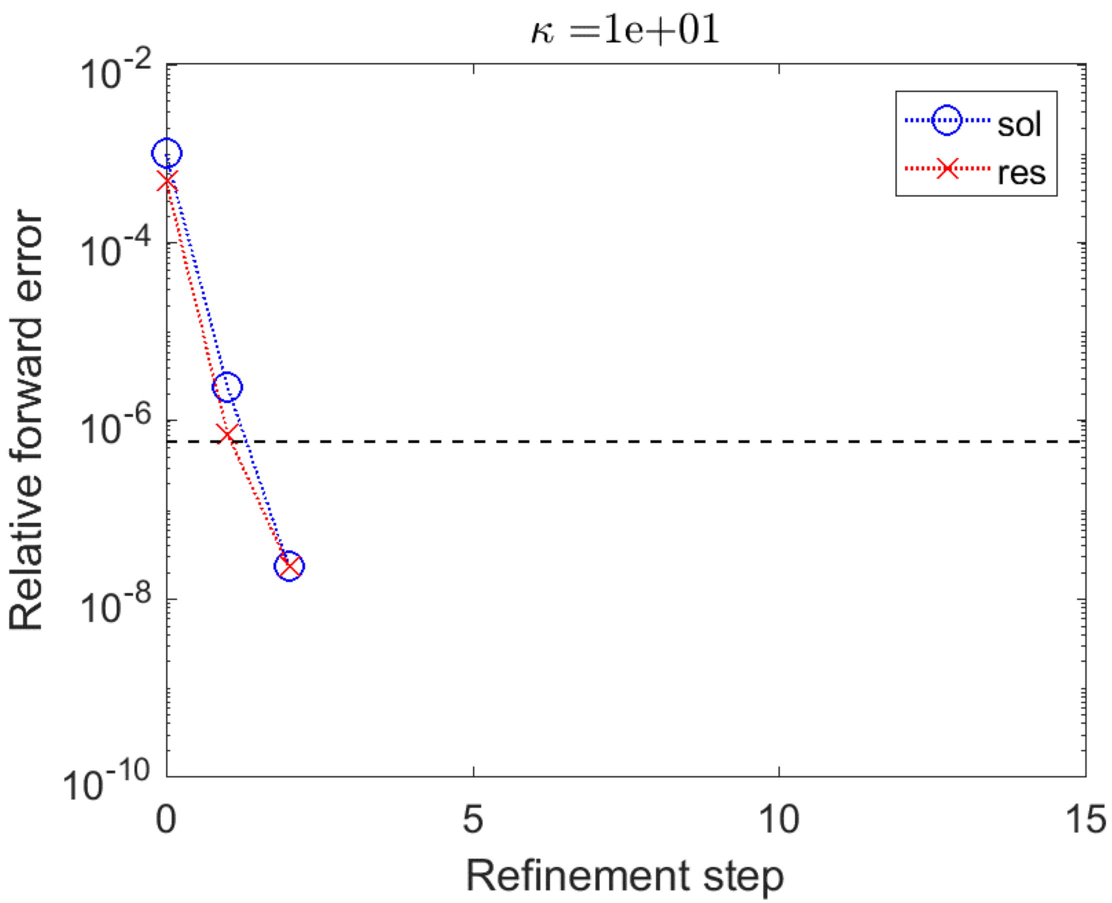
m n

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



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