Preconditioned GMRES-based Iterative Refinement

for the Solution of Sparse, Ill-Conditioned Linear Systems

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Iterative Refinement for $Ax = b$

A is $n \times n$, nonsingular

Solve $Ax_0 = b$ by LU factorization

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

$\quad r_i = b - Ax_i$

$\quad$ Solve $Ad_i = r_i$

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

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Notation/Setting

- Assume standard floating point arithmetic
  - u denotes unit roundoff
  - "Gamma notation": $\gamma_k = \frac{ku}{1-ku}$

- Condition numbers
  - $|A| = |(a_{ij})|$
  - $\kappa_\infty(A) = \|A^{-1}\|_\infty \|A\|_\infty$
  - $\mathrm{cond}(A, x) = \frac{\| \, |A^{-1}||A||x| \, \|_\infty}{\|x\|_\infty}$
  - $\mathrm{cond}(A) = \mathrm{cond}(A, e) = \| \, |A^{-1}||A| \, \|_\infty$
  - $1 \leq \mathrm{cond}(A, x) \leq \mathrm{cond}(A) \leq \kappa_\infty(A)$

Error Bounds ("Traditional" IR)

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Solve $Ax_0 = b$ by LU factorization	precision u
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- Early analyses by Wilkinson (1963), Moler (1967)
- If $\kappa_\infty(A)u < 1$, then error contracts (at a rate depending on $\kappa_\infty(A)$) until

$$\frac{\|x - x_i\|_\infty}{\|x\|_\infty} \approx u$$

Information in $\widehat{L}\widehat{U} \approx A$

- Empirically observed by Rump (1990) that if $\widehat{L}$ and $\widehat{U}$ are computed LU factors of A from GEPP, then $\kappa\left(\widehat{U}^{-1}\widehat{L}^{-1}A\right) \approx 1 + \kappa(A)u$

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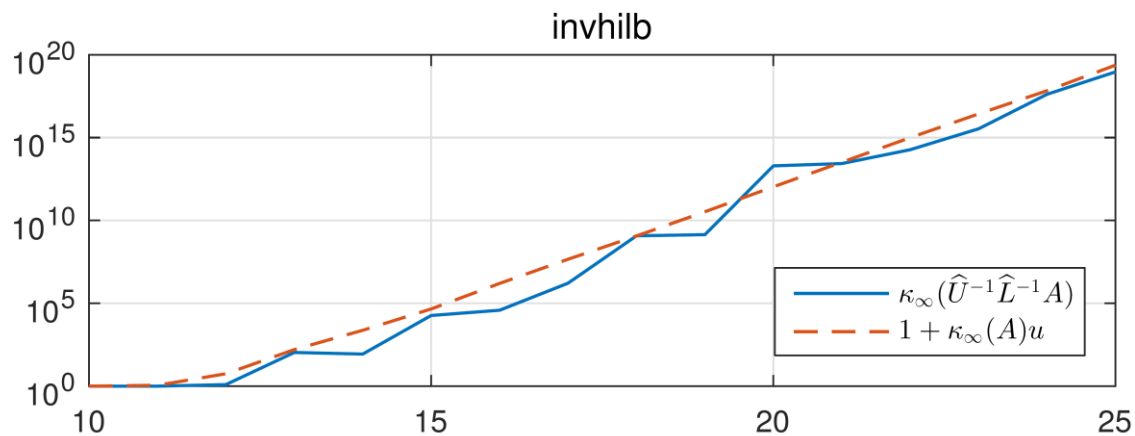
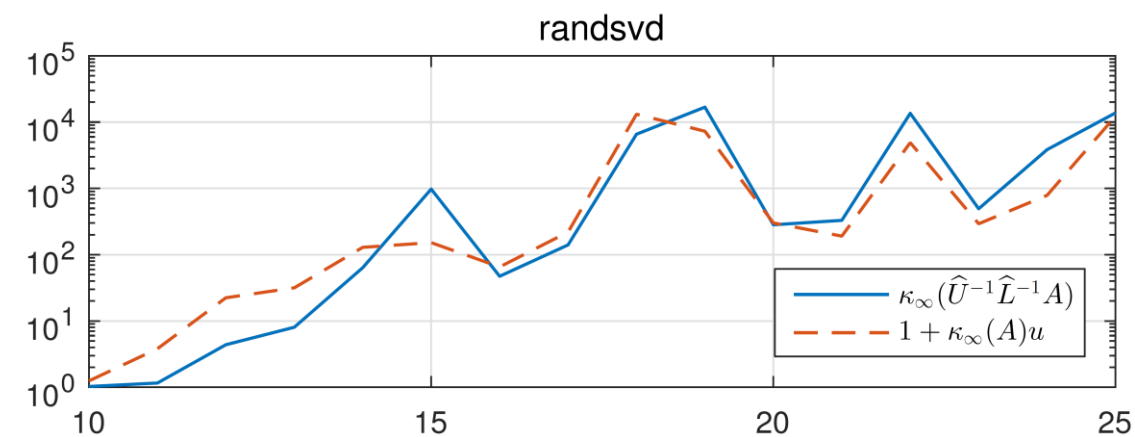
Examples: ill-conditioned problems ($10^{13} \leq \kappa_\infty(A) \leq 10^{35}$), u = double

```
A = invhilb(n)
```




```
A =
gallery('randsvd',
n,10^(n+5))
```



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- Need to define a few quantities...

The quantity θ_i

- Assume computed solution to $Ad_i = r_i$ satisfies

$$\frac{\left\|d_i - \hat{d}_i\right\|_\infty}{\|d_i\|_\infty} = \theta_i u$$

- θ_i depends on A, r_i, n, u, and the method of solving $Ad_i = r_i$

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- For a stable solver, 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,

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

Theorem (C. & Higham, 2017)

Let IR in precisions u and u^2 be applied to a linear system $Ax = b$ with nonsingular $A \in \mathbb{R}^{n\times n}$ and a given approximate solution x_0. Assume that the solver for the corrective term d_i satisfies $\left\|d_i - \hat{d}_i\right\|_\infty / \|d_i\|_\infty = \theta_i u$. Then for $i \geq 0$, the computed iterate $\hat{x}_{i+1}$ satisfies

$$\begin{aligned}\|x - \hat{x}_{i+1}\|_\infty \leq\ & (2\mu_i \kappa_\infty(A) u + \theta_i u)\, \|x - \hat{x}_i\|_\infty \\ & + n u^2 (1 + \theta_i u) \| \, |A^{-1}| \, (|b| + |A||\hat{x}_i|) \|_\infty + u \|\hat{x}_{i+1}\|\end{aligned}$$

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As long as for all i,

$$2\mu_i \kappa_\infty(A)u + \theta_i u < 1,$$

the error will contract until a limiting normwise relative error of order

$$2nu^2(1+\theta u)\mathrm{cond}(A,x) + u$$

is achieved, where θ is an upper bound on the θ_i terms.

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$\mu_i \kappa_\infty(A)u < 1$ (condition on iteration)

$\theta_i u < 1$ (condition on solver, data)

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- To compute the updates d_i, apply GMRES to

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GMRES-IR:

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

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(usually $\kappa_\infty(\tilde{A}) \approx 1 + \kappa_\infty(A)u$)