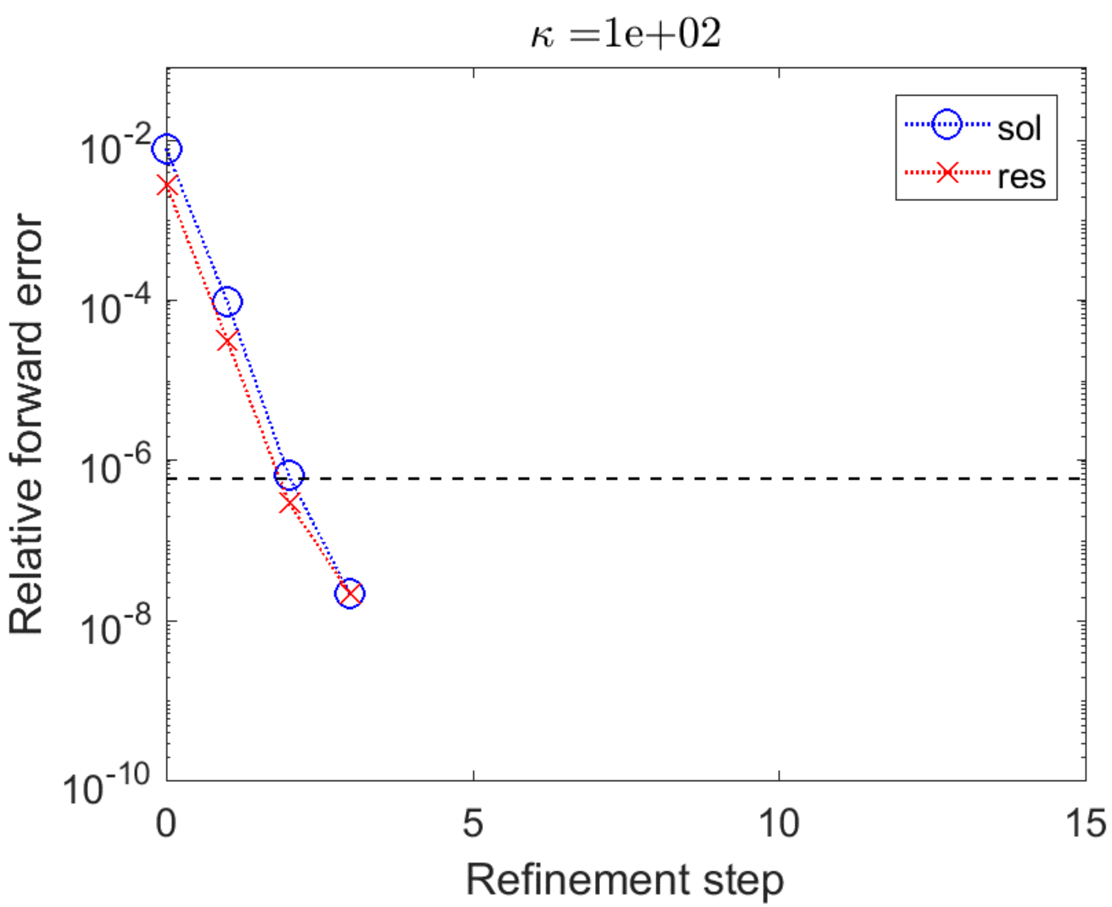

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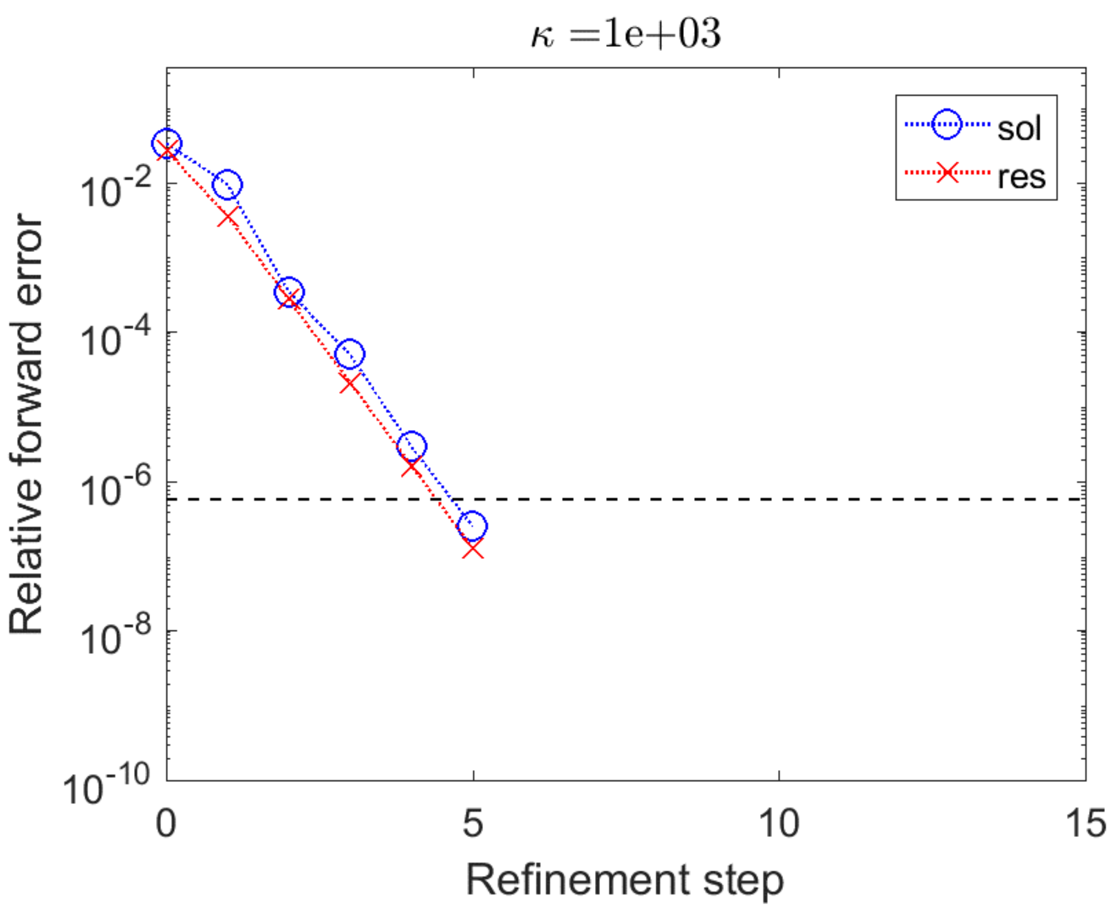