$\Longrightarrow$ Even if $\kappa_\infty(A) > u^{-1}$, $\theta_i u < 1$

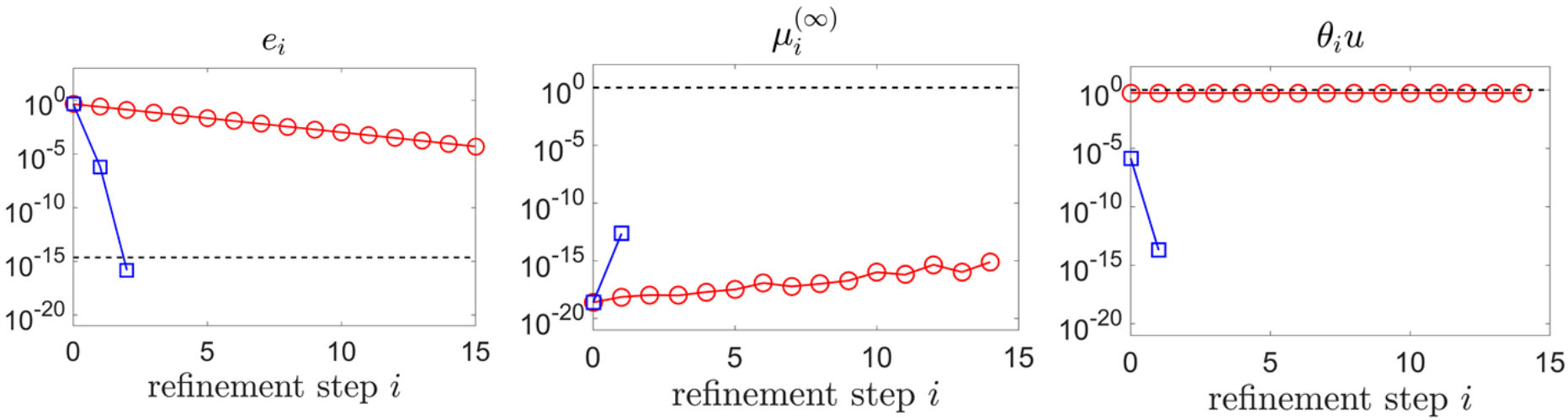
Numerical experiments

$u = 2^{-53}$ (double), $u^2 = 2^{-113}$ (quad)

UFSMC matrix: oscil_dcop_06, $n = 430$

$\mathrm{cond}(A) = 2 \cdot 10^{18}$, $\kappa_\infty(A) = 1 \cdot 10^{21}$, $\kappa(\tilde{A}) = 45$

$b = \mathrm{randn}(n, 1)$



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Standard IR steps	GMRES-IR steps	GMRES its.
–	2	7 (3,4)

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UFSMC matrix: oscil_dcop_43, $n = 430$

$\mathrm{cond}(A) = 1 \cdot 10^{18}$, $\kappa_\infty(A) = 8 \cdot 10^{20}$, $\kappa(\tilde{A}) = 2.1$

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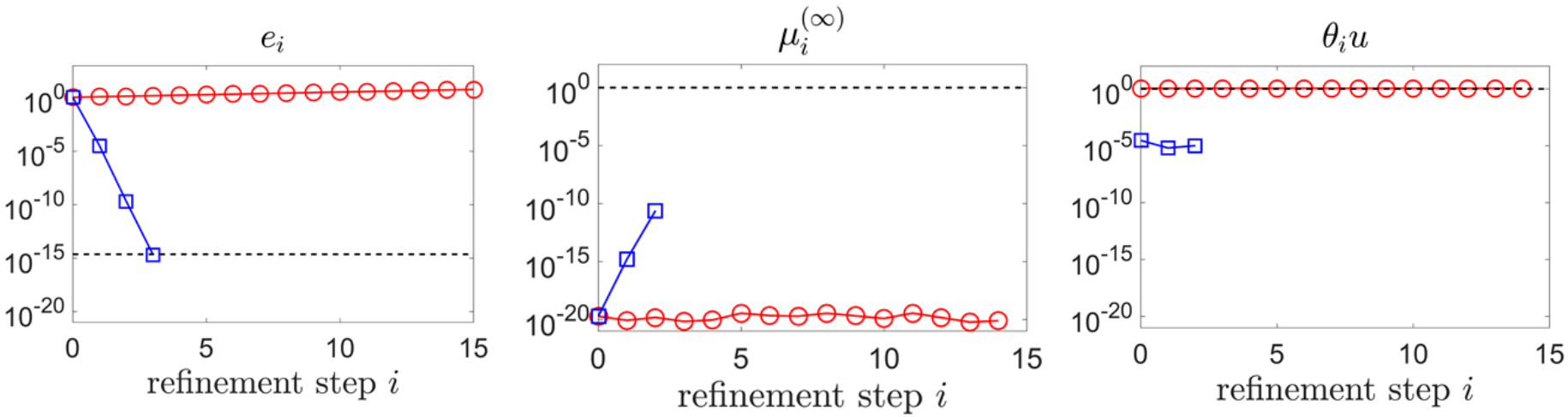