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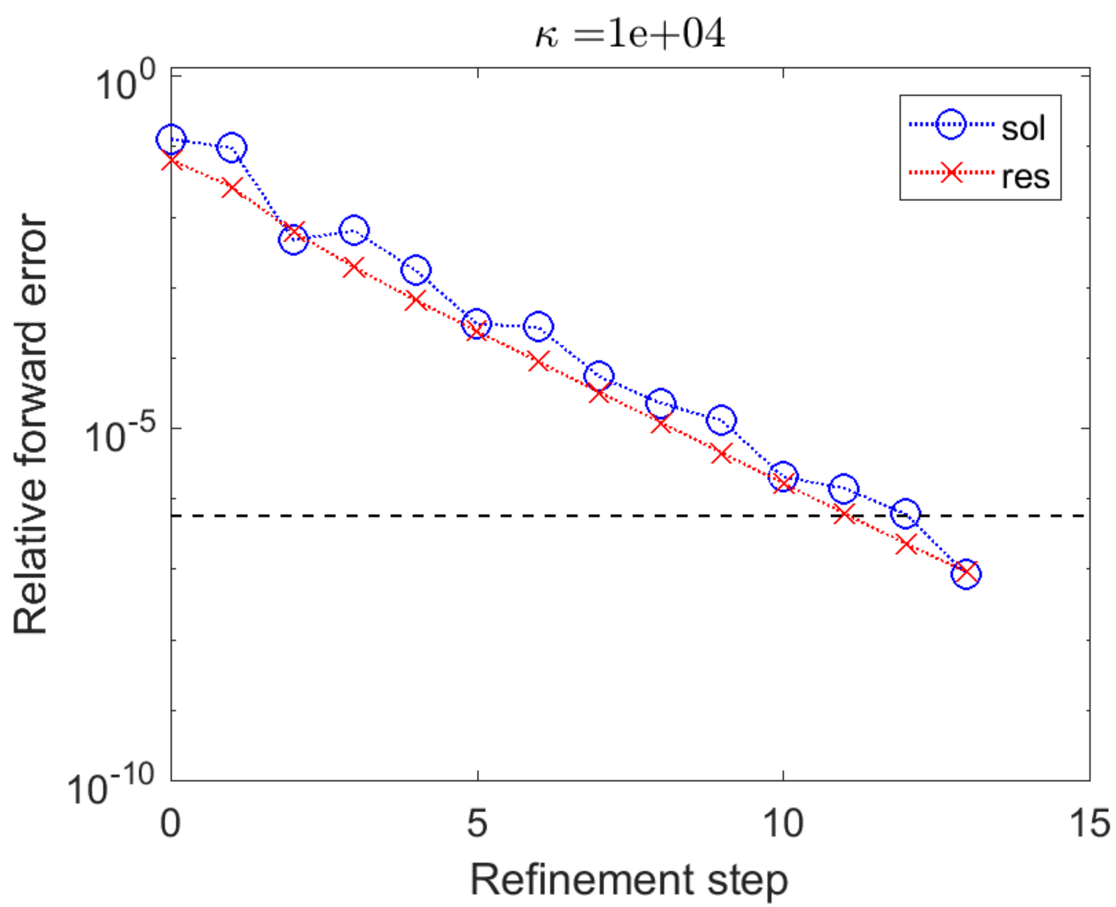

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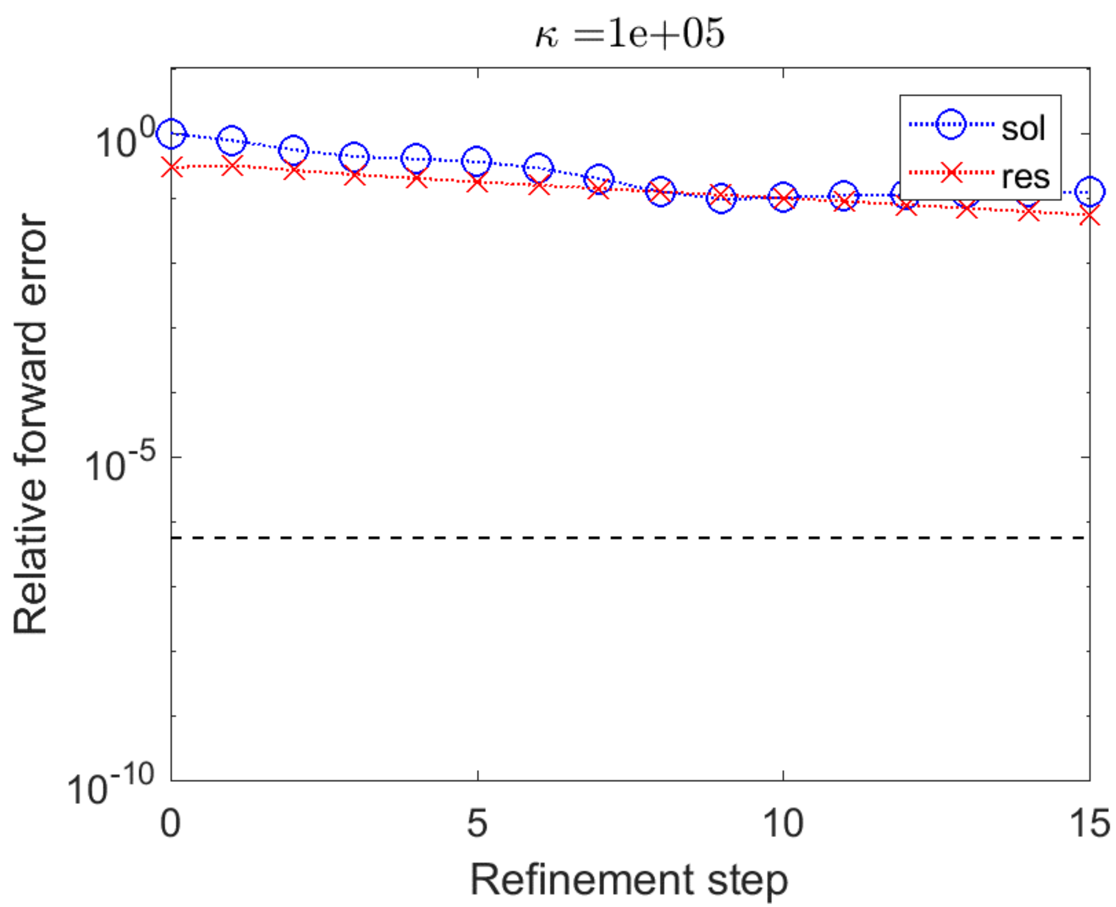

GMRES-IR for Least Squares

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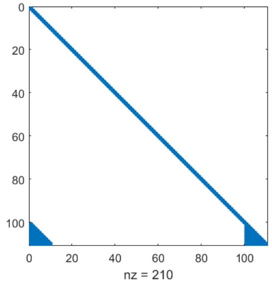

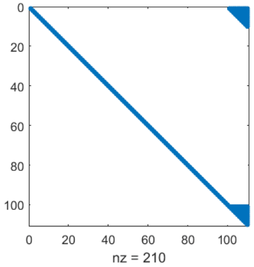

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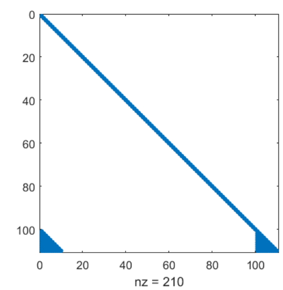