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Standard IR steps	GMRES-IR steps	GMRES its.
–	3	10 (2,4,4)

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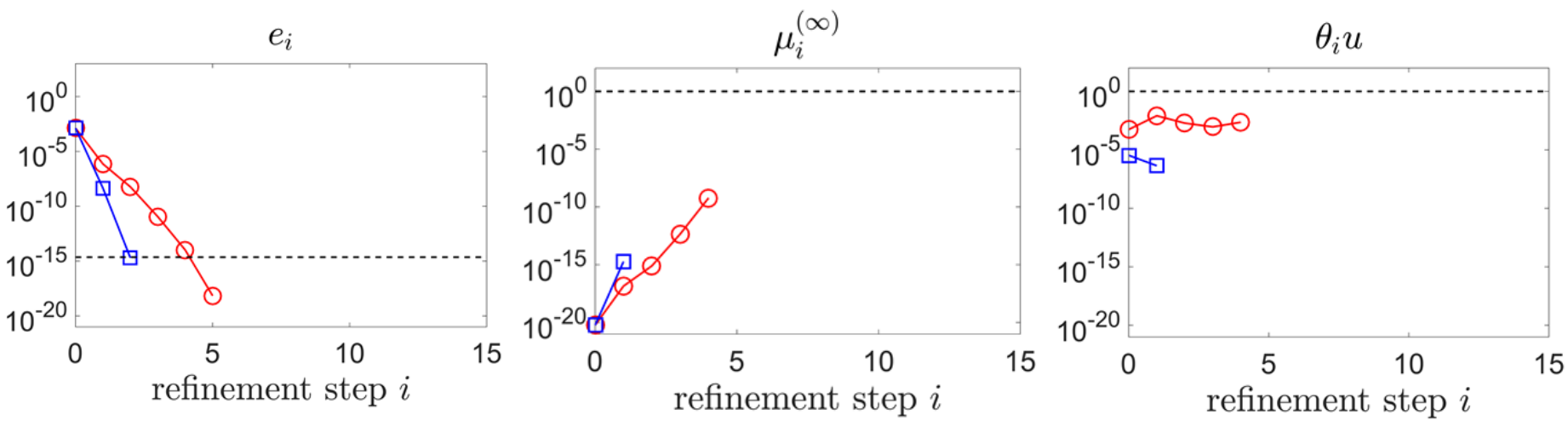
UFSMC matrix: mhda416, $n = 416$

$\mathrm{cond}(A) = 1 \cdot 10^{19}$, $\kappa_\infty(A) = 2 \cdot 10^{25}$, $\kappa(\tilde{A}) = 7 \cdot 10^{9}$

$b = \mathrm{randn}(n, 1)$



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Standard IR steps	GMRES-IR steps	GMRES its.
5	2	3 (1,2)

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- Decision to switch can be based on, e.g., stopping criteria for forward error of Demmel et al. (2006)

- Future work...

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- Incomplete LU factorizations
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- Other solvers
  - Left-preconditioned, unrestarted GMRES used here for theoretical purposes
  - In practice, many potential modifications may improve performance while still resulting in IR convergence
    - Restarted GMRES
    - Right, split preconditioned GMRES, FGMRES
    - Other Krylov subspace methods (not necessarily backward stable)

Extensions II: Iterative refinement in 3 precisions

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  - Half precision (FP16) defined as storage format in 2008 IEEE standard
  - Intel Ivy bridge, 2012: supports half precision for storage
  - NVIDIA Tesla P100, 2016: native hardware ISA support for 16-bit FP arithmetic
  - TSUBAME3.0 supercomputer, 2017: projected 12.2 double-precision petaflops, 64.3 half-precision petaflops
  - Intel Xeon Phi (Knights Mill), 2017: will support 16-bit FP
  - Google Tensorflow processor (TPU): quantizes 32-bit FP computations into 8-bit arithmetic

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  - TSUBAME3.0 supercomputer, 2017: projected 12.2 double-precision petaflops, 64.3 half-precision petaflops
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- Can we use lower precision in the most expensive part of solving $Ax = b$ using IR (the LU factorization) and still obtain accurate solutions?

Extensions II: Iterative refinement in 3 precisions

- Emerging architectures feature built-in support for multiprecision computation, rising interest in low-precision storage and computation (performance and energy savings!)
  - Half precision (FP16) defined as storage format in 2008 IEEE standard
  - Intel Ivy bridge, 2012: supports half precision for storage
  - NVIDIA Tesla P100, 2016: native hardware ISA support for 16-bit FP arithmetic
  - TSUBAME3.0 supercomputer, 2017: projected 12.2 double-precision petaflops, 64.3 half-precision petaflops
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- Can we use lower precision in the most expensive part of solving $Ax = b$ using IR (the LU factorization) and still obtain accurate solutions?
- Three precisions:

u_f = factorization precision, u = working precision, u_r = residual precision

$$u_f \geq u \geq u_r$$

Extensions II: Iterative refinement in 3 precisions

- Existing analyses:
  - **Wilkinson** (1963): fixed-point arithmetic.
  - **Moler** (1967): floating-point arithmetic.
  - **Higham** (1997, 2002): more general analysis for arbitrary solver.
  - **Langou et al.** (2006): lower precision LU.
- All the above support **at most two precisions** and require $\kappa_\infty(A)u < 1$.

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- All the above support **at most two precisions** and require $\kappa_\infty(A)u < 1$.

New analysis generalizes and extends existing types of IR: (u_f, u, u_r)

Traditional Wilkinson (1948)

SSD DDQ HHS	
HHD HHQ SSQ	

70s/80s Skeel (1980) Jankowski and Wozniakowski (1977)

SSS DDD	
HHH	

2000s Dongarra, Langou et al. (2006)

SDD HSS DQQ	
HDD HQQ SQQ	

New

HSD HSQ HDQ SDQ	

Extensions II: Iterative refinement in 3 precisions

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

Theorem (C. & Higham, 2017)

For IR in precisions $\boldsymbol{u_f} \geq \boldsymbol{u} \geq \boldsymbol{u_r}$, if

$$\phi_i = 2\boldsymbol{u_f} \min(\mathrm{cond}(A), \kappa_\infty(A)\mu_i) + \boldsymbol{u_f}\theta_i$$

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

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

- Analogous standard bounds would have $\mu_i = 1$, $u_f\theta_i = \kappa_\infty(A)u$

Extensions II: Iterative refinement in 3 precisions

Standard (LU-based) IR in three precisions:

				Backward error		
u_f	u	u_r	$\kappa_\infty(A)$	norm	comp	Forward error
H	S	S	10^4	S	S	$\mathrm{cond}(A,x)\cdot 10^{-8}$
H	S	D	10^4	S	S	S
H	D	D	10^4	D	D	$\mathrm{cond}(A,x)\cdot 10^{-16}$
H	D	Q	10^4	D	D	D
S	S	S	10^8	S	S	$\mathrm{cond}(A,x)\cdot 10^{-8}$
S	S	D	10^8	S	S	S
S	D	D	10^8	D	D	$\mathrm{cond}(A,x)\cdot 10^{-16}$
S	D	Q	10^8	D	D	D

Extensions II: Iterative refinement in 3 precisions

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

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

benefit of three precisions vs. $u_f \geq u, u = u_r$: no cond(A,x) term in forward error

Extensions II: Iterative refinement in 3 precisions

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If $\kappa_\infty(A) \leq 10^4$, can use lower precision factorization with no loss of accuracy!

Extensions II: Iterative refinement in 3 precisions

Benefits of GMRES-IR:

	u_f	u	u_r	$\kappa_\infty(A)$	Backward error norm	Backward error comp	Forward error
LU-IR	H	S	D	10^4	S	S	S
GMRES-IR	H	S	D	10^8	S	S	S
LU-IR	S	D	Q	10^8	D	D	D
GMRES-IR	S	D	Q	10^{16}	D	D	D
LU-IR	H	D	Q	10^4	D	D	D
GMRES-IR	H	D	Q	10^{12}	D	D	D