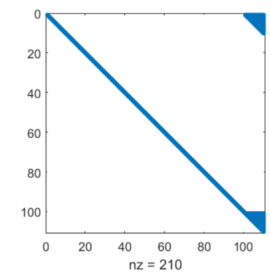

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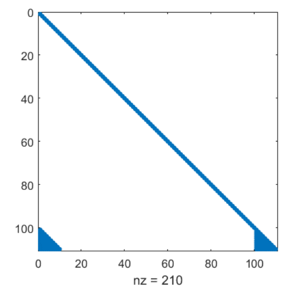

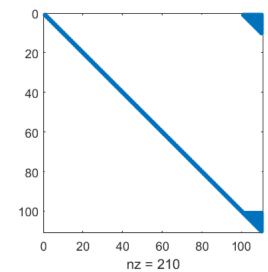

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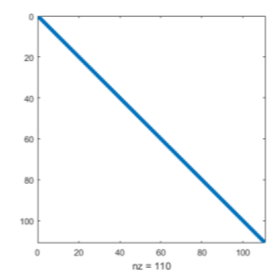

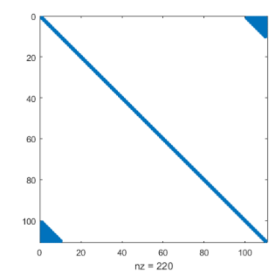

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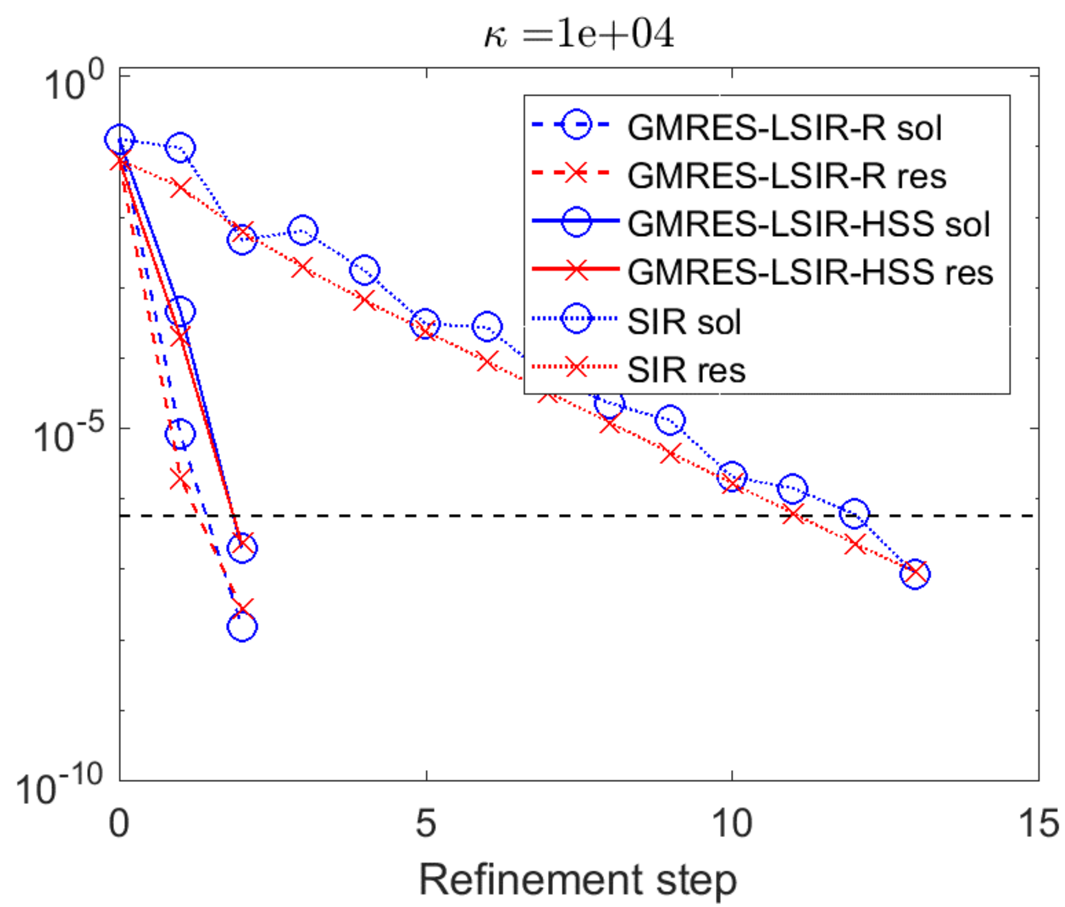
GMRES-LSIR and "Standard" LSIR with