Extensions II: Iterative refinement in 3 precisions

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

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

Extensions II: Iterative refinement in 3 precisions

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	u_f	u	u_r	$\kappa_\infty(A)$	Backward error norm	Backward error comp	Forward error
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Extensions II: Iterative refinement in 3 precisions

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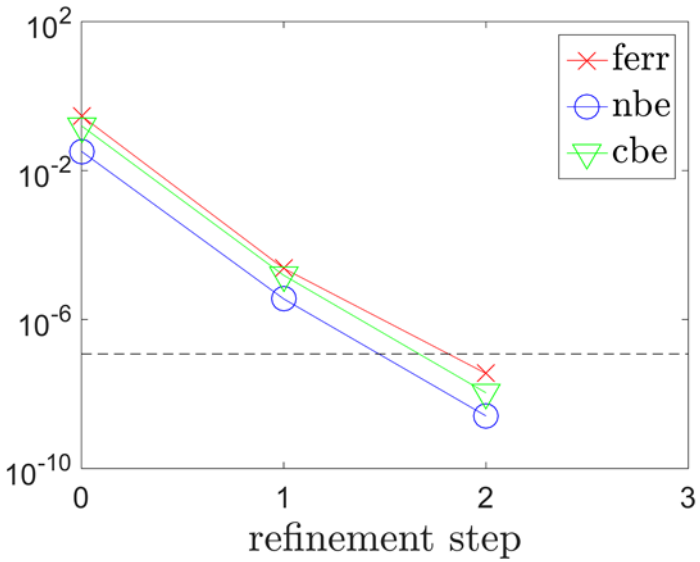
If $\kappa_\infty(A) \leq 10^{12}$, can use lower precision factorization with no loss of accuracy!

Numerical experiments

$u_f = 2^{-11}$ (half), $u = 2^{-24}$ (single), $u_r = 2^{-53}$ (double)

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



$\kappa_\infty(A) = 2 \cdot 10^2$
$\kappa_\infty(\tilde{A}) = 14$
GMRES its: 11 (5,6)

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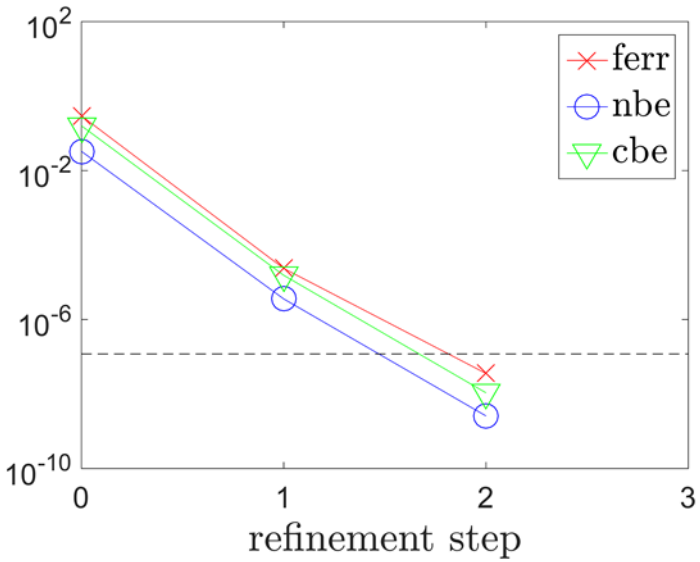

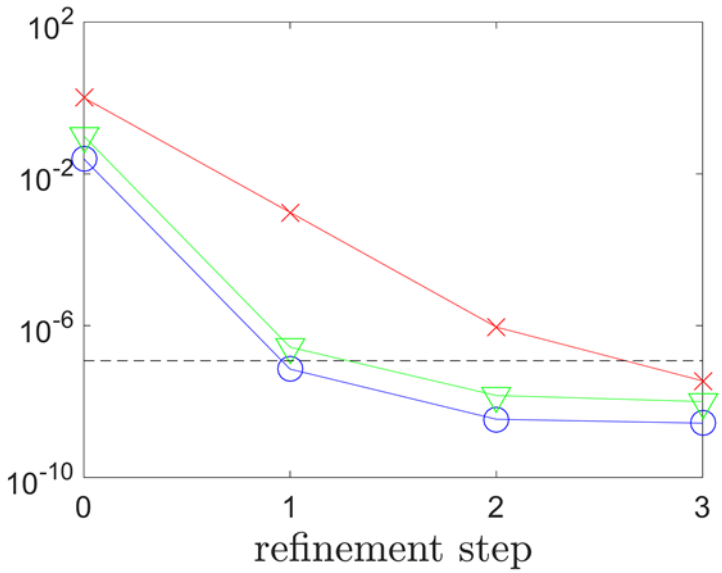

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GMRES its: 40 (7,24,9)

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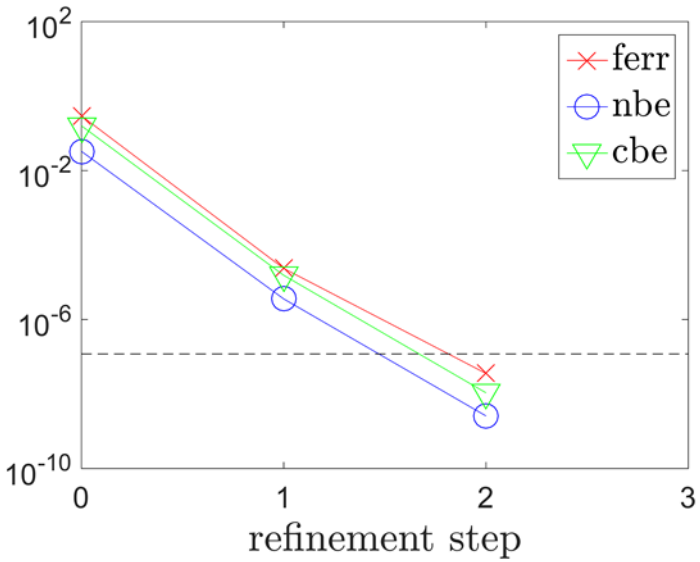

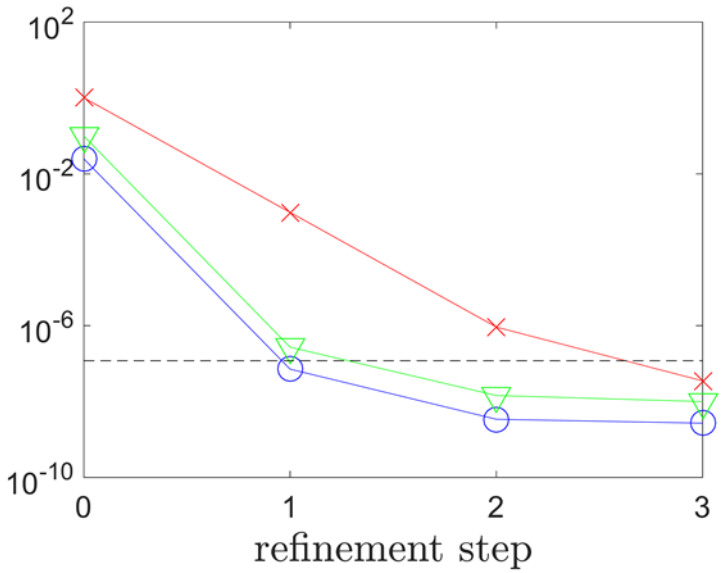

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GMRES convergence rate

- If LU factorization is computed in lower precision, can diminish effectiveness as a preconditioner
- Theory only guarantees that GMRES will converge to an accurate solution within n iterations
  - If close to n iterations, no expected performance benefit

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- If $\tilde{A}$ is normal, spectrum of $\tilde{A}$ determines GMRES convergence rate (Liesen & Tichý, 2004)
  - But small $\kappa_\infty(\tilde{A})$ may not mean fast GMRES convergence
    - e.g., if $\tilde{A}$ has a cluster of eigenvalues close to the origin

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  - But small $\kappa_\infty(\tilde{A})$ may not mean fast GMRES convergence
    - e.g., if $\tilde{A}$ has a cluster of eigenvalues close to the origin

$\Rightarrow$ Can only make guarantees on fast GMRES convergence in some cases, e.g., normality and no eigenvalue cluster near origin

- Potential fixes for slow GMRES convergence: apply additional preconditioner, deflation, other Krylov subspace methods

Thank you!