u_f: half, u: single, u_r: double



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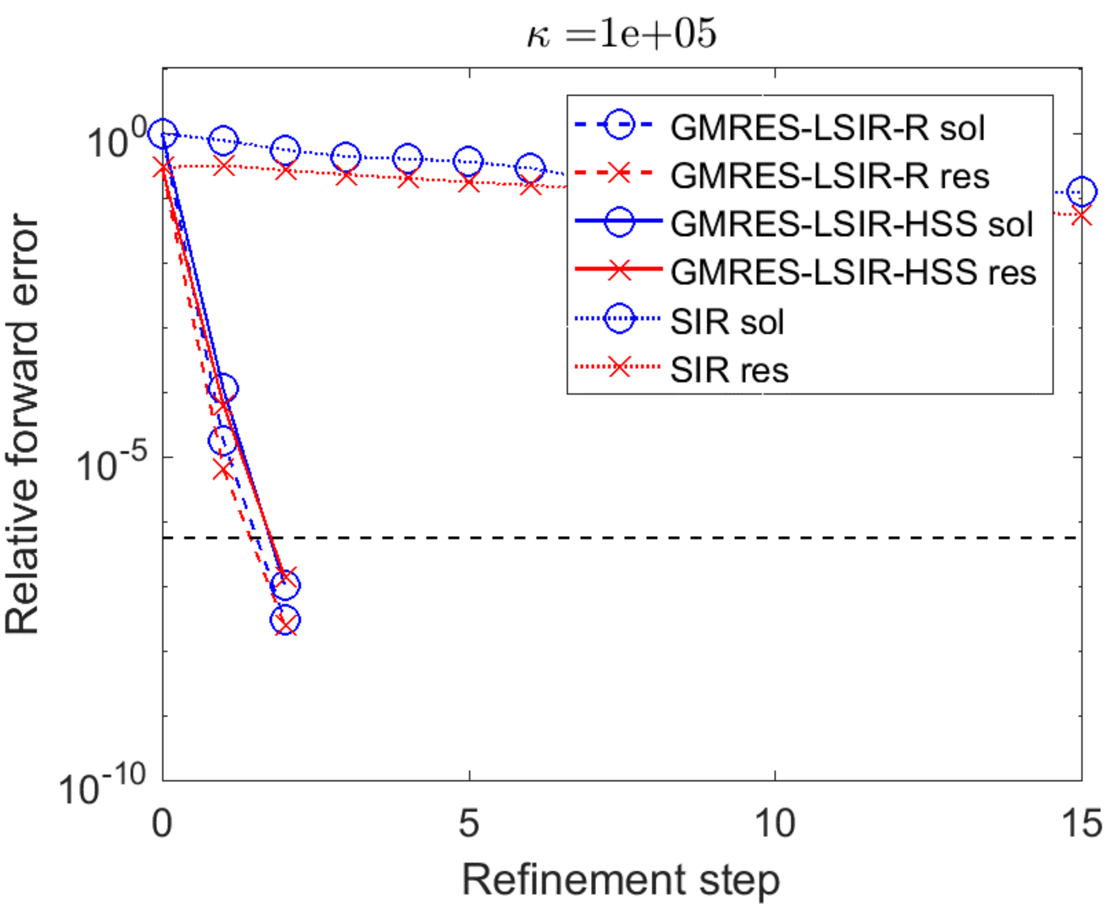

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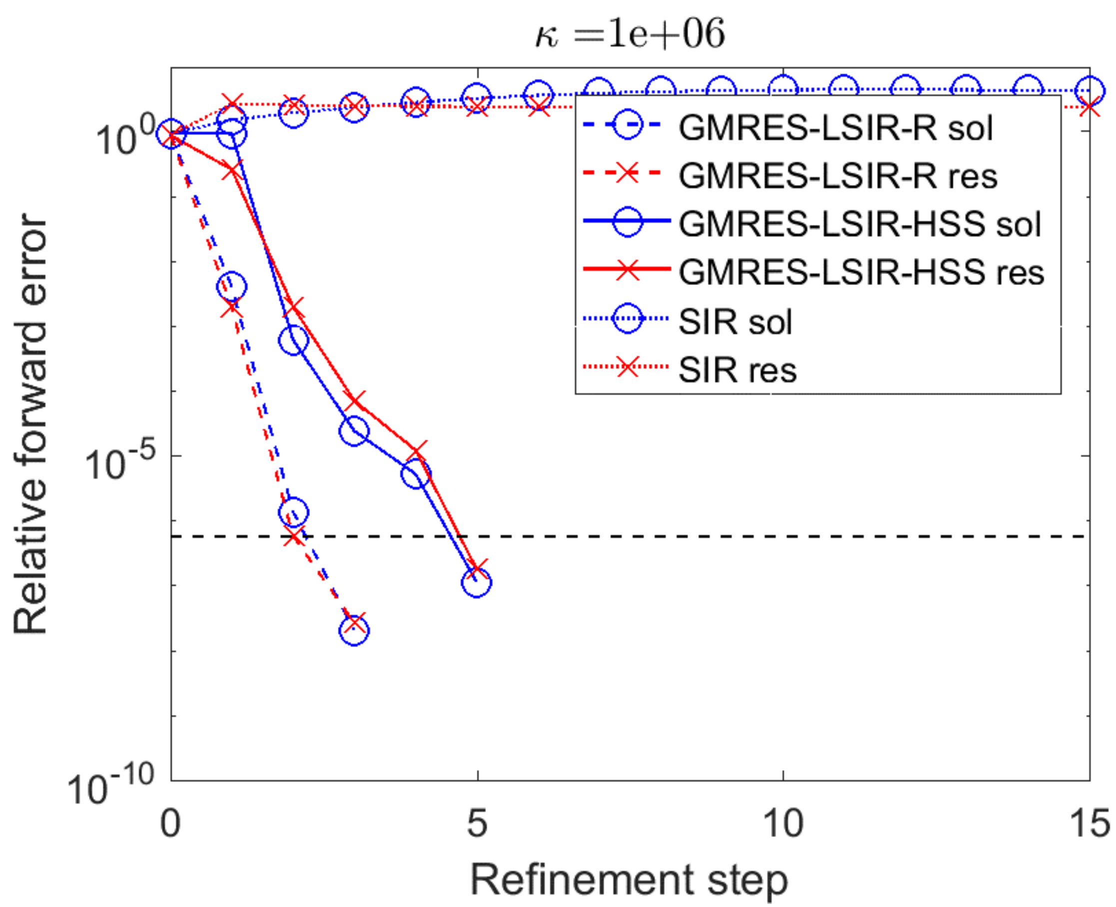

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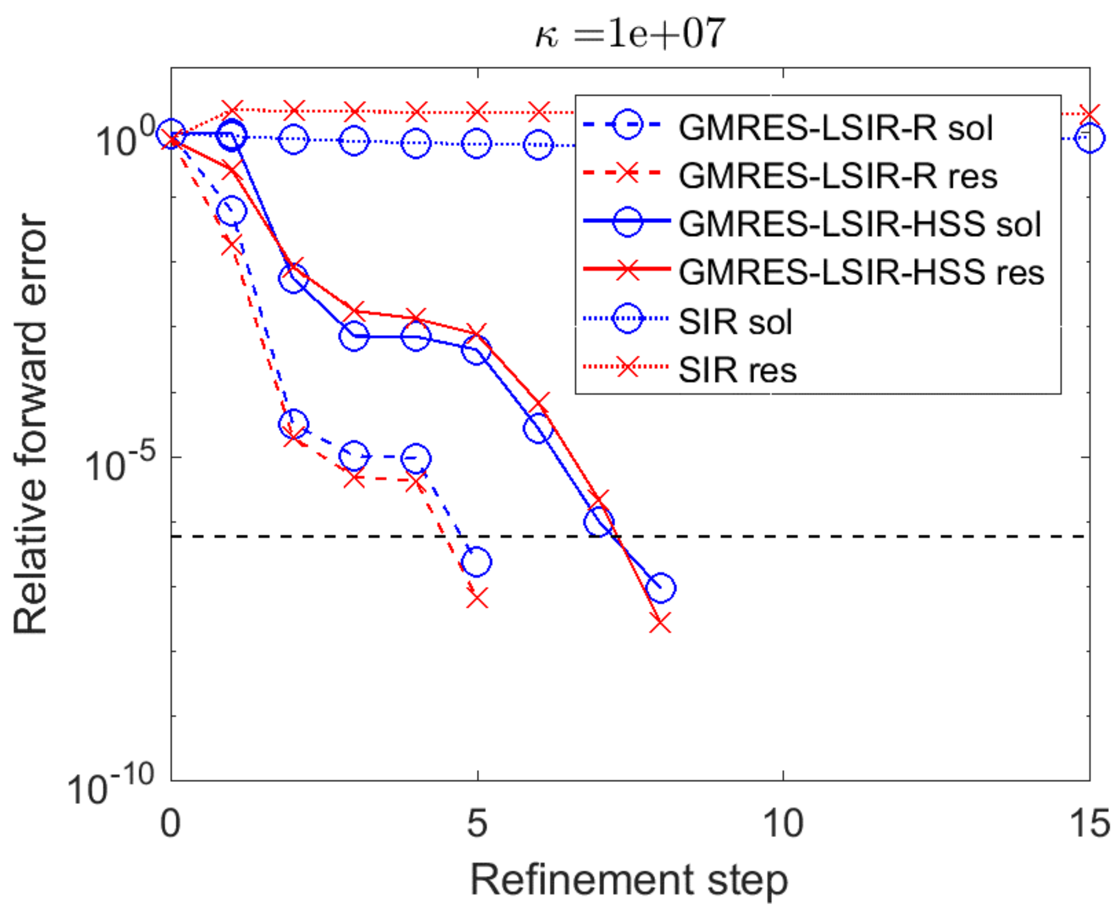