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Resources:

- E. Carson and N. J. Higham. A new analysis of iterative refinement and its application to accurate solution of ill-conditioned sparse linear systems. MIMS EPrint 2017.12.
- E. Carson and N. J. Higham. Accelerating the solution of linear systems by iterative refinement in three precisions. MIMS EPrint 2017.24.
- MATLAB code for iterative refinement in 3 precisions: https://github.com/eccarson/ir3/

IEEE Standard 754-1985 and 2008 Revision

Type	Size	Range	$u = 2^{-t}$
half	16 bits	$10^{\pm 5}$	$2^{-11} \approx 4.9 \times 10^{-4}$
single	32 bits	$10^{\pm 38}$	$2^{-24} \approx 6.0 \times 10^{-8}$
double	64 bits	$10^{\pm 308}$	$2^{-53} \approx 1.1 \times 10^{-16}$
quadruple	128 bits	$10^{\pm 4932}$	$2^{-113} \approx 9.6 \times 10^{-35}$

- Arithmetic ops ($+, -, *, /, \sqrt{}$) performed *as if* first calculated to infinite precision, then rounded.
- Default: round to nearest, round to even in case of tie.
- Half precision is a *storage format only*.

Summary of the sizes of the quantities in assumptions (2.3)–(2.5) for solution of the correction equation with LU factorization (section 7) and GMRES-IR (section 8). Note that $f(n) = O(n^2)$.

	$u_s\|E_i\|_\infty$	$u_s \max(c_1, c_2)$	$u_s\|G_i\|_\infty$
IR w/LU fact.	$3nu_f\||A^{-1}||\widehat{L}||\widehat{U}|\|_\infty$	$3nu_f \dfrac{\||\widehat{L}||\widehat{U}|\|_\infty}{\|A\|_\infty}$	$3nu_f\||\widehat{L}||\widehat{U}|\|_\infty$
GMRES-IR	$uf(n)(1+\gamma_n^f\kappa_\infty(A))^2$	$O(u)$	$O(u\|A\|_\infty)$

Different scenarios for iterative refinement in IEEE arithmetic. The columns represent different choices for u_f, u, and u_r, where in the notation of Algorithm 1.1 the data is stored at precision u, the solves in steps 1 and 4 are carried out in precision $u_f = u_s$, and residuals are computed at precision u_r. The last column indicates whether any existing backward or forward error analysis is applicable to this situation when LU factorization is used as the solver.

	Precision			
Usage	Half	Single	Double	Existing analysis?
Traditional		data, solve	residual	✓
Traditional			data, solve, residual	✓
2000s		solve	data, residual	✓
New	solve	data, residual		✓
New	solve	data	residual	×
New	solve		data, residual	✓

Summary of existing rounding error analyses for iterative refinement in floating point arithmetic indicating (a) whether the analyses apply to LU factorization only or to an arbitrary solver, (b) whether the backward or forward error analyses are componentwise ("comp") or normwise ("norm"), and (c) the assumptions on the precisions u_f, u_s, u, u_r in Algorithm 1.1 ($u_f = u$ and $u_s = u_f$ unless otherwise stated).

	Year	Solver	Forward error	Backward error	Precisions
Moler [26]	1967	LU	norm	–	$u \geq u_r$
Stewart [33]	1973	LU	norm	–	$u \geq u_r$
Jankowski et al. [21]	1977	arb.	norm	norm	$u = u_r$
Skeel [31]	1980	LU	comp	comp	$u \geq u_r$
Higham [16]	1991	arb.	comp	comp	$u = u_r$
Higham [17], [18]	1997	arb.	comp	comp	$u \geq u_r$
Tisseur [34]	2001	arb.	norm	norm	$u \geq u_r$
Langou et al. [23]	2006	LU	norm	norm	$u_f \geq u = u_r$
Carson and Higham [9]	2017	arb.	comp	–	$u \geq u_r$
This work	2017	arb.	comp	comp, norm	$u_f \geq u_s \geq u \geq u_r$