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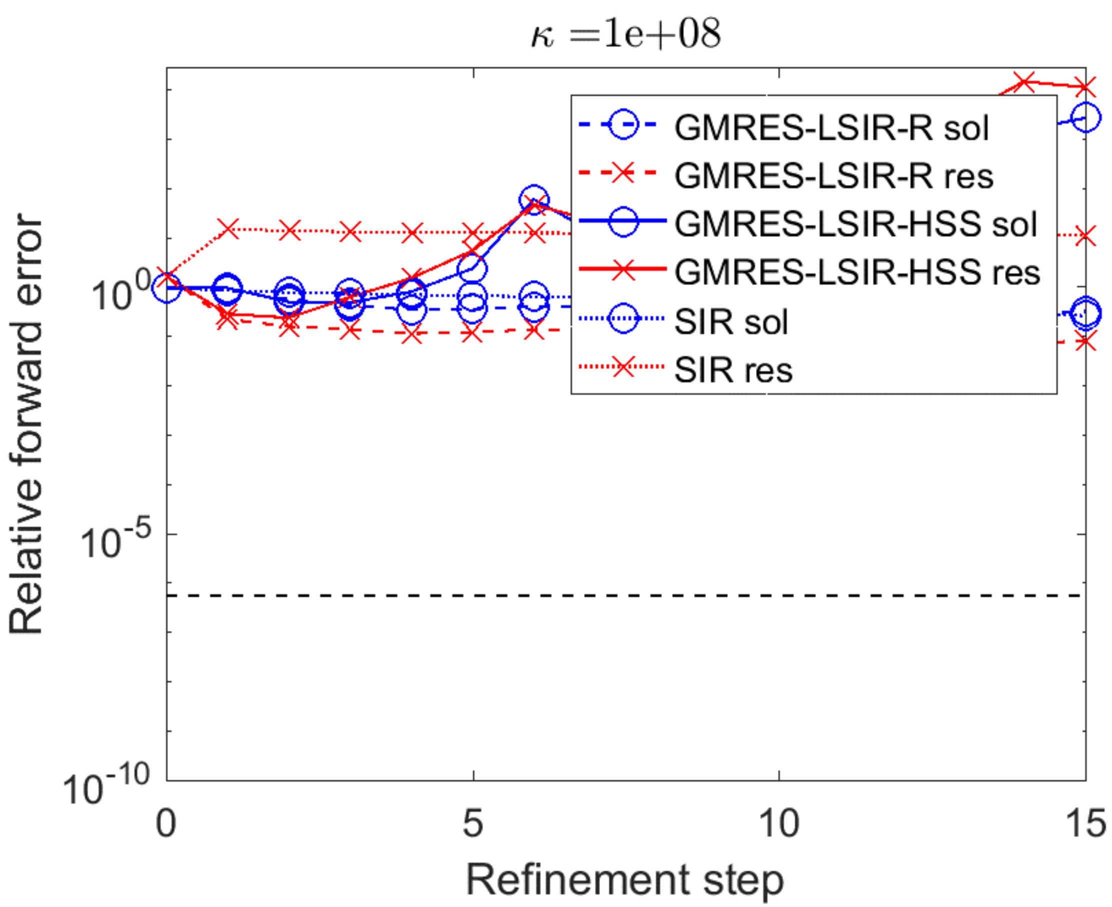

The rise of multiprecision hardware

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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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